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Systematic investigation of DFT-GIAO 15N NMR Chemical Shift Prediction using B3LYP/cc-pVDZ: Application to Studies of Regioisomers, Tautomers, Protonation States and N-oxides

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1. Linear Scaling Analysis with All Nitrogens

Linear scaling analysis was performed on all Ns including NH_2. Compared with the data set without NH2, the linear correlation is worse, suggesting that NH_2 should be considered separately.

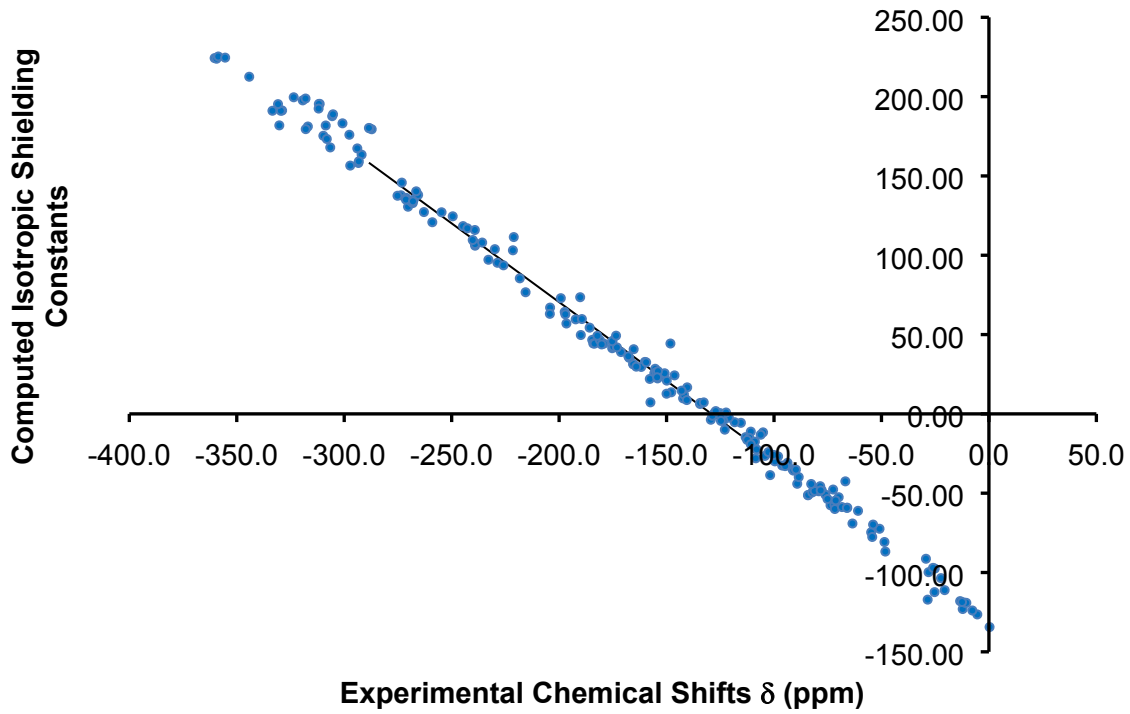
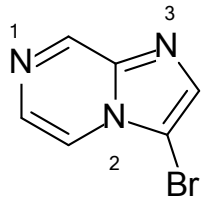


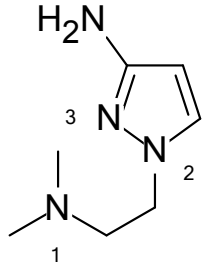
Figure S1. Linear correlation between experimental chemical shifts and calculated isotropic shielding constants for 202 ^{15}N chemical shifts including all NH_2.

When the linear scaling conversion without NH_2 was applied to the NH_2, a mean error of 16.5 ppm with 4.7 ppm standard deviation was observed.

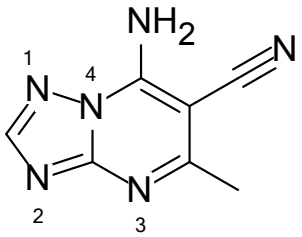
2. Calculated and Experimental Chemical Shifts for Compounds Used in Linear Regression Analysis



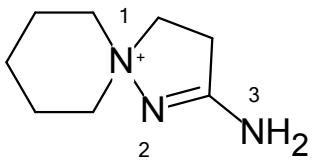
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-77.8	-48.00	-80.6	2.8
2	-175.30	41.3	-171.9	-3.4
3	-127.7	0.7	-130.4	2.7



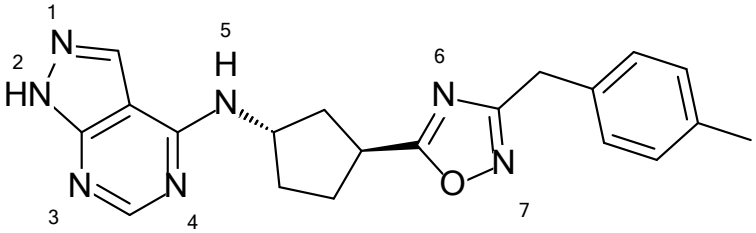
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-358.6	225.30	-360.1	1.5
2	-192.3	59.59	-190.6	-1.7
3	-110.8	-11.2	-118.2	7.4



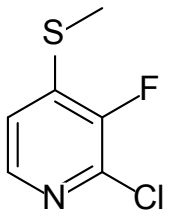
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-115.4	-5.63	-123.9	8.5
2	-149.9	21.0	-151.1	1.2
3	-142.3	9.8	-139.7	-2.6
4	-175.2	45.9	-176.6	1.4



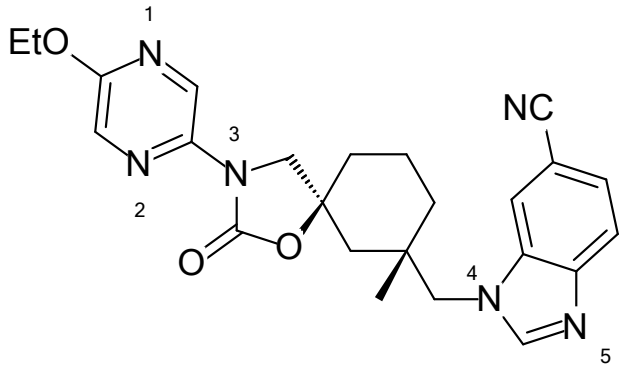
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-259	120.81	-253.3	-5.7
2	-121	-2.4	-127.2	6.2
3	-305.6	187.68	-321.7	16.1



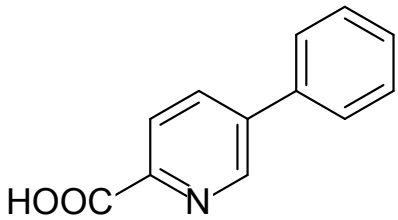
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-78.5	-45.58	-83.1	4.6
2	-190.2	73.5	-204.9	14.7
3	-160.1	32.8	-163.2	3.1
4	-155.7	25.6	-155.9	0.2
5	-273.2	145.79	-278.8	5.6
6	-140.4	16.7	-146.8	6.4
7	-25.2	-97.53	-29.9	4.7



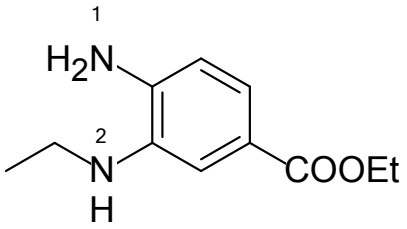
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-82.2	-49.51	-79.0	-3.2



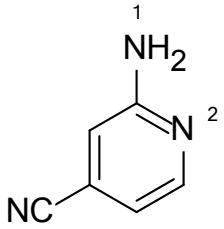
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-91.4	-34.88	-94.0	2.6
2	-69.9	-52.5	-75.9	6.0
3	-275.2	137.5	-270.3	-4.9
4	-225.9	93.7	-225.5	-0.4
5	-134.4	6.25	-136.1	1.7



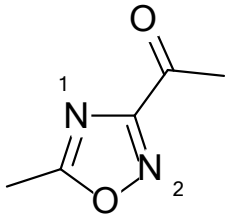
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-63.5	-69.10	-59.0	-4.5



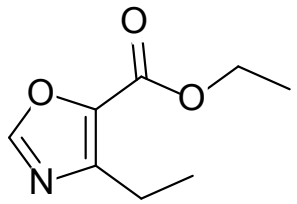
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-319.3	197.6	-331.8	12.5
2	-316.9	181.17	-315.0	-1.9



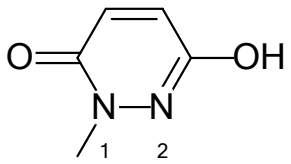
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-300.8	183.17	-317.0	16.2
2	-104.2	-26.5	-102.6	-1.6



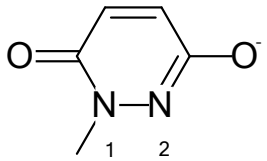
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-141.9	12.2	-142.1	0.2
2	-5.4	-126.43	-0.3	-5.1



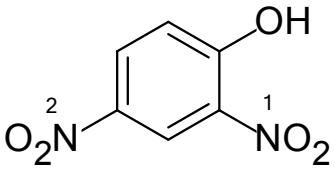
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-113.2	-14.66	-114.7	1.5



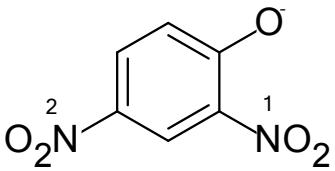
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-196.6	57.0	-187.9	-8.7
2	-98.1	-26.81	-102.2	4.1



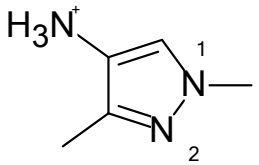
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-197.1	61.4	-192.5	-4.6
2	-111.5	-23.3	-105.8	-5.7



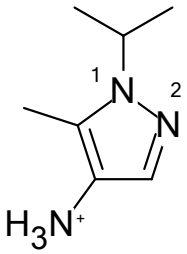
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-12.2	-123.02	-3.8	-8.4
2	-13.4	-118.0	-8.9	-4.5



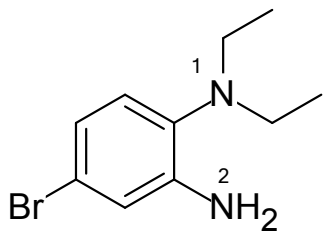
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-7.70	-123.60	-3.2	-4.5
2	-11.20	-119.1	-7.8	-3.4



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-189.9	49.72	-180.5	-9.4
2	-75.1	-53.7	-74.8	-0.3

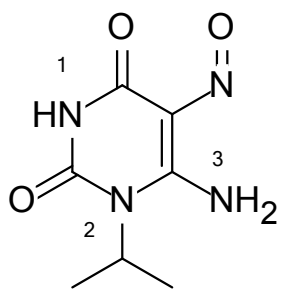


Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-157.80	21.10	-151.3	-6.5
2	-82.70	-42.3	-86.4	3.7

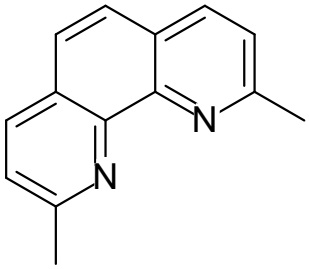


Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-330.8	195.27	-329.4	-1.4
2	-323.5	199.6	-333.8	10.3

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-91.0	-35.75	-93.1	2.1
2	-28.1	-99.8	-27.6	-0.5



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-229.9	103.84	-235.9	6.0
2	-240.2	109.6	-241.8	1.6
3	-288.5	180.26	-314.1	25.6



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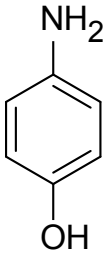
1	-73.53	-53.7	-74.7	1.2



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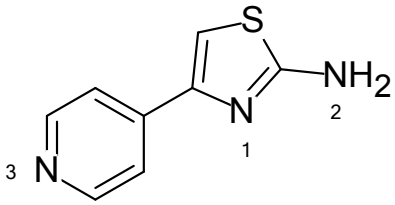
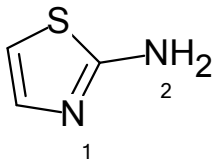
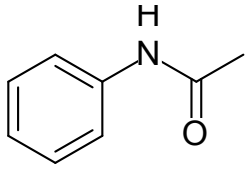
1	-327.03	201.8	-336.1	9.1



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-134.03	8.7	-138.6	4.5
2	-306.13	189.4	-323.4	17.3
3	-67.63	-60.4	-67.9	0.3



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-128.83	1.5	-131.2	2.4
2	-308.73	190.8	-324.8	16.1



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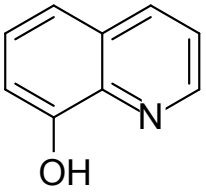
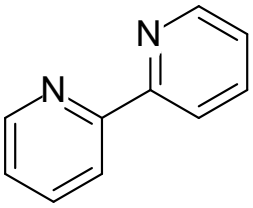
1	-245.62	116.4	-248.7	3.1

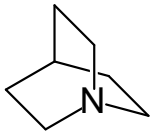


Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-83.73	-32.4	-96.5	12.8



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled

1	-71.53	-52.5	-76.0	4.4



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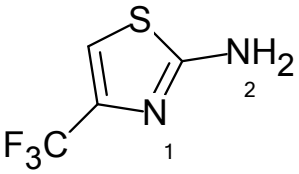
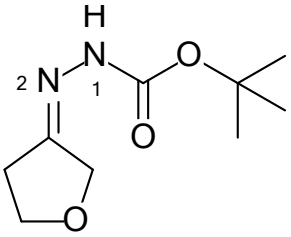
1	-365.83	230.7	-365.7	-0.2



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-139.63	11.7	-141.6	2.0
2	-304.06	187.7	-321.7	17.6



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-232.23	101.2	-233.2	1.0
2	-81.13	-42.3	-86.4	5.3

Chemical structures of proprietary compounds are not shown.

3

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-54.8	-74.63	-53.3	-1.5

2	-197.4	64.3	-195.4	-2.0
3	-215.6	76.7	-208.1	-7.5
4	-147.8	13.6	-143.6	-4.2
5	-73.7	-57.63	-70.7	-3.0
6	-184.6	46.7	-177.4	-7.2

8

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-228.70	95.26	-227.1	-1.6
2	-76.10	-50.9	-77.6	1.5
3	-171.20	39.0	-169.5	-1.7
4	-360.30	224.3	-359.1	-1.2

9

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-218.30	85.45	-217.1	-1.2
2	-81.50	-47.1	-81.5	0.0
3	-174.80	42.3	-172.9	-1.9
4	-359.40	223.9	-358.7	-0.7

600

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-291.90	163.40	-296.8	4.9
2	-173.10	41.9	-172.6	-0.5
3	-118.30	-5.3	-124.3	6.0
4	-152.70	25.0	-155.3	2.6
5	-155.30	28.43	-158.8	3.5

602

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-184.1	44.40	-175.1	-9.0
2	-84.2	-51.3	-77.2	-7.0
3	-328.9	191.3	-325.3	-3.6

603

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-183.50	44.30	-175.0	-8.5
2	-84.10	-51.1	-77.4	-6.7

3	-355.40	224.6	-359.4	4.0
4	-329.50	191.1	-325.1	-4.4

606

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-270.3	130.59	-263.3	-7.0
2	-249.5	124.6	-257.1	7.6
3	-273.6	137.8	-270.6	-3.0
4	-165.3	40.8	-171.4	6.1
5	-140.6	8.72	-138.6	-2.0
6	-268.1	132.9	-265.6	-2.5

611

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-244.7	118.4	-250.8	6.1
2	-267.6	135.3	-268.0	0.4
3	-265.6	138.07	-270.9	5.3
4	-112.5	-16.4	-112.9	0.4
5	-150.9	25.6	-155.9	5.0
6	-269.1	134.10	-266.8	-2.3

628

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-48.6	-80.8	-47.1	-1.5
2	0.3	-134.4	7.8	-7.5
3	-96.2	-32.6	-96.4	0.2
4	-79.2	-48.8	-79.8	0.6

629

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-71.9	-57.47	-70.9	-1.0
2	-48.2	-86.8	-40.9	-7.3
3	-179.2	44.29	-175.0	-4.2

651

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled

1	-50.9	-72.4	-55.6	4.7
2	-105.1	-11.6	-117.8	12.7
3	-239.2	115.92	-248.2	9.0

652

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-204.2	67.00	-198.2	-6.0
2	-89.2	-44.1	-84.6	-4.6

668

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-311.4	195.44	-329.6	18.2
2	-101.8	-38.6	-90.2	-11.6
3	-311.8	195.39	-329.5	17.7
4	-108.5	-28.0	-101.0	-7.5

682

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-123.6	-4.30	-125.3	1.7
2	-134.4	6.9	-136.7	2.3
3	-271.2	136.2	-269.0	-2.2
4	-161.8	29.6	-159.9	-1.9
5	-93.7	-30.84	-98.1	4.4
6	-60.9	-61.1	-67.2	6.3

683

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-266.5	140.30	-273.2	6.7
2	-239.1	106.03	-238.1	-1.0

686

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-129.4	-3.70	-125.9	-3.5
2	-20.6	-111.1	-16.0	-4.6
3	-29.3	-91.3	-36.2	6.9

691

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-344.2	212.53	-347.1	2.9
2	-317.9	179.5	-313.3	-4.6
3	-311.9	192.5	-326.6	14.7
4	-102.6	-24.1	-105.0	2.4
5	-154.2	22.37	-152.6	-1.6
6	-94.8	-32.9	-96.0	1.2

700

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-239.4	107.95	-240.1	0.7
2	-175.3	45.8	-176.5	1.2
3	-81.1	-48.57	-80.0	-1.1
4	-128.7	-1.2	-128.4	-0.3

707

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-297.2	156.52	-289.8	-7.4
2	-154.8	26.3	-156.6	1.8

711

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-199.2	72.94	-204.3	5.1
2	-287.2	179.4	-313.2	26.0

716

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-181	46.44	-177.2	-3.8
2	-72.5	-47.7	-80.9	8.4
3	-309.7	175.33	-309.0	-0.7

717

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-180.20	43.79	-174.5	-5.7
2	-132.70	7.2	-137.1	4.4

3	-154.00	26.9	-157.2	3.2

718

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-204.3	63.06	-194.2	-10.1
2	-99.6	-29.9	-99.1	-0.5
3	-165.5	31.3	-161.7	-3.8

720

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-239.1	107.03	-239.2	0.1
2	-288.2	180.0	-313.8	25.6
3	-125.1	0.50	-130.2	5.1

724

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-165.5	31.4	-161.8	-3.7
2	-71.3	-54.55	-73.9	2.6
3	-221.5	103.1	-235.2	13.7
4	-127.1	1.8	-131.5	4.4

726

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-242.7	116.99	-249.3	6.6
2	-25.3	-112.4	-14.7	-10.6
3	-308.6	181.8	-315.6	7.0

730

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-65.9	-59.15	-69.2	3.3
2	-22.3	-103.5	-23.8	1.5
3	-150.0	12.7	-142.7	-7.3
4	-318.0	198.8	-333.0	15.0

735

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-26.0	-97.07	-30.4	4.4
2	-146.3	24.3	-154.5	8.2
3	-262.9	127.2	-259.8	-3.1

738

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-293.4	158.2	-291.5	-1.9
2	-167.4	35.37	-165.9	-1.5
3	-78.3	-48.2	-80.3	2.0
4	-271.3	135.1	-267.9	-3.4
5	-100.1	-25.91	-103.2	3.1
6	-154.4	23.1	-153.3	-1.1
7	-108.9	-17.5	-111.8	2.9

743

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-53.9	-69.8	-58.3	4.4
2	-122.9	-9.9	-119.5	-3.4
3	-268.0	134.0	-266.8	-1.2
4	-308.1	173.3	-307.0	-1.1
5	-110.8	-19.1	-110.1	-0.7

745

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-143	14.64	-144.6	1.6
2	-297.6	176.0	-309.7	12.1
3	-106.2	-13.15	-116.2	10.0
4	-108.1	-22.4	-106.8	-1.3

746

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-173.5	49.30	-180.1	6.6
2	-293.2	159.2	-292.5	-0.7
3	-254.7	127.1	-259.7	5.0

749

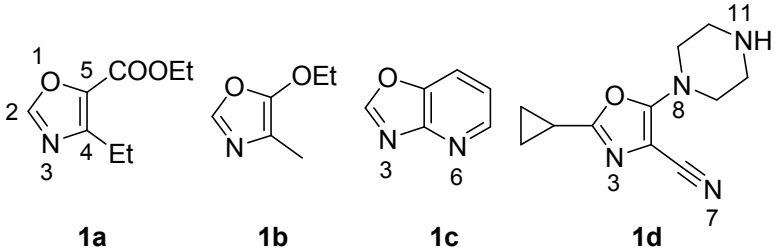
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-66.1	-59.24	-69.1	3.0
2	-54.3	-77.6	-50.3	-4.0
3	-189.4	59.78	-190.8	1.4

752

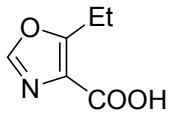
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-293.9	167.4	-300.9	7.0
2	-159.5	32.5	-163.0	3.5
3	-122.3	0.9	-130.6	8.3
4	-182.2	49.2	-180.0	-2.2
5	-306.5	168.0	-301.5	-5.0
6	-167.8	36.3	-166.8	-1.0
7	-124.8	-1.6	-128.1	3.3
8	-88.5	-39.8	-88.9	0.4
9	-164.1	29.8	-160.1	-4.0
10	-89.8	-35.1	-93.7	3.9
11	-124.7	-4.4	-125.2	0.5

3. Calculated and Experimental Chemical Shifts for Compounds 1-3

Table S1. Comparison of experimental and calculated ^{15}N chemical shift differences for oxazoles.



1a **1b** **1c** **1d**

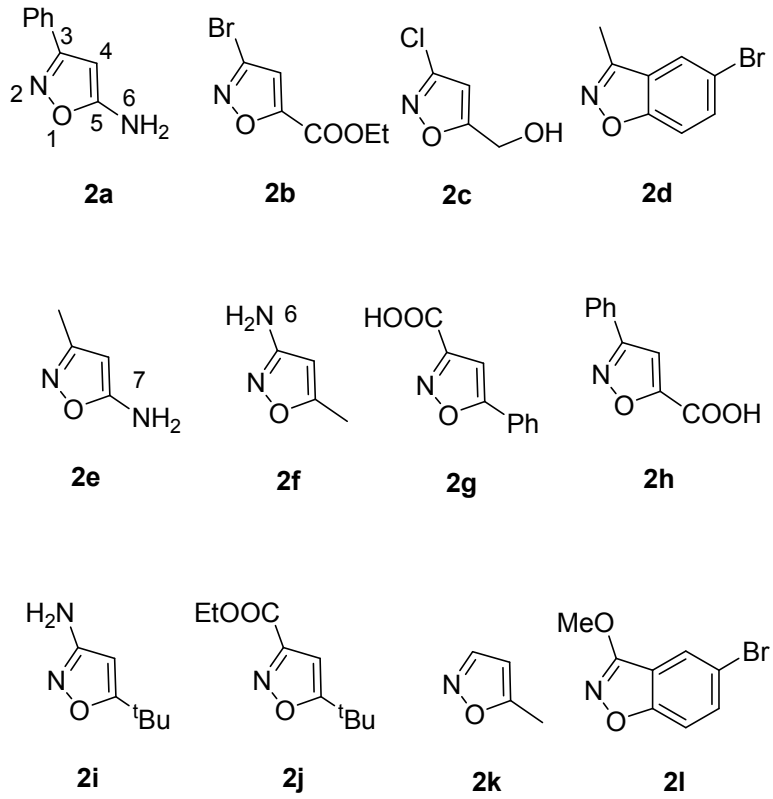


1e

Entry	Position	δ_{exp} - δ_{calc} (ppm)	
		Correct isomer[a]	Incorrect isomer[b]
1a	3	1.4	9.8
1b	3	4.0	26.8
1c	3	0.8	28.7
	6	3.2	5.0
1d	3	7.0	17.5
	7	1.5	0.7
	8	2.2	-19.3
	11	-8.4	-7.1
1e	3	2.2	-6.2

a. Calculated ^{15}N chemical shifts for the correct isomer.
b. Calculated values for the regiomer with 4- and 5-substituents exchanged.

Table S2. Comparison of experimental and calculated ^{15}N chemical shift differences for isoxazoles.

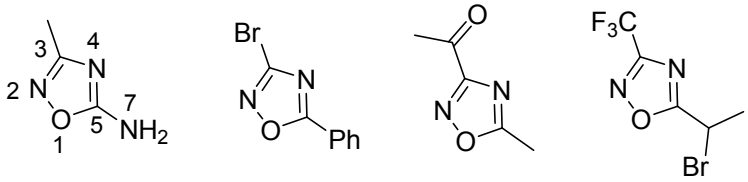


Entry	Position	δ_{exp} - δ_{calc} (ppm)	
		Correct isomer[a]	Incorrect isomer[b]
2a	2	1.7	17.1
	6[c]	-0.4	11.2
2b	2	0.1	-25.6
2c	2	3.1	-10.5
2d	2	1.7	12.2
2e	2	2.5	16.1
	7[c]	-1.0	10.0

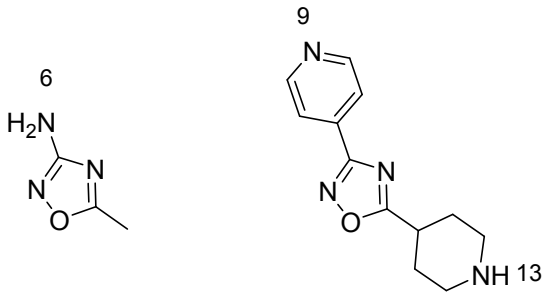
2f	2	2.0	-11.5
	6[c]	-2.2	-13.3
2g	2	0.2	5.8
2h	2	-4.8	-10.4
2i	2	2.6	-10.7
	6[c]	-2.5	-13.3
2j	2	-1.2	8.9
2k	2	3.1	11.7
2l	2	4.8	-8.2

a. Calculated ^{15}N chemical shifts for the correct isomer.
b. Calculated values for the regiomer with swapped 3- and 5-substituents.
c. Systematic error correction of -16.5 ppm was applied.

Table S3. Comparison of experimental and calculated ^{15}N chemical shift differences for oxadiazoles.



3a **3b** **3c** **3d**

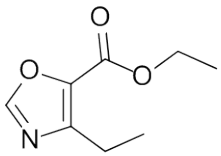


3e **3f**

Entry	Position	δ_{exp} - δ_{calc} (ppm)	
		Correct isomer[a]	Incorrect isomer[b]

3a	2	-1.3	23.6
	4	1.1	-32.7
	7[c]	2.3	13.3
3b	2	4.4	-14.8
	4	7.2	2.3
3c	2	0.5	-15.0
	4	-5.2	15.9
3d	2	-3.1	-0.9
	4	-0.7	-10.6
3e	2	0.2	-24.8
	4	3.1	36.9
	6[c]	-0.9	-11.8
3f	2	-1.3	4.2
	4	2.3	-1.0
	9	-1.0	-7.0
	13	6.8	5.8

a. Calculated ^{15}N chemical shifts for the correct isomer.
b. Calculated values for the regiomer with swapped 3- and 5-substituents.
c. Systematic error correction of -16.5 ppm was applied.



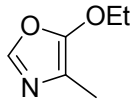
1a

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-113.2	-14.7	-114.6	1.4

1a incorrect isomer

Atom Number	Exptl. Chemical	Tensors	Linearly Scaled	Exptl. - Scaled

	Shifts		Chemical Shifts	
1	-	-6.5	-123.0	9.8

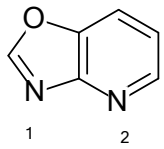


1b

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-111.63	-13.7	-115.7	4.0

1b incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	8.6	-138.5	26.8

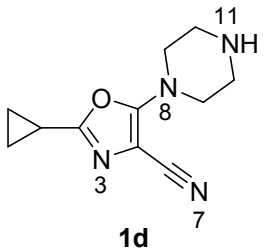


1c

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-83.92	-43.9	-84.8	0.8
2	-128.26	1.7	-131.4	3.2

1c incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-16.7	-112.6	28.7
2	-	3.5	-133.3	5.0

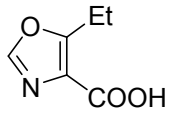


1d

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
3	-139.34	16.3	-146.3	7.0
7	-114.09	-13.1	-116.3	2.2
8	-307.81	165.9	-299.4	-8.4
11	-349.68	216.5	-351.1	1.5

1d incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	26.6	-156.9	17.5
2	-	-34.1	-94.8	-19.3
3	-	167.2	-300.7	-7.1
4	-	215.8	-350.4	0.7

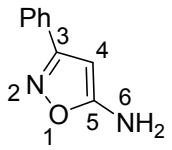


1e

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-120.6	-6.7	-122.8	2.2

1e incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-15.0	-114.3	-6.2

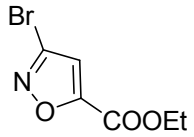


2a

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
2	-34.52	-91.4	-36.2	1.7
6	-322.45	204.2	-338.6	16.1

2a incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
2	-	-76.3	-51.6	17.1
6	-	215.5	-350.1	27.7

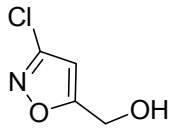


2b

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-1.23	-125.5	-1.3	0.1

2b incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-150.6	24.4	-25.6



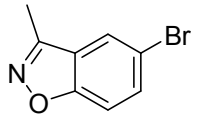
2c

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-14.11	-109.9	-17.3	3.1

2c incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled

1	-	-123.2	-3.7	-10.5

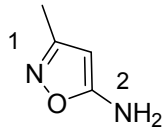


2d

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-2.82	-122.4	-4.5	1.7

2d incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-112.1	-15.0	12.2

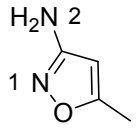


2e

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-33.5	-91.6	-36.0	2.5
2	-324.2	205.3	-339.7	15.5

2e incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-78.3	-49.6	16.1
2	-	216.1	-350.7	26.5



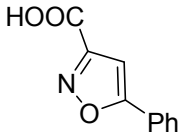
2f

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-47.4	-78.3	-49.6	2.0

2	-336.5	216.1	-350.7	14.3

2f incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-91.6	-36.0	-11.5
2	-	205.3	-339.7	3.2

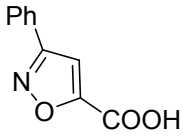


2g

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	6.9	-133.4	6.8	0.2

2g incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-127.9	1.2	5.8

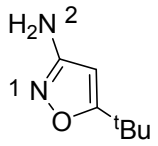


2h

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-3.7	-127.9	1.2	-4.8

2h incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-133.4	6.8	-10.4

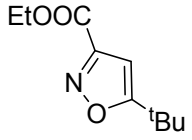


2i

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-48.68	-76.6	-51.3	2.6
2	-336.39	215.8	-350.4	14.0

2i incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-89.6	-38.0	-10.7
2	-	205.2	-339.6	3.2

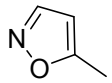


2j

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	7.35	-135.1	8.5	-1.2

2j incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-125.3	-1.5	8.9

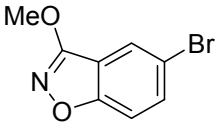


2k

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	1.08	-124.8	-2.0	3.1

2k incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-116.4	-10.6	11.7

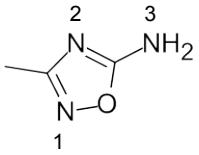


2l

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-43.6	-79.5	-48.4	4.8

2l incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-92.2	-35.4	-8.2



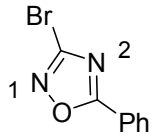
3a

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-43.03	-86.0	-41.7	-1.3
2	-188.33	58.4	-189.4	1.1
3	-319.03	203.5	-337.8	18.8

3a incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-61.6	-66.7	23.6

2	-	25.4	-155.7	-32.7
3	-	214.2	-348.8	29.8

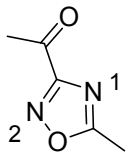


3b

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-25.03	-98	-29.4	4.4
2	-138.27	15.4	-145.4	7.2

3b incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-116.8	-10.2	-14.8
2	-	10.7	-140.6	2.3

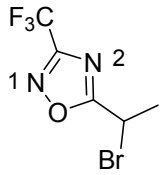


3c

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-141.9	12.4	-142.4	0.5
2	-5.4	-126.6	-0.2	-5.2

3c incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-2.7	-126.9	-15.0
2	-	-105.9	-21.3	15.9

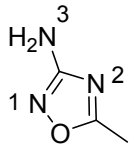


3d

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-13.84	-116.3	-10.7	-3.1
2	-142.95	12.3	-142.3	-0.7

3d incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-114.1	-13.0	-0.9
2	-	2.6	-132.3	-10.6

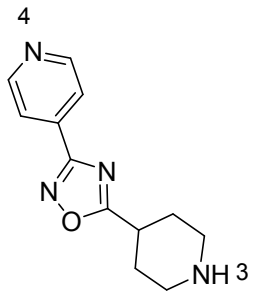


3e

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-66.46	-61.6	-66.7	0.2
2	-152.56	25.4	-155.7	3.1
3	-333.18	214.2	-348.8	15.6

3e incorrect isomer

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-86.0	-41.7	-24.8
2	-	58.4	-189.4	36.9
3	-	203.5	-337.8	4.7



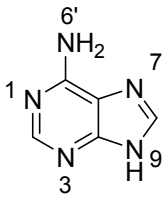
3f

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-22.53	-106	-21.2	-1.3
2	-146.23	18.4	-148.5	2.3
3	-345.19	217.3	-352.0	6.8
4	-55.62	-73.4	-54.6	-1.0

3f incorrect isomer

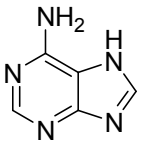
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-100.6	-26.8	4.2
2	-	15.2	-145.2	-1.0
3	-	216.4	-351.0	5.8
4	-	-79.2	-48.7	-7.0

4. Calculated and Experimental Chemical Shifts for Compounds 4



4a

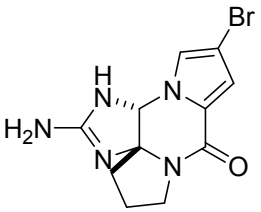
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-145.7	19.8	-149.9	4.2
3	-151.5	25.8	-156.1	4.6
7	-140.3	14.2	-144.2	3.9
9	-222.6	104.5	-236.6	14.0
6'	-301.2	185	-318.9	17.7



4b

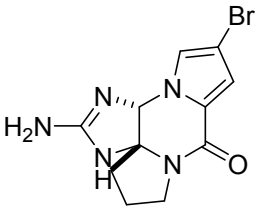
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	13	-143.0	-2.7
3	-	5.3	-135.1	-16.4
7	-	116.8	-249.2	108.9
9	-	8.1	-138.0	-84.6
6'	-	186.8	-320.8	19.6

5. Calculated and Experimental Chemical Shifts for Compounds 5 and 6



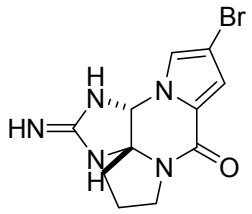
5a

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	76.7	-208.1	-3.1
7	-	121.2	-253.7	-5.6
13	-	160.1	-293.4	8.2
15	-	69	-200.3	-71.0
16	-	204.1	-338.5	35.2



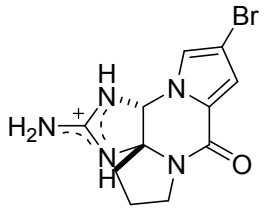
5b

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	70	-201.3	-10.0
7	-	126.4	-259.0	-0.3
13	-	75.6	-207.0	-78.2
15	-	151.4	-284.5	13.3
16	-	199.8	-334.1	30.8



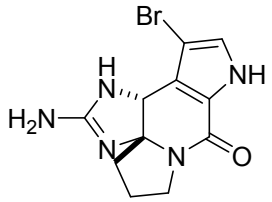
5c

Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	75.5	-206.9	-4.3
7	-	125.5	-258.1	-1.2
13	-	162.9	-296.3	11.1
15	-	162.8	-296.2	25.0
16	-	109.7	-241.9	-61.3



5d

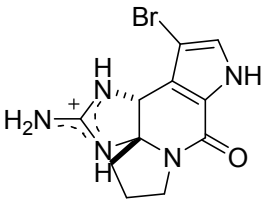
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-211.23	85	-216.6	5.4
7	-259.23	131.1	-263.8	4.5
13	-285.23	160.3	-293.6	8.4
15	-271.23	147.6	-280.7	9.4
16	-303.23	187.5	-321.5	18.2



6a

Atom Number	Exptl. Chemical	Tensors	Linearly Scaled	Exptl. - Scaled

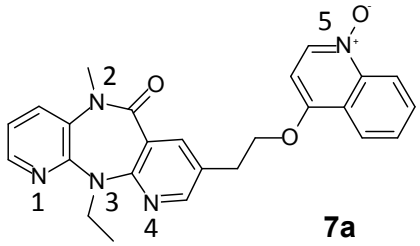
	Shifts	Chemical Shifts		
1	-	109.8	-242.0	30.8
7	-	118	-250.4	-8.9
13	-	166.9	-300.4	15.2
15	-	65.7	-196.9	-74.3
16	-	204.9	-339.3	36.0



6b

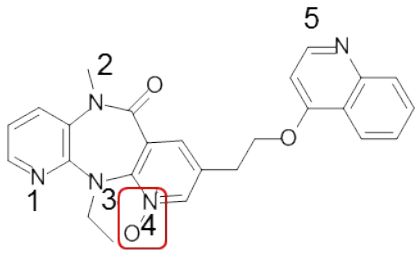
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	107.3	-239.4	28.2
7	-	128	-260.6	1.4
13	-	165.8	-299.3	14.0
15	-	145.9	-278.9	7.7
16	-	189.6	-323.6	20.4

6. Calculated and Experimental Chemical Shifts for Compounds 7

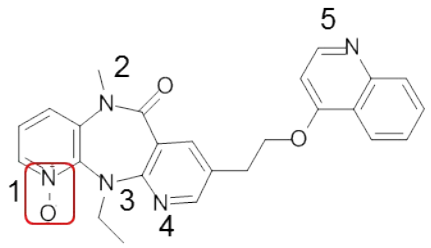


7a

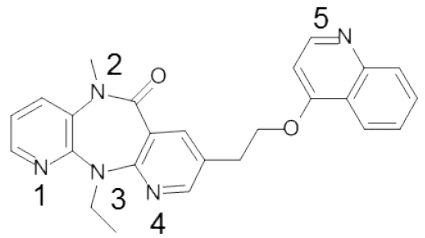
Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-86.47	-41.2	-87.5	1.1
2	-256.85	123.1	-255.6	-1.3
3	-273.34	136.5	-269.3	-4.0
4	-91.22	-34.2	-94.7	3.5
5	-113.34	-23.9	-105.2	-8.1



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-42.8	-85.9	-0.6
2	-	118.2	-250.6	-6.3
3	-	165.1	-298.6	25.2
4	-	-43.1	-85.6	-5.6
5	-	-38.0	-90.8	-22.5

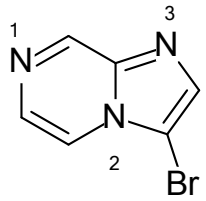


Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-46.7	-81.9	-4.6
2	-	122.8	-255.3	-1.6
3	-	158.7	-292.0	18.7
4	-	-34.4	-94.5	3.3
5	-	-37.9	-90.9	-22.4



Atom Number	Exptl. Chemical Shifts	Tensors	Linearly Scaled Chemical Shifts	Exptl. - Scaled
1	-	-41.3	-87.4	1.0
2	-	123	-255.5	-1.4
3	-	136.5	-269.3	-4.0
4	-	-35.1	-93.8	2.6
5	-	-37.6	-91.2	-22.1

7. Coordinates and Shielding Constants for Compounds Used in Linear Regression Analysis



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

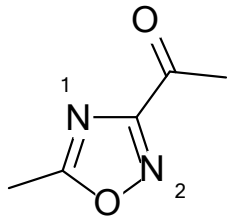
C	-1.370307827694	1.379871866060	-0.425088037361
N	-0.219410757809	0.669933173562	-0.170278013046
C	-0.154274085695	-0.705628535906	-0.444078858175
C	-1.314976366851	-1.310017758676	-0.985353593095
N	-2.425164244307	-0.645648204544	-1.234857045843
C	-2.433750930351	0.695991339730	-0.948827786917
N	1.042816605215	-1.211076964175	-0.129643797564
C	1.759440106744	-0.159672316784	0.350835587600
C	1.009686331583	1.011137955201	0.338429245927
Br	1.440497271064	2.758805242000	0.867715237955
H	-1.370476618521	2.444093505957	-0.197004232183
H	-1.283463344545	-2.381342542341	-1.205428507908
H	-3.358849956860	1.235412316066	-1.160261305453
H	2.787413818027	-0.263099076151	0.691911106063

SCF Done: E(RB3LYP) = -2969.46401718

Zero-point correction= 0.095913
Thermal correction to Energy= 0.103187
Thermal correction to Enthalpy= 0.104131
Thermal correction to Gibbs Free Energy= 0.062492
Sum of electronic and zero-point Energies= -2969.368104
Sum of electronic and thermal Energies= -2969.360830
Sum of electronic and thermal Enthalpies= -2969.359886
Sum of electronic and thermal Free Energies= -2969.401525

1	C	Isotropic =	74.9844	Anisotropy =	126.2858
2	N	Isotropic =	41.3261	Anisotropy =	242.6038
3	C	Isotropic =	51.3633	Anisotropy =	120.7110
4	C	Isotropic =	50.8025	Anisotropy =	142.3652
5	N	Isotropic =	-48.0466	Anisotropy =	520.7099

6 C Isotropic = 61.2819 Anisotropy = 140.2741
7 N Isotropic = 0.6870 Anisotropy = 366.3996
8 C Isotropic = 57.0388 Anisotropy = 114.2864
9 C Isotropic = 76.3853 Anisotropy = 43.5199
10 Br Isotropic = 2270.4124 Anisotropy = 930.9423
11 H Isotropic = 23.3797 Anisotropy = 10.8773
12 H Isotropic = 22.4531 Anisotropy = 6.4521
13 H Isotropic = 23.2915 Anisotropy = 6.2535
14 H Isotropic = 23.6679 Anisotropy = 7.4624



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.290857087194	0.911053751614	0.181910758680
N	0.571195401666	-0.359938973357	-0.272076469160
C	1.722303344096	-0.197320912261	-0.861751480662
C	2.569358356109	-1.196317962458	-1.558864645340
H	3.554657517278	-1.267482001234	-1.073359951301
H	2.731693565673	-0.896865007037	-2.605436603338
H	2.076250458850	-2.174798397449	-1.530193756635
O	2.163252948849	1.081533433796	-0.800287599817
N	1.205683371079	1.808976637091	-0.105120719696
C	-0.954931233203	1.260203350587	0.946283163930
C	-1.109906255477	2.693106104122	1.383456735391
H	-0.268723874469	2.982065071202	2.033954751577
H	-2.059616132703	2.813803006454	1.918791952431
H	-1.078370316348	3.362430509289	0.508991180789
O	-1.772404238594	0.389431389642	1.178832683151

SCF Done: E(RB3LYP) = -454.092890320

Zero-point correction= 0.110211
Thermal correction to Energy= 0.119020
Thermal correction to Enthalpy= 0.119964
Thermal correction to Gibbs Free Energy= 0.075379
Sum of electronic and zero-point Energies= -453.982679
Sum of electronic and thermal Energies= -453.973870
Sum of electronic and thermal Enthalpies= -453.972926
Sum of electronic and thermal Free Energies= -454.017511

1 C Isotropic = 26.1359 Anisotropy = 104.8786
2 N Isotropic = 12.7864 Anisotropy = 283.8691

3 C Isotropic = 12.3935 Anisotropy = 113.0052
4 C Isotropic = 180.0703 Anisotropy = 25.8843
5 H Isotropic = 28.8039 Anisotropy = 8.2265
6 H Isotropic = 28.8008 Anisotropy = 8.2094
7 H Isotropic = 28.8189 Anisotropy = 8.1681
8 O Isotropic = -70.7678 Anisotropy = 224.3385
9 N Isotropic = -127.4600 Anisotropy = 288.5047
10 C Isotropic = 2.0636 Anisotropy = 159.2151
11 C Isotropic = 163.7651 Anisotropy = 48.3537
12 H Isotropic = 28.5230 Anisotropy = 4.6761
13 H Isotropic = 29.4008 Anisotropy = 6.5925
14 H Isotropic = 28.4925 Anisotropy = 4.6395
15 O Isotropic = -293.5859 Anisotropy = 971.6973

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

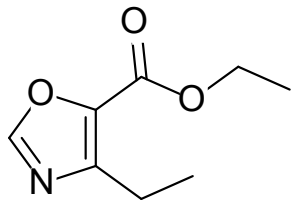
C	0.690722840115	0.423865419026	-0.171816867738
N	0.220918141336	1.717504508675	-0.099846113278
C	-0.191070734855	1.799669966819	1.135345286593
C	-0.809487246303	2.946409591602	1.844980339565
H	-1.812594781813	2.675534677603	2.208133515438
H	-0.886392847564	3.799040969784	1.160457721781
H	-0.201655076485	3.229684916184	2.717710807178
O	-0.004198420428	0.647573492771	1.817342607953
N	0.581151916109	-0.261349042463	0.944764169312
C	1.284637721996	-0.183159345540	-1.413738142672
C	1.348913762905	0.711637925918	-2.621687876595
H	1.941308027192	1.612231691133	-2.392123600717
H	0.338201933895	1.063806658011	-2.884181989686
H	1.793968145013	0.166812719732	-3.463083609149
O	1.677916618887	-1.334984149253	-1.399606247984

SCF Done: E(RB3LYP) = -454.092082918

Zero-point correction= 0.110205
Thermal correction to Energy= 0.118970
Thermal correction to Enthalpy= 0.119914
Thermal correction to Gibbs Free Energy= 0.075558
Sum of electronic and zero-point Energies= -453.981878
Sum of electronic and thermal Energies= -453.973113
Sum of electronic and thermal Enthalpies= -453.972169
Sum of electronic and thermal Free Energies= -454.016525

1 C Isotropic = 26.3802 Anisotropy = 107.0199
2 N Isotropic = 10.9773 Anisotropy = 275.0567
3 C Isotropic = 12.2911 Anisotropy = 113.5217
4 C Isotropic = 179.9853 Anisotropy = 25.6854
5 H Isotropic = 28.8012 Anisotropy = 8.3169
6 H Isotropic = 28.8112 Anisotropy = 7.8606
7 H Isotropic = 28.7972 Anisotropy = 8.3161
8 O Isotropic = -72.3613 Anisotropy = 246.7077
9 N Isotropic = -124.5191 Anisotropy = 278.6362

10	C	Isotropic =	0.6495	Anisotropy =	157.4740
11	C	Isotropic =	162.1159	Anisotropy =	46.0754
12	H	Isotropic =	28.5055	Anisotropy =	4.2743
13	H	Isotropic =	28.5005	Anisotropy =	4.2572
14	H	Isotropic =	29.4377	Anisotropy =	6.4964
15	O	Isotropic =	-278.0870	Anisotropy =	957.3572



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.290349306977	-0.251274362754	-1.597668315252
C	0.637936168216	1.067055742158	-1.870616780040
C	-0.735765974997	0.915813577336	-2.543508705231
H	-0.653659935880	0.347999891051	-3.483515960210
H	-1.160093572663	1.904956452246	-2.775354064829
H	-1.442681725329	0.384753011731	-1.885741041280
H	1.304327680901	1.646882968568	-2.532595400246
H	0.546298234792	1.616802986782	-0.924721369749
N	1.667896627417	-1.104009644980	-2.630998402607
C	2.180561323368	-2.140256646643	-2.033650542576
H	2.598832068531	-3.037395720454	-2.484282483774
O	2.187770569937	-2.075168956469	-0.689851956602
C	1.610810187561	-0.853694774411	-0.405002256910
C	1.452823862061	-0.433498504087	0.990999335930
O	0.956574271170	0.631093448247	1.320840333372
O	1.916553793569	-1.354255059891	1.850975861161
C	1.803171775057	-1.026590638565	3.262545805960
C	2.370042327102	-2.192431787363	4.044123406418
H	2.302528254880	-1.980036427070	5.122322361522
H	3.428207136299	-2.360789264043	3.790402964333
H	1.808304022924	-3.116707258461	3.837759338029
H	0.742659668088	-0.845312748795	3.496181747515
H	2.355053930022	-0.092616284136	3.450586125066

SCF Done: E(RB3LYP) = -591.944069890

Zero-point correction= 0.184886
Thermal correction to Energy= 0.197137
Thermal correction to Enthalpy= 0.198081
Thermal correction to Gibbs Free Energy= 0.144739
Sum of electronic and zero-point Energies= -591.759183
Sum of electronic and thermal Energies= -591.746933
Sum of electronic and thermal Enthalpies= -591.745989

Sum of electronic and thermal Free Energies= -591.799331

1	C	Isotropic =	37.1311	Anisotropy =	138.1929
2	C	Isotropic =	167.9363	Anisotropy =	13.4411
3	C	Isotropic =	175.8858	Anisotropy =	22.9214
4	H	Isotropic =	29.9246	Anisotropy =	8.1081
5	H	Isotropic =	30.0492	Anisotropy =	9.9856
6	H	Isotropic =	30.3862	Anisotropy =	7.4273
7	H	Isotropic =	28.8547	Anisotropy =	7.9676
8	H	Isotropic =	27.9072	Anisotropy =	8.5072
9	N	Isotropic =	-14.2688	Anisotropy =	353.8737
10	C	Isotropic =	42.7051	Anisotropy =	93.6659
11	H	Isotropic =	23.7950	Anisotropy =	4.2349
12	O	Isotropic =	30.2903	Anisotropy =	256.9284
13	C	Isotropic =	54.2126	Anisotropy =	83.1686
14	C	Isotropic =	35.7695	Anisotropy =	78.8664
15	O	Isotropic =	-28.2694	Anisotropy =	519.7425
16	O	Isotropic =	127.5299	Anisotropy =	132.5479
17	C	Isotropic =	128.4697	Anisotropy =	57.4265
18	C	Isotropic =	177.1790	Anisotropy =	20.0972
19	H	Isotropic =	30.0416	Anisotropy =	9.5372
20	H	Isotropic =	29.8991	Anisotropy =	7.7068
21	H	Isotropic =	29.9009	Anisotropy =	7.6506
22	H	Isotropic =	27.1568	Anisotropy =	5.9704
23	H	Isotropic =	27.1829	Anisotropy =	6.1105

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.656894159746	-0.142114970133	-1.340039933603
C	-0.740077941517	-0.617256686870	-1.586296402539
C	-1.781916518438	0.497938415966	-1.403437257421
H	-1.790514956991	0.865435808560	-0.364562099187
H	-2.789484985459	0.124597360976	-1.643442967152
H	-1.565097490789	1.351738235053	-2.064411431907
H	-0.949782957033	-1.457162239469	-0.911070980740
H	-0.793509826457	-0.997496611305	-2.621243126866
N	1.249196371582	0.825220136200	-2.146661739421
C	2.436124769728	0.995643435341	-1.641002388488
H	3.221783474640	1.666562961042	-1.980767612790
O	2.709015183260	0.236126358219	-0.564505664542
C	1.558194908144	-0.500432012526	-0.366794036392
C	1.491045136769	-1.458461779542	0.741368789343
O	0.512027536906	-2.147415695906	0.976421238774
O	2.626674859879	-1.483249219253	1.457079451295
C	2.654985636326	-2.404410897692	2.581049334624
C	4.005025089303	-2.259350707687	3.250228394035
H	4.155966370746	-1.231803777266	3.616006387795
H	4.820214535100	-2.506830394918	2.552642488227
H	4.065298252528	-2.944795637726	4.109719433450
H	2.486189455004	-3.424334357276	2.202175915356
H	1.825038937027	-2.154537723787	3.259864208148

SCF Done: E(RB3LYP) = -591.944090927

Zero-point correction= 0.184978
Thermal correction to Energy= 0.197181
Thermal correction to Enthalpy= 0.198125
Thermal correction to Gibbs Free Energy= 0.145190
Sum of electronic and zero-point Energies= -591.759113
Sum of electronic and thermal Energies= -591.746910
Sum of electronic and thermal Enthalpies= -591.745966
Sum of electronic and thermal Free Energies= -591.798901

1	C	Isotropic =	37.1076	Anisotropy =	138.1031
2	C	Isotropic =	168.0308	Anisotropy =	13.3678
3	C	Isotropic =	175.9012	Anisotropy =	22.8631
4	H	Isotropic =	30.3886	Anisotropy =	7.4435
5	H	Isotropic =	30.0547	Anisotropy =	9.9836
6	H	Isotropic =	29.9200	Anisotropy =	8.0993
7	H	Isotropic =	27.9048	Anisotropy =	8.5411
8	H	Isotropic =	28.8607	Anisotropy =	7.9760
9	N	Isotropic =	-14.2610	Anisotropy =	354.1947
10	C	Isotropic =	42.6523	Anisotropy =	93.8044
11	H	Isotropic =	23.7929	Anisotropy =	4.2377
12	O	Isotropic =	30.2693	Anisotropy =	256.8245
13	C	Isotropic =	54.1525	Anisotropy =	83.3539
14	C	Isotropic =	35.7749	Anisotropy =	78.6842
15	O	Isotropic =	-28.3625	Anisotropy =	519.6094
16	O	Isotropic =	127.3753	Anisotropy =	132.5011
17	C	Isotropic =	128.4718	Anisotropy =	57.4193
18	C	Isotropic =	177.1664	Anisotropy =	20.2259
19	H	Isotropic =	29.9002	Anisotropy =	7.6482
20	H	Isotropic =	29.8966	Anisotropy =	7.7118
21	H	Isotropic =	30.0417	Anisotropy =	9.5367
22	H	Isotropic =	27.1855	Anisotropy =	6.1243
23	H	Isotropic =	27.1582	Anisotropy =	5.9634

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.605227019995	-0.232311548401	-1.345386171031
C	-0.763213691687	0.333245135783	-1.132419791446
C	-1.870182320927	-0.588763492829	-1.668846540524
H	-1.878301966202	-1.551195344003	-1.132144016856
H	-1.723709177297	-0.797913473911	-2.740149427247
H	-2.857046530366	-0.117208112329	-1.542461582806
H	-0.815413999761	1.304574038349	-1.653929021274
H	-0.903628600916	0.521091476345	-0.059897505081
N	1.125427064978	-0.415610277554	-2.623276580670
C	2.306033583436	-0.927517669543	-2.429135899451
H	3.043778688060	-1.217733647330	-3.173665933700
O	2.639996769467	-1.111371677781	-1.138863539091
C	1.539858919263	-0.663471505758	-0.435138711777
C	1.546001364507	-0.711370023880	1.030496035583
O	0.611666084571	-0.335680155191	1.719202877288

O	2.693027070070	-1.213369664764	1.514958500296
C	2.792899044275	-1.300140424470	2.962468035227
C	4.149913878989	-1.886851231959	3.287440674642
H	4.959093639538	-1.247637264057	2.901378380441
H	4.259818988596	-2.892737470358	2.853174004033
H	4.263965270335	-1.967419845978	4.379548950521
H	1.968334126441	-1.928362536102	3.333373912340
H	2.664394774637	-0.290955284278	3.383513350580

SCF Done: E(RB3LYP) = -591.944085807

Zero-point correction= 0.184846
Thermal correction to Energy= 0.197123
Thermal correction to Enthalpy= 0.198068
Thermal correction to Gibbs Free Energy= 0.144507
Sum of electronic and zero-point Energies= -591.759240
Sum of electronic and thermal Energies= -591.746962
Sum of electronic and thermal Enthalpies= -591.746018
Sum of electronic and thermal Free Energies= -591.799579

1	C	Isotropic =	37.0141	Anisotropy =	138.1398
2	C	Isotropic =	168.0488	Anisotropy =	13.4060
3	C	Isotropic =	175.7864	Anisotropy =	23.1070
4	H	Isotropic =	30.3830	Anisotropy =	7.4046
5	H	Isotropic =	29.9425	Anisotropy =	8.0723
6	H	Isotropic =	30.0500	Anisotropy =	9.9958
7	H	Isotropic =	28.8639	Anisotropy =	7.9782
8	H	Isotropic =	27.9083	Anisotropy =	8.4274
9	N	Isotropic =	-14.4087	Anisotropy =	353.3998
10	C	Isotropic =	42.6582	Anisotropy =	93.6850
11	H	Isotropic =	23.7958	Anisotropy =	4.2369
12	O	Isotropic =	30.1339	Anisotropy =	256.7222
13	C	Isotropic =	54.1293	Anisotropy =	83.1980
14	C	Isotropic =	35.8100	Anisotropy =	78.8563
15	O	Isotropic =	-28.2862	Anisotropy =	519.6159
16	O	Isotropic =	127.5066	Anisotropy =	132.4920
17	C	Isotropic =	128.5031	Anisotropy =	57.4536
18	C	Isotropic =	177.1603	Anisotropy =	20.2012
19	H	Isotropic =	29.8961	Anisotropy =	7.7087
20	H	Isotropic =	29.8956	Anisotropy =	7.6553
21	H	Isotropic =	30.0403	Anisotropy =	9.5335
22	H	Isotropic =	27.1718	Anisotropy =	5.9939
23	H	Isotropic =	27.1778	Anisotropy =	6.0880

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.082307775353	0.882916302436	-0.218190358139
C	1.582136906374	1.869111272531	0.789536374729
C	0.448516578088	2.472933481241	1.633888226682
H	0.847008442193	3.231542895717	2.325199865498
H	-0.057471220594	1.696855528108	2.230647623478
H	-0.306222060719	2.954671011235	0.992646615631

H	2.100743134127	2.678430073364	0.246759133223
H	2.320685072166	1.371721451343	1.431800333616
N	0.237844558155	1.267196233899	-1.255575185717
C	0.003265571836	0.169746240469	-1.914519195860
H	-0.611898078522	0.036381457975	-2.801440367398
O	0.607943385051	-0.927445605849	-1.423749418101
C	1.305844107402	-0.468616143301	-0.324490496618
C	2.101031036222	-1.406871769812	0.474042457595
O	2.743295541333	-1.076622438129	1.457342015054
O	2.035661182864	-2.659267495079	-0.005097270503
C	2.793207808214	-3.663668864762	0.723054863881
C	2.575968480023	-4.988514782876	0.023770235496
H	3.136310858647	-5.777662169119	0.548623620078
H	2.929621679057	-4.947678175340	-1.018165282767
H	1.509879002243	-5.263941773559	0.022196092631
H	2.440279920577	-3.681033297097	1.765748825581
H	3.853190319912	-3.366023433393	0.729961291931

SCF Done: E(RB3LYP) = -591.944101729

Zero-point correction= 0.184926
Thermal correction to Energy= 0.197168
Thermal correction to Enthalpy= 0.198112
Thermal correction to Gibbs Free Energy= 0.144811
Sum of electronic and zero-point Energies= -591.759176
Sum of electronic and thermal Energies= -591.746934
Sum of electronic and thermal Enthalpies= -591.745990
Sum of electronic and thermal Free Energies= -591.799291

1	C	Isotropic =	37.1832	Anisotropy =	138.4097
2	C	Isotropic =	167.9540	Anisotropy =	13.4293
3	C	Isotropic =	175.8781	Anisotropy =	22.9323
4	H	Isotropic =	30.0483	Anisotropy =	9.9913
5	H	Isotropic =	30.3872	Anisotropy =	7.4393
6	H	Isotropic =	29.9199	Anisotropy =	8.0965
7	H	Isotropic =	28.8621	Anisotropy =	7.9745
8	H	Isotropic =	27.9049	Anisotropy =	8.5270
9	N	Isotropic =	-14.2859	Anisotropy =	354.1962
10	C	Isotropic =	42.7084	Anisotropy =	93.6758
11	H	Isotropic =	23.7944	Anisotropy =	4.2379
12	O	Isotropic =	30.3783	Anisotropy =	256.8860
13	C	Isotropic =	54.2056	Anisotropy =	83.2395
14	C	Isotropic =	35.7522	Anisotropy =	78.8441
15	O	Isotropic =	-28.1923	Anisotropy =	519.8326
16	O	Isotropic =	127.5481	Anisotropy =	132.3917
17	C	Isotropic =	128.5053	Anisotropy =	57.4719
18	C	Isotropic =	177.1596	Anisotropy =	20.2535
19	H	Isotropic =	30.0397	Anisotropy =	9.5399
20	H	Isotropic =	29.8941	Anisotropy =	7.7098
21	H	Isotropic =	29.8955	Anisotropy =	7.6451
22	H	Isotropic =	27.1698	Anisotropy =	5.9885
23	H	Isotropic =	27.1786	Anisotropy =	6.1022

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.563539162387	0.320381060459	-0.426438975427
C	-0.330685919571	0.219799882073	0.769301668154
C	-0.015753546699	1.292530764004	1.825680321434
H	1.001953358532	1.162319060176	2.227494283864
H	-0.727157846011	1.227088928440	2.663565252452
H	-0.085397920329	2.303477244926	1.393702852210
H	-0.240443097458	-0.781986448662	1.208231987164
H	-1.369698522618	0.344364792462	0.421858467946
N	0.382030433740	1.329973812896	-1.368174944789
C	1.323274633635	1.136941443761	-2.245876942088
H	1.529412612355	1.709307068930	-3.147372649946
O	2.129654572086	0.092666278156	-1.991228491316
C	1.644218954404	-0.437193513828	-0.813148682675
C	2.361681983373	-1.610704104340	-0.298741672647
O	3.307934144166	-2.129619770707	-0.860946026930
O	1.843294561064	-2.033733970093	0.869110375005
C	2.479287294978	-3.197931322326	1.464156583287
C	1.750914854991	-3.507150719584	2.754450871880
H	0.690876684291	-3.737929994023	2.565913477907
H	1.807637680075	-2.658847391524	3.454120196211
H	2.213962843021	-4.382636790258	3.235492801131
H	3.542078370127	-2.965867428361	1.633171796283
H	2.424844709459	-4.031138882574	0.746647450892

SCF Done: E(RB3LYP) = -591.943193594

Zero-point correction= 0.185094
Thermal correction to Energy= 0.197290
Thermal correction to Enthalpy= 0.198235
Thermal correction to Gibbs Free Energy= 0.145092
Sum of electronic and zero-point Energies= -591.758099
Sum of electronic and thermal Energies= -591.745903
Sum of electronic and thermal Enthalpies= -591.744959
Sum of electronic and thermal Free Energies= -591.798101

1	C	Isotropic =	39.4654	Anisotropy = 137.0447
2	C	Isotropic =	166.8570	Anisotropy = 14.2023
3	C	Isotropic =	175.0266	Anisotropy = 24.0704
4	H	Isotropic =	30.3294	Anisotropy = 6.8159
5	H	Isotropic =	30.0292	Anisotropy = 9.8142
6	H	Isotropic =	30.0720	Anisotropy = 8.2128
7	H	Isotropic =	28.1034	Anisotropy = 8.8942
8	H	Isotropic =	28.8469	Anisotropy = 7.9445
9	N	Isotropic =	-15.2256	Anisotropy = 343.0073
10	C	Isotropic =	41.8859	Anisotropy = 96.5306
11	H	Isotropic =	23.7228	Anisotropy = 4.0950
12	O	Isotropic =	26.1534	Anisotropy = 259.0615
13	C	Isotropic =	53.2697	Anisotropy = 80.4042
14	C	Isotropic =	36.3441	Anisotropy = 74.7646
15	O	Isotropic =	-42.7280	Anisotropy = 540.8550
16	O	Isotropic =	133.5115	Anisotropy = 148.1597
17	C	Isotropic =	128.4374	Anisotropy = 57.6799
18	C	Isotropic =	177.0275	Anisotropy = 19.9465

19	H	Isotropic =	29.8668	Anisotropy =	7.2223
20	H	Isotropic =	29.8650	Anisotropy =	7.1307
21	H	Isotropic =	30.0418	Anisotropy =	9.7629
22	H	Isotropic =	27.1632	Anisotropy =	6.4181
23	H	Isotropic =	27.1677	Anisotropy =	6.5492

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.995597808838	0.619404304891	-0.241846641746
C	1.804361985037	1.241861492634	0.852763408216
C	3.100819162423	1.882468328103	0.328630292945
H	3.764896231933	1.121854924592	-0.112466598722
H	3.643106983209	2.378678482484	1.148499194425
H	2.883254329892	2.635792395831	-0.445061439202
H	2.037002676183	0.482432170386	1.610106333019
H	1.181872143998	2.016510784393	1.330339709979
N	0.263031037054	1.409596548756	-1.123921526411
C	-0.293546128964	0.564063639712	-1.941777809935
H	-0.952369874922	0.774929852203	-2.780958151491
O	-0.009532281124	-0.727098047245	-1.701249574788
C	0.827230879629	-0.696455338996	-0.604361876704
C	1.300702857347	-2.001825141281	-0.126240826020
O	0.966283115471	-3.066411906017	-0.611605080966
O	2.150727828872	-1.869478511439	0.909016841778
C	2.676338033119	-3.106316180346	1.464083768425
C	3.615407941298	-2.737803185067	2.592503826809
H	3.085750471175	-2.187919938085	3.385969117951
H	4.446984953030	-2.115334979547	2.227383797221
H	4.037641237920	-3.654932600189	3.031697096157
H	3.188754284254	-3.658320325944	0.661261670353
H	1.831254324328	-3.720836769830	1.811044468706

SCF Done: E(RB3LYP) = -591.943154709

Zero-point correction= 0.184951
Thermal correction to Energy= 0.197228
Thermal correction to Enthalpy= 0.198173
Thermal correction to Gibbs Free Energy= 0.143997
Sum of electronic and zero-point Energies= -591.758204
Sum of electronic and thermal Energies= -591.745926
Sum of electronic and thermal Enthalpies= -591.744982
Sum of electronic and thermal Free Energies= -591.799158

1	C	Isotropic =	39.2703	Anisotropy =	136.8250
2	C	Isotropic =	166.8734	Anisotropy =	14.3199
3	C	Isotropic =	175.0461	Anisotropy =	24.0645
4	H	Isotropic =	30.3273	Anisotropy =	6.8073
5	H	Isotropic =	30.0345	Anisotropy =	9.8061
6	H	Isotropic =	30.0787	Anisotropy =	8.2132
7	H	Isotropic =	28.1190	Anisotropy =	8.7855
8	H	Isotropic =	28.8542	Anisotropy =	7.9626
9	N	Isotropic =	-15.3186	Anisotropy =	342.9918

10	C	Isotropic =	41.9905	Anisotropy =	96.6426
11	H	Isotropic =	23.7188	Anisotropy =	4.0984
12	O	Isotropic =	25.8991	Anisotropy =	258.1860
13	C	Isotropic =	53.2210	Anisotropy =	80.4124
14	C	Isotropic =	36.2714	Anisotropy =	74.5821
15	O	Isotropic =	-42.4573	Anisotropy =	541.9204
16	O	Isotropic =	133.2362	Anisotropy =	147.8831
17	C	Isotropic =	128.2957	Anisotropy =	57.8877
18	C	Isotropic =	177.0145	Anisotropy =	19.9807
19	H	Isotropic =	29.8723	Anisotropy =	7.2055
20	H	Isotropic =	29.8756	Anisotropy =	7.1232
21	H	Isotropic =	30.0291	Anisotropy =	9.7788
22	H	Isotropic =	27.1416	Anisotropy =	6.3855
23	H	Isotropic =	27.1804	Anisotropy =	6.6257

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.651000207658	-0.162935742875	-1.050835738025
C	-0.461863423641	0.260438609194	-0.144264713098
C	-1.661707080075	-0.699688972355	-0.204670955851
H	-2.038976259674	-0.794322707736	-1.235182311179
H	-2.482309175299	-0.328930748287	0.429001562914
H	-1.380532577444	-1.704495690543	0.149574421499
H	-0.785533428875	1.267158486677	-0.457597212435
H	-0.085258404347	0.333718394753	0.883726806148
N	0.529579122402	-0.037169169949	-2.432382751554
C	1.647104704994	-0.505462661406	-2.906918532933
H	1.955471726974	-0.583534861972	-3.946907484427
O	2.518275701367	-0.939056030068	-1.980321497418
C	1.877235145065	-0.722350157554	-0.777487593149
C	2.625153299698	-1.119568505601	0.422662483047
O	3.748407874526	-1.587081537678	0.399482354669
O	1.912349848704	-0.904217800012	1.543854766145
C	2.566506767731	-1.258504457264	2.793111242756
C	1.606732944535	-0.937304994704	3.918534073673
H	1.361057421757	0.135925552175	3.935938199204
H	2.070789674104	-1.200468284687	4.881689292916
H	0.672285967765	-1.510846161288	3.817522046478
H	3.504134718013	-0.686870876490	2.870924037478
H	2.824385224062	-2.328281682330	2.760477503142

SCF Done: E(RB3LYP) = -591.943160310

Zero-point correction= 0.185000
Thermal correction to Energy= 0.197245
Thermal correction to Enthalpy= 0.198189
Thermal correction to Gibbs Free Energy= 0.144579
Sum of electronic and zero-point Energies= -591.758161
Sum of electronic and thermal Energies= -591.745915
Sum of electronic and thermal Enthalpies= -591.744971
Sum of electronic and thermal Free Energies= -591.798581

1	C	Isotropic =	39.5054	Anisotropy =	136.8032
2	C	Isotropic =	167.0567	Anisotropy =	13.8882
3	C	Isotropic =	175.1976	Anisotropy =	23.8924
4	H	Isotropic =	30.0380	Anisotropy =	8.2549
5	H	Isotropic =	30.0347	Anisotropy =	9.7931
6	H	Isotropic =	30.3476	Anisotropy =	6.9235
7	H	Isotropic =	28.8541	Anisotropy =	7.9176
8	H	Isotropic =	28.1004	Anisotropy =	9.2581
9	N	Isotropic =	-14.9781	Anisotropy =	344.5539
10	C	Isotropic =	41.8342	Anisotropy =	96.7916
11	H	Isotropic =	23.7136	Anisotropy =	4.0967
12	O	Isotropic =	26.4218	Anisotropy =	257.9936
13	C	Isotropic =	53.2953	Anisotropy =	80.3033
14	C	Isotropic =	36.2879	Anisotropy =	74.6864
15	O	Isotropic =	-42.8973	Anisotropy =	541.6567
16	O	Isotropic =	133.6201	Anisotropy =	148.4795
17	C	Isotropic =	128.3352	Anisotropy =	57.8552
18	C	Isotropic =	176.9491	Anisotropy =	19.9620
19	H	Isotropic =	29.8793	Anisotropy =	7.2102
20	H	Isotropic =	30.0261	Anisotropy =	9.7709
21	H	Isotropic =	29.8727	Anisotropy =	7.1395
22	H	Isotropic =	27.1684	Anisotropy =	6.5512
23	H	Isotropic =	27.1587	Anisotropy =	6.4246

Conformer 8

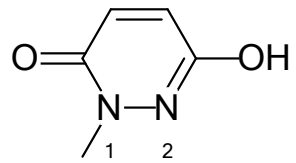
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.885090203167	0.404419111417	-0.815553526990
C	0.876560040114	1.355034857061	-0.250945919711
C	1.470793046827	2.250675489256	0.849392180950
H	0.719600838547	2.973502943040	1.203939515055
H	2.339183305987	2.814139714658	0.472770006132
H	1.801908060858	1.648099033615	1.710435686548
H	0.022851212321	0.788864106136	0.142839545928
H	0.511571502428	1.986353205033	-1.077882576248
N	2.866285596725	0.848505236551	-1.698211948183
C	3.571115918592	-0.211188459888	-1.970115494713
H	4.434125204943	-0.294102523130	-2.626674393907
O	3.163962807591	-1.334947428308	-1.356087051501
C	2.075274295783	-0.941234521279	-0.605148312121
C	1.429831246509	-1.997474022884	0.184952736472
O	1.780074663036	-3.162829946195	0.177134442449
O	0.409696124011	-1.513045441107	0.917575504592
C	-0.304737619629	-2.481733529980	1.733252283635
C	-1.403939094604	-1.741409669063	2.464408620567
H	-2.112031429204	-1.282891654709	1.756661973518
H	-0.988100094486	-0.951075611647	3.108413973194
H	-1.960472664417	-2.447415975379	3.100085490588
H	0.411906310231	-2.949788380668	2.425566655018
H	-0.701769475330	-3.269116532532	1.074130608728

SCF Done: E(RB3LYP) = -591.943151817

Zero-point correction= 0.184999
Thermal correction to Energy= 0.197233
Thermal correction to Enthalpy= 0.198177
Thermal correction to Gibbs Free Energy= 0.144676
Sum of electronic and zero-point Energies= -591.758152
Sum of electronic and thermal Energies= -591.745919
Sum of electronic and thermal Enthalpies= -591.744975
Sum of electronic and thermal Free Energies= -591.798475

1	C	Isotropic =	39.3103	Anisotropy =	136.8949
2	C	Isotropic =	166.8007	Anisotropy =	14.3032
3	C	Isotropic =	174.9818	Anisotropy =	24.1407
4	H	Isotropic =	30.0310	Anisotropy =	9.8056
5	H	Isotropic =	30.0814	Anisotropy =	8.2111
6	H	Isotropic =	30.3308	Anisotropy =	6.7969
7	H	Isotropic =	28.1324	Anisotropy =	8.7576
8	H	Isotropic =	28.8558	Anisotropy =	7.9613
9	N	Isotropic =	-15.2276	Anisotropy =	342.5875
10	C	Isotropic =	41.9535	Anisotropy =	96.8721
11	H	Isotropic =	23.7163	Anisotropy =	4.1070
12	O	Isotropic =	25.7532	Anisotropy =	257.8392
13	C	Isotropic =	53.2373	Anisotropy =	80.4858
14	C	Isotropic =	36.2594	Anisotropy =	74.6318
15	O	Isotropic =	-42.5037	Anisotropy =	542.4256
16	O	Isotropic =	133.3320	Anisotropy =	148.4375
17	C	Isotropic =	128.2474	Anisotropy =	57.8073
18	C	Isotropic =	176.9614	Anisotropy =	20.0451
19	H	Isotropic =	29.8769	Anisotropy =	7.2129
20	H	Isotropic =	29.8737	Anisotropy =	7.1128
21	H	Isotropic =	30.0287	Anisotropy =	9.7697
22	H	Isotropic =	27.1606	Anisotropy =	6.4348
23	H	Isotropic =	27.1680	Anisotropy =	6.5539



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

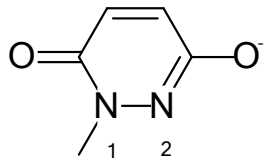
C	1.164304936748	0.780583359536	-0.186729644958
H	2.028262923512	1.439147477954	-0.289452964861
C	-0.131324999075	1.345811373075	0.048003317519
O	-0.217937598092	2.692130136588	0.131019736226
H	-1.152272963752	2.918168935619	0.288984629473
N	-1.212475534490	0.634053341774	0.182788180047
N	-1.101293067219	-0.715456044523	0.094743951921

C	-2.365143058263	-1.429781794550	0.259013977595
H	-2.791926559017	-1.205348110192	1.247739929361
H	-2.158600271546	-2.500534509011	0.169885347362
H	-3.074268215709	-1.112421652467	-0.519760147253
C	0.080699965326	-1.423292507170	-0.129912584191
C	1.256060705122	-0.569853677977	-0.271844848759
H	2.204347451170	-1.078845281096	-0.448830273262
O	0.104306285285	-2.658811047560	-0.198388606220

SCF Done: E(RB3LYP) = -454.111981855

Zero-point correction= 0.112891
Thermal correction to Energy= 0.120864
Thermal correction to Enthalpy= 0.121808
Thermal correction to Gibbs Free Energy= 0.079772
Sum of electronic and zero-point Energies= -453.999091
Sum of electronic and thermal Energies= -453.991118
Sum of electronic and thermal Enthalpies= -453.990174
Sum of electronic and thermal Free Energies= -454.032210

1	C	Isotropic =	69.3251	Anisotropy = 145.9459
2	H	Isotropic =	24.5849	Anisotropy = 5.1867
3	C	Isotropic =	43.7781	Anisotropy = 116.3303
4	O	Isotropic =	219.9799	Anisotropy = 91.1120
5	H	Isotropic =	26.8147	Anisotropy = 12.6933
6	N	Isotropic =	-26.8109	Anisotropy = 288.9499
7	N	Isotropic =	56.9649	Anisotropy = 136.0656
8	C	Isotropic =	156.8563	Anisotropy = 50.1115
9	H	Isotropic =	28.4684	Anisotropy = 8.3599
10	H	Isotropic =	26.8665	Anisotropy = 5.7628
11	H	Isotropic =	28.4686	Anisotropy = 8.3554
12	C	Isotropic =	36.9165	Anisotropy = 112.4909
13	C	Isotropic =	59.9038	Anisotropy = 147.6916
14	H	Isotropic =	24.7586	Anisotropy = 5.3210
15	O	Isotropic =	10.3874	Anisotropy = 485.8567



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

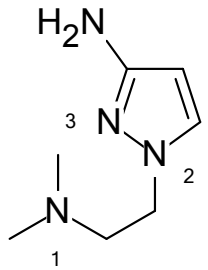
C	-0.236881214707	0.028945968055	0.917799411010
C	0.945269763011	-0.108808046262	1.566012985593
C	2.051425326552	-0.821908826392	0.945524006483
N	1.751551624049	-1.320537737989	-0.298403654337
N	0.567956050378	-1.204080290167	-1.002340449897
C	-0.454201921703	-0.532512607927	-0.423834214207

O	3.181587192025	-0.985680228875	1.465290424412
O	-1.565909233291	-0.389665712763	-1.012542057339
C	2.800557299115	-2.052085475230	-0.998359866060
H	-1.077311442926	0.564898528947	1.370647088052
H	1.125019657989	0.302288517344	2.562793322904
H	3.206260949227	-2.850945984927	-0.359112812861
H	2.355075354387	-2.475157644511	-1.905081148374
H	3.637270595894	-1.386110459302	-1.268883035378

SCF Done: E(RB3LYP) = -453.625727425

Zero-point correction= 0.099653
Thermal correction to Energy= 0.107380
Thermal correction to Enthalpy= 0.108324
Thermal correction to Gibbs Free Energy= 0.066544
Sum of electronic and zero-point Energies= -453.526075
Sum of electronic and thermal Energies= -453.518347
Sum of electronic and thermal Enthalpies= -453.517403
Sum of electronic and thermal Free Energies= -453.559183

1	C	Isotropic =	57.5956	Anisotropy =	128.6262
2	C	Isotropic =	65.8148	Anisotropy =	127.8786
3	C	Isotropic =	37.7299	Anisotropy =	120.8837
4	N	Isotropic =	61.4205	Anisotropy =	127.3519
5	N	Isotropic =	-23.2594	Anisotropy =	224.8971
6	C	Isotropic =	33.3568	Anisotropy =	120.3648
7	O	Isotropic =	32.2286	Anisotropy =	452.3914
8	O	Isotropic =	77.7517	Anisotropy =	357.0060
9	C	Isotropic =	149.7354	Anisotropy =	55.1064
10	H	Isotropic =	25.3085	Anisotropy =	5.7652
11	H	Isotropic =	25.3982	Anisotropy =	5.2435
12	H	Isotropic =	27.8971	Anisotropy =	7.7777
13	H	Isotropic =	28.5519	Anisotropy =	6.0919
14	H	Isotropic =	28.1101	Anisotropy =	8.4131



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.591165286542	-3.612584111425	-0.002275313058

H	2.275940237852	-4.261530288969	0.536736632920
C	1.533470493039	-3.364652046066	-1.401019374597
N	2.401286935183	-3.847495386753	-2.386072323681
H	1.980304774333	-3.794437268156	-3.312884602433
H	2.694611220617	-4.806521260815	-2.208734506943
N	0.546863121415	-2.516028026985	-1.709823448672
N	-0.037396919674	-2.209909650028	-0.515717397583
C	-1.120452886515	-1.242325069906	-0.471367803649
H	-1.832985185680	-1.504728544174	-1.266969215061
C	-0.617664712583	0.200161416527	-0.632324806711
H	-0.038628213675	0.280586295311	-1.579191075835
H	0.082668161647	0.409317378890	0.191643238307
N	-1.709992486371	1.169055840937	-0.562486924527
C	-1.224980450915	2.495997892292	-0.198066539124
H	-2.076382572566	3.188393332467	-0.103493566865
H	-0.521534182107	2.926127756642	-0.947762702517
H	-0.705362660158	2.455752494274	0.771900737633
C	-2.478239185323	1.228138135346	-1.802235271322
H	-1.871196144945	1.579602554604	-2.668310517725
H	-3.326929104436	1.919086174443	-1.679964141329
H	-2.887585622193	0.239266326566	-2.056217249803
H	-1.633941896258	-1.350644050212	0.494136207101
C	0.561706689117	-2.845092061618	0.521679189917
H	0.214065303655	-2.712997833191	1.543560775557

SCF Done: E(RB3LYP) = -494.177261421

Zero-point correction= 0.216263
Thermal correction to Energy= 0.228049
Thermal correction to Enthalpy= 0.228993
Thermal correction to Gibbs Free Energy= 0.177619
Sum of electronic and zero-point Energies= -493.960999
Sum of electronic and thermal Energies= -493.949212
Sum of electronic and thermal Enthalpies= -493.948268
Sum of electronic and thermal Free Energies= -493.999643

1	C	Isotropic =	101.9467	Anisotropy =	88.2923
2	H	Isotropic =	25.9729	Anisotropy =	2.5878
3	C	Isotropic =	38.9183	Anisotropy =	119.7566
4	N	Isotropic =	214.1352	Anisotropy =	73.7680
5	H	Isotropic =	28.4452	Anisotropy =	11.5364
6	H	Isotropic =	28.7220	Anisotropy =	12.2477
7	N	Isotropic =	-11.9065	Anisotropy =	238.6591
8	N	Isotropic =	60.1339	Anisotropy =	109.6679
9	C	Isotropic =	139.9875	Anisotropy =	54.4942
10	H	Isotropic =	27.5028	Anisotropy =	5.0676
11	C	Isotropic =	130.2787	Anisotropy =	65.8486
12	H	Isotropic =	29.1352	Anisotropy =	5.8589
13	H	Isotropic =	29.1043	Anisotropy =	5.8421
14	N	Isotropic =	224.4526	Anisotropy =	37.9133
15	C	Isotropic =	143.9043	Anisotropy =	69.8553
16	H	Isotropic =	29.1488	Anisotropy =	9.9003
17	H	Isotropic =	29.3813	Anisotropy =	8.3524
18	H	Isotropic =	29.1240	Anisotropy =	9.2921
19	C	Isotropic =	148.9382	Anisotropy =	62.0026
20	H	Isotropic =	29.7329	Anisotropy =	8.1187

21	H	Isotropic =	29.2192	Anisotropy =	9.5552
22	H	Isotropic =	28.8498	Anisotropy =	7.9469
23	H	Isotropic =	27.8788	Anisotropy =	4.2697
24	C	Isotropic =	63.1381	Anisotropy =	107.6258
25	H	Isotropic =	24.2736	Anisotropy =	4.2100

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.234852340890	-3.160431089151	1.065552851230
H	1.619838264595	-3.628592431995	1.967330510258
C	0.498507995093	-3.762525695666	0.008814950174
N	0.040088899636	-5.082018636603	-0.063444137484
H	-0.174492232793	-5.350659467053	-1.023008251027
H	0.705916084064	-5.746446895236	0.326867893321
N	0.202742083530	-2.878571215021	-0.950378424777
N	0.743941941343	-1.702385543510	-0.520881970343
C	0.543820247849	-0.492295446979	-1.299902197752
H	1.279322076768	0.252879042802	-0.966086462102
C	-0.876143760912	0.071355780371	-1.140990229446
H	-1.029377147923	0.310390140180	-0.076747754890
H	-1.612874053712	-0.719514757715	-1.405642511540
N	-1.068344234062	1.294551662597	-1.918223945436
C	-1.267404555326	1.021722359615	-3.338438482484
H	-1.342035929581	1.970848526571	-3.891782088976
H	-2.193186296090	0.434002797065	-3.537512632739
H	-0.416202113345	0.461226327259	-3.752322731591
C	-2.170502171569	2.092941556185	-1.392323150704
H	-3.153505901575	1.570831189686	-1.446619984794
H	-2.257185034339	3.029070092729	-1.966269292471
H	-1.980857728780	2.352140975860	-0.339138295764
H	0.758068490446	-0.735247026778	-2.350811903727
C	1.364195563583	-1.835191120638	0.677578462964
H	1.852407172211	-0.991231124577	1.159219780099

SCF Done: E(RB3LYP) = -494.177292828

Zero-point correction= 0.216307
Thermal correction to Energy= 0.228080
Thermal correction to Enthalpy= 0.229024
Thermal correction to Gibbs Free Energy= 0.177672
Sum of electronic and zero-point Energies= -493.960986
Sum of electronic and thermal Energies= -493.949213
Sum of electronic and thermal Enthalpies= -493.948269
Sum of electronic and thermal Free Energies= -493.999621

1	C	Isotropic =	101.8247	Anisotropy =	88.3537
2	H	Isotropic =	25.9699	Anisotropy =	2.5860
3	C	Isotropic =	38.8895	Anisotropy =	119.5932
4	N	Isotropic =	214.0989	Anisotropy =	73.6718
5	H	Isotropic =	28.4461	Anisotropy =	11.5305
6	H	Isotropic =	28.7209	Anisotropy =	12.2476
7	N	Isotropic =	-11.9498	Anisotropy =	238.3234

8	N	Isotropic =	60.1845	Anisotropy =	109.5203
9	C	Isotropic =	139.9869	Anisotropy =	54.6057
10	H	Isotropic =	27.8743	Anisotropy =	4.2902
11	C	Isotropic =	130.0230	Anisotropy =	66.0967
12	H	Isotropic =	29.0950	Anisotropy =	5.8617
13	H	Isotropic =	29.1491	Anisotropy =	5.8857
14	N	Isotropic =	224.5090	Anisotropy =	37.8900
15	C	Isotropic =	148.8874	Anisotropy =	62.0604
16	H	Isotropic =	29.2214	Anisotropy =	9.5575
17	H	Isotropic =	29.7368	Anisotropy =	8.1068
18	H	Isotropic =	28.8443	Anisotropy =	7.9459
19	C	Isotropic =	143.9009	Anisotropy =	69.8118
20	H	Isotropic =	29.3856	Anisotropy =	8.3435
21	H	Isotropic =	29.1520	Anisotropy =	9.9032
22	H	Isotropic =	29.1221	Anisotropy =	9.3068
23	H	Isotropic =	27.5079	Anisotropy =	5.0501
24	C	Isotropic =	63.2272	Anisotropy =	107.5008
25	H	Isotropic =	24.2731	Anisotropy =	4.2168

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	2.907128638800	-1.294234601532	-0.762471637227
H	3.950918723322	-1.564904972908	-0.895702468969
C	2.258169028197	-0.853586577791	0.423466283417
N	2.811235422149	-0.740784150175	1.702942277319
H	2.256828704675	-0.125175986257	2.296751941986
H	3.773006429877	-0.406541714812	1.682700469953
N	0.962340018463	-0.600865806411	0.210146327151
N	0.764710377377	-0.878255409599	-1.110704509710
C	-0.567014114467	-0.760357151025	-1.679285722812
H	-0.976937320432	0.229320599610	-1.424735456319
C	-1.512917725384	-1.849407184081	-1.152403073067
H	-1.502970101225	-1.790057922940	-0.053700255382
H	-1.110969050101	-2.851874965343	-1.428217766386
N	-2.885574602789	-1.656783118383	-1.611655897325
C	-3.833918832304	-2.377797411308	-0.769381804625
H	-3.689951579015	-3.482567833535	-0.795337638768
H	-4.862184789250	-2.166912800874	-1.103203945291
H	-3.736926162291	-2.047067303216	0.276332388547
C	-3.060053239525	-2.027400678308	-3.012611367859
H	-4.095054043244	-1.818906682689	-3.325285543415
H	-2.855683415719	-3.106798564873	-3.200851091472
H	-2.392564871884	-1.439166842863	-3.659697682588
H	-0.455496271541	-0.811724199326	-2.770828344277
C	1.903118223980	-1.293874719254	-1.718928799577
H	1.919000552331	-1.552034002107	-2.775166683304

SCF Done: E(RB3LYP) = -494.177609325

Zero-point correction= 0.216136
Thermal correction to Energy= 0.227994
Thermal correction to Enthalpy= 0.228939

Thermal correction to Gibbs Free Energy= 0.176946
Sum of electronic and zero-point Energies= -493.961473
Sum of electronic and thermal Energies= -493.949615
Sum of electronic and thermal Enthalpies= -493.948671
Sum of electronic and thermal Free Energies= -494.000664

1	C	Isotropic =	102.3860	Anisotropy =	87.7754
2	H	Isotropic =	26.0104	Anisotropy =	2.6011
3	C	Isotropic =	38.6295	Anisotropy =	119.8636
4	N	Isotropic =	213.8381	Anisotropy =	74.0150
5	H	Isotropic =	28.4220	Anisotropy =	11.5522
6	H	Isotropic =	28.7090	Anisotropy =	12.2315
7	N	Isotropic =	-10.6952	Anisotropy =	242.8758
8	N	Isotropic =	60.6860	Anisotropy =	109.4580
9	C	Isotropic =	139.4579	Anisotropy =	51.1299
10	H	Isotropic =	27.7227	Anisotropy =	4.6954
11	C	Isotropic =	130.2624	Anisotropy =	65.5234
12	H	Isotropic =	28.6046	Anisotropy =	7.8643
13	H	Isotropic =	29.5296	Anisotropy =	4.0136
14	N	Isotropic =	223.4406	Anisotropy =	38.4373
15	C	Isotropic =	143.8704	Anisotropy =	69.9375
16	H	Isotropic =	29.3947	Anisotropy =	8.3258
17	H	Isotropic =	29.1206	Anisotropy =	9.8670
18	H	Isotropic =	29.0715	Anisotropy =	9.2102
19	C	Isotropic =	148.8894	Anisotropy =	62.2070
20	H	Isotropic =	29.2151	Anisotropy =	9.5770
21	H	Isotropic =	29.7890	Anisotropy =	8.1810
22	H	Isotropic =	28.9328	Anisotropy =	8.2786
23	H	Isotropic =	27.6574	Anisotropy =	4.9236
24	C	Isotropic =	63.2434	Anisotropy =	106.1538
25	H	Isotropic =	24.3338	Anisotropy =	4.1505

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.176321767684	-3.762886407829	-2.530478818851
H	0.047144548190	-4.760665166487	-2.940702097018
C	0.320509256447	-2.535474766666	-3.233581849409
N	0.254027948938	-2.335603349357	-4.616073634623
H	0.688438522887	-1.454337397839	-4.887439933251
H	0.685965959502	-3.094848906233	-5.139648025703
N	0.469693099866	-1.503503525884	-2.396015517004
N	0.420082833361	-2.054877054288	-1.149457739396
C	0.502581464374	-1.197595827080	0.020477177197
H	0.664989380897	-1.852764123384	0.886937594716
C	-0.756090198824	-0.333819677364	0.188418274962
H	-1.643290748432	-0.996565248200	0.316661691910
H	-0.902415710802	0.220602983189	-0.750793539982
N	-0.621498368040	0.631611672838	1.275195660330
C	-0.728167220258	0.008990508184	2.590976023813
H	-1.723717531330	-0.460735669738	2.766163054161
H	-0.569024328593	0.767079270745	3.373597017341
H	0.039620323159	-0.768127114801	2.720386268484

C	-1.586232938589	1.718069377788	1.143208416401
H	-2.644071554885	1.374935393137	1.215712774100
H	-1.457936218343	2.220357065437	0.171807576643
H	-1.420606546909	2.460958246793	1.939415307554
H	1.380869145815	-0.541167127077	-0.079852525238
C	0.246331548325	-3.398876678478	-1.194269675421
H	0.191065565563	-3.993416477409	-0.285433481715

SCF Done: E(RB3LYP) = -494.177607917

Zero-point correction= 0.216183
Thermal correction to Energy= 0.228006
Thermal correction to Enthalpy= 0.228950
Thermal correction to Gibbs Free Energy= 0.177273
Sum of electronic and zero-point Energies= -493.961425
Sum of electronic and thermal Energies= -493.949602
Sum of electronic and thermal Enthalpies= -493.948658
Sum of electronic and thermal Free Energies= -494.000335

1	C	Isotropic =	102.5295	Anisotropy =	88.5881
2	H	Isotropic =	25.9963	Anisotropy =	2.6042
3	C	Isotropic =	38.5944	Anisotropy =	120.0578
4	N	Isotropic =	213.8557	Anisotropy =	73.9135
5	H	Isotropic =	28.4246	Anisotropy =	11.5605
6	H	Isotropic =	28.7031	Anisotropy =	12.2404
7	N	Isotropic =	-10.8632	Anisotropy =	242.6322
8	N	Isotropic =	60.6802	Anisotropy =	109.3085
9	C	Isotropic =	139.4093	Anisotropy =	51.0302
10	H	Isotropic =	27.6543	Anisotropy =	4.9462
11	C	Isotropic =	130.4210	Anisotropy =	65.3166
12	H	Isotropic =	29.5200	Anisotropy =	3.9814
13	H	Isotropic =	28.6116	Anisotropy =	7.8570
14	N	Isotropic =	223.4548	Anisotropy =	38.2784
15	C	Isotropic =	149.0134	Anisotropy =	62.0454
16	H	Isotropic =	29.7869	Anisotropy =	8.2030
17	H	Isotropic =	29.2149	Anisotropy =	9.5728
18	H	Isotropic =	28.9360	Anisotropy =	8.2692
19	C	Isotropic =	143.9075	Anisotropy =	69.9002
20	H	Isotropic =	29.3941	Anisotropy =	8.3354
21	H	Isotropic =	29.0692	Anisotropy =	9.2049
22	H	Isotropic =	29.1168	Anisotropy =	9.8601
23	H	Isotropic =	27.7315	Anisotropy =	4.6741
24	C	Isotropic =	63.1618	Anisotropy =	106.0789
25	H	Isotropic =	24.3265	Anisotropy =	4.1528

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.749802967498	-2.417542131668	-0.037392477707
H	-3.710343496402	-2.574062357570	0.445682179969
C	-2.425175785505	-2.560006136001	-1.414372940553
N	-3.296104330106	-2.865319835488	-2.465277649301
H	-2.791509272177	-3.214303626047	-3.279274438953

H	-4.005613319310	-3.544937794564	-2.197197070370
N	-1.135289859200	-2.293068648601	-1.645746611467
N	-0.619414876904	-1.974688381516	-0.423860777123
C	0.773357243696	-1.576317782661	-0.312582539394
H	1.027664919817	-1.593456193650	0.755828018424
C	1.025889553200	-0.195830784291	-0.935957324763
H	0.417785865797	0.568197674833	-0.398138406909
H	0.655660120542	-0.230401076063	-1.971648878294
N	2.445200964090	0.145235246538	-0.967091165228
C	2.961421942360	0.506539625870	0.349354881562
H	2.819838774033	-0.316432034238	1.065526798061
H	2.471782880934	1.415082376266	0.770432196029
H	4.042294768870	0.705437332185	0.281292858562
C	2.714796512021	1.205805168133	-1.931868563493
H	2.378675299053	0.898084419959	-2.934222268390
H	3.797953766060	1.400818971249	-1.976572203938
H	2.208437198119	2.165876961078	-1.679207985772
H	1.398948213403	-2.324104206648	-0.824120059867
C	-1.554771909231	-2.039402802083	0.555708982683
H	-1.306492205664	-1.819343985024	1.591325446230

SCF Done: E(RB3LYP) = -494.177614253

Zero-point correction= 0.216205
Thermal correction to Energy= 0.228004
Thermal correction to Enthalpy= 0.228949
Thermal correction to Gibbs Free Energy= 0.177425
Sum of electronic and zero-point Energies= -493.961409
Sum of electronic and thermal Energies= -493.949610
Sum of electronic and thermal Enthalpies= -493.948666
Sum of electronic and thermal Free Energies= -494.000190

1	C	Isotropic =	102.3701	Anisotropy =	87.9424
2	H	Isotropic =	26.0027	Anisotropy =	2.6083
3	C	Isotropic =	38.5398	Anisotropy =	119.6947
4	N	Isotropic =	213.7292	Anisotropy =	74.0307
5	H	Isotropic =	28.4201	Anisotropy =	11.5572
6	H	Isotropic =	28.7040	Anisotropy =	12.2309
7	N	Isotropic =	-10.8476	Anisotropy =	242.2152
8	N	Isotropic =	60.6543	Anisotropy =	109.3094
9	C	Isotropic =	139.3430	Anisotropy =	50.9119
10	H	Isotropic =	27.6482	Anisotropy =	4.9275
11	C	Isotropic =	130.4175	Anisotropy =	65.4363
12	H	Isotropic =	29.5157	Anisotropy =	3.9776
13	H	Isotropic =	28.6292	Anisotropy =	7.8571
14	N	Isotropic =	223.0378	Anisotropy =	38.6585
15	C	Isotropic =	148.9220	Anisotropy =	62.1488
16	H	Isotropic =	28.9399	Anisotropy =	8.2544
17	H	Isotropic =	29.7822	Anisotropy =	8.2060
18	H	Isotropic =	29.2145	Anisotropy =	9.5738
19	C	Isotropic =	143.9081	Anisotropy =	70.0101
20	H	Isotropic =	29.0708	Anisotropy =	9.2034
21	H	Isotropic =	29.1132	Anisotropy =	9.8605
22	H	Isotropic =	29.3966	Anisotropy =	8.3315
23	H	Isotropic =	27.7361	Anisotropy =	4.6602
24	C	Isotropic =	63.0771	Anisotropy =	106.2296

25 H Isotropic = 24.3250 Anisotropy = 4.1622

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.782184065326	-0.366049854299	-3.625271856863
H	-0.823763638683	0.161186946146	-4.574421157438
C	-0.936033961695	-1.758662909591	-3.386823538089
N	-1.101486116904	-2.771234620152	-4.337843478902
H	-1.492652993363	-3.614716061224	-3.920040635599
H	-1.692233950514	-2.480956674305	-5.115003838802
N	-0.835025693873	-2.048786438576	-2.084642035326
N	-0.615886803489	-0.848657125714	-1.474598244999
C	-0.382053742005	-0.804435712309	-0.040735223834
H	-0.488153793387	0.242774468678	0.275010900376
C	1.014992388589	-1.361325562679	0.323566068794
H	1.774662234769	-0.738173649088	-0.179883833690
H	1.092415943206	-2.375014138004	-0.102829656443
N	1.345405835087	-1.431639570545	1.740473491624
C	0.555069270018	-2.391934066921	2.497763095990
H	1.008811794539	-2.537983937209	3.491976631828
H	0.550981583581	-3.364007230349	1.979441942038
H	-0.502834696399	-2.087593686416	2.662355069683
C	1.436571314960	-0.138270385782	2.402663820068
H	2.078372636853	0.538020311110	1.815577323086
H	1.895434528972	-0.265468829260	3.397026430772
H	0.457008538149	0.367930586356	2.556476325708
H	-1.174481444136	-1.389921578888	0.449413695111
C	-0.576400970621	0.173944094025	-2.363936649057
H	-0.414584198327	1.199615624996	-2.040904646037

SCF Done: E(RB3LYP) = -494.175981074

Zero-point correction= 0.216288
Thermal correction to Energy= 0.228109
Thermal correction to Enthalpy= 0.229053
Thermal correction to Gibbs Free Energy= 0.177724
Sum of electronic and zero-point Energies= -493.959693
Sum of electronic and thermal Energies= -493.947872
Sum of electronic and thermal Enthalpies= -493.946928
Sum of electronic and thermal Free Energies= -493.998257

1 C Isotropic = 102.2114 Anisotropy = 87.7713
2 H Isotropic = 26.0015 Anisotropy = 2.6177
3 C Isotropic = 38.6996 Anisotropy = 119.4356
4 N Isotropic = 214.0042 Anisotropy = 74.1048
5 H Isotropic = 28.4447 Anisotropy = 11.5217
6 H Isotropic = 28.7340 Anisotropy = 12.2363
7 N Isotropic = -11.1945 Anisotropy = 240.6509
8 N Isotropic = 60.7609 Anisotropy = 108.9995
9 C Isotropic = 147.5923 Anisotropy = 53.2988
10 H Isotropic = 27.6892 Anisotropy = 5.4295
11 C Isotropic = 131.8700 Anisotropy = 58.7815

12	H	Isotropic =	28.7360	Anisotropy =	4.5903
13	H	Isotropic =	28.3578	Anisotropy =	6.4001
14	N	Isotropic =	230.9579	Anisotropy =	30.9262
15	C	Isotropic =	149.9015	Anisotropy =	61.2411
16	H	Isotropic =	29.0912	Anisotropy =	9.5140
17	H	Isotropic =	28.9910	Anisotropy =	8.6796
18	H	Isotropic =	28.8898	Anisotropy =	7.5472
19	C	Isotropic =	149.9307	Anisotropy =	60.9346
20	H	Isotropic =	29.0384	Anisotropy =	8.7858
21	H	Isotropic =	29.1000	Anisotropy =	9.5683
22	H	Isotropic =	28.9600	Anisotropy =	7.6972
23	H	Isotropic =	27.4673	Anisotropy =	5.8342
24	C	Isotropic =	63.4136	Anisotropy =	106.6092
25	H	Isotropic =	24.3322	Anisotropy =	4.2459

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.493613065499	0.373307798374	-1.751187398452
H	2.318848589058	1.068608625740	-1.623561588436
C	1.367054179404	-0.674103582911	-2.704292476446
N	2.317806222586	-1.087330433728	-3.643965555935
H	1.888893293925	-1.624530615539	-4.396628681930
H	2.831344994552	-0.304985347441	-4.045798263249
N	0.201967539994	-1.318091753092	-2.575569224320
N	-0.432726647546	-0.689200853234	-1.544446064728
C	-1.691028685352	-1.220454047412	-1.048584836737
H	-2.208327672326	-0.409687495417	-0.516650469731
C	-1.509222194844	-2.451516279610	-0.152040527110
H	-0.897472459846	-3.178838086945	-0.707398428506
H	-2.507770308260	-2.919899598373	0.006423826854
N	-0.835459909833	-2.149988172722	1.108825539174
C	-0.207416179170	-3.335117803519	1.682019364185
H	-0.939350082159	-4.129791962558	1.955530411119
H	0.342171336016	-3.059322392372	2.596001958466
H	0.510154525055	-3.765713293000	0.966548228409
C	-1.728941106168	-1.522920030192	2.076217478476
H	-2.167426478573	-0.601872091201	1.663773315959
H	-1.164371609432	-1.246612080976	2.980363274939
H	-2.566707630197	-2.190487049588	2.384437322169
H	-2.305566393921	-1.493495394547	-1.919172288231
C	0.312844593520	0.315724165564	-1.025731318458
H	-0.045050981979	0.913547774697	-0.191623597482

SCF Done: E(RB3LYP) = -494.178400192

Zero-point correction= 0.216374
Thermal correction to Energy= 0.228030
Thermal correction to Enthalpy= 0.228974
Thermal correction to Gibbs Free Energy= 0.177834
Sum of electronic and zero-point Energies= -493.962026
Sum of electronic and thermal Energies= -493.950370
Sum of electronic and thermal Enthalpies= -493.949426

Sum of electronic and thermal Free Energies= -494.000566

1	C	Isotropic =	102.3746	Anisotropy =	87.1663
2	H	Isotropic =	26.0009	Anisotropy =	2.7432
3	C	Isotropic =	38.8496	Anisotropy =	120.6079
4	N	Isotropic =	214.0212	Anisotropy =	74.5413
5	H	Isotropic =	28.4450	Anisotropy =	11.7421
6	H	Isotropic =	28.7163	Anisotropy =	12.2862
7	N	Isotropic =	-9.8965	Anisotropy =	233.6786
8	N	Isotropic =	58.6445	Anisotropy =	114.7710
9	C	Isotropic =	140.9650	Anisotropy =	47.8934
10	H	Isotropic =	27.6811	Anisotropy =	5.1183
11	C	Isotropic =	131.0944	Anisotropy =	45.4070
12	H	Isotropic =	28.8317	Anisotropy =	6.1380
13	H	Isotropic =	29.4669	Anisotropy =	6.3095
14	N	Isotropic =	227.1865	Anisotropy =	33.0680
15	C	Isotropic =	144.3688	Anisotropy =	69.0925
16	H	Isotropic =	29.4339	Anisotropy =	9.0784
17	H	Isotropic =	29.2351	Anisotropy =	9.9129
18	H	Isotropic =	29.4037	Anisotropy =	8.8652
19	C	Isotropic =	150.1574	Anisotropy =	60.6187
20	H	Isotropic =	28.7787	Anisotropy =	8.0402
21	H	Isotropic =	29.2657	Anisotropy =	9.5804
22	H	Isotropic =	29.9040	Anisotropy =	8.9359
23	H	Isotropic =	27.8006	Anisotropy =	7.4342
24	C	Isotropic =	62.1497	Anisotropy =	110.6221
25	H	Isotropic =	24.3147	Anisotropy =	4.4510

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.253749279040	-1.984128771431	-1.772152289515
H	-3.334498538459	-1.890953228465	-1.836247272210
C	-1.484975223367	-3.160000218353	-1.553066075251
N	-1.960228934178	-4.450909152630	-1.296953671500
H	-1.246805916183	-5.154443938328	-1.484397521863
H	-2.793938379590	-4.671880134103	-1.838587457432
N	-0.173768094252	-2.896910631507	-1.550854270084
N	-0.086352519306	-1.553504195752	-1.774325568235
C	1.210423172676	-0.901479667361	-1.704081694491
H	1.941670843822	-1.567808625814	-2.184477366193
C	1.657514265504	-0.610493590349	-0.265914740951
H	2.734151340846	-0.324311786543	-0.284350115784
H	1.584636732457	-1.551368757804	0.300854458977
N	0.831649281924	0.395017460688	0.399017950271
C	1.170634776787	1.750949164706	-0.018134955402
H	1.080030065454	1.857970267396	-1.109508612282
H	2.207730810748	2.042685625477	0.267673488790
H	0.475910924555	2.468620288390	0.445474448289
C	0.892965009807	0.272613363527	1.851041787378
H	0.211509614958	1.003652515496	2.314373092805
H	1.912460703845	0.453444776158	2.263250929925
H	0.575479650137	-0.735641509890	2.158817024758

H	1.156628308973	0.019647065697	-2.301433732017
C	-1.306670676375	-0.978799165618	-1.899963786796
H	-1.414517941742	0.089042846412	-2.070874051185

SCF Done: E(RB3LYP) = -494.178428405

Zero-point correction= 0.216386
Thermal correction to Energy= 0.228022
Thermal correction to Enthalpy= 0.228966
Thermal correction to Gibbs Free Energy= 0.178017
Sum of electronic and zero-point Energies= -493.962043
Sum of electronic and thermal Energies= -493.950406
Sum of electronic and thermal Enthalpies= -493.949462
Sum of electronic and thermal Free Energies= -494.000411

1	C	Isotropic =	102.0357	Anisotropy =	87.5629
2	H	Isotropic =	25.9800	Anisotropy =	2.7380
3	C	Isotropic =	38.9767	Anisotropy =	120.9750
4	N	Isotropic =	214.1666	Anisotropy =	74.2434
5	H	Isotropic =	28.4546	Anisotropy =	11.7532
6	H	Isotropic =	28.7195	Anisotropy =	12.2890
7	N	Isotropic =	-10.4809	Anisotropy =	231.0062
8	N	Isotropic =	58.6930	Anisotropy =	114.7398
9	C	Isotropic =	140.9613	Anisotropy =	47.6314
10	H	Isotropic =	27.8048	Anisotropy =	7.3635
11	C	Isotropic =	131.1624	Anisotropy =	45.2142
12	H	Isotropic =	29.4613	Anisotropy =	6.3257
13	H	Isotropic =	28.9025	Anisotropy =	6.1518
14	N	Isotropic =	226.9023	Anisotropy =	33.2227
15	C	Isotropic =	150.0961	Anisotropy =	60.4815
16	H	Isotropic =	28.7799	Anisotropy =	8.0311
17	H	Isotropic =	29.8931	Anisotropy =	8.9331
18	H	Isotropic =	29.2580	Anisotropy =	9.5722
19	C	Isotropic =	144.4071	Anisotropy =	69.0391
20	H	Isotropic =	29.2253	Anisotropy =	9.9058
21	H	Isotropic =	29.4213	Anisotropy =	9.0957
22	H	Isotropic =	29.4033	Anisotropy =	8.8472
23	H	Isotropic =	27.6789	Anisotropy =	5.2250
24	C	Isotropic =	62.2337	Anisotropy =	111.4800
25	H	Isotropic =	24.3105	Anisotropy =	4.5117

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.422057424052	-2.992818244718	-2.609419068228
H	0.195745690788	-3.871756868110	-3.206813576425
C	0.680750923470	-1.668635532508	-3.057559393490
N	0.628978140332	-1.189957929914	-4.370534279771
H	1.147737537388	-0.318355897720	-4.471127339758
H	0.980724526184	-1.866653499585	-5.045378411857
N	0.935682745171	-0.844074281604	-2.034582855872
N	0.844670393614	-1.628684791350	-0.922858775574
C	0.998911099663	-1.035119019754	0.395183731834

H	1.125525733896	-1.861758724755	1.108254205419
C	-0.175186240350	-0.150849813580	0.837667881790
H	-0.276117598689	0.704531374064	0.139321332880
H	0.107562526799	0.272060724874	1.814879709051
N	-1.432885444716	-0.891422797824	0.977870465959
C	-2.277001080529	-0.785373649448	-0.208689748991
H	-2.662723121655	0.248347414555	-0.368988496901
H	-3.145138346917	-1.456843420241	-0.110024083958
H	-1.717275536343	-1.079280419716	-1.107019255844
C	-2.176349451894	-0.514189990664	2.174873231331
H	-3.071276811356	-1.150219494343	2.268987912064
H	-2.518294355877	0.546540789740	2.166724908354
H	-1.556506121068	-0.666399875771	3.072000875883
H	1.923272101144	-0.435192255148	0.391878938970
C	0.539761032463	-2.912880296786	-1.229571008924
H	0.427024234430	-3.667583499694	-0.455226897942

SCF Done: E(RB3LYP) = -494.176074013

Zero-point correction= 0.216351
Thermal correction to Energy= 0.228065
Thermal correction to Enthalpy= 0.229009
Thermal correction to Gibbs Free Energy= 0.177701
Sum of electronic and zero-point Energies= -493.959723
Sum of electronic and thermal Energies= -493.948009
Sum of electronic and thermal Enthalpies= -493.947065
Sum of electronic and thermal Free Energies= -493.998373

1	C	Isotropic =	102.0963	Anisotropy =	89.3675
2	H	Isotropic =	25.9798	Anisotropy =	2.7416
3	C	Isotropic =	37.9019	Anisotropy =	121.4886
4	N	Isotropic =	213.8165	Anisotropy =	74.2869
5	H	Isotropic =	28.4046	Anisotropy =	11.7257
6	H	Isotropic =	28.6927	Anisotropy =	12.2875
7	N	Isotropic =	-8.6923	Anisotropy =	242.7311
8	N	Isotropic =	60.1439	Anisotropy =	113.0824
9	C	Isotropic =	135.8679	Anisotropy =	32.1875
10	H	Isotropic =	27.8119	Anisotropy =	6.0868
11	C	Isotropic =	133.4474	Anisotropy =	51.5393
12	H	Isotropic =	28.9159	Anisotropy =	5.1081
13	H	Isotropic =	29.2108	Anisotropy =	6.0242
14	N	Isotropic =	225.7283	Anisotropy =	46.0061
15	C	Isotropic =	146.6896	Anisotropy =	62.4813
16	H	Isotropic =	29.8468	Anisotropy =	7.8428
17	H	Isotropic =	29.6058	Anisotropy =	9.0458
18	H	Isotropic =	30.3296	Anisotropy =	8.0712
19	C	Isotropic =	144.4452	Anisotropy =	68.5270
20	H	Isotropic =	29.3164	Anisotropy =	9.9843
21	H	Isotropic =	29.2750	Anisotropy =	8.8625
22	H	Isotropic =	29.0772	Anisotropy =	9.5553
23	H	Isotropic =	27.6419	Anisotropy =	7.3255
24	C	Isotropic =	62.3285	Anisotropy =	107.9771
25	H	Isotropic =	24.2634	Anisotropy =	3.9832

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.938573087900	-3.348875364118	0.296212947469
H	-1.656972993147	-3.913922295638	0.883774058287
C	0.415324508588	-3.051870500604	0.612487646292
N	1.101317190620	-3.363860519015	1.790383482746
H	2.111027213077	-3.332319154058	1.654801160450
H	0.842836351317	-4.276404420245	2.161125694242
N	1.002637087053	-2.341320183779	-0.357880949210
N	0.034479744520	-2.175691067517	-1.303835469514
C	0.311998130591	-1.383633861246	-2.491060830273
H	1.246548269149	-1.758179864304	-2.939300054896
C	0.445155810746	0.124267278918	-2.237467538752
H	0.725452284926	0.575128908444	-3.202677494299
H	1.290884143280	0.307960770868	-1.543490214126
N	-0.796440048642	0.743013287364	-1.763178503472
C	-0.848270449986	0.847593150286	-0.307773641274
H	-0.094890334178	1.562735183834	0.097305641504
H	-0.667138260054	-0.131405292669	0.155863381794
H	-1.845459942252	1.196630397231	0.005472598155
C	-1.045290855080	2.041084841480	-2.380639482522
H	-1.079332520955	1.941468678828	-3.476632533538
H	-0.275158904401	2.805620879543	-2.126652298954
H	-2.020443710585	2.428723483405	-2.044361191171
H	-0.508858467614	-1.565639936353	-3.198810241889
C	-1.132874247170	-2.763398119732	-0.946178672966
H	-2.007476911903	-2.722396280924	-1.590597494082

SCF Done: E(RB3LYP) = -494.176058528

Zero-point correction= 0.216309
Thermal correction to Energy= 0.228019
Thermal correction to Enthalpy= 0.228963
Thermal correction to Gibbs Free Energy= 0.177819
Sum of electronic and zero-point Energies= -493.959750
Sum of electronic and thermal Energies= -493.948040
Sum of electronic and thermal Enthalpies= -493.947096
Sum of electronic and thermal Free Energies= -493.998240

1	C	Isotropic =	102.2041	Anisotropy =	89.0149
2	H	Isotropic =	25.9921	Anisotropy =	2.7447
3	C	Isotropic =	37.9808	Anisotropy =	121.5133
4	N	Isotropic =	213.7855	Anisotropy =	74.2776
5	H	Isotropic =	28.4025	Anisotropy =	11.7270
6	H	Isotropic =	28.6832	Anisotropy =	12.2914
7	N	Isotropic =	-8.4926	Anisotropy =	243.9511
8	N	Isotropic =	60.2211	Anisotropy =	113.2037
9	C	Isotropic =	135.8349	Anisotropy =	31.9582
10	H	Isotropic =	27.6254	Anisotropy =	7.3399
11	C	Isotropic =	133.4264	Anisotropy =	51.2400
12	H	Isotropic =	29.2095	Anisotropy =	6.0299
13	H	Isotropic =	28.8920	Anisotropy =	5.0710
14	N	Isotropic =	225.0321	Anisotropy =	45.9812
15	C	Isotropic =	146.8562	Anisotropy =	62.3118

16 H Isotropic = 29.8639 Anisotropy = 7.7827
17 H Isotropic = 30.3280 Anisotropy = 8.2274
18 H Isotropic = 29.5979 Anisotropy = 9.0421
19 C Isotropic = 144.2678 Anisotropy = 68.8001
20 H Isotropic = 29.0799 Anisotropy = 9.5589
21 H Isotropic = 29.2857 Anisotropy = 8.8250
22 H Isotropic = 29.3145 Anisotropy = 9.9815
23 H Isotropic = 27.8025 Anisotropy = 6.0011
24 C Isotropic = 62.4552 Anisotropy = 107.8247
25 H Isotropic = 24.2717 Anisotropy = 3.9560

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	2.436144567885	-0.778429357150	-0.379085398429
H	3.400153026372	-0.282077854611	-0.450780980784
C	2.051070803872	-2.031752074984	-0.928489894581
N	2.854884935353	-2.933932110394	-1.635684890777
H	2.290322050143	-3.591754958771	-2.172174081151
H	3.500510977156	-2.462552744494	-2.266940117171
N	0.786410794457	-2.334962402556	-0.618925500539
N	0.349524579102	-1.289240322619	0.139943953653
C	-1.030758142055	-1.250097177792	0.598364537792
H	-1.372859877978	-2.292109713132	0.642827971463
C	-1.959502228129	-0.383587188237	-0.262780284802
H	-1.627480749581	0.664990334357	-0.188155527939
H	-2.972554591391	-0.427961708887	0.206267184563
N	-1.991694840834	-0.736845300201	-1.677252687336
C	-2.710249011060	0.274570159822	-2.442819324998
H	-2.669657624643	0.029226995484	-3.515705796624
H	-2.241989128398	1.260993393182	-2.297661124126
H	-3.783927762884	0.361937216278	-2.154837472949
C	-2.545012312104	-2.064339584266	-1.917962579943
H	-3.582033198070	-2.182288304230	-1.525200306359
H	-1.907225911811	-2.834430454458	-1.461580868191
H	-2.572663601381	-2.256270706163	-3.001852363206
H	-1.047222322334	-0.854988797853	1.625571201217
C	1.305332345232	-0.340565462746	0.294119609869
H	1.121687223084	0.562848124419	0.871164741349

SCF Done: E(RB3LYP) = -494.176731523

Zero-point correction= 0.216461
Thermal correction to Energy= 0.228036
Thermal correction to Enthalpy= 0.228980
Thermal correction to Gibbs Free Energy= 0.178443
Sum of electronic and zero-point Energies= -493.960271
Sum of electronic and thermal Energies= -493.948696
Sum of electronic and thermal Enthalpies= -493.947752
Sum of electronic and thermal Free Energies= -493.998288

1 C Isotropic = 100.3391 Anisotropy = 90.0139
2 H Isotropic = 25.8297 Anisotropy = 2.4105

3	C	Isotropic =	40.4459	Anisotropy =	119.4943
4	N	Isotropic =	215.0461	Anisotropy =	73.7348
5	H	Isotropic =	28.5002	Anisotropy =	11.1829
6	H	Isotropic =	28.7775	Anisotropy =	12.0562
7	N	Isotropic =	-17.8189	Anisotropy =	227.2034
8	N	Isotropic =	57.2673	Anisotropy =	113.2413
9	C	Isotropic =	141.6242	Anisotropy =	53.0757
10	H	Isotropic =	27.4297	Anisotropy =	4.4697
11	C	Isotropic =	129.3323	Anisotropy =	44.1686
12	H	Isotropic =	28.7422	Anisotropy =	6.5964
13	H	Isotropic =	29.4583	Anisotropy =	6.3118
14	N	Isotropic =	225.8694	Anisotropy =	32.4411
15	C	Isotropic =	144.2060	Anisotropy =	70.3105
16	H	Isotropic =	29.2456	Anisotropy =	9.9244
17	H	Isotropic =	29.3303	Anisotropy =	9.4431
18	H	Isotropic =	29.5465	Anisotropy =	8.9988
19	C	Isotropic =	150.7209	Anisotropy =	58.6907
20	H	Isotropic =	29.9794	Anisotropy =	8.6733
21	H	Isotropic =	28.3617	Anisotropy =	7.1324
22	H	Isotropic =	29.3819	Anisotropy =	9.1763
23	H	Isotropic =	27.7174	Anisotropy =	7.3819
24	C	Isotropic =	64.9390	Anisotropy =	114.9300
25	H	Isotropic =	24.1837	Anisotropy =	4.5256

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.360592046783	-3.196858718272	0.894485655005
H	-0.856231605032	-3.868839993577	1.589911261738
C	0.120160212249	-3.484152347958	-0.412163491402
N	0.112895544620	-4.720765343805	-1.068434880427
H	0.222927637418	-4.606731920480	-2.075486549397
H	-0.739490647209	-5.248333338846	-0.887761593636
N	0.695642185217	-2.413794922153	-0.969195875377
N	0.602931643000	-1.433504003088	-0.025448972470
C	1.062976567192	-0.087250427879	-0.329715471426
H	1.549155099195	0.327794721021	0.566359717187
C	-0.049089878552	0.877737985945	-0.762104810963
H	0.433611901429	1.867983966437	-0.947640225868
H	-0.737557748648	1.020096151273	0.087016558325
N	-0.840910629178	0.429406786558	-1.901675495052
C	-0.061263533926	0.332255353094	-3.130079857952
H	0.417871095238	1.296750780567	-3.419454958528
H	-0.720340171645	0.023627949076	-3.956435429418
H	0.721733298127	-0.432355344641	-3.027421925115
C	-2.004145812959	1.288403436069	-2.087908114892
H	-2.613731868105	1.302295285998	-1.170484713170
H	-2.627164264567	0.900398513870	-2.909036724533
H	-1.736179171337	2.342501411629	-2.333898684379
H	1.834966556728	-0.190220937960	-1.103178534250
C	-0.030252087473	-1.864480020148	1.092936286475
H	-0.192152274999	-1.206515022728	1.943646829525

SCF Done: E(RB3LYP) = -494.176723580

Zero-point correction= 0.216349
Thermal correction to Energy= 0.228010
Thermal correction to Enthalpy= 0.228954
Thermal correction to Gibbs Free Energy= 0.177722
Sum of electronic and zero-point Energies= -493.960375
Sum of electronic and thermal Energies= -493.948714
Sum of electronic and thermal Enthalpies= -493.947769
Sum of electronic and thermal Free Energies= -493.999001

1	C	Isotropic =	100.2941	Anisotropy =	89.9367
2	H	Isotropic =	25.8287	Anisotropy =	2.4118
3	C	Isotropic =	40.2941	Anisotropy =	119.1889
4	N	Isotropic =	215.2126	Anisotropy =	73.4370
5	H	Isotropic =	28.4961	Anisotropy =	11.2038
6	H	Isotropic =	28.7748	Anisotropy =	12.0585
7	N	Isotropic =	-17.8315	Anisotropy =	227.7515
8	N	Isotropic =	57.2341	Anisotropy =	113.1852
9	C	Isotropic =	141.5625	Anisotropy =	53.0245
10	H	Isotropic =	27.7245	Anisotropy =	7.3804
11	C	Isotropic =	129.2713	Anisotropy =	43.9563
12	H	Isotropic =	29.4653	Anisotropy =	6.3123
13	H	Isotropic =	28.7608	Anisotropy =	6.5806
14	N	Isotropic =	225.5938	Anisotropy =	32.3103
15	C	Isotropic =	150.6927	Anisotropy =	58.7123
16	H	Isotropic =	29.9808	Anisotropy =	8.6791
17	H	Isotropic =	29.3822	Anisotropy =	9.1772
18	H	Isotropic =	28.3483	Anisotropy =	7.1024
19	C	Isotropic =	144.2035	Anisotropy =	70.5039
20	H	Isotropic =	29.3381	Anisotropy =	9.4390
21	H	Isotropic =	29.2446	Anisotropy =	9.9283
22	H	Isotropic =	29.5421	Anisotropy =	9.0085
23	H	Isotropic =	27.4333	Anisotropy =	4.4768
24	C	Isotropic =	64.8814	Anisotropy =	114.7961
25	H	Isotropic =	24.1946	Anisotropy =	4.5071

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	2.157484142763	-0.837523313542	0.012739921408
H	2.831890750053	-0.353108446611	0.713621985791
C	2.029670333661	-2.225918410672	-0.266457502697
N	2.795442029033	-3.272345608714	0.259174755439
H	2.323115759751	-4.169385139402	0.152447618429
H	3.020738124469	-3.130941393413	1.242300660049
N	1.103492340615	-2.455604027519	-1.203487029695
N	0.641590822489	-1.219241712035	-1.549040373951
C	-0.475709860021	-1.106429088307	-2.471299891720
H	-0.462298745075	-0.089262655861	-2.887414815980
C	-1.825762962784	-1.429768235164	-1.818924527289
H	-1.733524445403	-2.416915265835	-1.340922706832
H	-2.588661612976	-1.528559988425	-2.625155848260

N	-2.222012978644	-0.460436696035	-0.800140279123
C	-2.750432881406	0.768325846396	-1.381803987102
H	-2.015884942414	1.226733215437	-2.060639050726
H	-2.965405900800	1.495923031919	-0.583690829438
H	-3.690011207269	0.602562622153	-1.958024233145
C	-3.172793711378	-1.031600044179	0.146834643493
H	-3.401937274860	-0.295013293915	0.933190929052
H	-2.738803849537	-1.922382346395	0.626833193622
H	-4.136444156616	-1.331033098118	-0.326236800149
H	-0.298217314655	-1.807787835255	-3.300046012433
C	1.234571828920	-0.236131001855	-0.830084901437
H	0.966085712086	0.807722885346	-0.970004917306

SCF Done: E(RB3LYP) = -494.178448600

Zero-point correction= 0.216578
Thermal correction to Energy= 0.228152
Thermal correction to Enthalpy= 0.229096
Thermal correction to Gibbs Free Energy= 0.178444
Sum of electronic and zero-point Energies= -493.961870
Sum of electronic and thermal Energies= -493.950297
Sum of electronic and thermal Enthalpies= -493.949352
Sum of electronic and thermal Free Energies= -494.000005

1	C	Isotropic =	102.0950	Anisotropy =	87.1273
2	H	Isotropic =	25.9835	Anisotropy =	2.6509
3	C	Isotropic =	38.8567	Anisotropy =	120.9478
4	N	Isotropic =	213.8757	Anisotropy =	74.4894
5	H	Isotropic =	28.4376	Anisotropy =	11.5358
6	H	Isotropic =	28.7220	Anisotropy =	11.8472
7	N	Isotropic =	-9.8126	Anisotropy =	234.8761
8	N	Isotropic =	58.5394	Anisotropy =	112.9049
9	C	Isotropic =	140.8963	Anisotropy =	47.8855
10	H	Isotropic =	27.6978	Anisotropy =	5.2208
11	C	Isotropic =	131.0522	Anisotropy =	45.3698
12	H	Isotropic =	28.8114	Anisotropy =	6.1384
13	H	Isotropic =	29.4631	Anisotropy =	6.3005
14	N	Isotropic =	226.5798	Anisotropy =	32.3000
15	C	Isotropic =	150.1292	Anisotropy =	60.6434
16	H	Isotropic =	28.7953	Anisotropy =	8.0898
17	H	Isotropic =	29.2846	Anisotropy =	9.5507
18	H	Isotropic =	29.9009	Anisotropy =	8.9467
19	C	Isotropic =	144.3659	Anisotropy =	69.2934
20	H	Isotropic =	29.2554	Anisotropy =	9.8660
21	H	Isotropic =	29.4188	Anisotropy =	8.9025
22	H	Isotropic =	29.4317	Anisotropy =	9.0770
23	H	Isotropic =	27.8190	Anisotropy =	7.4870
24	C	Isotropic =	62.0277	Anisotropy =	110.9455
25	H	Isotropic =	24.3102	Anisotropy =	4.4019

Conformer 14

```
---------------------------------------------------------------------------
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)
---------------------------------------------------------------------------
```

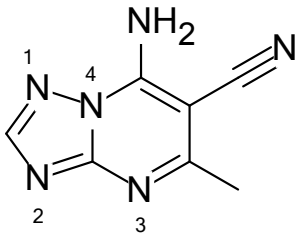
C	-1.836375155182	-0.772633999122	-2.563448135657
H	-2.626220011716	-0.232336586854	-3.078217791017
C	-0.484779613345	-0.947455894047	-2.966750855622
N	0.148945142795	-0.393450708824	-4.084776943710
H	1.000343771573	-0.902601352382	-4.319570495919
H	-0.458551383108	-0.369963533178	-4.901993735970
N	0.197621642637	-1.689136451894	-2.086770196295
N	-0.703637223596	-1.993354098315	-1.108712472127
C	-0.296519572152	-2.786452723713	0.043814155735
H	-1.075536546155	-3.542996649162	0.232582944504
C	-0.072163390433	-1.999464349152	1.356398696510
H	0.064111395901	-2.767277486489	2.140657217365
H	-0.999652226747	-1.456597150637	1.605537899549
N	1.036603796541	-1.061019636052	1.452816166786
C	2.346537366130	-1.644424987619	1.210549614358
H	3.129005405493	-0.938426658563	1.535489552142
H	2.545982126060	-1.889175384658	0.144028220734
H	2.460024597385	-2.570105322583	1.798328061407
C	0.852679736012	0.211440397930	0.764935512700
H	0.943048544820	0.148525203195	-0.338775866357
H	1.610966823736	0.929227950160	1.122612519349
H	-0.140440084034	0.623212468110	1.005347700249
H	0.614253118377	-3.320356022922	-0.258265232744
C	-1.926174968249	-1.467671737380	-1.366319252686
H	-2.766063292742	-1.626025285848	-0.693817283283

SCF Done: E(RB3LYP) = -494.174328653

Zero-point correction= 0.216472
Thermal correction to Energy= 0.228120
Thermal correction to Enthalpy= 0.229064
Thermal correction to Gibbs Free Energy= 0.178405
Sum of electronic and zero-point Energies= -493.957857
Sum of electronic and thermal Energies= -493.946209
Sum of electronic and thermal Enthalpies= -493.945265
Sum of electronic and thermal Free Energies= -493.995924

1	C	Isotropic =	100.4622	Anisotropy =	89.8858
2	H	Isotropic =	25.8412	Anisotropy =	2.4777
3	C	Isotropic =	39.8343	Anisotropy =	120.3429
4	N	Isotropic =	214.8711	Anisotropy =	72.8723
5	H	Isotropic =	28.4479	Anisotropy =	11.3862
6	H	Isotropic =	28.7517	Anisotropy =	12.4923
7	N	Isotropic =	-17.6767	Anisotropy =	225.8009
8	N	Isotropic =	55.8797	Anisotropy =	114.7823
9	C	Isotropic =	143.2633	Anisotropy =	56.8195
10	H	Isotropic =	28.0138	Anisotropy =	7.7906
11	C	Isotropic =	132.0436	Anisotropy =	38.2212
12	H	Isotropic =	28.5295	Anisotropy =	7.6449
13	H	Isotropic =	28.4416	Anisotropy =	6.5346
14	N	Isotropic =	232.3016	Anisotropy =	36.2240
15	C	Isotropic =	152.2415	Anisotropy =	57.2384
16	H	Isotropic =	29.1516	Anisotropy =	9.5351
17	H	Isotropic =	28.6737	Anisotropy =	6.9629
18	H	Isotropic =	29.1723	Anisotropy =	9.3885
19	C	Isotropic =	149.9095	Anisotropy =	61.9657

20	H	Isotropic =	29.3043	Anisotropy =	7.7447
21	H	Isotropic =	29.4358	Anisotropy =	9.7952
22	H	Isotropic =	29.4623	Anisotropy =	7.0832
23	H	Isotropic =	27.1639	Anisotropy =	3.5897
24	C	Isotropic =	64.3358	Anisotropy =	115.9200
25	H	Isotropic =	24.2081	Anisotropy =	4.3444



Conformer 1

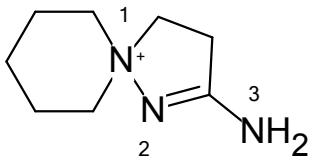
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.368535728679	-0.304255866373	-0.942212624170
C	-0.780273559396	-0.392926772728	-0.125631870938
N	-1.760239167827	-1.291496084090	-0.200458726767
H	-1.746447135229	-2.021764544096	-0.901725600075
H	-2.532274368279	-1.237546462466	0.455278533791
N	-0.860608649123	0.568353977446	0.839337702736
C	0.100214567900	1.559868463552	1.014798102319
N	1.198526574354	1.651742377220	0.238807135879
C	1.326313766907	0.739325970791	-0.716357503497
C	2.543534481431	0.823739435746	-1.593710970807
H	3.168069734045	1.667085056675	-1.276128548751
H	2.256743133859	0.961770153081	-2.648854310245
H	3.132215849982	-0.106111980487	-1.538925097284
N	-0.276769263926	2.332518358968	2.035352925165
C	-1.451010600033	1.770290957557	2.429736152602
H	-2.040685682544	2.159840492134	3.258256138747
N	-1.864578028246	0.702057546754	1.752399469220
C	0.547243350203	-1.263169035169	-1.978055861042
N	0.679079267243	-2.057242044516	-2.822895046886

SCF Done: E(RB3LYP) = -598.909860079

Zero-point correction= 0.136676
Thermal correction to Energy= 0.147411
Thermal correction to Enthalpy= 0.148355
Thermal correction to Gibbs Free Energy= 0.100281
Sum of electronic and zero-point Energies= -598.773184
Sum of electronic and thermal Energies= -598.762449
Sum of electronic and thermal Enthalpies= -598.761505
Sum of electronic and thermal Free Energies= -598.809579

1	C	Isotropic =	114.3169	Anisotropy =	69.8523
2	C	Isotropic =	44.7808	Anisotropy =	139.6647
3	N	Isotropic =	181.5692	Anisotropy =	45.1642
4	H	Isotropic =	25.8777	Anisotropy =	9.9182
5	H	Isotropic =	25.1189	Anisotropy =	12.3457
6	N	Isotropic =	45.9213	Anisotropy =	166.6170
7	C	Isotropic =	38.0910	Anisotropy =	99.2900
8	N	Isotropic =	9.7921	Anisotropy =	361.6562
9	C	Isotropic =	25.9697	Anisotropy =	184.0516
10	C	Isotropic =	166.5037	Anisotropy =	39.2582
11	H	Isotropic =	29.1156	Anisotropy =	7.9947
12	H	Isotropic =	28.5950	Anisotropy =	6.6243
13	H	Isotropic =	28.5946	Anisotropy =	6.5660
14	N	Isotropic =	20.9705	Anisotropy =	296.8249
15	C	Isotropic =	38.5265	Anisotropy =	122.2829
16	H	Isotropic =	23.2614	Anisotropy =	3.4317
17	N	Isotropic =	-5.6347	Anisotropy =	278.6944
18	C	Isotropic =	81.1515	Anisotropy =	304.6407
19	N	Isotropic =	-25.1579	Anisotropy =	351.4973



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

N	1.106014182145	0.599498458754	-0.788889980108
C	-0.374540319441	0.375652666082	-1.029602940118
H	-0.441161773810	-0.630816018189	-1.464282949725
H	-0.671468103365	1.102350209285	-1.796278779782
C	-1.195021247121	0.487109264881	0.250115844738
H	-2.244497006179	0.290662139370	-0.018935658498
H	-1.161355393248	1.519208300107	0.638696932646
C	-0.703022032319	-0.502073954963	1.311726629842
H	-0.881931651456	-1.534511529951	0.963125962318
H	-1.270249895676	-0.374427981767	2.246007391216
C	0.793123425975	-0.298869262952	1.571174121943
H	1.190131827470	-1.079696662978	2.238806499833
H	0.962568877591	0.661073405739	2.087629668720
C	1.607915004525	-0.360815363436	0.282342079668
H	1.549516938720	-1.351469749202	-0.187982439412
H	2.666651272080	-0.119396682159	0.443326001482
C	1.436224309778	2.055198716062	-0.461075811627
H	1.501273612774	2.190375284318	0.622286558932
H	0.620689320550	2.670100209759	-0.858373162424
C	2.740105927915	2.298615933022	-1.211640487734
H	3.633604116312	2.181686981038	-0.579576501360

H	2.778436775948	3.295707951262	-1.670419631262
C	2.692465082892	1.198932048079	-2.241658300703
N	3.536612022096	1.163506895383	-3.277299169651
H	3.481615672344	0.415841104864	-3.959353589300
H	4.156365831219	1.939934874190	-3.464914330880
N	1.796223222282	0.270022763404	-2.038413958752

SCF Done: E(RB3LYP) = -478.599488446

Zero-point correction= 0.245704
Thermal correction to Energy= 0.255921
Thermal correction to Enthalpy= 0.256865
Thermal correction to Gibbs Free Energy= 0.210780
Sum of electronic and zero-point Energies= -478.353784
Sum of electronic and thermal Energies= -478.343567
Sum of electronic and thermal Enthalpies= -478.342623
Sum of electronic and thermal Free Energies= -478.388709

1	N	Isotropic =	119.5343	Anisotropy =	105.1553
2	C	Isotropic =	121.6443	Anisotropy =	58.8888
3	H	Isotropic =	27.8606	Anisotropy =	6.8762
4	H	Isotropic =	28.1622	Anisotropy =	6.0893
5	C	Isotropic =	167.3541	Anisotropy =	11.2633
6	H	Isotropic =	29.5215	Anisotropy =	10.7260
7	H	Isotropic =	29.6099	Anisotropy =	6.7714
8	C	Isotropic =	167.8047	Anisotropy =	8.6177
9	H	Isotropic =	29.9029	Anisotropy =	9.1989
10	H	Isotropic =	29.6338	Anisotropy =	10.0012
11	C	Isotropic =	166.1094	Anisotropy =	12.0261
12	H	Isotropic =	29.4633	Anisotropy =	10.4627
13	H	Isotropic =	29.5212	Anisotropy =	7.0409
14	C	Isotropic =	126.7011	Anisotropy =	55.0208
15	H	Isotropic =	28.2940	Anisotropy =	6.5594
16	H	Isotropic =	28.2646	Anisotropy =	5.5359
17	C	Isotropic =	132.4843	Anisotropy =	72.8964
18	H	Isotropic =	27.3288	Anisotropy =	5.0854
19	H	Isotropic =	28.1923	Anisotropy =	6.8867
20	C	Isotropic =	159.0606	Anisotropy =	41.8801
21	H	Isotropic =	28.2686	Anisotropy =	7.9756
22	H	Isotropic =	28.5233	Anisotropy =	8.9708
23	C	Isotropic =	28.2785	Anisotropy =	126.0963
24	N	Isotropic =	188.4326	Anisotropy =	66.7286
25	H	Isotropic =	26.7351	Anisotropy =	12.3481
26	H	Isotropic =	27.0246	Anisotropy =	11.2311
27	N	Isotropic =	-14.7543	Anisotropy =	101.3876

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

N	1.326484156612	0.786378979522	-0.207084250396
C	0.058884013364	1.368101742514	0.389307625353
H	0.096198794952	2.444794594071	0.181547465297
H	0.141506836082	1.209212207974	1.475016551681

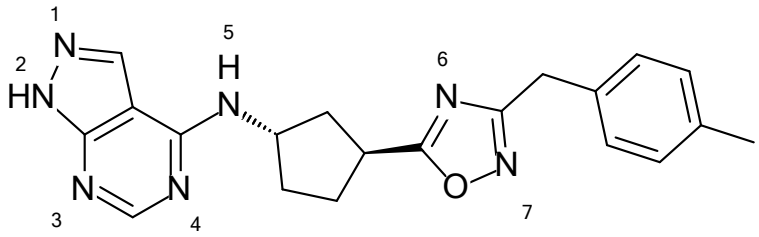
C	-1.196831608589	0.718672555812	-0.181578991422
H	-1.287593664783	0.987266078991	-1.245339405124
H	-2.058836071813	1.162280226207	0.341070557027
C	-1.178681259875	-0.805004631178	-0.017018451531
H	-2.058409756902	-1.248175042558	-0.508318288877
H	-1.244851572442	-1.065140669788	1.054746124993
C	0.108312776507	-1.389621902769	-0.608731668656
H	0.121874681589	-1.266528085929	-1.702654576733
H	0.185371112305	-2.468366719934	-0.400779686276
C	1.341531481373	-0.725364338515	-0.010128608303
H	2.272924860826	-1.087250868165	-0.464289479931
H	1.391241371438	-0.884288201940	1.076956990756
C	2.568990645480	1.423717251260	0.408792711379
H	2.910748772152	0.814285732657	1.251441485495
H	2.276358383022	2.417771857394	0.766436540654
C	3.533698302547	1.512281694770	-0.766165606783
H	4.232078233604	0.663007297459	-0.820954050831
H	4.124853227644	2.437766869311	-0.757792690864
C	2.571584719176	1.462341699242	-1.927578497147
N	2.953172636096	1.754797525837	-3.174535030015
H	2.286258332791	1.717673437000	-3.936861529324
H	3.872926113273	2.132695956170	-3.357862671512
N	1.352454483573	1.089904754585	-1.639062568909

SCF Done: E(RB3LYP) = -478.600417509

Zero-point correction= 0.245722
Thermal correction to Energy= 0.255938
Thermal correction to Enthalpy= 0.256883
Thermal correction to Gibbs Free Energy= 0.210822
Sum of electronic and zero-point Energies= -478.354696
Sum of electronic and thermal Energies= -478.344479
Sum of electronic and thermal Enthalpies= -478.343535
Sum of electronic and thermal Free Energies= -478.389595

1	N	Isotropic =	121.5467	Anisotropy =	107.3823
2	C	Isotropic =	123.2617	Anisotropy =	56.9358
3	H	Isotropic =	28.2418	Anisotropy =	5.8063
4	H	Isotropic =	28.0358	Anisotropy =	6.8954
5	C	Isotropic =	166.7631	Anisotropy =	10.1776
6	H	Isotropic =	29.0411	Anisotropy =	7.0435
7	H	Isotropic =	29.6221	Anisotropy =	10.3484
8	C	Isotropic =	167.4755	Anisotropy =	7.8890
9	H	Isotropic =	29.5946	Anisotropy =	9.8125
10	H	Isotropic =	29.8723	Anisotropy =	9.0370
11	C	Isotropic =	167.9734	Anisotropy =	11.0495
12	H	Isotropic =	29.2355	Anisotropy =	6.8329
13	H	Isotropic =	29.7115	Anisotropy =	10.5179
14	C	Isotropic =	124.3440	Anisotropy =	56.1042
15	H	Isotropic =	28.1335	Anisotropy =	5.1416
16	H	Isotropic =	28.2531	Anisotropy =	7.0971
17	C	Isotropic =	124.5583	Anisotropy =	85.6274
18	H	Isotropic =	27.6831	Anisotropy =	6.7726
19	H	Isotropic =	28.0464	Anisotropy =	7.0016
20	C	Isotropic =	160.1335	Anisotropy =	40.6113
21	H	Isotropic =	28.2964	Anisotropy =	7.9451

22	H	Isotropic =	28.6067	Anisotropy =	8.9177
23	C	Isotropic =	27.9517	Anisotropy =	123.4315
24	N	Isotropic =	187.2428	Anisotropy =	69.0792
25	H	Isotropic =	26.6306	Anisotropy =	12.1045
26	H	Isotropic =	26.9601	Anisotropy =	11.3090
27	N	Isotropic =	4.6413	Anisotropy =	133.8652



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.665628176218	-5.776111949964	4.613875028310
H	-3.409413983366	-6.562555867763	4.785669372965
N	-1.444213901904	-6.018821445317	5.088307754074
C	-0.603147672769	-4.995351740308	4.828164268338
C	-0.918123935667	-3.800323606223	4.148694208422
C	-2.266721500247	-3.686235331784	3.701169302041
N	-2.722324903714	-2.594877732299	3.044699594251
H	-2.065304988005	-1.842835712962	2.876159256301
N	-3.124317922666	-4.698833759398	3.945864078678
C	0.302194356990	-3.060592865372	4.139585819144
H	0.514218041408	-2.079738402586	3.717848153769
N	1.270241419244	-3.731357443240	4.750230869185
N	0.710713127647	-4.901142279271	5.163394933490
H	1.268502785638	-5.584816766802	5.661979344270
C	-4.417277980135	-0.766853876804	0.758899477924
H	-3.816372988756	0.084493128553	0.408748006678
H	-5.445966640108	-0.615168870758	0.399690709637
C	-4.396148727502	-0.926489699627	2.302618136979
H	-5.363168843003	-0.638567544136	2.738105304497
H	-3.637210458833	-0.284773096777	2.775730511041
C	-4.106850489083	-2.422367391060	2.596122030863
H	-4.754174296033	-2.830353476968	3.382853965593
C	-4.377002817860	-3.134290622284	1.253905889627
H	-5.462337245751	-3.287740758727	1.134346419331
H	-3.881339432306	-4.111849988025	1.186512998163
C	-3.889064271662	-2.111751762174	0.202214833321
H	-2.788265066311	-2.114304746775	0.185906532557
C	-5.386294084162	-2.772557345772	-2.971788245246
C	-6.500457022473	-2.853973536786	-3.973097732000
H	-7.309893185075	-3.459221995621	-3.537850673590
H	-6.121659713401	-3.387529880571	-4.857169371452

N	-5.560241658492	-2.334640973183	-1.674335234041
C	-4.353909185369	-2.416909943820	-1.180785188848
O	-3.453637934677	-2.866228185758	-2.073212406847
N	-4.152505906994	-3.104514456983	-3.271333022449
C	-8.017165316640	1.079555107840	-5.100541334599
C	-8.531540373064	2.441791481313	-5.500551856352
H	-8.629386146126	2.525609047230	-6.596032138640
H	-7.840698521840	3.239427099126	-5.179951296335
H	-9.516462446515	2.647436302412	-5.056419224414
C	-6.760662290049	0.627671760525	-5.543098667680
H	-6.151942065398	1.272657371036	-6.183101945564
C	-6.277826048931	-0.630170190919	-5.182261430383
H	-5.296434090590	-0.954260318136	-5.539407124470
C	-7.035540658805	-1.485480500449	-4.364849718295
C	-8.285389525248	-1.040021296507	-3.919863370323
H	-8.894869226359	-1.686281069903	-3.282810395791
C	-8.768027973132	0.222883508995	-4.283987045004
H	-9.749200115688	0.545081624780	-3.925129377123

SCF Done: E(RB3LYP) = -1233.33129207

Zero-point correction= 0.395608
Thermal correction to Energy= 0.419452
Thermal correction to Enthalpy= 0.420396
Thermal correction to Gibbs Free Energy= 0.334249
Sum of electronic and zero-point Energies= -1232.935684
Sum of electronic and thermal Energies= -1232.911840
Sum of electronic and thermal Enthalpies= -1232.910896
Sum of electronic and thermal Free Energies= -1232.997043

1	C	Isotropic =	38.0778	Anisotropy =	128.9991
2	H	Isotropic =	23.0863	Anisotropy =	5.9971
3	N	Isotropic =	32.3629	Anisotropy =	363.2523
4	C	Isotropic =	39.4652	Anisotropy =	138.3737
5	C	Isotropic =	91.4061	Anisotropy =	117.6575
6	C	Isotropic =	40.2494	Anisotropy =	139.2167
7	N	Isotropic =	144.5861	Anisotropy =	93.1413
8	H	Isotropic =	26.4968	Anisotropy =	9.7934
9	N	Isotropic =	24.8550	Anisotropy =	366.8564
10	C	Isotropic =	62.6545	Anisotropy =	122.3056
11	H	Isotropic =	23.6550	Anisotropy =	6.0766
12	N	Isotropic =	-45.6790	Anisotropy =	355.4149
13	N	Isotropic =	73.4916	Anisotropy =	91.4061
14	H	Isotropic =	22.1072	Anisotropy =	6.7885
15	C	Isotropic =	158.1519	Anisotropy =	35.2355
16	H	Isotropic =	29.2578	Anisotropy =	8.0868
17	H	Isotropic =	29.4393	Anisotropy =	10.1541
18	C	Isotropic =	158.7903	Anisotropy =	36.1294
19	H	Isotropic =	28.8731	Anisotropy =	9.1721
20	H	Isotropic =	29.7532	Anisotropy =	8.3101
21	C	Isotropic =	135.5788	Anisotropy =	23.5429
22	H	Isotropic =	26.7233	Anisotropy =	6.1151
23	C	Isotropic =	146.1813	Anisotropy =	33.7554
24	H	Isotropic =	29.5902	Anisotropy =	7.3049
25	H	Isotropic =	29.1737	Anisotropy =	6.6834
26	C	Isotropic =	152.0117	Anisotropy =	26.0457

27	H	Isotropic =	28.1775	Anisotropy =	6.5064
28	C	Isotropic =	20.3841	Anisotropy =	125.6790
29	C	Isotropic =	157.6690	Anisotropy =	25.2299
30	H	Isotropic =	27.8780	Anisotropy =	6.0244
31	H	Isotropic =	27.4279	Anisotropy =	6.6402
32	N	Isotropic =	17.1544	Anisotropy =	288.6282
33	C	Isotropic =	7.9267	Anisotropy =	118.0956
34	O	Isotropic =	-64.4331	Anisotropy =	193.7228
35	N	Isotropic =	-96.9512	Anisotropy =	206.7506
36	C	Isotropic =	53.8809	Anisotropy =	187.7559
37	C	Isotropic =	169.8628	Anisotropy =	37.2353
38	H	Isotropic =	28.8731	Anisotropy =	8.5648
39	H	Isotropic =	28.9072	Anisotropy =	7.8905
40	H	Isotropic =	29.4637	Anisotropy =	7.2550
41	C	Isotropic =	63.8397	Anisotropy =	161.2733
42	H	Isotropic =	24.2148	Anisotropy =	7.0099
43	C	Isotropic =	64.6500	Anisotropy =	165.3038
44	H	Isotropic =	24.2471	Anisotropy =	8.3903
45	C	Isotropic =	57.9635	Anisotropy =	176.5200
46	C	Isotropic =	63.4147	Anisotropy =	152.4925
47	H	Isotropic =	24.0986	Anisotropy =	6.7073
48	C	Isotropic =	63.6017	Anisotropy =	150.3337
49	H	Isotropic =	24.2268	Anisotropy =	6.3060

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.292093527416	-2.828658797026	4.722926109983
H	-0.599210735156	-2.778832601915	5.570839187615
N	-1.500785967918	-4.044570018586	4.213111110026
C	-2.351538805801	-3.997959028817	3.168879916081
C	-2.986480110971	-2.849640592478	2.637477691050
C	-2.683188275578	-1.628675907273	3.309123510630
N	-3.203438919231	-0.419207571769	3.000673692556
H	-2.835724488286	0.349547819599	3.554418999631
N	-1.814006318067	-1.649798457939	4.346753787957
C	-3.743165801504	-3.345595838652	1.527444176370
H	-4.365622790114	-2.809687700722	0.812141941696
N	-3.596832206886	-4.656589503710	1.400616314797
N	-2.757695399209	-5.042560427372	2.401859955806
H	-2.489794318354	-6.015075737132	2.499053762203
C	-5.756673513720	1.460148589546	1.004858946579
H	-5.883916059349	2.544917265605	0.889922980938
H	-6.759722142043	1.011047567465	0.953330981834
C	-5.062966448212	1.095003276429	2.332538938618
H	-5.774870604143	0.886555770388	3.143856429916
H	-4.406947088844	1.918349842900	2.664353512774
C	-4.192818477754	-0.122350790208	1.982933543540
H	-4.846255315014	-1.001063754152	1.879990064169
C	-3.629265502204	0.254855796180	0.597356627808
H	-3.189657530441	-0.593953549685	0.057535609618
H	-2.846422706926	1.017884457626	0.730886146186
C	-4.836275909338	0.877681959424	-0.136920236071

H	-4.522369744584	1.679803915720	-0.819270878816
C	-6.454826584915	-1.819704119699	-1.847837832447
C	-6.762942246466	-3.254118296014	-2.165404452833
H	-7.653155205096	-3.274074581786	-2.810199125979
H	-7.016735722220	-3.765718158161	-1.224690415906
N	-5.540873113939	-1.434901025018	-0.885350537978
C	-5.573451032609	-0.131335144081	-0.958844722340
O	-6.432462355457	0.315262715562	-1.890158910710
N	-7.021876658412	-0.821633503313	-2.480780977441
C	-3.419598592129	-5.257096887302	-4.130448255902
C	-2.269615141761	-5.947507965299	-4.824100281402
H	-1.641727629348	-6.500461706154	-4.110224596512
H	-1.628266758684	-5.222922462363	-5.352808425093
H	-2.632222555865	-6.663997996218	-5.580630736462
C	-3.647608050724	-5.412751067514	-2.756046574952
H	-2.974719636430	-6.041669930645	-2.166670230857
C	-4.720779036750	-4.777654188895	-2.119533125372
H	-4.860507966174	-4.921388347117	-1.045169465357
C	-5.600343648248	-3.963577995753	-2.843882754668
C	-5.374481739889	-3.799606582603	-4.220476552264
H	-6.045333362919	-3.164642107330	-4.805741309436
C	-4.304985822054	-4.436056886430	-4.851267996388
H	-4.154518432846	-4.295019747314	-5.925335543200

SCF Done: E(RB3LYP) = -1233.33240796

Zero-point correction= 0.396305
Thermal correction to Energy= 0.419726
Thermal correction to Enthalpy= 0.420670
Thermal correction to Gibbs Free Energy= 0.338883
Sum of electronic and zero-point Energies= -1232.936103
Sum of electronic and thermal Energies= -1232.912682
Sum of electronic and thermal Enthalpies= -1232.911738
Sum of electronic and thermal Free Energies= -1232.993525

1	C	Isotropic =	38.0296	Anisotropy =	127.8194
2	H	Isotropic =	23.1284	Anisotropy =	5.1795
3	N	Isotropic =	34.3932	Anisotropy =	362.6963
4	C	Isotropic =	38.4967	Anisotropy =	138.3956
5	C	Isotropic =	92.6371	Anisotropy =	119.6497
6	C	Isotropic =	38.3798	Anisotropy =	136.8807
7	N	Isotropic =	145.0264	Anisotropy =	75.4100
8	H	Isotropic =	26.5104	Anisotropy =	9.0842
9	N	Isotropic =	21.8691	Anisotropy =	335.0524
10	C	Isotropic =	58.7374	Anisotropy =	123.3991
11	H	Isotropic =	22.0946	Anisotropy =	8.2300
12	N	Isotropic =	-44.0609	Anisotropy =	343.2019
13	N	Isotropic =	74.3850	Anisotropy =	89.8058
14	H	Isotropic =	21.9779	Anisotropy =	6.5503
15	C	Isotropic =	160.9246	Anisotropy =	34.4000
16	H	Isotropic =	28.9322	Anisotropy =	10.2424
17	H	Isotropic =	29.7206	Anisotropy =	6.6018
18	C	Isotropic =	156.3026	Anisotropy =	34.3701
19	H	Isotropic =	29.2337	Anisotropy =	8.5960
20	H	Isotropic =	29.7123	Anisotropy =	8.9041
21	C	Isotropic =	134.9400	Anisotropy =	41.3759

22	H	Isotropic =	26.8855	Anisotropy =	5.6395
23	C	Isotropic =	153.2770	Anisotropy =	28.4417
24	H	Isotropic =	28.7761	Anisotropy =	4.9956
25	H	Isotropic =	29.6679	Anisotropy =	7.6725
26	C	Isotropic =	155.3039	Anisotropy =	16.6576
27	H	Isotropic =	27.9125	Anisotropy =	8.7251
28	C	Isotropic =	20.7561	Anisotropy =	125.2135
29	C	Isotropic =	157.3428	Anisotropy =	24.7816
30	H	Isotropic =	27.4073	Anisotropy =	7.1632
31	H	Isotropic =	27.6532	Anisotropy =	4.8574
32	N	Isotropic =	18.9654	Anisotropy =	263.5400
33	C	Isotropic =	6.0564	Anisotropy =	119.7116
34	O	Isotropic =	-57.5632	Anisotropy =	198.6661
35	N	Isotropic =	-98.9859	Anisotropy =	203.7588
36	C	Isotropic =	53.7179	Anisotropy =	187.9116
37	C	Isotropic =	169.6976	Anisotropy =	37.4733
38	H	Isotropic =	29.5068	Anisotropy =	6.8859
39	H	Isotropic =	28.9555	Anisotropy =	8.0256
40	H	Isotropic =	28.8637	Anisotropy =	8.9273
41	C	Isotropic =	63.0813	Anisotropy =	151.3678
42	H	Isotropic =	24.1944	Anisotropy =	7.9583
43	C	Isotropic =	62.5994	Anisotropy =	158.5500
44	H	Isotropic =	23.3736	Anisotropy =	6.0103
45	C	Isotropic =	58.1947	Anisotropy =	173.9738
46	C	Isotropic =	64.8178	Anisotropy =	160.6980
47	H	Isotropic =	24.1811	Anisotropy =	8.0691
48	C	Isotropic =	63.9851	Anisotropy =	159.7607
49	H	Isotropic =	24.2126	Anisotropy =	6.7393

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.550513729964	1.959688131562	3.070672667097
H	-7.488889797530	2.271268212307	2.597861732921
N	-6.416910459681	2.275490427846	4.358521800711
C	-5.231785439812	1.853174516808	4.848174331189
C	-4.227256382078	1.163309771835	4.138604574318
C	-4.517539621014	0.894322388496	2.769290075725
N	-3.647912273874	0.248542963420	1.959263822157
H	-2.774566579138	-0.063226172264	2.366797846868
N	-5.696874824874	1.305167485488	2.258217206985
C	-3.189273863512	0.956567546996	5.095606262992
H	-2.225917718768	0.463897249405	4.976583772771
N	-3.520855931706	1.465278160318	6.275164103023
N	-4.759739674717	2.005256537211	6.113733379771
H	-5.222780185215	2.459902035940	6.892195269138
C	-2.548930397109	-1.839433590303	-0.514990912018
H	-1.585553289145	-2.321897373869	-0.296799081308
H	-2.771042274442	-2.007785802916	-1.579685760416
C	-2.553313780070	-0.323909028945	-0.189525950808
H	-2.475056447196	0.276360996349	-1.106616664307
H	-1.699140753969	-0.039225766209	0.443937253795
C	-3.891432315331	-0.024664959952	0.540775814993

H	-4.406830146179	0.852893309261	0.131218885690
C	-4.743853356996	-1.294170110461	0.325666814739
H	-5.223078134582	-1.248719550993	-0.666166034191
H	-5.531034559820	-1.408222151522	1.082976972959
C	-3.702149060194	-2.434366083701	0.329827320400
H	-3.365287571698	-2.613758183274	1.362562214235
C	-5.022030701519	-5.331194196550	-1.287924077969
C	-5.569217650348	-6.135798111291	-2.430127377651
H	-6.449272064112	-5.609402838735	-2.830068999826
H	-5.911164140230	-7.101173995027	-2.029389162040
N	-4.638234202961	-4.010315775972	-1.402677565150
C	-4.228036398197	-3.726158757593	-0.195743058053
O	-4.327259683735	-4.767963589496	0.648922966969
N	-4.860932609660	-5.840693953261	-0.089187251847
C	-2.629898173597	-6.745572217843	-5.596784240543
C	-1.610159926552	-6.971066114662	-6.687490948744
H	-1.779994626964	-6.301224544458	-7.543107535914
H	-1.646374958344	-8.009326590655	-7.058663992739
H	-0.585412637850	-6.799635396624	-6.318282866717
C	-3.685851877825	-5.837724375132	-5.756481318262
H	-3.774109693717	-5.274181386742	-6.689196382516
C	-4.631742775291	-5.640386110192	-4.743343908623
H	-5.445183821383	-4.926587188895	-4.897355811008
C	-4.550172702230	-6.347552209886	-3.538306473217
C	-3.492266773966	-7.256553507794	-3.371642349589
H	-3.405025129440	-7.818164069704	-2.437437157021
C	-2.550925884443	-7.451218721145	-4.382575678211
H	-1.738604999023	-8.167117307176	-4.228604530754

SCF Done: E(RB3LYP) = -1233.33134362

Zero-point correction= 0.395587
Thermal correction to Energy= 0.418512
Thermal correction to Enthalpy= 0.419456
Thermal correction to Gibbs Free Energy= 0.337547
Sum of electronic and zero-point Energies= -1232.935756
Sum of electronic and thermal Energies= -1232.912832
Sum of electronic and thermal Enthalpies= -1232.911888
Sum of electronic and thermal Free Energies= -1232.993796

1	C	Isotropic =	37.9234	Anisotropy =	128.5474
2	H	Isotropic =	23.0956	Anisotropy =	5.9685
3	N	Isotropic =	32.8121	Anisotropy =	364.0651
4	C	Isotropic =	39.5896	Anisotropy =	138.5304
5	C	Isotropic =	91.4527	Anisotropy =	117.5953
6	C	Isotropic =	40.2715	Anisotropy =	139.6333
7	N	Isotropic =	143.1481	Anisotropy =	94.5657
8	H	Isotropic =	26.4991	Anisotropy =	9.8455
9	N	Isotropic =	24.9616	Anisotropy =	367.0520
10	C	Isotropic =	62.8192	Anisotropy =	122.6080
11	H	Isotropic =	23.6632	Anisotropy =	6.0641
12	N	Isotropic =	-45.6816	Anisotropy =	355.6419
13	N	Isotropic =	73.4688	Anisotropy =	91.4300
14	H	Isotropic =	22.1050	Anisotropy =	6.7904
15	C	Isotropic =	156.9912	Anisotropy =	35.2372
16	H	Isotropic =	29.2732	Anisotropy =	8.0736

17	H	Isotropic =	29.5835	Anisotropy =	9.9646
18	C	Isotropic =	158.8106	Anisotropy =	35.7202
19	H	Isotropic =	28.8594	Anisotropy =	9.0104
20	H	Isotropic =	29.7899	Anisotropy =	8.3519
21	C	Isotropic =	136.4377	Anisotropy =	24.0358
22	H	Isotropic =	26.6814	Anisotropy =	6.0811
23	C	Isotropic =	146.2995	Anisotropy =	33.2439
24	H	Isotropic =	29.4951	Anisotropy =	7.5943
25	H	Isotropic =	29.2230	Anisotropy =	6.6188
26	C	Isotropic =	152.1077	Anisotropy =	26.0987
27	H	Isotropic =	28.2245	Anisotropy =	6.6761
28	C	Isotropic =	20.1246	Anisotropy =	125.6558
29	C	Isotropic =	157.2973	Anisotropy =	25.4512
30	H	Isotropic =	27.8867	Anisotropy =	6.0045
31	H	Isotropic =	27.4546	Anisotropy =	6.6474
32	N	Isotropic =	17.7343	Anisotropy =	289.9187
33	C	Isotropic =	7.8539	Anisotropy =	118.3375
34	O	Isotropic =	-64.4605	Anisotropy =	192.3290
35	N	Isotropic =	-96.6887	Anisotropy =	207.0048
36	C	Isotropic =	53.7747	Anisotropy =	188.2576
37	C	Isotropic =	169.8149	Anisotropy =	37.2877
38	H	Isotropic =	29.4672	Anisotropy =	7.1929
39	H	Isotropic =	28.8559	Anisotropy =	8.6835
40	H	Isotropic =	28.9140	Anisotropy =	7.8153
41	C	Isotropic =	63.6683	Anisotropy =	150.7631
42	H	Isotropic =	24.2252	Anisotropy =	6.3117
43	C	Isotropic =	63.7650	Anisotropy =	152.4665
44	H	Isotropic =	24.1203	Anisotropy =	6.6584
45	C	Isotropic =	57.9940	Anisotropy =	176.4374
46	C	Isotropic =	64.5409	Anisotropy =	164.4126
47	H	Isotropic =	24.2534	Anisotropy =	8.2714
48	C	Isotropic =	63.3438	Anisotropy =	161.5806
49	H	Isotropic =	24.1910	Anisotropy =	6.9916

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.616644530137	-5.737660575215	0.483790899527
H	1.280130960682	-5.454713851591	1.309027034407
N	0.981889542159	-6.815045339902	-0.210430271981
C	0.104143280073	-7.082713271477	-1.200754171619
C	-1.063604833965	-6.354299788991	-1.507786409410
C	-1.320248001706	-5.225709426959	-0.675600058436
N	-2.404970536832	-4.436096978131	-0.842691095440
H	-3.049740248288	-4.684302316108	-1.583166134709
N	-0.454938071416	-4.936765958094	0.318716256243
C	-1.631433510585	-7.039267820267	-2.623252194088
H	-2.538486619531	-6.817855900493	-3.182813849133
N	-0.889001861895	-8.083044053142	-2.969140598294
N	0.159052302051	-8.099614606857	-2.101052842250
H	0.868033366155	-8.820317293475	-2.172200676842
C	-2.708956538438	-1.521945536503	-1.644297863416
H	-2.401841159392	-2.100098038492	-2.529086688149

H	-2.529841826926	-0.460884719457	-1.869619772934
C	-1.956428671769	-2.016574888486	-0.402857944703
H	-2.034894580387	-1.279814462495	0.414507108402
H	-0.890283574995	-2.211714480437	-0.582546887001
C	-2.727863933081	-3.286182476246	0.008791123275
H	-2.510266625618	-3.572349311074	1.046367496570
C	-4.199705122334	-2.874110126274	-0.185354393343
H	-4.556299085318	-2.401078642099	0.739133862991
H	-4.853656927084	-3.734416959554	-0.388683658310
C	-4.217503049694	-1.829368149909	-1.342228194104
H	-4.698707526951	-2.228731029850	-2.245852213470
C	-5.835953627816	1.110779246121	-0.103144318177
C	-6.291384934408	2.095902353831	0.932486604198
H	-6.683499102481	2.979633177115	0.408155307164
H	-5.412506398020	2.413926466133	1.513623031333
N	-5.134280355775	-0.040580581049	0.198415269704
C	-4.961911975368	-0.586697433780	-0.974781924517
O	-5.506110156851	0.134609101120	-1.971405880412
N	-6.088499875321	1.271925991421	-1.379897208519
C	-9.317594797762	0.433429914902	3.600879111082
C	-10.377298056993	-0.128744766253	4.518103324849
H	-10.886283671827	-0.992573326277	4.059976280555
H	-11.155689933558	0.622963175300	4.734401714491
H	-9.949216612811	-0.453809339953	5.477623942609
C	-8.005694470816	0.652372496086	4.043432574893
H	-7.736567135232	0.402321113124	5.073234109432
C	-7.032345214766	1.186037458909	3.190385894059
H	-6.017657680321	1.345969855009	3.564190198926
C	-7.343165294449	1.518940926728	1.866920186600
C	-8.655384660778	1.298142103470	1.416890103058
H	-8.920879506922	1.545102335884	0.385254002979
C	-9.623399696056	0.765840173882	2.268737183640
H	-10.638298516720	0.605715559859	1.894002628270

SCF Done: E(RB3LYP) = -1233.33062473

Zero-point correction= 0.395692
Thermal correction to Energy= 0.419396
Thermal correction to Enthalpy= 0.420340
Thermal correction to Gibbs Free Energy= 0.335241
Sum of electronic and zero-point Energies= -1232.934932
Sum of electronic and thermal Energies= -1232.911229
Sum of electronic and thermal Enthalpies= -1232.910285
Sum of electronic and thermal Free Energies= -1232.995384

1	C	Isotropic =	38.0509	Anisotropy = 128.6175
2	H	Isotropic =	23.0686	Anisotropy = 6.0158
3	N	Isotropic =	32.9885	Anisotropy = 363.3688
4	C	Isotropic =	39.8505	Anisotropy = 139.0623
5	C	Isotropic =	91.5142	Anisotropy = 117.6326
6	C	Isotropic =	39.7911	Anisotropy = 138.3186
7	N	Isotropic =	149.1867	Anisotropy = 86.8231
8	H	Isotropic =	26.5435	Anisotropy = 10.2032
9	N	Isotropic =	25.4164	Anisotropy = 368.7756
10	C	Isotropic =	63.1585	Anisotropy = 122.9466
11	H	Isotropic =	23.6952	Anisotropy = 6.1890

12	N	Isotropic =	-45.7915	Anisotropy =	354.9236
13	N	Isotropic =	73.4618	Anisotropy =	91.3835
14	H	Isotropic =	22.1214	Anisotropy =	6.8111
15	C	Isotropic =	157.8128	Anisotropy =	34.9951
16	H	Isotropic =	29.1313	Anisotropy =	8.5244
17	H	Isotropic =	29.7768	Anisotropy =	7.4221
18	C	Isotropic =	157.2924	Anisotropy =	27.6600
19	H	Isotropic =	29.6067	Anisotropy =	8.6308
20	H	Isotropic =	29.3520	Anisotropy =	8.4311
21	C	Isotropic =	134.4900	Anisotropy =	19.4328
22	H	Isotropic =	26.7627	Anisotropy =	5.9142
23	C	Isotropic =	153.3609	Anisotropy =	32.0632
24	H	Isotropic =	28.6967	Anisotropy =	10.5871
25	H	Isotropic =	29.4435	Anisotropy =	7.0332
26	C	Isotropic =	153.9170	Anisotropy =	21.7993
27	H	Isotropic =	27.7680	Anisotropy =	8.0400
28	C	Isotropic =	20.7193	Anisotropy =	125.4296
29	C	Isotropic =	157.1807	Anisotropy =	25.4561
30	H	Isotropic =	27.4039	Anisotropy =	6.7718
31	H	Isotropic =	27.8825	Anisotropy =	5.9025
32	N	Isotropic =	16.9775	Anisotropy =	279.9243
33	C	Isotropic =	6.3453	Anisotropy =	118.6349
34	O	Isotropic =	-58.8824	Anisotropy =	196.5610
35	N	Isotropic =	-99.3649	Anisotropy =	202.1652
36	C	Isotropic =	53.9062	Anisotropy =	187.7576
37	C	Isotropic =	170.0880	Anisotropy =	36.9212
38	H	Isotropic =	28.9519	Anisotropy =	7.7867
39	H	Isotropic =	28.8588	Anisotropy =	8.7663
40	H	Isotropic =	29.4545	Anisotropy =	7.1474
41	C	Isotropic =	63.6511	Anisotropy =	150.6268
42	H	Isotropic =	24.2244	Anisotropy =	6.3212
43	C	Isotropic =	63.5222	Anisotropy =	153.4665
44	H	Isotropic =	24.0569	Anisotropy =	6.6442
45	C	Isotropic =	57.9353	Anisotropy =	176.3969
46	C	Isotropic =	64.7641	Anisotropy =	165.2283
47	H	Isotropic =	24.2142	Anisotropy =	8.3378
48	C	Isotropic =	63.6745	Anisotropy =	160.3743
49	H	Isotropic =	24.2160	Anisotropy =	6.9279

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.772900498884	-3.143661275725	-0.333415938535
H	2.292031500902	-2.298892116988	-0.800453176875
N	2.489285574654	-4.258571855101	-0.192395575997
C	1.765996686488	-5.237323601165	0.391923753648
C	0.424738656128	-5.150318070037	0.819162342849
C	-0.209025138512	-3.892610069294	0.598999782584
N	-1.490661904303	-3.653951082585	0.958277716823
H	-1.983971672322	-4.399592853385	1.434437808787
N	0.493660473719	-2.899944131989	0.014677230251
C	0.137581861245	-6.437485432133	1.364074179940
H	-0.783375738657	-6.811590940840	1.807651298257

N	1.193283875197	-7.236424298040	1.280391857310
N	2.173438865585	-6.499279890984	0.690176099430
H	3.085629426793	-6.907181863768	0.521097452347
C	-4.018210951747	-2.896496104790	-0.717289554858
H	-3.888070447116	-3.880392143041	-1.190263103674
H	-4.763762021822	-2.346135086946	-1.307959130938
C	-2.680074490581	-2.127650532251	-0.634461888226
H	-2.850046088918	-1.046677622364	-0.766031824126
H	-1.951559226698	-2.442424596287	-1.393358985596
C	-2.160093356726	-2.358793861685	0.798683499633
H	-1.451256996155	-1.574730907173	1.098656892780
C	-3.450464459553	-2.325760517011	1.626397639736
H	-3.767019278698	-1.277798707898	1.730657793969
H	-3.335325768724	-2.745525694191	2.636783176544
C	-4.493004918017	-3.093226010498	0.766603006654
H	-4.477976414582	-4.163058338999	1.018009718207
C	-7.696426123070	-1.588145983998	1.251591323750
C	-8.692658282700	-0.466699389750	1.300534061209
H	-8.313144463225	0.296890899819	1.996727166313
H	-9.629326417908	-0.864230429589	1.716654726558
N	-6.362604078770	-1.407666485004	0.946076203543
C	-5.888161423279	-2.622739891171	1.008088509544
O	-6.824255393791	-3.533445172755	1.327387774317
N	-8.034388269841	-2.833487970143	1.490370488835
C	-9.379459338011	1.290864949211	-2.634182853891
C	-9.640919687321	1.909456596012	-3.986764233374
H	-8.794408174184	2.530237282283	-4.316946165250
H	-10.533162729540	2.559597772186	-3.958864647799
H	-9.825440595022	1.140323724948	-4.752687396639
C	-10.036381531501	0.113814242411	-2.237540083661
H	-10.730114146792	-0.373700248860	-2.928098831968
C	-9.820193461216	-0.444597992697	-0.975937852915
H	-10.343558924549	-1.362954442646	-0.696093200068
C	-8.937775985603	0.155852957667	-0.064817971439
C	-8.276180844248	1.326994716939	-0.457001431997
H	-7.580015999067	1.811131465181	0.232660364962
C	-8.493943333097	1.883849728916	-1.721242229041
H	-7.964589343730	2.798501276208	-2.002065791911

SCF Done: E(RB3LYP) = -1233.33027622

Zero-point correction= 0.395701
Thermal correction to Energy= 0.418579
Thermal correction to Enthalpy= 0.419523
Thermal correction to Gibbs Free Energy= 0.337670
Sum of electronic and zero-point Energies= -1232.934575
Sum of electronic and thermal Energies= -1232.911698
Sum of electronic and thermal Enthalpies= -1232.910753
Sum of electronic and thermal Free Energies= -1232.992606

1	C	Isotropic =	37.9580	Anisotropy =	128.2878
2	H	Isotropic =	23.0881	Anisotropy =	5.9814
3	N	Isotropic =	32.9037	Anisotropy =	363.6901
4	C	Isotropic =	39.5069	Anisotropy =	138.4028
5	C	Isotropic =	91.5339	Anisotropy =	118.2396
6	C	Isotropic =	39.7239	Anisotropy =	139.2514

7	N	Isotropic =	150.6261	Anisotropy =	72.2999
8	H	Isotropic =	26.5387	Anisotropy =	10.1282
9	N	Isotropic =	24.9001	Anisotropy =	367.1193
10	C	Isotropic =	63.1767	Anisotropy =	122.7620
11	H	Isotropic =	23.6378	Anisotropy =	6.1892
12	N	Isotropic =	-45.3220	Anisotropy =	356.2442
13	N	Isotropic =	73.6127	Anisotropy =	91.6877
14	H	Isotropic =	22.1184	Anisotropy =	6.8025
15	C	Isotropic =	158.8206	Anisotropy =	40.7040
16	H	Isotropic =	29.2166	Anisotropy =	7.8913
17	H	Isotropic =	29.8929	Anisotropy =	8.2514
18	C	Isotropic =	156.2174	Anisotropy =	32.6363
19	H	Isotropic =	29.4004	Anisotropy =	9.1329
20	H	Isotropic =	29.2394	Anisotropy =	7.7989
21	C	Isotropic =	133.6799	Anisotropy =	18.0538
22	H	Isotropic =	26.7882	Anisotropy =	6.1632
23	C	Isotropic =	149.6693	Anisotropy =	31.4320
24	H	Isotropic =	29.0712	Anisotropy =	8.2847
25	H	Isotropic =	29.2265	Anisotropy =	6.9485
26	C	Isotropic =	153.0914	Anisotropy =	24.4575
27	H	Isotropic =	27.8210	Anisotropy =	7.8818
28	C	Isotropic =	19.9319	Anisotropy =	124.8661
29	C	Isotropic =	157.7129	Anisotropy =	25.0247
30	H	Isotropic =	27.7905	Anisotropy =	5.9307
31	H	Isotropic =	27.4820	Anisotropy =	6.6671
32	N	Isotropic =	18.4109	Anisotropy =	283.6068
33	C	Isotropic =	5.7159	Anisotropy =	119.7631
34	O	Isotropic =	-65.0014	Anisotropy =	191.3938
35	N	Isotropic =	-95.8287	Anisotropy =	203.0049
36	C	Isotropic =	53.9237	Anisotropy =	187.9144
37	C	Isotropic =	169.6079	Anisotropy =	36.9801
38	H	Isotropic =	29.2520	Anisotropy =	7.3071
39	H	Isotropic =	28.8223	Anisotropy =	8.9093
40	H	Isotropic =	29.1379	Anisotropy =	7.4631
41	C	Isotropic =	64.2593	Anisotropy =	157.3767
42	H	Isotropic =	24.2238	Anisotropy =	6.7552
43	C	Isotropic =	64.3035	Anisotropy =	161.4849
44	H	Isotropic =	24.2110	Anisotropy =	7.9240
45	C	Isotropic =	57.9017	Anisotropy =	176.0923
46	C	Isotropic =	62.5902	Anisotropy =	155.4022
47	H	Isotropic =	24.0002	Anisotropy =	6.7827
48	C	Isotropic =	63.8760	Anisotropy =	154.5842
49	H	Isotropic =	24.1719	Anisotropy =	6.5816

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.361199332134	-6.044887971907	-1.218778507972
H	0.254543790631	-6.920511796951	-1.454770284050
N	-0.067435836618	-4.929273098309	-1.890449308556
C	-0.867107761646	-3.909761258610	-1.519522950978
C	-1.906565368035	-3.948149587026	-0.559287759142
C	-2.115566080808	-5.219551290315	0.051968955922

N	-3.076466079523	-5.498224112445	0.961924487123
H	-3.044834801887	-6.445078208451	1.329680659888
N	-1.310485737318	-6.252218328903	-0.291607929745
C	-2.407651125679	-2.607032592702	-0.526540689679
H	-3.197690249236	-2.172537515113	0.084439835334
N	-1.753256204955	-1.833970076370	-1.381207094911
N	-0.827040851664	-2.633082274388	-1.981043270130
H	-0.194432209300	-2.252186296455	-2.675055241829
C	-6.131110137322	-4.271650090809	2.751604428543
H	-6.666597227696	-4.728814476939	3.594489327736
H	-6.880740510819	-3.749503371825	2.138544958085
C	-5.371166103219	-5.317973103199	1.911173772971
H	-5.958839543648	-5.690574709040	1.060083020490
H	-5.095244714765	-6.186163629895	2.534232269442
C	-4.089148010763	-4.594089727744	1.471910484157
H	-4.344099543267	-3.885020561292	0.671152673720
C	-3.696452938943	-3.807204382995	2.739168579008
H	-2.951396615003	-3.022181204544	2.554108276314
H	-3.275185634508	-4.511132215990	3.473896397984
C	-5.039286473111	-3.254823944363	3.266043875986
H	-5.051017778396	-3.204023698322	4.363195019687
C	-5.476288156129	-0.052345972503	1.726058916197
C	-5.269943229662	1.008205081142	0.684342827488
H	-4.189848960124	1.207398805874	0.611256257158
H	-5.756192837143	1.928010351811	1.040061531269
N	-4.859115112229	-1.287767916670	1.685814643555
C	-5.311519643967	-1.873476863397	2.762185470210
O	-6.158571757520	-1.097830219799	3.458566978442
N	-6.264571589204	0.121776390658	2.759137959910
C	-6.853411540529	-0.140853672929	-3.216364382233
C	-7.413095276998	-0.524082693867	-4.565510911485
H	-6.639899509903	-0.962878918652	-5.213090513693
H	-7.830299686076	0.354119578894	-5.087400661030
H	-8.232063657117	-1.255327730407	-4.466331404940
C	-5.479645270209	-0.209385891163	-2.946031635731
H	-4.795311167251	-0.558842313027	-3.723900624040
C	-4.964450912158	0.160537050070	-1.697791492437
H	-3.887892049856	0.088440437373	-1.522479717364
C	-5.813551240868	0.610667574990	-0.679240394105
C	-7.191591375064	0.677137308369	-0.942493456981
H	-7.874621935632	1.021346426611	-0.161017919385
C	-7.700937852892	0.309036980990	-2.188218232535
H	-8.777794159837	0.373385730533	-2.368007223663

SCF Done: E(RB3LYP) = -1233.33236693

Zero-point correction= 0.396267
Thermal correction to Energy= 0.419738
Thermal correction to Enthalpy= 0.420682
Thermal correction to Gibbs Free Energy= 0.338290
Sum of electronic and zero-point Energies= -1232.936100
Sum of electronic and thermal Energies= -1232.912629
Sum of electronic and thermal Enthalpies= -1232.911685
Sum of electronic and thermal Free Energies= -1232.994077

1 C Isotropic = 38.0295 Anisotropy = 127.9277

2 H Isotropic = 23.1315 Anisotropy = 5.2087
3 N Isotropic = 34.3712 Anisotropy = 362.6485
4 C Isotropic = 38.5106 Anisotropy = 138.5772
5 C Isotropic = 92.7932 Anisotropy = 119.7330
6 C Isotropic = 38.2592 Anisotropy = 137.2549
7 N Isotropic = 145.0273 Anisotropy = 75.3328
8 H Isotropic = 26.5580 Anisotropy = 9.1841
9 N Isotropic = 21.8986 Anisotropy = 334.6568
10 C Isotropic = 58.4892 Anisotropy = 124.5864
11 H Isotropic = 22.1178 Anisotropy = 7.6444
12 N Isotropic = -44.3018 Anisotropy = 345.5039
13 N Isotropic = 74.2537 Anisotropy = 90.3698
14 H Isotropic = 21.9954 Anisotropy = 6.5813
15 C Isotropic = 160.8631 Anisotropy = 34.4260
16 H Isotropic = 29.0396 Anisotropy = 10.2934
17 H Isotropic = 29.9354 Anisotropy = 6.3414
18 C Isotropic = 156.4906 Anisotropy = 33.8261
19 H Isotropic = 29.3780 Anisotropy = 8.0199
20 H Isotropic = 29.7817 Anisotropy = 9.0678
21 C Isotropic = 135.3037 Anisotropy = 41.7293
22 H Isotropic = 26.9781 Anisotropy = 6.6086
23 C Isotropic = 152.7777 Anisotropy = 28.4557
24 H Isotropic = 28.7144 Anisotropy = 3.4324
25 H Isotropic = 29.6120 Anisotropy = 8.1006
26 C Isotropic = 155.3126 Anisotropy = 16.3235
27 H Isotropic = 27.8818 Anisotropy = 9.0830
28 C Isotropic = 20.4660 Anisotropy = 124.2758
29 C Isotropic = 157.4674 Anisotropy = 24.7031
30 H Isotropic = 27.6776 Anisotropy = 5.5133
31 H Isotropic = 27.3748 Anisotropy = 7.3503
32 N Isotropic = 18.9135 Anisotropy = 263.7319
33 C Isotropic = 5.5490 Anisotropy = 120.6857
34 O Isotropic = -57.9940 Anisotropy = 198.0373
35 N Isotropic = -97.8988 Anisotropy = 203.0261
36 C Isotropic = 53.9841 Anisotropy = 188.1164
37 C Isotropic = 170.0739 Anisotropy = 36.8880
38 H Isotropic = 29.5495 Anisotropy = 6.7101
39 H Isotropic = 28.8935 Anisotropy = 9.1551
40 H Isotropic = 29.0033 Anisotropy = 7.8915
41 C Isotropic = 63.6572 Anisotropy = 151.4114
42 H Isotropic = 24.3480 Anisotropy = 7.7377
43 C Isotropic = 62.6754 Anisotropy = 157.9641
44 H Isotropic = 23.5393 Anisotropy = 5.1079
45 C Isotropic = 58.1752 Anisotropy = 175.6309
46 C Isotropic = 64.3535 Anisotropy = 162.9895
47 H Isotropic = 24.1680 Anisotropy = 7.9655
48 C Isotropic = 63.7157 Anisotropy = 159.8784
49 H Isotropic = 24.2094 Anisotropy = 6.5683

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C -3.788663174546 2.358804987527 3.479382590226

H	-2.848913545231	2.374073970606	4.043195041442
N	-4.390432706157	3.537408861564	3.322535721270
C	-5.536253731414	3.414734756904	2.619202476734
C	-6.076652701581	2.222740052001	2.093378485169
C	-5.316629325837	1.042591683378	2.342283697759
N	-5.709842819238	-0.177848911262	1.911615368389
H	-6.569473440159	-0.232472204756	1.378734862741
N	-4.166269108443	1.141561974516	3.040711652183
C	-7.283033376367	2.629822788757	1.448781596514
H	-8.016603297218	2.031821881177	0.911140985116
N	-7.466548304992	3.938599895101	1.564178781796
N	-6.402860418437	4.403511128833	2.274599242080
H	-6.327041874134	5.390643022527	2.491231163472
C	-5.458903312388	-3.329589817403	0.645380170673
H	-6.306850978778	-3.601996148954	0.000898867496
H	-4.893147934050	-4.249894228952	0.854960183209
C	-5.898984832694	-2.646895995750	1.965866000458
H	-5.805934355655	-3.337938244846	2.815224388536
H	-6.953268313423	-2.331775568771	1.934449285513
C	-4.972222348055	-1.417880407753	2.167781856813
H	-4.578038443722	-1.350803887878	3.189447320273
C	-3.820097679959	-1.632011477781	1.162124162982
H	-3.082206634259	-2.327860754348	1.594502467544
H	-3.303545201406	-0.697158977946	0.906773698437
C	-4.513115970819	-2.312905008810	-0.039809966820
H	-5.095736053532	-1.559999125926	-0.592738059384
C	-2.125137642533	-4.058078276706	-2.040317594782
C	-1.109323802290	-5.117382481165	-2.351562068624
H	-0.322062967862	-5.074717333806	-1.583748922078
H	-0.647561366329	-4.869336175561	-3.318507161781
N	-2.781634208584	-3.967195906032	-0.829579934700
C	-3.560877235174	-2.933810366691	-1.003772628064
O	-3.436634064350	-2.385569258952	-2.225522580146
N	-2.471646593356	-3.143393957876	-2.915168172189
C	-2.869291408162	-9.108841676163	-2.469643655640
C	-3.476855892402	-10.490084180456	-2.527088335260
H	-3.301192498808	-11.047262280593	-1.595158278120
H	-3.049354572147	-11.078944438015	-3.356672646005
H	-4.564911946617	-10.441883759914	-2.697170681085
C	-2.046976115598	-8.713307714026	-1.405582135640
H	-1.845028197099	-9.415527767271	-0.592257937521
C	-1.478440060400	-7.434534583214	-1.364734274982
H	-0.841551965987	-7.155095466739	-0.521365280271
C	-1.714599353368	-6.511753950193	-2.390203247672
C	-2.539624434852	-6.902082884443	-3.458061502565
H	-2.743305400190	-6.196748537069	-4.268485220591
C	-3.105396424137	-8.176617436395	-3.496095513048
H	-3.742983967262	-8.455635810475	-4.339714269855

SCF Done: E(RB3LYP) = -1233.33136367

Zero-point correction= 0.395669
Thermal correction to Energy= 0.419497
Thermal correction to Enthalpy= 0.420442
Thermal correction to Gibbs Free Energy= 0.334392
Sum of electronic and zero-point Energies= -1232.935694

Sum of electronic and thermal Energies= -1232.911866
Sum of electronic and thermal Enthalpies= -1232.910922
Sum of electronic and thermal Free Energies= -1232.996972

1	C	Isotropic =	38.0246	Anisotropy =	128.4185
2	H	Isotropic =	23.0981	Anisotropy =	5.9889
3	N	Isotropic =	32.7847	Anisotropy =	363.8341
4	C	Isotropic =	39.2169	Anisotropy =	138.6948
5	C	Isotropic =	91.4713	Anisotropy =	117.9452
6	C	Isotropic =	40.1344	Anisotropy =	138.9433
7	N	Isotropic =	143.4410	Anisotropy =	94.4213
8	H	Isotropic =	26.4608	Anisotropy =	9.7763
9	N	Isotropic =	24.9069	Anisotropy =	366.8643
10	C	Isotropic =	63.3108	Anisotropy =	122.8047
11	H	Isotropic =	23.6476	Anisotropy =	6.0638
12	N	Isotropic =	-45.6763	Anisotropy =	355.3264
13	N	Isotropic =	73.3888	Anisotropy =	91.6928
14	H	Isotropic =	22.1089	Anisotropy =	6.7517
15	C	Isotropic =	157.0276	Anisotropy =	35.6185
16	H	Isotropic =	29.2620	Anisotropy =	8.0518
17	H	Isotropic =	29.4900	Anisotropy =	10.0111
18	C	Isotropic =	158.9639	Anisotropy =	35.9120
19	H	Isotropic =	28.8578	Anisotropy =	9.0629
20	H	Isotropic =	29.7679	Anisotropy =	8.3350
21	C	Isotropic =	136.1120	Anisotropy =	23.5837
22	H	Isotropic =	26.6697	Anisotropy =	6.1115
23	C	Isotropic =	146.1268	Anisotropy =	33.2488
24	H	Isotropic =	29.5369	Anisotropy =	7.4433
25	H	Isotropic =	29.2153	Anisotropy =	6.6199
26	C	Isotropic =	151.9950	Anisotropy =	25.8319
27	H	Isotropic =	28.2158	Anisotropy =	6.6122
28	C	Isotropic =	20.3706	Anisotropy =	125.7271
29	C	Isotropic =	157.7599	Anisotropy =	25.1340
30	H	Isotropic =	27.8708	Anisotropy =	6.0693
31	H	Isotropic =	27.4228	Anisotropy =	6.6581
32	N	Isotropic =	17.3161	Anisotropy =	289.3441
33	C	Isotropic =	8.0580	Anisotropy =	117.9864
34	O	Isotropic =	-64.2971	Anisotropy =	192.7641
35	N	Isotropic =	-96.8319	Anisotropy =	206.7028
36	C	Isotropic =	53.9161	Anisotropy =	187.4489
37	C	Isotropic =	170.0137	Anisotropy =	36.9678
38	H	Isotropic =	29.4579	Anisotropy =	7.1936
39	H	Isotropic =	28.8663	Anisotropy =	8.7105
40	H	Isotropic =	28.9685	Anisotropy =	7.7674
41	C	Isotropic =	63.6191	Anisotropy =	150.1666
42	H	Isotropic =	24.2574	Anisotropy =	6.2651
43	C	Isotropic =	63.7003	Anisotropy =	153.7892
44	H	Isotropic =	24.0786	Anisotropy =	6.6955
45	C	Isotropic =	57.8834	Anisotropy =	177.1014
46	C	Isotropic =	64.7526	Anisotropy =	165.4094
47	H	Isotropic =	24.2576	Anisotropy =	8.3522
48	C	Isotropic =	63.6517	Anisotropy =	160.4481
49	H	Isotropic =	24.2431	Anisotropy =	6.9563

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.884466637056	-2.324116386481	4.962336928211
H	-2.162505268890	-3.148054930686	4.994894545627
N	-2.747336613608	-1.394881958416	5.907513912686
C	-3.680524733914	-0.427087228080	5.784994060435
C	-4.692435403462	-0.354653824952	4.805304094787
C	-4.709464697651	-1.421977972528	3.860457316500
N	-5.623389408205	-1.494549697526	2.865631756355
H	-6.319291000603	-0.760211547174	2.817661499761
N	-3.785549703600	-2.399885158291	3.962540466241
C	-5.406015204944	0.841930042222	5.114379833889
H	-6.265467996342	1.284195940577	4.613706715343
N	-4.886313677592	1.445770583464	6.175077175200
N	-3.842167626408	0.668616254787	6.572893689040
H	-3.286986284698	0.933927828679	7.378175131680
C	-6.888998812986	-1.934863988476	-0.182681659638
H	-7.581963321949	-1.100971771282	-0.363846669634
H	-7.040261842723	-2.669105535869	-0.987083494882
C	-7.094053085138	-2.597173765474	1.208179248824
H	-7.450620500863	-3.630680624635	1.095397333183
H	-7.843726563807	-2.071909051116	1.819256737099
C	-5.713512367172	-2.602636679696	1.910077862467
H	-5.525838554407	-3.529998342593	2.466830392366
C	-4.707847592954	-2.452742805992	0.751091293608
H	-4.590200811707	-3.425806556304	0.245721461381
H	-3.718468827540	-2.115674952982	1.087609807692
C	-5.414662324611	-1.460038140959	-0.202019371862
H	-5.330807690909	-0.448357786337	0.223807738602
C	-4.117641006993	-1.738771529343	-3.518249945122
C	-3.924562652749	-2.363838893972	-4.868429966056
H	-3.303171746779	-1.683674652528	-5.469184305429
H	-4.908547735480	-2.435323329043	-5.356803965752
N	-4.948315401891	-2.264262757856	-2.548613528800
C	-4.805874844772	-1.420754188600	-1.562112287256
O	-3.956244855033	-0.418351688099	-1.850293472690
N	-3.497538667366	-0.638539495661	-3.162675231545
C	-2.096885090824	-6.319483249177	-4.631672157348
C	-1.466759495855	-7.690315289087	-4.564693545992
H	-0.446787339722	-7.645681622996	-4.155459329898
H	-1.406397071783	-8.149714834778	-5.566293668058
H	-2.059294717623	-8.373567332357	-3.934730305557
C	-1.347611765108	-5.156742476720	-4.392714873693
H	-0.286879539139	-5.243266315990	-4.142098223712
C	-1.932425941718	-3.889506196185	-4.470770360277
H	-1.323289646080	-3.002357215863	-4.276666733878
C	-3.289632949892	-3.743120674453	-4.791122834308
C	-4.043510286062	-4.901630550690	-5.027141977407
H	-5.104198697959	-4.813615194800	-5.276464016699
C	-3.456497946927	-6.167074871914	-4.949387865963
H	-4.067756046508	-7.053759583767	-5.139649209520

SCF Done: E(RB3LYP) = -1233.33128068

Zero-point correction= 0.395704
Thermal correction to Energy= 0.419490
Thermal correction to Enthalpy= 0.420434
Thermal correction to Gibbs Free Energy= 0.335676
Sum of electronic and zero-point Energies= -1232.935577
Sum of electronic and thermal Energies= -1232.911791
Sum of electronic and thermal Enthalpies= -1232.910846
Sum of electronic and thermal Free Energies= -1232.995605

1	C	Isotropic =	37.8803	Anisotropy =	128.4486
2	H	Isotropic =	23.1353	Anisotropy =	6.0152
3	N	Isotropic =	32.7343	Anisotropy =	364.4082
4	C	Isotropic =	39.5838	Anisotropy =	138.5337
5	C	Isotropic =	91.5579	Anisotropy =	118.3522
6	C	Isotropic =	40.0735	Anisotropy =	139.0585
7	N	Isotropic =	146.2921	Anisotropy =	91.2613
8	H	Isotropic =	26.5269	Anisotropy =	9.8387
9	N	Isotropic =	24.6965	Anisotropy =	366.9796
10	C	Isotropic =	62.9976	Anisotropy =	123.3403
11	H	Isotropic =	23.6245	Anisotropy =	6.1513
12	N	Isotropic =	-45.8215	Anisotropy =	355.3914
13	N	Isotropic =	73.5055	Anisotropy =	91.5251
14	H	Isotropic =	22.1257	Anisotropy =	6.7751
15	C	Isotropic =	159.6156	Anisotropy =	35.2173
16	H	Isotropic =	29.1125	Anisotropy =	8.8142
17	H	Isotropic =	29.1525	Anisotropy =	9.5404
18	C	Isotropic =	158.9313	Anisotropy =	36.1608
19	H	Isotropic =	28.9293	Anisotropy =	9.3065
20	H	Isotropic =	29.6932	Anisotropy =	8.6083
21	C	Isotropic =	134.9952	Anisotropy =	22.0406
22	H	Isotropic =	26.8298	Anisotropy =	5.8616
23	C	Isotropic =	147.0132	Anisotropy =	33.2051
24	H	Isotropic =	29.9302	Anisotropy =	8.1499
25	H	Isotropic =	29.2233	Anisotropy =	6.3526
26	C	Isotropic =	152.5268	Anisotropy =	25.0793
27	H	Isotropic =	28.1312	Anisotropy =	6.3057
28	C	Isotropic =	20.4940	Anisotropy =	125.5050
29	C	Isotropic =	157.2980	Anisotropy =	25.8538
30	H	Isotropic =	27.4324	Anisotropy =	6.7178
31	H	Isotropic =	27.8705	Anisotropy =	6.2417
32	N	Isotropic =	17.5861	Anisotropy =	286.3224
33	C	Isotropic =	7.8236	Anisotropy =	117.4764
34	O	Isotropic =	-63.1156	Anisotropy =	195.1310
35	N	Isotropic =	-97.6217	Anisotropy =	206.4559
36	C	Isotropic =	54.0774	Anisotropy =	187.8754
37	C	Isotropic =	170.0486	Anisotropy =	37.0236
38	H	Isotropic =	29.4801	Anisotropy =	7.2216
39	H	Isotropic =	28.8297	Anisotropy =	8.7784
40	H	Isotropic =	28.9160	Anisotropy =	7.6430
41	C	Isotropic =	63.7824	Anisotropy =	151.6911
42	H	Isotropic =	24.3082	Anisotropy =	6.3655
43	C	Isotropic =	64.2525	Anisotropy =	164.6994
44	H	Isotropic =	24.3205	Anisotropy =	8.1402
45	C	Isotropic =	57.6495	Anisotropy =	177.1598
46	C	Isotropic =	63.1297	Anisotropy =	153.9779
47	H	Isotropic =	24.0295	Anisotropy =	6.6984

48 C Isotropic = 64.1159 Anisotropy = 160.0710
49 H Isotropic = 24.1399 Anisotropy = 6.7654

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.312639622194	-3.848328411907	1.955926560391
H	-2.795407401381	-3.271248838980	2.753056974334
N	-1.545712808970	-4.862759205979	2.355851340803
C	-0.998538837662	-5.508103465082	1.303916193338
C	-1.178641992438	-5.196155675247	-0.059696449985
C	-2.028309310231	-4.084012285463	-0.329928218418
N	-2.284369111566	-3.668901814231	-1.592554919388
H	-1.876095365404	-4.207199597304	-2.349066755272
N	-2.586719045018	-3.425824780544	0.706651768392
C	-0.393921643938	-6.163448864127	-0.756026915749
H	-0.243624033182	-6.292082899301	-1.826485981713
N	0.207528638893	-6.988091434192	0.091271076955
N	-0.165866776121	-6.581900848359	1.335763891053
H	0.176841019706	-7.070008100508	2.155154197583
C	-3.707833092622	-0.760502646892	-3.483783072834
H	-3.594146010316	-0.461857281539	-4.534868385001
H	-3.807522204105	0.157827338841	-2.888172776563
C	-2.516294782056	-1.597177375948	-2.981978516981
H	-1.712383832757	-0.982301938072	-2.551603676450
H	-2.080699207419	-2.187667868480	-3.806988386687
C	-3.142566866081	-2.553982544807	-1.954603408594
H	-3.365651309829	-2.017235735311	-1.023402401842
C	-4.461067616724	-2.968570622511	-2.634244037224
H	-5.179759072748	-3.423326527655	-1.937320117760
H	-4.248747220205	-3.704941745929	-3.426238013103
C	-4.982393014819	-1.653449373314	-3.287312590617
H	-5.474003444280	-1.875432709609	-4.243242617365
C	-7.116601971136	-0.026398679741	-0.924401029715
C	-7.450883385055	0.725794563001	0.330555596906
H	-8.529270647144	0.938852352497	0.320927614655
H	-6.918549882494	1.689159849258	0.303383013857
N	-5.826547199676	-0.350830217911	-1.293823284118
C	-6.002882135684	-0.996436049348	-2.415530188541
O	-7.297516412420	-1.090656394896	-2.765031201005
N	-8.039269631233	-0.438070394325	-1.761100437423
C	-6.338831090818	-1.497190345729	3.917358544629
C	-5.937976532789	-2.279035274377	5.145707127023
H	-6.782440516672	-2.856793290513	5.549476229731
H	-5.563951190014	-1.614501526208	5.940978441287
H	-5.126911002537	-2.991287761125	4.914489710073
C	-5.506542695464	-0.489831532329	3.401292079874
H	-4.565474668349	-0.257262425187	3.907538117884
C	-5.862059050641	0.225764506741	2.255361641222
H	-5.195358400007	1.005317948470	1.877902954583
C	-7.066178199339	-0.039373753600	1.586766435108
C	-7.901522017362	-1.042093805107	2.098551267493
H	-8.847036481705	-1.266964829913	1.597539241430

C	-7.543291064609	-1.757129648468	3.245407755501
H	-8.216211861383	-2.529598038739	3.627475608242

SCF Done: E(RB3LYP) = -1233.33209692

Zero-point correction= 0.396140
Thermal correction to Energy= 0.419770
Thermal correction to Enthalpy= 0.420714
Thermal correction to Gibbs Free Energy= 0.336538
Sum of electronic and zero-point Energies= -1232.935957
Sum of electronic and thermal Energies= -1232.912327
Sum of electronic and thermal Enthalpies= -1232.911383
Sum of electronic and thermal Free Energies= -1232.995559

1	C	Isotropic =	38.1414	Anisotropy =	126.7690
2	H	Isotropic =	23.2680	Anisotropy =	6.6577
3	N	Isotropic =	32.5567	Anisotropy =	362.4547
4	C	Isotropic =	39.4866	Anisotropy =	137.6810
5	C	Isotropic =	91.4368	Anisotropy =	115.8397
6	C	Isotropic =	39.0868	Anisotropy =	138.6027
7	N	Isotropic =	150.6102	Anisotropy =	59.1858
8	H	Isotropic =	26.9346	Anisotropy =	9.9661
9	N	Isotropic =	28.0909	Anisotropy =	359.4595
10	C	Isotropic =	63.2697	Anisotropy =	123.1046
11	H	Isotropic =	23.7263	Anisotropy =	6.1575
12	N	Isotropic =	-45.8382	Anisotropy =	354.5041
13	N	Isotropic =	73.4370	Anisotropy =	91.1376
14	H	Isotropic =	22.1725	Anisotropy =	6.6109
15	C	Isotropic =	160.8300	Anisotropy =	32.3800
16	H	Isotropic =	29.1128	Anisotropy =	9.9843
17	H	Isotropic =	29.2270	Anisotropy =	6.7224
18	C	Isotropic =	157.2630	Anisotropy =	31.6606
19	H	Isotropic =	29.3405	Anisotropy =	7.7377
20	H	Isotropic =	29.8210	Anisotropy =	8.5676
21	C	Isotropic =	140.6501	Anisotropy =	40.7333
22	H	Isotropic =	26.2150	Anisotropy =	7.4609
23	C	Isotropic =	150.3001	Anisotropy =	35.2334
24	H	Isotropic =	29.8894	Anisotropy =	3.9972
25	H	Isotropic =	29.6764	Anisotropy =	7.9209
26	C	Isotropic =	155.2434	Anisotropy =	18.9529
27	H	Isotropic =	27.9754	Anisotropy =	8.9200
28	C	Isotropic =	20.2746	Anisotropy =	124.8787
29	C	Isotropic =	157.0763	Anisotropy =	24.8028
30	H	Isotropic =	27.4595	Anisotropy =	7.1118
31	H	Isotropic =	27.7484	Anisotropy =	5.9111
32	N	Isotropic =	17.6856	Anisotropy =	277.3982
33	C	Isotropic =	4.9202	Anisotropy =	122.8121
34	O	Isotropic =	-61.4412	Anisotropy =	189.2511
35	N	Isotropic =	-95.9757	Anisotropy =	200.0968
36	C	Isotropic =	53.6567	Anisotropy =	188.7616
37	C	Isotropic =	169.6586	Anisotropy =	37.0381
38	H	Isotropic =	29.3599	Anisotropy =	7.7294
39	H	Isotropic =	28.8654	Anisotropy =	8.0255
40	H	Isotropic =	28.6691	Anisotropy =	8.0861
41	C	Isotropic =	63.8389	Anisotropy =	159.3277
42	H	Isotropic =	23.9860	Anisotropy =	6.3680

43	C	Isotropic =	62.8359	Anisotropy =	155.5633
44	H	Isotropic =	23.9067	Anisotropy =	6.3479
45	C	Isotropic =	57.8962	Anisotropy =	176.2189
46	C	Isotropic =	64.2428	Anisotropy =	161.9847
47	H	Isotropic =	24.1839	Anisotropy =	7.6406
48	C	Isotropic =	63.6806	Anisotropy =	154.0213
49	H	Isotropic =	24.1946	Anisotropy =	6.2996

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.123624481693	-2.942246539485	-1.817612474062
H	-1.058976480414	-1.868770484987	-2.029372327249
N	-0.234258095332	-3.711771459357	-2.445636191808
C	-0.395649578758	-5.012044799874	-2.120284190456
C	-1.359156027375	-5.544633853930	-1.238958242350
C	-2.241524248220	-4.595858925672	-0.643381810908
N	-3.214942204434	-4.969703477693	0.218710470400
H	-3.284573669166	-5.958552696055	0.433913932281
N	-2.096734978760	-3.290867884604	-0.954350562805
C	-1.110323363220	-6.949798452445	-1.241893230110
H	-1.620809239034	-7.744504954124	-0.700586812677
N	-0.096923643413	-7.252727795037	-2.042644488042
N	0.328140139813	-6.071418686710	-2.568994453962
H	1.104208350312	-6.053747238337	-3.220541037999
C	-6.375860987216	-4.366831406215	1.967829703542
H	-6.534855480065	-5.374318787975	2.381059456176
H	-7.360334139117	-3.880591277012	1.911146232613
C	-5.653082041303	-4.447612638683	0.602281065922
H	-6.091505189679	-3.757292654411	-0.133499257665
H	-5.728769906569	-5.459587599420	0.176266680914
C	-4.162338784129	-4.075575504732	0.867855855183
H	-3.951012708374	-3.076674100032	0.474465957580
C	-4.017236867136	-4.053625348257	2.406210324434
H	-3.194802765089	-3.406981736029	2.743605431591
H	-3.821585021004	-5.073626277221	2.775906886617
C	-5.398204659330	-3.615240164462	2.922129773320
H	-5.568330793752	-3.916014343222	3.965536878426
C	-5.671072901795	-0.075688488964	2.450131716667
C	-5.393685492395	1.250850719248	1.807181006371
H	-4.310471106224	1.438504296408	1.857602911920
H	-5.895811901419	2.026599564110	2.403841484923
N	-5.062247208803	-1.252968742475	2.059076600905
C	-5.600374419991	-2.134242074087	2.858336414938
O	-6.489664265722	-1.591175525496	3.709553111166
N	-6.532000482493	-0.212217703124	3.429789181506
C	-6.742098844654	1.386705964110	-2.340821385437
C	-7.221885058906	1.437106562393	-3.771680698579
H	-7.905197910937	0.600637708934	-3.993713083589
H	-6.382191840827	1.387747523743	-4.480163779062
H	-7.780114702365	2.367208128675	-3.972510031407
C	-5.376633525723	1.360178782383	-2.025785378730
H	-4.638255536489	1.372224965847	-2.832027374826

C	-4.939859770944	1.318195934141	-0.696139750729
H	-3.868173468650	1.297445447704	-0.481775532723
C	-5.857872912492	1.303959642721	0.360015447301
C	-7.227960892712	1.329641975994	0.050066286871
H	-7.964466202550	1.314825192171	0.858213159123
C	-7.660460396352	1.370421403709	-1.275339886837
H	-8.732824295101	1.391487807838	-1.489193988681

SCF Done: E(RB3LYP) = -1233.33110493

Zero-point correction= 0.395905
Thermal correction to Energy= 0.419653
Thermal correction to Enthalpy= 0.420597
Thermal correction to Gibbs Free Energy= 0.334725
Sum of electronic and zero-point Energies= -1232.935200
Sum of electronic and thermal Energies= -1232.911452
Sum of electronic and thermal Enthalpies= -1232.910508
Sum of electronic and thermal Free Energies= -1232.996380

1	C	Isotropic =	37.6719	Anisotropy =	127.2830
2	H	Isotropic =	22.9951	Anisotropy =	6.0163
3	N	Isotropic =	32.7314	Anisotropy =	362.2116
4	C	Isotropic =	39.3465	Anisotropy =	137.9273
5	C	Isotropic =	91.5907	Anisotropy =	116.0085
6	C	Isotropic =	39.2881	Anisotropy =	137.7600
7	N	Isotropic =	142.8919	Anisotropy =	55.0929
8	H	Isotropic =	26.7454	Anisotropy =	10.0443
9	N	Isotropic =	29.3579	Anisotropy =	358.9577
10	C	Isotropic =	63.3564	Anisotropy =	123.0839
11	H	Isotropic =	23.6986	Anisotropy =	6.1225
12	N	Isotropic =	-45.2265	Anisotropy =	354.3257
13	N	Isotropic =	73.6071	Anisotropy =	90.8859
14	H	Isotropic =	22.1465	Anisotropy =	6.6604
15	C	Isotropic =	157.9617	Anisotropy =	32.0248
16	H	Isotropic =	29.1243	Anisotropy =	10.3796
17	H	Isotropic =	29.7623	Anisotropy =	7.9107
18	C	Isotropic =	160.3081	Anisotropy =	38.9192
19	H	Isotropic =	29.5138	Anisotropy =	7.0018
20	H	Isotropic =	30.0072	Anisotropy =	8.0810
21	C	Isotropic =	140.7776	Anisotropy =	35.0731
22	H	Isotropic =	25.4916	Anisotropy =	7.3206
23	C	Isotropic =	151.8256	Anisotropy =	31.1431
24	H	Isotropic =	29.1464	Anisotropy =	5.2431
25	H	Isotropic =	29.6293	Anisotropy =	8.2519
26	C	Isotropic =	151.0166	Anisotropy =	14.4604
27	H	Isotropic =	27.9066	Anisotropy =	8.9755
28	C	Isotropic =	20.6527	Anisotropy =	124.0692
29	C	Isotropic =	157.3343	Anisotropy =	24.8192
30	H	Isotropic =	27.8447	Anisotropy =	5.8600
31	H	Isotropic =	27.3594	Anisotropy =	7.2084
32	N	Isotropic =	16.3826	Anisotropy =	273.3074
33	C	Isotropic =	7.8241	Anisotropy =	120.7714
34	O	Isotropic =	-59.8503	Anisotropy =	191.2987
35	N	Isotropic =	-97.6295	Anisotropy =	208.8971
36	C	Isotropic =	53.9318	Anisotropy =	187.9848
37	C	Isotropic =	169.8391	Anisotropy =	36.9555

38	H	Isotropic =	28.9155	Anisotropy =	7.6491
39	H	Isotropic =	29.4756	Anisotropy =	6.9868
40	H	Isotropic =	28.8517	Anisotropy =	8.9260
41	C	Isotropic =	63.8697	Anisotropy =	151.4449
42	H	Isotropic =	24.1644	Anisotropy =	6.1432
43	C	Isotropic =	63.3393	Anisotropy =	153.1603
44	H	Isotropic =	23.9776	Anisotropy =	6.1370
45	C	Isotropic =	57.9493	Anisotropy =	177.1653
46	C	Isotropic =	64.5744	Anisotropy =	165.6266
47	H	Isotropic =	24.2178	Anisotropy =	8.1862
48	C	Isotropic =	63.6574	Anisotropy =	161.1448
49	H	Isotropic =	24.1752	Anisotropy =	6.7894

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-7.456096853121	2.691693306131	-0.362817596109
H	-8.003229851081	2.574000194915	-1.305194829692
N	-7.872395211963	3.678938049619	0.430303844076
C	-7.137503522901	3.742357280860	1.560907109026
C	-6.059966930177	2.902535917813	1.911187855586
C	-5.733849339936	1.890690740381	0.961444459377
N	-4.718467980585	1.018715560386	1.163664931627
H	-4.226652148360	1.077120761958	2.048798383790
N	-6.457019271697	1.808000234442	-0.174353727080
C	-5.629592682268	3.382904486654	3.184187981333
H	-4.822706527457	3.026323761556	3.821903577065
N	-6.366959203499	4.412581491645	3.578906506069
N	-7.277002913719	4.621179175207	2.588288258127
H	-7.956294903628	5.368866743438	2.669551677105
C	-2.651831289619	-1.579247481234	-0.510314464388
H	-1.615885303400	-1.945566562384	-0.481218546214
H	-2.994345407815	-1.613673873215	-1.557667635626
C	-2.821065623943	-0.165850885730	0.049817214276
H	-2.430689597844	0.618142857797	-0.615397863090
H	-2.299629668003	-0.079078946851	1.019777516122
C	-4.340802191413	-0.057774102441	0.262066791578
H	-4.829310048512	0.165466196587	-0.694136267960
C	-4.778009893126	-1.473140756402	0.744040010193
H	-5.719174127121	-1.776352232387	0.264390339146
H	-4.948377470416	-1.473004189455	1.830427364702
C	-3.599420999072	-2.430821631582	0.382361543974
H	-3.061248583306	-2.715909085389	1.296665574770
C	-4.368593253531	-5.693249374261	-0.851451291978
C	-4.323251586619	-7.192823735755	-0.881363618542
H	-5.041387547123	-7.538580070237	-1.638921663577
H	-4.661975559662	-7.565366627829	0.097364220443
N	-3.726971282990	-4.932738090560	0.108020660201
C	-4.017382394935	-3.712318278765	-0.253936069439
O	-4.785158633709	-3.663522969164	-1.359392537750
N	-5.017725465169	-4.995428736956	-1.752048722645
C	-0.322193499115	-8.697311797080	-1.758313379864
C	1.059436286135	-9.217558131431	-2.075912093039

H	1.012902081579	-10.078986673357	-2.763486957143
H	1.587818890494	-9.539613447010	-1.166732146040
H	1.672615845230	-8.446583447703	-2.571452638513
C	-1.144436262300	-8.176592402667	-2.773656957575
H	-0.775021746791	-8.147221567641	-3.802614079537
C	-2.424533462733	-7.698946566730	-2.492070247131
H	-3.040922567980	-7.297557327965	-3.301151920158
C	-2.931484400267	-7.726186398902	-1.182324709512
C	-2.116688028287	-8.241624877011	-0.167610413756
H	-2.487314662856	-8.273287386401	0.860219069153
C	-0.832399563489	-8.720219298245	-0.452815849215
H	-0.217355641898	-9.119849806650	0.357981337832

SCF Done: E(RB3LYP) = -1233.33196234

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.640360756959	-2.156958315761	4.313505756634
H	-7.614056966556	-2.563908090331	4.017714718870
N	-6.313703509599	-2.308400219741	5.596557084205
C	-5.102347767615	-1.774924325200	5.861905357614
C	-4.248510540677	-1.129610145266	4.943438739673
C	-4.735798728836	-1.047042478195	3.606358512516
N	-4.034187254142	-0.451566918346	2.614905739651
H	-3.133862742376	-0.053645762241	2.853574554788
N	-5.943167925258	-1.575345002251	3.317074789265
C	-3.110306979009	-0.751449195006	5.716599544523
H	-2.206884609632	-0.228418680430	5.408283291996
N	-3.247896903771	-1.126353687327	6.981656393240
N	-4.457636836783	-1.745208042049	7.058076417123
H	-4.783647299601	-2.119486602539	7.941679809620
C	-2.676498468662	0.032572151477	-0.411831772661
H	-1.647724830103	0.399087958351	-0.286447515632
H	-2.941710788528	0.151488422285	-1.472474394283
C	-3.696467154929	0.776503191561	0.492787599392
H	-4.371597007679	1.397799635023	-0.112235372077
H	-3.205907151461	1.453639877611	1.208547498748
C	-4.513097215058	-0.310862742418	1.236775239872
H	-5.583807355552	-0.075062590197	1.287547437454
C	-4.279202199165	-1.590581089686	0.408037622317
H	-4.927364511451	-1.570152658233	-0.483901307681
H	-4.496940695886	-2.507197823170	0.972169606366
C	-2.800762945717	-1.462278453419	-0.028910695574
H	-2.159115882701	-1.693244352888	0.835489088606
C	-2.125799031551	-3.478942831063	-2.898517491133
C	-2.167373823824	-3.859452675003	-4.348730211527
H	-1.532722056744	-4.748080756011	-4.482634883870
H	-1.721130442890	-3.040088300378	-4.932420588489
N	-2.683550014843	-2.318234860771	-2.400544862987
C	-2.424719126958	-2.401695509355	-1.123378854371

O	-1.751158241405	-3.520120263117	-0.798726997012
N	-1.554691106106	-4.237816494055	-1.993100437926
C	-6.217584743373	-4.653664140280	-5.766429619627
C	-7.619009666085	-4.940757049264	-6.250047992894
H	-8.336882214945	-4.945625180602	-5.412609302269
H	-7.681120620694	-5.932134500571	-6.729209670904
H	-7.955551720797	-4.189737497594	-6.979584332234
C	-5.587207722589	-5.508046966367	-4.843463933696
H	-6.120161164579	-6.389680238399	-4.476370734161
C	-4.293183182256	-5.252498807057	-4.390107357404
H	-3.828700242492	-5.932876287140	-3.671013622378
C	-3.579092138602	-4.131037395679	-4.844356472219
C	-4.202369281505	-3.276606750958	-5.760673493269
H	-3.668238282050	-2.397184629467	-6.129891680626
C	-5.501130816794	-3.535957291385	-6.215293497743
H	-5.963279331212	-2.853725637098	-6.933897707825

SCF Done: E(RB3LYP) = -1233.33126851

Zero-point correction= 0.395623
Thermal correction to Energy= 0.419441
Thermal correction to Enthalpy= 0.420385
Thermal correction to Gibbs Free Energy= 0.334757
Sum of electronic and zero-point Energies= -1232.935646
Sum of electronic and thermal Energies= -1232.911828
Sum of electronic and thermal Enthalpies= -1232.910883
Sum of electronic and thermal Free Energies= -1232.996512

1	C	Isotropic =	38.0697	Anisotropy =	128.8575
2	H	Isotropic =	23.1092	Anisotropy =	6.0331
3	N	Isotropic =	32.6319	Anisotropy =	363.9884
4	C	Isotropic =	39.5133	Anisotropy =	138.8150
5	C	Isotropic =	91.5323	Anisotropy =	118.0029
6	C	Isotropic =	40.0739	Anisotropy =	138.4924
7	N	Isotropic =	145.2609	Anisotropy =	92.8173
8	H	Isotropic =	26.5048	Anisotropy =	9.7937
9	N	Isotropic =	25.1446	Anisotropy =	367.8174
10	C	Isotropic =	63.2243	Anisotropy =	123.3036
11	H	Isotropic =	23.6446	Anisotropy =	6.1135
12	N	Isotropic =	-45.8338	Anisotropy =	355.0401
13	N	Isotropic =	73.5515	Anisotropy =	91.5445
14	H	Isotropic =	22.1180	Anisotropy =	6.7753
15	C	Isotropic =	159.1078	Anisotropy =	34.9633
16	H	Isotropic =	29.1284	Anisotropy =	8.7721
17	H	Isotropic =	29.1776	Anisotropy =	9.5065
18	C	Isotropic =	159.0719	Anisotropy =	35.9034
19	H	Isotropic =	28.8957	Anisotropy =	9.2626
20	H	Isotropic =	29.7166	Anisotropy =	8.5876
21	C	Isotropic =	135.1639	Anisotropy =	23.2712
22	H	Isotropic =	26.8059	Anisotropy =	5.8618
23	C	Isotropic =	146.5822	Anisotropy =	33.4602
24	H	Isotropic =	29.8927	Anisotropy =	8.1337
25	H	Isotropic =	29.2526	Anisotropy =	6.2695
26	C	Isotropic =	152.0519	Anisotropy =	25.9609
27	H	Isotropic =	28.1339	Anisotropy =	6.2855
28	C	Isotropic =	20.5492	Anisotropy =	126.0623

29	C	Isotropic =	157.5273	Anisotropy =	25.3245
30	H	Isotropic =	27.4028	Anisotropy =	6.7702
31	H	Isotropic =	27.9111	Anisotropy =	6.2392
32	N	Isotropic =	17.1511	Anisotropy =	287.5129
33	C	Isotropic =	7.8909	Anisotropy =	117.8089
34	O	Isotropic =	-63.4054	Anisotropy =	195.8949
35	N	Isotropic =	-97.7425	Anisotropy =	207.5782
36	C	Isotropic =	54.2225	Anisotropy =	187.8278
37	C	Isotropic =	169.8894	Anisotropy =	37.0932
38	H	Isotropic =	28.8695	Anisotropy =	7.8543
39	H	Isotropic =	28.8710	Anisotropy =	8.5765
40	H	Isotropic =	29.4669	Anisotropy =	7.2719
41	C	Isotropic =	63.9542	Anisotropy =	161.0639
42	H	Isotropic =	24.2237	Anisotropy =	6.9897
43	C	Isotropic =	64.9198	Anisotropy =	166.3554
44	H	Isotropic =	24.3271	Anisotropy =	8.3173
45	C	Isotropic =	57.5977	Anisotropy =	177.3871
46	C	Isotropic =	63.0882	Anisotropy =	152.2064
47	H	Isotropic =	24.1172	Anisotropy =	6.6404
48	C	Isotropic =	63.7328	Anisotropy =	150.8366
49	H	Isotropic =	24.2141	Anisotropy =	6.1868

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-7.115984403421	2.476953471447	-0.449545080966
H	-6.647074968592	3.366187479881	-0.886057066067
N	-8.418692366602	2.331023825715	-0.689266149756
C	-8.903237171061	1.211543200049	-0.110794717067
C	-8.174866141851	0.280143717664	0.657757433989
C	-6.789990389275	0.572617773985	0.825181270589
N	-5.963866101954	-0.223397782890	1.541833233375
H	-6.371472791903	-1.038190682774	1.984289612623
N	-6.282622714643	1.684777869230	0.254327505190
C	-9.136621341252	-0.703959876224	1.035560919545
H	-9.007654549878	-1.604040362879	1.634093766100
N	-10.335011976567	-0.409955756355	0.548291941839
N	-10.181887388499	0.751727844670	-0.144111894232
H	-10.975910967023	1.176237208842	-0.609321689591
C	-3.353452019545	-2.039195641367	2.345649945352
H	-3.811479654723	-2.979050021316	2.684682203131
H	-2.288420026514	-2.078787470131	2.617217450550
C	-4.025190903188	-0.783314124145	2.969426260916
H	-3.288242777812	-0.196790843887	3.536146506886
H	-4.833404264878	-1.037518398200	3.671604961760
C	-4.549969112366	0.071490461244	1.793975958250
H	-4.467760138111	1.149356919304	1.985876778964
C	-3.650316290317	-0.344917230937	0.614500535868
H	-2.667716561897	0.142982944382	0.723685641079
H	-4.069140603370	-0.061341568299	-0.360252731502
C	-3.502866746074	-1.871155263761	0.803850539530
H	-4.423573219934	-2.365517642487	0.462345929946
C	-1.138670059029	-3.572461476055	-1.263192528511

C	-0.676096188149	-4.570841805017	-2.281920662792
H	0.373670833844	-4.345275645144	-2.522846670112
H	-1.267227281146	-4.428887565499	-3.198923786247
N	-2.459686118502	-3.427990755213	-0.882179611300
C	-2.395940972266	-2.481961613774	0.015501019390
O	-1.140968212490	-2.035336291758	0.216086178486
N	-0.305344324466	-2.770483317624	-0.644705054578
C	-1.051516318221	-8.692419114459	-0.895788733515
C	-1.168194265048	-10.117041543218	-0.408816674457
H	-1.484702402311	-10.153253090422	0.647083264714
H	-0.199116317459	-10.640312801554	-0.469575504785
H	-1.898458263025	-10.687323001891	-1.001296300036
C	-0.177154222110	-7.787707069831	-0.266394935874
H	0.422810780639	-8.123382669229	0.584172539818
C	-0.060190837844	-6.470260024954	-0.708682148182
H	0.625801129680	-5.788262618991	-0.198781099153
C	-0.814612711069	-6.006940653267	-1.799766917473
C	-1.687876440165	-6.901783928713	-2.427815575996
H	-2.286630790137	-6.566399039886	-3.278785959227
C	-1.802316073012	-8.224653994630	-1.982735527088
H	-2.490845356462	-8.903642029632	-2.492914379384

SCF Done: E(RB3LYP) = -1233.33101683

Zero-point correction= 0.395654
Thermal correction to Energy= 0.419461
Thermal correction to Enthalpy= 0.420405
Thermal correction to Gibbs Free Energy= 0.335204
Sum of electronic and zero-point Energies= -1232.935363
Sum of electronic and thermal Energies= -1232.911556
Sum of electronic and thermal Enthalpies= -1232.910612
Sum of electronic and thermal Free Energies= -1232.995813

1	C	Isotropic =	38.0628	Anisotropy =	128.8736
2	H	Isotropic =	23.0884	Anisotropy =	5.9543
3	N	Isotropic =	32.4527	Anisotropy =	363.5261
4	C	Isotropic =	39.6850	Anisotropy =	138.5812
5	C	Isotropic =	91.5392	Anisotropy =	117.9345
6	C	Isotropic =	40.0666	Anisotropy =	139.0530
7	N	Isotropic =	147.5297	Anisotropy =	89.2569
8	H	Isotropic =	26.5266	Anisotropy =	9.5117
9	N	Isotropic =	25.2103	Anisotropy =	368.5220
10	C	Isotropic =	62.9598	Anisotropy =	123.0745
11	H	Isotropic =	23.6714	Anisotropy =	5.9896
12	N	Isotropic =	-45.4735	Anisotropy =	356.9277
13	N	Isotropic =	73.4691	Anisotropy =	91.6389
14	H	Isotropic =	22.1196	Anisotropy =	6.7566
15	C	Isotropic =	158.9065	Anisotropy =	38.6933
16	H	Isotropic =	29.1854	Anisotropy =	8.2163
17	H	Isotropic =	29.3964	Anisotropy =	8.0623
18	C	Isotropic =	158.8370	Anisotropy =	35.1924
19	H	Isotropic =	28.8972	Anisotropy =	9.7013
20	H	Isotropic =	29.6371	Anisotropy =	8.5001
21	C	Isotropic =	134.6014	Anisotropy =	21.2037
22	H	Isotropic =	26.7628	Anisotropy =	6.3950
23	C	Isotropic =	149.1010	Anisotropy =	31.3185

24	H	Isotropic =	29.3312	Anisotropy =	7.7549
25	H	Isotropic =	29.1130	Anisotropy =	6.8284
26	C	Isotropic =	151.2949	Anisotropy =	23.8673
27	H	Isotropic =	28.1268	Anisotropy =	6.6598
28	C	Isotropic =	21.0008	Anisotropy =	126.7668
29	C	Isotropic =	157.7925	Anisotropy =	25.6207
30	H	Isotropic =	27.4146	Anisotropy =	6.6949
31	H	Isotropic =	27.9755	Anisotropy =	6.0769
32	N	Isotropic =	11.2670	Anisotropy =	265.8121
33	C	Isotropic =	9.2774	Anisotropy =	119.1830
34	O	Isotropic =	-54.1621	Anisotropy =	213.8951
35	N	Isotropic =	-100.6956	Anisotropy =	213.5912
36	C	Isotropic =	54.1076	Anisotropy =	187.9518
37	C	Isotropic =	169.7538	Anisotropy =	37.4059
38	H	Isotropic =	28.8977	Anisotropy =	7.8590
39	H	Isotropic =	28.8745	Anisotropy =	8.5309
40	H	Isotropic =	29.4698	Anisotropy =	7.3259
41	C	Isotropic =	63.7827	Anisotropy =	161.2672
42	H	Isotropic =	24.2100	Anisotropy =	7.2558
43	C	Isotropic =	64.7568	Anisotropy =	167.0336
44	H	Isotropic =	24.3214	Anisotropy =	8.6455
45	C	Isotropic =	57.8373	Anisotropy =	176.5486
46	C	Isotropic =	63.4762	Anisotropy =	150.9176
47	H	Isotropic =	24.1868	Anisotropy =	6.7514
48	C	Isotropic =	63.8354	Anisotropy =	150.8916
49	H	Isotropic =	24.2361	Anisotropy =	6.2028

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-3.561254271821	-2.460293467354	3.026701149653
H	-4.488912693577	-1.881159454900	3.099475816175
N	-3.114686874200	-2.988449985546	4.166285390637
C	-1.971157776135	-3.678880063690	3.971770108953
C	-1.291824999726	-3.853467410523	2.747955150252
C	-1.894444479052	-3.230979674901	1.615971817408
N	-1.350108323799	-3.307538030647	0.378893544233
H	-0.522595644843	-3.883566861618	0.269149336484
N	-3.038639418887	-2.537275414454	1.787667971405
C	-0.153077478135	-4.647224211385	3.080044255785
H	0.644110411478	-5.017694170814	2.437984266852
N	-0.133356615777	-4.933722931595	4.375109781150
N	-1.239138300517	-4.342657498338	4.904930704410
H	-1.435748070996	-4.424588036382	5.895761473459
C	-1.631216376743	-1.875543321372	-3.071976546631
H	-0.964174635475	-1.942800314086	-3.942273620256
H	-2.110791247112	-0.886787155409	-3.098726105058
C	-0.880298788635	-2.066738856187	-1.741818783348
H	-0.490976168161	-1.123502914549	-1.331543516530
H	-0.025126990785	-2.752974455556	-1.872883103100
C	-1.920961882270	-2.726706245896	-0.824359261127
H	-2.660992256289	-1.985534255011	-0.495664697121
C	-2.603976591800	-3.744949965496	-1.757890246130

H	-3.566445913373	-4.105373597723	-1.367349635530
H	-1.945287270497	-4.618455855653	-1.889129473543
C	-2.732052539247	-2.993085342478	-3.116514317238
H	-2.568336476327	-3.687776584021	-3.950243968689
C	-5.929655346376	-1.395416550800	-3.186795897700
C	-6.979264633371	-0.409560199794	-2.763023177626
H	-7.840710690879	-0.520950241719	-3.436695749691
H	-6.571297280603	0.603269887596	-2.904161964033
N	-4.659047591887	-1.429512760026	-2.648354500835
C	-4.103520112317	-2.424912520739	-3.286213389121
O	-4.930888128589	-3.001662527567	-4.174806325802
N	-6.153847847951	-2.306329779059	-4.103919181020
C	-8.187399578740	-0.979600717171	1.391262356764
C	-8.613165996681	-1.187107364665	2.825208717332
H	-8.081620109154	-0.506381358701	3.506081260441
H	-8.414211777297	-2.220654632913	3.154849158664
H	-9.695452617673	-1.015101514514	2.949287565229
C	-7.221275833560	-0.024418382903	1.043745442850
H	-6.764497135800	0.587428051336	1.826292574221
C	-6.835047871881	0.164938593360	-0.288224109199
H	-6.081045018456	0.918817180354	-0.528304907848
C	-7.405108619771	-0.596765974882	-1.315530029562
C	-8.372266399977	-1.555633850878	-0.972919706711
H	-8.832018798341	-2.162960721146	-1.757405538179
C	-8.756257249876	-1.741937910982	0.355676649531
H	-9.515399688119	-2.492090628603	0.594553259737

SCF Done: E(RB3LYP) = -1233.33209913

Zero-point correction= 0.396037
Thermal correction to Energy= 0.419707
Thermal correction to Enthalpy= 0.420651
Thermal correction to Gibbs Free Energy= 0.335819
Sum of electronic and zero-point Energies= -1232.936062
Sum of electronic and thermal Energies= -1232.912392
Sum of electronic and thermal Enthalpies= -1232.911448
Sum of electronic and thermal Free Energies= -1232.996280

1	C	Isotropic =	38.0920	Anisotropy =	127.2280
2	H	Isotropic =	23.2907	Anisotropy =	6.7680
3	N	Isotropic =	32.3723	Anisotropy =	362.6360
4	C	Isotropic =	39.3250	Anisotropy =	137.7717
5	C	Isotropic =	91.3737	Anisotropy =	116.3380
6	C	Isotropic =	39.1756	Anisotropy =	138.4646
7	N	Isotropic =	150.4921	Anisotropy =	60.2887
8	H	Isotropic =	26.8825	Anisotropy =	9.8770
9	N	Isotropic =	27.9353	Anisotropy =	359.8554
10	C	Isotropic =	63.1411	Anisotropy =	122.9761
11	H	Isotropic =	23.7284	Anisotropy =	6.1371
12	N	Isotropic =	-45.5138	Anisotropy =	354.7724
13	N	Isotropic =	73.7012	Anisotropy =	91.0424
14	H	Isotropic =	22.1755	Anisotropy =	6.6218
15	C	Isotropic =	160.2410	Anisotropy =	32.7111
16	H	Isotropic =	29.1082	Anisotropy =	9.9742
17	H	Isotropic =	29.2775	Anisotropy =	6.5769
18	C	Isotropic =	157.3289	Anisotropy =	30.9324

19	H	Isotropic =	29.3027	Anisotropy =	7.9758
20	H	Isotropic =	29.7707	Anisotropy =	8.5553
21	C	Isotropic =	140.2799	Anisotropy =	40.6228
22	H	Isotropic =	26.2252	Anisotropy =	7.1132
23	C	Isotropic =	150.2644	Anisotropy =	35.2101
24	H	Isotropic =	29.8400	Anisotropy =	3.7694
25	H	Isotropic =	29.7241	Anisotropy =	7.8337
26	C	Isotropic =	155.1880	Anisotropy =	20.2931
27	H	Isotropic =	27.9564	Anisotropy =	8.9464
28	C	Isotropic =	20.2403	Anisotropy =	125.0243
29	C	Isotropic =	157.2424	Anisotropy =	24.6880
30	H	Isotropic =	27.4898	Anisotropy =	7.0612
31	H	Isotropic =	27.7271	Anisotropy =	5.8620
32	N	Isotropic =	17.9520	Anisotropy =	277.3577
33	C	Isotropic =	4.6969	Anisotropy =	123.2250
34	O	Isotropic =	-61.9425	Anisotropy =	188.5951
35	N	Isotropic =	-95.4209	Anisotropy =	200.3926
36	C	Isotropic =	53.4174	Anisotropy =	188.9062
37	C	Isotropic =	169.5240	Anisotropy =	37.3954
38	H	Isotropic =	29.3344	Anisotropy =	6.6119
39	H	Isotropic =	28.7722	Anisotropy =	7.3757
40	H	Isotropic =	28.8000	Anisotropy =	8.9781
41	C	Isotropic =	63.9523	Anisotropy =	151.7278
42	H	Isotropic =	24.0345	Anisotropy =	5.9439
43	C	Isotropic =	62.8032	Anisotropy =	156.9439
44	H	Isotropic =	23.8998	Anisotropy =	6.3840
45	C	Isotropic =	58.0104	Anisotropy =	176.3432
46	C	Isotropic =	64.3024	Anisotropy =	160.9549
47	H	Isotropic =	24.1686	Anisotropy =	7.6054
48	C	Isotropic =	63.8748	Anisotropy =	160.9923
49	H	Isotropic =	24.1583	Anisotropy =	6.7632

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.738438535588	-4.683338755957	3.701471367827
H	-1.625767035256	-5.687029079415	3.275902231622
N	-0.813748982327	-4.322959898364	4.590801806819
C	-1.038923563272	-3.076111382778	5.056914367431
C	-2.096976418503	-2.219436279749	4.688569092841
C	-3.004831561082	-2.745615221514	3.723888385753
N	-4.073124859277	-2.045738235715	3.278119011968
H	-4.209073522951	-1.114021496103	3.651255606775
N	-2.798390917111	-3.988762886012	3.241845995348
C	-1.886222857359	-1.037227748847	5.459389630949
H	-2.467452556972	-0.117397122151	5.489206820001
N	-0.807797009456	-1.152725052114	6.223357958358
N	-0.302698668310	-2.391150476853	5.971374599559
H	0.532868409232	-2.707699038199	6.449629876447
C	-6.335772994644	-0.780787096559	1.130287693165
H	-6.550650004971	0.266677179994	1.385496812469
H	-7.085248914946	-1.100987402166	0.391519929715
C	-6.352525206029	-1.719391427129	2.367352642352

H	-7.226144168555	-2.385535201673	2.338730577695
H	-6.415730439725	-1.161165349138	3.313815724031
C	-5.049105945227	-2.558053659824	2.312241852299
H	-5.217001303792	-3.615453270299	2.552762843407
C	-4.562104041402	-2.405453594367	0.856278580579
H	-5.137389440700	-3.085940538713	0.206757189205
H	-3.494953682485	-2.637362951514	0.739694800184
C	-4.924805500999	-0.942553067160	0.512743635147
H	-4.207748737536	-0.272955040199	1.012337838155
C	-5.104444578001	-0.472796351635	-3.023273900220
C	-5.671189750220	-0.633281571326	-4.402419642274
H	-5.107628668751	0.028426133576	-5.076944029231
H	-6.714719030904	-0.284148203801	-4.388350688902
N	-5.678258900677	-1.023333977647	-1.894742770706
C	-4.864767603096	-0.643611701877	-0.946286343782
O	-3.838541833956	0.096324323218	-1.403209415384
N	-4.004961931844	0.206726715944	-2.795902463872
C	-5.509605561445	-4.750815732295	-5.840170876412
C	-5.461214046592	-6.174390086474	-6.342171253827
H	-5.915875983158	-6.869364574159	-5.616289325809
H	-4.427447553439	-6.503246860968	-6.523150453907
H	-6.022974714595	-6.284778287783	-7.284722924238
C	-4.337668093555	-4.007127376807	-5.630428690922
H	-3.366475226006	-4.465557506340	-5.835393178497
C	-4.389686625154	-2.689523409245	-5.166914569823
H	-3.459644106096	-2.135674702974	-5.012072490115
C	-5.618566161481	-2.070106441789	-4.898123577905
C	-6.792164315388	-2.809628654496	-5.102594374588
H	-7.762802861862	-2.349086430447	-4.900237680053
C	-6.737591911944	-4.126146004444	-5.567151141777
H	-7.668662082594	-4.678845205716	-5.721127077859

SCF Done: E(RB3LYP) = -1233.33124674

Zero-point correction= 0.395739
Thermal correction to Energy= 0.419511
Thermal correction to Enthalpy= 0.420455
Thermal correction to Gibbs Free Energy= 0.335440
Sum of electronic and zero-point Energies= -1232.935507
Sum of electronic and thermal Energies= -1232.911736
Sum of electronic and thermal Enthalpies= -1232.910792
Sum of electronic and thermal Free Energies= -1232.995806

1	C	Isotropic =	37.8795	Anisotropy =	128.7911
2	H	Isotropic =	23.1257	Anisotropy =	5.9789
3	N	Isotropic =	32.8822	Anisotropy =	364.2534
4	C	Isotropic =	39.7402	Anisotropy =	138.1262
5	C	Isotropic =	91.6779	Anisotropy =	117.9210
6	C	Isotropic =	40.0943	Anisotropy =	139.2402
7	N	Isotropic =	144.7244	Anisotropy =	92.3378
8	H	Isotropic =	26.5090	Anisotropy =	9.8498
9	N	Isotropic =	25.0864	Anisotropy =	367.5149
10	C	Isotropic =	63.0967	Anisotropy =	123.0124
11	H	Isotropic =	23.6368	Anisotropy =	6.1037
12	N	Isotropic =	-45.8796	Anisotropy =	355.7176
13	N	Isotropic =	73.3432	Anisotropy =	91.9007

14	H	Isotropic =	22.1252	Anisotropy =	6.7398
15	C	Isotropic =	158.4655	Anisotropy =	35.7700
16	H	Isotropic =	29.1106	Anisotropy =	8.7040
17	H	Isotropic =	29.2638	Anisotropy =	9.2223
18	C	Isotropic =	159.4759	Anisotropy =	35.2854
19	H	Isotropic =	28.8688	Anisotropy =	9.3059
20	H	Isotropic =	29.7220	Anisotropy =	8.6634
21	C	Isotropic =	135.6556	Anisotropy =	23.4007
22	H	Isotropic =	26.7470	Anisotropy =	5.8906
23	C	Isotropic =	146.7620	Anisotropy =	33.0441
24	H	Isotropic =	29.8417	Anisotropy =	8.3922
25	H	Isotropic =	29.2961	Anisotropy =	6.1581
26	C	Isotropic =	152.2106	Anisotropy =	26.1604
27	H	Isotropic =	28.1746	Anisotropy =	6.4260
28	C	Isotropic =	20.3710	Anisotropy =	126.0466
29	C	Isotropic =	157.7247	Anisotropy =	25.2195
30	H	Isotropic =	27.3897	Anisotropy =	6.8084
31	H	Isotropic =	27.9021	Anisotropy =	6.2214
32	N	Isotropic =	17.1325	Anisotropy =	288.0234
33	C	Isotropic =	7.8204	Anisotropy =	117.8971
34	O	Isotropic =	-64.3476	Anisotropy =	193.8804
35	N	Isotropic =	-97.5435	Anisotropy =	207.6790
36	C	Isotropic =	54.1195	Anisotropy =	187.8264
37	C	Isotropic =	170.1375	Anisotropy =	37.0050
38	H	Isotropic =	28.8602	Anisotropy =	7.8871
39	H	Isotropic =	29.5131	Anisotropy =	7.2481
40	H	Isotropic =	28.8704	Anisotropy =	8.5499
41	C	Isotropic =	63.6823	Anisotropy =	151.3666
42	H	Isotropic =	24.3149	Anisotropy =	6.4413
43	C	Isotropic =	65.0950	Anisotropy =	167.1725
44	H	Isotropic =	24.3517	Anisotropy =	8.4085
45	C	Isotropic =	57.8792	Anisotropy =	177.1383
46	C	Isotropic =	63.4968	Anisotropy =	152.5652
47	H	Isotropic =	24.0675	Anisotropy =	6.7064
48	C	Isotropic =	63.4993	Anisotropy =	159.4380
49	H	Isotropic =	24.1595	Anisotropy =	6.7286

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.894033009750	-0.063598438059	4.290500409653
H	-7.460409511603	0.181121798930	5.196433120843
N	-7.258917431797	0.584493625127	3.182369909280
C	-6.512320173942	0.206266953509	2.126818642579
C	-5.457943672925	-0.739749167869	2.119208918534
C	-5.176108710452	-1.333254101283	3.385744246921
N	-4.200465099832	-2.235635324187	3.634646671295
H	-4.196837234364	-2.584873637159	4.589372576990
N	-5.925534329909	-0.978095961113	4.456032875380
C	-5.032863324696	-0.776403969214	0.752301266235
H	-4.254418594682	-1.371059779687	0.279784235375
N	-5.741849057292	0.059061272295	0.007598050461
N	-6.631239844988	0.650541547829	0.849251234833

H	-7.292732987873	1.332793355737	0.497125651436
C	-1.246244765149	-4.080157349236	2.313243075896
H	-0.489544261391	-4.756577503534	2.733716946795
H	-0.746702384874	-3.438488031489	1.571892628929
C	-1.929397484719	-3.209482729715	3.374203483389
H	-1.326262113930	-2.339719576909	3.672181242805
H	-2.147510526986	-3.799234000989	4.282336962626
C	-3.251467094567	-2.812810401540	2.701586881384
H	-3.033807942742	-2.061237029120	1.928888615821
C	-3.717459924974	-4.130034757754	2.037342707205
H	-4.404194850477	-3.963811642073	1.195753620602
H	-4.252039997397	-4.732217261813	2.787438340165
C	-2.404358751133	-4.867660658408	1.616789743207
H	-2.437254263381	-5.905589961597	1.972650848868
C	-1.998440079057	-4.580262857559	-1.922359652582
C	-1.792436869815	-3.863914652720	-3.225161345616
H	-1.768731356103	-4.616930039638	-4.025981395554
H	-0.806327735961	-3.374967645057	-3.196682877415
N	-2.029981391929	-3.939734141600	-0.699702427461
C	-2.239351228764	-4.923235653324	0.133798932850
O	-2.336268472000	-6.115354183728	-0.479077095892
N	-2.174945200524	-5.878761457238	-1.857876882000
C	-4.932107058670	-0.906097479222	-3.868535076468
C	-6.035376224407	0.114274529792	-4.010296118316
H	-5.683702353223	1.022027685709	-4.525944452542
H	-6.395860808156	0.424234532145	-3.014101736789
H	-6.893009227061	-0.290007503350	-4.568170122725
C	-5.163843576351	-2.272089409442	-4.094107393069
H	-6.153938864965	-2.602516550187	-4.419738661452
C	-4.153124013001	-3.218575500197	-3.903439629076
H	-4.365752026505	-4.276764571325	-4.078913374526
C	-2.873810913959	-2.828241333110	-3.482931873249
C	-2.631650285493	-1.463124129546	-3.273816250836
H	-1.639697368348	-1.133648016537	-2.953863795976
C	-3.643475899131	-0.519029284989	-3.465518329117
H	-3.429361700753	0.539180390444	-3.292033349700

SCF Done: E(RB3LYP) = -1233.33131979

Zero-point correction= 0.396461
Thermal correction to Energy= 0.419773
Thermal correction to Enthalpy= 0.420717
Thermal correction to Gibbs Free Energy= 0.339430
Sum of electronic and zero-point Energies= -1232.934858
Sum of electronic and thermal Energies= -1232.911547
Sum of electronic and thermal Enthalpies= -1232.910603
Sum of electronic and thermal Free Energies= -1232.991890

1	C	Isotropic =	38.1259	Anisotropy =	128.0593
2	H	Isotropic =	23.1903	Anisotropy =	5.2661
3	N	Isotropic =	34.8974	Anisotropy =	362.6019
4	C	Isotropic =	38.5197	Anisotropy =	137.4791
5	C	Isotropic =	93.2802	Anisotropy =	119.3435
6	C	Isotropic =	38.7910	Anisotropy =	137.7371
7	N	Isotropic =	142.7394	Anisotropy =	73.1866
8	H	Isotropic =	26.5688	Anisotropy =	9.0075

9	N	Isotropic =	21.2938	Anisotropy =	334.3918
10	C	Isotropic =	61.1152	Anisotropy =	115.2683
11	H	Isotropic =	24.1567	Anisotropy =	9.4529
12	N	Isotropic =	-42.8749	Anisotropy =	348.3210
13	N	Isotropic =	73.7987	Anisotropy =	91.0000
14	H	Isotropic =	22.1544	Anisotropy =	6.1642
15	C	Isotropic =	158.0109	Anisotropy =	31.1411
16	H	Isotropic =	29.0895	Anisotropy =	9.6216
17	H	Isotropic =	29.2901	Anisotropy =	6.6509
18	C	Isotropic =	155.2954	Anisotropy =	30.4541
19	H	Isotropic =	29.1689	Anisotropy =	8.4690
20	H	Isotropic =	29.7065	Anisotropy =	8.6806
21	C	Isotropic =	134.9612	Anisotropy =	43.0302
22	H	Isotropic =	27.1368	Anisotropy =	6.0589
23	C	Isotropic =	151.0082	Anisotropy =	38.9777
24	H	Isotropic =	29.5093	Anisotropy =	3.4253
25	H	Isotropic =	29.6442	Anisotropy =	7.2136
26	C	Isotropic =	155.0986	Anisotropy =	21.0540
27	H	Isotropic =	27.9254	Anisotropy =	8.8549
28	C	Isotropic =	19.8828	Anisotropy =	125.7155
29	C	Isotropic =	157.4327	Anisotropy =	25.2313
30	H	Isotropic =	27.3924	Anisotropy =	7.2023
31	H	Isotropic =	27.7741	Anisotropy =	6.0290
32	N	Isotropic =	19.0277	Anisotropy =	282.7537
33	C	Isotropic =	4.9698	Anisotropy =	122.6125
34	O	Isotropic =	-63.0998	Anisotropy =	190.6565
35	N	Isotropic =	-95.3687	Anisotropy =	201.1519
36	C	Isotropic =	53.3893	Anisotropy =	189.9683
37	C	Isotropic =	169.7140	Anisotropy =	37.0627
38	H	Isotropic =	28.9239	Anisotropy =	8.0761
39	H	Isotropic =	28.4897	Anisotropy =	8.5476
40	H	Isotropic =	29.3591	Anisotropy =	7.7413
41	C	Isotropic =	63.8116	Anisotropy =	153.5745
42	H	Isotropic =	24.2521	Anisotropy =	6.2800
43	C	Isotropic =	64.4958	Anisotropy =	163.3975
44	H	Isotropic =	24.2619	Anisotropy =	7.6981
45	C	Isotropic =	57.8038	Anisotropy =	177.8360
46	C	Isotropic =	62.8502	Anisotropy =	155.3898
47	H	Isotropic =	23.9244	Anisotropy =	6.2252
48	C	Isotropic =	63.4932	Anisotropy =	160.5766
49	H	Isotropic =	24.0015	Anisotropy =	6.3786

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.436298048190	0.809716344524	-2.459240172441
H	-6.238470015240	0.720199436837	-3.533499965862
N	-7.708483783381	1.013262761997	-2.118518966492
C	-7.849480493054	1.111452077588	-0.779479366506
C	-6.822380447914	1.019774617788	0.182358789724
C	-5.513525957153	0.798195332721	-0.336368981528
N	-4.426911617723	0.694735085276	0.462417963411
H	-4.571342308991	0.783798835072	1.460910204749

N	-5.348451435070	0.693506446580	-1.671433655567
C	-7.485989049858	1.190591193251	1.433834122687
H	-7.073387208059	1.190599435077	2.441123713780
N	-8.789325419106	1.368121613360	1.261312708677
N	-8.998067459861	1.318439170528	-0.082747619878
H	-9.932724581550	1.431294403566	-0.457938619693
C	-1.510003838088	-0.493918016881	1.655056340329
H	-1.535388213174	-0.528349945686	2.753394755212
H	-0.467907936803	-0.662255532950	1.344426817521
C	-2.034789471606	0.849933687699	1.080400700705
H	-1.211115220968	1.438378638234	0.652714114663
H	-2.500190874155	1.479512302921	1.854024183782
C	-3.060143071789	0.495230526012	-0.027685055514
H	-2.943292236608	1.116214294905	-0.924947262047
C	-2.771140328987	-0.985035400292	-0.352479486961
H	-1.895840986268	-1.045400133733	-1.020388587860
H	-3.616113511150	-1.481767405481	-0.847632925567
C	-2.414999598183	-1.585607704416	1.025314706849
H	-3.336050476484	-1.699982074362	1.616149770338
C	-1.284279926253	-4.972271952893	1.076904693236
C	-1.361154052177	-6.437836305149	1.388201349216
H	-1.512650152862	-6.551544295551	2.472234794056
H	-0.390186284161	-6.888777983618	1.136128057915
N	-2.263597260974	-4.065848986071	1.437369934648
C	-1.800306659936	-2.941291240084	0.962613394256
O	-0.615044605930	-3.085445271059	0.339419597274
N	-0.275967646707	-4.449224761377	0.421606733717
C	-4.580560501357	-8.422324024602	-0.788968376569
C	-5.684303153622	-9.114995995743	-1.552088411564
H	-5.346256802302	-10.088637148952	-1.945932838555
H	-6.009157685225	-8.515558795172	-2.418537254234
H	-6.562147124620	-9.296508070280	-0.914853085645
C	-3.407940686680	-8.002795334298	-1.442812366347
H	-3.299644367255	-8.176799470212	-2.517078803618
C	-2.379172508478	-7.370184786409	-0.744789754430
H	-1.480052394543	-7.051778605619	-1.279502011115
C	-2.484358431113	-7.134441343524	0.636095583130
C	-3.649958935300	-7.547698471186	1.291300782781
H	-3.757118966937	-7.375125271964	2.365393485457
C	-4.681091210293	-8.182464049313	0.588410833196
H	-5.580497053860	-8.496987827058	1.124665436689

SCF Done: E(RB3LYP) = -1233.33106968

Zero-point correction= 0.395748
Thermal correction to Energy= 0.419471
Thermal correction to Enthalpy= 0.420415
Thermal correction to Gibbs Free Energy= 0.335809
Sum of electronic and zero-point Energies= -1232.935322
Sum of electronic and thermal Energies= -1232.911599
Sum of electronic and thermal Enthalpies= -1232.910655
Sum of electronic and thermal Free Energies= -1232.995261

1	C	Isotropic =	38.0169	Anisotropy =	128.9961
2	H	Isotropic =	23.1458	Anisotropy =	5.8347
3	N	Isotropic =	32.7284	Anisotropy =	364.3096

4	C	Isotropic =	39.4928	Anisotropy =	138.7550
5	C	Isotropic =	91.4862	Anisotropy =	118.0856
6	C	Isotropic =	40.1885	Anisotropy =	139.1313
7	N	Isotropic =	145.0732	Anisotropy =	93.2886
8	H	Isotropic =	26.5373	Anisotropy =	9.4143
9	N	Isotropic =	24.8788	Anisotropy =	368.0093
10	C	Isotropic =	63.3282	Anisotropy =	123.5424
11	H	Isotropic =	23.6792	Anisotropy =	5.9553
12	N	Isotropic =	-46.1306	Anisotropy =	354.2031
13	N	Isotropic =	73.4388	Anisotropy =	91.6074
14	H	Isotropic =	22.1450	Anisotropy =	6.7102
15	C	Isotropic =	158.5949	Anisotropy =	35.8378
16	H	Isotropic =	29.1379	Anisotropy =	8.6405
17	H	Isotropic =	29.3311	Anisotropy =	8.4282
18	C	Isotropic =	158.8105	Anisotropy =	35.9661
19	H	Isotropic =	28.8165	Anisotropy =	9.6535
20	H	Isotropic =	29.6952	Anisotropy =	8.4657
21	C	Isotropic =	135.9142	Anisotropy =	22.8762
22	H	Isotropic =	26.7575	Anisotropy =	6.2916
23	C	Isotropic =	148.1608	Anisotropy =	31.6299
24	H	Isotropic =	29.4562	Anisotropy =	7.5743
25	H	Isotropic =	29.3553	Anisotropy =	5.9723
26	C	Isotropic =	150.5908	Anisotropy =	26.1817
27	H	Isotropic =	28.2125	Anisotropy =	6.6814
28	C	Isotropic =	20.9176	Anisotropy =	126.4825
29	C	Isotropic =	157.5551	Anisotropy =	25.5372
30	H	Isotropic =	27.9268	Anisotropy =	6.2819
31	H	Isotropic =	27.4609	Anisotropy =	6.6499
32	N	Isotropic =	11.7062	Anisotropy =	266.5292
33	C	Isotropic =	9.7356	Anisotropy =	118.8377
34	O	Isotropic =	-54.1569	Anisotropy =	215.4194
35	N	Isotropic =	-100.0018	Anisotropy =	212.4358
36	C	Isotropic =	54.0951	Anisotropy =	188.3365
37	C	Isotropic =	170.1599	Anisotropy =	36.8027
38	H	Isotropic =	28.8980	Anisotropy =	8.8124
39	H	Isotropic =	29.0050	Anisotropy =	7.6188
40	H	Isotropic =	29.5445	Anisotropy =	7.1361
41	C	Isotropic =	63.9148	Anisotropy =	161.1059
42	H	Isotropic =	24.2710	Anisotropy =	6.8903
43	C	Isotropic =	64.6853	Anisotropy =	164.7810
44	H	Isotropic =	24.3035	Anisotropy =	8.1182
45	C	Isotropic =	57.9023	Anisotropy =	176.3529
46	C	Isotropic =	63.2710	Anisotropy =	153.0296
47	H	Isotropic =	24.1527	Anisotropy =	6.6007
48	C	Isotropic =	63.8456	Anisotropy =	151.6147
49	H	Isotropic =	24.2902	Anisotropy =	6.0826

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.270083104125	0.567428580365	0.249694953786
H	1.210045207537	1.112257645089	0.104115269385
N	-0.598794461333	1.122763690147	1.097357198836

C	-1.711396444618	0.371914503041	1.219319577308
C	-1.992744311880	-0.848513897661	0.559441349767
C	-0.977214910758	-1.296970480490	-0.335875558214
N	-1.048218074095	-2.408948960157	-1.102180889241
H	-0.207866612181	-2.601862219060	-1.640285003661
N	0.157329684206	-0.568422883591	-0.457948157870
C	-3.275290198467	-1.236514865063	1.065225646729
H	-3.871277242356	-2.122297173284	0.849926346200
N	-3.733755998685	-0.345234825710	1.932336730611
N	-2.782670266314	0.626530453600	2.014207040548
H	-2.912482303410	1.419133956865	2.632157684227
C	-3.200235120024	-5.215709808241	-2.338279656891
H	-2.913310538485	-6.095096411499	-2.930321416256
H	-4.228462021021	-4.952976797788	-2.628523438692
C	-2.246835800807	-4.025231277623	-2.568577294712
H	-2.596894957383	-3.343561137891	-3.356789419802
H	-1.244080555375	-4.385079810898	-2.856809785457
C	-2.153930290380	-3.342432297372	-1.195489215867
H	-3.084462470456	-2.784492419797	-1.018676141673
C	-2.090160779685	-4.541315249270	-0.227330043406
H	-2.280256182181	-4.269123136524	0.819373779127
H	-1.085818476985	-4.989116476713	-0.287273516328
C	-3.130740307062	-5.532912923123	-0.793527318332
H	-2.824766211622	-6.575096382283	-0.630378493741
C	-6.236708714914	-4.732812707354	0.797055342301
C	-7.227765506809	-3.859209535477	1.509150713221
H	-6.750168962170	-3.478024902241	2.424591125144
H	-8.075749531016	-4.490302137944	1.812286807555
N	-4.974877373375	-4.307350464945	0.428968270235
C	-4.469078889397	-5.364417322819	-0.148276818354
O	-5.319806422899	-6.403620295926	-0.166234541819
N	-6.502748834092	-5.974190453334	0.469417545763
C	-8.603731814193	-0.535884118721	-0.962067183478
C	-9.096874146773	0.607981220209	-1.815704401624
H	-10.157478983917	0.831175093015	-1.607653563380
H	-9.025626898027	0.367028868821	-2.888905191608
H	-8.519652275994	1.526048111756	-1.632007670507
C	-9.078673435447	-1.843584204322	-1.167407738043
H	-9.806261780874	-2.033297012363	-1.961578840338
C	-8.639029631024	-2.903954760734	-0.374284414094
H	-9.023189778188	-3.911024771694	-0.558706058053
C	-7.707286148569	-2.695079536456	0.655862719841
C	-7.228076439842	-1.395887396145	0.863521816243
H	-6.493906567713	-1.201894489599	1.649852971328
C	-7.670802500449	-0.334644254566	0.064752967761
H	-7.278798824620	0.669845675768	0.246055915523

SCF Done: E(RB3LYP) = -1233.33234190

Zero-point correction= 0.396294
Thermal correction to Energy= 0.419773
Thermal correction to Enthalpy= 0.420717
Thermal correction to Gibbs Free Energy= 0.338136
Sum of electronic and zero-point Energies= -1232.936047
Sum of electronic and thermal Energies= -1232.912569
Sum of electronic and thermal Enthalpies= -1232.911625

Sum of electronic and thermal Free Energies= -1232.994206

1	C	Isotropic =	38.0809	Anisotropy =	127.7466
2	H	Isotropic =	23.1430	Anisotropy =	5.2044
3	N	Isotropic =	34.4100	Anisotropy =	362.5272
4	C	Isotropic =	38.7358	Anisotropy =	138.9317
5	C	Isotropic =	92.8259	Anisotropy =	119.5904
6	C	Isotropic =	38.3426	Anisotropy =	137.6840
7	N	Isotropic =	144.8285	Anisotropy =	74.7043
8	H	Isotropic =	26.5699	Anisotropy =	9.1724
9	N	Isotropic =	22.0592	Anisotropy =	335.0245
10	C	Isotropic =	58.5624	Anisotropy =	124.6288
11	H	Isotropic =	22.1898	Anisotropy =	7.6926
12	N	Isotropic =	-44.4624	Anisotropy =	345.5120
13	N	Isotropic =	74.2813	Anisotropy =	90.0519
14	H	Isotropic =	22.0048	Anisotropy =	6.5738
15	C	Isotropic =	160.7211	Anisotropy =	34.4448
16	H	Isotropic =	29.0256	Anisotropy =	10.2799
17	H	Isotropic =	29.9183	Anisotropy =	6.3410
18	C	Isotropic =	156.4899	Anisotropy =	33.5789
19	H	Isotropic =	29.3777	Anisotropy =	7.9743
20	H	Isotropic =	29.7660	Anisotropy =	9.0884
21	C	Isotropic =	135.1185	Anisotropy =	41.1404
22	H	Isotropic =	26.9649	Anisotropy =	6.7487
23	C	Isotropic =	152.4464	Anisotropy =	28.7281
24	H	Isotropic =	28.7590	Anisotropy =	3.3535
25	H	Isotropic =	29.6169	Anisotropy =	8.1536
26	C	Isotropic =	155.4721	Anisotropy =	16.8438
27	H	Isotropic =	27.8838	Anisotropy =	9.0566
28	C	Isotropic =	20.4139	Anisotropy =	124.3903
29	C	Isotropic =	157.8083	Anisotropy =	24.4064
30	H	Isotropic =	27.6992	Anisotropy =	5.5659
31	H	Isotropic =	27.3713	Anisotropy =	7.3602
32	N	Isotropic =	18.8380	Anisotropy =	264.0317
33	C	Isotropic =	5.5109	Anisotropy =	120.4126
34	O	Isotropic =	-58.3727	Anisotropy =	195.8505
35	N	Isotropic =	-97.9944	Anisotropy =	202.7567
36	C	Isotropic =	53.9084	Anisotropy =	187.9299
37	C	Isotropic =	169.8490	Anisotropy =	37.1176
38	H	Isotropic =	28.8774	Anisotropy =	9.1558
39	H	Isotropic =	29.0164	Anisotropy =	7.8517
40	H	Isotropic =	29.5350	Anisotropy =	6.7172
41	C	Isotropic =	63.7574	Anisotropy =	160.4040
42	H	Isotropic =	24.2054	Anisotropy =	6.5843
43	C	Isotropic =	64.0456	Anisotropy =	163.8465
44	H	Isotropic =	24.1883	Anisotropy =	8.0152
45	C	Isotropic =	58.1670	Anisotropy =	176.0149
46	C	Isotropic =	62.7628	Anisotropy =	156.9812
47	H	Isotropic =	23.5752	Anisotropy =	5.1266
48	C	Isotropic =	63.9373	Anisotropy =	151.6701
49	H	Isotropic =	24.3304	Anisotropy =	7.6527

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)

#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.011638613923	-6.616233368361	-0.196885344780
H	-6.980461723189	-6.375724667878	0.255709091617
N	-6.002548982759	-7.657767267865	-1.028954023301
C	-4.768228964116	-7.872540603878	-1.531712232665
C	-3.604775372485	-7.126633974886	-1.250738034605
C	-3.773356151887	-6.041102665024	-0.342201741245
N	-2.740123364483	-5.245499425104	0.020278171010
H	-1.840561782601	-5.432217728283	-0.409693505791
N	-4.998779050276	-5.808256219492	0.171353682890
C	-2.581177026388	-7.753966510942	-2.022093523083
H	-1.525047697170	-7.503496485088	-2.104885503443
N	-3.064010900167	-8.781066682226	-2.708877406586
N	-4.389367546015	-8.843311696288	-2.404368183754
H	-4.973805283718	-9.561015820069	-2.817189186991
C	-1.732592296119	-2.690643278147	2.526336470152
H	-0.860225441557	-2.455160283290	3.152448535627
H	-2.641336748292	-2.450679689381	3.102786787744
C	-1.778737502097	-4.144057528473	2.052437970024
H	-2.042197641699	-4.855482843656	2.848849295300
H	-0.795933794141	-4.440375760023	1.644829157048
C	-2.824693501348	-4.108097483700	0.922897250270
H	-3.831483385786	-4.146248177048	1.355544097381
C	-2.613740778000	-2.731514046270	0.223163727302
H	-3.576772863464	-2.241667187373	0.024191478332
H	-2.102067759749	-2.861929326306	-0.741526859172
C	-1.737020196801	-1.886719217928	1.194533534662
H	-0.705849703399	-1.833976287083	0.816660646403
C	-3.235491623791	1.315428912337	1.705258910674
C	-4.354127752747	2.283202615664	1.958057327709
H	-3.910377668396	3.274180806068	2.131612211917
H	-4.866960201045	1.979222278850	2.883492914788
N	-3.420493220946	-0.047455958876	1.588281310531
C	-2.208789815773	-0.482933149858	1.370467454189
O	-1.296162493821	0.504543228770	1.341766744796
N	-1.990741612098	1.707487375960	1.567800431310
C	-7.198139511506	2.425341994971	-1.348149786599
C	-8.178944033967	2.490469943501	-2.494517334546
H	-9.033065658377	1.816578927298	-2.333077737487
H	-7.699803098004	2.213813440549	-3.447903517595
H	-8.576095884010	3.512273391504	-2.620953852254
C	-5.959273208945	3.086671529731	-1.423491167719
H	-5.702407194457	3.646406846829	-2.327249323197
C	-5.052157989266	3.043540907541	-0.364174532712
H	-4.095356222399	3.565667829254	-0.451593432722
C	-5.351704662912	2.336888990225	0.812070957038
C	-6.582208057976	1.674028705525	0.891078189347
H	-6.838254357255	1.114892904886	1.794722151733
C	-7.490442477191	1.718782634440	-0.173002784324
H	-8.445419183488	1.193830068896	-0.084689485226

SCF Done: E(RB3LYP) = -1233.33230816

Zero-point correction= 0.396018
Thermal correction to Energy= 0.419688

Thermal correction to Enthalpy= 0.420633
Thermal correction to Gibbs Free Energy= 0.334905
Sum of electronic and zero-point Energies= -1232.936290
Sum of electronic and thermal Energies= -1232.912620
Sum of electronic and thermal Enthalpies= -1232.911676
Sum of electronic and thermal Free Energies= -1232.997404

1	C	Isotropic =	37.8328	Anisotropy =	127.9805
2	H	Isotropic =	23.0689	Anisotropy =	5.7255
3	N	Isotropic =	32.6817	Anisotropy =	364.3506
4	C	Isotropic =	39.6382	Anisotropy =	138.1507
5	C	Isotropic =	91.6322	Anisotropy =	116.4191
6	C	Isotropic =	39.4947	Anisotropy =	138.8639
7	N	Isotropic =	144.9840	Anisotropy =	55.4942
8	H	Isotropic =	26.7474	Anisotropy =	9.6847
9	N	Isotropic =	28.9282	Anisotropy =	360.0239
10	C	Isotropic =	63.4586	Anisotropy =	123.4620
11	H	Isotropic =	23.7146	Anisotropy =	6.0095
12	N	Isotropic =	-45.4285	Anisotropy =	355.1739
13	N	Isotropic =	73.7880	Anisotropy =	91.8654
14	H	Isotropic =	22.1553	Anisotropy =	6.6931
15	C	Isotropic =	154.4968	Anisotropy =	31.0253
16	H	Isotropic =	29.2291	Anisotropy =	8.7737
17	H	Isotropic =	29.6815	Anisotropy =	6.3978
18	C	Isotropic =	154.4222	Anisotropy =	28.5514
19	H	Isotropic =	29.3298	Anisotropy =	8.1940
20	H	Isotropic =	29.7135	Anisotropy =	7.7034
21	C	Isotropic =	139.9597	Anisotropy =	36.1713
22	H	Isotropic =	26.0067	Anisotropy =	7.7140
23	C	Isotropic =	152.2488	Anisotropy =	45.3528
24	H	Isotropic =	29.1074	Anisotropy =	8.1994
25	H	Isotropic =	29.6780	Anisotropy =	6.2041
26	C	Isotropic =	152.3095	Anisotropy =	25.0895
27	H	Isotropic =	28.0252	Anisotropy =	8.1775
28	C	Isotropic =	20.2120	Anisotropy =	124.9326
29	C	Isotropic =	157.2757	Anisotropy =	25.2633
30	H	Isotropic =	27.4541	Anisotropy =	6.8324
31	H	Isotropic =	27.8153	Anisotropy =	5.9046
32	N	Isotropic =	18.0580	Anisotropy =	284.7720
33	C	Isotropic =	6.6529	Anisotropy =	119.1538
34	O	Isotropic =	-64.0349	Anisotropy =	192.9066
35	N	Isotropic =	-96.6623	Anisotropy =	203.2033
36	C	Isotropic =	53.9473	Anisotropy =	188.1654
37	C	Isotropic =	169.9045	Anisotropy =	37.0278
38	H	Isotropic =	29.4721	Anisotropy =	7.0561
39	H	Isotropic =	28.9737	Anisotropy =	7.6147
40	H	Isotropic =	28.8633	Anisotropy =	8.8618
41	C	Isotropic =	63.8487	Anisotropy =	160.6757
42	H	Isotropic =	24.2326	Anisotropy =	6.7908
43	C	Isotropic =	64.6608	Anisotropy =	162.8530
44	H	Isotropic =	24.2432	Anisotropy =	7.9743
45	C	Isotropic =	57.9233	Anisotropy =	176.3877
46	C	Isotropic =	63.1126	Anisotropy =	154.3342
47	H	Isotropic =	24.0198	Anisotropy =	6.6229
48	C	Isotropic =	63.5956	Anisotropy =	151.6305
49	H	Isotropic =	24.2016	Anisotropy =	6.2320

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

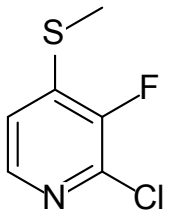
C	-3.383020296470	-7.038177672480	-1.552095751232
H	-4.448286406941	-7.254382659705	-1.692673991638
N	-2.537276034330	-7.944587996191	-2.042375658226
C	-1.254312163785	-7.588948516053	-1.819104988043
C	-0.807117306434	-6.425103999270	-1.159878948190
C	-1.830906870550	-5.550259568218	-0.692191576622
N	-1.545707544220	-4.399882258632	-0.038426567356
H	-0.566115412123	-4.162861631846	0.076311117292
N	-3.119879146862	-5.885691434429	-0.906498194542
C	0.616338471443	-6.523201674910	-1.184745417084
H	1.364409908138	-5.839871540088	-0.786648208345
N	1.006863995549	-7.633144940107	-1.797258579140
N	-0.134324515260	-8.270526984837	-2.177487635703
H	-0.084130054447	-9.155046403759	-2.669615061749
C	-3.092288471540	-1.742812850534	2.053648624931
H	-2.845466594420	-1.159562176133	2.952274311086
H	-4.173302432621	-1.957126651024	2.073273542900
C	-2.298918322152	-3.044065989139	1.926152069374
H	-2.623276909192	-3.824404688340	2.630155479464
H	-1.225487039347	-2.853494759718	2.102729315273
C	-2.524144644449	-3.444778657620	0.456969153508
H	-3.498623049736	-3.937685832410	0.358107024617
C	-2.543625466995	-2.098868129757	-0.326772960086
H	-3.350749262412	-2.090974394835	-1.072414716634
H	-1.595296415693	-1.950217822190	-0.863586492675
C	-2.741608277444	-0.981404157999	0.744665155846
H	-1.796369157191	-0.439801620229	0.891120433461
C	-5.467712588976	1.126905989056	-0.194276425310
C	-6.876491335727	1.452447834855	-0.594564034987
H	-7.127437099500	0.855475675619	-1.484382883602
H	-6.908427553250	2.513311975482	-0.883140786463
N	-5.022001689364	-0.156573326355	0.048169371197
C	-3.769503862239	0.031237898732	0.367423239709
O	-3.412799100404	1.327569674866	0.341943326223
N	-4.555090146510	2.056899368166	-0.036137827443
C	-9.750598364810	0.662913076964	2.593083089443
C	-10.743604210725	0.404394242149	3.701044818079
H	-11.430278079677	1.258017399405	3.828732103500
H	-10.233774615698	0.257818556262	4.668032474606
H	-11.349959506506	-0.490558839818	3.498535164490
C	-8.874355164143	1.761521434173	2.655844141095
H	-8.914964698652	2.433571591536	3.517738812679
C	-7.955900232566	2.011681728252	1.636338769806
H	-7.286402804448	2.872912339823	1.712559814196
C	-7.880334352652	1.171969757249	0.512649744060
C	-8.747392696729	0.075434997658	0.446651382384
H	-8.709081113934	-0.593649160568	-0.416949050415
C	-9.668611476248	-0.173410451517	1.471324124117
H	-10.336709887758	-1.035276751532	1.392899152147

SCF Done: E(RB3LYP) = -1233.33228550

Zero-point correction= 0.396063
Thermal correction to Energy= 0.419737
Thermal correction to Enthalpy= 0.420681
Thermal correction to Gibbs Free Energy= 0.335252
Sum of electronic and zero-point Energies= -1232.936223
Sum of electronic and thermal Energies= -1232.912549
Sum of electronic and thermal Enthalpies= -1232.911605
Sum of electronic and thermal Free Energies= -1232.997034

1	C	Isotropic =	37.8898	Anisotropy =	127.9525
2	H	Isotropic =	23.0577	Anisotropy =	5.8082
3	N	Isotropic =	32.3802	Anisotropy =	363.1853
4	C	Isotropic =	39.4947	Anisotropy =	137.9546
5	C	Isotropic =	91.4009	Anisotropy =	115.7942
6	C	Isotropic =	39.5687	Anisotropy =	138.7161
7	N	Isotropic =	145.1483	Anisotropy =	56.1167
8	H	Isotropic =	26.6973	Anisotropy =	9.8357
9	N	Isotropic =	28.7583	Anisotropy =	359.9275
10	C	Isotropic =	62.9141	Anisotropy =	122.5629
11	H	Isotropic =	23.6956	Anisotropy =	6.0173
12	N	Isotropic =	-45.7087	Anisotropy =	354.0768
13	N	Isotropic =	73.4302	Anisotropy =	90.1758
14	H	Isotropic =	22.1390	Anisotropy =	6.7206
15	C	Isotropic =	155.0741	Anisotropy =	30.0331
16	H	Isotropic =	29.3503	Anisotropy =	8.2565
17	H	Isotropic =	29.7672	Anisotropy =	8.1425
18	C	Isotropic =	154.7564	Anisotropy =	28.6988
19	H	Isotropic =	29.3776	Anisotropy =	7.8549
20	H	Isotropic =	29.7533	Anisotropy =	7.7932
21	C	Isotropic =	139.8119	Anisotropy =	37.1079
22	H	Isotropic =	26.0131	Anisotropy =	7.7072
23	C	Isotropic =	151.1270	Anisotropy =	46.3762
24	H	Isotropic =	29.0721	Anisotropy =	5.5472
25	H	Isotropic =	29.5323	Anisotropy =	6.7447
26	C	Isotropic =	152.7472	Anisotropy =	24.3436
27	H	Isotropic =	28.0323	Anisotropy =	8.2565
28	C	Isotropic =	20.0661	Anisotropy =	125.6106
29	C	Isotropic =	157.4211	Anisotropy =	25.0983
30	H	Isotropic =	27.8505	Anisotropy =	5.8811
31	H	Isotropic =	27.4143	Anisotropy =	6.8267
32	N	Isotropic =	17.8249	Anisotropy =	284.5416
33	C	Isotropic =	6.1766	Anisotropy =	120.0915
34	O	Isotropic =	-65.2243	Anisotropy =	192.1761
35	N	Isotropic =	-96.1149	Anisotropy =	203.5202
36	C	Isotropic =	53.8016	Anisotropy =	187.5464
37	C	Isotropic =	169.8052	Anisotropy =	37.2084
38	H	Isotropic =	28.8850	Anisotropy =	8.5571
39	H	Isotropic =	28.9045	Anisotropy =	7.8701
40	H	Isotropic =	29.4599	Anisotropy =	7.2008
41	C	Isotropic =	63.6081	Anisotropy =	161.0022
42	H	Isotropic =	24.2012	Anisotropy =	6.9593
43	C	Isotropic =	64.7055	Anisotropy =	165.1739
44	H	Isotropic =	24.2104	Anisotropy =	8.2992

45 C Isotropic = 58.0368 Anisotropy = 176.6045
46 C Isotropic = 63.5648 Anisotropy = 153.2519
47 H Isotropic = 24.0575 Anisotropy = 6.5959
48 C Isotropic = 63.6702 Anisotropy = 149.9992
49 H Isotropic = 24.2283 Anisotropy = 6.2746



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.846128595389	0.766232097935	-0.294403920081
F	1.034032755530	1.648998500317	-1.289848204071
C	1.273493896795	1.049471784120	1.007231581652
S	2.120662584678	2.532905034309	1.503510016019
C	1.335132698614	3.876972860245	0.529790672079
H	0.242511807898	3.830829652918	0.628045492274
H	1.635975404876	3.842601918008	-0.522981265768
H	1.705266586244	4.799927091656	0.997482792565
C	1.074073045667	0.037234344118	1.964858718949
H	1.383317215211	0.195549641150	2.998707670380
C	0.469329047242	-1.156569163163	1.585503664460
H	0.307998326166	-1.951052774999	2.318556455548
N	0.035703542050	-1.404561469934	0.336459864725
C	0.225882658451	-0.457885258866	-0.562274078172
Cl	-0.323858164810	-0.770224257815	-2.208909460559

SCF Done: E(RB3LYP) = -1244.67991576

Zero-point correction= 0.099154
Thermal correction to Energy= 0.108760
Thermal correction to Enthalpy= 0.109704
Thermal correction to Gibbs Free Energy= 0.062818
Sum of electronic and zero-point Energies= -1244.580762
Sum of electronic and thermal Energies= -1244.571156
Sum of electronic and thermal Enthalpies= -1244.570212
Sum of electronic and thermal Free Energies= -1244.617098

1 C Isotropic = 38.6132 Anisotropy = 87.3383
2 F Isotropic = 308.0960 Anisotropy = 115.1859
3 C Isotropic = 47.3223 Anisotropy = 158.2756
4 S Isotropic = 508.2109 Anisotropy = 298.9359

5 C Isotropic = 169.7066 Anisotropy = 33.3331
6 H Isotropic = 28.8860 Anisotropy = 8.7815
7 H Isotropic = 28.1195 Anisotropy = 8.5243
8 H Isotropic = 29.2239 Anisotropy = 11.7632
9 C Isotropic = 67.2714 Anisotropy = 141.1784
10 H Isotropic = 24.3432 Anisotropy = 7.9560
11 C Isotropic = 50.7095 Anisotropy = 151.3018
12 H Isotropic = 23.4628 Anisotropy = 5.1524
13 N Isotropic = -49.3577 Anisotropy = 439.9420
14 C Isotropic = 44.5947 Anisotropy = 72.2513
15 Cl Isotropic = 712.6039 Anisotropy = 433.8018

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.051831326167	0.579870648531	-0.240677280998
F	2.128552274757	0.689798688140	-1.037374443272
C	0.766455939861	1.555248102790	0.720896486989
S	1.720492611506	3.031332203119	0.993152334399
C	3.466490916379	2.524232635069	0.737820833218
H	4.051329357936	3.371220685203	1.122657655326
H	3.690299441849	2.364062351121	-0.322497206948
H	3.693498618326	1.626150373415	1.327309822355
C	-0.411494292529	1.369349666171	1.469052944792
H	-0.690779321950	2.092347683244	2.236474774587
C	-1.206046178755	0.252707053317	1.231555733121
H	-2.122783141458	0.095584386900	1.805549590932
N	-0.904783677647	-0.693305967933	0.323743774556
C	0.196955291323	-0.517623496593	-0.380086138002
Cl	0.602680834234	-1.740815012495	-1.584408881054

SCF Done: E(RB3LYP) = -1244.67990539

Zero-point correction= 0.099183
Thermal correction to Energy= 0.108758
Thermal correction to Enthalpy= 0.109702
Thermal correction to Gibbs Free Energy= 0.063038
Sum of electronic and zero-point Energies= -1244.580723
Sum of electronic and thermal Energies= -1244.571147
Sum of electronic and thermal Enthalpies= -1244.570203
Sum of electronic and thermal Free Energies= -1244.616868

1 C Isotropic = 38.7032 Anisotropy = 87.2676
2 F Isotropic = 308.1944 Anisotropy = 114.6050
3 C Isotropic = 47.2526 Anisotropy = 158.5295
4 S Isotropic = 507.6701 Anisotropy = 299.4684
5 C Isotropic = 169.5823 Anisotropy = 33.2759
6 H Isotropic = 29.2333 Anisotropy = 11.7514
7 H Isotropic = 28.1221 Anisotropy = 8.5048
8 H Isotropic = 28.8742 Anisotropy = 8.7370
9 C Isotropic = 67.5528 Anisotropy = 141.3957
10 H Isotropic = 24.3580 Anisotropy = 7.9426
11 C Isotropic = 50.7391 Anisotropy = 151.3103

12 H Isotropic = 23.4655 Anisotropy = 5.1512
13 N Isotropic = -48.9564 Anisotropy = 439.6877
14 C Isotropic = 44.5782 Anisotropy = 72.2641
15 Cl Isotropic = 712.6067 Anisotropy = 433.7999

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.170210974595	0.654036921482	-0.108472648529
F	2.399443719564	1.157755299511	-0.311170935290
C	0.191372175307	1.397166470015	0.559872415052
S	0.435421690416	3.024075430667	1.237238830229
C	1.499672572553	3.889575293764	0.016549829336
H	2.532268836004	3.524989642301	0.048856321494
H	1.462637582157	4.943244051601	0.326545167799
H	1.079784295985	3.791561980004	-0.993346928716
C	-1.047217352127	0.760618857185	0.763898056993
H	-1.853290306698	1.286538502298	1.276956252698
C	-1.237738003921	-0.534873617393	0.294469149684
H	-2.194582035907	-1.041376151501	0.444379102185
N	-0.297757200382	-1.227837423434	-0.373123689731
C	0.864875506008	-0.633298602211	-0.560632608886
Cl	2.113947546447	-1.532056654290	-1.422338314318

SCF Done: E(RB3LYP) = -1244.67988666

Zero-point correction= 0.099144
Thermal correction to Energy= 0.108753
Thermal correction to Enthalpy= 0.109698
Thermal correction to Gibbs Free Energy= 0.062770
Sum of electronic and zero-point Energies= -1244.580742
Sum of electronic and thermal Energies= -1244.571133
Sum of electronic and thermal Enthalpies= -1244.570189
Sum of electronic and thermal Free Energies= -1244.617117

1 C Isotropic = 38.4780 Anisotropy = 87.3973
2 F Isotropic = 307.6004 Anisotropy = 114.7690
3 C Isotropic = 47.3935 Anisotropy = 158.3380
4 S Isotropic = 509.2640 Anisotropy = 297.8981
5 C Isotropic = 169.5649 Anisotropy = 33.6488
6 H Isotropic = 28.1189 Anisotropy = 8.4967
7 H Isotropic = 29.2286 Anisotropy = 11.7599
8 H Isotropic = 28.8990 Anisotropy = 8.7943
9 C Isotropic = 67.1804 Anisotropy = 141.2080
10 H Isotropic = 24.3340 Anisotropy = 7.9433
11 C Isotropic = 50.6340 Anisotropy = 151.2384
12 H Isotropic = 23.4562 Anisotropy = 5.1589
13 N Isotropic = -49.6061 Anisotropy = 440.2244
14 C Isotropic = 44.6437 Anisotropy = 72.3183
15 Cl Isotropic = 712.6992 Anisotropy = 433.6016

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.856636762346	0.840733395268	0.285635819682
F	0.558092740092	1.958909475231	0.968223381707
C	0.912904556692	0.847265919994	-1.112113807110
S	0.650235862228	2.280869827710	-2.132658202416
C	-0.726419696121	3.189297306260	-1.324757378212
H	-1.021691056819	3.945370242531	-2.065510609298
H	-0.401680096131	3.677371668471	-0.399241614786
H	-1.570909192411	2.513048499216	-1.136789831268
C	1.281267396003	-0.362612738827	-1.729435855963
H	1.340995263413	-0.424483281028	-2.816691441981
C	1.554011678990	-1.477833385623	-0.943755483657
H	1.840441098397	-2.424404305701	-1.409099645114
N	1.468795045271	-1.478269094981	0.398694614599
C	1.127083234512	-0.343357551621	0.978034494528
Cl	1.024766403537	-0.321115976898	2.738635559291

SCF Done: E(RB3LYP) = -1244.67987678

Zero-point correction= 0.099147
Thermal correction to Energy= 0.108759
Thermal correction to Enthalpy= 0.109703
Thermal correction to Gibbs Free Energy= 0.062811
Sum of electronic and zero-point Energies= -1244.580730
Sum of electronic and thermal Energies= -1244.571118
Sum of electronic and thermal Enthalpies= -1244.570174
Sum of electronic and thermal Free Energies= -1244.617066

1	C	Isotropic =	38.4413	Anisotropy = 87.5096
2	F	Isotropic =	307.4493	Anisotropy = 115.0874
3	C	Isotropic =	47.4151	Anisotropy = 158.1472
4	S	Isotropic =	510.0819	Anisotropy = 297.8860
5	C	Isotropic =	169.6675	Anisotropy = 33.7244
6	H	Isotropic =	29.2244	Anisotropy = 11.7623
7	H	Isotropic =	28.1177	Anisotropy = 8.4891
8	H	Isotropic =	28.8978	Anisotropy = 8.8441
9	C	Isotropic =	67.1385	Anisotropy = 141.1656
10	H	Isotropic =	24.3261	Anisotropy = 7.9450
11	C	Isotropic =	50.6641	Anisotropy = 151.4208
12	H	Isotropic =	23.4521	Anisotropy = 5.1653
13	N	Isotropic =	-49.7796	Anisotropy = 440.5668
14	C	Isotropic =	44.7260	Anisotropy = 72.3404
15	Cl	Isotropic =	712.3601	Anisotropy = 434.1400

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.827251443914	0.655589983656	0.307635071952
F	0.126134418391	1.025075886086	1.392834338818
C	0.619326074930	1.278775925048	-0.927436609195

S	-0.519522493127	2.613967293600	-1.217439959006
C	-1.980765608050	2.228872548061	-0.174154728824
H	-2.309392338419	1.195310809212	-0.345136046428
H	-2.755367165075	2.922372481628	-0.530037688823
H	-1.778257282180	2.405087526830	0.888021765809
C	1.437719238513	0.850703087586	-1.989618711028
H	1.323905928454	1.294628754699	-2.979343545957
C	2.379455916642	-0.149148744367	-1.769964909560
H	3.021035811978	-0.491979272392	-2.585689178168
N	2.550298824120	-0.759945667574	-0.583628491569
C	1.785920889874	-0.356653277956	0.413099935950
Cl	2.005146340036	-1.136047334118	1.980018756029

SCF Done: E(RB3LYP) = -1244.67991917

Zero-point correction= 0.099173
Thermal correction to Energy= 0.108771
Thermal correction to Enthalpy= 0.109715
Thermal correction to Gibbs Free Energy= 0.062839
Sum of electronic and zero-point Energies= -1244.580746
Sum of electronic and thermal Energies= -1244.571148
Sum of electronic and thermal Enthalpies= -1244.570204
Sum of electronic and thermal Free Energies= -1244.617080

1	C	Isotropic = 38.5147	Anisotropy =	87.4128
2	F	Isotropic = 307.9803	Anisotropy =	114.9032
3	C	Isotropic = 47.2921	Anisotropy =	158.2417
4	S	Isotropic = 508.7546	Anisotropy =	297.6522
5	C	Isotropic = 169.5593	Anisotropy =	33.4643
6	H	Isotropic = 28.8824	Anisotropy =	8.7427
7	H	Isotropic = 29.2234	Anisotropy =	11.7588
8	H	Isotropic = 28.1264	Anisotropy =	8.5236
9	C	Isotropic = 67.3804	Anisotropy =	141.1755
10	H	Isotropic = 24.3470	Anisotropy =	7.9483
11	C	Isotropic = 50.7098	Anisotropy =	151.4072
12	H	Isotropic = 23.4596	Anisotropy =	5.1555
13	N	Isotropic = -49.2903	Anisotropy =	439.7969
14	C	Isotropic = 44.6859	Anisotropy =	72.2382
15	Cl	Isotropic = 712.6923	Anisotropy =	433.6788

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

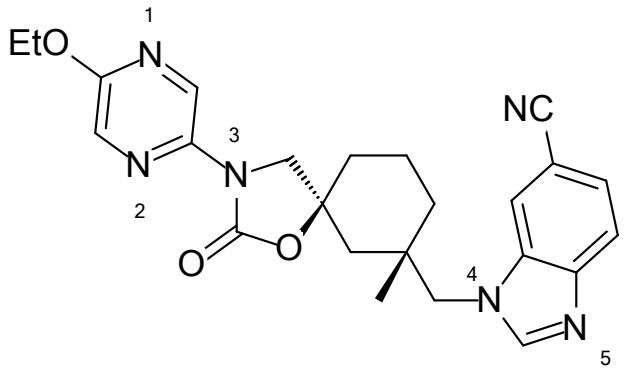
C	1.008788363181	0.729802204636	0.283729451640
F	1.079396229214	1.444756891866	1.419398667506
C	0.173814543589	1.129131472473	-0.765332829450
S	-0.894077747395	2.551287301863	-0.737407818586
C	0.039931111867	3.834246828118	0.186228301307
H	-0.519250382235	4.761237823966	-0.002576672571
H	1.055987920458	3.932302389339	-0.218055606133
H	0.064206610048	3.622976172084	1.260961105864
C	0.137122728022	0.284979839031	-1.891277361839
H	-0.491770299452	0.540809547197	-2.744856199418

C	0.917653467362	-0.866032527194	-1.911347279639
H	0.899884083694	-1.530040641758	-2.779290056283
N	1.738391190804	-1.223745707039	-0.907282356318
C	1.770252185566	-0.435148011401	0.149677344991
Cl	2.830649995277	-0.895063583181	1.482031308928

SCF Done: E(RB3LYP) = -1244.67986013

Zero-point correction= 0.099167
Thermal correction to Energy= 0.108766
Thermal correction to Enthalpy= 0.109710
Thermal correction to Gibbs Free Energy= 0.062855
Sum of electronic and zero-point Energies= -1244.580693
Sum of electronic and thermal Energies= -1244.571094
Sum of electronic and thermal Enthalpies= -1244.570150
Sum of electronic and thermal Free Energies= -1244.617005

1	C	Isotropic =	38.6649	Anisotropy =	87.1837
2	F	Isotropic =	308.3898	Anisotropy =	114.5392
3	C	Isotropic =	47.1085	Anisotropy =	158.1527
4	S	Isotropic =	507.2599	Anisotropy =	299.6789
5	C	Isotropic =	169.4819	Anisotropy =	33.3212
6	H	Isotropic =	29.2286	Anisotropy =	11.7559
7	H	Isotropic =	28.8641	Anisotropy =	8.7077
8	H	Isotropic =	28.1317	Anisotropy =	8.5297
9	C	Isotropic =	67.5867	Anisotropy =	141.3605
10	H	Isotropic =	24.3541	Anisotropy =	7.9604
11	C	Isotropic =	50.7381	Anisotropy =	151.2573
12	H	Isotropic =	23.4651	Anisotropy =	5.1509
13	N	Isotropic =	-49.1291	Anisotropy =	439.2231
14	C	Isotropic =	44.6701	Anisotropy =	72.3443
15	Cl	Isotropic =	712.1696	Anisotropy =	434.4875



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.071164604861	1.842846288796	-3.048226702298
C	-1.016177548168	2.112483636604	-3.964111193608
C	-0.555916030694	3.406651765796	-4.206033119689
H	0.239834106649	3.627057357924	-4.916503706435
C	-1.175757978498	4.441920794542	-3.486142962990
C	-2.220607324573	4.186491189450	-2.556819137496
H	-2.667195369888	5.024594329460	-2.020944454494
C	-2.672947407834	2.892950762971	-2.334930013857
H	-3.480076154534	2.690133136492	-1.629407630235
C	-0.742980856889	5.793827219054	-3.695402530932
N	-0.395207807972	6.893917687580	-3.861708360885
N	-0.665298712297	0.876030129216	-4.489115725143
C	0.342457792870	0.579383404669	-5.511443742707
H	-0.064478174084	-0.225842482135	-6.140876951857
H	0.431192221803	1.470287690537	-6.149741108677
C	-1.508891977186	-0.031371633453	-3.895397079167
H	-1.459431199070	-1.087708581843	-4.154281879602
N	-2.354934154720	0.489031208921	-3.030022478641
C	4.673014219814	0.877572147985	-5.206924542649
H	5.730333749634	0.707245299738	-4.949172898586
H	4.638191932606	1.776768528914	-5.847395941731
C	3.897391523779	1.197615998621	-3.928978584587
C	2.386996730904	1.314319552957	-4.196747830627
H	2.261256534340	2.246495426489	-4.773534696064
H	1.866596197127	1.461890288349	-3.236523505404
C	1.745612727262	0.151163377511	-4.997039749292
C	1.612014745071	-1.128535580893	-4.149652591432
H	1.102202003676	-1.919836697172	-4.723770721114
H	1.032614656411	-0.942477348429	-3.231817657318
H	2.590800748277	-1.510201417939	-3.835570505928
C	2.598056397251	-0.118543063331	-6.264216540317
H	2.490484093605	0.738524549175	-6.954310543529
H	2.196402782733	-0.998385604704	-6.793993944573
C	4.088481983636	-0.319415526146	-5.963785154267
H	4.638537651363	-0.460704875771	-6.907595025285
H	4.241868729706	-1.238754480280	-5.375457100847
O	4.134399194809	0.110845277034	-2.968276866851
C	4.527069650899	0.590898506315	-1.763677082692
N	4.666079415970	1.959940902435	-1.841805362703
C	4.444402651136	2.449524085693	-3.198802320268
H	3.728832125970	3.282265644362	-3.201913822329
H	5.386654685965	2.809071417301	-3.640461433935
O	4.711213747916	-0.130869163708	-0.803719414202
C	5.944170966772	4.521843060510	1.076203757371
O	6.361891693738	5.447405553641	1.961852730209
C	6.607006377024	5.015069601558	3.318995269632
C	7.048609871606	6.232779521773	4.104343141297
H	6.267342259280	7.008934511317	4.099338133393
H	7.970296710278	6.661965615011	3.680991249318
H	7.247384724236	5.948012580893	5.149155522033
H	7.378088861908	4.227455737626	3.312347406497
H	5.684186682611	4.573245756098	3.728849480734
C	5.704050316594	4.942639990135	-0.245927399210
H	5.854307332374	5.987553084270	-0.530929003147
N	5.291601330732	4.090546007226	-1.177915406703

C	5.110082083475	2.809271505318	-0.813215576314
C	5.347138786918	2.391832451025	0.506525731646
H	5.200655422919	1.353938581476	0.800354108093
N	5.764628879623	3.255195293031	1.443293470393

SCF Done: E(RB3LYP) = -1484.53186564

Zero-point correction= 0.478142
Thermal correction to Energy= 0.506874
Thermal correction to Enthalpy= 0.507818
Thermal correction to Gibbs Free Energy= 0.414919
Sum of electronic and zero-point Energies= -1484.053724
Sum of electronic and thermal Energies= -1484.024992
Sum of electronic and thermal Enthalpies= -1484.024048
Sum of electronic and thermal Free Energies= -1484.116946

1	C	Isotropic =	46.3192	Anisotropy =	145.0295
2	C	Isotropic =	57.1929	Anisotropy =	142.2308
3	C	Isotropic =	76.3510	Anisotropy =	157.4576
4	H	Isotropic =	23.6419	Anisotropy =	10.1748
5	C	Isotropic =	86.9533	Anisotropy =	125.7574
6	C	Isotropic =	66.9989	Anisotropy =	165.5845
7	H	Isotropic =	23.9502	Anisotropy =	5.8417
8	C	Isotropic =	72.3857	Anisotropy =	156.5308
9	H	Isotropic =	23.7357	Anisotropy =	4.7331
10	C	Isotropic =	75.7932	Anisotropy =	315.8223
11	N	Isotropic =	-1.5644	Anisotropy =	371.4570
12	N	Isotropic =	93.7916	Anisotropy =	118.2873
13	C	Isotropic =	131.6712	Anisotropy =	42.6385
14	H	Isotropic =	27.6061	Anisotropy =	5.9789
15	H	Isotropic =	27.5142	Anisotropy =	3.5767
16	C	Isotropic =	45.2878	Anisotropy =	100.0872
17	H	Isotropic =	23.5668	Anisotropy =	7.7252
18	N	Isotropic =	6.2251	Anisotropy =	348.1507
19	C	Isotropic =	152.2096	Anisotropy =	15.5217
20	H	Isotropic =	29.4674	Anisotropy =	7.2392
21	H	Isotropic =	29.7407	Anisotropy =	7.4022
22	C	Isotropic =	109.2761	Anisotropy =	64.5069
23	C	Isotropic =	143.9540	Anisotropy =	22.6041
24	H	Isotropic =	29.7694	Anisotropy =	6.6131
25	H	Isotropic =	29.9454	Anisotropy =	8.0526
26	C	Isotropic =	149.7374	Anisotropy =	14.7245
27	C	Isotropic =	169.0106	Anisotropy =	32.1766
28	H	Isotropic =	30.5856	Anisotropy =	10.4105
29	H	Isotropic =	30.5363	Anisotropy =	5.7337
30	H	Isotropic =	29.2836	Anisotropy =	6.2587
31	C	Isotropic =	153.9189	Anisotropy =	19.0932
32	H	Isotropic =	29.9140	Anisotropy =	6.8422
33	H	Isotropic =	29.7910	Anisotropy =	7.8767
34	C	Isotropic =	170.1492	Anisotropy =	12.6751
35	H	Isotropic =	29.6412	Anisotropy =	11.4567
36	H	Isotropic =	29.3072	Anisotropy =	6.9387
37	O	Isotropic =	138.1680	Anisotropy =	107.1465
38	C	Isotropic =	42.7029	Anisotropy =	82.6467
39	N	Isotropic =	137.5593	Anisotropy =	98.7244
40	C	Isotropic =	134.5036	Anisotropy =	37.5555

41	H	Isotropic =	27.8256	Anisotropy =	4.3887
42	H	Isotropic =	27.8279	Anisotropy =	5.4153
43	O	Isotropic =	61.6571	Anisotropy =	380.0310
44	C	Isotropic =	36.6419	Anisotropy =	121.5944
45	O	Isotropic =	196.3362	Anisotropy =	79.8364
46	C	Isotropic =	127.9084	Anisotropy =	54.2824
47	C	Isotropic =	176.3904	Anisotropy =	21.7261
48	H	Isotropic =	29.9414	Anisotropy =	7.6009
49	H	Isotropic =	29.9348	Anisotropy =	7.9096
50	H	Isotropic =	30.0827	Anisotropy =	9.5532
51	H	Isotropic =	27.3164	Anisotropy =	6.1456
52	H	Isotropic =	27.2991	Anisotropy =	5.7555
53	C	Isotropic =	63.0296	Anisotropy =	126.8519
54	H	Isotropic =	23.5563	Anisotropy =	7.4976
55	N	Isotropic =	-52.5595	Anisotropy =	484.1467
56	C	Isotropic =	50.4826	Anisotropy =	127.4050
57	C	Isotropic =	62.2858	Anisotropy =	142.1235
58	H	Isotropic =	22.4082	Anisotropy =	12.1922
59	N	Isotropic =	-34.7792	Anisotropy =	472.6882

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	7.197747332960	0.186948052034	-3.281885382799
C	6.180989186984	0.358645199110	-2.301950792631
C	4.990448297094	-0.367310068910	-2.329451055549
H	4.210459103792	-0.249807745040	-1.577836819111
C	4.832908645372	-1.278943862650	-3.387047557722
C	5.834138673243	-1.452578203691	-4.381065530962
H	5.662126768411	-2.170498062103	-5.183586691816
C	7.016190424856	-0.725984278411	-4.334060546016
H	7.791594394101	-0.859761635237	-5.089831625735
C	3.629025057968	-2.055576711901	-3.466570326461
N	2.653176388006	-2.689396144707	-3.535293599496
N	6.678325358925	1.311926178728	-1.423525043432
C	6.060446864323	1.808601320051	-0.191662193341
H	5.407281190632	1.008977358110	0.186808950160
H	6.867104124970	1.936667102904	0.544918345931
C	7.928756232008	1.632922204756	-1.895295313446
H	8.555971079556	2.347597299584	-1.364605641003
N	8.279621029634	1.000901630205	-2.996472177704
C	4.355173682896	5.421389208380	-2.041170551775
H	3.783548868890	6.348903306025	-2.202692133859
H	4.833409570094	5.164592684087	-3.003157784425
C	3.381220957537	4.294116322797	-1.699051417766
C	4.120623766424	2.996964895419	-1.326668171017
H	4.553579967206	2.620466578577	-2.267823874257
H	3.381195327088	2.248923510325	-0.994450972169
C	5.255388381340	3.137682725938	-0.281827834215
C	4.702522038299	3.356994957113	1.142595508927
H	4.144451332893	4.296695355554	1.226753053554
H	5.525744415204	3.376870940937	1.875642581393
H	4.016989790955	2.541519986857	1.425980275706

C	6.184140236639	4.305303974820	-0.693261537456
H	6.727038786165	4.030434511799	-1.614255919010
H	6.946209771000	4.461212639271	0.089023601750
C	5.426935384836	5.612242750803	-0.963609805368
H	6.136725195504	6.390157856992	-1.286583581161
H	4.957230317323	5.984687724761	-0.038597563068
O	2.567815802479	4.730276380881	-0.553656011395
C	1.253781248358	4.472254237417	-0.761206553313
N	1.080989551940	3.998756410812	-2.044994523515
C	2.327549105900	4.049091512863	-2.804479542696
H	2.496563433731	3.108999337902	-3.344567307994
H	2.301216177548	4.867759061868	-3.541044209562
O	0.410497969120	4.654359966594	0.094266414019
C	-2.427022689088	3.013709805832	-3.898635419450
O	-3.524459464741	2.670700952520	-4.601195801400
C	-4.781543515642	2.605636166242	-3.890769230947
C	-5.840998655680	2.189317449502	-4.890038915952
H	-6.819330067865	2.128134354040	-4.388663317126
H	-5.610187849937	1.202249763903	-5.320501463859
H	-5.917740746872	2.919404853011	-5.711006308533
H	-4.996835662694	3.592229311996	-3.448875146022
H	-4.690575661080	1.883716968878	-3.062935619697
C	-1.200105527949	3.071487773414	-4.587256408012
H	-1.153265571614	2.844638135066	-5.655888015347
N	-0.073233207841	3.399713287873	-3.964766454375
C	-0.145708733036	3.674491180257	-2.650806213221
C	-1.370224740741	3.616716978716	-1.965622180899
H	-1.428375509740	3.843958434952	-0.902597986762
N	-2.504893627683	3.285908112172	-2.598180658592

SCF Done: E(RB3LYP) = -1484.53191108

Zero-point correction= 0.478222
Thermal correction to Energy= 0.506936
Thermal correction to Enthalpy= 0.507880
Thermal correction to Gibbs Free Energy= 0.415563
Sum of electronic and zero-point Energies= -1484.053689
Sum of electronic and thermal Energies= -1484.024975
Sum of electronic and thermal Enthalpies= -1484.024031
Sum of electronic and thermal Free Energies= -1484.116348

1	C	Isotropic =	46.1925	Anisotropy =	144.3410
2	C	Isotropic =	57.0482	Anisotropy =	142.7036
3	C	Isotropic =	76.4780	Anisotropy =	157.6406
4	H	Isotropic =	23.7625	Anisotropy =	9.9740
5	C	Isotropic =	86.8859	Anisotropy =	125.9578
6	C	Isotropic =	66.7256	Anisotropy =	165.6668
7	H	Isotropic =	23.8854	Anisotropy =	6.0024
8	C	Isotropic =	72.1336	Anisotropy =	156.2660
9	H	Isotropic =	23.6653	Anisotropy =	4.8917
10	C	Isotropic =	75.9522	Anisotropy =	315.6237
11	N	Isotropic =	-1.8119	Anisotropy =	371.7526
12	N	Isotropic =	93.7644	Anisotropy =	119.5532
13	C	Isotropic =	134.4605	Anisotropy =	44.4237
14	H	Isotropic =	27.4715	Anisotropy =	3.6008
15	H	Isotropic =	27.6771	Anisotropy =	6.1898

16	C	Isotropic =	45.2863	Anisotropy =	99.1441
17	H	Isotropic =	23.5928	Anisotropy =	7.7813
18	N	Isotropic =	6.2291	Anisotropy =	350.2217
19	C	Isotropic =	153.0031	Anisotropy =	15.2634
20	H	Isotropic =	29.6369	Anisotropy =	7.6635
21	H	Isotropic =	30.1835	Anisotropy =	6.4354
22	C	Isotropic =	108.1603	Anisotropy =	63.9176
23	C	Isotropic =	146.0620	Anisotropy =	19.8105
24	H	Isotropic =	30.3247	Anisotropy =	10.5397
25	H	Isotropic =	29.5437	Anisotropy =	4.8078
26	C	Isotropic =	149.5513	Anisotropy =	16.5885
27	C	Isotropic =	166.3978	Anisotropy =	35.0332
28	H	Isotropic =	29.1119	Anisotropy =	6.3746
29	H	Isotropic =	30.5678	Anisotropy =	9.9956
30	H	Isotropic =	30.3857	Anisotropy =	7.8953
31	C	Isotropic =	156.8898	Anisotropy =	8.3601
32	H	Isotropic =	29.9278	Anisotropy =	7.9735
33	H	Isotropic =	29.8765	Anisotropy =	8.3337
34	C	Isotropic =	169.6969	Anisotropy =	12.7503
35	H	Isotropic =	29.7095	Anisotropy =	11.5184
36	H	Isotropic =	29.3106	Anisotropy =	7.0280
37	O	Isotropic =	136.5576	Anisotropy =	106.4483
38	C	Isotropic =	42.5234	Anisotropy =	82.4698
39	N	Isotropic =	137.1386	Anisotropy =	99.0659
40	C	Isotropic =	134.7071	Anisotropy =	37.6866
41	H	Isotropic =	27.9791	Anisotropy =	4.7678
42	H	Isotropic =	28.0255	Anisotropy =	5.2932
43	O	Isotropic =	60.8449	Anisotropy =	382.1270
44	C	Isotropic =	36.6466	Anisotropy =	121.3045
45	O	Isotropic =	196.3956	Anisotropy =	79.1070
46	C	Isotropic =	127.7370	Anisotropy =	54.0353
47	C	Isotropic =	176.4797	Anisotropy =	21.6260
48	H	Isotropic =	30.0448	Anisotropy =	9.5188
49	H	Isotropic =	29.9179	Anisotropy =	7.6663
50	H	Isotropic =	29.9045	Anisotropy =	7.9020
51	H	Isotropic =	27.2657	Anisotropy =	6.1582
52	H	Isotropic =	27.2327	Anisotropy =	5.7587
53	C	Isotropic =	62.9907	Anisotropy =	126.6644
54	H	Isotropic =	23.5582	Anisotropy =	7.5055
55	N	Isotropic =	-52.5026	Anisotropy =	483.9121
56	C	Isotropic =	50.1714	Anisotropy =	127.5172
57	C	Isotropic =	61.9462	Anisotropy =	142.0804
58	H	Isotropic =	22.2575	Anisotropy =	12.1160
59	N	Isotropic =	-34.8854	Anisotropy =	472.7531

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	6.942896669531	3.015185968343	-5.160840505500
C	6.028185503674	1.940484847977	-4.976875127053
C	6.153666676854	1.031218621161	-3.926704909589
H	5.470434456545	0.194987839679	-3.783431372860

C	7.224196576297	1.234870853016	-3.039654490739
C	8.136788366102	2.312414332617	-3.202003244169
H	8.949473713076	2.429015030551	-2.484401270682
C	8.003450568152	3.202577746427	-4.258766125435
H	8.704651235943	4.027326539747	-4.394534433343
C	7.401759579152	0.329801848440	-1.940537451946
N	7.550233277877	-0.403010567318	-1.046260111531
N	5.128923835820	2.044621021311	-6.029430358659
C	3.995232002529	1.171534856847	-6.346431314132
H	3.942961464227	1.099643910462	-7.442802942200
H	4.238949846193	0.167416631784	-5.970460304360
C	5.546893695901	3.124605598069	-6.768515654912
H	5.018602431772	3.413890996829	-7.675624252135
N	6.612172075565	3.736928368111	-6.293799025747
C	0.278610093521	0.619097554909	-4.165730205384
H	-0.715200785483	0.746339499247	-3.706967108486
H	0.645513919258	-0.378464077225	-3.866426242862
C	1.241156643229	1.655628472781	-3.575913444362
C	2.614320282743	1.602257090358	-4.258229418820
H	3.077451235089	0.660645959097	-3.916196127163
H	3.234283046640	2.423694690135	-3.864973008351
C	2.606601429275	1.617177485650	-5.808878749143
C	2.264046155449	3.012554421307	-6.365923224019
H	2.326172166186	3.014333488715	-7.466813790110
H	2.955474445198	3.778551547733	-5.981492541338
H	1.252381266945	3.325899347665	-6.080693452542
C	1.592660239583	0.562650954766	-6.324231177706
H	1.983453351285	-0.446904010735	-6.100107583337
H	1.520524250800	0.633047910818	-7.422463117007
C	0.201731884366	0.699364733157	-5.693325427715
H	-0.454661229830	-0.100691907026	-6.070610505537
H	-0.265571065433	1.651670968345	-5.992195124636
O	0.655019091442	2.988336156035	-3.776576762144
C	0.254139977202	3.534907916705	-2.603340907718
N	0.603043284522	2.696376401560	-1.566605340852
C	1.360958444251	1.540522746394	-2.035773801024
H	2.404928567027	1.596287094800	-1.690771151962
H	0.927169330932	0.606242165863	-1.655123855154
O	-0.318614932547	4.604964668509	-2.545800945812
C	0.095343464525	3.317880534718	2.441864782735
O	-0.013047192847	3.428729108043	3.780300497536
C	-0.726495229704	4.571281644415	4.304070396710
C	-0.698092321862	4.462933283600	5.814750723818
H	-1.187014712649	3.535693094539	6.152410005863
H	-1.232527956489	5.317473349198	6.257865433547
H	0.337087822668	4.469105438764	6.190517441045
H	-1.755802844096	4.565246661905	3.910021654274
H	-0.239748989030	5.493993299543	3.948385343895
C	0.796391935902	2.208025908162	1.932442113418
H	1.231033601222	1.468430455171	2.610490368483
N	0.950023636578	2.028507871058	0.625246065306
C	0.410017650408	2.945494413943	-0.196486032861
C	-0.292049024505	4.049904178404	0.313114771053
H	-0.727959922729	4.792044771936	-0.353302966232
N	-0.443352984250	4.227530262987	1.633335309584

SCF Done: E(RB3LYP) = -1484.53196812

Zero-point correction= 0.478190
Thermal correction to Energy= 0.506904
Thermal correction to Enthalpy= 0.507848
Thermal correction to Gibbs Free Energy= 0.415477
Sum of electronic and zero-point Energies= -1484.053778
Sum of electronic and thermal Energies= -1484.025064
Sum of electronic and thermal Enthalpies= -1484.024120
Sum of electronic and thermal Free Energies= -1484.116492

1	C	Isotropic =	46.1387	Anisotropy =	144.4089
2	C	Isotropic =	57.1903	Anisotropy =	141.2202
3	C	Isotropic =	76.8960	Anisotropy =	158.8365
4	H	Isotropic =	23.6227	Anisotropy =	10.2558
5	C	Isotropic =	86.8002	Anisotropy =	125.5008
6	C	Isotropic =	66.9873	Anisotropy =	165.7371
7	H	Isotropic =	23.8961	Anisotropy =	5.9516
8	C	Isotropic =	71.9569	Anisotropy =	155.4645
9	H	Isotropic =	23.7286	Anisotropy =	4.7781
10	C	Isotropic =	75.7432	Anisotropy =	315.9478
11	N	Isotropic =	-1.5509	Anisotropy =	371.4624
12	N	Isotropic =	93.2508	Anisotropy =	117.4660
13	C	Isotropic =	131.7958	Anisotropy =	42.0710
14	H	Isotropic =	27.5915	Anisotropy =	5.9460
15	H	Isotropic =	27.5026	Anisotropy =	3.5914
16	C	Isotropic =	45.4307	Anisotropy =	99.3494
17	H	Isotropic =	23.4927	Anisotropy =	7.8111
18	N	Isotropic =	5.7489	Anisotropy =	346.5451
19	C	Isotropic =	150.9143	Anisotropy =	16.0590
20	H	Isotropic =	29.4286	Anisotropy =	6.5715
21	H	Isotropic =	29.9138	Anisotropy =	7.2495
22	C	Isotropic =	109.3539	Anisotropy =	64.8550
23	C	Isotropic =	143.7123	Anisotropy =	22.9387
24	H	Isotropic =	29.6555	Anisotropy =	6.6784
25	H	Isotropic =	30.0145	Anisotropy =	7.7756
26	C	Isotropic =	149.4581	Anisotropy =	14.9407
27	C	Isotropic =	168.9282	Anisotropy =	32.4108
28	H	Isotropic =	30.5661	Anisotropy =	10.4243
29	H	Isotropic =	30.5322	Anisotropy =	5.8129
30	H	Isotropic =	29.2225	Anisotropy =	6.4092
31	C	Isotropic =	153.7721	Anisotropy =	18.4030
32	H	Isotropic =	29.9276	Anisotropy =	6.7629
33	H	Isotropic =	29.8209	Anisotropy =	7.8297
34	C	Isotropic =	170.3846	Anisotropy =	12.8418
35	H	Isotropic =	29.6966	Anisotropy =	11.4121
36	H	Isotropic =	29.3175	Anisotropy =	6.8790
37	O	Isotropic =	138.8253	Anisotropy =	114.2253
38	C	Isotropic =	42.6010	Anisotropy =	83.0827
39	N	Isotropic =	137.9390	Anisotropy =	98.3712
40	C	Isotropic =	134.4742	Anisotropy =	38.5077
41	H	Isotropic =	27.9862	Anisotropy =	6.3639
42	H	Isotropic =	27.6992	Anisotropy =	4.9644
43	O	Isotropic =	61.3122	Anisotropy =	379.5570
44	C	Isotropic =	36.7545	Anisotropy =	120.8775
45	O	Isotropic =	196.4787	Anisotropy =	79.1407

46	C	Isotropic =	127.9878	Anisotropy =	54.4436
47	C	Isotropic =	176.3260	Anisotropy =	21.8221
48	H	Isotropic =	29.9272	Anisotropy =	7.8257
49	H	Isotropic =	30.0603	Anisotropy =	9.5467
50	H	Isotropic =	29.9348	Anisotropy =	7.6832
51	H	Isotropic =	27.2818	Anisotropy =	6.1277
52	H	Isotropic =	27.3062	Anisotropy =	5.8871
53	C	Isotropic =	63.0708	Anisotropy =	126.3564
54	H	Isotropic =	23.5410	Anisotropy =	7.6912
55	N	Isotropic =	-52.6000	Anisotropy =	483.9159
56	C	Isotropic =	50.2713	Anisotropy =	127.3058
57	C	Isotropic =	62.1208	Anisotropy =	141.8765
58	H	Isotropic =	22.3541	Anisotropy =	12.3187
59	N	Isotropic =	-34.8597	Anisotropy =	472.3988

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	4.412610001248	4.230397644796	-7.015989822584
C	4.587709835870	3.168651823959	-6.085561455318
C	3.735085030341	2.065631700535	-6.045697097820
H	3.866607168220	1.243102086061	-5.343349495113
C	2.675958673397	2.054603908842	-6.969067794783
C	2.480533442903	3.113675699158	-7.896864384935
H	1.641248974368	3.059171483237	-8.590873317811
C	3.343196207369	4.201045919677	-7.926589599395
H	3.202501304259	5.014043805965	-8.640423872165
C	1.766998667297	0.944351732563	-6.976180382883
N	1.026290044595	0.044361905674	-6.986293538509
N	5.718653477632	3.507041214399	-5.354609554478
C	6.384013712441	2.720800729912	-4.313079545640
H	6.172036287639	1.662346847782	-4.523023212065
H	7.466721821051	2.860676726212	-4.445890936700
C	6.155580242811	4.699464006081	-5.880199075456
H	7.057161715936	5.177100344263	-5.499530496862
N	5.413146145332	5.173294224367	-6.859613439736
C	4.417201899359	4.770858998757	-0.952079515385
H	4.076645905422	5.043625730376	0.059559406857
H	3.907684492637	5.450878375891	-1.657642255402
C	3.945400030163	3.349343920781	-1.267049465659
C	4.498514048009	2.851731315531	-2.611857536379
H	3.955332185800	3.419791904234	-3.384999270038
H	4.218024010198	1.792398271011	-2.737658122240
C	6.020220647143	3.039557218372	-2.833793128886
C	6.848004568879	2.035824704184	-2.002939903056
H	7.922962770052	2.153130134847	-2.217661651434
H	6.565440139769	0.998609364728	-2.247242905495
H	6.695153533296	2.170543433338	-0.926080004179
C	6.411568946681	4.494780708781	-2.481600894064
H	5.964186620045	5.179673051252	-3.222833367493
H	7.505621342226	4.609828534592	-2.563026784064
C	5.934689255958	4.927333605585	-1.088776452348
H	6.212818079731	5.978511003700	-0.912907580238

H	6.439344658149	4.336481885122	-0.307027748051
O	4.425748283696	2.466066132410	-0.194897116945
C	3.408498297869	1.788942699520	0.389060313752
N	2.215582501176	2.171942554129	-0.184452886085
C	2.402849580276	3.207884754106	-1.194953261643
H	1.965379177594	2.899571508355	-2.154528485790
H	1.915085409806	4.144550574997	-0.886128258505
O	3.590898688253	0.980544771831	1.277897680747
C	-1.552993785291	0.912626938334	0.776404397549
O	-2.833790773874	0.571386781645	1.018699672943
C	-3.080487653278	-0.442454034289	2.018728124600
C	-4.581184835709	-0.628275728155	2.108135217275
H	-4.996444815216	-0.952761848460	1.141114330385
H	-5.077118220721	0.309284956557	2.404596701695
H	-4.815163179838	-1.396941792138	2.860896213512
H	-2.648244075914	-0.115072357254	2.978285646089
H	-2.567518230759	-1.372276533416	1.723301424912
C	-1.312250473476	1.901491744156	-0.196682868475
H	-2.144801431603	2.366992184443	-0.731316854363
N	-0.078076077316	2.295058073448	-0.491155576538
C	0.935707970947	1.713970111241	0.173995146167
C	0.693977961266	0.725598393553	1.142125996260
H	1.516047781410	0.255791544070	1.679065385611
N	-0.553457985524	0.332254606354	1.436253256654

SCF Done: E(RB3LYP) = -1484.53202478

Zero-point correction= 0.478303
Thermal correction to Energy= 0.507005
Thermal correction to Enthalpy= 0.507949
Thermal correction to Gibbs Free Energy= 0.415861
Sum of electronic and zero-point Energies= -1484.053722
Sum of electronic and thermal Energies= -1484.025020
Sum of electronic and thermal Enthalpies= -1484.024075
Sum of electronic and thermal Free Energies= -1484.116164

1	C	Isotropic =	46.2360	Anisotropy =	144.4971
2	C	Isotropic =	57.2268	Anisotropy =	143.0885
3	C	Isotropic =	76.4952	Anisotropy =	157.3367
4	H	Isotropic =	23.7117	Anisotropy =	10.0701
5	C	Isotropic =	86.8563	Anisotropy =	125.9152
6	C	Isotropic =	66.8001	Anisotropy =	165.5398
7	H	Isotropic =	23.8733	Anisotropy =	5.9592
8	C	Isotropic =	72.2663	Anisotropy =	155.9318
9	H	Isotropic =	23.6604	Anisotropy =	4.8838
10	C	Isotropic =	75.9407	Anisotropy =	315.5849
11	N	Isotropic =	-1.9149	Anisotropy =	371.9532
12	N	Isotropic =	93.9925	Anisotropy =	119.8421
13	C	Isotropic =	134.3450	Anisotropy =	44.8409
14	H	Isotropic =	27.4880	Anisotropy =	3.6030
15	H	Isotropic =	27.6504	Anisotropy =	6.1545
16	C	Isotropic =	45.2109	Anisotropy =	99.2781
17	H	Isotropic =	23.6106	Anisotropy =	7.7143
18	N	Isotropic =	6.6461	Anisotropy =	352.4155
19	C	Isotropic =	152.0360	Anisotropy =	15.6765
20	H	Isotropic =	29.6224	Anisotropy =	7.2587

21	H	Isotropic =	30.2585	Anisotropy =	6.3236
22	C	Isotropic =	108.3631	Anisotropy =	64.6146
23	C	Isotropic =	145.7141	Anisotropy =	19.7174
24	H	Isotropic =	30.2322	Anisotropy =	10.6189
25	H	Isotropic =	29.5469	Anisotropy =	4.4297
26	C	Isotropic =	149.5442	Anisotropy =	15.9497
27	C	Isotropic =	166.3424	Anisotropy =	35.3985
28	H	Isotropic =	30.5677	Anisotropy =	10.0385
29	H	Isotropic =	30.3636	Anisotropy =	7.8912
30	H	Isotropic =	29.0748	Anisotropy =	6.4561
31	C	Isotropic =	156.6270	Anisotropy =	8.3927
32	H	Isotropic =	29.9440	Anisotropy =	7.8491
33	H	Isotropic =	29.8861	Anisotropy =	8.2926
34	C	Isotropic =	169.5858	Anisotropy =	13.7210
35	H	Isotropic =	29.7320	Anisotropy =	11.4857
36	H	Isotropic =	29.2976	Anisotropy =	6.9028
37	O	Isotropic =	136.6152	Anisotropy =	108.2396
38	C	Isotropic =	42.7615	Anisotropy =	83.4129
39	N	Isotropic =	137.7153	Anisotropy =	99.4834
40	C	Isotropic =	134.3015	Anisotropy =	39.0840
41	H	Isotropic =	28.0027	Anisotropy =	5.8968
42	H	Isotropic =	27.9826	Anisotropy =	4.6277
43	O	Isotropic =	61.8750	Anisotropy =	377.2019
44	C	Isotropic =	36.7242	Anisotropy =	120.9419
45	O	Isotropic =	196.4206	Anisotropy =	79.4233
46	C	Isotropic =	127.9433	Anisotropy =	54.3153
47	C	Isotropic =	176.3588	Anisotropy =	21.7848
48	H	Isotropic =	29.9060	Anisotropy =	7.6980
49	H	Isotropic =	29.9203	Anisotropy =	7.8421
50	H	Isotropic =	30.0480	Anisotropy =	9.5156
51	H	Isotropic =	27.2556	Anisotropy =	6.0952
52	H	Isotropic =	27.2620	Anisotropy =	5.8991
53	C	Isotropic =	63.0479	Anisotropy =	126.3455
54	H	Isotropic =	23.5669	Anisotropy =	7.6704
55	N	Isotropic =	-52.6368	Anisotropy =	483.8821
56	C	Isotropic =	50.1595	Anisotropy =	127.1636
57	C	Isotropic =	62.1190	Anisotropy =	142.1535
58	H	Isotropic =	22.2445	Anisotropy =	12.2273
59	N	Isotropic =	-34.8279	Anisotropy =	472.6765

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	6.853411393296	-2.617819502860	-2.094476039272
C	6.552566830615	-1.253550809040	-1.824361404867
C	7.120621037756	-0.566302424882	-0.751946737780
H	6.906022398614	0.480912719332	-0.543254285944
C	8.001810976752	-1.292250279744	0.067058913349
C	8.301295390662	-2.659418529636	-0.181811176710
H	8.988906033484	-3.179493316185	0.485859460725
C	7.733276913437	-3.325890780044	-1.258989316064
H	7.964018817804	-4.372972527823	-1.460862763533
C	8.615500872947	-0.636402645723	1.186004949450

N	9.116787518473	-0.108625389326	2.096494110299
N	5.675736166447	-0.868956920928	-2.829565341277
C	5.079130536673	0.448660103455	-3.060533407390
H	5.790751147309	1.200361332275	-2.688861216057
H	5.011966104106	0.581042896251	-4.150677539030
C	5.516889989112	-1.976524743891	-3.626708014196
H	4.885399861459	-1.935431816133	-4.512807314917
N	6.187507890806	-3.039198837632	-3.231574461125
C	2.192505797901	2.637043104425	-0.666923503506
H	1.273564350769	3.026576457449	-0.199703129327
H	3.017065782102	3.303249271485	-0.357841250418
C	2.064659116950	2.741818653187	-2.191229329091
C	3.262438979100	2.109273727253	-2.907995609861
H	4.110721081855	2.798568134574	-2.748593239946
H	3.062797783512	2.102636447880	-3.992175444022
C	3.676813190755	0.689659070363	-2.432182691815
C	2.691015158786	-0.378081012257	-2.944490622138
H	2.995238856291	-1.384272854853	-2.616824884869
H	2.645081049432	-0.374524926237	-4.046200007156
H	1.673791449197	-0.196944425484	-2.576944666591
C	3.759002991630	0.670964780474	-0.886296361024
H	4.610603365617	1.298588299627	-0.567104633494
H	3.970598727200	-0.352510416775	-0.537291783990
C	2.492202181109	1.207642766336	-0.207169597482
H	2.625727858727	1.193513272893	0.886095753151
H	1.629710435089	0.556658757948	-0.423940867079
O	0.836388485870	2.037847584306	-2.592485453975
C	-0.141424821912	2.914389451289	-2.928175384914
N	0.370037511223	4.194928084454	-2.910323759541
C	1.808558640592	4.193650851811	-2.659883215891
H	2.361673862144	4.443099762964	-3.579302275247
H	2.075199147552	4.929819901259	-1.890850592796
O	-1.272063821585	2.558885565406	-3.195363203280
C	-1.536944588234	7.665734133170	-3.924634522343
O	-2.067304669745	8.861344467295	-4.248176309237
C	-3.483830813444	8.913054173591	-4.530193861341
C	-3.820317873298	10.350032146697	-4.871570189131
H	-3.586858988977	11.020113485857	-4.029336816322
H	-4.894937451580	10.436201141078	-5.095157316205
H	-3.254602409005	10.687677367809	-5.754076863076
H	-4.040309574680	8.558154102760	-3.647447980782
H	-3.710429920368	8.228102559960	-5.363390151504
C	-0.156065992026	7.614677451996	-3.653530682795
H	0.452685123607	8.521494024373	-3.706035002848
N	0.442758324699	6.473986609310	-3.329459509814
C	-0.318380448252	5.367555038539	-3.268175788321
C	-1.695898195924	5.420676998808	-3.536057379158
H	-2.309911162303	4.523125892878	-3.488069326970
N	-2.295688400128	6.573891568635	-3.864150961515

SCF Done: E(RB3LYP) = -1484.53210892

Zero-point correction= 0.478369
Thermal correction to Energy= 0.507030
Thermal correction to Enthalpy= 0.507974
Thermal correction to Gibbs Free Energy= 0.416292

Sum of electronic and zero-point Energies= -1484.053740
Sum of electronic and thermal Energies= -1484.025079
Sum of electronic and thermal Enthalpies= -1484.024135
Sum of electronic and thermal Free Energies= -1484.115817

1	C	Isotropic =	46.3210	Anisotropy =	143.9560
2	C	Isotropic =	57.3140	Anisotropy =	141.1844
3	C	Isotropic =	76.4133	Anisotropy =	157.1017
4	H	Isotropic =	23.5764	Anisotropy =	10.9941
5	C	Isotropic =	86.7810	Anisotropy =	125.0384
6	C	Isotropic =	66.4357	Anisotropy =	165.5102
7	H	Isotropic =	23.8461	Anisotropy =	5.9667
8	C	Isotropic =	72.3250	Anisotropy =	155.7800
9	H	Isotropic =	23.6773	Anisotropy =	5.0088
10	C	Isotropic =	75.7023	Anisotropy =	316.2382
11	N	Isotropic =	-1.5289	Anisotropy =	371.4877
12	N	Isotropic =	93.7372	Anisotropy =	116.4579
13	C	Isotropic =	132.4639	Anisotropy =	42.5645
14	H	Isotropic =	27.5296	Anisotropy =	4.1899
15	H	Isotropic =	27.5919	Anisotropy =	4.9089
16	C	Isotropic =	45.4127	Anisotropy =	98.2524
17	H	Isotropic =	23.5670	Anisotropy =	7.9050
18	N	Isotropic =	6.4730	Anisotropy =	346.9340
19	C	Isotropic =	151.6687	Anisotropy =	15.3029
20	H	Isotropic =	29.3853	Anisotropy =	6.5390
21	H	Isotropic =	29.9197	Anisotropy =	7.3655
22	C	Isotropic =	108.6027	Anisotropy =	64.3606
23	C	Isotropic =	144.9953	Anisotropy =	30.7289
24	H	Isotropic =	29.7553	Anisotropy =	4.3078
25	H	Isotropic =	29.6233	Anisotropy =	4.7756
26	C	Isotropic =	149.6640	Anisotropy =	15.4212
27	C	Isotropic =	169.4580	Anisotropy =	26.8203
28	H	Isotropic =	30.8091	Anisotropy =	7.5089
29	H	Isotropic =	30.4903	Anisotropy =	8.6355
30	H	Isotropic =	29.2628	Anisotropy =	7.1025
31	C	Isotropic =	153.5819	Anisotropy =	16.2121
32	H	Isotropic =	29.8257	Anisotropy =	8.8009
33	H	Isotropic =	30.1090	Anisotropy =	8.2371
34	C	Isotropic =	170.3341	Anisotropy =	13.2870
35	H	Isotropic =	29.8186	Anisotropy =	10.6790
36	H	Isotropic =	29.6043	Anisotropy =	6.2709
37	O	Isotropic =	137.4124	Anisotropy =	115.1745
38	C	Isotropic =	42.1224	Anisotropy =	82.2501
39	N	Isotropic =	137.7267	Anisotropy =	97.7034
40	C	Isotropic =	134.6326	Anisotropy =	38.0989
41	H	Isotropic =	27.8172	Anisotropy =	4.5517
42	H	Isotropic =	27.6167	Anisotropy =	5.3072
43	O	Isotropic =	60.5698	Anisotropy =	382.1935
44	C	Isotropic =	36.6790	Anisotropy =	121.2121
45	O	Isotropic =	196.0710	Anisotropy =	79.8123
46	C	Isotropic =	127.7526	Anisotropy =	54.2980
47	C	Isotropic =	176.4556	Anisotropy =	21.5128
48	H	Isotropic =	29.9073	Anisotropy =	7.8206
49	H	Isotropic =	30.0407	Anisotropy =	9.4369
50	H	Isotropic =	29.9072	Anisotropy =	7.7625
51	H	Isotropic =	27.2488	Anisotropy =	5.9839

52	H	Isotropic =	27.2568	Anisotropy =	5.9565
53	C	Isotropic =	62.8785	Anisotropy =	126.0807
54	H	Isotropic =	23.4905	Anisotropy =	7.4446
55	N	Isotropic =	-52.4954	Anisotropy =	483.8470
56	C	Isotropic =	50.1035	Anisotropy =	127.2763
57	C	Isotropic =	61.9208	Anisotropy =	142.2439
58	H	Isotropic =	22.2628	Anisotropy =	12.2066
59	N	Isotropic =	-34.8728	Anisotropy =	472.0115

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	3.845969310083	-2.657895922155	-2.522728104519
C	4.243964252960	-1.399699069678	-1.991664672360
C	3.605907676302	-0.818611505233	-0.896173870806
H	3.909291531987	0.140314776386	-0.477250463264
C	2.531691192552	-1.533903062305	-0.340526839977
C	2.113942265859	-2.786305356144	-0.867521943967
H	1.272228701291	-3.300448183063	-0.402510443471
C	2.765272454108	-3.353088234698	-1.954657061195
H	2.453625617102	-4.316968000888	-2.359853307716
C	1.837090134131	-0.985321877538	0.788834669381
N	1.269671751269	-0.543817422396	1.706353433187
N	5.321714391059	-0.999538905860	-2.770118680045
C	6.153596456428	0.195680235129	-2.610014766513
H	6.139770189450	0.458933349842	-1.542167827236
H	7.185663983835	-0.096141710645	-2.853344100964
C	5.517627325555	-2.012018322120	-3.678800319955
H	6.332282687442	-1.961530495869	-4.399683209779
N	4.666133149527	-3.012092768151	-3.579320516310
C	3.927883374476	2.616310275542	-5.537022032120
H	3.574592473803	3.460775370270	-6.149676655251
H	3.274176124186	1.756169382534	-5.766331712682
C	3.729629238612	2.960177845694	-4.061038901440
C	4.327315452013	1.882308170895	-3.140548322967
H	3.665360737275	1.006437764488	-3.240183175388
H	4.248243453873	2.224386710309	-2.094846776531
C	5.779086948773	1.445902565994	-3.458103234439
C	6.805284579005	2.521816903552	-3.043296581451
H	7.832451797882	2.158908765356	-3.212395147541
H	6.705104011441	2.767005723522	-1.973184429599
H	6.672290638666	3.453483232614	-3.605124909595
C	5.897922120893	1.130461456925	-4.968590636366
H	5.312697294242	0.222530452230	-5.196555666348
H	6.948579704807	0.899679849294	-5.213061098796
C	5.382510977634	2.264419205993	-5.864890218463
H	5.457344380615	1.962748736758	-6.921608734043
H	6.012758986173	3.161668407738	-5.752440897221
O	4.401055275425	4.242725432456	-3.800214147198
C	3.592212892654	5.092115103604	-3.121513114486
N	2.344432350336	4.521194803780	-2.985651269813
C	2.252279593209	3.254369696223	-3.705746326986
H	1.810666429390	2.474651459428	-3.072066984859

H	1.622174619073	3.362712836071	-4.602602786949
O	3.971836396096	6.175495018299	-2.723444063814
C	-0.990433867835	6.158650718184	-1.279750522543
O	-2.145952686565	6.608571780356	-0.752726145844
C	-2.115142895413	7.867056061468	-0.042726779095
C	-3.524494214255	8.144287067265	0.438396944362
H	-3.873880961728	7.347880242208	1.114067093163
H	-4.223353314870	8.214529051890	-0.409854905123
H	-3.548160543356	9.098760393266	0.986693403427
H	-1.749235361034	8.654737816474	-0.721314455167
H	-1.401706328225	7.791424082589	0.793992802852
C	-1.020857498413	4.932718077920	-1.971854912919
H	-1.956163446874	4.374811677972	-2.069840902755
N	0.075503064003	4.422338400029	-2.521585758906
C	1.218376026191	5.118549162446	-2.392407622915
C	1.247545065851	6.339644365939	-1.699507369974
H	2.173307509908	6.903063438005	-1.597191649197
N	0.138216531123	6.851524969809	-1.147423369510

SCF Done: E(RB3LYP) = -1484.53192846

Zero-point correction= 0.478049
Thermal correction to Energy= 0.506819
Thermal correction to Enthalpy= 0.507763
Thermal correction to Gibbs Free Energy= 0.415226
Sum of electronic and zero-point Energies= -1484.053879
Sum of electronic and thermal Energies= -1484.025109
Sum of electronic and thermal Enthalpies= -1484.024165
Sum of electronic and thermal Free Energies= -1484.116703

1	C	Isotropic =	46.0247	Anisotropy =	143.5725
2	C	Isotropic =	56.9360	Anisotropy =	142.1697
3	C	Isotropic =	76.5914	Anisotropy =	158.0671
4	H	Isotropic =	23.7443	Anisotropy =	9.9749
5	C	Isotropic =	86.9313	Anisotropy =	126.0243
6	C	Isotropic =	66.8800	Anisotropy =	165.9928
7	H	Isotropic =	23.8805	Anisotropy =	6.0130
8	C	Isotropic =	72.3091	Anisotropy =	155.8874
9	H	Isotropic =	23.6942	Anisotropy =	4.8337
10	C	Isotropic =	75.8238	Anisotropy =	315.8297
11	N	Isotropic =	-1.5361	Anisotropy =	371.2984
12	N	Isotropic =	93.7254	Anisotropy =	119.0905
13	C	Isotropic =	134.4099	Anisotropy =	44.4818
14	H	Isotropic =	27.4815	Anisotropy =	3.5452
15	H	Isotropic =	27.6754	Anisotropy =	6.1626
16	C	Isotropic =	45.3857	Anisotropy =	99.0005
17	H	Isotropic =	23.5777	Anisotropy =	7.7799
18	N	Isotropic =	6.0068	Anisotropy =	349.7047
19	C	Isotropic =	152.6162	Anisotropy =	15.2982
20	H	Isotropic =	29.6566	Anisotropy =	7.5877
21	H	Isotropic =	30.2398	Anisotropy =	6.3781
22	C	Isotropic =	108.1370	Anisotropy =	63.9241
23	C	Isotropic =	145.1831	Anisotropy =	19.9392
24	H	Isotropic =	30.3395	Anisotropy =	10.6151
25	H	Isotropic =	29.5480	Anisotropy =	4.6826
26	C	Isotropic =	149.6739	Anisotropy =	16.5639

27	C	Isotropic =	166.2126	Anisotropy =	35.1413
28	H	Isotropic =	30.5794	Anisotropy =	10.0404
29	H	Isotropic =	30.3856	Anisotropy =	7.8659
30	H	Isotropic =	29.0787	Anisotropy =	6.3697
31	C	Isotropic =	157.1142	Anisotropy =	7.9889
32	H	Isotropic =	29.9397	Anisotropy =	7.8672
33	H	Isotropic =	29.8893	Anisotropy =	8.3759
34	C	Isotropic =	169.8671	Anisotropy =	13.5851
35	H	Isotropic =	29.7094	Anisotropy =	11.4885
36	H	Isotropic =	29.2753	Anisotropy =	7.1254
37	O	Isotropic =	136.1690	Anisotropy =	106.8358
38	C	Isotropic =	42.3969	Anisotropy =	82.8769
39	N	Isotropic =	137.1496	Anisotropy =	98.4953
40	C	Isotropic =	134.3597	Anisotropy =	37.7916
41	H	Isotropic =	27.9848	Anisotropy =	5.0610
42	H	Isotropic =	28.0359	Anisotropy =	5.1026
43	O	Isotropic =	61.0606	Anisotropy =	381.3031
44	C	Isotropic =	36.7093	Anisotropy =	120.8344
45	O	Isotropic =	196.5700	Anisotropy =	79.3363
46	C	Isotropic =	128.0316	Anisotropy =	54.2983
47	C	Isotropic =	176.3473	Anisotropy =	21.7936
48	H	Isotropic =	29.8976	Anisotropy =	7.6906
49	H	Isotropic =	29.9163	Anisotropy =	7.8677
50	H	Isotropic =	30.0422	Anisotropy =	9.5042
51	H	Isotropic =	27.2659	Anisotropy =	6.1290
52	H	Isotropic =	27.2441	Anisotropy =	5.8220
53	C	Isotropic =	63.1826	Anisotropy =	126.4407
54	H	Isotropic =	23.5559	Anisotropy =	7.5469
55	N	Isotropic =	-52.5237	Anisotropy =	484.4991
56	C	Isotropic =	50.2365	Anisotropy =	127.6144
57	C	Isotropic =	61.8880	Anisotropy =	142.1083
58	H	Isotropic =	22.2543	Anisotropy =	12.1129
59	N	Isotropic =	-35.0051	Anisotropy =	472.2014

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.486372713667	1.360118410151	1.557315359092
C	-0.420745315214	1.294636349893	0.463478629813
C	-1.310748442940	0.233823343705	0.297877677891
H	-2.013829519804	0.178786616305	-0.532320989504
C	-1.264511726031	-0.784367372021	1.264847108535
C	-0.355531037653	-0.739260137935	2.357076109180
H	-0.356527480024	-1.556662283280	3.078821038488
C	0.519535611935	0.327505021284	2.509536413296
H	1.215531473616	0.371591931522	3.348584137763
C	-2.158199303496	-1.900771278417	1.147175353928
N	-2.882410081061	-2.809705559909	1.056882678485
N	-0.197803845062	2.455127810592	-0.264644748450
C	-0.893808092543	2.911625770617	-1.470951847107
H	-1.902061770423	2.473114734542	-1.450978202765
H	-1.017186624786	4.000916654268	-1.380701717902
C	0.783486267877	3.135805479308	0.414612242420

H	1.132940246168	4.105484578140	0.063589263171
N	1.226370580257	2.527428999365	1.496064198335
C	0.767892411513	3.899685169102	-5.365055868283
H	1.235438904987	3.849278609677	-6.361096702098
H	0.564654205924	4.965261197150	-5.157396410117
C	1.773420856637	3.415336144997	-4.321191956788
C	1.142052991399	3.323913056759	-2.920478547296
H	0.988964666671	4.367233449276	-2.593627594355
H	1.880479217009	2.881790604225	-2.231729882077
C	-0.213639273169	2.575468758210	-2.827109107616
C	-0.039899022594	1.051009029290	-2.959765381496
H	0.408653619793	0.778244084033	-3.922624185915
H	-1.014304383106	0.542095048484	-2.879479297062
H	0.619712348298	0.655070362068	-2.171860506640
C	-1.163866219248	3.117984685537	-3.925895221375
H	-1.443765131037	4.157224156139	-3.673270871013
H	-2.098490130774	2.532622342999	-3.921216230653
C	-0.541999365592	3.106081231618	-5.327347426343
H	-1.252797922572	3.537673743470	-6.049676093635
H	-0.356058394835	2.070453766584	-5.656243882520
O	2.243802501959	2.082379667582	-4.726606331170
C	3.594262793566	1.994224736676	-4.648152281335
N	4.112350564673	3.231737296871	-4.329621035926
C	3.072039833214	4.256200585256	-4.301159136296
H	3.156485576670	4.876560295436	-3.399919035768
H	3.152804508594	4.916147095085	-5.179377914219
O	4.191844763183	0.954378651416	-4.842120729649
C	8.044327759087	4.278112173448	-3.934801148558
O	9.305860074527	4.727424416550	-3.786036338602
C	10.373178624043	3.753476147668	-3.819657799954
C	11.672364805348	4.504398681201	-3.613172323568
H	11.827036686557	5.250653082797	-4.408195917811
H	12.516082657299	3.797312857206	-3.633052529395
H	11.677575488967	5.022673547058	-2.641460867858
H	10.350962760144	3.228198984537	-4.788477986617
H	10.201484521438	3.003026996242	-3.030939598705
C	7.003689897015	5.226083602226	-3.899287807809
H	7.225568194930	6.287365285017	-3.757602040997
N	5.733172331224	4.862674316431	-4.035339553799
C	5.475302499905	3.554616348850	-4.207614305253
C	6.514391337902	2.610602393539	-4.244413948515
H	6.304338172772	1.552331610250	-4.389037070285
N	7.795190613195	2.982156720911	-4.107511837303

SCF Done: E(RB3LYP) = -1484.53199528

Zero-point correction= 0.478280
Thermal correction to Energy= 0.506946
Thermal correction to Enthalpy= 0.507890
Thermal correction to Gibbs Free Energy= 0.415605
Sum of electronic and zero-point Energies= -1484.053715
Sum of electronic and thermal Energies= -1484.025049
Sum of electronic and thermal Enthalpies= -1484.024105
Sum of electronic and thermal Free Energies= -1484.116390

1 C Isotropic = 46.3528 Anisotropy = 144.8863

2	C	Isotropic =	57.0170	Anisotropy =	142.0558
3	C	Isotropic =	76.0110	Anisotropy =	157.4157
4	H	Isotropic =	23.6545	Anisotropy =	10.9050
5	C	Isotropic =	86.9090	Anisotropy =	125.3090
6	C	Isotropic =	66.8613	Anisotropy =	165.0981
7	H	Isotropic =	23.8872	Anisotropy =	5.8026
8	C	Isotropic =	72.2786	Anisotropy =	156.2471
9	H	Isotropic =	23.7071	Anisotropy =	5.2653
10	C	Isotropic =	75.7741	Anisotropy =	316.3245
11	N	Isotropic =	-1.5587	Anisotropy =	371.9662
12	N	Isotropic =	93.4223	Anisotropy =	119.4687
13	C	Isotropic =	132.1284	Anisotropy =	41.9191
14	H	Isotropic =	27.4869	Anisotropy =	4.8776
15	H	Isotropic =	27.6722	Anisotropy =	4.9901
16	C	Isotropic =	46.0349	Anisotropy =	99.7306
17	H	Isotropic =	23.6196	Anisotropy =	6.9686
18	N	Isotropic =	6.2671	Anisotropy =	349.6589
19	C	Isotropic =	152.5594	Anisotropy =	15.8007
20	H	Isotropic =	29.4601	Anisotropy =	7.3374
21	H	Isotropic =	29.7515	Anisotropy =	7.6367
22	C	Isotropic =	109.0002	Anisotropy =	64.4051
23	C	Isotropic =	144.8153	Anisotropy =	24.3545
24	H	Isotropic =	29.8622	Anisotropy =	5.0589
25	H	Isotropic =	29.5856	Anisotropy =	7.5235
26	C	Isotropic =	149.8319	Anisotropy =	14.3916
27	C	Isotropic =	169.0011	Anisotropy =	31.4529
28	H	Isotropic =	29.3629	Anisotropy =	6.6755
29	H	Isotropic =	30.5983	Anisotropy =	10.2196
30	H	Isotropic =	30.9275	Anisotropy =	5.6903
31	C	Isotropic =	153.7441	Anisotropy =	19.5863
32	H	Isotropic =	29.9822	Anisotropy =	7.0355
33	H	Isotropic =	29.7453	Anisotropy =	7.7768
34	C	Isotropic =	170.1008	Anisotropy =	13.2295
35	H	Isotropic =	29.6413	Anisotropy =	11.4446
36	H	Isotropic =	29.3271	Anisotropy =	6.6036
37	O	Isotropic =	136.8594	Anisotropy =	105.8033
38	C	Isotropic =	42.5965	Anisotropy =	82.1943
39	N	Isotropic =	137.3564	Anisotropy =	99.3365
40	C	Isotropic =	134.7782	Anisotropy =	37.2460
41	H	Isotropic =	27.6374	Anisotropy =	4.7417
42	H	Isotropic =	27.8324	Anisotropy =	5.7811
43	O	Isotropic =	60.7911	Anisotropy =	381.6112
44	C	Isotropic =	36.7014	Anisotropy =	121.5086
45	O	Isotropic =	195.9232	Anisotropy =	79.8218
46	C	Isotropic =	127.7911	Anisotropy =	54.3010
47	C	Isotropic =	176.3738	Anisotropy =	21.7287
48	H	Isotropic =	29.9156	Anisotropy =	7.9147
49	H	Isotropic =	30.0592	Anisotropy =	9.4744
50	H	Isotropic =	29.9298	Anisotropy =	7.6683
51	H	Isotropic =	27.3046	Anisotropy =	6.0366
52	H	Isotropic =	27.2595	Anisotropy =	5.8064
53	C	Isotropic =	62.6683	Anisotropy =	126.7822
54	H	Isotropic =	23.5066	Anisotropy =	7.3626
55	N	Isotropic =	-52.5940	Anisotropy =	484.0573
56	C	Isotropic =	50.1930	Anisotropy =	127.4890
57	C	Isotropic =	62.2354	Anisotropy =	141.8398

58 H Isotropic = 22.3728 Anisotropy = 12.2288
59 N Isotropic = -34.8013 Anisotropy = 472.2663

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	6.503948229266	-0.612879998339	-4.584947862109
C	5.195138279223	-0.139718481139	-4.879275642135
C	4.967795582488	1.106553495974	-5.462708264305
H	3.969594275818	1.472272793929	-5.701072355187
C	6.101679327771	1.889492008559	-5.737492826533
C	7.415125137920	1.436622467051	-5.436435370440
H	8.262106212332	2.083863187007	-5.666090597564
C	7.623098334272	0.189394747652	-4.863143020515
H	8.628958473023	-0.167076386942	-4.636180462338
C	5.929825127562	3.181320020140	-6.337853941844
N	5.795991413530	4.231507260322	-6.825631080661
N	4.341167907028	-1.162538667835	-4.488768529609
C	2.884014757665	-1.221858768582	-4.627107847428
H	2.615375518495	-0.598281835267	-5.492333448552
H	2.627468340054	-2.258687980341	-4.889302574182
C	5.155614787697	-2.165000545656	-4.018734771105
H	4.733064916808	-3.106579257460	-3.671199994771
N	6.442661144281	-1.886161446909	-4.047133538249
C	2.076090494958	0.181210566843	-0.544315705846
H	1.581808251674	0.533603123495	0.375400512410
H	3.163598332785	0.210808535859	-0.355766439437
C	1.780228368733	1.164713239805	-1.682725998198
C	2.349651182118	0.674114552067	-3.019013866081
H	3.442715939479	0.797306764327	-2.938803740294
H	2.008106604437	1.354365296485	-3.816562215218
C	2.033471812503	-0.795704544920	-3.395273244794
C	0.568342531375	-0.957819284167	-3.854071398407
H	0.376783241612	-1.996749020732	-4.169056279035
H	0.350528167938	-0.298899207104	-4.710564731888
H	-0.139900902073	-0.703714126826	-3.056844312755
C	2.329568013141	-1.717262754497	-2.187993854650
H	3.418842380657	-1.746690208595	-2.012131072331
H	2.019737440889	-2.747810168767	-2.430656373949
C	1.655608456209	-1.249653586684	-0.891158777165
H	1.933531392082	-1.924711941813	-0.066350836352
H	0.558572254517	-1.303364006854	-0.982040199391
O	0.319488435314	1.296020159440	-1.800260599746
C	-0.105721892057	2.481565052732	-1.299694177813
N	0.987843009374	3.248789443204	-0.956616287595
C	2.237731240927	2.604107123582	-1.350226865025
H	2.679954312557	3.115403295467	-2.220043780922
H	2.968404535676	2.628255931184	-0.531763116539
O	-1.283603002145	2.762139450151	-1.199743066787
C	1.007069576268	7.078310107992	0.474620248166
O	1.123535637703	8.338773919047	0.936441158991
C	-0.088527531822	9.028824658131	1.315449425072
C	0.311324400023	10.412506507484	1.784663350851

H	0.990439230572	10.354192425874	2.649672982034
H	-0.585775941550	10.975248983743	2.085940374797
H	0.816487655150	10.970378065596	0.980641865911
H	-0.596050454921	8.456077009014	2.108763578383
H	-0.767208819660	9.068281689731	0.447966505023
C	2.187435814536	6.403930903491	0.107530082279
H	3.159014515124	6.896976162009	0.200292302139
N	2.156168090415	5.160492387393	-0.359160667275
C	0.954940761170	4.566409471551	-0.467059189718
C	-0.221021917482	5.239403611630	-0.097627585766
H	-1.193227407393	4.757993685254	-0.187203835865
N	-0.184591976045	6.494734116211	0.371437960315

SCF Done: E(RB3LYP) = -1484.53208256

Zero-point correction= 0.478149
Thermal correction to Energy= 0.506890
Thermal correction to Enthalpy= 0.507834
Thermal correction to Gibbs Free Energy= 0.415688
Sum of electronic and zero-point Energies= -1484.053934
Sum of electronic and thermal Energies= -1484.025193
Sum of electronic and thermal Enthalpies= -1484.024249
Sum of electronic and thermal Free Energies= -1484.116395

1	C	Isotropic =	46.3668	Anisotropy =	145.1451
2	C	Isotropic =	57.0400	Anisotropy =	142.1889
3	C	Isotropic =	76.6465	Anisotropy =	157.4719
4	H	Isotropic =	23.7025	Anisotropy =	10.1670
5	C	Isotropic =	86.8425	Anisotropy =	125.8104
6	C	Isotropic =	66.5344	Anisotropy =	165.6507
7	H	Isotropic =	23.8486	Anisotropy =	5.9108
8	C	Isotropic =	72.2609	Anisotropy =	156.9041
9	H	Isotropic =	23.6558	Anisotropy =	4.8918
10	C	Isotropic =	75.7912	Anisotropy =	315.8326
11	N	Isotropic =	-1.6059	Anisotropy =	371.4727
12	N	Isotropic =	93.4541	Anisotropy =	119.2177
13	C	Isotropic =	134.1223	Anisotropy =	45.1091
14	H	Isotropic =	27.4568	Anisotropy =	3.6691
15	H	Isotropic =	27.6315	Anisotropy =	6.2150
16	C	Isotropic =	45.5752	Anisotropy =	99.0227
17	H	Isotropic =	23.5472	Anisotropy =	7.7344
18	N	Isotropic =	5.7172	Anisotropy =	349.9596
19	C	Isotropic =	152.1348	Anisotropy =	14.9963
20	H	Isotropic =	29.5712	Anisotropy =	6.7381
21	H	Isotropic =	30.4253	Anisotropy =	6.2250
22	C	Isotropic =	108.3387	Anisotropy =	64.0105
23	C	Isotropic =	146.9122	Anisotropy =	19.6222
24	H	Isotropic =	30.0990	Anisotropy =	11.1142
25	H	Isotropic =	29.6068	Anisotropy =	4.5815
26	C	Isotropic =	149.8011	Anisotropy =	15.2514
27	C	Isotropic =	166.1730	Anisotropy =	36.0476
28	H	Isotropic =	30.5624	Anisotropy =	10.0395
29	H	Isotropic =	30.3700	Anisotropy =	8.0153
30	H	Isotropic =	29.1111	Anisotropy =	6.5704
31	C	Isotropic =	156.8327	Anisotropy =	7.0186
32	H	Isotropic =	29.9449	Anisotropy =	8.0677

33	H	Isotropic =	29.8561	Anisotropy =	8.2943
34	C	Isotropic =	170.4156	Anisotropy =	13.0617
35	H	Isotropic =	29.7981	Anisotropy =	11.4630
36	H	Isotropic =	29.3688	Anisotropy =	6.9651
37	O	Isotropic =	136.9932	Anisotropy =	115.1301
38	C	Isotropic =	42.2426	Anisotropy =	82.6714
39	N	Isotropic =	137.7104	Anisotropy =	97.4038
40	C	Isotropic =	134.7667	Anisotropy =	38.5517
41	H	Isotropic =	28.0549	Anisotropy =	6.8221
42	H	Isotropic =	27.9176	Anisotropy =	4.5076
43	O	Isotropic =	60.1984	Anisotropy =	382.0889
44	C	Isotropic =	36.8829	Anisotropy =	121.3464
45	O	Isotropic =	196.3715	Anisotropy =	79.4763
46	C	Isotropic =	127.9104	Anisotropy =	54.3523
47	C	Isotropic =	176.4212	Anisotropy =	21.6813
48	H	Isotropic =	29.9291	Anisotropy =	7.8030
49	H	Isotropic =	30.0561	Anisotropy =	9.5309
50	H	Isotropic =	29.9239	Anisotropy =	7.7186
51	H	Isotropic =	27.2866	Anisotropy =	6.1294
52	H	Isotropic =	27.2649	Anisotropy =	5.9081
53	C	Isotropic =	63.0602	Anisotropy =	126.1759
54	H	Isotropic =	23.5758	Anisotropy =	7.8474
55	N	Isotropic =	-52.4951	Anisotropy =	483.7368
56	C	Isotropic =	50.1593	Anisotropy =	126.9132
57	C	Isotropic =	61.8794	Anisotropy =	141.7779
58	H	Isotropic =	22.2762	Anisotropy =	12.2776
59	N	Isotropic =	-34.8663	Anisotropy =	472.0214

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	5.137884345540	-1.847748848788	-0.779209040469
C	5.545969270735	-0.541704883394	-1.169735985187
C	5.803226716847	-0.211446961347	-2.500212296587
H	6.131442233013	0.780159196695	-2.809388850173
C	5.623743274214	-1.231374917275	-3.449917108689
C	5.201373338729	-2.536332285793	-3.076684224533
H	5.073087977012	-3.292014225221	-3.852275566136
C	4.959296355680	-2.850798254052	-1.746418070484
H	4.642990394800	-3.852420819938	-1.451297137032
C	5.874012456962	-0.948296421154	-4.834115249296
N	6.075907870917	-0.723697292017	-5.959984442422
N	5.630168996788	0.181403641857	0.012478850403
C	6.037998952942	1.577276846346	0.196100456935
H	6.609169062389	1.624051275995	1.135039919304
H	6.736399316366	1.823451040589	-0.616790722325
C	5.296980510122	-0.701172435508	1.011183549430
H	5.307236944562	-0.388401313187	2.053963911956
N	4.991512801926	-1.913018419307	0.594768123662
C	3.981375523168	5.200924710578	-1.034775771021
H	3.277447995426	6.042286916879	-1.139609938507
H	4.756890849633	5.333661329377	-1.809325004846
C	3.248544297078	3.889371237932	-1.341428833898

C	4.147910506054	2.670265694620	-1.104101104870
H	4.892084193799	2.690689939597	-1.918938690710
H	3.547816948577	1.756788634324	-1.242270039150
C	4.895453108917	2.629797629053	0.254108825981
C	3.943129661675	2.291066033525	1.417629210922
H	3.171411547077	3.059819305376	1.545745027380
H	4.503521371655	2.206924180518	2.363445961459
H	3.418056873861	1.338906489272	1.243287102743
C	5.586276883208	3.996369163919	0.500196207294
H	6.415418077673	4.112071316916	-0.221775619458
H	6.042921997727	3.998351776057	1.504021664234
C	4.636817407560	5.191243791627	0.348897084082
H	5.196680880257	6.128186912694	0.497036314685
H	3.858970060276	5.167011421555	1.129171177119
O	2.074952045212	3.803975954098	-0.458833717203
C	0.931920864173	4.058949293106	-1.141727631381
N	1.223281148461	4.186643385125	-2.483509753283
C	2.625745773267	3.885309262373	-2.757021675205
H	2.721295724308	2.908083911847	-3.256509376606
H	3.072481188644	4.646974635265	-3.408553087354
O	-0.149097511142	4.145498996978	-0.594197441396
C	-1.390222564290	4.783970578021	-5.569697177762
O	-2.165420730948	4.966891961820	-6.656413267054
C	-3.566922943230	5.247775781683	-6.442157811790
C	-4.207412965217	5.396649562331	-7.806869617500
H	-4.101024257365	4.471342365606	-8.394478751259
H	-3.746720163650	6.223359360142	-8.370037076777
H	-5.280902020212	5.612178367463	-7.691198345705
H	-3.662714711122	6.166052931834	-5.840092025370
H	-4.015435850368	4.423264380937	-5.864434402327
C	-0.025593131013	4.506789221637	-5.779065405434
H	0.378254795742	4.446180680188	-6.793403620766
N	0.803953808852	4.311787977054	-4.760015449259
C	0.293765170015	4.390152464619	-3.518661061509
C	-1.066811760347	4.669366105667	-3.311516533635
H	-1.479075620596	4.730495009591	-2.305859425942
N	-1.900625292338	4.864056404292	-4.343147037278

SCF Done: E(RB3LYP) = -1484.53204200

Zero-point correction= 0.478299
Thermal correction to Energy= 0.506950
Thermal correction to Enthalpy= 0.507894
Thermal correction to Gibbs Free Energy= 0.416223
Sum of electronic and zero-point Energies= -1484.053743
Sum of electronic and thermal Energies= -1484.025092
Sum of electronic and thermal Enthalpies= -1484.024148
Sum of electronic and thermal Free Energies= -1484.115819

1	C	Isotropic =	46.1323	Anisotropy =	144.7699
2	C	Isotropic =	57.1379	Anisotropy =	142.1651
3	C	Isotropic =	76.3657	Anisotropy =	157.2792
4	H	Isotropic =	23.6156	Anisotropy =	10.2625
5	C	Isotropic =	86.9724	Anisotropy =	125.6133
6	C	Isotropic =	66.8790	Anisotropy =	165.5516
7	H	Isotropic =	23.8807	Anisotropy =	5.9490

8	C	Isotropic =	72.2009	Anisotropy =	156.2988
9	H	Isotropic =	23.6893	Anisotropy =	4.8659
10	C	Isotropic =	75.7209	Anisotropy =	315.9906
11	N	Isotropic =	-1.5280	Anisotropy =	371.4827
12	N	Isotropic =	93.8651	Anisotropy =	118.2526
13	C	Isotropic =	131.9571	Anisotropy =	41.8406
14	H	Isotropic =	27.5938	Anisotropy =	5.9415
15	H	Isotropic =	27.4739	Anisotropy =	3.5888
16	C	Isotropic =	45.1630	Anisotropy =	99.9249
17	H	Isotropic =	23.5532	Anisotropy =	7.7497
18	N	Isotropic =	6.5444	Anisotropy =	348.2061
19	C	Isotropic =	151.4657	Anisotropy =	15.9489
20	H	Isotropic =	29.3919	Anisotropy =	6.4485
21	H	Isotropic =	29.9104	Anisotropy =	7.3477
22	C	Isotropic =	109.1135	Anisotropy =	64.4539
23	C	Isotropic =	144.8921	Anisotropy =	21.6427
24	H	Isotropic =	29.6007	Anisotropy =	6.7406
25	H	Isotropic =	30.0614	Anisotropy =	7.7555
26	C	Isotropic =	149.8746	Anisotropy =	15.0801
27	C	Isotropic =	168.9182	Anisotropy =	32.1585
28	H	Isotropic =	29.3161	Anisotropy =	6.4937
29	H	Isotropic =	30.5620	Anisotropy =	10.3511
30	H	Isotropic =	30.5832	Anisotropy =	5.8352
31	C	Isotropic =	153.7931	Anisotropy =	18.3597
32	H	Isotropic =	29.9259	Anisotropy =	6.8457
33	H	Isotropic =	29.7935	Anisotropy =	7.8674
34	C	Isotropic =	170.6915	Anisotropy =	13.0226
35	H	Isotropic =	29.6896	Anisotropy =	11.4756
36	H	Isotropic =	29.3357	Anisotropy =	6.8498
37	O	Isotropic =	138.1730	Anisotropy =	114.8748
38	C	Isotropic =	42.3888	Anisotropy =	82.7278
39	N	Isotropic =	137.7820	Anisotropy =	97.7670
40	C	Isotropic =	134.4867	Anisotropy =	37.9034
41	H	Isotropic =	28.0354	Anisotropy =	6.6562
42	H	Isotropic =	27.6693	Anisotropy =	5.0837
43	O	Isotropic =	60.3167	Anisotropy =	382.1966
44	C	Isotropic =	36.7909	Anisotropy =	120.5149
45	O	Isotropic =	196.4150	Anisotropy =	79.8335
46	C	Isotropic =	128.0916	Anisotropy =	54.4980
47	C	Isotropic =	176.2179	Anisotropy =	21.9408
48	H	Isotropic =	29.9316	Anisotropy =	7.6960
49	H	Isotropic =	29.9273	Anisotropy =	7.7864
50	H	Isotropic =	30.0664	Anisotropy =	9.5227
51	H	Isotropic =	27.2926	Anisotropy =	6.1332
52	H	Isotropic =	27.2915	Anisotropy =	5.8735
53	C	Isotropic =	62.9603	Anisotropy =	126.1354
54	H	Isotropic =	23.5359	Anisotropy =	7.7110
55	N	Isotropic =	-52.6243	Anisotropy =	483.4676
56	C	Isotropic =	49.9897	Anisotropy =	127.2934
57	C	Isotropic =	62.0903	Anisotropy =	141.6426
58	H	Isotropic =	22.3679	Anisotropy =	12.3177
59	N	Isotropic =	-34.8325	Anisotropy =	472.2542

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	7.090716093038	2.003027463876	0.381118078630
C	6.799672234736	2.212682981118	-0.995766155423
C	6.646077264777	1.154424381898	-1.891251998899
H	6.441583150032	1.302437859971	-2.950876351563
C	6.774064058869	-0.141989205784	-1.364779160921
C	7.048181783374	-0.367411918676	0.011627881432
H	7.134694804788	-1.393023624194	0.371735505788
C	7.209470928375	0.697780371239	0.887123745053
H	7.428707409551	0.532550271961	1.943056403684
C	6.625744350802	-1.268571455084	-2.240920845475
N	6.506588031688	-2.186780883093	-2.949077014530
N	6.758186841808	3.591641655858	-1.153022123460
C	6.530370406345	4.354195902679	-2.384287569802
H	7.196608392189	5.229096707887	-2.351799662994
H	6.866945338552	3.726703831875	-3.222178543516
C	7.034434534710	4.114292046633	0.087184990569
H	7.088410640686	5.191221448260	0.237029047277
N	7.232452245183	3.216215092151	1.030487050357
C	2.861142137785	4.675038472078	-4.678831281677
H	1.850022023081	4.915388775859	-5.045306742364
H	3.321097480438	4.004529593813	-5.425624880446
C	2.750096706327	3.891841636549	-3.365254536964
C	4.127930031557	3.618096783329	-2.753050294751
H	4.596957849811	2.863784946958	-3.408098596880
H	3.988922037945	3.143224742024	-1.769018893586
C	5.076096475736	4.840522767003	-2.636820581884
C	4.644041492444	5.786241912874	-1.499487805834
H	5.364940450465	6.613251777902	-1.390277419260
H	4.581314324643	5.255380834982	-0.536664043353
H	3.653784019350	6.218013315969	-1.688890319387
C	5.108628144479	5.599865032463	-3.989097296149
H	5.633451924129	4.976176881799	-4.735921017346
H	5.706413434584	6.519620279105	-3.875556519026
C	3.713731527859	5.938124267831	-4.529396373098
H	3.808002187276	6.436813132031	-5.506953002733
H	3.204295637603	6.653002669640	-3.863118583435
O	1.949755403997	4.691010763118	-2.423594107081
C	0.682945412107	4.213739291143	-2.342940825866
N	0.599204805144	3.030488228858	-3.047075184848
C	1.912455331042	2.603581857944	-3.523654822231
H	2.297727353399	1.773996944611	-2.909153388784
H	1.862731729031	2.264814911549	-4.565823659033
O	-0.192422243670	4.787200791884	-1.726052693276
C	-2.656915616517	0.597619692291	-3.482579027212
O	-3.665380170568	-0.272345495400	-3.686331413360
C	-4.987408658016	0.118688499956	-3.252258364280
C	-5.928365343929	-1.014822017982	-3.604879574945
H	-5.631669362626	-1.945759894647	-3.096791719085
H	-5.936240449126	-1.196622357322	-4.691052591966
H	-6.951625430846	-0.758828338385	-3.289198337988
H	-5.268663124330	1.058230777630	-3.755210390165
H	-4.967419020097	0.315159616113	-2.167867504570
C	-1.370766338429	0.221169442817	-3.915145295959

H	-1.209206991138	-0.748079043918	-4.394840263220
N	-0.325257912482	1.025123853420	-3.755801670115
C	-0.539101988022	2.213944150444	-3.165674199210
C	-1.821560184239	2.586006457793	-2.730950296604
H	-1.992179736728	3.545840856445	-2.246513699815
N	-2.873703858971	1.771430260854	-2.893966058420

SCF Done: E(RB3LYP) = -1484.53193643

Zero-point correction= 0.478132
Thermal correction to Energy= 0.506820
Thermal correction to Enthalpy= 0.507764
Thermal correction to Gibbs Free Energy= 0.416020
Sum of electronic and zero-point Energies= -1484.053804
Sum of electronic and thermal Energies= -1484.025117
Sum of electronic and thermal Enthalpies= -1484.024172
Sum of electronic and thermal Free Energies= -1484.115916

1	C	Isotropic =	46.7706	Anisotropy =	144.3314
2	C	Isotropic =	57.3307	Anisotropy =	141.6903
3	C	Isotropic =	76.2521	Anisotropy =	157.7752
4	H	Isotropic =	23.6264	Anisotropy =	10.2806
5	C	Isotropic =	86.6137	Anisotropy =	126.0186
6	C	Isotropic =	66.7580	Anisotropy =	165.5728
7	H	Isotropic =	23.8839	Anisotropy =	5.9284
8	C	Isotropic =	72.3614	Anisotropy =	156.1287
9	H	Isotropic =	23.6885	Anisotropy =	4.8448
10	C	Isotropic =	75.6561	Anisotropy =	316.2520
11	N	Isotropic =	-1.6356	Anisotropy =	371.3940
12	N	Isotropic =	93.7169	Anisotropy =	118.0320
13	C	Isotropic =	131.9232	Anisotropy =	42.0862
14	H	Isotropic =	27.5577	Anisotropy =	5.9698
15	H	Isotropic =	27.4755	Anisotropy =	3.8399
16	C	Isotropic =	45.4921	Anisotropy =	99.8591
17	H	Isotropic =	23.4960	Anisotropy =	7.7487
18	N	Isotropic =	6.0722	Anisotropy =	348.6027
19	C	Isotropic =	151.8804	Anisotropy =	15.5773
20	H	Isotropic =	29.4258	Anisotropy =	6.3734
21	H	Isotropic =	29.9794	Anisotropy =	7.3587
22	C	Isotropic =	108.8699	Anisotropy =	64.1463
23	C	Isotropic =	145.6197	Anisotropy =	21.7457
24	H	Isotropic =	29.6729	Anisotropy =	7.1804
25	H	Isotropic =	30.1846	Anisotropy =	7.6573
26	C	Isotropic =	149.5484	Anisotropy =	14.4086
27	C	Isotropic =	168.3695	Anisotropy =	33.3188
28	H	Isotropic =	30.5298	Anisotropy =	10.4532
29	H	Isotropic =	30.4784	Anisotropy =	6.0346
30	H	Isotropic =	29.2862	Anisotropy =	6.4357
31	C	Isotropic =	153.9302	Anisotropy =	18.2524
32	H	Isotropic =	29.9007	Anisotropy =	6.8883
33	H	Isotropic =	29.7423	Anisotropy =	7.8812
34	C	Isotropic =	171.0668	Anisotropy =	12.4241
35	H	Isotropic =	29.6661	Anisotropy =	11.4760
36	H	Isotropic =	29.3147	Anisotropy =	6.9621
37	O	Isotropic =	138.7241	Anisotropy =	116.4543
38	C	Isotropic =	42.1412	Anisotropy =	82.2930

39	N	Isotropic =	137.5924	Anisotropy =	96.5085
40	C	Isotropic =	134.9063	Anisotropy =	37.9589
41	H	Isotropic =	28.1269	Anisotropy =	6.8555
42	H	Isotropic =	27.6704	Anisotropy =	5.1858
43	O	Isotropic =	59.7723	Anisotropy =	384.3057
44	C	Isotropic =	36.6667	Anisotropy =	120.6894
45	O	Isotropic =	196.3538	Anisotropy =	79.0011
46	C	Isotropic =	127.8926	Anisotropy =	54.4577
47	C	Isotropic =	176.4051	Anisotropy =	21.7111
48	H	Isotropic =	29.9352	Anisotropy =	7.7297
49	H	Isotropic =	29.9287	Anisotropy =	7.7883
50	H	Isotropic =	30.0661	Anisotropy =	9.5379
51	H	Isotropic =	27.2951	Anisotropy =	6.0522
52	H	Isotropic =	27.2989	Anisotropy =	5.9656
53	C	Isotropic =	62.8820	Anisotropy =	126.2182
54	H	Isotropic =	23.5472	Anisotropy =	7.7522
55	N	Isotropic =	-52.4258	Anisotropy =	483.0428
56	C	Isotropic =	50.2579	Anisotropy =	126.9144
57	C	Isotropic =	61.9991	Anisotropy =	141.6902
58	H	Isotropic =	22.3935	Anisotropy =	12.3186
59	N	Isotropic =	-34.7785	Anisotropy =	472.3445

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.753883037108	-0.124255161575	-7.184518025642
C	0.138092302414	0.753830669547	-6.508855887181
C	0.219227791218	2.112181434379	-6.813635089290
H	0.904195187677	2.790043037387	-6.305418197003
C	-0.635726746453	2.582720563300	-7.824391531507
C	-1.540176902463	1.720114282151	-8.502066273672
H	-2.185074972719	2.135387002642	-9.277103473232
C	-1.603810676067	0.369187875981	-8.188580967797
H	-2.291579510295	-0.299358132643	-8.708558704417
C	-0.596036418527	3.971646866727	-8.182488612752
N	-0.567504998308	5.098964123147	-8.477676549630
N	0.820421790660	-0.046339406075	-5.603112288566
C	1.893414996802	0.346259544864	-4.686756197301
H	2.638218248888	-0.463274894026	-4.693119701083
H	2.380246657170	1.232208969674	-5.119928330307
C	0.330437757863	-1.316492692938	-5.787506561232
H	0.720488704775	-2.152210558853	-5.208963333276
N	-0.607581760616	-1.414729058840	-6.707589728627
C	2.140147229467	-0.127649078411	-0.377759454755
H	2.036649118144	0.001343568213	0.711357797064
H	2.878344613929	-0.933358767530	-0.538648025057
C	2.723643180355	1.153067039441	-0.974532025968
C	2.771141157311	1.094876357419	-2.509337452435
H	3.571650031905	0.377185057630	-2.761192331319
H	3.098988950414	2.075764847621	-2.892657502272
C	1.466325586275	0.647240350176	-3.222019139289
C	0.399761746126	1.758518771514	-3.207804479974
H	0.786079066541	2.681442477724	-3.670285362458

H	0.095063875798	2.013551228049	-2.185514349235
H	-0.497866145074	1.445998329329	-3.763880029070
C	0.934540811125	-0.640107246964	-2.543964036020
H	1.627095603541	-1.472657590089	-2.766499271957
H	-0.040544498987	-0.913865873753	-2.978160925925
C	0.804479800212	-0.513752846051	-1.020419420989
H	0.457162945041	-1.470753611129	-0.599935943758
H	0.039242252210	0.235793269307	-0.760289152420
O	1.867682586538	2.275502234177	-0.563188595221
C	2.594712697198	3.278112603997	-0.013987056022
N	3.916131201000	2.893674727025	0.063746439372
C	4.105901364096	1.514919467542	-0.376022828055
H	4.913444525066	1.448437002367	-1.117112329928
H	4.371721034317	0.869328736585	0.475275833328
O	2.095023309867	4.329261629059	0.335179366952
C	7.049215650660	4.981254949820	1.656839933298
O	8.145434942755	5.579084191883	2.163167508878
C	8.010532423896	6.937538764834	2.637731304531
C	9.370059005495	7.371923342535	3.145230968738
H	9.708471383021	6.724217721695	3.969152368296
H	9.313194125882	8.406085504513	3.518724754834
H	10.121035475210	7.334994695026	2.340533734814
H	7.246089258686	6.967580760950	3.431211359316
H	7.656816720398	7.574791019685	1.810969135407
C	7.180115449684	3.657061459755	1.196314703134
H	8.143810712972	3.143463609062	1.252698876413
N	6.146308160684	2.998076766382	0.684803360145
C	4.967775017842	3.642008990308	0.620918651750
C	4.839476782933	4.963520074492	1.078472404489
H	3.884335860603	5.483150242232	1.027154605954
N	5.885438571953	5.624030758735	1.595286057929

SCF Done: E(RB3LYP) = -1484.53211748

Zero-point correction= 0.478194
Thermal correction to Energy= 0.506912
Thermal correction to Enthalpy= 0.507857
Thermal correction to Gibbs Free Energy= 0.415481
Sum of electronic and zero-point Energies= -1484.053923
Sum of electronic and thermal Energies= -1484.025205
Sum of electronic and thermal Enthalpies= -1484.024261
Sum of electronic and thermal Free Energies= -1484.116636

1	C	Isotropic =	46.2729	Anisotropy =	144.4851
2	C	Isotropic =	56.9586	Anisotropy =	141.4080
3	C	Isotropic =	76.1904	Anisotropy =	156.6540
4	H	Isotropic =	23.6572	Anisotropy =	10.9215
5	C	Isotropic =	87.0453	Anisotropy =	125.5605
6	C	Isotropic =	66.9333	Anisotropy =	164.9241
7	H	Isotropic =	23.8781	Anisotropy =	5.9851
8	C	Isotropic =	72.3084	Anisotropy =	156.2286
9	H	Isotropic =	23.6687	Anisotropy =	5.0556
10	C	Isotropic =	75.8174	Anisotropy =	316.0064
11	N	Isotropic =	-1.6282	Anisotropy =	371.8642
12	N	Isotropic =	93.8155	Anisotropy =	117.9423
13	C	Isotropic =	132.7303	Anisotropy =	43.0372

14	H	Isotropic =	27.6992	Anisotropy =	4.8337
15	H	Isotropic =	27.5144	Anisotropy =	5.1288
16	C	Isotropic =	45.9234	Anisotropy =	99.5694
17	H	Isotropic =	23.5484	Anisotropy =	8.0016
18	N	Isotropic =	5.8811	Anisotropy =	348.9658
19	C	Isotropic =	151.9558	Anisotropy =	15.7950
20	H	Isotropic =	29.4575	Anisotropy =	7.1671
21	H	Isotropic =	29.7829	Anisotropy =	7.6101
22	C	Isotropic =	108.6308	Anisotropy =	64.2069
23	C	Isotropic =	143.5390	Anisotropy =	31.4775
24	H	Isotropic =	29.9645	Anisotropy =	4.6536
25	H	Isotropic =	29.4724	Anisotropy =	5.3035
26	C	Isotropic =	149.9144	Anisotropy =	15.4376
27	C	Isotropic =	169.5072	Anisotropy =	25.6636
28	H	Isotropic =	30.5240	Anisotropy =	8.1948
29	H	Isotropic =	29.3760	Anisotropy =	6.9651
30	H	Isotropic =	31.1149	Anisotropy =	7.1813
31	C	Isotropic =	154.9535	Anisotropy =	17.7208
32	H	Isotropic =	29.8921	Anisotropy =	7.6221
33	H	Isotropic =	29.8089	Anisotropy =	7.3100
34	C	Isotropic =	170.1217	Anisotropy =	13.0810
35	H	Isotropic =	29.6943	Anisotropy =	11.2453
36	H	Isotropic =	29.5287	Anisotropy =	6.1370
37	O	Isotropic =	136.6842	Anisotropy =	106.5163
38	C	Isotropic =	42.5395	Anisotropy =	82.7185
39	N	Isotropic =	137.4405	Anisotropy =	99.1635
40	C	Isotropic =	134.1449	Anisotropy =	38.3240
41	H	Isotropic =	27.6509	Anisotropy =	4.5825
42	H	Isotropic =	27.7754	Anisotropy =	5.5169
43	O	Isotropic =	61.3292	Anisotropy =	379.3817
44	C	Isotropic =	36.7520	Anisotropy =	121.2163
45	O	Isotropic =	196.2459	Anisotropy =	79.6819
46	C	Isotropic =	127.8503	Anisotropy =	53.9707
47	C	Isotropic =	176.4503	Anisotropy =	21.5482
48	H	Isotropic =	29.9054	Anisotropy =	7.8729
49	H	Isotropic =	30.0278	Anisotropy =	9.4472
50	H	Isotropic =	29.9018	Anisotropy =	7.7498
51	H	Isotropic =	27.2522	Anisotropy =	5.9997
52	H	Isotropic =	27.2328	Anisotropy =	5.9493
53	C	Isotropic =	62.7773	Anisotropy =	126.1957
54	H	Isotropic =	23.4720	Anisotropy =	7.3993
55	N	Isotropic =	-52.6995	Anisotropy =	483.6314
56	C	Isotropic =	50.1425	Anisotropy =	127.2062
57	C	Isotropic =	61.9973	Anisotropy =	142.2509
58	H	Isotropic =	22.2443	Anisotropy =	12.1795
59	N	Isotropic =	-34.8286	Anisotropy =	472.5614

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	6.376840353999	3.103225457884	-5.405546315481
C	5.215142787051	2.291958584178	-5.535608795168
C	5.152608061765	0.996778390069	-5.021993887795

H	4.274688504086	0.361106966898	-5.129708730079
C	6.293741960457	0.528939084061	-4.348838660600
C	7.455934041849	1.333303550122	-4.197276170158
H	8.314472674166	0.925371103443	-3.662889055490
C	7.504795597809	2.617000750228	-4.723613879143
H	8.396481998772	3.236854636462	-4.618452232291
C	6.285461861587	-0.796432348910	-3.799193255953
N	6.283756412682	-1.872356031537	-3.350657970619
N	4.312113444829	3.062704466171	-6.255315308146
C	2.964391514545	2.698451983350	-6.701899169694
H	2.826531121120	3.136621931983	-7.701439523112
H	2.946266050211	1.606048081654	-6.826055074106
C	4.962686443807	4.242726557728	-6.522821470525
H	4.476681045156	5.024615455495	-7.104052946881
N	6.184577210879	4.319291148543	-6.036350438458
C	-0.601616065112	2.059873462962	-4.293675988303
H	-1.485401374989	2.201351330317	-3.651630716947
H	-0.508051536925	0.975294813956	-4.480294811259
C	0.644377482371	2.499256693251	-3.525103709778
C	1.901258812725	2.452151672813	-4.410310007548
H	2.105661908699	1.380771525642	-4.575349456073
H	2.753294627173	2.854070446484	-3.838339914847
C	1.788551372599	3.149340799488	-5.790546715853
C	1.794657059584	4.684953552566	-5.664399182473
H	0.917812168974	5.049189974630	-5.115574924545
H	1.794033920493	5.155097308397	-6.661793778413
H	2.682558114542	5.039927641804	-5.118201940452
C	0.494330135263	2.665671457607	-6.495786771465
H	0.616314252538	1.602339462533	-6.772796329397
H	0.362456647997	3.221146045970	-7.439346013084
C	-0.759985821803	2.802816495700	-5.624035557112
H	-1.631073945759	2.402466720004	-6.166324148968
H	-0.977806582770	3.865430729121	-5.428178931140
O	0.431778660415	3.878376523968	-3.063523655708
C	0.703052387553	4.005320781297	-1.742146735450
N	1.006653308956	2.766729183047	-1.218439773974
C	0.844691596940	1.707046116936	-2.209586289349
H	1.731486276689	1.060477900646	-2.240198275356
H	-0.026187411324	1.078615142404	-1.966355857158
O	0.665187616973	5.076231022895	-1.169379147570
C	1.800921412434	1.820598999784	2.678518781049
O	2.060815576740	1.401041986434	3.932289320505
C	2.197382692939	2.406045188153	4.961896181175
C	2.475515115450	1.680287994183	6.262120211844
H	1.648685652669	0.999107946590	6.517458291043
H	2.586912188488	2.411011235741	7.078114401005
H	3.404359834873	1.092521390379	6.194205752915
H	1.269611255829	2.998985063060	5.011744056418
H	3.016170416643	3.091876596439	4.689813590467
C	1.661752559784	0.840820446725	1.676801560340
H	1.765942588631	-0.219924112839	1.920945039570
N	1.401289296878	1.172804601472	0.417203872296
C	1.276521763859	2.480549286426	0.131418579052
C	1.420448200917	3.456732195395	1.130720773144
H	1.319126530174	4.515190058181	0.897741626765
N	1.681510217119	3.116814551617	2.401039478331

SCF Done: E(RB3LYP) = -1484.53189729

Zero-point correction= 0.478168
Thermal correction to Energy= 0.506862
Thermal correction to Enthalpy= 0.507806
Thermal correction to Gibbs Free Energy= 0.415477
Sum of electronic and zero-point Energies= -1484.053729
Sum of electronic and thermal Energies= -1484.025035
Sum of electronic and thermal Enthalpies= -1484.024091
Sum of electronic and thermal Free Energies= -1484.116421

1	C	Isotropic =	46.0011	Anisotropy =	144.9832
2	C	Isotropic =	57.1193	Anisotropy =	142.0072
3	C	Isotropic =	76.4101	Anisotropy =	158.0526
4	H	Isotropic =	23.6737	Anisotropy =	10.1668
5	C	Isotropic =	87.1572	Anisotropy =	125.6973
6	C	Isotropic =	67.1395	Anisotropy =	165.3312
7	H	Isotropic =	23.9487	Anisotropy =	5.8410
8	C	Isotropic =	72.4419	Anisotropy =	156.3627
9	H	Isotropic =	23.7402	Anisotropy =	4.7225
10	C	Isotropic =	75.7482	Anisotropy =	315.8014
11	N	Isotropic =	-1.3440	Anisotropy =	371.3250
12	N	Isotropic =	93.7102	Anisotropy =	117.8443
13	C	Isotropic =	131.6657	Anisotropy =	42.3202
14	H	Isotropic =	27.6156	Anisotropy =	5.9838
15	H	Isotropic =	27.5108	Anisotropy =	3.6472
16	C	Isotropic =	45.3772	Anisotropy =	99.7989
17	H	Isotropic =	23.5539	Anisotropy =	7.7299
18	N	Isotropic =	6.6162	Anisotropy =	349.4744
19	C	Isotropic =	151.8516	Anisotropy =	16.2427
20	H	Isotropic =	29.5157	Anisotropy =	7.2293
21	H	Isotropic =	29.7790	Anisotropy =	7.3731
22	C	Isotropic =	109.2704	Anisotropy =	64.8104
23	C	Isotropic =	144.0003	Anisotropy =	22.5132
24	H	Isotropic =	29.8352	Anisotropy =	6.6140
25	H	Isotropic =	29.9847	Anisotropy =	8.0517
26	C	Isotropic =	150.0224	Anisotropy =	14.9682
27	C	Isotropic =	168.7991	Anisotropy =	31.9258
28	H	Isotropic =	29.2495	Anisotropy =	6.1742
29	H	Isotropic =	30.5575	Anisotropy =	10.3917
30	H	Isotropic =	30.5325	Anisotropy =	5.6666
31	C	Isotropic =	154.6042	Anisotropy =	18.2817
32	H	Isotropic =	29.9021	Anisotropy =	6.9508
33	H	Isotropic =	29.7906	Anisotropy =	7.8679
34	C	Isotropic =	170.0393	Anisotropy =	12.8258
35	H	Isotropic =	29.6266	Anisotropy =	11.4720
36	H	Isotropic =	29.2860	Anisotropy =	6.9779
37	O	Isotropic =	138.0450	Anisotropy =	107.2902
38	C	Isotropic =	42.6621	Anisotropy =	82.7281
39	N	Isotropic =	137.5372	Anisotropy =	98.8396
40	C	Isotropic =	134.3938	Anisotropy =	37.6276
41	H	Isotropic =	27.8199	Anisotropy =	4.3258
42	H	Isotropic =	27.8557	Anisotropy =	5.4370
43	O	Isotropic =	61.4998	Anisotropy =	380.5293
44	C	Isotropic =	36.7936	Anisotropy =	121.1350

45	O	Isotropic =	196.4396	Anisotropy =	78.9548
46	C	Isotropic =	128.0644	Anisotropy =	54.3441
47	C	Isotropic =	176.3049	Anisotropy =	21.9229
48	H	Isotropic =	29.9391	Anisotropy =	7.8945
49	H	Isotropic =	30.0748	Anisotropy =	9.5427
50	H	Isotropic =	29.9381	Anisotropy =	7.6162
51	H	Isotropic =	27.3162	Anisotropy =	6.1204
52	H	Isotropic =	27.3233	Anisotropy =	5.8022
53	C	Isotropic =	63.1117	Anisotropy =	126.6384
54	H	Isotropic =	23.5535	Anisotropy =	7.4973
55	N	Isotropic =	-52.4692	Anisotropy =	484.5142
56	C	Isotropic =	50.2773	Anisotropy =	127.7176
57	C	Isotropic =	62.0145	Anisotropy =	142.2710
58	H	Isotropic =	22.4248	Anisotropy =	12.1830
59	N	Isotropic =	-34.8068	Anisotropy =	472.2606

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	8.833645009278	1.296294880687	-1.737097768181
C	7.738836926694	2.178396453460	-1.518275628708
C	7.795128212936	3.215436152784	-0.587627701423
H	6.966610736910	3.902366782141	-0.421685070400
C	8.988633781814	3.343881282273	0.142558786657
C	10.085986931851	2.462056422681	-0.055036851821
H	10.989194574442	2.601566206123	0.539790052498
C	10.015882611412	1.439943331720	-0.991852741465
H	10.856674909466	0.763828536842	-1.154045906062
C	9.103023325912	4.392906311097	1.114760017062
N	9.201707707792	5.243370784028	1.905826652319
N	6.757107861123	1.767612484820	-2.409633264316
C	5.436453840878	2.356883832553	-2.641481976350
H	5.516215064666	3.433282315597	-2.429118210389
H	5.227736922519	2.257080176079	-3.717047751999
C	7.301327087353	0.711266037950	-3.099213599451
H	6.736407733357	0.212656356872	-3.885365474701
N	8.525371394318	0.388724139573	-2.734749846896
C	1.979494671698	2.521850668157	-0.003077597994
H	1.062799549498	2.275392215557	0.555595560569
H	2.174815407948	3.597447780247	0.154858230581
C	1.717760048456	2.319712817055	-1.495143543264
C	2.996278304234	2.503530969096	-2.329937988437
H	3.215388375276	3.585467198626	-2.317292397039
H	2.778736740389	2.241893614036	-3.379145937835
C	4.256154378294	1.742775127288	-1.835358033265
C	4.160037547304	0.233986750402	-2.131965929888
H	4.040330389972	0.053205903629	-3.213122922931
H	3.299033924642	-0.223189696109	-1.629976962699
H	5.067024332436	-0.291298168227	-1.794428032249
C	4.436060009236	2.002084037523	-0.319746605561
H	4.696722485758	3.065357100468	-0.169584544285
H	5.282682383720	1.410064013587	0.063341462616
C	3.172846200010	1.701831434225	0.497737998440

H	3.356675917137	1.932983694795	1.558874093027
H	2.929822443879	0.627681498951	0.451272782474
O	1.211619245034	0.951707308223	-1.685976551870
C	0.123367677218	0.940987694244	-2.494017783653
N	-0.244408929381	2.239395956389	-2.777826374357
C	0.562185628805	3.199145164437	-2.028813562832
H	0.916745004318	4.007440726238	-2.680704911684
H	-0.027262105199	3.649355694548	-1.214345313924
O	-0.398551273630	-0.089334284732	-2.871039369243
C	-3.436082693637	3.514974095597	-4.991187184961
O	-4.457553785032	4.039975321087	-5.695782021951
C	-5.299273218053	3.129065244426	-6.437865571831
C	-6.351425275205	3.962354286101	-7.140218076707
H	-5.886442368968	4.682751557630	-7.831331941384
H	-6.962462543869	4.519926031703	-6.413171603213
H	-7.017507020959	3.305621946815	-7.720968974623
H	-5.747395058269	2.402866617738	-5.740253517897
H	-4.677505929028	2.564271283344	-7.151475080209
C	-2.612992978427	4.402881112235	-4.272163951605
H	-2.808345863129	5.478561425479	-4.291689142578
N	-1.584200772833	3.964230919269	-3.555276717156
C	-1.355347713034	2.639531661784	-3.541146529767
C	-2.178264690269	1.755209345497	-4.257416461924
H	-1.995214795668	0.682284638806	-4.240699778135
N	-3.215888283395	2.202476806561	-4.978982927125

SCF Done: E(RB3LYP) = -1484.53182743

Zero-point correction= 0.477981
Thermal correction to Energy= 0.506747
Thermal correction to Enthalpy= 0.507691
Thermal correction to Gibbs Free Energy= 0.415022
Sum of electronic and zero-point Energies= -1484.053846
Sum of electronic and thermal Energies= -1484.025080
Sum of electronic and thermal Enthalpies= -1484.024136
Sum of electronic and thermal Free Energies= -1484.116805

1	C	Isotropic =	45.9663	Anisotropy = 144.0544
2	C	Isotropic =	56.9237	Anisotropy = 141.0695
3	C	Isotropic =	76.6380	Anisotropy = 155.7804
4	H	Isotropic =	23.6454	Anisotropy = 11.0069
5	C	Isotropic =	87.1119	Anisotropy = 124.9702
6	C	Isotropic =	66.7726	Anisotropy = 165.7027
7	H	Isotropic =	23.8358	Anisotropy = 6.0219
8	C	Isotropic =	71.9762	Anisotropy = 156.9468
9	H	Isotropic =	23.6429	Anisotropy = 5.1046
10	C	Isotropic =	75.7129	Anisotropy = 316.0787
11	N	Isotropic =	-1.4734	Anisotropy = 371.6766
12	N	Isotropic =	93.5065	Anisotropy = 116.9980
13	C	Isotropic =	132.3201	Anisotropy = 42.9504
14	H	Isotropic =	27.6004	Anisotropy = 4.3414
15	H	Isotropic =	27.6514	Anisotropy = 4.8083
16	C	Isotropic =	45.4881	Anisotropy = 97.8926
17	H	Isotropic =	23.5818	Anisotropy = 7.8821
18	N	Isotropic =	6.4821	Anisotropy = 348.0107
19	C	Isotropic =	152.6672	Anisotropy = 15.3106

20	H	Isotropic =	29.4638	Anisotropy =	7.3548
21	H	Isotropic =	29.7434	Anisotropy =	7.4450
22	C	Isotropic =	108.3168	Anisotropy =	64.0477
23	C	Isotropic =	144.1065	Anisotropy =	30.7155
24	H	Isotropic =	29.9652	Anisotropy =	4.4867
25	H	Isotropic =	29.5340	Anisotropy =	5.7178
26	C	Isotropic =	149.7832	Anisotropy =	15.5262
27	C	Isotropic =	169.6438	Anisotropy =	26.2191
28	H	Isotropic =	30.5098	Anisotropy =	8.5219
29	H	Isotropic =	29.2573	Anisotropy =	6.7390
30	H	Isotropic =	30.7938	Anisotropy =	7.5920
31	C	Isotropic =	153.7134	Anisotropy =	16.5657
32	H	Isotropic =	29.8658	Anisotropy =	8.7791
33	H	Isotropic =	30.1307	Anisotropy =	8.1279
34	C	Isotropic =	169.8607	Anisotropy =	13.1933
35	H	Isotropic =	29.7582	Anisotropy =	10.7228
36	H	Isotropic =	29.5852	Anisotropy =	6.3256
37	O	Isotropic =	135.7610	Anisotropy =	104.9760
38	C	Isotropic =	42.3576	Anisotropy =	82.4387
39	N	Isotropic =	137.1202	Anisotropy =	98.8502
40	C	Isotropic =	134.3084	Anisotropy =	37.7097
41	H	Isotropic =	27.6001	Anisotropy =	4.8686
42	H	Isotropic =	27.8127	Anisotropy =	5.6290
43	O	Isotropic =	60.4942	Anisotropy =	381.4804
44	C	Isotropic =	36.4842	Anisotropy =	120.7256
45	O	Isotropic =	196.3712	Anisotropy =	79.4166
46	C	Isotropic =	127.9560	Anisotropy =	54.1712
47	C	Isotropic =	176.3305	Anisotropy =	21.7401
48	H	Isotropic =	29.9038	Anisotropy =	7.7506
49	H	Isotropic =	29.8954	Anisotropy =	7.8537
50	H	Isotropic =	30.0322	Anisotropy =	9.4380
51	H	Isotropic =	27.2460	Anisotropy =	6.0213
52	H	Isotropic =	27.2441	Anisotropy =	5.9586
53	C	Isotropic =	62.9336	Anisotropy =	126.3755
54	H	Isotropic =	23.4872	Anisotropy =	7.4141
55	N	Isotropic =	-52.5837	Anisotropy =	483.3824
56	C	Isotropic =	50.2092	Anisotropy =	127.2419
57	C	Isotropic =	61.9383	Anisotropy =	141.8478
58	H	Isotropic =	22.2496	Anisotropy =	12.1513
59	N	Isotropic =	-34.9492	Anisotropy =	472.6179

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.060074958073	1.640900222732	-5.845003135553
C	0.264073476430	1.467344281731	-6.334991314024
C	0.622264034567	0.389008053543	-7.143681106809
H	1.631737167483	0.251364467841	-7.529010438983
C	-0.391822129923	-0.534345682631	-7.448269216680
C	-1.716973254541	-0.380897012850	-6.956830411393
H	-2.466968035001	-1.127644465410	-7.219286127334
C	-2.057326388489	0.702044079546	-6.157746624093
H	-3.073592758855	0.829423556484	-5.781795395744

C	-0.081317057444	-1.664107225455	-8.276615577326
N	0.166138923864	-2.583640693059	-8.948929730039
N	0.976792045877	2.556293485713	-5.852010028964
C	2.381458479606	2.896690805253	-6.096655492288
H	2.658479204330	2.455867512149	-7.065206790493
H	2.433377347946	3.988961179077	-6.215640225312
C	0.071759256289	3.304199412342	-5.138371113610
H	0.371097840317	4.239002361949	-4.667138452154
N	-1.145716066682	2.802492441636	-5.098456285545
C	5.552387521412	3.556294712147	-3.214162551170
H	6.333900012948	3.450386298069	-2.444407381599
H	5.488081936573	4.630669964569	-3.460386216341
C	4.201135111464	3.139719215838	-2.621153815353
C	3.087913397684	3.160537471988	-3.675949546350
H	2.892273265348	4.227785762379	-3.881846446695
H	2.171995914465	2.750129495111	-3.221719725326
C	3.400840727518	2.441752953270	-5.015563169686
C	3.347627914347	0.909774073135	-4.862715292904
H	2.355656274796	0.578432047652	-4.517913694002
H	4.080360139882	0.550914306778	-4.129613417030
H	3.558627304067	0.418565066879	-5.826563275046
C	4.793228192951	2.892603851651	-5.527904189374
H	4.732083273822	3.950735253347	-5.842623918436
H	5.054071430820	2.313028769506	-6.429167832524
C	5.900018507712	2.761523461213	-4.475148517056
H	6.851038860077	3.129232272490	-4.891769882695
H	6.062348848898	1.703085535543	-4.214871699111
O	4.338820809358	1.774050788289	-2.092682670977
C	4.399058731959	1.778691663167	-0.738404944717
N	4.176055287943	3.059249415013	-0.278027280809
C	3.830622476743	3.967586499719	-1.368138199822
H	2.759670362634	4.223494463970	-1.334312801628
H	4.406781112758	4.899277130460	-1.301814133751
O	4.616378005650	0.773041501584	-0.092371315231
C	3.932046409938	4.314603145636	3.605067795856
O	3.821253575010	4.826970008793	4.846325007790
C	4.123821694671	3.956719590405	5.959983657151
C	3.907186477417	4.757579467288	7.227279776181
H	4.569246885418	5.637205740398	7.256145828347
H	4.127469698449	4.129608529334	8.104418334163
H	2.864015358375	5.102746855124	7.301545467386
H	5.163913998920	3.603371935480	5.868866331128
H	3.467483083514	3.072415711345	5.914835488446
C	3.631292567284	5.158604865192	2.518732994971
H	3.321084699839	6.193045164631	2.689992502555
N	3.713779685199	4.726944114635	1.264962450317
C	4.096872362182	3.453315233716	1.069421546106
C	4.398996169532	2.613687114992	2.153873972106
H	4.706750406767	1.581886755176	1.994253963777
N	4.313064377960	3.053317013497	3.417354267696

SCF Done: E(RB3LYP) = -1484.53215698

Zero-point correction= 0.478218
Thermal correction to Energy= 0.506890
Thermal correction to Enthalpy= 0.507834

Thermal correction to Gibbs Free Energy= 0.416018
Sum of electronic and zero-point Energies= -1484.053939
Sum of electronic and thermal Energies= -1484.025267
Sum of electronic and thermal Enthalpies= -1484.024323
Sum of electronic and thermal Free Energies= -1484.116139

1	C	Isotropic =	46.5213	Anisotropy =	144.8910
2	C	Isotropic =	56.9895	Anisotropy =	141.2571
3	C	Isotropic =	76.1898	Anisotropy =	157.0761
4	H	Isotropic =	23.6204	Anisotropy =	10.8811
5	C	Isotropic =	86.7673	Anisotropy =	125.3633
6	C	Isotropic =	66.8810	Anisotropy =	165.0757
7	H	Isotropic =	23.8816	Anisotropy =	5.8224
8	C	Isotropic =	72.5608	Anisotropy =	156.1107
9	H	Isotropic =	23.6904	Anisotropy =	5.2138
10	C	Isotropic =	75.7089	Anisotropy =	316.4691
11	N	Isotropic =	-1.4702	Anisotropy =	371.6956
12	N	Isotropic =	93.6500	Anisotropy =	118.9568
13	C	Isotropic =	132.0583	Anisotropy =	41.8865
14	H	Isotropic =	27.4433	Anisotropy =	4.8410
15	H	Isotropic =	27.5898	Anisotropy =	4.9519
16	C	Isotropic =	46.1480	Anisotropy =	98.9987
17	H	Isotropic =	23.5610	Anisotropy =	7.2318
18	N	Isotropic =	6.1771	Anisotropy =	348.8391
19	C	Isotropic =	151.7449	Anisotropy =	15.3945
20	H	Isotropic =	29.3941	Anisotropy =	6.4583
21	H	Isotropic =	29.9559	Anisotropy =	7.5416
22	C	Isotropic =	109.0425	Anisotropy =	63.9007
23	C	Isotropic =	145.6425	Anisotropy =	23.7107
24	H	Isotropic =	29.6714	Anisotropy =	4.9375
25	H	Isotropic =	29.7305	Anisotropy =	6.6598
26	C	Isotropic =	149.4741	Anisotropy =	14.3675
27	C	Isotropic =	168.5565	Anisotropy =	32.5087
28	H	Isotropic =	30.8603	Anisotropy =	6.0274
29	H	Isotropic =	29.3488	Anisotropy =	7.0624
30	H	Isotropic =	30.5775	Anisotropy =	10.1832
31	C	Isotropic =	153.4780	Anisotropy =	18.8497
32	H	Isotropic =	29.9719	Anisotropy =	6.9536
33	H	Isotropic =	29.7242	Anisotropy =	7.7043
34	C	Isotropic =	170.6621	Anisotropy =	12.9340
35	H	Isotropic =	29.7200	Anisotropy =	11.3858
36	H	Isotropic =	29.3514	Anisotropy =	6.4360
37	O	Isotropic =	138.0515	Anisotropy =	115.9566
38	C	Isotropic =	42.2466	Anisotropy =	82.3285
39	N	Isotropic =	137.8653	Anisotropy =	97.7539
40	C	Isotropic =	134.8030	Anisotropy =	38.2894
41	H	Isotropic =	27.8572	Anisotropy =	5.0739
42	H	Isotropic =	27.6169	Anisotropy =	5.3806
43	O	Isotropic =	60.2379	Anisotropy =	382.0304
44	C	Isotropic =	36.6631	Anisotropy =	121.0123
45	O	Isotropic =	196.4247	Anisotropy =	79.5021
46	C	Isotropic =	127.8649	Anisotropy =	54.1633
47	C	Isotropic =	176.5122	Anisotropy =	21.7091
48	H	Isotropic =	29.9055	Anisotropy =	7.8409
49	H	Isotropic =	30.0568	Anisotropy =	9.4776
50	H	Isotropic =	29.9328	Anisotropy =	7.7682

51	H	Isotropic =	27.2822	Anisotropy =	6.0577
52	H	Isotropic =	27.2759	Anisotropy =	5.8513
53	C	Isotropic =	63.0965	Anisotropy =	125.9243
54	H	Isotropic =	23.5022	Anisotropy =	7.4348
55	N	Isotropic =	-52.8046	Anisotropy =	483.8385
56	C	Isotropic =	50.0841	Anisotropy =	127.0978
57	C	Isotropic =	61.8331	Anisotropy =	142.2200
58	H	Isotropic =	22.3349	Anisotropy =	12.3939
59	N	Isotropic =	-34.6893	Anisotropy =	472.4171

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	8.232614466279	0.636656083268	-5.230299640729
C	6.883802026796	0.432121800736	-4.826972434936
C	6.408933722881	-0.815181835641	-4.422722634557
H	5.376511226031	-0.981445310166	-4.117389255810
C	7.334876941431	-1.871937876978	-4.422876291820
C	8.688581299427	-1.681452024251	-4.813223725861
H	9.368655119001	-2.533586163709	-4.792642059400
C	9.142663259557	-0.433576210980	-5.217919753108
H	10.178828338322	-0.281632920739	-5.523900991946
C	6.903733292497	-3.178859777199	-4.016772742726
N	6.558835770739	-4.242716811124	-3.688037820172
N	6.271986755495	1.670620782248	-4.961870353657
C	4.868242001735	2.015187209540	-4.725324571733
H	4.570759889997	2.717500369909	-5.517925746725
H	4.279010709130	1.098029465563	-4.871645382498
C	7.245896881184	2.515942690673	-5.435438405958
H	7.018850163267	3.558414124050	-5.652711832232
N	8.425421616492	1.954339155972	-5.605556365432
C	3.226912335117	5.054725501581	-2.102822549907
H	2.840132413504	5.623358266104	-1.241702969815
H	3.020701803516	5.657895663859	-3.004275961396
C	2.439531657787	3.745883413905	-2.236057962782
C	3.003584026306	2.854585692319	-3.347037926668
H	2.721670611743	3.340112507946	-4.298389429040
H	2.479625135527	1.884991543878	-3.322150862039
C	4.540444568910	2.631307775426	-3.335958692351
C	4.958156151504	1.653772334701	-2.220766147901
H	6.040367176320	1.454578101234	-2.260884597534
H	4.427588836925	0.692816676678	-2.320500403874
H	4.723061900165	2.051073055529	-1.225598092522
C	5.256245396975	3.995134902852	-3.170590782313
H	5.110743213952	4.588530201378	-4.092002738586
H	6.341297872548	3.835378297360	-3.063796484863
C	4.733548991856	4.812568803519	-1.981735043159
H	5.259928308409	5.779136804101	-1.939277760079
H	4.951884070611	4.296442644933	-1.032761210376
O	2.528311370665	3.029257150237	-0.954372990107
C	1.361958810653	3.109899459401	-0.268599089063
N	0.414649452837	3.731788204243	-1.054686200479
C	0.920726203205	3.987597474097	-2.400380845954

H	0.461239414220	3.296388755191	-3.124790621193
H	0.695744745199	5.013861127080	-2.717399680394
O	1.238146526618	2.677940731829	0.860133033605
C	-3.518641734203	4.410282091900	-0.170857798720
O	-4.827391062934	4.670576490715	0.015692882610
C	-5.384199736446	4.410533906065	1.323860184814
C	-6.853351219550	4.774822262136	1.265459222286
H	-6.985539155999	5.838257183921	1.011481131185
H	-7.320010548193	4.592411426339	2.245856915795
H	-7.380029493005	4.167617968111	0.512622501233
H	-4.840958882485	5.009674162134	2.072705742663
H	-5.232851048193	3.348074777993	1.574992820234
C	-2.978185942606	4.658314276037	-1.447292072024
H	-3.609609359199	5.049685802003	-2.249646565695
N	-1.697465786117	4.425650020141	-1.712624483823
C	-0.933203494493	3.945620269491	-0.716168989723
C	-1.473107312137	3.701406427165	0.557030907629
H	-0.853273863988	3.310981724777	1.362240487554
N	-2.766685835788	3.936093370518	0.819633132068

SCF Done: E(RB3LYP) = -1484.53230962

Zero-point correction= 0.478179
Thermal correction to Energy= 0.506883
Thermal correction to Enthalpy= 0.507827
Thermal correction to Gibbs Free Energy= 0.415964
Sum of electronic and zero-point Energies= -1484.054131
Sum of electronic and thermal Energies= -1484.025426
Sum of electronic and thermal Enthalpies= -1484.024482
Sum of electronic and thermal Free Energies= -1484.116346

1	C	Isotropic =	46.4134	Anisotropy =	144.7450
2	C	Isotropic =	57.0658	Anisotropy =	141.5478
3	C	Isotropic =	76.2520	Anisotropy =	157.3815
4	H	Isotropic =	23.6384	Anisotropy =	10.9487
5	C	Isotropic =	86.9212	Anisotropy =	125.1810
6	C	Isotropic =	66.8238	Anisotropy =	165.2468
7	H	Isotropic =	23.8584	Anisotropy =	5.9648
8	C	Isotropic =	72.2390	Anisotropy =	155.5141
9	H	Isotropic =	23.6677	Anisotropy =	5.0572
10	C	Isotropic =	75.7770	Anisotropy =	316.0742
11	N	Isotropic =	-1.7477	Anisotropy =	372.0137
12	N	Isotropic =	94.0143	Anisotropy =	118.4034
13	C	Isotropic =	132.3756	Anisotropy =	43.1410
14	H	Isotropic =	27.6855	Anisotropy =	4.9175
15	H	Isotropic =	27.4494	Anisotropy =	5.0239
16	C	Isotropic =	45.8958	Anisotropy =	99.1246
17	H	Isotropic =	23.5312	Anisotropy =	7.9480
18	N	Isotropic =	6.2634	Anisotropy =	349.5754
19	C	Isotropic =	151.3641	Anisotropy =	15.8356
20	H	Isotropic =	29.3972	Anisotropy =	6.4433
21	H	Isotropic =	29.9665	Anisotropy =	7.5600
22	C	Isotropic =	108.4346	Anisotropy =	63.3504
23	C	Isotropic =	144.8860	Anisotropy =	31.1208
24	H	Isotropic =	29.8007	Anisotropy =	4.5019
25	H	Isotropic =	29.5438	Anisotropy =	4.5141

26	C	Isotropic =	149.5395	Anisotropy =	15.8651
27	C	Isotropic =	168.9671	Anisotropy =	26.8153
28	H	Isotropic =	31.0399	Anisotropy =	7.4488
29	H	Isotropic =	30.4719	Anisotropy =	8.3713
30	H	Isotropic =	29.3974	Anisotropy =	7.1761
31	C	Isotropic =	154.7986	Anisotropy =	16.6934
32	H	Isotropic =	29.9209	Anisotropy =	7.6065
33	H	Isotropic =	29.8368	Anisotropy =	7.3724
34	C	Isotropic =	170.2454	Anisotropy =	13.4669
35	H	Isotropic =	29.7726	Anisotropy =	11.1671
36	H	Isotropic =	29.5499	Anisotropy =	6.0063
37	O	Isotropic =	137.6515	Anisotropy =	115.0091
38	C	Isotropic =	42.2502	Anisotropy =	82.3806
39	N	Isotropic =	137.8394	Anisotropy =	98.7921
40	C	Isotropic =	134.6686	Anisotropy =	37.9816
41	H	Isotropic =	27.8008	Anisotropy =	4.5763
42	H	Isotropic =	27.6058	Anisotropy =	5.3913
43	O	Isotropic =	60.4139	Anisotropy =	382.4065
44	C	Isotropic =	36.7080	Anisotropy =	121.0669
45	O	Isotropic =	196.4201	Anisotropy =	79.3056
46	C	Isotropic =	127.8411	Anisotropy =	54.2072
47	C	Isotropic =	176.3714	Anisotropy =	21.6629
48	H	Isotropic =	29.8989	Anisotropy =	7.8278
49	H	Isotropic =	30.0372	Anisotropy =	9.4283
50	H	Isotropic =	29.9144	Anisotropy =	7.7708
51	H	Isotropic =	27.2531	Anisotropy =	5.9843
52	H	Isotropic =	27.2477	Anisotropy =	5.9626
53	C	Isotropic =	62.9064	Anisotropy =	126.3181
54	H	Isotropic =	23.4875	Anisotropy =	7.4171
55	N	Isotropic =	-52.7182	Anisotropy =	483.4715
56	C	Isotropic =	50.0189	Anisotropy =	127.2835
57	C	Isotropic =	61.7890	Anisotropy =	141.9931
58	H	Isotropic =	22.2610	Anisotropy =	12.2292
59	N	Isotropic =	-34.7518	Anisotropy =	472.5508

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.630556373928	3.042846723571	1.557086939515
C	-1.115587778635	2.428088377819	0.369623681828
C	-2.432761224166	2.580356663083	-0.062606796327
H	-2.814827816190	2.105477100285	-0.965407638545
C	-3.266032162227	3.388534938347	0.728833804407
C	-2.792325555638	4.021490590766	1.910357087293
H	-3.478027835935	4.642462480253	2.487634509857
C	-1.479852899845	3.852358109189	2.329947191415
H	-1.111928969017	4.329492566467	3.239516577834
C	-4.631812399218	3.581628407719	0.333533860523
N	-5.742157201156	3.741774251924	0.016916410893
N	-0.039223696042	1.711870155320	-0.136386444903
C	-0.011756282532	0.839772630431	-1.313276141401
H	0.648843272313	-0.005808278305	-1.070489588261
H	-1.024232121770	0.428483828235	-1.434959262405

C	0.988916264349	1.911921701364	0.753728085801
H	1.953890119893	1.429483540216	0.605050617386
N	0.692627214123	2.698029633900	1.768294766754
C	1.502619617783	3.927270385694	-4.065132160336
H	1.882346193513	4.435500719392	-4.965464715066
H	1.535524298869	4.662103477769	-3.241297685209
C	2.455738371706	2.790072597191	-3.700735589511
C	1.913413346531	1.948269477451	-2.532749956888
H	1.997547587725	2.593212365244	-1.642455901520
H	2.584852262770	1.088825341334	-2.366372574464
C	0.445982651280	1.469840698613	-2.661586003688
C	0.304932822491	0.330171834617	-3.693040070143
H	-0.735340230706	-0.033353557892	-3.723599243186
H	0.953232740543	-0.521126200773	-3.427680909993
H	0.587244014779	0.653424228372	-4.701423636939
C	-0.448816075578	2.672154363292	-3.043390034936
H	-0.493638538918	3.372725664462	-2.192053327231
H	-1.478945111815	2.321855984965	-3.223532704879
C	0.063975237360	3.440602068164	-4.269705049655
H	-0.590652187650	4.305146954306	-4.462724099743
H	0.014570821793	2.806520767756	-5.170110383083
O	2.611786124140	1.930588519903	-4.884655468518
C	3.914625518676	1.621175934063	-5.093942410331
N	4.697502879325	2.329213393957	-4.206247392130
C	3.899368751643	3.272851300075	-3.427781262492
H	4.163505136659	3.226548903116	-2.363878042528
H	4.065948478677	4.304155649280	-3.777864475696
O	4.268785636000	0.834739599174	-5.949684384063
C	8.774447602866	2.327573778110	-3.907682814056
O	10.107832336763	2.402743158927	-3.728581758255
C	10.937853260293	1.485013404758	-4.475422797428
C	12.375182370673	1.760238340414	-4.084478000330
H	13.045062278877	1.080406250890	-4.633424706080
H	12.527294904283	1.599943024670	-3.005589519415
H	12.658464457184	2.796399581552	-4.327385439420
H	10.767273303385	1.640755228617	-5.553178266529
H	10.637445693157	0.451633782255	-4.237291753810
C	7.964754045710	3.217603102052	-3.176114646841
H	8.415427407243	3.941297742664	-2.491425713901
N	6.641557079382	3.204529977635	-3.294475245145
C	6.101652875872	2.308461274968	-4.138703173272
C	6.910752521662	1.422928606427	-4.869205157115
H	6.472087830299	0.701723606910	-5.556489553272
N	8.245617130377	1.440275249041	-4.747011634565

SCF Done: E(RB3LYP) = -1484.53191092

Zero-point correction= 0.478153
Thermal correction to Energy= 0.506857
Thermal correction to Enthalpy= 0.507801
Thermal correction to Gibbs Free Energy= 0.415931
Sum of electronic and zero-point Energies= -1484.053758
Sum of electronic and thermal Energies= -1484.025054
Sum of electronic and thermal Enthalpies= -1484.024110
Sum of electronic and thermal Free Energies= -1484.115980

1	C	Isotropic =	46.3097	Anisotropy =	144.4818
2	C	Isotropic =	56.6727	Anisotropy =	142.2633
3	C	Isotropic =	75.9083	Anisotropy =	157.9378
4	H	Isotropic =	23.6774	Anisotropy =	10.9817
5	C	Isotropic =	86.7951	Anisotropy =	125.3211
6	C	Isotropic =	66.7765	Anisotropy =	165.0932
7	H	Isotropic =	23.8722	Anisotropy =	5.8767
8	C	Isotropic =	72.3172	Anisotropy =	156.1086
9	H	Isotropic =	23.6805	Anisotropy =	5.1824
10	C	Isotropic =	75.7408	Anisotropy =	316.4041
11	N	Isotropic =	-1.6052	Anisotropy =	371.8742
12	N	Isotropic =	93.2543	Anisotropy =	119.5145
13	C	Isotropic =	134.1776	Anisotropy =	44.6715
14	H	Isotropic =	27.6216	Anisotropy =	5.2878
15	H	Isotropic =	27.5448	Anisotropy =	4.4341
16	C	Isotropic =	45.6633	Anisotropy =	98.2318
17	H	Isotropic =	23.6575	Anisotropy =	7.1237
18	N	Isotropic =	5.7846	Anisotropy =	348.8713
19	C	Isotropic =	153.8807	Anisotropy =	14.5359
20	H	Isotropic =	29.6104	Anisotropy =	7.7363
21	H	Isotropic =	30.2016	Anisotropy =	6.3216
22	C	Isotropic =	108.0237	Anisotropy =	63.9113
23	C	Isotropic =	146.6750	Anisotropy =	21.7466
24	H	Isotropic =	30.0247	Anisotropy =	8.2019
25	H	Isotropic =	29.6234	Anisotropy =	5.8055
26	C	Isotropic =	149.5233	Anisotropy =	16.1202
27	C	Isotropic =	166.3134	Anisotropy =	35.1866
28	H	Isotropic =	30.5215	Anisotropy =	9.7577
29	H	Isotropic =	30.4680	Anisotropy =	8.1964
30	H	Isotropic =	29.1065	Anisotropy =	6.4905
31	C	Isotropic =	156.2750	Anisotropy =	7.1167
32	H	Isotropic =	30.3478	Anisotropy =	10.3900
33	H	Isotropic =	29.8269	Anisotropy =	8.3598
34	C	Isotropic =	169.8795	Anisotropy =	13.9309
35	H	Isotropic =	29.8067	Anisotropy =	10.9044
36	H	Isotropic =	29.3448	Anisotropy =	7.0607
37	O	Isotropic =	136.4185	Anisotropy =	107.1905
38	C	Isotropic =	42.3768	Anisotropy =	82.4602
39	N	Isotropic =	137.0323	Anisotropy =	99.5799
40	C	Isotropic =	134.4921	Anisotropy =	37.6853
41	H	Isotropic =	27.7073	Anisotropy =	4.6609
42	H	Isotropic =	27.9316	Anisotropy =	5.4050
43	O	Isotropic =	60.6614	Anisotropy =	381.9977
44	C	Isotropic =	36.5465	Anisotropy =	121.0211
45	O	Isotropic =	196.3265	Anisotropy =	79.5720
46	C	Isotropic =	127.8063	Anisotropy =	54.1003
47	C	Isotropic =	176.4169	Anisotropy =	21.5586
48	H	Isotropic =	30.0433	Anisotropy =	9.4698
49	H	Isotropic =	29.9154	Anisotropy =	7.7146
50	H	Isotropic =	29.9043	Anisotropy =	7.8707
51	H	Isotropic =	27.2577	Anisotropy =	6.0821
52	H	Isotropic =	27.2261	Anisotropy =	5.8304
53	C	Isotropic =	63.0840	Anisotropy =	126.1460
54	H	Isotropic =	23.5258	Anisotropy =	7.4401
55	N	Isotropic =	-52.5203	Anisotropy =	483.9089
56	C	Isotropic =	50.2314	Anisotropy =	127.3480

57	C	Isotropic =	61.8867	Anisotropy =	141.8214
58	H	Isotropic =	22.2305	Anisotropy =	12.2212
59	N	Isotropic =	-34.9606	Anisotropy =	471.8679

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	7.179071249902	1.989263362642	-4.870725532219
C	6.039141886368	1.154024373930	-4.703642584263
C	5.909458708756	0.284028075347	-3.621202470804
H	5.050950690986	-0.373641031062	-3.491633743760
C	6.955742524749	0.282541794165	-2.683356784933
C	8.092675959107	1.123343778038	-2.828221850036
H	8.876138657739	1.087639864614	-2.070622272158
C	8.211238793006	1.975145303946	-3.917879786209
H	9.084607759565	2.617470998645	-4.040359748755
C	6.875264244378	-0.592452849885	-1.549051697654
N	6.815411783821	-1.301369558601	-0.625664136584
N	5.235580452049	1.411056196626	-5.806373941866
C	3.950388615535	0.799900909420	-6.157483650486
H	3.934525281409	0.693453221518	-7.252135351859
H	3.944960259559	-0.216361399386	-5.737328131025
C	5.919522725374	2.338117595906	-6.555145987626
H	5.513072272451	2.698477372672	-7.498831984001
N	7.071912250015	2.717368865058	-6.041928670518
C	0.110818289185	1.193625394136	-4.163800758166
H	-0.848234889005	1.559410833004	-3.762568859945
H	0.229059418323	0.153354001027	-3.813092451939
C	1.255981256789	2.014221728505	-3.558627440428
C	2.610206114140	1.624790817666	-4.163444596790
H	2.832277657017	0.620765483196	-3.762816779285
H	3.381586409551	2.304504567101	-3.767994114364
C	2.674799495200	1.568405129290	-5.711928276465
C	2.680820464654	2.977977877203	-6.334362045580
H	2.792479051784	2.915460302903	-7.429417685561
H	3.507873177313	3.587822342298	-5.938827620569
H	1.752589850136	3.520180185733	-6.116833990829
C	1.472554224737	0.745978536678	-6.244773038299
H	1.613389785392	-0.314172905898	-5.964575412785
H	1.467347186440	0.779876180819	-7.347086617986
C	0.122194999470	1.221863785988	-5.694866269420
H	-0.681956320176	0.575625318898	-6.080761330538
H	-0.100335128748	2.241353774873	-6.049277892741
O	0.994215923153	3.434827660263	-3.832895486141
C	0.590659084592	4.083015887217	-2.712963703147
N	0.674594931718	3.225834489272	-1.636219406595
C	1.273192110706	1.948346637008	-2.012900760039
H	2.293866766644	1.863985788216	-1.607276769553
H	0.682254309784	1.108171147428	-1.626326916267
O	0.226457882722	5.241984018810	-2.726172218075
C	-0.097933617145	4.053964914725	2.291960119597
O	-0.316466961288	4.224438449267	3.610549772580
C	-0.894145941084	5.478267838359	4.038354915617

C	-1.037806308181	5.414663008565	5.544982559370
H	-1.695655064621	4.583300730779	5.843219785327
H	-1.477111555670	6.353877085092	5.915295089688
H	-0.058164681571	5.276054153325	6.028674663545
H	-1.866308736403	5.616605700390	3.537705245739
H	-0.236710877331	6.304480769777	3.722149615133
C	0.462273095848	2.831490443217	1.874166423702
H	0.706654454372	2.055509357066	2.604754754763
N	0.708228960090	2.586664355192	0.591825588369
C	0.401790178200	3.549147880086	-0.295391491292
C	-0.158317593880	4.767169391022	0.122784904923
H	-0.403373062344	5.546909416011	-0.596188875142
N	-0.403768455282	5.010150651900	1.418175694344

SCF Done: E(RB3LYP) = -1484.53194928

Zero-point correction= 0.478131
Thermal correction to Energy= 0.506855
Thermal correction to Enthalpy= 0.507799
Thermal correction to Gibbs Free Energy= 0.415117
Sum of electronic and zero-point Energies= -1484.053818
Sum of electronic and thermal Energies= -1484.025095
Sum of electronic and thermal Enthalpies= -1484.024150
Sum of electronic and thermal Free Energies= -1484.116832

1	C	Isotropic =	46.2436	Anisotropy =	144.8210
2	C	Isotropic =	57.0894	Anisotropy =	141.9209
3	C	Isotropic =	75.8807	Anisotropy =	156.1277
4	H	Isotropic =	23.6537	Anisotropy =	10.2317
5	C	Isotropic =	86.9940	Anisotropy =	125.6113
6	C	Isotropic =	66.6439	Anisotropy =	165.1565
7	H	Isotropic =	23.8974	Anisotropy =	5.9378
8	C	Isotropic =	72.4372	Anisotropy =	157.6915
9	H	Isotropic =	23.6467	Anisotropy =	4.9199
10	C	Isotropic =	75.6761	Anisotropy =	315.9996
11	N	Isotropic =	-1.4498	Anisotropy =	371.3952
12	N	Isotropic =	93.4586	Anisotropy =	118.2739
13	C	Isotropic =	131.5896	Anisotropy =	42.6181
14	H	Isotropic =	27.6127	Anisotropy =	5.8866
15	H	Isotropic =	27.4767	Anisotropy =	3.5512
16	C	Isotropic =	45.2858	Anisotropy =	99.0380
17	H	Isotropic =	23.5531	Anisotropy =	7.7066
18	N	Isotropic =	6.9431	Anisotropy =	350.3047
19	C	Isotropic =	151.5707	Anisotropy =	16.1479
20	H	Isotropic =	29.4349	Anisotropy =	6.4814
21	H	Isotropic =	29.9575	Anisotropy =	7.3123
22	C	Isotropic =	109.2196	Anisotropy =	64.3378
23	C	Isotropic =	144.5597	Anisotropy =	22.1538
24	H	Isotropic =	29.6383	Anisotropy =	6.7581
25	H	Isotropic =	30.0469	Anisotropy =	7.7554
26	C	Isotropic =	149.6037	Anisotropy =	14.9170
27	C	Isotropic =	168.8544	Anisotropy =	32.3000
28	H	Isotropic =	30.5721	Anisotropy =	10.3962
29	H	Isotropic =	30.5598	Anisotropy =	5.8105
30	H	Isotropic =	29.2434	Anisotropy =	6.4088
31	C	Isotropic =	154.0813	Anisotropy =	18.0187

32	H	Isotropic =	29.9413	Anisotropy =	6.8515
33	H	Isotropic =	29.8068	Anisotropy =	7.8549
34	C	Isotropic =	170.4881	Anisotropy =	12.9473
35	H	Isotropic =	29.6893	Anisotropy =	11.4236
36	H	Isotropic =	29.3104	Anisotropy =	6.8689
37	O	Isotropic =	138.8511	Anisotropy =	115.4758
38	C	Isotropic =	42.4121	Anisotropy =	82.7656
39	N	Isotropic =	137.8828	Anisotropy =	97.6353
40	C	Isotropic =	134.5489	Anisotropy =	38.1561
41	H	Isotropic =	28.0373	Anisotropy =	6.6382
42	H	Isotropic =	27.6720	Anisotropy =	5.0371
43	O	Isotropic =	60.3686	Anisotropy =	381.0202
44	C	Isotropic =	36.7561	Anisotropy =	120.8569
45	O	Isotropic =	196.4651	Anisotropy =	79.0989
46	C	Isotropic =	127.9380	Anisotropy =	54.3637
47	C	Isotropic =	176.3645	Anisotropy =	21.7508
48	H	Isotropic =	29.9355	Anisotropy =	7.7946
49	H	Isotropic =	30.0600	Anisotropy =	9.5478
50	H	Isotropic =	29.9358	Anisotropy =	7.7155
51	H	Isotropic =	27.2905	Anisotropy =	6.0937
52	H	Isotropic =	27.3034	Anisotropy =	5.9162
53	C	Isotropic =	62.9390	Anisotropy =	126.4359
54	H	Isotropic =	23.5403	Anisotropy =	7.7085
55	N	Isotropic =	-52.5060	Anisotropy =	483.8617
56	C	Isotropic =	50.1361	Anisotropy =	127.0097
57	C	Isotropic =	62.0081	Anisotropy =	141.8101
58	H	Isotropic =	22.3659	Anisotropy =	12.3260
59	N	Isotropic =	-34.8454	Anisotropy =	472.1623

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.082870881022	-1.973113434880	-0.619303063050
C	-0.044717336025	-1.615015146774	-1.990006611060
C	-1.259556703647	-1.695541573702	-2.670159125093
H	-1.364159404376	-1.431841813906	-3.721843176175
C	-2.367899179622	-2.139369480212	-1.929533053804
C	-2.259494478714	-2.487922388075	-0.555562017093
H	-3.150590735927	-2.823275309045	-0.024033291409
C	-1.040334323381	-2.408457064676	0.103654423462
H	-0.948637618159	-2.681050662956	1.156083484564
C	-3.644442424065	-2.242660797585	-2.576588488642
N	-4.683791503348	-2.328395271213	-3.097306080823
N	1.231553587549	-1.243203869680	-2.390170352109
C	1.680025436256	-0.851883182216	-3.728707217152
H	2.692678779975	-1.261290070428	-3.858577783849
H	1.032441095133	-1.367712742834	-4.452472148874
C	2.029691837240	-1.412033436916	-1.283842279708
H	3.099458615915	-1.214523520995	-1.336505078915
N	1.396817208210	-1.833897797255	-0.208490601418
C	1.236050625821	3.461923106833	-3.027770140152
H	1.255667656489	4.558660345365	-3.133546713703
H	0.879732390857	3.244294436174	-2.005717816335

C	2.666352955781	2.920087305290	-3.138821727161
C	2.693488843991	1.387944255954	-3.108252481593
H	2.455441585210	1.113237149886	-2.066822991232
H	3.723719495427	1.045352352503	-3.300919490721
C	1.702562070127	0.668971967034	-4.058777960617
C	2.177202595128	0.745410408303	-5.525847908861
H	3.176955964419	0.294747330243	-5.638547659968
H	2.244409695379	1.780592976125	-5.880162747987
H	1.483088795121	0.197786122049	-6.184305394340
C	0.293984309493	1.290266611408	-3.905883023020
H	-0.105901984289	1.036004678814	-2.909303498177
H	-0.387182087668	0.840642222179	-4.647678463965
C	0.291311028745	2.818629137164	-4.046759446989
H	-0.730041407717	3.201778477717	-3.894243266368
H	0.586715488573	3.114384793997	-5.066569151689
O	3.233152712595	3.390184801560	-4.412573908832
C	4.128949723538	4.386925846692	-4.209479163310
N	4.322757043687	4.554777149878	-2.854346195808
C	3.611778161866	3.539233793571	-2.082900432165
H	4.318258904143	2.802735081960	-1.668052959230
H	3.061445623480	3.991960313700	-1.248306136309
O	4.646113189057	4.995495401974	-5.125009278161
C	6.917183921333	7.107642876508	-0.993107900474
O	7.743451147547	7.900665785047	-0.283269841346
C	8.477962394790	8.917895673118	-1.000510450360
C	9.321060602210	9.661577085484	0.014801305559
H	10.028553139291	8.980844009328	0.513697976394
H	8.687837658915	10.132094976905	0.783239743245
H	9.898077751016	10.451805399092	-0.490010613505
H	7.764200969376	9.585185083053	-1.510532884015
H	9.096056999012	8.437075591023	-1.776098621665
C	6.196216331803	6.121235035310	-0.293104595631
H	6.312016000081	6.013458400312	0.788849141202
N	5.361777707343	5.299755291168	-0.920471542737
C	5.228684613490	5.444436214020	-2.250418511773
C	5.946938320277	6.430020723961	-2.946739718702
H	5.840354235244	6.544331674888	-4.024029934240
N	6.788831094987	7.256167677754	-2.309503134109

SCF Done: E(RB3LYP) = -1484.53202918

Zero-point correction= 0.477920
Thermal correction to Energy= 0.506729
Thermal correction to Enthalpy= 0.507674
Thermal correction to Gibbs Free Energy= 0.415314
Sum of electronic and zero-point Energies= -1484.054109
Sum of electronic and thermal Energies= -1484.025300
Sum of electronic and thermal Enthalpies= -1484.024356
Sum of electronic and thermal Free Energies= -1484.116715

1	C	Isotropic =	46.2170	Anisotropy =	144.3136
2	C	Isotropic =	56.6943	Anisotropy =	142.2787
3	C	Isotropic =	76.0887	Anisotropy =	157.4905
4	H	Isotropic =	23.6613	Anisotropy =	10.8961
5	C	Isotropic =	86.8372	Anisotropy =	125.3619
6	C	Isotropic =	66.7955	Anisotropy =	165.4751

7	H	Isotropic =	23.8536	Anisotropy =	5.8931
8	C	Isotropic =	72.2560	Anisotropy =	156.0797
9	H	Isotropic =	23.6709	Anisotropy =	5.1220
10	C	Isotropic =	75.7956	Anisotropy =	316.2509
11	N	Isotropic =	-1.7193	Anisotropy =	372.1087
12	N	Isotropic =	93.2421	Anisotropy =	119.6471
13	C	Isotropic =	134.1208	Anisotropy =	45.0653
14	H	Isotropic =	27.5866	Anisotropy =	5.4097
15	H	Isotropic =	27.5091	Anisotropy =	4.3412
16	C	Isotropic =	45.4744	Anisotropy =	98.7055
17	H	Isotropic =	23.6046	Anisotropy =	7.3152
18	N	Isotropic =	5.6792	Anisotropy =	349.0443
19	C	Isotropic =	152.1360	Anisotropy =	14.9811
20	H	Isotropic =	29.5806	Anisotropy =	6.8233
21	H	Isotropic =	30.4618	Anisotropy =	6.0427
22	C	Isotropic =	108.4827	Anisotropy =	64.1856
23	C	Isotropic =	147.4735	Anisotropy =	22.1495
24	H	Isotropic =	29.7964	Anisotropy =	8.6123
25	H	Isotropic =	29.7001	Anisotropy =	5.0680
26	C	Isotropic =	149.0085	Anisotropy =	16.2477
27	C	Isotropic =	166.1015	Anisotropy =	36.3767
28	H	Isotropic =	30.4385	Anisotropy =	8.3328
29	H	Isotropic =	29.0361	Anisotropy =	6.7495
30	H	Isotropic =	30.4823	Anisotropy =	9.7333
31	C	Isotropic =	155.3888	Anisotropy =	6.3280
32	H	Isotropic =	30.3321	Anisotropy =	10.4423
33	H	Isotropic =	29.7849	Anisotropy =	8.1693
34	C	Isotropic =	170.2092	Anisotropy =	14.0468
35	H	Isotropic =	29.8865	Anisotropy =	10.8589
36	H	Isotropic =	29.3560	Anisotropy =	6.9365
37	O	Isotropic =	137.6989	Anisotropy =	116.1236
38	C	Isotropic =	42.2301	Anisotropy =	82.6323
39	N	Isotropic =	137.8168	Anisotropy =	97.3605
40	C	Isotropic =	134.5318	Anisotropy =	38.9447
41	H	Isotropic =	27.8948	Anisotropy =	5.1803
42	H	Isotropic =	27.8177	Anisotropy =	4.9448
43	O	Isotropic =	60.4112	Anisotropy =	382.1850
44	C	Isotropic =	36.6980	Anisotropy =	121.0751
45	O	Isotropic =	196.0652	Anisotropy =	79.3987
46	C	Isotropic =	127.7669	Anisotropy =	54.3484
47	C	Isotropic =	176.3812	Anisotropy =	21.6308
48	H	Isotropic =	29.9159	Anisotropy =	7.7638
49	H	Isotropic =	29.9206	Anisotropy =	7.7904
50	H	Isotropic =	30.0294	Anisotropy =	9.4974
51	H	Isotropic =	27.2623	Anisotropy =	6.0229
52	H	Isotropic =	27.2560	Anisotropy =	5.9562
53	C	Isotropic =	63.1175	Anisotropy =	126.5253
54	H	Isotropic =	23.5345	Anisotropy =	7.6337
55	N	Isotropic =	-52.2456	Anisotropy =	484.9881
56	C	Isotropic =	50.2544	Anisotropy =	127.4611
57	C	Isotropic =	61.8225	Anisotropy =	141.2739
58	H	Isotropic =	22.2851	Anisotropy =	12.2226
59	N	Isotropic =	-35.2476	Anisotropy =	470.6217

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	3.985004648176	2.017851557045	-7.711154491330
C	4.037535100817	2.151841187133	-6.295453152176
C	4.822974031089	3.121389583632	-5.672418656191
H	4.863266591361	3.243953587928	-4.591332185889
C	5.578876706632	3.957886345582	-6.510956705335
C	5.547126397584	3.826268090236	-7.925569373430
H	6.154665027654	4.498137976819	-8.532616956974
C	4.753170641464	2.861441729700	-8.530477837480
H	4.717198867776	2.758917830976	-9.616057686911
C	6.405007235461	4.972805238757	-5.922504682252
N	7.077932030247	5.798741907363	-5.449541197172
N	3.168342607326	1.185241824537	-5.806480260581
C	2.791517017183	0.909207494366	-4.416176418894
H	2.861692688034	1.862690390903	-3.876399297104
H	1.728159894614	0.629550079484	-4.429387541219
C	2.648060861266	0.560821542299	-6.915113947255
H	1.910862014410	-0.233518469764	-6.809258855790
N	3.103984446959	1.011438046277	-8.064941600649
C	4.569343632727	0.793185444455	-1.008813079627
H	5.082784613692	-0.113493682586	-0.647824536059
H	4.668919464232	1.558887611345	-0.222599699522
C	3.089226767511	0.440077552388	-1.201145202302
C	2.904920711339	-0.557001142356	-2.352324630571
H	1.829622539877	-0.741172549585	-2.510567952761
H	3.334031962445	-1.507207517407	-1.995953145137
C	3.601286246722	-0.213470381493	-3.699960046299
C	3.591343754146	-1.488731705889	-4.562743311225
H	4.112514815198	-1.335382866907	-5.519514061807
H	2.563234378813	-1.822958196720	-4.778616161469
H	4.104276295310	-2.306760487288	-4.034240554818
C	5.065085007099	0.209331708699	-3.424454458667
H	5.534923700494	0.558847798584	-4.358070383114
H	5.625368790267	-0.693140460788	-3.123579519296
C	5.212633270023	1.262405126976	-2.318661731001
H	4.764462864360	2.223479064948	-2.626688662385
H	6.279682096527	1.473943912210	-2.147904654698
O	2.641316079592	-0.257809298510	0.012659284202
C	1.913091535420	0.564185747596	0.805811038794
N	1.692060162547	1.753386589757	0.141967359668
C	2.171808102889	1.686570970741	-1.236385859933
H	1.323113685482	1.573478705248	-1.929086234801
H	2.711156073524	2.604398882270	-1.503006682058
O	1.542459668950	0.241963838112	1.916879693096
C	-0.521846187327	4.951252416498	1.401096665490
O	-1.234275694302	6.050187845684	1.717369359725
C	-1.751006249170	6.149187702703	3.063681947246
C	-2.492951732809	7.465891587316	3.164088875154
H	-1.819170420651	8.313836350772	2.964455209839
H	-2.904926633712	7.582358142477	4.178474275944
H	-3.326440975225	7.504897261297	2.445297312511
H	-0.912166231043	6.094107497050	3.776448671448
H	-2.410907063394	5.288458189230	3.260189913448

C	-0.014586709254	4.854120569645	0.091040637244
H	-0.200063123744	5.649864316904	-0.635559513879
N	0.697837401791	3.802211460705	-0.297564474280
C	0.919275905581	2.832572086615	0.606619424822
C	0.413647066411	2.931354165932	1.912896704701
H	0.590343399409	2.143322251256	2.642803340547
N	-0.306235779799	3.993807548842	2.300075688465

SCF Done: E(RB3LYP) = -1484.52800553

Zero-point correction= 0.478413
Thermal correction to Energy= 0.506995
Thermal correction to Enthalpy= 0.507939
Thermal correction to Gibbs Free Energy= 0.416852
Sum of electronic and zero-point Energies= -1484.049592
Sum of electronic and thermal Energies= -1484.021010
Sum of electronic and thermal Enthalpies= -1484.020066
Sum of electronic and thermal Free Energies= -1484.111154

1	C	Isotropic =	46.4949	Anisotropy =	143.9560
2	C	Isotropic =	57.1754	Anisotropy =	140.8943
3	C	Isotropic =	77.1700	Anisotropy =	155.3205
4	H	Isotropic =	23.6020	Anisotropy =	11.4037
5	C	Isotropic =	86.5837	Anisotropy =	125.0086
6	C	Isotropic =	66.7265	Anisotropy =	166.0017
7	H	Isotropic =	23.8206	Anisotropy =	6.0665
8	C	Isotropic =	71.9548	Anisotropy =	155.6981
9	H	Isotropic =	23.6522	Anisotropy =	4.8833
10	C	Isotropic =	75.8950	Anisotropy =	315.6605
11	N	Isotropic =	-2.0189	Anisotropy =	372.1890
12	N	Isotropic =	93.3369	Anisotropy =	114.0639
13	C	Isotropic =	139.9278	Anisotropy =	42.5953
14	H	Isotropic =	27.1862	Anisotropy =	7.5642
15	H	Isotropic =	27.6136	Anisotropy =	5.2478
16	C	Isotropic =	44.8351	Anisotropy =	98.1866
17	H	Isotropic =	23.5806	Anisotropy =	8.1007
18	N	Isotropic =	5.7935	Anisotropy =	348.9638
19	C	Isotropic =	153.0034	Anisotropy =	15.1449
20	H	Isotropic =	29.7882	Anisotropy =	7.8530
21	H	Isotropic =	29.3081	Anisotropy =	6.4286
22	C	Isotropic =	108.3881	Anisotropy =	70.1274
23	C	Isotropic =	141.6837	Anisotropy =	29.1590
24	H	Isotropic =	29.4593	Anisotropy =	4.0180
25	H	Isotropic =	29.4891	Anisotropy =	5.4933
26	C	Isotropic =	149.2872	Anisotropy =	11.4197
27	C	Isotropic =	161.7478	Anisotropy =	38.8277
28	H	Isotropic =	30.5332	Anisotropy =	6.7859
29	H	Isotropic =	30.1761	Anisotropy =	9.5384
30	H	Isotropic =	30.5404	Anisotropy =	9.2682
31	C	Isotropic =	157.0512	Anisotropy =	19.6360
32	H	Isotropic =	29.8921	Anisotropy =	6.2280
33	H	Isotropic =	30.2605	Anisotropy =	7.9371
34	C	Isotropic =	169.4897	Anisotropy =	15.6993
35	H	Isotropic =	29.2857	Anisotropy =	7.3505
36	H	Isotropic =	29.5087	Anisotropy =	10.8739
37	O	Isotropic =	124.5431	Anisotropy =	111.5310

38	C	Isotropic =	42.3296	Anisotropy =	81.7241
39	N	Isotropic =	136.3850	Anisotropy =	98.9060
40	C	Isotropic =	137.1311	Anisotropy =	33.8677
41	H	Isotropic =	27.7736	Anisotropy =	7.3975
42	H	Isotropic =	27.1563	Anisotropy =	5.6498
43	O	Isotropic =	61.2624	Anisotropy =	395.4980
44	C	Isotropic =	36.6986	Anisotropy =	121.3321
45	O	Isotropic =	196.2318	Anisotropy =	79.3468
46	C	Isotropic =	127.8362	Anisotropy =	54.5054
47	C	Isotropic =	176.4265	Anisotropy =	21.6126
48	H	Isotropic =	29.9113	Anisotropy =	7.7245
49	H	Isotropic =	30.0460	Anisotropy =	9.5712
50	H	Isotropic =	29.9147	Anisotropy =	7.7224
51	H	Isotropic =	27.2373	Anisotropy =	6.0124
52	H	Isotropic =	27.2567	Anisotropy =	6.1445
53	C	Isotropic =	63.0567	Anisotropy =	126.3355
54	H	Isotropic =	23.5112	Anisotropy =	8.2281
55	N	Isotropic =	-51.9113	Anisotropy =	483.3986
56	C	Isotropic =	50.1527	Anisotropy =	126.8342
57	C	Isotropic =	61.9678	Anisotropy =	141.9913
58	H	Isotropic =	22.2458	Anisotropy =	11.8381
59	N	Isotropic =	-35.0513	Anisotropy =	472.4133

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=100,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	7.554996650192	2.736035553231	-4.250846266608
C	6.708191784818	2.032051060188	-3.350333263082
C	5.804068817918	1.062218338446	-3.782859675011
H	5.157871225994	0.511873151692	-3.099838932292
C	5.757739549660	0.816380661037	-5.165500851039
C	6.588435957531	1.520251161006	-6.079351551413
H	6.511946853146	1.294825217829	-7.143463856140
C	7.487583002553	2.478005116331	-5.630149711757
H	8.132467104995	3.017233894098	-6.325622098693
C	4.847376882522	-0.171695257342	-5.669276040117
N	4.109864333725	-0.973484255207	-6.083938918283
N	7.030921167001	2.518585742500	-2.090509800277
C	6.501073266548	2.086091637869	-0.795154084496
H	6.200337124976	1.033851807694	-0.903626903039
H	7.338340395376	2.106207907097	-0.082058255632
C	8.030767874770	3.439353703919	-2.294668140157
H	8.489406858944	3.956488374022	-1.453245425947
N	8.371535159050	3.610124710618	-3.555521323623
C	3.465866318732	5.266168947926	-0.535065376352
H	2.615629711414	5.880433128464	-0.199011918439
H	3.823803313321	5.702275644269	-1.484574875141
C	2.965327335924	3.854853829162	-0.839756041390
C	4.123623895919	2.901120791571	-1.181213729223
H	4.482861640469	3.214243883631	-2.175192227167
H	3.721984767626	1.880027760951	-1.294523194256
C	5.320280072984	2.905755388770	-0.197748662948
C	4.978012174592	2.190942088068	1.126860374116

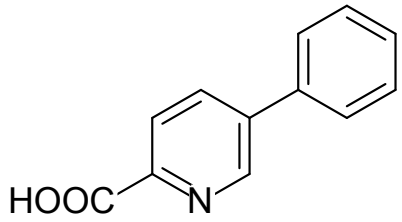
H	4.650034400158	1.155359619935	0.938872983611
H	4.170295866816	2.695776006907	1.669128893789
H	5.863392697388	2.151222307383	1.782583573013
C	5.756080734555	4.367100986719	0.064427158527
H	6.188605750261	4.786683023667	-0.860463069236
H	6.556142786410	4.381023869146	0.823681234324
C	4.596755456200	5.273732981017	0.498750123480
H	4.963550746085	6.303628724764	0.633003920556
H	4.203270693368	4.953589600591	1.477283187197
O	2.264562629208	3.355019845702	0.353140814128
C	1.077571521593	2.790685592461	0.023168945499
N	0.842271785917	2.981536692984	-1.322210430587
C	1.867425151758	3.826179761236	-1.929446875548
H	2.224170369147	3.394059166882	-2.872935665759
H	1.466757904211	4.829920839588	-2.142685877474
O	0.377493962375	2.221607266451	0.836994648957
C	-2.462228992570	1.888083405363	-3.466033656239
O	-3.506652355168	1.579994029826	-4.259712112845
C	-4.553563182181	0.755143416114	-3.700848363152
C	-5.594027997316	0.556037139832	-4.783618360117
H	-6.414717075228	-0.068523860796	-4.398124251743
H	-5.158501568430	0.052895794436	-5.661112793818
H	-6.015368252890	1.520800151187	-5.106983257074
H	-4.973884500730	1.257313706058	-2.814261175530
H	-4.119022348769	-0.200999954398	-3.366579788562
C	-1.439909211680	2.688542815602	-4.010983357614
H	-1.503909320061	3.041756118258	-5.043830422060
N	-0.377139725895	3.035446304501	-3.293231637887
C	-0.311648927194	2.593364846881	-2.025388665661
C	-1.331941711560	1.794837490132	-1.483473432342
H	-1.279692120691	1.441173214214	-0.455299649647
N	-2.402858405784	1.447879109515	-2.211401891782

SCF Done: E(RB3LYP) = -1484.53199826

Zero-point correction= 0.478294
Thermal correction to Energy= 0.506978
Thermal correction to Enthalpy= 0.507923
Thermal correction to Gibbs Free Energy= 0.415916
Sum of electronic and zero-point Energies= -1484.053705
Sum of electronic and thermal Energies= -1484.025020
Sum of electronic and thermal Enthalpies= -1484.024076
Sum of electronic and thermal Free Energies= -1484.116082

1	C	Isotropic =	46.3720	Anisotropy = 145.0493
2	C	Isotropic =	57.0672	Anisotropy = 142.9604
3	C	Isotropic =	76.5823	Anisotropy = 157.8273
4	H	Isotropic =	23.7822	Anisotropy = 9.9599
5	C	Isotropic =	86.8944	Anisotropy = 125.6779
6	C	Isotropic =	66.8502	Anisotropy = 165.8039
7	H	Isotropic =	23.8737	Anisotropy = 6.0280
8	C	Isotropic =	72.2426	Anisotropy = 156.4119
9	H	Isotropic =	23.6575	Anisotropy = 4.8966
10	C	Isotropic =	75.9028	Anisotropy = 315.6856
11	N	Isotropic =	-1.6437	Anisotropy = 371.5749
12	N	Isotropic =	93.9204	Anisotropy = 119.4560

13	C	Isotropic =	134.2358	Anisotropy =	44.5723
14	H	Isotropic =	27.4805	Anisotropy =	3.6080
15	H	Isotropic =	27.6740	Anisotropy =	6.2064
16	C	Isotropic =	45.1323	Anisotropy =	99.1269
17	H	Isotropic =	23.6037	Anisotropy =	7.7480
18	N	Isotropic =	6.6526	Anisotropy =	351.2089
19	C	Isotropic =	153.3607	Anisotropy =	14.8135
20	H	Isotropic =	29.6523	Anisotropy =	7.6929
21	H	Isotropic =	30.2096	Anisotropy =	6.4096
22	C	Isotropic =	107.9294	Anisotropy =	63.4502
23	C	Isotropic =	146.0169	Anisotropy =	19.3296
24	H	Isotropic =	30.3540	Anisotropy =	10.5676
25	H	Isotropic =	29.5342	Anisotropy =	4.7501
26	C	Isotropic =	149.9497	Anisotropy =	15.9761
27	C	Isotropic =	166.6803	Anisotropy =	34.6878
28	H	Isotropic =	30.3639	Anisotropy =	7.9042
29	H	Isotropic =	29.0950	Anisotropy =	6.3402
30	H	Isotropic =	30.6068	Anisotropy =	10.0507
31	C	Isotropic =	156.9540	Anisotropy =	8.0183
32	H	Isotropic =	29.9219	Anisotropy =	7.9073
33	H	Isotropic =	29.8892	Anisotropy =	8.3749
34	C	Isotropic =	170.0301	Anisotropy =	13.0137
35	H	Isotropic =	29.7252	Anisotropy =	11.5211
36	H	Isotropic =	29.3214	Anisotropy =	7.0199
37	O	Isotropic =	136.1522	Anisotropy =	106.1429
38	C	Isotropic =	42.3957	Anisotropy =	82.3658
39	N	Isotropic =	137.0755	Anisotropy =	98.5708
40	C	Isotropic =	134.6826	Anisotropy =	37.1522
41	H	Isotropic =	27.9773	Anisotropy =	4.7985
42	H	Isotropic =	28.0330	Anisotropy =	5.2905
43	O	Isotropic =	60.7852	Anisotropy =	381.5812
44	C	Isotropic =	36.5747	Anisotropy =	120.7797
45	O	Isotropic =	196.3379	Anisotropy =	79.5051
46	C	Isotropic =	127.8262	Anisotropy =	54.1348
47	C	Isotropic =	176.4078	Anisotropy =	21.6594
48	H	Isotropic =	30.0430	Anisotropy =	9.4972
49	H	Isotropic =	29.9060	Anisotropy =	7.6752
50	H	Isotropic =	29.9154	Anisotropy =	7.8760
51	H	Isotropic =	27.2549	Anisotropy =	6.1494
52	H	Isotropic =	27.2404	Anisotropy =	5.7806
53	C	Isotropic =	63.0588	Anisotropy =	126.4000
54	H	Isotropic =	23.5597	Anisotropy =	7.5058
55	N	Isotropic =	-52.4833	Anisotropy =	484.1425
56	C	Isotropic =	50.1179	Anisotropy =	127.4150
57	C	Isotropic =	61.9567	Anisotropy =	142.0789
58	H	Isotropic =	22.2532	Anisotropy =	12.1371
59	N	Isotropic =	-34.9921	Anisotropy =	472.4329



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.107811070315	0.636733043150	-0.327385569058
C	-0.002356160122	-0.020978061628	-0.879656575500
H	-0.134249534064	-0.069965588522	-1.961875610767
C	-0.926497135562	-0.638156843403	-0.039019752050
H	-1.791084388730	-1.160300718459	-0.445989410635
C	-0.716529596063	-0.586233761545	1.344342364175
N	0.334607039066	0.042748426967	1.899857246142
C	1.206386479380	0.631259370078	1.081887490040
H	2.036565300885	1.153664775797	1.567163658335
C	-1.663873426116	-1.237737194372	2.309189000839
O	-1.538883807605	-1.236013547359	3.515634116331
O	-2.694750846797	-1.841635315300	1.678807818711
H	-3.256277665791	-2.237437189921	2.371024037532
C	4.059829189327	2.596520397111	-2.772761274979
H	4.808257820449	3.093637500533	-3.393624960452
C	2.710732546386	2.618005477761	-3.143144368313
H	2.399741179703	3.138886714079	-4.051370464158
C	1.753406158990	1.981006533182	-2.350748567415
H	0.701593701327	2.024711920405	-2.640907005776
C	2.126161952066	1.311646101885	-1.168814731921
C	3.487370283394	1.298026296664	-0.807026820027
H	3.805897516172	0.763945200531	0.090319648523
C	4.443835422935	1.933212101820	-1.602462370588
H	5.495516900454	1.902904360544	-1.309257898986

SCF Done: E(RB3LYP) = -667.968726092

Zero-point correction= 0.183996
Thermal correction to Energy= 0.195694
Thermal correction to Enthalpy= 0.196638
Thermal correction to Gibbs Free Energy= 0.144754
Sum of electronic and zero-point Energies= -667.784731
Sum of electronic and thermal Energies= -667.773032
Sum of electronic and thermal Enthalpies= -667.772088
Sum of electronic and thermal Free Energies= -667.823972

1	C	Isotropic =	50.6847	Anisotropy =	183.1234
2	C	Isotropic =	58.1175	Anisotropy =	179.9439
3	H	Isotropic =	23.4246	Anisotropy =	8.9632

4	C	Isotropic =	65.0674	Anisotropy =	174.1206
5	H	Isotropic =	23.1706	Anisotropy =	8.7008
6	C	Isotropic =	46.6723	Anisotropy =	143.0050
7	N	Isotropic =	-71.7793	Anisotropy =	540.5025
8	C	Isotropic =	44.4693	Anisotropy =	151.7858
9	H	Isotropic =	22.4176	Anisotropy =	9.2568
10	C	Isotropic =	31.8098	Anisotropy =	82.1648
11	O	Isotropic =	-44.0727	Anisotropy =	528.2036
12	O	Isotropic =	146.9186	Anisotropy =	175.5498
13	H	Isotropic =	25.2948	Anisotropy =	11.2353
14	C	Isotropic =	63.9073	Anisotropy =	178.2107
15	H	Isotropic =	23.8777	Anisotropy =	4.7074
16	C	Isotropic =	63.3095	Anisotropy =	175.1963
17	H	Isotropic =	23.8384	Anisotropy =	5.1983
18	C	Isotropic =	64.8621	Anisotropy =	166.5586
19	H	Isotropic =	23.7743	Anisotropy =	8.3134
20	C	Isotropic =	54.0910	Anisotropy =	176.6410
21	C	Isotropic =	65.4998	Anisotropy =	165.6202
22	H	Isotropic =	23.7331	Anisotropy =	7.8344
23	C	Isotropic =	63.4618	Anisotropy =	174.9540
24	H	Isotropic =	23.8439	Anisotropy =	5.1181

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

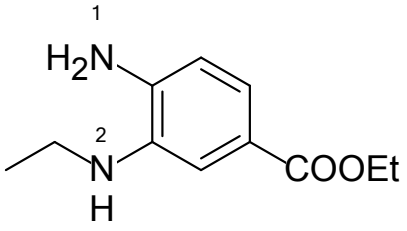
C	1.177687494281	0.752230488809	-0.040791690879
C	0.035665745319	1.275919553852	-0.669429097291
H	0.067725902897	2.256213155802	-1.148101592310
C	-1.150404420535	0.547136055667	-0.654947074428
H	-2.058245823803	0.924250151627	-1.124976061974
C	-1.169578330487	-0.693216484666	-0.007294637138
N	-0.091107549451	-1.222136010803	0.596103771053
C	1.038516254447	-0.513336129520	0.569953338324
H	1.904584417100	-0.980172075352	1.048721905807
C	-2.452706761762	-1.467021111161	0.011892726583
O	-3.480866526392	-1.075585482367	-0.509552447782
O	-2.361412476521	-2.639162831769	0.662450820031
H	-3.244699709037	-3.051008106557	0.610757917916
C	4.930905356903	2.860405673999	0.017682511009
H	5.882879523398	3.395416303324	0.031928167885
C	4.100924741419	2.929910008303	-1.106560356131
H	4.405634205740	3.513847939667	-1.977784311781
C	2.882719745387	2.247462170859	-1.124740082727
H	2.255926817297	2.292718016842	-2.017623412725
C	2.471072335121	1.478410353997	-0.018928963649
C	3.316054134274	1.416571518958	1.106392785152
H	3.008110461792	0.848992476485	1.986777221125
C	4.532972075682	2.101974954554	1.123774117819
H	5.169612386930	2.048599409452	2.009594446113

SCF Done: E(RB3LYP) = -667.969819287

Zero-point correction= 0.184105

Thermal correction to Energy= 0.195751
Thermal correction to Enthalpy= 0.196695
Thermal correction to Gibbs Free Energy= 0.145094
Sum of electronic and zero-point Energies= -667.785714
Sum of electronic and thermal Energies= -667.774068
Sum of electronic and thermal Enthalpies= -667.773124
Sum of electronic and thermal Free Energies= -667.824726

1	C	Isotropic =	50.3003	Anisotropy =	183.8311
2	C	Isotropic =	58.3337	Anisotropy =	179.7629
3	H	Isotropic =	23.4076	Anisotropy =	8.8856
4	C	Isotropic =	65.6629	Anisotropy =	179.1719
5	H	Isotropic =	23.1520	Anisotropy =	8.0363
6	C	Isotropic =	46.3906	Anisotropy =	142.7019
7	N	Isotropic =	-67.4378	Anisotropy =	533.5105
8	C	Isotropic =	45.0208	Anisotropy =	150.9776
9	H	Isotropic =	22.4894	Anisotropy =	9.2752
10	C	Isotropic =	29.1999	Anisotropy =	87.7817
11	O	Isotropic =	-36.0520	Anisotropy =	495.4353
12	O	Isotropic =	146.8958	Anisotropy =	156.2650
13	H	Isotropic =	25.3622	Anisotropy =	10.9751
14	C	Isotropic =	63.8266	Anisotropy =	177.9676
15	H	Isotropic =	23.8879	Anisotropy =	4.6990
16	C	Isotropic =	63.1449	Anisotropy =	174.7384
17	H	Isotropic =	23.8497	Anisotropy =	5.1675
18	C	Isotropic =	65.0665	Anisotropy =	166.6846
19	H	Isotropic =	23.7767	Anisotropy =	8.3189
20	C	Isotropic =	54.0884	Anisotropy =	176.7842
21	C	Isotropic =	65.6107	Anisotropy =	165.9243
22	H	Isotropic =	23.7274	Anisotropy =	7.8445
23	C	Isotropic =	63.4532	Anisotropy =	174.8464
24	H	Isotropic =	23.8585	Anisotropy =	5.1133



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.656213867844	-2.109473073242	-1.254475464303
H	0.692134990246	-2.320480622133	-2.322579737990
C	1.323655409606	-2.941170974965	-0.353576281921
H	1.877971507442	-3.809650376804	-0.718702938515
C	1.281709952761	-2.697721939812	1.026595051158
N	1.959829606122	-3.493525706259	1.946917161669

H	1.443609806486	-3.636539728621	2.815063074967
H	2.283718857841	-4.382360872049	1.573720241967
C	0.563756915657	-1.562822561434	1.517635310014
N	0.553293503460	-1.365716527272	2.904661943451
H	1.468359447573	-1.558420687148	3.313823050209
C	-0.054331551148	-0.165405586943	3.470059891941
H	-1.122214025152	-0.156099070413	3.194424707081
C	0.086644004345	-0.163023666095	4.988046117376
H	-0.376157177495	-1.061282527121	5.426842428258
H	-0.399409033352	0.725820741774	5.418253906661
H	1.147985792674	-0.143205339356	5.288719458079
H	0.388196702331	0.760135911517	3.046489487819
C	-0.108835421719	-0.747702728508	0.606579358438
H	-0.668637942269	0.122359620060	0.946089550373
C	-0.078180610850	-1.015015378747	-0.778150815210
C	-0.824534025280	-0.101954125882	-1.675240952097
O	-1.483070463609	0.857232193899	-1.299958810537
O	-0.707129120489	-0.435418347862	-2.980992539593
C	-1.410497535699	0.407156186913	-3.924457838374
C	-1.143877667511	-0.139521570311	-5.311635114161
H	-1.663993922015	0.478322001982	-6.060194312748
H	-1.508247635970	-1.174635584536	-5.405416027236
H	-0.066802576498	-0.126127463534	-5.541222366108
H	-1.051270946970	1.442573531313	-3.812978293815
H	-2.483940708362	0.398644271591	-3.677019246853

SCF Done: E(RB3LYP) = -688.833969697

Zero-point correction= 0.260448
Thermal correction to Energy= 0.276043
Thermal correction to Enthalpy= 0.276987
Thermal correction to Gibbs Free Energy= 0.216972
Sum of electronic and zero-point Energies= -688.573521
Sum of electronic and thermal Energies= -688.557927
Sum of electronic and thermal Enthalpies= -688.556983
Sum of electronic and thermal Free Energies= -688.616997

1	C	Isotropic = 71.8368	Anisotropy =	162.9932
2	H	Isotropic = 24.0048	Anisotropy =	7.6030
3	C	Isotropic = 80.4203	Anisotropy =	127.8029
4	H	Isotropic = 24.8480	Anisotropy =	6.1669
5	C	Isotropic = 51.4689	Anisotropy =	155.7475
6	N	Isotropic = 197.5409	Anisotropy =	43.5076
7	H	Isotropic = 28.4072	Anisotropy =	9.1405
8	H	Isotropic = 28.0437	Anisotropy =	12.3221
9	C	Isotropic = 56.1860	Anisotropy =	141.0699
10	N	Isotropic = 181.1858	Anisotropy =	44.7169
11	H	Isotropic = 29.3143	Anisotropy =	7.6909
12	C	Isotropic = 150.2918	Anisotropy =	28.9687
13	H	Isotropic = 28.3683	Anisotropy =	6.6313
14	C	Isotropic = 175.7242	Anisotropy =	25.1394
15	H	Isotropic = 29.9930	Anisotropy =	7.9154
16	H	Isotropic = 29.9508	Anisotropy =	9.8879
17	H	Isotropic = 30.1499	Anisotropy =	8.0152
18	H	Isotropic = 28.3913	Anisotropy =	7.1870
19	C	Isotropic = 80.9039	Anisotropy =	152.4467

20	H	Isotropic =	24.3355	Anisotropy =	11.0410
21	C	Isotropic =	72.5129	Anisotropy =	134.0095
22	C	Isotropic =	27.7151	Anisotropy =	82.8547
23	O	Isotropic =	-22.9961	Anisotropy =	533.8303
24	O	Isotropic =	140.3650	Anisotropy =	143.6748
25	C	Isotropic =	129.5127	Anisotropy =	55.4584
26	C	Isotropic =	176.7840	Anisotropy =	21.0232
27	H	Isotropic =	30.0571	Anisotropy =	9.6786
28	H	Isotropic =	29.9101	Anisotropy =	7.5449
29	H	Isotropic =	29.9116	Anisotropy =	7.4873
30	H	Isotropic =	27.2434	Anisotropy =	6.2957
31	H	Isotropic =	27.2527	Anisotropy =	6.2792

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.168702740485	-2.142468359353	0.393188271628
H	-2.048990011331	-2.677532657234	0.039104201170
C	-0.685751643690	-2.365506864725	1.683760707968
H	-1.194235950621	-3.073483257456	2.343323068941
C	0.437567617326	-1.679357117101	2.166539528688
N	0.958885801453	-1.902348029854	3.438758011949
H	0.337748411440	-2.412475946045	4.061741392320
H	1.301024722337	-1.054002906618	3.890212041227
C	1.114362846689	-0.752769673648	1.313407943069
N	2.228673191041	-0.092184767321	1.846902969996
H	2.803426032790	-0.724432837319	2.405422087335
C	3.040184947925	0.778289531408	1.002226260040
H	2.399403671052	1.596290326436	0.632468190118
C	4.204749974454	1.355329189457	1.799109381424
H	4.798847790986	2.038388229974	1.173108881159
H	4.877215543876	0.556417342412	2.155053559857
H	3.841390639833	1.912670898993	2.677122639644
H	3.420499267184	0.246343532745	0.105468095780
C	0.613537564465	-0.531509931372	0.029997251945
H	1.102378660562	0.169609904231	-0.644638172720
C	-0.530181074503	-1.211968102562	-0.437804855773
C	-0.999275206889	-0.914391353739	-1.811530297738
O	-0.478434486055	-0.104295158886	-2.564538593455
O	-2.084151176399	-1.641177683086	-2.164817991352
C	-2.608505059647	-1.409701480234	-3.493847454327
C	-3.785671429950	-2.342693744509	-3.688853000319
H	-4.573475683068	-2.146188281386	-2.944720193840
H	-3.474464842118	-3.395311390862	-3.598712244885
H	-4.214414850932	-2.194409806827	-4.692271504459
H	-1.809131114018	-1.594423671267	-4.228745260073
H	-2.902801413710	-0.351495934249	-3.580494915316

SCF Done: E(RB3LYP) = -688.833983694

Zero-point correction= 0.260464
Thermal correction to Energy= 0.276053
Thermal correction to Enthalpy= 0.276997

Thermal correction to Gibbs Free Energy= 0.217039
Sum of electronic and zero-point Energies= -688.573520
Sum of electronic and thermal Energies= -688.557930
Sum of electronic and thermal Enthalpies= -688.556986
Sum of electronic and thermal Free Energies= -688.616944

1	C	Isotropic =	71.8785	Anisotropy =	162.9067
2	H	Isotropic =	24.0086	Anisotropy =	7.6109
3	C	Isotropic =	80.5057	Anisotropy =	127.8403
4	H	Isotropic =	24.8513	Anisotropy =	6.1635
5	C	Isotropic =	51.3573	Anisotropy =	155.6214
6	N	Isotropic =	197.5630	Anisotropy =	43.4082
7	H	Isotropic =	28.0438	Anisotropy =	12.3163
8	H	Isotropic =	28.4002	Anisotropy =	9.1558
9	C	Isotropic =	56.1013	Anisotropy =	140.6336
10	N	Isotropic =	181.2340	Anisotropy =	44.6188
11	H	Isotropic =	29.3065	Anisotropy =	7.6997
12	C	Isotropic =	150.4164	Anisotropy =	28.7520
13	H	Isotropic =	28.3704	Anisotropy =	6.6368
14	C	Isotropic =	175.7176	Anisotropy =	25.1486
15	H	Isotropic =	29.9531	Anisotropy =	9.8855
16	H	Isotropic =	30.1538	Anisotropy =	8.0129
17	H	Isotropic =	29.9990	Anisotropy =	7.8997
18	H	Isotropic =	28.3829	Anisotropy =	7.2091
19	C	Isotropic =	80.8722	Anisotropy =	152.3900
20	H	Isotropic =	24.3350	Anisotropy =	11.0310
21	C	Isotropic =	72.5298	Anisotropy =	133.9901
22	C	Isotropic =	27.7262	Anisotropy =	82.7800
23	O	Isotropic =	-22.7054	Anisotropy =	534.1657
24	O	Isotropic =	140.4008	Anisotropy =	143.3573
25	C	Isotropic =	129.5373	Anisotropy =	55.5419
26	C	Isotropic =	176.8335	Anisotropy =	20.9455
27	H	Isotropic =	29.9077	Anisotropy =	7.5564
28	H	Isotropic =	29.9191	Anisotropy =	7.4762
29	H	Isotropic =	30.0581	Anisotropy =	9.6847
30	H	Isotropic =	27.2149	Anisotropy =	6.2158
31	H	Isotropic =	27.2802	Anisotropy =	6.3675

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.115476421085	-1.921266635575	1.363443513609
H	0.808400194854	-2.480666040236	1.990786970890
C	-1.237270495433	-1.854479599483	1.701746448697
H	-1.601513423692	-2.358766337576	2.600564227856
C	-2.146326651476	-1.129755225257	0.918050827743
N	-3.505461027708	-1.066148128949	1.216145940778
H	-3.917247949386	-0.152085388549	1.027883002697
H	-3.743249224351	-1.378312229015	2.154332326114
C	-1.684198299225	-0.469861812784	-0.263259885362
N	-2.632934024756	0.240864748638	-1.009869068675
H	-3.516864554875	-0.266425177299	-1.067238020847
C	-2.262534617614	0.836740080156	-2.289543759913

H	-1.843731461386	0.084087028991	-2.989532976884
C	-3.466360035381	1.524721402922	-2.923307743371
H	-4.269926435472	0.800248180538	-3.139024839212
H	-3.181308013951	2.000909611228	-3.873751516547
H	-3.874208946275	2.298167248018	-2.253204135100
H	-1.463256967054	1.574903704954	-2.108733008189
C	-0.327582104276	-0.536046390660	-0.582742996385
H	0.058840690117	-0.042157531992	-1.472854841651
C	0.582409906383	-1.248514731771	0.226112643496
C	2.006742577356	-1.261558656151	-0.182361495823
O	2.453452004789	-0.688826087676	-1.165766989473
O	2.787254520934	-1.983310383698	0.654161648569
C	4.195613672411	-2.044307603624	0.325987791408
C	4.876434603663	-2.881073953832	1.389261706882
H	5.954035568601	-2.950043889968	1.173324324712
H	4.463464540874	-3.901770285317	1.413618330429
H	4.752429370190	-2.429958936395	2.386308798575
H	4.596670417341	-1.019039675049	0.288231335912
H	4.307739743710	-2.482917304586	-0.678338560934

SCF Done: E(RB3LYP) = -688.833984463

Zero-point correction= 0.260431
Thermal correction to Energy= 0.276040
Thermal correction to Enthalpy= 0.276984
Thermal correction to Gibbs Free Energy= 0.216921
Sum of electronic and zero-point Energies= -688.573554
Sum of electronic and thermal Energies= -688.557945
Sum of electronic and thermal Enthalpies= -688.557001
Sum of electronic and thermal Free Energies= -688.617063

1	C	Isotropic =	71.9202	Anisotropy =	162.9536
2	H	Isotropic =	24.0145	Anisotropy =	7.5901
3	C	Isotropic =	80.4551	Anisotropy =	127.5800
4	H	Isotropic =	24.8530	Anisotropy =	6.1624
5	C	Isotropic =	51.4488	Anisotropy =	155.6192
6	N	Isotropic =	197.6499	Anisotropy =	43.4228
7	H	Isotropic =	28.4043	Anisotropy =	9.1468
8	H	Isotropic =	28.0476	Anisotropy =	12.3216
9	C	Isotropic =	56.1776	Anisotropy =	140.9859
10	N	Isotropic =	181.1967	Anisotropy =	44.7472
11	H	Isotropic =	29.3069	Anisotropy =	7.6924
12	C	Isotropic =	150.2361	Anisotropy =	28.8871
13	H	Isotropic =	28.3814	Anisotropy =	7.1897
14	C	Isotropic =	175.7713	Anisotropy =	25.1122
15	H	Isotropic =	30.1595	Anisotropy =	8.0124
16	H	Isotropic =	29.9541	Anisotropy =	9.8951
17	H	Isotropic =	29.9956	Anisotropy =	7.9099
18	H	Isotropic =	28.3609	Anisotropy =	6.6214
19	C	Isotropic =	80.8063	Anisotropy =	152.5013
20	H	Isotropic =	24.3268	Anisotropy =	11.0543
21	C	Isotropic =	72.4970	Anisotropy =	134.1530
22	C	Isotropic =	27.7570	Anisotropy =	82.8768
23	O	Isotropic =	-23.0165	Anisotropy =	533.4545
24	O	Isotropic =	140.2996	Anisotropy =	143.5190
25	C	Isotropic =	129.4991	Anisotropy =	55.4813

26	C	Isotropic =	176.8136	Anisotropy =	20.9597
27	H	Isotropic =	30.0596	Anisotropy =	9.6806
28	H	Isotropic =	29.9103	Anisotropy =	7.4949
29	H	Isotropic =	29.9177	Anisotropy =	7.5356
30	H	Isotropic =	27.2362	Anisotropy =	6.2327
31	H	Isotropic =	27.2569	Anisotropy =	6.3373

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.858402338187	-2.448865141937	0.174564742164
H	-0.920134276332	-3.491416331170	-0.135161359180
C	-1.771792908212	-1.937451197769	1.098136243358
H	-2.546574029317	-2.584916977371	1.516914432749
C	-1.704865640987	-0.602689293669	1.522087564357
N	-2.618882458891	-0.057239655923	2.420699743053
H	-3.181716488785	-0.745164063765	2.914867617986
H	-2.197070288046	0.598853491715	3.078094804706
C	-0.698591473109	0.256393928561	0.979862818273
N	-0.674182024393	1.579624478247	1.438967702460
H	-1.617404417921	1.958111130966	1.533657260252
C	0.243419266511	2.545855252761	0.844137618346
H	0.110045904793	2.619526571063	-0.255228006068
C	0.058062570918	3.916940392804	1.484509301535
H	0.217905555753	3.866287311764	2.573311271560
H	-0.959337680199	4.304199103043	1.305300004493
H	0.771025794328	4.639956376700	1.059926029246
H	1.274475528131	2.191773179301	1.011297016630
C	0.214140932771	-0.271366834877	0.065875369067
H	0.994820723589	0.353444887500	-0.365372612976
C	0.150811369216	-1.621798769594	-0.336813459382
C	1.161356012694	-2.101513566115	-1.308574348046
O	2.056422798775	-1.413706502064	-1.777996268048
O	0.997618568289	-3.403329039794	-1.637576339765
C	1.944192705588	-3.950841081372	-2.585878329159
C	1.592185436228	-5.409754888168	-2.790934587550
H	0.570675213045	-5.517827720814	-3.188184623345
H	1.660284496832	-5.969058728599	-1.844639131485
H	2.291899585874	-5.862615664515	-3.510610846326
H	2.962567119630	-3.824230750316	-2.185657092919
H	1.880854441416	-3.375839896595	-3.523472535984

SCF Done: E(RB3LYP) = -688.833987951

Zero-point correction= 0.260454
Thermal correction to Energy= 0.276056
Thermal correction to Enthalpy= 0.277000
Thermal correction to Gibbs Free Energy= 0.216875
Sum of electronic and zero-point Energies= -688.573534
Sum of electronic and thermal Energies= -688.557932
Sum of electronic and thermal Enthalpies= -688.556988
Sum of electronic and thermal Free Energies= -688.617113

1	C	Isotropic =	71.9166	Anisotropy =	163.0013
2	H	Isotropic =	24.0038	Anisotropy =	7.6045
3	C	Isotropic =	80.4713	Anisotropy =	127.8784
4	H	Isotropic =	24.8506	Anisotropy =	6.1625
5	C	Isotropic =	51.4611	Anisotropy =	155.5340
6	N	Isotropic =	197.6694	Anisotropy =	43.4548
7	H	Isotropic =	28.0457	Anisotropy =	12.3214
8	H	Isotropic =	28.4073	Anisotropy =	9.1604
9	C	Isotropic =	56.0865	Anisotropy =	140.6800
10	N	Isotropic =	181.2559	Anisotropy =	44.8924
11	H	Isotropic =	29.3046	Anisotropy =	7.6972
12	C	Isotropic =	150.3907	Anisotropy =	28.8694
13	H	Isotropic =	28.3872	Anisotropy =	7.2052
14	C	Isotropic =	175.6694	Anisotropy =	25.2186
15	H	Isotropic =	29.9933	Anisotropy =	7.9110
16	H	Isotropic =	30.1534	Anisotropy =	8.0024
17	H	Isotropic =	29.9489	Anisotropy =	9.8846
18	H	Isotropic =	28.3702	Anisotropy =	6.6409
19	C	Isotropic =	80.8858	Anisotropy =	152.2920
20	H	Isotropic =	24.3327	Anisotropy =	11.0354
21	C	Isotropic =	72.4994	Anisotropy =	134.0765
22	C	Isotropic =	27.7189	Anisotropy =	82.8025
23	O	Isotropic =	-22.8597	Anisotropy =	533.6613
24	O	Isotropic =	140.4502	Anisotropy =	143.4601
25	C	Isotropic =	129.4472	Anisotropy =	55.5351
26	C	Isotropic =	176.8083	Anisotropy =	20.9483
27	H	Isotropic =	29.9079	Anisotropy =	7.4758
28	H	Isotropic =	29.9231	Anisotropy =	7.5420
29	H	Isotropic =	30.0580	Anisotropy =	9.6856
30	H	Isotropic =	27.2250	Anisotropy =	6.2153
31	H	Isotropic =	27.2618	Anisotropy =	6.3611

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.543983039665	0.110084998321	-1.309839322687
H	-0.477893169590	0.328890019160	-2.374887089044
C	-1.377604570265	0.871783106544	-0.489226729617
H	-1.961075069051	1.692729739163	-0.913898611894
C	-1.470823356601	0.617429396161	0.886404453492
N	-2.316759166233	1.340889919966	1.723983961365
H	-1.917137698913	1.521700767712	2.644943797845
H	-2.675036113674	2.200578870163	1.315556511913
C	-0.716828404633	-0.456530168802	1.454214485288
N	-0.845793430604	-0.667257492367	2.833188258100
H	-1.813848834065	-0.554480291109	3.136713555782
C	-0.208800746506	-1.820147347858	3.461486997775
H	0.880247607734	-1.740529389159	3.306612679193
C	-0.516252985710	-1.849407877974	4.954473843201
H	-0.010122881900	-2.700577202405	5.434848525457
H	-1.599128403028	-1.957759085586	5.135461365022
H	-0.179169547694	-0.921315616777	5.442944725897
H	-0.525087500329	-2.773994386754	2.990307239539

C	0.121863819545	-1.201292885515	0.624081412161
H	0.713183715447	-2.023432404234	1.024139589179
C	0.223411396160	-0.923089795516	-0.755157550203
C	1.140167421751	-1.760119216016	-1.564280457040
O	1.835517523451	-2.661320440486	-1.118397043394
O	1.135480871747	-1.427665852356	-2.875516130157
C	2.006778759702	-2.197658722227	-3.737369208252
C	1.831191327513	-1.674751145504	-5.148111004165
H	2.102992844048	-0.609325996630	-5.211460262075
H	0.789089086833	-1.790156079548	-5.485217536319
H	2.480835615079	-2.237929731261	-5.836149347034
H	1.737451179621	-3.262638592961	-3.655461407836
H	3.044293749830	-2.088217096146	-3.383499701491

SCF Done: E(RB3LYP) = -688.833946679

Zero-point correction= 0.260426
Thermal correction to Energy= 0.276039
Thermal correction to Enthalpy= 0.276983
Thermal correction to Gibbs Free Energy= 0.216853
Sum of electronic and zero-point Energies= -688.573521
Sum of electronic and thermal Energies= -688.557908
Sum of electronic and thermal Enthalpies= -688.556963
Sum of electronic and thermal Free Energies= -688.617094

1	C	Isotropic =	71.8651	Anisotropy =	162.9561
2	H	Isotropic =	24.0085	Anisotropy =	7.6125
3	C	Isotropic =	80.4851	Anisotropy =	127.7757
4	H	Isotropic =	24.8531	Anisotropy =	6.1591
5	C	Isotropic =	51.5054	Anisotropy =	155.4960
6	N	Isotropic =	197.6376	Anisotropy =	43.3912
7	H	Isotropic =	28.4166	Anisotropy =	9.1578
8	H	Isotropic =	28.0437	Anisotropy =	12.3153
9	C	Isotropic =	56.1106	Anisotropy =	141.0842
10	N	Isotropic =	181.0670	Anisotropy =	44.8348
11	H	Isotropic =	29.3073	Anisotropy =	7.7059
12	C	Isotropic =	150.1837	Anisotropy =	28.8628
13	H	Isotropic =	28.3638	Anisotropy =	6.6190
14	C	Isotropic =	175.7670	Anisotropy =	25.0853
15	H	Isotropic =	29.9506	Anisotropy =	9.8910
16	H	Isotropic =	30.1536	Anisotropy =	8.0141
17	H	Isotropic =	29.9990	Anisotropy =	7.9124
18	H	Isotropic =	28.3965	Anisotropy =	7.1829
19	C	Isotropic =	81.0784	Anisotropy =	152.5809
20	H	Isotropic =	24.3384	Anisotropy =	11.0283
21	C	Isotropic =	72.4468	Anisotropy =	134.0256
22	C	Isotropic =	27.7410	Anisotropy =	82.7927
23	O	Isotropic =	-22.8241	Anisotropy =	533.7158
24	O	Isotropic =	140.4029	Anisotropy =	143.6482
25	C	Isotropic =	129.5585	Anisotropy =	55.4172
26	C	Isotropic =	176.7978	Anisotropy =	21.0101
27	H	Isotropic =	29.9035	Anisotropy =	7.5511
28	H	Isotropic =	29.9153	Anisotropy =	7.4810
29	H	Isotropic =	30.0634	Anisotropy =	9.6763
30	H	Isotropic =	27.2295	Anisotropy =	6.2574
31	H	Isotropic =	27.2636	Anisotropy =	6.3211

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.824755449926	-0.062817189480	-1.325379367845
H	1.723758718045	-0.037139113747	-1.940000515968
C	-0.117141395975	0.963256144852	-1.419729260259
H	0.043883859499	1.791471786840	-2.114802336782
C	-1.288717408314	0.945389240631	-0.649729470219
N	-2.233242283040	1.968092102909	-0.702007309857
H	-3.194745139931	1.633561149070	-0.636977230111
H	-2.127164472544	2.595200423432	-1.495507680466
C	-1.510011793141	-0.129219572791	0.266977126157
N	-2.696910824701	-0.099696828164	1.010690790591
H	-2.912296867553	0.845647106621	1.329854099332
C	-2.934142153824	-1.093574310666	2.052455888354
H	-2.117355859156	-1.106783198806	2.803739634574
C	-4.270390089312	-0.834396860297	2.739087080312
H	-4.274930716437	0.147426935175	3.242319377203
H	-4.466255176940	-1.602589854298	3.502539514218
H	-5.095551380917	-0.848265746361	2.009334913023
H	-2.943529234527	-2.091365307003	1.582688063932
C	-0.565171355838	-1.153193180094	0.342751123080
H	-0.702997661492	-1.988727987800	1.027408785376
C	0.599114814877	-1.136541623022	-0.453511259428
C	1.546438532622	-2.267624220426	-0.315936400420
O	1.383993487656	-3.224287397771	0.427703783270
O	2.635193240863	-2.141688929191	-1.108827231709
C	3.608721007469	-3.210326260489	-1.036464375053
C	4.731654025047	-2.871406075377	-1.994812097018
H	4.358269467525	-2.787609570104	-3.027544060952
H	5.494559082633	-3.665004109451	-1.967078118089
H	5.213102416638	-1.920088273488	-1.718863268669
H	3.114751526902	-4.159313972548	-1.299052804886
H	3.965178183940	-3.296845308158	0.002252608311

SCF Done: E(RB3LYP) = -688.833967619

Zero-point correction= 0.260476
Thermal correction to Energy= 0.276076
Thermal correction to Enthalpy= 0.277020
Thermal correction to Gibbs Free Energy= 0.216810
Sum of electronic and zero-point Energies= -688.573492
Sum of electronic and thermal Energies= -688.557892
Sum of electronic and thermal Enthalpies= -688.556948
Sum of electronic and thermal Free Energies= -688.617158

1	C	Isotropic = 71.8346	Anisotropy =	162.9904
2	H	Isotropic = 24.0083	Anisotropy =	7.5960
3	C	Isotropic = 80.5221	Anisotropy =	127.9768
4	H	Isotropic = 24.8531	Anisotropy =	6.1510
5	C	Isotropic = 51.4272	Anisotropy =	155.6888
6	N	Isotropic = 197.6192	Anisotropy =	43.4346

7	H	Isotropic =	28.4154	Anisotropy =	9.1500
8	H	Isotropic =	28.0509	Anisotropy =	12.3087
9	C	Isotropic =	56.0928	Anisotropy =	140.9203
10	N	Isotropic =	181.0937	Anisotropy =	44.5534
11	H	Isotropic =	29.3027	Anisotropy =	7.6907
12	C	Isotropic =	150.4053	Anisotropy =	28.6827
13	H	Isotropic =	28.3907	Anisotropy =	7.1929
14	C	Isotropic =	175.6343	Anisotropy =	25.2582
15	H	Isotropic =	30.1535	Anisotropy =	8.0062
16	H	Isotropic =	29.9495	Anisotropy =	9.8826
17	H	Isotropic =	29.9948	Anisotropy =	7.9000
18	H	Isotropic =	28.3679	Anisotropy =	6.6386
19	C	Isotropic =	80.9262	Anisotropy =	152.4944
20	H	Isotropic =	24.3288	Anisotropy =	11.0485
21	C	Isotropic =	72.4696	Anisotropy =	134.0678
22	C	Isotropic =	27.7144	Anisotropy =	82.8020
23	O	Isotropic =	-22.7403	Anisotropy =	534.3668
24	O	Isotropic =	140.4197	Anisotropy =	143.7244
25	C	Isotropic =	129.3622	Anisotropy =	55.4336
26	C	Isotropic =	176.8567	Anisotropy =	20.8538
27	H	Isotropic =	29.9193	Anisotropy =	7.5548
28	H	Isotropic =	30.0567	Anisotropy =	9.6820
29	H	Isotropic =	29.9178	Anisotropy =	7.4847
30	H	Isotropic =	27.2459	Anisotropy =	6.2645
31	H	Isotropic =	27.2401	Anisotropy =	6.2956

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.911482290116	-2.470475326762	0.028398705058
H	1.339319701608	-3.274465228181	-0.569295026055
C	1.036656467707	-2.488834832630	1.418656779230
H	1.569646977338	-3.307354760803	1.909422896885
C	0.505173243585	-1.459742638858	2.208650326302
N	0.588273448033	-1.467321503585	3.599168357776
H	0.749028083112	-0.543342532719	4.000408492695
H	1.252604246317	-2.139492046756	3.974624909473
C	-0.198115011809	-0.384619147107	1.581119566936
N	-0.708670046900	0.617700272331	2.416042823014
H	-1.105916367421	0.222977709073	3.269460896531
C	-1.549152500013	1.674532722930	1.862492586768
H	-2.425566978140	1.262845502443	1.320005180335
C	-2.015719954586	2.616098798641	2.967074180766
H	-1.155968601822	3.056515364890	3.496675255520
H	-2.637681818911	2.083760704238	3.706695138423
H	-2.621899300132	3.432569455541	2.545998383080
H	-0.956548642023	2.234928236722	1.120035732580
C	-0.304154177860	-0.372828628272	0.189858172943
H	-0.828698027146	0.432699030085	-0.321613626484
C	0.252478575828	-1.403184226605	-0.596600262871
C	0.096459064963	-1.310639611189	-2.067225351459
O	-0.463112610282	-0.393621345192	-2.650710475233
O	0.642973281088	-2.360856855438	-2.721587392103

C	0.534736479519	-2.344717959985	-4.164847705830
C	1.197691958004	-3.602776709621	-4.686471626276
H	0.700378941206	-4.503450620559	-4.293481137004
H	2.260599394069	-3.637305955482	-4.400050883769
H	1.135720611139	-3.626294780799	-5.785665638011
H	1.020854162613	-1.433197814812	-4.547599121194
H	-0.530502889199	-2.294785271539	-4.441080138027

SCF Done: E(RB3LYP) = -688.833978777

Zero-point correction= 0.260495
Thermal correction to Energy= 0.276077
Thermal correction to Enthalpy= 0.277021
Thermal correction to Gibbs Free Energy= 0.217052
Sum of electronic and zero-point Energies= -688.573484
Sum of electronic and thermal Energies= -688.557902
Sum of electronic and thermal Enthalpies= -688.556957
Sum of electronic and thermal Free Energies= -688.616927

1	C	Isotropic =	71.9393	Anisotropy =	162.8794
2	H	Isotropic =	24.0157	Anisotropy =	7.5885
3	C	Isotropic =	80.4056	Anisotropy =	127.8038
4	H	Isotropic =	24.8478	Anisotropy =	6.1678
5	C	Isotropic =	51.4586	Anisotropy =	155.3818
6	N	Isotropic =	197.7511	Anisotropy =	43.3943
7	H	Isotropic =	28.4103	Anisotropy =	9.1896
8	H	Isotropic =	28.0372	Anisotropy =	12.3233
9	C	Isotropic =	55.9702	Anisotropy =	140.7871
10	N	Isotropic =	181.2779	Anisotropy =	45.2258
11	H	Isotropic =	29.2877	Anisotropy =	7.7156
12	C	Isotropic =	150.3606	Anisotropy =	28.9034
13	H	Isotropic =	28.3909	Anisotropy =	7.1616
14	C	Isotropic =	175.7547	Anisotropy =	25.1644
15	H	Isotropic =	29.9967	Anisotropy =	7.9224
16	H	Isotropic =	30.1566	Anisotropy =	8.0101
17	H	Isotropic =	29.9523	Anisotropy =	9.8867
18	H	Isotropic =	28.3599	Anisotropy =	6.6546
19	C	Isotropic =	80.8872	Anisotropy =	152.4260
20	H	Isotropic =	24.3332	Anisotropy =	11.0459
21	C	Isotropic =	72.4713	Anisotropy =	134.1466
22	C	Isotropic =	27.6946	Anisotropy =	82.8037
23	O	Isotropic =	-23.0164	Anisotropy =	533.5650
24	O	Isotropic =	140.3500	Anisotropy =	143.7591
25	C	Isotropic =	129.4147	Anisotropy =	55.4780
26	C	Isotropic =	176.8648	Anisotropy =	20.8770
27	H	Isotropic =	29.9161	Anisotropy =	7.4877
28	H	Isotropic =	29.9146	Anisotropy =	7.5556
29	H	Isotropic =	30.0580	Anisotropy =	9.6809
30	H	Isotropic =	27.2541	Anisotropy =	6.2993
31	H	Isotropic =	27.2365	Anisotropy =	6.2723

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.785322464663	-2.263338921260	-0.976703104281
H	0.714810700428	-2.838956799446	-1.898830264916
C	1.820146963446	-2.511723920459	-0.073331589620
H	2.557734350081	-3.289370835618	-0.287807710178
C	1.924191795973	-1.793311769685	1.126114785203
N	2.960855444185	-1.999473815194	2.033281812496
H	2.664849403811	-1.934076855627	3.007264829240
H	3.490360423841	-2.853696469912	1.877960497074
C	0.967876064700	-0.770711038532	1.416938265885
N	1.116668621072	-0.084856945941	2.629386274361
H	2.098434774402	0.114326349864	2.825323334376
C	0.257721051490	1.053618409632	2.939181348282
H	-0.787646412537	0.702659149360	2.959467076080
C	0.629760027750	1.645701278813	4.293827064980
H	0.549254191372	0.887523220742	5.088991134724
H	-0.036437365267	2.485571312919	4.543222370516
H	1.664547531739	2.028315377435	4.289210157598
H	0.311872879156	1.837013893941	2.154821879068
C	-0.067442727470	-0.541288106037	0.510047980737
H	-0.814265485071	0.227214166976	0.702581004598
C	-0.175014196945	-1.285612647734	-0.683409655140
C	-1.307839589715	-0.982364547687	-1.589180081028
O	-2.166347040531	-0.139545826017	-1.372134223619
O	-1.304498283281	-1.743532857877	-2.707507725183
C	-2.381317900352	-1.510827696821	-3.646187259280
C	-2.195488846892	-2.473055614183	-4.801074188225
H	-2.999131540763	-2.326330683700	-5.539482480309
H	-2.232020863730	-3.517786216965	-4.454362291218
H	-1.230120584234	-2.305388678067	-5.304055190492
H	-2.345383776930	-0.459936977140	-3.974936800918
H	-3.342352074392	-1.665715935782	-3.130537250810

SCF Done: E(RB3LYP) = -688.833945335

Zero-point correction= 0.260419
Thermal correction to Energy= 0.276018
Thermal correction to Enthalpy= 0.276962
Thermal correction to Gibbs Free Energy= 0.217009
Sum of electronic and zero-point Energies= -688.573526
Sum of electronic and thermal Energies= -688.557927
Sum of electronic and thermal Enthalpies= -688.556983
Sum of electronic and thermal Free Energies= -688.616936

1	C	Isotropic =	71.8400	Anisotropy = 163.1853
2	H	Isotropic =	24.0046	Anisotropy = 7.6070
3	C	Isotropic =	80.3814	Anisotropy = 127.4132
4	H	Isotropic =	24.8640	Anisotropy = 6.1440
5	C	Isotropic =	51.3963	Anisotropy = 155.3153
6	N	Isotropic =	197.6370	Anisotropy = 43.3139
7	H	Isotropic =	28.4106	Anisotropy = 9.1436
8	H	Isotropic =	28.0458	Anisotropy = 12.3205
9	C	Isotropic =	56.1238	Anisotropy = 140.8077
10	N	Isotropic =	181.1435	Anisotropy = 44.7368
11	H	Isotropic =	29.2997	Anisotropy = 7.7164
12	C	Isotropic =	150.3287	Anisotropy = 28.8188

13	H	Isotropic =	28.3626	Anisotropy =	6.6129
14	C	Isotropic =	175.6504	Anisotropy =	25.2284
15	H	Isotropic =	29.9925	Anisotropy =	7.9070
16	H	Isotropic =	29.9507	Anisotropy =	9.8843
17	H	Isotropic =	30.1516	Anisotropy =	8.0025
18	H	Isotropic =	28.3895	Anisotropy =	7.2188
19	C	Isotropic =	81.2150	Anisotropy =	152.9558
20	H	Isotropic =	24.3382	Anisotropy =	11.0394
21	C	Isotropic =	72.5303	Anisotropy =	134.1492
22	C	Isotropic =	27.8128	Anisotropy =	83.0619
23	O	Isotropic =	-22.8023	Anisotropy =	533.5607
24	O	Isotropic =	140.2959	Anisotropy =	143.9136
25	C	Isotropic =	129.4592	Anisotropy =	55.3839
26	C	Isotropic =	176.8871	Anisotropy =	20.8175
27	H	Isotropic =	30.0619	Anisotropy =	9.6797
28	H	Isotropic =	29.9261	Anisotropy =	7.5423
29	H	Isotropic =	29.9097	Anisotropy =	7.5009
30	H	Isotropic =	27.2575	Anisotropy =	6.3337
31	H	Isotropic =	27.2338	Anisotropy =	6.2184

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.677839685326	-0.458049042156	-0.027728937388
H	2.644329490224	-0.580856315842	-0.515086041227
C	1.557528810155	0.371336634673	1.088737607213
H	2.432412189790	0.903383544876	1.471207301774
C	0.322398041192	0.554810875647	1.726381970160
N	0.177135643849	1.351199877933	2.859892335071
H	-0.696428966355	1.877787543060	2.874442690030
H	0.966756509932	1.964640829613	3.045232615105
C	-0.829390592282	-0.137575148956	1.237949018479
N	-2.038595295013	0.083727117228	1.909548426182
H	-1.901225619372	0.115647297831	2.920479789912
C	-3.229327631687	-0.677068770997	1.545739425742
H	-3.056780822685	-1.771413466276	1.613063526531
C	-4.404256015017	-0.279293340427	2.432065828410
H	-4.609232697192	0.800079882870	2.351049929202
H	-4.198593741532	-0.510124031463	3.491148648524
H	-5.311125339856	-0.830112790001	2.139532838051
H	-3.467781171665	-0.461833302684	0.490647594689
C	-0.696573566521	-0.953623328160	0.114031671763
H	-1.553356759854	-1.493466841819	-0.286210416955
C	0.547104130358	-1.114757669531	-0.531973669934
C	0.598776680113	-1.997566185494	-1.720873831000
O	-0.364453845589	-2.581886996519	-2.195517464370
O	1.841246052681	-2.101334360787	-2.245477194764
C	1.977322576955	-2.947562801602	-3.411802466114
C	3.435370487462	-2.929323148675	-3.821715525120
H	4.077512808725	-3.314783106752	-3.014206089763
H	3.763083226457	-1.907918812520	-4.071382306271
H	3.578915963397	-3.564510970027	-4.709696016057
H	1.320303078264	-2.563503234132	-4.208330667245

H 1.633286689741 -3.962499938909 -3.156820590630

SCF Done: E(RB3LYP) = -688.833977423

Zero-point correction= 0.260505
Thermal correction to Energy= 0.276092
Thermal correction to Enthalpy= 0.277037
Thermal correction to Gibbs Free Energy= 0.217007
Sum of electronic and zero-point Energies= -688.573472
Sum of electronic and thermal Energies= -688.557885
Sum of electronic and thermal Enthalpies= -688.556941
Sum of electronic and thermal Free Energies= -688.616970

1 C Isotropic = 71.9327 Anisotropy = 162.9670
2 H Isotropic = 24.0140 Anisotropy = 7.5928
3 C Isotropic = 80.5132 Anisotropy = 127.6744
4 H Isotropic = 24.8553 Anisotropy = 6.1522
5 C Isotropic = 51.4235 Anisotropy = 155.4933
6 N Isotropic = 197.6739 Anisotropy = 43.4515
7 H Isotropic = 28.3982 Anisotropy = 9.1449
8 H Isotropic = 28.0449 Anisotropy = 12.3316
9 C Isotropic = 56.0795 Anisotropy = 140.8126
10 N Isotropic = 181.2241 Anisotropy = 44.3312
11 H Isotropic = 29.3078 Anisotropy = 7.6856
12 C Isotropic = 150.3504 Anisotropy = 28.7867
13 H Isotropic = 28.3856 Anisotropy = 7.2100
14 C Isotropic = 175.6555 Anisotropy = 25.2145
15 H Isotropic = 29.9951 Anisotropy = 7.9091
16 H Isotropic = 30.1542 Anisotropy = 7.9995
17 H Isotropic = 29.9510 Anisotropy = 9.8865
18 H Isotropic = 28.3703 Anisotropy = 6.6179
19 C Isotropic = 80.9588 Anisotropy = 152.6666
20 H Isotropic = 24.3304 Anisotropy = 11.0440
21 C Isotropic = 72.5080 Anisotropy = 134.1066
22 C Isotropic = 27.7514 Anisotropy = 82.9874
23 O Isotropic = -22.9592 Anisotropy = 533.4118
24 O Isotropic = 140.3666 Anisotropy = 143.6507
25 C Isotropic = 129.4922 Anisotropy = 55.4394
26 C Isotropic = 176.8637 Anisotropy = 20.9140
27 H Isotropic = 29.9142 Anisotropy = 7.4862
28 H Isotropic = 29.9138 Anisotropy = 7.5570
29 H Isotropic = 30.0586 Anisotropy = 9.6788
30 H Isotropic = 27.2561 Anisotropy = 6.2977
31 H Isotropic = 27.2353 Anisotropy = 6.2671

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C -1.400667318533 -0.753099529633 0.864188975286
H -2.476589562486 -0.599960162383 0.789578760174
C -0.780750362814 -0.768238621195 2.114898123624
H -1.375328957864 -0.632106608871 3.021908661330
C 0.600213699236 -0.977103819616 2.237539519439

N	1.250437997771	-0.969091461509	3.469341958851
H	1.997722029840	-1.660225842226	3.536273206051
H	0.628741001033	-1.037152305323	4.271255606979
C	1.391100155683	-1.152565837673	1.059319493956
N	2.764934720107	-1.359413181168	1.238418534520
H	3.138507676850	-0.758854566786	1.974374938366
C	3.654620057340	-1.423297349393	0.083623088272
H	3.576847009802	-0.514275850272	-0.548479747282
C	5.097078435081	-1.622030095226	0.535338449620
H	5.442985754103	-0.770987018698	1.146322630663
H	5.765489270861	-1.702376949088	-0.335376095772
H	5.196653002892	-2.538591650875	1.138351652345
H	3.341447353864	-2.271465079379	-0.547994422003
C	0.756209197746	-1.146348110762	-0.183212427724
H	1.327115578877	-1.280534772329	-1.100628744713
C	-0.637468941934	-0.957384319145	-0.293339502293
C	-1.231832832941	-0.971067789849	-1.650607443414
O	-0.602303737320	-1.146408258032	-2.683810566889
O	-2.569068421963	-0.766698136635	-1.641529410510
C	-3.227458585449	-0.768283047141	-2.930493999890
C	-4.704238527946	-0.533072629714	-2.689465360255
H	-5.240676157243	-0.528800739494	-3.651139221584
H	-4.874811226026	0.436074314995	-2.194868236827
H	-5.132945154268	-1.327645676724	-2.058708401608
H	-3.039325012257	-1.734677755823	-3.424714652287
H	-2.781478142042	0.019202849967	-3.558655366426

SCF Done: E(RB3LYP) = -688.833987918

Zero-point correction= 0.260462
Thermal correction to Energy= 0.276055
Thermal correction to Enthalpy= 0.276999
Thermal correction to Gibbs Free Energy= 0.216969
Sum of electronic and zero-point Energies= -688.573526
Sum of electronic and thermal Energies= -688.557933
Sum of electronic and thermal Enthalpies= -688.556989
Sum of electronic and thermal Free Energies= -688.617018

1	C	Isotropic =	71.8896	Anisotropy =	162.9974
2	H	Isotropic =	24.0095	Anisotropy =	7.5937
3	C	Isotropic =	80.4586	Anisotropy =	128.0319
4	H	Isotropic =	24.8478	Anisotropy =	6.1595
5	C	Isotropic =	51.3664	Anisotropy =	155.4685
6	N	Isotropic =	197.6129	Anisotropy =	43.3753
7	H	Isotropic =	28.4093	Anisotropy =	9.1422
8	H	Isotropic =	28.0390	Anisotropy =	12.3205
9	C	Isotropic =	56.0629	Anisotropy =	140.8783
10	N	Isotropic =	181.0905	Anisotropy =	44.4225
11	H	Isotropic =	29.3004	Anisotropy =	7.6834
12	C	Isotropic =	150.1808	Anisotropy =	29.1356
13	H	Isotropic =	28.3915	Anisotropy =	7.1929
14	C	Isotropic =	175.7193	Anisotropy =	25.1860
15	H	Isotropic =	30.1523	Anisotropy =	8.0038
16	H	Isotropic =	29.9508	Anisotropy =	9.8905
17	H	Isotropic =	29.9902	Anisotropy =	7.9121
18	H	Isotropic =	28.3637	Anisotropy =	6.6180

19	C	Isotropic =	80.9108	Anisotropy =	152.3398
20	H	Isotropic =	24.3376	Anisotropy =	11.0403
21	C	Isotropic =	72.4970	Anisotropy =	134.0219
22	C	Isotropic =	27.7188	Anisotropy =	82.8305
23	O	Isotropic =	-23.0807	Anisotropy =	533.5496
24	O	Isotropic =	140.3261	Anisotropy =	143.5287
25	C	Isotropic =	129.4669	Anisotropy =	55.4041
26	C	Isotropic =	176.7810	Anisotropy =	20.9925
27	H	Isotropic =	30.0586	Anisotropy =	9.6777
28	H	Isotropic =	29.9147	Anisotropy =	7.4916
29	H	Isotropic =	29.9193	Anisotropy =	7.5396
30	H	Isotropic =	27.2421	Anisotropy =	6.2496
31	H	Isotropic =	27.2490	Anisotropy =	6.3106

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.453401539085	-0.857355920445	0.797663189252
H	-2.534552915892	-0.802276931921	0.676251564630
C	-0.891462473861	-0.855033274720	2.075558869138
H	-1.536110080707	-0.791649843051	2.956050840537
C	0.497554661978	-0.912255712512	2.257685072285
N	1.085042391635	-0.938563273064	3.520369042783
H	1.953345160472	-0.405825765767	3.573519607253
H	0.459713047292	-0.677440162598	4.278664754245
C	1.352070715641	-1.001120478512	1.114743531634
N	2.731724997519	-1.054677154166	1.351600345008
H	2.948884926120	-1.650205853080	2.151636497600
C	3.657525015045	-1.271043062941	0.244559456925
H	3.545950646531	-0.436357022589	-0.467759388823
C	5.092806988818	-1.325173668574	0.755528259279
H	5.355082774395	-0.397439445444	1.288576568307
H	5.794635786619	-1.457017755647	-0.081984832900
H	5.235953338077	-2.170968417077	1.449342450934
H	3.419591911117	-2.198167926529	-0.317396963064
C	0.776949082846	-0.991219480358	-0.156574945811
H	1.398476325869	-1.053293039886	-1.048523757430
C	-0.620866619193	-0.910192687137	-0.328478129650
C	-1.147933533920	-0.900379617674	-1.713340581196
O	-0.457022561257	-0.946007001899	-2.720845980272
O	-2.498169770987	-0.835019254690	-1.761841740906
C	-3.093407928158	-0.819599696374	-3.081059108387
C	-4.595458514371	-0.739652124954	-2.902845326043
H	-5.085946152908	-0.728109179716	-3.888702930644
H	-4.881340154527	0.177616042024	-2.364421787568
H	-4.973077838543	-1.607519868484	-2.339646657030
H	-2.789899081689	-1.731909845811	-3.618758168374
H	-2.697638604876	0.043337423594	-3.639819751712

SCF Done: E(RB3LYP) = -688.833974764

Zero-point correction= 0.260463
Thermal correction to Energy= 0.276059

Thermal correction to Enthalpy= 0.277003
Thermal correction to Gibbs Free Energy= 0.216960
Sum of electronic and zero-point Energies= -688.573512
Sum of electronic and thermal Energies= -688.557916
Sum of electronic and thermal Enthalpies= -688.556971
Sum of electronic and thermal Free Energies= -688.617015

1	C	Isotropic =	71.7927	Anisotropy =	163.0109
2	H	Isotropic =	24.0065	Anisotropy =	7.6046
3	C	Isotropic =	80.5928	Anisotropy =	128.0881
4	H	Isotropic =	24.8554	Anisotropy =	6.1519
5	C	Isotropic =	51.4178	Anisotropy =	155.4528
6	N	Isotropic =	197.6285	Anisotropy =	43.2511
7	H	Isotropic =	28.4049	Anisotropy =	9.1480
8	H	Isotropic =	28.0487	Anisotropy =	12.3083
9	C	Isotropic =	56.0561	Anisotropy =	140.7172
10	N	Isotropic =	181.2744	Anisotropy =	44.9519
11	H	Isotropic =	29.3023	Anisotropy =	7.7069
12	C	Isotropic =	150.2360	Anisotropy =	28.8009
13	H	Isotropic =	28.3611	Anisotropy =	6.6269
14	C	Isotropic =	175.7069	Anisotropy =	25.1202
15	H	Isotropic =	29.9991	Anisotropy =	7.9102
16	H	Isotropic =	29.9514	Anisotropy =	9.8840
17	H	Isotropic =	30.1568	Anisotropy =	8.0087
18	H	Isotropic =	28.3831	Anisotropy =	7.1852
19	C	Isotropic =	80.8507	Anisotropy =	152.3161
20	H	Isotropic =	24.3328	Anisotropy =	11.0503
21	C	Isotropic =	72.4985	Anisotropy =	134.0544
22	C	Isotropic =	27.7535	Anisotropy =	82.8859
23	O	Isotropic =	-22.9970	Anisotropy =	533.7502
24	O	Isotropic =	140.3853	Anisotropy =	143.3851
25	C	Isotropic =	129.4343	Anisotropy =	55.4496
26	C	Isotropic =	176.7752	Anisotropy =	20.9828
27	H	Isotropic =	30.0544	Anisotropy =	9.6850
28	H	Isotropic =	29.9235	Anisotropy =	7.5385
29	H	Isotropic =	29.9161	Anisotropy =	7.4807
30	H	Isotropic =	27.2502	Anisotropy =	6.3125
31	H	Isotropic =	27.2442	Anisotropy =	6.2587

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.950754158532	-2.235138881849	-0.792614071958
H	-0.905384922013	-3.094620989346	-1.460328950615
C	-2.160789683765	-1.873215402446	-0.198218227283
H	-3.063819661367	-2.455965036517	-0.397697190188
C	-2.241373009885	-0.779377659198	0.675123835448
N	-3.439499898481	-0.378527719697	1.261704388043
H	-3.330399171852	-0.053142912479	2.222258069405
H	-4.186322524877	-1.066094401650	1.200635870381
C	-1.069006479904	-0.004823215085	0.940173677670
N	-1.204694241899	1.077581081233	1.819186715807
H	-2.078275353045	1.580160668054	1.657276255956

C	-0.085802270183	1.988332817061	2.039130714478
H	0.286839542001	2.421295912423	1.087550336300
C	-0.490116293231	3.104066348898	2.996167937084
H	-1.306854529807	3.713381237330	2.573251839949
H	0.361799752163	3.773791464079	3.188703496816
H	-0.834242689444	2.690992844566	3.957720374263
H	0.750269681057	1.411918294267	2.469402834292
C	0.135855613657	-0.385259720566	0.348051961899
H	1.048704003883	0.179663677966	0.530690438917
C	0.209822069821	-1.501765726665	-0.510897049477
C	1.529532340670	-1.840911205104	-1.093065083605
O	2.564526919052	-1.227989586774	-0.874873135737
O	1.482337758706	-2.918856834449	-1.909027334643
C	2.732313695721	-3.318166956118	-2.519694839799
C	2.454428541836	-4.539422173844	-3.371522451265
H	2.066438741789	-5.368388909890	-2.758932631372
H	3.385458398252	-4.874139692663	-3.854999634681
H	1.718787317433	-4.312900016472	-4.159235214082
H	3.465614398151	-3.527897338900	-1.724848295509
H	3.120196114093	-2.478049966167	-3.117534636494

SCF Done: E(RB3LYP) = -688.833955743

Zero-point correction= 0.260467
Thermal correction to Energy= 0.276063
Thermal correction to Enthalpy= 0.277007
Thermal correction to Gibbs Free Energy= 0.216936
Sum of electronic and zero-point Energies= -688.573489
Sum of electronic and thermal Energies= -688.557893
Sum of electronic and thermal Enthalpies= -688.556949
Sum of electronic and thermal Free Energies= -688.617019

1	C	Isotropic =	71.9051	Anisotropy =	162.7871
2	H	Isotropic =	24.0107	Anisotropy =	7.6033
3	C	Isotropic =	80.5257	Anisotropy =	127.9786
4	H	Isotropic =	24.8484	Anisotropy =	6.1658
5	C	Isotropic =	51.4298	Anisotropy =	155.4977
6	N	Isotropic =	197.6880	Anisotropy =	43.4213
7	H	Isotropic =	28.3946	Anisotropy =	9.1638
8	H	Isotropic =	28.0368	Anisotropy =	12.3340
9	C	Isotropic =	55.9606	Anisotropy =	140.5592
10	N	Isotropic =	181.3113	Anisotropy =	45.2762
11	H	Isotropic =	29.3038	Anisotropy =	7.7048
12	C	Isotropic =	150.3170	Anisotropy =	28.8060
13	H	Isotropic =	28.3909	Anisotropy =	7.1730
14	C	Isotropic =	175.7442	Anisotropy =	25.1548
15	H	Isotropic =	30.1585	Anisotropy =	8.0096
16	H	Isotropic =	29.9520	Anisotropy =	9.8899
17	H	Isotropic =	29.9934	Anisotropy =	7.9206
18	H	Isotropic =	28.3692	Anisotropy =	6.6630
19	C	Isotropic =	80.9279	Anisotropy =	152.3602
20	H	Isotropic =	24.3350	Anisotropy =	11.0262
21	C	Isotropic =	72.5291	Anisotropy =	134.0787
22	C	Isotropic =	27.7022	Anisotropy =	82.6636
23	O	Isotropic =	-22.8400	Anisotropy =	533.4242
24	O	Isotropic =	140.4448	Anisotropy =	143.4587

25	C	Isotropic =	129.5138	Anisotropy =	55.5093
26	C	Isotropic =	176.8087	Anisotropy =	20.9787
27	H	Isotropic =	29.9162	Anisotropy =	7.5342
28	H	Isotropic =	30.0603	Anisotropy =	9.6764
29	H	Isotropic =	29.9115	Anisotropy =	7.4961
30	H	Isotropic =	27.2330	Anisotropy =	6.2451
31	H	Isotropic =	27.2615	Anisotropy =	6.3413

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.476915043144	-2.124788197202	-1.321978156751
H	0.499062329053	-2.269426053087	-2.401431586910
C	0.948735902138	-3.126256311858	-0.471636873175
H	1.347169488294	-4.054854309107	-0.888443817798
C	0.941919253768	-2.959032423663	0.920411562910
N	1.378265348054	-3.952224511577	1.794017577086
H	1.909401212116	-4.697001993357	1.349828886603
H	1.881023344064	-3.587333541605	2.603021216427
C	0.420607092691	-1.750790146538	1.479696881355
N	0.439786592654	-1.633965540829	2.875710355276
H	0.181708996074	-2.513164002371	3.325484495119
C	-0.185672640432	-0.486295997090	3.524747079655
H	-1.252669727822	-0.380477906955	3.238015290571
C	-0.062343079922	-0.600851414242	5.039959828050
H	0.994084371685	-0.674572040576	5.343526875690
H	-0.589466313862	-1.494568065968	5.414965440442
H	-0.505914970720	0.279265774912	5.529884752079
H	0.323947965727	0.427785843407	3.176700354749
C	-0.037227817827	-0.754178949750	0.617162717558
H	-0.438941824691	0.179198262004	1.008424129507
C	-0.006348904788	-0.924880957854	-0.782806610616
C	-0.510451371392	0.184620027305	-1.625687516013
O	-0.939859226295	1.245309666106	-1.195436651045
O	-0.451546996258	-0.091186713143	-2.948704834770
C	-0.927738958168	0.943248141981	-3.841989933905
C	-0.768605754619	0.431681618330	-5.258756437026
H	0.287061615958	0.212331057954	-5.483324274769
H	-1.121535392741	1.194322733279	-5.970396520445
H	-1.357348546735	-0.485714155335	-5.416038711174
H	-0.344134307893	1.860913543040	-3.666544641407
H	-1.979042721255	1.165916563789	-3.599540877271

SCF Done: E(RB3LYP) = -688.833982207

Zero-point correction= 0.260575
Thermal correction to Energy= 0.276144
Thermal correction to Enthalpy= 0.277088
Thermal correction to Gibbs Free Energy= 0.217075
Sum of electronic and zero-point Energies= -688.573407
Sum of electronic and thermal Energies= -688.557838
Sum of electronic and thermal Enthalpies= -688.556894
Sum of electronic and thermal Free Energies= -688.616907

1	C	Isotropic =	71.9263	Anisotropy =	162.8795
2	H	Isotropic =	24.0140	Anisotropy =	7.5913
3	C	Isotropic =	80.4006	Anisotropy =	127.8451
4	H	Isotropic =	24.8476	Anisotropy =	6.1695
5	C	Isotropic =	51.3415	Anisotropy =	155.4214
6	N	Isotropic =	197.7602	Anisotropy =	43.3119
7	H	Isotropic =	28.0340	Anisotropy =	12.3259
8	H	Isotropic =	28.4090	Anisotropy =	9.1602
9	C	Isotropic =	56.0883	Anisotropy =	140.7136
10	N	Isotropic =	181.2864	Anisotropy =	44.4357
11	H	Isotropic =	29.3086	Anisotropy =	7.6969
12	C	Isotropic =	150.4004	Anisotropy =	28.7975
13	H	Isotropic =	28.3835	Anisotropy =	7.2022
14	C	Isotropic =	175.6833	Anisotropy =	25.2217
15	H	Isotropic =	29.9933	Anisotropy =	7.9145
16	H	Isotropic =	30.1556	Anisotropy =	8.0080
17	H	Isotropic =	29.9512	Anisotropy =	9.8815
18	H	Isotropic =	28.3662	Anisotropy =	6.6281
19	C	Isotropic =	80.8599	Anisotropy =	152.4033
20	H	Isotropic =	24.3320	Anisotropy =	11.0414
21	C	Isotropic =	72.5344	Anisotropy =	134.1603
22	C	Isotropic =	27.7380	Anisotropy =	82.9020
23	O	Isotropic =	-22.9434	Anisotropy =	533.8101
24	O	Isotropic =	140.3738	Anisotropy =	143.5694
25	C	Isotropic =	129.5402	Anisotropy =	55.4698
26	C	Isotropic =	176.8167	Anisotropy =	20.9772
27	H	Isotropic =	29.9148	Anisotropy =	7.5432
28	H	Isotropic =	30.0621	Anisotropy =	9.6792
29	H	Isotropic =	29.9125	Anisotropy =	7.4891
30	H	Isotropic =	27.2426	Anisotropy =	6.2601
31	H	Isotropic =	27.2523	Anisotropy =	6.3122

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.768046911627	0.356397642454	0.463922801595
H	2.821667105333	0.557007579207	0.268168518925
C	1.054675481161	1.127844407136	1.380980944071
H	1.547501534060	1.948103006105	1.909242239268
C	-0.304001602904	0.883380475147	1.627751510859
N	-1.037731690715	1.616197043165	2.557953277449
H	-0.586900922251	2.475298098797	2.862887608057
H	-1.996229281592	1.801033131040	2.261617105644
C	-0.958986727224	-0.188848266649	0.946085705504
N	-2.316840110321	-0.388561304412	1.228994114302
H	-2.509860738577	-0.271772890698	2.224539101106
C	-3.022465772608	-1.536770096230	0.669194992742
H	-2.523577565937	-2.494082002232	0.927311159798
C	-4.469153856594	-1.557282791812	1.149699441086
H	-4.987690923780	-0.625242172704	0.873924541204
H	-4.522551423004	-1.667288226381	2.246221513019
H	-5.011223929811	-2.404084345553	0.701978153293

H	-2.996110455927	-1.456737824843	-0.430546450669
C	-0.234861306030	-0.945710920315	0.022266480203
H	-0.715476287769	-1.764565302026	-0.508580007901
C	1.126732721659	-0.676138807101	-0.232658247804
C	1.916174854092	-1.464545272636	-1.208003374896
O	3.100186216060	-1.285257124359	-1.452414205548
O	1.187105365331	-2.427728589551	-1.818465357922
C	1.886805126775	-3.248050383299	-2.784073007181
C	0.897925655761	-4.258444868361	-3.327770892608
H	0.050700393709	-3.756731013057	-3.821215618416
H	0.504499671702	-4.898789432681	-2.522701117800
H	1.396215340027	-4.902863189024	-4.068735445464
H	2.740491173904	-3.733827229433	-2.285397165874
H	2.289845043847	-2.597849329692	-3.576728316043

SCF Done: E(RB3LYP) = -688.833785451

Zero-point correction= 0.260351
Thermal correction to Energy= 0.275975
Thermal correction to Enthalpy= 0.276919
Thermal correction to Gibbs Free Energy= 0.216764
Sum of electronic and zero-point Energies= -688.573434
Sum of electronic and thermal Energies= -688.557811
Sum of electronic and thermal Enthalpies= -688.556867
Sum of electronic and thermal Free Energies= -688.617021

1	C	Isotropic =	71.0270	Anisotropy =	165.9337
2	H	Isotropic =	23.9714	Anisotropy =	6.4341
3	C	Isotropic =	80.2137	Anisotropy =	128.5779
4	H	Isotropic =	24.7914	Anisotropy =	5.8515
5	C	Isotropic =	51.3467	Anisotropy =	155.4168
6	N	Isotropic =	197.6424	Anisotropy =	43.8633
7	H	Isotropic =	28.0443	Anisotropy =	12.4602
8	H	Isotropic =	28.4070	Anisotropy =	9.0170
9	C	Isotropic =	56.2503	Anisotropy =	140.5162
10	N	Isotropic =	181.0918	Anisotropy =	44.7264
11	H	Isotropic =	29.3115	Anisotropy =	7.8531
12	C	Isotropic =	150.3039	Anisotropy =	28.5433
13	H	Isotropic =	28.4088	Anisotropy =	7.1768
14	C	Isotropic =	175.6972	Anisotropy =	25.2112
15	H	Isotropic =	29.9929	Anisotropy =	7.9597
16	H	Isotropic =	30.1560	Anisotropy =	8.0715
17	H	Isotropic =	29.9558	Anisotropy =	9.7665
18	H	Isotropic =	28.3963	Anisotropy =	6.7265
19	C	Isotropic =	81.7712	Anisotropy =	150.1340
20	H	Isotropic =	24.3651	Anisotropy =	11.9909
21	C	Isotropic =	72.5654	Anisotropy =	134.2694
22	C	Isotropic =	27.9264	Anisotropy =	82.8148
23	O	Isotropic =	-23.8236	Anisotropy =	533.4061
24	O	Isotropic =	139.6634	Anisotropy =	142.7593
25	C	Isotropic =	129.5457	Anisotropy =	55.5518
26	C	Isotropic =	176.7859	Anisotropy =	20.5726
27	H	Isotropic =	29.8895	Anisotropy =	7.2080
28	H	Isotropic =	29.8899	Anisotropy =	7.2514
29	H	Isotropic =	30.0517	Anisotropy =	9.7918
30	H	Isotropic =	27.2331	Anisotropy =	6.5455

31 H Isotropic = 27.2596 Anisotropy = 6.6190

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.115666919970	-0.215700220227	-1.203365909531
H	1.712866228724	-0.400358928666	-2.095497467719
C	1.081004109281	1.059124911540	-0.635644306337
H	1.658221235730	1.872644819249	-1.082670456443
C	0.330765419406	1.318734079867	0.520073575244
N	0.255414245756	2.586318599776	1.092479114124
H	0.958184480504	3.239950571746	0.756256673143
H	0.240682310630	2.569761463370	2.112306439531
C	-0.432452637898	0.264889060747	1.112697088272
N	-1.162969989239	0.577172599746	2.266596389968
H	-1.604902330987	1.494067400002	2.189696092267
C	-2.058448428250	-0.412157018507	2.857209615842
H	-1.457539306561	-1.287986029390	3.154380327789
C	-2.761842044006	0.169304733958	4.078423279656
H	-3.412443138072	-0.586556854587	4.544022103052
H	-3.393603774093	1.030209447092	3.800967634045
H	-2.029805825617	0.509812926740	4.827935073436
H	-2.808707081803	-0.778737954924	2.126033683100
C	-0.379364802899	-1.006729803113	0.540794922942
H	-0.945292806810	-1.833047343954	0.968024211359
C	0.396823387795	-1.261767497862	-0.609148558471
C	0.401257316459	-2.642020065983	-1.148184209124
O	-0.211264941157	-3.581116764112	-0.660805825496
O	1.164765713848	-2.770929023739	-2.257426928576
C	1.224944524900	-4.091853475612	-2.846032826759
C	2.130260268986	-4.010620122828	-4.057662599685
H	1.735963720862	-3.297344652606	-4.798424113085
H	2.200755119229	-5.000401707834	-4.535107869782
H	3.145131415459	-3.692331973354	-3.771815507991
H	0.204416756594	-4.408506772710	-3.114048438637
H	1.606303933259	-4.799774403824	-2.093071206136

SCF Done: E(RB3LYP) = -688.833972518

Zero-point correction= 0.260505
Thermal correction to Energy= 0.276097
Thermal correction to Enthalpy= 0.277042
Thermal correction to Gibbs Free Energy= 0.217089
Sum of electronic and zero-point Energies= -688.573467
Sum of electronic and thermal Energies= -688.557875
Sum of electronic and thermal Enthalpies= -688.556931
Sum of electronic and thermal Free Energies= -688.616884

1 C Isotropic = 71.8707 Anisotropy = 163.1233
2 H Isotropic = 24.0080 Anisotropy = 7.5974
3 C Isotropic = 80.4946 Anisotropy = 127.6650
4 H Isotropic = 24.8560 Anisotropy = 6.1576
5 C Isotropic = 51.3950 Anisotropy = 155.4987

6	N	Isotropic =	197.6353	Anisotropy =	43.4560
7	H	Isotropic =	28.0405	Anisotropy =	12.3230
8	H	Isotropic =	28.4010	Anisotropy =	9.1524
9	C	Isotropic =	56.1317	Anisotropy =	140.7611
10	N	Isotropic =	181.3241	Anisotropy =	44.7922
11	H	Isotropic =	29.3112	Anisotropy =	7.6956
12	C	Isotropic =	150.2518	Anisotropy =	28.8925
13	H	Isotropic =	28.3681	Anisotropy =	6.6186
14	C	Isotropic =	175.6800	Anisotropy =	25.1479
15	H	Isotropic =	29.9512	Anisotropy =	9.8892
16	H	Isotropic =	30.1527	Anisotropy =	8.0048
17	H	Isotropic =	29.9952	Anisotropy =	7.9069
18	H	Isotropic =	28.3844	Anisotropy =	7.1951
19	C	Isotropic =	80.9914	Anisotropy =	152.5596
20	H	Isotropic =	24.3365	Anisotropy =	11.0392
21	C	Isotropic =	72.5443	Anisotropy =	134.0477
22	C	Isotropic =	27.7189	Anisotropy =	82.9029
23	O	Isotropic =	-23.1217	Anisotropy =	532.8410
24	O	Isotropic =	140.2657	Anisotropy =	143.5284
25	C	Isotropic =	129.4587	Anisotropy =	55.4343
26	C	Isotropic =	176.8398	Anisotropy =	20.8749
27	H	Isotropic =	29.9120	Anisotropy =	7.4941
28	H	Isotropic =	30.0595	Anisotropy =	9.6778
29	H	Isotropic =	29.9219	Anisotropy =	7.5422
30	H	Isotropic =	27.2499	Anisotropy =	6.3078
31	H	Isotropic =	27.2404	Anisotropy =	6.2595

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.422412900843	-0.077520164840	-0.565172851202
H	2.116376696659	0.074472985198	-1.390917965901
C	1.606208005649	0.604721165046	0.638743202035
H	2.444447256231	1.297017664406	0.752082481337
C	0.718894483967	0.435672396916	1.711087432404
N	0.891843772302	1.080879699139	2.933247085684
H	0.014675266917	1.381061828155	3.358616842633
H	1.558843862716	1.848191004115	2.911441150477
C	-0.379018763745	-0.470612063520	1.577632376098
N	-1.236758456321	-0.600033291724	2.677808296680
H	-0.715962178909	-0.615440011486	3.555606382857
C	-2.306747787445	-1.592445100979	2.661200167749
H	-1.918460202569	-2.615035982406	2.473212636826
C	-3.080239600102	-1.561632045021	3.974577660802
H	-3.498533613964	-0.559548328881	4.160199041382
H	-2.429287550572	-1.823983291392	4.825838799439
H	-3.907919279061	-2.286716547251	3.950738145391
H	-2.984334216768	-1.356116510301	1.823707916097
C	-0.556508013734	-1.137109929179	0.364678460687
H	-1.384345583491	-1.831014347638	0.227523413501
C	0.330190906491	-0.942655750919	-0.715110508573
C	0.066300483712	-1.685354102864	-1.969859562027
O	-0.874674014535	-2.446255055356	-2.143217059337

O	0.986206848254	-1.437686795949	-2.930397783696
C	0.799319819506	-2.122659701012	-4.191658004879
C	1.930763220550	-1.706186427418	-5.108574465762
H	1.921090524527	-0.618118278865	-5.278843085780
H	1.823519582937	-2.208750696737	-6.082488751526
H	2.907369725240	-1.984547898895	-4.682289187542
H	-0.185843992215	-1.849534618332	-4.602076345632
H	0.794779896929	-3.209029802011	-4.009265920220

SCF Done: E(RB3LYP) = -688.833976767

Zero-point correction= 0.260427
Thermal correction to Energy= 0.276032
Thermal correction to Enthalpy= 0.276977
Thermal correction to Gibbs Free Energy= 0.216966
Sum of electronic and zero-point Energies= -688.573550
Sum of electronic and thermal Energies= -688.557944
Sum of electronic and thermal Enthalpies= -688.557000
Sum of electronic and thermal Free Energies= -688.617011

1	C	Isotropic =	71.8192	Anisotropy =	162.8656
2	H	Isotropic =	24.0099	Anisotropy =	7.6070
3	C	Isotropic =	80.5111	Anisotropy =	127.7063
4	H	Isotropic =	24.8540	Anisotropy =	6.1601
5	C	Isotropic =	51.3991	Anisotropy =	155.7846
6	N	Isotropic =	197.6546	Anisotropy =	43.4458
7	H	Isotropic =	28.4003	Anisotropy =	9.1495
8	H	Isotropic =	28.0403	Anisotropy =	12.3276
9	C	Isotropic =	56.0139	Anisotropy =	140.7523
10	N	Isotropic =	181.4035	Anisotropy =	44.4955
11	H	Isotropic =	29.2975	Anisotropy =	7.7149
12	C	Isotropic =	150.2353	Anisotropy =	28.9298
13	H	Isotropic =	28.3771	Anisotropy =	7.2088
14	C	Isotropic =	175.7925	Anisotropy =	25.0575
15	H	Isotropic =	30.0016	Anisotropy =	7.9108
16	H	Isotropic =	30.1585	Anisotropy =	8.0130
17	H	Isotropic =	29.9521	Anisotropy =	9.8919
18	H	Isotropic =	28.3605	Anisotropy =	6.6195
19	C	Isotropic =	80.8764	Anisotropy =	152.2401
20	H	Isotropic =	24.3326	Anisotropy =	11.0381
21	C	Isotropic =	72.5746	Anisotropy =	134.1354
22	C	Isotropic =	27.7035	Anisotropy =	82.8238
23	O	Isotropic =	-22.9856	Anisotropy =	533.1780
24	O	Isotropic =	140.4137	Anisotropy =	143.3885
25	C	Isotropic =	129.4444	Anisotropy =	55.5318
26	C	Isotropic =	176.8034	Anisotropy =	20.9017
27	H	Isotropic =	29.9182	Anisotropy =	7.5362
28	H	Isotropic =	30.0550	Anisotropy =	9.6859
29	H	Isotropic =	29.9169	Anisotropy =	7.4904
30	H	Isotropic =	27.2518	Anisotropy =	6.2937
31	H	Isotropic =	27.2382	Anisotropy =	6.3004

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)

#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.078138182863	-1.693299106940	0.369329500756
H	-3.128735284497	-1.556540989791	0.112135312161
C	-1.697481749129	-2.615848920760	1.343461280557
H	-2.454080801633	-3.208376581160	1.864243021684
C	-0.348901559465	-2.786433637260	1.688220303375
N	0.067313600798	-3.718681441024	2.635498162461
H	0.841172089932	-3.390564999875	3.213381318991
H	-0.681060482269	-4.088295031951	3.216425703559
C	0.650511089422	-2.019357279173	1.012719673339
N	1.981208700315	-2.225966873056	1.400265415217
H	2.173380002184	-3.216243955938	1.556616144438
C	3.066874309833	-1.566927641878	0.681808103657
H	2.930660503258	-0.476369042612	0.774602622519
C	4.414370026718	-1.970373985746	1.269849996654
H	4.466453062610	-1.718725228951	2.341096025911
H	5.232862609098	-1.450823680112	0.748778758900
H	4.584889701375	-3.055293878206	1.164433280795
H	3.043320219422	-1.796002821791	-0.403972230811
C	0.253630350348	-1.092767186705	0.045961575269
H	0.998850017734	-0.499019142626	-0.478846661175
C	-1.108779933767	-0.915126287440	-0.276716536029
C	-1.556255791725	0.064158571615	-1.294934206493
O	-2.720188281075	0.248080051653	-1.619428844112
O	-0.531454721136	0.754136743596	-1.847595294793
C	-0.884660523176	1.730649994828	-2.855935847798
C	0.399276128531	2.369366279634	-3.343598438244
H	0.930184007749	2.869529409989	-2.518406750974
H	0.169509105807	3.123001826384	-4.112907916305
H	1.071139417492	1.617651351577	-3.786870790669
H	-1.569436299999	2.469545755283	-2.410212407390
H	-1.426951331892	1.222057728435	-3.668760275450

SCF Done: E(RB3LYP) = -688.833790563

Zero-point correction= 0.260367
Thermal correction to Energy= 0.275995
Thermal correction to Enthalpy= 0.276939
Thermal correction to Gibbs Free Energy= 0.216712
Sum of electronic and zero-point Energies= -688.573424
Sum of electronic and thermal Energies= -688.557796
Sum of electronic and thermal Enthalpies= -688.556851
Sum of electronic and thermal Free Energies= -688.617079

1	C	Isotropic =	70.8578	Anisotropy = 166.2391
2	H	Isotropic =	23.9609	Anisotropy = 6.4563
3	C	Isotropic =	80.2842	Anisotropy = 128.6035
4	H	Isotropic =	24.7922	Anisotropy = 5.8577
5	C	Isotropic =	51.4056	Anisotropy = 155.8990
6	N	Isotropic =	197.5930	Anisotropy = 43.9265
7	H	Isotropic =	28.3923	Anisotropy = 9.0016
8	H	Isotropic =	28.0474	Anisotropy = 12.4621
9	C	Isotropic =	56.3859	Anisotropy = 140.5826
10	N	Isotropic =	181.1747	Anisotropy = 44.3041
11	H	Isotropic =	29.3243	Anisotropy = 7.8506

12	C	Isotropic =	150.4084	Anisotropy =	28.4651
13	H	Isotropic =	28.4006	Anisotropy =	6.7228
14	C	Isotropic =	175.7293	Anisotropy =	25.1765
15	H	Isotropic =	29.9981	Anisotropy =	7.9575
16	H	Isotropic =	29.9572	Anisotropy =	9.7649
17	H	Isotropic =	30.1563	Anisotropy =	8.0732
18	H	Isotropic =	28.3975	Anisotropy =	7.2126
19	C	Isotropic =	81.6981	Anisotropy =	149.9850
20	H	Isotropic =	24.3627	Anisotropy =	11.9864
21	C	Isotropic =	72.5604	Anisotropy =	134.1736
22	C	Isotropic =	27.8882	Anisotropy =	82.6880
23	O	Isotropic =	-23.5903	Anisotropy =	533.3657
24	O	Isotropic =	139.7053	Anisotropy =	142.6939
25	C	Isotropic =	129.4986	Anisotropy =	55.5978
26	C	Isotropic =	176.8498	Anisotropy =	20.5046
27	H	Isotropic =	29.8972	Anisotropy =	7.2155
28	H	Isotropic =	30.0539	Anisotropy =	9.7902
29	H	Isotropic =	29.8987	Anisotropy =	7.2610
30	H	Isotropic =	27.2554	Anisotropy =	6.6142
31	H	Isotropic =	27.2317	Anisotropy =	6.5475

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.616787635363	-0.679295170848	-1.624006024692
H	-2.085361927689	-1.110826075976	-2.508757527011
C	-2.093478727092	0.510981351554	-1.075323724466
H	-2.948678684610	1.020143540155	-1.527184622223
C	-1.504328081993	1.063324961631	0.071157328062
N	-1.935279672189	2.264614998591	0.628609830801
H	-2.839776409992	2.583729061169	0.290720710454
H	-1.911238981950	2.268695993637	1.648387671634
C	-0.384122640383	0.407281514971	0.669970645349
N	0.161805885066	1.001056664583	1.815908077161
H	0.204904478690	2.016754155857	1.723364009543
C	1.373142462510	0.456688745521	2.420014114168
H	2.213263584311	0.413749201318	1.696000691546
C	1.776659012298	1.281190315325	3.637469754242
H	2.670337042714	0.850882149747	4.114505727890
H	0.962925091524	1.308506928590	4.379520935882
H	2.015983746208	2.319971074539	3.353110170540
H	1.169289302049	-0.583231702890	2.725572927595
C	0.075695024231	-0.789315787194	0.115497211976
H	0.925975361940	-1.304803081782	0.556843720118
C	-0.539354366737	-1.345985991116	-1.026300992621
C	-0.075645285391	-2.616946792853	-1.630951457051
O	-0.558302108490	-3.128973962672	-2.630334039441
O	0.957491405863	-3.174154198471	-0.957301484488
C	1.468720099934	-4.421814470761	-1.483678375576
C	2.609236264973	-4.862017732532	-0.589381584833
H	2.263703590947	-5.015197268095	0.445086821651
H	3.416651595986	-4.113019956438	-0.580979911679
H	3.024518397856	-5.812676325487	-0.958698810544

H	1.797306625388	-4.261241853598	-2.522747714783
H	0.651265549390	-5.160000286475	-1.503294079202

SCF Done: E(RB3LYP) = -688.833833082

Zero-point correction= 0.260506
Thermal correction to Energy= 0.276091
Thermal correction to Enthalpy= 0.277035
Thermal correction to Gibbs Free Energy= 0.216925
Sum of electronic and zero-point Energies= -688.573327
Sum of electronic and thermal Energies= -688.557742
Sum of electronic and thermal Enthalpies= -688.556798
Sum of electronic and thermal Free Energies= -688.616908

1	C	Isotropic =	70.9356	Anisotropy =	166.1231
2	H	Isotropic =	23.9677	Anisotropy =	6.4549
3	C	Isotropic =	80.3283	Anisotropy =	128.5926
4	H	Isotropic =	24.7932	Anisotropy =	5.8410
5	C	Isotropic =	51.3220	Anisotropy =	155.6812
6	N	Isotropic =	197.5667	Anisotropy =	43.8816
7	H	Isotropic =	28.0456	Anisotropy =	12.4578
8	H	Isotropic =	28.3963	Anisotropy =	8.9900
9	C	Isotropic =	56.3683	Anisotropy =	140.6481
10	N	Isotropic =	180.9887	Anisotropy =	43.6992
11	H	Isotropic =	29.3145	Anisotropy =	7.8485
12	C	Isotropic =	150.4586	Anisotropy =	28.3641
13	H	Isotropic =	28.4028	Anisotropy =	7.2267
14	C	Isotropic =	175.6117	Anisotropy =	25.2905
15	H	Isotropic =	29.9560	Anisotropy =	9.7528
16	H	Isotropic =	29.9964	Anisotropy =	7.9362
17	H	Isotropic =	30.1453	Anisotropy =	8.0821
18	H	Isotropic =	28.4051	Anisotropy =	6.7067
19	C	Isotropic =	81.9095	Anisotropy =	150.3228
20	H	Isotropic =	24.3695	Anisotropy =	11.9693
21	C	Isotropic =	72.6178	Anisotropy =	134.1708
22	C	Isotropic =	27.9322	Anisotropy =	82.9132
23	O	Isotropic =	-24.0516	Anisotropy =	531.8350
24	O	Isotropic =	139.6382	Anisotropy =	142.8230
25	C	Isotropic =	129.4754	Anisotropy =	55.5322
26	C	Isotropic =	176.7882	Anisotropy =	20.4523
27	H	Isotropic =	29.9017	Anisotropy =	7.2135
28	H	Isotropic =	29.8945	Anisotropy =	7.2585
29	H	Isotropic =	30.0482	Anisotropy =	9.7913
30	H	Isotropic =	27.2358	Anisotropy =	6.5509
31	H	Isotropic =	27.2520	Anisotropy =	6.5892

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.924736267792	0.254330769883	-0.098139316790
H	2.950588875845	0.289926709522	-0.465525050846
C	1.414299716801	1.285555127836	0.689850363776
H	2.044024110249	2.139729728501	0.951732985413

C	0.099891236342	1.239129599109	1.176389169935
N	-0.449718286258	2.265497605080	1.940840340800
H	0.231834468294	2.923669231505	2.310095021364
H	-1.065228354738	1.932863479833	2.683119247724
C	-0.734903751026	0.129154303226	0.837952875405
N	-2.038482854572	0.132969616872	1.351950613266
H	-2.451505048125	1.065550329848	1.310523166911
C	-2.988498240724	-0.901365370488	0.955329347701
H	-2.587537887995	-1.879060110994	1.271380633858
C	-4.341261483059	-0.660520835941	1.615946703613
H	-5.049753367824	-1.457721818216	1.344218420292
H	-4.776304590527	0.299802524866	1.291004282598
H	-4.243815876703	-0.638088782964	2.713017333389
H	-3.108547821588	-0.951304070657	-0.146940876136
C	-0.206695737694	-0.901253988533	0.056958578691
H	-0.825445379608	-1.755109833887	-0.210050333679
C	1.124650137455	-0.852925248115	-0.408789864681
C	1.709637233882	-1.934368812959	-1.236097881939
O	2.849019314772	-1.933580978894	-1.678466094195
O	0.843980434619	-2.949531760125	-1.463619384098
C	1.337877220841	-4.046235905827	-2.268831393089
C	0.214196818890	-5.051957800024	-2.410321117427
H	-0.659535922222	-4.601254393905	-2.906737908015
H	-0.100848705867	-5.433673913678	-1.426451719577
H	0.554510377829	-5.904754849157	-3.018211642764
H	2.220315528761	-4.481491402691	-1.773384816810
H	1.664231566157	-3.652049149027	-3.244261684687

SCF Done: E(RB3LYP) = -688.833807793

Zero-point correction= 0.260540
Thermal correction to Energy= 0.276090
Thermal correction to Enthalpy= 0.277034
Thermal correction to Gibbs Free Energy= 0.217295
Sum of electronic and zero-point Energies= -688.573267
Sum of electronic and thermal Energies= -688.557718
Sum of electronic and thermal Enthalpies= -688.556774
Sum of electronic and thermal Free Energies= -688.616512

1	C	Isotropic = 70.9645	Anisotropy =	166.0159
2	H	Isotropic = 23.9666	Anisotropy =	6.4450
3	C	Isotropic = 80.3702	Anisotropy =	128.6592
4	H	Isotropic = 24.7947	Anisotropy =	5.8470
5	C	Isotropic = 51.4023	Anisotropy =	155.5275
6	N	Isotropic = 197.6328	Anisotropy =	43.8929
7	H	Isotropic = 28.0466	Anisotropy =	12.4586
8	H	Isotropic = 28.4033	Anisotropy =	9.0177
9	C	Isotropic = 56.2832	Anisotropy =	140.4298
10	N	Isotropic = 181.0526	Anisotropy =	44.6971
11	H	Isotropic = 29.3178	Anisotropy =	7.8479
12	C	Isotropic = 150.4955	Anisotropy =	28.5216
13	H	Isotropic = 28.4040	Anisotropy =	6.7419
14	C	Isotropic = 175.6668	Anisotropy =	25.3035
15	H	Isotropic = 29.9590	Anisotropy =	9.7637
16	H	Isotropic = 30.1515	Anisotropy =	8.0687
17	H	Isotropic = 29.9937	Anisotropy =	7.9524

18	H	Isotropic =	28.4056	Anisotropy =	7.1980
19	C	Isotropic =	81.7935	Anisotropy =	149.9655
20	H	Isotropic =	24.3660	Anisotropy =	11.9788
21	C	Isotropic =	72.5882	Anisotropy =	134.2740
22	C	Isotropic =	27.9014	Anisotropy =	82.8161
23	O	Isotropic =	-23.9023	Anisotropy =	532.2608
24	O	Isotropic =	139.6155	Anisotropy =	142.4912
25	C	Isotropic =	129.4726	Anisotropy =	55.6192
26	C	Isotropic =	176.8281	Anisotropy =	20.5372
27	H	Isotropic =	29.8985	Anisotropy =	7.2619
28	H	Isotropic =	29.9007	Anisotropy =	7.2159
29	H	Isotropic =	30.0491	Anisotropy =	9.7909
30	H	Isotropic =	27.2600	Anisotropy =	6.6271
31	H	Isotropic =	27.2321	Anisotropy =	6.5390

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.204422938960	-2.373068443042	1.691144673018
H	0.843975624670	-3.117510757420	2.165916736272
C	-1.025479253598	-2.029276451104	2.251751231942
H	-1.363041627102	-2.510715148359	3.173235130291
C	-1.858291270717	-1.082121701365	1.638774927304
N	-3.078845723788	-0.694673818492	2.186761364091
H	-3.420638790579	-1.307811078470	2.922579648905
H	-3.804201880307	-0.535610376574	1.487350317397
C	-1.427094044973	-0.443123982871	0.434859601655
N	-2.299470119820	0.493086478463	-0.135852947151
H	-2.737284323796	1.076035394502	0.578608231460
C	-1.883454601387	1.273977438388	-1.296077142500
H	-1.661405595694	0.575898954506	-2.120572400068
C	-2.992198007253	2.232138162826	-1.716516006073
H	-3.213779005491	2.959072135511	-0.916738911879
H	-3.919242076309	1.682907265434	-1.945654742264
H	-2.692160552762	2.799740780468	-2.610513795447
H	-0.947963693167	1.838489898724	-1.100538972044
C	-0.198038982153	-0.805384947770	-0.120882481926
H	0.146536398168	-0.331678024729	-1.037441674184
C	0.621363518795	-1.775947127570	0.494316738457
C	1.927605512941	-2.179959010691	-0.077355533547
O	2.683734130215	-2.999015996153	0.423817909778
O	2.214167681410	-1.541731847682	-1.235821972472
C	3.476651841252	-1.877475850684	-1.859297461306
C	3.589818649579	-1.061027008834	-3.130050396985
H	2.766673408121	-1.293726036298	-3.823754586105
H	4.541372020148	-1.290083920953	-3.634777052456
H	3.567157599375	0.017873845979	-2.909952511220
H	3.496206709840	-2.960168656793	-2.061275317203
H	4.292043515422	-1.655750168948	-1.152522605739

SCF Done: E(RB3LYP) = -688.833840454

Zero-point correction= 0.260531

Thermal correction to Energy= 0.276091
Thermal correction to Enthalpy= 0.277036
Thermal correction to Gibbs Free Energy= 0.217120
Sum of electronic and zero-point Energies= -688.573309
Sum of electronic and thermal Energies= -688.557749
Sum of electronic and thermal Enthalpies= -688.556805
Sum of electronic and thermal Free Energies= -688.616721

1	C	Isotropic =	70.9143	Anisotropy =	165.8893
2	H	Isotropic =	23.9689	Anisotropy =	6.4456
3	C	Isotropic =	80.3021	Anisotropy =	128.6135
4	H	Isotropic =	24.7894	Anisotropy =	5.8492
5	C	Isotropic =	51.4377	Anisotropy =	155.6202
6	N	Isotropic =	197.7355	Anisotropy =	43.6945
7	H	Isotropic =	28.0459	Anisotropy =	12.4593
8	H	Isotropic =	28.4042	Anisotropy =	9.0250
9	C	Isotropic =	56.2787	Anisotropy =	140.5540
10	N	Isotropic =	181.2258	Anisotropy =	44.2723
11	H	Isotropic =	29.3136	Anisotropy =	7.8840
12	C	Isotropic =	150.3610	Anisotropy =	28.4831
13	H	Isotropic =	28.3935	Anisotropy =	6.7116
14	C	Isotropic =	175.7239	Anisotropy =	25.1268
15	H	Isotropic =	30.1652	Anisotropy =	8.0764
16	H	Isotropic =	30.0068	Anisotropy =	7.9436
17	H	Isotropic =	29.9630	Anisotropy =	9.7565
18	H	Isotropic =	28.4043	Anisotropy =	7.2181
19	C	Isotropic =	81.5811	Anisotropy =	149.7901
20	H	Isotropic =	24.3679	Anisotropy =	11.9818
21	C	Isotropic =	72.5579	Anisotropy =	134.3628
22	C	Isotropic =	27.8237	Anisotropy =	82.5321
23	O	Isotropic =	-23.2153	Anisotropy =	534.8810
24	O	Isotropic =	139.6256	Anisotropy =	142.7556
25	C	Isotropic =	129.3773	Anisotropy =	55.7274
26	C	Isotropic =	176.7980	Anisotropy =	20.5833
27	H	Isotropic =	29.9077	Anisotropy =	7.2071
28	H	Isotropic =	30.0419	Anisotropy =	9.8033
29	H	Isotropic =	29.8995	Anisotropy =	7.2428
30	H	Isotropic =	27.2363	Anisotropy =	6.5878
31	H	Isotropic =	27.2447	Anisotropy =	6.5977

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.404081712404	0.772436471013	0.321675507522
H	2.448472685511	1.083947283666	0.350199192238
C	0.383000523610	1.677712016471	0.609717369849
H	0.622755436160	2.713856415924	0.862209487162
C	-0.962908913938	1.287013253429	0.560824738032
N	-2.005246542068	2.158265569151	0.869220709347
H	-2.826181081420	2.032610657362	0.276817014541
H	-1.735442473415	3.138278519936	0.901379990192
C	-1.289385199525	-0.065993240772	0.235168088159
N	-2.649223665870	-0.401038051954	0.197181531862

H	-3.162085862920	0.039548028756	0.961792069272
C	-3.060223872549	-1.786153300458	-0.006712559567
H	-2.612030137918	-2.465690971291	0.747806962080
C	-4.580186919078	-1.899385554051	0.028696360083
H	-5.039862585649	-1.253009495109	-0.735835921500
H	-4.977917786000	-1.601019420540	1.013579012336
H	-4.893252500090	-2.937912434852	-0.157862996530
H	-2.684500710876	-2.117917068665	-0.989245096775
C	-0.256928643472	-0.958845744620	-0.060737492281
H	-0.484894646466	-1.992229083523	-0.312543362018
C	1.092771195800	-0.547630976089	-0.029273870289
C	2.205646135292	-1.474831483091	-0.342708503106
O	3.390276295067	-1.175375290969	-0.315234364525
O	1.778677848173	-2.716648986258	-0.670167780773
C	2.804800434208	-3.686349592488	-0.989125283722
C	2.113551582505	-4.998577197718	-1.296710794573
H	1.536163991999	-5.354069677848	-0.428822065912
H	2.864799192930	-5.763516222745	-1.547910944754
H	1.428767778475	-4.893427333701	-2.152861425933
H	3.491430932186	-3.772378755640	-0.132167387423
H	3.388005796930	-3.316858333328	-1.847608182995

SCF Done: E(RB3LYP) = -688.833807933

Zero-point correction= 0.260467
Thermal correction to Energy= 0.276068
Thermal correction to Enthalpy= 0.277012
Thermal correction to Gibbs Free Energy= 0.216894
Sum of electronic and zero-point Energies= -688.573341
Sum of electronic and thermal Energies= -688.557740
Sum of electronic and thermal Enthalpies= -688.556796
Sum of electronic and thermal Free Energies= -688.616914

1	C	Isotropic =	70.9578	Anisotropy =	166.0321
2	H	Isotropic =	23.9671	Anisotropy =	6.4455
3	C	Isotropic =	80.1742	Anisotropy =	128.5914
4	H	Isotropic =	24.7871	Anisotropy =	5.8580
5	C	Isotropic =	51.4277	Anisotropy =	155.6423
6	N	Isotropic =	197.6549	Anisotropy =	43.8424
7	H	Isotropic =	28.4083	Anisotropy =	9.0196
8	H	Isotropic =	28.0485	Anisotropy =	12.4637
9	C	Isotropic =	56.3870	Anisotropy =	140.7714
10	N	Isotropic =	181.1373	Anisotropy =	44.7556
11	H	Isotropic =	29.3143	Anisotropy =	7.8734
12	C	Isotropic =	150.4016	Anisotropy =	28.5556
13	H	Isotropic =	28.4058	Anisotropy =	7.1851
14	C	Isotropic =	175.7130	Anisotropy =	25.1950
15	H	Isotropic =	29.9943	Anisotropy =	7.9513
16	H	Isotropic =	30.1559	Anisotropy =	8.0709
17	H	Isotropic =	29.9563	Anisotropy =	9.7644
18	H	Isotropic =	28.3939	Anisotropy =	6.7410
19	C	Isotropic =	81.7279	Anisotropy =	149.9481
20	H	Isotropic =	24.3606	Anisotropy =	11.9895
21	C	Isotropic =	72.5392	Anisotropy =	134.3229
22	C	Isotropic =	27.9259	Anisotropy =	82.7149
23	O	Isotropic =	-23.6944	Anisotropy =	533.1597

24	O	Isotropic =	139.6754	Anisotropy =	142.4469
25	C	Isotropic =	129.5954	Anisotropy =	55.6014
26	C	Isotropic =	176.7579	Anisotropy =	20.6501
27	H	Isotropic =	29.8953	Anisotropy =	7.2491
28	H	Isotropic =	30.0557	Anisotropy =	9.7918
29	H	Isotropic =	29.8876	Anisotropy =	7.2039
30	H	Isotropic =	27.2227	Anisotropy =	6.5152
31	H	Isotropic =	27.2710	Anisotropy =	6.6487

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-2.022435056184	-1.425093368219	-0.960308374913
H	-2.559827902564	-1.634107009298	-1.885574955533
C	-2.701387333205	-1.346317820787	0.255378811093
H	-3.784633639907	-1.488414610707	0.289689571296
C	-2.017727966149	-1.064352182260	1.446900409125
N	-2.660691866627	-1.007003537123	2.681141325588
H	-3.674441323270	-0.951728628297	2.622791363326
H	-2.296823103199	-0.276758504758	3.293394776440
C	-0.600539237339	-0.879913650743	1.416112960229
N	0.031687096387	-0.599882460700	2.634943651358
H	-0.356757622326	-1.163439034861	3.392305796528
C	1.487044572302	-0.520411244695	2.705684335238
H	1.821079343132	0.297016770878	2.044831213071
C	1.935597284880	-0.242752346133	4.136014632028
H	1.488755405107	0.690749370075	4.513585270193
H	3.031226415133	-0.149835506412	4.184363268650
H	1.638583822998	-1.062457442358	4.812059244999
H	1.969810675879	-1.446513771972	2.329891280735
C	0.064343841598	-0.950553550141	0.189849874229
H	1.142225309286	-0.811458054419	0.144755452626
C	-0.638253590254	-1.213875357302	-1.005469922529
C	0.044259887138	-1.291373564976	-2.318656457931
O	-0.511756681327	-1.536619886613	-3.379081289902
O	1.375040432362	-1.059896675925	-2.233762062220
C	2.118286228607	-1.119874804586	-3.474341289510
C	3.569757873369	-0.830867383155	-3.151894920055
H	4.169027322899	-0.867021179112	-4.075030822282
H	3.974383218961	-1.575618962263	-2.448609819827
H	3.683702896507	0.169496971620	-2.705532984932
H	1.697240500576	-0.383101180719	-4.176713534957
H	1.985713195230	-2.118531394038	-3.920066802159

SCF Done: E(RB3LYP) = -688.833810133

Zero-point correction= 0.260440
Thermal correction to Energy= 0.276047
Thermal correction to Enthalpy= 0.276991
Thermal correction to Gibbs Free Energy= 0.216820
Sum of electronic and zero-point Energies= -688.573371
Sum of electronic and thermal Energies= -688.557764
Sum of electronic and thermal Enthalpies= -688.556819

Sum of electronic and thermal Free Energies= -688.616990

1	C	Isotropic =	70.9507	Anisotropy =	166.1661
2	H	Isotropic =	23.9662	Anisotropy =	6.4477
3	C	Isotropic =	80.2867	Anisotropy =	128.6037
4	H	Isotropic =	24.7903	Anisotropy =	5.8496
5	C	Isotropic =	51.4014	Anisotropy =	155.5183
6	N	Isotropic =	197.6518	Anisotropy =	43.7382
7	H	Isotropic =	28.0450	Anisotropy =	12.4598
8	H	Isotropic =	28.4074	Anisotropy =	9.0214
9	C	Isotropic =	56.2422	Anisotropy =	140.7124
10	N	Isotropic =	181.0839	Anisotropy =	44.8457
11	H	Isotropic =	29.3111	Anisotropy =	7.8581
12	C	Isotropic =	150.2976	Anisotropy =	28.6503
13	H	Isotropic =	28.3962	Anisotropy =	6.7275
14	C	Isotropic =	175.7379	Anisotropy =	25.1306
15	H	Isotropic =	29.9989	Anisotropy =	7.9546
16	H	Isotropic =	29.9591	Anisotropy =	9.7614
17	H	Isotropic =	30.1557	Anisotropy =	8.0761
18	H	Isotropic =	28.4067	Anisotropy =	7.1704
19	C	Isotropic =	81.6629	Anisotropy =	150.0266
20	H	Isotropic =	24.3603	Anisotropy =	11.9938
21	C	Isotropic =	72.5508	Anisotropy =	134.2548
22	C	Isotropic =	27.9019	Anisotropy =	82.7254
23	O	Isotropic =	-23.7946	Anisotropy =	533.5756
24	O	Isotropic =	139.6917	Anisotropy =	142.5825
25	C	Isotropic =	129.5223	Anisotropy =	55.5685
26	C	Isotropic =	176.8120	Anisotropy =	20.5468
27	H	Isotropic =	30.0542	Anisotropy =	9.7869
28	H	Isotropic =	29.8916	Anisotropy =	7.2581
29	H	Isotropic =	29.8990	Anisotropy =	7.2105
30	H	Isotropic =	27.2428	Anisotropy =	6.5721
31	H	Isotropic =	27.2443	Anisotropy =	6.5830

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.688573537672	0.651838248922	-1.517290322590
H	1.247023558958	0.848427382278	-2.432787896503
C	0.071946369678	1.691814161914	-0.822193220740
H	0.138794064382	2.717128830404	-1.195064658044
C	-0.658402965343	1.443665005488	0.349003482544
N	-1.261883773909	2.462007440061	1.082829947336
H	-1.333387597401	3.348238571588	0.589214048570
H	-2.165109133654	2.196433150864	1.475381063696
C	-0.750104662201	0.107569823275	0.848988137734
N	-1.494224192018	-0.084079590663	2.020840750988
H	-1.322978981844	0.661747410583	2.696455280960
C	-1.537601409914	-1.396220720837	2.657736802908
H	-0.521377588524	-1.773881374684	2.895708729656
C	-2.383744426361	-1.343394014629	3.924873938010
H	-2.444341567561	-2.339533852406	4.388974988980
H	-3.405868944385	-0.999495066607	3.699995192097

H	-1.945854185519	-0.653913277180	4.666592852142
H	-1.978550249572	-2.112442482669	1.944208675966
C	-0.136504019550	-0.925156855653	0.136457980338
H	-0.196388030265	-1.948804384605	0.499503113861
C	0.577740223532	-0.665172468538	-1.052733428601
C	1.235315308086	-1.743079769171	-1.828479377493
O	1.880127655826	-1.569665338088	-2.852180547313
O	1.052300837132	-2.969206987553	-1.285532738999
C	1.667005281905	-4.078595021894	-1.983253935474
C	1.337552950465	-5.341272081604	-1.214267871027
H	0.248903364356	-5.500059415186	-1.163172711107
H	1.732512505816	-5.293096747906	-0.187307062270
H	1.789615148659	-6.210319878625	-1.717278164781
H	2.752927141508	-3.903050728690	-2.042433403321
H	1.278083780045	-4.109689968189	-3.013379647522

SCF Done: E(RB3LYP) = -688.833802893

Zero-point correction= 0.260459
Thermal correction to Energy= 0.276048
Thermal correction to Enthalpy= 0.276992
Thermal correction to Gibbs Free Energy= 0.217034
Sum of electronic and zero-point Energies= -688.573344
Sum of electronic and thermal Energies= -688.557755
Sum of electronic and thermal Enthalpies= -688.556811
Sum of electronic and thermal Free Energies= -688.616769

1	C	Isotropic =	70.9542	Anisotropy =	166.0075
2	H	Isotropic =	23.9671	Anisotropy =	6.4478
3	C	Isotropic =	80.3032	Anisotropy =	128.5982
4	H	Isotropic =	24.7916	Anisotropy =	5.8452
5	C	Isotropic =	51.4255	Anisotropy =	155.6988
6	N	Isotropic =	197.5784	Anisotropy =	43.8016
7	H	Isotropic =	28.0463	Anisotropy =	12.4573
8	H	Isotropic =	28.4077	Anisotropy =	8.9998
9	C	Isotropic =	56.3412	Anisotropy =	140.4494
10	N	Isotropic =	181.0268	Anisotropy =	44.0728
11	H	Isotropic =	29.3220	Anisotropy =	7.8389
12	C	Isotropic =	150.2689	Anisotropy =	28.4936
13	H	Isotropic =	28.4019	Anisotropy =	7.1927
14	C	Isotropic =	175.7405	Anisotropy =	25.1017
15	H	Isotropic =	29.9566	Anisotropy =	9.7645
16	H	Isotropic =	30.0021	Anisotropy =	7.9463
17	H	Isotropic =	30.1563	Anisotropy =	8.0749
18	H	Isotropic =	28.4006	Anisotropy =	6.7212
19	C	Isotropic =	81.6421	Anisotropy =	149.8730
20	H	Isotropic =	24.3632	Anisotropy =	11.9926
21	C	Isotropic =	72.5938	Anisotropy =	134.2264
22	C	Isotropic =	27.8898	Anisotropy =	82.7528
23	O	Isotropic =	-23.6702	Anisotropy =	533.5306
24	O	Isotropic =	139.8179	Anisotropy =	142.4432
25	C	Isotropic =	129.4829	Anisotropy =	55.6083
26	C	Isotropic =	176.7914	Anisotropy =	20.6314
27	H	Isotropic =	29.8988	Anisotropy =	7.1999
28	H	Isotropic =	29.8920	Anisotropy =	7.2559
29	H	Isotropic =	30.0470	Anisotropy =	9.7962

30 H Isotropic = 27.2491 Anisotropy = 6.5873
31 H Isotropic = 27.2470 Anisotropy = 6.5770

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.330001158863	1.145296799718	0.602071451820
H	-0.730677357995	2.113871286166	0.302029046142
C	0.239001212274	0.970456388305	1.863355918253
H	0.293216316102	1.809121216644	2.562300368172
C	0.768789391474	-0.268957412805	2.250474499365
N	1.319447822780	-0.485826130098	3.511157425651
H	2.134773648443	-1.098527347013	3.495033982256
H	1.521081343376	0.363720149798	4.032461258712
C	0.700745835932	-1.374341734673	1.346429904439
N	1.247697057166	-2.588315127415	1.783510483010
H	1.023591901598	-2.765490994799	2.763540910575
C	1.111986363609	-3.791053581140	0.968496098291
H	1.607405435862	-3.609944998149	-0.000120147899
C	1.762011655017	-4.980877245270	1.665616582835
H	1.264399605137	-5.199047809002	2.625804191272
H	2.826360275774	-4.782834207635	1.869359699401
H	1.688165169090	-5.882090080975	1.038146595325
H	0.049639196304	-4.018606846345	0.741367844463
C	0.138332447002	-1.181384789371	0.082675138242
H	0.079901433360	-2.009016707436	-0.620865992945
C	-0.371576162104	0.076821745637	-0.303136495086
C	-0.968368578610	0.308002649173	-1.639742441314
O	-1.442291624584	1.369621884114	-2.016677549949
O	-0.939103287103	-0.793199141555	-2.426054466598
C	-1.503870299306	-0.651384345399	-3.751237268312
C	-1.368413448943	-1.987780410841	-4.451190394368
H	-1.911791825612	-2.776049781285	-3.906801134431
H	-0.311161695402	-2.285106572714	-4.533791173211
H	-1.787560609601	-1.918473699586	-5.467126772164
H	-0.965238586345	0.148973871467	-4.283003332602
H	-2.556151475834	-0.339247027518	-3.657604229341

SCF Done: E(RB3LYP) = -688.833812151

Zero-point correction= 0.260490
Thermal correction to Energy= 0.276074
Thermal correction to Enthalpy= 0.277018
Thermal correction to Gibbs Free Energy= 0.216971
Sum of electronic and zero-point Energies= -688.573323
Sum of electronic and thermal Energies= -688.557738
Sum of electronic and thermal Enthalpies= -688.556794
Sum of electronic and thermal Free Energies= -688.616841

1 C Isotropic = 70.9308 Anisotropy = 166.0190
2 H Isotropic = 23.9694 Anisotropy = 6.4343
3 C Isotropic = 80.3287 Anisotropy = 128.7569
4 H Isotropic = 24.7912 Anisotropy = 5.8498

5	C	Isotropic =	51.3351	Anisotropy =	155.7489
6	N	Isotropic =	197.6084	Anisotropy =	43.8990
7	H	Isotropic =	28.4055	Anisotropy =	8.9933
8	H	Isotropic =	28.0407	Anisotropy =	12.4628
9	C	Isotropic =	56.3384	Anisotropy =	140.5273
10	N	Isotropic =	180.9704	Anisotropy =	44.1845
11	H	Isotropic =	29.3231	Anisotropy =	7.8418
12	C	Isotropic =	150.3582	Anisotropy =	28.3538
13	H	Isotropic =	28.3994	Anisotropy =	6.7204
14	C	Isotropic =	175.7085	Anisotropy =	25.1867
15	H	Isotropic =	30.1550	Anisotropy =	8.0746
16	H	Isotropic =	29.9974	Anisotropy =	7.9550
17	H	Isotropic =	29.9571	Anisotropy =	9.7626
18	H	Isotropic =	28.4063	Anisotropy =	7.2109
19	C	Isotropic =	81.7388	Anisotropy =	149.8872
20	H	Isotropic =	24.3643	Anisotropy =	11.9835
21	C	Isotropic =	72.6090	Anisotropy =	134.2891
22	C	Isotropic =	27.9000	Anisotropy =	82.6730
23	O	Isotropic =	-23.7459	Anisotropy =	533.1664
24	O	Isotropic =	139.6299	Anisotropy =	142.6218
25	C	Isotropic =	129.4709	Anisotropy =	55.6407
26	C	Isotropic =	176.7981	Anisotropy =	20.5811
27	H	Isotropic =	29.8950	Anisotropy =	7.2618
28	H	Isotropic =	29.9007	Anisotropy =	7.2049
29	H	Isotropic =	30.0472	Anisotropy =	9.7976
30	H	Isotropic =	27.2500	Anisotropy =	6.5953
31	H	Isotropic =	27.2433	Anisotropy =	6.5770

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

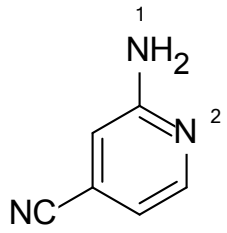
C	-0.078232427994	1.272412517702	0.096333870835
H	-0.512452739213	2.173076591994	-0.338339532362
C	0.772196356243	1.352970964957	1.198835076233
H	1.015476641390	2.325500780868	1.634631308627
C	1.345115824594	0.199560866931	1.753941039044
N	2.175780301265	0.240544258230	2.871259955463
H	2.946530247862	-0.426058512873	2.825612882617
H	2.519361495403	1.168705827588	3.104850734261
C	1.031422358485	-1.078462336007	1.195418333034
N	1.632622274867	-2.196820484110	1.788205640558
H	1.646298889225	-2.116008014093	2.805745053934
C	1.271107785599	-3.542273857997	1.354281211733
H	1.527623994482	-3.642102422547	0.286271602350
C	2.031981949892	-4.584070647816	2.166690193235
H	1.770566660881	-4.521877309873	3.236725293750
H	3.119752635289	-4.438189960772	2.071462836678
H	1.783939011985	-5.598833323586	1.820158712344
H	0.178887039944	-3.722752564706	1.434499187566
C	0.187442591418	-1.142572127178	0.084545562651
H	-0.061468262041	-2.105044561140	-0.356985729033
C	-0.365257046909	0.027565222231	-0.478660991576
C	-1.257951102475	-0.014063798788	-1.660822440574

O	-1.778950182963	0.964773326018	-2.174823371410
O	-1.447637911909	-1.268381987683	-2.132592613559
C	-2.306456815061	-1.395836102319	-3.290750823337
C	-2.373339855711	-2.865533748902	-3.650924551648
H	-1.373371845468	-3.259182853330	-3.891903557796
H	-3.019491389156	-3.002266133425	-4.532048469516
H	-2.791412951714	-3.457240929968	-2.821432841820
H	-1.889595413870	-0.788906455020	-4.110041250018
H	-3.298808114340	-0.985842224388	-3.044352322267

SCF Done: E(RB3LYP) = -688.833787086

Zero-point correction= 0.260419
Thermal correction to Energy= 0.276026
Thermal correction to Enthalpy= 0.276970
Thermal correction to Gibbs Free Energy= 0.216911
Sum of electronic and zero-point Energies= -688.573368
Sum of electronic and thermal Energies= -688.557761
Sum of electronic and thermal Enthalpies= -688.556817
Sum of electronic and thermal Free Energies= -688.616876

1	C	Isotropic =	70.9251	Anisotropy =	166.0070
2	H	Isotropic =	23.9673	Anisotropy =	6.4425
3	C	Isotropic =	80.2664	Anisotropy =	128.8191
4	H	Isotropic =	24.7876	Anisotropy =	5.8490
5	C	Isotropic =	51.4316	Anisotropy =	155.7352
6	N	Isotropic =	197.5892	Anisotropy =	43.8525
7	H	Isotropic =	28.4021	Anisotropy =	9.0000
8	H	Isotropic =	28.0444	Anisotropy =	12.4626
9	C	Isotropic =	56.3424	Anisotropy =	140.5658
10	N	Isotropic =	181.0586	Anisotropy =	44.3303
11	H	Isotropic =	29.3141	Anisotropy =	7.8473
12	C	Isotropic =	150.4382	Anisotropy =	28.4677
13	H	Isotropic =	28.3965	Anisotropy =	6.7367
14	C	Isotropic =	175.6631	Anisotropy =	25.2351
15	H	Isotropic =	30.1609	Anisotropy =	8.0696
16	H	Isotropic =	29.9977	Anisotropy =	7.9492
17	H	Isotropic =	29.9590	Anisotropy =	9.7613
18	H	Isotropic =	28.4021	Anisotropy =	7.2046
19	C	Isotropic =	81.6455	Anisotropy =	149.9471
20	H	Isotropic =	24.3610	Anisotropy =	11.9857
21	C	Isotropic =	72.5676	Anisotropy =	134.3144
22	C	Isotropic =	27.8879	Anisotropy =	82.7296
23	O	Isotropic =	-23.7359	Anisotropy =	533.7493
24	O	Isotropic =	139.6154	Anisotropy =	142.6894
25	C	Isotropic =	129.5076	Anisotropy =	55.6160
26	C	Isotropic =	176.8503	Anisotropy =	20.5342
27	H	Isotropic =	29.9010	Anisotropy =	7.2089
28	H	Isotropic =	30.0492	Anisotropy =	9.7960
29	H	Isotropic =	29.8900	Anisotropy =	7.2631
30	H	Isotropic =	27.2461	Anisotropy =	6.5731
31	H	Isotropic =	27.2439	Anisotropy =	6.5919



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

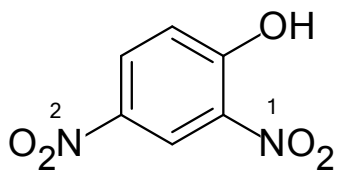
N	1.187626324042	0.748628743740	0.037197121849
C	0.005478869400	1.396966972244	0.058848726147
N	0.053716330948	2.763964248873	0.147756527112
H	-0.760979519073	3.289736494217	-0.148180140526
H	0.945109963414	3.184491509341	-0.094859298542
C	-1.233402949862	0.711757522492	0.042256134337
H	-2.176329487437	1.258812125853	0.057741667317
C	-1.212396489754	-0.681754322494	0.006642791266
C	0.017545177485	-1.369026503538	-0.009473087807
H	0.063012782453	-2.456542042141	-0.037682176174
C	1.172302888882	-0.591206959272	0.007137157042
H	2.152919876343	-1.077780319121	-0.008756854862
C	-2.450352305379	-1.415788747872	-0.013626226188
N	-3.448281461461	-2.014598722322	-0.029752340971

SCF Done: E(RB3LYP) = -395.927570828

Zero-point correction= 0.103572
Thermal correction to Energy= 0.110963
Thermal correction to Enthalpy= 0.111907
Thermal correction to Gibbs Free Energy= 0.071760
Sum of electronic and zero-point Energies= -395.823999
Sum of electronic and thermal Energies= -395.816608
Sum of electronic and thermal Enthalpies= -395.815663
Sum of electronic and thermal Free Energies= -395.855811

1	N	Isotropic =	-26.4787	Anisotropy =	437.7500
2	C	Isotropic =	34.5022	Anisotropy =	157.3954
3	N	Isotropic =	183.1740	Anisotropy =	91.8650
4	H	Isotropic =	27.3600	Anisotropy =	9.7716
5	H	Isotropic =	27.2909	Anisotropy =	11.2187
6	C	Isotropic =	82.7944	Anisotropy =	132.4658
7	H	Isotropic =	24.9313	Anisotropy =	7.6390
8	C	Isotropic =	71.2742	Anisotropy =	147.9050
9	C	Isotropic =	77.9240	Anisotropy =	151.7070
10	H	Isotropic =	24.8139	Anisotropy =	5.4631
11	C	Isotropic =	43.2183	Anisotropy =	163.1013
12	H	Isotropic =	23.2271	Anisotropy =	5.3424
13	C	Isotropic =	78.1602	Anisotropy =	316.6147

14 N Isotropic = -8.2362 Anisotropy = 383.0102



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

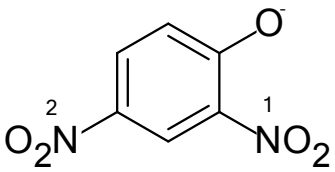
C	1.179817027960	0.744389329115	-0.033655184721
H	2.130129919956	1.275602185310	-0.031827626585
C	-0.018836486469	1.429168121068	-0.085737681613
H	-0.046165744658	2.518092395342	-0.126234390927
C	-1.251285227473	0.738358688749	-0.089006093469
O	-2.369970909288	1.449822693141	-0.141879985287
H	-3.118456375784	0.797622868818	-0.137370814046
C	-1.214990445954	-0.683305613216	-0.035418550077
C	-0.007066055428	-1.381723515078	0.017914794540
H	-0.005013761242	-2.467994076906	0.057588414297
C	1.174940522428	-0.661344045883	0.017948163811
N	-2.445943037120	-1.456516930782	-0.037700578435
O	-3.525120065927	-0.833606383482	-0.090808062594
O	-2.386697449105	-2.673412795327	0.011180676258
N	2.447646010037	-1.385706957098	0.073067987697
O	3.481160436832	-0.722708160431	0.069505353617
O	2.411241641235	-2.612037803340	0.119453577534

SCF Done: E(RB3LYP) = -716.545972031

Zero-point correction= 0.109928
Thermal correction to Energy= 0.120001
Thermal correction to Enthalpy= 0.120945
Thermal correction to Gibbs Free Energy= 0.073191
Sum of electronic and zero-point Energies= -716.436044
Sum of electronic and thermal Energies= -716.425971
Sum of electronic and thermal Enthalpies= -716.425027
Sum of electronic and thermal Free Energies= -716.472781

1 C Isotropic = 59.8426 Anisotropy = 183.4071
2 H Isotropic = 23.0411 Anisotropy = 5.3837
3 C Isotropic = 72.1604 Anisotropy = 141.8133
4 H Isotropic = 24.2914 Anisotropy = 5.3121
5 C Isotropic = 30.9914 Anisotropy = 150.0755
6 O Isotropic = 186.3559 Anisotropy = 194.3129
7 H Isotropic = 19.3165 Anisotropy = 18.5742
8 C Isotropic = 59.2472 Anisotropy = 99.3830
9 C Isotropic = 69.7448 Anisotropy = 172.2523
10 H Isotropic = 22.5688 Anisotropy = 5.1158

11 C Isotropic = 52.5677 Anisotropy = 92.3572
12 N Isotropic = -123.0196 Anisotropy = 268.4158
13 O Isotropic = -216.0588 Anisotropy = 552.2707
14 O Isotropic = -276.7698 Anisotropy = 695.8476
15 N Isotropic = -118.0271 Anisotropy = 268.8617
16 O Isotropic = -257.8335 Anisotropy = 700.0381
17 O Isotropic = -250.4912 Anisotropy = 685.9584



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

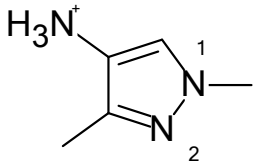
C	-0.266334093424	1.406835874487	-0.485041513234
C	1.073614817220	1.189059506343	-0.173069488322
C	1.515477348581	0.794361132981	1.178728579845
C	0.405311211400	0.656547452615	2.126704338188
C	-0.906035003630	0.868536458113	1.808342798846
C	-1.253067696383	1.250409556116	0.481650341334
O	2.688855342789	0.591686413924	1.540386528794
N	2.016890761171	1.376005455183	-1.257083464239
N	-2.626601498983	1.474390437437	0.133011409019
O	-2.907606954884	1.805709776682	-1.027797347009
O	-3.488126657120	1.327415188482	1.012501645515
O	1.590279943661	1.782441359245	-2.350942405095
O	3.209494796108	1.127326442286	-1.070897941698
H	-0.536636485857	1.699397795704	-1.496086012710
H	0.693146942739	0.364325277880	3.139389657251
H	-1.698712773387	0.752681872522	2.547112873515

SCF Done: E(RB3LYP) = -716.076126210

Zero-point correction= 0.096576
Thermal correction to Energy= 0.106788
Thermal correction to Enthalpy= 0.107732
Thermal correction to Gibbs Free Energy= 0.058785
Sum of electronic and zero-point Energies= -715.979550
Sum of electronic and thermal Energies= -715.969338
Sum of electronic and thermal Enthalpies= -715.968394
Sum of electronic and thermal Free Energies= -716.017342

1 C Isotropic = 65.8555 Anisotropy = 167.2328
2 C Isotropic = 55.8794 Anisotropy = 97.1663
3 C Isotropic = 23.1425 Anisotropy = 140.3708
4 C Isotropic = 63.8046 Anisotropy = 119.7015
5 C Isotropic = 66.1454 Anisotropy = 163.2232

6 C Isotropic = 62.6901 Anisotropy = 83.3165
7 O Isotropic = -98.9780 Anisotropy = 723.4761
8 N Isotropic = -123.6217 Anisotropy = 276.6919
9 N Isotropic = -119.0849 Anisotropy = 275.9051
10 O Isotropic = -210.5415 Anisotropy = 618.1621
11 O Isotropic = -221.8820 Anisotropy = 635.1475
12 O Isotropic = -216.6637 Anisotropy = 589.2525
13 O Isotropic = -264.6168 Anisotropy = 681.1045
14 H Isotropic = 22.5981 Anisotropy = 5.2401
15 H Isotropic = 25.3911 Anisotropy = 4.6701
16 H Isotropic = 23.7845 Anisotropy = 5.2435



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

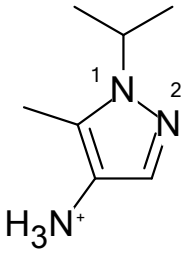
C	-0.316108235973	-0.248814834561	0.278822401140
N	-1.086550455128	-1.123635678615	1.155147477011
H	-0.724135772418	-2.086064978189	1.146568613904
H	-2.076178441974	-1.184317474084	0.875873732887
H	-1.073782372123	-0.814504229994	2.138664669140
C	-0.638355274319	1.074020363398	-0.108203744877
C	-1.825342731665	1.912966367578	0.247386196772
H	-2.767191733725	1.445410724161	-0.083774541703
H	-1.738438338393	2.893275568270	-0.239746215638
H	-1.898703298298	2.070841618930	1.335598567144
N	0.327576111961	1.537083504817	-0.906915390497
N	1.235052060696	0.543602147912	-1.022192194620
C	2.421205931672	0.740357510738	-1.843045052185
H	3.042870139845	-0.161124953278	-1.788375178311
H	2.989943475237	1.603048000266	-1.469219362707
H	2.126743076968	0.922489686523	-2.886176073142
C	0.891512322693	-0.559672715224	-0.323253089603
H	1.503733534943	-1.456740628647	-0.300670814716

SCF Done: E(RB3LYP) = -360.654482546

Zero-point correction= 0.157937
Thermal correction to Energy= 0.166454
Thermal correction to Enthalpy= 0.167399
Thermal correction to Gibbs Free Energy= 0.124813
Sum of electronic and zero-point Energies= -360.496545
Sum of electronic and thermal Energies= -360.488028

Sum of electronic and thermal Enthalpies= -360.487084
Sum of electronic and thermal Free Energies= -360.529670

1	C	Isotropic =	85.2339	Anisotropy =	63.4663
2	N	Isotropic =	225.8546	Anisotropy =	18.1190
3	H	Isotropic =	25.3637	Anisotropy =	14.6975
4	H	Isotropic =	25.5669	Anisotropy =	13.9717
5	H	Isotropic =	25.5686	Anisotropy =	14.7320
6	C	Isotropic =	49.8863	Anisotropy =	128.1276
7	C	Isotropic =	180.3373	Anisotropy =	23.2347
8	H	Isotropic =	29.1082	Anisotropy =	8.4948
9	H	Isotropic =	29.0404	Anisotropy =	8.2506
10	H	Isotropic =	29.1217	Anisotropy =	8.4879
11	N	Isotropic =	-53.6683	Anisotropy =	295.0051
12	N	Isotropic =	49.7157	Anisotropy =	143.9607
13	C	Isotropic =	152.6546	Anisotropy =	61.1191
14	H	Isotropic =	27.8173	Anisotropy =	7.3620
15	H	Isotropic =	27.5621	Anisotropy =	8.3146
16	H	Isotropic =	27.5689	Anisotropy =	8.3972
17	C	Isotropic =	65.2666	Anisotropy =	104.0681
18	H	Isotropic =	23.7972	Anisotropy =	3.8685



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-2.156535944805	0.795064811181	-0.527309900495
N	-0.921917882323	1.287056295826	-0.568135898185
N	-0.135462224400	0.347629954481	0.003797663688
C	-0.824627431650	-0.751702053190	0.417956535432
C	-2.146058833051	-0.474295916776	0.078298284402
C	1.320227886982	0.592485444325	0.099644786564
C	1.935609407946	0.658909869491	-1.300203412905
C	1.590374666900	1.847107977535	0.932758951686
C	-0.203679955389	-1.938918672269	1.081054416039
N	-3.303648261376	-1.333285294557	0.304415978349
H	-2.998333256019	1.358313310429	-0.925873650391
H	1.725950708424	-0.281250230043	0.627845358470
H	1.742870539850	-0.268536699567	-1.861170452304
H	1.518094469857	1.504397702784	-1.867560029175
H	3.024891958121	0.795035725302	-1.220365836780

H	2.676181532027	1.993093963580	1.038089254684
H	1.163297445504	2.736442694400	0.445649715570
H	1.153777609984	1.755080394682	1.939057424293
H	-0.964378977772	-2.693765428715	1.320979681818
H	0.544480960235	-2.416591965022	0.429708564024
H	0.293802091121	-1.657947499259	2.022237351373
H	-3.476212727905	-1.527851460877	1.301653941912
H	-4.160349639723	-0.889698097871	-0.052604553265
H	-3.231454142536	-2.242394825870	-0.174704174803

SCF Done: E(RB3LYP) = -439.287542255

Zero-point correction= 0.214258
Thermal correction to Energy= 0.225255
Thermal correction to Enthalpy= 0.226199
Thermal correction to Gibbs Free Energy= 0.177960
Sum of electronic and zero-point Energies= -439.073285
Sum of electronic and thermal Energies= -439.062287
Sum of electronic and thermal Enthalpies= -439.061343
Sum of electronic and thermal Free Energies= -439.109582

1	C	Isotropic =	62.0913	Anisotropy =	117.1606
2	N	Isotropic =	-42.0800	Anisotropy =	350.3783
3	N	Isotropic =	21.1001	Anisotropy =	156.8376
4	C	Isotropic =	57.4786	Anisotropy =	120.5287
5	C	Isotropic =	85.0171	Anisotropy =	59.8933
6	C	Isotropic =	136.6134	Anisotropy =	41.0766
7	C	Isotropic =	168.3583	Anisotropy =	33.0709
8	C	Isotropic =	168.7721	Anisotropy =	32.3215
9	C	Isotropic =	183.1487	Anisotropy =	12.0202
10	N	Isotropic =	225.1445	Anisotropy =	20.5044
11	H	Isotropic =	23.8537	Anisotropy =	3.2240
12	H	Isotropic =	27.1093	Anisotropy =	6.1069
13	H	Isotropic =	30.0832	Anisotropy =	8.2616
14	H	Isotropic =	29.6774	Anisotropy =	6.8558
15	H	Isotropic =	30.0122	Anisotropy =	9.5222
16	H	Isotropic =	30.0126	Anisotropy =	9.4517
17	H	Isotropic =	29.5762	Anisotropy =	6.9197
18	H	Isotropic =	30.0881	Anisotropy =	8.4173
19	H	Isotropic =	29.0960	Anisotropy =	8.1651
20	H	Isotropic =	29.0278	Anisotropy =	8.8142
21	H	Isotropic =	29.0291	Anisotropy =	8.8809
22	H	Isotropic =	25.4480	Anisotropy =	14.4805
23	H	Isotropic =	25.4679	Anisotropy =	14.6899
24	H	Isotropic =	25.4534	Anisotropy =	14.4116

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

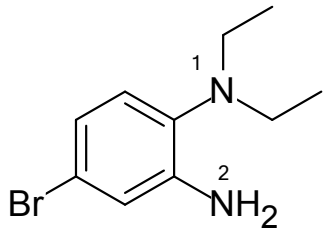
C	-1.820183471482	0.871956489576	-1.313558421383
N	-0.588831439640	1.303709193329	-1.061090310765
N	-0.079365339730	0.457976188258	-0.132596173417
C	-0.959319771424	-0.519187551074	0.233417711339

C	-2.094169262908	-0.261728921859	-0.530974235819
C	1.289271033486	0.755269839407	0.359076949959
C	1.261901618474	1.332744766069	1.777086099020
C	2.241488263462	-0.431289136595	0.198478610587
C	-0.703644861698	-1.612840931527	1.221842030557
N	-3.339423959737	-1.023022634908	-0.516362860565
H	-2.455528829404	1.378365690670	-2.037493336064
H	1.607079391071	1.548542760616	-0.331062728157
H	0.573443357878	2.189164252788	1.836352266974
H	0.957281388544	0.585547759814	2.525951523028
H	2.270721286941	1.682347664171	2.045693054239
H	2.192235853412	-0.843200169471	-0.820837627184
H	3.270818877127	-0.085095855363	0.378412710722
H	2.035815214206	-1.238270423684	0.916835519286
H	-0.269394481575	-1.228553550118	2.154971879602
H	-1.642287653721	-2.120168272875	1.483702188636
H	-0.018418374781	-2.372061739274	0.814385556860
H	-3.195105575127	-2.032905851954	-0.657842970411
H	-3.870460719372	-0.911940084368	0.360414894596
H	-3.965822544000	-0.714469481629	-1.271962331641

SCF Done: E(RB3LYP) = -439.283530953

Zero-point correction= 0.214190
Thermal correction to Energy= 0.225197
Thermal correction to Enthalpy= 0.226141
Thermal correction to Gibbs Free Energy= 0.178043
Sum of electronic and zero-point Energies= -439.069341
Sum of electronic and thermal Energies= -439.058334
Sum of electronic and thermal Enthalpies= -439.057389
Sum of electronic and thermal Free Energies= -439.105488

1	C	Isotropic =	63.3634	Anisotropy =	116.6751
2	N	Isotropic =	-55.3921	Anisotropy =	299.6978
3	N	Isotropic =	21.5187	Anisotropy =	156.9429
4	C	Isotropic =	57.0679	Anisotropy =	125.4280
5	C	Isotropic =	83.0518	Anisotropy =	60.9865
6	C	Isotropic =	128.4363	Anisotropy =	60.4067
7	C	Isotropic =	170.7753	Anisotropy =	29.4909
8	C	Isotropic =	171.4387	Anisotropy =	27.7174
9	C	Isotropic =	182.1452	Anisotropy =	9.9495
10	N	Isotropic =	225.0767	Anisotropy =	19.9647
11	H	Isotropic =	24.0168	Anisotropy =	3.2038
12	H	Isotropic =	26.7492	Anisotropy =	5.6350
13	H	Isotropic =	30.0153	Anisotropy =	8.1632
14	H	Isotropic =	29.6474	Anisotropy =	5.8334
15	H	Isotropic =	30.0044	Anisotropy =	9.7580
16	H	Isotropic =	29.9079	Anisotropy =	7.9967
17	H	Isotropic =	29.9056	Anisotropy =	9.7137
18	H	Isotropic =	29.5861	Anisotropy =	5.6394
19	H	Isotropic =	28.7407	Anisotropy =	7.3306
20	H	Isotropic =	29.0810	Anisotropy =	8.2962
21	H	Isotropic =	28.9256	Anisotropy =	8.4529
22	H	Isotropic =	25.4517	Anisotropy =	13.9028
23	H	Isotropic =	25.4852	Anisotropy =	14.5937
24	H	Isotropic =	25.4707	Anisotropy =	14.8143



Conformer1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.074252506479	0.319381835987	-1.235938173182
H	1.960195823792	0.817996655909	-1.628016676888
C	-0.201941674740	0.861859974770	-1.438728538455
H	-0.287649269796	1.795863681772	-1.996166719436
C	-1.360197547608	0.247099018594	-0.948457731490
N	-2.676635582137	0.777913599559	-1.115255480682
C	-3.489076540179	0.078762380428	-2.134430993676
H	-3.446195576051	-0.998062552389	-1.910290941603
H	-4.536622347345	0.390848536449	-1.983002195626
C	-3.084287289071	0.317706550586	-3.593497657787
H	-2.043419894392	0.006078134514	-3.778044521611
H	-3.180446490935	1.377553174856	-3.880030466895
H	-3.735451206586	-0.268437955067	-4.262932155135
C	-2.816666742334	2.238977510339	-1.139263480491
C	-2.435195010062	2.889467481881	0.188942094317
H	-1.370568106025	2.739482846103	0.426896745919
H	-3.031945485724	2.467453655744	1.013650976972
H	-2.619090250783	3.974924168957	0.145158654921
H	-3.879313373481	2.441722429740	-1.349543967614
H	-2.250078791488	2.715092976432	-1.965709065001
C	-1.229256586125	-0.963199168599	-0.206497988343
N	-2.370502975239	-1.591811223075	0.279470687701
H	-2.213164590979	-2.201694176186	1.077299621914
H	-3.126092679754	-0.927939159526	0.449013745489
C	0.046766929188	-1.522086779516	-0.013412436648
H	0.149996455367	-2.445827360496	0.557920883725
C	1.170371266759	-0.877530811187	-0.529801136326
Br	2.905935029248	-1.663725426579	-0.235513084069

SCF Done: E(RB3LYP) = -3073.78278399

Zero-point correction= 0.235339
Thermal correction to Energy= 0.249215
Thermal correction to Enthalpy= 0.250159
Thermal correction to Gibbs Free Energy= 0.194192
Sum of electronic and zero-point Energies= -3073.547445
Sum of electronic and thermal Energies= -3073.533569
Sum of electronic and thermal Enthalpies= -3073.532625

Sum of electronic and thermal Free Energies= -3073.588592

1	C	Isotropic =	74.6208	Anisotropy =	124.0129
2	H	Isotropic =	24.8928	Anisotropy =	7.9453
3	C	Isotropic =	67.9145	Anisotropy =	170.3225
4	H	Isotropic =	24.4697	Anisotropy =	9.1766
5	C	Isotropic =	59.5362	Anisotropy =	128.6969
6	N	Isotropic =	195.2529	Anisotropy =	66.6199
7	C	Isotropic =	142.4245	Anisotropy =	49.3651
8	H	Isotropic =	28.0823	Anisotropy =	5.9451
9	H	Isotropic =	28.5585	Anisotropy =	7.7425
10	C	Isotropic =	182.2258	Anisotropy =	13.7829
11	H	Isotropic =	30.6000	Anisotropy =	5.5944
12	H	Isotropic =	30.1295	Anisotropy =	7.4978
13	H	Isotropic =	30.8477	Anisotropy =	11.0014
14	C	Isotropic =	145.3696	Anisotropy =	45.3395
15	C	Isotropic =	176.7042	Anisotropy =	24.6118
16	H	Isotropic =	30.3530	Anisotropy =	4.5440
17	H	Isotropic =	30.6159	Anisotropy =	8.4236
18	H	Isotropic =	30.4500	Anisotropy =	10.8532
19	H	Isotropic =	28.7682	Anisotropy =	7.1592
20	H	Isotropic =	27.7029	Anisotropy =	6.5624
21	C	Isotropic =	47.1365	Anisotropy =	154.7097
22	N	Isotropic =	199.6183	Anisotropy =	56.7157
23	H	Isotropic =	28.4156	Anisotropy =	12.6890
24	H	Isotropic =	27.4899	Anisotropy =	8.2697
25	C	Isotropic =	77.5623	Anisotropy =	106.0645
26	H	Isotropic =	24.8605	Anisotropy =	10.0667
27	C	Isotropic =	57.2016	Anisotropy =	91.1503
28	Br	Isotropic =	2115.6497	Anisotropy =	1298.1029

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

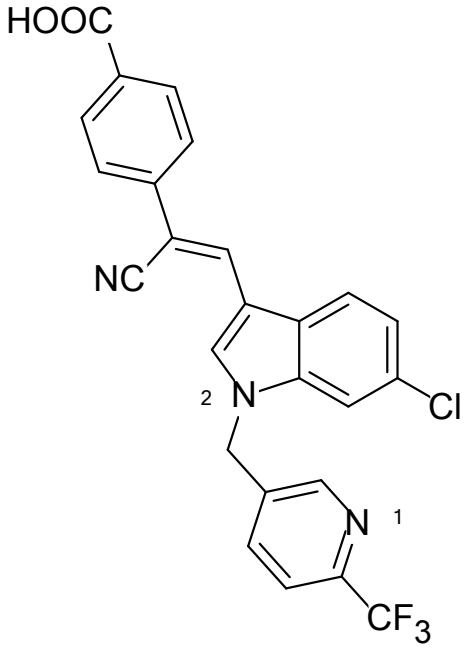
C	-0.225533668579	-1.134078245401	0.394387112285
H	-0.417917923671	-1.766428492203	1.260634120840
C	-0.580127501033	0.221689242547	0.404299484706
H	-1.051615277402	0.629570831106	1.299730943914
C	-0.347102602151	1.061541215340	-0.691180784326
N	-0.673244356970	2.452756301683	-0.712952689873
C	-0.580978425436	3.186817646779	0.555039033778
H	-0.940740081430	4.207315007652	0.345982024530
H	-1.255356721820	2.784421417859	1.338739403761
C	0.847276316448	3.258042942607	1.091507048177
H	1.520055623783	3.713051551820	0.346714503831
H	1.239736233402	2.259902823907	1.340874889806
H	0.877350813450	3.868804293302	2.008052598992
C	-1.869877409759	2.784790195319	-1.516069314154
C	-3.216788168846	2.365428790239	-0.916289478905
H	-4.033911593827	2.638988559612	-1.604186227306
H	-3.411994495336	2.863637369997	0.047182515644
H	-3.263121673390	1.276309083359	-0.754046816460
H	-1.744038240641	2.318822533124	-2.505383900237

H	-1.858235826735	3.876300977286	-1.677950909959
C	0.286305784090	0.516897628066	-1.846589321167
N	0.517628956402	1.335608914970	-2.946700490394
H	1.266978901508	1.024051740743	-3.558820282493
H	0.626750045148	2.312998492314	-2.676058851560
C	0.629833563538	-0.846610080554	-1.869915502130
H	1.119680434620	-1.263970318199	-2.751010202192
C	0.368059050579	-1.645655506970	-0.757336757751
Br	0.865818244059	-3.507264916304	-0.815242151360

SCF Done: E(RB3LYP) = -3073.78273539

Zero-point correction= 0.235211
Thermal correction to Energy= 0.249134
Thermal correction to Enthalpy= 0.250079
Thermal correction to Gibbs Free Energy= 0.193889
Sum of electronic and zero-point Energies= -3073.547524
Sum of electronic and thermal Energies= -3073.533601
Sum of electronic and thermal Enthalpies= -3073.532657
Sum of electronic and thermal Free Energies= -3073.588847

1	C	Isotropic =	74.6055	Anisotropy =	124.1268
2	H	Isotropic =	24.8878	Anisotropy =	7.9527
3	C	Isotropic =	68.0117	Anisotropy =	170.4668
4	H	Isotropic =	24.4630	Anisotropy =	9.2122
5	C	Isotropic =	59.5764	Anisotropy =	128.9972
6	N	Isotropic =	195.2852	Anisotropy =	66.0504
7	C	Isotropic =	145.3953	Anisotropy =	45.2137
8	H	Isotropic =	28.7787	Anisotropy =	7.1303
9	H	Isotropic =	27.7081	Anisotropy =	6.5429
10	C	Isotropic =	176.6921	Anisotropy =	24.6513
11	H	Isotropic =	30.6197	Anisotropy =	8.4493
12	H	Isotropic =	30.3438	Anisotropy =	4.5300
13	H	Isotropic =	30.4523	Anisotropy =	10.8463
14	C	Isotropic =	142.5849	Anisotropy =	49.2098
15	C	Isotropic =	182.1327	Anisotropy =	13.9197
16	H	Isotropic =	30.8540	Anisotropy =	10.9671
17	H	Isotropic =	30.1455	Anisotropy =	7.4515
18	H	Isotropic =	30.6054	Anisotropy =	5.6416
19	H	Isotropic =	28.0725	Anisotropy =	5.8976
20	H	Isotropic =	28.5735	Anisotropy =	7.7439
21	C	Isotropic =	47.2067	Anisotropy =	154.9473
22	N	Isotropic =	199.5595	Anisotropy =	56.8247
23	H	Isotropic =	28.4080	Anisotropy =	12.6861
24	H	Isotropic =	27.4991	Anisotropy =	8.2521
25	C	Isotropic =	77.4953	Anisotropy =	105.9309
26	H	Isotropic =	24.8566	Anisotropy =	10.0641
27	C	Isotropic =	57.2514	Anisotropy =	91.0074
28	Br	Isotropic =	2116.0648	Anisotropy =	1297.5172



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.845543623208	-1.438886828461	0.120688429045
H	-1.464384308910	-2.306053718333	-0.120327861026
C	-1.281936320570	-0.148022402072	-0.187445171008
C	-2.646563774214	0.082568104873	-0.812929172301
H	-3.372139428994	0.358589109158	-0.034140692801
H	-3.010245716448	-0.848136093042	-1.272172755236
C	-0.431456620623	0.920773915432	0.143057210153
H	-0.726576727845	1.949299773753	-0.084735129645
N	0.757717000649	0.771809131465	0.732189420951
C	1.147948640816	-0.477198797580	1.020286024387
C	2.501759983481	-0.575220250738	1.690276942085
F	2.854877763255	-1.856089963736	1.935667537376
F	2.520293552229	0.078372217506	2.873832946150
F	3.476767729999	-0.030016564486	0.929282012028
C	0.394050881601	-1.614747954394	0.740292469889
H	0.762495445358	-2.608438706104	0.991266132144
C	-3.099901302356	3.145198134020	-2.799641765214
C	-3.544055480927	4.479530465122	-3.088202807504
H	-3.302939549807	4.812696086307	-4.099637053713
C	-4.199262360044	5.399092393112	-2.306224328240
C	-3.246310498108	2.372682313395	-1.645234139366
H	-3.731708414914	2.615230812490	-0.705353320019
N	-2.671174576759	1.144456277598	-1.813789874136
C	-2.126985171670	1.067769147708	-3.092108887488
C	-2.375835839602	2.304146471273	-3.741754723416

C	-1.927342089949	2.478112967938	-5.061752821302
H	-2.096723140744	3.413551561501	-5.598029275555
C	-1.255299132227	1.437349298585	-5.696999039431
H	-0.899740510547	1.553175340307	-6.720726212106
C	-1.030211844934	0.224280335558	-5.017326681745
Cl	-0.173994223123	-1.070413454213	-5.860158210028
C	-1.453464644451	0.006655140175	-3.710137625040
H	-1.261797878803	-0.939608275242	-3.206587361122
C	-5.364200948893	9.331289687876	-3.649189840352
C	-5.020275366625	8.336267189349	-4.579447787085
H	-5.057247139641	8.573503845296	-5.643294452840
C	-4.652168527679	7.065105535868	-4.155921617665
H	-4.419938700493	6.310923322953	-4.908269017690
C	-4.604298980343	6.744629818096	-2.781195898128
C	-4.961583401494	7.748563240736	-1.856758726802
H	-4.940875174584	7.531260552259	-0.787590551547
C	-5.333775981660	9.021828946967	-2.280895330711
H	-5.600087445806	9.781396029466	-1.546244217976
C	-5.755780918211	10.672319973559	-4.154753516653
O	-5.797063686032	10.983721950842	-5.331882338472
O	-6.069992345696	11.538847598566	-3.167009266585
H	-6.309836283667	12.380148624822	-3.598035028166
C	-4.512052184804	5.078677918079	-0.945810720565
N	-4.765670731987	4.812559776392	0.161814094471

SCF Done: E(RB3LYP) = -2036.27406239

Zero-point correction= 0.349595
Thermal correction to Energy= 0.378178
Thermal correction to Enthalpy= 0.379122
Thermal correction to Gibbs Free Energy= 0.283978
Sum of electronic and zero-point Energies= -2035.924468
Sum of electronic and thermal Energies= -2035.895884
Sum of electronic and thermal Enthalpies= -2035.894940
Sum of electronic and thermal Free Energies= -2035.990084

1	C	Isotropic =	56.7080	Anisotropy =	183.4160
2	H	Isotropic =	23.4142	Anisotropy =	7.5844
3	C	Isotropic =	55.2640	Anisotropy =	179.3806
4	C	Isotropic =	140.3433	Anisotropy =	40.4611
5	H	Isotropic =	26.0249	Anisotropy =	5.6111
6	H	Isotropic =	26.2604	Anisotropy =	8.0602
7	C	Isotropic =	45.1685	Anisotropy =	168.4112
8	H	Isotropic =	23.0472	Anisotropy =	11.2157
9	N	Isotropic =	-59.5231	Anisotropy =	532.9476
10	C	Isotropic =	42.6570	Anisotropy =	146.7509
11	C	Isotropic =	64.6361	Anisotropy =	15.6472
12	F	Isotropic =	282.0204	Anisotropy =	125.4335
13	F	Isotropic =	261.9192	Anisotropy =	120.8331
14	F	Isotropic =	262.9908	Anisotropy =	119.3987
15	C	Isotropic =	70.9985	Anisotropy =	171.1633
16	H	Isotropic =	23.6378	Anisotropy =	8.2400
17	C	Isotropic =	79.9128	Anisotropy =	115.2635
18	C	Isotropic =	56.8235	Anisotropy =	173.2590
19	H	Isotropic =	23.2222	Anisotropy =	12.0774
20	C	Isotropic =	90.5877	Anisotropy =	77.4077

21	C	Isotropic =	56.6773	Anisotropy =	112.4341
22	H	Isotropic =	22.5482	Anisotropy =	11.3532
23	N	Isotropic =	97.3525	Anisotropy =	121.8349
24	C	Isotropic =	56.9429	Anisotropy =	128.9643
25	C	Isotropic =	63.9992	Anisotropy =	153.6470
26	C	Isotropic =	73.3721	Anisotropy =	164.0541
27	H	Isotropic =	23.5729	Anisotropy =	7.5206
28	C	Isotropic =	69.9187	Anisotropy =	139.4381
29	H	Isotropic =	24.2164	Anisotropy =	7.6317
30	C	Isotropic =	53.4360	Anisotropy =	100.9170
31	Cl	Isotropic =	735.7356	Anisotropy =	456.7106
32	C	Isotropic =	81.3735	Anisotropy =	127.9652
33	H	Isotropic =	24.3915	Anisotropy =	11.6854
34	C	Isotropic =	65.6891	Anisotropy =	148.4837
35	C	Isotropic =	61.3837	Anisotropy =	178.9395
36	H	Isotropic =	23.3283	Anisotropy =	7.7610
37	C	Isotropic =	70.9468	Anisotropy =	165.1040
38	H	Isotropic =	23.5642	Anisotropy =	9.4847
39	C	Isotropic =	51.4172	Anisotropy =	182.4175
40	C	Isotropic =	66.8243	Anisotropy =	161.1865
41	H	Isotropic =	23.7521	Anisotropy =	9.7984
42	C	Isotropic =	61.3873	Anisotropy =	175.0950
43	H	Isotropic =	23.3123	Anisotropy =	8.0238
44	C	Isotropic =	29.6172	Anisotropy =	87.0944
45	O	Isotropic =	-32.5963	Anisotropy =	494.2496
46	O	Isotropic =	149.7261	Anisotropy =	169.5511
47	H	Isotropic =	25.4942	Anisotropy =	11.9630
48	C	Isotropic =	76.4940	Anisotropy =	307.6015
49	N	Isotropic =	-23.0491	Anisotropy =	348.3899

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.621246857260	4.018679642297	2.248321180357
H	1.241240547140	4.917275319385	2.282961724089
C	0.114632369798	3.552120733178	1.032618995578
C	0.460923010380	4.251304959127	-0.270304173084
H	1.311616982245	3.745916231283	-0.749870274441
H	0.778058267935	5.284561166547	-0.067405130658
C	-0.682677367114	2.395432943559	1.063105761350
H	-1.109090073654	1.995835759076	0.138340598362
N	-0.975675864789	1.721872505825	2.178672815580
C	-0.471275952191	2.189048974231	3.328503372662
C	-0.833205069264	1.374847300355	4.552176305800
F	-2.171757236880	1.279580516864	4.712552745807
F	-0.331026239392	1.912254642851	5.685627411670
F	-0.360676943544	0.110497361399	4.465986210129
C	0.328130260767	3.325985585512	3.425235767796
H	0.707163604820	3.665722400858	4.388104893155
C	-1.846690579384	3.803910717277	-3.099629344666
C	-2.326473614518	3.270817362251	-4.343370567575
H	-3.295859562254	3.671437250526	-4.646396036051
C	-1.766668446894	2.363608392875	-5.209386147694

C	-0.675282216042	3.531709650951	-2.389056821391
H	0.138094286366	2.853408114828	-2.626029413881
N	-0.626194397141	4.274682526464	-1.243037443773
C	-1.767919944998	5.065750481802	-1.163255127058
C	-2.558426097224	4.798993024829	-2.310381218151
C	-3.772953547984	5.486855758525	-2.470867758358
H	-4.410630933774	5.313222196800	-3.339501039693
C	-4.168264963637	6.408370312259	-1.504891597786
H	-5.107131881287	6.951641635868	-1.611542898832
C	-3.353112216628	6.645233420992	-0.380710403034
Cl	-3.890477626872	7.823678006202	0.820197851259
C	-2.143746474710	5.988109502937	-0.178624166798
H	-1.534945347423	6.185993443300	0.702327394593
C	-3.617682790257	1.043701005637	-8.877677299468
C	-4.378257456337	1.697940434815	-7.894174515651
H	-5.441577699244	1.861987799448	-8.072592509500
C	-3.792679967619	2.118634175524	-6.706415839250
H	-4.421725523626	2.598443796725	-5.956233808707
C	-2.417445772349	1.908506392201	-6.462112271687
C	-1.666128979369	1.241205039799	-7.452294684222
H	-0.602420197893	1.058211960163	-7.291927949492
C	-2.253256933440	0.816607077265	-8.641641592773
H	-1.649222406473	0.308055949195	-9.392745274139
C	-4.293639890284	0.610668460200	-10.127742435441
O	-5.474022610137	0.786161284857	-10.373223890238
O	-3.460909900250	-0.010925869299	-10.991047224868
H	-3.994579400093	-0.252647393221	-11.770699744477
C	-0.474046217206	1.816925836494	-4.923853290984
N	0.578872155463	1.373616209166	-4.685581134369

SCF Done: E(RB3LYP) = -2036.27405078

Zero-point correction= 0.349666
Thermal correction to Energy= 0.378229
Thermal correction to Enthalpy= 0.379173
Thermal correction to Gibbs Free Energy= 0.284199
Sum of electronic and zero-point Energies= -2035.924385
Sum of electronic and thermal Energies= -2035.895822
Sum of electronic and thermal Enthalpies= -2035.894877
Sum of electronic and thermal Free Energies= -2035.989851

1	C	Isotropic =	56.7688	Anisotropy =	183.6130
2	H	Isotropic =	23.4153	Anisotropy =	7.6355
3	C	Isotropic =	55.1287	Anisotropy =	179.2846
4	C	Isotropic =	140.2569	Anisotropy =	40.8982
5	H	Isotropic =	26.0356	Anisotropy =	5.6938
6	H	Isotropic =	26.2218	Anisotropy =	8.0893
7	C	Isotropic =	45.4274	Anisotropy =	168.2408
8	H	Isotropic =	23.1119	Anisotropy =	11.3034
9	N	Isotropic =	-59.5369	Anisotropy =	533.1668
10	C	Isotropic =	42.6550	Anisotropy =	146.8648
11	C	Isotropic =	64.6187	Anisotropy =	15.6108
12	F	Isotropic =	263.1557	Anisotropy =	119.2531
13	F	Isotropic =	281.9445	Anisotropy =	125.5567
14	F	Isotropic =	261.5482	Anisotropy =	120.9087
15	C	Isotropic =	70.9215	Anisotropy =	171.3935

16	H	Isotropic =	23.6334	Anisotropy =	8.2373
17	C	Isotropic =	79.7787	Anisotropy =	115.0617
18	C	Isotropic =	56.9365	Anisotropy =	173.8212
19	H	Isotropic =	23.1904	Anisotropy =	12.1048
20	C	Isotropic =	90.6066	Anisotropy =	77.3660
21	C	Isotropic =	56.5136	Anisotropy =	112.6639
22	H	Isotropic =	22.5528	Anisotropy =	11.4323
23	N	Isotropic =	97.9497	Anisotropy =	120.5257
24	C	Isotropic =	57.1780	Anisotropy =	128.9797
25	C	Isotropic =	64.3921	Anisotropy =	154.4595
26	C	Isotropic =	73.2480	Anisotropy =	164.1667
27	H	Isotropic =	23.5602	Anisotropy =	7.5352
28	C	Isotropic =	69.8404	Anisotropy =	139.2992
29	H	Isotropic =	24.2137	Anisotropy =	7.6061
30	C	Isotropic =	53.3323	Anisotropy =	100.4309
31	Cl	Isotropic =	735.3475	Anisotropy =	457.1254
32	C	Isotropic =	81.5533	Anisotropy =	127.7566
33	H	Isotropic =	24.3757	Anisotropy =	11.6654
34	C	Isotropic =	65.6478	Anisotropy =	148.3661
35	C	Isotropic =	61.4674	Anisotropy =	179.7061
36	H	Isotropic =	23.2919	Anisotropy =	7.8135
37	C	Isotropic =	70.9866	Anisotropy =	165.1911
38	H	Isotropic =	23.5551	Anisotropy =	9.4419
39	C	Isotropic =	51.5184	Anisotropy =	182.3258
40	C	Isotropic =	66.7452	Anisotropy =	160.3123
41	H	Isotropic =	23.7819	Anisotropy =	9.7958
42	C	Isotropic =	61.8064	Anisotropy =	175.6445
43	H	Isotropic =	23.3397	Anisotropy =	7.9729
44	C	Isotropic =	29.7964	Anisotropy =	87.4007
45	O	Isotropic =	-32.3516	Anisotropy =	494.1873
46	O	Isotropic =	150.2615	Anisotropy =	168.6507
47	H	Isotropic =	25.4933	Anisotropy =	11.9608
48	C	Isotropic =	76.4753	Anisotropy =	307.7839
49	N	Isotropic =	-23.1094	Anisotropy =	348.2545

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.076847709901	-1.788045391029	-0.818482124622
H	-1.892400111895	-2.509666942404	-0.903508906743
C	-1.171966145136	-0.535397403193	-1.429323203557
C	-2.385285852595	-0.167967539014	-2.265562230915
H	-3.215413486748	-0.853177961891	-2.040743974781
H	-2.153471858200	-0.286994445483	-3.333743426689
C	-0.088645034574	0.346448622045	-1.273608199724
H	-0.118245838565	1.341307866157	-1.727963700367
N	1.016147383058	0.054332499593	-0.582761321105
C	1.080781425543	-1.155770063817	-0.010743882929
C	2.359516767228	-1.423821375253	0.753639100136
F	2.360736784620	-2.647238599795	1.327045081389
F	2.550600543328	-0.519225617670	1.739634829786
F	3.444614902486	-1.357821686823	-0.050557832275
C	0.072072532822	-2.112900426676	-0.093124522401

H	0.174345141639	-3.080143297579	0.396898401600
C	-3.243970727058	3.401264420981	-2.502862965319
C	-3.326273453683	4.703505733773	-3.102234199652
H	-3.875680403123	5.431299265755	-2.500986724343
C	-2.815520256588	5.183188481036	-4.283192927112
C	-2.686210614913	2.216270658238	-2.987584869922
H	-2.189472637433	2.018850125542	-3.932178695490
N	-2.842739048241	1.205927255358	-2.080266805934
C	-3.512638903947	1.696485659741	-0.963737504190
C	-3.782509088962	3.070433323916	-1.191871599945
C	-4.463956169325	3.800822020214	-0.203929307082
H	-4.688661500592	4.860367789007	-0.338545748257
C	-4.858738220345	3.160728223354	0.967672877941
H	-5.388189841544	3.710227688916	1.745882048409
C	-4.573962442793	1.793954427766	1.154470809145
Cl	-5.092135817287	1.020004176819	2.655309344356
C	-3.899730839585	1.031186669615	0.206428731316
H	-3.688338122934	-0.022675426625	0.379825606413
C	-3.352359119710	9.235833271872	-5.660877390636
C	-2.313514624216	8.439888326044	-6.167818939398
H	-1.628295604148	8.849420871177	-6.909658898777
C	-2.152178247370	7.129720344718	-5.724150303001
H	-1.334664480516	6.529512961168	-6.127160230122
C	-3.016500469432	6.574031695740	-4.757922268366
C	-4.067758416733	7.379455914981	-4.267985041372
H	-4.784255212006	6.975824637213	-3.551957342154
C	-4.227605218342	8.687861450037	-4.708547193297
H	-5.044563508399	9.301994752248	-4.327927443440
C	-3.568815638639	10.638386052101	-6.101206091729
O	-4.457966832060	11.363458341631	-5.691532996542
O	-2.667336719008	11.049099543645	-7.019738198233
H	-2.892175791774	11.972145257203	-7.240015506669
C	-2.023117871593	4.329839853955	-5.116690237008
N	-1.379373600813	3.631417995693	-5.794824076393

SCF Done: E(RB3LYP) = -2036.27403114

Zero-point correction= 0.349610
Thermal correction to Energy= 0.378186
Thermal correction to Enthalpy= 0.379130
Thermal correction to Gibbs Free Energy= 0.284194
Sum of electronic and zero-point Energies= -2035.924422
Sum of electronic and thermal Energies= -2035.895846
Sum of electronic and thermal Enthalpies= -2035.894901
Sum of electronic and thermal Free Energies= -2035.989837

1	C	Isotropic =	56.5574	Anisotropy = 183.0579
2	H	Isotropic =	23.4142	Anisotropy = 7.5579
3	C	Isotropic =	55.3560	Anisotropy = 179.5548
4	C	Isotropic =	140.3919	Anisotropy = 39.5697
5	H	Isotropic =	26.2922	Anisotropy = 7.9780
6	H	Isotropic =	26.0338	Anisotropy = 5.5853
7	C	Isotropic =	45.0113	Anisotropy = 168.4657
8	H	Isotropic =	22.9695	Anisotropy = 11.0751
9	N	Isotropic =	-59.5205	Anisotropy = 532.9312
10	C	Isotropic =	42.6109	Anisotropy = 146.7853

11	C	Isotropic =	64.5770	Anisotropy =	15.6162
12	F	Isotropic =	282.2411	Anisotropy =	125.1754
13	F	Isotropic =	262.8888	Anisotropy =	119.5559
14	F	Isotropic =	262.0701	Anisotropy =	121.0687
15	C	Isotropic =	70.9696	Anisotropy =	170.9989
16	H	Isotropic =	23.6389	Anisotropy =	8.2848
17	C	Isotropic =	79.6495	Anisotropy =	115.3424
18	C	Isotropic =	56.2730	Anisotropy =	172.6482
19	H	Isotropic =	23.3215	Anisotropy =	12.1104
20	C	Isotropic =	90.1578	Anisotropy =	78.6360
21	C	Isotropic =	57.0306	Anisotropy =	111.6851
22	H	Isotropic =	22.5703	Anisotropy =	11.2250
23	N	Isotropic =	96.9771	Anisotropy =	121.8809
24	C	Isotropic =	56.9736	Anisotropy =	128.6228
25	C	Isotropic =	64.0668	Anisotropy =	153.9591
26	C	Isotropic =	73.6839	Anisotropy =	164.1761
27	H	Isotropic =	23.6182	Anisotropy =	7.5121
28	C	Isotropic =	69.8604	Anisotropy =	139.5497
29	H	Isotropic =	24.2277	Anisotropy =	7.6247
30	C	Isotropic =	53.3253	Anisotropy =	100.6486
31	Cl	Isotropic =	735.5669	Anisotropy =	457.3306
32	C	Isotropic =	81.4580	Anisotropy =	128.0698
33	H	Isotropic =	24.3719	Anisotropy =	11.6431
34	C	Isotropic =	65.7556	Anisotropy =	148.7345
35	C	Isotropic =	62.1593	Anisotropy =	176.0808
36	H	Isotropic =	23.3101	Anisotropy =	8.0068
37	C	Isotropic =	66.4565	Anisotropy =	160.5401
38	H	Isotropic =	23.7924	Anisotropy =	9.6709
39	C	Isotropic =	50.7995	Anisotropy =	182.2844
40	C	Isotropic =	69.9513	Anisotropy =	162.9113
41	H	Isotropic =	23.6464	Anisotropy =	9.3350
42	C	Isotropic =	61.6616	Anisotropy =	180.5297
43	H	Isotropic =	23.2892	Anisotropy =	7.7901
44	C	Isotropic =	29.8212	Anisotropy =	87.6149
45	O	Isotropic =	-31.9600	Anisotropy =	497.2939
46	O	Isotropic =	150.1604	Anisotropy =	168.7682
47	H	Isotropic =	25.4796	Anisotropy =	11.9829
48	C	Isotropic =	76.2420	Anisotropy =	308.1019
49	N	Isotropic =	-21.9242	Anisotropy =	348.0060

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.760953731848	3.292568838089	-0.292026165312
H	-7.060223218589	4.128364035856	0.344425707744
C	-5.516098483514	3.294398739766	-0.927456402097
C	-4.583945440379	4.484975924984	-0.786606284360
H	-4.784320167924	5.006528036808	0.161095722184
H	-4.780119494230	5.206704241493	-1.592806580432
C	-5.192909446266	2.183851670828	-1.724538765669
H	-4.227731410780	2.135559950772	-2.236775179175
N	-6.003696865007	1.137669663066	-1.907831823878
C	-7.192246870933	1.165901566128	-1.291349246307

C	-8.059105822932	-0.049937078209	-1.539101992032
F	-9.256294128041	0.045361910961	-0.920011027469
F	-7.468321049614	-1.182301740084	-1.094605213465
F	-8.302632082280	-0.229831829359	-2.856367754733
C	-7.623802858554	2.210344740312	-0.475726066711
H	-8.599592051733	2.179740928748	0.007069173184
C	-1.037803893362	3.997456470688	-1.628222722369
C	0.156059859751	4.082188731396	-2.421476138154
H	1.042606736183	3.681384897988	-1.925580060592
C	0.359236104436	4.561251562886	-3.692191584822
C	-2.337533705230	4.429430615601	-1.900687943902
H	-2.733269129437	4.928653112891	-2.779374013711
N	-3.165921366004	4.150397658675	-0.849539635239
C	-2.432997772176	3.524958562318	0.154362063830
C	-1.092931073459	3.411311150763	-0.296940945738
C	-0.141409912265	2.816076043273	0.548226392339
H	0.900117672356	2.708044345507	0.239952428850
C	-0.535098509440	2.356933828415	1.802296113562
H	0.188368109928	1.892768482433	2.472481521069
C	-1.876009933568	2.489780292743	2.213083623870
Cl	-2.333597271476	1.893864715666	3.811620167905
C	-2.853186926491	3.069067567247	1.410141617972
H	-3.884212768169	3.153801764838	1.750138120641
C	4.197483137758	4.613920307410	-5.661592520284
C	4.120851303754	4.506255516863	-4.262453142753
H	5.035357719467	4.440609392509	-3.673409700535
C	2.885696463731	4.498939964465	-3.622215988232
H	2.862466121487	4.446000909235	-2.533338412431
C	1.684561007768	4.587619047042	-4.358052144508
C	1.775379206262	4.708464693023	-5.761119826760
H	0.864950853074	4.786118425962	-6.357783042744
C	3.010303162102	4.718410618337	-6.401639502358
H	3.069494116521	4.804720413536	-7.487193592681
C	5.493436681633	4.629538466057	-6.388536166509
O	5.608434108218	4.721070170862	-7.597868891577
O	6.561175131696	4.529700788700	-5.566868419382
H	7.354388890650	4.549372611654	-6.133923256199
C	-0.749303618728	5.054199981980	-4.453207651841
N	-1.654557384346	5.456519288877	-5.070204848189

SCF Done: E(RB3LYP) = -2036.27401621

Zero-point correction= 0.349617
Thermal correction to Energy= 0.378203
Thermal correction to Enthalpy= 0.379147
Thermal correction to Gibbs Free Energy= 0.284108
Sum of electronic and zero-point Energies= -2035.924399
Sum of electronic and thermal Energies= -2035.895814
Sum of electronic and thermal Enthalpies= -2035.894870
Sum of electronic and thermal Free Energies= -2035.989909

1	C	Isotropic = 57.1820	Anisotropy =	184.6725
2	H	Isotropic = 23.4391	Anisotropy =	7.7240
3	C	Isotropic = 54.9482	Anisotropy =	178.4044
4	C	Isotropic = 140.6966	Anisotropy =	43.6516
5	H	Isotropic = 26.1777	Anisotropy =	8.1991

6	H	Isotropic =	26.0034	Anisotropy =	5.5756
7	C	Isotropic =	46.0126	Anisotropy =	168.6017
8	H	Isotropic =	23.1962	Anisotropy =	11.6214
9	N	Isotropic =	-59.0122	Anisotropy =	535.4132
10	C	Isotropic =	42.9279	Anisotropy =	147.0203
11	C	Isotropic =	64.5914	Anisotropy =	15.6187
12	F	Isotropic =	281.8706	Anisotropy =	125.8181
13	F	Isotropic =	261.6911	Anisotropy =	120.4098
14	F	Isotropic =	263.2320	Anisotropy =	120.3797
15	C	Isotropic =	71.0550	Anisotropy =	170.6328
16	H	Isotropic =	23.6686	Anisotropy =	8.1438
17	C	Isotropic =	79.6749	Anisotropy =	115.3713
18	C	Isotropic =	56.4212	Anisotropy =	172.9686
19	H	Isotropic =	23.2706	Anisotropy =	12.0960
20	C	Isotropic =	90.2247	Anisotropy =	77.9759
21	C	Isotropic =	56.7685	Anisotropy =	112.4671
22	H	Isotropic =	22.5825	Anisotropy =	11.3937
23	N	Isotropic =	99.0840	Anisotropy =	118.7220
24	C	Isotropic =	57.2541	Anisotropy =	128.9141
25	C	Isotropic =	64.1010	Anisotropy =	153.9146
26	C	Isotropic =	73.6176	Anisotropy =	164.0810
27	H	Isotropic =	23.5765	Anisotropy =	7.4804
28	C	Isotropic =	69.8634	Anisotropy =	139.7069
29	H	Isotropic =	24.2058	Anisotropy =	7.5914
30	C	Isotropic =	53.1495	Anisotropy =	100.7782
31	Cl	Isotropic =	735.4055	Anisotropy =	457.1292
32	C	Isotropic =	81.4998	Anisotropy =	128.5204
33	H	Isotropic =	24.4163	Anisotropy =	11.6856
34	C	Isotropic =	65.4126	Anisotropy =	148.6095
35	C	Isotropic =	61.8256	Anisotropy =	175.2349
36	H	Isotropic =	23.3327	Anisotropy =	8.3753
37	C	Isotropic =	70.4344	Anisotropy =	163.7966
38	H	Isotropic =	23.6459	Anisotropy =	9.4249
39	C	Isotropic =	50.9701	Anisotropy =	182.0371
40	C	Isotropic =	66.8608	Anisotropy =	161.2403
41	H	Isotropic =	23.7366	Anisotropy =	9.7007
42	C	Isotropic =	61.0119	Anisotropy =	180.4591
43	H	Isotropic =	23.2859	Anisotropy =	7.4068
44	C	Isotropic =	29.7126	Anisotropy =	87.2389
45	O	Isotropic =	-32.3623	Anisotropy =	494.6282
46	O	Isotropic =	149.6555	Anisotropy =	169.2020
47	H	Isotropic =	25.4889	Anisotropy =	11.9280
48	C	Isotropic =	76.4040	Anisotropy =	307.9469
49	N	Isotropic =	-22.4752	Anisotropy =	348.2138

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.948127559056	0.156201115232	-0.550429790971
H	2.954742697846	0.563910203523	-0.667289969770
C	0.832368173550	0.994612899371	-0.607413650170
C	0.992502505395	2.494794619301	-0.782227904335
H	2.003906097974	2.723060852083	-1.148603572531

H	0.882698945355	2.998322058636	0.188963782727
C	-0.433141563471	0.402317837699	-0.456182008156
H	-1.337094763116	1.017126765493	-0.498744843616
N	-0.625193284016	-0.904665382489	-0.262007471335
C	0.463596370161	-1.684181094217	-0.208527297134
C	0.174384725498	-3.152905527936	0.015740563761
F	-0.468384493797	-3.360990384556	1.186944770936
F	1.303293566910	-3.894753398947	0.042230530591
F	-0.615686981465	-3.660023384147	-0.956848641526
C	1.767769422835	-1.213868691448	-0.344413416119
H	2.617899413721	-1.893053783501	-0.297689533809
C	-1.766262956757	4.301381832498	-2.413974521880
C	-2.927732344651	5.140108441931	-2.504829143122
H	-3.286230564964	5.277869045261	-3.526636202198
C	-3.658041071610	5.776382294817	-1.530864642268
C	-1.022653469040	3.897869252807	-1.302336722037
H	-1.160928581838	4.134511752612	-0.252259751122
N	0.014884047531	3.094842863379	-1.685356132614
C	-0.010259974481	2.946399951152	-3.068640460957
C	-1.114171371374	3.688025975025	-3.561950497667
C	-1.354603973922	3.706113271036	-4.946020212511
H	-2.193288941670	4.263606329900	-5.366807096933
C	-0.506206877176	3.001291680936	-5.795605662748
H	-0.676209603686	3.003427984171	-6.872153226271
C	0.581207754856	2.279565298624	-5.265818225065
Cl	1.635305014767	1.400939092412	-6.377935888790
C	0.857190455250	2.230596083651	-3.903241921791
H	1.703031069142	1.661368364186	-3.521263463924
C	-7.133436428329	8.222725985223	-2.287146685701
C	-6.812388466507	7.816369782465	-0.983198670245
H	-7.447586635436	8.114298178557	-0.149285561271
C	-5.685970408326	7.031519405236	-0.749051684427
H	-5.458754614349	6.724223479425	0.272938876427
C	-4.844362542509	6.623305714119	-1.805381766295
C	-5.172586110449	7.049676230305	-3.111594611713
H	-4.538380619416	6.785516870489	-3.957845176042
C	-6.297504982383	7.830426475096	-3.346094265390
H	-6.540420579835	8.156137719668	-4.358177323667
C	-8.321950020171	9.060045829415	-2.592139853745
O	-8.635030083547	9.438142739988	-3.707236572243
O	-9.044200945299	9.373048027486	-1.494105034675
H	-9.793934548825	9.917913461838	-1.797542407430
C	-3.284733987217	5.622044971961	-0.156618163680
N	-2.974616030214	5.492500910234	0.960931123453

SCF Done: E(RB3LYP) = -2036.27403890

Zero-point correction= 0.349675
Thermal correction to Energy= 0.378246
Thermal correction to Enthalpy= 0.379191
Thermal correction to Gibbs Free Energy= 0.283941
Sum of electronic and zero-point Energies= -2035.924364
Sum of electronic and thermal Energies= -2035.895793
Sum of electronic and thermal Enthalpies= -2035.894848
Sum of electronic and thermal Free Energies= -2035.990098

1	C	Isotropic =	56.4534	Anisotropy =	183.0471
2	H	Isotropic =	23.4027	Anisotropy =	7.5466
3	C	Isotropic =	55.3429	Anisotropy =	179.4892
4	C	Isotropic =	140.1780	Anisotropy =	39.6240
5	H	Isotropic =	26.2822	Anisotropy =	8.0037
6	H	Isotropic =	26.0253	Anisotropy =	5.6564
7	C	Isotropic =	44.8971	Anisotropy =	168.4465
8	H	Isotropic =	23.0047	Anisotropy =	11.0643
9	N	Isotropic =	-59.6734	Anisotropy =	532.7799
10	C	Isotropic =	42.7142	Anisotropy =	147.0127
11	C	Isotropic =	64.6635	Anisotropy =	15.5949
12	F	Isotropic =	262.1542	Anisotropy =	120.7231
13	F	Isotropic =	282.2346	Anisotropy =	125.3894
14	F	Isotropic =	262.8749	Anisotropy =	119.4664
15	C	Isotropic =	70.9701	Anisotropy =	171.2866
16	H	Isotropic =	23.6365	Anisotropy =	8.2323
17	C	Isotropic =	79.9386	Anisotropy =	115.0622
18	C	Isotropic =	57.2500	Anisotropy =	174.2004
19	H	Isotropic =	23.1312	Anisotropy =	12.1263
20	C	Isotropic =	90.7643	Anisotropy =	76.2506
21	C	Isotropic =	56.6567	Anisotropy =	111.7475
22	H	Isotropic =	22.5347	Anisotropy =	11.3656
23	N	Isotropic =	96.4371	Anisotropy =	122.7418
24	C	Isotropic =	56.9588	Anisotropy =	128.9767
25	C	Isotropic =	64.0316	Anisotropy =	153.9893
26	C	Isotropic =	73.5255	Anisotropy =	163.7396
27	H	Isotropic =	23.5783	Anisotropy =	7.4980
28	C	Isotropic =	70.0000	Anisotropy =	139.6170
29	H	Isotropic =	24.2152	Anisotropy =	7.6331
30	C	Isotropic =	53.2983	Anisotropy =	100.6611
31	Cl	Isotropic =	735.7047	Anisotropy =	456.9720
32	C	Isotropic =	81.3606	Anisotropy =	128.3207
33	H	Isotropic =	24.3785	Anisotropy =	11.6980
34	C	Isotropic =	65.6810	Anisotropy =	148.0603
35	C	Isotropic =	61.5708	Anisotropy =	175.4448
36	H	Isotropic =	23.3123	Anisotropy =	8.0196
37	C	Isotropic =	66.9214	Anisotropy =	160.0749
38	H	Isotropic =	23.7473	Anisotropy =	9.8827
39	C	Isotropic =	51.9231	Anisotropy =	182.5785
40	C	Isotropic =	71.4651	Anisotropy =	165.9912
41	H	Isotropic =	23.5354	Anisotropy =	9.5469
42	C	Isotropic =	61.5787	Anisotropy =	179.3449
43	H	Isotropic =	23.3375	Anisotropy =	7.7703
44	C	Isotropic =	29.6812	Anisotropy =	87.4996
45	O	Isotropic =	-32.3146	Anisotropy =	494.7047
46	O	Isotropic =	149.9729	Anisotropy =	169.6568
47	H	Isotropic =	25.5004	Anisotropy =	11.9760
48	C	Isotropic =	76.4586	Anisotropy =	307.7050
49	N	Isotropic =	-23.4227	Anisotropy =	348.0062

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.590845778525	0.779872284659	0.057189649702
H	-1.473744648933	1.027395960410	-0.535132983164
C	0.689376054011	1.118084825841	-0.390512400511
C	0.934214280857	1.793472527206	-1.728240697468
H	0.903695461008	1.046040692598	-2.534179138197
H	1.938607013179	2.241147999479	-1.746458400354
C	1.775830039686	0.775003253487	0.430468225836
H	2.795090137024	1.029832761759	0.121713225770
N	1.657874574849	0.142396590308	1.601361303928
C	0.420268266978	-0.170824320315	2.004219436251
C	0.352138264095	-0.881338765474	3.339333794881
F	1.013152717338	-2.060538149042	3.311154466875
F	-0.920348683909	-1.145544303819	3.708843951425
F	0.910900075543	-0.145196670329	4.325562784784
C	-0.734713198618	0.122442400071	1.280076071045
H	-1.718071811600	-0.153654301240	1.658140560518
C	-1.801128959205	3.856935211407	-3.066622500829
C	-2.930212000003	4.179769924044	-3.892764339243
H	-3.347976290311	5.170029208647	-3.699385133626
C	-3.551740176121	3.464097575138	-4.886476872557
C	-1.032591612517	2.692557425961	-3.000509135339
H	-1.119616013181	1.771126866926	-3.567286544732
N	-0.047781218371	2.820342289181	-2.061322966578
C	-0.136645216539	4.079997559136	-1.476822923591
C	-1.224682193500	4.760456459558	-2.081611176178
C	-1.520471607530	6.069623656431	-1.665989442451
H	-2.348339343105	6.628987822022	-2.105453078851
C	-0.742131101315	6.663993205747	-0.676429485773
H	-0.956289330296	7.678466527319	-0.340336983722
C	0.331319719233	5.954742208805	-0.102815875242
Cl	1.295545482518	6.745883460217	1.147859362683
C	0.661154170388	4.657339456156	-0.481002805763
H	1.494275292073	4.131067655232	-0.017874520544
C	-6.972402162992	4.885547150088	-7.098006468362
C	-6.646762386500	5.450406946681	-5.853716917584
H	-7.274660946561	6.248952590974	-5.456970784778
C	-5.552526479866	4.991430241612	-5.130334363227
H	-5.347704113690	5.431267431212	-4.153814181965
C	-4.735772399211	3.954920756466	-5.633089908443
C	-5.079766900490	3.386056209132	-6.877144160811
H	-4.472096163831	2.578202351933	-7.288256313143
C	-6.177840778215	3.843847805731	-7.601131902771
H	-6.419189533656	3.392929625844	-8.563464282406
C	-8.154946224209	5.410697866587	-7.828453637566
O	-8.873591710733	6.309023410138	-7.427422342761
O	-8.367374923328	4.787607621992	-9.008109379488
H	-9.156475158125	5.200620396575	-9.405428558559
C	-3.045782796205	2.177918057854	-5.261246103015
N	-2.631439687591	1.129302239656	-5.562566124107

SCF Done: E(RB3LYP) = -2036.27439209

Zero-point correction= 0.349614
Thermal correction to Energy= 0.378177
Thermal correction to Enthalpy= 0.379121
Thermal correction to Gibbs Free Energy= 0.284430

Sum of electronic and zero-point Energies= -2035.924778
Sum of electronic and thermal Energies= -2035.896215
Sum of electronic and thermal Enthalpies= -2035.895271
Sum of electronic and thermal Free Energies= -2035.989962

1	C	Isotropic =	58.3949	Anisotropy =	196.7178
2	H	Isotropic =	23.9381	Anisotropy =	11.7285
3	C	Isotropic =	55.0581	Anisotropy =	177.7809
4	C	Isotropic =	141.2259	Anisotropy =	38.6339
5	H	Isotropic =	26.1227	Anisotropy =	6.0587
6	H	Isotropic =	26.2049	Anisotropy =	8.1580
7	C	Isotropic =	44.4678	Anisotropy =	155.0249
8	H	Isotropic =	22.5191	Anisotropy =	8.4069
9	N	Isotropic =	-60.1814	Anisotropy =	525.8584
10	C	Isotropic =	42.1737	Anisotropy =	147.2228
11	C	Isotropic =	64.6175	Anisotropy =	15.3343
12	F	Isotropic =	261.8844	Anisotropy =	121.2204
13	F	Isotropic =	281.9558	Anisotropy =	124.9416
14	F	Isotropic =	262.8037	Anisotropy =	119.7826
15	C	Isotropic =	70.7193	Anisotropy =	172.2465
16	H	Isotropic =	23.8161	Anisotropy =	10.0211
17	C	Isotropic =	79.6965	Anisotropy =	114.9358
18	C	Isotropic =	56.5838	Anisotropy =	172.9758
19	H	Isotropic =	23.2891	Anisotropy =	12.0712
20	C	Isotropic =	90.2910	Anisotropy =	77.9702
21	C	Isotropic =	56.5098	Anisotropy =	112.3903
22	H	Isotropic =	22.5822	Anisotropy =	11.4341
23	N	Isotropic =	97.1768	Anisotropy =	121.1415
24	C	Isotropic =	57.1545	Anisotropy =	128.9266
25	C	Isotropic =	64.1441	Anisotropy =	154.0484
26	C	Isotropic =	73.4077	Anisotropy =	164.3000
27	H	Isotropic =	23.6096	Anisotropy =	7.4837
28	C	Isotropic =	69.8680	Anisotropy =	138.9576
29	H	Isotropic =	24.2370	Anisotropy =	7.5853
30	C	Isotropic =	53.3659	Anisotropy =	100.1993
31	Cl	Isotropic =	735.6426	Anisotropy =	456.7021
32	C	Isotropic =	81.5766	Anisotropy =	128.6639
33	H	Isotropic =	24.3821	Anisotropy =	11.6336
34	C	Isotropic =	65.5188	Anisotropy =	148.6176
35	C	Isotropic =	61.8434	Anisotropy =	181.1821
36	H	Isotropic =	23.2935	Anisotropy =	7.8181
37	C	Isotropic =	70.0644	Anisotropy =	162.3949
38	H	Isotropic =	23.6473	Anisotropy =	9.3470
39	C	Isotropic =	50.9590	Anisotropy =	182.1591
40	C	Isotropic =	66.3594	Anisotropy =	159.6000
41	H	Isotropic =	23.8064	Anisotropy =	9.6979
42	C	Isotropic =	62.0312	Anisotropy =	176.9887
43	H	Isotropic =	23.2794	Anisotropy =	8.0295
44	C	Isotropic =	29.8300	Anisotropy =	88.0166
45	O	Isotropic =	-31.3248	Anisotropy =	498.2990
46	O	Isotropic =	150.0737	Anisotropy =	169.0160
47	H	Isotropic =	25.4792	Anisotropy =	11.9858
48	C	Isotropic =	76.2443	Anisotropy =	308.1164
49	N	Isotropic =	-21.9444	Anisotropy =	347.2714

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	0.768812623271	1.221784795883	-1.380163685378
H	-0.076616009461	1.358673724333	-2.057045705124
C	0.620502691404	1.409622168229	-0.003043321530
C	-0.712045682162	1.759039645255	0.634993245018
H	-0.551024864627	2.155423876298	1.648289956234
H	-1.323620247836	0.851435294987	0.741242347079
C	1.754962495151	1.224421558725	0.803498215703
H	1.684492917753	1.371649457776	1.886265304575
N	2.955959610008	0.873060415144	0.335224156639
C	3.068084899123	0.696591326712	-0.987085420638
C	4.453680167959	0.306743273484	-1.456309962719
F	5.369987771521	1.249011965624	-1.139565218873
F	4.505715202637	0.132122895229	-2.795162862705
F	4.868267190906	-0.846447897303	-0.885831718475
C	2.016792081538	0.858234882691	-1.888759857003
H	2.166145471609	0.704495630126	-2.956531497838
C	-3.144643481404	3.568427842708	-1.447684156967
C	-4.306579003443	3.744094492573	-2.272474651235
H	-4.465181919119	4.776282699531	-2.591385478899
C	-5.229126488393	2.836522152969	-2.732560905505
C	-2.631975924032	2.421104320093	-0.837833671308
H	-3.004071949345	1.401804310654	-0.854978651083
N	-1.501514555900	2.718759763216	-0.129703968546
C	-1.232900616899	4.078624510808	-0.250793476237
C	-2.242096148738	4.646301987697	-1.070257993060
C	-2.200196140216	6.024447532444	-1.340209758818
H	-2.956678894475	6.501020928478	-1.966253206281
C	-1.175340138054	6.795301397411	-0.798245786619
H	-1.125596040648	7.865867530660	-0.996533960994
C	-0.193262568557	6.193089269429	0.012484781486
Cl	1.088945172692	7.207197575602	0.681216455928
C	-0.192432385299	4.833150520804	0.305505062103
H	0.581998927397	4.392370730025	0.931290486629
C	-8.609325698626	3.859277501719	-5.212357055945
C	-7.928288327607	4.856452845098	-4.494338848499
H	-8.270635884348	5.889039346100	-4.572025884921
C	-6.844733340176	4.534715781848	-3.686067341199
H	-6.359498907924	5.331412936853	-3.121663511765
C	-6.394635500182	3.200648732134	-3.574586693545
C	-7.093400266997	2.206295986045	-4.290888571549
H	-6.774599336759	1.165029098599	-4.220957300028
C	-8.181509943552	2.527734048684	-5.098414216606
H	-8.701282558846	1.741480173706	-5.645464693711
C	-9.764271208851	4.255587258523	-6.058778651271
O	-10.172611259755	5.396674223096	-6.183036696561
O	-10.335834246778	3.210370043431	-6.695948620833
H	-11.074659572417	3.571288545968	-7.220296349325
C	-5.078744205774	1.448652166811	-2.412568207716
N	-4.952263905767	0.319070733090	-2.147872452085

SCF Done: E(RB3LYP) = -2036.27442850

Zero-point correction= 0.349582
Thermal correction to Energy= 0.378167
Thermal correction to Enthalpy= 0.379111
Thermal correction to Gibbs Free Energy= 0.283997
Sum of electronic and zero-point Energies= -2035.924846
Sum of electronic and thermal Energies= -2035.896261
Sum of electronic and thermal Enthalpies= -2035.895317
Sum of electronic and thermal Free Energies= -2035.990432

1	C	Isotropic =	58.3438	Anisotropy =	196.7858
2	H	Isotropic =	23.9077	Anisotropy =	11.6902
3	C	Isotropic =	55.0758	Anisotropy =	177.7985
4	C	Isotropic =	141.0756	Anisotropy =	38.6082
5	H	Isotropic =	26.2127	Anisotropy =	8.1857
6	H	Isotropic =	26.1231	Anisotropy =	5.9318
7	C	Isotropic =	44.3793	Anisotropy =	154.9595
8	H	Isotropic =	22.5132	Anisotropy =	8.4014
9	N	Isotropic =	-60.2794	Anisotropy =	525.8819
10	C	Isotropic =	42.1484	Anisotropy =	147.3403
11	C	Isotropic =	64.5839	Anisotropy =	15.3209
12	F	Isotropic =	262.0133	Anisotropy =	120.4086
13	F	Isotropic =	282.2257	Anisotropy =	124.7608
14	F	Isotropic =	262.9209	Anisotropy =	120.6241
15	C	Isotropic =	70.7175	Anisotropy =	172.4080
16	H	Isotropic =	23.8089	Anisotropy =	10.0042
17	C	Isotropic =	79.9504	Anisotropy =	115.2490
18	C	Isotropic =	56.8412	Anisotropy =	173.2789
19	H	Isotropic =	23.2403	Anisotropy =	12.0698
20	C	Isotropic =	90.5985	Anisotropy =	77.6642
21	C	Isotropic =	56.5311	Anisotropy =	112.3412
22	H	Isotropic =	22.5749	Anisotropy =	11.4232
23	N	Isotropic =	97.2947	Anisotropy =	122.1970
24	C	Isotropic =	57.1482	Anisotropy =	128.5559
25	C	Isotropic =	64.2041	Anisotropy =	154.0221
26	C	Isotropic =	73.5174	Anisotropy =	163.8328
27	H	Isotropic =	23.5985	Anisotropy =	7.4700
28	C	Isotropic =	70.0164	Anisotropy =	139.7988
29	H	Isotropic =	24.2130	Anisotropy =	7.6251
30	C	Isotropic =	53.3443	Anisotropy =	100.6904
31	Cl	Isotropic =	735.5439	Anisotropy =	456.8303
32	C	Isotropic =	81.4687	Anisotropy =	128.2154
33	H	Isotropic =	24.3867	Anisotropy =	11.7073
34	C	Isotropic =	65.6057	Anisotropy =	148.4436
35	C	Isotropic =	61.3552	Anisotropy =	179.5359
36	H	Isotropic =	23.2947	Anisotropy =	7.8061
37	C	Isotropic =	70.9418	Anisotropy =	164.7352
38	H	Isotropic =	23.5897	Anisotropy =	9.4481
39	C	Isotropic =	51.3725	Anisotropy =	182.4058
40	C	Isotropic =	66.7999	Anisotropy =	160.8573
41	H	Isotropic =	23.7855	Anisotropy =	9.7700
42	C	Isotropic =	61.7620	Anisotropy =	175.6537
43	H	Isotropic =	23.3399	Anisotropy =	7.9905
44	C	Isotropic =	29.7620	Anisotropy =	87.3086
45	O	Isotropic =	-32.5013	Anisotropy =	494.5705
46	O	Isotropic =	150.1064	Anisotropy =	168.8278

47	H	Isotropic =	25.4918	Anisotropy =	11.9663
48	C	Isotropic =	76.4172	Anisotropy =	307.7323
49	N	Isotropic =	-22.8242	Anisotropy =	347.9427

Conformer 8

#B3LYP/CC-pVDZ nmr=(giao) freq=(noraman) symmetry=(none) scf=(maxcycle=1000)
#scrf=(check) geom=(allcheck) guess=(tcheck)

C	-0.150371272689	0.205566080911	-2.229847773455
H	-0.658509567323	0.954442248811	-2.840496516103
C	0.574359341104	0.578564502375	-1.093865202619
C	0.739116055066	2.026931684615	-0.670129683367
H	1.486500034153	2.520085710992	-1.307948360720
H	1.117039332391	2.076585825133	0.361405426632
C	1.195597006928	-0.441945606640	-0.356542940650
H	1.767417164023	-0.193552016139	0.543652049859
N	1.140273311254	-1.737545641740	-0.678459871429
C	0.440920047259	-2.065535536009	-1.771547098256
C	0.410672927742	-3.547785887234	-2.078521161209
F	-0.291612103148	-3.819858903162	-3.200179062146
F	-0.153146251529	-4.253460471504	-1.072474871941
F	1.654808934516	-4.046276142379	-2.253839240132
C	-0.223175046519	-1.143507997620	-2.580204346612
H	-0.780060365466	-1.467165533289	-3.458472858140
C	-2.009699215236	4.320095746669	-1.517665444154
C	-2.697445881435	5.344085663790	-2.252161392708
H	-3.666097941303	5.614863028752	-1.827043497550
C	-2.349718455391	6.016830657996	-3.397811958996
C	-0.747819287658	3.755823143307	-1.717822413322
H	-0.005583427245	3.970446876552	-2.480057441628
N	-0.486862608021	2.813521742656	-0.762776627865
C	-1.574529726080	2.726867118930	0.100698068936
C	-2.550294822420	3.657607641593	-0.339791069516
C	-3.753297300842	3.768936895115	0.377402277648
H	-4.531102222520	4.470921769321	0.071379490361
C	-3.956133239457	2.968668995586	1.498446133389
H	-4.882855019124	3.040375123574	2.067702516281
C	-2.960639618850	2.058459569718	1.904477862968
Cl	-3.257052198288	1.062665630199	3.332849319554
C	-1.755536854134	1.911826527137	1.225219986090
H	-1.004867488286	1.197215141674	1.559312610076
C	-4.784283140361	9.068444646055	-5.235195443338
C	-4.984021167805	8.715098108841	-3.890349674475
H	-5.759904796620	9.227588015288	-3.320511505681
C	-4.197771835423	7.740313184789	-3.288060430023
H	-4.360808083710	7.513539116429	-2.233995610616
C	-3.186916673885	7.074175495539	-4.015384107702
C	-2.986541287177	7.446205852954	-5.361181432741
H	-2.208537065490	6.954702421252	-5.947708526455
C	-3.772542315109	8.424826695994	-5.964409022967
H	-3.602643222091	8.689467538257	-7.007859137400
C	-5.650336035886	10.119354634012	-5.829478911107
O	-6.537125458048	10.704650869097	-5.233366940353
O	-5.359933274459	10.374027723090	-7.123970091950

H	-5.977317953723	11.069128793186	-7.418519466536
C	-1.127534040913	5.692856204498	-4.070299506205
N	-0.129967890774	5.427137111030	-4.614667101725

SCF Done: E(RB3LYP) = -2036.27438892

Zero-point correction= 0.349591
Thermal correction to Energy= 0.378208
Thermal correction to Enthalpy= 0.379152
Thermal correction to Gibbs Free Energy= 0.283535
Sum of electronic and zero-point Energies= -2035.924798
Sum of electronic and thermal Energies= -2035.896181
Sum of electronic and thermal Enthalpies= -2035.895237
Sum of electronic and thermal Free Energies= -2035.990854

1	C	Isotropic =	57.9624	Anisotropy =	196.6014
2	H	Isotropic =	23.8055	Anisotropy =	11.4526
3	C	Isotropic =	55.2022	Anisotropy =	178.0737
4	C	Isotropic =	141.2365	Anisotropy =	37.5911
5	H	Isotropic =	26.1381	Anisotropy =	5.8959
6	H	Isotropic =	26.2494	Anisotropy =	8.0643
7	C	Isotropic =	44.2519	Anisotropy =	154.2923
8	H	Isotropic =	22.5086	Anisotropy =	8.3576
9	N	Isotropic =	-60.2686	Anisotropy =	525.5383
10	C	Isotropic =	42.0302	Anisotropy =	147.4644
11	C	Isotropic =	64.6553	Anisotropy =	15.4404
12	F	Isotropic =	282.2409	Anisotropy =	124.7796
13	F	Isotropic =	261.8102	Anisotropy =	120.5328
14	F	Isotropic =	262.7068	Anisotropy =	120.8041
15	C	Isotropic =	70.6170	Anisotropy =	172.2683
16	H	Isotropic =	23.7865	Anisotropy =	9.9634
17	C	Isotropic =	79.9537	Anisotropy =	115.8627
18	C	Isotropic =	56.5250	Anisotropy =	173.0369
19	H	Isotropic =	23.2601	Anisotropy =	12.1320
20	C	Isotropic =	90.4067	Anisotropy =	78.0470
21	C	Isotropic =	56.9110	Anisotropy =	112.0269
22	H	Isotropic =	22.5820	Anisotropy =	11.2998
23	N	Isotropic =	96.4700	Anisotropy =	123.1524
24	C	Isotropic =	57.2378	Anisotropy =	128.8342
25	C	Isotropic =	64.4735	Anisotropy =	154.9689
26	C	Isotropic =	73.2443	Anisotropy =	163.1176
27	H	Isotropic =	23.6103	Anisotropy =	7.4935
28	C	Isotropic =	69.9996	Anisotropy =	139.6382
29	H	Isotropic =	24.2263	Anisotropy =	7.6167
30	C	Isotropic =	53.3438	Anisotropy =	100.5131
31	Cl	Isotropic =	735.3736	Anisotropy =	457.2829
32	C	Isotropic =	81.7406	Anisotropy =	128.1878
33	H	Isotropic =	24.3322	Anisotropy =	11.6504
34	C	Isotropic =	65.5106	Anisotropy =	148.5386
35	C	Isotropic =	61.2103	Anisotropy =	179.4683
36	H	Isotropic =	23.3040	Anisotropy =	7.7832
37	C	Isotropic =	70.8907	Anisotropy =	164.7273
38	H	Isotropic =	23.5986	Anisotropy =	9.4393
39	C	Isotropic =	51.0181	Anisotropy =	182.2162
40	C	Isotropic =	66.8805	Anisotropy =	160.9922
41	H	Isotropic =	23.7558	Anisotropy =	9.7789

42	C	Isotropic =	61.6922	Anisotropy =	175.1886
43	H	Isotropic =	23.3685	Anisotropy =	7.9440
44	C	Isotropic =	29.6849	Anisotropy =	87.3749
45	O	Isotropic =	-32.8572	Anisotropy =	493.2237
46	O	Isotropic =	150.1883	Anisotropy =	168.5437
47	H	Isotropic =	25.4924	Anisotropy =	11.9529
48	C	Isotropic =	76.3406	Anisotropy =	307.8518
49	N	Isotropic =	-22.2158	Anisotropy =	347.7639

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-5.073589498344	2.414595148248	-0.875686607523
H	-4.466843295137	2.999257138895	-1.569736981052
C	-4.594259382355	2.090571549224	0.396622467540
C	-3.246203027900	2.567096602695	0.907048037541
H	-2.930781442864	1.957222990005	1.766116636421
H	-3.329017414095	3.603150852342	1.265922462119
C	-5.428173536053	1.327057546010	1.229574376853
H	-5.086919561287	1.042363028771	2.230354833189
N	-6.647134584689	0.904719554579	0.882260691150
C	-7.082042738829	1.232816393401	-0.340600769387
C	-8.467701535281	0.722178228563	-0.673094869130
F	-8.536503573917	-0.624902187570	-0.586073983359
F	-8.848532017487	1.062615059721	-1.923950033930
F	-9.397267198222	1.214934393576	0.176281964434
C	-6.343169748110	1.978208897541	-1.258532790194
H	-6.745260192174	2.212794431388	-2.243245602664
C	-0.676204417829	3.286248265072	-1.623515628131
C	0.139599041825	4.093866874161	-2.485745552453
H	0.828537215723	3.516375787250	-3.105618626643
C	0.206304800324	5.456418033671	-2.644810981536
C	-1.668066481238	3.653511510926	-0.711201851842
H	-2.039314445575	4.639157442096	-0.449483395577
N	-2.191029514815	2.548399287031	-0.100322046259
C	-1.556600581367	1.412249391623	-0.593248536840
C	-0.598540224084	1.834450105166	-1.550599981024
C	0.188248504458	0.864857709618	-2.194777281037
H	0.937705629109	1.146514520226	-2.936634009068
C	0.008805410303	-0.479330791130	-1.879737093851
H	0.608980824887	-1.246174556989	-2.369350587819
C	-0.952915687754	-0.856837310233	-0.922209163172
Cl	-1.148173709103	-2.572657370800	-0.551117479999
C	-1.754957480359	0.066598499740	-0.259524157296
H	-2.494431629241	-0.253849958422	0.472702426669
C	2.854882119865	7.439838255576	-5.414419178420
C	2.565973858767	6.073102859550	-5.563198448535
H	3.018733433481	5.525631845258	-6.390644246139
C	1.706286811207	5.429188033091	-4.681611184259
H	1.481961533546	4.375017894196	-4.846438265545
C	1.111180239740	6.128830505905	-3.608839515114
C	1.398762225695	7.503527227284	-3.476449013619
H	0.949366649338	8.073765235032	-2.661748877571

C	2.257580035973	8.150170382564	-4.361885500379
H	2.468416414742	9.211744909780	-4.234369076324
C	3.777858553655	8.080624330577	-6.386553242072
O	4.316768482930	7.502811290569	-7.313932078848
O	3.972230571927	9.395209103562	-6.143682430641
H	4.587173381736	9.718951099530	-6.827853381456
C	-0.618472298733	6.306622813071	-1.839872770859
N	-1.293680522388	6.995377148058	-1.182818676349

SCF Done: E(RB3LYP) = -2036.27439404

Zero-point correction= 0.349618
Thermal correction to Energy= 0.378195
Thermal correction to Enthalpy= 0.379139
Thermal correction to Gibbs Free Energy= 0.283679
Sum of electronic and zero-point Energies= -2035.924776
Sum of electronic and thermal Energies= -2035.896199
Sum of electronic and thermal Enthalpies= -2035.895255
Sum of electronic and thermal Free Energies= -2035.990715

1	C	Isotropic =	58.6997	Anisotropy =	196.9166
2	H	Isotropic =	23.9475	Anisotropy =	11.7617
3	C	Isotropic =	55.0224	Anisotropy =	177.4514
4	C	Isotropic =	141.2683	Anisotropy =	39.2674
5	H	Isotropic =	26.2110	Anisotropy =	8.1750
6	H	Isotropic =	26.1123	Anisotropy =	6.0495
7	C	Isotropic =	44.3840	Anisotropy =	155.5047
8	H	Isotropic =	22.5168	Anisotropy =	8.4400
9	N	Isotropic =	-60.5376	Anisotropy =	524.8443
10	C	Isotropic =	42.3015	Anisotropy =	147.9989
11	C	Isotropic =	64.6036	Anisotropy =	15.3238
12	F	Isotropic =	262.3304	Anisotropy =	119.9878
13	F	Isotropic =	282.7179	Anisotropy =	124.3414
14	F	Isotropic =	261.8837	Anisotropy =	121.3456
15	C	Isotropic =	70.6773	Anisotropy =	171.9108
16	H	Isotropic =	23.8182	Anisotropy =	10.0169
17	C	Isotropic =	79.9135	Anisotropy =	115.1233
18	C	Isotropic =	56.6803	Anisotropy =	173.0745
19	H	Isotropic =	23.2446	Anisotropy =	12.0634
20	C	Isotropic =	90.3927	Anisotropy =	77.8236
21	C	Isotropic =	56.6848	Anisotropy =	112.3337
22	H	Isotropic =	22.5714	Anisotropy =	11.4723
23	N	Isotropic =	97.3937	Anisotropy =	121.8691
24	C	Isotropic =	57.1576	Anisotropy =	128.8582
25	C	Isotropic =	64.2615	Anisotropy =	154.3361
26	C	Isotropic =	73.4090	Anisotropy =	163.6560
27	H	Isotropic =	23.5880	Anisotropy =	7.4946
28	C	Isotropic =	69.9453	Anisotropy =	139.4353
29	H	Isotropic =	24.2209	Anisotropy =	7.5996
30	C	Isotropic =	53.2850	Anisotropy =	100.6726
31	Cl	Isotropic =	735.6206	Anisotropy =	456.9752
32	C	Isotropic =	81.4830	Anisotropy =	128.3519
33	H	Isotropic =	24.3697	Anisotropy =	11.6329
34	C	Isotropic =	65.6844	Anisotropy =	148.3078
35	C	Isotropic =	61.5145	Anisotropy =	179.4737
36	H	Isotropic =	23.3151	Anisotropy =	7.7996

37	C	Isotropic =	70.8375	Anisotropy =	164.8191
38	H	Isotropic =	23.5762	Anisotropy =	9.4495
39	C	Isotropic =	51.2103	Anisotropy =	182.4380
40	C	Isotropic =	66.6624	Anisotropy =	160.9398
41	H	Isotropic =	23.7673	Anisotropy =	9.7796
42	C	Isotropic =	61.7303	Anisotropy =	175.3299
43	H	Isotropic =	23.3388	Anisotropy =	7.9479
44	C	Isotropic =	29.7029	Anisotropy =	87.3376
45	O	Isotropic =	-32.6365	Anisotropy =	494.3803
46	O	Isotropic =	150.1787	Anisotropy =	168.8757
47	H	Isotropic =	25.4952	Anisotropy =	11.9696
48	C	Isotropic =	76.5348	Anisotropy =	307.6115
49	N	Isotropic =	-23.1084	Anisotropy =	348.3048

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	2.702339855560	3.897187942810	-0.281178004012
H	2.889209542710	4.869020293627	0.181209946199
C	1.554904159127	3.686365588209	-1.049649423774
C	0.572522548345	4.816413352270	-1.302770698955
H	0.762624373266	5.262387019283	-2.289689773323
H	0.720590321554	5.613219603580	-0.559384045983
C	1.373546226061	2.409770127719	-1.608539465070
H	0.486560411068	2.193810433256	-2.211545906499
N	2.231551884103	1.398683489985	-1.449877738593
C	3.325288561479	1.631392335151	-0.711735721069
C	4.259204302684	0.447564731576	-0.578829344607
F	4.744394599728	0.059112170213	-1.780014898289
F	3.634188094968	-0.625801673838	-0.046290578053
F	5.320694146934	0.725392205469	0.209589953881
C	3.612501608314	2.852238800854	-0.105252530960
H	4.514348666711	2.985196820041	0.490722804385
C	-2.925324540342	3.919362482776	-2.006118306976
C	-4.098464342711	3.696560445109	-2.803125385072
H	-4.967088426893	3.379375398803	-2.222827947141
C	-4.307854932323	3.829994469486	-4.153988049756
C	-1.640292680540	4.320815353581	-2.378107236317
H	-1.245055205517	4.557545829432	-3.360707398809
N	-0.828287461339	4.406533572945	-1.282104984777
C	-1.557285328175	4.064774734717	-0.147217641309
C	-2.878200538434	3.753608591266	-0.560541019244
C	-3.822678964540	3.382695401296	0.411264103507
H	-4.850222016628	3.137214097109	0.136598908037
C	-3.440817858256	3.329962381965	1.749120027795
H	-4.159191194851	3.044297100315	2.517437441435
C	-2.119046129302	3.647614789876	2.118165516104
Cl	-1.675716469797	3.568906781979	3.826032986883
C	-1.149830523950	4.019345446966	1.191982755239
H	-0.133798392999	4.254976368928	1.504857794380
C	-8.066077991296	3.041001836532	-6.124079069810
C	-7.837978386425	2.576272885366	-4.818050029092
H	-8.623637480158	2.011787507109	-4.314560997663

C	-6.628076504056	2.817907180348	-4.179037435305
H	-6.479976114200	2.418241049402	-3.175591966920
C	-5.601160566892	3.544260959340	-4.821676979671
C	-5.837664802890	3.996711350457	-6.136829761983
H	-5.062865130007	4.556024583943	-6.663636851020
C	-7.049114939368	3.752176990693	-6.778893128805
H	-7.207805029158	4.117103295198	-7.793429539582
C	-9.375763798559	2.751546483032	-6.762797665614
O	-10.284000245724	2.136590940001	-6.232415214052
O	-9.472914165331	3.244288164147	-8.016969981931
H	-10.359471690991	3.004108012903	-8.344651248155
C	-3.240197653106	4.283809211762	-4.993989528045
N	-2.366379797851	4.652423063012	-5.674066741610

SCF Done: E(RB3LYP) = -2036.27397086

Zero-point correction= 0.349671
Thermal correction to Energy= 0.378277
Thermal correction to Enthalpy= 0.379221
Thermal correction to Gibbs Free Energy= 0.282952
Sum of electronic and zero-point Energies= -2035.924300
Sum of electronic and thermal Energies= -2035.895694
Sum of electronic and thermal Enthalpies= -2035.894750
Sum of electronic and thermal Free Energies= -2035.991019

1	C	Isotropic =	56.4311	Anisotropy =	183.7988
2	H	Isotropic =	23.3917	Anisotropy =	7.6147
3	C	Isotropic =	55.2854	Anisotropy =	179.3654
4	C	Isotropic =	140.3061	Anisotropy =	40.3644
5	H	Isotropic =	26.0094	Anisotropy =	5.7531
6	H	Isotropic =	26.2576	Anisotropy =	8.0575
7	C	Isotropic =	45.0340	Anisotropy =	168.4039
8	H	Isotropic =	23.0244	Anisotropy =	11.1256
9	N	Isotropic =	-59.7558	Anisotropy =	532.2757
10	C	Isotropic =	42.6336	Anisotropy =	146.8780
11	C	Isotropic =	64.6175	Anisotropy =	15.5974
12	F	Isotropic =	261.6228	Anisotropy =	121.0336
13	F	Isotropic =	263.4010	Anisotropy =	119.5404
14	F	Isotropic =	282.4216	Anisotropy =	125.0052
15	C	Isotropic =	70.9761	Anisotropy =	171.0954
16	H	Isotropic =	23.6338	Anisotropy =	8.2354
17	C	Isotropic =	79.8745	Anisotropy =	115.0853
18	C	Isotropic =	57.1196	Anisotropy =	173.6688
19	H	Isotropic =	23.2026	Anisotropy =	12.0885
20	C	Isotropic =	90.6503	Anisotropy =	77.2362
21	C	Isotropic =	56.4954	Anisotropy =	111.9298
22	H	Isotropic =	22.5475	Anisotropy =	11.4175
23	N	Isotropic =	97.2869	Anisotropy =	121.1838
24	C	Isotropic =	56.6392	Anisotropy =	129.0051
25	C	Isotropic =	64.0432	Anisotropy =	154.0689
26	C	Isotropic =	73.3945	Anisotropy =	164.1460
27	H	Isotropic =	23.5845	Anisotropy =	7.5059
28	C	Isotropic =	70.1029	Anisotropy =	139.0971
29	H	Isotropic =	24.2293	Anisotropy =	7.6010
30	C	Isotropic =	53.6410	Anisotropy =	100.1468
31	Cl	Isotropic =	735.2883	Anisotropy =	457.2215

32	C	Isotropic =	81.3371	Anisotropy =	128.3538
33	H	Isotropic =	24.3941	Anisotropy =	11.7178
34	C	Isotropic =	65.6236	Anisotropy =	148.1668
35	C	Isotropic =	61.5514	Anisotropy =	180.1461
36	H	Isotropic =	23.3020	Anisotropy =	7.8238
37	C	Isotropic =	70.8547	Anisotropy =	164.4159
38	H	Isotropic =	23.5711	Anisotropy =	9.4462
39	C	Isotropic =	51.5811	Anisotropy =	182.5188
40	C	Isotropic =	66.4984	Anisotropy =	159.7725
41	H	Isotropic =	23.7713	Anisotropy =	9.8119
42	C	Isotropic =	61.9829	Anisotropy =	176.5629
43	H	Isotropic =	23.3047	Anisotropy =	8.0121
44	C	Isotropic =	29.7862	Anisotropy =	87.8140
45	O	Isotropic =	-31.9605	Anisotropy =	496.0270
46	O	Isotropic =	150.4357	Anisotropy =	168.5643
47	H	Isotropic =	25.4933	Anisotropy =	11.9555
48	C	Isotropic =	76.4423	Anisotropy =	307.8310
49	N	Isotropic =	-22.9326	Anisotropy =	347.9307

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.660917208953	2.289243383426	1.487922571054
H	1.956358363411	3.145494045861	2.098424458360
C	0.480442047394	2.323863401491	0.741588556984
C	-0.441017987679	3.529577490984	0.802442578384
H	0.111149354148	4.403223268018	1.178255669326
H	-1.258675195874	3.339376991937	1.512633107216
C	0.165286369521	1.190746739807	-0.027464434141
H	-0.745468250444	1.172294398943	-0.633248062807
N	0.924424763984	0.093407762861	-0.082406054232
C	2.049108978842	0.087501341334	0.645787077396
C	2.859521756781	-1.186551983845	0.539967126155
F	3.998268162141	-1.126345317835	1.264878672440
F	3.211630788899	-1.449493306373	-0.738152118823
F	2.161766929725	-2.258249739431	0.979606841267
C	2.466637292939	1.148828597991	1.445826180924
H	3.393974588667	1.093013800530	2.014289066812
C	-2.635596559046	4.149592048478	-2.084842922558
C	-3.862162784581	4.176686968285	-2.830778472476
H	-3.764089414514	4.625180906654	-3.821649438725
C	-5.118552892736	3.722237467758	-2.512797985197
C	-2.374866800892	3.695877737411	-0.789895917604
H	-3.048370863985	3.258519213610	-0.059886831994
N	-1.056889859521	3.875136751006	-0.474996988109
C	-0.405289808089	4.457237872645	-1.557805456721
C	-1.362508523852	4.644896116934	-2.587797495217
C	-0.950537088762	5.230344497636	-3.796744948784
H	-1.654190323483	5.392165605540	-4.615284957050
C	0.379458420884	5.611610331528	-3.952198888852
H	0.718073560847	6.067379821874	-4.882503144440
C	1.298298767403	5.409501152813	-2.903836841298
Cl	2.975896598159	5.908094448849	-3.142314834011

C	0.937528386182	4.832132420641	-1.690723396817
H	1.669361614595	4.682271632850	-0.898497657268
C	-8.542355223581	4.068904868606	-5.115588212728
C	-7.413021428958	4.879991358650	-5.316096620538
H	-7.419169576339	5.599817040263	-6.135346950187
C	-6.309790821349	4.780559466903	-4.477007357267
H	-5.463553453047	5.447456942787	-4.643979989684
C	-6.292369496271	3.855836071888	-3.409839119153
C	-7.436458682346	3.055153857358	-3.210430421136
H	-7.456520779369	2.335727566554	-2.390086829825
C	-8.543235240936	3.156051790430	-4.049668706885
H	-9.412538836301	2.521405964444	-3.879036314400
C	-9.697269353059	4.217264068450	-6.038578852155
O	-9.742713115686	5.000063915389	-6.971032972607
O	-10.719181882375	3.383959876366	-5.744690318886
H	-11.419136769625	3.556127464467	-6.401592776095
C	-5.341401015316	3.064122788739	-1.260545277458
N	-5.519451925459	2.529511088492	-0.238524340192

SCF Done: E(RB3LYP) = -2036.27401851

Zero-point correction= 0.349670
Thermal correction to Energy= 0.378258
Thermal correction to Enthalpy= 0.379202
Thermal correction to Gibbs Free Energy= 0.283879
Sum of electronic and zero-point Energies= -2035.924348
Sum of electronic and thermal Energies= -2035.895761
Sum of electronic and thermal Enthalpies= -2035.894817
Sum of electronic and thermal Free Energies= -2035.990140

1	C	Isotropic =	56.7026	Anisotropy =	183.5996
2	H	Isotropic =	23.4175	Anisotropy =	7.5781
3	C	Isotropic =	55.2705	Anisotropy =	179.3371
4	C	Isotropic =	140.1999	Anisotropy =	40.6240
5	H	Isotropic =	26.2687	Anisotropy =	8.0666
6	H	Isotropic =	26.0288	Anisotropy =	5.6066
7	C	Isotropic =	45.2288	Anisotropy =	168.5038
8	H	Isotropic =	23.0427	Anisotropy =	11.2007
9	N	Isotropic =	-59.3552	Anisotropy =	533.7697
10	C	Isotropic =	42.6917	Anisotropy =	146.8677
11	C	Isotropic =	64.6098	Anisotropy =	15.6622
12	F	Isotropic =	281.9851	Anisotropy =	125.6460
13	F	Isotropic =	263.0219	Anisotropy =	119.4011
14	F	Isotropic =	261.8313	Anisotropy =	120.8838
15	C	Isotropic =	70.9994	Anisotropy =	171.2009
16	H	Isotropic =	23.6397	Anisotropy =	8.2143
17	C	Isotropic =	79.8853	Anisotropy =	115.2627
18	C	Isotropic =	56.4160	Anisotropy =	173.1468
19	H	Isotropic =	23.2527	Anisotropy =	12.0844
20	C	Isotropic =	90.3096	Anisotropy =	77.8546
21	C	Isotropic =	56.7582	Anisotropy =	111.9926
22	H	Isotropic =	22.5557	Anisotropy =	11.3258
23	N	Isotropic =	97.3742	Anisotropy =	121.2109
24	C	Isotropic =	57.1573	Anisotropy =	128.8371
25	C	Isotropic =	64.3729	Anisotropy =	154.4371
26	C	Isotropic =	73.4912	Anisotropy =	163.7914

27	H	Isotropic =	23.5988	Anisotropy =	7.4938
28	C	Isotropic =	69.7998	Anisotropy =	139.7718
29	H	Isotropic =	24.2182	Anisotropy =	7.6218
30	C	Isotropic =	53.1964	Anisotropy =	100.7225
31	Cl	Isotropic =	735.7476	Anisotropy =	456.7518
32	C	Isotropic =	81.4137	Anisotropy =	128.3331
33	H	Isotropic =	24.4031	Anisotropy =	11.7295
34	C	Isotropic =	65.5463	Anisotropy =	148.7302
35	C	Isotropic =	61.7847	Anisotropy =	180.6815
36	H	Isotropic =	23.2889	Anisotropy =	7.8046
37	C	Isotropic =	70.4633	Anisotropy =	163.1997
38	H	Isotropic =	23.6373	Anisotropy =	9.3708
39	C	Isotropic =	51.1599	Anisotropy =	182.2256
40	C	Isotropic =	66.4232	Anisotropy =	159.9148
41	H	Isotropic =	23.7904	Anisotropy =	9.7070
42	C	Isotropic =	61.8545	Anisotropy =	176.7274
43	H	Isotropic =	23.2938	Anisotropy =	8.0326
44	C	Isotropic =	29.8028	Anisotropy =	87.6930
45	O	Isotropic =	-32.1981	Anisotropy =	495.7211
46	O	Isotropic =	150.4956	Anisotropy =	168.4551
47	H	Isotropic =	25.4897	Anisotropy =	11.9795
48	C	Isotropic =	76.3214	Anisotropy =	307.8751
49	N	Isotropic =	-22.5559	Anisotropy =	347.6815

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-6.240317894119	2.072251758699	0.547822732550
H	-6.901741494248	2.914097050123	0.764574229068
C	-5.230280449004	2.192951307970	-0.409633853923
C	-5.063213625047	3.476241895689	-1.204434128959
H	-5.573464934362	4.303015458038	-0.689502283793
H	-5.540160660427	3.371023122031	-2.189487407846
C	-4.410624609763	1.073533907414	-0.633239069335
H	-3.601442263288	1.121504558548	-1.367943573004
N	-4.544768410323	-0.088164809873	0.011554528672
C	-5.524542799236	-0.176150605886	0.921393354622
C	-5.623832987779	-1.519980571970	1.610900039658
F	-6.604709180973	-1.542774223593	2.539705712265
F	-4.471419273167	-1.846608728111	2.237036246605
F	-5.883450939833	-2.513420236885	0.730813915446
C	-6.398368386070	0.863816116820	1.230629418675
H	-7.175014652533	0.739978505762	1.984067652368
C	-1.705792390902	4.205554464027	-2.519675863675
C	-0.656945314034	4.285197895863	-3.496919789090
H	0.284958783082	4.668280756783	-3.098760736504
C	-0.648642360959	3.976713022354	-4.835190946374
C	-3.023069671093	3.756944410911	-2.639466608232
H	-3.548170076605	3.372191437417	-3.507844826248
N	-3.673455360173	3.853958157128	-1.441229006420
C	-2.801214375846	4.374215163921	-0.490257430310
C	-1.556720129062	4.609143599615	-1.129088320282
C	-0.500108312047	5.149229192037	-0.376854539733

H	0.472907710753	5.347025078614	-0.830233795673
C	-0.699779995162	5.438477782418	0.970304870555
H	0.107541478874	5.857505664800	1.570735898181
C	-1.951670899885	5.190822241036	1.566872829645
Cl	-2.162444016865	5.572725235549	3.278467536086
C	-3.026200453587	4.656910163617	0.862885118518
H	-3.982283047705	4.470669559160	1.349595090511
C	2.807389476400	4.368758989224	-7.388610399845
C	2.956378431820	4.340417194959	-5.991981215744
H	3.957991831155	4.414743671850	-5.566914216818
C	1.849551435170	4.205260808156	-5.162691923110
H	2.006519223000	4.156828950640	-4.084814417367
C	0.548209892372	4.103902041513	-5.702029089849
C	0.411863750162	4.121363669607	-7.105904131810
H	-0.579780846498	4.037899277580	-7.553640663404
C	1.521047896628	4.253709054752	-7.937558906202
H	1.388698977543	4.270261852326	-9.019135719987
C	4.023133088830	4.510610967815	-8.230850990950
O	5.157984132697	4.607352673638	-7.798418803649
O	3.750723866741	4.524121512237	-9.554002487576
H	4.604458383908	4.621961102468	-10.015113420453
C	-1.849870112077	3.517074590554	-5.465218788792
N	-2.830768436466	3.141385312656	-5.973831818467

SCF Done: E(RB3LYP) = -2036.27402772

Zero-point correction= 0.349656
Thermal correction to Energy= 0.378236
Thermal correction to Enthalpy= 0.379180
Thermal correction to Gibbs Free Energy= 0.283738
Sum of electronic and zero-point Energies= -2035.924371
Sum of electronic and thermal Energies= -2035.895792
Sum of electronic and thermal Enthalpies= -2035.894848
Sum of electronic and thermal Free Energies= -2035.990289

1	C	Isotropic =	56.7380	Anisotropy =	182.9030
2	H	Isotropic =	23.4070	Anisotropy =	7.5954
3	C	Isotropic =	55.2604	Anisotropy =	179.2016
4	C	Isotropic =	140.3805	Anisotropy =	40.3768
5	H	Isotropic =	26.2382	Anisotropy =	8.0174
6	H	Isotropic =	26.0162	Anisotropy =	5.7352
7	C	Isotropic =	45.0323	Anisotropy =	168.3177
8	H	Isotropic =	23.0267	Anisotropy =	11.1513
9	N	Isotropic =	-59.8282	Anisotropy =	532.5602
10	C	Isotropic =	42.5882	Anisotropy =	146.6872
11	C	Isotropic =	64.6799	Anisotropy =	15.6104
12	F	Isotropic =	281.9366	Anisotropy =	125.2688
13	F	Isotropic =	262.9211	Anisotropy =	119.2266
14	F	Isotropic =	261.4086	Anisotropy =	120.7869
15	C	Isotropic =	71.1071	Anisotropy =	170.6951
16	H	Isotropic =	23.6562	Anisotropy =	8.2261
17	C	Isotropic =	79.7906	Anisotropy =	115.4245
18	C	Isotropic =	56.7609	Anisotropy =	173.1877
19	H	Isotropic =	23.2573	Anisotropy =	12.0518
20	C	Isotropic =	90.5197	Anisotropy =	77.7834
21	C	Isotropic =	56.8341	Anisotropy =	112.0902

22	H	Isotropic =	22.5533	Anisotropy =	11.3744
23	N	Isotropic =	97.4134	Anisotropy =	121.1420
24	C	Isotropic =	56.9473	Anisotropy =	128.9446
25	C	Isotropic =	64.1531	Anisotropy =	154.0900
26	C	Isotropic =	73.2895	Anisotropy =	164.0289
27	H	Isotropic =	23.5952	Anisotropy =	7.5182
28	C	Isotropic =	70.1066	Anisotropy =	139.4380
29	H	Isotropic =	24.2196	Anisotropy =	7.6170
30	C	Isotropic =	53.5455	Anisotropy =	100.3797
31	Cl	Isotropic =	735.2856	Anisotropy =	457.2796
32	C	Isotropic =	81.5666	Anisotropy =	128.1751
33	H	Isotropic =	24.3655	Anisotropy =	11.6059
34	C	Isotropic =	65.5936	Anisotropy =	148.6327
35	C	Isotropic =	61.4906	Anisotropy =	179.8192
36	H	Isotropic =	23.3177	Anisotropy =	7.7838
37	C	Isotropic =	70.5264	Anisotropy =	164.7407
38	H	Isotropic =	23.5930	Anisotropy =	9.3956
39	C	Isotropic =	51.3487	Anisotropy =	182.4355
40	C	Isotropic =	66.8600	Anisotropy =	160.4009
41	H	Isotropic =	23.7757	Anisotropy =	9.7614
42	C	Isotropic =	61.7048	Anisotropy =	175.2612
43	H	Isotropic =	23.3110	Anisotropy =	8.0044
44	C	Isotropic =	29.6685	Anisotropy =	87.3436
45	O	Isotropic =	-32.3699	Anisotropy =	494.5383
46	O	Isotropic =	150.0261	Anisotropy =	168.9530
47	H	Isotropic =	25.4849	Anisotropy =	11.9688
48	C	Isotropic =	76.4020	Anisotropy =	307.8840
49	N	Isotropic =	-22.6705	Anisotropy =	348.0485

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-5.569793045344	0.880255491601	0.919782201712
H	-5.313034710659	-0.032075431402	1.462756500098
C	-4.750248982547	1.346506153410	-0.111052180691
C	-3.517212674670	0.567311058098	-0.534035317013
H	-3.752395497382	-0.056415039098	-1.408481294020
H	-3.212309007843	-0.115857373372	0.272004793686
C	-5.135400341869	2.531212072287	-0.761212273080
H	-4.522520987989	2.939537900991	-1.570099588761
N	-6.232091157943	3.227791251513	-0.451819385975
C	-7.000965688256	2.754993963384	0.538375505998
C	-8.229508901999	3.588102340063	0.834882841246
F	-9.070504972366	3.630935223573	-0.223732155727
F	-7.907125615682	4.867359834802	1.127239652161
F	-8.931106909527	3.101853951600	1.882208114241
C	-6.722907203684	1.593445200620	1.255682389963
H	-7.379942054802	1.256377501097	2.056211255531
C	-0.804582367034	2.438667631733	-2.169203970180
C	0.012166518394	2.906517014570	-3.253544903595
H	0.841027938654	3.542915421539	-2.936359056595
C	-0.088995415608	2.703408434359	-4.607959852954
C	-1.910699264733	1.586038720412	-2.171875201098

H	-2.397197009886	1.084519803309	-3.002366529034
N	-2.379576239452	1.404845647266	-0.900659160124
C	-1.591403477229	2.134681585620	-0.016243065237
C	-0.591689867105	2.796363318981	-0.774420562614
C	0.345015096801	3.601671772956	-0.105059436359
H	1.129472038399	4.128763998477	-0.651084663548
C	0.270435209676	3.728234295933	1.279449039269
H	0.987603940884	4.348604361440	1.816792169240
C	-0.736983900958	3.052799844273	1.995818664656
Cl	-0.796343258778	3.239702715993	3.751202348325
C	-1.686971360964	2.247007253676	1.376537020249
H	-2.458971470395	1.741378747202	1.954399725241
C	2.656649609604	4.337606744002	-7.506872263425
C	3.026206423295	4.241470746852	-6.154928802239
H	4.017617231373	4.581993221391	-5.853896401981
C	2.151157070175	3.708013597852	-5.216312087506
H	2.482622848322	3.620860193877	-4.181202153911
C	0.867110340215	3.259573410030	-5.596257144003
C	0.511289355058	3.349840739946	-6.958219763434
H	-0.471736108900	3.005678199978	-7.283903241538
C	1.388768010112	3.881898039243	-7.899616738050
H	1.088244912819	3.946797887239	-8.945109016442
C	3.630336477624	4.912225767502	-8.470945635354
O	4.741355727661	5.315707131567	-8.175886832369
O	3.160996463297	4.949610524861	-9.737210643486
H	3.865785292507	5.340744513219	-10.286141772077
C	-1.175513425561	1.931679501079	-5.132324806302
N	-2.061329585708	1.300585114456	-5.555516322897

SCF Done: E(RB3LYP) = -2036.27402382

Zero-point correction= 0.349516
Thermal correction to Energy= 0.378144
Thermal correction to Enthalpy= 0.379088
Thermal correction to Gibbs Free Energy= 0.283464
Sum of electronic and zero-point Energies= -2035.924508
Sum of electronic and thermal Energies= -2035.895880
Sum of electronic and thermal Enthalpies= -2035.894936
Sum of electronic and thermal Free Energies= -2035.990560

1	C	Isotropic =	56.4666	Anisotropy = 183.3541
2	H	Isotropic =	23.4233	Anisotropy = 7.5897
3	C	Isotropic =	55.2454	Anisotropy = 179.3205
4	C	Isotropic =	140.3336	Anisotropy = 40.7974
5	H	Isotropic =	26.0425	Anisotropy = 5.6371
6	H	Isotropic =	26.2745	Anisotropy = 8.0708
7	C	Isotropic =	45.1596	Anisotropy = 168.1647
8	H	Isotropic =	23.0838	Anisotropy = 11.2225
9	N	Isotropic =	-58.7176	Anisotropy = 535.5241
10	C	Isotropic =	42.6427	Anisotropy = 146.9460
11	C	Isotropic =	64.6253	Anisotropy = 15.6513
12	F	Isotropic =	261.5249	Anisotropy = 121.6220
13	F	Isotropic =	263.7218	Anisotropy = 119.3163
14	F	Isotropic =	282.3948	Anisotropy = 124.6502
15	C	Isotropic =	70.8741	Anisotropy = 171.6447
16	H	Isotropic =	23.5991	Anisotropy = 8.2730

17	C	Isotropic =	79.7708	Anisotropy =	115.3592
18	C	Isotropic =	56.5735	Anisotropy =	173.0420
19	H	Isotropic =	23.2580	Anisotropy =	12.1202
20	C	Isotropic =	90.2681	Anisotropy =	77.6991
21	C	Isotropic =	56.7226	Anisotropy =	111.8796
22	H	Isotropic =	22.5617	Anisotropy =	11.3009
23	N	Isotropic =	97.4793	Anisotropy =	121.1667
24	C	Isotropic =	57.1037	Anisotropy =	128.8280
25	C	Isotropic =	64.0919	Anisotropy =	154.3202
26	C	Isotropic =	73.3746	Anisotropy =	164.1648
27	H	Isotropic =	23.5866	Anisotropy =	7.5176
28	C	Isotropic =	69.8361	Anisotropy =	139.6768
29	H	Isotropic =	24.2190	Anisotropy =	7.6153
30	C	Isotropic =	53.3504	Anisotropy =	100.5321
31	Cl	Isotropic =	735.5919	Anisotropy =	456.9906
32	C	Isotropic =	81.5575	Anisotropy =	128.0248
33	H	Isotropic =	24.4257	Anisotropy =	11.7191
34	C	Isotropic =	65.5416	Anisotropy =	148.5402
35	C	Isotropic =	61.2849	Anisotropy =	179.0667
36	H	Isotropic =	23.3187	Anisotropy =	7.7513
37	C	Isotropic =	70.9073	Anisotropy =	164.9247
38	H	Isotropic =	23.5895	Anisotropy =	9.4208
39	C	Isotropic =	51.1402	Anisotropy =	182.0684
40	C	Isotropic =	66.9312	Anisotropy =	161.3575
41	H	Isotropic =	23.7618	Anisotropy =	9.7509
42	C	Isotropic =	61.5551	Anisotropy =	175.0471
43	H	Isotropic =	23.3455	Anisotropy =	7.9610
44	C	Isotropic =	29.7520	Anisotropy =	87.2733
45	O	Isotropic =	-32.3211	Anisotropy =	494.9797
46	O	Isotropic =	149.7924	Anisotropy =	169.4220
47	H	Isotropic =	25.5039	Anisotropy =	11.9621
48	C	Isotropic =	76.3150	Anisotropy =	307.9371
49	N	Isotropic =	-22.4729	Anisotropy =	348.0808

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.137266485328	5.348445934407	0.279251808865
H	-1.921264743457	4.854245701470	-0.297310972869
C	0.164462276245	5.446581792205	-0.218958944682
C	0.561788844629	4.934632107282	-1.592223076194
H	1.643803275484	4.738426982444	-1.621315018727
H	0.359111750679	5.706044703363	-2.349343122326
C	1.121178404430	6.087078367544	0.586048323436
H	2.155918429576	6.174846062887	0.238686461276
N	0.857956011870	6.613934997844	1.784699718021
C	-0.398719455120	6.509061974147	2.235483435734
C	-0.633383126546	7.124546677524	3.598419247450
F	0.170084180951	6.578583774311	4.538160109568
F	-1.907685113498	6.960723941136	4.016858337592
F	-0.381645611559	8.453197867127	3.595292004841
C	-1.430412012571	5.888028471249	1.533323600286
H	-2.434458558225	5.826569262710	1.950768978379

C	-1.591630824190	2.376503669847	-3.122676443718
C	-2.603233159235	1.848460302377	-3.994008297219
H	-2.761126596664	0.773843558303	-3.882360438042
C	-3.381680579946	2.461129098613	-4.945081545690
C	-1.130833685952	3.684574797129	-2.957968481097
H	-1.438343867541	4.596701151350	-3.459363866904
N	-0.147681755369	3.730782686098	-2.009169630316
C	0.072091563300	2.447333777502	-1.518351248487
C	-0.815192628565	1.569724656450	-2.192584732568
C	-0.783677919718	0.200810084545	-1.877635139574
H	-1.447788240927	-0.509116657862	-2.373918644646
C	0.112631593931	-0.257699272919	-0.915974632274
H	0.151516327233	-1.315739941742	-0.657302378202
C	0.978123961700	0.646822439270	-0.270211155655
Cl	2.099380419930	0.023435469792	0.943821342729
C	0.982898476069	2.009770264392	-0.548647881640
H	1.659878684028	2.687991954453	-0.031510859601
C	-6.325867986169	0.409394721372	-7.340605056740
C	-5.833373089182	1.664005483569	-7.731574809969
H	-6.189006949316	2.124379906681	-8.653127257672
C	-4.888484066065	2.322509933539	-6.948577280722
H	-4.515223572764	3.295128959490	-7.273581354570
C	-4.400964457959	1.750255726630	-5.755070144912
C	-4.915714453988	0.494275808772	-5.364959404825
H	-4.596443665188	0.032173440693	-4.430345755454
C	-5.856645762308	-0.164363567563	-6.147252604082
H	-6.251775396971	-1.132362811091	-5.836826100856
C	-7.334651755115	-0.334690017721	-8.138351149139
O	-7.789982926496	-1.423693064781	-7.836620809562
O	-7.711506202689	0.320761599942	-9.257817053068
H	-8.367734755431	-0.244302889852	-9.706311946559
C	-3.214111167402	3.858842496844	-5.208383935030
N	-3.075483628600	4.998477618227	-5.418232194585

SCF Done: E(RB3LYP) = -2036.27436908

Zero-point correction= 0.349578
Thermal correction to Energy= 0.378194
Thermal correction to Enthalpy= 0.379138
Thermal correction to Gibbs Free Energy= 0.283426
Sum of electronic and zero-point Energies= -2035.924791
Sum of electronic and thermal Energies= -2035.896175
Sum of electronic and thermal Enthalpies= -2035.895231
Sum of electronic and thermal Free Energies= -2035.990943

1	C	Isotropic = 58.7679	Anisotropy =	196.5602
2	H	Isotropic = 24.0654	Anisotropy =	12.0490
3	C	Isotropic = 54.8158	Anisotropy =	177.1980
4	C	Isotropic = 141.2686	Anisotropy =	40.7119
5	H	Isotropic = 26.1418	Anisotropy =	8.2751
6	H	Isotropic = 26.0874	Anisotropy =	6.1319
7	C	Isotropic = 44.6874	Anisotropy =	155.9238
8	H	Isotropic = 22.5355	Anisotropy =	8.5391
9	N	Isotropic = -59.6290	Anisotropy =	527.0377
10	C	Isotropic = 42.4238	Anisotropy =	147.1287
11	C	Isotropic = 64.5613	Anisotropy =	15.0788

12	F	Isotropic =	262.8063	Anisotropy =	119.8872
13	F	Isotropic =	282.4086	Anisotropy =	124.1467
14	F	Isotropic =	261.6821	Anisotropy =	121.7025
15	C	Isotropic =	70.4729	Anisotropy =	172.5070
16	H	Isotropic =	23.8132	Anisotropy =	10.1094
17	C	Isotropic =	79.8898	Anisotropy =	115.4862
18	C	Isotropic =	56.7411	Anisotropy =	173.3640
19	H	Isotropic =	23.2409	Anisotropy =	12.1042
20	C	Isotropic =	90.3303	Anisotropy =	77.8771
21	C	Isotropic =	56.4742	Anisotropy =	112.1825
22	H	Isotropic =	22.5929	Anisotropy =	11.4991
23	N	Isotropic =	98.5302	Anisotropy =	119.7759
24	C	Isotropic =	57.2904	Anisotropy =	129.1045
25	C	Isotropic =	64.1202	Anisotropy =	154.0728
26	C	Isotropic =	73.5320	Anisotropy =	164.0304
27	H	Isotropic =	23.5826	Anisotropy =	7.4883
28	C	Isotropic =	69.8134	Anisotropy =	139.3973
29	H	Isotropic =	24.2180	Anisotropy =	7.5909
30	C	Isotropic =	53.2731	Anisotropy =	100.6825
31	Cl	Isotropic =	735.6595	Anisotropy =	456.7389
32	C	Isotropic =	81.3820	Anisotropy =	128.4239
33	H	Isotropic =	24.4111	Anisotropy =	11.6594
34	C	Isotropic =	65.5225	Anisotropy =	148.4795
35	C	Isotropic =	61.6104	Anisotropy =	175.1789
36	H	Isotropic =	23.3500	Anisotropy =	7.9333
37	C	Isotropic =	66.9543	Anisotropy =	161.3056
38	H	Isotropic =	23.7649	Anisotropy =	9.7839
39	C	Isotropic =	51.1009	Anisotropy =	182.1030
40	C	Isotropic =	70.9593	Anisotropy =	165.1045
41	H	Isotropic =	23.5747	Anisotropy =	9.4131
42	C	Isotropic =	61.1953	Anisotropy =	179.2870
43	H	Isotropic =	23.3235	Anisotropy =	7.7731
44	C	Isotropic =	29.7506	Anisotropy =	87.4439
45	O	Isotropic =	-32.1992	Anisotropy =	495.6212
46	O	Isotropic =	149.3415	Anisotropy =	170.0209
47	H	Isotropic =	25.4990	Anisotropy =	11.9582
48	C	Isotropic =	76.3638	Anisotropy =	308.0154
49	N	Isotropic =	-22.4685	Anisotropy =	347.9859

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.280733046014	2.481195356588	-1.323956547494
H	0.529499275447	2.834233878679	-2.032832264156
C	1.014328380210	1.402960760580	-0.475683219304
C	-0.291797094882	0.629713996649	-0.519920133063
H	-0.429275158518	0.069133686656	0.416028916578
H	-0.258246576316	-0.111195887758	-1.331857388324
C	2.027041244383	1.012156900488	0.415400980967
H	1.855454519123	0.178517060962	1.104372851004
N	3.224168650499	1.600371572889	0.491182161146
C	3.453411207144	2.627719478615	-0.336185234211
C	4.825274096396	3.253338129825	-0.200557196438

F	5.030345314095	3.742989097884	1.042982275750
F	5.004566880561	4.274381512603	-1.067009984203
F	5.808436473166	2.354749325822	-0.431743873774
C	2.524468927406	3.111457540643	-1.256604896610
H	2.763044682605	3.954353747513	-1.903738188499
C	-3.229350506703	2.431102054706	-1.805517469006
C	-4.223272713192	2.825157591318	-2.763662424617
H	-4.956930475989	3.531285458693	-2.369312042381
C	-4.389794742373	2.478924690350	-4.082184097889
C	-2.159644375816	1.540964355524	-1.924881298259
H	-1.844076746834	0.946379464744	-2.776209794842
N	-1.467912266939	1.461988669972	-0.748645413624
C	-2.063889231005	2.301373607704	0.187558877049
C	-3.173283467472	2.926318807360	-0.437885438964
C	-3.955199007748	3.823920512201	0.308455292244
H	-4.817368766188	4.326049886442	-0.134242377708
C	-3.624156746766	4.075751466481	1.637087829714
H	-4.218475381513	4.768727123173	2.232527002814
C	-2.514837785214	3.433425079933	2.221285983258
Cl	-2.129723794572	3.780397003642	3.909747621530
C	-1.711057517945	2.538977711318	1.521939678932
H	-0.856798058345	2.060076347328	1.998039591419
C	-7.589972790565	3.944169973381	-6.577957065065
C	-7.688821998978	4.020786308048	-5.178730309919
H	-8.587718792394	4.451961437853	-4.736629112445
C	-6.667009995756	3.542135845527	-4.367701110243
H	-6.792107850399	3.590111667869	-3.285627648289
C	-5.500435234932	2.978033368958	-4.929248754802
C	-5.417282524200	2.895302847045	-6.334995205048
H	-4.531502101725	2.458707782764	-6.799360641819
C	-6.442642191580	3.371687900450	-7.148188905491
H	-6.351683314684	3.302085857092	-8.231936102007
C	-8.712525712254	4.466589770993	-7.399278123557
O	-9.725473308787	4.970364109631	-6.947129525510
O	-8.504127304318	4.330082633687	-8.727034105252
H	-9.288567097630	4.699293820866	-9.173600338262
C	-3.448136260320	1.601986339517	-4.710874680052
N	-2.678965804194	0.885794346791	-5.218298151279

SCF Done: E(RB3LYP) = -2036.27437742

Zero-point correction= 0.349583
Thermal correction to Energy= 0.378195
Thermal correction to Enthalpy= 0.379139
Thermal correction to Gibbs Free Energy= 0.282919
Sum of electronic and zero-point Energies= -2035.924795
Sum of electronic and thermal Energies= -2035.896182
Sum of electronic and thermal Enthalpies= -2035.895238
Sum of electronic and thermal Free Energies= -2035.991458

1	C	Isotropic = 58.6880	Anisotropy =	196.5903
2	H	Isotropic = 23.9383	Anisotropy =	11.8457
3	C	Isotropic = 54.9851	Anisotropy =	177.4938
4	C	Isotropic = 141.4398	Anisotropy =	39.1106
5	H	Isotropic = 26.1983	Anisotropy =	8.1515
6	H	Isotropic = 26.1213	Anisotropy =	5.9252

7	C	Isotropic =	44.4818	Anisotropy =	155.3590
8	H	Isotropic =	22.5212	Anisotropy =	8.4516
9	N	Isotropic =	-60.2554	Anisotropy =	525.8476
10	C	Isotropic =	42.2493	Anisotropy =	147.2287
11	C	Isotropic =	64.5882	Anisotropy =	15.2770
12	F	Isotropic =	261.9274	Anisotropy =	120.6370
13	F	Isotropic =	282.1811	Anisotropy =	124.5348
14	F	Isotropic =	262.4874	Anisotropy =	120.7868
15	C	Isotropic =	70.6419	Anisotropy =	172.0437
16	H	Isotropic =	23.8111	Anisotropy =	10.0681
17	C	Isotropic =	79.8421	Anisotropy =	115.5740
18	C	Isotropic =	56.6450	Anisotropy =	173.0325
19	H	Isotropic =	23.2344	Anisotropy =	12.1115
20	C	Isotropic =	90.3226	Anisotropy =	77.6244
21	C	Isotropic =	56.7060	Anisotropy =	112.4573
22	H	Isotropic =	22.5774	Anisotropy =	11.4089
23	N	Isotropic =	97.3911	Anisotropy =	121.3163
24	C	Isotropic =	57.1949	Anisotropy =	128.8063
25	C	Isotropic =	64.3566	Anisotropy =	154.7001
26	C	Isotropic =	73.5075	Anisotropy =	163.8290
27	H	Isotropic =	23.5990	Anisotropy =	7.4745
28	C	Isotropic =	69.8676	Anisotropy =	139.4682
29	H	Isotropic =	24.2199	Anisotropy =	7.6001
30	C	Isotropic =	53.1595	Anisotropy =	100.4490
31	Cl	Isotropic =	735.3842	Anisotropy =	457.1785
32	C	Isotropic =	81.6551	Anisotropy =	128.5179
33	H	Isotropic =	24.3520	Anisotropy =	11.6352
34	C	Isotropic =	65.5030	Anisotropy =	148.2952
35	C	Isotropic =	61.3643	Anisotropy =	179.6845
36	H	Isotropic =	23.3078	Anisotropy =	7.7836
37	C	Isotropic =	70.6478	Anisotropy =	164.2994
38	H	Isotropic =	23.5888	Anisotropy =	9.4405
39	C	Isotropic =	51.2006	Anisotropy =	182.3482
40	C	Isotropic =	66.7503	Anisotropy =	160.7048
41	H	Isotropic =	23.7686	Anisotropy =	9.7711
42	C	Isotropic =	61.9040	Anisotropy =	175.9678
43	H	Isotropic =	23.3397	Anisotropy =	7.9836
44	C	Isotropic =	29.7121	Anisotropy =	87.3986
45	O	Isotropic =	-32.4412	Anisotropy =	494.9105
46	O	Isotropic =	149.9272	Anisotropy =	168.9917
47	H	Isotropic =	25.4883	Anisotropy =	11.9621
48	C	Isotropic =	76.4003	Anisotropy =	307.7962
49	N	Isotropic =	-22.5623	Anisotropy =	347.8150

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.137317389693	1.471370559785	1.794936560391
H	1.148351065663	0.408264621238	2.045683010720
C	0.538942215854	1.914540434982	0.612509426431
C	-0.054682257185	0.919822003046	-0.370002957166
H	-0.307248027224	-0.014992594018	0.151590973349
H	0.691178544939	0.664109636745	-1.136685505885

C	0.552242053843	3.296019285440	0.357124712533
H	0.091494335567	3.693485555991	-0.551800030225
N	1.102049655662	4.198891461473	1.173824175592
C	1.673264808539	3.744546788256	2.297003970147
C	2.275101333120	4.819560701896	3.176399109583
F	1.341148725237	5.704590088813	3.592451584647
F	3.219203120873	5.530250555470	2.520168959142
F	2.857383148511	4.304145545725	4.281334726748
C	1.721674255674	2.399872157305	2.659056423175
H	2.194095002383	2.084639343814	3.588395992169
C	-2.575653128710	2.165491096415	-2.750612291816
C	-2.823650945136	2.576969538416	-4.106848048110
H	-1.900632369215	2.795552328421	-4.651262345184
C	-3.965653257753	2.702854862375	-4.858792832088
C	-1.286506888659	1.774937809916	-2.382224952151
H	-0.393542351214	1.725954478342	-3.001592746596
N	-1.238339371259	1.402916385206	-1.073072057401
C	-2.505265230996	1.567215788819	-0.520910789724
C	-3.378595450533	2.050085676601	-1.537110290770
C	-4.703935957682	2.355215499280	-1.173021438726
H	-5.411085194544	2.752946656565	-1.896668133844
C	-5.128658063253	2.142255999350	0.136184731392
H	-6.154957151344	2.371911455197	0.422875530303
C	-4.237338324434	1.633012969640	1.097520352907
Cl	-4.818717807559	1.370598624109	2.743628081483
C	-2.910879945822	1.341905965279	0.799434882160
H	-2.228719671081	0.972307343919	1.563506487264
C	-3.883490550390	4.175978001551	-8.915845974007
C	-4.931399966595	3.350450028557	-8.478817624230
H	-5.725195604045	3.069432512407	-9.170594518235
C	-4.958753058833	2.885201450603	-7.166565295127
H	-5.779096228430	2.240002432544	-6.848443021204
C	-3.940129829270	3.222927613984	-6.251428730915
C	-2.902865284920	4.070769867766	-6.697311926541
H	-2.124128577782	4.395598499890	-6.006245022794
C	-2.872274026076	4.531489225621	-8.008721004004
H	-2.069205143420	5.188403940254	-8.344900861219
C	-3.808648123065	4.700210406944	-10.304338407345
O	-2.922431270482	5.422592939352	-10.724963707624
O	-4.837267690519	4.292556251802	-11.079404156013
H	-4.696656665756	4.684760303375	-11.961189772030
C	-5.239323624580	2.249419772996	-4.389283663648
N	-6.294488617792	1.862358128544	-4.074671585512

SCF Done: E(RB3LYP) = -2036.26971177

Zero-point correction= 0.349674
Thermal correction to Energy= 0.378219
Thermal correction to Enthalpy= 0.379163
Thermal correction to Gibbs Free Energy= 0.283616
Sum of electronic and zero-point Energies= -2035.920038
Sum of electronic and thermal Energies= -2035.891493
Sum of electronic and thermal Enthalpies= -2035.890549
Sum of electronic and thermal Free Energies= -2035.986096

1 C Isotropic = 56.9503 Anisotropy = 184.4152

2 H Isotropic = 23.4208 Anisotropy = 7.6809
3 C Isotropic = 55.2522 Anisotropy = 178.9354
4 C Isotropic = 140.7846 Anisotropy = 41.6847
5 H Isotropic = 26.2321 Anisotropy = 8.0213
6 H Isotropic = 26.0390 Anisotropy = 5.6686
7 C Isotropic = 45.7223 Anisotropy = 168.3456
8 H Isotropic = 23.1694 Anisotropy = 11.5340
9 N Isotropic = -59.6803 Anisotropy = 533.0783
10 C Isotropic = 42.7693 Anisotropy = 147.0564
11 C Isotropic = 64.6171 Anisotropy = 15.5830
12 F Isotropic = 261.6857 Anisotropy = 120.2280
13 F Isotropic = 263.0592 Anisotropy = 119.8995
14 F Isotropic = 281.9760 Anisotropy = 125.4571
15 C Isotropic = 70.9222 Anisotropy = 171.3162
16 H Isotropic = 23.6331 Anisotropy = 8.2358
17 C Isotropic = 77.9391 Anisotropy = 117.0941
18 C Isotropic = 50.9251 Anisotropy = 159.1206
19 H Isotropic = 23.6233 Anisotropy = 12.0883
20 C Isotropic = 89.5500 Anisotropy = 80.9806
21 C Isotropic = 49.5341 Anisotropy = 103.8956
22 H Isotropic = 23.6434 Anisotropy = 7.2170
23 N Isotropic = 98.6737 Anisotropy = 123.0891
24 C Isotropic = 55.1326 Anisotropy = 126.2137
25 C Isotropic = 68.5581 Anisotropy = 151.5535
26 C Isotropic = 66.9620 Anisotropy = 163.4790
27 H Isotropic = 22.7969 Anisotropy = 9.0181
28 C Isotropic = 70.7864 Anisotropy = 138.3648
29 H Isotropic = 24.2224 Anisotropy = 7.8700
30 C Isotropic = 53.0116 Anisotropy = 101.9026
31 Cl Isotropic = 735.7427 Anisotropy = 453.2483
32 C Isotropic = 81.7219 Anisotropy = 128.5628
33 H Isotropic = 24.4373 Anisotropy = 11.4781
34 C Isotropic = 65.4294 Anisotropy = 149.0593
35 C Isotropic = 61.8867 Anisotropy = 175.1281
36 H Isotropic = 23.3403 Anisotropy = 7.8746
37 C Isotropic = 66.8384 Anisotropy = 163.0700
38 H Isotropic = 23.7248 Anisotropy = 9.7498
39 C Isotropic = 49.5153 Anisotropy = 184.4672
40 C Isotropic = 69.6990 Anisotropy = 162.8667
41 H Isotropic = 23.7940 Anisotropy = 9.1458
42 C Isotropic = 61.3603 Anisotropy = 179.3646
43 H Isotropic = 23.3408 Anisotropy = 7.7302
44 C Isotropic = 29.6747 Anisotropy = 87.5491
45 O Isotropic = -32.3481 Anisotropy = 494.8143
46 O Isotropic = 149.5209 Anisotropy = 169.6366
47 H Isotropic = 25.4947 Anisotropy = 11.9562
48 C Isotropic = 76.2405 Anisotropy = 307.4008
49 N Isotropic = -17.8229 Anisotropy = 351.4703

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C -0.153909036646 0.153367779563 -1.549561477607

H	-0.116059641333	1.130208293263	-2.035514438808
C	-1.341696744621	-0.583184998741	-1.513635434736
C	-2.617826897448	-0.102562946321	-2.180777555939
H	-3.474872593150	-0.691837487325	-1.823691211531
H	-2.552751785978	-0.258955240894	-3.267116366720
C	-1.314953785874	-1.827187313780	-0.863312583804
H	-2.225882182610	-2.432099889383	-0.804579069048
N	-0.226063950661	-2.347805421961	-0.289817411621
C	0.897745676879	-1.622686437100	-0.342885132572
C	2.094145057310	-2.265433530075	0.326358800464
F	1.870160621634	-2.489139030604	1.640672601141
F	3.201541529658	-1.496759268303	0.234577082796
F	2.390373980286	-3.462450684988	-0.227217951308
C	0.993010627950	-0.371879631283	-0.952391110533
H	1.934036158549	0.176302813096	-0.962315371531
C	-3.114190514705	3.536433286384	-2.388263432411
C	-3.135209937928	4.834557057397	-3.001148190658
H	-3.495440993458	5.625592335329	-2.340183182835
C	-2.766003933972	5.240973004763	-4.260098868791
C	-2.756976118988	2.292630966467	-2.914361464844
H	-2.415248018785	2.033443793639	-3.911282527858
N	-2.898223477026	1.314229152392	-1.970703213502
C	-3.356017943444	1.885180075951	-0.787432713869
C	-3.504855363403	3.278223824567	-1.009963154722
C	-3.969343122977	4.086468589804	0.041190754677
H	-4.097432154474	5.162666567296	-0.087620729072
C	-4.272548547976	3.502716386288	1.268237337821
H	-4.634326182943	4.112767112460	2.095762942208
C	-4.112541286043	2.114717056309	1.447641668898
Cl	-4.509754570465	1.414724796080	3.019855236183
C	-3.653792748446	1.275338860620	0.437587334278
H	-3.534487946915	0.205980975844	0.604514252980
C	-3.039973551713	9.309476754583	-5.672590823632
C	-2.251603222204	8.367522791510	-6.351100299099
H	-1.696069752387	8.663630630550	-7.240683482663
C	-2.173143409297	7.055410942486	-5.890884188877
H	-1.550369381353	6.340669317405	-6.431335913206
C	-2.873875236469	6.640695546274	-4.738876063027
C	-3.674187791768	7.595130049156	-4.073065858676
H	-4.262677157148	7.311811012546	-3.200159381645
C	-3.750300283634	8.905189566933	-4.529954990411
H	-4.374009248814	9.634349766606	-4.011534466073
C	-3.160509582751	10.720478245349	-6.121842638798
O	-3.831723797423	11.570076515032	-5.563290516326
O	-2.440262796791	10.984694010837	-7.233801831533
H	-2.583657505989	11.926177831600	-7.443835705412
C	-2.229034849175	4.287637154541	-5.184156686300
N	-1.793266605079	3.507049017840	-5.934352571448

SCF Done: E(RB3LYP) = -2036.27444396

Zero-point correction= 0.349641
Thermal correction to Energy= 0.378204
Thermal correction to Enthalpy= 0.379148
Thermal correction to Gibbs Free Energy= 0.284314
Sum of electronic and zero-point Energies= -2035.924803

Sum of electronic and thermal Energies= -2035.896240
Sum of electronic and thermal Enthalpies= -2035.895296
Sum of electronic and thermal Free Energies= -2035.990130

1	C	Isotropic =	57.9130	Anisotropy =	196.7401
2	H	Isotropic =	23.7944	Anisotropy =	11.4815
3	C	Isotropic =	55.2400	Anisotropy =	177.9775
4	C	Isotropic =	141.2867	Anisotropy =	37.5628
5	H	Isotropic =	26.2567	Anisotropy =	8.0691
6	H	Isotropic =	26.1403	Anisotropy =	5.9076
7	C	Isotropic =	44.2298	Anisotropy =	154.5398
8	H	Isotropic =	22.5036	Anisotropy =	8.3592
9	N	Isotropic =	-60.4069	Anisotropy =	525.4785
10	C	Isotropic =	42.0178	Anisotropy =	147.4275
11	C	Isotropic =	64.6557	Anisotropy =	15.4671
12	F	Isotropic =	262.1918	Anisotropy =	120.1375
13	F	Isotropic =	282.2625	Anisotropy =	124.7261
14	F	Isotropic =	262.5453	Anisotropy =	120.6249
15	C	Isotropic =	70.7104	Anisotropy =	172.2682
16	H	Isotropic =	23.7904	Anisotropy =	9.9581
17	C	Isotropic =	79.7917	Anisotropy =	114.9275
18	C	Isotropic =	56.9366	Anisotropy =	173.2012
19	H	Isotropic =	23.2518	Anisotropy =	12.0726
20	C	Isotropic =	90.6374	Anisotropy =	77.3481
21	C	Isotropic =	56.6879	Anisotropy =	112.2336
22	H	Isotropic =	22.5579	Anisotropy =	11.3885
23	N	Isotropic =	96.4882	Anisotropy =	123.3089
24	C	Isotropic =	57.1727	Anisotropy =	128.4456
25	C	Isotropic =	64.1952	Anisotropy =	153.6464
26	C	Isotropic =	73.7177	Anisotropy =	163.8981
27	H	Isotropic =	23.6123	Anisotropy =	7.4797
28	C	Isotropic =	69.8976	Anisotropy =	139.4371
29	H	Isotropic =	24.2276	Anisotropy =	7.6279
30	C	Isotropic =	53.3050	Anisotropy =	100.6974
31	Cl	Isotropic =	735.4600	Anisotropy =	457.2077
32	C	Isotropic =	81.5618	Anisotropy =	128.0782
33	H	Isotropic =	24.3365	Anisotropy =	11.6535
34	C	Isotropic =	65.6748	Anisotropy =	148.5938
35	C	Isotropic =	61.8471	Anisotropy =	176.2845
36	H	Isotropic =	23.3123	Anisotropy =	8.0231
37	C	Isotropic =	66.4917	Anisotropy =	160.1572
38	H	Isotropic =	23.7835	Anisotropy =	9.7598
39	C	Isotropic =	51.4244	Anisotropy =	182.3486
40	C	Isotropic =	70.6577	Anisotropy =	164.1322
41	H	Isotropic =	23.6133	Anisotropy =	9.4382
42	C	Isotropic =	61.7716	Anisotropy =	179.9736
43	H	Isotropic =	23.3095	Anisotropy =	7.8019
44	C	Isotropic =	29.9332	Anisotropy =	87.5289
45	O	Isotropic =	-32.0892	Anisotropy =	496.0183
46	O	Isotropic =	150.3541	Anisotropy =	168.3559
47	H	Isotropic =	25.4885	Anisotropy =	11.9792
48	C	Isotropic =	76.3722	Anisotropy =	307.6366
49	N	Isotropic =	-22.8001	Anisotropy =	347.8236

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-4.757932854949	1.310968143459	-0.928880328033
H	-4.289758020149	1.773244858752	-1.800198859128
C	-4.001792016601	0.557155679454	-0.026272824782
C	-2.518954872043	0.300424579949	-0.225315963355
H	-2.372300891979	-0.458318462658	-1.007230061595
H	-2.078903769098	-0.103148040247	0.698098108023
C	-4.670856820639	0.000644646771	1.075239968423
H	-4.114146182635	-0.588801699818	1.811247430949
N	-5.980068122059	0.141244277619	1.303850098715
C	-6.679727999057	0.864464772040	0.421399289995
C	-8.154689634268	0.991173959939	0.738872192401
F	-8.814482547427	1.712183118180	-0.194006796194
F	-8.357833031589	1.597517663883	1.930118335549
F	-8.755163552337	-0.217570130706	0.809977177174
C	-6.125969191095	1.472237118138	-0.705307885556
H	-6.743098028945	2.053368887687	-1.389154570398
C	-0.604186483157	2.932139128262	-1.940184424110
C	0.075979726683	3.574264502621	-3.029336369827
H	0.529299283648	4.530641972622	-2.760695260628
C	0.232894641690	3.195626229466	-4.340243640634
C	-1.269216462063	1.704908127680	-1.886468362165
H	-1.418221944984	0.962861954453	-2.664256834210
N	-1.765774617847	1.482807719553	-0.632814737027
C	-1.441878637922	2.562155142043	0.183301446862
C	-0.712068895610	3.492228894179	-0.600910309207
C	-0.257622715613	4.677283814208	0.001779889162
H	0.307104868842	5.419599761065	-0.565196813622
C	-0.531881626978	4.907654344456	1.347163434587
H	-0.187965016967	5.821037445256	1.832283838278
C	-1.258362135735	3.957647206424	2.091400202223
Cl	-1.584267461119	4.288249828755	3.795572340249
C	-1.730013401680	2.771816198314	1.537751147948
H	-2.293586321194	2.056975617112	2.135262636876
C	2.405402851003	5.487815729319	-7.280713274445
C	2.591467313876	5.733345179020	-5.910037078569
H	3.295717461750	6.507810281007	-5.604039309519
C	1.902712602689	4.993880537224	-4.956216706225
H	2.095238700873	5.192825463449	-3.901625208819
C	0.991746728060	3.985316875203	-5.340523540413
C	0.821261886114	3.740062136950	-6.719229031932
H	0.129159837129	2.963355846624	-7.048617765914
C	1.513544034966	4.478830058749	-7.675471618864
H	1.359639163859	4.273422091091	-8.734610109651
C	3.170324634538	6.303284440939	-8.259152281884
O	3.955924992110	7.185561613904	-7.961300291756
O	2.909836936555	5.970780597861	-9.542328432375
H	3.454487528765	6.556623952699	-10.100170858329
C	-0.370963464954	1.983353216065	-4.805889666803
N	-0.863636472456	0.993954720982	-5.180578321446

SCF Done: E(RB3LYP) = -2036.27441816

Zero-point correction= 0.349569
Thermal correction to Energy= 0.378189
Thermal correction to Enthalpy= 0.379133
Thermal correction to Gibbs Free Energy= 0.283499
Sum of electronic and zero-point Energies= -2035.924850
Sum of electronic and thermal Energies= -2035.896229
Sum of electronic and thermal Enthalpies= -2035.895285
Sum of electronic and thermal Free Energies= -2035.990919

1	C	Isotropic =	57.8394	Anisotropy =	196.6122
2	H	Isotropic =	23.7830	Anisotropy =	11.4246
3	C	Isotropic =	55.2702	Anisotropy =	178.2749
4	C	Isotropic =	141.1173	Anisotropy =	37.2826
5	H	Isotropic =	26.1369	Anisotropy =	5.9077
6	H	Isotropic =	26.2600	Anisotropy =	8.0516
7	C	Isotropic =	44.1659	Anisotropy =	154.2833
8	H	Isotropic =	22.4927	Anisotropy =	8.3320
9	N	Isotropic =	-60.5093	Anisotropy =	525.2342
10	C	Isotropic =	42.0056	Anisotropy =	147.6401
11	C	Isotropic =	64.6046	Anisotropy =	15.4572
12	F	Isotropic =	281.9600	Anisotropy =	125.3460
13	F	Isotropic =	261.9840	Anisotropy =	120.3014
14	F	Isotropic =	262.7524	Anisotropy =	120.6055
15	C	Isotropic =	70.7339	Anisotropy =	172.3596
16	H	Isotropic =	23.7885	Anisotropy =	9.9496
17	C	Isotropic =	79.8854	Anisotropy =	115.0669
18	C	Isotropic =	56.7133	Anisotropy =	173.0644
19	H	Isotropic =	23.2515	Anisotropy =	12.0763
20	C	Isotropic =	90.3958	Anisotropy =	77.2754
21	C	Isotropic =	56.7273	Anisotropy =	111.7752
22	H	Isotropic =	22.5558	Anisotropy =	11.3754
23	N	Isotropic =	96.1883	Anisotropy =	123.5333
24	C	Isotropic =	57.0320	Anisotropy =	128.7516
25	C	Isotropic =	64.1562	Anisotropy =	153.7642
26	C	Isotropic =	73.6349	Anisotropy =	163.8096
27	H	Isotropic =	23.6207	Anisotropy =	7.4730
28	C	Isotropic =	69.8937	Anisotropy =	139.3302
29	H	Isotropic =	24.2321	Anisotropy =	7.6227
30	C	Isotropic =	53.3071	Anisotropy =	100.6676
31	Cl	Isotropic =	735.7180	Anisotropy =	456.7480
32	C	Isotropic =	81.5001	Anisotropy =	128.1965
33	H	Isotropic =	24.3331	Anisotropy =	11.6585
34	C	Isotropic =	65.5212	Anisotropy =	148.2972
35	C	Isotropic =	61.4873	Anisotropy =	180.1341
36	H	Isotropic =	23.3127	Anisotropy =	7.7818
37	C	Isotropic =	70.6279	Anisotropy =	164.2046
38	H	Isotropic =	23.5911	Anisotropy =	9.4656
39	C	Isotropic =	51.3408	Anisotropy =	182.4878
40	C	Isotropic =	66.7374	Anisotropy =	160.2577
41	H	Isotropic =	23.7701	Anisotropy =	9.7879
42	C	Isotropic =	61.7714	Anisotropy =	176.1159
43	H	Isotropic =	23.3039	Anisotropy =	8.0358
44	C	Isotropic =	29.7413	Anisotropy =	87.2999
45	O	Isotropic =	-32.4568	Anisotropy =	494.3455
46	O	Isotropic =	149.9761	Anisotropy =	169.0614
47	H	Isotropic =	25.4953	Anisotropy =	11.9687

48 C Isotropic = 76.3417 Anisotropy = 307.7659
49 N Isotropic = -22.6454 Anisotropy = 347.5139

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-0.031473025414	0.978125636012	-0.044772711641
H	-0.855687719894	0.926831275109	-0.758918875342
C	1.026894486331	1.871293370145	-0.235929755495
C	1.120776080266	2.774370014845	-1.452496799878
H	1.445958055908	2.192063493264	-2.326505693233
H	1.880069896248	3.552338170116	-1.286125266245
C	2.045654843548	1.886782781795	0.729916133452
H	2.888370696751	2.577646802061	0.622521160248
N	2.066335069833	1.097480452838	1.807909221689
C	1.042699353140	0.249192224558	1.963132813317
C	1.121322016788	-0.611848099422	3.205951929925
F	1.111282464901	0.136933677288	4.332038009131
F	2.257633689610	-1.342765089538	3.234865782535
F	0.086267252474	-1.476050620828	3.291665742757
C	-0.029133286055	0.147195387793	1.076570338449
H	-0.838306885249	-0.559831893167	1.254231859360
C	-2.053984546338	3.887013266186	-2.941774619071
C	-3.140606778356	3.902259994682	-3.879949594453
H	-3.901759889252	4.652665672194	-3.656892676229
C	-3.369303147150	3.149538363087	-5.005723493092
C	-0.916405190287	3.078188617822	-2.886026261438
H	-0.600406106855	2.279103259716	-3.548890016604
N	-0.140825457355	3.414626226567	-1.812170062224
C	-0.745929195326	4.461082029993	-1.123139854066
C	-1.948081444757	4.786606916902	-1.802209234898
C	-2.746820719869	5.829335674646	-1.303492030952
H	-3.678185474577	6.113594314108	-1.796642707848
C	-2.341270614280	6.513357709888	-0.160714764905
H	-2.947521017449	7.324818495163	0.241632433895
C	-1.139691544929	6.159457044923	0.483729953307
Cl	-0.661395037705	7.052665367553	1.930447000712
C	-0.316882685858	5.134917325820	0.027258535208
H	0.604893058503	4.879167067350	0.547260198881
C	-6.836061925224	3.581856526921	-7.538631378093
C	-5.692755184113	2.910558856507	-7.998431104565
H	-5.672911545653	2.500085512234	-9.007762383080
C	-4.581031816646	2.769524186094	-7.171509133009
H	-3.700614701900	2.248542144197	-7.551320178521
C	-4.570985387658	3.296091801996	-5.862819864791
C	-5.733637691245	3.955684556205	-5.406850083809
H	-5.786077212403	4.344761593528	-4.389705183517
C	-6.841891898152	4.099520928224	-6.232651769588
H	-7.736474908434	4.607885375717	-5.871097385425
C	-8.048394226856	3.759552513453	-8.378870279772
O	-9.061640339951	4.333102689915	-8.020131264193
O	-7.923780253778	3.214625286961	-9.608692705235
H	-8.762705054251	3.383274177542	-10.076493566061

C	-2.406125073916	2.171245301030	-5.413405681837
N	-1.618909977167	1.374043620005	-5.740184733757

SCF Done: E(RB3LYP) = -2036.27434566

Zero-point correction= 0.349535
Thermal correction to Energy= 0.378199
Thermal correction to Enthalpy= 0.379144
Thermal correction to Gibbs Free Energy= 0.282396
Sum of electronic and zero-point Energies= -2035.924811
Sum of electronic and thermal Energies= -2035.896146
Sum of electronic and thermal Enthalpies= -2035.895202
Sum of electronic and thermal Free Energies= -2035.991950

1	C	Isotropic =	57.8650	Anisotropy =	196.6397
2	H	Isotropic =	23.8196	Anisotropy =	11.4224
3	C	Isotropic =	55.2621	Anisotropy =	178.1801
4	C	Isotropic =	141.1790	Anisotropy =	37.4966
5	H	Isotropic =	26.1301	Anisotropy =	6.0419
6	H	Isotropic =	26.2450	Anisotropy =	8.0543
7	C	Isotropic =	44.1610	Anisotropy =	154.3024
8	H	Isotropic =	22.4970	Anisotropy =	8.3628
9	N	Isotropic =	-60.2572	Anisotropy =	525.7190
10	C	Isotropic =	42.0638	Anisotropy =	147.6844
11	C	Isotropic =	64.6047	Anisotropy =	15.4298
12	F	Isotropic =	261.3288	Anisotropy =	120.9434
13	F	Isotropic =	263.2364	Anisotropy =	120.2420
14	F	Isotropic =	282.1260	Anisotropy =	125.0356
15	C	Isotropic =	70.7326	Anisotropy =	172.3221
16	H	Isotropic =	23.7987	Anisotropy =	9.9384
17	C	Isotropic =	79.9868	Anisotropy =	115.6291
18	C	Isotropic =	56.6791	Anisotropy =	173.2318
19	H	Isotropic =	23.2733	Anisotropy =	12.0751
20	C	Isotropic =	90.6390	Anisotropy =	78.0581
21	C	Isotropic =	56.9126	Anisotropy =	111.9994
22	H	Isotropic =	22.5543	Anisotropy =	11.4104
23	N	Isotropic =	96.4493	Anisotropy =	123.6851
24	C	Isotropic =	56.8243	Anisotropy =	128.4381
25	C	Isotropic =	63.9231	Anisotropy =	153.7393
26	C	Isotropic =	73.6297	Anisotropy =	163.8612
27	H	Isotropic =	23.6009	Anisotropy =	7.4997
28	C	Isotropic =	70.2278	Anisotropy =	139.9298
29	H	Isotropic =	24.2077	Anisotropy =	7.6534
30	C	Isotropic =	53.6462	Anisotropy =	101.0672
31	Cl	Isotropic =	735.5826	Anisotropy =	456.8288
32	C	Isotropic =	81.3082	Anisotropy =	127.5734
33	H	Isotropic =	24.3430	Anisotropy =	11.6321
34	C	Isotropic =	65.6163	Anisotropy =	148.5252
35	C	Isotropic =	61.4457	Anisotropy =	174.2905
36	H	Isotropic =	23.3491	Anisotropy =	7.9402
37	C	Isotropic =	67.3564	Anisotropy =	161.7276
38	H	Isotropic =	23.7759	Anisotropy =	9.7848
39	C	Isotropic =	51.2621	Anisotropy =	182.2609
40	C	Isotropic =	71.0148	Anisotropy =	165.5891
41	H	Isotropic =	23.5746	Anisotropy =	9.4316
42	C	Isotropic =	60.8814	Anisotropy =	178.5968

43	H	Isotropic =	23.3333	Anisotropy =	7.7771
44	C	Isotropic =	29.6113	Anisotropy =	86.9105
45	O	Isotropic =	-32.6959	Anisotropy =	493.5802
46	O	Isotropic =	149.6490	Anisotropy =	169.5918
47	H	Isotropic =	25.4971	Anisotropy =	11.9704
48	C	Isotropic =	76.4485	Anisotropy =	307.7376
49	N	Isotropic =	-22.9384	Anisotropy =	348.1260

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-5.302942270265	3.477064570883	-1.300099684437
H	-4.540283920785	3.776424423977	-2.021597966925
C	-4.994899543881	3.355345094737	0.058157647908
C	-3.619353477361	3.677478231916	0.613517001173
H	-3.524279599548	3.284255181501	1.636093293365
H	-3.488700648351	4.767315730705	0.677120782030
C	-6.025567844885	2.957546828235	0.924507320836
H	-5.824809024106	2.842075379949	1.994768543001
N	-7.276078777066	2.699997496567	0.530337573575
C	-7.543647164822	2.829013985631	-0.774778843308
C	-8.976332142175	2.523437469475	-1.157026249307
F	-9.194503201851	2.685516537317	-2.480388643451
F	-9.846917953753	3.326881728074	-0.506011144466
F	-9.315207629984	1.251398501796	-0.848650980672
C	-6.602765900230	3.208700380710	-1.731735591622
H	-6.875339146635	3.294756363056	-2.782677069583
C	-0.740235104984	3.118429364859	-1.607968838601
C	0.322670950167	3.467625981588	-2.507518704073
H	0.920520593736	2.612918650016	-2.829845391877
C	0.713415457588	4.684867405419	-3.010019219629
C	-1.694559178200	3.921130441721	-0.978417211508
H	-1.839918532927	4.995221435588	-1.031119079175
N	-2.517951665771	3.162626513946	-0.194533266418
C	-2.129108906607	1.829407571265	-0.282244473975
C	-1.016569630075	1.761291041252	-1.159692764589
C	-0.427096377168	0.510947083675	-1.410754130500
H	0.429852798522	0.414253715332	-2.079780764473
C	-0.945622675689	-0.624414859065	-0.793939472916
H	-0.502216967107	-1.603192725216	-0.976374419126
C	-2.050118300989	-0.513453559071	0.073223870255
Cl	-2.675603287828	-1.977873102173	0.837423938667
C	-2.667913848141	0.701830808404	0.350037872049
H	-3.523775814851	0.757772021251	1.020922025478
C	4.026427238371	5.259341969102	-5.716546082589
C	3.510586811817	3.972403718924	-5.489416622740
H	3.959176056818	3.125174157135	-6.009410918191
C	2.438901724920	3.778516695447	-4.626671801967
H	2.051669857378	2.767726774859	-4.496986079921
C	1.847221402121	4.867478531991	-3.948792706132
C	2.367534723204	6.156077944667	-4.192270950473
H	1.930195020970	7.019683714052	-3.688778246366
C	3.439387589769	6.351410483319	-5.059723990879

H	3.824823292933	7.357035506912	-5.226386430223
C	5.170843291693	5.412310512719	-6.651370093692
O	5.711601753755	4.493195848161	-7.240604457999
O	5.569547953161	6.695315841164	-6.793425569711
H	6.317675697877	6.688915774227	-7.418990393684
C	0.012752368388	5.869896383350	-2.614634491608
N	-0.563316047153	6.831700450653	-2.290597121531

SCF Done: E(RB3LYP) = -2036.27436390

Zero-point correction= 0.349683
Thermal correction to Energy= 0.378281
Thermal correction to Enthalpy= 0.379225
Thermal correction to Gibbs Free Energy= 0.283482
Sum of electronic and zero-point Energies= -2035.924681
Sum of electronic and thermal Energies= -2035.896083
Sum of electronic and thermal Enthalpies= -2035.895138
Sum of electronic and thermal Free Energies= -2035.990882

1	C	Isotropic =	57.9327	Anisotropy =	197.3462
2	H	Isotropic =	23.7783	Anisotropy =	11.4746
3	C	Isotropic =	55.2845	Anisotropy =	178.0304
4	C	Isotropic =	141.0683	Anisotropy =	37.6728
5	H	Isotropic =	26.2441	Anisotropy =	8.0737
6	H	Isotropic =	26.1208	Anisotropy =	6.0218
7	C	Isotropic =	44.3290	Anisotropy =	154.0267
8	H	Isotropic =	22.5008	Anisotropy =	8.3714
9	N	Isotropic =	-60.6803	Anisotropy =	524.2921
10	C	Isotropic =	42.0723	Anisotropy =	147.5993
11	C	Isotropic =	64.5780	Anisotropy =	15.3756
12	F	Isotropic =	282.2103	Anisotropy =	124.7727
13	F	Isotropic =	262.7663	Anisotropy =	120.3075
14	F	Isotropic =	262.2861	Anisotropy =	119.8194
15	C	Isotropic =	70.2868	Anisotropy =	172.0851
16	H	Isotropic =	23.7856	Anisotropy =	9.9309
17	C	Isotropic =	79.9182	Anisotropy =	115.1477
18	C	Isotropic =	57.1960	Anisotropy =	174.0912
19	H	Isotropic =	23.1789	Anisotropy =	12.0854
20	C	Isotropic =	90.7283	Anisotropy =	76.9427
21	C	Isotropic =	56.6170	Anisotropy =	112.1867
22	H	Isotropic =	22.5422	Anisotropy =	11.4640
23	N	Isotropic =	96.3378	Anisotropy =	123.3212
24	C	Isotropic =	57.0260	Anisotropy =	128.7401
25	C	Isotropic =	64.2005	Anisotropy =	154.0226
26	C	Isotropic =	73.4654	Anisotropy =	163.8243
27	H	Isotropic =	23.5867	Anisotropy =	7.4845
28	C	Isotropic =	69.9943	Anisotropy =	139.4273
29	H	Isotropic =	24.2241	Anisotropy =	7.6265
30	C	Isotropic =	53.3667	Anisotropy =	100.4683
31	Cl	Isotropic =	735.3877	Anisotropy =	457.1529
32	C	Isotropic =	81.6052	Anisotropy =	128.0457
33	H	Isotropic =	24.3371	Anisotropy =	11.6568
34	C	Isotropic =	65.7396	Anisotropy =	148.3439
35	C	Isotropic =	61.2903	Anisotropy =	179.1746
36	H	Isotropic =	23.3210	Anisotropy =	7.7970
37	C	Isotropic =	71.4000	Anisotropy =	166.3493

38	H	Isotropic =	23.5307	Anisotropy =	9.5301
39	C	Isotropic =	51.7411	Anisotropy =	182.6769
40	C	Isotropic =	67.0174	Anisotropy =	160.5283
41	H	Isotropic =	23.7674	Anisotropy =	9.8586
42	C	Isotropic =	61.4819	Anisotropy =	174.6778
43	H	Isotropic =	23.3399	Anisotropy =	7.9752
44	C	Isotropic =	29.6235	Anisotropy =	87.2736
45	O	Isotropic =	-32.4537	Anisotropy =	494.2287
46	O	Isotropic =	149.9248	Anisotropy =	169.1634
47	H	Isotropic =	25.4932	Anisotropy =	11.9626
48	C	Isotropic =	76.4617	Anisotropy =	307.6707
49	N	Isotropic =	-23.4310	Anisotropy =	347.9225

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-4.851784296281	1.082474193754	1.737002502391
H	-4.381562841531	0.377582663315	2.426359962821
C	-4.285689920084	1.336483348083	0.485538344696
C	-3.035226969883	0.604625358833	0.028954463412
H	-3.306206997920	-0.197916901602	-0.672045729249
H	-2.544699287491	0.125307018808	0.887983131060
C	-4.939975308196	2.260912636925	-0.346906853194
H	-4.532199741745	2.497929401450	-1.334114788294
N	-6.062707644131	2.900870609716	-0.011977914656
C	-6.585328626718	2.634076154950	1.192961335161
C	-7.860553513873	3.387412602196	1.505291256879
F	-8.338757581228	3.090612322292	2.733535116786
F	-8.837486819548	3.100824492695	0.615523720516
F	-7.674025352743	4.725483125834	1.460617239863
C	-6.028175044743	1.740698298620	2.104842043609
H	-6.492171347937	1.565073616566	3.074405627581
C	-0.846294472341	2.407481181115	-2.324884785422
C	-0.467416452236	2.576273207067	-3.702733569622
H	-1.200111013651	2.149100354578	-4.393218204827
C	0.634856588652	3.120610729450	-4.314550091017
C	-1.842626351346	1.485652231467	-1.996795253674
H	-2.398351995610	0.827845362581	-2.661649967498
N	-2.064520945408	1.455459698191	-0.653494589289
C	-1.232193029262	2.392052044028	-0.047601541721
C	-0.449563710006	3.017649873491	-1.059961064626
C	0.419365757209	4.054964611606	-0.671857213793
H	1.023281335699	4.588417160348	-1.401622933792
C	0.518574208441	4.408502657943	0.671527262955
H	1.193392387991	5.207322096692	0.979104224173
C	-0.252281456176	3.740342899992	1.639613457613
Cl	-0.090841849683	4.214615892083	3.332502004729
C	-1.146342496607	2.728437563210	1.308313615003
H	-1.751855088802	2.240468541484	2.070423398114
C	0.946623578530	3.445208269378	-8.608063449799
C	2.101715654194	3.402541481856	-7.811372999630
H	3.085268965964	3.442965108245	-8.278982576844
C	1.996841532426	3.304963633379	-6.426148710171

H	2.907110840041	3.268075739591	-5.825601683890
C	0.738309789359	3.241567207953	-5.792602446646
C	-0.415799320013	3.305183665080	-6.603402240929
H	-1.406808692247	3.310413556851	-6.148134241646
C	-0.311775546225	3.396944398493	-7.986786320632
H	-1.208281013050	3.449323103310	-8.605699718487
C	1.003531127960	3.553388111312	-10.089125710399
O	0.028466715467	3.598999703781	-10.818033340896
O	2.265883514861	3.596972593822	-10.568039594296
H	2.195485523016	3.666130081301	-11.538276592003
C	1.794913979025	3.517760668248	-3.576442477278
N	2.781193227879	3.819397629638	-3.030142103142

SCF Done: E(RB3LYP) = -2036.26963555

Zero-point correction= 0.349676
Thermal correction to Energy= 0.378233
Thermal correction to Enthalpy= 0.379177
Thermal correction to Gibbs Free Energy= 0.282905
Sum of electronic and zero-point Energies= -2035.919959
Sum of electronic and thermal Energies= -2035.891403
Sum of electronic and thermal Enthalpies= -2035.890459
Sum of electronic and thermal Free Energies= -2035.986730

1	C	Isotropic =	56.4856	Anisotropy =	182.5622
2	H	Isotropic =	23.4190	Anisotropy =	7.5157
3	C	Isotropic =	55.5488	Anisotropy =	179.4709
4	C	Isotropic =	140.8685	Anisotropy =	38.4813
5	H	Isotropic =	26.0681	Anisotropy =	5.6932
6	H	Isotropic =	26.3253	Anisotropy =	7.7279
7	C	Isotropic =	44.8799	Anisotropy =	168.1370
8	H	Isotropic =	22.9394	Anisotropy =	11.1914
9	N	Isotropic =	-59.1331	Anisotropy =	534.1626
10	C	Isotropic =	42.6957	Anisotropy =	147.2879
11	C	Isotropic =	64.6021	Anisotropy =	15.4192
12	F	Isotropic =	282.4742	Anisotropy =	124.7676
13	F	Isotropic =	261.8890	Anisotropy =	121.0335
14	F	Isotropic =	262.6892	Anisotropy =	119.7421
15	C	Isotropic =	71.0843	Anisotropy =	171.1239
16	H	Isotropic =	23.6370	Anisotropy =	8.3345
17	C	Isotropic =	77.9862	Anisotropy =	116.8685
18	C	Isotropic =	51.0169	Anisotropy =	159.2645
19	H	Isotropic =	23.6184	Anisotropy =	12.0166
20	C	Isotropic =	89.4646	Anisotropy =	81.3196
21	C	Isotropic =	49.7812	Anisotropy =	103.8622
22	H	Isotropic =	23.6118	Anisotropy =	7.1269
23	N	Isotropic =	96.8802	Anisotropy =	126.0437
24	C	Isotropic =	54.8292	Anisotropy =	126.0222
25	C	Isotropic =	68.4927	Anisotropy =	150.9917
26	C	Isotropic =	67.0659	Anisotropy =	164.0426
27	H	Isotropic =	22.8314	Anisotropy =	9.0432
28	C	Isotropic =	70.7856	Anisotropy =	138.2426
29	H	Isotropic =	24.2393	Anisotropy =	7.9058
30	C	Isotropic =	53.0986	Anisotropy =	102.0143
31	Cl	Isotropic =	735.9272	Anisotropy =	453.3255
32	C	Isotropic =	81.7450	Anisotropy =	127.9467

33	H	Isotropic =	24.3474	Anisotropy =	11.3636
34	C	Isotropic =	65.4765	Anisotropy =	149.4347
35	C	Isotropic =	62.1677	Anisotropy =	175.8077
36	H	Isotropic =	23.3340	Anisotropy =	7.8751
37	C	Isotropic =	66.4805	Anisotropy =	162.5997
38	H	Isotropic =	23.7478	Anisotropy =	9.7045
39	C	Isotropic =	49.5153	Anisotropy =	184.4793
40	C	Isotropic =	69.3016	Anisotropy =	162.3696
41	H	Isotropic =	23.8153	Anisotropy =	9.1387
42	C	Isotropic =	61.4203	Anisotropy =	180.0287
43	H	Isotropic =	23.3044	Anisotropy =	7.7898
44	C	Isotropic =	29.7443	Anisotropy =	87.5501
45	O	Isotropic =	-32.3816	Anisotropy =	495.5035
46	O	Isotropic =	150.1225	Anisotropy =	168.8975
47	H	Isotropic =	25.4998	Anisotropy =	11.9706
48	C	Isotropic =	76.3305	Anisotropy =	307.3880
49	N	Isotropic =	-17.6885	Anisotropy =	351.1772

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.427396930205	-1.904540539769	-0.638287424721
H	-2.256156489697	-2.401591003423	-0.129101309852
C	-1.620289425326	-0.674673598854	-1.272827181725
C	-2.996515656057	-0.034780114309	-1.312381603868
H	-3.609045634252	-0.415238549145	-0.481532545784
H	-3.512627545634	-0.317514863396	-2.241443929408
C	-0.509212458804	-0.086547366348	-1.899955618255
H	-0.608560238918	0.879417672976	-2.403508097432
N	0.708509756083	-0.635161147773	-1.925113756200
C	0.862570642738	-1.816959643278	-1.313459375213
C	2.264803879731	-2.383297905511	-1.379829548724
F	3.165807010780	-1.554698122875	-0.805830371582
F	2.667340151992	-2.571262591539	-2.656700075766
F	2.360346813532	-3.575300880806	-0.750879759843
C	-0.162372393438	-2.495623718572	-0.657229281834
H	0.019377949346	-3.452580112714	-0.170098240341
C	-3.183444520466	3.595622126823	-1.908458418873
C	-3.459898094136	4.631354979864	-2.868334861962
H	-4.006294636011	4.261428288584	-3.740600095836
C	-3.134526023319	5.964051610666	-2.925375133137
C	-3.290623386141	2.257364807690	-2.291348363577
H	-3.564005699924	1.853517590598	-3.263823293897
N	-2.980057383991	1.422901903918	-1.260437295566
C	-2.690300238241	2.195436810529	-0.139314928198
C	-2.810551286175	3.568345487246	-0.497973613685
C	-2.645575858100	4.529949712181	0.516900309691
H	-2.752960458429	5.592108568697	0.310989324687
C	-2.335838661160	4.122703184373	1.812246501952
H	-2.201179054998	4.862437330497	2.601480949353
C	-2.197606554794	2.755477529806	2.111869626944
Cl	-1.796877485329	2.282007624465	3.764770432439
C	-2.375497574517	1.763369088533	1.154189912103

H	-2.278732449944	0.709307026655	1.409527420824
C	-4.496711037739	8.519713963189	-6.126538877923
C	-3.333447286412	8.837222272943	-5.407695669569
H	-2.762669503538	9.729281063494	-5.664844574805
C	-2.902459053398	8.014992620699	-4.369647516662
H	-1.992624010285	8.277276367076	-3.827423578742
C	-3.613605231535	6.848355269574	-4.019824547800
C	-4.793390139699	6.551464849705	-4.736135304155
H	-5.398803123892	5.686579198476	-4.462168071906
C	-5.221310504165	7.369038185836	-5.776098694409
H	-6.135504394944	7.134133986703	-6.322501228165
C	-5.000394435717	9.363455028529	-7.241334947346
O	-6.004347026932	9.126939698720	-7.889621631923
O	-4.224988221105	10.443747275722	-7.479180273983
H	-4.635025173322	10.925044789818	-8.221692651375
C	-2.230521846250	6.563506333175	-1.991527265072
N	-1.469269077268	7.093147910551	-1.282955518880

SCF Done: E(RB3LYP) = -2036.26981790

Zero-point correction= 0.349524
Thermal correction to Energy= 0.378109
Thermal correction to Enthalpy= 0.379053
Thermal correction to Gibbs Free Energy= 0.283193
Sum of electronic and zero-point Energies= -2035.920294
Sum of electronic and thermal Energies= -2035.891709
Sum of electronic and thermal Enthalpies= -2035.890765
Sum of electronic and thermal Free Energies= -2035.986625

1	C	Isotropic =	56.9101	Anisotropy =	184.1607
2	H	Isotropic =	23.4242	Anisotropy =	7.6399
3	C	Isotropic =	55.1185	Anisotropy =	178.9218
4	C	Isotropic =	140.7995	Anisotropy =	41.6064
5	H	Isotropic =	26.2435	Anisotropy =	8.1234
6	H	Isotropic =	26.0510	Anisotropy =	5.9301
7	C	Isotropic =	45.4410	Anisotropy =	168.3810
8	H	Isotropic =	23.1399	Anisotropy =	11.3295
9	N	Isotropic =	-59.5846	Anisotropy =	533.3459
10	C	Isotropic =	42.6961	Anisotropy =	146.9250
11	C	Isotropic =	64.6654	Anisotropy =	15.6491
12	F	Isotropic =	262.4080	Anisotropy =	119.8083
13	F	Isotropic =	262.4543	Anisotropy =	120.7942
14	F	Isotropic =	282.0601	Anisotropy =	125.0151
15	C	Isotropic =	71.0551	Anisotropy =	171.3683
16	H	Isotropic =	23.6363	Anisotropy =	8.2506
17	C	Isotropic =	78.0666	Anisotropy =	117.4768
18	C	Isotropic =	51.0218	Anisotropy =	159.5484
19	H	Isotropic =	23.6585	Anisotropy =	11.8878
20	C	Isotropic =	89.3673	Anisotropy =	81.6541
21	C	Isotropic =	49.6824	Anisotropy =	103.7677
22	H	Isotropic =	23.6557	Anisotropy =	7.0950
23	N	Isotropic =	98.8103	Anisotropy =	121.9166
24	C	Isotropic =	55.1106	Anisotropy =	126.0753
25	C	Isotropic =	68.4579	Anisotropy =	151.0212
26	C	Isotropic =	67.2217	Anisotropy =	163.9078
27	H	Isotropic =	22.8916	Anisotropy =	8.9372

28	C	Isotropic =	70.6836	Anisotropy =	138.5228
29	H	Isotropic =	24.2118	Anisotropy =	7.8592
30	C	Isotropic =	52.9595	Anisotropy =	102.1466
31	Cl	Isotropic =	735.8634	Anisotropy =	453.5780
32	C	Isotropic =	81.5802	Anisotropy =	128.1680
33	H	Isotropic =	24.4191	Anisotropy =	11.6326
34	C	Isotropic =	65.4784	Anisotropy =	149.7715
35	C	Isotropic =	62.5405	Anisotropy =	177.5125
36	H	Isotropic =	23.2725	Anisotropy =	7.9885
37	C	Isotropic =	66.1423	Anisotropy =	160.8650
38	H	Isotropic =	23.7877	Anisotropy =	9.6699
39	C	Isotropic =	49.5973	Anisotropy =	184.4309
40	C	Isotropic =	68.5599	Anisotropy =	160.3633
41	H	Isotropic =	23.8880	Anisotropy =	9.1163
42	C	Isotropic =	61.8006	Anisotropy =	182.0355
43	H	Isotropic =	23.2680	Anisotropy =	7.7524
44	C	Isotropic =	29.7738	Anisotropy =	88.0222
45	O	Isotropic =	-31.8133	Anisotropy =	496.7979
46	O	Isotropic =	150.7040	Anisotropy =	167.7475
47	H	Isotropic =	25.4675	Anisotropy =	11.9736
48	C	Isotropic =	76.4812	Anisotropy =	307.1301
49	N	Isotropic =	-17.4398	Anisotropy =	350.9031

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	-1.660689378774	3.139624970142	3.193928870473
H	-1.931774336189	4.057152220598	3.721047369555
C	-1.987558869529	2.972867834505	1.845344954124
C	-2.776474856768	4.040616160824	1.108093915544
H	-2.614824976164	5.019390391041	1.583592059012
H	-3.852320078345	3.825676530331	1.184982872736
C	-1.599156905233	1.772808067662	1.227135459733
H	-1.824711594812	1.598985905795	0.171104092264
N	-0.944914231275	0.790458596535	1.853230713475
C	-0.651629235129	0.974599877434	3.146927079932
C	0.087790319357	-0.176537941612	3.794522343573
F	1.280440156595	-0.401899688406	3.198456362337
F	-0.612542365145	-1.329651665651	3.710966953858
F	0.332201491500	0.049406654311	5.103932229145
C	-0.981349215151	2.121789923386	3.866360862833
H	-0.712880515688	2.222744411040	4.917058867833
C	-2.688126282394	4.018344340398	-2.573961505677
C	-3.394697263408	3.677615758197	-3.780493457345
H	-4.464282340906	3.520931135451	-3.613666153340
C	-2.984953449152	3.465224009450	-5.073526695754
C	-3.284543223174	3.777153111140	-1.335159760837
H	-4.260161869531	3.342276353108	-1.128927142804
N	-2.463723983090	4.146485288509	-0.312344176703
C	-1.300350392629	4.686604898941	-0.853110201769
C	-1.398625418031	4.631356968097	-2.272718748389
C	-0.361059418282	5.211538562562	-3.026723390378
H	-0.393095911939	5.226303440363	-4.113382292098

C	0.732610513544	5.778612041509	-2.377170939584
H	1.541927679294	6.224867375960	-2.955035938493
C	0.799063624250	5.783030318849	-0.972292043793
Cl	2.206492713536	6.505689184783	-0.188768406724
C	-0.209382440024	5.247342937585	-0.179115435399
H	-0.146230872098	5.273828577353	0.907548840309
C	-5.779478541954	2.619807552273	-8.252275560277
C	-6.185783228753	3.346172654394	-7.121317121406
H	-7.216674449420	3.697284443970	-7.062341492652
C	-5.284779750162	3.632035637291	-6.101606514838
H	-5.619258224534	4.231584970909	-5.254066128183
C	-3.947220544182	3.185918593549	-6.171477948427
C	-3.546145816530	2.470157442631	-7.318483277590
H	-2.516087344566	2.120739206754	-7.404914948494
C	-4.446779214606	2.187762426460	-8.342318421339
H	-4.116096685862	1.625807546183	-9.215533406723
C	-6.778871307186	2.347563992328	-9.318109267456
O	-7.943114488344	2.704453270682	-9.282954171505
O	-6.268097352034	1.650124147393	-10.356084659665
H	-6.995050228540	1.523327966965	-10.993757144787
C	-1.599867746701	3.397958821192	-5.428164515490
N	-0.487212151842	3.293464776839	-5.764592978814

SCF Done: E(RB3LYP) = -2036.26983158

Zero-point correction= 0.349499
Thermal correction to Energy= 0.378079
Thermal correction to Enthalpy= 0.379024
Thermal correction to Gibbs Free Energy= 0.283619
Sum of electronic and zero-point Energies= -2035.920333
Sum of electronic and thermal Energies= -2035.891752
Sum of electronic and thermal Enthalpies= -2035.890808
Sum of electronic and thermal Free Energies= -2035.986213

1	C	Isotropic =	56.9168	Anisotropy =	184.7994
2	H	Isotropic =	23.4178	Anisotropy =	7.6996
3	C	Isotropic =	55.1156	Anisotropy =	178.7050
4	C	Isotropic =	140.8482	Anisotropy =	42.7253
5	H	Isotropic =	26.2091	Anisotropy =	8.1864
6	H	Isotropic =	26.0387	Anisotropy =	5.9303
7	C	Isotropic =	45.7384	Anisotropy =	167.8131
8	H	Isotropic =	23.1961	Anisotropy =	11.4668
9	N	Isotropic =	-59.8018	Anisotropy =	532.8057
10	C	Isotropic =	42.6726	Anisotropy =	146.6515
11	C	Isotropic =	64.6874	Anisotropy =	15.5878
12	F	Isotropic =	261.9937	Anisotropy =	120.6638
13	F	Isotropic =	262.8800	Anisotropy =	120.1337
14	F	Isotropic =	282.3988	Anisotropy =	125.1633
15	C	Isotropic =	70.9079	Anisotropy =	171.4739
16	H	Isotropic =	23.6177	Anisotropy =	8.2323
17	C	Isotropic =	77.8861	Anisotropy =	116.9385
18	C	Isotropic =	50.9251	Anisotropy =	159.3421
19	H	Isotropic =	23.6450	Anisotropy =	11.9068
20	C	Isotropic =	88.9654	Anisotropy =	81.3646
21	C	Isotropic =	49.7459	Anisotropy =	103.9301
22	H	Isotropic =	23.6621	Anisotropy =	7.1239

23	N	Isotropic =	99.4050	Anisotropy =	121.1371
24	C	Isotropic =	55.0404	Anisotropy =	126.3855
25	C	Isotropic =	68.3865	Anisotropy =	150.9956
26	C	Isotropic =	67.2277	Anisotropy =	164.2557
27	H	Isotropic =	22.8805	Anisotropy =	8.9135
28	C	Isotropic =	70.8338	Anisotropy =	138.2068
29	H	Isotropic =	24.2091	Anisotropy =	7.8602
30	C	Isotropic =	53.0880	Anisotropy =	101.9840
31	Cl	Isotropic =	735.5842	Anisotropy =	453.9581
32	C	Isotropic =	81.7196	Anisotropy =	127.9559
33	H	Isotropic =	24.4291	Anisotropy =	11.6087
34	C	Isotropic =	65.3890	Anisotropy =	149.4392
35	C	Isotropic =	60.9470	Anisotropy =	179.2784
36	H	Isotropic =	23.3432	Anisotropy =	7.6335
37	C	Isotropic =	69.2043	Anisotropy =	162.8367
38	H	Isotropic =	23.8203	Anisotropy =	9.2273
39	C	Isotropic =	49.5178	Anisotropy =	184.4947
40	C	Isotropic =	67.1279	Anisotropy =	163.4935
41	H	Isotropic =	23.7251	Anisotropy =	9.7364
42	C	Isotropic =	61.9975	Anisotropy =	174.7842
43	H	Isotropic =	23.3358	Anisotropy =	7.8949
44	C	Isotropic =	29.5070	Anisotropy =	87.3176
45	O	Isotropic =	-32.8908	Anisotropy =	493.8625
46	O	Isotropic =	149.4327	Anisotropy =	169.4907
47	H	Isotropic =	25.4800	Anisotropy =	11.9535
48	C	Isotropic =	76.3194	Anisotropy =	307.3728
49	N	Isotropic =	-17.3113	Anisotropy =	350.8092

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.971050698040	4.451365123436	1.052121556727
H	1.937357021630	5.410475087902	1.573811857888
C	1.029066621370	4.147081765972	0.065093174187
C	-0.018889075076	5.171045752756	-0.333929598659
H	0.382085071971	5.821973096477	-1.124637688600
H	-0.250934122438	5.821219689464	0.522700105046
C	1.123653837048	2.891650774862	-0.557031152861
H	0.404589709999	2.603526444102	-1.328936324004
N	2.058945538184	1.983538325089	-0.262931255257
C	2.953073914736	2.305411056993	0.680360717533
C	3.982484338447	1.232809920114	0.964986782399
F	4.893358616652	1.633115531069	1.879265779714
F	4.660592768277	0.883212786398	-0.150417108791
F	3.408560947793	0.104387107151	1.441033264742
C	2.959024910598	3.517442728438	1.368919692611
H	3.706778155068	3.725804966750	2.132922599936
C	-2.904647441611	3.984163485184	-2.289973721829
C	-3.495066600897	3.888158401162	-3.598828021984
H	-3.039222209993	4.576546170624	-4.316265921918
C	-4.468415216801	3.078202447252	-4.129366354057
C	-1.669875152114	4.618010909595	-2.139887803012
H	-1.048925636004	5.076307470804	-2.906548578981

N	-1.259528603167	4.597677198379	-0.841040734566
C	-2.242333036174	3.974447503348	-0.077320545782
C	-3.298992890991	3.576535468787	-0.945309833080
C	-4.444810219149	3.000295625546	-0.365060566920
H	-5.295471704713	2.701199575639	-0.972532081979
C	-4.497706802312	2.802517056489	1.012516117753
H	-5.379499243890	2.351521228692	1.467609430940
C	-3.416228248525	3.185422964620	1.826105582384
Cl	-3.521609519250	2.910595176484	3.566848800299
C	-2.271637391978	3.781568279368	1.308704032517
H	-1.450846024583	4.083745375699	1.957477116190
C	-5.828757288436	3.496686663649	-8.204518203706
C	-5.948510723970	2.267965915338	-7.536171484348
H	-6.377764771620	1.409186567961	-8.051824019994
C	-5.517131918265	2.140235122015	-6.218336982222
H	-5.613697842949	1.175049278615	-5.718741986454
C	-4.947518498235	3.230365612003	-5.528273752181
C	-4.851706737069	4.466104756215	-6.204276024922
H	-4.464434762865	5.345488941918	-5.688291434818
C	-5.277736866591	4.593045261839	-7.521728473110
H	-5.203340844135	5.551845747996	-8.036179872024
C	-6.275653611020	3.685715070987	-9.609187174323
O	-6.197379242567	4.733347043622	-10.225961399419
O	-6.788954730865	2.562129052692	-10.155950215324
H	-7.048406538330	2.787443018570	-11.068630760960
C	-5.010546204897	1.969974217286	-3.403569049771
N	-5.457512428332	1.031643234650	-2.872668485010

SCF Done: E(RB3LYP) = -2036.26983712

Zero-point correction= 0.349676
Thermal correction to Energy= 0.378190
Thermal correction to Enthalpy= 0.379134
Thermal correction to Gibbs Free Energy= 0.284284
Sum of electronic and zero-point Energies= -2035.920161
Sum of electronic and thermal Energies= -2035.891647
Sum of electronic and thermal Enthalpies= -2035.890703
Sum of electronic and thermal Free Energies= -2035.985553

1	C	Isotropic =	57.2728	Anisotropy =	185.1613
2	H	Isotropic =	23.4540	Anisotropy =	7.7490
3	C	Isotropic =	54.9579	Anisotropy =	178.0821
4	C	Isotropic =	140.9805	Anisotropy =	44.1751
5	H	Isotropic =	26.0682	Anisotropy =	6.0104
6	H	Isotropic =	26.1776	Anisotropy =	8.1620
7	C	Isotropic =	46.2711	Anisotropy =	167.9203
8	H	Isotropic =	23.2901	Anisotropy =	11.6581
9	N	Isotropic =	-58.8677	Anisotropy =	535.6477
10	C	Isotropic =	42.6287	Anisotropy =	146.8631
11	C	Isotropic =	64.5693	Anisotropy =	15.7591
12	F	Isotropic =	281.7457	Anisotropy =	126.0541
13	F	Isotropic =	263.5215	Anisotropy =	119.7224
14	F	Isotropic =	261.0545	Anisotropy =	121.0344
15	C	Isotropic =	70.9824	Anisotropy =	171.5190
16	H	Isotropic =	23.6444	Anisotropy =	8.2068
17	C	Isotropic =	77.9166	Anisotropy =	117.4481

18	C	Isotropic =	50.8870	Anisotropy =	159.1265
19	H	Isotropic =	23.6428	Anisotropy =	11.9610
20	C	Isotropic =	89.2116	Anisotropy =	81.2173
21	C	Isotropic =	49.6750	Anisotropy =	103.8032
22	H	Isotropic =	23.6863	Anisotropy =	7.1828
23	N	Isotropic =	100.0575	Anisotropy =	120.3233
24	C	Isotropic =	55.1181	Anisotropy =	126.1611
25	C	Isotropic =	68.4879	Anisotropy =	151.1457
26	C	Isotropic =	66.9965	Anisotropy =	164.1611
27	H	Isotropic =	22.8516	Anisotropy =	8.9393
28	C	Isotropic =	70.6773	Anisotropy =	138.5297
29	H	Isotropic =	24.1945	Anisotropy =	7.8555
30	C	Isotropic =	52.9972	Anisotropy =	101.9173
31	Cl	Isotropic =	735.6295	Anisotropy =	453.4323
32	C	Isotropic =	81.9295	Anisotropy =	128.0860
33	H	Isotropic =	24.4381	Anisotropy =	11.5726
34	C	Isotropic =	65.3702	Anisotropy =	149.4133
35	C	Isotropic =	62.1812	Anisotropy =	176.1987
36	H	Isotropic =	23.3157	Anisotropy =	7.9526
37	C	Isotropic =	66.4117	Anisotropy =	161.8561
38	H	Isotropic =	23.7484	Anisotropy =	9.7245
39	C	Isotropic =	49.6220	Anisotropy =	184.4753
40	C	Isotropic =	68.8951	Anisotropy =	161.9700
41	H	Isotropic =	23.8104	Anisotropy =	9.2118
42	C	Isotropic =	61.5183	Anisotropy =	180.8987
43	H	Isotropic =	23.2992	Anisotropy =	7.6911
44	C	Isotropic =	29.6927	Anisotropy =	87.5338
45	O	Isotropic =	-32.4571	Anisotropy =	495.0784
46	O	Isotropic =	150.0166	Anisotropy =	168.6208
47	H	Isotropic =	25.4810	Anisotropy =	11.9612
48	C	Isotropic =	76.3135	Anisotropy =	307.1645
49	N	Isotropic =	-17.3531	Anisotropy =	350.8199

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	2.883846912275	1.452772578903	-1.816713205147
H	3.594134524965	1.925987741098	-2.498369741716
C	1.508204638917	1.592738460577	-2.017314015883
C	0.975430955155	2.359191401098	-3.215635014349
H	0.750866293861	1.660957345296	-4.034996130277
H	1.744553616080	3.050139271442	-3.590092893775
C	0.651217398985	0.965074280362	-1.097666847445
H	-0.433736625818	1.049573050291	-1.208583507200
N	1.075756406655	0.249292147092	-0.052988897228
C	2.399768061543	0.128517809475	0.111877167061
C	2.810995237487	-0.686764903882	1.319053952089
F	4.152376228052	-0.821571296512	1.408716411536
F	2.284394705878	-1.930769322493	1.285442140425
F	2.388922279224	-0.116450439723	2.470573603429
C	3.347021248593	0.703296049847	-0.732970199035
H	4.413265005498	0.577710932321	-0.549647241579
C	-2.443891820874	3.707263553581	-2.958432167487

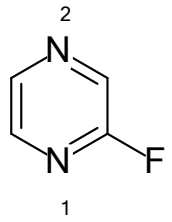
C	-3.823690215974	3.523316866714	-3.323507064181
H	-4.034193329498	2.505908050531	-3.665149662935
C	-4.903041043139	4.370718065723	-3.371219032366
C	-1.495341741572	2.770714288589	-3.374082569556
H	-1.648437527046	1.876445608239	-3.974474116806
N	-0.246609515267	3.110923792513	-2.949735569338
C	-0.338126582673	4.281749659214	-2.202764580933
C	-1.701834741780	4.691918746906	-2.177617578454
C	-2.033565067555	5.824508383567	-1.410143664075
H	-3.060899695622	6.170871663216	-1.329670992398
C	-1.032651014498	6.524080016125	-0.740556617891
H	-1.282231650257	7.404420056749	-0.148226406461
C	0.305407540825	6.098505098202	-0.820831685646
Cl	1.544156149874	7.018113145080	0.037451088678
C	0.684524524275	4.971323323992	-1.541112598088
H	1.722615586403	4.643892169971	-1.569589957617
C	-8.856315262308	2.993900066184	-4.426135670565
C	-8.497467009060	4.338520159774	-4.610605107205
H	-9.217621599564	5.039849664268	-5.031592594828
C	-7.223626730461	4.779923531153	-4.261617152237
H	-6.963407082437	5.828054788931	-4.417283370986
C	-6.266411405695	3.894576356848	-3.724094718605
C	-6.645839577006	2.549173733185	-3.525393105364
H	-5.951506144232	1.844806568099	-3.065767049770
C	-7.915844463220	2.106721803409	-3.878233011228
H	-8.202249661270	1.066554670429	-3.718410420463
C	-10.202806697253	2.473108760255	-4.778763108592
O	-10.558929558760	1.317484703113	-4.630986280623
O	-11.017921919957	3.420106403735	-5.292131080441
H	-11.866764958201	2.982499055424	-5.489837305589
C	-4.768232433618	5.782977400949	-3.181910941155
N	-4.710572239936	6.943834740138	-3.076061487702

SCF Done: E(RB3LYP) = -2036.26971526

Zero-point correction= 0.349646
Thermal correction to Energy= 0.378193
Thermal correction to Enthalpy= 0.379137
Thermal correction to Gibbs Free Energy= 0.283638
Sum of electronic and zero-point Energies= -2035.920070
Sum of electronic and thermal Energies= -2035.891522
Sum of electronic and thermal Enthalpies= -2035.890578
Sum of electronic and thermal Free Energies= -2035.986077

1	C	Isotropic = 56.8411	Anisotropy =	184.0403
2	H	Isotropic = 23.4259	Anisotropy =	7.6421
3	C	Isotropic = 55.2904	Anisotropy =	179.0858
4	C	Isotropic = 140.9428	Anisotropy =	41.0009
5	H	Isotropic = 26.0426	Anisotropy =	5.6784
6	H	Isotropic = 26.2503	Anisotropy =	7.9786
7	C	Isotropic = 45.5643	Anisotropy =	168.1889
8	H	Isotropic = 23.1346	Anisotropy =	11.5153
9	N	Isotropic = -59.5956	Anisotropy =	533.3468
10	C	Isotropic = 42.6926	Anisotropy =	146.9864
11	C	Isotropic = 64.6510	Anisotropy =	15.6014
12	F	Isotropic = 282.1027	Anisotropy =	125.5648

13	F	Isotropic =	263.6625	Anisotropy =	119.6385
14	F	Isotropic =	261.0666	Anisotropy =	120.5519
15	C	Isotropic =	71.0367	Anisotropy =	171.3673
16	H	Isotropic =	23.6412	Anisotropy =	8.2267
17	C	Isotropic =	77.9843	Anisotropy =	116.6645
18	C	Isotropic =	50.9935	Anisotropy =	159.2705
19	H	Isotropic =	23.6090	Anisotropy =	12.0143
20	C	Isotropic =	89.2267	Anisotropy =	81.1195
21	C	Isotropic =	49.6617	Anisotropy =	104.0582
22	H	Isotropic =	23.6352	Anisotropy =	7.1895
23	N	Isotropic =	98.5516	Anisotropy =	123.2874
24	C	Isotropic =	55.1659	Anisotropy =	126.0211
25	C	Isotropic =	68.3606	Anisotropy =	150.6983
26	C	Isotropic =	67.5022	Anisotropy =	163.6284
27	H	Isotropic =	22.8413	Anisotropy =	8.9744
28	C	Isotropic =	70.6470	Anisotropy =	138.5739
29	H	Isotropic =	24.2210	Anisotropy =	7.8736
30	C	Isotropic =	52.8829	Anisotropy =	102.4303
31	Cl	Isotropic =	736.0920	Anisotropy =	453.1912
32	C	Isotropic =	81.3552	Anisotropy =	128.6329
33	H	Isotropic =	24.4136	Anisotropy =	11.4401
34	C	Isotropic =	65.5042	Anisotropy =	149.2467
35	C	Isotropic =	61.5672	Anisotropy =	173.8062
36	H	Isotropic =	23.3512	Anisotropy =	7.8578
37	C	Isotropic =	66.9167	Anisotropy =	163.1121
38	H	Isotropic =	23.7336	Anisotropy =	9.7370
39	C	Isotropic =	49.6523	Anisotropy =	184.6392
40	C	Isotropic =	69.6884	Anisotropy =	163.9099
41	H	Isotropic =	23.7719	Anisotropy =	9.1737
42	C	Isotropic =	61.2747	Anisotropy =	179.3124
43	H	Isotropic =	23.3286	Anisotropy =	7.7524
44	C	Isotropic =	29.5330	Anisotropy =	87.1085
45	O	Isotropic =	-32.8098	Anisotropy =	493.8195
46	O	Isotropic =	149.6940	Anisotropy =	169.2749
47	H	Isotropic =	25.5006	Anisotropy =	11.9435
48	C	Isotropic =	76.3342	Anisotropy =	307.4071
49	N	Isotropic =	-17.7568	Anisotropy =	351.1624



Conformer 1

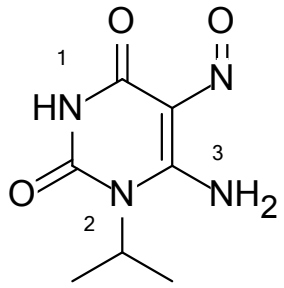
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.496754653824	-0.184658021349	0.128957333886
C	-1.585301139910	0.549819528116	0.076965978040
C	-1.595423688887	1.948046066529	0.033626433413
N	-0.446800408812	2.626786502665	0.043873393883
C	0.681729374002	1.898900267043	0.096805596590
C	0.658085513566	0.504918883641	0.138994187167
F	-2.755502919489	-0.110401183394	0.065820750007
H	-2.536626259088	2.501875565055	-0.008864897130
H	1.629470684072	2.442928438789	0.105714441683
H	1.583253498371	-0.075926047096	0.181836782461

SCF Done: E(RB3LYP) = -363.584582555

Zero-point correction= 0.068595
Thermal correction to Energy= 0.073471
Thermal correction to Enthalpy= 0.074415
Thermal correction to Gibbs Free Energy= 0.039887
Sum of electronic and zero-point Energies= -363.515987
Sum of electronic and thermal Energies= -363.511112
Sum of electronic and thermal Enthalpies= -363.510168
Sum of electronic and thermal Free Energies= -363.544695

1	N	Isotropic = -35.7839	Anisotropy =	453.1973
2	C	Isotropic = 30.9792	Anisotropy =	93.6717
3	C	Isotropic = 59.1225	Anisotropy =	137.6674
4	N	Isotropic = -99.8291	Anisotropy =	591.0521
5	C	Isotropic = 50.1163	Anisotropy =	162.2699
6	C	Isotropic = 50.0625	Anisotropy =	151.1959
7	F	Isotropic = 268.3885	Anisotropy =	69.0777
8	H	Isotropic = 23.0281	Anisotropy =	6.1404
9	H	Isotropic = 22.9117	Anisotropy =	5.3799
10	H	Isotropic = 23.1927	Anisotropy =	4.9323



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=75,noeigen,calcfc)
#symmetry=(none) scf=(maxcycle=1000) scrf=(cpcm,solvent=dmso)

C	1.219313781898	0.656504914526	0.611813201716

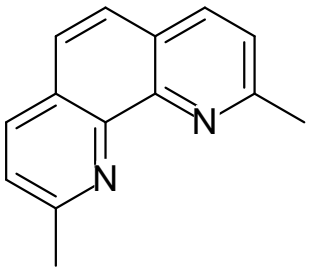
N	2.312091868238	1.090082889796	1.300797761058
C	0.112289728329	1.607859452819	0.553336316378
N	-0.989946461187	1.131641851536	-0.165645150400
H	-1.788379146519	1.758263736585	-0.238097917009
C	-1.144330420937	-0.079921312388	-0.795460687278
N	-0.046843801317	-0.974214543437	-0.710305242162
C	-0.234372728154	-2.297221780687	-1.400367217301
C	-0.275370431554	-3.471181560005	-0.414853741576
H	0.694888927398	-3.715299581042	0.042964575136
H	-0.613241959849	-4.367570386199	-0.957096293959
H	-0.992992110511	-3.272650725053	0.395234207163
C	0.716338075837	-2.480105248080	-2.589379872639
H	1.767807906761	-2.647659937326	-2.311571705287
H	0.676399488959	-1.605918772448	-3.256334613827
H	0.388515158321	-3.360756637914	-3.162755588550
H	-1.242502129159	-2.192028827307	-1.812646070239
C	1.095916769151	-0.625628935484	-0.032807283157
N	2.124217350017	-1.454876537716	0.052294441522
H	2.922584008463	-1.062664415260	0.591682709520
H	2.130002050786	-2.372932946587	-0.368619203466
O	-2.168682226959	-0.365241487237	-1.391595992197
O	0.075335972103	2.722131155142	1.053872719028
O	3.318540329886	0.336959633767	1.407970647528

SCF Done: E(RB3LYP) = -717.488574932

Zero-point correction= 0.184460
Thermal correction to Energy= 0.197622
Thermal correction to Enthalpy= 0.198566
Thermal correction to Gibbs Free Energy= 0.144858
Sum of electronic and zero-point Energies= -717.304115
Sum of electronic and thermal Energies= -717.290953
Sum of electronic and thermal Enthalpies= -717.290009
Sum of electronic and thermal Free Energies= -717.343716

1	C	Isotropic =	50.7632	Anisotropy =	146.3814
2	N	Isotropic =	-478.2150	Anisotropy =	932.4017
3	C	Isotropic =	36.4621	Anisotropy =	103.5708
4	N	Isotropic =	103.8412	Anisotropy =	48.3101
5	H	Isotropic =	24.5883	Anisotropy =	5.3388
6	C	Isotropic =	48.0152	Anisotropy =	71.1541
7	N	Isotropic =	109.5933	Anisotropy =	88.8755
8	C	Isotropic =	142.8842	Anisotropy =	44.3516
9	C	Isotropic =	172.9376	Anisotropy =	28.8822
10	H	Isotropic =	29.8643	Anisotropy =	6.2956
11	H	Isotropic =	30.0516	Anisotropy =	9.9155
12	H	Isotropic =	30.1380	Anisotropy =	8.6027
13	C	Isotropic =	172.8689	Anisotropy =	28.8762
14	H	Isotropic =	29.8714	Anisotropy =	6.2984
15	H	Isotropic =	30.1422	Anisotropy =	8.6051
16	H	Isotropic =	30.0415	Anisotropy =	9.9042
17	H	Isotropic =	26.0120	Anisotropy =	6.9970
18	C	Isotropic =	49.4082	Anisotropy =	113.3107
19	N	Isotropic =	180.2581	Anisotropy =	110.5644
20	H	Isotropic =	17.2761	Anisotropy =	23.4006
21	H	Isotropic =	26.6011	Anisotropy =	10.2791

22 O Isotropic = 14.0630 Anisotropy = 438.4188
23 O Isotropic = -17.7651 Anisotropy = 553.5953
24 O Isotropic = -643.8670 Anisotropy = 1478.9108



Conformer 1

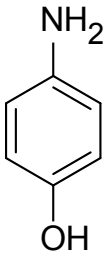
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.084405757140	0.458654690280	-2.800559859551
N	1.387455928382	0.006526329005	-1.588381385181
C	0.609536880359	0.368285459591	-0.534443319204
C	-0.524897769220	1.217874622522	-0.677381994212
C	-0.826232023505	1.684992093767	-1.980935380697
C	-0.028397049676	1.309922422852	-3.039234166670
C	0.949505912051	-0.132750573176	0.793282270943
C	0.134856299300	0.246695833372	1.898621706275
C	-0.999008703318	1.105429404872	1.707365213831
C	-1.317343254905	1.573581036378	0.465072974182
N	2.031439689471	-0.944088237714	0.928644155280
C	2.346856749070	-1.404171712939	2.134725849360
C	1.592988252735	-1.078856587631	3.294888396886
C	0.494069621648	-0.257513599735	3.173354683563
C	1.972517083154	0.037562275906	-3.943600508530
C	3.552661491404	-2.302120931975	2.244815555631
H	-1.689204611225	2.337984805371	-2.131462025709
H	-0.240265876575	1.656841365859	-4.052383203289
H	-1.602057603729	1.375627615780	2.577202730731
H	-2.180435091014	2.227070559311	0.319213256403
H	1.889335596243	-1.479977552190	4.265993926392
H	-0.105877474561	0.011416036037	4.046009726918
H	1.392396803659	-0.482717661805	-4.723964754403
H	2.438298844165	0.914435277071	-4.424038986210
H	2.763677368114	-0.631169735460	-3.580369664213
H	4.012856279741	-2.439090500520	1.257625687038
H	4.301015135664	-1.875373122014	2.933428290290
H	3.273225765426	-3.289219612816	2.649830824145

SCF Done: E(RB3LYP) = -650.296600730

Zero-point correction= 0.224159
Thermal correction to Energy= 0.237003
Thermal correction to Enthalpy= 0.237948
Thermal correction to Gibbs Free Energy= 0.184653
Sum of electronic and zero-point Energies= -650.072442
Sum of electronic and thermal Energies= -650.059597
Sum of electronic and thermal Enthalpies= -650.058653
Sum of electronic and thermal Free Energies= -650.111948

1	C	Isotropic =	32.8158	Anisotropy =	175.9694
2	N	Isotropic =	-53.6807	Anisotropy =	483.1099
3	C	Isotropic =	46.0316	Anisotropy =	166.7541
4	C	Isotropic =	64.6022	Anisotropy =	193.2270
5	C	Isotropic =	56.9460	Anisotropy =	169.3278
6	C	Isotropic =	69.8491	Anisotropy =	155.7584
7	C	Isotropic =	46.0819	Anisotropy =	166.7769
8	C	Isotropic =	64.6364	Anisotropy =	193.2776
9	C	Isotropic =	66.2811	Anisotropy =	146.6450
10	C	Isotropic =	66.3433	Anisotropy =	146.6099
11	N	Isotropic =	-53.6880	Anisotropy =	483.0891
12	C	Isotropic =	32.8076	Anisotropy =	175.8556
13	C	Isotropic =	69.8117	Anisotropy =	155.8876
14	C	Isotropic =	56.8627	Anisotropy =	169.3613
15	C	Isotropic =	165.7392	Anisotropy =	43.3378
16	C	Isotropic =	165.6926	Anisotropy =	43.3352
17	H	Isotropic =	23.2586	Anisotropy =	7.3173
18	H	Isotropic =	23.8016	Anisotropy =	7.9740
19	H	Isotropic =	23.6453	Anisotropy =	6.8617
20	H	Isotropic =	23.6520	Anisotropy =	6.8531
21	H	Isotropic =	23.7939	Anisotropy =	7.9849
22	H	Isotropic =	23.2501	Anisotropy =	7.3326
23	H	Isotropic =	28.3456	Anisotropy =	7.2787
24	H	Isotropic =	28.3379	Anisotropy =	7.2790
25	H	Isotropic =	28.8816	Anisotropy =	7.4905
26	H	Isotropic =	28.8841	Anisotropy =	7.4865
27	H	Isotropic =	28.3406	Anisotropy =	7.2676
28	H	Isotropic =	28.3400	Anisotropy =	7.2724



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

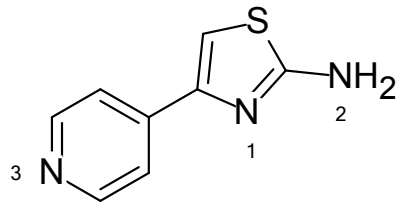
C	-0.218439290954	-0.611600841151	0.910609298402
C	0.901691324338	0.178871474714	0.626617536975
C	1.928849122103	-0.311932289537	-0.185295371156
C	1.865728584892	-1.604333729513	-0.737209912873
C	0.734276894812	-2.389631504335	-0.440775950655
C	-0.291820126930	-1.901912830438	0.369901176400
N	2.861637635858	-2.070516156098	-1.613241275592
O	-1.257690824200	-0.186377826779	1.701633424306
H	0.978038920720	1.187021442276	1.044586317384
H	2.794683903508	0.322112103272	-0.394537447176
H	0.657312630146	-3.399321022170	-0.853402769425
H	-1.162639837320	-2.521689941631	0.594863339857
H	3.773342248474	-1.650005252892	-1.445207136957
H	2.956621494087	-3.084089117492	-1.610505328140
H	-1.071802679532	0.716975491775	2.000974098650

SCF Done: E(RB3LYP) = -362.855383307

Zero-point correction= 0.120578
Thermal correction to Energy= 0.127610
Thermal correction to Enthalpy= 0.128554
Thermal correction to Gibbs Free Energy= 0.089844
Sum of electronic and zero-point Energies= -362.734806
Sum of electronic and thermal Energies= -362.727774
Sum of electronic and thermal Enthalpies= -362.726829
Sum of electronic and thermal Free Energies= -362.765539

1	C	Isotropic =	45.3106	Anisotropy =	127.7373
2	C	Isotropic =	79.3158	Anisotropy =	127.3964
3	C	Isotropic =	79.0584	Anisotropy =	133.1117
4	C	Isotropic =	51.9577	Anisotropy =	158.5632
5	C	Isotropic =	78.4082	Anisotropy =	134.9855
6	C	Isotropic =	79.1889	Anisotropy =	138.8188
7	N	Isotropic =	201.8051	Anisotropy =	84.5208
8	O	Isotropic =	233.7784	Anisotropy =	60.8277

9 H Isotropic = 25.0258 Anisotropy = 4.7938
10 H Isotropic = 25.0076 Anisotropy = 5.6008
11 H Isotropic = 24.9263 Anisotropy = 5.5675
12 H Isotropic = 24.8896 Anisotropy = 4.7888
13 H Isotropic = 28.6281 Anisotropy = 11.1707
14 H Isotropic = 28.6210 Anisotropy = 11.2453
15 H Isotropic = 27.9215 Anisotropy = 13.2220



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

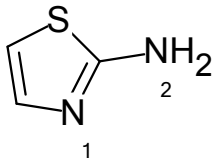
C	1.961241028820	3.341702159102	-0.440781777550
C	0.798108223703	2.583838060250	-0.319511368983
C	0.898987317097	1.202384157431	-0.072656243428
C	2.196915682831	0.674162738143	0.036323001832
C	3.295249169102	1.523577538592	-0.102115029245
N	3.205713694745	2.842495951320	-0.337678551515
C	-0.280361081098	0.328155716098	0.068621731889
N	-0.083280084180	-1.024307716877	0.316339089787
C	-1.219713545715	-1.658961504724	0.413566992766
S	-2.657323426721	-0.634155297501	0.204285380160
C	-1.589250481526	0.727107858913	-0.027691950260
N	-1.340696572955	-2.985905823760	0.726885394629
H	1.887451409530	4.417344325464	-0.632609712882
H	-0.171027760447	3.075130258295	-0.417787140128
H	2.334742074994	-0.389519069644	0.226952854554
H	4.308575482736	1.116192401597	-0.018082725403
H	-1.997913783227	1.714834192692	-0.222080624696
H	-0.493472292031	-3.526872297702	0.570791704887
H	-2.182925055660	-3.458973647689	0.414318973587

SCF Done: E(RB3LYP) = -871.567202107

Zero-point correction= 0.140712
Thermal correction to Energy= 0.150567
Thermal correction to Enthalpy= 0.151511
Thermal correction to Gibbs Free Energy= 0.104450
Sum of electronic and zero-point Energies= -871.426490

Sum of electronic and thermal Energies= -871.416635
Sum of electronic and thermal Enthalpies= -871.415691
Sum of electronic and thermal Free Energies= -871.462752

1	C	Isotropic =	43.4336	Anisotropy =	161.9152
2	C	Isotropic =	74.1239	Anisotropy =	154.4073
3	C	Isotropic =	51.6829	Anisotropy =	186.0971
4	C	Isotropic =	71.4983	Anisotropy =	157.8470
5	C	Isotropic =	42.3279	Anisotropy =	163.2058
6	N	Isotropic =	-60.4298	Anisotropy =	531.8926
7	C	Isotropic =	45.7035	Anisotropy =	84.6737
8	N	Isotropic =	8.7487	Anisotropy =	276.3219
9	C	Isotropic =	22.1249	Anisotropy =	99.2696
10	S	Isotropic =	329.9530	Anisotropy =	186.2703
11	C	Isotropic =	78.1814	Anisotropy =	91.7066
12	N	Isotropic =	189.3546	Anisotropy =	91.9961
13	H	Isotropic =	22.8875	Anisotropy =	6.6311
14	H	Isotropic =	23.9701	Anisotropy =	8.6430
15	H	Isotropic =	23.6545	Anisotropy =	8.7875
16	H	Isotropic =	22.8265	Anisotropy =	6.6459
17	H	Isotropic =	24.2226	Anisotropy =	4.9426
18	H	Isotropic =	26.9326	Anisotropy =	12.5168
19	H	Isotropic =	27.1914	Anisotropy =	10.7771



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

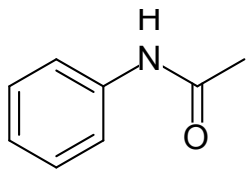
C	1.465580693149	1.893841777620	0.665813369254
N	0.129539038476	1.552809836897	0.776977577462
C	-0.098320682771	0.403266348007	0.194191547348
S	1.329291153053	-0.353336668293	-0.541523928012
C	2.275029332486	1.023406183583	0.000513308692
N	-1.313087563500	-0.238300491355	0.200304712855
H	1.806546660037	2.833487830007	1.103793914531
H	3.339148568368	1.092669428901	-0.211839662156
H	-1.497062471000	-0.864634111724	-0.577973307806
H	-2.095084728298	0.382569866356	0.397102467832

SCF Done: E(RB3LYP) = -624.450385595

Zero-point correction= 0.071489

Thermal correction to Energy= 0.076855
Thermal correction to Enthalpy= 0.077799
Thermal correction to Gibbs Free Energy= 0.042603
Sum of electronic and zero-point Energies= -624.378897
Sum of electronic and thermal Energies= -624.373530
Sum of electronic and thermal Enthalpies= -624.372586
Sum of electronic and thermal Free Energies= -624.407782

1	C	Isotropic =	56.5153	Anisotropy =	96.2909
2	N	Isotropic =	1.4613	Anisotropy =	293.4627
3	C	Isotropic =	21.1542	Anisotropy =	100.5052
4	S	Isotropic =	352.4213	Anisotropy =	168.5522
5	C	Isotropic =	79.1127	Anisotropy =	83.0778
6	N	Isotropic =	190.7910	Anisotropy =	92.4238
7	H	Isotropic =	24.5249	Anisotropy =	5.5015
8	H	Isotropic =	24.9546	Anisotropy =	3.0008
9	H	Isotropic =	27.3348	Anisotropy =	10.4700
10	H	Isotropic =	27.1433	Anisotropy =	12.4239



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.483109177044	1.654686332485	1.060633925145
C	0.575836629969	1.158105975366	0.119122515804
C	-0.397651245072	0.223739969721	0.519314845552
C	-0.437751322346	-0.193502400956	1.863916683180
C	0.474736441497	0.311106252825	2.790104442977
C	1.443827022722	1.240693483084	2.395241223432
N	-1.351201366873	-0.332595397115	-0.357898843049
C	-1.548739744525	-0.092045176500	-1.697853670552
C	-2.724012940076	-0.846335681385	-2.293292123502
O	-0.859345540985	0.677262581969	-2.362318792404
H	2.233957924738	2.379615871226	0.736860844822
H	0.609125278927	1.480571211139	-0.917628821199
H	-1.192029154368	-0.919018302566	2.180858261200
H	0.425525255932	-0.026676452564	3.827773315761
H	2.158687458652	1.635968879955	3.119728787325
H	-1.990318651577	-0.992763473997	0.071920539576
H	-2.613109947190	-0.868522072528	-3.384424595203
H	-2.800573735632	-1.873747006118	-1.906566736213
H	-3.661891540838	-0.320834594043	-2.047231802652

SCF Done: E(RB3LYP) = -440.302956556

Zero-point correction= 0.154429
Thermal correction to Energy= 0.163614
Thermal correction to Enthalpy= 0.164558
Thermal correction to Gibbs Free Energy= 0.118739
Sum of electronic and zero-point Energies= -440.148528
Sum of electronic and thermal Energies= -440.139343
Sum of electronic and thermal Enthalpies= -440.138398
Sum of electronic and thermal Free Energies= -440.184218

1	C	Isotropic =	63.8781	Anisotropy =	174.6519
2	C	Isotropic =	76.4235	Anisotropy =	160.9676
3	C	Isotropic =	52.5821	Anisotropy =	147.6573
4	C	Isotropic =	76.8410	Anisotropy =	137.0708
5	C	Isotropic =	64.4034	Anisotropy =	172.9385
6	C	Isotropic =	70.9206	Anisotropy =	166.9196
7	N	Isotropic =	116.4133	Anisotropy =	108.8618
8	C	Isotropic =	26.1818	Anisotropy =	108.1971
9	C	Isotropic =	167.5938	Anisotropy =	46.9637
10	O	Isotropic =	-70.7637	Anisotropy =	599.3171
11	H	Isotropic =	24.1235	Anisotropy =	4.8117
12	H	Isotropic =	22.7804	Anisotropy =	9.9070
13	H	Isotropic =	24.7635	Anisotropy =	6.6151
14	H	Isotropic =	24.1222	Anisotropy =	4.6933
15	H	Isotropic =	24.3775	Anisotropy =	4.0564
16	H	Isotropic =	24.8647	Anisotropy =	7.6426
17	H	Isotropic =	29.7625	Anisotropy =	7.1639
18	H	Isotropic =	29.3419	Anisotropy =	5.9374
19	H	Isotropic =	28.9716	Anisotropy =	6.0477

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.346776712451	0.096591335055	2.484639407229
C	-0.548841026483	0.285215080008	1.427107782139
C	-0.074849826279	0.252812933999	0.102319252652
C	1.296004315726	0.030130155292	-0.131838108289
C	2.175856169135	-0.156109402947	0.934086112240
C	1.707509052898	-0.124493052130	2.252791355679
N	-0.901571725843	0.431400556493	-1.025642926046
C	-2.254979441766	0.671766574508	-1.087410543629
C	-2.783353685111	0.842928899487	-2.500628541590
O	-2.979029298668	0.755955548317	-0.098974485509
H	-0.034138840784	0.123863267979	3.508499100671
H	-1.605809180796	0.456896189882	1.609216259376
H	1.669740354921	0.004900154487	-1.159202279628

H	3.235194647151	-0.327086005083	0.729518845578
H	2.395725932730	-0.270510040725	3.087752994084
H	-0.419421850630	0.385945571839	-1.917144931768
H	-2.432592698516	1.799410306212	-2.922207877530
H	-2.435292356066	0.036158558366	-3.164279225221
H	-3.879467254071	0.848013368961	-2.470172190438

SCF Done: E(RB3LYP) = -440.302967429

Zero-point correction= 0.154475
Thermal correction to Energy= 0.163651
Thermal correction to Enthalpy= 0.164595
Thermal correction to Gibbs Free Energy= 0.118901
Sum of electronic and zero-point Energies= -440.148492
Sum of electronic and thermal Energies= -440.139316
Sum of electronic and thermal Enthalpies= -440.138372
Sum of electronic and thermal Free Energies= -440.184067

1	C	Isotropic =	63.8765	Anisotropy =	174.7169
2	C	Isotropic =	76.4052	Anisotropy =	160.8111
3	C	Isotropic =	52.6066	Anisotropy =	147.7115
4	C	Isotropic =	77.0009	Anisotropy =	136.8157
5	C	Isotropic =	64.3341	Anisotropy =	172.8591
6	C	Isotropic =	71.0180	Anisotropy =	166.8985
7	N	Isotropic =	117.1041	Anisotropy =	107.0566
8	C	Isotropic =	26.0485	Anisotropy =	108.3518
9	C	Isotropic =	167.6742	Anisotropy =	47.7105
10	O	Isotropic =	-74.4333	Anisotropy =	596.8870
11	H	Isotropic =	24.1241	Anisotropy =	4.8134
12	H	Isotropic =	22.7949	Anisotropy =	9.8981
13	H	Isotropic =	24.7735	Anisotropy =	6.6047
14	H	Isotropic =	24.1188	Anisotropy =	4.6964
15	H	Isotropic =	24.3804	Anisotropy =	4.0590
16	H	Isotropic =	24.9124	Anisotropy =	7.6687
17	H	Isotropic =	28.9970	Anisotropy =	5.9671
18	H	Isotropic =	29.2047	Anisotropy =	5.9090
19	H	Isotropic =	29.8294	Anisotropy =	7.2148

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.199382710003	2.007794495685	1.015125151641
C	0.028694161775	1.552381488319	0.401099535108
C	-0.383049128726	0.220460093439	0.572537821593
C	0.376733369968	-0.629658526471	1.396096798651
C	1.532515056801	-0.160380156061	2.022081740496
C	1.957253435731	1.158793746785	1.826992642449
N	-1.569231407854	-0.293139857633	-0.004476556423

C	-2.114378466365	-0.144549255716	-1.262421915282
C	-1.414169551229	0.740686680642	-2.270726829953
O	-3.150899568974	-0.744331006185	-1.539428832999
H	1.507739399724	3.045330448856	0.868428251965
H	-0.573514104488	2.242532310352	-0.188292819443
H	0.054983417268	-1.664090007532	1.538477671539
H	2.108881047732	-0.834784449060	2.659314877309
H	2.865622100418	1.523446757120	2.310615087370
H	-2.052827221505	-1.007720553855	0.534991898535
H	-0.319294879567	0.697921828040	-2.189729831516
H	-1.732087093695	0.419270328899	-3.270813496059
H	-1.725023277019	1.789235634376	-2.136801194983

SCF Done: E(RB3LYP) = -440.296828142

Zero-point correction= 0.154583
Thermal correction to Energy= 0.163539
Thermal correction to Enthalpy= 0.164483
Thermal correction to Gibbs Free Energy= 0.119827
Sum of electronic and zero-point Energies= -440.142245
Sum of electronic and thermal Energies= -440.133289
Sum of electronic and thermal Enthalpies= -440.132345
Sum of electronic and thermal Free Energies= -440.177001

1	C	Isotropic =	63.9302	Anisotropy =	174.2260
2	C	Isotropic =	71.2928	Anisotropy =	158.6542
3	C	Isotropic =	53.5271	Anisotropy =	146.2943
4	C	Isotropic =	71.8980	Anisotropy =	145.8391
5	C	Isotropic =	63.6282	Anisotropy =	174.0019
6	C	Isotropic =	69.3220	Anisotropy =	170.7146
7	N	Isotropic =	113.0024	Anisotropy =	104.3911
8	C	Isotropic =	26.4678	Anisotropy =	117.6748
9	C	Isotropic =	171.1995	Anisotropy =	29.9231
10	O	Isotropic =	-70.4016	Anisotropy =	540.3267
11	H	Isotropic =	24.0479	Anisotropy =	5.0439
12	H	Isotropic =	24.3808	Anisotropy =	7.7768
13	H	Isotropic =	24.4851	Anisotropy =	6.6143
14	H	Isotropic =	24.0390	Anisotropy =	4.5500
15	H	Isotropic =	24.2618	Anisotropy =	4.1891
16	H	Isotropic =	25.0313	Anisotropy =	6.7073
17	H	Isotropic =	29.2767	Anisotropy =	4.1272
18	H	Isotropic =	29.7362	Anisotropy =	7.9617
19	H	Isotropic =	29.1060	Anisotropy =	6.5340

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

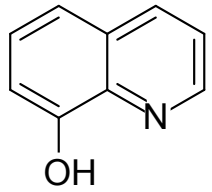
C	0.555402636488	0.300523728545	2.400849948719

C	-0.452117584784	0.302878985478	1.431455460181
C	-0.177019329657	0.761479294640	0.132632172021
C	1.108416625192	1.249467361511	-0.162893682648
C	2.102083434197	1.263125517178	0.817176677268
C	1.834792595986	0.778632431552	2.102622969824
N	-1.161019296726	0.807625419350	-0.884312192643
C	-2.119583285486	-0.105497166388	-1.270018856430
C	-2.251140678269	-1.403848269383	-0.503346155589
O	-2.836952469811	0.151182621386	-2.234550458937
H	0.326614920879	-0.063284344756	3.405022480517
H	-1.455390362835	-0.028591744656	1.696671518992
H	1.323609859923	1.614434302960	-1.170011331398
H	3.094298028373	1.647025761075	0.569813254110
H	2.614417745827	0.782276220610	2.866934026680
H	-1.078977806013	1.573834610562	-1.548913389657
H	-2.730770913658	-2.134138268124	-1.167577291121
H	-1.285632691930	-1.790884878399	-0.149686915632
H	-2.903381427696	-1.263171583140	0.373361765742

SCF Done: E(RB3LYP) = -440.296824651

Zero-point correction= 0.154619
Thermal correction to Energy= 0.163561
Thermal correction to Enthalpy= 0.164505
Thermal correction to Gibbs Free Energy= 0.119994
Sum of electronic and zero-point Energies= -440.142206
Sum of electronic and thermal Energies= -440.133264
Sum of electronic and thermal Enthalpies= -440.132320
Sum of electronic and thermal Free Energies= -440.176831

1	C	Isotropic =	63.9134	Anisotropy =	174.2135
2	C	Isotropic =	70.9625	Anisotropy =	158.5169
3	C	Isotropic =	53.6032	Anisotropy =	146.1157
4	C	Isotropic =	71.7875	Anisotropy =	146.0455
5	C	Isotropic =	63.5997	Anisotropy =	174.1926
6	C	Isotropic =	69.2115	Anisotropy =	170.8140
7	N	Isotropic =	113.2228	Anisotropy =	104.5566
8	C	Isotropic =	26.4300	Anisotropy =	117.7963
9	C	Isotropic =	171.3322	Anisotropy =	29.7723
10	O	Isotropic =	-69.8960	Anisotropy =	540.3561
11	H	Isotropic =	24.0428	Anisotropy =	5.0451
12	H	Isotropic =	24.3744	Anisotropy =	7.7465
13	H	Isotropic =	24.4813	Anisotropy =	6.6109
14	H	Isotropic =	24.0306	Anisotropy =	4.5605
15	H	Isotropic =	24.2529	Anisotropy =	4.2000
16	H	Isotropic =	25.0412	Anisotropy =	6.7100
17	H	Isotropic =	29.7505	Anisotropy =	7.9683
18	H	Isotropic =	29.2923	Anisotropy =	4.1915
19	H	Isotropic =	29.1144	Anisotropy =	6.5519



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

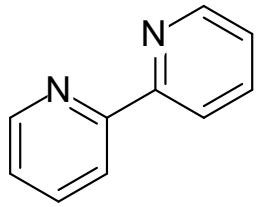
C	-0.567435163055	0.809567423458	0.843737065196
C	0.674412171162	0.392816742358	0.264037883146
C	0.735678895998	-0.811484271144	-0.499075675573
C	-0.447555910419	-1.582169272090	-0.671488847031
C	-1.630600892614	-1.153265531807	-0.099810507748
C	-1.703497938145	0.041890194854	0.660313882213
N	1.745707236455	1.204619692658	0.490948323366
C	2.907746296047	0.848868780241	-0.030449167312
C	3.087096897278	-0.325554861356	-0.805914877169
C	2.006482800545	-1.150725242477	-1.038824752211
O	-0.583064595020	1.956539458349	1.560341532371
H	-0.407046654460	-2.504032242704	-1.254643665604
H	-2.540013873684	-1.743546874144	-0.231297724611
H	-2.646758923885	0.364210626920	1.104063689661
H	3.757403134120	1.511457587262	0.161046243789
H	4.074178056501	-0.559975305550	-1.207230283023
H	2.113431023814	-2.061519560738	-1.632658983770
H	0.343047439363	2.282302655908	1.523325864309

SCF Done: E(RB3LYP) = -477.195957201

Zero-point correction= 0.140160
Thermal correction to Energy= 0.147771
Thermal correction to Enthalpy= 0.148715
Thermal correction to Gibbs Free Energy= 0.107860
Sum of electronic and zero-point Energies= -477.055797
Sum of electronic and thermal Energies= -477.048187
Sum of electronic and thermal Enthalpies= -477.047242
Sum of electronic and thermal Free Energies= -477.088097

1	C	Isotropic =	39.7295	Anisotropy =	137.7748
2	C	Isotropic =	54.6336	Anisotropy =	167.5720
3	C	Isotropic =	63.3446	Anisotropy =	194.3073
4	C	Isotropic =	76.4201	Anisotropy =	139.2587
5	C	Isotropic =	64.0976	Anisotropy =	173.8477
6	C	Isotropic =	84.6023	Anisotropy =	136.5618
7	N	Isotropic =	-32.3740	Anisotropy =	493.0357

8 C Isotropic = 46.4218 Anisotropy = 161.6019
9 C Isotropic = 70.0836 Anisotropy = 163.4222
10 C Isotropic = 56.6427 Anisotropy = 177.0332
11 O Isotropic = 231.0834 Anisotropy = 125.1884
12 H Isotropic = 24.0952 Anisotropy = 5.7773
13 H Isotropic = 23.8475 Anisotropy = 5.1183
14 H Isotropic = 24.3611 Anisotropy = 5.7268
15 H Isotropic = 22.6314 Anisotropy = 5.8601
16 H Isotropic = 23.9225 Anisotropy = 5.6054
17 H Isotropic = 23.2336 Anisotropy = 7.0538
18 H Isotropic = 23.3646 Anisotropy = 16.3319



Conformer 1

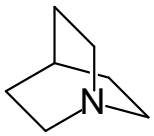
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.578304392103	3.667534803736	-0.452439327095
C	0.706937674355	2.279869587749	-0.489075689116
C	-0.289717905015	1.488674703684	0.106408321009
N	-1.368218338095	2.023614621261	0.712621449963
C	-1.477609175264	3.357317731671	0.739477561278
C	-0.538061815214	4.225756195642	0.175258872867
C	-0.194329872080	-0.001825478331	0.092600787847
C	-1.190985741525	-0.793021239498	0.688083049890
C	-1.062351528120	-2.180686373080	0.651446356650
C	0.054015610037	-2.738906952572	0.023749115991
C	0.993563012211	-1.870467638533	-0.540468216077
N	0.884171802319	-0.536764601338	-0.513610764358
H	1.339286248751	4.304893181221	-0.907571156349
H	1.556482107359	1.792962225517	-0.965048592010
H	-2.365534658783	3.757155386779	1.239597636564
H	-0.682139765340	5.305924286086	0.229087247367
H	-2.040531553018	-0.306115221544	1.164054386874
H	-1.823333579090	-2.818045360255	1.106576771115
H	0.198094094017	-3.819075257857	-0.030079716849
H	1.881488990392	-2.270304600338	-1.040588095561

SCF Done: E(RB3LYP) = -495.422924606

Zero-point correction= 0.157666
Thermal correction to Energy= 0.166289
Thermal correction to Enthalpy= 0.167234
Thermal correction to Gibbs Free Energy= 0.123116
Sum of electronic and zero-point Energies= -495.265259
Sum of electronic and thermal Energies= -495.256635
Sum of electronic and thermal Enthalpies= -495.255691
Sum of electronic and thermal Free Energies= -495.299809

1	C	Isotropic =	56.3788	Anisotropy =	192.1093
2	C	Isotropic =	71.8615	Anisotropy =	174.4511
3	C	Isotropic =	36.5235	Anisotropy =	163.4101
4	N	Isotropic =	-52.5226	Anisotropy =	514.0152
5	C	Isotropic =	43.7726	Anisotropy =	161.7975
6	C	Isotropic =	68.1750	Anisotropy =	167.8529
7	C	Isotropic =	36.5183	Anisotropy =	163.3974
8	C	Isotropic =	71.8511	Anisotropy =	174.4206
9	C	Isotropic =	56.3840	Anisotropy =	192.1261
10	C	Isotropic =	68.1698	Anisotropy =	167.8360
11	C	Isotropic =	43.7637	Anisotropy =	161.7704
12	N	Isotropic =	-52.5264	Anisotropy =	514.0028
13	H	Isotropic =	23.5609	Anisotropy =	5.4466
14	H	Isotropic =	22.7774	Anisotropy =	8.6229
15	H	Isotropic =	22.6854	Anisotropy =	6.1639
16	H	Isotropic =	24.1253	Anisotropy =	4.9848
17	H	Isotropic =	22.7755	Anisotropy =	8.6258
18	H	Isotropic =	23.5601	Anisotropy =	5.4478
19	H	Isotropic =	24.1263	Anisotropy =	4.9834
20	H	Isotropic =	22.6878	Anisotropy =	6.1602



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

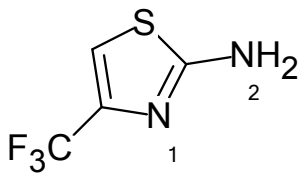
C	1.427353134821	1.403219114833	0.375512051935
C	1.487397803568	1.193104530724	-1.150196756025
C	1.614754123112	-0.338058726743	-1.421648507865
N	1.648107333821	-1.117782026444	-0.170526324314
C	2.713089560753	0.833754571000	1.006098117114
C	2.798430755462	-0.681097944477	0.642043735446
C	0.402780889211	-0.878579271770	0.582284247837

C	0.216790705921	0.630089360950	0.934839712486
H	1.333243629745	2.475828151052	0.607966793965
H	2.346239730287	1.741908339553	-1.571565078508
H	0.579588295733	1.604197920456	-1.622664951516
H	2.534845799550	-0.564132849995	-1.984737179527
H	0.768084537037	-0.704282401604	-2.024690983244
H	2.690577553479	0.976507038782	2.099439068864
H	3.592642093293	1.381292738451	0.628052194762
H	3.715757324541	-0.899274040415	0.071466627464
H	2.826316835031	-1.304900816120	1.550249394987
H	0.435779674844	-1.496435161373	1.494368108265
H	-0.436956481371	-1.247952032590	-0.028568546076
H	-0.715764003440	1.025763026579	0.498745377820
H	0.148850704600	0.775490479152	2.025972896130

SCF Done: E(RB3LYP) = -329.323204705

Zero-point correction= 0.193577
Thermal correction to Energy= 0.200146
Thermal correction to Enthalpy= 0.201090
Thermal correction to Gibbs Free Energy= 0.163007
Sum of electronic and zero-point Energies= -329.129628
Sum of electronic and thermal Energies= -329.123059
Sum of electronic and thermal Enthalpies= -329.122115
Sum of electronic and thermal Free Energies= -329.160198

1	C	Isotropic =	166.1027	Anisotropy =	0.3693
2	C	Isotropic =	161.1905	Anisotropy =	7.9319
3	C	Isotropic =	141.2962	Anisotropy =	43.4902
4	N	Isotropic =	230.6560	Anisotropy =	21.8083
5	C	Isotropic =	161.1994	Anisotropy =	8.0449
6	C	Isotropic =	141.3966	Anisotropy =	43.6009
7	C	Isotropic =	141.3510	Anisotropy =	43.3146
8	C	Isotropic =	161.1705	Anisotropy =	7.9147
9	H	Isotropic =	29.8410	Anisotropy =	9.8627
10	H	Isotropic =	30.0406	Anisotropy =	8.9298
11	H	Isotropic =	30.0221	Anisotropy =	8.9330
12	H	Isotropic =	28.7546	Anisotropy =	9.0309
13	H	Isotropic =	28.7589	Anisotropy =	9.0567
14	H	Isotropic =	30.0403	Anisotropy =	8.9406
15	H	Isotropic =	30.0450	Anisotropy =	8.9219
16	H	Isotropic =	28.7710	Anisotropy =	9.0271
17	H	Isotropic =	28.7569	Anisotropy =	9.0424
18	H	Isotropic =	28.7463	Anisotropy =	9.0471
19	H	Isotropic =	28.7460	Anisotropy =	9.0658
20	H	Isotropic =	30.0160	Anisotropy =	8.9416
21	H	Isotropic =	30.0265	Anisotropy =	8.9483



Conformer 1

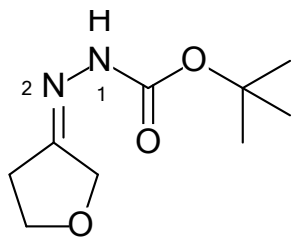
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.393139850408	-0.338534888486	-0.381528763929
C	2.000645770948	0.783755026775	-0.675347895570
S	1.104522417512	2.252574518900	-0.222147662734
C	-0.169070066181	1.230121230775	0.399260440523
C	0.181855213820	-0.074022303418	0.221195219015
C	-0.669810156623	-1.233350909011	0.633343763587
F	-0.034708769139	-2.043081867475	1.514824956162
F	-1.818078838197	-0.827135860639	1.218802261700
F	-1.012385087818	-2.014611433437	-0.419735155730
N	3.252018475377	0.862355109753	-1.215900511222
H	-1.070702916473	1.646559487589	0.839020787787
H	3.486285507684	1.703913613052	-1.732729404733
H	3.572208598681	0.005718275620	-1.660768034856

SCF Done: E(RB3LYP) = -961.511959100

Zero-point correction= 0.076025
Thermal correction to Energy= 0.084960
Thermal correction to Enthalpy= 0.085904
Thermal correction to Gibbs Free Energy= 0.041083
Sum of electronic and zero-point Energies= -961.435934
Sum of electronic and thermal Energies= -961.426999
Sum of electronic and thermal Enthalpies= -961.426055
Sum of electronic and thermal Free Energies= -961.470876

1	N	Isotropic =	11.7292	Anisotropy =	278.0758
2	C	Isotropic =	20.4187	Anisotropy =	101.2779
3	S	Isotropic =	336.2398	Anisotropy =	174.1172
4	C	Isotropic =	74.7985	Anisotropy =	96.1812
5	C	Isotropic =	52.3115	Anisotropy =	76.5373
6	C	Isotropic =	65.9364	Anisotropy =	11.6447
7	F	Isotropic =	262.0664	Anisotropy =	126.0266
8	F	Isotropic =	277.9475	Anisotropy =	133.6200
9	F	Isotropic =	261.6419	Anisotropy =	126.6591
10	N	Isotropic =	187.6948	Anisotropy =	91.9338
11	H	Isotropic =	24.4580	Anisotropy =	3.9027
12	H	Isotropic =	27.1189	Anisotropy =	10.6701
13	H	Isotropic =	26.9376	Anisotropy =	12.3502



Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.238308148867	1.656724359772	4.039034657052
O	5.281255585019	2.157640461015	3.195079753233
C	5.195713664775	1.435002124031	1.970724738296
C	3.715130104103	1.159444507892	1.786107337157
C	3.032898737495	1.435242263123	3.110821563881
N	3.233808450223	0.780755601861	0.662781704530
N	1.887297761749	0.559096345141	0.602493509909
C	1.234133845968	0.143288502491	-0.538924761798
O	0.024017410865	-0.037560555522	-0.532946368201
O	2.074113723591	-0.016422895805	-1.569188959978
C	1.581930549800	-0.460511607339	-2.896170243460
C	0.964008268766	-1.856642574014	-2.786799528570
C	0.605215254477	0.571678906745	-3.464629854355
C	2.869747299340	-0.501394577622	-3.719609931951
H	4.061285925734	2.397082610699	4.830383414422
H	4.545907910300	0.701095077274	4.507114409009
H	5.759628938387	0.480322986710	2.029777330887
H	5.627653728127	2.044302446357	1.163756729143
H	2.410060527542	2.343816140779	3.035305865850
H	2.384934208012	0.606978216951	3.439952534416
H	1.281707956535	0.689124490585	1.412548949220
H	0.718800165758	-2.226434961032	-3.794783321443
H	1.680154498656	-2.558004283825	-2.330394722519
H	0.047362487845	-1.841612220075	-2.184133629153
H	-0.314224409686	0.620919605620	-2.867902752876
H	1.070904485281	1.569543243210	-3.485824625752
H	0.342565439970	0.294999221860	-4.497754599585
H	3.337848414970	0.494001248277	-3.758341169897
H	3.589375960199	-1.208662591354	-3.279831402008
H	2.647994957331	-0.823412093803	-4.748256625460

SCF Done: E(RB3LYP) = -687.789646123

Zero-point correction= 0.250903
Thermal correction to Energy= 0.266009

Thermal correction to Enthalpy= 0.266953
Thermal correction to Gibbs Free Energy= 0.207974
Sum of electronic and zero-point Energies= -687.538743
Sum of electronic and thermal Energies= -687.523637
Sum of electronic and thermal Enthalpies= -687.522693
Sum of electronic and thermal Free Energies= -687.581672

1	C	Isotropic =	123.3811	Anisotropy =	78.0133
2	O	Isotropic =	282.7990	Anisotropy =	84.3000
3	C	Isotropic =	122.3211	Anisotropy =	63.5658
4	C	Isotropic =	38.1140	Anisotropy =	90.7683
5	C	Isotropic =	163.7484	Anisotropy =	18.3384
6	N	Isotropic =	-43.2949	Anisotropy =	358.8618
7	N	Isotropic =	99.3149	Anisotropy =	60.2960
8	C	Isotropic =	44.2689	Anisotropy =	59.4932
9	O	Isotropic =	60.1471	Anisotropy =	343.2891
10	O	Isotropic =	143.1713	Anisotropy =	99.9053
11	C	Isotropic =	107.5319	Anisotropy =	74.1809
12	C	Isotropic =	165.8916	Anisotropy =	38.2771
13	C	Isotropic =	165.8511	Anisotropy =	38.3518
14	C	Isotropic =	160.3721	Anisotropy =	44.5855
15	H	Isotropic =	27.2512	Anisotropy =	7.6239
16	H	Isotropic =	27.6725	Anisotropy =	7.9735
17	H	Isotropic =	27.2830	Anisotropy =	6.6495
18	H	Isotropic =	27.1517	Anisotropy =	6.0662
19	H	Isotropic =	29.1325	Anisotropy =	7.9373
20	H	Isotropic =	29.0991	Anisotropy =	6.4259
21	H	Isotropic =	24.9756	Anisotropy =	5.4199
22	H	Isotropic =	30.2201	Anisotropy =	8.6014
23	H	Isotropic =	30.2083	Anisotropy =	7.2411
24	H	Isotropic =	28.8657	Anisotropy =	6.1826
25	H	Isotropic =	28.8678	Anisotropy =	6.1830
26	H	Isotropic =	30.2005	Anisotropy =	7.2405
27	H	Isotropic =	30.2157	Anisotropy =	8.6125
28	H	Isotropic =	30.0077	Anisotropy =	7.2478
29	H	Isotropic =	30.0086	Anisotropy =	7.2424
30	H	Isotropic =	30.1999	Anisotropy =	8.1505

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	2.044554883047	4.830368264359	1.198668062556
O	3.348793372390	4.584975253888	1.737135360727
C	3.886200653257	3.482448265373	1.013092612609
C	2.687243154109	2.611953682796	0.686654098482
C	1.443101575458	3.439902062739	0.937038411929
N	2.819301222280	1.401041620012	0.295324749717
N	1.676722656648	0.702140548164	0.027132808671

C	1.669040416727	-0.608067559112	-0.403514851039
O	0.612770856559	-1.183249880960	-0.628782859537
O	2.906364663682	-1.105385657354	-0.523819951895
C	3.129219766073	-2.500915969027	-0.975044892500
C	4.654396849687	-2.606930451866	-0.949846834350
C	2.500422549689	-3.480396103972	0.018808277790
C	2.594547877679	-2.683065770063	-2.397444944285
H	2.118621127630	5.403205177091	0.253443006459
H	1.485059609927	5.427285595315	1.931006045426
H	4.634459550795	2.973679654944	1.637797165383
H	4.381264173779	3.821240665715	0.078739643179
H	0.741800219882	3.428984876142	0.087226958164
H	0.907009711482	3.059572521501	1.824108566249
H	0.751708909862	1.118323183833	0.132032928381
H	5.106425133688	-1.868017693679	-1.628916588023
H	5.038997938888	-2.428433864028	0.065901837088
H	4.966659173239	-3.612451180238	-1.269777164130
H	2.870930704275	-3.283867757740	1.037221869693
H	1.406197019104	-3.401687605087	0.017044478194
H	2.782822463666	-4.509049957468	-0.255124655210
H	3.036177889736	-1.933249891086	-3.072551163732
H	2.874119440793	-3.682330512336	-2.766522901747
H	1.501826435972	-2.588921517857	-2.427030074249

SCF Done: E(RB3LYP) = -687.789652035

Zero-point correction= 0.250905
Thermal correction to Energy= 0.266013
Thermal correction to Enthalpy= 0.266958
Thermal correction to Gibbs Free Energy= 0.207990
Sum of electronic and zero-point Energies= -687.538747
Sum of electronic and thermal Energies= -687.523639
Sum of electronic and thermal Enthalpies= -687.522694
Sum of electronic and thermal Free Energies= -687.581662

1	C	Isotropic =	123.2502	Anisotropy =	77.8139
2	O	Isotropic =	282.8654	Anisotropy =	84.5090
3	C	Isotropic =	122.3296	Anisotropy =	63.6064
4	C	Isotropic =	38.1469	Anisotropy =	90.9652
5	C	Isotropic =	163.7305	Anisotropy =	18.1405
6	N	Isotropic =	-43.3413	Anisotropy =	358.8786
7	N	Isotropic =	99.3231	Anisotropy =	60.2022
8	C	Isotropic =	44.1635	Anisotropy =	59.4214
9	O	Isotropic =	59.9288	Anisotropy =	343.1032
10	O	Isotropic =	143.0931	Anisotropy =	100.3012
11	C	Isotropic =	107.7752	Anisotropy =	73.9208
12	C	Isotropic =	160.3602	Anisotropy =	44.5629
13	C	Isotropic =	165.8806	Anisotropy =	38.1736
14	C	Isotropic =	165.9099	Anisotropy =	38.2508
15	H	Isotropic =	27.6727	Anisotropy =	7.9669
16	H	Isotropic =	27.2450	Anisotropy =	7.6205

17	H	Isotropic =	27.1447	Anisotropy =	6.0660
18	H	Isotropic =	27.2798	Anisotropy =	6.6487
19	H	Isotropic =	29.0962	Anisotropy =	6.4317
20	H	Isotropic =	29.1343	Anisotropy =	7.9425
21	H	Isotropic =	24.9773	Anisotropy =	5.4083
22	H	Isotropic =	29.9999	Anisotropy =	7.2549
23	H	Isotropic =	30.0056	Anisotropy =	7.2438
24	H	Isotropic =	30.2079	Anisotropy =	8.1405
25	H	Isotropic =	30.2038	Anisotropy =	7.2345
26	H	Isotropic =	28.8385	Anisotropy =	6.1917
27	H	Isotropic =	30.2212	Anisotropy =	8.5918
28	H	Isotropic =	30.2047	Anisotropy =	7.2643
29	H	Isotropic =	30.2247	Anisotropy =	8.5968
30	H	Isotropic =	28.8617	Anisotropy =	6.1765

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	6.863996645004	-0.662954875736	0.654213250865
O	7.302952915633	0.544664964237	0.021689934831
C	6.267656767078	1.503761018796	0.214339641243
C	4.983425093455	0.696528443944	0.190806381663
C	5.361255568780	-0.762908188907	0.344855100679
N	3.839881588162	1.249886858765	0.041055507238
N	2.746564733382	0.433776248888	0.034240902570
C	1.486320134859	0.967979375457	-0.135951002915
O	1.242239608283	2.151143840571	-0.284264608459
O	0.601977285914	-0.053213344145	-0.105917764566
C	-0.852006397102	0.181298074573	-0.264234866024
C	-1.423952845293	-1.233246709932	-0.163789586663
C	-1.367337036749	1.058267373314	0.879625571589
C	-1.137244054159	0.785405584722	-1.641632876198
H	7.030152609290	-0.608329622087	1.747992707739
H	7.458750871146	-1.491346434204	0.247169057770
H	6.322003396347	2.255847977175	-0.585857795019
H	6.378894230389	2.021220570398	1.190407823524
H	4.793035748517	-1.271795908790	1.140065248580
H	5.179158441862	-1.303270293207	-0.600702178180
H	2.825283783050	-0.576533705134	0.142643889667
H	-2.518993822024	-1.203628231102	-0.268947304950
H	-1.014459028534	-1.875293769950	-0.958536314117
H	-1.178975637533	-1.683290194648	0.810340677861
H	-1.102766472198	0.614158908650	1.852162985476
H	-0.947671461269	2.070600190485	0.825390119107
H	-2.464968372325	1.126686929587	0.821831158439
H	-2.226010082424	0.843706692026	-1.796692004608
H	-0.714750325228	1.794212133844	-1.730427526014
H	-0.712403886313	0.149796092411	-2.434456131129

SCF Done: E(RB3LYP) = -687.790412348

Zero-point correction= 0.250830
Thermal correction to Energy= 0.265968
Thermal correction to Enthalpy= 0.266912
Thermal correction to Gibbs Free Energy= 0.207903
Sum of electronic and zero-point Energies= -687.539583
Sum of electronic and thermal Energies= -687.524445
Sum of electronic and thermal Enthalpies= -687.523500
Sum of electronic and thermal Free Energies= -687.582510

1	C	Isotropic =	123.4145	Anisotropy =	77.8495
2	O	Isotropic =	283.5621	Anisotropy =	82.9308
3	C	Isotropic =	122.3215	Anisotropy =	63.1685
4	C	Isotropic =	36.9575	Anisotropy =	92.9326
5	C	Isotropic =	163.5798	Anisotropy =	17.8384
6	N	Isotropic =	-41.7271	Anisotropy =	364.7899
7	N	Isotropic =	101.1818	Anisotropy =	84.5488
8	C	Isotropic =	44.8188	Anisotropy =	70.4044
9	O	Isotropic =	56.9646	Anisotropy =	395.3199
10	O	Isotropic =	146.3576	Anisotropy =	81.5804
11	C	Isotropic =	108.2664	Anisotropy =	73.3272
12	C	Isotropic =	160.2734	Anisotropy =	45.0362
13	C	Isotropic =	165.8870	Anisotropy =	38.1460
14	C	Isotropic =	165.8912	Anisotropy =	38.2382
15	H	Isotropic =	27.6634	Anisotropy =	7.8920
16	H	Isotropic =	27.2480	Anisotropy =	7.4400
17	H	Isotropic =	27.1044	Anisotropy =	5.9840
18	H	Isotropic =	27.2450	Anisotropy =	6.7997
19	H	Isotropic =	29.1506	Anisotropy =	6.4395
20	H	Isotropic =	29.1628	Anisotropy =	7.7719
21	H	Isotropic =	24.6047	Anisotropy =	9.3916
22	H	Isotropic =	30.2235	Anisotropy =	8.1473
23	H	Isotropic =	30.0613	Anisotropy =	7.3523
24	H	Isotropic =	30.0653	Anisotropy =	7.3445
25	H	Isotropic =	30.2134	Anisotropy =	7.2539
26	H	Isotropic =	28.8720	Anisotropy =	6.0831
27	H	Isotropic =	30.2297	Anisotropy =	8.5648
28	H	Isotropic =	30.2279	Anisotropy =	8.5749
29	H	Isotropic =	28.8746	Anisotropy =	6.0792
30	H	Isotropic =	30.2067	Anisotropy =	7.2622

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.150149159731	3.417138079129	2.876126346938
O	4.449666577397	3.386639612124	1.472664385259

C	3.546324880149	2.476967908299	0.844519479607
C	3.012214385543	1.589338654515	1.949678388196
C	3.734808456416	1.982638875425	3.215351558664
N	2.044964264067	0.750891666148	1.957386939026
N	1.423445764302	0.499384385439	0.720689426940
C	2.086325563712	-0.135413136028	-0.320996962440
O	3.299001744727	-0.192403138925	-0.443985777165
O	1.161672271021	-0.646088356726	-1.158531950730
C	1.548629133146	-1.332516642287	-2.416244179154
C	0.190665695536	-1.694006124493	-3.018719182665
C	2.308374908279	-0.366285775622	-3.327970632263
C	2.353948923262	-2.593116182362	-2.092684607048
H	3.323265209926	4.125141059345	3.083530836401
H	5.050469872114	3.760741926116	3.403491993791
H	4.082121743512	1.907641807042	0.073134217681
H	2.696108803001	3.001075429301	0.360528255906
H	3.103583465753	1.881397828512	4.108107721628
H	4.629813371438	1.348507555620	3.340679051290
H	0.479727713772	0.146352906037	0.859230749381
H	0.332852193446	-2.224900793725	-3.972058660724
H	-0.375567806682	-2.346930086069	-2.337132395899
H	-0.404030222526	-0.787612356500	-3.209160123088
H	3.282385548717	-0.095780157753	-2.901217837397
H	2.472722681286	-0.842782600192	-4.307140106600
H	1.721343224210	0.551580998024	-3.488756581249
H	2.531457456212	-3.160927204486	-3.019464877254
H	3.322786983686	-2.343394247865	-1.642077714129
H	1.793138034848	-3.238281888042	-1.398307762902

SCF Done: E(RB3LYP) = -687.785194840

Zero-point correction= 0.251179
Thermal correction to Energy= 0.266151
Thermal correction to Enthalpy= 0.267095
Thermal correction to Gibbs Free Energy= 0.208846
Sum of electronic and zero-point Energies= -687.534016
Sum of electronic and thermal Energies= -687.519044
Sum of electronic and thermal Enthalpies= -687.518099
Sum of electronic and thermal Free Energies= -687.576349

1 C Isotropic = 124.4290 Anisotropy = 73.1972
2 O Isotropic = 288.9164 Anisotropy = 95.0042
3 C Isotropic = 123.2488 Anisotropy = 61.5554
4 C Isotropic = 14.1591 Anisotropy = 131.8187
5 C Isotropic = 155.0653 Anisotropy = 26.5842
6 N Isotropic = -46.2483 Anisotropy = 329.9968
7 N Isotropic = 109.4445 Anisotropy = 90.2426
8 C Isotropic = 43.6240 Anisotropy = 63.4535
9 O Isotropic = 51.0099 Anisotropy = 395.3596
10 O Isotropic = 141.2469 Anisotropy = 81.6188
11 C Isotropic = 107.3904 Anisotropy = 74.8088

12	C	Isotropic =	160.3958	Anisotropy =	45.0520
13	C	Isotropic =	166.1936	Anisotropy =	37.7996
14	C	Isotropic =	165.6196	Anisotropy =	38.4045
15	H	Isotropic =	27.7357	Anisotropy =	8.5606
16	H	Isotropic =	27.3783	Anisotropy =	7.6342
17	H	Isotropic =	26.8348	Anisotropy =	10.3415
18	H	Isotropic =	27.2673	Anisotropy =	5.7502
19	H	Isotropic =	29.1111	Anisotropy =	7.0507
20	H	Isotropic =	28.6853	Anisotropy =	7.4064
21	H	Isotropic =	24.7748	Anisotropy =	5.7951
22	H	Isotropic =	30.2248	Anisotropy =	8.2486
23	H	Isotropic =	30.0364	Anisotropy =	7.5832
24	H	Isotropic =	30.0429	Anisotropy =	7.4481
25	H	Isotropic =	28.9261	Anisotropy =	5.9854
26	H	Isotropic =	30.2255	Anisotropy =	8.4984
27	H	Isotropic =	30.2237	Anisotropy =	7.0845
28	H	Isotropic =	30.2319	Anisotropy =	8.6110
29	H	Isotropic =	28.9636	Anisotropy =	5.7487
30	H	Isotropic =	30.1914	Anisotropy =	7.3791

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	5.832722376345	2.847732913863	1.763699613611
O	5.994090045480	1.628208375287	1.024240044070
C	4.704443412590	1.043346951387	0.842332965714
C	3.704927301773	2.159545053822	1.064370176074
C	4.501347740152	3.424788598413	1.274016310416
N	2.434457846300	2.128725282806	1.218244258047
N	1.809784970132	0.880983690179	1.044454533324
C	1.773048197013	0.235918897979	-0.184319902863
O	2.547904639543	0.442017440667	-1.104132657947
O	0.758046039702	-0.650886040516	-0.162322281648
C	0.490870775891	-1.555156043038	-1.308481560391
C	-0.708743740075	-2.362188598164	-0.811180763550
C	0.119828918973	-0.732246876250	-2.544306681191
C	1.697291237357	-2.465429943800	-1.549145351836
H	6.702791370072	3.484627854516	1.553601880353
H	5.795364152329	2.642609531472	2.852091820436
H	4.507935853045	0.231978146002	1.573665627334
H	4.638088826816	0.617554206840	-0.167907663578
H	4.643576967986	3.936296274706	0.306014549724
H	4.012065489870	4.118212456689	1.970710019731
H	0.914718490148	0.858552564673	1.526868068258
H	-1.018372047589	-3.086033518426	-1.580044747203
H	-0.452498149272	-2.915014986830	0.105449506226
H	-1.559878354313	-1.699097467786	-0.593522949505
H	-0.193843914518	-1.410310187001	-3.353401278459

H	-0.720633233962	-0.057648555642	-2.317706933757
H	0.970830702481	-0.135105614427	-2.895163351717
H	1.440125961403	-3.215796239669	-2.313062457108
H	2.566502028012	-1.893688523447	-1.898043603574
H	1.967636096315	-2.998125644307	-0.623887188992

SCF Done: E(RB3LYP) = -687.785223331

Zero-point correction= 0.251231
Thermal correction to Energy= 0.266172
Thermal correction to Enthalpy= 0.267116
Thermal correction to Gibbs Free Energy= 0.208990
Sum of electronic and zero-point Energies= -687.533993
Sum of electronic and thermal Energies= -687.519051
Sum of electronic and thermal Enthalpies= -687.518107
Sum of electronic and thermal Free Energies= -687.576233

1	C	Isotropic =	124.5570	Anisotropy =	72.7913
2	O	Isotropic =	289.0735	Anisotropy =	94.1208
3	C	Isotropic =	123.2980	Anisotropy =	61.9810
4	C	Isotropic =	14.6513	Anisotropy =	132.0166
5	C	Isotropic =	154.9113	Anisotropy =	26.5541
6	N	Isotropic =	-46.2762	Anisotropy =	330.5981
7	N	Isotropic =	109.4857	Anisotropy =	89.9638
8	C	Isotropic =	43.6090	Anisotropy =	63.4479
9	O	Isotropic =	51.2097	Anisotropy =	394.9463
10	O	Isotropic =	141.1338	Anisotropy =	81.9877
11	C	Isotropic =	107.3737	Anisotropy =	74.6820
12	C	Isotropic =	160.4182	Anisotropy =	45.1064
13	C	Isotropic =	165.7248	Anisotropy =	38.1344
14	C	Isotropic =	166.2068	Anisotropy =	37.8379
15	H	Isotropic =	27.3717	Anisotropy =	7.6483
16	H	Isotropic =	27.7365	Anisotropy =	8.6006
17	H	Isotropic =	27.2787	Anisotropy =	5.7622
18	H	Isotropic =	26.8418	Anisotropy =	10.3216
19	H	Isotropic =	28.6722	Anisotropy =	7.4105
20	H	Isotropic =	29.1089	Anisotropy =	7.0330
21	H	Isotropic =	24.7682	Anisotropy =	5.8166
22	H	Isotropic =	30.2246	Anisotropy =	8.2281
23	H	Isotropic =	30.0449	Anisotropy =	7.4580
24	H	Isotropic =	30.0410	Anisotropy =	7.5823
25	H	Isotropic =	30.2397	Anisotropy =	8.5912
26	H	Isotropic =	30.2053	Anisotropy =	7.3709
27	H	Isotropic =	28.9614	Anisotropy =	5.7668
28	H	Isotropic =	30.2267	Anisotropy =	8.4963
29	H	Isotropic =	28.9418	Anisotropy =	5.9949
30	H	Isotropic =	30.2193	Anisotropy =	7.0937

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.016874472140	2.285709172323	3.923852019536
O	2.993981674975	3.215382500489	3.533113595733
C	2.646477834797	2.923201726490	2.184200975290
C	2.974133448272	1.451759141015	1.987943651336
C	3.611819579237	0.961716084474	3.267937776997
N	2.808891970474	0.709153517438	0.958582748283
N	2.219955671106	1.279244901444	-0.136790614459
C	1.973568300518	0.594667474898	-1.309353312297
O	1.422469854125	1.150784659715	-2.249548881896
O	2.404233695061	-0.671221255793	-1.253612742264
C	2.236849787596	-1.586959114585	-2.409174080552
C	2.865606397747	-2.879840049480	-1.888800994701
C	0.748654899736	-1.786985975058	-2.705244449624
C	3.011289602090	-1.054550884031	-3.617244631796
H	4.037475992373	2.257230602760	5.021431586994
H	5.005946985646	2.622784948375	3.555740812965
H	3.229050089689	3.543862587087	1.470104182609
H	1.577110868525	3.153316416538	2.039368779681
H	2.859657513171	0.443037034495	3.887602414205
H	4.448320838646	0.272674555990	3.088164067829
H	1.889763260884	2.243669557340	-0.143192129756
H	2.807180037685	-3.662814482591	-2.659864625217
H	3.924033860706	-2.721085745850	-1.631913436595
H	2.337416938878	-3.233966873186	-0.990507215900
H	0.284146761968	-0.857360368262	-3.057108388486
H	0.631428304420	-2.557955023485	-3.482857880886
H	0.220984015879	-2.129801584044	-1.801296649966
H	2.984939503334	-1.802512686892	-4.425183868877
H	2.576992919887	-0.118130307898	-3.988991666267
H	4.064964920435	-0.877710529716	-3.349617041920

SCF Done: E(RB3LYP) = -687.788377268

Zero-point correction= 0.250851
Thermal correction to Energy= 0.265933
Thermal correction to Enthalpy= 0.266877
Thermal correction to Gibbs Free Energy= 0.208072
Sum of electronic and zero-point Energies= -687.537526
Sum of electronic and thermal Energies= -687.522445
Sum of electronic and thermal Enthalpies= -687.521500
Sum of electronic and thermal Free Energies= -687.580306

1	C	Isotropic =	123.6820	Anisotropy =	74.2351
2	O	Isotropic =	289.7794	Anisotropy =	91.3560
3	C	Isotropic =	127.5720	Anisotropy =	56.4627
4	C	Isotropic =	37.5102	Anisotropy =	94.8763
5	C	Isotropic =	156.7604	Anisotropy =	25.2053
6	N	Isotropic =	-43.7452	Anisotropy =	347.7127

7	N	Isotropic =	101.0235	Anisotropy =	62.5499
8	C	Isotropic =	44.3130	Anisotropy =	59.4306
9	O	Isotropic =	60.1723	Anisotropy =	342.1799
10	O	Isotropic =	143.4173	Anisotropy =	101.7569
11	C	Isotropic =	107.4185	Anisotropy =	74.6578
12	C	Isotropic =	160.3965	Anisotropy =	44.4727
13	C	Isotropic =	165.9307	Anisotropy =	38.1762
14	C	Isotropic =	165.8075	Anisotropy =	38.3353
15	H	Isotropic =	27.3875	Anisotropy =	7.4470
16	H	Isotropic =	27.7546	Anisotropy =	8.0148
17	H	Isotropic =	27.3378	Anisotropy =	6.2309
18	H	Isotropic =	27.0286	Anisotropy =	6.0005
19	H	Isotropic =	28.7771	Anisotropy =	7.5451
20	H	Isotropic =	29.1310	Anisotropy =	6.7873
21	H	Isotropic =	25.1598	Anisotropy =	5.4614
22	H	Isotropic =	30.1856	Anisotropy =	8.1243
23	H	Isotropic =	29.9818	Anisotropy =	7.2068
24	H	Isotropic =	29.9941	Anisotropy =	7.2525
25	H	Isotropic =	28.8734	Anisotropy =	6.1441
26	H	Isotropic =	30.2235	Anisotropy =	8.6325
27	H	Isotropic =	30.2035	Anisotropy =	7.2761
28	H	Isotropic =	30.2154	Anisotropy =	8.6156
29	H	Isotropic =	28.8607	Anisotropy =	6.1994
30	H	Isotropic =	30.1964	Anisotropy =	7.2433

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	5.489165763393	2.636803798754	-2.753484844135
O	5.850164404958	3.166536206820	-1.468004447644
C	5.190872676757	2.379104838398	-0.482575576095
C	3.959667115776	1.811342334519	-1.170194952065
C	4.012964038692	2.250983011856	-2.615461157178
N	3.032661058034	1.065112993338	-0.698909730258
N	3.106581483067	0.735795159913	0.626886147810
C	2.174553632530	-0.056554840920	1.265485596752
O	2.283736332486	-0.306069671155	2.458304495353
O	1.213031581092	-0.473126670166	0.432885987471
C	0.103669091975	-1.333200309245	0.913821725655
C	-0.719920651753	-1.535984887376	-0.358298672723
C	0.657611457194	-2.666530939600	1.421456540149
C	-0.710234514869	-0.591544713210	1.976645599646
H	6.108241102334	1.749915081734	-2.993229790173
H	5.683205387562	3.417914399075	-3.500560186083
H	4.947836794148	3.025102880352	0.378313638684
H	5.840896264900	1.554969629378	-0.118243118049
H	3.684616049668	1.465530747834	-3.309737644498
H	3.371475251640	3.137361813781	-2.762527867902

H	3.848131845753	1.077121201316	1.237441330366
H	-1.593588245849	-2.169923121039	-0.143805566699
H	-1.076391908778	-0.570442336029	-0.748350727415
H	-0.116287094421	-2.025663655377	-1.137658163252
H	1.273871230405	-3.146161208529	0.644807420886
H	1.266626005685	-2.527076531230	2.323314944887
H	-0.178791036243	-3.342085553453	1.660044998924
H	-0.118102249428	-0.422311540168	2.884598488693
H	-1.053700069633	0.379941163681	1.587700198719
H	-1.598032797078	-1.188259283251	2.238665330175

SCF Done: E(RB3LYP) = -687.788377564

Zero-point correction= 0.250829
Thermal correction to Energy= 0.265937
Thermal correction to Enthalpy= 0.266881
Thermal correction to Gibbs Free Energy= 0.207864
Sum of electronic and zero-point Energies= -687.537549
Sum of electronic and thermal Energies= -687.522441
Sum of electronic and thermal Enthalpies= -687.521497
Sum of electronic and thermal Free Energies= -687.580514

1	C	Isotropic =	123.6205	Anisotropy =	74.3043
2	O	Isotropic =	289.3989	Anisotropy =	91.9609
3	C	Isotropic =	127.5769	Anisotropy =	56.6153
4	C	Isotropic =	37.4891	Anisotropy =	94.7588
5	C	Isotropic =	156.7871	Anisotropy =	25.0781
6	N	Isotropic =	-43.7951	Anisotropy =	347.9736
7	N	Isotropic =	101.0284	Anisotropy =	62.5827
8	C	Isotropic =	44.4133	Anisotropy =	59.4243
9	O	Isotropic =	60.4852	Anisotropy =	342.7524
10	O	Isotropic =	143.5239	Anisotropy =	101.9729
11	C	Isotropic =	107.3879	Anisotropy =	74.3726
12	C	Isotropic =	160.3292	Anisotropy =	44.5670
13	C	Isotropic =	165.8622	Anisotropy =	38.2070
14	C	Isotropic =	165.8668	Anisotropy =	38.2742
15	H	Isotropic =	27.7529	Anisotropy =	8.0077
16	H	Isotropic =	27.3833	Anisotropy =	7.4456
17	H	Isotropic =	27.0440	Anisotropy =	5.9778
18	H	Isotropic =	27.3269	Anisotropy =	6.2168
19	H	Isotropic =	29.1399	Anisotropy =	6.7903
20	H	Isotropic =	28.7736	Anisotropy =	7.5449
21	H	Isotropic =	25.1616	Anisotropy =	5.4501
22	H	Isotropic =	30.1818	Anisotropy =	8.1362
23	H	Isotropic =	29.9885	Anisotropy =	7.2552
24	H	Isotropic =	29.9855	Anisotropy =	7.2119
25	H	Isotropic =	30.1984	Anisotropy =	7.2728
26	H	Isotropic =	28.8676	Anisotropy =	6.1886
27	H	Isotropic =	30.2115	Anisotropy =	8.6254
28	H	Isotropic =	28.8707	Anisotropy =	6.1512
29	H	Isotropic =	30.2176	Anisotropy =	7.2763

30 H Isotropic = 30.2187 Anisotropy = 8.6266

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.149994945487	4.288488566663	2.379840250146
O	4.614497416301	4.285952889636	1.020509263372
C	3.958323794132	3.216694062088	0.348085526729
C	3.607261446764	2.207975065784	1.429903333869
C	4.027429136239	2.807569069529	2.752293970082
N	3.029124860965	1.070781798099	1.328783711611
N	2.693827781385	0.646365317583	0.074232910990
C	2.068649167385	-0.572414180535	-0.094377546736
O	1.757382193745	-1.328408471092	0.806959315293
O	1.875199826048	-0.752605286259	-1.419207734168
C	1.213930626386	-1.970581047278	-1.943601659984
C	2.044211159776	-3.207666230235	-1.592055526671
C	-0.219170585463	-2.056115712471	-1.413111133301
C	1.221569590701	-1.721990813114	-3.452241995689
H	3.167930471368	4.796278544717	2.451355879989
H	4.882229901589	4.845297484691	2.979587068017
H	4.641534736787	2.811974836301	-0.418121744733
H	3.036382199561	3.563800936972	-0.165747898937
H	3.309324256979	2.602136346672	3.557813182587
H	5.011750972773	2.406748235776	3.051092083067
H	2.911894781063	1.181822512413	-0.764678901806
H	1.614903615839	-4.090058623125	-2.091994791140
H	3.080994868638	-3.086212041324	-1.943160703733
H	2.054234629909	-3.386117083543	-0.509493475302
H	-0.737824528227	-2.898936276634	-1.896342778804
H	-0.232211324084	-2.210511728940	-0.326911611139
H	-0.772094075280	-1.133271130306	-1.649068184125
H	0.748711115197	-2.567247010599	-3.974758965682
H	0.665132755379	-0.804652632374	-3.698078246580
H	2.252264262654	-1.615027399095	-3.823513597222

SCF Done: E(RB3LYP) = -687.789154960

Zero-point correction= 0.250703
Thermal correction to Energy= 0.265892
Thermal correction to Enthalpy= 0.266836
Thermal correction to Gibbs Free Energy= 0.207482
Sum of electronic and zero-point Energies= -687.538452
Sum of electronic and thermal Energies= -687.523263
Sum of electronic and thermal Enthalpies= -687.522319
Sum of electronic and thermal Free Energies= -687.581673

1 C Isotropic = 123.6695 Anisotropy = 74.3493

2	O	Isotropic =	289.6350	Anisotropy =	91.3758
3	C	Isotropic =	127.5550	Anisotropy =	57.1621
4	C	Isotropic =	36.2012	Anisotropy =	96.4103
5	C	Isotropic =	156.7829	Anisotropy =	25.3750
6	N	Isotropic =	-42.2060	Anisotropy =	354.1351
7	N	Isotropic =	102.9506	Anisotropy =	85.9132
8	C	Isotropic =	44.9032	Anisotropy =	70.6723
9	O	Isotropic =	57.0474	Anisotropy =	397.2397
10	O	Isotropic =	146.4483	Anisotropy =	82.2271
11	C	Isotropic =	108.2357	Anisotropy =	73.5612
12	C	Isotropic =	165.8087	Anisotropy =	38.3672
13	C	Isotropic =	166.0618	Anisotropy =	38.0319
14	C	Isotropic =	160.4001	Anisotropy =	44.8967
15	H	Isotropic =	27.7587	Anisotropy =	8.0833
16	H	Isotropic =	27.3765	Anisotropy =	7.5808
17	H	Isotropic =	27.0785	Anisotropy =	6.4096
18	H	Isotropic =	27.3596	Anisotropy =	6.5294
19	H	Isotropic =	29.1003	Anisotropy =	7.0120
20	H	Isotropic =	28.7304	Anisotropy =	7.7433
21	H	Isotropic =	24.7579	Anisotropy =	9.6915
22	H	Isotropic =	30.2305	Anisotropy =	8.5630
23	H	Isotropic =	30.2146	Anisotropy =	7.2645
24	H	Isotropic =	28.8636	Anisotropy =	6.0803
25	H	Isotropic =	30.2355	Anisotropy =	8.5527
26	H	Isotropic =	28.8708	Anisotropy =	6.0457
27	H	Isotropic =	30.2224	Anisotropy =	7.2808
28	H	Isotropic =	30.2337	Anisotropy =	8.1716
29	H	Isotropic =	30.0772	Anisotropy =	7.3565
30	H	Isotropic =	30.0794	Anisotropy =	7.3447

Conformer9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.643572386135	4.291383818699	1.960423748039
O	4.300181838914	4.530692110333	0.586214821935
C	3.845420861198	3.297404722216	0.040076023130
C	3.313219862132	2.500068643936	1.219737373526
C	3.574651426696	3.316473466595	2.464631243600
N	2.774037827349	1.339806301313	1.244793125623
N	2.598113757859	0.701858974933	0.049473244633
C	2.024259257702	-0.552999420266	0.019420502174
O	1.659115782613	-1.177862490642	0.997784134937
O	1.951696893245	-0.939235814089	-1.272952733979
C	1.386056896553	-2.255527495148	-1.652511887822
C	1.515254377876	-2.238756191365	-3.175896018739
C	2.230188479113	-3.380010385564	-1.047325694235
C	-0.083283131615	-2.332742655672	-1.231095579794

H	4.647889835667	5.261451016961	2.475026004986
H	5.653716484323	3.842381974854	2.033513090139
H	4.670533860126	2.742812139348	-0.456007535972
H	3.076487553007	3.512953218509	-0.721329312966
H	2.661696307435	3.866679513253	2.752043542583
H	3.891310105535	2.699798309799	3.316797925072
H	2.852198110971	1.123416408899	-0.842699371069
H	1.122878856760	-3.176779764639	-3.596913622203
H	0.947004596845	-1.399360628170	-3.604912481992
H	2.569537480869	-2.136629463453	-3.475312934847
H	1.878647452890	-4.349504051160	-1.433798762202
H	3.287499190219	-3.261321169305	-1.332092773277
H	2.155525720964	-3.389348684645	0.047395651738
H	-0.526354434674	-3.263163066192	-1.619496137873
H	-0.184033045888	-2.323228276451	-0.138567377310
H	-0.647414590817	-1.484231062887	-1.649168207835

SCF Done: E(RB3LYP) = -687.789201246

Zero-point correction= 0.250818
Thermal correction to Energy= 0.265946
Thermal correction to Enthalpy= 0.266891
Thermal correction to Gibbs Free Energy= 0.207869
Sum of electronic and zero-point Energies= -687.538383
Sum of electronic and thermal Energies= -687.523255
Sum of electronic and thermal Enthalpies= -687.522311
Sum of electronic and thermal Free Energies= -687.581333

1	C	Isotropic =	123.6973	Anisotropy =	74.1355
2	O	Isotropic =	289.6342	Anisotropy =	91.4328
3	C	Isotropic =	127.6206	Anisotropy =	57.1815
4	C	Isotropic =	36.4345	Anisotropy =	96.9734
5	C	Isotropic =	156.8048	Anisotropy =	25.0826
6	N	Isotropic =	-42.1571	Anisotropy =	354.0216
7	N	Isotropic =	102.9809	Anisotropy =	85.7119
8	C	Isotropic =	44.8603	Anisotropy =	70.5001
9	O	Isotropic =	57.0139	Anisotropy =	397.0769
10	O	Isotropic =	146.1758	Anisotropy =	81.7036
11	C	Isotropic =	108.2023	Anisotropy =	73.5751
12	C	Isotropic =	160.3620	Anisotropy =	44.9033
13	C	Isotropic =	165.9430	Anisotropy =	38.2240
14	C	Isotropic =	165.9320	Anisotropy =	38.0548
15	H	Isotropic =	27.3842	Anisotropy =	7.5707
16	H	Isotropic =	27.7647	Anisotropy =	8.0920
17	H	Isotropic =	27.3591	Anisotropy =	6.5399
18	H	Isotropic =	27.0729	Anisotropy =	6.4156
19	H	Isotropic =	28.7333	Anisotropy =	7.7511
20	H	Isotropic =	29.0840	Anisotropy =	7.0130
21	H	Isotropic =	24.7465	Anisotropy =	9.6718
22	H	Isotropic =	30.2314	Anisotropy =	8.1708
23	H	Isotropic =	30.0633	Anisotropy =	7.3537

24	H	Isotropic =	30.0782	Anisotropy =	7.3642
25	H	Isotropic =	30.2342	Anisotropy =	8.5552
26	H	Isotropic =	30.2181	Anisotropy =	7.2655
27	H	Isotropic =	28.8666	Anisotropy =	6.0290
28	H	Isotropic =	30.2288	Anisotropy =	8.5507
29	H	Isotropic =	28.8545	Anisotropy =	6.0700
30	H	Isotropic =	30.2168	Anisotropy =	7.2781

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	5.653286139240	2.799531503571	-0.395752796530
O	6.524600948161	2.077184757882	0.485424439556
C	6.247356833443	0.692270763041	0.305960707904
C	4.798348323742	0.621150472994	-0.150804429831
C	4.323015465540	2.039360392262	-0.340264941165
N	4.251780183380	-0.510927086027	-0.387336181439
N	2.919359736966	-0.488462103992	-0.828313140139
C	1.889264232674	-0.038335013992	-0.014112206363
O	2.033518088434	0.679805321146	0.961137081271
O	0.727473889467	-0.518910710340	-0.503400376902
C	-0.576544350987	-0.164246362868	0.108033411607
C	-0.638055077876	-0.688153999912	1.544978462540
C	-0.799353318217	1.347527414696	0.023935197850
C	-1.567416821881	-0.910721773024	-0.785630387029
H	6.062937696033	2.808465647673	-1.425232491823
H	5.591620558362	3.833883999620	-0.031567287745
H	6.422338946878	0.168616746015	1.257918746675
H	6.903733402535	0.239325345812	-0.464984951705
H	3.696555098483	2.139784309692	-1.239320230479
H	3.719156235891	2.343119048402	0.528157993699
H	2.687010508163	-1.343930410102	-1.326583675738
H	-1.650236813083	-0.528966854444	1.948793298984
H	-0.426647068340	-1.768771488802	1.568718550017
H	0.083717504409	-0.170439825274	2.189173358678
H	-0.084074574172	1.892038899685	0.653231285126
H	-0.695564419368	1.693088035463	-1.016609201795
H	-1.819742714634	1.584852523230	0.363316438702
H	-2.595410539162	-0.735878969092	-0.433968951937
H	-1.490713363539	-0.562680106376	-1.827021283914
H	-1.370864730540	-1.993510476939	-0.763566438075

SCF Done: E(RB3LYP) = -687.785284835

Zero-point correction= 0.251169
Thermal correction to Energy= 0.266138
Thermal correction to Enthalpy= 0.267082
Thermal correction to Gibbs Free Energy= 0.208886

Sum of electronic and zero-point Energies= -687.534116
Sum of electronic and thermal Energies= -687.519147
Sum of electronic and thermal Enthalpies= -687.518203
Sum of electronic and thermal Free Energies= -687.576399

1	C	Isotropic =	123.5327	Anisotropy =	76.0071
2	O	Isotropic =	286.1353	Anisotropy =	87.6166
3	C	Isotropic =	122.1678	Anisotropy =	63.1535
4	C	Isotropic =	14.2904	Anisotropy =	126.5996
5	C	Isotropic =	156.0355	Anisotropy =	30.6804
6	N	Isotropic =	-45.7914	Anisotropy =	339.1663
7	N	Isotropic =	109.1358	Anisotropy =	93.5829
8	C	Isotropic =	43.6264	Anisotropy =	64.7455
9	O	Isotropic =	47.7704	Anisotropy =	395.2520
10	O	Isotropic =	142.6232	Anisotropy =	83.4504
11	C	Isotropic =	107.5973	Anisotropy =	74.3395
12	C	Isotropic =	165.6142	Anisotropy =	38.3039
13	C	Isotropic =	166.1332	Anisotropy =	37.8599
14	C	Isotropic =	160.3222	Anisotropy =	45.1535
15	H	Isotropic =	27.7871	Anisotropy =	8.0103
16	H	Isotropic =	27.3349	Anisotropy =	7.1405
17	H	Isotropic =	27.0525	Anisotropy =	6.1164
18	H	Isotropic =	27.2132	Anisotropy =	6.9126
19	H	Isotropic =	28.9744	Anisotropy =	4.7328
20	H	Isotropic =	28.7470	Anisotropy =	8.2226
21	H	Isotropic =	24.6446	Anisotropy =	5.7291
22	H	Isotropic =	30.2299	Anisotropy =	8.6134
23	H	Isotropic =	30.1964	Anisotropy =	7.4107
24	H	Isotropic =	28.9480	Anisotropy =	5.7071
25	H	Isotropic =	28.9120	Anisotropy =	5.9901
26	H	Isotropic =	30.2104	Anisotropy =	7.0343
27	H	Isotropic =	30.2203	Anisotropy =	8.5143
28	H	Isotropic =	30.2138	Anisotropy =	8.2454
29	H	Isotropic =	30.0365	Anisotropy =	7.4279
30	H	Isotropic =	30.0313	Anisotropy =	7.6052

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.369028055789	1.652934864516	-3.504737776798
O	0.054845505087	2.073737470864	-3.113071984352
C	-0.402192731691	1.156036814760	-2.125277660941
C	0.852555082924	0.616946226014	-1.455724953641
C	2.032615906103	1.181185492307	-2.205547396361
N	0.759822401216	-0.233158969336	-0.504428233460
N	1.963995367792	-0.699145667230	0.046272404151
C	2.823798203513	0.143935195066	0.736865935419
O	2.836097554945	1.359711372418	0.640232305153

O	3.632530419393	-0.617337290537	1.502847425794
C	4.727912993495	-0.019689355489	2.305098642701
C	5.730421313520	0.674657443308	1.380659760674
C	4.149640882368	0.926006232533	3.360545537117
C	5.355065797851	-1.248919642111	2.963536979136
H	1.868690415633	2.510669227569	-3.974882302541
H	1.309010227985	0.828312404818	-4.242380170470
H	-0.973198348935	0.318785089919	-2.576242553805
H	-1.065279646665	1.687684322861	-1.426165553284
H	2.458436050981	2.023226688265	-1.639398293677
H	2.824858698191	0.429244714099	-2.339299034200
H	1.828823594116	-1.594170826856	0.509772153023
H	6.090385439640	-0.024433719243	0.609499801179
H	5.280950007870	1.546545491494	0.888734526955
H	6.598096952365	1.011009317839	1.969561243599
H	3.395959880471	0.404576156548	3.971319023370
H	4.957686496916	1.262857964114	4.028737669191
H	3.685379517518	1.805989215141	2.898176942533
H	5.730443244865	-1.949064817322	2.201795417895
H	6.197226835488	-0.943725060884	3.602820544031
H	4.616343881259	-1.774456355443	3.587709601606

SCF Done: E(RB3LYP) = -687.785269585

Zero-point correction= 0.251185
Thermal correction to Energy= 0.266155
Thermal correction to Enthalpy= 0.267099
Thermal correction to Gibbs Free Energy= 0.208816
Sum of electronic and zero-point Energies= -687.534085
Sum of electronic and thermal Energies= -687.519114
Sum of electronic and thermal Enthalpies= -687.518170
Sum of electronic and thermal Free Energies= -687.576454

1	C	Isotropic =	123.5421	Anisotropy =	76.0042
2	O	Isotropic =	286.2151	Anisotropy =	88.1571
3	C	Isotropic =	122.2513	Anisotropy =	63.1597
4	C	Isotropic =	14.2851	Anisotropy =	126.4453
5	C	Isotropic =	156.2917	Anisotropy =	30.5024
6	N	Isotropic =	-45.8309	Anisotropy =	339.2813
7	N	Isotropic =	109.0633	Anisotropy =	93.7221
8	C	Isotropic =	43.5872	Anisotropy =	64.8467
9	O	Isotropic =	47.6303	Anisotropy =	395.0997
10	O	Isotropic =	142.6624	Anisotropy =	83.6020
11	C	Isotropic =	107.5763	Anisotropy =	74.4117
12	C	Isotropic =	166.1285	Anisotropy =	38.1826
13	C	Isotropic =	165.5330	Anisotropy =	38.2062
14	C	Isotropic =	160.4318	Anisotropy =	45.0252
15	H	Isotropic =	27.3236	Anisotropy =	7.1381
16	H	Isotropic =	27.7874	Anisotropy =	8.0126
17	H	Isotropic =	27.2188	Anisotropy =	6.9099
18	H	Isotropic =	27.0552	Anisotropy =	6.1181

19	H	Isotropic =	28.7346	Anisotropy =	8.2687
20	H	Isotropic =	28.9786	Anisotropy =	4.7671
21	H	Isotropic =	24.6384	Anisotropy =	5.7368
22	H	Isotropic =	30.2058	Anisotropy =	7.0324
23	H	Isotropic =	28.9257	Anisotropy =	5.9796
24	H	Isotropic =	30.2123	Anisotropy =	8.5312
25	H	Isotropic =	30.1863	Anisotropy =	7.3809
26	H	Isotropic =	30.2308	Anisotropy =	8.6268
27	H	Isotropic =	28.9293	Anisotropy =	5.7436
28	H	Isotropic =	30.0598	Anisotropy =	7.4420
29	H	Isotropic =	30.2071	Anisotropy =	8.2494
30	H	Isotropic =	30.0428	Anisotropy =	7.5874

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.113147534307	3.241959713188	-2.333121520228
O	3.411159496000	2.073194117131	-2.781853019639
C	3.540143780600	1.070351386136	-1.775747470238
C	3.869446799554	1.808454890110	-0.493528815986
C	3.872304692900	3.280861721052	-0.820689660901
N	4.201020304589	1.357036212833	0.655322163854
N	4.169058734015	-0.063989391782	0.763448894543
C	3.004536342638	-0.783439026519	1.010949952174
O	3.043380134126	-1.890277685171	1.527677908296
O	1.911487634836	-0.131230713534	0.585628499217
C	0.552363377350	-0.708217345152	0.762998320856
C	0.262674588867	-0.905830663880	2.252729960151
C	-0.344886655306	0.382754880748	0.178302608064
C	0.428383106593	-2.005979909350	-0.037725658020
H	3.705853868164	4.106163697146	-2.874841890249
H	5.194965275248	3.157470271509	-2.557123525654
H	4.357418156607	0.354866423006	-1.999305157460
H	2.598888249011	0.507223895318	-1.710210310220
H	2.874605998426	3.702030303169	-0.606623938045
H	4.621391205926	3.839660898481	-0.244342011560
H	4.904369202785	-0.382402612374	1.391218187459
H	-0.787004233161	-1.213152227426	2.380568542927
H	0.910991602130	-1.676591730340	2.687501123055
H	0.411722165570	0.037649288027	2.800917561130
H	-0.204153783497	1.331868926544	0.717401556314
H	-0.120297970249	0.547392686696	-0.886545006600
H	-1.400486545957	0.084677380161	0.267462954591
H	0.678722858970	-1.831858694958	-1.095984777301
H	1.090779065466	-2.783837924396	0.361926081856
H	-0.611284986507	-2.365988766375	0.012098447615

SCF Done: E(RB3LYP) = -687.781905486

Zero-point correction= 0.251259
Thermal correction to Energy= 0.266159
Thermal correction to Enthalpy= 0.267104
Thermal correction to Gibbs Free Energy= 0.209161
Sum of electronic and zero-point Energies= -687.530647
Sum of electronic and thermal Energies= -687.515746
Sum of electronic and thermal Enthalpies= -687.514802
Sum of electronic and thermal Free Energies= -687.572745

1	C	Isotropic =	124.4684	Anisotropy =	73.8382
2	O	Isotropic =	289.4599	Anisotropy =	90.0183
3	C	Isotropic =	123.9196	Anisotropy =	58.7736
4	C	Isotropic =	6.6568	Anisotropy =	139.2763
5	C	Isotropic =	155.4802	Anisotropy =	25.5805
6	N	Isotropic =	-54.0505	Anisotropy =	330.8578
7	N	Isotropic =	110.2639	Anisotropy =	72.2748
8	C	Isotropic =	42.8220	Anisotropy =	61.3748
9	O	Isotropic =	53.6800	Anisotropy =	347.2682
10	O	Isotropic =	140.6336	Anisotropy =	105.0888
11	C	Isotropic =	106.7561	Anisotropy =	76.3615
12	C	Isotropic =	166.0556	Anisotropy =	38.4357
13	C	Isotropic =	160.3587	Anisotropy =	44.1090
14	C	Isotropic =	165.8306	Anisotropy =	37.5605
15	H	Isotropic =	27.3814	Anisotropy =	7.6895
16	H	Isotropic =	27.7355	Anisotropy =	8.8945
17	H	Isotropic =	27.0856	Anisotropy =	5.3095
18	H	Isotropic =	26.7905	Anisotropy =	10.4741
19	H	Isotropic =	28.7466	Anisotropy =	6.8947
20	H	Isotropic =	29.0488	Anisotropy =	7.2942
21	H	Isotropic =	25.5486	Anisotropy =	6.2508
22	H	Isotropic =	30.2902	Anisotropy =	8.8437
23	H	Isotropic =	28.9637	Anisotropy =	6.3385
24	H	Isotropic =	30.3225	Anisotropy =	7.2751
25	H	Isotropic =	30.0795	Anisotropy =	6.6408
26	H	Isotropic =	30.0310	Anisotropy =	6.4567
27	H	Isotropic =	30.2334	Anisotropy =	8.3051
28	H	Isotropic =	30.2056	Anisotropy =	6.7677
29	H	Isotropic =	28.9105	Anisotropy =	6.3552
30	H	Isotropic =	30.2431	Anisotropy =	8.7935

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	3.078870272184	3.985796796387	1.706598252552
O	3.043765314989	2.723151178793	2.388338854802
C	3.444723142625	1.713740769796	1.463664208413
C	3.210202878841	2.297091216815	0.084550409702

C	2.614742127004	3.669011145145	0.281487994223
N	3.523906426444	1.841667107163	-1.067771020950
N	4.106199599590	0.540738444384	-1.051932153749
C	3.357062511575	-0.629523924290	-0.986323756735
O	3.797460122968	-1.686631536147	-1.413088640704
O	2.173022598527	-0.434652825449	-0.385583957944
C	1.201269987078	-1.548337288533	-0.220197132606
C	1.797394074990	-2.632452509931	0.679994490713
C	0.023406765136	-0.856086986423	0.465571476255
C	0.789233930413	-2.083915340795	-1.593505711220
H	4.107024102201	4.398610874204	1.702756684675
H	2.421301386348	4.678087079102	2.249301983500
H	2.852471157468	0.806549148241	1.646658193964
H	4.517926289810	1.453539513201	1.566355837261
H	2.942377455474	4.384553029020	-0.484194907088
H	1.513775644350	3.595368604061	0.248629323496
H	4.797086967087	0.459638208005	-1.795060006968
H	1.030877592384	-3.396578627326	0.883862936830
H	2.659592722920	-3.115749061832	0.203937231175
H	2.114669567539	-2.202519790467	1.643036645530
H	-0.790063553117	-1.579126471234	0.628361757396
H	0.322814671935	-0.446064893700	1.442150535119
H	-0.360309221680	-0.033927009601	-0.157325662588
H	0.406318649945	-1.266797934204	-2.224901352223
H	1.632959086875	-2.563645827239	-2.104821006440
H	-0.015802271905	-2.824813087147	-1.468371506389

SCF Done: E(RB3LYP) = -687.781882342

Zero-point correction= 0.251240
Thermal correction to Energy= 0.266158
Thermal correction to Enthalpy= 0.267102
Thermal correction to Gibbs Free Energy= 0.209075
Sum of electronic and zero-point Energies= -687.530643
Sum of electronic and thermal Energies= -687.515724
Sum of electronic and thermal Enthalpies= -687.514780
Sum of electronic and thermal Free Energies= -687.572808

1 C Isotropic = 124.4558 Anisotropy = 74.1220
2 O Isotropic = 289.4882 Anisotropy = 91.1424
3 C Isotropic = 123.9117 Anisotropy = 58.6373
4 C Isotropic = 6.7700 Anisotropy = 139.2891
5 C Isotropic = 155.4850 Anisotropy = 25.9392
6 N Isotropic = -54.1399 Anisotropy = 330.9014
7 N Isotropic = 110.0858 Anisotropy = 72.1612
8 C Isotropic = 42.7933 Anisotropy = 61.3647
9 O Isotropic = 53.6198 Anisotropy = 347.1037
10 O Isotropic = 140.3684 Anisotropy = 104.7917
11 C Isotropic = 106.5966 Anisotropy = 76.2795
12 C Isotropic = 165.8173 Anisotropy = 37.6529
13 C Isotropic = 160.3590 Anisotropy = 44.0465

14	C	Isotropic =	166.0857	Anisotropy =	38.4925
15	H	Isotropic =	27.7634	Anisotropy =	8.8637
16	H	Isotropic =	27.3853	Anisotropy =	7.6648
17	H	Isotropic =	26.7705	Anisotropy =	10.4958
18	H	Isotropic =	27.0749	Anisotropy =	5.2823
19	H	Isotropic =	29.0767	Anisotropy =	7.2976
20	H	Isotropic =	28.7241	Anisotropy =	6.8850
21	H	Isotropic =	25.5474	Anisotropy =	6.1891
22	H	Isotropic =	30.2396	Anisotropy =	8.7983
23	H	Isotropic =	28.8913	Anisotropy =	6.3706
24	H	Isotropic =	30.1881	Anisotropy =	6.7822
25	H	Isotropic =	30.2179	Anisotropy =	8.2827
26	H	Isotropic =	30.0159	Anisotropy =	6.4455
27	H	Isotropic =	30.0701	Anisotropy =	6.6295
28	H	Isotropic =	30.3240	Anisotropy =	7.2603
29	H	Isotropic =	28.9578	Anisotropy =	6.3353
30	H	Isotropic =	30.2892	Anisotropy =	8.8436

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.383050446072	1.289694838725	-1.612055670742
O	-1.086682618969	0.879995579199	-0.430838472376
C	-0.500368599090	-0.342385991155	0.004165916567
C	0.933593754867	-0.310328681944	-0.498997393592
C	1.082658133579	0.934286058771	-1.336036721488
N	1.735054846134	-1.273118611141	-0.246600086020
N	3.034695654816	-1.151940606883	-0.799776752420
C	4.035319974171	-0.346541508445	-0.268715933584
O	5.213930973074	-0.569079110974	-0.505880265107
O	3.538537642087	0.659288583218	0.467502411184
C	4.438332544372	1.641545717361	1.129593345143
C	5.350045117265	0.921870772799	2.126273303251
C	5.222028220933	2.422326599248	0.072752201590
C	3.451136856062	2.551507275181	1.861001681575
H	-0.563428020113	2.363667958203	-1.753724445984
H	-0.761935600362	0.744487925651	-2.498961364134
H	-1.023236999789	-1.222560353088	-0.422139587804
H	-0.566975118949	-0.399785462239	1.101035529448
H	1.572998256978	1.718554508461	-0.738673398673
H	1.696089522969	0.753615634581	-2.230682030731
H	3.412694840344	-2.071285522485	-1.017227780912
H	4.751230100370	0.332118173196	2.837990641099
H	6.052435680449	0.253962438912	1.612732883095
H	5.923326468431	1.668348460657	2.697995182762
H	4.533916517091	2.893521767788	-0.646439839719
H	5.800979694965	3.219876240993	0.564281122188
H	5.913366804640	1.767489240975	-0.471906440533

H	2.838420495187	1.972150522063	2.568297575678
H	4.000306961782	3.320249617983	2.425338438063
H	2.781188342778	3.058557934388	1.149905952175

SCF Done: E(RB3LYP) = -687.781967431

Zero-point correction= 0.251178
Thermal correction to Energy= 0.266140
Thermal correction to Enthalpy= 0.267084
Thermal correction to Gibbs Free Energy= 0.208888
Sum of electronic and zero-point Energies= -687.530790
Sum of electronic and thermal Energies= -687.515828
Sum of electronic and thermal Enthalpies= -687.514883
Sum of electronic and thermal Free Energies= -687.573080

1	C	Isotropic =	123.6257	Anisotropy =	75.9129
2	O	Isotropic =	286.2568	Anisotropy =	88.2004
3	C	Isotropic =	122.4986	Anisotropy =	62.2973
4	C	Isotropic =	8.6751	Anisotropy =	132.6780
5	C	Isotropic =	157.3570	Anisotropy =	28.4114
6	N	Isotropic =	-52.4960	Anisotropy =	340.1890
7	N	Isotropic =	108.9206	Anisotropy =	71.8118
8	C	Isotropic =	42.8070	Anisotropy =	60.0460
9	O	Isotropic =	57.0137	Anisotropy =	341.3532
10	O	Isotropic =	139.1812	Anisotropy =	104.8296
11	C	Isotropic =	106.5780	Anisotropy =	76.2467
12	C	Isotropic =	165.9675	Anisotropy =	38.5360
13	C	Isotropic =	165.8750	Anisotropy =	37.2553
14	C	Isotropic =	160.3020	Anisotropy =	43.7462
15	H	Isotropic =	27.3216	Anisotropy =	7.0340
16	H	Isotropic =	27.7757	Anisotropy =	8.3285
17	H	Isotropic =	27.2206	Anisotropy =	7.2384
18	H	Isotropic =	27.0370	Anisotropy =	5.8752
19	H	Isotropic =	28.7946	Anisotropy =	10.6766
20	H	Isotropic =	28.7464	Anisotropy =	4.5631
21	H	Isotropic =	25.3445	Anisotropy =	6.5096
22	H	Isotropic =	30.2923	Anisotropy =	7.3613
23	H	Isotropic =	28.8706	Anisotropy =	6.3766
24	H	Isotropic =	30.2897	Anisotropy =	8.8893
25	H	Isotropic =	30.2088	Anisotropy =	6.6110
26	H	Isotropic =	30.2323	Anisotropy =	8.8119
27	H	Isotropic =	28.8687	Anisotropy =	6.2951
28	H	Isotropic =	30.0630	Anisotropy =	6.5483
29	H	Isotropic =	30.2302	Anisotropy =	8.3329
30	H	Isotropic =	30.0224	Anisotropy =	6.3961

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.956518338609	0.180483095261	2.461071305689
O	4.887889681830	-1.240915389333	2.279477033388
C	4.878197796851	-1.484443053476	0.876675924057
C	4.275038592964	-0.238154342354	0.249173046237
C	4.059598160277	0.757882420976	1.359719998539
N	4.111210265900	-0.160114489412	-1.015705251012
N	3.576750844509	1.063226882482	-1.493543578705
C	2.229743495253	1.400839386726	-1.428485171163
O	1.750298015722	2.226791958318	-2.191701096328
O	1.590851469054	0.747255412152	-0.446215965121
C	0.138159979699	0.955426692496	-0.205820848537
C	-0.140686330905	0.011314033275	0.963953850935
C	-0.122529036618	2.409448822805	0.193072942392
C	-0.657938639103	0.531830356318	-1.442637181333
H	5.999628701031	0.536744636724	2.349853510005
H	4.613423703947	0.404753752411	3.479929329345
H	4.288712011992	-2.391632214843	0.675792826149
H	5.902161364816	-1.640464914606	0.480392074142
H	4.307015908465	1.781780996798	1.044004209448
H	3.001736583579	0.740588404516	1.664364958003
H	3.934902443639	1.263232728733	-2.424760242767
H	-1.209308732623	0.046809155347	1.224563689141
H	0.118708456436	-1.024712526464	0.698317974140
H	0.440927557352	0.302547055759	1.851903774573
H	0.501208197094	2.688822597448	1.056625321007
H	0.091114700114	3.094059007879	-0.637039095139
H	-1.178710098534	2.522717636387	0.484058678698
H	-1.734206678189	0.573450638259	-1.213412835250
H	-0.453817222885	1.191504178986	-2.295068067117
H	-0.407889530278	-0.503252919568	-1.723761113415

SCF Done: E(RB3LYP) = -687.781959918

Zero-point correction= 0.251129
Thermal correction to Energy= 0.266111
Thermal correction to Enthalpy= 0.267055
Thermal correction to Gibbs Free Energy= 0.208699
Sum of electronic and zero-point Energies= -687.530831
Sum of electronic and thermal Energies= -687.515849
Sum of electronic and thermal Enthalpies= -687.514905
Sum of electronic and thermal Free Energies= -687.573261

1	C	Isotropic =	123.6102	Anisotropy =	75.8957
2	O	Isotropic =	286.2026	Anisotropy =	88.4750
3	C	Isotropic =	122.3313	Anisotropy =	62.2432
4	C	Isotropic =	8.5942	Anisotropy =	132.5412
5	C	Isotropic =	157.4155	Anisotropy =	28.3429
6	N	Isotropic =	-52.7616	Anisotropy =	340.1779
7	N	Isotropic =	108.9286	Anisotropy =	71.8109
8	C	Isotropic =	42.8874	Anisotropy =	60.3255

9	O	Isotropic =	56.5098	Anisotropy =	341.0599
10	O	Isotropic =	139.3471	Anisotropy =	105.4629
11	C	Isotropic =	106.7285	Anisotropy =	76.0095
12	C	Isotropic =	160.1272	Anisotropy =	44.0329
13	C	Isotropic =	165.7394	Anisotropy =	37.4471
14	C	Isotropic =	165.9846	Anisotropy =	38.6565
15	H	Isotropic =	27.7737	Anisotropy =	8.3418
16	H	Isotropic =	27.3200	Anisotropy =	7.0235
17	H	Isotropic =	27.0397	Anisotropy =	5.8676
18	H	Isotropic =	27.2188	Anisotropy =	7.2197
19	H	Isotropic =	28.7331	Anisotropy =	4.5818
20	H	Isotropic =	28.7868	Anisotropy =	10.7065
21	H	Isotropic =	25.3322	Anisotropy =	6.4970
22	H	Isotropic =	30.2258	Anisotropy =	8.3388
23	H	Isotropic =	30.0558	Anisotropy =	6.5196
24	H	Isotropic =	30.0112	Anisotropy =	6.3849
25	H	Isotropic =	30.2010	Anisotropy =	6.6463
26	H	Isotropic =	28.8601	Anisotropy =	6.2899
27	H	Isotropic =	30.2321	Anisotropy =	8.7897
28	H	Isotropic =	30.2877	Anisotropy =	8.8906
29	H	Isotropic =	28.9387	Anisotropy =	6.3681
30	H	Isotropic =	30.3021	Anisotropy =	7.3417

Conformer16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	2.072577551430	2.982844937664	2.683223083273
O	2.011774067688	3.570943275599	1.376936763499
C	2.427621200818	2.560921560268	0.463184262833
C	3.473287428600	1.761214655125	1.213403410253
C	3.353613350528	2.136093127224	2.676409598016
N	4.369308600455	0.957025224797	0.785152732890
N	4.361851410888	0.748480115357	-0.624191480115
C	3.511865271042	-0.150170808789	-1.258704819565
O	3.798848694758	-0.633230427432	-2.344199587832
O	2.386534272906	-0.358061666722	-0.557357081454
C	1.336561195260	-1.289911261534	-1.048549453674
C	1.913106204133	-2.702319724433	-1.173435531787
C	0.294813895656	-1.228795405115	0.068594018783
C	0.755860589274	-0.772433847784	-2.366169445028
H	1.182725932991	2.347500575162	2.860899443848
H	2.078585068036	3.797470995686	3.419322406637
H	2.833076320658	3.027421223719	-0.447203524094
H	1.587226700345	1.901327614710	0.173473624146
H	3.312128031782	1.256461623165	3.333675715518
H	4.229596359655	2.739757643803	2.966489863326
H	5.312657206573	0.613792180957	-0.961673247857

H	1.100820663834	-3.406033840874	-1.413547897289
H	2.671257019996	-2.755901543046	-1.964401752696
H	2.367289204956	-3.016709893325	-0.220644135394
H	-0.541289572547	-1.905587258294	-0.163720644725
H	0.735455231806	-1.536793550049	1.028918043841
H	-0.105712900814	-0.209308609538	0.177213287505
H	0.385447578256	0.257615283167	-2.245233296834
H	1.507203770946	-0.789772287654	-3.165434010338
H	-0.093280349909	-1.407599911814	-2.663770345689

SCF Done: E(RB3LYP) = -687.781585609

Zero-point correction= 0.251166
Thermal correction to Energy= 0.266123
Thermal correction to Enthalpy= 0.267067
Thermal correction to Gibbs Free Energy= 0.208823
Sum of electronic and zero-point Energies= -687.530420
Sum of electronic and thermal Energies= -687.515463
Sum of electronic and thermal Enthalpies= -687.514518
Sum of electronic and thermal Free Energies= -687.572763

1	C	Isotropic =	123.8819	Anisotropy =	76.8204
2	O	Isotropic =	283.7956	Anisotropy =	86.4072
3	C	Isotropic =	122.8877	Anisotropy =	60.6023
4	C	Isotropic =	7.2910	Anisotropy =	135.5246
5	C	Isotropic =	157.1220	Anisotropy =	25.4776
6	N	Isotropic =	-54.4809	Anisotropy =	333.4037
7	N	Isotropic =	108.9749	Anisotropy =	68.3958
8	C	Isotropic =	42.6428	Anisotropy =	61.6916
9	O	Isotropic =	54.4597	Anisotropy =	346.8494
10	O	Isotropic =	139.9497	Anisotropy =	105.6891
11	C	Isotropic =	106.7306	Anisotropy =	76.0604
12	C	Isotropic =	165.9458	Anisotropy =	38.4593
13	C	Isotropic =	160.4195	Anisotropy =	43.5853
14	C	Isotropic =	165.7767	Anisotropy =	37.7282
15	H	Isotropic =	27.6843	Anisotropy =	6.9450
16	H	Isotropic =	27.3500	Anisotropy =	7.7676
17	H	Isotropic =	26.8416	Anisotropy =	5.1105
18	H	Isotropic =	27.2049	Anisotropy =	10.9689
19	H	Isotropic =	28.9766	Anisotropy =	6.7187
20	H	Isotropic =	28.7509	Anisotropy =	8.3710
21	H	Isotropic =	25.5511	Anisotropy =	6.3731
22	H	Isotropic =	30.2913	Anisotropy =	8.8341
23	H	Isotropic =	28.9386	Anisotropy =	6.3631
24	H	Isotropic =	30.3066	Anisotropy =	7.2689
25	H	Isotropic =	30.2283	Anisotropy =	8.2995
26	H	Isotropic =	30.0602	Anisotropy =	6.5699
27	H	Isotropic =	29.9822	Anisotropy =	6.4343
28	H	Isotropic =	30.2124	Anisotropy =	6.7257
29	H	Isotropic =	28.8943	Anisotropy =	6.3419
30	H	Isotropic =	30.2393	Anisotropy =	8.7979

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	5.511798626201	2.588507951526	0.737319327226
O	4.445445025838	2.792999767357	1.674152338203
C	3.477851707009	1.783023302441	1.406260191485
C	4.282667967968	0.576042102117	0.969591041446
C	5.682890351959	1.064354011974	0.659829237576
N	3.960231327306	-0.658859748915	0.904813877878
N	2.613319050737	-0.946564276085	1.268029186492
C	1.538212614396	-0.805074485978	0.398246373429
O	0.509038481630	-1.445380407250	0.556651223201
O	1.778147929978	0.110392505547	-0.553549794704
C	0.764662336239	0.415236971120	-1.598831629097
C	0.474614841867	-0.842799048986	-2.420898833527
C	-0.493113041666	0.998203444262	-0.951659448641
C	1.476989642176	1.465381773222	-2.451256180973
H	6.396318543553	3.119693546594	1.112809841395
H	5.239291555271	3.004158175021	-0.252766433791
H	2.785651984897	2.085100248618	0.597191588148
H	2.887259554554	1.584453475015	2.313268391070
H	6.372180739848	0.702339608126	1.440704461295
H	6.048084258732	0.703936096142	-0.311948491998
H	2.561979544505	-1.853333448545	1.727502293667
H	1.409165498716	-1.258310712855	-2.829398568845
H	-0.021012958099	-1.610473660757	-1.813903352849
H	-0.181713906256	-0.581899015269	-3.265809842854
H	-0.237865535040	1.874678034088	-0.335626776882
H	-1.188692439290	1.325677059432	-1.740297003781
H	-0.996670935565	0.254262272107	-0.322039258833
H	0.832886662886	1.761220876848	-3.293142512701
H	1.705414489448	2.364400881744	-1.858708454209
H	2.418036080204	1.064122701338	-2.857112788827

SCF Done: E(RB3LYP) = -687.781584432

Zero-point correction= 0.251258
Thermal correction to Energy= 0.266180
Thermal correction to Enthalpy= 0.267125
Thermal correction to Gibbs Free Energy= 0.208957
Sum of electronic and zero-point Energies= -687.530327
Sum of electronic and thermal Energies= -687.515404
Sum of electronic and thermal Enthalpies= -687.514460
Sum of electronic and thermal Free Energies= -687.572627

1 C Isotropic = 124.0186 Anisotropy = 76.9622
2 O Isotropic = 283.7815 Anisotropy = 85.9008

3	C	Isotropic =	122.9105	Anisotropy =	60.4980
4	C	Isotropic =	7.3692	Anisotropy =	135.4717
5	C	Isotropic =	157.0222	Anisotropy =	25.5629
6	N	Isotropic =	-54.2986	Anisotropy =	333.1033
7	N	Isotropic =	109.0600	Anisotropy =	68.4503
8	C	Isotropic =	42.5891	Anisotropy =	61.4465
9	O	Isotropic =	54.2540	Anisotropy =	346.0573
10	O	Isotropic =	139.7750	Anisotropy =	105.8318
11	C	Isotropic =	106.6608	Anisotropy =	76.2871
12	C	Isotropic =	166.0269	Anisotropy =	38.4840
13	C	Isotropic =	165.8186	Anisotropy =	37.5209
14	C	Isotropic =	160.3184	Anisotropy =	43.7080
15	H	Isotropic =	27.3494	Anisotropy =	7.7758
16	H	Isotropic =	27.6853	Anisotropy =	6.9569
17	H	Isotropic =	27.2026	Anisotropy =	11.0305
18	H	Isotropic =	26.8558	Anisotropy =	5.1005
19	H	Isotropic =	28.7442	Anisotropy =	8.3826
20	H	Isotropic =	28.9739	Anisotropy =	6.7135
21	H	Isotropic =	25.5464	Anisotropy =	6.3768
22	H	Isotropic =	30.3101	Anisotropy =	7.2715
23	H	Isotropic =	28.9401	Anisotropy =	6.3503
24	H	Isotropic =	30.2906	Anisotropy =	8.8419
25	H	Isotropic =	30.2104	Anisotropy =	6.7301
26	H	Isotropic =	30.2399	Anisotropy =	8.7924
27	H	Isotropic =	28.8804	Anisotropy =	6.3435
28	H	Isotropic =	30.2262	Anisotropy =	8.2903
29	H	Isotropic =	29.9788	Anisotropy =	6.4139
30	H	Isotropic =	30.0568	Anisotropy =	6.5553

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.687815107387	3.345152367883	-1.550639253779
O	1.863468206236	2.999400089885	-2.931811885538
C	2.500361943329	1.727506029452	-2.946105221080
C	1.914316669981	0.991115378457	-1.758534400133
C	1.318958184553	2.033682999324	-0.838374461012
N	1.915925376553	-0.285508068574	-1.711122208021
N	1.320275251813	-0.848200373096	-0.548357631597
C	1.983365089189	-0.974067046549	0.667079527168
O	1.644687493108	-1.815190696113	1.487047902376
O	2.962126806296	-0.066022540768	0.804295276511
C	3.813304918459	-0.031568377338	2.023053807792
C	4.774717936488	1.117142514900	1.718133484506
C	2.957028178033	0.284477862102	3.251161236046
C	4.573264022251	-1.352986058189	2.160245126807
H	0.909246741560	4.117667255174	-1.495589886428
H	2.628920010569	3.759475375930	-1.138740751933

H	3.599478948197	1.824838889858	-2.819553973974
H	2.300819773541	1.227055337335	-3.903794187884
H	0.228346107548	1.875917520740	-0.789224875806
H	1.717605375314	1.963973484749	0.181371776245
H	0.865427818869	-1.728648457974	-0.780358188837
H	5.342109815637	0.915136643907	0.796983786055
H	4.227605738281	2.063960217858	1.592651043047
H	5.488264940468	1.237077321853	2.547388429567
H	2.250405241199	-0.527457396381	3.462898816258
H	3.612836471355	0.421604242948	4.125304320054
H	2.393448245585	1.218237210777	3.098085958947
H	5.142140627966	-1.565777472598	1.241546701443
H	5.287532133615	-1.276976631714	2.994935518943
H	3.888966826620	-2.187627623838	2.357034214259

SCF Done: E(RB3LYP) = -687.781427675

Zero-point correction= 0.251277
Thermal correction to Energy= 0.266200
Thermal correction to Enthalpy= 0.267144
Thermal correction to Gibbs Free Energy= 0.209019
Sum of electronic and zero-point Energies= -687.530150
Sum of electronic and thermal Energies= -687.515228
Sum of electronic and thermal Enthalpies= -687.514284
Sum of electronic and thermal Free Energies= -687.572409

1	C	Isotropic =	123.6560	Anisotropy =	78.7352
2	O	Isotropic =	285.3525	Anisotropy =	84.1915
3	C	Isotropic =	121.7509	Anisotropy =	59.2717
4	C	Isotropic =	8.4404	Anisotropy =	134.4114
5	C	Isotropic =	158.9731	Anisotropy =	20.7474
6	N	Isotropic =	-53.3370	Anisotropy =	336.2354
7	N	Isotropic =	110.8153	Anisotropy =	75.7412
8	C	Isotropic =	43.0143	Anisotropy =	61.0973
9	O	Isotropic =	55.0841	Anisotropy =	344.0977
10	O	Isotropic =	140.1102	Anisotropy =	105.6243
11	C	Isotropic =	106.7541	Anisotropy =	75.8565
12	C	Isotropic =	160.3885	Anisotropy =	44.0262
13	C	Isotropic =	165.7526	Anisotropy =	37.3697
14	C	Isotropic =	166.0828	Anisotropy =	38.6323
15	H	Isotropic =	27.2931	Anisotropy =	7.2546
16	H	Isotropic =	27.6117	Anisotropy =	6.7016
17	H	Isotropic =	27.3135	Anisotropy =	6.3634
18	H	Isotropic =	27.1444	Anisotropy =	6.0940
19	H	Isotropic =	28.8355	Anisotropy =	7.3280
20	H	Isotropic =	28.6135	Anisotropy =	9.6518
21	H	Isotropic =	25.4763	Anisotropy =	6.6261
22	H	Isotropic =	30.0646	Anisotropy =	6.6225
23	H	Isotropic =	30.0531	Anisotropy =	6.5107
24	H	Isotropic =	30.2226	Anisotropy =	8.3096
25	H	Isotropic =	28.8561	Anisotropy =	6.3501

26	H	Isotropic =	30.2448	Anisotropy =	8.7797
27	H	Isotropic =	30.1999	Anisotropy =	6.7047
28	H	Isotropic =	30.3086	Anisotropy =	7.3242
29	H	Isotropic =	30.2859	Anisotropy =	8.8572
30	H	Isotropic =	28.9430	Anisotropy =	6.3255

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	4.060093226478	3.065179866575	1.560340803019
O	3.004657537329	4.035478462185	1.611631991805
C	1.827705319732	3.366909568489	1.174399058050
C	2.306048816406	2.410226437210	0.100978453928
C	3.795024153347	2.230279842898	0.297012897576
N	1.506746126013	1.975149933954	-0.795555657283
N	2.091170898955	1.097173925905	-1.750324576147
C	2.290514953697	-0.259214028070	-1.519646117502
O	2.372534979235	-1.052082818680	-2.446547525828
O	2.407612738351	-0.536391570912	-0.211593428155
C	2.606892470635	-1.930382308473	0.264847784758
C	3.936769971132	-2.477925656855	-0.257509071977
C	2.648177803270	-1.754143142597	1.782905448121
C	1.412789315953	-2.794836158788	-0.146879548263
H	4.031692625650	2.423380647261	2.462643939507
H	5.014050600531	3.608899059574	1.544684565084
H	1.102749376299	4.103951942222	0.802046249176
H	1.357667338196	2.794313397342	2.001884234293
H	4.074784693410	1.174996347151	0.405248441921
H	4.316613141485	2.631617009223	-0.588175100032
H	1.651023098814	1.226353882526	-2.658913578710
H	3.921405599039	-2.585358087414	-1.349151213514
H	4.766294702458	-1.810787054862	0.024897019403
H	4.124601239267	-3.465006909767	0.193463104857
H	3.489218627074	-1.109366636788	2.080291939898
H	1.713366860319	-1.301691803801	2.147164798881
H	2.773597758988	-2.733505414318	2.268896100804
H	1.364382402658	-2.916187237211	-1.236051508280
H	1.507753163245	-3.789501288170	0.315953581837
H	0.472220462032	-2.342330205806	0.204626912772

SCF Done: E(RB3LYP) = -687.781467060

Zero-point correction= 0.251248
Thermal correction to Energy= 0.266187
Thermal correction to Enthalpy= 0.267131
Thermal correction to Gibbs Free Energy= 0.209000
Sum of electronic and zero-point Energies= -687.530219
Sum of electronic and thermal Energies= -687.515280

Sum of electronic and thermal Enthalpies= -687.514336
Sum of electronic and thermal Free Energies= -687.572467

1	C	Isotropic =	123.5144	Anisotropy =	79.0782
2	O	Isotropic =	284.5720	Anisotropy =	84.6397
3	C	Isotropic =	121.7842	Anisotropy =	59.2235
4	C	Isotropic =	8.3299	Anisotropy =	134.5460
5	C	Isotropic =	159.0266	Anisotropy =	20.4706
6	N	Isotropic =	-53.5663	Anisotropy =	336.6168
7	N	Isotropic =	110.8426	Anisotropy =	75.9296
8	C	Isotropic =	42.8966	Anisotropy =	61.0552
9	O	Isotropic =	55.0566	Anisotropy =	344.4256
10	O	Isotropic =	140.2119	Anisotropy =	104.8240
11	C	Isotropic =	106.8722	Anisotropy =	75.8186
12	C	Isotropic =	165.6809	Anisotropy =	37.5924
13	C	Isotropic =	160.3256	Anisotropy =	43.8069
14	C	Isotropic =	166.0388	Anisotropy =	38.4705
15	H	Isotropic =	27.6153	Anisotropy =	6.6849
16	H	Isotropic =	27.3143	Anisotropy =	7.2409
17	H	Isotropic =	27.1435	Anisotropy =	6.0949
18	H	Isotropic =	27.3173	Anisotropy =	6.3577
19	H	Isotropic =	28.6251	Anisotropy =	9.6156
20	H	Isotropic =	28.8211	Anisotropy =	7.3138
21	H	Isotropic =	25.4838	Anisotropy =	6.6082
22	H	Isotropic =	28.8640	Anisotropy =	6.3653
23	H	Isotropic =	30.1983	Anisotropy =	6.7175
24	H	Isotropic =	30.2338	Anisotropy =	8.7915
25	H	Isotropic =	30.0440	Anisotropy =	6.5076
26	H	Isotropic =	30.0759	Anisotropy =	6.6149
27	H	Isotropic =	30.2260	Anisotropy =	8.3156
28	H	Isotropic =	28.9503	Anisotropy =	6.3558
29	H	Isotropic =	30.2812	Anisotropy =	8.8572
30	H	Isotropic =	30.3195	Anisotropy =	7.3139

8. Coordinates and Shielding Constants for Compounds 1-3

1a

Comformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.871698642613	0.754194932585	0.444615818374
O	-2.674509344019	-0.349029095618	0.655723712846
C	-2.532680365381	-0.616617027862	1.966643402245
N	-1.735925907193	0.187766802807	2.608280502167
C	-1.292807408145	1.089150952114	1.644889127166
C	-0.334580113921	2.187054175214	1.983174118918
C	-1.778663754272	1.338341806752	-0.897206224040
C	1.028964755463	1.654816312430	2.452223443280
O	-1.093098654877	2.312581386209	-1.160537193119
O	-2.532560282497	0.676574421680	-1.789466505471
C	-2.504663248777	1.182690032355	-3.151740002840
C	-3.416550229692	0.302575666650	-3.979543011926
H	-3.090151903028	-1.464447154829	2.358076575984
H	-0.216393097270	2.833423033755	1.103710624347
H	-0.782973578378	2.795188605281	2.788018490027
H	1.527785000610	1.083919333234	1.652422770415
H	1.687749533375	2.488598677237	2.740308044290
H	0.914110994973	0.990613108565	3.323135649833
H	-2.835965472086	2.232585295019	-3.142397829889
H	-1.464687095176	1.159872321155	-3.512453932334
H	-4.449543650860	0.336542669145	-3.599834783377
H	-3.419737201500	0.654392594517	-5.022797531272
H	-3.072660334736	-0.743378848395	-3.968245265627

SCF Done: E(RB3LYP) = -591.944096879

Zero-point correction= 0.184937
Thermal correction to Energy= 0.197166
Thermal correction to Enthalpy= 0.198111
Thermal correction to Gibbs Free Energy= 0.144867
Sum of electronic and zero-point Energies= -591.759159

Sum of electronic and thermal Energies= -591.746930
Sum of electronic and thermal Enthalpies= -591.745986
Sum of electronic and thermal Free Energies= -591.799230

1	C	Isotropic =	54.1616	Anisotropy =	83.2135
2	O	Isotropic =	30.2199	Anisotropy =	257.2053
3	C	Isotropic =	42.6914	Anisotropy =	93.5498
4	N	Isotropic =	-14.2818	Anisotropy =	354.4915
5	C	Isotropic =	37.2047	Anisotropy =	138.2205
6	C	Isotropic =	168.0481	Anisotropy =	13.4043
7	C	Isotropic =	35.7487	Anisotropy =	78.8098
8	C	Isotropic =	175.9711	Anisotropy =	22.7972
9	O	Isotropic =	-28.3272	Anisotropy =	519.9033
10	O	Isotropic =	127.3250	Anisotropy =	132.7072
11	C	Isotropic =	128.4813	Anisotropy =	57.4833
12	C	Isotropic =	177.1552	Anisotropy =	20.1677
13	H	Isotropic =	23.7955	Anisotropy =	4.2326
14	H	Isotropic =	27.8955	Anisotropy =	8.5769
15	H	Isotropic =	28.8679	Anisotropy =	7.9669
16	H	Isotropic =	30.3890	Anisotropy =	7.4590
17	H	Isotropic =	30.0544	Anisotropy =	9.9916
18	H	Isotropic =	29.9128	Anisotropy =	8.1036
19	H	Isotropic =	27.1688	Anisotropy =	6.0753
20	H	Isotropic =	27.1721	Anisotropy =	6.0099
21	H	Isotropic =	29.8976	Anisotropy =	7.7105
22	H	Isotropic =	30.0384	Anisotropy =	9.5433
23	H	Isotropic =	29.8986	Anisotropy =	7.6452

Comformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.438214205944	0.728746514615	0.285404360975
O	-0.936002893872	-0.539428261165	0.072159034214
C	-0.175624866595	-0.781624095576	1.155352303851
N	-0.137962665498	0.183873792954	2.027083221870
C	-0.948143907068	1.178819008476	1.487645677821
C	-1.180941856245	2.471630843184	2.203443411365
C	-2.326617191481	1.335554695194	-0.711033506021
C	-1.920634714262	2.280946246415	3.537355023853
O	-2.803155227157	2.452692676434	-0.595065520918
O	-2.548851190084	0.519656839208	-1.753851971694
C	-3.420675306743	1.036069553889	-2.795887460756
C	-3.556054011387	-0.043441696368	-3.848376598237
H	0.327790630466	-1.744806107097	1.196688758402
H	-0.198580097220	2.936490775342	2.396749968218
H	-1.743749010434	3.143046238820	1.541842149163
H	-2.027174999779	3.245210978323	4.057984473698
H	-2.928275930378	1.865202318453	3.375500034920
H	-1.370691432390	1.592439069302	4.197914725449
H	-4.388950163486	1.300369410825	-2.343664554710
H	-2.974207561167	1.957446501914	-3.200986843714
H	-3.999647571565	-0.956775102875	-3.422405431173
H	-4.210123639201	0.313396896974	-4.658935013892

H -2.576182188511 -0.298037097241 -4.281326242686

SCF Done: E(RB3LYP) = -591.944097633

Zero-point correction= 0.184936
Thermal correction to Energy= 0.197167
Thermal correction to Enthalpy= 0.198111
Thermal correction to Gibbs Free Energy= 0.144919
Sum of electronic and zero-point Energies= -591.759161
Sum of electronic and thermal Energies= -591.746931
Sum of electronic and thermal Enthalpies= -591.745987
Sum of electronic and thermal Free Energies= -591.799179

1 C Isotropic = 54.2365 Anisotropy = 83.4028
2 O Isotropic = 30.6050 Anisotropy = 256.9810
3 C Isotropic = 42.7180 Anisotropy = 93.7095
4 N Isotropic = -14.4002 Anisotropy = 354.2724
5 C Isotropic = 37.1134 Anisotropy = 138.5401
6 C Isotropic = 167.9553 Anisotropy = 13.4646
7 C Isotropic = 35.7565 Anisotropy = 78.7396
8 C Isotropic = 175.9655 Anisotropy = 22.8438
9 O Isotropic = -28.3445 Anisotropy = 519.4430
10 O Isotropic = 127.4759 Anisotropy = 132.2801
11 C Isotropic = 128.4719 Anisotropy = 57.4535
12 C Isotropic = 177.1741 Anisotropy = 20.1753
13 H Isotropic = 23.7953 Anisotropy = 4.2370
14 H Isotropic = 28.8666 Anisotropy = 7.9648
15 H Isotropic = 27.8995 Anisotropy = 8.5394
16 H Isotropic = 30.0462 Anisotropy = 9.9928
17 H Isotropic = 30.3840 Anisotropy = 7.4417
18 H Isotropic = 29.9247 Anisotropy = 8.1137
19 H Isotropic = 27.1478 Anisotropy = 5.9315
20 H Isotropic = 27.2002 Anisotropy = 6.1646
21 H Isotropic = 29.9062 Anisotropy = 7.6584
22 H Isotropic = 30.0395 Anisotropy = 9.5410
23 H Isotropic = 29.8949 Anisotropy = 7.7044

Comformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.422396520050	1.079740710270	0.410341873186
O	-1.457701982659	1.872866224901	1.539963233961
C	-0.494128980162	1.367102847583	2.330717010637
N	0.146348721599	0.349020095870	1.833866097467
C	-0.434711201736	0.140545703768	0.586495531991
C	0.021261278258	-0.964958841790	-0.312460405261
C	-2.351453644621	1.344963413744	-0.692739231239
C	-0.198743605160	-2.354975651254	0.305381019661
O	-2.372281979484	0.690139927931	-1.722066063349
O	-3.158241587310	2.387215681904	-0.428897221636
C	-4.125865806325	2.745806145613	-1.455358577345
C	-5.403521824758	1.936301198061	-1.318694880847
H	-0.344078077789	1.850988099791	3.293123525023

H	-0.505777117606	-0.878241919720	-1.271570577183
H	1.098247879140	-0.822072069555	-0.508863236372
H	0.311115561723	-2.438265948608	1.277886307319
H	-1.271010432712	-2.552661815352	0.465364880736
H	0.198526864958	-3.137380275426	-0.359565810043
H	-4.305946105112	3.815642750633	-1.285781901967
H	-3.662023770285	2.605493386243	-2.441503796229
H	-5.216845018638	0.868243373224	-1.506587133262
H	-5.836445248943	2.050633198356	-0.312626837538
H	-6.142307402330	2.291543763811	-2.055053807710

SCF Done: E(RB3LYP) = -591.943688353

Zero-point correction= 0.185161
Thermal correction to Energy= 0.197285
Thermal correction to Enthalpy= 0.198229
Thermal correction to Gibbs Free Energy= 0.145277
Sum of electronic and zero-point Energies= -591.758528
Sum of electronic and thermal Energies= -591.746404
Sum of electronic and thermal Enthalpies= -591.745460
Sum of electronic and thermal Free Energies= -591.798411

1	C	Isotropic =	54.1628	Anisotropy =	82.6692
2	O	Isotropic =	30.4978	Anisotropy =	257.1167
3	C	Isotropic =	42.5946	Anisotropy =	93.9437
4	N	Isotropic =	-14.2847	Anisotropy =	354.7478
5	C	Isotropic =	36.8810	Anisotropy =	138.5152
6	C	Isotropic =	168.1095	Anisotropy =	13.3594
7	C	Isotropic =	35.9072	Anisotropy =	78.3673
8	C	Isotropic =	176.0657	Anisotropy =	22.6031
9	O	Isotropic =	-18.2766	Anisotropy =	517.6235
10	O	Isotropic =	128.0177	Anisotropy =	152.3096
11	C	Isotropic =	129.7697	Anisotropy =	64.3559
12	C	Isotropic =	175.9863	Anisotropy =	22.9115
13	H	Isotropic =	23.7824	Anisotropy =	4.2874
14	H	Isotropic =	27.8820	Anisotropy =	8.6913
15	H	Isotropic =	28.8615	Anisotropy =	8.0074
16	H	Isotropic =	29.8964	Anisotropy =	8.1648
17	H	Isotropic =	30.3816	Anisotropy =	7.3934
18	H	Isotropic =	30.0575	Anisotropy =	9.9644
19	H	Isotropic =	27.4201	Anisotropy =	7.5013
20	H	Isotropic =	26.4444	Anisotropy =	5.5502
21	H	Isotropic =	29.8781	Anisotropy =	6.0022
22	H	Isotropic =	30.0828	Anisotropy =	7.6519
23	H	Isotropic =	30.2410	Anisotropy =	9.9141

Comformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.799336641337	0.505938830637	-0.231046963244
O	-2.769578943528	-0.012917567328	-1.065120676868
C	-2.586436906796	-1.344010168390	-0.999453987339
N	-1.614442150438	-1.727226655630	-0.223583904225

C	-1.084474337312	-0.546526614017	0.288329825467
C	0.063825836057	-0.556880969375	1.247451738629
C	-1.692720785275	1.957899525311	-0.056001154214
C	-0.278338225680	-1.264924575614	2.567907748501
O	-0.858352193709	2.485889028949	0.660814126858
O	-2.613142446092	2.618504345341	-0.779456463111
C	-2.601890466239	4.071107380826	-0.690100136995
C	-3.433649538093	4.559281836412	0.483083957818
H	-3.256595916841	-1.962031157874	-1.592584927347
H	0.907177158217	-1.079753424042	0.763494601417
H	0.376900540960	0.479013449123	1.432297004862
H	-1.083817330412	-0.737061417720	3.103620163414
H	-0.611937830531	-2.298346035708	2.385201145929
H	0.604717180415	-1.299487236667	3.224567697229
H	-1.559916787452	4.411820621799	-0.616544826505
H	-3.026101654090	4.397829354805	-1.648798959612
H	-2.991059835897	4.244406886304	1.440117485469
H	-3.475796917357	5.660304963826	0.468908271816
H	-4.463321808570	4.173579599030	0.422948232051

SCF Done: E(RB3LYP) = -591.943675449

Zero-point correction= 0.185165
Thermal correction to Energy= 0.197287
Thermal correction to Enthalpy= 0.198231
Thermal correction to Gibbs Free Energy= 0.145392
Sum of electronic and zero-point Energies= -591.758511
Sum of electronic and thermal Energies= -591.746388
Sum of electronic and thermal Enthalpies= -591.745444
Sum of electronic and thermal Free Energies= -591.798283

1	C	Isotropic =	54.1586	Anisotropy =	82.6854
2	O	Isotropic =	30.3179	Anisotropy =	257.2505
3	C	Isotropic =	42.6588	Anisotropy =	93.8081
4	N	Isotropic =	-14.4281	Anisotropy =	354.6068
5	C	Isotropic =	36.8486	Anisotropy =	138.4308
6	C	Isotropic =	167.9955	Anisotropy =	13.4455
7	C	Isotropic =	35.8457	Anisotropy =	78.2100
8	C	Isotropic =	176.0528	Anisotropy =	22.6056
9	O	Isotropic =	-18.1148	Anisotropy =	517.6118
10	O	Isotropic =	127.9819	Anisotropy =	152.3144
11	C	Isotropic =	129.8995	Anisotropy =	64.3315
12	C	Isotropic =	175.8996	Anisotropy =	23.0735
13	H	Isotropic =	23.7783	Anisotropy =	4.2871
14	H	Isotropic =	28.8674	Anisotropy =	7.9953
15	H	Isotropic =	27.8868	Anisotropy =	8.6614
16	H	Isotropic =	30.3799	Anisotropy =	7.3876
17	H	Isotropic =	29.9024	Anisotropy =	8.1640
18	H	Isotropic =	30.0543	Anisotropy =	9.9645
19	H	Isotropic =	26.4350	Anisotropy =	5.5189
20	H	Isotropic =	27.4284	Anisotropy =	7.5066
21	H	Isotropic =	29.8737	Anisotropy =	6.0169
22	H	Isotropic =	30.2423	Anisotropy =	9.9190
23	H	Isotropic =	30.0731	Anisotropy =	7.6436

Comformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.603712453589	0.895376840605	0.518070173728
O	-1.854636026842	1.417313996256	1.771377612277
C	-1.010605068311	0.753992584742	2.582161555334
N	-0.256643356261	-0.125605369444	1.989277952726
C	-0.621280697298	-0.056713485452	0.647929966098
C	0.033542263606	-0.918086611671	-0.385131041170
C	-2.356483623624	1.389636879150	-0.639253724586
C	1.530619673772	-0.608975153426	-0.546170791342
O	-2.186891317896	0.974989990014	-1.774200420651
O	-3.236972993530	2.344485873122	-0.293262404604
C	-4.044104733986	2.913905060850	-1.362205104627
C	-5.296940034993	2.091375217815	-1.607685285322
H	-1.040355660600	1.011021670493	3.638544912453
H	-0.088245683473	-1.971236207865	-0.077632111006
H	-0.493590657281	-0.785540498223	-1.338963838344
H	2.061215564953	-0.721656041561	0.412259113906
H	1.987769728584	-1.295874680247	-1.275124244924
H	1.686142300288	0.422322698317	-0.902014598390
H	-4.287786567758	3.921707716856	-1.000610078872
H	-3.426806259031	2.990243436438	-2.267939341931
H	-5.886146485092	1.985851814535	-0.683370922990
H	-5.923559905138	2.595356924462	-2.361050672298
H	-5.044468006499	1.089037344232	-1.985136705465

SCF Done: E(RB3LYP) = -591.943680557

Zero-point correction= 0.185175
Thermal correction to Energy= 0.197296
Thermal correction to Enthalpy= 0.198240
Thermal correction to Gibbs Free Energy= 0.145462
Sum of electronic and zero-point Energies= -591.758505
Sum of electronic and thermal Energies= -591.746385
Sum of electronic and thermal Enthalpies= -591.745441
Sum of electronic and thermal Free Energies= -591.798218

1	C	Isotropic =	54.2200	Anisotropy = 82.7074
2	O	Isotropic =	30.2687	Anisotropy = 257.3118
3	C	Isotropic =	42.6445	Anisotropy = 93.8467
4	N	Isotropic =	-14.4224	Anisotropy = 354.0088
5	C	Isotropic =	36.9055	Anisotropy = 138.6667
6	C	Isotropic =	167.9356	Anisotropy = 13.2970
7	C	Isotropic =	35.8801	Anisotropy = 78.3854
8	C	Isotropic =	175.8775	Anisotropy = 22.9225
9	O	Isotropic =	-18.2713	Anisotropy = 517.8553
10	O	Isotropic =	128.3004	Anisotropy = 153.0276
11	C	Isotropic =	129.9852	Anisotropy = 64.2791
12	C	Isotropic =	175.9316	Anisotropy = 23.1505
13	H	Isotropic =	23.7813	Anisotropy = 4.2840
14	H	Isotropic =	28.8549	Anisotropy = 7.8838
15	H	Isotropic =	27.8854	Anisotropy = 8.6487
16	H	Isotropic =	29.9249	Anisotropy = 8.1515

17	H	Isotropic =	30.0477	Anisotropy =	9.9783
18	H	Isotropic =	30.3918	Anisotropy =	7.4432
19	H	Isotropic =	27.4256	Anisotropy =	7.4105
20	H	Isotropic =	26.4356	Anisotropy =	5.4248
21	H	Isotropic =	30.0711	Anisotropy =	7.7229
22	H	Isotropic =	30.2478	Anisotropy =	9.9171
23	H	Isotropic =	29.8733	Anisotropy =	6.0192

Comformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.657885378934	0.707088093826	0.485693918707
O	-1.837745878384	-0.459698540508	1.201658196218
C	-1.313238511865	-0.191112144973	2.410943014171
N	-0.823479922872	1.007303954202	2.543592515989
C	-1.034811937791	1.613976331851	1.308995846919
C	-0.595228180111	3.018948488795	1.043057413249
C	-2.116818159517	0.784790519414	-0.904902486892
C	0.931435636336	3.181571600738	1.116662383017
O	-1.994785094361	1.783776325378	-1.594749335957
O	-2.672997728297	-0.368698558010	-1.313634514504
C	-3.163997909600	-0.415116714680	-2.682801234155
C	-4.596698474729	0.080639713396	-2.772365444746
H	-1.350312715133	-0.987822349973	3.150396192836
H	-0.969382652445	3.323600932197	0.056937092684
H	-1.066359620626	3.672542197947	1.797637918518
H	1.315053743214	2.860043416730	2.097627850011
H	1.431717375295	2.579059284273	0.341363611156
H	1.212502957049	4.235444919015	0.966353707917
H	-2.491032954146	0.175550694259	-3.319416675642
H	-3.086790282419	-1.476021193480	-2.955595904523
H	-4.965041899318	-0.048715282531	-3.802789898338
H	-5.253404779074	-0.489550466252	-2.096898742778
H	-4.663347632270	1.148598778385	-2.515115423858

SCF Done: E(RB3LYP) = -591.943673738

Zero-point correction= 0.185136
Thermal correction to Energy= 0.197270
Thermal correction to Enthalpy= 0.198214
Thermal correction to Gibbs Free Energy= 0.145228
Sum of electronic and zero-point Energies= -591.758537
Sum of electronic and thermal Energies= -591.746404
Sum of electronic and thermal Enthalpies= -591.745460
Sum of electronic and thermal Free Energies= -591.798446

1	C	Isotropic =	54.1991	Anisotropy =	82.6616
2	O	Isotropic =	30.3008	Anisotropy =	257.7731
3	C	Isotropic =	42.7038	Anisotropy =	93.8802
4	N	Isotropic =	-14.5117	Anisotropy =	353.7692
5	C	Isotropic =	36.8628	Anisotropy =	138.6637
6	C	Isotropic =	168.0511	Anisotropy =	13.3134
7	C	Isotropic =	35.8152	Anisotropy =	78.2992

8 C Isotropic = 175.9531 Anisotropy = 22.8501
9 O Isotropic = -17.6579 Anisotropy = 517.4404
10 O Isotropic = 128.2173 Anisotropy = 152.7613
11 C Isotropic = 130.0745 Anisotropy = 64.3376
12 C Isotropic = 175.9302 Anisotropy = 23.1829
13 H Isotropic = 23.7812 Anisotropy = 4.2862
14 H Isotropic = 27.8830 Anisotropy = 8.6794
15 H Isotropic = 28.8509 Anisotropy = 7.8975
16 H Isotropic = 29.9265 Anisotropy = 8.1638
17 H Isotropic = 30.3936 Anisotropy = 7.4425
18 H Isotropic = 30.0560 Anisotropy = 9.9839
19 H Isotropic = 26.4207 Anisotropy = 5.3719
20 H Isotropic = 27.4348 Anisotropy = 7.4301
21 H Isotropic = 30.2422 Anisotropy = 9.9193
22 H Isotropic = 30.0668 Anisotropy = 7.7266
23 H Isotropic = 29.8977 Anisotropy = 6.0658

Comformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.648917585820	1.681558577967	0.468290328962
O	-1.686301788340	2.860260063080	1.184942367180
C	-0.752933929180	2.702121587687	2.138602576003
N	-0.126662603086	1.561748645640	2.109159109795
C	-0.685657480432	0.878211344471	1.032418242777
C	-0.230133450994	-0.504136533373	0.684426709962
C	-2.593072821666	1.586510678210	-0.652782392160
C	-0.753004997665	-1.557902800101	1.675200583195
O	-3.354259437098	2.478313984682	-0.978532411379
O	-2.510889013011	0.392075863951	-1.267955837593
C	-3.399009979225	0.197204200436	-2.402549793774
C	-3.149636277311	-1.193838684009	-2.944450345870
H	-0.610918793287	3.529359818233	2.830169528447
H	-0.555217588400	-0.748141614024	-0.334847306091
H	0.872489365318	-0.507088412726	0.697580962178
H	-0.446301840522	-1.316667413189	2.705315326942
H	-1.853357506604	-1.610079735285	1.649825844739
H	-0.355650042494	-2.553263106555	1.422568596825
H	-4.436724469514	0.328848128175	-2.059452605341
H	-3.187971153893	0.977866596082	-3.149650509851
H	-2.107992966832	-1.306604362321	-3.283201965645
H	-3.356360468895	-1.959200069385	-2.180367226524
H	-3.813295171047	-1.376086757646	-3.803879782775

SCF Done: E(RB3LYP) = -591.943137974

Zero-point correction= 0.184941
Thermal correction to Energy= 0.197201
Thermal correction to Enthalpy= 0.198145
Thermal correction to Gibbs Free Energy= 0.144350
Sum of electronic and zero-point Energies= -591.758197
Sum of electronic and thermal Energies= -591.745937
Sum of electronic and thermal Enthalpies= -591.744993

Sum of electronic and thermal Free Energies= -591.798788

1	C	Isotropic =	53.2118	Anisotropy =	80.4746
2	O	Isotropic =	26.2547	Anisotropy =	258.8602
3	C	Isotropic =	41.8503	Anisotropy =	96.6879
4	N	Isotropic =	-15.1381	Anisotropy =	343.5494
5	C	Isotropic =	39.4612	Anisotropy =	137.0891
6	C	Isotropic =	166.9442	Anisotropy =	14.1855
7	C	Isotropic =	36.3288	Anisotropy =	74.7623
8	C	Isotropic =	175.0877	Anisotropy =	24.0052
9	O	Isotropic =	-42.8618	Anisotropy =	541.1884
10	O	Isotropic =	133.4848	Anisotropy =	148.3111
11	C	Isotropic =	128.4174	Anisotropy =	57.7189
12	C	Isotropic =	177.0371	Anisotropy =	19.9324
13	H	Isotropic =	23.7208	Anisotropy =	4.0931
14	H	Isotropic =	28.1050	Anisotropy =	9.0111
15	H	Isotropic =	28.8521	Anisotropy =	7.9356
16	H	Isotropic =	30.0591	Anisotropy =	8.2322
17	H	Isotropic =	30.3369	Anisotropy =	6.8430
18	H	Isotropic =	30.0298	Anisotropy =	9.8085
19	H	Isotropic =	27.1570	Anisotropy =	6.4060
20	H	Isotropic =	27.1728	Anisotropy =	6.5661
21	H	Isotropic =	29.8712	Anisotropy =	7.2128
22	H	Isotropic =	29.8675	Anisotropy =	7.1410
23	H	Isotropic =	30.0365	Anisotropy =	9.7645

Comformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.839465346578	0.250740971940	0.670044617153
O	-2.163879176752	-0.642141132334	1.670882370983
C	-1.198616906976	-0.478582943034	2.591280447661
N	-0.298948666124	0.412272067477	2.289998404663
C	-0.687445870425	0.901290308544	1.045449285135
C	0.101740690508	1.975317627762	0.364699937172
C	-2.752004403144	0.279937077456	-0.480183776380
C	-0.146633688967	3.362426667496	0.981312290665
O	-3.722296740853	-0.444977923235	-0.597803744225
O	-2.380960869979	1.209028701939	-1.380749506393
C	-3.214902003244	1.315139037967	-2.567065457907
C	-2.633322451697	2.407579010564	-3.438380190175
H	-1.259067255738	-1.097862406209	3.483221159723
H	1.169519352005	1.718627963462	0.461833200623
H	-0.146045251483	1.987636819158	-0.704394948380
H	0.489532368120	4.118380357481	0.495178318743
H	-1.198461015303	3.665725654967	0.855904315942
H	0.082660591764	3.361925102433	2.058771421332
H	-3.224380663729	0.338948324456	-3.076054533741
H	-4.244561321211	1.541171433951	-2.249910131709
H	-1.603847307747	2.164611807191	-3.744386250303
H	-3.246320730521	2.516538621056	-4.346470133092
H	-2.624913331925	3.373316849513	-2.909617097490

SCF Done: E(RB3LYP) = -591.943144665

Zero-point correction= 0.184958
Thermal correction to Energy= 0.197216
Thermal correction to Enthalpy= 0.198160
Thermal correction to Gibbs Free Energy= 0.144415
Sum of electronic and zero-point Energies= -591.758186
Sum of electronic and thermal Energies= -591.745929
Sum of electronic and thermal Enthalpies= -591.744985
Sum of electronic and thermal Free Energies= -591.798730

1	C	Isotropic =	53.2502	Anisotropy =	80.4805
2	O	Isotropic =	25.9595	Anisotropy =	258.8572
3	C	Isotropic =	41.9147	Anisotropy =	96.6854
4	N	Isotropic =	-15.3484	Anisotropy =	342.3524
5	C	Isotropic =	39.4516	Anisotropy =	137.1338
6	C	Isotropic =	166.9152	Anisotropy =	14.4352
7	C	Isotropic =	36.3338	Anisotropy =	74.8044
8	C	Isotropic =	174.9638	Anisotropy =	24.1817
9	O	Isotropic =	-42.6170	Anisotropy =	541.2950
10	O	Isotropic =	133.2111	Anisotropy =	148.2107
11	C	Isotropic =	128.3996	Anisotropy =	57.7520
12	C	Isotropic =	177.0700	Anisotropy =	19.9648
13	H	Isotropic =	23.7202	Anisotropy =	4.0957
14	H	Isotropic =	28.8481	Anisotropy =	7.9707
15	H	Isotropic =	28.1190	Anisotropy =	8.6955
16	H	Isotropic =	30.0286	Anisotropy =	9.8185
17	H	Isotropic =	30.3224	Anisotropy =	6.7812
18	H	Isotropic =	30.0859	Anisotropy =	8.2014
19	H	Isotropic =	27.1760	Anisotropy =	6.5722
20	H	Isotropic =	27.1536	Anisotropy =	6.4089
21	H	Isotropic =	29.8646	Anisotropy =	7.2145
22	H	Isotropic =	30.0370	Anisotropy =	9.7676
23	H	Isotropic =	29.8694	Anisotropy =	7.1319

Comformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.883897649777	0.269191278654	0.545410659995
O	-1.788153432522	-1.008925287998	1.056922678941
C	-1.324370323934	-0.835580035544	2.306066376473
N	-1.116819600601	0.403145736192	2.647140831865
C	-1.474076549383	1.144463116630	1.523966174818
C	-1.352345777834	2.636078243773	1.520688671417
C	-2.370533981763	0.370059281981	-0.836397334241
C	0.107612340768	3.101795321594	1.389075789545
O	-2.715618998033	-0.586263126872	-1.505205372220
O	-2.383864568616	1.650435772162	-1.256705217774
C	-2.857227972121	1.891912521719	-2.612322908638
C	-1.734871379779	1.747605548215	-3.625088734789
H	-1.172126859139	-1.731680205076	2.903224553775
H	-1.955955699271	3.048184458034	0.702070865337
H	-1.769986880666	3.008760647687	2.470646628631

H	0.167305071048	4.199859095273	1.445452402894
H	0.729649942650	2.681943136894	2.195421739966
H	0.536442460595	2.782825563879	0.425531545553
H	-3.684018542554	1.199992546509	-2.823806838082
H	-3.241079572658	2.920002182293	-2.579037122677
H	-0.895816645755	2.418200199104	-3.382276945668
H	-1.364661692294	0.712017445796	-3.659927002197
H	-2.110033688363	2.013226559102	-4.626591442922

SCF Done: E(RB3LYP) = -591.942834295

Zero-point correction= 0.185183
Thermal correction to Energy= 0.197339
Thermal correction to Enthalpy= 0.198283
Thermal correction to Gibbs Free Energy= 0.144965
Sum of electronic and zero-point Energies= -591.757652
Sum of electronic and thermal Energies= -591.745495
Sum of electronic and thermal Enthalpies= -591.744551
Sum of electronic and thermal Free Energies= -591.797869

1	C	Isotropic =	53.0845	Anisotropy =	79.9289
2	O	Isotropic =	25.5943	Anisotropy =	258.8181
3	C	Isotropic =	41.7497	Anisotropy =	96.9221
4	N	Isotropic =	-15.0671	Anisotropy =	343.2578
5	C	Isotropic =	39.2516	Anisotropy =	137.2578
6	C	Isotropic =	166.8490	Anisotropy =	14.3923
7	C	Isotropic =	36.3426	Anisotropy =	74.5843
8	C	Isotropic =	175.0539	Anisotropy =	24.0656
9	O	Isotropic =	-32.6587	Anisotropy =	539.5656
10	O	Isotropic =	135.1006	Anisotropy =	137.3260
11	C	Isotropic =	129.8172	Anisotropy =	64.8043
12	C	Isotropic =	175.8725	Anisotropy =	23.1065
13	H	Isotropic =	23.7102	Anisotropy =	4.1228
14	H	Isotropic =	28.0829	Anisotropy =	8.0781
15	H	Isotropic =	28.8412	Anisotropy =	8.0657
16	H	Isotropic =	30.0130	Anisotropy =	9.9621
17	H	Isotropic =	30.0633	Anisotropy =	8.1244
18	H	Isotropic =	30.3093	Anisotropy =	6.8829
19	H	Isotropic =	26.4383	Anisotropy =	5.8836
20	H	Isotropic =	27.4285	Anisotropy =	7.1836
21	H	Isotropic =	30.0441	Anisotropy =	7.2305
22	H	Isotropic =	29.8666	Anisotropy =	6.2114
23	H	Isotropic =	30.2449	Anisotropy =	10.0518

Comformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.521825262364	0.513696068281	0.720737418355
O	-0.738754292300	-0.228218978821	1.581782904210
C	-1.441259381414	-1.355166597330	1.786066144930
N	-2.578943817866	-1.414080618101	1.157009323246
C	-2.660015390251	-0.212384501106	0.458089692886
C	-3.839151586847	0.086008186149	-0.413948793319

C	-0.973161504504	1.817103472920	0.324400888773
C	-3.843836323028	-0.760023702734	-1.698228756710
O	0.084307944840	2.259128230501	0.733434798626
O	-1.789983591515	2.449524682081	-0.540678742506
C	-1.363188717536	3.760536893793	-1.008478315242
C	-0.449510571143	3.647559416965	-2.216297876334
H	-1.000688833200	-2.096422094611	2.448800852700
H	-4.750640804793	-0.131155057720	0.167865422066
H	-3.846087117507	1.154732366066	-0.662560111033
H	-4.752202572594	-0.558794526824	-2.287095673620
H	-2.968493763450	-0.528155890776	-2.326047165225
H	-3.818657768342	-1.835418046168	-1.461413623610
H	-2.302738854880	4.270060470915	-1.259647384575
H	-0.872795038040	4.287000253579	-0.178176842436
H	-0.935721974751	3.082324501806	-3.026693963730
H	-0.214317373404	4.656385309365	-2.592168503271
H	0.495796594889	3.149870161771	-1.952531694179

SCF Done: E(RB3LYP) = -591.942871107

Zero-point correction= 0.185297
Thermal correction to Energy= 0.197393
Thermal correction to Enthalpy= 0.198337
Thermal correction to Gibbs Free Energy= 0.145503
Sum of electronic and zero-point Energies= -591.757574
Sum of electronic and thermal Energies= -591.745478
Sum of electronic and thermal Enthalpies= -591.744534
Sum of electronic and thermal Free Energies= -591.797368

1	C	Isotropic =	53.2328	Anisotropy =	79.6203
2	O	Isotropic =	25.9676	Anisotropy =	257.8530
3	C	Isotropic =	41.8181	Anisotropy =	96.7282
4	N	Isotropic =	-15.0284	Anisotropy =	345.2345
5	C	Isotropic =	39.3619	Anisotropy =	136.8361
6	C	Isotropic =	166.9905	Anisotropy =	14.1325
7	C	Isotropic =	36.3076	Anisotropy =	74.6845
8	C	Isotropic =	175.0354	Anisotropy =	23.9770
9	O	Isotropic =	-32.8321	Anisotropy =	539.7340
10	O	Isotropic =	135.2696	Anisotropy =	137.6576
11	C	Isotropic =	129.8910	Anisotropy =	64.7402
12	C	Isotropic =	175.9643	Anisotropy =	23.0852
13	H	Isotropic =	23.7064	Anisotropy =	4.1127
14	H	Isotropic =	28.8360	Anisotropy =	8.0214
15	H	Isotropic =	28.0533	Anisotropy =	8.4456
16	H	Isotropic =	30.0083	Anisotropy =	9.9502
17	H	Isotropic =	30.3342	Anisotropy =	6.9479
18	H	Isotropic =	30.0303	Anisotropy =	8.1493
19	H	Isotropic =	27.4262	Anisotropy =	7.1931
20	H	Isotropic =	26.4355	Anisotropy =	5.8861
21	H	Isotropic =	30.0463	Anisotropy =	7.2606
22	H	Isotropic =	30.2414	Anisotropy =	10.0525
23	H	Isotropic =	29.8688	Anisotropy =	6.2120

Comformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.543838867795	0.296344933071	0.507852317459
O	-1.186408384604	-0.904398271514	1.086518177808
C	-0.664467792854	-0.560352710980	2.275939304485
N	-0.651209044792	0.717971957957	2.520034601155
C	-1.219062881633	1.300383628849	1.389985576649
C	-1.360700367175	2.786478604748	1.283871898605
C	-2.146346782421	0.207924033683	-0.828362129496
C	-0.021790504782	3.480058462536	0.980503221468
O	-2.350783391621	-0.840037657507	-1.412146836177
O	-2.429825629979	1.431299636043	-1.317724369014
C	-3.035112341862	1.485232976177	-2.640625559408
C	-4.545449248457	1.344129647170	-2.567119578866
H	-0.311782985196	-1.369614759241	2.911113074024
H	-2.095685801266	3.027021456474	0.505234794821
H	-1.753051171194	3.155184464755	2.246063521688
H	-0.150423960260	4.573541186353	0.965144434551
H	0.732239888985	3.233367928608	1.744726622455
H	0.370082986808	3.165822626709	-0.000190258602
H	-2.740047912329	2.470062476131	-3.025937656422
H	-2.585616804219	0.699647894651	-3.263408485893
H	-4.973312143072	1.465918197567	-3.575293874249
H	-4.832153215353	0.351009427111	-2.189819799126
H	-4.982433644928	2.113933860648	-1.912058997915

SCF Done: E(RB3LYP) = -591.942863184

Zero-point correction= 0.185221
Thermal correction to Energy= 0.197361
Thermal correction to Enthalpy= 0.198306
Thermal correction to Gibbs Free Energy= 0.145037
Sum of electronic and zero-point Energies= -591.757642
Sum of electronic and thermal Energies= -591.745502
Sum of electronic and thermal Enthalpies= -591.744558
Sum of electronic and thermal Free Energies= -591.797827

1	C	Isotropic =	53.1845	Anisotropy = 79.8810
2	O	Isotropic =	25.6606	Anisotropy = 258.5684
3	C	Isotropic =	41.7901	Anisotropy = 96.7912
4	N	Isotropic =	-15.2054	Anisotropy = 343.0717
5	C	Isotropic =	39.1789	Anisotropy = 137.3206
6	C	Isotropic =	166.8385	Anisotropy = 14.4968
7	C	Isotropic =	36.2760	Anisotropy = 73.8438
8	C	Isotropic =	174.8853	Anisotropy = 24.4841
9	O	Isotropic =	-32.6508	Anisotropy = 539.6463
10	O	Isotropic =	134.7249	Anisotropy = 147.6713
11	C	Isotropic =	129.7549	Anisotropy = 64.8417
12	C	Isotropic =	175.8125	Anisotropy = 23.4433
13	H	Isotropic =	23.7120	Anisotropy = 4.1127
14	H	Isotropic =	28.0663	Anisotropy = 8.6265
15	H	Isotropic =	28.8401	Anisotropy = 7.8937
16	H	Isotropic =	30.0221	Anisotropy = 9.9850
17	H	Isotropic =	30.0768	Anisotropy = 8.1489
18	H	Isotropic =	30.3386	Anisotropy = 6.8429

19	H	Isotropic =	27.4060	Anisotropy =	6.9307
20	H	Isotropic =	26.4242	Anisotropy =	5.7210
21	H	Isotropic =	30.2415	Anisotropy =	10.0457
22	H	Isotropic =	29.8806	Anisotropy =	6.3171
23	H	Isotropic =	30.0637	Anisotropy =	7.3532

Comformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-2.065978939210	0.832871635501	0.792297166837
O	-2.817932776922	0.749774399412	1.946269396168
C	-1.919783631763	0.861201808522	2.939537740927
N	-0.685943184784	1.002628664923	2.550002507840
C	-0.749270526970	0.985064744056	1.159278371803
C	0.488526646348	1.145561626561	0.333501198897
C	-2.814585806714	0.745318012891	-0.467731759789
C	0.958965071509	2.608445816652	0.265694710105
O	-4.018436281126	0.579660304327	-0.531735667014
O	-1.996848126754	0.882174306437	-1.530493917910
C	-2.613812392097	0.812683119315	-2.847365089115
C	-2.733246664675	-0.621940735425	-3.331071332214
H	-2.303083891786	0.820535963628	3.956463642829
H	1.278789807566	0.528219308395	0.791326794789
H	0.303195409226	0.761849329167	-0.678007719162
H	0.205020655499	3.240537592960	-0.230302726254
H	1.134138371462	3.013619541939	1.275009876967
H	1.899024728406	2.683751325065	-0.302738750592
H	-3.594122263956	1.306497900869	-2.800737696458
H	-1.939730187870	1.398930112737	-3.485611206530
H	-1.750909207970	-1.119530694799	-3.336693526098
H	-3.420847538683	-1.198600230112	-2.694287757695
H	-3.129239268736	-0.628743853021	-4.359394258331

SCF Done: E(RB3LYP) = -591.942864343

Zero-point correction= 0.185248
Thermal correction to Energy= 0.197365
Thermal correction to Enthalpy= 0.198309
Thermal correction to Gibbs Free Energy= 0.145322
Sum of electronic and zero-point Energies= -591.757617
Sum of electronic and thermal Energies= -591.745500
Sum of electronic and thermal Enthalpies= -591.744556
Sum of electronic and thermal Free Energies= -591.797542

1	C	Isotropic =	53.0936	Anisotropy =	80.0176
2	O	Isotropic =	25.5624	Anisotropy =	259.7150
3	C	Isotropic =	41.8435	Anisotropy =	96.5971
4	N	Isotropic =	-15.3752	Anisotropy =	342.2068
5	C	Isotropic =	39.1269	Anisotropy =	137.6235
6	C	Isotropic =	166.6475	Anisotropy =	14.7485
7	C	Isotropic =	36.3295	Anisotropy =	73.7333
8	C	Isotropic =	174.8577	Anisotropy =	24.4441
9	O	Isotropic =	-32.3507	Anisotropy =	539.8823

10	O	Isotropic =	134.2614	Anisotropy =	148.5182
11	C	Isotropic =	129.8075	Anisotropy =	64.8792
12	C	Isotropic =	175.7765	Anisotropy =	23.5072
13	H	Isotropic =	23.7149	Anisotropy =	4.1185
14	H	Isotropic =	28.8386	Anisotropy =	7.9137
15	H	Isotropic =	28.0830	Anisotropy =	8.3763
16	H	Isotropic =	30.3335	Anisotropy =	6.7818
17	H	Isotropic =	30.0998	Anisotropy =	8.1500
18	H	Isotropic =	30.0190	Anisotropy =	9.9908
19	H	Isotropic =	26.4228	Anisotropy =	5.7303
20	H	Isotropic =	27.4085	Anisotropy =	6.9254
21	H	Isotropic =	30.0665	Anisotropy =	7.3250
22	H	Isotropic =	29.8749	Anisotropy =	6.3333
23	H	Isotropic =	30.2448	Anisotropy =	10.0490

Comformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.666026196094	0.721476099745	0.292688339752
O	-2.644218246468	-0.070619624930	0.864805223127
C	-1.964324686155	-1.028642273448	1.520257097110
N	-0.669609384117	-0.939946412534	1.426109305686
C	-0.445849941358	0.182588336172	0.638000674681
C	0.940669765734	0.640070953582	0.312337450147
C	-1.968928472439	1.919277420804	-0.503847321057
C	1.502135644802	1.604910178754	1.371148842852
O	-1.061670867836	2.667736172487	-0.832937439563
O	-3.219461657052	2.233745046940	-0.887263809646
C	-4.390636215174	1.385925337948	-0.713444362806
C	-5.512694381337	2.032043281121	-1.499390841084
H	-2.553406736410	-1.770792097773	2.053906295211
H	1.581503977407	-0.253321067238	0.246432106924
H	0.934653164875	1.136726458055	-0.667428348139
H	0.896890262027	2.523665010724	1.415622784646
H	1.503352365153	1.141737286441	2.370882376120
H	2.537538233018	1.885875952564	1.122465494327
H	-4.167388178182	0.375650243168	-1.085677034865
H	-4.631951362021	1.322152315178	0.356944595498
H	-5.260032493210	2.093084108963	-2.569217905751
H	-6.429572848015	1.431907392862	-1.391695610729
H	-5.717701747148	3.047979880415	-1.127847912442

SCF Done: E(RB3LYP) = -591.933207558

Zero-point correction= 0.184903
Thermal correction to Energy= 0.197073
Thermal correction to Enthalpy= 0.198017
Thermal correction to Gibbs Free Energy= 0.144992
Sum of electronic and zero-point Energies= -591.748305
Sum of electronic and thermal Energies= -591.736135
Sum of electronic and thermal Enthalpies= -591.735191
Sum of electronic and thermal Free Energies= -591.788216

1	C	Isotropic =	54.0458	Anisotropy =	82.8384
2	O	Isotropic =	29.5001	Anisotropy =	264.2415
3	C	Isotropic =	43.2181	Anisotropy =	92.3278
4	N	Isotropic =	-15.7427	Anisotropy =	346.0440
5	C	Isotropic =	33.5029	Anisotropy =	142.2087
6	C	Isotropic =	165.6694	Anisotropy =	17.0120
7	C	Isotropic =	37.1323	Anisotropy =	74.1415
8	C	Isotropic =	175.7603	Anisotropy =	23.1909
9	O	Isotropic =	-47.9167	Anisotropy =	515.3547
10	O	Isotropic =	129.5485	Anisotropy =	143.4514
11	C	Isotropic =	123.3902	Anisotropy =	61.5309
12	C	Isotropic =	175.3255	Anisotropy =	22.7292
13	H	Isotropic =	23.7557	Anisotropy =	4.2404
14	H	Isotropic =	28.8177	Anisotropy =	8.0174
15	H	Isotropic =	28.1247	Anisotropy =	5.9290
16	H	Isotropic =	30.1556	Anisotropy =	6.7507
17	H	Isotropic =	30.2822	Anisotropy =	7.9267
18	H	Isotropic =	30.0784	Anisotropy =	10.2176
19	H	Isotropic =	26.8649	Anisotropy =	4.4193
20	H	Isotropic =	26.5642	Anisotropy =	4.4005
21	H	Isotropic =	29.9523	Anisotropy =	7.7592
22	H	Isotropic =	30.0901	Anisotropy =	9.2142
23	H	Isotropic =	29.8769	Anisotropy =	7.7210

Comformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.667582457248	0.723746105052	0.308865040412
O	-2.476780795990	-0.355666287102	0.610764360219
C	-2.184300571288	-0.651059718807	1.890228544897
N	-1.288636132310	0.118622865647	2.436594207261
C	-0.934713664472	1.017794357774	1.437847963557
C	0.103480087825	2.069748194355	1.669299793806
C	-1.641113379326	1.359292125402	-1.016335289108
C	1.521009674213	1.578200420027	1.329178635814
O	-0.768202477842	2.173110699709	-1.275843881578
O	-2.546981259477	1.075474864444	-1.969536867402
C	-3.743637616400	0.268411928014	-1.775576491180
C	-4.592582936645	0.447842363976	-3.017078862640
H	-2.716362165349	-1.488989467032	2.334489530642
H	-0.133554506637	2.950122155206	1.056198073054
H	0.054437233434	2.360980415974	2.730356078980
H	1.782874467664	0.681908586075	1.914079150197
H	1.594852074848	1.328445412489	0.259437094166
H	2.261966396573	2.361745176802	1.552562038778
H	-3.449622181605	-0.781381366602	-1.635848644820
H	-4.271580088981	0.610149471267	-0.873541218690
H	-5.510066080142	-0.154019458129	-2.925083882089
H	-4.879594713860	1.502491647802	-3.149049918757
H	-4.049258906985	0.116199507657	-3.915425455519

SCF Done: E(RB3LYP) = -591.933192704

Zero-point correction= 0.184862
Thermal correction to Energy= 0.197046
Thermal correction to Enthalpy= 0.197991
Thermal correction to Gibbs Free Energy= 0.144932
Sum of electronic and zero-point Energies= -591.748330
Sum of electronic and thermal Energies= -591.736146
Sum of electronic and thermal Enthalpies= -591.735202
Sum of electronic and thermal Free Energies= -591.788261

1	C	Isotropic =	54.0311	Anisotropy =	83.0144
2	O	Isotropic =	29.5381	Anisotropy =	264.1610
3	C	Isotropic =	43.2305	Anisotropy =	92.2342
4	N	Isotropic =	-15.7030	Anisotropy =	345.9732
5	C	Isotropic =	33.5935	Anisotropy =	142.0804
6	C	Isotropic =	165.5961	Anisotropy =	16.9760
7	C	Isotropic =	37.0535	Anisotropy =	74.4155
8	C	Isotropic =	175.8165	Anisotropy =	23.0863
9	O	Isotropic =	-49.3561	Anisotropy =	516.5996
10	O	Isotropic =	129.6133	Anisotropy =	143.7234
11	C	Isotropic =	123.4393	Anisotropy =	61.7897
12	C	Isotropic =	175.2714	Anisotropy =	22.7565
13	H	Isotropic =	23.7587	Anisotropy =	4.2476
14	H	Isotropic =	28.1636	Anisotropy =	5.8443
15	H	Isotropic =	28.8080	Anisotropy =	8.0194
16	H	Isotropic =	30.2937	Anisotropy =	7.9384
17	H	Isotropic =	30.1242	Anisotropy =	6.7337
18	H	Isotropic =	30.0821	Anisotropy =	10.2095
19	H	Isotropic =	26.5642	Anisotropy =	4.4925
20	H	Isotropic =	26.9023	Anisotropy =	4.5017
21	H	Isotropic =	30.0942	Anisotropy =	9.2220
22	H	Isotropic =	29.9558	Anisotropy =	7.7484
23	H	Isotropic =	29.8790	Anisotropy =	7.7194

Comformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.877121840349	0.791008714773	0.204624072333
O	-2.605771721152	-0.073134648283	-0.591625535391
C	-2.554536550548	-1.253779519093	0.054286230884
N	-1.873831850368	-1.238882010137	1.162193268808
C	-1.425562886182	0.071516832596	1.287744831443
C	-0.612549475733	0.505708198430	2.465762158558
C	-1.721927486448	2.221858692379	-0.102936986249
C	-1.490521210259	0.900596386052	3.665678205366
O	-1.337093548843	2.984329432215	0.769335999706
O	-2.000366821248	2.732349765715	-1.316028554826
C	-2.183777080803	1.962579230417	-2.539778793780
C	-3.653827873878	1.855191938320	-2.898364447948
H	-3.078538802865	-2.087895906457	-0.406367348268
H	0.046140123099	-0.331426634463	2.746985403656
H	0.016298205632	1.358435516215	2.175662000776
H	-2.121429851492	1.766709128007	3.412258880912
H	-2.147734318948	0.069511908216	3.967689953507

H	-0.861817782439	1.171675953777	4.528224231037
H	-1.636927855351	2.543601861890	-3.296161314366
H	-1.703915386468	0.980504371698	-2.447326435086
H	-4.203369204691	1.255966126659	-2.158001460544
H	-4.112453794513	2.854349438307	-2.960691222047
H	-3.755232986153	1.368245222768	-3.881783138481

SCF Done: E(RB3LYP) = -591.932097515

Zero-point correction= 0.185079
Thermal correction to Energy= 0.197125
Thermal correction to Enthalpy= 0.198069
Thermal correction to Gibbs Free Energy= 0.145657
Sum of electronic and zero-point Energies= -591.747018
Sum of electronic and thermal Energies= -591.734973
Sum of electronic and thermal Enthalpies= -591.734029
Sum of electronic and thermal Free Energies= -591.786441

1	C	Isotropic =	54.8049	Anisotropy =	83.2989
2	O	Isotropic =	32.1796	Anisotropy =	255.5533
3	C	Isotropic =	43.5411	Anisotropy =	91.1824
4	N	Isotropic =	-16.0207	Anisotropy =	348.7995
5	C	Isotropic =	33.9214	Anisotropy =	141.1026
6	C	Isotropic =	165.8266	Anisotropy =	16.4140
7	C	Isotropic =	36.3728	Anisotropy =	72.8957
8	C	Isotropic =	175.7259	Anisotropy =	23.3178
9	O	Isotropic =	-54.1105	Anisotropy =	520.3714
10	O	Isotropic =	128.5869	Anisotropy =	147.3460
11	C	Isotropic =	124.0328	Anisotropy =	72.8018
12	C	Isotropic =	173.9686	Anisotropy =	25.1622
13	H	Isotropic =	23.7680	Anisotropy =	4.2715
14	H	Isotropic =	28.8333	Anisotropy =	8.0784
15	H	Isotropic =	28.2336	Anisotropy =	5.8159
16	H	Isotropic =	30.1597	Anisotropy =	6.8631
17	H	Isotropic =	30.2571	Anisotropy =	7.8904
18	H	Isotropic =	30.0746	Anisotropy =	10.2209
19	H	Isotropic =	27.1231	Anisotropy =	7.1683
20	H	Isotropic =	26.5512	Anisotropy =	3.6032
21	H	Isotropic =	29.5874	Anisotropy =	5.5347
22	H	Isotropic =	29.7978	Anisotropy =	8.0642
23	H	Isotropic =	30.1097	Anisotropy =	9.6208

Comformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.697324047442	0.772404844710	0.218098094407
O	-0.321734563496	0.683496674244	0.110409083957
C	-0.053530959309	-0.627152611341	0.264338854072
N	-1.098635563641	-1.378274354239	0.450392614049
C	-2.177125848597	-0.500606640861	0.428569608023
C	-3.577012284138	-0.984631662147	0.636734874150
C	-2.421651397603	2.052583632851	0.167301359393
C	-3.943724520609	-1.082141124551	2.127482534196

O	-3.576508077317	2.103723081209	0.559856030532
O	-1.855078883577	3.184394522271	-0.288683275141
C	-0.613625851505	3.268187592634	-1.047284930195
C	0.530215075509	3.734042314403	-0.166411904831
H	0.992112374764	-0.922265690676	0.218695234612
H	-4.274065627812	-0.301846150435	0.132202217218
H	-3.662852098225	-1.977620740127	0.167280650987
H	-3.907491198991	-0.087499874356	2.598501422732
H	-4.962169877162	-1.483816417156	2.246521161836
H	-3.248028239219	-1.745907609386	2.665348425108
H	-0.400935040142	2.309434340764	-1.535911645010
H	-0.835895891495	4.010801797363	-1.826875752056
H	0.770695879262	2.987395987951	0.604162704520
H	1.427345749779	3.893112047566	-0.786372581407
H	0.278780890966	4.686766039309	0.325175218849

SCF Done: E(RB3LYP) = -591.932079318

Zero-point correction= 0.185106
Thermal correction to Energy= 0.197131
Thermal correction to Enthalpy= 0.198075
Thermal correction to Gibbs Free Energy= 0.145681
Sum of electronic and zero-point Energies= -591.746973
Sum of electronic and thermal Energies= -591.734949
Sum of electronic and thermal Enthalpies= -591.734004
Sum of electronic and thermal Free Energies= -591.786398

1	C	Isotropic =	54.7714	Anisotropy = 83.2196
2	O	Isotropic =	32.2577	Anisotropy = 255.0154
3	C	Isotropic =	43.4139	Anisotropy = 91.3686
4	N	Isotropic =	-15.9611	Anisotropy = 348.6104
5	C	Isotropic =	34.0265	Anisotropy = 140.9854
6	C	Isotropic =	165.8726	Anisotropy = 16.3825
7	C	Isotropic =	36.3773	Anisotropy = 72.8000
8	C	Isotropic =	175.7096	Anisotropy = 23.2669
9	O	Isotropic =	-54.0958	Anisotropy = 519.2337
10	O	Isotropic =	128.4179	Anisotropy = 146.7847
11	C	Isotropic =	124.1954	Anisotropy = 72.9009
12	C	Isotropic =	173.8853	Anisotropy = 25.2037
13	H	Isotropic =	23.7673	Anisotropy = 4.2804
14	H	Isotropic =	28.2281	Anisotropy = 5.8152
15	H	Isotropic =	28.8269	Anisotropy = 8.0857
16	H	Isotropic =	30.1647	Anisotropy = 6.8502
17	H	Isotropic =	30.0676	Anisotropy = 10.2302
18	H	Isotropic =	30.2610	Anisotropy = 7.8853
19	H	Isotropic =	26.5312	Anisotropy = 3.6030
20	H	Isotropic =	27.1214	Anisotropy = 7.1715
21	H	Isotropic =	29.5857	Anisotropy = 5.5213
22	H	Isotropic =	30.1031	Anisotropy = 9.6017
23	H	Isotropic =	29.8051	Anisotropy = 8.0584

Comformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.658024983563	0.752319671794	0.211178778259
O	-0.475697953228	0.404593222252	-0.416297640570
C	-0.141173971405	-0.783525412301	0.119860136936
N	-0.971602127330	-1.228398802988	1.016617015628
C	-1.960215991946	-0.255256433649	1.102420889731
C	-3.121738643168	-0.411401204254	2.033050894428
C	-2.382748702565	2.003966151085	-0.059483139812
C	-4.344268075749	-1.048428474132	1.349997682368
O	-3.405877686342	2.242935105075	0.563830642610
O	-1.978401596723	2.911839514508	-0.966454196374
C	-0.834178645167	2.801776970473	-1.861952544226
C	0.431896667778	3.341084062237	-1.221645975407
H	0.774864840730	-1.244513462371	-0.241935558596
H	-2.791911288033	-1.043186788748	2.872346908798
H	-3.399573272621	0.575414369014	2.427331625092
H	-5.160730909809	-1.183582686146	2.076668547573
H	-4.711845372904	-0.404327642059	0.536164110190
H	-4.095963900632	-2.034825979367	0.926437280353
H	-0.720745396966	1.767719152599	-2.207536533550
H	-1.131719304800	3.422238617619	-2.718605614521
H	0.756974087143	2.717278295875	-0.375959476598
H	1.241215398952	3.350823689608	-1.969667149070
H	0.279316828346	4.372038063877	-0.866206683243

SCF Done: E(RB3LYP) = -591.931605059

Zero-point correction= 0.185229
Thermal correction to Energy= 0.197226
Thermal correction to Enthalpy= 0.198170
Thermal correction to Gibbs Free Energy= 0.145736
Sum of electronic and zero-point Energies= -591.746377
Sum of electronic and thermal Energies= -591.734379
Sum of electronic and thermal Enthalpies= -591.733435
Sum of electronic and thermal Free Energies= -591.785869

1	C	Isotropic =	54.5841	Anisotropy =	82.5947
2	O	Isotropic =	32.0565	Anisotropy =	258.2418
3	C	Isotropic =	43.4211	Anisotropy =	92.0067
4	N	Isotropic =	-16.2133	Anisotropy =	345.1126
5	C	Isotropic =	33.0873	Anisotropy =	142.0243
6	C	Isotropic =	165.3202	Anisotropy =	18.1742
7	C	Isotropic =	37.3328	Anisotropy =	74.7133
8	C	Isotropic =	175.9875	Anisotropy =	22.6941
9	O	Isotropic =	-45.3728	Anisotropy =	516.0651
10	O	Isotropic =	126.5844	Anisotropy =	146.7481
11	C	Isotropic =	124.4901	Anisotropy =	72.2650
12	C	Isotropic =	174.0037	Anisotropy =	24.8042
13	H	Isotropic =	23.7630	Anisotropy =	4.2991
14	H	Isotropic =	28.8226	Anisotropy =	7.9447
15	H	Isotropic =	28.0279	Anisotropy =	6.0726
16	H	Isotropic =	30.1056	Anisotropy =	10.2661
17	H	Isotropic =	30.1901	Anisotropy =	6.5525
18	H	Isotropic =	30.3265	Anisotropy =	7.9439
19	H	Isotropic =	26.1048	Anisotropy =	3.7722
20	H	Isotropic =	27.1042	Anisotropy =	7.0405

21 H Isotropic = 29.8346 Anisotropy = 5.0180
22 H Isotropic = 30.1208 Anisotropy = 9.6755
23 H Isotropic = 29.8672 Anisotropy = 8.1516

Comformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.749588796462	0.714870854276	0.060527970109
O	-0.586645285480	0.263786370311	-0.536805798808
C	-0.689987229699	-1.077878976584	-0.515967934982
N	-1.784580457114	-1.530417430740	0.020975959370
C	-2.492496881953	-0.395780805921	0.399830292259
C	-3.820724024668	-0.505862041003	1.079777734541
C	-2.066447122853	2.139762247381	0.247273219731
C	-3.692886183905	-0.558718177316	2.612155470856
O	-3.102698380223	2.446252516766	0.817183700783
O	-1.267768784759	3.137563613382	-0.173567124567
C	0.000055495983	3.003306564795	-0.879236348475
C	-0.201457429040	2.842400620797	-2.375125340962
H	0.136464357306	-1.640248921815	-0.944008717836
H	-4.442063982638	0.353571334925	0.794735806447
H	-4.305603219512	-1.425079823581	0.715490406760
H	-4.684475606584	-0.683322456706	3.074846968228
H	-3.058041991802	-1.401359971546	2.929898699449
H	-3.248749257499	0.372827936027	2.996273101414
H	0.505174107737	3.952844585049	-0.655171221775
H	0.590200695899	2.187475481374	-0.446258324327
H	-0.814994499638	3.664222587695	-2.775964749990
H	0.779129302491	2.867783765377	-2.877527111264
H	-0.684444825587	1.885070127060	-2.620926656961

SCF Done: E(RB3LYP) = -591.931589486

Zero-point correction= 0.185163
Thermal correction to Energy= 0.197185
Thermal correction to Enthalpy= 0.198129
Thermal correction to Gibbs Free Energy= 0.145524
Sum of electronic and zero-point Energies= -591.746427
Sum of electronic and thermal Energies= -591.734404
Sum of electronic and thermal Enthalpies= -591.733460
Sum of electronic and thermal Free Energies= -591.786066

1 C Isotropic = 54.3932 Anisotropy = 82.5682
2 O Isotropic = 32.6470 Anisotropy = 257.3498
3 C Isotropic = 43.2843 Anisotropy = 92.0815
4 N Isotropic = -15.7734 Anisotropy = 346.6496
5 C Isotropic = 33.0305 Anisotropy = 141.4079
6 C Isotropic = 165.4291 Anisotropy = 17.8959
7 C Isotropic = 37.4356 Anisotropy = 75.4248
8 C Isotropic = 175.7115 Anisotropy = 23.1370
9 O Isotropic = -46.1537 Anisotropy = 516.6289
10 O Isotropic = 126.2155 Anisotropy = 147.3201
11 C Isotropic = 124.6826 Anisotropy = 72.1912

12	C	Isotropic =	174.0534	Anisotropy =	24.6994
13	H	Isotropic =	23.7542	Anisotropy =	4.2960
14	H	Isotropic =	28.0239	Anisotropy =	6.0891
15	H	Isotropic =	28.8295	Anisotropy =	7.9138
16	H	Isotropic =	30.0880	Anisotropy =	10.2624
17	H	Isotropic =	30.2948	Anisotropy =	7.9197
18	H	Isotropic =	30.2157	Anisotropy =	6.6566
19	H	Isotropic =	27.1046	Anisotropy =	7.0472
20	H	Isotropic =	26.0245	Anisotropy =	3.8924
21	H	Isotropic =	29.8970	Anisotropy =	8.1587
22	H	Isotropic =	30.1371	Anisotropy =	9.6923
23	H	Isotropic =	29.9309	Anisotropy =	4.9515

1a incorrect isomer

Comformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.054550659010	0.673987574430	0.163212518056
N	1.419097590698	0.786784796526	-0.125078227413
C	1.981280616172	-0.046903369809	0.685809708016
O	1.113475716258	-0.715780805440	1.498239388091
C	-0.128433884157	-0.252739525583	1.161200731545
C	-1.297935696844	-0.800707131899	1.900400532262
C	-0.996111546491	1.448172582637	-0.524557825329
C	-1.285824673761	-0.447657891990	3.397749127341
O	-2.189041215580	1.351858676058	-0.282526171937
O	-0.487512534473	2.275849911513	-1.451716017037
C	-1.446505821444	3.083879450271	-2.182666673930
C	-0.666797630160	3.936610199133	-3.161212421688
H	3.036393052025	-0.280765687464	0.801731149174
H	-2.200480687128	-0.407827779505	1.415018243371
H	-1.303371241784	-1.898138688282	1.780673473682
H	-2.158248878246	-0.895253542980	3.897604557625
H	-0.377202767132	-0.828640824778	3.889414704131
H	-1.324992256435	0.642946150258	3.547166001036
H	-2.157309020611	2.413626549035	-2.690795499328
H	-2.015308800138	3.692833545597	-1.462793837471
H	-1.361935893138	4.565706903137	-3.738503674610
H	0.040032664045	4.596138154653	-2.633939167644
H	-0.100347750687	3.309360754487	-3.867100617944

SCF Done: E(RB3LYP) = -591.946196470

Zero-point correction= 0.184901
Thermal correction to Energy= 0.197136
Thermal correction to Enthalpy= 0.198080
Thermal correction to Gibbs Free Energy= 0.144793
Sum of electronic and zero-point Energies= -591.761296
Sum of electronic and thermal Energies= -591.749061
Sum of electronic and thermal Enthalpies= -591.748116
Sum of electronic and thermal Free Energies= -591.801404

1	C	Isotropic =	64.3423	Anisotropy =	82.8737
2	N	Isotropic =	-5.3926	Anisotropy =	348.6642
3	C	Isotropic =	46.3799	Anisotropy =	84.4341
4	O	Isotropic =	9.0554	Anisotropy =	280.6089
5	C	Isotropic =	27.5408	Anisotropy =	125.5177
6	C	Isotropic =	169.3635	Anisotropy =	14.8601
7	C	Isotropic =	31.4322	Anisotropy =	85.1176
8	C	Isotropic =	176.5840	Anisotropy =	22.7153
9	O	Isotropic =	-30.7531	Anisotropy =	527.2588
10	O	Isotropic =	124.3589	Anisotropy =	132.1671
11	C	Isotropic =	128.7468	Anisotropy =	56.4409
12	C	Isotropic =	177.0910	Anisotropy =	20.3226
13	H	Isotropic =	23.9221	Anisotropy =	4.1999
14	H	Isotropic =	27.6655	Anisotropy =	8.7857
15	H	Isotropic =	28.7247	Anisotropy =	8.1097
16	H	Isotropic =	30.0492	Anisotropy =	10.0493
17	H	Isotropic =	29.9907	Anisotropy =	8.1130
18	H	Isotropic =	30.3287	Anisotropy =	7.4936
19	H	Isotropic =	27.1896	Anisotropy =	6.0154
20	H	Isotropic =	27.1738	Anisotropy =	5.9016
21	H	Isotropic =	30.0380	Anisotropy =	9.5078
22	H	Isotropic =	29.8881	Anisotropy =	7.6594
23	H	Isotropic =	29.8897	Anisotropy =	7.7127

Comformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.237487835642	0.470230064891	0.136909778403
N	-0.381474752296	-0.715867770175	-0.591292832258
C	-0.220471489083	-1.646686814248	0.289791722061
O	0.021506335991	-1.191988078280	1.552848185680
C	0.011941426043	0.172049363731	1.454922326711
C	0.242164996520	0.959288252992	2.696645045326
C	-0.341026911873	1.815692925386	-0.458882824150
C	-0.853254543920	0.751739516612	3.756562974429
O	-0.211389075275	2.855811994287	0.167426556217
O	-0.595505858633	1.764496128305	-1.776348693635
C	-0.714435402000	3.041717004408	-2.455483721871
C	-1.004425705797	2.753179430078	-3.913305635514
H	-0.251573068982	-2.725070006166	0.157543605354
H	1.221015042422	0.669194112749	3.116879369790
H	0.305690072395	2.014946769832	2.403056525217
H	-0.929258549732	-0.307143288168	4.048862995220
H	-0.621571154198	1.339325897022	4.657880706974
H	-1.836151958201	1.074428700631	3.378252713224
H	-1.520459505543	3.620915803831	-1.978550184166
H	0.224985717151	3.600554915736	-2.321825240605
H	-1.943310412909	2.188598429751	-4.024410236813
H	-1.103308656094	3.700835544416	-4.465068288474
H	-0.189378710345	2.170371102378	-4.370074847121

SCF Done: E(RB3LYP) = -591.946189042

Zero-point correction= 0.184924
Thermal correction to Energy= 0.197136
Thermal correction to Enthalpy= 0.198080
Thermal correction to Gibbs Free Energy= 0.144995
Sum of electronic and zero-point Energies= -591.761265
Sum of electronic and thermal Energies= -591.749053
Sum of electronic and thermal Enthalpies= -591.748109
Sum of electronic and thermal Free Energies= -591.801194

1	C	Isotropic =	64.4311	Anisotropy =	82.7983
2	N	Isotropic =	-5.3861	Anisotropy =	348.4652
3	C	Isotropic =	46.2928	Anisotropy =	84.5167
4	O	Isotropic =	9.1996	Anisotropy =	281.0953
5	C	Isotropic =	27.6042	Anisotropy =	125.5079
6	C	Isotropic =	169.3912	Anisotropy =	14.8690
7	C	Isotropic =	31.4668	Anisotropy =	85.2144
8	C	Isotropic =	176.6230	Anisotropy =	22.6082
9	O	Isotropic =	-30.5710	Anisotropy =	526.2921
10	O	Isotropic =	124.2313	Anisotropy =	132.1248
11	C	Isotropic =	128.7817	Anisotropy =	56.4157
12	C	Isotropic =	177.0561	Anisotropy =	20.3606
13	H	Isotropic =	23.9206	Anisotropy =	4.1974
14	H	Isotropic =	28.7219	Anisotropy =	8.1067
15	H	Isotropic =	27.6576	Anisotropy =	8.8453
16	H	Isotropic =	29.9794	Anisotropy =	8.1189
17	H	Isotropic =	30.0501	Anisotropy =	10.0424
18	H	Isotropic =	30.3319	Anisotropy =	7.5048
19	H	Isotropic =	27.1767	Anisotropy =	5.8967
20	H	Isotropic =	27.1930	Anisotropy =	6.0200
21	H	Isotropic =	29.8869	Anisotropy =	7.6491
22	H	Isotropic =	30.0377	Anisotropy =	9.5057
23	H	Isotropic =	29.8835	Anisotropy =	7.7201

Comformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.566377894959	0.771998864538	0.576065714323
N	-1.742988010024	0.351929732708	1.206215348526
C	-1.338242840972	-0.490719262010	2.097606571114
O	0.012872022624	-0.676292256967	2.126044497431
C	0.511129997242	0.138134249120	1.146988828334
C	1.983423520284	0.140791008896	0.930061556891
C	-0.528951088533	1.751208447491	-0.526810804136
C	2.522697466583	-1.211924811788	0.433574827770
O	0.497456284660	2.125294382912	-1.072376052221
O	-1.759152065777	2.183886168902	-0.854232174904
C	-1.849572686216	3.156185928484	-1.930800786483
C	-1.913424946223	2.476444544871	-3.287903317657
H	-1.923680639114	-1.059624292720	2.815237480330
H	2.203215322154	0.936718834043	0.207051808473
H	2.475494425104	0.406501806459	1.881812340813
H	2.081823444563	-1.480088100808	-0.539541270501
H	3.615637131497	-1.161224905647	0.314266975981

H	2.293382344227	-2.018029821456	1.147775375336
H	-2.774488631645	3.707268744195	-1.713640001521
H	-0.992764593137	3.840973189985	-1.863883879941
H	-2.068831059800	3.235030897666	-4.071966809166
H	-0.976294530171	1.942619076492	-3.506499167422
H	-2.749002972366	1.760327574636	-3.330227061371

SCF Done: E(RB3LYP) = -591.945708563

Zero-point correction= 0.185105
Thermal correction to Energy= 0.197243
Thermal correction to Enthalpy= 0.198187
Thermal correction to Gibbs Free Energy= 0.145123
Sum of electronic and zero-point Energies= -591.760603
Sum of electronic and thermal Energies= -591.748465
Sum of electronic and thermal Enthalpies= -591.747521
Sum of electronic and thermal Free Energies= -591.800586

1	C	Isotropic =	64.2514	Anisotropy =	82.2906
2	N	Isotropic =	-5.4452	Anisotropy =	349.1320
3	C	Isotropic =	46.3785	Anisotropy =	84.4014
4	O	Isotropic =	8.8389	Anisotropy =	280.5927
5	C	Isotropic =	27.2532	Anisotropy =	125.9046
6	C	Isotropic =	169.2804	Anisotropy =	14.8522
7	C	Isotropic =	31.5133	Anisotropy =	84.4070
8	C	Isotropic =	176.5027	Anisotropy =	22.7115
9	O	Isotropic =	-20.5135	Anisotropy =	525.0725
10	O	Isotropic =	125.2877	Anisotropy =	157.8205
11	C	Isotropic =	130.1083	Anisotropy =	63.6125
12	C	Isotropic =	175.8119	Anisotropy =	22.9771
13	H	Isotropic =	23.9172	Anisotropy =	4.2910
14	H	Isotropic =	27.6444	Anisotropy =	8.7728
15	H	Isotropic =	28.7202	Anisotropy =	8.1565
16	H	Isotropic =	30.3262	Anisotropy =	7.3840
17	H	Isotropic =	30.0486	Anisotropy =	10.0342
18	H	Isotropic =	29.9978	Anisotropy =	8.1370
19	H	Isotropic =	27.4359	Anisotropy =	7.5134
20	H	Isotropic =	26.4288	Anisotropy =	5.4402
21	H	Isotropic =	30.2430	Anisotropy =	9.8879
22	H	Isotropic =	29.8532	Anisotropy =	5.9617
23	H	Isotropic =	30.0800	Anisotropy =	7.6527

Comformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.038709886555	0.972355242289	0.558480381461
N	0.992220359880	1.677328555961	1.189490719092
C	1.588905660365	0.784829310369	1.907765938010
O	1.048788575789	-0.464649941647	1.818500201405
C	-0.000697548593	-0.344450298939	0.950051217311
C	-0.789976833149	-1.567788942131	0.641960573675
C	-1.001837398960	1.585869472707	-0.375477802291
C	0.026551709158	-2.645101696775	-0.092615983997

O	-1.900790450963	0.972563408938	-0.929394555669
O	-0.772753241432	2.900740096262	-0.537767465502
C	-1.661612691169	3.617396400880	-1.437041790107
C	-1.178406753695	3.536042609870	-2.874993752047
H	2.448818946761	0.898366021187	2.562794654742
H	-1.176516710167	-1.981025322371	1.589880772485
H	-1.651679030131	-1.254073817446	0.038930605268
H	-0.598426429913	-3.532484268935	-0.275056611657
H	0.388687724642	-2.273137937394	-1.064138559338
H	0.899220708293	-2.957856724407	0.501668487328
H	-2.677224671607	3.211690032047	-1.329916199797
H	-1.640425787986	4.650273280786	-1.064164640217
H	-1.823846426681	4.158635862003	-3.515421400565
H	-0.144689446701	3.905283221321	-2.964157191711
H	-1.219390377186	2.501375435424	-3.247467597879

SCF Done: E(RB3LYP) = -591.945693968

Zero-point correction= 0.185132
Thermal correction to Energy= 0.197258
Thermal correction to Enthalpy= 0.198202
Thermal correction to Gibbs Free Energy= 0.145262
Sum of electronic and zero-point Energies= -591.760562
Sum of electronic and thermal Energies= -591.748436
Sum of electronic and thermal Enthalpies= -591.747492
Sum of electronic and thermal Free Energies= -591.800432

1	C	Isotropic =	64.2353	Anisotropy =	82.3007
2	N	Isotropic =	-5.3525	Anisotropy =	349.1318
3	C	Isotropic =	46.2526	Anisotropy =	84.4387
4	O	Isotropic =	8.9894	Anisotropy =	280.6035
5	C	Isotropic =	27.2876	Anisotropy =	125.9736
6	C	Isotropic =	169.2802	Anisotropy =	14.8744
7	C	Isotropic =	31.5090	Anisotropy =	84.4669
8	C	Isotropic =	176.5595	Anisotropy =	22.6803
9	O	Isotropic =	-20.3194	Anisotropy =	524.7638
10	O	Isotropic =	125.2664	Anisotropy =	158.0670
11	C	Isotropic =	130.1831	Anisotropy =	63.5510
12	C	Isotropic =	175.9077	Anisotropy =	23.1051
13	H	Isotropic =	23.9194	Anisotropy =	4.2901
14	H	Isotropic =	28.7220	Anisotropy =	8.1493
15	H	Isotropic =	27.6499	Anisotropy =	8.7879
16	H	Isotropic =	30.0467	Anisotropy =	10.0235
17	H	Isotropic =	30.3215	Anisotropy =	7.3948
18	H	Isotropic =	29.9896	Anisotropy =	8.1560
19	H	Isotropic =	26.4264	Anisotropy =	5.4178
20	H	Isotropic =	27.4434	Anisotropy =	7.5169
21	H	Isotropic =	30.2456	Anisotropy =	9.8915
22	H	Isotropic =	30.0709	Anisotropy =	7.6712
23	H	Isotropic =	29.8558	Anisotropy =	5.9776

Comformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.293151923040	0.393670612861	0.105052066988
N	-0.509628412613	-0.874606893048	-0.444957202964
C	-0.006725140114	-1.684858397871	0.426241899414
O	0.533176439332	-1.073262280804	1.519529376662
C	0.350133732088	0.266044356469	1.312842393896
C	0.838080401099	1.202771068847	2.361243249102
C	-0.705003820182	1.651984598265	-0.545834598641
C	0.130947409524	1.017626702820	3.714736853901
O	-0.514848451007	2.760664740028	-0.070627210464
O	-1.318350152138	1.428919548885	-1.721383815716
C	-1.770448095560	2.596551916907	-2.459396796969
C	-0.664744542791	3.161626341297	-3.334624580673
H	0.041591858937	-2.770415057601	0.401390826426
H	1.923834589642	1.048091661552	2.489084783369
H	0.689887138935	2.220981041533	1.979472851589
H	0.544775232090	1.719076733934	4.454999143332
H	-0.950217203670	1.208714795404	3.625823156731
H	0.267851859305	-0.005111586443	4.098951711944
H	-2.607878977035	2.221172878176	-3.062811744996
H	-2.141952187039	3.345500278915	-1.746255432905
H	-0.270190785787	2.391709707882	-4.016095902999
H	-1.064211995791	3.989135438605	-3.942871307437
H	0.162223025814	3.552341793387	-2.722719719588

SCF Done: E(RB3LYP) = -591.945697254

Zero-point correction= 0.185061
Thermal correction to Energy= 0.197217
Thermal correction to Enthalpy= 0.198161
Thermal correction to Gibbs Free Energy= 0.144933
Sum of electronic and zero-point Energies= -591.760637
Sum of electronic and thermal Energies= -591.748480
Sum of electronic and thermal Enthalpies= -591.747536
Sum of electronic and thermal Free Energies= -591.800765

1	C	Isotropic =	64.2882	Anisotropy =	82.3571
2	N	Isotropic =	-5.3495	Anisotropy =	348.9202
3	C	Isotropic =	46.3063	Anisotropy =	84.5018
4	O	Isotropic =	9.0852	Anisotropy =	281.7319
5	C	Isotropic =	27.3763	Anisotropy =	125.8329
6	C	Isotropic =	169.3564	Anisotropy =	14.7838
7	C	Isotropic =	31.4948	Anisotropy =	84.5577
8	C	Isotropic =	176.6746	Anisotropy =	22.6003
9	O	Isotropic =	-20.4741	Anisotropy =	525.1110
10	O	Isotropic =	125.1214	Anisotropy =	158.4025
11	C	Isotropic =	130.1441	Anisotropy =	63.6235
12	C	Isotropic =	175.8840	Anisotropy =	23.2054
13	H	Isotropic =	23.9190	Anisotropy =	4.2832
14	H	Isotropic =	28.7137	Anisotropy =	8.0234
15	H	Isotropic =	27.6386	Anisotropy =	9.0274
16	H	Isotropic =	30.0503	Anisotropy =	10.0297
17	H	Isotropic =	30.3384	Anisotropy =	7.5534
18	H	Isotropic =	29.9725	Anisotropy =	8.1642
19	H	Isotropic =	27.4369	Anisotropy =	7.4244
20	H	Isotropic =	26.4311	Anisotropy =	5.3368

21 H Isotropic = 30.0818 Anisotropy = 7.7256
22 H Isotropic = 30.2489 Anisotropy = 9.8994
23 H Isotropic = 29.8555 Anisotropy = 5.9592

Comformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.023180773408	0.516836943262	-0.087733587189
N	0.783723092771	-0.094430663895	-1.053714177707
C	0.988270878542	-1.281268216376	-0.586766090031
O	0.387388695159	-1.526581011520	0.613007915979
C	-0.265568172102	-0.368956572734	0.934682857022
C	-1.016695925018	-0.330650041895	2.218790123725
C	-0.520103019597	1.902084523329	-0.189432616332
C	-0.106889825821	-0.448812715514	3.453930062407
O	-1.214303484187	2.441787969908	0.657897254359
O	-0.112538159297	2.497799928504	-1.323841050214
C	-0.537314856749	3.871740241067	-1.534387872496
C	-1.904298682075	3.934885749065	-2.194074656208
H	1.565612147788	-2.094868324727	-1.018179001654
H	-1.577702987158	0.612461720577	2.238813425215
H	-1.748117726012	-1.157390129804	2.219516621683
H	-0.714014957273	-0.436660359749	4.371864507522
H	0.468171197658	-1.387726344299	3.436617333020
H	0.606128033132	0.389424632221	3.501021378393
H	-0.531810990225	4.396795982691	-0.569078010398
H	0.241707339757	4.293893198331	-2.183402646253
H	-1.911170318943	3.371041410270	-3.140056852798
H	-2.681733240506	3.526272695972	-1.531092551177
H	-2.157118266438	4.984289385315	-2.415882366868

SCF Done: E(RB3LYP) = -591.945719442

Zero-point correction= 0.185144
Thermal correction to Energy= 0.197272
Thermal correction to Enthalpy= 0.198216
Thermal correction to Gibbs Free Energy= 0.145111
Sum of electronic and zero-point Energies= -591.760575
Sum of electronic and thermal Energies= -591.748448
Sum of electronic and thermal Enthalpies= -591.747503
Sum of electronic and thermal Free Energies= -591.800608

1 C Isotropic = 64.3151 Anisotropy = 82.4427
2 N Isotropic = -5.4077 Anisotropy = 348.7730
3 C Isotropic = 46.2876 Anisotropy = 84.5376
4 O Isotropic = 8.8728 Anisotropy = 280.3175
5 C Isotropic = 27.2873 Anisotropy = 126.0606
6 C Isotropic = 169.2464 Anisotropy = 14.6615
7 C Isotropic = 31.4383 Anisotropy = 84.3831
8 C Isotropic = 176.4919 Anisotropy = 22.8368
9 O Isotropic = -20.6171 Anisotropy = 524.5302
10 O Isotropic = 125.3165 Anisotropy = 158.6179
11 C Isotropic = 130.1218 Anisotropy = 63.6262

12	C	Isotropic =	175.8997	Anisotropy =	23.1087
13	H	Isotropic =	23.9193	Anisotropy =	4.2924
14	H	Isotropic =	27.6577	Anisotropy =	8.8095
15	H	Isotropic =	28.7191	Anisotropy =	8.0234
16	H	Isotropic =	30.0434	Anisotropy =	10.0434
17	H	Isotropic =	29.9998	Anisotropy =	8.1603
18	H	Isotropic =	30.3309	Anisotropy =	7.4760
19	H	Isotropic =	26.4289	Anisotropy =	5.3338
20	H	Isotropic =	27.4334	Anisotropy =	7.4266
21	H	Isotropic =	30.0883	Anisotropy =	7.7299
22	H	Isotropic =	29.8611	Anisotropy =	5.9602
23	H	Isotropic =	30.2517	Anisotropy =	9.8945

Comformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.543536482759	0.521940397914	-0.100561735787
N	1.878806176617	0.193775653535	-0.355737727727
C	2.414581369635	0.115247298962	0.816611644489
O	1.554617285644	0.359134897318	1.845711107253
C	0.346643920390	0.619478000456	1.256882367961
C	-0.790377555658	0.945559097932	2.162432187734
C	-0.399998441364	0.707299951033	-1.220768027174
C	-0.777336054693	2.410500220293	2.635578889478
O	-0.112364674579	0.539438148563	-2.390392225790
O	-1.621829173000	1.091553985742	-0.796281137947
C	-2.622553095341	1.292935975196	-1.829353058110
C	-3.906670591126	1.716095206235	-1.148158362932
H	3.441951732579	-0.118230270020	1.083861245414
H	-1.724505779675	0.730950441630	1.628261438956
H	-0.736465190900	0.272591345951	3.033677472568
H	-0.876788948092	3.098049602434	1.781121082173
H	-1.616150414418	2.592403865506	3.324893752376
H	0.158905263229	2.649941074570	3.163886371732
H	-2.253427300405	2.058928287845	-2.528877642705
H	-2.741479162618	0.353462437306	-2.391172733071
H	-4.264410434837	0.937451498898	-0.456446629295
H	-3.765500217635	2.650571661797	-0.583032084697
H	-4.685955196510	1.886671220904	-1.907156194900

SCF Done: E(RB3LYP) = -591.945050351

Zero-point correction= 0.184948
Thermal correction to Energy= 0.197181
Thermal correction to Enthalpy= 0.198125
Thermal correction to Gibbs Free Energy= 0.144644
Sum of electronic and zero-point Energies= -591.760103
Sum of electronic and thermal Energies= -591.747870
Sum of electronic and thermal Enthalpies= -591.746925
Sum of electronic and thermal Free Energies= -591.800406

1	C	Isotropic =	63.7338	Anisotropy =	80.1523
2	N	Isotropic =	-8.6837	Anisotropy =	349.5525

3	C	Isotropic =	46.0408	Anisotropy =	85.8613
4	O	Isotropic =	8.1160	Anisotropy =	259.2575
5	C	Isotropic =	28.5857	Anisotropy =	125.0452
6	C	Isotropic =	168.1537	Anisotropy =	15.0619
7	C	Isotropic =	32.7165	Anisotropy =	78.2850
8	C	Isotropic =	175.6449	Anisotropy =	23.7536
9	O	Isotropic =	-49.5992	Anisotropy =	554.1246
10	O	Isotropic =	130.5292	Anisotropy =	153.9384
11	C	Isotropic =	128.7235	Anisotropy =	56.9737
12	C	Isotropic =	176.9244	Anisotropy =	20.1128
13	H	Isotropic =	23.9004	Anisotropy =	4.4205
14	H	Isotropic =	27.9777	Anisotropy =	8.3172
15	H	Isotropic =	28.6818	Anisotropy =	7.9723
16	H	Isotropic =	30.2406	Anisotropy =	6.6855
17	H	Isotropic =	30.0429	Anisotropy =	9.8176
18	H	Isotropic =	30.1456	Anisotropy =	8.2808
19	H	Isotropic =	27.1660	Anisotropy =	6.4507
20	H	Isotropic =	27.1751	Anisotropy =	6.5992
21	H	Isotropic =	29.8733	Anisotropy =	7.1575
22	H	Isotropic =	29.8773	Anisotropy =	7.0237
23	H	Isotropic =	30.0339	Anisotropy =	9.7848

Comformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.097618223767	0.755936342658	1.027496064461
N	0.449563557701	0.547089798224	2.297295571996
C	0.639883575582	-0.729018395059	2.353474597543
O	0.264604363965	-1.403728910394	1.230049518447
C	-0.213629158659	-0.448597221471	0.374301412780
C	-0.679483291689	-0.909550964543	-0.963579307431
C	-0.450080977061	2.119527026682	0.585090049941
C	0.469126144582	-1.057332770154	-1.978018122583
O	-0.351489408941	3.111578172612	1.281594664084
O	-0.891920379881	2.139099226706	-0.690054361247
C	-1.276939964408	3.438507118858	-1.211977681490
C	-1.735174381050	3.242063618364	-2.641450571097
H	1.049459711822	-1.323459327627	3.165977466620
H	-1.188786306627	-1.877806325427	-0.832004644558
H	-1.417710429579	-0.187791471555	-1.335943894087
H	0.079440709095	-1.425329433173	-2.939595491026
H	0.961667494699	-0.088101877636	-2.152471958281
H	1.227762511272	-1.770698892809	-1.619362542536
H	-2.074487998557	3.850522504303	-0.574310874187
H	-0.409725045649	4.113493079933	-1.144493122097
H	-0.928199384577	2.822201741963	-3.261950533518
H	-2.604073165726	2.567279849379	-2.690713255520
H	-2.029009952549	4.213207110168	-3.069222986214

SCF Done: E(RB3LYP) = -591.945081424

Zero-point correction= 0.185009
Thermal correction to Energy= 0.197195

Thermal correction to Enthalpy= 0.198139
Thermal correction to Gibbs Free Energy= 0.145139
Sum of electronic and zero-point Energies= -591.760073
Sum of electronic and thermal Energies= -591.747887
Sum of electronic and thermal Enthalpies= -591.746943
Sum of electronic and thermal Free Energies= -591.799943

1	C	Isotropic =	63.7460	Anisotropy =	80.3425
2	N	Isotropic =	-8.8913	Anisotropy =	349.5225
3	C	Isotropic =	46.1246	Anisotropy =	85.6604
4	O	Isotropic =	7.6854	Anisotropy =	257.5460
5	C	Isotropic =	28.3969	Anisotropy =	125.3233
6	C	Isotropic =	168.0476	Anisotropy =	15.1475
7	C	Isotropic =	32.7252	Anisotropy =	78.2909
8	C	Isotropic =	175.5957	Anisotropy =	23.7087
9	O	Isotropic =	-49.2766	Anisotropy =	553.8935
10	O	Isotropic =	130.2574	Anisotropy =	153.8022
11	C	Isotropic =	128.6680	Anisotropy =	56.9643
12	C	Isotropic =	176.9051	Anisotropy =	20.0690
13	H	Isotropic =	23.9036	Anisotropy =	4.4291
14	H	Isotropic =	28.6765	Anisotropy =	7.9818
15	H	Isotropic =	28.0051	Anisotropy =	7.9059
16	H	Isotropic =	30.0511	Anisotropy =	9.8115
17	H	Isotropic =	30.2186	Anisotropy =	6.6002
18	H	Isotropic =	30.1748	Anisotropy =	8.2840
19	H	Isotropic =	27.1831	Anisotropy =	6.6225
20	H	Isotropic =	27.1573	Anisotropy =	6.4400
21	H	Isotropic =	29.8814	Anisotropy =	6.9990
22	H	Isotropic =	29.8712	Anisotropy =	7.1483
23	H	Isotropic =	30.0299	Anisotropy =	9.7945

Comformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.243874715409	0.591930667114	-0.051315523687
N	-0.949127979289	-0.278708136317	-0.889070046315
C	-0.086212907262	-0.632866264600	-1.782994806369
O	1.144672654108	-0.069754149465	-1.625875816831
C	1.047986311866	0.714377352522	-0.512549471175
C	2.267422604222	1.444974588392	-0.071464644771
C	-0.755207892715	1.250858366044	1.169832360366
C	3.163254994958	0.601132965730	0.853441119391
O	0.013788363980	1.747611883523	1.978975392693
O	-2.072623145076	1.316267810791	1.437180171780
C	-3.130527226503	0.984477456858	0.493882691007
C	-4.417146732112	1.533725717828	1.075979996863
H	-0.213944744358	-1.306954741462	-2.625855826257
H	2.830132070518	1.749450875353	-0.968328923822
H	1.944541010167	2.351522063090	0.457805201513
H	2.619050595458	0.332811278376	1.771591827668
H	3.489924758997	-0.325844431264	0.356401450255
H	4.060059819213	1.173889274200	1.135808266003
H	-2.901877912064	1.434822626794	-0.482796378288

H	-3.169080977744	-0.105510265061	0.367610383812
H	-5.256755712488	1.295276070687	0.404382103541
H	-4.624824103847	1.086737169065	2.060771153933
H	-4.363969134620	2.627461821801	1.191979318691

SCF Done: E(RB3LYP) = -591.935826173

Zero-point correction= 0.184913
Thermal correction to Energy= 0.197064
Thermal correction to Enthalpy= 0.198008
Thermal correction to Gibbs Free Energy= 0.145306
Sum of electronic and zero-point Energies= -591.750913
Sum of electronic and thermal Energies= -591.738762
Sum of electronic and thermal Enthalpies= -591.737818
Sum of electronic and thermal Free Energies= -591.790520

1	C	Isotropic =	63.9839	Anisotropy =	83.5960
2	N	Isotropic =	-5.7374	Anisotropy =	351.4579
3	C	Isotropic =	47.3909	Anisotropy =	82.4366
4	O	Isotropic =	8.5100	Anisotropy =	280.8020
5	C	Isotropic =	24.4876	Anisotropy =	129.7657
6	C	Isotropic =	167.5690	Anisotropy =	15.8198
7	C	Isotropic =	32.2889	Anisotropy =	81.7277
8	C	Isotropic =	176.2812	Anisotropy =	23.0582
9	O	Isotropic =	-53.3676	Anisotropy =	520.3069
10	O	Isotropic =	125.8211	Anisotropy =	149.0810
11	C	Isotropic =	121.7885	Anisotropy =	57.5862
12	C	Isotropic =	175.0998	Anisotropy =	22.9754
13	H	Isotropic =	23.8932	Anisotropy =	4.1605
14	H	Isotropic =	28.6654	Anisotropy =	7.9879
15	H	Isotropic =	28.0935	Anisotropy =	6.0562
16	H	Isotropic =	30.0799	Anisotropy =	6.8937
17	H	Isotropic =	30.2712	Anisotropy =	8.0825
18	H	Isotropic =	30.0726	Anisotropy =	10.2085
19	H	Isotropic =	26.9492	Anisotropy =	4.6441
20	H	Isotropic =	26.2809	Anisotropy =	5.1420
21	H	Isotropic =	30.1146	Anisotropy =	9.1305
22	H	Isotropic =	29.8961	Anisotropy =	7.6328
23	H	Isotropic =	30.0089	Anisotropy =	7.6502

Comformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.112554868530	0.774526461427	-0.159509816275
N	-0.359890265336	0.166918285884	-1.395232891690
C	0.480730658410	-0.812921019103	-1.444722331332
O	1.273956705070	-0.925251398347	-0.342442647808
C	0.898322196623	0.094775585342	0.483287137874
C	1.622381687227	0.242947992348	1.775364406210
C	-0.773937293875	1.980854959372	0.382584903282
C	2.880094400806	1.122512311027	1.654972861587
O	-0.290574374816	2.583803820269	1.329067986061
O	-1.914851488893	2.459724742971	-0.147086988068

C	-2.737126947124	1.760889504594	-1.124003212820
C	-4.067202159458	2.485343190168	-1.167659700212
H	0.631883591476	-1.543404490218	-2.235084714638
H	0.930290456900	0.691091901363	2.501182891329
H	1.896029869636	-0.762225006921	2.133442189906
H	2.604800603657	2.140763103409	1.341471976464
H	3.391740039363	1.184692884141	2.627814213378
H	3.588524268870	0.708786121409	0.920065034451
H	-2.228522597197	1.777015298028	-2.096984307790
H	-2.856131390990	0.711879807610	-0.816931603217
H	-4.565564220244	2.457096716506	-0.186144818119
H	-3.932081661059	3.537966538435	-1.461702815529
H	-4.725707210517	2.002072690287	-1.906367753044

SCF Done: E(RB3LYP) = -591.935851624

Zero-point correction= 0.184836
Thermal correction to Energy= 0.197024
Thermal correction to Enthalpy= 0.197968
Thermal correction to Gibbs Free Energy= 0.145030
Sum of electronic and zero-point Energies= -591.751016
Sum of electronic and thermal Energies= -591.738828
Sum of electronic and thermal Enthalpies= -591.737884
Sum of electronic and thermal Free Energies= -591.790821

1	C	Isotropic =	63.8858	Anisotropy =	83.4883
2	N	Isotropic =	-5.8415	Anisotropy =	351.2404
3	C	Isotropic =	47.4278	Anisotropy =	82.4045
4	O	Isotropic =	8.2621	Anisotropy =	279.3949
5	C	Isotropic =	24.3730	Anisotropy =	129.8942
6	C	Isotropic =	167.5439	Anisotropy =	15.8641
7	C	Isotropic =	32.3944	Anisotropy =	81.6130
8	C	Isotropic =	176.4309	Anisotropy =	22.9298
9	O	Isotropic =	-53.3247	Anisotropy =	519.8495
10	O	Isotropic =	125.7129	Anisotropy =	149.3508
11	C	Isotropic =	121.7338	Anisotropy =	57.5401
12	C	Isotropic =	175.1249	Anisotropy =	22.9008
13	H	Isotropic =	23.8908	Anisotropy =	4.1758
14	H	Isotropic =	28.1108	Anisotropy =	6.0220
15	H	Isotropic =	28.6672	Anisotropy =	7.9600
16	H	Isotropic =	30.0447	Anisotropy =	6.8629
17	H	Isotropic =	30.0846	Anisotropy =	10.2079
18	H	Isotropic =	30.2848	Anisotropy =	8.0980
19	H	Isotropic =	26.2986	Anisotropy =	5.0982
20	H	Isotropic =	26.9190	Anisotropy =	4.6583
21	H	Isotropic =	30.0115	Anisotropy =	7.6338
22	H	Isotropic =	29.8957	Anisotropy =	7.6403
23	H	Isotropic =	30.1133	Anisotropy =	9.1289

Comformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.063779073607	0.299649029243	0.673524526241

N	0.602674964501	-0.354833837402	1.714224944858
C	1.411276278629	-1.162545742867	1.112961921558
O	1.346786443457	-1.113572574063	-0.247951203503
C	0.394455702094	-0.173142187309	-0.533863007061
C	0.128648332602	0.104998969742	-1.973104990513
C	-1.084498947828	1.323240317050	0.972836034528
C	1.152528752173	1.072643095982	-2.593943588637
O	-1.455607666626	1.606518344741	2.095789509148
O	-1.554526245773	1.905429339409	-0.152303797755
C	-2.584721331627	2.918910851398	0.011534159560
C	-1.980639934652	4.290985685023	0.255706137812
H	2.120742354663	-1.864792085054	1.542914161453
H	0.146357572036	-0.854570143488	-2.514937131774
H	-0.882524208504	0.522494291556	-2.058876831233
H	0.932476470417	1.221440986452	-3.662265630054
H	1.115964076179	2.052891123394	-2.093562563671
H	2.177115145596	0.678319153661	-2.506211519738
H	-3.142266985917	2.887581724441	-0.934068262393
H	-3.246312781559	2.617784155770	0.835452332889
H	-2.784527275944	5.043830576764	0.294190800110
H	-1.437155603841	4.318929686243	1.212061073096
H	-1.288696036467	4.567229239315	-0.555307074920

SCF Done: E(RB3LYP) = -591.944748484

Zero-point correction= 0.185189
Thermal correction to Energy= 0.197301
Thermal correction to Enthalpy= 0.198245
Thermal correction to Gibbs Free Energy= 0.145266
Sum of electronic and zero-point Energies= -591.759559
Sum of electronic and thermal Energies= -591.747447
Sum of electronic and thermal Enthalpies= -591.746503
Sum of electronic and thermal Free Energies= -591.799483

1	C	Isotropic =	63.6147	Anisotropy =	79.5171
2	N	Isotropic =	-8.8966	Anisotropy =	349.9898
3	C	Isotropic =	46.0160	Anisotropy =	85.6079
4	O	Isotropic =	8.1518	Anisotropy =	259.9743
5	C	Isotropic =	28.5170	Anisotropy =	125.3805
6	C	Isotropic =	168.1428	Anisotropy =	15.2173
7	C	Isotropic =	32.7005	Anisotropy =	77.7387
8	C	Isotropic =	175.6305	Anisotropy =	23.7997
9	O	Isotropic =	-39.1379	Anisotropy =	551.2395
10	O	Isotropic =	132.3363	Anisotropy =	137.4289
11	C	Isotropic =	130.2415	Anisotropy =	64.1409
12	C	Isotropic =	175.8096	Anisotropy =	23.4045
13	H	Isotropic =	23.8947	Anisotropy =	4.3882
14	H	Isotropic =	28.6780	Anisotropy =	8.0755
15	H	Isotropic =	27.9698	Anisotropy =	7.4165
16	H	Isotropic =	30.0252	Anisotropy =	10.0044
17	H	Isotropic =	30.2020	Anisotropy =	6.8602
18	H	Isotropic =	30.1481	Anisotropy =	8.1636
19	H	Isotropic =	27.4584	Anisotropy =	7.1661
20	H	Isotropic =	26.4305	Anisotropy =	5.8187
21	H	Isotropic =	30.2436	Anisotropy =	10.0520
22	H	Isotropic =	29.8464	Anisotropy =	6.2949

23 H Isotropic = 30.0579 Anisotropy = 7.1540

Comformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.639688592452	0.146928551584	-0.244393731433
N	-0.862982139910	-0.959600899870	-1.069793423922
C	-0.310454108047	-1.941344419687	-0.438334160561
O	0.265551761603	-1.594328931911	0.747656104506
C	0.052063788004	-0.248802973466	0.876320278682
C	0.603793448148	0.412272169572	2.092100698971
C	-1.129033358397	1.482116400166	-0.640373430228
C	2.086586574752	0.798189879854	1.942276673844
O	-1.794683789684	1.696828288256	-1.635275706079
O	-0.746379611070	2.435129110517	0.238048561988
C	-1.184511729414	3.795078369597	-0.033861661002
C	-0.228976117718	4.510693383836	-0.973025172273
H	-0.249007977430	-2.988557325987	-0.722783829480
H	0.002911256633	1.307768980242	2.296406851887
H	0.481328822900	-0.279103794555	2.941324167051
H	2.219399766296	1.522495182048	1.123667737319
H	2.453618949921	1.257242174995	2.873134162211
H	2.708359116765	-0.084947240011	1.726628981848
H	-2.202937973064	3.761128811730	-0.445053463732
H	-1.206938010973	4.270285730474	0.955893750025
H	0.796132962462	4.507748443473	-0.570553723397
H	-0.222799501794	4.037130418603	-1.966211153034
H	-0.549043537531	5.558399690544	-1.092908513191

SCF Done: E(RB3LYP) = -591.944738922

Zero-point correction= 0.185198
Thermal correction to Energy= 0.197299
Thermal correction to Enthalpy= 0.198243
Thermal correction to Gibbs Free Energy= 0.145454
Sum of electronic and zero-point Energies= -591.759541
Sum of electronic and thermal Energies= -591.747440
Sum of electronic and thermal Enthalpies= -591.746496
Sum of electronic and thermal Free Energies= -591.799285

1 C Isotropic = 63.5167 Anisotropy = 79.6669
2 N Isotropic = -8.9771 Anisotropy = 349.9288
3 C Isotropic = 46.0915 Anisotropy = 85.4916
4 O Isotropic = 7.8066 Anisotropy = 258.6267
5 C Isotropic = 28.3477 Anisotropy = 125.5832
6 C Isotropic = 167.9995 Anisotropy = 15.4000
7 C Isotropic = 32.7033 Anisotropy = 77.8010
8 C Isotropic = 175.5529 Anisotropy = 23.7704
9 O Isotropic = -38.9815 Anisotropy = 551.2498
10 O Isotropic = 132.1488 Anisotropy = 137.2467
11 C Isotropic = 130.1403 Anisotropy = 64.1561
12 C Isotropic = 175.8883 Anisotropy = 23.2681
13 H Isotropic = 23.8994 Anisotropy = 4.4032

14	H	Isotropic =	27.9957	Anisotropy =	7.1284
15	H	Isotropic =	28.6743	Anisotropy =	8.0818
16	H	Isotropic =	30.1809	Anisotropy =	6.8481
17	H	Isotropic =	30.0274	Anisotropy =	10.0104
18	H	Isotropic =	30.1668	Anisotropy =	8.1567
19	H	Isotropic =	26.4402	Anisotropy =	5.8519
20	H	Isotropic =	27.4487	Anisotropy =	7.1470
21	H	Isotropic =	30.0624	Anisotropy =	7.1583
22	H	Isotropic =	29.8355	Anisotropy =	6.2817
23	H	Isotropic =	30.2462	Anisotropy =	10.0500

Comformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.463449633287	0.536252701307	0.058107296397
N	1.745785430004	0.001826863331	-0.100501427602
C	1.684196460793	-1.146680395717	0.486868017201
O	0.468938779822	-1.434418336748	1.033690596475
C	-0.319353105734	-0.349566250217	0.760805701342
C	-1.732118281201	-0.402542937373	1.230694174129
C	0.137444377330	1.863901437159	-0.498243754248
C	-2.658979448311	-1.151504288953	0.255847124428
O	0.938819479503	2.578374686952	-1.069390223699
O	-1.161815052841	2.181710723398	-0.304266422561
C	-1.605360216980	3.474013411092	-0.802275171797
C	-1.361678910510	4.575954105614	0.214394918467
H	2.461577764287	-1.897429811734	0.602721462695
H	-1.745477056918	-0.898498828193	2.214575875185
H	-2.085548947645	0.627592510646	1.366339783259
H	-3.681868957909	-1.189915257347	0.661012430259
H	-2.692416006541	-0.641511511468	-0.719484149390
H	-2.314959591013	-2.185150566597	0.093693472113
H	-1.090389437183	3.680069520847	-1.750711631529
H	-2.677548981505	3.332310422831	-0.992722149975
H	-1.778080167052	5.523228571328	-0.164747292392
H	-1.851285628625	4.343895501785	1.173183108787
H	-0.285072135060	4.720157728058	0.390768262460

SCF Done: E(RB3LYP) = -591.944788019

Zero-point correction= 0.185116
Thermal correction to Energy= 0.197296
Thermal correction to Enthalpy= 0.198241
Thermal correction to Gibbs Free Energy= 0.143682
Sum of electronic and zero-point Energies= -591.759672
Sum of electronic and thermal Energies= -591.747492
Sum of electronic and thermal Enthalpies= -591.746547
Sum of electronic and thermal Free Energies= -591.801106

1	C	Isotropic =	63.6529	Anisotropy =	79.7709
2	N	Isotropic =	-8.9089	Anisotropy =	349.8063
3	C	Isotropic =	46.0831	Anisotropy =	85.5797
4	O	Isotropic =	7.6467	Anisotropy =	258.4095

5 C Isotropic = 28.3425 Anisotropy = 125.6969
6 C Isotropic = 167.9835 Anisotropy = 15.2453
7 C Isotropic = 32.7605 Anisotropy = 77.1352
8 C Isotropic = 175.4754 Anisotropy = 24.1582
9 O Isotropic = -38.6316 Anisotropy = 551.6654
10 O Isotropic = 131.8866 Anisotropy = 153.2275
11 C Isotropic = 130.1176 Anisotropy = 64.1867
12 C Isotropic = 175.6093 Anisotropy = 23.7259
13 H Isotropic = 23.9004 Anisotropy = 4.4066
14 H Isotropic = 28.6670 Anisotropy = 7.9117
15 H Isotropic = 27.9530 Anisotropy = 7.8970
16 H Isotropic = 30.0342 Anisotropy = 10.0206
17 H Isotropic = 30.2323 Anisotropy = 6.6189
18 H Isotropic = 30.1765 Anisotropy = 8.2385
19 H Isotropic = 26.3988 Anisotropy = 5.6561
20 H Isotropic = 27.4310 Anisotropy = 6.8545
21 H Isotropic = 30.2462 Anisotropy = 10.0478
22 H Isotropic = 30.0748 Anisotropy = 7.2849
23 H Isotropic = 29.8729 Anisotropy = 6.3430

Comformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.977628629110	0.956112777298	0.666559138107
N	-2.101365411256	1.058351697244	1.492415818572
C	-1.842424184329	0.264896722983	2.477885302751
O	-0.635971727987	-0.364084888584	2.391693793207
C	-0.075193100491	0.081941409715	1.225862567910
C	1.259980038538	-0.469290407955	0.860889349345
C	-0.904167353925	1.727417104941	-0.589872923953
C	1.168750438935	-1.819491841935	0.126797659191
O	-1.755822752062	2.513586469487	-0.958012005922
O	0.219935316594	1.443721724929	-1.284632815117
C	0.411453404908	2.146131159295	-2.543541608283
C	1.081857357341	3.493033363292	-2.334462453603
H	-2.448460660583	0.040388720670	3.351778266419
H	1.772050204676	0.266692584311	0.227879744351
H	1.845385616931	-0.585962455680	1.787049417205
H	0.648277454173	-2.571924585574	0.740007541342
H	0.622702536088	-1.709954792311	-0.823045004371
H	2.178388939675	-2.197452523258	-0.096253359431
H	1.044227767029	1.468916325168	-3.132543945750
H	-0.564522547114	2.254489362324	-3.036506561318
H	2.043058317980	3.378741204639	-1.809210160192
H	1.277608712919	3.960655079017	-3.312985785604
H	0.437230261072	4.169545789984	-1.753341974857

SCF Done: E(RB3LYP) = -591.944779316

Zero-point correction= 0.185124
Thermal correction to Energy= 0.197267
Thermal correction to Enthalpy= 0.198211
Thermal correction to Gibbs Free Energy= 0.144997

Sum of electronic and zero-point Energies= -591.759656
Sum of electronic and thermal Energies= -591.747512
Sum of electronic and thermal Enthalpies= -591.746568
Sum of electronic and thermal Free Energies= -591.799782

1	C	Isotropic =	63.5567	Anisotropy =	79.6162
2	N	Isotropic =	-8.8331	Anisotropy =	350.3389
3	C	Isotropic =	46.0491	Anisotropy =	85.1321
4	O	Isotropic =	7.7702	Anisotropy =	258.0299
5	C	Isotropic =	28.2857	Anisotropy =	125.6966
6	C	Isotropic =	167.9582	Anisotropy =	15.2963
7	C	Isotropic =	32.8247	Anisotropy =	77.1994
8	C	Isotropic =	175.4482	Anisotropy =	24.1232
9	O	Isotropic =	-38.6680	Anisotropy =	551.6447
10	O	Isotropic =	131.5937	Anisotropy =	152.6902
11	C	Isotropic =	130.0850	Anisotropy =	64.2465
12	C	Isotropic =	175.6389	Anisotropy =	23.7057
13	H	Isotropic =	23.9056	Anisotropy =	4.4032
14	H	Isotropic =	27.9603	Anisotropy =	7.8024
15	H	Isotropic =	28.6666	Anisotropy =	7.9212
16	H	Isotropic =	30.1825	Anisotropy =	8.2375
17	H	Isotropic =	30.2305	Anisotropy =	6.5941
18	H	Isotropic =	30.0345	Anisotropy =	10.0239
19	H	Isotropic =	27.4301	Anisotropy =	6.8382
20	H	Isotropic =	26.4081	Anisotropy =	5.6750
21	H	Isotropic =	30.0724	Anisotropy =	7.2903
22	H	Isotropic =	30.2426	Anisotropy =	10.0476
23	H	Isotropic =	29.8615	Anisotropy =	6.3429

Comformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.413647715178	0.707082160765	0.044510922937
N	-0.325791482792	-0.019469514561	-1.148059107238
C	0.052668242205	-1.198837440213	-0.779158138273
O	0.234528231355	-1.331890943001	0.563711874395
C	-0.068608087374	-0.111109668329	1.096407240719
C	0.013400443923	0.037689474231	2.575029698881
C	-0.864863357085	2.108640229155	0.198178891385
C	-1.278556438994	-0.401047646639	3.287951686359
O	-1.218920278653	2.527984886917	1.289687298170
O	-0.913274519015	2.959881485479	-0.843015317463
C	-0.311789650213	2.737936277600	-2.150793104452
C	-1.365702275778	2.346262882796	-3.168155807707
H	0.240371225346	-2.077340016207	-1.390810092747
H	0.865517759686	-0.560742525926	2.935184004339
H	0.215363496694	1.094056186308	2.797331451547
H	-1.163056799486	-0.295994614102	4.377723437940
H	-2.124414980756	0.225223739490	2.966199955749
H	-1.518765899087	-1.453173388125	3.067877114591
H	0.135901699776	3.711257725430	-2.400180912492
H	0.485591743074	1.989129604848	-2.079572060088
H	-2.181004175543	3.086388853425	-3.192128809772

H	-0.909826940877	2.304336928493	-4.170916616841
H	-1.781050241228	1.355355322165	-2.934363609938

SCF Done: E(RB3LYP) = -591.935188287

Zero-point correction= 0.185073
Thermal correction to Energy= 0.197095
Thermal correction to Enthalpy= 0.198040
Thermal correction to Gibbs Free Energy= 0.145721
Sum of electronic and zero-point Energies= -591.750115
Sum of electronic and thermal Energies= -591.738093
Sum of electronic and thermal Enthalpies= -591.737149
Sum of electronic and thermal Free Energies= -591.789467

1	C	Isotropic =	64.7292	Anisotropy =	83.3769
2	N	Isotropic =	-4.3985	Anisotropy =	344.6336
3	C	Isotropic =	47.0418	Anisotropy =	83.3103
4	O	Isotropic =	7.4004	Anisotropy =	282.8331
5	C	Isotropic =	24.6392	Anisotropy =	128.5460
6	C	Isotropic =	167.7955	Anisotropy =	15.6100
7	C	Isotropic =	31.9659	Anisotropy =	80.8472
8	C	Isotropic =	176.2867	Anisotropy =	23.1789
9	O	Isotropic =	-55.2493	Anisotropy =	521.6608
10	O	Isotropic =	123.9676	Anisotropy =	149.6427
11	C	Isotropic =	123.7101	Anisotropy =	72.5938
12	C	Isotropic =	173.8519	Anisotropy =	25.4374
13	H	Isotropic =	23.8708	Anisotropy =	3.9835
14	H	Isotropic =	28.6827	Anisotropy =	8.0762
15	H	Isotropic =	28.1218	Anisotropy =	6.0099
16	H	Isotropic =	30.0840	Anisotropy =	10.2343
17	H	Isotropic =	30.0954	Anisotropy =	6.9336
18	H	Isotropic =	30.2663	Anisotropy =	8.0087
19	H	Isotropic =	27.1555	Anisotropy =	7.1076
20	H	Isotropic =	26.1831	Anisotropy =	3.4386
21	H	Isotropic =	29.8654	Anisotropy =	7.8859
22	H	Isotropic =	30.1991	Anisotropy =	9.6646
23	H	Isotropic =	29.3610	Anisotropy =	5.7076

Comformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.179429341147	0.715956358298	0.092255295012
N	-0.555107947115	-0.620714522610	0.264754227124
C	0.154066176258	-1.027324772213	1.265832956848
O	0.975275389065	-0.076361805440	1.790755577338
C	0.767393212285	1.043225012678	1.036009371838
C	1.563325857416	2.257089487485	1.364803625721
C	-0.650054749379	1.638363319539	-0.965520069820
C	2.939214189532	2.269054327604	0.674690830331
O	-0.012738352705	2.644266172887	-1.238205770382
O	-1.774379822674	1.401695852854	-1.665910786494
C	-2.798410875778	0.425053681112	-1.321449138731
C	-2.707997227126	-0.788556293213	-2.225911322879

H	0.177275869874	-2.009211936818	1.731074216780
H	0.985744238351	3.136069045373	1.048203953363
H	1.688228055213	2.301659486798	2.458551001552
H	3.536023324028	1.387797825480	0.958124801280
H	2.817386881623	2.272061265267	-0.419044753020
H	3.499838427403	3.171066192737	0.964685467746
H	-2.721916262543	0.151442792895	-0.262849178937
H	-3.742075750116	0.967459764667	-1.481008117621
H	-1.780945104273	-1.347589940763	-2.033289367159
H	-3.563531047821	-1.455716603075	-2.031044335423
H	-2.739305140372	-0.490284711543	-3.285688484468

SCF Done: E(RB3LYP) = -591.935213050

Zero-point correction= 0.185159
Thermal correction to Energy= 0.197156
Thermal correction to Enthalpy= 0.198100
Thermal correction to Gibbs Free Energy= 0.145916
Sum of electronic and zero-point Energies= -591.750054
Sum of electronic and thermal Energies= -591.738057
Sum of electronic and thermal Enthalpies= -591.737113
Sum of electronic and thermal Free Energies= -591.789297

1	C	Isotropic =	64.6651	Anisotropy =	83.4851
2	N	Isotropic =	-4.5270	Anisotropy =	344.3654
3	C	Isotropic =	47.0377	Anisotropy =	83.3504
4	O	Isotropic =	7.3213	Anisotropy =	281.6314
5	C	Isotropic =	24.7830	Anisotropy =	128.4689
6	C	Isotropic =	167.7567	Anisotropy =	15.5510
7	C	Isotropic =	31.8224	Anisotropy =	80.5833
8	C	Isotropic =	176.2326	Anisotropy =	23.2294
9	O	Isotropic =	-56.2425	Anisotropy =	522.8439
10	O	Isotropic =	124.2333	Anisotropy =	149.4438
11	C	Isotropic =	123.8209	Anisotropy =	72.9452
12	C	Isotropic =	173.8742	Anisotropy =	25.3854
13	H	Isotropic =	23.8718	Anisotropy =	3.9924
14	H	Isotropic =	28.1526	Anisotropy =	5.9808
15	H	Isotropic =	28.6732	Anisotropy =	8.0667
16	H	Isotropic =	30.2727	Anisotropy =	8.0013
17	H	Isotropic =	30.0870	Anisotropy =	6.9340
18	H	Isotropic =	30.0795	Anisotropy =	10.2339
19	H	Isotropic =	26.2205	Anisotropy =	3.4427
20	H	Isotropic =	27.1557	Anisotropy =	7.1136
21	H	Isotropic =	29.3752	Anisotropy =	5.7349
22	H	Isotropic =	30.2022	Anisotropy =	9.6487
23	H	Isotropic =	29.8671	Anisotropy =	7.8867

Comformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.138214509400	0.861718470168	0.210756512067
N	0.864499656418	1.698357875458	0.713426937365
C	1.499380044098	0.967218659123	1.568614202984

O	1.014689931190	-0.299274461246	1.685986029590
C	-0.033287415073	-0.373825371758	0.814435897710
C	-0.774611903040	-1.663709409428	0.744111541354
C	-1.161414658954	1.191094482187	-0.807565639069
C	-2.008380823790	-1.695502634971	1.664409227802
O	-1.985083890868	0.351134448593	-1.140578552503
O	-1.243325960208	2.397161189105	-1.399101410021
C	-0.387107410299	3.549943197471	-1.151706359486
C	0.852910112133	3.518554062647	-2.025624199987
H	2.353181462869	1.227992993308	2.188348597005
H	-1.090780431619	-1.815885960464	-0.296510032114
H	-0.077572273940	-2.471024258120	1.017909287531
H	-2.728927873858	-0.918133242495	1.368665567062
H	-2.506640953057	-2.674616729026	1.591992231649
H	-1.726946979250	-1.530178931646	2.716364149316
H	-1.032669551249	4.398575772192	-1.418862257774
H	-0.133665855895	3.609207584050	-0.088157379805
H	1.404646918816	4.465710926823	-1.909095819078
H	1.523015645331	2.695722894720	-1.735373592316
H	0.582666719644	3.405838443307	-3.087364939282

SCF Done: E(RB3LYP) = -591.934606697

Zero-point correction= 0.185198
Thermal correction to Energy= 0.197195
Thermal correction to Enthalpy= 0.198139
Thermal correction to Gibbs Free Energy= 0.145800
Sum of electronic and zero-point Energies= -591.749409
Sum of electronic and thermal Energies= -591.737412
Sum of electronic and thermal Enthalpies= -591.736468
Sum of electronic and thermal Free Energies= -591.788806

1	C	Isotropic =	64.4815	Anisotropy =	83.3588
2	N	Isotropic =	-4.3064	Anisotropy =	345.2044
3	C	Isotropic =	47.1150	Anisotropy =	83.8463
4	O	Isotropic =	7.4109	Anisotropy =	280.5245
5	C	Isotropic =	23.6446	Anisotropy =	129.9455
6	C	Isotropic =	167.2560	Anisotropy =	17.1508
7	C	Isotropic =	33.3021	Anisotropy =	83.5237
8	C	Isotropic =	176.7485	Anisotropy =	22.2397
9	O	Isotropic =	-47.1095	Anisotropy =	517.0486
10	O	Isotropic =	121.6847	Anisotropy =	150.3895
11	C	Isotropic =	124.3862	Anisotropy =	72.2284
12	C	Isotropic =	174.0153	Anisotropy =	24.6785
13	H	Isotropic =	23.8683	Anisotropy =	4.0044
14	H	Isotropic =	27.9384	Anisotropy =	6.3124
15	H	Isotropic =	28.6697	Anisotropy =	7.8357
16	H	Isotropic =	30.1118	Anisotropy =	6.6074
17	H	Isotropic =	30.1245	Anisotropy =	10.2699
18	H	Isotropic =	30.3399	Anisotropy =	8.1050
19	H	Isotropic =	27.1416	Anisotropy =	7.0034
20	H	Isotropic =	25.4027	Anisotropy =	3.7487
21	H	Isotropic =	30.2191	Anisotropy =	9.7498
22	H	Isotropic =	29.7560	Anisotropy =	5.1082
23	H	Isotropic =	29.9417	Anisotropy =	7.9472

Comformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.502804939449	0.578639580445	0.300912345615
N	1.844291070140	0.195182728877	0.396902817001
C	1.811838048699	-0.899304302408	1.081550097573
O	0.561669877302	-1.288783824490	1.460727873220
C	-0.284128600210	-0.336088554988	0.960889373313
C	-1.740594649410	-0.525999928886	1.210664636275
C	0.129534827227	1.804175898022	-0.432535377565
C	-2.406277672681	-1.460644351483	0.184244709996
O	0.929888410612	2.561788846454	-0.946792601857
O	-1.210594003821	1.974358794467	-0.471443836607
C	-1.704646425857	3.153595251259	-1.164239824447
C	-1.734786748257	4.366451397891	-0.250234701116
H	2.636467434197	-1.536000790130	1.391293562593
H	-1.860901259990	-0.938906762599	2.225176603819
H	-2.223255524082	0.459367782640	1.187645833241
H	-2.332821160228	-1.039907095089	-0.830644287873
H	-1.929767284959	-2.453612625824	0.182006004280
H	-3.471808922467	-1.591906869839	0.427890461492
H	-1.075370322428	3.330930252267	-2.047360748954
H	-2.714500454240	2.868235788863	-1.487740789286
H	-0.718641159290	4.651738171858	0.061020216133
H	-2.182336371636	5.218603293059	-0.786904624668
H	-2.340234048068	4.169097319634	0.648292257825

SCF Done: E(RB3LYP) = -591.944783367

Zero-point correction= 0.185175
Thermal correction to Energy= 0.197295
Thermal correction to Enthalpy= 0.198239
Thermal correction to Gibbs Free Energy= 0.145206
Sum of electronic and zero-point Energies= -591.759609
Sum of electronic and thermal Energies= -591.747489
Sum of electronic and thermal Enthalpies= -591.746545
Sum of electronic and thermal Free Energies= -591.799578

1	C	Isotropic = 63.6565	Anisotropy =	79.6266
2	N	Isotropic = -8.8369	Anisotropy =	349.7539
3	C	Isotropic = 46.0721	Anisotropy =	85.5899
4	O	Isotropic = 7.6705	Anisotropy =	258.1487
5	C	Isotropic = 28.2987	Anisotropy =	125.7380
6	C	Isotropic = 167.9254	Anisotropy =	15.3353
7	C	Isotropic = 32.7848	Anisotropy =	77.2490
8	C	Isotropic = 175.4861	Anisotropy =	24.1570
9	O	Isotropic = -39.0078	Anisotropy =	552.0426
10	O	Isotropic = 131.8664	Anisotropy =	152.7756
11	C	Isotropic = 130.0190	Anisotropy =	64.2839
12	C	Isotropic = 175.6846	Anisotropy =	23.6779
13	H	Isotropic = 23.9016	Anisotropy =	4.4000
14	H	Isotropic = 28.6663	Anisotropy =	7.9067
15	H	Isotropic = 27.9565	Anisotropy =	7.8599

16	H	Isotropic =	30.2341	Anisotropy =	6.6147
17	H	Isotropic =	30.1801	Anisotropy =	8.2339
18	H	Isotropic =	30.0349	Anisotropy =	10.0232
19	H	Isotropic =	26.4202	Anisotropy =	5.6959
20	H	Isotropic =	27.4280	Anisotropy =	6.8329
21	H	Isotropic =	29.8472	Anisotropy =	6.3276
22	H	Isotropic =	30.2409	Anisotropy =	10.0500
23	H	Isotropic =	30.0745	Anisotropy =	7.3046

Comformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

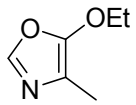
C	0.299034177960	0.514896040967	0.625542627263
N	1.073141540152	-0.066210265764	1.634616244732
C	1.900121201813	-0.828000675108	0.999342074245
O	1.754138722495	-0.809829454288	-0.355994322785
C	0.723879297600	0.057349707264	-0.599827529093
C	0.326088119854	0.253796986612	-2.022038290566
C	-0.780473917037	1.461062751899	0.969200335006
C	-0.636202332566	-0.835670815439	-2.529408475644
O	-1.037103502245	1.818694077093	2.102862989243
O	-1.453457172845	1.871924823093	-0.128397155817
C	-2.538989330915	2.816871370422	0.079818553869
C	-2.033914833499	4.249154296983	0.106386887418
H	2.684293809302	-1.466812463092	1.397221278984
H	-0.145101401512	1.240818958538	-2.111672969816
H	1.242001234820	0.258014171911	-2.634677473734
H	-0.876798373618	-0.663368380180	-3.589764625082
H	-0.187745547392	-1.837420173074	-2.437562140937
H	-1.575761687822	-0.823879940775	-1.955279244616
H	-3.210282934566	2.642719923289	-0.771608844402
H	-3.057603034168	2.555332408645	1.012515099349
H	-2.890091975037	4.938185863693	0.187860046708
H	-1.372610270488	4.419323715375	0.969302709855
H	-1.483931790285	4.490997071937	-0.816587774179

SCF Done: E(RB3LYP) = -591.944817432

Zero-point correction= 0.185221
Thermal correction to Energy= 0.197321
Thermal correction to Enthalpy= 0.198266
Thermal correction to Gibbs Free Energy= 0.145374
Sum of electronic and zero-point Energies= -591.759596
Sum of electronic and thermal Energies= -591.747496
Sum of electronic and thermal Enthalpies= -591.746552
Sum of electronic and thermal Free Energies= -591.799444

1	C	Isotropic =	63.6378	Anisotropy =	79.6850
2	N	Isotropic =	-8.8667	Anisotropy =	349.9313
3	C	Isotropic =	45.9996	Anisotropy =	85.6241
4	O	Isotropic =	7.8548	Anisotropy =	258.4001
5	C	Isotropic =	28.3821	Anisotropy =	125.6979
6	C	Isotropic =	168.0366	Anisotropy =	15.2168

7 C Isotropic = 32.8039 Anisotropy = 77.2083
8 C Isotropic = 175.4330 Anisotropy = 24.1940
9 O Isotropic = -38.9226 Anisotropy = 551.8899
10 O Isotropic = 132.1401 Anisotropy = 153.0019
11 C Isotropic = 130.1046 Anisotropy = 64.1774
12 C Isotropic = 175.7445 Anisotropy = 23.6089
13 H Isotropic = 23.9006 Anisotropy = 4.4039
14 H Isotropic = 27.9475 Anisotropy = 7.9569
15 H Isotropic = 28.6664 Anisotropy = 7.9064
16 H Isotropic = 30.0309 Anisotropy = 10.0195
17 H Isotropic = 30.1718 Anisotropy = 8.2301
18 H Isotropic = 30.2422 Anisotropy = 6.6302
19 H Isotropic = 27.4287 Anisotropy = 6.8507
20 H Isotropic = 26.4069 Anisotropy = 5.6801
21 H Isotropic = 30.2485 Anisotropy = 10.0489
22 H Isotropic = 29.8660 Anisotropy = 6.3398
23 H Isotropic = 30.0835 Anisotropy = 7.2991



1b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.267568426465	-0.376740238362	0.052929633960
C	1.585189128329	-1.406601392036	-0.339606396064
O	0.268053003260	-1.158728753689	-0.567626644072
C	0.126917483049	0.180938294235	-0.269338920515
C	1.339510981681	0.671279783512	0.115821927338
O	-1.066163369758	0.749566384126	-0.461498130771
C	1.703688886985	2.058884272281	0.528402541265
C	-2.160883442902	0.213130049873	0.339665297266
C	-3.402934885696	1.010018595895	0.006530282621
H	1.925441754968	-2.426671171605	-0.500306143121
H	2.452556190530	2.495405289082	-0.153415704009
H	0.815330750926	2.706451259803	0.523398057923
H	2.137778051811	2.072152465668	1.541671739090
H	-2.287248096029	-0.854407468768	0.097624424186
H	-1.887078542168	0.303095899965	1.404638008231
H	-4.254703251755	0.631072090624	0.592233220838
H	-3.262494106822	2.075453974812	0.246565976674
H	-3.649758962874	0.919910664585	-1.062859170840

SCF Done: E(RB3LYP) = -439.260792603

Zero-point correction= 0.145846
Thermal correction to Energy= 0.155074

Thermal correction to Enthalpy= 0.156019
Thermal correction to Gibbs Free Energy= 0.110704
Sum of electronic and zero-point Energies= -439.114946
Sum of electronic and thermal Energies= -439.105718
Sum of electronic and thermal Enthalpies= -439.104774
Sum of electronic and thermal Free Energies= -439.150088

1	N	Isotropic =	-13.6614	Anisotropy =	350.4419
2	C	Isotropic =	52.6678	Anisotropy =	83.6854
3	O	Isotropic =	29.8343	Anisotropy =	254.1160
4	C	Isotropic =	38.2739	Anisotropy =	62.7086
5	C	Isotropic =	76.4804	Anisotropy =	89.8923
6	O	Isotropic =	248.4458	Anisotropy =	69.1816
7	C	Isotropic =	180.8912	Anisotropy =	18.0768
8	C	Isotropic =	119.7348	Anisotropy =	79.5885
9	C	Isotropic =	175.7193	Anisotropy =	22.2525
10	H	Isotropic =	24.1780	Anisotropy =	4.7245
11	H	Isotropic =	29.3593	Anisotropy =	9.5312
12	H	Isotropic =	29.2765	Anisotropy =	6.4841
13	H	Isotropic =	29.3430	Anisotropy =	9.2338
14	H	Isotropic =	27.0098	Anisotropy =	5.6639
15	H	Isotropic =	27.6494	Anisotropy =	5.6045
16	H	Isotropic =	30.1292	Anisotropy =	9.3752
17	H	Isotropic =	29.8893	Anisotropy =	7.4981
18	H	Isotropic =	29.8629	Anisotropy =	7.5719

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.042960093488	1.606661180359	1.815351917972
C	-1.140783645680	1.080937910162	1.861618611978
O	-1.299715592355	-0.022746056607	1.082688454583
C	-0.069523533875	-0.182815720070	0.479402416716
C	0.760627491078	0.807723700675	0.915053977950
O	0.116658510446	-1.252077993759	-0.300355349104
C	2.188558891277	1.060586810124	0.560962115135
C	-0.758417718808	-1.365004815248	-1.464951596067
C	-0.362835183258	-0.403057372458	-2.569769754612
H	-2.009304577280	1.408147281636	2.427917615114
H	2.320300233206	2.067146521262	0.130904553491
H	2.838550501222	0.997609230327	1.449674883827
H	2.538583677017	0.321701033569	-0.173916896084
H	-0.643334620155	-2.410781405081	-1.780075629167
H	-1.799957404893	-1.211132526947	-1.141585194579
H	0.676361583226	-0.577003000892	-2.890087588017
H	-1.023355949283	-0.551131427017	-3.439315173456
H	-0.460372755373	0.644796649963	-2.244127365681

SCF Done: E(RB3LYP) = -439.259984887

Zero-point correction= 0.145957
Thermal correction to Energy= 0.155100
Thermal correction to Enthalpy= 0.156044

Thermal correction to Gibbs Free Energy= 0.110830
Sum of electronic and zero-point Energies= -439.114027
Sum of electronic and thermal Energies= -439.104885
Sum of electronic and thermal Enthalpies= -439.103941
Sum of electronic and thermal Free Energies= -439.149155

1	N	Isotropic =	-13.7881	Anisotropy =	349.2855
2	C	Isotropic =	52.6308	Anisotropy =	83.7829
3	O	Isotropic =	32.2898	Anisotropy =	250.4579
4	C	Isotropic =	40.1987	Anisotropy =	59.5296
5	C	Isotropic =	74.4957	Anisotropy =	93.1626
6	O	Isotropic =	244.4129	Anisotropy =	103.1403
7	C	Isotropic =	180.9420	Anisotropy =	17.8909
8	C	Isotropic =	121.6647	Anisotropy =	80.8237
9	C	Isotropic =	176.7453	Anisotropy =	20.4584
10	H	Isotropic =	24.1560	Anisotropy =	4.7609
11	H	Isotropic =	29.3733	Anisotropy =	8.9814
12	H	Isotropic =	29.3829	Anisotropy =	9.7170
13	H	Isotropic =	29.3186	Anisotropy =	6.2172
14	H	Isotropic =	27.1857	Anisotropy =	7.0535
15	H	Isotropic =	27.0661	Anisotropy =	6.3648
16	H	Isotropic =	30.0903	Anisotropy =	7.6032
17	H	Isotropic =	30.3933	Anisotropy =	9.9771
18	H	Isotropic =	30.0987	Anisotropy =	4.6694

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.160100001608	-0.025803560116	-0.263006258465
C	1.608965808956	-1.065775764288	-0.805131118846
O	0.312032828862	-1.268881600690	-0.446717808862
C	0.035614692436	-0.220832319543	0.405515953768
C	1.154488966935	0.549909988762	0.525408736897
O	-1.160444401940	-0.186486703109	1.000747716596
C	1.362860431292	1.785891905372	1.336179087277
C	-2.325130551391	-0.174311418456	0.119745789283
C	-2.510516299051	1.167069746228	-0.565338705158
H	2.039761921591	-1.779069958606	-1.503435719413
H	1.673155602954	2.631857244105	0.700897447664
H	0.435559496947	2.065524583452	1.856224844537
H	2.151395384690	1.639961439340	2.093348572547
H	-2.227375574038	-0.995091743333	-0.608106070325
H	-3.163373648877	-0.403594079284	0.791165502473
H	-2.615035103089	1.976345259167	0.174212599857
H	-1.661372963222	1.402172777792	-1.226666694403
H	-3.423266594664	1.140544203206	-1.182143875426

SCF Done: E(RB3LYP) = -439.259983944

Zero-point correction= 0.145924
Thermal correction to Energy= 0.155093
Thermal correction to Enthalpy= 0.156037
Thermal correction to Gibbs Free Energy= 0.110738

Sum of electronic and zero-point Energies= -439.114060
Sum of electronic and thermal Energies= -439.104891
Sum of electronic and thermal Enthalpies= -439.103947
Sum of electronic and thermal Free Energies= -439.149246

1	N	Isotropic =	-13.8658	Anisotropy =	349.1225
2	C	Isotropic =	52.8060	Anisotropy =	83.2785
3	O	Isotropic =	33.2187	Anisotropy =	251.6958
4	C	Isotropic =	40.1400	Anisotropy =	59.8953
5	C	Isotropic =	74.9285	Anisotropy =	92.2286
6	O	Isotropic =	243.4897	Anisotropy =	103.7715
7	C	Isotropic =	181.0002	Anisotropy =	17.9215
8	C	Isotropic =	122.1549	Anisotropy =	80.1427
9	C	Isotropic =	176.6695	Anisotropy =	20.5640
10	H	Isotropic =	24.1635	Anisotropy =	4.7702
11	H	Isotropic =	29.3761	Anisotropy =	9.0103
12	H	Isotropic =	29.3240	Anisotropy =	6.2636
13	H	Isotropic =	29.3880	Anisotropy =	9.7123
14	H	Isotropic =	27.0033	Anisotropy =	6.4068
15	H	Isotropic =	27.1903	Anisotropy =	7.0663
16	H	Isotropic =	30.1022	Anisotropy =	7.6358
17	H	Isotropic =	30.1235	Anisotropy =	4.6096
18	H	Isotropic =	30.3830	Anisotropy =	9.9533

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.718827395253	0.232290571831	1.675466486938
C	0.850151348107	1.166888179055	1.903954172440
O	-0.143050960766	1.253631209188	0.979220302793
C	0.148796522774	0.245124925119	0.084562659156
C	1.281353736641	-0.390988637822	0.499176553310
O	-0.623218163582	0.115421540409	-0.997447691282
C	1.999043042948	-1.537381793873	-0.132508489964
C	-2.031006344427	-0.169910375473	-0.743335078701
C	-2.713665774479	-0.325837059907	-2.084449679337
H	0.811702448845	1.872736914063	2.730037256203
H	3.024354124530	-1.255564746134	-0.424981034089
H	2.080291807604	-2.388795839140	0.563053513168
H	1.465125882950	-1.874517049700	-1.032396543145
H	-2.094914520892	-1.091026680407	-0.139406351200
H	-2.462229352170	0.661846264889	-0.163395200261
H	-3.783107744259	-0.539496786059	-1.933440538020
H	-2.624777714855	0.597619541772	-2.677673273715
H	-2.270645734222	-1.155680177811	-2.656757064294

SCF Done: E(RB3LYP) = -439.260798655

Zero-point correction= 0.145807
Thermal correction to Energy= 0.155063
Thermal correction to Enthalpy= 0.156008
Thermal correction to Gibbs Free Energy= 0.110460
Sum of electronic and zero-point Energies= -439.114992

Sum of electronic and thermal Energies= -439.105735
Sum of electronic and thermal Enthalpies= -439.104791
Sum of electronic and thermal Free Energies= -439.150339

1	N	Isotropic =	-13.7811	Anisotropy =	350.4051
2	C	Isotropic =	52.7576	Anisotropy =	83.2959
3	O	Isotropic =	29.9260	Anisotropy =	254.1987
4	C	Isotropic =	38.1828	Anisotropy =	62.8477
5	C	Isotropic =	76.6164	Anisotropy =	89.5477
6	O	Isotropic =	248.0323	Anisotropy =	69.0652
7	C	Isotropic =	180.9546	Anisotropy =	17.9621
8	C	Isotropic =	119.9190	Anisotropy =	79.2704
9	C	Isotropic =	175.7380	Anisotropy =	22.2209
10	H	Isotropic =	24.1806	Anisotropy =	4.7305
11	H	Isotropic =	29.3630	Anisotropy =	9.5299
12	H	Isotropic =	29.3454	Anisotropy =	9.2570
13	H	Isotropic =	29.2770	Anisotropy =	6.4851
14	H	Isotropic =	27.6528	Anisotropy =	5.6204
15	H	Isotropic =	26.9990	Anisotropy =	5.6651
16	H	Isotropic =	30.1300	Anisotropy =	9.3751
17	H	Isotropic =	29.8658	Anisotropy =	7.5734
18	H	Isotropic =	29.8929	Anisotropy =	7.5020

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.169765923153	-1.515112831179	-0.662697665560
C	0.267488916583	-1.000778382705	-1.439131887205
O	-0.400928748969	0.055623560841	-0.907715827358
C	0.152259206793	0.200491334879	0.350985146792
C	1.111268048969	-0.755893253751	0.512666528874
O	-0.256102664629	1.215511493974	1.115708701172
C	1.994868207563	-1.007076105830	1.689251062598
C	-1.624666414207	1.143684232245	1.626566406433
C	-2.624367207478	1.779588483984	0.677569050351
H	-0.019170368763	-1.306671252498	-2.442428151780
H	1.772184107518	-0.293973504039	2.495692442294
H	1.857101383579	-2.028456009121	2.080691561893
H	3.058636529847	-0.901860470904	1.418532065141
H	-1.865748003080	0.088160874094	1.833571498491
H	-1.584568992370	1.686772420907	2.581522860846
H	-2.684763298878	1.228795703945	-0.272790485121
H	-3.623216217227	1.778355115956	1.143712366382
H	-2.345830408405	2.823478589201	0.463084325755

SCF Done: E(RB3LYP) = -439.259736843

Zero-point correction= 0.145931
Thermal correction to Energy= 0.155080
Thermal correction to Enthalpy= 0.156024
Thermal correction to Gibbs Free Energy= 0.110663
Sum of electronic and zero-point Energies= -439.113806
Sum of electronic and thermal Energies= -439.104657

Sum of electronic and thermal Enthalpies= -439.103713
Sum of electronic and thermal Free Energies= -439.149074

1	N	Isotropic =	-13.6853	Anisotropy =	351.6593
2	C	Isotropic =	52.2139	Anisotropy =	85.0789
3	O	Isotropic =	24.3995	Anisotropy =	239.9793
4	C	Isotropic =	36.9666	Anisotropy =	63.9223
5	C	Isotropic =	75.4585	Anisotropy =	91.7987
6	O	Isotropic =	249.8875	Anisotropy =	88.2159
7	C	Isotropic =	180.7906	Anisotropy =	18.2690
8	C	Isotropic =	117.8009	Anisotropy =	85.7619
9	C	Isotropic =	174.0170	Anisotropy =	24.3614
10	H	Isotropic =	24.1861	Anisotropy =	4.7767
11	H	Isotropic =	29.2975	Anisotropy =	6.3917
12	H	Isotropic =	29.3534	Anisotropy =	9.2126
13	H	Isotropic =	29.3690	Anisotropy =	9.5570
14	H	Isotropic =	27.7431	Anisotropy =	5.6989
15	H	Isotropic =	27.0387	Anisotropy =	6.6377
16	H	Isotropic =	29.5453	Anisotropy =	6.2856
17	H	Isotropic =	30.2708	Anisotropy =	9.7848
18	H	Isotropic =	29.8355	Anisotropy =	7.2981

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.916413900252	0.078494724563	2.140186247450
C	0.061717141206	1.030053077237	1.927490840266
O	-0.455906585125	1.055315474140	0.671768517627
C	0.147239298721	-0.017048589591	0.041345203138
C	0.986081699297	-0.623057601562	0.929993134645
O	-0.109914003947	-0.225604169234	-1.251662221733
C	1.865894945131	-1.811911336858	0.727940285547
C	-1.467833111831	-0.649498085304	-1.591342934964
C	-2.380901885128	0.530390714305	-1.871627573951
H	-0.290196220131	1.793430037676	2.617203750005
H	1.616226247834	-2.617799054393	1.437588097322
H	1.754972413994	-2.202936162576	-0.293460704974
H	2.926439750724	-1.554600290367	0.886209937480
H	-1.340134179404	-1.272941583136	-2.487766470345
H	-1.850873336832	-1.283679854533	-0.775206772714
H	-3.364955278307	0.161233094930	-2.203795213734
H	-2.527272309655	1.148240761525	-0.973346724039
H	-1.962888486798	1.163018843180	-2.670577397027

SCF Done: E(RB3LYP) = -439.259721307

Zero-point correction= 0.145829
Thermal correction to Energy= 0.154108
Thermal correction to Enthalpy= 0.155052
Thermal correction to Gibbs Free Energy= 0.112565
Sum of electronic and zero-point Energies= -439.113892
Sum of electronic and thermal Energies= -439.105614
Sum of electronic and thermal Enthalpies= -439.104669

Sum of electronic and thermal Free Energies= -439.147156

1	N	Isotropic =	-13.6757	Anisotropy =	351.7465
2	C	Isotropic =	52.3401	Anisotropy =	84.9380
3	O	Isotropic =	24.8565	Anisotropy =	239.6410
4	C	Isotropic =	37.0843	Anisotropy =	63.8549
5	C	Isotropic =	75.6968	Anisotropy =	91.4246
6	O	Isotropic =	249.8047	Anisotropy =	88.2951
7	C	Isotropic =	180.8202	Anisotropy =	18.2553
8	C	Isotropic =	117.8299	Anisotropy =	85.6933
9	C	Isotropic =	173.9820	Anisotropy =	24.3984
10	H	Isotropic =	24.1883	Anisotropy =	4.7755
11	H	Isotropic =	29.3557	Anisotropy =	9.2214
12	H	Isotropic =	29.3008	Anisotropy =	6.4062
13	H	Isotropic =	29.3720	Anisotropy =	9.5553
14	H	Isotropic =	27.0390	Anisotropy =	6.6432
15	H	Isotropic =	27.7398	Anisotropy =	5.7117
16	H	Isotropic =	30.2603	Anisotropy =	9.7763
17	H	Isotropic =	29.5404	Anisotropy =	6.3159
18	H	Isotropic =	29.8310	Anisotropy =	7.3154

1b incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.099598929546	-1.669951538970	0.555530182068
C	-1.750213529226	-0.593905703333	1.042497001924
N	-1.155631539164	0.543536307444	0.822700860992
C	-0.009867143789	0.189765989194	0.128924193043
C	0.042961939302	-1.166855475934	-0.045146445375
O	0.910997224366	1.076993467650	-0.305939294364
C	0.997400751888	-2.100843882706	-0.690917729149
C	0.667050032365	2.465259067115	-0.002134359308
C	1.817469532553	3.262908625586	-0.581360327989
H	-2.688614383166	-0.772429680231	1.561255668893
H	0.527084589423	-2.668957813941	-1.511360082206
H	1.833918492567	-1.523920924387	-1.110047235599
H	1.409258504558	-2.830857504129	0.026421216920
H	-0.298958031861	2.770836793036	-0.438207258646
H	0.594748836004	2.593058988312	1.091189178843
H	1.878393075102	3.128519916699	-1.672868801804
H	1.671896416685	4.333912785957	-0.371497930952
H	2.775514161939	2.949580582639	-0.137358837291

SCF Done: E(RB3LYP) = -439.262931265

Zero-point correction= 0.145834
Thermal correction to Energy= 0.155147
Thermal correction to Enthalpy= 0.156091
Thermal correction to Gibbs Free Energy= 0.110047
Sum of electronic and zero-point Energies= -439.117097
Sum of electronic and thermal Energies= -439.107784

Sum of electronic and thermal Enthalpies= -439.106840
Sum of electronic and thermal Free Energies= -439.152884

1	O	Isotropic =	27.0818	Anisotropy =	257.7343
2	C	Isotropic =	49.1421	Anisotropy =	89.9516
3	N	Isotropic =	8.0492	Anisotropy =	314.5404
4	C	Isotropic =	43.6428	Anisotropy =	73.8608
5	C	Isotropic =	64.4383	Anisotropy =	75.4486
6	O	Isotropic =	245.5814	Anisotropy =	58.0670
7	C	Isotropic =	182.3472	Anisotropy =	17.2117
8	C	Isotropic =	126.8799	Anisotropy =	59.9169
9	C	Isotropic =	175.8012	Anisotropy =	22.2911
10	H	Isotropic =	24.0705	Anisotropy =	4.6162
11	H	Isotropic =	29.1446	Anisotropy =	9.7998
12	H	Isotropic =	29.0434	Anisotropy =	6.6830
13	H	Isotropic =	29.1419	Anisotropy =	9.8070
14	H	Isotropic =	27.2433	Anisotropy =	6.3702
15	H	Isotropic =	27.2728	Anisotropy =	6.3846
16	H	Isotropic =	29.9504	Anisotropy =	7.5860
17	H	Isotropic =	30.0994	Anisotropy =	9.3170
18	H	Isotropic =	29.9515	Anisotropy =	7.5832

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.142177956178	-1.528348003603	0.032929413504
C	-1.837457403689	-0.458555720018	0.470461917891
N	-1.117022002615	0.602313383672	0.691694804954
C	0.170680649233	0.202366159685	0.368973600840
C	0.174109078639	-1.101227494827	-0.044831238356
O	1.262393833276	0.990390280009	0.501909576821
C	1.220578182252	-2.048793084641	-0.499745533451
C	1.038433743105	2.416408728582	0.572345275232
C	0.719584153022	3.021650542419	-0.785623907103
H	-2.910952693776	-0.579103731633	0.592264182161
H	2.184744519433	-1.522523164670	-0.540630965777
H	1.327674928089	-2.907946811484	0.184260722534
H	1.002280058344	-2.447880375006	-1.504465809772
H	0.237885164267	2.623579037550	1.298744635339
H	1.983585365900	2.813600743236	0.968552562755
H	0.636300599923	4.116859329270	-0.692972294895
H	1.515499327858	2.795746963565	-1.513038294495
H	-0.235679547084	2.639983217893	-1.178478648181

SCF Done: E(RB3LYP) = -439.262255436

Zero-point correction= 0.146081
Thermal correction to Energy= 0.155249
Thermal correction to Enthalpy= 0.156193
Thermal correction to Gibbs Free Energy= 0.110351
Sum of electronic and zero-point Energies= -439.116174
Sum of electronic and thermal Energies= -439.107007
Sum of electronic and thermal Enthalpies= -439.106062

Sum of electronic and thermal Free Energies= -439.151904

1	O	Isotropic =	27.5274	Anisotropy =	258.9139
2	C	Isotropic =	48.8400	Anisotropy =	90.0449
3	N	Isotropic =	9.4401	Anisotropy =	324.6323
4	C	Isotropic =	44.6861	Anisotropy =	70.7811
5	C	Isotropic =	63.0092	Anisotropy =	77.1024
6	O	Isotropic =	246.0092	Anisotropy =	81.1054
7	C	Isotropic =	182.4856	Anisotropy =	17.3431
8	C	Isotropic =	128.3424	Anisotropy =	69.2663
9	C	Isotropic =	176.0470	Anisotropy =	22.8487
10	H	Isotropic =	24.0496	Anisotropy =	4.5861
11	H	Isotropic =	29.0789	Anisotropy =	6.6384
12	H	Isotropic =	29.1875	Anisotropy =	10.0132
13	H	Isotropic =	29.1835	Anisotropy =	9.6154
14	H	Isotropic =	26.5336	Anisotropy =	6.3350
15	H	Isotropic =	27.3495	Anisotropy =	7.3647
16	H	Isotropic =	30.3890	Anisotropy =	9.7750
17	H	Isotropic =	30.2326	Anisotropy =	7.8789
18	H	Isotropic =	29.9824	Anisotropy =	5.0689

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	2.074152895912	-0.397373451482	0.405481510044
C	1.988323433320	0.921967370982	0.138943441668
N	0.774559287251	1.390276751712	0.106399204624
C	-0.015909067098	0.282646582683	0.371635949890
C	0.764292803971	-0.826362353185	0.551276732060
O	-1.363628708341	0.324891860346	0.482242838599
C	0.495689739229	-2.253010792998	0.855502547211
C	-2.034156467169	1.469163729607	-0.091880468286
C	-2.125032505754	1.388653308251	-1.607548376664
H	2.919960040753	1.458325096326	-0.022775631760
H	0.914845320462	-2.921719017144	0.085032471820
H	0.920451363981	-2.556641552529	1.827503503807
H	-0.591456854696	-2.410975204431	0.893295127997
H	-3.033811321020	1.446744737774	0.364392984816
H	-1.522012392337	2.389452809458	0.227965883382
H	-2.620131249993	0.456159479878	-1.922119868903
H	-2.713910875746	2.238761534475	-1.989072599221
H	-1.126605442727	1.431469110278	-2.069905251084

SCF Done: E(RB3LYP) = -439.262271041

Zero-point correction= 0.146145
Thermal correction to Energy= 0.155277
Thermal correction to Enthalpy= 0.156221
Thermal correction to Gibbs Free Energy= 0.110716
Sum of electronic and zero-point Energies= -439.116126
Sum of electronic and thermal Energies= -439.106994
Sum of electronic and thermal Enthalpies= -439.106050
Sum of electronic and thermal Free Energies= -439.151555

1	O	Isotropic =	27.5272	Anisotropy =	258.9128
2	C	Isotropic =	48.9198	Anisotropy =	89.9859
3	N	Isotropic =	9.4802	Anisotropy =	324.2703
4	C	Isotropic =	44.6038	Anisotropy =	70.9599
5	C	Isotropic =	63.1772	Anisotropy =	76.8757
6	O	Isotropic =	245.8304	Anisotropy =	80.3964
7	C	Isotropic =	182.4505	Anisotropy =	17.3766
8	C	Isotropic =	128.2103	Anisotropy =	69.0758
9	C	Isotropic =	176.0147	Anisotropy =	22.8949
10	H	Isotropic =	24.0484	Anisotropy =	4.5896
11	H	Isotropic =	29.1830	Anisotropy =	9.6217
12	H	Isotropic =	29.1855	Anisotropy =	10.0071
13	H	Isotropic =	29.0809	Anisotropy =	6.6413
14	H	Isotropic =	27.3427	Anisotropy =	7.3751
15	H	Isotropic =	26.5343	Anisotropy =	6.3306
16	H	Isotropic =	30.2412	Anisotropy =	7.8880
17	H	Isotropic =	30.3801	Anisotropy =	9.7694
18	H	Isotropic =	29.9728	Anisotropy =	5.0924

Conformer 4

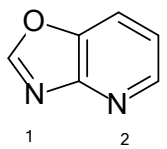
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	2.056052634179	-0.677778096889	-0.278864990980
C	1.440267222147	-1.728915798153	0.293704734791
N	0.206327796274	-1.513393508595	0.632102358257
C	-0.025779793505	-0.198807758015	0.251831392558
C	1.104919260089	0.338435486938	-0.314806162525
O	-1.267388999822	0.271561497594	0.504868432439
C	1.572030826482	1.617864196854	-0.918877551734
C	-1.571735879463	1.628843045243	0.148494754652
C	-3.008566916007	1.893396092491	0.552184336575
H	2.021180686720	-2.639812341594	0.416670505481
H	1.899537206131	1.464728420633	-1.961065501744
H	0.780389910563	2.374607680505	-0.922137343192
H	2.430957389714	2.027049512998	-0.360619757888
H	-0.880490509594	2.311170627852	0.674019656292
H	-1.434930114056	1.763919593749	-0.938974784854
H	-3.693516044363	1.209290246504	0.027389258922
H	-3.140428604810	1.756849196843	1.636854787025
H	-3.285196070681	2.927511905041	0.295305875929

SCF Done: E(RB3LYP) = -439.259681028

Zero-point correction= 0.146273
Thermal correction to Energy= 0.155399
Thermal correction to Enthalpy= 0.156343
Thermal correction to Gibbs Free Energy= 0.111368
Sum of electronic and zero-point Energies= -439.113408
Sum of electronic and thermal Energies= -439.104282
Sum of electronic and thermal Enthalpies= -439.103338
Sum of electronic and thermal Free Energies= -439.148313

1	O	Isotropic =	24.9303	Anisotropy =	229.8499
2	C	Isotropic =	48.4545	Anisotropy =	92.6913
3	N	Isotropic =	1.7757	Anisotropy =	297.5193
4	C	Isotropic =	43.6088	Anisotropy =	71.4795
5	C	Isotropic =	64.9521	Anisotropy =	76.0531
6	O	Isotropic =	230.6780	Anisotropy =	58.7752
7	C	Isotropic =	180.0301	Anisotropy =	20.5810
8	C	Isotropic =	125.6602	Anisotropy =	59.1129
9	C	Isotropic =	175.1498	Anisotropy =	23.5527
10	H	Isotropic =	24.1140	Anisotropy =	4.6810
11	H	Isotropic =	29.0230	Anisotropy =	9.4139
12	H	Isotropic =	28.8841	Anisotropy =	6.7459
13	H	Isotropic =	29.0163	Anisotropy =	9.4068
14	H	Isotropic =	27.3345	Anisotropy =	4.7857
15	H	Isotropic =	27.3118	Anisotropy =	4.8342
16	H	Isotropic =	29.9275	Anisotropy =	7.8372
17	H	Isotropic =	29.9286	Anisotropy =	7.8296
18	H	Isotropic =	30.0692	Anisotropy =	9.0825



1c

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.618048501569	-0.977713838221	0.747356946805
C	2.839195740010	-0.434194963640	0.332056870896
C	2.880864955840	0.805539943414	-0.335541438224
N	1.808147860359	1.558639013203	-0.628974748027
C	0.647255821170	1.033670062431	-0.229895598938
C	0.517315531639	-0.193677911766	0.439647046380
O	-0.814494470380	-0.396313673855	0.683122103895
C	-1.412115394924	0.717031333347	0.148320072610
N	-0.626757452957	1.588290660188	-0.397230965142
H	1.542971162219	-1.933410425700	1.266665747726
H	3.770786647469	-0.968496309667	0.523191531885
H	3.848240694750	1.208265797905	-0.649684954432
H	-2.495499596764	0.755170312360	0.237657384566

SCF Done: E(RB3LYP) = -415.793936336

Zero-point correction= 0.094034
Thermal correction to Energy= 0.099633
Thermal correction to Enthalpy= 0.100577

Thermal correction to Gibbs Free Energy= 0.064109
Sum of electronic and zero-point Energies= -415.699903
Sum of electronic and thermal Energies= -415.694303
Sum of electronic and thermal Enthalpies= -415.693359
Sum of electronic and thermal Free Energies= -415.729828

1	C	Isotropic =	74.6962	Anisotropy =	165.3677
2	C	Isotropic =	71.3871	Anisotropy =	163.0567
3	C	Isotropic =	46.7087	Anisotropy =	161.1910
4	N	Isotropic =	-43.9265	Anisotropy =	480.3153
5	C	Isotropic =	38.2197	Anisotropy =	125.3085
6	C	Isotropic =	50.2160	Anisotropy =	129.4202
7	O	Isotropic =	59.2137	Anisotropy =	236.9817
8	C	Isotropic =	38.7393	Anisotropy =	91.6459
9	N	Isotropic =	1.6780	Anisotropy =	339.3809
10	H	Isotropic =	23.4905	Anisotropy =	5.2997
11	H	Isotropic =	24.0245	Anisotropy =	5.3710
12	H	Isotropic =	22.6878	Anisotropy =	6.0238
13	H	Isotropic =	23.2693	Anisotropy =	3.9106

1c incorrect isomer

Conformer 1

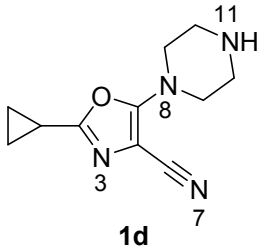
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.713565056221	-0.969910293040	0.248973249341
C	2.825485975857	-0.289964373450	-0.099238049537
C	2.853767075188	1.080038381812	-0.416349378469
C	1.680655390315	1.842269905346	-0.386553107879
C	0.519135321538	1.155788818690	-0.028432487649
C	0.636151208014	-0.212596440293	0.263320976119
O	-0.618611433608	-0.672739357227	0.585425585789
C	-1.408748826467	0.438865812786	0.468725021526
N	-0.818174764683	1.537150398779	0.116180922477
H	3.750725433004	-0.872009362640	-0.127265593950
H	3.804841102536	1.541129320496	-0.686684133259
H	1.673261822293	2.906334545856	-0.628086359104
H	-2.464873360206	0.292762642883	0.685043354594

SCF Done: E(RB3LYP) = -415.796857291

Zero-point correction= 0.094080
Thermal correction to Energy= 0.099672
Thermal correction to Enthalpy= 0.100616
Thermal correction to Gibbs Free Energy= 0.064165
Sum of electronic and zero-point Energies= -415.702777
Sum of electronic and thermal Energies= -415.697185
Sum of electronic and thermal Enthalpies= -415.696241
Sum of electronic and thermal Free Energies= -415.732692

1	N	Isotropic =	-16.6707	Anisotropy =	441.7006
2	C	Isotropic =	48.2678	Anisotropy =	157.6136
3	C	Isotropic =	70.6795	Anisotropy =	165.2189
4	C	Isotropic =	64.5512	Anisotropy =	175.3754
5	C	Isotropic =	60.4296	Anisotropy =	137.0886
6	C	Isotropic =	34.0088	Anisotropy =	111.2379
7	O	Isotropic =	44.7716	Anisotropy =	241.9448
8	C	Isotropic =	41.1872	Anisotropy =	89.4270
9	N	Isotropic =	3.4838	Anisotropy =	346.1927
10	H	Isotropic =	22.9081	Anisotropy =	5.7362
11	H	Isotropic =	23.9513	Anisotropy =	5.3189
12	H	Isotropic =	23.2804	Anisotropy =	5.4123
13	H	Isotropic =	23.3731	Anisotropy =	3.8388



1d

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.641340138668	1.664679683388	0.257880316902
O	1.708833377973	2.296239027655	-0.306349677528
C	1.938866751977	3.427858006114	0.465900534295
N	1.111371168879	3.552111987163	1.446499886987
C	0.248645517292	2.441381857927	1.348053089745
C	3.049720756616	4.303469119183	0.079943603583
C	-0.810077545455	2.261999158542	2.266148730012
N	-1.677008627348	2.140508463409	3.041485503966
N	0.254381928071	0.493357480304	-0.292587433144
C	0.665088839787	0.140552205194	-1.663565155734
C	0.726141241163	-1.376851329469	-1.811693991525
N	-0.567091582100	-1.950570789298	-1.440599867253
C	-0.855077895834	-1.678423664603	-0.033357114001
C	-0.967643507744	-0.170213408744	0.179814382698
C	3.416575108451	4.499354198302	-1.384662648900
C	4.338345517040	3.723641054397	-0.487875066861
H	3.134811044476	5.166748268287	0.740659891288
H	1.644884924222	0.585144867751	-1.868876523637
H	-0.068438776434	0.553676689871	-2.381593874181
H	1.563558965963	-1.763179172815	-1.189827210941
H	0.945701434999	-1.619849048027	-2.862474158932
H	-0.548727407699	-2.958992872636	-1.594441186077
H	-0.073734753049	-2.076110609672	0.651160615935
H	-1.813304203629	-2.144961728700	0.241047619173
H	-1.841454887647	0.221954496130	-0.373909645348
H	-1.106823260329	0.043878075256	1.245998842489

H	3.705466674478	5.508353151391	-1.685386834300
H	2.833445352246	3.943508136765	-2.121653071617
H	4.381681672601	2.639971875158	-0.614559880454
H	5.269782032365	4.191764821776	-0.163459676642

SCF Done: E(RB3LYP) = -721.814795154

Zero-point correction= 0.245947
Thermal correction to Energy= 0.260188
Thermal correction to Enthalpy= 0.261132
Thermal correction to Gibbs Free Energy= 0.203253
Sum of electronic and zero-point Energies= -721.568848
Sum of electronic and thermal Energies= -721.554607
Sum of electronic and thermal Enthalpies= -721.553663
Sum of electronic and thermal Free Energies= -721.611542

1	C	Isotropic =	33.0179	Anisotropy = 95.3886
2	O	Isotropic =	61.5696	Anisotropy = 186.5557
3	C	Isotropic =	40.2441	Anisotropy = 66.6396
4	N	Isotropic =	8.7144	Anisotropy = 293.4756
5	C	Isotropic =	106.9084	Anisotropy = 38.0140
6	C	Isotropic =	179.3844	Anisotropy = 74.6847
7	C	Isotropic =	78.4670	Anisotropy = 299.7530
8	N	Isotropic =	-12.8334	Anisotropy = 327.6271
9	N	Isotropic =	165.6466	Anisotropy = 51.2265
10	C	Isotropic =	144.5311	Anisotropy = 23.9714
11	C	Isotropic =	144.4562	Anisotropy = 25.5893
12	N	Isotropic =	216.4781	Anisotropy = 35.2880
13	C	Isotropic =	144.7254	Anisotropy = 25.5121
14	C	Isotropic =	144.5452	Anisotropy = 20.8782
15	C	Isotropic =	181.8636	Anisotropy = 44.0331
16	C	Isotropic =	181.4957	Anisotropy = 44.5124
17	H	Isotropic =	29.8528	Anisotropy = 13.1446
18	H	Isotropic =	27.8266	Anisotropy = 7.6042
19	H	Isotropic =	28.5100	Anisotropy = 8.1580
20	H	Isotropic =	28.6479	Anisotropy = 7.5869
21	H	Isotropic =	28.6406	Anisotropy = 8.5915
22	H	Isotropic =	30.3842	Anisotropy = 15.6688
23	H	Isotropic =	28.6002	Anisotropy = 7.6944
24	H	Isotropic =	28.5845	Anisotropy = 8.6728
25	H	Isotropic =	28.4069	Anisotropy = 8.0315
26	H	Isotropic =	27.6852	Anisotropy = 9.0361
27	H	Isotropic =	30.4841	Anisotropy = 14.6017
28	H	Isotropic =	30.5385	Anisotropy = 10.8291
29	H	Isotropic =	30.5644	Anisotropy = 10.7925
30	H	Isotropic =	30.4728	Anisotropy = 14.5697

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.077661755733	1.341477584756	-0.037584998428
O	1.178524471938	2.355486642145	0.866877567904
C	2.464709328214	2.281574180354	1.386676543579

N	3.162795212707	1.321915821726	0.883168682990
C	2.312003415745	0.691441861893	-0.047495451344
C	2.849216674201	3.270271719202	2.398849570632
C	2.759491514530	-0.412704183090	-0.806672556765
N	3.158044185505	-1.325100513081	-1.420027056567
N	-0.116075282397	1.174545622203	-0.647719669650
C	-0.245669757367	0.218560384459	-1.755428615975
C	-1.681583933564	-0.295626126002	-1.835230745191
N	-2.598376569997	0.837627189576	-1.950560500334
C	-2.517324302930	1.674609526932	-0.754157785597
C	-1.112910353746	2.260405002473	-0.641938156124
C	1.837112550728	3.779135547053	3.416273781995
C	2.323598134348	4.697942401727	2.332389663088
H	3.875700314119	3.126811074883	2.737623188143
H	0.439406362046	-0.621478846318	-1.591217815193
H	0.028509740108	0.713537615738	-2.706155700832
H	-1.884074939103	-0.923511527893	-0.939766032088
H	-1.776675678247	-0.936023913449	-2.725143433497
H	-3.552207987225	0.492536804687	-2.060598099895
H	-2.746317703683	1.115194280230	0.179587950626
H	-3.238159212363	2.502128999498	-0.837307488475
H	-0.922993043958	2.935729660889	-1.497593299614
H	-1.011656491352	2.833980964686	0.285721347814
H	2.201252286993	3.931733258514	4.434144871565
H	0.818620811394	3.393070341106	3.339566487751
H	1.636048310330	4.936407169570	1.518419249057
H	3.026970187292	5.490621455533	2.594778500425

SCF Done: E(RB3LYP) = -721.814821482

Zero-point correction= 0.245959
Thermal correction to Energy= 0.260189
Thermal correction to Enthalpy= 0.261133
Thermal correction to Gibbs Free Energy= 0.203361
Sum of electronic and zero-point Energies= -721.568863
Sum of electronic and thermal Energies= -721.554632
Sum of electronic and thermal Enthalpies= -721.553688
Sum of electronic and thermal Free Energies= -721.611460

1 C Isotropic = 33.0711 Anisotropy = 95.9390
2 O Isotropic = 61.5983 Anisotropy = 186.5198
3 C Isotropic = 40.3402 Anisotropy = 66.9481
4 N Isotropic = 8.8234 Anisotropy = 293.4916
5 C Isotropic = 106.8066 Anisotropy = 37.6987
6 C Isotropic = 179.3711 Anisotropy = 74.8608
7 C Isotropic = 78.4954 Anisotropy = 299.7366
8 N Isotropic = -12.8845 Anisotropy = 326.9687
9 N Isotropic = 165.5427 Anisotropy = 51.1207
10 C Isotropic = 144.5296 Anisotropy = 21.1170
11 C Isotropic = 144.8433 Anisotropy = 25.5607
12 N Isotropic = 216.5929 Anisotropy = 34.9348
13 C Isotropic = 144.4433 Anisotropy = 25.6841
14 C Isotropic = 144.6159 Anisotropy = 23.7552
15 C Isotropic = 181.8298 Anisotropy = 44.2389
16 C Isotropic = 181.8577 Anisotropy = 44.0824
17 H Isotropic = 29.8465 Anisotropy = 13.1352

18	H	Isotropic =	27.6785	Anisotropy =	9.0785
19	H	Isotropic =	28.4178	Anisotropy =	8.0444
20	H	Isotropic =	28.6030	Anisotropy =	7.7159
21	H	Isotropic =	28.5881	Anisotropy =	8.6782
22	H	Isotropic =	30.3759	Anisotropy =	15.6741
23	H	Isotropic =	28.6499	Anisotropy =	7.5804
24	H	Isotropic =	28.6288	Anisotropy =	8.6010
25	H	Isotropic =	28.5109	Anisotropy =	8.1402
26	H	Isotropic =	27.8322	Anisotropy =	7.6346
27	H	Isotropic =	30.4887	Anisotropy =	14.5769
28	H	Isotropic =	30.5434	Anisotropy =	10.8435
29	H	Isotropic =	30.5424	Anisotropy =	10.8134
30	H	Isotropic =	30.4995	Anisotropy =	14.5950

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.691611335524	1.527328700140	0.075461291753
O	1.479422420232	2.438285218707	-0.561675396759
C	2.268737847480	3.018230453279	0.420551162990
N	2.044321047782	2.546962269868	1.599046613293
C	1.037739048419	1.576179092773	1.425970185877
C	3.208531438551	4.057509369251	-0.021669180243
C	0.548846651111	0.833648661052	2.524049588849
N	0.164163147222	0.235227527582	3.452127272133
N	-0.211174006974	0.858288441144	-0.675968129905
C	-0.973591702358	-0.251150554156	-0.088323654945
C	-2.308573464777	-0.408083411843	-0.813638766264
N	-2.067118047995	-0.576918363746	-2.245474715077
C	-1.431047636592	0.620637734085	-2.793169998439
C	-0.064011978528	0.807794224180	-2.141793851629
C	4.488403910784	4.283139452937	0.766703088966
C	3.394046195971	5.307223609856	0.831482665180
H	3.249088674608	4.178110535398	-1.104704508439
H	-1.152070752196	-0.045149658137	0.973683707687
H	-0.390489995713	-1.187845904719	-0.170419994074
H	-2.942915409917	0.476653281570	-0.585287211532
H	-2.819248643103	-1.300061912434	-0.420333199963
H	-2.954197503717	-0.740170213080	-2.722264404494
H	-2.033338399700	1.541341439232	-2.629545534044
H	-1.290647659746	0.496820588721	-3.877712207897
H	0.595836199118	-0.037397286996	-2.415162556662
H	0.399490788276	1.738709133415	-2.486071760727
H	5.388167700165	4.513077016692	0.192621465896
H	4.635677350520	3.641756897139	1.638050480995
H	2.800191440704	5.360671370421	1.746413736722
H	3.527080004849	6.251872287671	0.300193810750

SCF Done: E(RB3LYP) = -721.814230986

Zero-point correction= 0.245879
Thermal correction to Energy= 0.260202
Thermal correction to Enthalpy= 0.261146

Thermal correction to Gibbs Free Energy= 0.202456
Sum of electronic and zero-point Energies= -721.568352
Sum of electronic and thermal Energies= -721.554029
Sum of electronic and thermal Enthalpies= -721.553085
Sum of electronic and thermal Free Energies= -721.611775

1	C	Isotropic =	32.8368	Anisotropy =	96.2464
2	O	Isotropic =	44.4965	Anisotropy =	175.7063
3	C	Isotropic =	37.8223	Anisotropy =	68.3098
4	N	Isotropic =	20.2693	Anisotropy =	298.1347
5	C	Isotropic =	106.5497	Anisotropy =	37.8498
6	C	Isotropic =	181.0799	Anisotropy =	69.0315
7	C	Isotropic =	78.4111	Anisotropy =	299.7779
8	N	Isotropic =	-13.2557	Anisotropy =	327.4299
9	N	Isotropic =	166.2300	Anisotropy =	50.5993
10	C	Isotropic =	144.5526	Anisotropy =	20.6655
11	C	Isotropic =	144.7226	Anisotropy =	25.6981
12	N	Isotropic =	216.6157	Anisotropy =	35.2245
13	C	Isotropic =	144.3659	Anisotropy =	25.3682
14	C	Isotropic =	144.4784	Anisotropy =	23.9495
15	C	Isotropic =	180.1683	Anisotropy =	44.0533
16	C	Isotropic =	178.0394	Anisotropy =	45.9734
17	H	Isotropic =	29.9095	Anisotropy =	11.9543
18	H	Isotropic =	27.6723	Anisotropy =	9.0359
19	H	Isotropic =	28.3935	Anisotropy =	7.9625
20	H	Isotropic =	28.5744	Anisotropy =	7.7275
21	H	Isotropic =	28.5662	Anisotropy =	8.5863
22	H	Isotropic =	30.3624	Anisotropy =	15.6453
23	H	Isotropic =	28.6016	Anisotropy =	7.7372
24	H	Isotropic =	28.5902	Anisotropy =	8.7015
25	H	Isotropic =	28.4435	Anisotropy =	8.3639
26	H	Isotropic =	27.6468	Anisotropy =	6.6150
27	H	Isotropic =	30.4100	Anisotropy =	14.2499
28	H	Isotropic =	30.4963	Anisotropy =	10.6937
29	H	Isotropic =	30.6572	Anisotropy =	10.3684
30	H	Isotropic =	30.3959	Anisotropy =	14.2086

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.728371560402	1.472588566129	0.030635436230
O	2.056239731681	1.251946815033	0.238054745243
C	2.296012357805	1.566785530203	1.568535494843
N	1.242831322046	1.966502085706	2.194527513861
C	0.205019115146	1.925319495198	1.242512682547
C	3.669987727813	1.370449640416	2.050347315433
C	-1.109755232533	2.312218157890	1.584971671076
N	-2.188775891015	2.636530300900	1.898199958107
N	0.239015516493	1.189448233762	-1.196604948400
C	1.151219322847	1.019082178886	-2.341491388111
C	0.522891199251	0.081082195737	-3.367786140489
N	-0.787485397955	0.599781229980	-3.758560562096
C	-1.686870154636	0.621299248475	-2.606060789689

C	-1.133892269107	1.574418113127	-1.548374449582
C	3.909464091265	0.538314270996	3.308602292358
C	4.098684379387	2.026793654484	3.347883706459
H	4.407048730381	1.283227547146	1.250866081635
H	2.102977745843	0.612467681279	-1.982628871892
H	1.341252733034	2.004559024725	-2.807410275338
H	0.469842868926	-0.940907079434	-2.931876706905
H	1.176975753764	0.037255961270	-4.251885292327
H	-1.184494576535	0.007023045368	-4.487920554893
H	-1.820393503959	-0.382005296843	-2.144681502262
H	-2.677578884888	0.982112872045	-2.921584524712
H	-1.140034320201	2.609939831307	-1.938060949916
H	-1.762755249513	1.537376054447	-0.651165105921
H	4.792656273593	-0.103934824373	3.314243047550
H	3.023157573285	0.124036347483	3.793807961678
H	3.340397201265	2.621264987544	3.861280325552
H	5.114770276116	2.423794131115	3.388223829961

SCF Done: E(RB3LYP) = -721.814246330

Zero-point correction= 0.245923
Thermal correction to Energy= 0.260232
Thermal correction to Enthalpy= 0.261176
Thermal correction to Gibbs Free Energy= 0.202565
Sum of electronic and zero-point Energies= -721.568324
Sum of electronic and thermal Energies= -721.554015
Sum of electronic and thermal Enthalpies= -721.553070
Sum of electronic and thermal Free Energies= -721.611681

1	C	Isotropic =	32.8915	Anisotropy =	96.6571
2	O	Isotropic =	45.4979	Anisotropy =	177.4758
3	C	Isotropic =	38.3089	Anisotropy =	67.2619
4	N	Isotropic =	18.4745	Anisotropy =	298.7937
5	C	Isotropic =	107.0200	Anisotropy =	37.8675
6	C	Isotropic =	181.0147	Anisotropy =	68.2428
7	C	Isotropic =	78.3237	Anisotropy =	299.8912
8	N	Isotropic =	-13.3121	Anisotropy =	326.2955
9	N	Isotropic =	165.8246	Anisotropy =	50.8121
10	C	Isotropic =	144.5670	Anisotropy =	23.9921
11	C	Isotropic =	144.3438	Anisotropy =	25.1363
12	N	Isotropic =	216.5743	Anisotropy =	35.2034
13	C	Isotropic =	144.7304	Anisotropy =	25.5044
14	C	Isotropic =	144.7567	Anisotropy =	20.8934
15	C	Isotropic =	177.4502	Anisotropy =	46.5666
16	C	Isotropic =	182.5306	Anisotropy =	42.1698
17	H	Isotropic =	29.8899	Anisotropy =	12.0334
18	H	Isotropic =	27.6394	Anisotropy =	6.6211
19	H	Isotropic =	28.4476	Anisotropy =	8.3816
20	H	Isotropic =	28.5916	Anisotropy =	7.7019
21	H	Isotropic =	28.5990	Anisotropy =	8.7009
22	H	Isotropic =	30.3654	Anisotropy =	15.6370
23	H	Isotropic =	28.5656	Anisotropy =	7.6899
24	H	Isotropic =	28.5779	Anisotropy =	8.5919
25	H	Isotropic =	28.3990	Anisotropy =	8.0243
26	H	Isotropic =	27.6415	Anisotropy =	9.1586
27	H	Isotropic =	30.4204	Anisotropy =	14.1790

28 H Isotropic = 30.7896 Anisotropy = 10.2173
29 H Isotropic = 30.3663 Anisotropy = 11.0450
30 H Isotropic = 30.4534 Anisotropy = 14.3317

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.718448097022	1.539118380493	0.042000177691
O	2.061801431507	1.471004528076	-0.173543035191
C	2.635114626133	2.413803562871	0.667794342349
N	1.771159221232	3.058055823075	1.374596211223
C	0.518427445534	2.531122343698	1.002711347949
C	4.100626716893	2.514741411920	0.637592636949
C	-0.674823708333	3.019280773208	1.580268764294
N	-1.645253983445	3.442842480408	2.076656176953
N	-0.061994229193	0.671772523161	-0.639886447424
C	0.464376792066	-0.031579447791	-1.823258463510
C	-0.259382557211	-1.363498673215	-1.998300627141
N	-1.700153164637	-1.124397491311	-2.073786067416
C	-2.181936856201	-0.549946675582	-0.818744991938
C	-1.523690002375	0.810442918991	-0.598278021688
C	4.872001707675	2.570853499193	1.953152993443
C	4.762752241096	3.800215903717	1.099812706680
H	4.560236515219	1.970222320932	-0.188120120551
H	1.539761432281	-0.194216621745	-1.692762582212
H	0.308421137306	0.595543992243	-2.721443275639
H	0.022206093422	-2.036291520102	-1.158462119082
H	0.083459642695	-1.829934649525	-2.934332161412
H	-2.182572712674	-2.005605668242	-2.251649856425
H	-1.966319657055	-1.195206863778	0.061227286204
H	-3.271915767046	-0.408685782918	-0.874975960455
H	-1.851906121566	1.516521152623	-1.384352037870
H	-1.822592331306	1.212940665034	0.376676528397
H	5.825395119540	2.039634591190	1.989117620337
H	4.275250772512	2.529934996727	2.866838712414
H	4.091893235618	4.593438581225	1.435786665388
H	5.641748863292	4.130892945423	0.543143597679

SCF Done: E(RB3LYP) = -721.814227668

Zero-point correction= 0.245846
Thermal correction to Energy= 0.260183
Thermal correction to Enthalpy= 0.261127
Thermal correction to Gibbs Free Energy= 0.202259
Sum of electronic and zero-point Energies= -721.568382
Sum of electronic and thermal Energies= -721.554044
Sum of electronic and thermal Enthalpies= -721.553100
Sum of electronic and thermal Free Energies= -721.611969

1 C Isotropic = 32.9640 Anisotropy = 96.4023
2 O Isotropic = 44.9425 Anisotropy = 175.7799
3 C Isotropic = 38.0176 Anisotropy = 67.7691
4 N Isotropic = 19.5670 Anisotropy = 298.2240

5	C	Isotropic =	106.8499	Anisotropy =	37.7372
6	C	Isotropic =	181.0795	Anisotropy =	68.6822
7	C	Isotropic =	78.3950	Anisotropy =	299.7801
8	N	Isotropic =	-13.3715	Anisotropy =	326.5534
9	N	Isotropic =	166.0544	Anisotropy =	50.6896
10	C	Isotropic =	144.5505	Anisotropy =	23.9430
11	C	Isotropic =	144.3953	Anisotropy =	25.4440
12	N	Isotropic =	216.5092	Anisotropy =	34.9600
13	C	Isotropic =	144.6924	Anisotropy =	25.4273
14	C	Isotropic =	144.6523	Anisotropy =	20.7254
15	C	Isotropic =	177.4899	Anisotropy =	46.1281
16	C	Isotropic =	181.1098	Anisotropy =	43.2014
17	H	Isotropic =	29.9155	Anisotropy =	12.0211
18	H	Isotropic =	27.6478	Anisotropy =	6.6235
19	H	Isotropic =	28.4396	Anisotropy =	8.3792
20	H	Isotropic =	28.5967	Anisotropy =	7.7216
21	H	Isotropic =	28.5954	Anisotropy =	8.7122
22	H	Isotropic =	30.3591	Anisotropy =	15.6322
23	H	Isotropic =	28.5796	Anisotropy =	7.6969
24	H	Isotropic =	28.5728	Anisotropy =	8.5915
25	H	Isotropic =	28.4086	Anisotropy =	8.0121
26	H	Isotropic =	27.6534	Anisotropy =	9.1431
27	H	Isotropic =	30.3884	Anisotropy =	14.1769
28	H	Isotropic =	30.7192	Anisotropy =	10.2472
29	H	Isotropic =	30.4235	Anisotropy =	10.8303
30	H	Isotropic =	30.4080	Anisotropy =	14.2820

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.848063349844	1.456557092829	-0.054795765816
O	0.764316165399	2.550159112599	0.752738265352
C	2.019011861055	2.702377873213	1.326052471027
N	2.866053112461	1.810324910042	0.941695590695
C	2.157432030654	0.985069272601	0.046209955207
C	2.175063164962	3.811134989838	2.277242772716
C	2.789383855261	-0.106271242301	-0.590598656496
N	3.338942558990	-1.003114257838	-1.101608727126
N	-0.278308545193	1.073044244103	-0.695480837978
C	-0.222253306110	0.007186493969	-1.704236623481
C	-1.571124881485	-0.704623354359	-1.783592801941
N	-2.623215430074	0.275180669055	-2.049197616824
C	-2.715769796404	1.229024907357	-0.944137898041
C	-1.408026726320	2.008320227631	-0.839735439076
C	3.569566644656	4.300049463534	2.618623292649
C	2.788227826398	3.538234405609	3.648915194925
H	1.370461846252	4.546153748767	2.230214619957
H	0.559686006621	-0.710626461155	-1.429955841344
H	0.030411175196	0.441606004123	-2.689970924812
H	-1.733007342847	-1.264728687957	-0.836367161534
H	-1.535376742463	-1.435240537045	-2.605836363324
H	-3.515833526081	-0.206659043629	-2.158671738013
H	-2.918007770393	0.738279960490	0.033352817680

H	-3.533770353957	1.938487357126	-1.141273403403
H	-1.264989814445	2.615934088077	-1.753350176596
H	-1.429727754667	2.678446152536	0.026512704217
H	3.697375589166	5.376318151706	2.749261142165
H	4.395178424297	3.784226360048	2.124246953817
H	3.083420654064	2.506790021076	3.852882711362
H	2.364617725163	4.082788077956	4.495381484037

SCF Done: E(RB3LYP) = -721.814280706

Zero-point correction= 0.245961
Thermal correction to Energy= 0.260242
Thermal correction to Enthalpy= 0.261187
Thermal correction to Gibbs Free Energy= 0.202818
Sum of electronic and zero-point Energies= -721.568320
Sum of electronic and thermal Energies= -721.554038
Sum of electronic and thermal Enthalpies= -721.553094
Sum of electronic and thermal Free Energies= -721.611463

1	C	Isotropic =	32.9005	Anisotropy =	96.3100
2	O	Isotropic =	45.2369	Anisotropy =	177.6292
3	C	Isotropic =	38.2479	Anisotropy =	67.3686
4	N	Isotropic =	18.9282	Anisotropy =	299.2150
5	C	Isotropic =	106.9194	Anisotropy =	37.9503
6	C	Isotropic =	181.1327	Anisotropy =	68.5909
7	C	Isotropic =	78.3409	Anisotropy =	299.8753
8	N	Isotropic =	-13.2102	Anisotropy =	327.0809
9	N	Isotropic =	166.0800	Anisotropy =	50.9277
10	C	Isotropic =	144.6848	Anisotropy =	20.7148
11	C	Isotropic =	144.7269	Anisotropy =	25.4614
12	N	Isotropic =	216.5245	Anisotropy =	34.8749
13	C	Isotropic =	144.3950	Anisotropy =	25.2708
14	C	Isotropic =	144.5083	Anisotropy =	24.0110
15	C	Isotropic =	181.9660	Anisotropy =	42.4621
16	C	Isotropic =	177.3917	Anisotropy =	46.4094
17	H	Isotropic =	29.9036	Anisotropy =	12.0433
18	H	Isotropic =	27.6590	Anisotropy =	9.0993
19	H	Isotropic =	28.4039	Anisotropy =	8.0102
20	H	Isotropic =	28.5763	Anisotropy =	7.6945
21	H	Isotropic =	28.5700	Anisotropy =	8.6018
22	H	Isotropic =	30.3535	Anisotropy =	15.6258
23	H	Isotropic =	28.6014	Anisotropy =	7.7307
24	H	Isotropic =	28.6012	Anisotropy =	8.6970
25	H	Isotropic =	28.4497	Anisotropy =	8.3782
26	H	Isotropic =	27.6464	Anisotropy =	6.6233
27	H	Isotropic =	30.4477	Anisotropy =	14.3045
28	H	Isotropic =	30.3861	Anisotropy =	10.9669
29	H	Isotropic =	30.7613	Anisotropy =	10.2257
30	H	Isotropic =	30.4138	Anisotropy =	14.1846

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.753723811174	1.592464915645	-0.013687256650
O	2.079083739137	1.306308187951	0.119154423547
C	2.483674743125	1.897994721305	1.306928339410
N	1.534132572540	2.523212536096	1.914085891422
C	0.399270386584	2.362760412017	1.094370438918
C	3.899227226356	1.741899103380	1.668184166935
C	-0.841865548096	2.934792684255	1.452287551789
N	-1.856257029963	3.419064012388	1.774812470348
N	0.113176165196	1.070120377421	-1.082916986550
C	0.879085108872	0.561211726607	-2.234524816478
C	0.083768433628	-0.533300073685	-2.940149537454
N	-1.228140939694	-0.009704130360	-3.319495567097
C	-1.989545299396	0.357018740125	-2.126326428524
C	-1.264201177578	1.479333832501	-1.386752844209
C	4.300877471495	1.801097002706	3.132420702100
C	4.663283335602	2.938933053952	2.224314176406
H	4.443942231072	1.057136506423	1.017324573127
H	1.838888282099	0.169461498958	-1.880674240978
H	1.074811457656	1.390970296986	-2.940009515326
H	0.016862865276	-1.415890580331	-2.266544660439
H	0.630827562964	-0.838867608752	-3.844919599685
H	-1.739439963552	-0.720151671879	-3.843670273607
H	-2.131319509313	-0.495817965401	-1.426464387072
H	-2.985604087364	0.718107245064	-2.424225661676
H	-1.250365094381	2.391552082820	-2.012736142761
H	-1.789946277935	1.707672247798	-0.452227373856
H	5.088532377328	1.117851848119	3.456058336569
H	3.491320836751	1.960016030791	3.847780487321
H	4.099203741994	3.868745466316	2.323247045041
H	5.703342578423	3.049757500784	1.910676689428

SCF Done: E(RB3LYP) = -721.814244945

Zero-point correction= 0.245839
Thermal correction to Energy= 0.260192
Thermal correction to Enthalpy= 0.261136
Thermal correction to Gibbs Free Energy= 0.201886
Sum of electronic and zero-point Energies= -721.568406
Sum of electronic and thermal Energies= -721.554053
Sum of electronic and thermal Enthalpies= -721.553109
Sum of electronic and thermal Free Energies= -721.612359

1	C	Isotropic =	32.9849	Anisotropy =	96.4472
2	O	Isotropic =	44.6416	Anisotropy =	175.6400
3	C	Isotropic =	37.9748	Anisotropy =	67.9661
4	N	Isotropic =	20.1151	Anisotropy =	298.1870
5	C	Isotropic =	106.8559	Anisotropy =	37.5546
6	C	Isotropic =	181.0754	Anisotropy =	68.8729
7	C	Isotropic =	78.3711	Anisotropy =	299.8311
8	N	Isotropic =	-13.4320	Anisotropy =	326.4048
9	N	Isotropic =	165.8803	Anisotropy =	50.8119
10	C	Isotropic =	144.4936	Anisotropy =	24.2533
11	C	Isotropic =	144.2920	Anisotropy =	25.1496
12	N	Isotropic =	216.4196	Anisotropy =	35.0204
13	C	Isotropic =	144.7008	Anisotropy =	25.4882
14	C	Isotropic =	144.4903	Anisotropy =	20.9584

15	C	Isotropic =	180.2417	Anisotropy =	43.6406
16	C	Isotropic =	177.7978	Anisotropy =	46.2474
17	H	Isotropic =	29.9110	Anisotropy =	11.9942
18	H	Isotropic =	27.6442	Anisotropy =	6.6149
19	H	Isotropic =	28.4391	Anisotropy =	8.3580
20	H	Isotropic =	28.5985	Anisotropy =	7.7097
21	H	Isotropic =	28.5954	Anisotropy =	8.7041
22	H	Isotropic =	30.3611	Anisotropy =	15.6273
23	H	Isotropic =	28.5732	Anisotropy =	7.7113
24	H	Isotropic =	28.5792	Anisotropy =	8.5771
25	H	Isotropic =	28.3966	Anisotropy =	7.9737
26	H	Isotropic =	27.6498	Anisotropy =	9.1407
27	H	Isotropic =	30.3966	Anisotropy =	14.2480
28	H	Isotropic =	30.4728	Anisotropy =	10.6874
29	H	Isotropic =	30.6841	Anisotropy =	10.3408
30	H	Isotropic =	30.3852	Anisotropy =	14.2080

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.774531534257	1.427802193331	0.082366388316
O	1.883802607003	1.908838751184	-0.545119217409
C	2.684431119732	2.450961550957	0.450037259780
N	2.173393273866	2.345607476456	1.628623436902
C	0.945383457152	1.680086414916	1.443799595813
C	3.970509779431	3.016981473893	0.021175091335
C	0.110649547110	1.378612249357	2.543141656370
N	-0.558056757420	1.142086886786	3.472807841337
N	-0.193882388962	0.895535411991	-0.696047603086
C	-1.338895340663	0.215392427745	-0.076663000006
C	-2.552656572857	0.292765030827	-1.000550253751
N	-2.202600701875	-0.257143773901	-2.309110777556
C	-1.150798704079	0.547726010105	-2.929398033183
C	0.111072731720	0.473216289743	-2.075060772528
C	5.244474834007	2.628040561699	0.767222613703
C	4.678574186007	4.008699813368	0.925399206018
H	4.048899328821	3.160260952671	-1.057236065295
H	-1.571125179419	0.696286118969	0.880878317541
H	-1.082436808685	-0.843505377866	0.116317411129
H	-2.890855011211	1.351030989760	-1.054793038869
H	-3.368456777355	-0.300271219191	-0.560183424271
H	-3.028156910054	-0.259018945911	-2.908628843021
H	-1.438923230116	1.615493600474	-3.048324319920
H	-0.924128880484	0.145747212929	-3.928555115520
H	0.490969659950	-0.566022690710	-2.064264375859
H	0.889688463361	1.126015311082	-2.484423324598
H	6.146667337432	2.496128622711	0.166333118279
H	5.126300798293	1.930340411196	1.598982380454
H	4.176356820235	4.247092914646	1.865176163183
H	5.189027784804	4.842423330785	0.439477684713

SCF Done: E(RB3LYP) = -721.814297612

Zero-point correction= 0.245997
Thermal correction to Energy= 0.260263
Thermal correction to Enthalpy= 0.261207
Thermal correction to Gibbs Free Energy= 0.202934
Sum of electronic and zero-point Energies= -721.568300
Sum of electronic and thermal Energies= -721.554034
Sum of electronic and thermal Enthalpies= -721.553090
Sum of electronic and thermal Free Energies= -721.611364

1	C	Isotropic =	32.8722	Anisotropy =	96.4081
2	O	Isotropic =	44.7607	Anisotropy =	178.2879
3	C	Isotropic =	38.0062	Anisotropy =	67.8085
4	N	Isotropic =	19.1761	Anisotropy =	298.4397
5	C	Isotropic =	106.7942	Anisotropy =	38.1290
6	C	Isotropic =	181.1615	Anisotropy =	68.9179
7	C	Isotropic =	78.4085	Anisotropy =	299.8499
8	N	Isotropic =	-13.1649	Anisotropy =	327.6711
9	N	Isotropic =	165.9755	Anisotropy =	50.7021
10	C	Isotropic =	144.5249	Anisotropy =	20.6422
11	C	Isotropic =	144.8243	Anisotropy =	25.6046
12	N	Isotropic =	216.6654	Anisotropy =	35.3511
13	C	Isotropic =	144.3934	Anisotropy =	25.5366
14	C	Isotropic =	144.3802	Anisotropy =	24.1757
15	C	Isotropic =	177.4053	Anisotropy =	46.6295
16	C	Isotropic =	181.6568	Anisotropy =	42.6960
17	H	Isotropic =	29.8970	Anisotropy =	12.0380
18	H	Isotropic =	27.6687	Anisotropy =	9.0645
19	H	Isotropic =	28.3972	Anisotropy =	7.9445
20	H	Isotropic =	28.5755	Anisotropy =	7.7479
21	H	Isotropic =	28.5693	Anisotropy =	8.5859
22	H	Isotropic =	30.3704	Anisotropy =	15.6426
23	H	Isotropic =	28.5980	Anisotropy =	7.7409
24	H	Isotropic =	28.5934	Anisotropy =	8.7037
25	H	Isotropic =	28.4369	Anisotropy =	8.3394
26	H	Isotropic =	27.6455	Anisotropy =	6.6191
27	H	Isotropic =	30.4214	Anisotropy =	14.1899
28	H	Isotropic =	30.7439	Anisotropy =	10.2544
29	H	Isotropic =	30.3992	Anisotropy =	10.9127
30	H	Isotropic =	30.4333	Anisotropy =	14.2885

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.993674386624	1.224085922155	0.042820333577
O	1.425475304425	2.488879003973	0.308267873173
C	2.437476138363	2.360302512444	1.251326561671
N	2.669891845805	1.137101351352	1.585139548049
C	1.767413099371	0.365949902866	0.824568553372
C	3.088882069070	3.585809053660	1.724250070342
C	1.752393320157	-1.042946556494	0.926895899796
N	1.763314790532	-2.207420794253	1.033770496505
N	-0.037624964122	1.091682426104	-0.819523669018
C	-0.450347178373	-0.243506219256	-1.271673431689

C	-1.934949790689	-0.235267089598	-1.630600545740
N	-2.189112133498	0.806155366564	-2.624682269240
C	-1.883244357849	2.123016776773	-2.066845032932
C	-0.397032497431	2.194732901699	-1.728544112643
C	2.294925287956	4.873638193832	1.897703816818
C	3.300565329571	4.767145591405	0.787312999776
H	3.871419478279	3.374649696539	2.453661528127
H	-0.266694407101	-0.970281606071	-0.471728677640
H	0.146972681415	-0.536334593821	-2.155681437823
H	-2.524893243769	-0.094514868347	-0.698195124415
H	-2.199938767185	-1.216597917979	-2.052491807438
H	-3.169239626931	0.774996419605	-2.906339114542
H	-2.469535446758	2.349856957571	-1.149132008719
H	-2.112154379038	2.898407318359	-2.813654450549
H	0.198711934532	2.110976999901	-2.657148126890
H	-0.160416217305	3.148727623082	-1.245187212956
H	2.539245409283	5.485310040316	2.768439454256
H	1.236152339584	4.843717122063	1.632406215985
H	2.925762600579	4.664793368359	-0.233067739363
H	4.245966994506	5.304575097197	0.883991410149

SCF Done: E(RB3LYP) = -721.814817553

Zero-point correction= 0.246022
Thermal correction to Energy= 0.260237
Thermal correction to Enthalpy= 0.261181
Thermal correction to Gibbs Free Energy= 0.203506
Sum of electronic and zero-point Energies= -721.568795
Sum of electronic and thermal Energies= -721.554580
Sum of electronic and thermal Enthalpies= -721.553636
Sum of electronic and thermal Free Energies= -721.611311

1	C	Isotropic =	33.1771	Anisotropy =	95.6460
2	O	Isotropic =	61.7369	Anisotropy =	186.2286
3	C	Isotropic =	40.3898	Anisotropy =	66.6099
4	N	Isotropic =	8.8097	Anisotropy =	294.0251
5	C	Isotropic =	106.9539	Anisotropy =	37.6861
6	C	Isotropic =	179.3945	Anisotropy =	74.8701
7	C	Isotropic =	78.4838	Anisotropy =	299.7290
8	N	Isotropic =	-12.9317	Anisotropy =	327.0666
9	N	Isotropic =	165.4801	Anisotropy =	51.2924
10	C	Isotropic =	144.5914	Anisotropy =	21.0721
11	C	Isotropic =	144.7687	Anisotropy =	25.4483
12	N	Isotropic =	216.4997	Anisotropy =	35.1484
13	C	Isotropic =	144.3993	Anisotropy =	25.6151
14	C	Isotropic =	144.5820	Anisotropy =	23.8437
15	C	Isotropic =	181.6619	Anisotropy =	44.4791
16	C	Isotropic =	181.6974	Anisotropy =	44.3823
17	H	Isotropic =	29.8514	Anisotropy =	13.1233
18	H	Isotropic =	27.6673	Anisotropy =	9.0869
19	H	Isotropic =	28.4096	Anisotropy =	8.0518
20	H	Isotropic =	28.5905	Anisotropy =	7.6986
21	H	Isotropic =	28.5824	Anisotropy =	8.6804
22	H	Isotropic =	30.3796	Anisotropy =	15.6641
23	H	Isotropic =	28.6455	Anisotropy =	7.5697
24	H	Isotropic =	28.6440	Anisotropy =	8.5822

25 H Isotropic = 28.5076 Anisotropy = 8.1387
26 H Isotropic = 27.8212 Anisotropy = 7.6477
27 H Isotropic = 30.4949 Anisotropy = 14.5821
28 H Isotropic = 30.5506 Anisotropy = 10.8291
29 H Isotropic = 30.5436 Anisotropy = 10.8253
30 H Isotropic = 30.5009 Anisotropy = 14.6033

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.654800617375	1.793556925376	0.017348300883
O	1.990690574078	1.594071403351	0.195980269525
C	2.442344927391	2.666934445102	0.954450399729
N	1.511257180903	3.506934630660	1.252985696796
C	0.340161202515	2.989684361608	0.662793917133
C	3.866557205599	2.706279430360	1.300547165049
C	-0.891989848961	3.670747910097	0.779402881367
N	-1.897599664119	4.256548084383	0.893971609360
N	-0.027444787670	0.842266896359	-0.656952719642
C	0.689163489729	-0.139506820058	-1.490575974612
C	-0.118528676658	-1.430996335272	-1.579480030086
N	-1.458273688904	-1.130097483779	-2.082904054882
C	-2.165296589114	-0.258820937484	-1.145653336312
C	-1.427675570650	1.074086257330	-1.035798304568
C	4.918634515466	2.185939671084	0.330395918786
C	4.634044625247	1.424125267479	1.593058694901
H	4.117296834111	3.588797054635	1.889895098577
H	1.672430134366	-0.333844841571	-1.048683645807
H	0.833589212029	0.278238740397	-2.504923841073
H	-0.132866512146	-1.912852136200	-0.577094520663
H	0.388441607371	-2.115919739354	-2.276051784918
H	-1.981108502842	-1.998452664741	-2.199622842320
H	-2.253012603258	-0.700842860523	-0.128731723126
H	-3.182614755009	-0.067734162056	-1.519425804514
H	-1.465973444402	1.604238717166	-2.006090215264
H	-1.909531810556	1.702263352186	-0.277397721747
H	5.845934045211	2.758067547996	0.261672606921
H	4.560504395283	1.765231577888	-0.611375133545
H	4.082792117767	0.485277055012	1.509661557445
H	5.363173769847	1.465118652570	2.404637536607

SCF Done: E(RB3LYP) = -721.814822715

Zero-point correction= 0.245991
Thermal correction to Energy= 0.260220
Thermal correction to Enthalpy= 0.261164
Thermal correction to Gibbs Free Energy= 0.203358
Sum of electronic and zero-point Energies= -721.568832
Sum of electronic and thermal Energies= -721.554603
Sum of electronic and thermal Enthalpies= -721.553658
Sum of electronic and thermal Free Energies= -721.611465

1 C Isotropic = 33.0715 Anisotropy = 95.6992

2	O	Isotropic =	61.5241	Anisotropy =	185.9612
3	C	Isotropic =	40.3266	Anisotropy =	66.5282
4	N	Isotropic =	8.6297	Anisotropy =	293.4734
5	C	Isotropic =	106.9062	Anisotropy =	37.6133
6	C	Isotropic =	179.4805	Anisotropy =	74.7221
7	C	Isotropic =	78.4830	Anisotropy =	299.7397
8	N	Isotropic =	-12.9525	Anisotropy =	326.8711
9	N	Isotropic =	165.5472	Anisotropy =	51.0910
10	C	Isotropic =	144.6076	Anisotropy =	23.7824
11	C	Isotropic =	144.5020	Anisotropy =	25.5877
12	N	Isotropic =	216.5380	Anisotropy =	35.3109
13	C	Isotropic =	144.7827	Anisotropy =	25.5673
14	C	Isotropic =	144.5358	Anisotropy =	21.0484
15	C	Isotropic =	181.9876	Anisotropy =	43.9823
16	C	Isotropic =	181.8686	Anisotropy =	44.1996
17	H	Isotropic =	29.8514	Anisotropy =	13.1382
18	H	Isotropic =	27.8258	Anisotropy =	7.6332
19	H	Isotropic =	28.5056	Anisotropy =	8.1259
20	H	Isotropic =	28.6417	Anisotropy =	7.5875
21	H	Isotropic =	28.6343	Anisotropy =	8.5919
22	H	Isotropic =	30.3838	Anisotropy =	15.6741
23	H	Isotropic =	28.5954	Anisotropy =	7.7113
24	H	Isotropic =	28.5824	Anisotropy =	8.6738
25	H	Isotropic =	28.4154	Anisotropy =	8.0504
26	H	Isotropic =	27.6586	Anisotropy =	9.1138
27	H	Isotropic =	30.5047	Anisotropy =	14.5795
28	H	Isotropic =	30.5353	Anisotropy =	10.8506
29	H	Isotropic =	30.5402	Anisotropy =	10.8303
30	H	Isotropic =	30.4966	Anisotropy =	14.5752

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.571874027381	1.526260252829	0.071299465137
O	1.332868203217	0.492292566957	0.526500109668
C	2.030137115735	0.980463854345	1.622429189979
N	1.767112187621	2.214764256065	1.884479628359
C	0.820152134482	2.607078207805	0.917800703602
C	2.909305796593	0.029127767423	2.315534141443
C	0.287562422088	3.915737186073	0.912426300065
N	-0.135595440185	5.005616360486	0.933766459595
N	-0.163053245774	1.309027903196	-1.042227975253
C	-1.120982981562	2.325369845831	-1.496617502875
C	-1.324571461247	2.211324781676	-3.006009572810
N	-1.738148512225	0.849196399618	-3.339239304096
C	-0.682848755586	-0.099345491729	-2.984586193114
C	-0.462609334646	-0.067747222058	-1.475120680082
C	2.783962008488	-0.141358628058	3.828292489986
C	3.978991005460	0.558887650007	3.250442479831
H	3.134483137839	-0.865023586509	1.732632265862
H	-0.735935653299	3.321736764274	-1.249333871024
H	-2.087597690101	2.184373298369	-0.976970595820
H	-0.382741471172	2.512288553510	-3.515426770219

H	-2.112380979831	2.917627827733	-3.308783156430
H	-1.929273949075	0.787444860132	-4.339549248684
H	0.282691168403	0.120850480149	-3.491074337706
H	-0.991983222631	-1.115174606054	-3.274195095937
H	-1.374872781946	-0.423400916903	-0.959585537800
H	0.372974825036	-0.719099792061	-1.196713722526
H	2.907147071951	-1.152488987820	4.221907939333
H	2.026464471406	0.468200052189	4.325478563588
H	4.032198453641	1.644191389163	3.356742128945
H	4.938771449936	0.038798973362	3.247051698983

SCF Done: E(RB3LYP) = -721.814265616

Zero-point correction= 0.245846
Thermal correction to Energy= 0.260179
Thermal correction to Enthalpy= 0.261123
Thermal correction to Gibbs Free Energy= 0.202210
Sum of electronic and zero-point Energies= -721.568419
Sum of electronic and thermal Energies= -721.554087
Sum of electronic and thermal Enthalpies= -721.553143
Sum of electronic and thermal Free Energies= -721.612055

1	C	Isotropic =	32.7523	Anisotropy =	96.5248
2	O	Isotropic =	44.7036	Anisotropy =	178.9968
3	C	Isotropic =	38.1703	Anisotropy =	67.3933
4	N	Isotropic =	18.5109	Anisotropy =	298.8824
5	C	Isotropic =	106.7169	Anisotropy =	38.0659
6	C	Isotropic =	181.0337	Anisotropy =	68.4920
7	C	Isotropic =	78.4661	Anisotropy =	299.8113
8	N	Isotropic =	-13.1810	Anisotropy =	328.1172
9	N	Isotropic =	166.0098	Anisotropy =	50.8735
10	C	Isotropic =	144.5357	Anisotropy =	20.6875
11	C	Isotropic =	144.6936	Anisotropy =	25.8128
12	N	Isotropic =	216.3699	Anisotropy =	35.2297
13	C	Isotropic =	144.4483	Anisotropy =	25.5251
14	C	Isotropic =	144.4841	Anisotropy =	24.0805
15	C	Isotropic =	177.4309	Anisotropy =	46.6411
16	C	Isotropic =	182.3107	Anisotropy =	42.1545
17	H	Isotropic =	29.8932	Anisotropy =	12.0549
18	H	Isotropic =	27.6782	Anisotropy =	9.0295
19	H	Isotropic =	28.3991	Anisotropy =	7.9313
20	H	Isotropic =	28.5783	Anisotropy =	7.7353
21	H	Isotropic =	28.5672	Anisotropy =	8.5878
22	H	Isotropic =	30.3554	Anisotropy =	15.6496
23	H	Isotropic =	28.6010	Anisotropy =	7.7587
24	H	Isotropic =	28.5921	Anisotropy =	8.7033
25	H	Isotropic =	28.4408	Anisotropy =	8.3325
26	H	Isotropic =	27.6509	Anisotropy =	6.6134
27	H	Isotropic =	30.4295	Anisotropy =	14.1988
28	H	Isotropic =	30.7793	Anisotropy =	10.2354
29	H	Isotropic =	30.3723	Anisotropy =	11.0042
30	H	Isotropic =	30.4433	Anisotropy =	14.3179

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.754508719773	1.305876495641	0.189298309766
O	0.854732255152	2.595596267749	0.616208667965
C	2.212239801114	2.870662990072	0.695040942132
N	2.954695759260	1.871669971698	0.359947461853
C	2.058308506669	0.833469554238	0.037696130850
C	2.583109521421	4.212091494089	1.165601909343
C	2.531923510739	-0.435937209606	-0.363295149883
N	2.954076679525	-1.475835789843	-0.691499522293
N	-0.489064733617	0.820076997718	-0.023504935211
C	-1.656590883675	1.481308683727	0.587141182215
C	-2.900894580146	1.215911581785	-0.254934488763
N	-3.082289025309	-0.227260622162	-0.408524662232
C	-1.953822233502	-0.801982153771	-1.139014880309
C	-0.672577097271	-0.604214898257	-0.331713352846
C	3.963191521795	4.753478413388	0.841047536942
C	3.645664310293	4.355185589238	2.252374270728
H	1.749504031678	4.915065588660	1.187871748644
H	-1.462459640061	2.557365466875	0.654277672737
H	-1.809061197745	1.085339817430	1.609146444405
H	-2.792311622311	1.742462756567	-1.228715022040
H	-3.774010294605	1.640953813280	0.263072798452
H	-3.945934683747	-0.409120479538	-0.920426417118
H	-1.814281491457	-0.346399769820	-2.144136901384
H	-2.118667135776	-1.881208807728	-1.277820489759
H	-0.729806011971	-1.184166803146	0.608887372752
H	0.187577593303	-0.962815282841	-0.909393590218
H	4.032125260249	5.815977863550	0.599951486394
H	4.614862779659	4.095855162274	0.262233540140
H	4.080808444352	3.427624044466	2.630263585240
H	3.487781936210	5.138779264267	2.996358351501

SCF Done: E(RB3LYP) = -721.814236598

Zero-point correction= 0.245814
Thermal correction to Energy= 0.260166
Thermal correction to Enthalpy= 0.261110
Thermal correction to Gibbs Free Energy= 0.202114
Sum of electronic and zero-point Energies= -721.568422
Sum of electronic and thermal Energies= -721.554071
Sum of electronic and thermal Enthalpies= -721.553127
Sum of electronic and thermal Free Energies= -721.612123

1 C Isotropic = 32.7686 Anisotropy = 96.4560
2 O Isotropic = 44.4548 Anisotropy = 178.6471
3 C Isotropic = 37.9161 Anisotropy = 67.9251
4 N Isotropic = 19.4427 Anisotropy = 298.6808
5 C Isotropic = 106.5531 Anisotropy = 38.0500
6 C Isotropic = 181.1093 Anisotropy = 68.9170
7 C Isotropic = 78.4396 Anisotropy = 299.8586
8 N Isotropic = -13.1725 Anisotropy = 328.2628
9 N Isotropic = 166.2004 Anisotropy = 50.6528
10 C Isotropic = 144.3783 Anisotropy = 24.1745
11 C Isotropic = 144.3879 Anisotropy = 25.5731

12	N	Isotropic =	216.5852	Anisotropy =	35.1364
13	C	Isotropic =	144.7725	Anisotropy =	25.7913
14	C	Isotropic =	144.5174	Anisotropy =	20.5625
15	C	Isotropic =	181.3515	Anisotropy =	42.6154
16	C	Isotropic =	177.4611	Anisotropy =	46.1112
17	H	Isotropic =	29.8959	Anisotropy =	12.0416
18	H	Isotropic =	27.6532	Anisotropy =	6.6091
19	H	Isotropic =	28.4412	Anisotropy =	8.3288
20	H	Isotropic =	28.5961	Anisotropy =	7.7550
21	H	Isotropic =	28.5876	Anisotropy =	8.7134
22	H	Isotropic =	30.3598	Anisotropy =	15.6402
23	H	Isotropic =	28.5769	Anisotropy =	7.7486
24	H	Isotropic =	28.5678	Anisotropy =	8.5891
25	H	Isotropic =	28.4003	Anisotropy =	7.9220
26	H	Isotropic =	27.6815	Anisotropy =	9.0199
27	H	Isotropic =	30.4254	Anisotropy =	14.2703
28	H	Isotropic =	30.4098	Anisotropy =	10.8642
29	H	Isotropic =	30.7365	Anisotropy =	10.2485
30	H	Isotropic =	30.4114	Anisotropy =	14.1853

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.640007694753	1.523962709208	0.005321545361
O	1.640278154365	0.704650317502	0.434466953956
C	2.011971622596	1.173910859422	1.685860482442
N	1.332965070327	2.200933777632	2.067421614825
C	0.425549933720	2.456716026060	1.020200505112
C	3.075058488701	0.430625429176	2.375654042675
C	-0.503027447017	3.518078969627	1.107400829912
N	-1.260054974846	4.403465846713	1.209106784658
N	0.147123291775	1.300797446126	-1.233495941995
C	-1.026701059542	2.050942367194	-1.698877437513
C	-1.007697709748	2.154201977184	-3.222523673352
N	-0.923147372884	0.813591133829	-3.799369778247
C	0.331852993008	0.173312832558	-3.406551047193
C	0.355853851720	-0.001953286684	-1.891108482025
C	2.904825916542	0.080669079599	3.851175246465
C	3.894550056346	1.132225173093	3.444253887987
H	3.579242879665	-0.300897078076	1.743146334031
H	-1.011682549766	3.055531705319	-1.259804751662
H	-1.950528798349	1.538146389545	-1.370492867610
H	-0.159132962364	2.807185952102	-3.523764420515
H	-1.939370305187	2.637319553030	-3.553794743956
H	-0.968254417971	0.878285730566	-4.816574927961
H	1.227792966852	0.756994738794	-3.712978571141
H	0.398416684262	-0.819433324765	-3.877080488226
H	-0.447369761420	-0.699162870631	-1.585670020459
H	1.318250388291	-0.414181411151	-1.568750229250
H	3.276811414678	-0.894223821769	4.173035735227
H	1.976806611840	0.410381357592	4.322957976969
H	3.637681648186	2.174967581053	3.641702329189
H	4.959047691467	0.893444840152	3.485713112296

SCF Done: E(RB3LYP) = -721.814294562

Zero-point correction= 0.245987
Thermal correction to Energy= 0.260263
Thermal correction to Enthalpy= 0.261207
Thermal correction to Gibbs Free Energy= 0.202702
Sum of electronic and zero-point Energies= -721.568307
Sum of electronic and thermal Energies= -721.554031
Sum of electronic and thermal Enthalpies= -721.553087
Sum of electronic and thermal Free Energies= -721.611592

1	C	Isotropic =	32.9416	Anisotropy =	96.4652
2	O	Isotropic =	44.5091	Anisotropy =	178.0083
3	C	Isotropic =	37.9439	Anisotropy =	68.0537
4	N	Isotropic =	19.8807	Anisotropy =	298.9913
5	C	Isotropic =	106.6028	Anisotropy =	38.0057
6	C	Isotropic =	181.1867	Anisotropy =	68.9860
7	C	Isotropic =	78.4079	Anisotropy =	299.8622
8	N	Isotropic =	-13.1036	Anisotropy =	328.0299
9	N	Isotropic =	166.2002	Anisotropy =	50.6405
10	C	Isotropic =	144.4096	Anisotropy =	20.6281
11	C	Isotropic =	144.7424	Anisotropy =	25.6537
12	N	Isotropic =	216.4756	Anisotropy =	34.9463
13	C	Isotropic =	144.4577	Anisotropy =	25.4128
14	C	Isotropic =	144.4086	Anisotropy =	24.1504
15	C	Isotropic =	177.6231	Anisotropy =	46.5787
16	C	Isotropic =	180.8485	Anisotropy =	43.3296
17	H	Isotropic =	29.9099	Anisotropy =	12.0289
18	H	Isotropic =	27.6807	Anisotropy =	8.9957
19	H	Isotropic =	28.3942	Anisotropy =	7.9229
20	H	Isotropic =	28.5762	Anisotropy =	7.7443
21	H	Isotropic =	28.5632	Anisotropy =	8.5966
22	H	Isotropic =	30.3521	Anisotropy =	15.6428
23	H	Isotropic =	28.5989	Anisotropy =	7.7567
24	H	Isotropic =	28.5925	Anisotropy =	8.7076
25	H	Isotropic =	28.4404	Anisotropy =	8.3440
26	H	Isotropic =	27.6511	Anisotropy =	6.6035
27	H	Isotropic =	30.4056	Anisotropy =	14.1991
28	H	Isotropic =	30.7234	Anisotropy =	10.3092
29	H	Isotropic =	30.4419	Anisotropy =	10.7807
30	H	Isotropic =	30.4086	Anisotropy =	14.2719

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.661762331665	1.474068922836	0.119888966611
O	1.439818871705	2.278741827776	-0.657006901043
C	2.438829607472	2.765745447263	0.173049223497
N	2.346426412336	2.339462881728	1.386049792616
C	1.205947275838	1.512123860401	1.403606305586
C	3.404948637926	3.689931191626	-0.435940944484
C	0.787349782876	0.878431892128	2.595078622896

N	0.466134525868	0.368318058127	3.596999198277
N	-0.358949810452	0.828929805719	-0.487352201319
C	-0.877603241412	1.311273963008	-1.779956130641
C	-1.486998022011	0.149804649698	-2.559083007840
N	-2.513314938474	-0.495825660557	-1.740803121051
C	-1.912671224239	-1.068433689378	-0.537158844589
C	-1.312057249444	0.049660642750	0.313058170734
C	4.766232213104	3.867603701875	0.211549571959
C	3.764975314855	4.982227445556	0.292326854698
H	3.346192434362	3.730368440101	-1.524342584252
H	-0.057081964305	1.763852290264	-2.347363323714
H	-1.650037380691	2.082771901350	-1.599352756243
H	-0.672434366014	-0.546427033542	-2.857471131942
H	-1.947030407011	0.544662939813	-3.477672125588
H	-2.963366328084	-1.235568800196	-2.280471065619
H	-1.114453238719	-1.808852108606	-0.764820613339
H	-2.689197391264	-1.579553535157	0.051900883283
H	-2.117314525096	0.711659162434	0.683947067053
H	-0.791967166448	-0.381393786529	1.176812631004
H	5.621123503212	3.978216179937	-0.458308822092
H	4.949041633792	3.282565282454	1.115162661207
H	3.269003191827	5.153004396045	1.250165617939
H	3.916601516825	5.869909731077	-0.325231993605

SCF Done: E(RB3LYP) = -721.814252884

Zero-point correction= 0.245821
Thermal correction to Energy= 0.260166
Thermal correction to Enthalpy= 0.261110
Thermal correction to Gibbs Free Energy= 0.202006
Sum of electronic and zero-point Energies= -721.568432
Sum of electronic and thermal Energies= -721.554087
Sum of electronic and thermal Enthalpies= -721.553143
Sum of electronic and thermal Free Energies= -721.612247

1	C	Isotropic =	32.8732	Anisotropy =	96.0850
2	O	Isotropic =	44.5489	Anisotropy =	178.1529
3	C	Isotropic =	37.8700	Anisotropy =	68.1772
4	N	Isotropic =	19.3536	Anisotropy =	297.8950
5	C	Isotropic =	106.6057	Anisotropy =	37.9906
6	C	Isotropic =	181.1412	Anisotropy =	69.0358
7	C	Isotropic =	78.4086	Anisotropy =	299.8607
8	N	Isotropic =	-12.9363	Anisotropy =	328.2446
9	N	Isotropic =	166.3348	Anisotropy =	50.6209
10	C	Isotropic =	144.4981	Anisotropy =	24.3414
11	C	Isotropic =	144.3009	Anisotropy =	25.5008
12	N	Isotropic =	216.4357	Anisotropy =	35.3511
13	C	Isotropic =	144.8332	Anisotropy =	25.4275
14	C	Isotropic =	144.7028	Anisotropy =	20.6838
15	C	Isotropic =	181.1716	Anisotropy =	43.1472
16	C	Isotropic =	177.4670	Anisotropy =	46.3662
17	H	Isotropic =	29.8945	Anisotropy =	11.9920
18	H	Isotropic =	27.6411	Anisotropy =	6.6254
19	H	Isotropic =	28.4397	Anisotropy =	8.3459
20	H	Isotropic =	28.5912	Anisotropy =	7.7291
21	H	Isotropic =	28.6030	Anisotropy =	8.6817

22	H	Isotropic =	30.3753	Anisotropy =	15.6123
23	H	Isotropic =	28.5664	Anisotropy =	7.7595
24	H	Isotropic =	28.5671	Anisotropy =	8.5786
25	H	Isotropic =	28.3876	Anisotropy =	7.9294
26	H	Isotropic =	27.6863	Anisotropy =	8.9680
27	H	Isotropic =	30.4199	Anisotropy =	14.2684
28	H	Isotropic =	30.4207	Anisotropy =	10.8580
29	H	Isotropic =	30.7187	Anisotropy =	10.2884
30	H	Isotropic =	30.4185	Anisotropy =	14.1904

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.673471720487	1.477171766336	-0.010364129966
O	1.581398758663	0.959790632206	0.863532451024
C	2.669238140193	0.563594786201	0.098973986972
N	2.516325868448	0.791000741693	-1.160564414623
C	1.247930291349	1.392940007204	-1.278758014870
C	3.810023108349	-0.006169837567	0.828557913845
C	0.751895491661	1.799750635468	-2.537704127733
N	0.369195468617	2.126706030284	-3.593138047123
N	-0.511972666527	1.881946241565	0.497971936329
C	-0.639924339458	2.168345258781	1.938420741381
C	-2.084511970850	1.958175516302	2.381676109073
N	-2.967252157018	2.784078303723	1.558520672876
C	-2.894141085343	2.361534355486	0.160862264755
C	-1.475892572556	2.580026993733	-0.362582088021
C	5.213562742150	0.533479811003	0.562174445765
C	4.832174582852	-0.832528581621	0.071701781829
H	3.575147608111	-0.294982424152	1.853853395584
H	-0.341555555835	3.216407527268	2.130793468632
H	0.031603919749	1.505466827930	2.494908499792
H	-2.177616994211	2.261566211547	3.435516171474
H	-2.324154715466	0.873923966330	2.316408856163
H	-3.927428482505	2.691972760829	1.890930440645
H	-3.588408624554	2.966749066207	-0.441547993191
H	-3.163746799811	1.291646102724	0.019806583006
H	-1.394597845761	2.192197862642	-1.384974732962
H	-1.245424781676	3.662089304101	-0.378592041280
H	5.881605415473	0.615226815527	1.422135034662
H	5.294127481712	1.335536419539	-0.174543915034
H	4.654995661180	-0.956255340943	-0.998539552108
H	5.239002332575	-1.705537760343	0.585544303105

SCF Done: E(RB3LYP) = -721.814260378

Zero-point correction= 0.245898
Thermal correction to Energy= 0.260225
Thermal correction to Enthalpy= 0.261169
Thermal correction to Gibbs Free Energy= 0.202039
Sum of electronic and zero-point Energies= -721.568362
Sum of electronic and thermal Energies= -721.554035

Sum of electronic and thermal Enthalpies= -721.553091
Sum of electronic and thermal Free Energies= -721.612221

1	C	Isotropic =	32.7746	Anisotropy =	96.3617
2	O	Isotropic =	44.5483	Anisotropy =	179.1320
3	C	Isotropic =	38.0042	Anisotropy =	67.6974
4	N	Isotropic =	18.7398	Anisotropy =	298.7857
5	C	Isotropic =	106.6105	Anisotropy =	38.1411
6	C	Isotropic =	181.0432	Anisotropy =	68.6193
7	C	Isotropic =	78.4621	Anisotropy =	299.8169
8	N	Isotropic =	-13.0360	Anisotropy =	328.5272
9	N	Isotropic =	166.1036	Anisotropy =	50.7699
10	C	Isotropic =	144.4134	Anisotropy =	24.3068
11	C	Isotropic =	144.4118	Anisotropy =	25.5264
12	N	Isotropic =	216.6075	Anisotropy =	34.9362
13	C	Isotropic =	144.7543	Anisotropy =	25.5248
14	C	Isotropic =	144.5876	Anisotropy =	20.5590
15	C	Isotropic =	177.4056	Anisotropy =	46.3291
16	C	Isotropic =	182.0027	Anisotropy =	42.4131
17	H	Isotropic =	29.8938	Anisotropy =	12.0455
18	H	Isotropic =	28.4420	Anisotropy =	8.3307
19	H	Isotropic =	27.6485	Anisotropy =	6.6317
20	H	Isotropic =	28.5919	Anisotropy =	8.7086
21	H	Isotropic =	28.5984	Anisotropy =	7.7513
22	H	Isotropic =	30.3532	Anisotropy =	15.6517
23	H	Isotropic =	28.5675	Anisotropy =	8.5843
24	H	Isotropic =	28.5824	Anisotropy =	7.7549
25	H	Isotropic =	27.6881	Anisotropy =	8.9814
26	H	Isotropic =	28.3997	Anisotropy =	7.9207
27	H	Isotropic =	30.4236	Anisotropy =	14.1894
28	H	Isotropic =	30.7608	Anisotropy =	10.2410
29	H	Isotropic =	30.3884	Anisotropy =	10.9589
30	H	Isotropic =	30.4345	Anisotropy =	14.2997

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.761628621792	1.394946331002	-0.045865605512
O	0.651766501043	1.908993042361	1.210602236722
C	1.949508840779	2.087284467535	1.668953597854
N	2.844877808409	1.725485304913	0.815498109120
C	2.126506945891	1.268756971323	-0.307235989407
C	2.096034212745	2.668089358522	3.010439752908
C	2.798965208277	0.782724000541	-1.450618556761
N	3.383085703370	0.388225589807	-2.383719213323
N	-0.385486120866	1.172808800756	-0.725288092860
C	-1.674826336678	1.134428533355	-0.012379772276
C	-2.801100413854	1.540069627107	-0.958662814792
N	-2.779008045205	0.673196288619	-2.136112814286
C	-1.529216777095	0.854853000292	-2.872899430686
C	-0.354756223611	0.431716362680	-1.993025361423
C	3.043016763847	3.848135134779	3.215539861963
C	3.408350233909	2.494768973032	3.751346643299

H	1.173759410073	2.663533620342	3.592781966314
H	-1.630105391711	1.816262661853	0.843784287386
H	-1.856217817022	0.109111670361	0.362179047115
H	-2.682703764013	2.616239718704	-1.213705818320
H	-3.761614191996	1.420597046609	-0.434775076341
H	-3.566834635237	0.902521430242	-2.742488257616
H	-1.369033875335	1.906833838617	-3.196984228982
H	-1.539853223393	0.222399349210	-3.773501365831
H	-0.412353498274	-0.654154366862	-1.788595114225
H	0.589018831450	0.637865795737	-2.511576048137
H	2.722380311573	4.621372712636	3.916818622798
H	3.572591993252	4.205947327920	2.330043556370
H	4.186555356627	1.934896649410	3.228745303832
H	3.348693571253	2.324730758593	4.828050575099

SCF Done: E(RB3LYP) = -721.814239749

Zero-point correction= 0.245914
Thermal correction to Energy= 0.260225
Thermal correction to Enthalpy= 0.261169
Thermal correction to Gibbs Free Energy= 0.202528
Sum of electronic and zero-point Energies= -721.568326
Sum of electronic and thermal Energies= -721.554015
Sum of electronic and thermal Enthalpies= -721.553071
Sum of electronic and thermal Free Energies= -721.611711

1	C	Isotropic =	32.8429	Anisotropy =	96.6156
2	O	Isotropic =	44.9700	Anisotropy =	176.7009
3	C	Isotropic =	38.1444	Anisotropy =	67.7355
4	N	Isotropic =	18.9116	Anisotropy =	298.1563
5	C	Isotropic =	106.9297	Anisotropy =	38.1371
6	C	Isotropic =	181.0304	Anisotropy =	68.6679
7	C	Isotropic =	78.4571	Anisotropy =	299.7962
8	N	Isotropic =	-13.5144	Anisotropy =	326.7433
9	N	Isotropic =	165.8328	Anisotropy =	50.8282
10	C	Isotropic =	144.5629	Anisotropy =	23.8368
11	C	Isotropic =	144.2722	Anisotropy =	25.6599
12	N	Isotropic =	216.5921	Anisotropy =	35.6973
13	C	Isotropic =	144.7377	Anisotropy =	25.7913
14	C	Isotropic =	144.6617	Anisotropy =	20.7332
15	C	Isotropic =	177.4668	Anisotropy =	46.6039
16	C	Isotropic =	181.6847	Anisotropy =	42.6460
17	H	Isotropic =	29.8995	Anisotropy =	12.0333
18	H	Isotropic =	27.6486	Anisotropy =	6.6379
19	H	Isotropic =	28.4430	Anisotropy =	8.3688
20	H	Isotropic =	28.6011	Anisotropy =	7.7079
21	H	Isotropic =	28.5915	Anisotropy =	8.6921
22	H	Isotropic =	30.3771	Anisotropy =	15.6343
23	H	Isotropic =	28.5765	Anisotropy =	7.7068
24	H	Isotropic =	28.5730	Anisotropy =	8.5788
25	H	Isotropic =	28.4040	Anisotropy =	8.0216
26	H	Isotropic =	27.6434	Anisotropy =	9.1796
27	H	Isotropic =	30.4117	Anisotropy =	14.1941
28	H	Isotropic =	30.7600	Anisotropy =	10.2468
29	H	Isotropic =	30.3888	Anisotropy =	10.9181
30	H	Isotropic =	30.4328	Anisotropy =	14.2998

1d incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.918782974978	-1.194589984442	0.173025980817
N	1.885418414388	-0.363759647700	-0.369900511606
C	2.537839191841	0.137164888981	0.648150146474
O	2.107004949115	-0.280936034136	1.848477962248
C	1.052004310886	-1.163572911429	1.564720532862
C	3.657190417586	1.081982162262	0.621344039519
C	0.424103344478	-1.772458287539	2.658608679566
N	-0.093627260074	-2.276310179598	3.580749362333
N	0.030586285160	-1.840394284366	-0.626740587568
C	-0.898626929496	-2.831601492663	-0.080538941348
C	-2.173683289471	-2.875249001677	-0.922582018166
N	-1.827961400445	-3.129374150447	-2.320510830745
C	-1.002867299725	-2.039452882090	-2.843424394018
C	0.307043789682	-1.982122171647	-2.063286813338
C	3.700829829887	2.144606121937	-0.471583600105
C	4.664383292894	1.001059788838	-0.521000015586
H	4.028398722038	1.351466525920	1.610273816486
H	-1.153097434601	-2.565425567345	0.952478362673
H	-0.422194396972	-3.831264896670	-0.074756459838
H	-2.721269209591	-1.916901328127	-0.782499800836
H	-2.816588453199	-3.688107741454	-0.551574899452
H	-2.682929888680	-3.204294549437	-2.872453362971
H	-1.504453047282	-1.048773456242	-2.773056311036
H	-0.778260103751	-2.229704239492	-3.904217572766
H	0.877414591604	-2.915330629942	-2.237879367394
H	0.920267870233	-1.134214568887	-2.385800255674
H	4.068408595287	3.129039098233	-0.175918493443
H	2.869491848448	2.142604162908	-1.179075038196
H	4.491243526937	0.218650916038	-1.262315863448
H	5.708656757848	1.182154340213	-0.259543745444

SCF Done: E(RB3LYP) = -721.814488592

Zero-point correction= 0.246135
Thermal correction to Energy= 0.260309
Thermal correction to Enthalpy= 0.261253
Thermal correction to Gibbs Free Energy= 0.203817
Sum of electronic and zero-point Energies= -721.568353
Sum of electronic and thermal Energies= -721.554180
Sum of electronic and thermal Enthalpies= -721.553236
Sum of electronic and thermal Free Energies= -721.610672

1	C	Isotropic =	36.4154	Anisotropy =	102.1703
2	N	Isotropic =	31.4507	Anisotropy =	276.2887
3	C	Isotropic =	23.3684	Anisotropy =	101.7959
4	O	Isotropic =	58.7695	Anisotropy =	155.0768
5	C	Isotropic =	88.7623	Anisotropy =	47.4012

6	C	Isotropic =	179.3224	Anisotropy =	74.2814
7	C	Isotropic =	80.6721	Anisotropy =	292.1960
8	N	Isotropic =	-33.9549	Anisotropy =	269.9220
9	N	Isotropic =	167.0526	Anisotropy =	48.7330
10	C	Isotropic =	144.0328	Anisotropy =	21.3510
11	C	Isotropic =	144.3804	Anisotropy =	25.0054
12	N	Isotropic =	215.6430	Anisotropy =	36.0552
13	C	Isotropic =	143.9835	Anisotropy =	24.6267
14	C	Isotropic =	144.8939	Anisotropy =	22.1535
15	C	Isotropic =	177.5889	Anisotropy =	42.8401
16	C	Isotropic =	177.3804	Anisotropy =	42.6761
17	H	Isotropic =	29.8392	Anisotropy =	12.5771
18	H	Isotropic =	27.8933	Anisotropy =	9.0202
19	H	Isotropic =	28.4541	Anisotropy =	8.0316
20	H	Isotropic =	28.6192	Anisotropy =	7.6796
21	H	Isotropic =	28.6085	Anisotropy =	8.5752
22	H	Isotropic =	30.4145	Anisotropy =	15.5816
23	H	Isotropic =	28.6823	Anisotropy =	7.5891
24	H	Isotropic =	28.6497	Anisotropy =	8.6263
25	H	Isotropic =	28.6418	Anisotropy =	8.3335
26	H	Isotropic =	27.3521	Anisotropy =	8.0140
27	H	Isotropic =	30.2649	Anisotropy =	14.3492
28	H	Isotropic =	30.3698	Anisotropy =	10.6566
29	H	Isotropic =	30.3784	Anisotropy =	10.6239
30	H	Isotropic =	30.2793	Anisotropy =	14.3511

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.062726319532	-1.214016683652	-0.070317743082
N	1.115895072861	-0.212289993786	0.885156275141
C	2.355426127678	0.207861197894	0.892884533642
O	3.164225595810	-0.421879604889	0.026520314605
C	2.343285303242	-1.366252538921	-0.610916128501
C	2.940687244342	1.264495487270	1.721896521586
C	2.949561210112	-2.188863667228	-1.568771365065
N	3.466734119277	-2.871519604038	-2.367963337912
N	-0.110622738494	-1.835157878028	-0.359212020167
C	-1.240798845781	-1.732195716057	0.575284825289
C	-2.558652112785	-1.835499730291	-0.186272720592
N	-2.575682787753	-3.081799373402	-0.952916552801
C	-1.506492323762	-3.076060767274	-1.950395883828
C	-0.151830669038	-2.999572942771	-1.246552211104
C	2.417137344242	1.464457897698	3.140298789445
C	2.087102585668	2.474506061930	2.087052467851
H	4.003841359958	1.425730403743	1.542893605133
H	-1.167744838114	-0.777971920773	1.107398560632
H	-1.181901946685	-2.553153567290	1.316401690875
H	-2.672784977598	-0.933944134437	-0.828302552739
H	-3.388647090611	-1.841866898471	0.536895216127
H	-3.476022394302	-3.180848942455	-1.422764544156
H	-1.584341181481	-2.222069758916	-2.659353577238
H	-1.549338021366	-4.006181855971	-2.537493536410

H	0.016164223687	-3.924646308632	-0.661359830265
H	0.644639722187	-2.917213154429	-1.996050853216
H	3.159185546371	1.719603352220	3.899179246569
H	1.625433424890	0.785193801709	3.461936017598
H	1.070215504887	2.484611639000	1.690193244585
H	2.597189223027	3.439455200247	2.105851547996

SCF Done: E(RB3LYP) = -721.814455923

Zero-point correction= 0.246056
Thermal correction to Energy= 0.260285
Thermal correction to Enthalpy= 0.261229
Thermal correction to Gibbs Free Energy= 0.203318
Sum of electronic and zero-point Energies= -721.568400
Sum of electronic and thermal Energies= -721.554171
Sum of electronic and thermal Enthalpies= -721.553227
Sum of electronic and thermal Free Energies= -721.611138

1	C	Isotropic =	36.3977	Anisotropy =	102.3760
2	N	Isotropic =	31.4758	Anisotropy =	276.7126
3	C	Isotropic =	23.2987	Anisotropy =	101.9147
4	O	Isotropic =	58.8086	Anisotropy =	154.6723
5	C	Isotropic =	88.6678	Anisotropy =	47.6438
6	C	Isotropic =	179.1956	Anisotropy =	74.2096
7	C	Isotropic =	80.5613	Anisotropy =	292.3856
8	N	Isotropic =	-33.8450	Anisotropy =	269.6528
9	N	Isotropic =	167.1177	Anisotropy =	48.3607
10	C	Isotropic =	144.9628	Anisotropy =	21.9535
11	C	Isotropic =	143.9659	Anisotropy =	24.7671
12	N	Isotropic =	215.7967	Anisotropy =	35.7090
13	C	Isotropic =	144.3756	Anisotropy =	25.3210
14	C	Isotropic =	144.0627	Anisotropy =	21.3657
15	C	Isotropic =	177.5648	Anisotropy =	42.7855
16	C	Isotropic =	177.3270	Anisotropy =	43.0147
17	H	Isotropic =	29.8373	Anisotropy =	12.6104
18	H	Isotropic =	27.3639	Anisotropy =	8.0095
19	H	Isotropic =	28.6566	Anisotropy =	8.3291
20	H	Isotropic =	28.6806	Anisotropy =	7.5893
21	H	Isotropic =	28.6495	Anisotropy =	8.6387
22	H	Isotropic =	30.4044	Anisotropy =	15.5793
23	H	Isotropic =	28.6140	Anisotropy =	7.6826
24	H	Isotropic =	28.6152	Anisotropy =	8.5893
25	H	Isotropic =	28.4609	Anisotropy =	8.0267
26	H	Isotropic =	27.8898	Anisotropy =	9.0348
27	H	Isotropic =	30.2514	Anisotropy =	14.3835
28	H	Isotropic =	30.3826	Anisotropy =	10.6088
29	H	Isotropic =	30.3961	Anisotropy =	10.6102
30	H	Isotropic =	30.2464	Anisotropy =	14.3707

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.878641195509	-1.150683319637	-0.093059352224

N	1.248800083466	0.181196794416	-0.211476324626
C	2.186146760474	0.370888167787	0.681138915825
O	2.492876719354	-0.716227206428	1.409742670182
C	1.641360187160	-1.724321702524	0.927505022047
C	2.903278090555	1.620502514020	0.941910447097
C	1.738967001782	-2.980785385289	1.538576035030
N	1.828607957503	-4.027576987440	2.056563598607
N	-0.056199415144	-1.684742212418	-0.921408734109
C	-0.954028662842	-0.800699850748	-1.678261584623
C	-1.366676668750	-1.470847991485	-2.985331945309
N	-1.973942829509	-2.769578016770	-2.690663219043
C	-0.997337737242	-3.649190666907	-2.049765662919
C	-0.562023175746	-3.043369201660	-0.715563304671
C	4.369733779149	1.586430721600	1.360263854034
C	3.328553737984	1.974510747995	2.363631708184
H	2.578594939720	2.432217471488	0.291401134944
H	-0.434162258765	0.144297556768	-1.867347338721
H	-1.858152050516	-0.589789220212	-1.074347624950
H	-0.472554260280	-1.553961819181	-3.642234896394
H	-2.103277648782	-0.832088958841	-3.496520751227
H	-2.297877693437	-3.198817954100	-3.557871512357
H	-0.091375334025	-3.812830947713	-2.674515669302
H	-1.458178503517	-4.630722247687	-1.860342999316
H	-1.421574092018	-3.023358268596	-0.017605909517
H	0.226295206987	-3.664536365663	-0.273263601517
H	5.009731650600	2.364486345282	0.940156020695
H	4.830271876477	0.601181728243	1.455369552473
H	3.077121500877	1.254515007246	3.144785916513
H	3.238119642975	3.024691268454	2.647235555197

SCF Done: E(RB3LYP) = -721.814369606

Zero-point correction= 0.246039
Thermal correction to Energy= 0.260242
Thermal correction to Enthalpy= 0.261187
Thermal correction to Gibbs Free Energy= 0.203540
Sum of electronic and zero-point Energies= -721.568330
Sum of electronic and thermal Energies= -721.554127
Sum of electronic and thermal Enthalpies= -721.553183
Sum of electronic and thermal Free Energies= -721.610830

1	C	Isotropic =	36.5678	Anisotropy =	102.1448
2	N	Isotropic =	18.7395	Anisotropy =	271.1275
3	C	Isotropic =	25.2891	Anisotropy =	102.6677
4	O	Isotropic =	78.8518	Anisotropy =	156.1830
5	C	Isotropic =	88.6474	Anisotropy =	47.2613
6	C	Isotropic =	178.3225	Anisotropy =	74.0240
7	C	Isotropic =	80.6005	Anisotropy =	292.3104
8	N	Isotropic =	-34.6263	Anisotropy =	269.8895
9	N	Isotropic =	167.1947	Anisotropy =	48.6769
10	C	Isotropic =	144.9710	Anisotropy =	22.0906
11	C	Isotropic =	143.9261	Anisotropy =	24.6349
12	N	Isotropic =	215.7292	Anisotropy =	36.0599
13	C	Isotropic =	144.2343	Anisotropy =	25.5225
14	C	Isotropic =	144.1393	Anisotropy =	21.0429
15	C	Isotropic =	179.2773	Anisotropy =	41.0557

16	C	Isotropic =	179.1005	Anisotropy =	41.2072
17	H	Isotropic =	29.6877	Anisotropy =	12.4119
18	H	Isotropic =	27.2058	Anisotropy =	7.2730
19	H	Isotropic =	28.5945	Anisotropy =	8.5035
20	H	Isotropic =	28.6424	Anisotropy =	7.7027
21	H	Isotropic =	28.6165	Anisotropy =	8.7078
22	H	Isotropic =	30.3966	Anisotropy =	15.5569
23	H	Isotropic =	28.6062	Anisotropy =	7.6704
24	H	Isotropic =	28.6029	Anisotropy =	8.4953
25	H	Isotropic =	28.4535	Anisotropy =	7.9573
26	H	Isotropic =	27.9156	Anisotropy =	9.0384
27	H	Isotropic =	30.3070	Anisotropy =	14.3312
28	H	Isotropic =	30.3618	Anisotropy =	10.4701
29	H	Isotropic =	30.3800	Anisotropy =	10.4618
30	H	Isotropic =	30.3163	Anisotropy =	14.3273

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.914709996228	-1.251254901366	0.056948535638
N	1.132703364106	-0.682756236684	1.303476735638
C	1.604791503015	0.514942124223	1.070819296156
O	1.727975600196	0.824332591271	-0.231445873358
C	1.271965948094	-0.314395017992	-0.916262994376
C	1.996721388649	1.508615214371	2.072284210566
C	1.271917922474	-0.253603286166	-2.315517841489
N	1.275607750281	-0.192256161812	-3.485291854877
N	0.462183607797	-2.527369263518	-0.051381724796
C	0.088239373699	-3.090584714308	-1.350334981922
C	0.304147158370	-4.603754431612	-1.348017811260
N	-0.433046050584	-5.200923607441	-0.235324489741
C	0.075627149116	-4.692006645000	1.039204136097
C	-0.157314043194	-3.185758992080	1.107697870327
C	1.771559994218	2.993494467789	1.803992025692
C	3.166124273030	2.449015041485	1.798812827269
H	1.860601351842	1.149767013809	3.092198585895
H	0.701734524297	-2.635386408281	-2.137277423320
H	-0.974795282216	-2.866825000968	-1.565401671119
H	1.397396308813	-4.803798924192	-1.296234624737
H	-0.069369361187	-5.016907612980	-2.297490335444
H	-0.325821274485	-6.215257001772	-0.264278415908
H	1.160770003048	-4.893455644978	1.180046376183
H	-0.467161944417	-5.174632161606	1.866487374959
H	-1.246323559734	-2.984149823136	1.106526535459
H	0.273659688801	-2.761608549129	2.020708884844
H	1.445344940537	3.593917131049	2.655195685931
H	1.321275928641	3.256367319795	0.844832604594
H	3.669281239032	2.339737264819	0.836146962414
H	3.818232501534	2.667386216411	2.646481394685

SCF Done: E(RB3LYP) = -721.814364630

Zero-point correction= 0.246079

Thermal correction to Energy= 0.260283
Thermal correction to Enthalpy= 0.261227
Thermal correction to Gibbs Free Energy= 0.203520
Sum of electronic and zero-point Energies= -721.568286
Sum of electronic and thermal Energies= -721.554081
Sum of electronic and thermal Enthalpies= -721.553137
Sum of electronic and thermal Free Energies= -721.610845

1	C	Isotropic =	36.5507	Anisotropy =	102.1579
2	N	Isotropic =	18.8667	Anisotropy =	271.1106
3	C	Isotropic =	25.3172	Anisotropy =	102.6398
4	O	Isotropic =	78.8290	Anisotropy =	156.4881
5	C	Isotropic =	88.7327	Anisotropy =	47.2072
6	C	Isotropic =	178.3341	Anisotropy =	73.9335
7	C	Isotropic =	80.5782	Anisotropy =	292.3047
8	N	Isotropic =	-34.6842	Anisotropy =	269.6740
9	N	Isotropic =	167.0065	Anisotropy =	48.7703
10	C	Isotropic =	144.0352	Anisotropy =	21.2144
11	C	Isotropic =	144.3866	Anisotropy =	25.1884
12	N	Isotropic =	215.7801	Anisotropy =	36.0338
13	C	Isotropic =	143.9527	Anisotropy =	24.6354
14	C	Isotropic =	145.0729	Anisotropy =	22.4145
15	C	Isotropic =	179.1093	Anisotropy =	40.9756
16	C	Isotropic =	179.3007	Anisotropy =	40.7642
17	H	Isotropic =	29.6842	Anisotropy =	12.3909
18	H	Isotropic =	27.9168	Anisotropy =	9.0500
19	H	Isotropic =	28.4533	Anisotropy =	7.9362
20	H	Isotropic =	28.6015	Anisotropy =	7.6823
21	H	Isotropic =	28.6070	Anisotropy =	8.5010
22	H	Isotropic =	30.3974	Anisotropy =	15.5545
23	H	Isotropic =	28.6380	Anisotropy =	7.7127
24	H	Isotropic =	28.6123	Anisotropy =	8.7165
25	H	Isotropic =	28.5976	Anisotropy =	8.5276
26	H	Isotropic =	27.2102	Anisotropy =	7.2795
27	H	Isotropic =	30.3204	Anisotropy =	14.3069
28	H	Isotropic =	30.3733	Anisotropy =	10.4562
29	H	Isotropic =	30.3554	Anisotropy =	10.4706
30	H	Isotropic =	30.3179	Anisotropy =	14.3174

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.723536098477	-1.169850462222	0.187012742164
N	0.871610781078	-0.087066197812	-0.664320213105
C	1.072050138916	0.949736163570	0.108926339106
O	1.070030343328	0.675609598988	1.422759548895
C	0.833398528942	-0.706393716367	1.501651474141
C	1.296202620336	2.340493717954	-0.293556217679
C	0.758505756360	-1.263863657343	2.784400456286
N	0.697861458493	-1.719490546852	3.861845940543
N	0.544965210769	-2.422395705975	-0.308258381248
C	0.120688877474	-2.602344140322	-1.704104187116
C	0.649309977453	-3.927556920427	-2.244466041031

N	0.200777365609	-5.016085821537	-1.375169692596
C	0.756840078520	-4.851290141281	-0.033019940697
C	0.239885310095	-3.548468390621	0.576972176007
C	0.595345378838	2.870068565188	-1.540134886231
C	2.070041895263	2.620678288840	-1.577696541957
H	1.433591724078	3.024135182873	0.544370845656
H	0.496201607345	-1.759840259278	-2.294268156503
H	-0.985694732599	-2.602091766103	-1.755943376367
H	1.757733580595	-3.867077743643	-2.319891691710
H	0.250052239200	-4.083379969708	-3.258481414506
H	0.508231685116	-5.909064812710	-1.761412149875
H	1.869158397007	-4.825904893831	-0.028493652892
H	0.436290716203	-5.691791631588	0.601355774642
H	-0.854155892278	-3.619540498508	0.733123360644
H	0.717011760652	-3.386999762321	1.551247084175
H	0.237646499507	3.900387990734	-1.493812144371
H	-0.055088998273	2.166434683988	-2.063089934912
H	2.426180068283	1.746444287232	-2.125938495130
H	2.748451525214	3.475688559080	-1.558078624332

SCF Done: E(RB3LYP) = -721.814465381

Zero-point correction= 0.246039
Thermal correction to Energy= 0.260272
Thermal correction to Enthalpy= 0.261216
Thermal correction to Gibbs Free Energy= 0.203253
Sum of electronic and zero-point Energies= -721.568427
Sum of electronic and thermal Energies= -721.554193
Sum of electronic and thermal Enthalpies= -721.553249
Sum of electronic and thermal Free Energies= -721.611212

1	C	Isotropic =	36.4085	Anisotropy =	102.1280
2	N	Isotropic =	31.4160	Anisotropy =	276.3603
3	C	Isotropic =	23.2076	Anisotropy =	101.9075
4	O	Isotropic =	58.7549	Anisotropy =	155.1669
5	C	Isotropic =	88.6312	Anisotropy =	47.4881
6	C	Isotropic =	179.3686	Anisotropy =	74.1974
7	C	Isotropic =	80.6218	Anisotropy =	292.3144
8	N	Isotropic =	-33.7975	Anisotropy =	270.1879
9	N	Isotropic =	167.2229	Anisotropy =	48.5176
10	C	Isotropic =	145.0526	Anisotropy =	21.9383
11	C	Isotropic =	143.9710	Anisotropy =	24.8878
12	N	Isotropic =	215.8946	Anisotropy =	36.2006
13	C	Isotropic =	144.4794	Anisotropy =	25.1734
14	C	Isotropic =	144.0729	Anisotropy =	21.0444
15	C	Isotropic =	177.8181	Anisotropy =	42.6203
16	C	Isotropic =	177.4462	Anisotropy =	42.9964
17	H	Isotropic =	29.8400	Anisotropy =	12.5945
18	H	Isotropic =	27.3632	Anisotropy =	8.0122
19	H	Isotropic =	28.6463	Anisotropy =	8.3270
20	H	Isotropic =	28.6818	Anisotropy =	7.5897
21	H	Isotropic =	28.6557	Anisotropy =	8.6247
22	H	Isotropic =	30.4240	Anisotropy =	15.5877
23	H	Isotropic =	28.6199	Anisotropy =	7.6995
24	H	Isotropic =	28.6105	Anisotropy =	8.5768
25	H	Isotropic =	28.4542	Anisotropy =	8.0182

26 H Isotropic = 27.8904 Anisotropy = 9.0248
27 H Isotropic = 30.2587 Anisotropy = 14.3889
28 H Isotropic = 30.3768 Anisotropy = 10.6357
29 H Isotropic = 30.3958 Anisotropy = 10.6261
30 H Isotropic = 30.2515 Anisotropy = 14.3664

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.123600692967	-1.229507809364	0.113899408807
N	0.986455427301	-0.066731592890	-0.626596865918
C	1.328926447865	0.909252685091	0.175508977248
O	1.695034035376	0.518657147574	1.406203535573
C	1.578636496274	-0.880616333884	1.389225510125
C	1.354960600023	2.344740746155	-0.115958201237
C	1.922643923002	-1.559041048932	2.565348976159
N	2.212357337959	-2.116473462697	3.554034679256
N	0.799534795811	-2.435860272200	-0.421164757774
C	1.098270528737	-3.681109604928	0.289768493550
C	0.097776834219	-4.766088259763	-0.107240777006
N	0.102513834064	-4.926658105969	-1.560485983321
C	-0.327336065606	-3.686312963269	-2.207432271930
C	0.666489835890	-2.576429903035	-1.878361664066
C	0.307790332774	2.925527958573	-1.060422070636
C	1.725899611140	2.805081620457	-1.521834981884
H	1.680632119918	2.958095250649	0.724409861608
H	1.039082827972	-3.508776341214	1.371266877665
H	2.125699843031	-4.015484787148	0.046798716334
H	-0.902686810686	-4.486528530109	0.291343997666
H	0.395976699599	-5.714030439502	0.366215371036
H	-0.531139043381	-5.683346007204	-1.819471290480
H	-1.342873002651	-3.363466754897	-1.887229554271
H	-0.348590781901	-3.833295891694	-3.298245224336
H	1.652544705508	-2.827125057999	-2.316076589698
H	0.336292323789	-1.618095162806	-2.292576805577
H	-0.079741135909	3.913709233367	-0.805528756202
H	-0.421828045291	2.220534346388	-1.463327598220
H	1.964375722232	2.017988944962	-2.239722872570
H	2.334799909973	3.708470396290	-1.590848139902

SCF Done: E(RB3LYP) = -721.814455055

Zero-point correction= 0.246005
Thermal correction to Energy= 0.260251
Thermal correction to Enthalpy= 0.261195
Thermal correction to Gibbs Free Energy= 0.203182
Sum of electronic and zero-point Energies= -721.568450
Sum of electronic and thermal Energies= -721.554204
Sum of electronic and thermal Enthalpies= -721.553260
Sum of electronic and thermal Free Energies= -721.611273

1 C Isotropic = 36.3127 Anisotropy = 102.4009
2 N Isotropic = 31.4057 Anisotropy = 276.4628

3	C	Isotropic =	23.3000	Anisotropy =	101.7145
4	O	Isotropic =	58.5368	Anisotropy =	155.7348
5	C	Isotropic =	88.6382	Anisotropy =	47.6635
6	C	Isotropic =	179.2134	Anisotropy =	74.1152
7	C	Isotropic =	80.6378	Anisotropy =	292.3235
8	N	Isotropic =	-33.9738	Anisotropy =	269.9588
9	N	Isotropic =	167.1478	Anisotropy =	48.6035
10	C	Isotropic =	144.1978	Anisotropy =	21.1846
11	C	Isotropic =	144.4291	Anisotropy =	25.3697
12	N	Isotropic =	215.7239	Anisotropy =	36.0262
13	C	Isotropic =	143.9517	Anisotropy =	24.7863
14	C	Isotropic =	145.1147	Anisotropy =	21.8709
15	C	Isotropic =	177.5005	Anisotropy =	42.7989
16	C	Isotropic =	177.7013	Anisotropy =	42.5892
17	H	Isotropic =	29.8337	Anisotropy =	12.5896
18	H	Isotropic =	27.8747	Anisotropy =	9.0974
19	H	Isotropic =	28.4736	Anisotropy =	8.0088
20	H	Isotropic =	28.6107	Anisotropy =	7.6986
21	H	Isotropic =	28.6183	Anisotropy =	8.5624
22	H	Isotropic =	30.4234	Anisotropy =	15.5693
23	H	Isotropic =	28.6689	Anisotropy =	7.6062
24	H	Isotropic =	28.6564	Anisotropy =	8.6124
25	H	Isotropic =	28.6546	Anisotropy =	8.2887
26	H	Isotropic =	27.3691	Anisotropy =	8.0138
27	H	Isotropic =	30.2491	Anisotropy =	14.3695
28	H	Isotropic =	30.3877	Anisotropy =	10.6188
29	H	Isotropic =	30.3778	Anisotropy =	10.6195
30	H	Isotropic =	30.2561	Anisotropy =	14.3755

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.722968564904	-1.209762323327	0.098407927110
N	0.747966542452	0.176380451949	0.049847238162
C	1.886125687714	0.530999533650	0.588548172995
O	2.648991977445	-0.493090496500	1.008601109416
C	1.902739945292	-1.644452177263	0.707534314140
C	2.379690885859	1.898076670599	0.765507852310
C	2.466465344165	-2.875559211729	1.066346542483
N	2.947026603634	-3.899548366232	1.370469170119
N	-0.321042433253	-1.901443316923	-0.429267417789
C	-1.593211092298	-1.211070136759	-0.688169002591
C	-2.332789236150	-1.890466081512	-1.836406578266
N	-2.517031717903	-3.307257087161	-1.519355304256
C	-1.218418037046	-3.968813399400	-1.401250062584
C	-0.432449870660	-3.350160280536	-0.245380123584
C	3.872721630911	2.191536266894	0.660911668520
C	3.203064090152	2.259362047654	1.998194595062
H	1.686016837569	2.645498006925	0.381220494044
H	-1.378846276121	-0.163262233952	-0.923598132074
H	-2.222964618782	-1.244123700988	0.222390175778
H	-1.758603195772	-1.732218388189	-2.776241451570
H	-3.317379923102	-1.413298380926	-1.957804368669

H	-3.058250963497	-3.754629913046	-2.259759117252
H	-0.608218123301	-3.884853336251	-2.327790815004
H	-1.370350132065	-5.039066746554	-1.193714715411
H	-0.942730083193	-3.570968286692	0.712408605060
H	0.571291877548	-3.791341906644	-0.210452795703
H	4.147939780987	3.123374146967	0.163524545635
H	4.526917545146	1.341234306215	0.458815187887
H	3.399456531742	1.455750494286	2.710595335417
H	3.007961857624	3.238843845442	2.438676950617

SCF Done: E(RB3LYP) = -721.814318181

Zero-point correction= 0.245974
Thermal correction to Energy= 0.260205
Thermal correction to Enthalpy= 0.261149
Thermal correction to Gibbs Free Energy= 0.203270
Sum of electronic and zero-point Energies= -721.568344
Sum of electronic and thermal Energies= -721.554113
Sum of electronic and thermal Enthalpies= -721.553169
Sum of electronic and thermal Free Energies= -721.611049

1	C	Isotropic =	36.3504	Anisotropy =	102.3865
2	N	Isotropic =	18.4141	Anisotropy =	271.5647
3	C	Isotropic =	25.2794	Anisotropy =	102.6295
4	O	Isotropic =	78.4640	Anisotropy =	156.7020
5	C	Isotropic =	88.5310	Anisotropy =	47.4184
6	C	Isotropic =	178.4848	Anisotropy =	74.1555
7	C	Isotropic =	80.6495	Anisotropy =	292.3630
8	N	Isotropic =	-34.5007	Anisotropy =	271.2003
9	N	Isotropic =	167.3491	Anisotropy =	48.5110
10	C	Isotropic =	144.9680	Anisotropy =	22.2303
11	C	Isotropic =	143.9552	Anisotropy =	24.9595
12	N	Isotropic =	215.8786	Anisotropy =	35.6141
13	C	Isotropic =	144.4596	Anisotropy =	25.4332
14	C	Isotropic =	144.1643	Anisotropy =	20.9119
15	C	Isotropic =	179.1963	Anisotropy =	40.6097
16	C	Isotropic =	179.1210	Anisotropy =	41.0178
17	H	Isotropic =	29.6833	Anisotropy =	12.4044
18	H	Isotropic =	27.2160	Anisotropy =	7.2733
19	H	Isotropic =	28.6027	Anisotropy =	8.4801
20	H	Isotropic =	28.6372	Anisotropy =	7.7337
21	H	Isotropic =	28.6130	Anisotropy =	8.7220
22	H	Isotropic =	30.3960	Anisotropy =	15.5370
23	H	Isotropic =	28.6024	Anisotropy =	7.7298
24	H	Isotropic =	28.5959	Anisotropy =	8.5022
25	H	Isotropic =	28.4630	Anisotropy =	7.9158
26	H	Isotropic =	27.9261	Anisotropy =	8.9875
27	H	Isotropic =	30.3147	Anisotropy =	14.2983
28	H	Isotropic =	30.3501	Anisotropy =	10.4782
29	H	Isotropic =	30.3770	Anisotropy =	10.4682
30	H	Isotropic =	30.3235	Anisotropy =	14.3076

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.948966568935	-1.348212789996	-0.129927617774
N	1.693283173842	-0.355772998057	-0.751004570828
C	2.482149493303	0.128522695833	0.173420504505
O	2.348858103349	-0.447821833501	1.380507255330
C	1.356801953782	-1.426521592985	1.204108085562
C	3.460787331790	1.205224381569	0.009633196325
C	1.030994045266	-2.205626974330	2.321572838696
N	0.766312709208	-2.851318479475	3.262358443444
N	-0.008963066058	-2.025316239396	-0.815111989452
C	-0.699077216937	-3.169271843094	-0.215567812169
C	-2.100572802483	-3.307322224503	-0.809577342226
N	-2.007121850684	-3.398847455950	-2.265857971239
C	-1.428727772809	-2.170874678892	-2.812765342851
C	-0.006443074487	-2.006956922635	-2.285231713306
C	4.776264276720	1.165126094128	0.781345913027
C	3.733750852624	2.171627152829	1.157761930152
H	3.478756310598	1.602629219314	-1.004859371154
H	-0.775753600242	-3.022435423021	0.868714381491
H	-0.123219474283	-4.096773461124	-0.401391456857
H	-2.713359959037	-2.442274565118	-0.471801528435
H	-2.564532634890	-4.223969005378	-0.414523341859
H	-2.939104701412	-3.540054281093	-2.656576491994
H	-2.016309359296	-1.263883999114	-2.547739866251
H	-1.395207459147	-2.241827073812	-3.910847036726
H	0.620890201374	-2.838125113735	-2.662448830336
H	0.431711447035	-1.061151637716	-2.621003958409
H	5.662854878192	1.503845111339	0.242165280902
H	4.929308154086	0.313382875415	1.446877859964
H	3.174094250130	2.008338266014	2.080799255055
H	3.889059221533	3.216432796484	0.882491297412

SCF Done: E(RB3LYP) = -721.814337688

Zero-point correction= 0.246063
Thermal correction to Energy= 0.260271
Thermal correction to Enthalpy= 0.261215
Thermal correction to Gibbs Free Energy= 0.203550
Sum of electronic and zero-point Energies= -721.568275
Sum of electronic and thermal Energies= -721.554066
Sum of electronic and thermal Enthalpies= -721.553122
Sum of electronic and thermal Free Energies= -721.610787

1	C	Isotropic = 36.4334	Anisotropy =	102.2658
2	N	Isotropic = 18.6008	Anisotropy =	271.1525
3	C	Isotropic = 25.3076	Anisotropy =	102.4323
4	O	Isotropic = 78.7952	Anisotropy =	157.1332
5	C	Isotropic = 88.6641	Anisotropy =	47.2800
6	C	Isotropic = 178.2884	Anisotropy =	73.8005
7	C	Isotropic = 80.6635	Anisotropy =	292.2344
8	N	Isotropic = -34.7076	Anisotropy =	270.4990
9	N	Isotropic = 167.2701	Anisotropy =	48.4583
10	C	Isotropic = 144.2182	Anisotropy =	20.8824
11	C	Isotropic = 144.3980	Anisotropy =	25.2872
12	N	Isotropic = 215.7898	Anisotropy =	35.3508

13	C	Isotropic =	143.9544	Anisotropy =	24.7856
14	C	Isotropic =	144.9818	Anisotropy =	22.3780
15	C	Isotropic =	179.1687	Anisotropy =	41.5142
16	C	Isotropic =	179.1992	Anisotropy =	40.6697
17	H	Isotropic =	29.6861	Anisotropy =	12.3920
18	H	Isotropic =	27.9180	Anisotropy =	9.0247
19	H	Isotropic =	28.4551	Anisotropy =	7.9468
20	H	Isotropic =	28.6082	Anisotropy =	7.6809
21	H	Isotropic =	28.6056	Anisotropy =	8.5098
22	H	Isotropic =	30.3857	Anisotropy =	15.5386
23	H	Isotropic =	28.6382	Anisotropy =	7.7179
24	H	Isotropic =	28.6182	Anisotropy =	8.7327
25	H	Isotropic =	28.5990	Anisotropy =	8.4989
26	H	Isotropic =	27.2103	Anisotropy =	7.2631
27	H	Isotropic =	30.3106	Anisotropy =	14.3318
28	H	Isotropic =	30.3807	Anisotropy =	10.4749
29	H	Isotropic =	30.3542	Anisotropy =	10.4570
30	H	Isotropic =	30.3052	Anisotropy =	14.3106

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.616516330130	-1.142175153798	-0.044260066661
N	1.562330210580	-0.185999648309	-0.376073015546
C	1.093479412024	0.950430001622	0.072986295683
O	-0.098109995624	0.860812226879	0.683937711595
C	-0.437973389400	-0.499860687501	0.612015624784
C	1.711234584611	2.275645349916	-0.018908298750
C	-1.665789409847	-0.876371184428	1.171120789034
N	-2.694595129165	-1.179961569468	1.641767834731
N	0.823894541553	-2.453341506926	-0.335383455356
C	1.848825048389	-2.826594697867	-1.321152692631
C	2.395610619693	-4.215235411624	-1.005468642835
N	1.288344084130	-5.170759022898	-0.958536121207
C	0.365582422215	-4.821168771612	0.120754034245
C	-0.238994521847	-3.443692613775	-0.149879108742
C	2.528762113759	2.621862595684	-1.259415057808
C	3.230758580509	2.387749198186	0.040944364269
H	1.121788927049	3.068935785783	0.441111427961
H	2.645916446767	-2.076193037041	-1.296836446609
H	1.401969321788	-2.830963982000	-2.334598367729
H	2.963067127975	-4.167509757891	-0.049600573158
H	3.097685053889	-4.510645206705	-1.800261087054
H	1.654831862105	-6.109691896444	-0.799532986890
H	0.858398795176	-4.800767417919	1.118102367114
H	-0.446756482414	-5.562868608610	0.161975221454
H	-0.874268008615	-3.487717519482	-1.055958046127
H	-0.868972181811	-3.149618453979	0.698472185339
H	2.436729080205	3.644329290688	-1.630567116027
H	2.596598714143	1.845270816252	-2.023618521376
H	3.778606079113	1.451662245202	0.164345055752
H	3.632259762919	3.246018638063	0.582966692546

SCF Done: E(RB3LYP) = -721.814450472

Zero-point correction= 0.246000
Thermal correction to Energy= 0.260242
Thermal correction to Enthalpy= 0.261186
Thermal correction to Gibbs Free Energy= 0.203170
Sum of electronic and zero-point Energies= -721.568450
Sum of electronic and thermal Energies= -721.554209
Sum of electronic and thermal Enthalpies= -721.553264
Sum of electronic and thermal Free Energies= -721.611280

1	C	Isotropic =	36.3386	Anisotropy =	102.3728
2	N	Isotropic =	31.4620	Anisotropy =	276.7699
3	C	Isotropic =	23.2409	Anisotropy =	101.9489
4	O	Isotropic =	58.5876	Anisotropy =	155.2253
5	C	Isotropic =	88.5636	Anisotropy =	47.6826
6	C	Isotropic =	179.2936	Anisotropy =	74.0867
7	C	Isotropic =	80.6441	Anisotropy =	292.3913
8	N	Isotropic =	-33.8393	Anisotropy =	270.2044
9	N	Isotropic =	167.1592	Anisotropy =	48.6840
10	C	Isotropic =	144.9942	Anisotropy =	21.7178
11	C	Isotropic =	143.9615	Anisotropy =	24.8088
12	N	Isotropic =	215.8182	Anisotropy =	36.2094
13	C	Isotropic =	144.3590	Anisotropy =	25.6065
14	C	Isotropic =	144.4108	Anisotropy =	21.2011
15	C	Isotropic =	177.4881	Anisotropy =	42.7541
16	C	Isotropic =	177.5939	Anisotropy =	42.6962
17	H	Isotropic =	29.8358	Anisotropy =	12.5902
18	H	Isotropic =	27.3702	Anisotropy =	8.0287
19	H	Isotropic =	28.6551	Anisotropy =	8.2702
20	H	Isotropic =	28.6794	Anisotropy =	7.6041
21	H	Isotropic =	28.6612	Anisotropy =	8.6157
22	H	Isotropic =	30.4326	Anisotropy =	15.5523
23	H	Isotropic =	28.6038	Anisotropy =	7.7048
24	H	Isotropic =	28.6061	Anisotropy =	8.5763
25	H	Isotropic =	28.4676	Anisotropy =	8.0640
26	H	Isotropic =	27.8767	Anisotropy =	9.0721
27	H	Isotropic =	30.2565	Anisotropy =	14.3785
28	H	Isotropic =	30.3894	Anisotropy =	10.5844
29	H	Isotropic =	30.3757	Anisotropy =	10.6609
30	H	Isotropic =	30.2597	Anisotropy =	14.3699

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.049549159493	-1.272161437008	-0.239833230028
N	1.041291848816	0.053672347523	0.161432464741
C	2.290291944728	0.443676010222	0.129336248094
O	3.160199024992	-0.499603382562	-0.264061630598
C	2.370927100685	-1.632037416949	-0.522047248847
C	2.829128841322	1.763239344169	0.467942621543
C	3.036975914493	-2.778300484418	-0.974166487656
N	3.604766925108	-3.730830327772	-1.351534024177

N	-0.101038189862	-1.994492605474	-0.273116785044
C	-0.129692903235	-3.340140355128	-0.850404870531
C	-1.236263415996	-4.168998478070	-0.198657185233
N	-2.512902446755	-3.467657553989	-0.327018734815
C	-2.458760339642	-2.188568009225	0.381875995946
C	-1.397521594989	-1.301354103595	-0.261581820916
C	2.171783779027	2.566257509358	1.585430147347
C	1.992554236610	3.001925673797	0.165338310687
H	3.910799048023	1.838191199771	0.354959441053
H	0.837517695300	-3.830134528340	-0.684564276363
H	-0.304926818722	-3.277634785034	-1.942084533977
H	-0.955868513911	-4.360622626838	0.860898690507
H	-1.299682674369	-5.141071836293	-0.711247674945
H	-3.256746392032	-4.044498751327	0.066958843191
H	-2.220350791267	-2.306108433629	1.462323498003
H	-3.436118297215	-1.687866541622	0.304519534569
H	-1.699064517365	-1.066028786939	-1.301047138373
H	-1.285404166102	-0.361012683455	0.288324788596
H	2.842304251231	3.137939639673	2.229839993809
H	1.324215676256	2.093864939608	2.085689856410
H	1.022928325121	2.825727647069	-0.304107641346
H	2.536817290256	3.879748816477	-0.187997151649

SCF Done: E(RB3LYP) = -721.814431549

Zero-point correction= 0.245992
Thermal correction to Energy= 0.260244
Thermal correction to Enthalpy= 0.261188
Thermal correction to Gibbs Free Energy= 0.203016
Sum of electronic and zero-point Energies= -721.568440
Sum of electronic and thermal Energies= -721.554187
Sum of electronic and thermal Enthalpies= -721.553243
Sum of electronic and thermal Free Energies= -721.611416

1	C	Isotropic =	36.3115	Anisotropy =	102.2864
2	N	Isotropic =	31.2356	Anisotropy =	276.1682
3	C	Isotropic =	23.2141	Anisotropy =	101.8368
4	O	Isotropic =	58.6564	Anisotropy =	155.2246
5	C	Isotropic =	88.5967	Anisotropy =	47.6887
6	C	Isotropic =	179.2695	Anisotropy =	74.1154
7	C	Isotropic =	80.6950	Anisotropy =	292.2922
8	N	Isotropic =	-33.9277	Anisotropy =	270.4805
9	N	Isotropic =	167.1913	Anisotropy =	48.5543
10	C	Isotropic =	144.1465	Anisotropy =	21.1077
11	C	Isotropic =	144.3429	Anisotropy =	25.4748
12	N	Isotropic =	215.7866	Anisotropy =	36.0325
13	C	Isotropic =	143.9622	Anisotropy =	24.9420
14	C	Isotropic =	145.1825	Anisotropy =	21.7945
15	C	Isotropic =	177.3785	Anisotropy =	42.9993
16	C	Isotropic =	177.5724	Anisotropy =	42.8547
17	H	Isotropic =	29.8364	Anisotropy =	12.5830
18	H	Isotropic =	27.8911	Anisotropy =	9.0407
19	H	Isotropic =	28.4731	Anisotropy =	8.0059
20	H	Isotropic =	28.6174	Anisotropy =	7.6886
21	H	Isotropic =	28.6154	Anisotropy =	8.5650
22	H	Isotropic =	30.4208	Anisotropy =	15.5725

23	H	Isotropic =	28.6714	Anisotropy =	7.6063
24	H	Isotropic =	28.6455	Anisotropy =	8.6297
25	H	Isotropic =	28.6525	Anisotropy =	8.3240
26	H	Isotropic =	27.3689	Anisotropy =	8.0097
27	H	Isotropic =	30.2551	Anisotropy =	14.3682
28	H	Isotropic =	30.3891	Anisotropy =	10.6153
29	H	Isotropic =	30.3813	Anisotropy =	10.6226
30	H	Isotropic =	30.2530	Anisotropy =	14.3829

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.127752107638	-1.269869176199	-0.113604112006
N	1.082509778804	-0.450790577317	1.002763682482
C	1.997222423280	0.465311812802	0.809960884272
O	2.673155736681	0.345917318552	-0.343376404577
C	2.129219669674	-0.790328966388	-0.963468066249
C	2.354515538196	1.579224744339	1.691912625223
C	2.677446282421	-1.161307877131	-2.197981696465
N	3.143719341354	-1.461683703663	-3.229694866941
N	0.261443045451	-2.308425256901	-0.248787465635
C	-0.456883574217	-2.814426964691	0.930102588660
C	-1.785681604436	-3.433426621399	0.507588477027
N	-1.537726613050	-4.474287819176	-0.490798037032
C	-0.943726603310	-3.887230123385	-1.691066448830
C	0.410969560131	-3.272701273732	-1.341164744170
C	2.269801080232	1.381908237325	3.201790205606
C	1.261117376465	2.249346370990	2.517235111557
H	3.157199273204	2.206517997921	1.303799915055
H	-0.615073843651	-1.982963134071	1.624970725859
H	0.159705526724	-3.582364693159	1.436893590003
H	-2.452577814692	-2.626876483907	0.129867373923
H	-2.265724679263	-3.882399959037	1.390659942118
H	-2.418481802638	-4.927449983852	-0.736033966277
H	-1.583343005202	-3.097612668989	-2.144033321791
H	-0.792199740058	-4.673218101272	-2.446607873349
H	1.116860428488	-4.072748646712	-1.044318005103
H	0.818320600140	-2.763938135742	-2.223439005577
H	3.052902729134	1.855478707543	3.796867749791
H	1.947779138649	0.395931608034	3.542092465632
H	0.251095803741	1.855085916410	2.390518662372
H	1.335443840111	3.332437452809	2.631370014421

SCF Done: E(RB3LYP) = -721.814448333

Zero-point correction= 0.245984
Thermal correction to Energy= 0.260244
Thermal correction to Enthalpy= 0.261188
Thermal correction to Gibbs Free Energy= 0.202950
Sum of electronic and zero-point Energies= -721.568465
Sum of electronic and thermal Energies= -721.554204
Sum of electronic and thermal Enthalpies= -721.553260
Sum of electronic and thermal Free Energies= -721.611499

1	C	Isotropic =	36.3250	Anisotropy =	102.4819
2	N	Isotropic =	31.2567	Anisotropy =	276.9181
3	C	Isotropic =	23.3242	Anisotropy =	101.7660
4	O	Isotropic =	58.6017	Anisotropy =	156.7214
5	C	Isotropic =	88.6261	Anisotropy =	47.8266
6	C	Isotropic =	179.1992	Anisotropy =	74.1412
7	C	Isotropic =	80.6272	Anisotropy =	292.4064
8	N	Isotropic =	-33.7342	Anisotropy =	270.8876
9	N	Isotropic =	167.2636	Anisotropy =	48.2388
10	C	Isotropic =	145.2803	Anisotropy =	21.9025
11	C	Isotropic =	143.9888	Anisotropy =	25.1876
12	N	Isotropic =	215.8274	Anisotropy =	35.4036
13	C	Isotropic =	144.3554	Anisotropy =	25.4804
14	C	Isotropic =	144.2537	Anisotropy =	20.9337
15	C	Isotropic =	177.7107	Anisotropy =	42.5970
16	C	Isotropic =	177.5127	Anisotropy =	42.8685
17	H	Isotropic =	29.8340	Anisotropy =	12.5837
18	H	Isotropic =	27.3871	Anisotropy =	8.0017
19	H	Isotropic =	28.6605	Anisotropy =	8.3147
20	H	Isotropic =	28.6816	Anisotropy =	7.6271
21	H	Isotropic =	28.6506	Anisotropy =	8.6266
22	H	Isotropic =	30.4060	Anisotropy =	15.5790
23	H	Isotropic =	28.6201	Anisotropy =	7.6948
24	H	Isotropic =	28.6064	Anisotropy =	8.5727
25	H	Isotropic =	28.4713	Anisotropy =	8.0053
26	H	Isotropic =	27.8966	Anisotropy =	9.0286
27	H	Isotropic =	30.2547	Anisotropy =	14.3811
28	H	Isotropic =	30.3818	Anisotropy =	10.6162
29	H	Isotropic =	30.3961	Anisotropy =	10.6292
30	H	Isotropic =	30.2504	Anisotropy =	14.3808

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

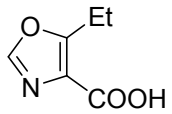
C	0.726130699473	-1.352904168146	-0.082700257216
N	1.823409320864	-1.737968594312	0.670503840988
C	1.345977348585	-2.455585745667	1.655399069306
O	0.012109148951	-2.603132773893	1.644051355395
C	-0.418428111171	-1.897548213648	0.508405945757
C	2.089647767411	-3.095883451690	2.743282037756
C	-1.793483837084	-1.905315267530	0.242506258290
N	-2.945674004324	-1.919236350102	0.031205356698
N	0.876700426045	-0.549573557351	-1.167811034363
C	2.201641909287	-0.385795220381	-1.782634838278
C	2.321318583243	1.006937723340	-2.409478471137
N	1.229560618230	1.338792316389	-3.329427634419
C	-0.068860389145	1.139518003642	-2.683590008248
C	-0.250669448091	-0.248692492912	-2.052256382117
C	3.327874576638	-2.400711200041	3.300421343604
C	3.489855567389	-3.631222158873	2.464853547529
H	1.459921234251	-3.650124551822	3.439458124153
H	2.341684108999	-1.159333175886	-2.565204126301

H	2.965844849793	-0.540756336987	-1.012754211821
H	3.280531649495	1.080842053090	-2.945356883413
H	2.331698938211	1.763534787494	-1.604479590721
H	1.289509603410	0.725485636941	-4.147105132657
H	-0.870403489636	1.307373006177	-3.419597528291
H	-0.178064364126	1.903705675389	-1.893458621738
H	-1.185616663530	-0.272046269706	-1.478079034864
H	-0.321280112035	-1.019144108556	-2.846881713005
H	3.480436481476	-2.473560804880	4.378881263309
H	3.585319265314	-1.440436422561	2.849594644554
H	3.857506734484	-3.509622769631	1.444264314684
H	3.756921587591	-4.568845567885	2.955928366565

SCF Done: E(RB3LYP) = -721.814054147

Zero-point correction= 0.246031
Thermal correction to Energy= 0.260293
Thermal correction to Enthalpy= 0.261238
Thermal correction to Gibbs Free Energy= 0.203241
Sum of electronic and zero-point Energies= -721.568023
Sum of electronic and thermal Energies= -721.553761
Sum of electronic and thermal Enthalpies= -721.552816
Sum of electronic and thermal Free Energies= -721.610814

1	C	Isotropic =	36.3610	Anisotropy =	101.8174
2	N	Isotropic =	32.0373	Anisotropy =	277.5955
3	C	Isotropic =	23.2228	Anisotropy =	102.0992
4	O	Isotropic =	59.5118	Anisotropy =	155.8999
5	C	Isotropic =	88.6701	Anisotropy =	47.7049
6	C	Isotropic =	179.2506	Anisotropy =	74.2039
7	C	Isotropic =	80.6071	Anisotropy =	292.1551
8	N	Isotropic =	-34.2470	Anisotropy =	268.1885
9	N	Isotropic =	167.1973	Anisotropy =	48.9425
10	C	Isotropic =	144.8148	Anisotropy =	17.8709
11	C	Isotropic =	144.9296	Anisotropy =	24.1271
12	N	Isotropic =	221.3992	Anisotropy =	58.3210
13	C	Isotropic =	145.3724	Anisotropy =	24.3622
14	C	Isotropic =	143.4212	Anisotropy =	17.5935
15	C	Isotropic =	177.2993	Anisotropy =	43.1004
16	C	Isotropic =	177.4969	Anisotropy =	42.8350
17	H	Isotropic =	29.8429	Anisotropy =	12.5962
18	H	Isotropic =	28.8291	Anisotropy =	8.1423
19	H	Isotropic =	27.3978	Anisotropy =	7.8481
20	H	Isotropic =	28.6504	Anisotropy =	8.7582
21	H	Isotropic =	28.7229	Anisotropy =	7.2924
22	H	Isotropic =	31.1236	Anisotropy =	12.5370
23	H	Isotropic =	28.6141	Anisotropy =	8.6773
24	H	Isotropic =	28.6802	Anisotropy =	7.4155
25	H	Isotropic =	27.9321	Anisotropy =	8.8197
26	H	Isotropic =	28.6074	Anisotropy =	7.7448
27	H	Isotropic =	30.2476	Anisotropy =	14.3651
28	H	Isotropic =	30.4034	Anisotropy =	10.5941
29	H	Isotropic =	30.3785	Anisotropy =	10.6465
30	H	Isotropic =	30.2488	Anisotropy =	14.3815



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Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.652248863385	1.092663606411	0.067403704379
C	0.202524408416	-0.061428313122	0.662846309292
O	1.052163783485	-0.321304205088	1.700893086689
C	1.969902314843	0.688690046025	1.680396870822
N	1.787892885298	1.555675600877	0.740519063223
C	0.061190212929	1.772922419444	-1.095627319656
C	-0.917087146043	-1.011668475869	0.423875161215
O	-0.926301088407	1.385839616925	-1.698130771388
O	0.732490389147	2.889858460803	-1.436479637598
C	-0.440935008988	-2.427995497840	0.058263340735
H	2.743632448750	0.659511705443	2.443177130040
H	-1.537345969813	-1.055400478641	1.336197887238
H	-1.535431306104	-0.588136194925	-0.378091325166
H	0.268370312172	3.264799375745	-2.208519470307
H	-1.307815454953	-3.090316351656	-0.086466680854
H	0.146216826593	-2.420177990352	-0.873626557780
H	0.186633529289	-2.855333324179	0.855669209115

SCF Done: E(RB3LYP) = -513.326109294

Zero-point correction= 0.129263
Thermal correction to Energy= 0.138480
Thermal correction to Enthalpy= 0.139425
Thermal correction to Gibbs Free Energy= 0.093703
Sum of electronic and zero-point Energies= -513.196847
Sum of electronic and thermal Energies= -513.187629
Sum of electronic and thermal Enthalpies= -513.186685
Sum of electronic and thermal Free Energies= -513.232406

1	C	Isotropic =	65.5862	Anisotropy = 83.2669
2	C	Isotropic =	26.3811	Anisotropy = 127.4187
3	O	Isotropic =	7.5898	Anisotropy = 284.7301
4	C	Isotropic =	46.2525	Anisotropy = 84.6128
5	N	Isotropic =	-5.7976	Anisotropy = 347.4974
6	C	Isotropic =	32.4573	Anisotropy = 90.8108
7	C	Isotropic =	169.3255	Anisotropy = 14.9010
8	O	Isotropic =	-25.3389	Anisotropy = 466.2943
9	O	Isotropic =	139.9595	Anisotropy = 165.4497
10	C	Isotropic =	176.7240	Anisotropy = 22.3810
11	H	Isotropic =	23.8878	Anisotropy = 4.2948
12	H	Isotropic =	28.7096	Anisotropy = 8.0782
13	H	Isotropic =	27.6726	Anisotropy = 8.6942
14	H	Isotropic =	25.5791	Anisotropy = 11.0313
15	H	Isotropic =	30.0432	Anisotropy = 9.9868
16	H	Isotropic =	30.3222	Anisotropy = 7.6427

17 H Isotropic = 29.9667 Anisotropy = 8.0410

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.315817709382	0.915027233655	-0.419795923457
C	1.093178557360	0.455214479950	0.617689194293
O	2.389589569416	0.509139331739	0.185056300088
C	2.328769422198	1.000266641529	-1.085817085421
N	1.133963250555	1.260911531190	-1.499594543998
C	-1.145943140923	1.067906162291	-0.518237003428
C	0.859519350578	-0.074366259124	1.990058410666
O	-1.730081084704	1.516689773619	-1.484324174045
O	-1.787760276263	0.645032450775	0.595477573375
C	0.980822240812	-1.607151689608	2.067020806456
H	3.274389731457	1.121718509568	-1.607715041873
H	1.596283340243	0.390679362333	2.665713466983
H	-0.139382920435	0.243842458834	2.313337301567
H	-2.740489304458	0.788295713879	0.440871777292
H	1.974780069823	-1.944536943316	1.733989751694
H	0.833369510005	-1.945288159426	3.104065803979
H	0.221813974954	-2.092850597890	1.433903385829

SCF Done: E(RB3LYP) = -513.324956253

Zero-point correction= 0.129257
Thermal correction to Energy= 0.138488
Thermal correction to Enthalpy= 0.139432
Thermal correction to Gibbs Free Energy= 0.093405
Sum of electronic and zero-point Energies= -513.195700
Sum of electronic and thermal Energies= -513.186468
Sum of electronic and thermal Enthalpies= -513.185524
Sum of electronic and thermal Free Energies= -513.231551

1 C Isotropic = 64.9995 Anisotropy = 79.7252
2 C Isotropic = 27.6929 Anisotropy = 126.6467
3 O Isotropic = 7.7151 Anisotropy = 265.0954
4 C Isotropic = 45.5946 Anisotropy = 85.8978
5 N Isotropic = -8.6408 Anisotropy = 349.9517
6 C Isotropic = 34.3367 Anisotropy = 83.9454
7 C Isotropic = 168.2244 Anisotropy = 15.2812
8 O Isotropic = -45.3259 Anisotropy = 494.2901
9 O Isotropic = 147.4657 Anisotropy = 180.4407
10 C Isotropic = 175.5990 Anisotropy = 24.0973
11 H Isotropic = 23.8623 Anisotropy = 4.2448
12 H Isotropic = 28.6446 Anisotropy = 7.9238
13 H Isotropic = 27.9065 Anisotropy = 7.5863
14 H Isotropic = 25.5129 Anisotropy = 11.6416
15 H Isotropic = 30.0868 Anisotropy = 7.9413
16 H Isotropic = 30.0128 Anisotropy = 10.0439
17 H Isotropic = 30.2436 Anisotropy = 7.2646

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.214085693093	0.541807770801	0.116116810156
C	1.069201778405	0.566238676411	0.607490904790
O	1.041360551289	-0.092561044224	1.804072900512
C	-0.256188539746	-0.479598801235	1.975212602959
N	-1.046786422533	-0.134699413736	1.013988878759
C	-0.685523658894	1.124604398733	-1.149971785660
C	2.374375861200	1.105352914102	0.138995991793
O	0.020774035609	1.724054815596	-1.943648945802
O	-2.002708013669	0.926230804923	-1.351090466340
C	3.428414206905	0.011575103716	-0.103786900963
H	-0.485451613459	-1.027282739979	2.885606578695
H	2.178935852866	1.671225912936	-0.780995131628
H	2.749010409213	1.816827234050	0.895648013257
H	-2.215793554591	1.344466396989	-2.206515563466
H	4.376855576778	0.468083649477	-0.424926458205
H	3.620219819157	-0.566996941216	0.813112701510
H	3.099579404564	-0.687958737344	-0.888520130366

SCF Done: E(RB3LYP) = -513.326107047

Zero-point correction= 0.129340
Thermal correction to Energy= 0.138531
Thermal correction to Enthalpy= 0.139476
Thermal correction to Gibbs Free Energy= 0.093951
Sum of electronic and zero-point Energies= -513.196767
Sum of electronic and thermal Energies= -513.187576
Sum of electronic and thermal Enthalpies= -513.186631
Sum of electronic and thermal Free Energies= -513.232156

1	C	Isotropic =	65.6094	Anisotropy =	83.2297
2	C	Isotropic =	26.4641	Anisotropy =	127.5749
3	O	Isotropic =	7.8574	Anisotropy =	284.8229
4	C	Isotropic =	46.2213	Anisotropy =	84.6755
5	N	Isotropic =	-5.6770	Anisotropy =	347.8971
6	C	Isotropic =	32.4022	Anisotropy =	90.8857
7	C	Isotropic =	169.2688	Anisotropy =	14.9711
8	O	Isotropic =	-25.4111	Anisotropy =	466.3283
9	O	Isotropic =	139.8883	Anisotropy =	165.4076
10	C	Isotropic =	176.7043	Anisotropy =	22.3565
11	H	Isotropic =	23.8909	Anisotropy =	4.2851
12	H	Isotropic =	27.6691	Anisotropy =	8.6997
13	H	Isotropic =	28.6990	Anisotropy =	8.0877
14	H	Isotropic =	25.5768	Anisotropy =	11.0249
15	H	Isotropic =	30.0405	Anisotropy =	9.9847
16	H	Isotropic =	29.9680	Anisotropy =	8.0364
17	H	Isotropic =	30.3277	Anisotropy =	7.6542

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.406567992077	1.070448043674	0.473687271155
C	1.130807786404	0.049627303263	-0.096520121952
O	2.202750121958	-0.170804738283	0.723296080921
C	2.073036432181	0.728081772235	1.741124892327
N	1.034545255716	1.490014790868	1.649828684285
C	-0.843576499004	1.707093201919	0.026657657072
C	1.000464782180	-0.822698020720	-1.297278541445
O	-1.387302435742	2.636995347482	0.588262397911
O	-1.340419031996	1.134900589037	-1.094968617668
C	0.321978542273	-2.169310699082	-0.986072249533
H	2.843998078823	0.712210955423	2.507074670831
H	0.422476756352	-0.278612954491	-2.055362800259
H	2.010123613256	-0.997059815869	-1.702463857285
H	-2.156768979121	1.620135614527	-1.319023867062
H	0.277896532836	-2.788510738668	-1.895169679541
H	0.878529826913	-2.727452660076	-0.216901467649
H	-0.706058775105	-2.012957991239	-0.624020452110

SCF Done: E(RB3LYP) = -513.324931561

Zero-point correction= 0.129245
Thermal correction to Energy= 0.138481
Thermal correction to Enthalpy= 0.139425
Thermal correction to Gibbs Free Energy= 0.093344
Sum of electronic and zero-point Energies= -513.195687
Sum of electronic and thermal Energies= -513.186451
Sum of electronic and thermal Enthalpies= -513.185506
Sum of electronic and thermal Free Energies= -513.231588

1	C	Isotropic =	64.9269	Anisotropy =	80.5038
2	C	Isotropic =	27.3381	Anisotropy =	127.1840
3	O	Isotropic =	6.8647	Anisotropy =	260.5720
4	C	Isotropic =	45.7850	Anisotropy =	85.5262
5	N	Isotropic =	-9.0398	Anisotropy =	350.2451
6	C	Isotropic =	34.4031	Anisotropy =	83.7674
7	C	Isotropic =	168.0620	Anisotropy =	15.5120
8	O	Isotropic =	-44.4010	Anisotropy =	493.6223
9	O	Isotropic =	147.0085	Anisotropy =	179.6420
10	C	Isotropic =	175.4956	Anisotropy =	24.1891
11	H	Isotropic =	23.8719	Anisotropy =	4.2803
12	H	Isotropic =	27.9630	Anisotropy =	7.0160
13	H	Isotropic =	28.6441	Anisotropy =	7.8681
14	H	Isotropic =	25.5030	Anisotropy =	11.6103
15	H	Isotropic =	30.0242	Anisotropy =	10.0901
16	H	Isotropic =	30.1562	Anisotropy =	7.9259
17	H	Isotropic =	30.1935	Anisotropy =	7.0670

1e incorrect isomer

Conformer 1

```
---------------------------------------------------------------------------
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)
---------------------------------------------------------------------------
C        0.099031534472      0.062690686241     -0.010862330766
C        1.220795785296      0.852850718820     -0.087149918618
N        2.338301169846      0.027504828098     -0.017651614895
C        1.854738383434     -1.176222298414      0.091041195238
O        0.511828211306     -1.249888941952      0.103092010293
C       -1.330623910121      0.369938538415     -0.032504500750
C        1.349571852653      2.338072087537     -0.207544763405
O       -1.782385834486      1.497332923623     -0.133527123955
O       -2.097786896513     -0.732271539784      0.072582560094
C        2.019184591967      2.972128347668      1.022309126534
H        2.398910209268     -2.114568766120      0.170148778990
H        1.956146733571      2.555438883766     -1.103737137088
H        0.351229638538      2.765820609800     -0.368352297435
H       -3.025340560106     -0.430174656713      0.050026444167
H        1.410509381740      2.818784308603      1.927994882426
H        3.012400522332      2.531324080091      1.200963353180
H        2.145339186802      4.055600190323      0.873321335991

SCF Done:  E(RB3LYP) =  -513.323778036

Zero-point correction=                          0.129321
Thermal correction to Energy=                   0.138509
Thermal correction to Enthalpy=                 0.139453
Thermal correction to Gibbs Free Energy=        0.094110
Sum of electronic and zero-point Energies=          -513.194457
Sum of electronic and thermal Energies=             -513.185269
Sum of electronic and thermal Enthalpies=           -513.184325
Sum of electronic and thermal Free Energies=        -513.229668

1  C    Isotropic =    55.2617   Anisotropy =    83.0324
2  C    Isotropic =    35.4375   Anisotropy =   140.8518
3  N    Isotropic =   -14.7603   Anisotropy =   355.3601
4  C    Isotropic =    42.1361   Anisotropy =    94.4146
5  O    Isotropic =    30.1217   Anisotropy =   255.5885
6  C    Isotropic =    37.2179   Anisotropy =    84.5448
7  C    Isotropic =   167.9255   Anisotropy =    13.3635
8  O    Isotropic =   -23.4398   Anisotropy =   462.0800
9  O    Isotropic =   144.0324   Anisotropy =   162.7737
10  C    Isotropic =   175.9675   Anisotropy =    22.7450
11  H    Isotropic =    23.7510   Anisotropy =     4.0435
12  H    Isotropic =    28.8410   Anisotropy =     7.9271
13  H    Isotropic =    27.9116   Anisotropy =     8.3873
14  H    Isotropic =    25.5440   Anisotropy =    11.4473
15  H    Isotropic =    30.3773   Anisotropy =     7.5667
16  H    Isotropic =    29.9144   Anisotropy =     8.0255
17  H    Isotropic =    30.0398   Anisotropy =     9.9278
```

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.511689609218	0.724440447686	0.610079393278
C	0.851247570190	0.328382866015	-0.661267220720
N	2.085772790314	-0.309695177485	-0.601700208410
C	2.420239550636	-0.267121712813	0.655660093957
O	1.529229961134	0.339522503458	1.460077627280
C	-0.651039250321	1.428785186284	1.149228752809
C	0.109516846687	0.480835848297	-1.950922731996
O	-1.592843138045	1.803433543412	0.472462567556
O	-0.568442956046	1.619463469603	2.480162421449
C	-0.334430052498	-0.869598968695	-2.536371391465
H	3.320880047744	-0.656133702096	1.125096994712
H	-0.757453095581	1.133316140395	-1.783315090623
H	0.777255259812	0.986457867861	-2.669618648268
H	-1.380160900194	2.091421925605	2.745828522835
H	-0.828366789253	-0.721491647080	-3.509062857613
H	0.529185129350	-1.536163274292	-2.686781514373
H	-1.044470583146	-1.378055316155	-1.864406710407

SCF Done: E(RB3LYP) = -513.323785332

Zero-point correction= 0.129273
Thermal correction to Energy= 0.138495
Thermal correction to Enthalpy= 0.139439
Thermal correction to Gibbs Free Energy= 0.093785
Sum of electronic and zero-point Energies= -513.194512
Sum of electronic and thermal Energies= -513.185291
Sum of electronic and thermal Enthalpies= -513.184346
Sum of electronic and thermal Free Energies= -513.230000

1	C	Isotropic =	55.1817	Anisotropy = 83.0112
2	C	Isotropic =	35.3844	Anisotropy = 140.9975
3	N	Isotropic =	-14.9259	Anisotropy = 354.5801
4	C	Isotropic =	42.1797	Anisotropy = 94.3208
5	O	Isotropic =	30.0444	Anisotropy = 255.9923
6	C	Isotropic =	37.1990	Anisotropy = 84.5277
7	C	Isotropic =	167.8432	Anisotropy = 13.3753
8	O	Isotropic =	-23.5035	Anisotropy = 462.4241
9	O	Isotropic =	144.0739	Anisotropy = 162.7853
10	C	Isotropic =	175.8232	Anisotropy = 22.9116
11	H	Isotropic =	23.7531	Anisotropy = 4.0459
12	H	Isotropic =	27.9193	Anisotropy = 8.2910
13	H	Isotropic =	28.8427	Anisotropy = 7.9290
14	H	Isotropic =	25.5452	Anisotropy = 11.4530
15	H	Isotropic =	30.0340	Anisotropy = 9.9324
16	H	Isotropic =	29.9357	Anisotropy = 8.0023
17	H	Isotropic =	30.3741	Anisotropy = 7.5320

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.086017591995	0.176266626467	-0.286060722153
C	1.296751612921	0.579407391398	0.227621198919
N	2.157527935767	-0.514287220876	0.215195640009
C	1.452412250411	-1.485309845555	-0.288709882017
O	0.192483008243	-1.158254267836	-0.620276477067
C	-1.214479076823	0.797976245144	-0.547908557218
C	1.748730128867	1.902449625092	0.761083168446
O	-2.165828519321	0.221616191391	-1.038082841308
O	-1.239088708794	2.096226775443	-0.177977910100
C	1.982198279989	1.869556958024	2.280645826079
H	1.758422994374	-2.512696613398	-0.472233043825
H	2.693093929564	2.163650081221	0.254089726678
H	1.009177973928	2.671194022075	0.503969876722
H	-2.131967151727	2.430397662757	-0.386619812614
H	2.371540670134	2.838473166974	2.629545700904
H	1.044183442528	1.661474007824	2.820099648855
H	2.710843637943	1.088729193855	2.549448459688

SCF Done: E(RB3LYP) = -513.322804796

Zero-point correction= 0.129251
Thermal correction to Energy= 0.138500
Thermal correction to Enthalpy= 0.139444
Thermal correction to Gibbs Free Energy= 0.093464
Sum of electronic and zero-point Energies= -513.193553
Sum of electronic and thermal Energies= -513.184305
Sum of electronic and thermal Enthalpies= -513.183360
Sum of electronic and thermal Free Energies= -513.229341

1	C	Isotropic =	54.4111	Anisotropy = 79.4354
2	C	Isotropic =	38.0824	Anisotropy = 138.3851
3	N	Isotropic =	-14.9181	Anisotropy = 348.2428
4	C	Isotropic =	41.0748	Anisotropy = 97.5321
5	O	Isotropic =	26.5212	Anisotropy = 257.6565
6	C	Isotropic =	38.0510	Anisotropy = 80.2479
7	C	Isotropic =	167.0720	Anisotropy = 13.8540
8	O	Isotropic =	-39.0017	Anisotropy = 484.6636
9	O	Isotropic =	150.9556	Anisotropy = 174.4624
10	C	Isotropic =	175.3389	Anisotropy = 23.7443
11	H	Isotropic =	23.6626	Anisotropy = 3.8513
12	H	Isotropic =	28.8029	Anisotropy = 7.9211
13	H	Isotropic =	28.0602	Anisotropy = 8.0742
14	H	Isotropic =	25.5329	Anisotropy = 11.8897
15	H	Isotropic =	30.0099	Anisotropy = 9.9541
16	H	Isotropic =	30.3321	Anisotropy = 7.4335
17	H	Isotropic =	29.9570	Anisotropy = 7.9586

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

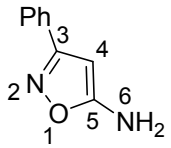
C	0.341303388724	1.088812077955	-0.034388613859
C	1.006467463705	-0.100817535844	-0.220186205514

N	2.344281585478	0.187123998475	-0.474235859148
C	2.417060278432	1.486138837711	-0.434562337809
O	1.256295342898	2.111287645904	-0.176705034162
C	-1.034336738723	1.496798135110	0.260462266313
C	0.524599169580	-1.516455952477	-0.163967972275
O	-1.404243767516	2.650370894586	0.360174663257
O	-1.853682984576	0.434537531915	0.413497943659
C	0.998308854073	-2.243544850554	1.105911354458
H	3.291432783358	2.114965127679	-0.585648108042
H	-0.571104628593	-1.532323557382	-0.224580403439
H	0.918164575393	-2.039680960234	-1.051368887438
H	-2.743146015399	0.790528918956	0.599401683370
H	0.675931183335	-3.296145668972	1.087559412160
H	2.096624619522	-2.221446760707	1.185807551236
H	0.580354890309	-1.771257882120	2.009408547232

SCF Done: E(RB3LYP) = -513.322814080

Zero-point correction= 0.129294
Thermal correction to Energy= 0.138525
Thermal correction to Enthalpy= 0.139469
Thermal correction to Gibbs Free Energy= 0.093502
Sum of electronic and zero-point Energies= -513.193520
Sum of electronic and thermal Energies= -513.184289
Sum of electronic and thermal Enthalpies= -513.183345
Sum of electronic and thermal Free Energies= -513.229313

1	C	Isotropic =	54.3422	Anisotropy =	79.6035
2	C	Isotropic =	37.9892	Anisotropy =	138.7919
3	N	Isotropic =	-15.2920	Anisotropy =	345.6572
4	C	Isotropic =	41.1121	Anisotropy =	97.5201
5	O	Isotropic =	26.2014	Anisotropy =	258.4804
6	C	Isotropic =	38.0557	Anisotropy =	80.1871
7	C	Isotropic =	166.8737	Anisotropy =	14.2820
8	O	Isotropic =	-38.6521	Anisotropy =	484.5298
9	O	Isotropic =	150.7330	Anisotropy =	174.0305
10	C	Isotropic =	175.0310	Anisotropy =	24.1840
11	H	Isotropic =	23.6666	Anisotropy =	3.8594
12	H	Isotropic =	28.0774	Anisotropy =	7.7112
13	H	Isotropic =	28.8032	Anisotropy =	7.9105
14	H	Isotropic =	25.5249	Anisotropy =	11.8755
15	H	Isotropic =	30.0030	Anisotropy =	9.9861
16	H	Isotropic =	30.0144	Anisotropy =	7.9052
17	H	Isotropic =	30.3157	Anisotropy =	7.3166



2a

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.250811391182	1.412866387056	0.452558426997
C	-0.267700183116	0.559749908367	0.206577552612
C	-0.712245688333	-0.794918005595	0.244101116037
C	-2.052893588275	-0.687821414741	0.534617998885
O	-2.394660601205	0.609800408723	0.662136226369
N	-3.037469214289	-1.604062663710	0.776834062835
C	1.094024916550	1.064431196488	-0.069386489262
C	2.171210144799	0.174542095071	-0.222789177982
C	3.457889872380	0.654090233360	-0.483889904477
C	3.687995589070	2.028743970787	-0.595262703071
C	2.620974262031	2.923124558686	-0.443202152759
C	1.335748405271	2.446949261987	-0.183294098237
H	-0.148832945702	-1.705455296807	0.074480436562
H	-2.874471028945	-2.520685284402	0.370652297207
H	-3.983723155166	-1.268293710258	0.613003782040
H	2.009121093132	-0.901002919557	-0.134329866117
H	4.283520834648	-0.051361423468	-0.599907678282
H	4.693553974655	2.402694363421	-0.799910672141
H	2.791922023357	3.998499024343	-0.529572438099
H	0.504036680320	3.143059310246	-0.068186719118

SCF Done: E(RB3LYP) = -532.503447072

Zero-point correction= 0.155330
Thermal correction to Energy= 0.164872
Thermal correction to Enthalpy= 0.165816
Thermal correction to Gibbs Free Energy= 0.119581
Sum of electronic and zero-point Energies= -532.348117
Sum of electronic and thermal Energies= -532.338575
Sum of electronic and thermal Enthalpies= -532.337631
Sum of electronic and thermal Free Energies= -532.383866

1	N	Isotropic =	-91.3660	Anisotropy = 176.6122
2	C	Isotropic =	30.2858	Anisotropy = 134.9568
3	C	Isotropic =	115.5148	Anisotropy = 63.8675
4	C	Isotropic =	23.8082	Anisotropy = 114.1150
5	O	Isotropic =	-6.1572	Anisotropy = 175.8217
6	N	Isotropic =	204.1952	Anisotropy = 67.6411
7	C	Isotropic =	61.8679	Anisotropy = 169.7330
8	C	Isotropic =	66.1598	Anisotropy = 166.4521
9	C	Isotropic =	64.0412	Anisotropy = 173.9811
10	C	Isotropic =	63.4367	Anisotropy = 177.2967
11	C	Isotropic =	64.2653	Anisotropy = 174.2940
12	C	Isotropic =	68.1601	Anisotropy = 171.5558
13	H	Isotropic =	25.9502	Anisotropy = 5.0921
14	H	Isotropic =	27.4504	Anisotropy = 11.9805
15	H	Isotropic =	27.3498	Anisotropy = 11.9113
16	H	Isotropic =	23.8675	Anisotropy = 8.4329
17	H	Isotropic =	23.9565	Anisotropy = 5.1204
18	H	Isotropic =	23.9848	Anisotropy = 4.6258
19	H	Isotropic =	23.9938	Anisotropy = 4.9969

20 H Isotropic = 23.3411 Anisotropy = 7.8798

2a incorrect isomer

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

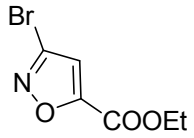
N	-1.748463766107	-1.156511329160	0.008299868366
C	-2.372254616372	0.009823529064	0.077049015109
C	-1.450919473986	1.102307816265	0.147120063285
C	-0.220469038869	0.502067987607	0.107751838481
O	-0.376136399781	-0.839866092162	0.018784625118
C	1.149747763578	1.019572360439	0.138961156274
N	-3.749222251771	0.095357147330	0.008582831552
C	1.386510764464	2.404549140325	0.232510195270
C	2.691569395161	2.896514872698	0.263016696658
C	3.779399218561	2.017215533901	0.200515236712
C	3.552163499413	0.639766894379	0.107416917603
C	2.248539010668	0.141408793980	0.076836022140
H	-1.686191092832	2.159821667876	0.212045518522
H	-4.141635278242	0.870286030073	0.536966777925
H	-4.222643409249	-0.777501334592	0.232468311914
H	0.546945608257	3.100284688770	0.281875710340
H	2.860630822014	3.972928317342	0.335853424881
H	4.800007913693	2.405113468052	0.224316059786
H	4.395600872471	-0.052339029308	0.058395248769
H	2.074440458930	-0.932640462880	0.004584481296

SCF Done: E(RB3LYP) = -532.503520124

Zero-point correction= 0.155600
Thermal correction to Energy= 0.165064
Thermal correction to Enthalpy= 0.166008
Thermal correction to Gibbs Free Energy= 0.120068
Sum of electronic and zero-point Energies= -532.347920
Sum of electronic and thermal Energies= -532.338457
Sum of electronic and thermal Enthalpies= -532.337512
Sum of electronic and thermal Free Energies= -532.383452

1 N Isotropic = -76.2905 Anisotropy = 180.8921
2 C Isotropic = 28.9952 Anisotropy = 131.1005
3 C Isotropic = 100.8215 Anisotropy = 82.8735
4 C Isotropic = 23.8034 Anisotropy = 113.5141
5 O Isotropic = 5.0246 Anisotropy = 184.1124
6 C Isotropic = 64.3786 Anisotropy = 164.5007
7 N Isotropic = 215.4731 Anisotropy = 59.0632
8 C Isotropic = 67.2894 Anisotropy = 164.9739
9 C Isotropic = 63.7789 Anisotropy = 175.0901
10 C Isotropic = 63.1026 Anisotropy = 177.8675
11 C Isotropic = 63.9486 Anisotropy = 176.0769
12 C Isotropic = 68.1220 Anisotropy = 172.9856
13 H Isotropic = 25.2732 Anisotropy = 5.2451
14 H Isotropic = 28.2561 Anisotropy = 11.8685

15	H	Isotropic =	27.9947	Anisotropy =	12.4012
16	H	Isotropic =	23.7383	Anisotropy =	8.1835
17	H	Isotropic =	23.9296	Anisotropy =	5.0665
18	H	Isotropic =	23.9755	Anisotropy =	4.6190
19	H	Isotropic =	23.9323	Anisotropy =	5.0858
20	H	Isotropic =	23.4953	Anisotropy =	8.4217



2b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.344609249058	0.928493260825	-0.779330807935
C	0.173363235852	-0.226943828630	-0.097445774186
C	1.253897757471	-0.471920704880	0.700155561413
C	2.091694549914	0.645074416736	0.433620933448
N	1.571349388781	1.483248687234	-0.437583235308
Br	3.782892648422	0.998639258045	1.181745642360
C	-1.064676422639	-1.025375256918	-0.283656951834
O	-1.893696193686	-0.462092940825	-1.162510213312
O	-1.254957681497	-2.064145799765	0.315633459738
C	-3.141886007862	-1.172483675192	-1.417848707063
C	-3.910400050908	-0.377666936284	-2.450312620527
H	1.425997955296	-1.309203440647	1.366779079009
H	-2.895115180570	-2.186466723544	-1.767149614573
H	-3.687116102448	-1.261447210110	-0.465931584554
H	-3.340965654343	-0.294748933413	-3.388836567827
H	-4.862729264687	-0.885592870818	-2.667027471625
H	-4.134362226152	0.635542698184	-2.082621127223

SCF Done: E(RB3LYP) = -3086.81557935

Zero-point correction= 0.118058
Thermal correction to Energy= 0.128822
Thermal correction to Enthalpy= 0.129766
Thermal correction to Gibbs Free Energy= 0.078967
Sum of electronic and zero-point Energies= -3086.697522
Sum of electronic and thermal Energies= -3086.686757
Sum of electronic and thermal Enthalpies= -3086.685813
Sum of electronic and thermal Free Energies= -3086.736612

1	O	Isotropic =	-62.9232	Anisotropy =	288.5299
2	C	Isotropic =	28.6691	Anisotropy =	110.2348
3	C	Isotropic =	78.6740	Anisotropy =	107.8702
4	C	Isotropic =	30.7897	Anisotropy =	100.0839
5	N	Isotropic =	-125.4816	Anisotropy =	268.1220
6	Br	Isotropic =	2163.6250	Anisotropy =	1129.5236

7 C Isotropic = 38.3132 Anisotropy = 73.3224
8 O Isotropic = 123.3546 Anisotropy = 124.9358
9 O Isotropic = -52.6736 Anisotropy = 541.5287
10 C Isotropic = 126.6519 Anisotropy = 60.9431
11 C Isotropic = 177.3517 Anisotropy = 19.6790
12 H Isotropic = 24.4172 Anisotropy = 6.2568
13 H Isotropic = 27.0823 Anisotropy = 5.9926
14 H Isotropic = 27.1163 Anisotropy = 6.0886
15 H Isotropic = 29.8733 Anisotropy = 7.6384
16 H Isotropic = 30.0234 Anisotropy = 9.5485
17 H Isotropic = 29.8644 Anisotropy = 7.6458

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	2.798468121879	0.322092450518	-0.038240918049
C	1.763820097561	-0.545948769649	-0.098565535030
C	0.584105025909	0.106052764084	0.120244319830
C	1.008623351044	1.448577938955	0.318371208539
N	2.313530779393	1.593916373387	0.227815409716
Br	-0.079486333027	2.942189150033	0.680139779110
C	2.105234067509	-1.964800554529	-0.374885706000
O	0.996379203272	-2.708533513794	-0.413785600253
O	3.238997653722	-2.363459074223	-0.537428962856
C	1.182548129438	-4.131244859120	-0.675365190111
C	-0.187762141206	-4.771705830647	-0.689662160049
H	-0.421487336263	-0.298124733439	0.138946225848
H	1.705403521525	-4.238168070561	-1.637843267336
H	1.829513809655	-4.543607787495	0.113812787951
H	-0.084047175210	-5.850150587898	-0.884943908481
H	-0.694679966504	-4.642883976429	0.279081105215
H	-0.819200808699	-4.336320919191	-1.479409588045

SCF Done: E(RB3LYP) = -3086.81556178

Zero-point correction= 0.118112
Thermal correction to Energy= 0.128864
Thermal correction to Enthalpy= 0.129809
Thermal correction to Gibbs Free Energy= 0.079019
Sum of electronic and zero-point Energies= -3086.697450
Sum of electronic and thermal Energies= -3086.686697
Sum of electronic and thermal Enthalpies= -3086.685753
Sum of electronic and thermal Free Energies= -3086.736543

1 O Isotropic = -65.4673 Anisotropy = 289.4877
2 C Isotropic = 29.4528 Anisotropy = 111.6133
3 C Isotropic = 80.1034 Anisotropy = 104.9640
4 C Isotropic = 30.7988 Anisotropy = 99.4750
5 N Isotropic = -125.4348 Anisotropy = 279.1179
6 Br Isotropic = 2159.9566 Anisotropy = 1134.8435
7 C Isotropic = 38.5138 Anisotropy = 73.0827
8 O Isotropic = 126.1455 Anisotropy = 141.2891
9 O Isotropic = -54.0717 Anisotropy = 578.9484

10 C Isotropic = 126.7898 Anisotropy = 60.7239
11 C Isotropic = 177.2540 Anisotropy = 19.8595
12 H Isotropic = 24.5947 Anisotropy = 7.2847
13 H Isotropic = 27.0973 Anisotropy = 6.0763
14 H Isotropic = 27.1212 Anisotropy = 6.1388
15 H Isotropic = 30.0261 Anisotropy = 9.6097
16 H Isotropic = 29.8982 Anisotropy = 7.5479
17 H Isotropic = 29.9075 Anisotropy = 7.5463

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.088495057978	1.036895738131	0.474432070980
C	0.149837550635	-0.122682518249	-0.179690055742
C	1.452057892047	-0.499553666484	-0.018267834225
C	1.974739100365	0.542429643053	0.795049219035
N	1.079507492699	1.459207282725	1.095964705347
Br	3.736998920873	0.705184691991	1.437127950710
C	-0.941361009737	-0.792968086748	-0.931661526503
O	-2.087630463380	-0.114919685948	-0.848721787756
O	-0.758993820468	-1.834464746277	-1.528912609862
C	-3.240326518378	-0.675052114896	-1.549389150179
C	-3.277952387484	-0.216323906553	-2.995640957959
H	1.956208407601	-1.374278662249	-0.412908686019
H	-3.197696567511	-1.769775341802	-1.468774548313
H	-4.099386323589	-0.298001493806	-0.979950192746
H	-4.200105529912	-0.588744668027	-3.469689839612
H	-3.275371407633	0.882684543705	-3.060658124093
H	-2.418750278148	-0.609587008566	-3.559528633063

SCF Done: E(RB3LYP) = -3086.81516645

Zero-point correction= 0.118328
Thermal correction to Energy= 0.128972
Thermal correction to Enthalpy= 0.129916
Thermal correction to Gibbs Free Energy= 0.079543
Sum of electronic and zero-point Energies= -3086.696839
Sum of electronic and thermal Energies= -3086.686194
Sum of electronic and thermal Enthalpies= -3086.685250
Sum of electronic and thermal Free Energies= -3086.735623

1 O Isotropic = -62.9317 Anisotropy = 289.4947
2 C Isotropic = 28.5181 Anisotropy = 110.0109
3 C Isotropic = 78.6271 Anisotropy = 108.1078
4 C Isotropic = 30.7748 Anisotropy = 99.9510
5 N Isotropic = -125.5912 Anisotropy = 268.6212
6 Br Isotropic = 2163.5618 Anisotropy = 1129.5524
7 C Isotropic = 38.2599 Anisotropy = 73.4612
8 O Isotropic = 123.6066 Anisotropy = 172.6181
9 O Isotropic = -42.6485 Anisotropy = 538.7123
10 C Isotropic = 127.9708 Anisotropy = 67.3247
11 C Isotropic = 176.3080 Anisotropy = 22.4255
12 H Isotropic = 24.4117 Anisotropy = 6.3830

13 H Isotropic = 26.4156 Anisotropy = 5.5256
14 H Isotropic = 27.3093 Anisotropy = 7.1994
15 H Isotropic = 30.2137 Anisotropy = 9.9009
16 H Isotropic = 30.0338 Anisotropy = 7.6576
17 H Isotropic = 29.8891 Anisotropy = 6.2179

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.000044992737	1.181331759332	0.310964872793
C	0.112622176572	-0.146039726346	0.076943985889
C	1.407574184225	-0.469163312717	-0.209989893446
C	2.063758087023	0.788893334284	-0.126714278461
N	1.248647418267	1.775754944740	0.180269692678
Br	3.893792756443	1.132879850107	-0.404382878584
C	-1.084453409512	-1.021747957716	0.151446961029
O	-2.184725826572	-0.330740416973	0.455198533250
O	-1.014866932756	-2.216687335549	-0.053492116922
C	-3.431996867120	-1.084059967491	0.557336738449
C	-3.614924640822	-1.654576270381	1.951903484117
H	1.825563801555	-1.441901406053	-0.442504787510
H	-4.204333478537	-0.342648915727	0.316180774358
H	-3.426145613118	-1.871502129293	-0.208582124799
H	-4.599769787138	-2.144254867745	2.016265436272
H	-2.842797049802	-2.405066347040	2.178645635260
H	-3.574239811445	-0.858881235432	2.711679965628

SCF Done: E(RB3LYP) = -3086.81514975

Zero-point correction= 0.118292
Thermal correction to Energy= 0.128958
Thermal correction to Enthalpy= 0.129902
Thermal correction to Gibbs Free Energy= 0.079364
Sum of electronic and zero-point Energies= -3086.696858
Sum of electronic and thermal Energies= -3086.686192
Sum of electronic and thermal Enthalpies= -3086.685248
Sum of electronic and thermal Free Energies= -3086.735786

1 O Isotropic = -63.0056 Anisotropy = 289.4129
2 C Isotropic = 28.5133 Anisotropy = 110.0071
3 C Isotropic = 78.5143 Anisotropy = 108.0460
4 C Isotropic = 30.7776 Anisotropy = 99.9869
5 N Isotropic = -125.6529 Anisotropy = 268.3752
6 Br Isotropic = 2162.6177 Anisotropy = 1130.5490
7 C Isotropic = 38.2405 Anisotropy = 73.4439
8 O Isotropic = 123.5928 Anisotropy = 172.3640
9 O Isotropic = -42.7354 Anisotropy = 538.6678
10 C Isotropic = 127.9875 Anisotropy = 67.3891
11 C Isotropic = 176.2573 Anisotropy = 22.4907
12 H Isotropic = 24.4066 Anisotropy = 6.4007
13 H Isotropic = 27.3073 Anisotropy = 7.1918
14 H Isotropic = 26.4208 Anisotropy = 5.5321
15 H Isotropic = 30.2160 Anisotropy = 9.8967

16 H Isotropic = 29.8912 Anisotropy = 6.2038
17 H Isotropic = 30.0365 Anisotropy = 7.6464

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.157472612517	-0.105821577198	-1.458146283629
C	-0.029105749705	0.283383891035	-0.176859665198
C	1.169899993850	0.377186566269	0.469843472418
C	2.094767876361	0.007440669385	-0.544743934477
N	1.513722197258	-0.280785457836	-1.689983468137
Br	3.968456966962	-0.097389696377	-0.388092758053
C	-1.433144077396	0.515525845598	0.248875074923
O	-1.465554835157	0.896188124782	1.530505659095
O	-2.387041245437	0.374658752715	-0.486726037811
C	-2.778886346439	1.161412674250	2.111249369037
C	-3.397641560639	-0.108466292071	2.666191484723
H	1.366279366890	0.661097234354	1.497297087708
H	-2.571538287219	1.893100636684	2.902516696464
H	-3.412343709970	1.622225741869	1.341201167402
H	-4.346015259742	0.139880569859	3.168931787340
H	-3.613078821224	-0.829154674495	1.862952133815
H	-2.730139120913	-0.582653008823	3.402148214381

SCF Done: E(RB3LYP) = -3086.81514189

Zero-point correction= 0.118304
Thermal correction to Energy= 0.128972
Thermal correction to Enthalpy= 0.129916
Thermal correction to Gibbs Free Energy= 0.079346
Sum of electronic and zero-point Energies= -3086.696838
Sum of electronic and thermal Energies= -3086.686170
Sum of electronic and thermal Enthalpies= -3086.685226
Sum of electronic and thermal Free Energies= -3086.735796

1 O Isotropic = -65.9234 Anisotropy = 289.7623
2 C Isotropic = 29.3629 Anisotropy = 111.3212
3 C Isotropic = 80.0500 Anisotropy = 105.2947
4 C Isotropic = 30.7707 Anisotropy = 99.5576
5 N Isotropic = -125.6578 Anisotropy = 279.2964
6 Br Isotropic = 2159.4127 Anisotropy = 1135.3030
7 C Isotropic = 38.4364 Anisotropy = 74.0113
8 O Isotropic = 126.5302 Anisotropy = 154.0693
9 O Isotropic = -43.9681 Anisotropy = 576.3357
10 C Isotropic = 128.1313 Anisotropy = 67.2818
11 C Isotropic = 176.2480 Anisotropy = 22.4687
12 H Isotropic = 24.5804 Anisotropy = 7.1744
13 H Isotropic = 27.3512 Anisotropy = 7.1865
14 H Isotropic = 26.4169 Anisotropy = 5.5392
15 H Isotropic = 30.2160 Anisotropy = 9.9361
16 H Isotropic = 29.9208 Anisotropy = 6.2063
17 H Isotropic = 30.0419 Anisotropy = 7.5674

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.097177924260	-0.529728060997	1.333019783737
C	-0.032112513997	-0.122244919298	0.045534119855
C	1.167949116296	0.480739196828	-0.201251179782
C	1.817827787135	0.397074801908	1.060597869354
N	1.084688322992	-0.196972474678	1.978154490106
Br	3.537470602284	1.028819362837	1.495271903633
C	-1.222296428641	-0.398989827401	-0.799093111207
O	-1.017828611302	0.054273369565	-2.040469829655
O	-2.219915507703	-0.953029190714	-0.388353518389
C	-2.099013171850	-0.137864039917	-3.003042229182
C	-2.005175328467	-1.498405783680	-3.669359469678
H	1.532445301285	0.914030791868	-1.125517788603
H	-3.056211936416	-0.003878479845	-2.480854473715
H	-1.955782791843	0.678613575360	-3.722221380591
H	-2.163565522849	-2.308778690428	-2.942006302194
H	-2.783109878540	-1.576140838389	-4.445669483712
H	-1.023631514125	-1.635328793019	-4.148879399977

SCF Done: E(RB3LYP) = -3086.81514068

Zero-point correction= 0.118279
Thermal correction to Energy= 0.128958
Thermal correction to Enthalpy= 0.129902
Thermal correction to Gibbs Free Energy= 0.079264
Sum of electronic and zero-point Energies= -3086.696861
Sum of electronic and thermal Energies= -3086.686183
Sum of electronic and thermal Enthalpies= -3086.685239
Sum of electronic and thermal Free Energies= -3086.735877

1	O	Isotropic =	-65.7998	Anisotropy =	289.5550
2	C	Isotropic =	29.3504	Anisotropy =	111.3296
3	C	Isotropic =	80.0336	Anisotropy =	105.1234
4	C	Isotropic =	30.7913	Anisotropy =	99.7497
5	N	Isotropic =	-125.6161	Anisotropy =	279.3883
6	Br	Isotropic =	2159.8404	Anisotropy =	1134.5592
7	C	Isotropic =	38.4452	Anisotropy =	74.1013
8	O	Isotropic =	126.5104	Anisotropy =	153.8598
9	O	Isotropic =	-44.2259	Anisotropy =	576.2373
10	C	Isotropic =	128.0198	Anisotropy =	67.3562
11	C	Isotropic =	176.2266	Anisotropy =	22.5139
12	H	Isotropic =	24.5783	Anisotropy =	7.1808
13	H	Isotropic =	26.4400	Anisotropy =	5.5547
14	H	Isotropic =	27.3537	Anisotropy =	7.1576
15	H	Isotropic =	29.8990	Anisotropy =	6.1927
16	H	Isotropic =	30.2215	Anisotropy =	9.9277
17	H	Isotropic =	30.0427	Anisotropy =	7.5619

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.205888247894	-0.075466580698	-0.935019523474
C	0.596098747907	-0.817710478516	0.129717152369
C	1.396083447922	-0.069631785700	0.947979384819
C	1.448821786369	1.181389289370	0.278470892310
N	0.751037714927	1.198487287289	-0.837229885836
Br	2.380939322833	2.721987139221	0.825371114528
C	0.186926690556	-2.238965627196	0.336867783371
O	-0.587119529819	-2.895541840780	-0.530461768193
O	0.582033633905	-2.804687355512	1.337106097062
C	-1.122072418205	-2.347406381920	-1.775118818372
C	-1.916506770128	-3.458607626497	-2.427054283984
H	1.869913388912	-0.365964823597	1.876323863479
H	-1.754337096757	-1.479948438768	-1.540060494108
H	-0.286659316663	-2.019674311909	-2.409531479479
H	-1.274060120898	-4.324932737085	-2.647006662704
H	-2.741733558787	-3.786446457397	-1.776500320103
H	-2.344034169969	-3.093259270305	-3.373543051687

SCF Done: E(RB3LYP) = -3086.80454115

Zero-point correction= 0.117951
Thermal correction to Energy= 0.128711
Thermal correction to Enthalpy= 0.129655
Thermal correction to Gibbs Free Energy= 0.078630
Sum of electronic and zero-point Energies= -3086.686590
Sum of electronic and thermal Energies= -3086.675830
Sum of electronic and thermal Enthalpies= -3086.674886
Sum of electronic and thermal Free Energies= -3086.725911

1	O	Isotropic =	-60.6723	Anisotropy = 294.6967
2	C	Isotropic =	27.9085	Anisotropy = 106.1859
3	C	Isotropic =	75.1791	Anisotropy = 108.0909
4	C	Isotropic =	30.3978	Anisotropy = 102.5802
5	N	Isotropic =	-127.1027	Anisotropy = 259.2118
6	Br	Isotropic =	2163.3411	Anisotropy = 1122.7530
7	C	Isotropic =	40.2412	Anisotropy = 69.1594
8	O	Isotropic =	124.8419	Anisotropy = 133.2543
9	O	Isotropic =	-66.9894	Anisotropy = 528.9440
10	C	Isotropic =	122.3265	Anisotropy = 64.4070
11	C	Isotropic =	175.5646	Anisotropy = 22.1279
12	H	Isotropic =	24.2768	Anisotropy = 6.3346
13	H	Isotropic =	26.5929	Anisotropy = 4.1620
14	H	Isotropic =	26.6166	Anisotropy = 4.1033
15	H	Isotropic =	29.8939	Anisotropy = 7.8182
16	H	Isotropic =	29.8863	Anisotropy = 7.8136
17	H	Isotropic =	30.0609	Anisotropy = 9.0838

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.656179774156	-0.865752951352	0.812252522394
C	0.872175685052	-0.769104257384	-0.522335620528
C	1.119084570955	0.532282873439	-0.858287464912
C	1.025831302560	1.203521510069	0.390103604319
N	0.757248551393	0.394233794290	1.392079185598
Br	1.249930592405	3.045079122216	0.704925673995
C	0.885769200560	-1.948519767778	-1.440886299425
O	0.427036443467	-3.148840840442	-1.079218976028
O	1.338117225160	-1.790372826445	-2.557403548812
C	-0.290121922890	-3.464507881532	0.155094334747
C	0.650021044188	-4.033353297142	1.199992508661
H	1.334850420316	0.943482217847	-1.837364566778
H	-0.832320572005	-2.581181003695	0.513029973130
H	-1.023976300439	-4.215224217589	-0.167965754140
H	1.374860669984	-3.280656865833	1.542810146763
H	0.062317313497	-4.366355901304	2.070550583938
H	1.196326001640	-4.901699707365	0.800693697078

SCF Done: E(RB3LYP) = -3086.80331976

Zero-point correction= 0.118068
Thermal correction to Energy= 0.128733
Thermal correction to Enthalpy= 0.129677
Thermal correction to Gibbs Free Energy= 0.078957
Sum of electronic and zero-point Energies= -3086.685252
Sum of electronic and thermal Energies= -3086.674587
Sum of electronic and thermal Enthalpies= -3086.673643
Sum of electronic and thermal Free Energies= -3086.724362

1	O	Isotropic =	-57.5378	Anisotropy =	285.6520
2	C	Isotropic =	28.6303	Anisotropy =	107.7967
3	C	Isotropic =	75.2907	Anisotropy =	106.8413
4	C	Isotropic =	30.3571	Anisotropy =	103.1121
5	N	Isotropic =	-125.9896	Anisotropy =	256.3613
6	Br	Isotropic =	2161.4411	Anisotropy =	1123.0535
7	C	Isotropic =	39.6608	Anisotropy =	68.3334
8	O	Isotropic =	122.5292	Anisotropy =	165.3331
9	O	Isotropic =	-71.1529	Anisotropy =	532.3265
10	C	Isotropic =	123.1654	Anisotropy =	74.8188
11	C	Isotropic =	174.0470	Anisotropy =	24.7088
12	H	Isotropic =	24.3288	Anisotropy =	6.1976
13	H	Isotropic =	26.3128	Anisotropy =	2.9601
14	H	Isotropic =	27.0329	Anisotropy =	6.8630
15	H	Isotropic =	29.6771	Anisotropy =	5.6945
16	H	Isotropic =	30.0678	Anisotropy =	9.4174
17	H	Isotropic =	29.7906	Anisotropy =	8.0960

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.128228104592	0.822291881235	0.243661496418
C	0.103773414803	-0.505179055266	0.389309491422
C	1.423238158255	-0.773094502315	0.155777995277

C	1.958756813169	0.510091768853	-0.135130030966
N	1.056893599460	1.467087154067	-0.093451235615
Br	3.746018265536	0.922661478441	-0.556369758674
C	-0.971336933953	-1.496122397386	0.700945202308
O	-2.178227042987	-1.132522453903	1.140714074898
O	-0.720357231664	-2.673759236161	0.539021692280
C	-2.577599425411	0.212112855262	1.553394570311
C	-3.317959632133	0.923690549248	0.437692169239
H	1.929553717151	-1.730739391764	0.184677367386
H	-3.238102563888	0.025031399284	2.410911357242
H	-1.704157392621	0.774577324332	1.904320145968
H	-3.703799327881	1.884068210515	0.815775270350
H	-2.656992519580	1.131376012802	-0.416468744112
H	-4.172163793665	0.321558402756	0.091658936268

SCF Done: E(RB3LYP) = -3086.80331938

Zero-point correction= 0.118131
Thermal correction to Energy= 0.128769
Thermal correction to Enthalpy= 0.129714
Thermal correction to Gibbs Free Energy= 0.079096
Sum of electronic and zero-point Energies= -3086.685189
Sum of electronic and thermal Energies= -3086.674550
Sum of electronic and thermal Enthalpies= -3086.673606
Sum of electronic and thermal Free Energies= -3086.724223

1	O	Isotropic =	-57.5150	Anisotropy =	285.4039
2	C	Isotropic =	28.6764	Anisotropy =	108.2293
3	C	Isotropic =	75.4554	Anisotropy =	106.8336
4	C	Isotropic =	30.3645	Anisotropy =	102.8971
5	N	Isotropic =	-125.7954	Anisotropy =	256.6359
6	Br	Isotropic =	2161.0716	Anisotropy =	1123.8650
7	C	Isotropic =	39.5844	Anisotropy =	68.1845
8	O	Isotropic =	122.4949	Anisotropy =	165.5985
9	O	Isotropic =	-71.6008	Anisotropy =	533.1983
10	C	Isotropic =	123.1110	Anisotropy =	74.8208
11	C	Isotropic =	174.1214	Anisotropy =	24.6052
12	H	Isotropic =	24.3385	Anisotropy =	6.1763
13	H	Isotropic =	27.0273	Anisotropy =	6.8721
14	H	Isotropic =	26.3310	Anisotropy =	2.9259
15	H	Isotropic =	30.0700	Anisotropy =	9.4198
16	H	Isotropic =	29.6766	Anisotropy =	5.7100
17	H	Isotropic =	29.7843	Anisotropy =	8.1106

2b incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.042195576879	1.248462691888	-0.049954710075
C	0.386820573997	0.309301740656	0.773647431005
C	1.392512072505	-0.512311474997	0.189758272398
C	1.522408554431	0.023027896617	-1.056443341733

O	0.683961200263	1.066943328573	-1.222104933965
Br	2.612678572453	-0.424655101315	-2.505410927426
C	-0.147272017900	0.153763558003	2.159662557053
O	-1.091975532679	1.054219738605	2.440210940103
O	0.258970236710	-0.712072236336	2.908534411519
C	-1.689726365710	0.995356056394	3.770168006277
C	-0.880407321976	1.798683973616	4.772152010966
H	1.917623727452	-1.350766486801	0.631759356515
H	-2.691819011190	1.419102343477	3.625055709613
H	-1.776484847237	-0.058608809245	4.067591619738
H	-0.763266814998	2.841238474621	4.438147438425
H	-1.403895274649	1.803041262873	5.741631949855
H	0.116737825407	1.358073043372	4.922224209731

SCF Done: E(RB3LYP) = -3086.81339959

Zero-point correction= 0.118275
Thermal correction to Energy= 0.128939
Thermal correction to Enthalpy= 0.129883
Thermal correction to Gibbs Free Energy= 0.079381
Sum of electronic and zero-point Energies= -3086.695125
Sum of electronic and thermal Energies= -3086.684461
Sum of electronic and thermal Enthalpies= -3086.683517
Sum of electronic and thermal Free Energies= -3086.734019

1	N	Isotropic =	-150.1914	Anisotropy = 297.7173
2	C	Isotropic =	33.3702	Anisotropy = 122.7930
3	C	Isotropic =	84.2861	Anisotropy = 102.1562
4	C	Isotropic =	26.3876	Anisotropy = 76.5066
5	O	Isotropic =	-69.0921	Anisotropy = 251.7518
6	Br	Isotropic =	2087.2421	Anisotropy = 1174.2728
7	C	Isotropic =	34.4310	Anisotropy = 78.6976
8	O	Isotropic =	126.9492	Anisotropy = 163.6172
9	O	Isotropic =	-55.9573	Anisotropy = 559.1396
10	C	Isotropic =	128.2749	Anisotropy = 66.7795
11	C	Isotropic =	176.3131	Anisotropy = 22.4162
12	H	Isotropic =	24.6757	Anisotropy = 6.9278
13	H	Isotropic =	27.3519	Anisotropy = 7.2445
14	H	Isotropic =	26.3881	Anisotropy = 5.4167
15	H	Isotropic =	30.0546	Anisotropy = 7.7206
16	H	Isotropic =	30.2210	Anisotropy = 9.8504
17	H	Isotropic =	29.8819	Anisotropy = 6.1737

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.702218129604	-0.202158128577	1.219581543161
C	0.773713264316	-0.635217608273	0.386072308807
C	0.460745213104	0.316271545723	-0.626056970738
C	1.287771946174	1.354585444990	-0.318764282808
O	2.032496584751	1.071734938492	0.769972992904
Br	1.551182845203	3.024737526267	-1.112644809238
C	0.141781990000	-1.981402887361	0.521018393803

O	0.625054360103	-2.669100765412	1.556295102788
O	-0.714593322754	-2.370272211615	-0.247539078580
C	0.063076483357	-3.997641125805	1.765322282310
C	0.765371397260	-4.602351644539	2.961239766813
H	-0.256132190002	0.229552613472	-1.434017371787
H	-1.020821666069	-3.892087447696	1.925613746626
H	0.216531831938	-4.586251140574	0.848104217085
H	0.363176778237	-5.609522075008	3.150514752921
H	1.847840116125	-4.690277423481	2.780599879083
H	0.607186238650	-3.991349610603	3.863297526850

SCF Done: E(RB3LYP) = -3086.81385555

Zero-point correction= 0.118014
Thermal correction to Energy= 0.128793
Thermal correction to Enthalpy= 0.129737
Thermal correction to Gibbs Free Energy= 0.078844
Sum of electronic and zero-point Energies= -3086.695841
Sum of electronic and thermal Energies= -3086.685063
Sum of electronic and thermal Enthalpies= -3086.684119
Sum of electronic and thermal Free Energies= -3086.735012

1	N	Isotropic =	-149.8826	Anisotropy =	297.4275
2	C	Isotropic =	33.4676	Anisotropy =	123.0539
3	C	Isotropic =	84.3185	Anisotropy =	102.0440
4	C	Isotropic =	26.3959	Anisotropy =	76.4642
5	O	Isotropic =	-68.7377	Anisotropy =	251.0105
6	Br	Isotropic =	2086.8319	Anisotropy =	1175.2808
7	C	Isotropic =	34.5002	Anisotropy =	79.0146
8	O	Isotropic =	126.3317	Anisotropy =	134.9608
9	O	Isotropic =	-66.4612	Anisotropy =	561.9706
10	C	Isotropic =	126.8926	Anisotropy =	60.1499
11	C	Isotropic =	177.3666	Anisotropy =	19.8039
12	H	Isotropic =	24.6893	Anisotropy =	6.8068
13	H	Isotropic =	27.1138	Anisotropy =	6.0043
14	H	Isotropic =	27.0716	Anisotropy =	5.8764
15	H	Isotropic =	30.0384	Anisotropy =	9.4898
16	H	Isotropic =	29.9084	Anisotropy =	7.6945
17	H	Isotropic =	29.8992	Anisotropy =	7.7016

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.144303016964	1.276242793103	1.096723181883
C	0.578843970809	0.097210275296	0.910608598944
C	0.987005992053	-0.518905162733	-0.306557847388
C	1.846530980567	0.401062317944	-0.827641225416
O	1.956104732772	1.472415796397	-0.015058740637
Br	2.850962850458	0.428283508994	-2.402200867846
C	-0.379407509895	-0.494855475422	1.891326572302
O	-0.584566879859	0.304352668412	2.940638495665
O	-0.885674082122	-1.584674358404	1.713746871146
C	-1.503624254899	-0.174002287703	3.968462252146

C	-2.940128432656	0.181945739647	3.630525914116
H	0.685132634102	-1.478052106188	-0.710505425514
H	-1.368006148701	-1.258397460673	4.080951919463
H	-1.163149710887	0.334345629090	4.879732684915
H	-3.051356656917	1.266469842340	3.476654158466
H	-3.276562988161	-0.343458218849	2.724129008301
H	-3.594527513629	-0.117713501251	4.464734449455

SCF Done: E(RB3LYP) = -3086.81340084

Zero-point correction= 0.118288
Thermal correction to Energy= 0.128944
Thermal correction to Enthalpy= 0.129888
Thermal correction to Gibbs Free Energy= 0.079421
Sum of electronic and zero-point Energies= -3086.695113
Sum of electronic and thermal Energies= -3086.684457
Sum of electronic and thermal Enthalpies= -3086.683512
Sum of electronic and thermal Free Energies= -3086.733980

1	N	Isotropic =	-150.1350	Anisotropy =	297.8316
2	C	Isotropic =	33.3418	Anisotropy =	122.8446
3	C	Isotropic =	84.3260	Anisotropy =	102.1372
4	C	Isotropic =	26.4071	Anisotropy =	76.4898
5	O	Isotropic =	-68.9173	Anisotropy =	252.0468
6	Br	Isotropic =	2087.6586	Anisotropy =	1173.8345
7	C	Isotropic =	34.4557	Anisotropy =	78.7433
8	O	Isotropic =	126.8780	Anisotropy =	163.2167
9	O	Isotropic =	-56.2501	Anisotropy =	558.9493
10	C	Isotropic =	128.1597	Anisotropy =	66.8936
11	C	Isotropic =	176.2479	Anisotropy =	22.3791
12	H	Isotropic =	24.6793	Anisotropy =	6.9208
13	H	Isotropic =	26.3992	Anisotropy =	5.4530
14	H	Isotropic =	27.3441	Anisotropy =	7.2445
15	H	Isotropic =	30.0599	Anisotropy =	7.7003
16	H	Isotropic =	29.8768	Anisotropy =	6.1466
17	H	Isotropic =	30.2167	Anisotropy =	9.8519

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.802106046746	0.151058852261	-0.640037097504
C	-0.005932149834	-0.392863066665	0.263411580527
C	1.302552698777	0.171028862001	0.245863494948
C	1.209172885619	1.097609843315	-0.749249756936
O	-0.027989161134	1.102894298241	-1.287249742969
Br	2.446117449474	2.303918150155	-1.460028084293
C	-0.543335811786	-1.473393081879	1.145130982777
O	0.403638784408	-1.893251706118	1.991877318358
O	-1.677083489175	-1.899117191202	1.090233685113
C	0.020867704682	-2.951705386915	2.917106729489
C	1.231918687136	-3.273089573754	3.765153262250
H	2.155627724598	-0.075273171730	0.866713730136
H	-0.828164432813	-2.592848353581	3.518763833715

H	-0.319915613418	-3.817026573827	2.328401309293
H	2.070012208920	-3.621389999278	3.141896795441
H	1.559845891636	-2.390961490096	4.336559189110
H	0.976632669656	-4.071620410928	4.478742770544

SCF Done: E(RB3LYP) = -3086.81346393

Zero-point correction= 0.118085
Thermal correction to Energy= 0.128825
Thermal correction to Enthalpy= 0.129769
Thermal correction to Gibbs Free Energy= 0.078978
Sum of electronic and zero-point Energies= -3086.695379
Sum of electronic and thermal Energies= -3086.684639
Sum of electronic and thermal Enthalpies= -3086.683695
Sum of electronic and thermal Free Energies= -3086.734486

1	N	Isotropic =	-151.0767	Anisotropy = 299.1246
2	C	Isotropic =	33.5692	Anisotropy = 125.9832
3	C	Isotropic =	84.8081	Anisotropy = 100.5634
4	C	Isotropic =	26.2519	Anisotropy = 76.7821
5	O	Isotropic =	-68.2811	Anisotropy = 269.6641
6	Br	Isotropic =	2083.5485	Anisotropy = 1179.8331
7	C	Isotropic =	35.5572	Anisotropy = 77.4574
8	O	Isotropic =	117.7554	Anisotropy = 139.3922
9	O	Isotropic =	-50.8527	Anisotropy = 569.8562
10	C	Isotropic =	127.1696	Anisotropy = 59.9142
11	C	Isotropic =	177.2814	Anisotropy = 19.8719
12	H	Isotropic =	24.7732	Anisotropy = 8.2728
13	H	Isotropic =	27.1226	Anisotropy = 6.0873
14	H	Isotropic =	27.1108	Anisotropy = 6.0522
15	H	Isotropic =	29.8970	Anisotropy = 7.5136
16	H	Isotropic =	29.8932	Anisotropy = 7.5145
17	H	Isotropic =	30.0342	Anisotropy = 9.5847

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.437820296815	1.190345486899	0.586437560826
C	1.154982398979	0.974528711559	0.817761539784
C	0.655165801361	-0.152876907883	0.104070942861
C	1.757628464486	-0.585427646679	-0.570443555838
O	2.824243739628	0.194959991839	-0.299796397511
Br	2.028166411604	-2.007117722993	-1.751391061079
C	0.424848649922	1.888679532865	1.748135384251
O	-0.854712796722	1.507409451234	1.855670658717
O	0.936269402856	2.829666199853	2.316210811335
C	-1.712552356201	2.297364891568	2.732308872779
C	-2.314500836590	3.478466746440	1.992561949586
H	-0.347999774807	-0.561900239415	0.098908977651
H	-2.482710904772	1.585746431786	3.056598838540
H	-1.120420021782	2.618717491358	3.600047905090
H	-3.018469568800	4.003218513425	2.658090490829
H	-1.535795896820	4.192249230188	1.684351702797

H -2.866283009158 3.144609837957 1.100215379382

SCF Done: E(RB3LYP) = -3086.81302971

Zero-point correction= 0.118329
Thermal correction to Energy= 0.128966
Thermal correction to Enthalpy= 0.129910
Thermal correction to Gibbs Free Energy= 0.079420
Sum of electronic and zero-point Energies= -3086.694701
Sum of electronic and thermal Energies= -3086.684063
Sum of electronic and thermal Enthalpies= -3086.683119
Sum of electronic and thermal Free Energies= -3086.733609

1 N Isotropic = -151.6471 Anisotropy = 299.2200
2 C Isotropic = 33.3541 Anisotropy = 125.5723
3 C Isotropic = 84.8692 Anisotropy = 100.4873
4 C Isotropic = 26.3055 Anisotropy = 76.8275
5 O Isotropic = -68.5925 Anisotropy = 269.9516
6 Br Isotropic = 2082.8599 Anisotropy = 1180.7855
7 C Isotropic = 35.4874 Anisotropy = 77.2734
8 O Isotropic = 118.2607 Anisotropy = 161.0549
9 O Isotropic = -40.6844 Anisotropy = 566.6931
10 C Isotropic = 128.3819 Anisotropy = 66.7308
11 C Isotropic = 176.2126 Anisotropy = 22.4884
12 H Isotropic = 24.7656 Anisotropy = 7.9833
13 H Isotropic = 27.3744 Anisotropy = 7.1180
14 H Isotropic = 26.4194 Anisotropy = 5.4473
15 H Isotropic = 30.2291 Anisotropy = 9.8981
16 H Isotropic = 29.8977 Anisotropy = 6.2648
17 H Isotropic = 30.0531 Anisotropy = 7.5322

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.325076039064	-1.042464436781	0.338851638723
C	1.021094942076	-0.846745764514	0.422478121782
C	0.658521527648	0.511888081933	0.192800724448
C	1.865259217682	1.103220600430	-0.033960039182
O	2.865805032464	0.202021061075	0.047672821541
Br	2.343973282095	2.867123512681	-0.420535833778
C	0.133008153194	-2.009279713538	0.729542474478
O	-1.144424886973	-1.609125453751	0.779326910340
O	0.531048248908	-3.140302848116	0.908549438720
C	-2.149038019919	-2.625638505728	1.071818357514
C	-2.606525450047	-3.326277596228	-0.194840845243
H	-0.327516738089	0.960592738483	0.197240165900
H	-1.726426426335	-3.332646187476	1.798771852658
H	-2.964854245720	-2.060698732762	1.540917834560
H	-1.786074109509	-3.902663956237	-0.648149790492
H	-3.422717607258	-4.024355305491	0.050894181192
H	-2.982988959283	-2.600537493983	-0.932268013160

SCF Done: E(RB3LYP) = -3086.81301266

Zero-point correction= 0.118246
Thermal correction to Energy= 0.128923
Thermal correction to Enthalpy= 0.129867
Thermal correction to Gibbs Free Energy= 0.079146
Sum of electronic and zero-point Energies= -3086.694767
Sum of electronic and thermal Energies= -3086.684090
Sum of electronic and thermal Enthalpies= -3086.683146
Sum of electronic and thermal Free Energies= -3086.733867

1	N	Isotropic =	-151.7187	Anisotropy =	298.9963
2	C	Isotropic =	33.3606	Anisotropy =	125.5978
3	C	Isotropic =	84.8437	Anisotropy =	100.2555
4	C	Isotropic =	26.3434	Anisotropy =	76.7725
5	O	Isotropic =	-68.6340	Anisotropy =	269.7998
6	Br	Isotropic =	2083.8347	Anisotropy =	1179.2727
7	C	Isotropic =	35.4930	Anisotropy =	77.2801
8	O	Isotropic =	118.1572	Anisotropy =	161.0884
9	O	Isotropic =	-40.6897	Anisotropy =	566.8263
10	C	Isotropic =	128.4189	Anisotropy =	66.7026
11	C	Isotropic =	176.2181	Anisotropy =	22.5836
12	H	Isotropic =	24.7669	Anisotropy =	7.9935
13	H	Isotropic =	26.4215	Anisotropy =	5.4570
14	H	Isotropic =	27.3759	Anisotropy =	7.1169
15	H	Isotropic =	29.8909	Anisotropy =	6.2668
16	H	Isotropic =	30.2286	Anisotropy =	9.8964
17	H	Isotropic =	30.0505	Anisotropy =	7.5324

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.150547394567	0.877209566188	0.312030699913
C	0.627856869232	0.119782521457	1.065654211155
C	1.742076671434	-0.394577003159	0.337576202703
C	1.552570142515	0.124925170700	-0.906134080650
O	0.436087489818	0.882561985848	-0.945578996142
Br	2.526883042072	-0.023892983046	-2.491282110007
C	0.405059419482	-0.189112218406	2.517914517979
O	-0.634841510769	0.294709013647	3.202962539120
O	1.205643941816	-0.906742159281	3.085207732698
C	-1.674337664962	1.162864785194	2.660688745994
C	-2.628524595628	1.455175787347	3.799239936576
H	2.535633409147	-1.037910661253	0.697297101828
H	-1.207722369365	2.078281307616	2.271408951717
H	-2.173698759995	0.645106087838	1.829944503469
H	-2.110885173289	1.965007350619	4.626306735583
H	-3.436407114342	2.110493662986	3.438592069555
H	-3.079336402599	0.527367785703	4.183701238507

SCF Done: E(RB3LYP) = -3086.80362742

Zero-point correction= 0.117920
Thermal correction to Energy= 0.128693

Thermal correction to Enthalpy= 0.129637
Thermal correction to Gibbs Free Energy= 0.078571
Sum of electronic and zero-point Energies= -3086.685708
Sum of electronic and thermal Energies= -3086.674935
Sum of electronic and thermal Enthalpies= -3086.673991
Sum of electronic and thermal Free Energies= -3086.725056

1	N	Isotropic =	-146.9719	Anisotropy =	306.2460
2	C	Isotropic =	32.3844	Anisotropy =	118.8897
3	C	Isotropic =	81.8778	Anisotropy =	100.4988
4	C	Isotropic =	26.1765	Anisotropy =	78.6655
5	O	Isotropic =	-69.3453	Anisotropy =	236.9845
6	Br	Isotropic =	2090.7545	Anisotropy =	1162.0629
7	C	Isotropic =	35.9753	Anisotropy =	75.2543
8	O	Isotropic =	120.8343	Anisotropy =	134.1464
9	O	Isotropic =	-80.9652	Anisotropy =	551.0814
10	C	Isotropic =	121.1783	Anisotropy =	60.7458
11	C	Isotropic =	175.6709	Anisotropy =	21.9132
12	H	Isotropic =	24.5759	Anisotropy =	6.8403
13	H	Isotropic =	26.6779	Anisotropy =	4.2374
14	H	Isotropic =	26.6935	Anisotropy =	4.2252
15	H	Isotropic =	29.9229	Anisotropy =	7.7392
16	H	Isotropic =	30.0914	Anisotropy =	9.0462
17	H	Isotropic =	29.9242	Anisotropy =	7.7357

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.344890935316	0.541362954849	1.207326481938
C	0.359189635968	1.093250299595	0.006751983590
C	1.159480835402	0.353082535564	-0.913189661100
C	1.607259448450	-0.684194959572	-0.153362787840
O	1.140487657820	-0.592308676272	1.109427322605
Br	2.708460001667	-2.140043525651	-0.542873330762
C	-0.309147666199	2.387504767789	-0.363560594558
O	-1.274208979311	2.939619204316	0.376497188949
O	0.047667041849	2.944691753437	-1.382998268937
C	-1.887197125142	2.359304686916	1.568117775323
C	-1.249103544371	2.913241157273	2.827165992272
H	1.356651452352	0.572173182437	-1.955534193447
H	-2.938727233786	2.667145887813	1.486281023639
H	-1.832750387774	1.265185404532	1.523315183575
H	-0.204056009242	2.583366858468	2.920352400898
H	-1.282457299101	4.013725746871	2.831226607317
H	-1.805308763898	2.547882721635	3.705556876538

SCF Done: E(RB3LYP) = -3086.80254780

Zero-point correction= 0.118140
Thermal correction to Energy= 0.128769
Thermal correction to Enthalpy= 0.129713
Thermal correction to Gibbs Free Energy= 0.079218
Sum of electronic and zero-point Energies= -3086.684408

Sum of electronic and thermal Energies= -3086.673779
Sum of electronic and thermal Enthalpies= -3086.672835
Sum of electronic and thermal Free Energies= -3086.723330

1	N	Isotropic =	-142.9358	Anisotropy =	297.4734
2	C	Isotropic =	33.8604	Anisotropy =	119.2798
3	C	Isotropic =	81.9275	Anisotropy =	99.7204
4	C	Isotropic =	26.2095	Anisotropy =	79.2306
5	O	Isotropic =	-66.6434	Anisotropy =	234.6410
6	Br	Isotropic =	2087.8587	Anisotropy =	1164.1609
7	C	Isotropic =	35.5298	Anisotropy =	74.3229
8	O	Isotropic =	117.8499	Anisotropy =	167.6736
9	O	Isotropic =	-83.8390	Anisotropy =	553.9093
10	C	Isotropic =	122.7799	Anisotropy =	75.1052
11	C	Isotropic =	174.3771	Anisotropy =	24.2435
12	H	Isotropic =	24.6486	Anisotropy =	6.5615
13	H	Isotropic =	27.0841	Anisotropy =	6.8271
14	H	Isotropic =	26.1940	Anisotropy =	2.7359
15	H	Isotropic =	29.7337	Anisotropy =	5.8182
16	H	Isotropic =	29.8695	Anisotropy =	7.9788
17	H	Isotropic =	30.2054	Anisotropy =	9.4653

Conformer 9

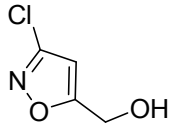
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.190045777095	0.040444639664	0.708691311287
C	0.358751815109	1.098966318994	0.138929732314
C	1.664937429036	0.820166607088	-0.362121195248
C	1.839448019790	-0.489032843956	-0.031196604433
O	0.750989395589	-0.974431686064	0.601741644744
Br	3.257972429595	-1.672901288962	-0.295510609964
C	-0.310577186134	2.431886237341	-0.047413394973
O	-1.395984841032	2.798059480462	0.639733244761
O	0.167374676248	3.204115898976	-0.855053877030
C	-2.043030534236	2.033369544680	1.702268297651
C	-3.208760404632	1.230660517134	1.158145364586
H	2.340987180441	1.491207763348	-0.877818317666
H	-1.306064828195	1.400293757139	2.210232854526
H	-2.385729052893	2.810678813993	2.399009232561
H	-2.861950351494	0.437027063877	0.480346956458
H	-3.744670216734	0.757299161121	1.996716960975
H	-3.915657753362	1.881750015167	0.620938399451

SCF Done: E(RB3LYP) = -3086.80255419

Zero-point correction= 0.118180
Thermal correction to Energy= 0.128798
Thermal correction to Enthalpy= 0.129743
Thermal correction to Gibbs Free Energy= 0.079293
Sum of electronic and zero-point Energies= -3086.684374
Sum of electronic and thermal Energies= -3086.673756
Sum of electronic and thermal Enthalpies= -3086.672812
Sum of electronic and thermal Free Energies= -3086.723261

1	N	Isotropic =	-142.9028	Anisotropy = 297.9626
2	C	Isotropic =	33.7922	Anisotropy = 119.1725
3	C	Isotropic =	81.9583	Anisotropy = 99.6072
4	C	Isotropic =	26.2223	Anisotropy = 79.2593
5	O	Isotropic =	-66.7927	Anisotropy = 234.7369
6	Br	Isotropic =	2088.4743	Anisotropy = 1163.2367
7	C	Isotropic =	35.5332	Anisotropy = 74.4638
8	O	Isotropic =	117.9476	Anisotropy = 168.3757
9	O	Isotropic =	-83.6506	Anisotropy = 554.2547
10	C	Isotropic =	122.9701	Anisotropy = 74.9581
11	C	Isotropic =	174.3636	Anisotropy = 24.2732
12	H	Isotropic =	24.6512	Anisotropy = 6.5635
13	H	Isotropic =	26.1805	Anisotropy = 2.7813
14	H	Isotropic =	27.0750	Anisotropy = 6.8412
15	H	Isotropic =	29.7382	Anisotropy = 5.7825
16	H	Isotropic =	30.2083	Anisotropy = 9.4704
17	H	Isotropic =	29.8725	Anisotropy = 7.9886



2c

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.428279705085	2.034844957368	0.302260494406
C	0.378797505899	1.172827589219	-0.273153734506
C	-0.175190556952	-0.132237458456	-0.389672200519
C	-1.411472270601	0.012924260288	0.170318253752
O	-1.576479398842	1.294171053583	0.581663245418
Cl	1.947298811853	1.681459257606	-0.799347405983
C	-2.553520018112	-0.925173419955	0.423249592679
O	-2.766062853277	-1.166233321665	1.807498810088
H	0.279104599637	-1.020300274364	-0.815464909649
H	-3.460706843610	-0.529349153776	-0.069480423038
H	-2.313290525284	-1.892148100767	-0.039517405664
H	-3.112118745627	-0.348235389081	2.197555683016

SCF Done: E(RB3LYP) = -820.207264296

Zero-point correction= 0.080970
Thermal correction to Energy= 0.088372
Thermal correction to Enthalpy= 0.089316
Thermal correction to Gibbs Free Energy= 0.047720
Sum of electronic and zero-point Energies= -820.126294
Sum of electronic and thermal Energies= -820.118893
Sum of electronic and thermal Enthalpies= -820.117948
Sum of electronic and thermal Free Energies= -820.159544

1 N Isotropic = -111.3345 Anisotropy = 259.3599
2 C Isotropic = 30.9392 Anisotropy = 96.5362
3 C Isotropic = 89.4789 Anisotropy = 87.1745
4 C Isotropic = 16.3080 Anisotropy = 135.7227
5 O Isotropic = -50.6111 Anisotropy = 267.9173
6 Cl Isotropic = 784.8174 Anisotropy = 356.7440
7 C Isotropic = 135.7995 Anisotropy = 51.1668
8 O Isotropic = 305.4440 Anisotropy = 41.5321
9 H Isotropic = 25.2516 Anisotropy = 4.1225
10 H Isotropic = 26.5514 Anisotropy = 6.0459
11 H Isotropic = 26.8544 Anisotropy = 6.0650
12 H Isotropic = 30.6668 Anisotropy = 16.1369

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.847453135681	0.758483006951	-1.279393482784
C	0.234118674133	1.055859571110	-0.595662459836
C	0.079652948727	0.893207897380	0.808974045986
C	-1.211977541397	0.467126305597	0.923866637252
O	-1.775198464953	0.386450172887	-0.306728279305
Cl	1.659080957143	1.583046651314	-1.424965239054
C	-2.073887504376	0.068966012228	2.084327097377
O	-2.375477096412	-1.319883300316	2.088917892045
H	0.812270206938	1.063008253889	1.590460303267
H	-1.523047015008	0.281680160710	3.010735752453
H	-2.989222012462	0.688996995360	2.083474463791
H	-2.978150016652	-1.491481727108	1.348443268809

SCF Done: E(RB3LYP) = -820.207278018

Zero-point correction= 0.081011
Thermal correction to Energy= 0.088394
Thermal correction to Enthalpy= 0.089338
Thermal correction to Gibbs Free Energy= 0.047965
Sum of electronic and zero-point Energies= -820.126267
Sum of electronic and thermal Energies= -820.118885
Sum of electronic and thermal Enthalpies= -820.117940
Sum of electronic and thermal Free Energies= -820.159313

1 N Isotropic = -111.3610 Anisotropy = 259.3010
2 C Isotropic = 30.9149 Anisotropy = 96.4927
3 C Isotropic = 89.4018 Anisotropy = 87.1856
4 C Isotropic = 16.2877 Anisotropy = 135.8197
5 O Isotropic = -50.6654 Anisotropy = 267.8576
6 Cl Isotropic = 784.8866 Anisotropy = 356.6428
7 C Isotropic = 135.8341 Anisotropy = 51.1297
8 O Isotropic = 305.0956 Anisotropy = 40.9859
9 H Isotropic = 25.2481 Anisotropy = 4.1337
10 H Isotropic = 26.8603 Anisotropy = 6.0575
11 H Isotropic = 26.5567 Anisotropy = 6.0376
12 H Isotropic = 30.6757 Anisotropy = 16.1193

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.049806946580	0.177823455363	0.041696593424
C	0.242930513329	1.095866570044	-0.439038233084
C	-1.103413513139	0.962541204172	-0.000332474181
C	-1.041544522454	-0.137585753406	0.803908696310
O	0.220124174670	-0.616771492835	0.842874493436
Cl	0.865789369515	2.312449792293	-1.502323461689
C	-2.079688688849	-0.856504802900	1.601191790834
O	-3.304563204774	-0.179434435398	1.397206372762
H	-1.961649502820	1.577769705346	-0.241849890637
H	-2.117211376535	-1.912551299269	1.268991914967
H	-1.770804820276	-0.864924932019	2.664972524051
H	-3.982565375247	-0.640088011391	1.913011673806

SCF Done: E(RB3LYP) = -820.206839172

Zero-point correction= 0.080401
Thermal correction to Energy= 0.087989
Thermal correction to Enthalpy= 0.088933
Thermal correction to Gibbs Free Energy= 0.046863
Sum of electronic and zero-point Energies= -820.126438
Sum of electronic and thermal Energies= -820.118850
Sum of electronic and thermal Enthalpies= -820.117906
Sum of electronic and thermal Free Energies= -820.159976

1	N	Isotropic =	-108.2929	Anisotropy = 244.8197
2	C	Isotropic =	30.7980	Anisotropy = 96.5007
3	C	Isotropic =	91.3975	Anisotropy = 93.7720
4	C	Isotropic =	14.8760	Anisotropy = 126.8986
5	O	Isotropic =	-39.1950	Anisotropy = 255.5152
6	Cl	Isotropic =	787.2276	Anisotropy = 354.0787
7	C	Isotropic =	133.0316	Anisotropy = 52.0318
8	O	Isotropic =	324.2322	Anisotropy = 92.4909
9	H	Isotropic =	25.1955	Anisotropy = 6.0634
10	H	Isotropic =	26.4182	Anisotropy = 6.6640
11	H	Isotropic =	26.4152	Anisotropy = 6.6575
12	H	Isotropic =	30.6669	Anisotropy = 19.9982

2c incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.123368612853	0.498946254523	1.267174559626
C	-0.140152789454	1.035341483484	0.064213390956
C	1.152551797825	1.034525149166	-0.543519147940
C	1.931145075306	0.462869961971	0.415789029567

O	1.214244106109	0.134944112933	1.503752840647
Cl	3.607871714495	0.101955137855	0.465237131363
C	-1.422797149932	1.557784789564	-0.526974967777
O	-1.567776888438	1.202623016407	-1.892645727944
H	1.441696305447	1.395011891032	-1.524099916312
H	-2.268996775883	1.224865605893	0.099876253077
H	-1.404403842634	2.659026709753	-0.503016195608
H	-1.668412939987	0.238675887419	-1.937637249656

SCF Done: E(RB3LYP) = -820.206262751

Zero-point correction= 0.081036
Thermal correction to Energy= 0.088341
Thermal correction to Enthalpy= 0.089285
Thermal correction to Gibbs Free Energy= 0.048104
Sum of electronic and zero-point Energies= -820.125227
Sum of electronic and thermal Energies= -820.117922
Sum of electronic and thermal Enthalpies= -820.116978
Sum of electronic and thermal Free Energies= -820.158159

1	N	Isotropic =	-123.2428	Anisotropy = 227.7596
2	C	Isotropic =	23.4597	Anisotropy = 147.2744
3	C	Isotropic =	91.6151	Anisotropy = 96.6374
4	C	Isotropic =	29.1101	Anisotropy = 74.1456
5	O	Isotropic =	-46.2240	Anisotropy = 223.5013
6	Cl	Isotropic =	747.4867	Anisotropy = 378.6805
7	C	Isotropic =	133.5890	Anisotropy = 51.4254
8	O	Isotropic =	304.8098	Anisotropy = 33.0627
9	H	Isotropic =	25.0830	Anisotropy = 5.6817
10	H	Isotropic =	26.7263	Anisotropy = 6.9054
11	H	Isotropic =	26.7674	Anisotropy = 5.6776
12	H	Isotropic =	30.8792	Anisotropy = 15.1935

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

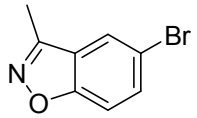
N	0.626681846092	0.936126332355	1.644497873896
C	-0.007663410715	0.300605709858	0.680756813832
C	0.799961999586	0.150812989330	-0.487835006960
C	1.969052885948	0.742486562286	-0.118363886750
O	1.907930606440	1.216730403131	1.137210493781
Cl	3.448871999435	0.976889139948	-0.954737543216
C	-1.423110581212	-0.175180855680	0.875085307711
O	-2.228897423238	0.053592833373	-0.269646170626
H	0.545529364275	-0.314052727546	-1.433461259643
H	-1.415028836531	-1.266794314981	1.023511925678
H	-1.833274389332	0.282521778898	1.792767226459
H	-2.323814060748	1.013172149029	-0.377235774161

SCF Done: E(RB3LYP) = -820.206280670

Zero-point correction= 0.081048
Thermal correction to Energy= 0.088336

Thermal correction to Enthalpy= 0.089280
Thermal correction to Gibbs Free Energy= 0.048207
Sum of electronic and zero-point Energies= -820.125232
Sum of electronic and thermal Energies= -820.117945
Sum of electronic and thermal Enthalpies= -820.117000
Sum of electronic and thermal Free Energies= -820.158073

1	N	Isotropic =	-123.0960	Anisotropy =	227.8616
2	C	Isotropic =	23.3500	Anisotropy =	147.0488
3	C	Isotropic =	91.6209	Anisotropy =	96.5307
4	C	Isotropic =	29.1354	Anisotropy =	74.1207
5	O	Isotropic =	-46.1761	Anisotropy =	223.6331
6	Cl	Isotropic =	747.6675	Anisotropy =	378.4811
7	C	Isotropic =	133.5829	Anisotropy =	51.4464
8	O	Isotropic =	305.1766	Anisotropy =	33.1949
9	H	Isotropic =	25.0892	Anisotropy =	5.6934
10	H	Isotropic =	26.7706	Anisotropy =	5.6873
11	H	Isotropic =	26.7228	Anisotropy =	6.9156
12	H	Isotropic =	30.8720	Anisotropy =	15.2287



2d

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.115473051174	-0.906848991837	-1.107838396333
C	1.121309614640	-0.808429673394	-0.142439421701
C	1.228568973698	0.275555677772	0.736453583873
C	0.306059967532	1.333924182029	0.682224029605
C	-0.695386783424	1.238523651319	-0.276923116095
C	-0.799187096201	0.142349303183	-1.162122581856
C	2.389547982215	-0.048421613585	1.532771672668
N	2.903172451557	-1.194704830734	1.160487772182
O	2.115121078621	-1.696634071739	0.098375197306
Br	-1.996262037838	2.646807301814	-0.413786936292
C	3.001668532994	0.740113701371	2.643767001515
H	0.046608802126	-1.758371187046	-1.784837889295
H	0.370973828717	2.187003504410	1.357067352221
H	-1.605094311865	0.118608239280	-1.895792689771
H	3.880425321938	0.219094487635	3.045824834216
H	3.308687579034	1.735536837114	2.285689553837
H	2.273113045083	0.891943482407	3.455820033921

SCF Done: E(RB3LYP) = -3012.59056917

Zero-point correction= 0.122187
Thermal correction to Energy= 0.131232
Thermal correction to Enthalpy= 0.132176
Thermal correction to Gibbs Free Energy= 0.086775
Sum of electronic and zero-point Energies= -3012.468382
Sum of electronic and thermal Energies= -3012.459337
Sum of electronic and thermal Enthalpies= -3012.458393
Sum of electronic and thermal Free Energies= -3012.503795

1	C	Isotropic =	81.8358	Anisotropy =	144.5590
2	C	Isotropic =	30.9685	Anisotropy =	138.5756
3	C	Isotropic =	67.9283	Anisotropy =	128.1198
4	C	Isotropic =	68.3736	Anisotropy =	142.3444
5	C	Isotropic =	56.5082	Anisotropy =	99.3596
6	C	Isotropic =	60.8892	Anisotropy =	148.7703
7	C	Isotropic =	35.0421	Anisotropy =	141.3064
8	N	Isotropic =	-122.4494	Anisotropy =	218.2861
9	O	Isotropic =	-2.7821	Anisotropy =	185.8868
10	Br	Isotropic =	2086.1774	Anisotropy =	1327.7938
11	C	Isotropic =	181.0225	Anisotropy =	20.5639
12	H	Isotropic =	23.9684	Anisotropy =	4.9368
13	H	Isotropic =	23.7229	Anisotropy =	10.8993
14	H	Isotropic =	23.9161	Anisotropy =	9.3341
15	H	Isotropic =	28.8577	Anisotropy =	8.8522
16	H	Isotropic =	28.9131	Anisotropy =	8.0224
17	H	Isotropic =	28.9119	Anisotropy =	8.0198

2d incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

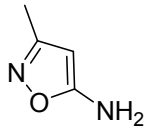
C	0.020420204082	-1.108974263260	-0.774001127130
C	1.312734680266	-0.495067956943	-0.793654884161
C	1.491102044225	0.829067574748	-0.259187898139
C	0.395600397130	1.553555200744	0.296568658466
C	-0.822818650755	0.926746217717	0.294056984477
C	-1.019857830824	-0.396830033625	-0.235502977982
C	2.839896514507	1.081473216827	-0.447377410121
O	3.392763937044	0.007877758499	-1.034870359077
N	2.449294252248	-1.000524415210	-1.263672204332
Br	-2.356519672554	1.826523636047	1.020926383995
C	3.721689150877	2.236742672809	-0.140943965462
H	-0.125937041227	-2.112117547850	-1.176022327807
H	0.525938698772	2.556668022110	0.701952424618
H	-2.019726498600	-0.830567247766	-0.202353525100
H	4.540777707047	1.936538868161	0.531805075883
H	4.176009236990	2.637831213843	-1.061036298119
H	3.144722870772	3.035737083148	0.342693449991

SCF Done: E(RB3LYP) = -3012.57546154

Zero-point correction= 0.121733

Thermal correction to Energy= 0.131023
Thermal correction to Enthalpy= 0.131967
Thermal correction to Gibbs Free Energy= 0.085386
Sum of electronic and zero-point Energies= -3012.453728
Sum of electronic and thermal Energies= -3012.444438
Sum of electronic and thermal Enthalpies= -3012.443494
Sum of electronic and thermal Free Energies= -3012.490076

1	C	Isotropic =	76.4737	Anisotropy =	147.8652
2	C	Isotropic =	37.4031	Anisotropy =	159.5697
3	C	Isotropic =	74.4299	Anisotropy =	120.1975
4	C	Isotropic =	68.8581	Anisotropy =	140.0199
5	C	Isotropic =	56.2071	Anisotropy =	93.6720
6	C	Isotropic =	58.6625	Anisotropy =	143.2160
7	C	Isotropic =	22.3687	Anisotropy =	130.1960
8	O	Isotropic =	-78.1378	Anisotropy =	297.5214
9	N	Isotropic =	-112.0858	Anisotropy =	240.7045
10	Br	Isotropic =	2078.0744	Anisotropy =	1314.3247
11	C	Isotropic =	180.2376	Anisotropy =	21.0828
12	H	Isotropic =	24.0426	Anisotropy =	5.3106
13	H	Isotropic =	23.7880	Anisotropy =	10.6835
14	H	Isotropic =	24.2439	Anisotropy =	9.0095
15	H	Isotropic =	28.6590	Anisotropy =	9.4433
16	H	Isotropic =	28.6613	Anisotropy =	9.4589
17	H	Isotropic =	28.5523	Anisotropy =	7.2750



2e

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-2.115944396802	1.235817258574	-0.001806535244
C	-1.321769901947	0.185120458577	0.280741409046
C	-0.004016980665	0.581453228302	0.304796872816
C	-0.068019936316	1.973558888900	0.008463690902
N	-1.304619991868	2.392675286012	-0.177586377536
N	-1.941163332383	-1.029014443417	0.410228198786
C	1.067282372444	2.943720293298	-0.101090128198
H	0.872365307145	-0.026195903415	0.506372365636
H	-1.412269085065	-1.718509708020	0.936580503244
H	-2.912436677758	-0.979219090420	0.709386702910
H	1.632910840886	2.990306149856	0.843147483900
H	1.770754982938	2.633139800373	-0.889946793660
H	0.692536799390	3.949067781381	-0.338017392603

SCF Done: E(RB3LYP) = -340.749783560

Zero-point correction= 0.101708
Thermal correction to Energy= 0.108322
Thermal correction to Enthalpy= 0.109266
Thermal correction to Gibbs Free Energy= 0.071517
Sum of electronic and zero-point Energies= -340.648075
Sum of electronic and thermal Energies= -340.641462
Sum of electronic and thermal Enthalpies= -340.640517
Sum of electronic and thermal Free Energies= -340.678266

1	O	Isotropic =	-8.5381	Anisotropy = 161.5900
2	C	Isotropic =	24.4456	Anisotropy = 115.9919
3	C	Isotropic =	112.9148	Anisotropy = 59.3310
4	C	Isotropic =	30.7725	Anisotropy = 148.0268
5	N	Isotropic =	-91.5689	Anisotropy = 157.0422
6	N	Isotropic =	205.2581	Anisotropy = 67.8885
7	C	Isotropic =	179.3691	Anisotropy = 23.8822
8	H	Isotropic =	26.5057	Anisotropy = 3.1861
9	H	Isotropic =	27.6541	Anisotropy = 11.9226
10	H	Isotropic =	27.5235	Anisotropy = 11.7496
11	H	Isotropic =	29.3094	Anisotropy = 8.1289
12	H	Isotropic =	29.3079	Anisotropy = 8.2098
13	H	Isotropic =	29.4725	Anisotropy = 7.6653

2e incorrect isomer

Conformer 1

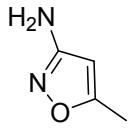
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.280479450001	0.520879715967	1.176224896151
C	-1.541996671133	0.369542631837	-0.111497245317
C	-0.835962623462	1.324952229042	-0.914609630735
C	-0.124738644416	2.055344785705	-0.008658768669
O	-0.364992904200	1.596339039556	1.239266660396
N	-2.349223196364	-0.656719747664	-0.568227851194
C	0.818735953761	3.199367875540	-0.139171402094
H	-0.858469765799	1.437373986820	-1.994517933496
H	-2.880552247778	-0.419780913951	-1.402208861871
H	-2.956928785184	-1.043394905317	0.151290754040
H	0.933501213233	3.478605169903	-1.194701061353
H	0.452929124106	4.075197480282	0.420593112625
H	1.809137997238	2.938002652280	0.267027331518

SCF Done: E(RB3LYP) = -340.748750072

Zero-point correction= 0.101916
Thermal correction to Energy= 0.108535
Thermal correction to Enthalpy= 0.109479
Thermal correction to Gibbs Free Energy= 0.071532
Sum of electronic and zero-point Energies= -340.646834
Sum of electronic and thermal Energies= -340.640215
Sum of electronic and thermal Enthalpies= -340.639271
Sum of electronic and thermal Free Energies= -340.677218

1 N Isotropic = -78.2848 Anisotropy = 175.4461
2 C Isotropic = 29.8224 Anisotropy = 133.1508
3 C Isotropic = 98.1425 Anisotropy = 74.1972
4 C Isotropic = 22.0720 Anisotropy = 125.9991
5 O Isotropic = -10.1600 Anisotropy = 192.0884
6 N Isotropic = 216.0716 Anisotropy = 58.7541
7 C Isotropic = 179.2412 Anisotropy = 24.3405
8 H Isotropic = 25.9096 Anisotropy = 3.8524
9 H Isotropic = 28.4483 Anisotropy = 11.7861
10 H Isotropic = 28.1525 Anisotropy = 12.1997
11 H Isotropic = 29.1324 Anisotropy = 7.4470
12 H Isotropic = 29.1557 Anisotropy = 8.5371
13 H Isotropic = 29.1587 Anisotropy = 8.5956



2f

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.698191045358	1.502239194738	0.983155656902
C	-1.606463004575	0.400141410395	0.206939431198
C	-0.511225036723	0.493271768670	-0.600380618474
C	0.067974504600	1.758459243475	-0.253836506676
N	-0.630314654427	2.378648503028	0.682902605032
N	1.248711072025	2.287600956551	-0.743197619480
C	-2.657805890104	-0.639406573819	0.380245624425
H	-0.157027136521	-0.226384253178	-1.332487392415
H	1.424435599596	2.063859121032	-1.719499114156
H	1.341820605371	3.287905317968	-0.578083148934
H	-2.480729650368	-1.476933320280	-0.307128511160
H	-2.661608553310	-1.024309954304	1.412751497160
H	-3.657806810206	-0.222451414276	0.179488096579

SCF Done: E(RB3LYP) = -340.748761041

Zero-point correction= 0.101940
Thermal correction to Energy= 0.108558
Thermal correction to Enthalpy= 0.109502
Thermal correction to Gibbs Free Energy= 0.071541
Sum of electronic and zero-point Energies= -340.646821
Sum of electronic and thermal Energies= -340.640203
Sum of electronic and thermal Enthalpies= -340.639259
Sum of electronic and thermal Free Energies= -340.677220

1 O Isotropic = -10.0801 Anisotropy = 191.9592

2 C Isotropic = 22.1048 Anisotropy = 125.9608
3 C Isotropic = 98.2094 Anisotropy = 74.0573
4 C Isotropic = 29.7737 Anisotropy = 133.1156
5 N Isotropic = -78.3607 Anisotropy = 175.5101
6 N Isotropic = 216.1274 Anisotropy = 58.7862
7 C Isotropic = 179.1881 Anisotropy = 24.3600
8 H Isotropic = 25.9162 Anisotropy = 3.8410
9 H Isotropic = 28.4475 Anisotropy = 11.7893
10 H Isotropic = 28.1523 Anisotropy = 12.2031
11 H Isotropic = 29.1350 Anisotropy = 7.4330
12 H Isotropic = 29.1564 Anisotropy = 8.6110
13 H Isotropic = 29.1549 Anisotropy = 8.5179

2f incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

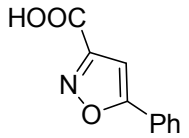
O	-1.718277425475	0.889441357019	1.005570518505
C	-1.397154274707	0.229452911787	-0.123877980942
C	-0.393131567993	0.893989038039	-0.790608935526
C	-0.132069570104	2.023340170632	0.037912012280
N	-0.899534037046	2.049505536204	1.110230651014
C	0.872420671949	3.112177746616	-0.180233379211
N	-2.144775226108	-0.880344141832	-0.413853220685
H	0.085729491054	0.616435617040	-1.724240964563
H	0.835849833155	3.839380210931	0.642651042820
H	1.890934308769	2.696606758738	-0.240218250744
H	0.676826605406	3.639516443458	-1.127504118259
H	-1.697401811169	-1.536463970472	-1.047532843466
H	-2.546726997730	-1.343617678160	0.398035468778

SCF Done: E(RB3LYP) = -340.749739667

Zero-point correction= 0.101658
Thermal correction to Energy= 0.108283
Thermal correction to Enthalpy= 0.109227
Thermal correction to Gibbs Free Energy= 0.071451
Sum of electronic and zero-point Energies= -340.648082
Sum of electronic and thermal Energies= -340.641457
Sum of electronic and thermal Enthalpies= -340.640512
Sum of electronic and thermal Free Energies= -340.678289

1 O Isotropic = -8.5508 Anisotropy = 161.6470
2 C Isotropic = 24.5319 Anisotropy = 115.9636
3 C Isotropic = 113.0462 Anisotropy = 59.6019
4 C Isotropic = 30.8159 Anisotropy = 148.2505
5 N Isotropic = -91.5841 Anisotropy = 157.2925
6 C Isotropic = 179.3505 Anisotropy = 23.9092
7 N Isotropic = 205.2682 Anisotropy = 67.8538
8 H Isotropic = 26.5041 Anisotropy = 3.1844
9 H Isotropic = 29.4711 Anisotropy = 7.6588
10 H Isotropic = 29.3102 Anisotropy = 8.1304

11 H Isotropic = 29.3064 Anisotropy = 8.2163
12 H Isotropic = 27.6612 Anisotropy = 11.9298
13 H Isotropic = 27.5273 Anisotropy = 11.7448



2g

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.934698977124	1.109659276347	-1.100410162257
C	-0.990423137103	1.167260929575	-0.121646381509
C	-1.612126605572	1.454621520756	1.067656435134
C	-2.984263033301	1.560154627477	0.714541496165
N	-3.185784469176	1.356140765998	-0.575633632646
C	0.399025037029	0.926117880189	-0.508674964788
C	1.420417713069	0.986337734565	0.458614836806
C	2.746708266721	0.754774134936	0.094620416462
C	3.072382205295	0.461004455140	-1.234956652287
C	2.061950277730	0.400297588703	-2.200949472545
C	0.732629120595	0.630837371399	-1.844172182144
C	-4.151150714447	1.857111224907	1.591868874939
O	-3.756360294522	2.038173420092	2.864680792952
O	-5.300881816545	1.926937527486	1.217204985489
H	-1.172911517339	1.574230093369	2.051262376153
H	1.177907007630	1.214891808582	1.497826657712
H	3.530565730885	0.804063330281	0.852972211670
H	4.111709023616	0.280031059739	-1.516777067645
H	2.309767830556	0.171911211698	-3.239518191288
H	-0.052620372869	0.582088524221	-2.599100543890
H	-4.555041275128	2.227175514539	3.393210167519

SCF Done: E(RB3LYP) = -665.725344380

Zero-point correction= 0.153538
Thermal correction to Energy= 0.164504
Thermal correction to Enthalpy= 0.165448
Thermal correction to Gibbs Free Energy= 0.114901
Sum of electronic and zero-point Energies= -665.571807
Sum of electronic and thermal Energies= -665.560840
Sum of electronic and thermal Enthalpies= -665.559896
Sum of electronic and thermal Free Energies= -665.610443

1 O Isotropic = -51.0106 Anisotropy = 279.5952
2 C Isotropic = 19.3777 Anisotropy = 115.2621
3 C Isotropic = 91.9056 Anisotropy = 103.8333
4 C Isotropic = 35.2340 Anisotropy = 119.7465

5	N	Isotropic =	-135.1829	Anisotropy =	304.1385
6	C	Isotropic =	65.6061	Anisotropy =	162.6035
7	C	Isotropic =	66.5922	Anisotropy =	166.2534
8	C	Isotropic =	63.4338	Anisotropy =	176.2066
9	C	Isotropic =	61.5895	Anisotropy =	180.4010
10	C	Isotropic =	63.5077	Anisotropy =	177.0054
11	C	Isotropic =	67.4639	Anisotropy =	173.1546
12	C	Isotropic =	36.1651	Anisotropy =	84.4423
13	O	Isotropic =	139.3125	Anisotropy =	174.1506
14	O	Isotropic =	-45.7819	Anisotropy =	515.6631
15	H	Isotropic =	24.4388	Anisotropy =	6.3769
16	H	Isotropic =	23.6112	Anisotropy =	8.0768
17	H	Isotropic =	23.8540	Anisotropy =	5.1246
18	H	Isotropic =	23.8651	Anisotropy =	4.7690
19	H	Isotropic =	23.8417	Anisotropy =	5.1421
20	H	Isotropic =	23.2917	Anisotropy =	8.0418
21	H	Isotropic =	25.1266	Anisotropy =	11.3740

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.974518381504	2.543633722199	-0.348577885470
C	-0.895651435007	1.230098176594	0.001920730641
C	-2.032905472969	0.892851778436	0.691512312951
C	-2.780887807702	2.099203590948	0.719363764944
N	-2.160546869710	3.089625357883	0.102889502314
C	0.302691917459	0.494647445029	-0.400141469329
C	0.443165980318	-0.863776620324	-0.057455055770
C	1.583774431295	-1.569959219047	-0.438704517018
C	2.597484673919	-0.933522552591	-1.165026712498
C	2.463881244265	0.416269200635	-1.508486837223
C	1.325374011384	1.129318116959	-1.130381426707
C	-4.113493283179	2.275041937521	1.357173655564
O	-4.592609301832	3.520808672977	1.230842200116
O	-4.691307956904	1.373267212723	1.927714594762
H	-2.313734225644	-0.062032989325	1.121035275676
H	-0.340988829717	-1.369394572618	0.508726952056
H	1.682061653752	-2.622988778983	-0.167371317530
H	3.489391653443	-1.489163632207	-1.462242700122
H	3.251210658183	0.918054619750	-2.074785779698
H	1.224232319810	2.181088141643	-1.399892986514
H	-5.461434979659	3.540670391798	1.675957698854

SCF Done: E(RB3LYP) = -665.726100179

Zero-point correction= 0.153570
Thermal correction to Energy= 0.164530
Thermal correction to Enthalpy= 0.165474
Thermal correction to Gibbs Free Energy= 0.114965
Sum of electronic and zero-point Energies= -665.572530
Sum of electronic and thermal Energies= -665.561570
Sum of electronic and thermal Enthalpies= -665.560626
Sum of electronic and thermal Free Energies= -665.611135

1	O	Isotropic =	-51.0433	Anisotropy =	258.6501
2	C	Isotropic =	19.7451	Anisotropy =	116.4144
3	C	Isotropic =	91.0986	Anisotropy =	106.5287
4	C	Isotropic =	35.2115	Anisotropy =	117.6776
5	N	Isotropic =	-132.5964	Anisotropy =	303.4744
6	C	Isotropic =	65.6412	Anisotropy =	162.5868
7	C	Isotropic =	66.3864	Anisotropy =	166.2420
8	C	Isotropic =	63.4542	Anisotropy =	176.2072
9	C	Isotropic =	61.6101	Anisotropy =	180.1703
10	C	Isotropic =	63.5761	Anisotropy =	177.0480
11	C	Isotropic =	67.4963	Anisotropy =	172.9385
12	C	Isotropic =	35.1253	Anisotropy =	87.1169
13	O	Isotropic =	146.0892	Anisotropy =	167.4379
14	O	Isotropic =	-58.6848	Anisotropy =	505.8823
15	H	Isotropic =	24.3509	Anisotropy =	6.0245
16	H	Isotropic =	23.5974	Anisotropy =	8.0953
17	H	Isotropic =	23.8548	Anisotropy =	5.1064
18	H	Isotropic =	23.8695	Anisotropy =	4.7648
19	H	Isotropic =	23.8405	Anisotropy =	5.1643
20	H	Isotropic =	23.2968	Anisotropy =	8.0340
21	H	Isotropic =	25.1460	Anisotropy =	11.5481

2g incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.629455206818	-0.801597227164	0.566969809659
C	1.354875181170	-0.995929897096	0.255170357468
C	0.832527147084	0.136112918731	-0.446832756723
C	1.890418158064	0.992443149996	-0.517689189940
O	2.971952258903	0.447802018144	0.083212570764
C	0.667396928975	-2.246589993099	0.629575849669
C	-0.693041069446	-2.430068469155	0.328272383986
C	-1.342767207164	-3.614757746733	0.684029947296
C	-0.643591392841	-4.629822026777	1.344077893408
C	0.712238703656	-4.454219553336	1.647903869275
C	1.364409555522	-3.273212002407	1.294551477123
C	1.981904774967	2.337182051346	-1.126658171932
O	3.201169580180	2.878248492117	-0.991697190817
O	1.043196070669	2.869753120710	-1.680858432695
H	-0.164094674230	0.299307985695	-0.841406790215
H	-1.253433079050	-1.647159961555	-0.185255840285
H	-2.400072373644	-3.743233964624	0.443636111764
H	-1.152457258135	-5.555443772192	1.621323797571
H	1.264378578360	-5.243110238544	2.163030701152
H	2.420395344148	-3.136610368369	1.530489976280
H	3.176749565995	3.757095484314	-1.416336372808

SCF Done: E(RB3LYP) = -665.723446970

Zero-point correction= 0.153576

Thermal correction to Energy= 0.164536
Thermal correction to Enthalpy= 0.165480
Thermal correction to Gibbs Free Energy= 0.114872
Sum of electronic and zero-point Energies= -665.569870
Sum of electronic and thermal Energies= -665.558911
Sum of electronic and thermal Enthalpies= -665.557967
Sum of electronic and thermal Free Energies= -665.608575

1	N	Isotropic =	-127.9207	Anisotropy =	264.0153
2	C	Isotropic =	28.8990	Anisotropy =	134.8140
3	C	Isotropic =	82.7255	Anisotropy =	119.8916
4	C	Isotropic =	29.8368	Anisotropy =	104.0886
5	O	Isotropic =	-43.3927	Anisotropy =	277.2245
6	C	Isotropic =	64.0577	Anisotropy =	166.0379
7	C	Isotropic =	65.3667	Anisotropy =	167.2866
8	C	Isotropic =	63.6286	Anisotropy =	175.3888
9	C	Isotropic =	61.8549	Anisotropy =	179.6082
10	C	Isotropic =	63.8050	Anisotropy =	176.1736
11	C	Isotropic =	67.3014	Anisotropy =	171.7346
12	C	Isotropic =	39.2909	Anisotropy =	80.3094
13	O	Isotropic =	144.7650	Anisotropy =	157.7202
14	O	Isotropic =	-45.2462	Anisotropy =	485.5427
15	H	Isotropic =	23.8915	Anisotropy =	6.8427
16	H	Isotropic =	23.6811	Anisotropy =	8.0652
17	H	Isotropic =	23.8584	Anisotropy =	5.1762
18	H	Isotropic =	23.8719	Anisotropy =	4.7832
19	H	Isotropic =	23.8754	Anisotropy =	5.0976
20	H	Isotropic =	23.1021	Anisotropy =	7.4093
21	H	Isotropic =	25.1203	Anisotropy =	11.5002

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

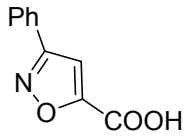
N	1.567567396615	0.136128129960	1.307945257023
C	1.185893034542	-0.797590251525	0.446938656612
C	1.500481930861	-0.401421370179	-0.892100097162
C	2.086690973135	0.820125632337	-0.740517759637
O	2.134003906576	1.155070563486	0.567305977420
C	0.534870828468	-2.036661366832	0.913733918719
C	0.163854620899	-3.035605001241	-0.002548731130
C	-0.451246615065	-4.209182170661	0.440800512881
C	-0.703420509067	-4.400122253821	1.802721038901
C	-0.336760569753	-3.409145954153	2.721909398734
C	0.277287118387	-2.236255785448	2.283395069910
C	2.650592827453	1.795075872482	-1.699928827018
O	2.538741434526	1.342323720549	-2.959883725472
O	3.144725251466	2.855932134656	-1.385488109468
H	1.322178079892	-0.930008731614	-1.821839322163
H	0.355051702929	-2.903079061983	-1.068578027851
H	-0.733703762217	-4.976647597880	-0.282654094226
H	-1.184388321108	-5.317708459898	2.148114378280
H	-0.531278776263	-3.551502757457	3.787013372382
H	0.562106046765	-1.464235315525	2.999118369661

H 2.923443400959 2.019400024747 -3.548667256396

SCF Done: E(RB3LYP) = -665.723185057

Zero-point correction= 0.153485
Thermal correction to Energy= 0.164493
Thermal correction to Enthalpy= 0.165437
Thermal correction to Gibbs Free Energy= 0.114347
Sum of electronic and zero-point Energies= -665.569700
Sum of electronic and thermal Energies= -665.558692
Sum of electronic and thermal Enthalpies= -665.557748
Sum of electronic and thermal Free Energies= -665.608838

1 N Isotropic = -127.7984 Anisotropy = 276.4199
2 C Isotropic = 28.6602 Anisotropy = 133.1209
3 C Isotropic = 84.3383 Anisotropy = 116.1131
4 C Isotropic = 30.7378 Anisotropy = 105.3214
5 O Isotropic = -46.6034 Anisotropy = 277.8246
6 C Isotropic = 63.9760 Anisotropy = 166.1485
7 C Isotropic = 65.5640 Anisotropy = 167.9223
8 C Isotropic = 63.5763 Anisotropy = 175.1655
9 C Isotropic = 61.9959 Anisotropy = 179.7981
10 C Isotropic = 63.6544 Anisotropy = 175.4077
11 C Isotropic = 67.4181 Anisotropy = 171.9977
12 C Isotropic = 39.4474 Anisotropy = 79.4630
13 O Isotropic = 147.4874 Anisotropy = 173.0457
14 O Isotropic = -48.2305 Anisotropy = 524.3577
15 H Isotropic = 24.0489 Anisotropy = 7.0389
16 H Isotropic = 23.6809 Anisotropy = 8.0869
17 H Isotropic = 23.8655 Anisotropy = 5.1891
18 H Isotropic = 23.8733 Anisotropy = 4.7827
19 H Isotropic = 23.8945 Anisotropy = 5.0483
20 H Isotropic = 23.1089 Anisotropy = 7.4053
21 H Isotropic = 25.1993 Anisotropy = 11.8610



2h

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N 2.629455206818 -0.801597227164 0.566969809659
C 1.354875181170 -0.995929897096 0.255170357468
C 0.832527147084 0.136112918731 -0.446832756723
C 1.890418158064 0.992443149996 -0.517689189940
O 2.971952258903 0.447802018144 0.083212570764

C	0.667396928975	-2.246589993099	0.629575849669
C	-0.693041069446	-2.430068469155	0.328272383986
C	-1.342767207164	-3.614757746733	0.684029947296
C	-0.643591392841	-4.629822026777	1.344077893408
C	0.712238703656	-4.454219553336	1.647903869275
C	1.364409555522	-3.273212002407	1.294551477123
C	1.981904774967	2.337182051346	-1.126658171932
O	3.201169580180	2.878248492117	-0.991697190817
O	1.043196070669	2.869753120710	-1.680858432695
H	-0.164094674230	0.299307985695	-0.841406790215
H	-1.253433079050	-1.647159961555	-0.185255840285
H	-2.400072373644	-3.743233964624	0.443636111764
H	-1.152457258135	-5.555443772192	1.621323797571
H	1.264378578360	-5.243110238544	2.163030701152
H	2.420395344148	-3.136610368369	1.530489976280
H	3.176749565995	3.757095484314	-1.416336372808

SCF Done: E(RB3LYP) = -665.723446970

Zero-point correction= 0.153576
Thermal correction to Energy= 0.164536
Thermal correction to Enthalpy= 0.165480
Thermal correction to Gibbs Free Energy= 0.114872
Sum of electronic and zero-point Energies= -665.569870
Sum of electronic and thermal Energies= -665.558911
Sum of electronic and thermal Enthalpies= -665.557967
Sum of electronic and thermal Free Energies= -665.608575

1	N	Isotropic =	-127.9207	Anisotropy = 264.0153
2	C	Isotropic =	28.8990	Anisotropy = 134.8140
3	C	Isotropic =	82.7255	Anisotropy = 119.8916
4	C	Isotropic =	29.8368	Anisotropy = 104.0886
5	O	Isotropic =	-43.3927	Anisotropy = 277.2245
6	C	Isotropic =	64.0577	Anisotropy = 166.0379
7	C	Isotropic =	65.3667	Anisotropy = 167.2866
8	C	Isotropic =	63.6286	Anisotropy = 175.3888
9	C	Isotropic =	61.8549	Anisotropy = 179.6082
10	C	Isotropic =	63.8050	Anisotropy = 176.1736
11	C	Isotropic =	67.3014	Anisotropy = 171.7346
12	C	Isotropic =	39.2909	Anisotropy = 80.3094
13	O	Isotropic =	144.7650	Anisotropy = 157.7202
14	O	Isotropic =	-45.2462	Anisotropy = 485.5427
15	H	Isotropic =	23.8915	Anisotropy = 6.8427
16	H	Isotropic =	23.6811	Anisotropy = 8.0652
17	H	Isotropic =	23.8584	Anisotropy = 5.1762
18	H	Isotropic =	23.8719	Anisotropy = 4.7832
19	H	Isotropic =	23.8754	Anisotropy = 5.0976
20	H	Isotropic =	23.1021	Anisotropy = 7.4093
21	H	Isotropic =	25.1203	Anisotropy = 11.5002

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.567567396615	0.136128129960	1.307945257023
C	1.185893034542	-0.797590251525	0.446938656612
C	1.500481930861	-0.401421370179	-0.892100097162
C	2.086690973135	0.820125632337	-0.740517759637
O	2.134003906576	1.155070563486	0.567305977420
C	0.534870828468	-2.036661366832	0.913733918719
C	0.163854620899	-3.035605001241	-0.002548731130
C	-0.451246615065	-4.209182170661	0.440800512881
C	-0.703420509067	-4.400122253821	1.802721038901
C	-0.336760569753	-3.409145954153	2.721909398734
C	0.277287118387	-2.236255785448	2.283395069910
C	2.650592827453	1.795075872482	-1.699928827018
O	2.538741434526	1.342323720549	-2.959883725472
O	3.144725251466	2.855932134656	-1.385488109468
H	1.322178079892	-0.930008731614	-1.821839322163
H	0.355051702929	-2.903079061983	-1.068578027851
H	-0.733703762217	-4.976647597880	-0.282654094226
H	-1.184388321108	-5.317708459898	2.148114378280
H	-0.531278776263	-3.551502757457	3.787013372382
H	0.562106046765	-1.464235315525	2.999118369661
H	2.923443400959	2.019400024747	-3.548667256396

SCF Done: E(RB3LYP) = -665.723185057

Zero-point correction= 0.153485
Thermal correction to Energy= 0.164493
Thermal correction to Enthalpy= 0.165437
Thermal correction to Gibbs Free Energy= 0.114347
Sum of electronic and zero-point Energies= -665.569700
Sum of electronic and thermal Energies= -665.558692
Sum of electronic and thermal Enthalpies= -665.557748
Sum of electronic and thermal Free Energies= -665.608838

1	N	Isotropic =	-127.7984	Anisotropy =	276.4199
2	C	Isotropic =	28.6602	Anisotropy =	133.1209
3	C	Isotropic =	84.3383	Anisotropy =	116.1131
4	C	Isotropic =	30.7378	Anisotropy =	105.3214
5	O	Isotropic =	-46.6034	Anisotropy =	277.8246
6	C	Isotropic =	63.9760	Anisotropy =	166.1485
7	C	Isotropic =	65.5640	Anisotropy =	167.9223
8	C	Isotropic =	63.5763	Anisotropy =	175.1655
9	C	Isotropic =	61.9959	Anisotropy =	179.7981
10	C	Isotropic =	63.6544	Anisotropy =	175.4077
11	C	Isotropic =	67.4181	Anisotropy =	171.9977
12	C	Isotropic =	39.4474	Anisotropy =	79.4630
13	O	Isotropic =	147.4874	Anisotropy =	173.0457
14	O	Isotropic =	-48.2305	Anisotropy =	524.3577
15	H	Isotropic =	24.0489	Anisotropy =	7.0389
16	H	Isotropic =	23.6809	Anisotropy =	8.0869
17	H	Isotropic =	23.8655	Anisotropy =	5.1891
18	H	Isotropic =	23.8733	Anisotropy =	4.7827
19	H	Isotropic =	23.8945	Anisotropy =	5.0483
20	H	Isotropic =	23.1089	Anisotropy =	7.4053
21	H	Isotropic =	25.1993	Anisotropy =	11.8610

2h incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.934698977124	1.109659276347	-1.100410162257
C	-0.990423137103	1.167260929575	-0.121646381509
C	-1.612126605572	1.454621520756	1.067656435134
C	-2.984263033301	1.560154627477	0.714541496165
N	-3.185784469176	1.356140765998	-0.575633632646
C	0.399025037029	0.926117880189	-0.508674964788
C	1.420417713069	0.986337734565	0.458614836806
C	2.746708266721	0.754774134936	0.094620416462
C	3.072382205295	0.461004455140	-1.234956652287
C	2.061950277730	0.400297588703	-2.200949472545
C	0.732629120595	0.630837371399	-1.844172182144
C	-4.151150714447	1.857111224907	1.591868874939
O	-3.756360294522	2.038173420092	2.864680792952
O	-5.300881816545	1.926937527486	1.217204985489
H	-1.172911517339	1.574230093369	2.051262376153
H	1.177907007630	1.214891808582	1.497826657712
H	3.530565730885	0.804063330281	0.852972211670
H	4.111709023616	0.280031059739	-1.516777067645
H	2.309767830556	0.171911211698	-3.239518191288
H	-0.052620372869	0.582088524221	-2.599100543890
H	-4.555041275128	2.227175514539	3.393210167519

SCF Done: E(RB3LYP) = -665.725344380

Zero-point correction= 0.153538
Thermal correction to Energy= 0.164504
Thermal correction to Enthalpy= 0.165448
Thermal correction to Gibbs Free Energy= 0.114901
Sum of electronic and zero-point Energies= -665.571807
Sum of electronic and thermal Energies= -665.560840
Sum of electronic and thermal Enthalpies= -665.559896
Sum of electronic and thermal Free Energies= -665.610443

1	O	Isotropic =	-51.0106	Anisotropy =	279.5952
2	C	Isotropic =	19.3777	Anisotropy =	115.2621
3	C	Isotropic =	91.9056	Anisotropy =	103.8333
4	C	Isotropic =	35.2340	Anisotropy =	119.7465
5	N	Isotropic =	-135.1829	Anisotropy =	304.1385
6	C	Isotropic =	65.6061	Anisotropy =	162.6035
7	C	Isotropic =	66.5922	Anisotropy =	166.2534
8	C	Isotropic =	63.4338	Anisotropy =	176.2066
9	C	Isotropic =	61.5895	Anisotropy =	180.4010
10	C	Isotropic =	63.5077	Anisotropy =	177.0054
11	C	Isotropic =	67.4639	Anisotropy =	173.1546
12	C	Isotropic =	36.1651	Anisotropy =	84.4423
13	O	Isotropic =	139.3125	Anisotropy =	174.1506
14	O	Isotropic =	-45.7819	Anisotropy =	515.6631
15	H	Isotropic =	24.4388	Anisotropy =	6.3769
16	H	Isotropic =	23.6112	Anisotropy =	8.0768

17 H Isotropic = 23.8540 Anisotropy = 5.1246
18 H Isotropic = 23.8651 Anisotropy = 4.7690
19 H Isotropic = 23.8417 Anisotropy = 5.1421
20 H Isotropic = 23.2917 Anisotropy = 8.0418
21 H Isotropic = 25.1266 Anisotropy = 11.3740

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

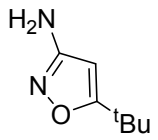
O	-0.974518381504	2.543633722199	-0.348577885470
C	-0.895651435007	1.230098176594	0.001920730641
C	-2.032905472969	0.892851778436	0.691512312951
C	-2.780887807702	2.099203590948	0.719363764944
N	-2.160546869710	3.089625357883	0.102889502314
C	0.302691917459	0.494647445029	-0.400141469329
C	0.443165980318	-0.863776620324	-0.057455055770
C	1.583774431295	-1.569959219047	-0.438704517018
C	2.597484673919	-0.933522552591	-1.165026712498
C	2.463881244265	0.416269200635	-1.508486837223
C	1.325374011384	1.129318116959	-1.130381426707
C	-4.113493283179	2.275041937521	1.357173655564
O	-4.592609301832	3.520808672977	1.230842200116
O	-4.691307956904	1.373267212723	1.927714594762
H	-2.313734225644	-0.062032989325	1.121035275676
H	-0.340988829717	-1.369394572618	0.508726952056
H	1.682061653752	-2.622988778983	-0.167371317530
H	3.489391653443	-1.489163632207	-1.462242700122
H	3.251210658183	0.918054619750	-2.074785779698
H	1.224232319810	2.181088141643	-1.399892986514
H	-5.461434979659	3.540670391798	1.675957698854

SCF Done: E(RB3LYP) = -665.726100179

Zero-point correction= 0.153570
Thermal correction to Energy= 0.164530
Thermal correction to Enthalpy= 0.165474
Thermal correction to Gibbs Free Energy= 0.114965
Sum of electronic and zero-point Energies= -665.572530
Sum of electronic and thermal Energies= -665.561570
Sum of electronic and thermal Enthalpies= -665.560626
Sum of electronic and thermal Free Energies= -665.611135

1 O Isotropic = -51.0433 Anisotropy = 258.6501
2 C Isotropic = 19.7451 Anisotropy = 116.4144
3 C Isotropic = 91.0986 Anisotropy = 106.5287
4 C Isotropic = 35.2115 Anisotropy = 117.6776
5 N Isotropic = -132.5964 Anisotropy = 303.4744
6 C Isotropic = 65.6412 Anisotropy = 162.5868
7 C Isotropic = 66.3864 Anisotropy = 166.2420
8 C Isotropic = 63.4542 Anisotropy = 176.2072
9 C Isotropic = 61.6101 Anisotropy = 180.1703
10 C Isotropic = 63.5761 Anisotropy = 177.0480
11 C Isotropic = 67.4963 Anisotropy = 172.9385

12	C	Isotropic =	35.1253	Anisotropy =	87.1169
13	O	Isotropic =	146.0892	Anisotropy =	167.4379
14	O	Isotropic =	-58.6848	Anisotropy =	505.8823
15	H	Isotropic =	24.3509	Anisotropy =	6.0245
16	H	Isotropic =	23.5974	Anisotropy =	8.0953
17	H	Isotropic =	23.8548	Anisotropy =	5.1064
18	H	Isotropic =	23.8695	Anisotropy =	4.7648
19	H	Isotropic =	23.8405	Anisotropy =	5.1643
20	H	Isotropic =	23.2968	Anisotropy =	8.0340
21	H	Isotropic =	25.1460	Anisotropy =	11.5481



2i

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	1.435948530452	-0.470276247430	0.145938145111
C	0.152939031802	-0.064871586480	0.004954415663
C	-0.057771719164	1.052988380826	0.759169471545
C	1.212229636874	1.302420481350	1.376984771540
N	2.118559315891	0.409379181554	1.017439062501
N	1.498393442600	2.290121603181	2.301673852398
C	-0.725374388841	-0.890102324111	-0.906257042653
C	-2.144981210959	-0.298453311915	-0.927089859769
C	-0.128990047049	-0.870725407614	-2.332361687276
C	-0.771068712748	-2.343502814897	-0.382083165521
H	-0.972257653856	1.625273487930	0.874950572839
H	0.992921212006	3.158313049341	2.144315898272
H	2.495316801774	2.464791392189	2.411788544550
H	-2.144130486036	0.737995555359	-1.299609695725
H	-2.787248891835	-0.896378923409	-1.592371224978
H	-2.598333346224	-0.304366002000	0.076628659052
H	0.894736764848	-1.274341266008	-2.340123932033
H	-0.747315982698	-1.484466895733	-3.006751622842
H	-0.097116662348	0.154979242672	-2.733329624207
H	-1.395740959769	-2.962468339300	-1.045662610103
H	0.236333688368	-2.784856803756	-0.346204831820
H	-1.200808363087	-2.384892451750	0.631521903456

SCF Done: E(RB3LYP) = -458.690962351

Zero-point correction= 0.185673
Thermal correction to Energy= 0.196211
Thermal correction to Enthalpy= 0.197155
Thermal correction to Gibbs Free Energy= 0.150231
Sum of electronic and zero-point Energies= -458.505289

Sum of electronic and thermal Energies= -458.494751
Sum of electronic and thermal Enthalpies= -458.493807
Sum of electronic and thermal Free Energies= -458.540732

1	O	Isotropic =	-5.3716	Anisotropy =	194.4230
2	C	Isotropic =	10.9099	Anisotropy =	130.4535
3	C	Isotropic =	101.3699	Anisotropy =	77.4918
4	C	Isotropic =	29.9131	Anisotropy =	132.5991
5	N	Isotropic =	-76.6290	Anisotropy =	174.8408
6	N	Isotropic =	215.7604	Anisotropy =	59.7550
7	C	Isotropic =	153.7388	Anisotropy =	10.1327
8	C	Isotropic =	163.3372	Anisotropy =	38.6288
9	C	Isotropic =	161.1632	Anisotropy =	41.5221
10	C	Isotropic =	161.3649	Anisotropy =	41.2421
11	H	Isotropic =	25.9445	Anisotropy =	6.6952
12	H	Isotropic =	28.4092	Anisotropy =	11.7261
13	H	Isotropic =	28.1239	Anisotropy =	12.5274
14	H	Isotropic =	29.9471	Anisotropy =	7.8928
15	H	Isotropic =	30.2408	Anisotropy =	8.0325
16	H	Isotropic =	29.9514	Anisotropy =	7.9021
17	H	Isotropic =	29.7418	Anisotropy =	7.7333
18	H	Isotropic =	30.1966	Anisotropy =	8.3359
19	H	Isotropic =	30.3001	Anisotropy =	8.1986
20	H	Isotropic =	30.2037	Anisotropy =	8.3329
21	H	Isotropic =	29.7188	Anisotropy =	7.7596
22	H	Isotropic =	30.2862	Anisotropy =	8.2521

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	1.472502453521	-0.599306779470	0.414241862155
C	0.190342820268	-0.197698631189	0.256022538946
C	0.109629324016	1.152659794469	0.437939262544
C	1.458000592046	1.548066773831	0.724783398493
N	2.284632495335	0.516063620152	0.723321404842
N	1.915376786259	2.839670429391	0.911961046436
C	-0.822892870519	-1.268747086803	-0.074898665155
C	-0.832774200142	-2.320538349175	1.057703413383
C	-2.216911711994	-0.632927175068	-0.209162594189
C	-0.424515343994	-1.944086075408	-1.407115992403
H	-0.766533251825	1.789736381816	0.377077836635
H	1.249801080913	3.447109395954	1.383184396182
H	2.828918114889	2.884981933890	1.359007561083
H	-1.124676953610	-1.865275774078	2.017600117184
H	-1.554089687292	-3.119593164184	0.823119812309
H	0.160034663248	-2.778455020145	1.182830054218
H	-2.958468052148	-1.409366347798	-0.453701202067
H	-2.530246577762	-0.148371749360	0.728922192695
H	-2.239389985590	0.121107465668	-1.011594143341
H	-1.145329973388	-2.739493906780	-1.655056804024
H	-0.419095737626	-1.215582566995	-2.233591715882
H	0.577136015393	-2.394853168715	-1.339963780045

SCF Done: E(RB3LYP) = -458.690968374

Zero-point correction= 0.185683
Thermal correction to Energy= 0.196219
Thermal correction to Enthalpy= 0.197163
Thermal correction to Gibbs Free Energy= 0.150261
Sum of electronic and zero-point Energies= -458.505286
Sum of electronic and thermal Energies= -458.494749
Sum of electronic and thermal Enthalpies= -458.493805
Sum of electronic and thermal Free Energies= -458.540708

1	O	Isotropic =	-5.4709	Anisotropy =	194.8522
2	C	Isotropic =	10.8465	Anisotropy =	130.5252
3	C	Isotropic =	101.5950	Anisotropy =	77.3626
4	C	Isotropic =	29.8743	Anisotropy =	132.3881
5	N	Isotropic =	-76.6059	Anisotropy =	175.0521
6	N	Isotropic =	215.7115	Anisotropy =	59.6556
7	C	Isotropic =	154.0258	Anisotropy =	10.2371
8	C	Isotropic =	161.4347	Anisotropy =	41.1051
9	C	Isotropic =	163.3882	Anisotropy =	38.5013
10	C	Isotropic =	161.3072	Anisotropy =	41.3218
11	H	Isotropic =	25.9482	Anisotropy =	6.7071
12	H	Isotropic =	28.4091	Anisotropy =	11.7277
13	H	Isotropic =	28.1209	Anisotropy =	12.5241
14	H	Isotropic =	30.2920	Anisotropy =	8.2382
15	H	Isotropic =	30.2118	Anisotropy =	8.3118
16	H	Isotropic =	29.7157	Anisotropy =	7.7740
17	H	Isotropic =	30.2523	Anisotropy =	8.0087
18	H	Isotropic =	29.9558	Anisotropy =	7.9147
19	H	Isotropic =	29.9384	Anisotropy =	7.8956
20	H	Isotropic =	30.2071	Anisotropy =	8.3358
21	H	Isotropic =	30.2779	Anisotropy =	8.2444
22	H	Isotropic =	29.7279	Anisotropy =	7.7733

2i incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.334152141172	1.346295901696	0.095450268644
C	-0.010391660645	0.072143960053	-0.008511178182
C	1.368215664069	-0.107229412002	-0.333252413541
C	1.854122251356	1.176723251568	-0.414508520469
O	0.868830360147	2.060636123664	-0.165763632261
N	3.104101384609	1.698535076772	-0.617181746617
C	-1.053421092294	-1.013683160477	0.210275703095
C	-1.153887919044	-1.872873844632	-1.069278322838
C	-0.603288449185	-1.902250677367	1.391127139841
C	-2.429233555638	-0.400630685863	0.525891768794
H	1.916268118281	-1.030820785285	-0.486668394114
H	3.741265690834	1.084015157762	-1.115852817760

H	3.111910553687	2.644662889461	-0.991613813679
H	-1.892497616323	-2.678473186280	-0.925695798153
H	-1.473605383629	-1.265389750311	-1.931207603980
H	-0.188658003857	-2.340159513576	-1.320206037737
H	-1.339098699598	-2.705331088399	1.560528419336
H	0.372796874262	-2.373020380178	1.194646775754
H	-0.518412464582	-1.314481741335	2.319285577617
H	-2.394308970203	0.216686884967	1.436301823058
H	-2.782343479336	0.237743993833	-0.298099820043
H	-3.167101461739	-1.203679014070	0.681192623237

SCF Done: E(RB3LYP) = -458.690752327

Zero-point correction= 0.185303
Thermal correction to Energy= 0.195889
Thermal correction to Enthalpy= 0.196833
Thermal correction to Gibbs Free Energy= 0.149874
Sum of electronic and zero-point Energies= -458.505449
Sum of electronic and thermal Energies= -458.494864
Sum of electronic and thermal Enthalpies= -458.493919
Sum of electronic and thermal Free Energies= -458.540879

1	N	Isotropic =	-89.5781	Anisotropy = 156.5390
2	C	Isotropic =	18.8168	Anisotropy = 150.8499
3	C	Isotropic =	114.7832	Anisotropy = 63.3705
4	C	Isotropic =	24.6187	Anisotropy = 115.4165
5	O	Isotropic =	-4.0184	Anisotropy = 162.5255
6	N	Isotropic =	205.1881	Anisotropy = 68.5879
7	C	Isotropic =	154.2459	Anisotropy = 9.0740
8	C	Isotropic =	160.0968	Anisotropy = 41.7411
9	C	Isotropic =	159.8228	Anisotropy = 42.0484
10	C	Isotropic =	164.2674	Anisotropy = 34.2364
11	H	Isotropic =	26.3549	Anisotropy = 5.7141
12	H	Isotropic =	27.6447	Anisotropy = 11.9197
13	H	Isotropic =	27.5315	Anisotropy = 12.0946
14	H	Isotropic =	30.1989	Anisotropy = 8.2776
15	H	Isotropic =	30.2730	Anisotropy = 8.1622
16	H	Isotropic =	29.9551	Anisotropy = 7.4823
17	H	Isotropic =	30.1928	Anisotropy = 8.3249
18	H	Isotropic =	29.9578	Anisotropy = 7.4755
19	H	Isotropic =	30.2717	Anisotropy = 8.1634
20	H	Isotropic =	29.9260	Anisotropy = 8.4702
21	H	Isotropic =	29.9508	Anisotropy = 8.4592
22	H	Isotropic =	30.4395	Anisotropy = 7.7629

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

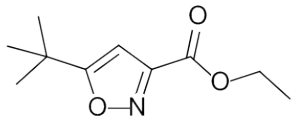
N	1.399626420775	-0.675634265345	0.077255262021
C	0.195347594661	-0.139600612659	0.116357615086
C	0.237098951117	1.283615756555	0.011828962460
C	1.579485267411	1.563922044813	-0.091994268988
O	2.294297895455	0.423007745887	-0.056447368835

N	2.295548162957	2.730183879746	-0.146728211895
C	-1.039148044344	-1.017958587108	0.255448526144
C	-1.950622193589	-0.791849791142	-0.971002740496
C	-0.650116119787	-2.504522465614	0.338679097515
C	-1.796388209889	-0.612317578631	1.539337269957
H	-0.585661776586	1.990702304109	0.008754631414
H	1.775363702328	3.526948005687	-0.502891309741
H	3.210644498458	2.644196487732	-0.583389515177
H	-2.861343864561	-1.406649455799	-0.883058057449
H	-2.260683504336	0.261526012508	-1.056206434379
H	-1.436885322411	-1.073289061858	-1.904273488230
H	-1.557223750970	-3.120929102808	0.442022981079
H	-0.112634830973	-2.830013626011	-0.564778451137
H	0.000774084194	-2.700566386649	1.204175530860
H	-1.168481554398	-0.758611076861	2.432914754744
H	-2.107832539064	0.443684784685	1.509846486320
H	-2.702394866447	-1.229725011238	1.652968728729

SCF Done: E(RB3LYP) = -458.690752230

Zero-point correction= 0.185306
Thermal correction to Energy= 0.195884
Thermal correction to Enthalpy= 0.196828
Thermal correction to Gibbs Free Energy= 0.149737
Sum of electronic and zero-point Energies= -458.505446
Sum of electronic and thermal Energies= -458.494868
Sum of electronic and thermal Enthalpies= -458.493924
Sum of electronic and thermal Free Energies= -458.541015

1	N	Isotropic =	-89.6224	Anisotropy =	156.6232
2	C	Isotropic =	18.8360	Anisotropy =	150.8674
3	C	Isotropic =	114.8619	Anisotropy =	63.3992
4	C	Isotropic =	24.5890	Anisotropy =	115.4843
5	O	Isotropic =	-4.0148	Anisotropy =	163.2708
6	N	Isotropic =	205.2083	Anisotropy =	68.6321
7	C	Isotropic =	154.2435	Anisotropy =	9.3284
8	C	Isotropic =	159.9929	Anisotropy =	41.8949
9	C	Isotropic =	164.3150	Anisotropy =	34.2233
10	C	Isotropic =	160.0064	Anisotropy =	41.9578
11	H	Isotropic =	26.3597	Anisotropy =	5.7013
12	H	Isotropic =	27.6466	Anisotropy =	11.9226
13	H	Isotropic =	27.5300	Anisotropy =	12.0971
14	H	Isotropic =	30.1971	Anisotropy =	8.2852
15	H	Isotropic =	29.9659	Anisotropy =	7.4692
16	H	Isotropic =	30.2755	Anisotropy =	8.1453
17	H	Isotropic =	30.4425	Anisotropy =	7.7615
18	H	Isotropic =	29.9370	Anisotropy =	8.4636
19	H	Isotropic =	29.9316	Anisotropy =	8.4796
20	H	Isotropic =	30.2582	Anisotropy =	8.1875
21	H	Isotropic =	29.9565	Anisotropy =	7.4883
22	H	Isotropic =	30.2018	Anisotropy =	8.3152



2g

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.539681650846	-1.023368849789	0.403118302119
C	-1.237078303533	-1.030404814721	0.615317071062
C	-0.526977340189	-0.292731697478	-0.374107889612
C	-1.507080302021	0.166186176813	-1.208843477651
O	-2.710347500799	-0.269856601586	-0.746112668104
C	-0.617959556417	-1.740174064060	1.770192671379
O	-1.526839940600	-2.342704357072	2.545549321728
O	0.583452321828	-1.744572696835	1.957257587627
C	-1.028578176667	-3.065605379772	3.708655243192
C	-0.650949865107	-4.492113996623	3.350905680023
C	-1.521931729610	1.006572458192	-2.462039758751
C	-0.079000545577	1.398565631412	-2.824225664531
C	-2.149488499473	0.185683296339	-3.612007367361
C	-2.364774792854	2.277133891762	-2.206875034591
H	0.544206211638	-0.140598758871	-0.434903411009
H	-0.176223469682	-2.512663285873	4.126860619760
H	-1.867351707477	-3.034835293414	4.416364636061
H	-0.359909589107	-5.032672333812	4.265871752447
H	-1.501012949127	-5.021304163909	2.892887870593
H	0.199907465729	-4.514184361525	2.653421802339
H	0.391504086373	1.988916784991	-2.022371131816
H	0.544806287043	0.510676591251	-3.012193972141
H	-0.080582983509	2.010727921795	-3.739116282129
H	-2.175846719172	0.792250535844	-4.530923601159
H	-1.562338364016	-0.723626638933	-3.816396381564
H	-3.179570643898	-0.116682270061	-3.369736799734
H	-1.931936939046	2.882745799492	-1.395007027080
H	-2.393991268456	2.894304254953	-3.118665155085
H	-3.398993535429	2.020586221492	-1.931846936011

SCF Done: E(RB3LYP) = -670.534522029

Zero-point correction= 0.239523
Thermal correction to Energy= 0.254494
Thermal correction to Enthalpy= 0.255438
Thermal correction to Gibbs Free Energy= 0.196602
Sum of electronic and zero-point Energies= -670.294999
Sum of electronic and thermal Energies= -670.280028
Sum of electronic and thermal Enthalpies= -670.279084
Sum of electronic and thermal Free Energies= -670.337920

1 N Isotropic = -134.5007 Anisotropy = 302.0366

2	C	Isotropic =	35.0499	Anisotropy =	117.5791
3	C	Isotropic =	91.5309	Anisotropy =	102.0111
4	C	Isotropic =	7.0953	Anisotropy =	134.2640
5	O	Isotropic =	-62.6938	Anisotropy =	277.9208
6	C	Isotropic =	33.4524	Anisotropy =	80.1865
7	O	Isotropic =	127.7403	Anisotropy =	159.0926
8	O	Isotropic =	-51.9080	Anisotropy =	555.4728
9	C	Isotropic =	128.8851	Anisotropy =	65.8822
10	C	Isotropic =	176.1694	Anisotropy =	22.6459
11	C	Isotropic =	153.3972	Anisotropy =	9.8939
12	C	Isotropic =	163.4365	Anisotropy =	38.3538
13	C	Isotropic =	161.1112	Anisotropy =	41.0260
14	C	Isotropic =	161.1291	Anisotropy =	41.1352
15	H	Isotropic =	24.9834	Anisotropy =	7.8630
16	H	Isotropic =	26.3988	Anisotropy =	5.4632
17	H	Isotropic =	27.3785	Anisotropy =	7.3334
18	H	Isotropic =	30.2273	Anisotropy =	9.9317
19	H	Isotropic =	30.0527	Anisotropy =	7.6571
20	H	Isotropic =	29.8740	Anisotropy =	6.0728
21	H	Isotropic =	29.8559	Anisotropy =	8.0249
22	H	Isotropic =	29.8530	Anisotropy =	7.9943
23	H	Isotropic =	30.1560	Anisotropy =	8.1218
24	H	Isotropic =	30.0945	Anisotropy =	8.4130
25	H	Isotropic =	30.2113	Anisotropy =	8.0611
26	H	Isotropic =	29.6343	Anisotropy =	7.9747
27	H	Isotropic =	30.2125	Anisotropy =	8.1090
28	H	Isotropic =	30.0925	Anisotropy =	8.4337
29	H	Isotropic =	29.6375	Anisotropy =	7.9787

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.919949358203	-1.799354647693	0.170461172607
C	-0.988232581607	-0.943436449166	0.546142714568
C	-0.957055406459	0.214591641122	-0.281935507012
C	-1.949318197663	-0.007457412124	-1.195291011699
O	-2.525660849505	-1.210623528610	-0.925935713839
C	-0.092181326449	-1.196724184581	1.709404135017
O	-0.338421400067	-2.368657631454	2.302956438039
O	0.761467868108	-0.403705929474	2.056876345106
C	0.494052385104	-2.694021616773	3.451705296116
C	0.057893579248	-4.052696208851	3.955765883306
C	-2.500323274214	0.765666113885	-2.368268709467
C	-2.337210442848	-0.080573738136	-3.651757132674
C	-3.998653369103	1.055938316522	-2.121247876012
C	-1.726523012801	2.087732540606	-2.509671617685
H	-0.292567749432	1.066194604121	-0.193857861535
H	1.547285437103	-2.686048375193	3.131481894617
H	0.363857440110	-1.906048263364	4.209492148029
H	0.667016957355	-4.333264820632	4.828942276722
H	-0.999731040461	-4.039733489351	4.261676823025
H	0.190070823027	-4.822764490211	3.179960869070
H	-2.873593966697	-1.038061125475	-3.569282064777

H	-2.745655154943	0.469350941648	-4.514228386106
H	-1.275803534626	-0.296325330549	-3.852297587387
H	-4.416857672410	1.607698858027	-2.977842545236
H	-4.570726234610	0.123633964355	-2.000088190885
H	-4.139603762274	1.667352967171	-1.215899890950
H	-0.654698035978	1.909950479739	-2.689594362767
H	-2.123134068900	2.659010551093	-3.363039105772
H	-1.827754050806	2.711746263349	-1.607938432419

SCF Done: E(RB3LYP) = -670.535020549

Zero-point correction= 0.239315
Thermal correction to Energy= 0.254361
Thermal correction to Enthalpy= 0.255305
Thermal correction to Gibbs Free Energy= 0.196354
Sum of electronic and zero-point Energies= -670.295706
Sum of electronic and thermal Energies= -670.280660
Sum of electronic and thermal Enthalpies= -670.279715
Sum of electronic and thermal Free Energies= -670.338667

1	N	Isotropic =	-134.0393	Anisotropy =	302.2776
2	C	Isotropic =	35.2067	Anisotropy =	117.6976
3	C	Isotropic =	91.6273	Anisotropy =	101.9803
4	C	Isotropic =	7.0767	Anisotropy =	134.1112
5	O	Isotropic =	-62.2203	Anisotropy =	277.2891
6	C	Isotropic =	33.4940	Anisotropy =	80.8308
7	O	Isotropic =	127.1601	Anisotropy =	138.5218
8	O	Isotropic =	-62.3283	Anisotropy =	558.4055
9	C	Isotropic =	127.5202	Anisotropy =	59.0128
10	C	Isotropic =	177.2264	Anisotropy =	19.9704
11	C	Isotropic =	153.4217	Anisotropy =	9.9670
12	C	Isotropic =	161.2445	Anisotropy =	41.0082
13	C	Isotropic =	161.1236	Anisotropy =	41.1752
14	C	Isotropic =	163.5340	Anisotropy =	38.2210
15	H	Isotropic =	24.9901	Anisotropy =	7.7326
16	H	Isotropic =	27.1087	Anisotropy =	5.9844
17	H	Isotropic =	27.1251	Anisotropy =	6.0401
18	H	Isotropic =	30.0352	Anisotropy =	9.5645
19	H	Isotropic =	29.8871	Anisotropy =	7.6459
20	H	Isotropic =	29.8940	Anisotropy =	7.6339
21	H	Isotropic =	29.6337	Anisotropy =	7.9702
22	H	Isotropic =	30.0947	Anisotropy =	8.4039
23	H	Isotropic =	30.2195	Anisotropy =	8.1102
24	H	Isotropic =	30.0935	Anisotropy =	8.4128
25	H	Isotropic =	29.6236	Anisotropy =	7.9549
26	H	Isotropic =	30.2063	Anisotropy =	8.1161
27	H	Isotropic =	29.8498	Anisotropy =	8.0212
28	H	Isotropic =	30.1565	Anisotropy =	8.1159
29	H	Isotropic =	29.8528	Anisotropy =	8.0233

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.314107967379	-1.593748219696	0.258240962679
C	-1.142711532311	-1.075104190169	0.575456305963
C	-0.622290784678	-0.248305880495	-0.460512382881
C	-1.575958714705	-0.305980221701	-1.437784588586
O	-2.587766590392	-1.109302535803	-1.009986101823
C	-0.474001072075	-1.347005240224	1.879236477901
O	-1.193199997342	-2.159908524883	2.661598576038
O	0.607049771153	-0.868410882403	2.163293135847
C	-0.630470375104	-2.492177907174	3.964293817562
C	-0.997298330224	-1.449343731620	5.005158988597
C	-1.723512805410	0.304536666061	-2.809924284246
C	-0.485107659177	1.164266547949	-3.116630662130
C	-1.850435631578	-0.828215982028	-3.854375352334
C	-2.994806340163	1.183898665482	-2.835573451035
H	0.315699871029	0.294369768638	-0.457203844825
H	-1.070821606648	-3.470080829603	4.199047097114
H	0.458331928102	-2.596409098958	3.860039564986
H	-0.627788894613	-1.772808014086	5.991507503089
H	-0.540769016269	-0.476272825213	4.769271538020
H	-2.089410492738	-1.324487575858	5.069480433186
H	-0.373527971051	1.984788192948	-2.390542280415
H	0.436849901980	0.562072176894	-3.103189244173
H	-0.583660842503	1.610300690616	-4.118250823579
H	-1.972093345480	-0.395522404393	-4.859832645415
H	-0.951531333135	-1.464820500727	-3.859913220738
H	-2.722913579385	-1.465624033892	-3.645826336039
H	-2.923790670035	2.003089874405	-2.102723163294
H	-3.121137581231	1.626548609309	-3.836099899770
H	-3.893398338636	0.591967406623	-2.604826119701

SCF Done: E(RB3LYP) = -670.534518439

Zero-point correction= 0.239470
Thermal correction to Energy= 0.254483
Thermal correction to Enthalpy= 0.255427
Thermal correction to Gibbs Free Energy= 0.196224
Sum of electronic and zero-point Energies= -670.295048
Sum of electronic and thermal Energies= -670.280036
Sum of electronic and thermal Enthalpies= -670.279091
Sum of electronic and thermal Free Energies= -670.338294

1	N	Isotropic =	-134.5527	Anisotropy = 302.1836
2	C	Isotropic =	35.0878	Anisotropy = 117.5657
3	C	Isotropic =	91.6460	Anisotropy = 102.2402
4	C	Isotropic =	7.0802	Anisotropy = 134.3136
5	O	Isotropic =	-62.6409	Anisotropy = 277.5588
6	C	Isotropic =	33.4392	Anisotropy = 80.1102
7	O	Isotropic =	127.7866	Anisotropy = 158.9320
8	O	Isotropic =	-52.0494	Anisotropy = 555.5043
9	C	Isotropic =	128.8191	Anisotropy = 65.9264
10	C	Isotropic =	176.1891	Anisotropy = 22.5520
11	C	Isotropic =	153.4812	Anisotropy = 9.8636
12	C	Isotropic =	163.5742	Anisotropy = 38.2948
13	C	Isotropic =	161.1940	Anisotropy = 41.1766
14	C	Isotropic =	161.0831	Anisotropy = 41.1835
15	H	Isotropic =	24.9752	Anisotropy = 7.8596

16	H	Isotropic =	27.3751	Anisotropy =	7.3284
17	H	Isotropic =	26.3975	Anisotropy =	5.4825
18	H	Isotropic =	30.2261	Anisotropy =	9.9285
19	H	Isotropic =	29.8689	Anisotropy =	6.0618
20	H	Isotropic =	30.0538	Anisotropy =	7.6567
21	H	Isotropic =	29.8411	Anisotropy =	8.0046
22	H	Isotropic =	29.8472	Anisotropy =	8.0407
23	H	Isotropic =	30.1534	Anisotropy =	8.1162
24	H	Isotropic =	30.1060	Anisotropy =	8.4172
25	H	Isotropic =	30.2064	Anisotropy =	8.1222
26	H	Isotropic =	29.6276	Anisotropy =	7.9718
27	H	Isotropic =	30.2142	Anisotropy =	8.0414
28	H	Isotropic =	30.0982	Anisotropy =	8.4081
29	H	Isotropic =	29.6463	Anisotropy =	7.9528

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.090243046288	-2.072299014643	0.405715849452
C	-1.227854968229	-1.446892101949	0.645782106535
C	-1.421261511106	-0.335232895360	-0.224510608455
C	-0.305122171289	-0.337569654496	-1.014033117707
O	0.489926943442	-1.375465689412	-0.637163689209
C	-2.116014642171	-1.951093903858	1.732966172260
O	-3.218487373766	-1.193335977733	1.825667346273
O	-1.872531377611	-2.911751482915	2.433394737811
C	-4.177649099998	-1.572990153694	2.851737027510
C	-5.333153952761	-0.598750208380	2.775884933116
C	0.192017764982	0.524569352392	-2.148296491172
C	0.358497600550	-0.352080176653	-3.410845718928
C	-0.828604320325	1.643607808451	-2.417020049572
C	1.555189777422	1.138464149665	-1.754592830024
H	-2.262544678241	0.347151478691	-0.246437568608
H	-4.493433037349	-2.610782590468	2.664250192614
H	-3.670232446320	-1.543708349202	3.828244703888
H	-5.819718977831	-0.639159456569	1.789031436125
H	-6.081478623659	-0.857033576989	3.540988288092
H	-4.993344353451	0.432404265751	2.959044562901
H	0.735012217840	0.262104509523	-4.243942122872
H	1.073288767199	-1.170524893462	-3.236392054225
H	-0.603306787817	-0.793820674535	-3.716062929557
H	-0.473646715095	2.278194789111	-3.243587010364
H	-1.810230899865	1.233863039950	-2.702099478543
H	-0.964538681018	2.284759460918	-1.532068791300
H	2.299241472428	0.355693889787	-1.543104306222
H	1.935384861324	1.760959055058	-2.579784938432
H	1.459428259004	1.773809001018	-0.859885651389

SCF Done: E(RB3LYP) = -670.534512041

Zero-point correction= 0.239394
Thermal correction to Energy= 0.254408
Thermal correction to Enthalpy= 0.255353

Thermal correction to Gibbs Free Energy= 0.196495
Sum of electronic and zero-point Energies= -670.295118
Sum of electronic and thermal Energies= -670.280104
Sum of electronic and thermal Enthalpies= -670.279159
Sum of electronic and thermal Free Energies= -670.338017

1	N	Isotropic =	-136.1985	Anisotropy =	302.9258
2	C	Isotropic =	35.0682	Anisotropy =	120.0918
3	C	Isotropic =	92.4154	Anisotropy =	100.0900
4	C	Isotropic =	6.8031	Anisotropy =	133.1534
5	O	Isotropic =	-61.9208	Anisotropy =	294.6634
6	C	Isotropic =	34.4959	Anisotropy =	79.4335
7	O	Isotropic =	119.6377	Anisotropy =	141.8559
8	O	Isotropic =	-49.0455	Anisotropy =	565.2812
9	C	Isotropic =	127.7980	Anisotropy =	58.7370
10	C	Isotropic =	177.2149	Anisotropy =	19.9278
11	C	Isotropic =	153.4249	Anisotropy =	9.8479
12	C	Isotropic =	161.1238	Anisotropy =	41.2953
13	C	Isotropic =	163.5465	Anisotropy =	38.2210
14	C	Isotropic =	161.1764	Anisotropy =	41.1554
15	H	Isotropic =	25.0922	Anisotropy =	9.0134
16	H	Isotropic =	27.1404	Anisotropy =	6.1970
17	H	Isotropic =	27.1506	Anisotropy =	6.2273
18	H	Isotropic =	29.8943	Anisotropy =	7.4123
19	H	Isotropic =	30.0369	Anisotropy =	9.6726
20	H	Isotropic =	29.8905	Anisotropy =	7.4110
21	H	Isotropic =	30.0867	Anisotropy =	8.4627
22	H	Isotropic =	29.6313	Anisotropy =	8.0661
23	H	Isotropic =	30.2057	Anisotropy =	8.0923
24	H	Isotropic =	30.1584	Anisotropy =	8.0448
25	H	Isotropic =	29.8600	Anisotropy =	7.9545
26	H	Isotropic =	29.8753	Anisotropy =	7.9520
27	H	Isotropic =	29.6249	Anisotropy =	8.0853
28	H	Isotropic =	30.0989	Anisotropy =	8.4323
29	H	Isotropic =	30.2121	Anisotropy =	8.0994

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.123516507714	-1.116692781613	1.274699455051
C	-1.100845183452	-1.351265056240	0.840219648998
C	-1.297689234151	-0.874920431332	-0.488164332449
C	-0.089640386456	-0.330849980282	-0.824905136799
O	0.759471943298	-0.475368119123	0.228259793131
C	-2.069155146355	-2.044411486900	1.738429459746
O	-3.252099199101	-2.192467701649	1.124312184994
O	-1.819400433448	-2.419991254607	2.865034756024
C	-4.297978899102	-2.855558705769	1.888045225896
C	-5.528587135631	-2.922057536389	1.009687204465
C	0.455757620199	0.355417429708	-2.053131801115
C	0.914297580324	1.781665367374	-1.671649546797
C	1.658858623883	-0.453882617573	-2.589931604575
C	-0.646952231467	0.428158908963	-3.123286190431

H	-2.200444124310	-0.935632630068	-1.084075559397
H	-3.936672109736	-3.854559039090	2.176608915187
H	-4.473293649761	-2.278648256421	2.809160266813
H	-5.328736437405	-3.497709452936	0.092644181372
H	-6.344357202985	-3.417951317780	1.558079867502
H	-5.866242998568	-1.913321655972	0.725615254094
H	1.322128076329	2.291097937609	-2.558819565801
H	0.072130642195	2.379070378200	-1.288153474861
H	1.697823411112	1.755126538322	-0.899324752237
H	2.075870127195	0.043773896891	-3.479630366595
H	2.455673848152	-0.532117766056	-1.834822653197
H	1.354358708395	-1.472887130914	-2.876578029765
H	-1.516770085126	1.001945383493	-2.766824042471
H	-0.256581366838	0.928860460706	-4.022606466435
H	-0.991181264905	-0.575833380552	-3.416922690344

SCF Done: E(RB3LYP) = -670.534533312

Zero-point correction= 0.239405
Thermal correction to Energy= 0.254425
Thermal correction to Enthalpy= 0.255369
Thermal correction to Gibbs Free Energy= 0.196343
Sum of electronic and zero-point Energies= -670.295129
Sum of electronic and thermal Energies= -670.280108
Sum of electronic and thermal Enthalpies= -670.279164
Sum of electronic and thermal Free Energies= -670.338191

1	N	Isotropic =	-136.2216	Anisotropy =	302.4242
2	C	Isotropic =	35.0521	Anisotropy =	119.9399
3	C	Isotropic =	92.1656	Anisotropy =	99.8446
4	C	Isotropic =	6.7992	Anisotropy =	133.1817
5	O	Isotropic =	-61.8980	Anisotropy =	294.5344
6	C	Isotropic =	34.4604	Anisotropy =	79.2143
7	O	Isotropic =	119.5173	Anisotropy =	142.2176
8	O	Isotropic =	-48.7667	Anisotropy =	566.1259
9	C	Isotropic =	127.7493	Anisotropy =	58.8536
10	C	Isotropic =	177.1744	Anisotropy =	19.9680
11	C	Isotropic =	153.6448	Anisotropy =	9.7245
12	C	Isotropic =	161.2306	Anisotropy =	41.1552
13	C	Isotropic =	161.1770	Anisotropy =	41.2407
14	C	Isotropic =	163.5605	Anisotropy =	38.1595
15	H	Isotropic =	25.0866	Anisotropy =	9.0470
16	H	Isotropic =	27.1316	Anisotropy =	6.2035
17	H	Isotropic =	27.1528	Anisotropy =	6.2505
18	H	Isotropic =	29.8879	Anisotropy =	7.4084
19	H	Isotropic =	30.0258	Anisotropy =	9.6851
20	H	Isotropic =	29.8889	Anisotropy =	7.4030
21	H	Isotropic =	30.1030	Anisotropy =	8.4149
22	H	Isotropic =	30.2125	Anisotropy =	8.1004
23	H	Isotropic =	29.6309	Anisotropy =	8.0824
24	H	Isotropic =	30.0974	Anisotropy =	8.4252
25	H	Isotropic =	29.6405	Anisotropy =	8.0790
26	H	Isotropic =	30.2144	Anisotropy =	8.1026
27	H	Isotropic =	29.8592	Anisotropy =	7.9614
28	H	Isotropic =	30.1658	Anisotropy =	8.0396
29	H	Isotropic =	29.8566	Anisotropy =	7.9585

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.425730891422	0.553706601871	1.070695840585
C	-1.129113878830	-0.711896298208	0.840152444330
C	-1.219756505219	-1.039291224112	-0.543740096525
C	-1.596172717910	0.134338828605	-1.135239813137
O	-1.719066535312	1.085967500771	-0.170476686393
C	-0.759505357026	-1.589487090599	1.988456247383
O	-0.491352146831	-2.831740876326	1.554865166811
O	-0.707733378855	-1.222889864182	3.144171705823
C	-0.115848164604	-3.817585648467	2.559671615846
C	-1.340413945960	-4.485060128076	3.160177555244
C	-1.885734121678	0.560056706661	-2.553812139826
C	-0.915631473713	1.697849926243	-2.946867057922
C	-1.690432057586	-0.643035041018	-3.492428875858
C	-3.344724301341	1.063994639633	-2.640026455913
H	-1.031411285474	-1.999876164766	-1.008089462639
H	0.506101460596	-4.534279777499	2.007615496526
H	0.492265254005	-3.319480421562	3.327284164103
H	-1.019757277044	-5.277449232640	3.855425175663
H	-1.950709871183	-3.761535440751	3.721423769744
H	-1.962715552347	-4.944262848485	2.376421615060
H	0.131477282434	1.359003529613	-2.901602176966
H	-1.126371901133	2.027894436233	-3.976305529516
H	-1.026314096141	2.564950491066	-2.278265477551
H	-1.898373566772	-0.339602463096	-4.529993470359
H	-0.657622981135	-1.023043012092	-3.451253337170
H	-2.373718526563	-1.468207614288	-3.237541447089
H	-3.511729123503	1.917674983055	-1.965941769119
H	-3.566156930148	1.388837687267	-3.668836271103
H	-4.055447409305	0.266997815149	-2.369970730032

SCF Done: E(RB3LYP) = -670.534074040

Zero-point correction= 0.239543
Thermal correction to Energy= 0.254502
Thermal correction to Enthalpy= 0.255446
Thermal correction to Gibbs Free Energy= 0.196479
Sum of electronic and zero-point Energies= -670.294531
Sum of electronic and thermal Energies= -670.279572
Sum of electronic and thermal Enthalpies= -670.278628
Sum of electronic and thermal Free Energies= -670.337595

1	N	Isotropic = -136.6304	Anisotropy =	303.3452
2	C	Isotropic = 34.8531	Anisotropy =	119.5871
3	C	Isotropic = 92.0609	Anisotropy =	100.3665
4	C	Isotropic = 6.8774	Anisotropy =	132.9248
5	O	Isotropic = -62.0256	Anisotropy =	295.2028
6	C	Isotropic = 34.4267	Anisotropy =	78.7535
7	O	Isotropic = 120.2507	Anisotropy =	157.8852
8	O	Isotropic = -38.6513	Anisotropy =	563.0730

9	C	Isotropic =	129.0637	Anisotropy =	65.6490
10	C	Isotropic =	176.0465	Anisotropy =	22.7683
11	C	Isotropic =	153.5814	Anisotropy =	9.8499
12	C	Isotropic =	161.2678	Anisotropy =	41.0818
13	C	Isotropic =	163.4874	Anisotropy =	38.1219
14	C	Isotropic =	161.1114	Anisotropy =	41.1720
15	H	Isotropic =	25.0662	Anisotropy =	8.8595
16	H	Isotropic =	27.4025	Anisotropy =	7.1346
17	H	Isotropic =	26.4168	Anisotropy =	5.5393
18	H	Isotropic =	30.2370	Anisotropy =	9.9859
19	H	Isotropic =	29.8978	Anisotropy =	6.1962
20	H	Isotropic =	30.0617	Anisotropy =	7.4463
21	H	Isotropic =	30.2070	Anisotropy =	8.1169
22	H	Isotropic =	30.0998	Anisotropy =	8.4376
23	H	Isotropic =	29.6290	Anisotropy =	8.0928
24	H	Isotropic =	30.1603	Anisotropy =	8.0728
25	H	Isotropic =	29.8555	Anisotropy =	7.9447
26	H	Isotropic =	29.8551	Anisotropy =	7.9755
27	H	Isotropic =	29.6305	Anisotropy =	8.0486
28	H	Isotropic =	30.0929	Anisotropy =	8.4273
29	H	Isotropic =	30.2038	Anisotropy =	8.0536

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.327194593935	0.501849872768	-0.078769392455
C	-1.922132190360	-0.616816918440	0.493292526044
C	-0.831411135935	-1.210802609206	-0.205159981778
C	-0.607701301249	-0.359018283568	-1.250816573596
O	-1.501451059026	0.664198199825	-1.175205121087
C	-2.614158204244	-1.091029716017	1.726768839156
O	-2.064757168220	-2.239522988527	2.153590386132
O	-3.541911042380	-0.516541706765	2.257795989589
C	-2.629221587013	-2.837987878764	3.355893699785
C	-1.981812483790	-2.273281715434	4.607969358786
C	0.370680823410	-0.326955613956	-2.399493086229
C	1.285556198176	-1.561025693765	-2.319195874650
C	-0.414561970164	-0.338786984549	-3.731043924490
C	1.217160660682	0.963279684554	-2.303587007522
H	-0.308826018742	-2.126397172240	0.044597952739
H	-3.715438198547	-2.672992085989	3.350893946937
H	-2.420878543391	-3.909704616968	3.240638516082
H	-0.889157788345	-2.406745807436	4.580786331825
H	-2.207186628839	-1.202240816482	4.721880974066
H	-2.372655521628	-2.803216052562	5.491399483647
H	2.003250073899	-1.543381120637	-3.153698061544
H	1.859275708796	-1.577067564753	-1.379348052504
H	0.707909192298	-2.496044602701	-2.388810746961
H	0.288299491246	-0.301660939154	-4.578137458993
H	-1.019900907039	-1.254168992188	-3.825734091157
H	-1.087853094274	0.528631497473	-3.804198974155
H	1.791624131604	0.991135881332	-1.364196030527
H	1.928285815378	1.004799546238	-3.143570453307

H 0.581757341631 1.860815197912 -2.345853173834

SCF Done: E(RB3LYP) = -670.534075606

Zero-point correction= 0.239558
Thermal correction to Energy= 0.254504
Thermal correction to Enthalpy= 0.255448
Thermal correction to Gibbs Free Energy= 0.196632
Sum of electronic and zero-point Energies= -670.294517
Sum of electronic and thermal Energies= -670.279572
Sum of electronic and thermal Enthalpies= -670.278627
Sum of electronic and thermal Free Energies= -670.337444

1 N Isotropic = -136.6010 Anisotropy = 302.9991
2 C Isotropic = 34.9161 Anisotropy = 119.4781
3 C Isotropic = 92.0190 Anisotropy = 100.2913
4 C Isotropic = 6.8340 Anisotropy = 132.9251
5 O Isotropic = -62.2282 Anisotropy = 295.1309
6 C Isotropic = 34.4520 Anisotropy = 78.8831
7 O Isotropic = 120.3724 Anisotropy = 157.5228
8 O Isotropic = -38.5990 Anisotropy = 562.7648
9 C Isotropic = 129.0826 Anisotropy = 65.6547
10 C Isotropic = 176.1171 Anisotropy = 22.6001
11 C Isotropic = 153.3510 Anisotropy = 10.1026
12 C Isotropic = 163.4716 Anisotropy = 38.2237
13 C Isotropic = 161.2664 Anisotropy = 41.1001
14 C Isotropic = 161.0850 Anisotropy = 41.2626
15 H Isotropic = 25.0718 Anisotropy = 8.8499
16 H Isotropic = 26.4276 Anisotropy = 5.5326
17 H Isotropic = 27.4055 Anisotropy = 7.1400
18 H Isotropic = 30.0619 Anisotropy = 7.4561
19 H Isotropic = 29.8942 Anisotropy = 6.2118
20 H Isotropic = 30.2358 Anisotropy = 9.9780
21 H Isotropic = 30.1530 Anisotropy = 8.0852
22 H Isotropic = 29.8563 Anisotropy = 7.9610
23 H Isotropic = 29.8610 Anisotropy = 7.9481
24 H Isotropic = 30.0905 Anisotropy = 8.4529
25 H Isotropic = 30.2083 Anisotropy = 8.1175
26 H Isotropic = 29.6243 Anisotropy = 8.0860
27 H Isotropic = 30.2120 Anisotropy = 8.0355
28 H Isotropic = 30.0921 Anisotropy = 8.4405
29 H Isotropic = 29.6377 Anisotropy = 8.0402

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N -1.530708067218 -1.791808434130 -0.273279771353
C -0.893564637571 -1.094472174089 0.650544768491
C -0.986699201616 0.308569608134 0.408683466634
C -1.731041698744 0.402359993879 -0.732007317084
O -2.056245255538 -0.854410215153 -1.141810216051
C -0.148900072263 -1.670686689458 1.815248651164
O -0.101598685281 -2.986375927252 2.061135114487

O	0.434981881771	-0.915064182423	2.569179627292
C	-0.755516529317	-4.017352222874	1.265960324350
C	-0.460856207531	-5.337712767997	1.946482478435
C	-2.237293130765	1.546105656703	-1.575714681510
C	-3.782405300945	1.500170767810	-1.608970899695
C	-1.765317059074	2.875024492434	-0.960935076534
C	-1.679431529746	1.401137866679	-3.010172230361
H	-0.556587474535	1.101722407492	1.007927388044
H	-1.833726673287	-3.809498012495	1.224722071343
H	-0.357454622275	-3.985410720479	0.242249939512
H	0.622985398555	-5.526577982798	1.987958264540
H	-0.859781856120	-5.349639801422	2.972556877400
H	-0.934177332794	-6.154889881339	1.380288216093
H	-4.203708642821	1.610340777148	-0.597257034500
H	-4.165489734024	2.322897316668	-2.232914315847
H	-4.143567388768	0.550533983296	-2.031851114206
H	-2.132630611225	3.714933202659	-1.570400589431
H	-2.150878670167	3.005333007451	0.062366400057
H	-0.666230027858	2.935733870317	-0.927713995383
H	-1.995238885530	0.450790383047	-3.466409881245
H	-2.051939167730	2.225406127106	-3.638396179671
H	-0.578528817582	1.436459551088	-3.012860284972

SCF Done: E(RB3LYP) = -670.525143919

Zero-point correction= 0.239189
Thermal correction to Energy= 0.254250
Thermal correction to Enthalpy= 0.255194
Thermal correction to Gibbs Free Energy= 0.195755
Sum of electronic and zero-point Energies= -670.285955
Sum of electronic and thermal Energies= -670.270894
Sum of electronic and thermal Enthalpies= -670.269950
Sum of electronic and thermal Free Energies= -670.329389

1	N	Isotropic =	-131.8784	Anisotropy =	310.7565
2	C	Isotropic =	34.0378	Anisotropy =	114.3393
3	C	Isotropic =	89.0420	Anisotropy =	99.9396
4	C	Isotropic =	7.8803	Anisotropy =	136.7975
5	O	Isotropic =	-63.5578	Anisotropy =	262.4296
6	C	Isotropic =	34.8084	Anisotropy =	76.6163
7	O	Isotropic =	121.9433	Anisotropy =	137.6915
8	O	Isotropic =	-76.2953	Anisotropy =	546.0865
9	C	Isotropic =	121.4328	Anisotropy =	59.6198
10	C	Isotropic =	175.4626	Anisotropy =	22.3725
11	C	Isotropic =	153.4698	Anisotropy =	10.0259
12	C	Isotropic =	161.0939	Anisotropy =	41.2526
13	C	Isotropic =	163.4459	Anisotropy =	38.5693
14	C	Isotropic =	161.2576	Anisotropy =	41.0955
15	H	Isotropic =	24.8914	Anisotropy =	7.7275
16	H	Isotropic =	26.6647	Anisotropy =	4.1573
17	H	Isotropic =	26.6338	Anisotropy =	4.2919
18	H	Isotropic =	29.9114	Anisotropy =	7.7669
19	H	Isotropic =	29.9258	Anisotropy =	7.7510
20	H	Isotropic =	30.0793	Anisotropy =	9.0249
21	H	Isotropic =	30.2080	Anisotropy =	8.0680
22	H	Isotropic =	30.0818	Anisotropy =	8.4356

23	H	Isotropic =	29.6434	Anisotropy =	7.9221
24	H	Isotropic =	30.1438	Anisotropy =	8.1807
25	H	Isotropic =	29.8481	Anisotropy =	8.0633
26	H	Isotropic =	29.8494	Anisotropy =	8.1000
27	H	Isotropic =	29.6301	Anisotropy =	7.9330
28	H	Isotropic =	30.0945	Anisotropy =	8.4302
29	H	Isotropic =	30.1993	Anisotropy =	8.1060

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.356764484682	-0.563864435485	-0.098863685331
C	-1.601427169964	-1.206892681360	0.772934512612
C	-0.269872894605	-1.376960237003	0.290799743970
C	-0.280091724448	-0.778710387218	-0.936986528703
O	-1.529986144268	-0.295246658222	-1.173593176158
C	-2.073889007766	-1.767259237866	2.081075444356
O	-3.218980979799	-1.387694501627	2.662237989533
O	-1.383686073466	-2.598523106980	2.639876460574
C	-4.117944134894	-0.340477544252	2.190077392741
C	-5.259410294442	-0.928733527706	1.382954135069
C	0.749244766170	-0.561879408926	-2.018566081686
C	0.910117274058	0.955987416432	-2.264044102977
C	2.090719893418	-1.165076459148	-1.567601430414
C	0.269869304478	-1.253446284981	-3.315628204627
H	0.548395237105	-1.872352469487	0.799215847328
H	-4.484334362633	0.117262847750	3.119623653436
H	-3.554989106738	0.408720669798	1.621182485656
H	-4.895108500797	-1.361030476594	0.439599916637
H	-5.786171993388	-1.706253401788	1.957872146171
H	-5.980722373924	-0.131468076663	1.140500843234
H	1.650871186857	1.126983601524	-3.060835062471
H	-0.041446547134	1.412947549800	-2.575132102799
H	1.258371097044	1.469754392884	-1.354094195415
H	2.847537979453	-1.009557098845	-2.351710530669
H	2.456367507980	-0.689013435409	-0.644342141700
H	2.006059671421	-2.248444887172	-1.388941254610
H	-0.695254242833	-0.845549215215	-3.652353852324
H	1.009125868323	-1.094167004957	-4.116285111938
H	0.152460249473	-2.338435941284	-3.166373109494

SCF Done: E(RB3LYP) = -670.524097933

Zero-point correction= 0.239347
Thermal correction to Energy= 0.254288
Thermal correction to Enthalpy= 0.255232
Thermal correction to Gibbs Free Energy= 0.196537
Sum of electronic and zero-point Energies= -670.284751
Sum of electronic and thermal Energies= -670.269810
Sum of electronic and thermal Enthalpies= -670.268866
Sum of electronic and thermal Free Energies= -670.327561

1 N Isotropic = -127.5999 Anisotropy = 301.4448

2	C	Isotropic =	35.4584	Anisotropy =	114.5284
3	C	Isotropic =	89.0807	Anisotropy =	99.0830
4	C	Isotropic =	7.7193	Anisotropy =	137.6430
5	O	Isotropic =	-61.0714	Anisotropy =	259.3588
6	C	Isotropic =	34.4371	Anisotropy =	75.9500
7	O	Isotropic =	119.0461	Anisotropy =	165.5138
8	O	Isotropic =	-79.4689	Anisotropy =	549.2084
9	C	Isotropic =	123.3085	Anisotropy =	74.1350
10	C	Isotropic =	174.2915	Anisotropy =	24.4626
11	C	Isotropic =	153.5001	Anisotropy =	10.0204
12	C	Isotropic =	161.2418	Anisotropy =	40.9350
13	C	Isotropic =	163.5649	Anisotropy =	38.3603
14	C	Isotropic =	161.1910	Anisotropy =	41.0830
15	H	Isotropic =	24.9531	Anisotropy =	7.5155
16	H	Isotropic =	27.1000	Anisotropy =	6.9297
17	H	Isotropic =	26.0907	Anisotropy =	2.6495
18	H	Isotropic =	29.6520	Anisotropy =	5.7940
19	H	Isotropic =	29.8722	Anisotropy =	8.0724
20	H	Isotropic =	30.1997	Anisotropy =	9.4564
21	H	Isotropic =	30.0944	Anisotropy =	8.4274
22	H	Isotropic =	29.6321	Anisotropy =	7.9058
23	H	Isotropic =	30.1988	Anisotropy =	8.1237
24	H	Isotropic =	30.1504	Anisotropy =	8.1745
25	H	Isotropic =	29.8587	Anisotropy =	8.0136
26	H	Isotropic =	29.8458	Anisotropy =	8.1575
27	H	Isotropic =	29.6290	Anisotropy =	7.8567
28	H	Isotropic =	30.0875	Anisotropy =	8.4315
29	H	Isotropic =	30.2061	Anisotropy =	8.1210

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.424211917318	-1.360361627985	0.501335963075
C	-1.696464946327	-1.125649196369	0.766815697825
C	-2.364553094358	-0.530450856064	-0.343809446280
C	-1.392856018693	-0.416761334821	-1.296769927440
O	-0.231552889510	-0.917524804033	-0.794158000733
C	-2.398952623143	-1.495678661458	2.038881777482
O	-1.745496851790	-1.783908855816	3.171475799513
O	-3.614896415457	-1.528685355536	2.042400967964
C	-0.303792465258	-1.702419591737	3.377215215651
C	0.345870714594	-3.061511050250	3.201031091220
C	-1.350970454939	0.117356489131	-2.707334338795
C	-0.932780900837	-1.021396039084	-3.665630020150
C	-2.745840474613	0.641052332489	-3.090291736652
C	-0.318724796875	1.266157606853	-2.779078869198
H	-3.407211435117	-0.241784450482	-0.397967159947
H	0.129160501462	-0.950055597613	2.707703966759
H	-0.214814017433	-1.351683362293	4.414926116517
H	0.281902727500	-3.397022520132	2.155652655730
H	1.410834384934	-2.992975320745	3.476427874820
H	-0.130615165979	-3.811093627910	3.851854002617
H	0.057900884248	-1.421076162143	-3.401188514574

H	-1.657911694254	-1.849974484146	-3.637055103041
H	-0.885884984372	-0.640063579642	-4.697739876401
H	-2.723562951032	1.033546102066	-4.118523078104
H	-3.501983566875	-0.158545620188	-3.049548443258
H	-3.067296057054	1.456165318244	-2.423174413543
H	0.686179583912	0.917113175575	-2.497320307168
H	-0.271262936238	1.659444171513	-3.806667026003
H	-0.598232139175	2.092506902577	-2.106594867887

SCF Done: E(RB3LYP) = -670.524115782

Zero-point correction= 0.239370
Thermal correction to Energy= 0.254311
Thermal correction to Enthalpy= 0.255255
Thermal correction to Gibbs Free Energy= 0.196355
Sum of electronic and zero-point Energies= -670.284746
Sum of electronic and thermal Energies= -670.269805
Sum of electronic and thermal Enthalpies= -670.268861
Sum of electronic and thermal Free Energies= -670.327761

1	N	Isotropic =	-127.5186	Anisotropy =	301.0146
2	C	Isotropic =	35.4811	Anisotropy =	114.6924
3	C	Isotropic =	89.0582	Anisotropy =	98.7271
4	C	Isotropic =	7.7107	Anisotropy =	137.6857
5	O	Isotropic =	-60.9217	Anisotropy =	259.3528
6	C	Isotropic =	34.3825	Anisotropy =	75.9734
7	O	Isotropic =	119.0051	Anisotropy =	165.5119
8	O	Isotropic =	-79.3205	Anisotropy =	549.5209
9	C	Isotropic =	123.2759	Anisotropy =	74.3461
10	C	Isotropic =	174.3074	Anisotropy =	24.4130
11	C	Isotropic =	153.4050	Anisotropy =	10.0414
12	C	Isotropic =	161.3021	Anisotropy =	41.0741
13	C	Isotropic =	163.5054	Anisotropy =	38.3659
14	C	Isotropic =	161.1930	Anisotropy =	41.0918
15	H	Isotropic =	24.9559	Anisotropy =	7.5222
16	H	Isotropic =	26.1039	Anisotropy =	2.6268
17	H	Isotropic =	27.1076	Anisotropy =	6.9412
18	H	Isotropic =	29.6562	Anisotropy =	5.7966
19	H	Isotropic =	30.1994	Anisotropy =	9.4564
20	H	Isotropic =	29.8750	Anisotropy =	8.0706
21	H	Isotropic =	29.6341	Anisotropy =	7.8585
22	H	Isotropic =	30.2056	Anisotropy =	8.1380
23	H	Isotropic =	30.0860	Anisotropy =	8.4218
24	H	Isotropic =	30.1494	Anisotropy =	8.1803
25	H	Isotropic =	29.8517	Anisotropy =	8.1535
26	H	Isotropic =	29.8624	Anisotropy =	7.9913
27	H	Isotropic =	29.6298	Anisotropy =	7.8940
28	H	Isotropic =	30.0961	Anisotropy =	8.4400
29	H	Isotropic =	30.2010	Anisotropy =	8.1042

2g incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.339430848823	-0.988164325152	0.695444437719
C	-1.671490886717	-0.844775883034	0.518790521095
C	-1.940709752774	-0.525743683904	-0.779128931396
C	-0.651315000970	-0.482171279812	-1.399085732601
N	0.295612648345	-0.756780937581	-0.521237017768
C	-2.600141759745	-1.033416130220	1.657480562686
O	-1.957079235438	-1.345480091264	2.786705494621
O	-3.803984128047	-0.910244628394	1.541176988557
C	-2.789392398435	-1.550392124300	3.964205996913
C	-1.870482011888	-1.912847862564	5.110384434631
C	-0.324349735822	-0.174497258702	-2.850337103144
C	-0.855229338387	1.236897096089	-3.186833742224
C	1.194560954714	-0.226096810545	-3.089815098243
C	-1.027344306048	-1.219709162278	-3.745012479067
H	-2.916551081528	-0.349862154371	-1.219124946116
H	-3.351224782171	-0.623400003469	4.156234181483
H	-3.514642352341	-2.347740290829	3.741140938861
H	-1.313612912614	-2.837400163990	4.892998422341
H	-1.148632405357	-1.105512719960	5.308686231158
H	-2.467464537146	-2.074414384269	6.021173395888
H	-0.645279789953	1.473117123619	-4.242410848434
H	-1.943808861061	1.309442840396	-3.035346124373
H	-0.370187402119	2.003138931818	-2.561317124947
H	1.724852335392	0.507187014356	-2.463535714622
H	1.603688816032	-1.221949512784	-2.861796295271
H	1.409512699428	0.002016931394	-4.145376294216
H	-2.120195153464	-1.202709294079	-3.608485410167
H	-0.816663742773	-1.006533212844	-4.805330026921
H	-0.669535030290	-2.237508023327	-3.522078716444

SCF Done: E(RB3LYP) = -670.532845479

Zero-point correction= 0.239140
Thermal correction to Energy= 0.254218
Thermal correction to Enthalpy= 0.255162
Thermal correction to Gibbs Free Energy= 0.196079
Sum of electronic and zero-point Energies= -670.293705
Sum of electronic and thermal Energies= -670.278627
Sum of electronic and thermal Enthalpies= -670.277683
Sum of electronic and thermal Free Energies= -670.336766

1	O	Isotropic =	-39.3116	Anisotropy = 263.3302
2	C	Isotropic =	30.0287	Anisotropy = 105.2404
3	C	Isotropic =	82.2549	Anisotropy = 118.7816
4	C	Isotropic =	17.9972	Anisotropy = 152.2468
5	N	Isotropic =	-125.4402	Anisotropy = 248.0946
6	C	Isotropic =	37.3917	Anisotropy = 74.7091
7	O	Isotropic =	124.9414	Anisotropy = 126.9543
8	O	Isotropic =	-47.8429	Anisotropy = 536.2847
9	C	Isotropic =	127.3021	Anisotropy = 59.6601
10	C	Isotropic =	177.3286	Anisotropy = 19.7338
11	C	Isotropic =	154.0288	Anisotropy = 8.9862
12	C	Isotropic =	160.2906	Anisotropy = 41.4661
13	C	Isotropic =	163.8724	Anisotropy = 33.8423

14	C	Isotropic =	160.2670	Anisotropy =	41.4409
15	H	Isotropic =	24.3068	Anisotropy =	7.6411
16	H	Isotropic =	27.1448	Anisotropy =	6.1644
17	H	Isotropic =	27.1061	Anisotropy =	6.0667
18	H	Isotropic =	29.8833	Anisotropy =	7.6022
19	H	Isotropic =	29.8772	Anisotropy =	7.6096
20	H	Isotropic =	30.0196	Anisotropy =	9.6149
21	H	Isotropic =	30.0771	Anisotropy =	8.4407
22	H	Isotropic =	29.8857	Anisotropy =	7.8039
23	H	Isotropic =	30.2010	Anisotropy =	8.0261
24	H	Isotropic =	29.7825	Anisotropy =	8.5871
25	H	Isotropic =	29.7835	Anisotropy =	8.5975
26	H	Isotropic =	30.2701	Anisotropy =	7.7851
27	H	Isotropic =	29.8842	Anisotropy =	7.7833
28	H	Isotropic =	30.0746	Anisotropy =	8.4475
29	H	Isotropic =	30.2090	Anisotropy =	8.0249

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.918383374332	-1.763411995057	-0.382207855301
C	-1.411022468525	-0.983285570185	0.605197593517
C	-1.562752565460	0.296513711522	0.160011204734
C	-1.118437443404	0.244409071912	-1.199570457142
N	-0.737037569255	-0.978782572776	-1.517278897502
C	-1.700916251102	-1.562132547758	1.937576048169
O	-1.418438400917	-2.867274666533	1.991955668706
O	-2.144347196547	-0.896521400898	2.853134146184
C	-1.671973920153	-3.527253050472	3.265231070766
C	-1.283428676459	-4.980979960232	3.106279101276
C	-1.061827175145	1.380738350978	-2.206260351865
C	-0.488691534388	0.892859662400	-3.547929450343
C	-2.493780526895	1.921222076977	-2.418376732510
C	-0.165352056275	2.501726088323	-1.635069125185
H	-1.935998863097	1.144571100658	0.724137801476
H	-1.080893517372	-3.019150391359	4.042449569782
H	-2.737406699220	-3.403805539649	3.512819054481
H	-1.462000513085	-5.513385532663	4.053228204025
H	-1.880839331110	-5.465756619607	2.318728767665
H	-0.217183898369	-5.079066668764	2.850007628510
H	-0.456519439035	1.730779538266	-4.261608120467
H	0.532918267207	0.501089986760	-3.429294469012
H	-1.107524594345	0.093309201676	-3.982370598009
H	-3.157343792274	1.139896170967	-2.821820392760
H	-2.931685500840	2.291387617090	-1.477902838724
H	-2.474990813268	2.758402748783	-3.134527170903
H	0.863527719783	2.143312935900	-1.471979305406
H	-0.126371034343	3.345521895223	-2.342526703889
H	-0.551798831776	2.883396358517	-0.676783390269

SCF Done: E(RB3LYP) = -670.532865297

Zero-point correction= 0.239179

Thermal correction to Energy= 0.254243
Thermal correction to Enthalpy= 0.255187
Thermal correction to Gibbs Free Energy= 0.196047
Sum of electronic and zero-point Energies= -670.293686
Sum of electronic and thermal Energies= -670.278622
Sum of electronic and thermal Enthalpies= -670.277678
Sum of electronic and thermal Free Energies= -670.336818

1	O	Isotropic =	-39.3363	Anisotropy =	263.0169
2	C	Isotropic =	30.1014	Anisotropy =	105.3195
3	C	Isotropic =	82.4572	Anisotropy =	118.9066
4	C	Isotropic =	18.0237	Anisotropy =	152.4396
5	N	Isotropic =	-125.4518	Anisotropy =	248.1746
6	C	Isotropic =	37.4208	Anisotropy =	74.7578
7	O	Isotropic =	124.9611	Anisotropy =	126.5422
8	O	Isotropic =	-47.6613	Anisotropy =	536.3171
9	C	Isotropic =	127.3158	Anisotropy =	59.6500
10	C	Isotropic =	177.2329	Anisotropy =	19.8953
11	C	Isotropic =	154.0659	Anisotropy =	8.7969
12	C	Isotropic =	164.0864	Anisotropy =	33.7228
13	C	Isotropic =	160.1948	Anisotropy =	41.5612
14	C	Isotropic =	160.4142	Anisotropy =	41.1955
15	H	Isotropic =	24.3153	Anisotropy =	7.6304
16	H	Isotropic =	27.1262	Anisotropy =	6.1065
17	H	Isotropic =	27.1353	Anisotropy =	6.1248
18	H	Isotropic =	30.0224	Anisotropy =	9.6244
19	H	Isotropic =	29.8761	Anisotropy =	7.5992
20	H	Isotropic =	29.8771	Anisotropy =	7.5883
21	H	Isotropic =	30.2744	Anisotropy =	7.7748
22	H	Isotropic =	29.8036	Anisotropy =	8.6097
23	H	Isotropic =	29.7629	Anisotropy =	8.6203
24	H	Isotropic =	30.2069	Anisotropy =	8.0330
25	H	Isotropic =	29.8873	Anisotropy =	7.7774
26	H	Isotropic =	30.0788	Anisotropy =	8.4466
27	H	Isotropic =	30.1970	Anisotropy =	8.0420
28	H	Isotropic =	30.0885	Anisotropy =	8.4181
29	H	Isotropic =	29.8740	Anisotropy =	7.8098

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.904676664907	0.277938482289	1.437923347032
C	-1.757045737646	-0.350554732422	0.599339350626
C	-1.060850650932	-1.114876698508	-0.290100977512
C	0.308360802470	-0.904038353267	0.071634685565
N	0.394973266157	-0.077332997846	1.097055338464
C	-3.202262161616	-0.094184452946	0.802528978517
O	-3.928790635641	-0.776820154896	-0.092107671070
O	-3.648944188378	0.635998011510	1.663606632755
C	-5.373185252782	-0.613774276685	-0.006875071955
C	-5.989642105783	-1.456036334980	-1.102380207003
C	1.546344082989	-1.500952881824	-0.575694895222
C	1.458649996779	-3.040546329428	-0.480522206814

C	1.578543534973	-1.074800787909	-2.060414549550
C	2.821805960745	-1.011089351910	0.131447062385
H	-1.467130714164	-1.733502453409	-1.083020877658
H	-5.698696253851	-0.930051234997	0.996052554504
H	-5.608229687821	0.455702798266	-0.119834318406
H	-5.735326977855	-2.519508242016	-0.973790967806
H	-7.085488875929	-1.356063680303	-1.068105521398
H	-5.643435973695	-1.128419668604	-2.094851935656
H	2.341065110282	-3.495302390075	-0.958609882006
H	1.428738120564	-3.372219528876	0.569575791302
H	0.562235836751	-3.428976459703	-0.989231221292
H	2.459851901896	-1.512723008617	-2.556009899207
H	0.682441328369	-1.418134018386	-2.601148409621
H	1.639662944304	0.020830724141	-2.157738609764
H	3.705346294189	-1.456363974680	-0.351902846593
H	2.915345755998	0.084196232328	0.078937884133
H	2.828050944533	-1.298954236247	1.193688443250

SCF Done: E(RB3LYP) = -670.532729806

Zero-point correction= 0.239115
Thermal correction to Energy= 0.254220
Thermal correction to Enthalpy= 0.255165
Thermal correction to Gibbs Free Energy= 0.195585
Sum of electronic and zero-point Energies= -670.293615
Sum of electronic and thermal Energies= -670.278509
Sum of electronic and thermal Enthalpies= -670.277565
Sum of electronic and thermal Free Energies= -670.337145

1	O	Isotropic =	-42.5299	Anisotropy =	263.4968
2	C	Isotropic =	30.7141	Anisotropy =	106.2002
3	C	Isotropic =	83.9982	Anisotropy =	116.1001
4	C	Isotropic =	17.8413	Anisotropy =	150.6975
5	N	Isotropic =	-124.9856	Anisotropy =	258.9995
6	C	Isotropic =	37.5689	Anisotropy =	74.7149
7	O	Isotropic =	128.4857	Anisotropy =	144.1724
8	O	Isotropic =	-50.1070	Anisotropy =	572.7515
9	C	Isotropic =	127.5454	Anisotropy =	59.4587
10	C	Isotropic =	177.1873	Anisotropy =	20.0153
11	C	Isotropic =	154.0236	Anisotropy =	8.7394
12	C	Isotropic =	160.2573	Anisotropy =	41.2752
13	C	Isotropic =	160.1645	Anisotropy =	41.3001
14	C	Isotropic =	163.9651	Anisotropy =	34.0261
15	H	Isotropic =	24.4821	Anisotropy =	8.4750
16	H	Isotropic =	27.1496	Anisotropy =	6.2742
17	H	Isotropic =	27.1382	Anisotropy =	6.2370
18	H	Isotropic =	29.8910	Anisotropy =	7.4442
19	H	Isotropic =	30.0350	Anisotropy =	9.6909
20	H	Isotropic =	29.8941	Anisotropy =	7.4412
21	H	Isotropic =	30.0804	Anisotropy =	8.3724
22	H	Isotropic =	30.2019	Anisotropy =	8.0217
23	H	Isotropic =	29.8865	Anisotropy =	7.7867
24	H	Isotropic =	30.0766	Anisotropy =	8.3691
25	H	Isotropic =	29.8949	Anisotropy =	7.7668
26	H	Isotropic =	30.2092	Anisotropy =	8.0208
27	H	Isotropic =	30.2688	Anisotropy =	7.8154

28 H Isotropic = 29.7790 Anisotropy = 8.7413
29 H Isotropic = 29.7866 Anisotropy = 8.7231

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.552828774904	0.453533363528	0.303400720349
C	-1.860665106783	-0.846710121258	0.101256401071
C	-0.748038350913	-1.538880239965	-0.275494482016
C	0.286175409324	-0.549333323972	-0.290459007520
N	-0.195431397974	0.630774668840	0.053684901774
C	-3.249773338782	-1.323525029091	0.296363275856
O	-4.069700029344	-0.333872465040	0.668383676924
O	-3.564813017100	-2.485021037459	0.123403601421
C	-5.467801010448	-0.682700754884	0.892438937251
C	-5.694211910863	-1.152429640762	2.318144401801
C	1.753293386720	-0.739100485452	-0.636034043200
C	2.516731500207	0.591809155194	-0.523088227115
C	2.359278680598	-1.770179516474	0.342138764306
C	1.854135360231	-1.275566276745	-2.081252175605
H	-0.684183248585	-2.597038537655	-0.505965622161
H	-6.007949191771	0.249523645311	0.682021694641
H	-5.758932817612	-1.448507426681	0.160583156748
H	-6.770408038933	-1.327157661616	2.477067311416
H	-5.160490262856	-2.094448104950	2.515230721966
H	-5.356934652621	-0.393534594698	3.041058999449
H	3.576230564978	0.432404430603	-0.777357606074
H	2.107876272810	1.349189503352	-1.208917228590
H	2.465206715235	0.999339834799	0.497905603569
H	3.422034031339	-1.933565610344	0.101598675705
H	2.293743482174	-1.415973110157	1.383213779967
H	1.845654497177	-2.742391990541	0.277341961925
H	2.911117930450	-1.439591662501	-2.345732428421
H	1.324904067591	-2.234679719921	-2.195998075567
H	1.427469250653	-0.559787291461	-2.801817689871

SCF Done: E(RB3LYP) = -670.532423691

Zero-point correction= 0.239412
Thermal correction to Energy= 0.254359
Thermal correction to Enthalpy= 0.255303
Thermal correction to Gibbs Free Energy= 0.196651
Sum of electronic and zero-point Energies= -670.293011
Sum of electronic and thermal Energies= -670.278065
Sum of electronic and thermal Enthalpies= -670.277121
Sum of electronic and thermal Free Energies= -670.335772

1 O Isotropic = -39.3676 Anisotropy = 264.0117
2 C Isotropic = 29.9778 Anisotropy = 105.0102
3 C Isotropic = 82.2686 Anisotropy = 119.1263
4 C Isotropic = 18.0302 Anisotropy = 152.3493
5 N Isotropic = -125.5116 Anisotropy = 248.9072
6 C Isotropic = 37.3962 Anisotropy = 74.4208

7	O	Isotropic =	125.4177	Anisotropy =	167.0128
8	O	Isotropic =	-37.1616	Anisotropy =	533.3504
9	C	Isotropic =	128.7679	Anisotropy =	66.2180
10	C	Isotropic =	176.1566	Anisotropy =	22.6854
11	C	Isotropic =	154.0290	Anisotropy =	8.9297
12	C	Isotropic =	163.9125	Anisotropy =	33.9366
13	C	Isotropic =	160.2619	Anisotropy =	41.3595
14	C	Isotropic =	160.3003	Anisotropy =	41.3592
15	H	Isotropic =	24.2945	Anisotropy =	7.7621
16	H	Isotropic =	27.3557	Anisotropy =	7.3034
17	H	Isotropic =	26.4230	Anisotropy =	5.5411
18	H	Isotropic =	30.2212	Anisotropy =	9.9738
19	H	Isotropic =	29.9052	Anisotropy =	6.1296
20	H	Isotropic =	30.0487	Anisotropy =	7.6089
21	H	Isotropic =	30.2610	Anisotropy =	7.7963
22	H	Isotropic =	29.7838	Anisotropy =	8.6235
23	H	Isotropic =	29.7807	Anisotropy =	8.6183
24	H	Isotropic =	30.0762	Anisotropy =	8.4295
25	H	Isotropic =	30.2015	Anisotropy =	7.9802
26	H	Isotropic =	29.8837	Anisotropy =	7.7724
27	H	Isotropic =	30.0757	Anisotropy =	8.4429
28	H	Isotropic =	29.8830	Anisotropy =	7.7930
29	H	Isotropic =	30.2008	Anisotropy =	8.0431

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.405895030516	-1.133958664206	-1.119389589693
C	-1.755126984105	-0.464417921648	0.001285052983
C	-0.784841894755	-0.599249239225	0.949665073877
C	0.205454585330	-1.416645510335	0.317228079503
N	-0.167113482995	-1.731919163427	-0.909440823598
C	-3.039087097073	0.272446612005	0.060010629391
O	-3.722045361603	0.177384859909	-1.086509837195
O	-3.389911737675	0.882730981016	1.051290130925
C	-5.007014345929	0.864009276269	-1.148879172809
C	-6.125079085892	-0.013830023241	-0.615628796507
C	1.525105305609	-1.899380933486	0.894633520123
C	1.235386603362	-2.710541267884	2.177134835900
C	2.272127956326	-2.783696772294	-0.118900109798
C	2.389178433845	-0.667418823710	1.245157413851
H	-0.785106669894	-0.175569946848	1.948279624435
H	-4.927527868330	1.806246165490	-0.589509004811
H	-5.136551696937	1.081585997515	-2.216977548342
H	-6.164708427357	-0.972379664155	-1.155880415058
H	-5.993413093276	-0.214911157247	0.458228734954
H	-7.089382301136	0.501012835126	-0.753629001771
H	2.181814328345	-3.059562927293	2.620224314223
H	0.713544861690	-2.103215251400	2.933490154270
H	0.613954461159	-3.593291445041	1.957470852907
H	3.225175428637	-3.120877233252	0.317627236898
H	1.682278872773	-3.673192182684	-0.387672240662
H	2.492946368361	-2.233697390201	-1.046132920681

H	3.344298387555	-0.994580748254	1.686548350445
H	2.612931028081	-0.071097866205	0.346330990161
H	1.886948456399	-0.012872595297	1.974904466081

SCF Done: E(RB3LYP) = -670.532440392

Zero-point correction= 0.239558
Thermal correction to Energy= 0.254458
Thermal correction to Enthalpy= 0.255403
Thermal correction to Gibbs Free Energy= 0.196854
Sum of electronic and zero-point Energies= -670.292883
Sum of electronic and thermal Energies= -670.277982
Sum of electronic and thermal Enthalpies= -670.277038
Sum of electronic and thermal Free Energies= -670.335586

1	O	Isotropic =	-39.4474	Anisotropy =	263.9831
2	C	Isotropic =	30.0325	Anisotropy =	104.9680
3	C	Isotropic =	82.2780	Anisotropy =	119.0894
4	C	Isotropic =	18.0723	Anisotropy =	152.2610
5	N	Isotropic =	-125.5888	Anisotropy =	248.8565
6	C	Isotropic =	37.3895	Anisotropy =	74.4178
7	O	Isotropic =	125.3822	Anisotropy =	167.3556
8	O	Isotropic =	-37.4607	Anisotropy =	533.6302
9	C	Isotropic =	128.8128	Anisotropy =	66.2316
10	C	Isotropic =	176.2083	Anisotropy =	22.7072
11	C	Isotropic =	154.2155	Anisotropy =	8.7000
12	C	Isotropic =	160.4093	Anisotropy =	41.1717
13	C	Isotropic =	163.8867	Anisotropy =	33.7464
14	C	Isotropic =	160.1676	Anisotropy =	41.4718
15	H	Isotropic =	24.2950	Anisotropy =	7.7509
16	H	Isotropic =	26.4348	Anisotropy =	5.5601
17	H	Isotropic =	27.3525	Anisotropy =	7.2942
18	H	Isotropic =	30.0472	Anisotropy =	7.6016
19	H	Isotropic =	29.8838	Anisotropy =	6.1062
20	H	Isotropic =	30.2268	Anisotropy =	9.9797
21	H	Isotropic =	30.0856	Anisotropy =	8.4037
22	H	Isotropic =	29.8626	Anisotropy =	7.8220
23	H	Isotropic =	30.1989	Anisotropy =	7.9935
24	H	Isotropic =	30.2714	Anisotropy =	7.7788
25	H	Isotropic =	29.8116	Anisotropy =	8.6109
26	H	Isotropic =	29.7557	Anisotropy =	8.6271
27	H	Isotropic =	30.0762	Anisotropy =	8.4488
28	H	Isotropic =	30.2013	Anisotropy =	8.0403
29	H	Isotropic =	29.8926	Anisotropy =	7.7823

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.196047752315	0.422337355277	0.967964531017
C	-0.824585821740	-0.767869005074	0.852646072604
C	-1.213125587810	-0.969220464010	-0.439006454277
C	-0.767959915521	0.208537522229	-1.120748856010
N	-0.165578138542	1.030283840283	-0.281551456313

C	-0.957741521819	-1.574193822930	2.088645741724
O	-1.602060758712	-2.720183205851	1.832401920464
O	-0.536309121521	-1.230184974741	3.174082239063
C	-1.802111279935	-3.612595207603	2.965403812326
C	-2.561477380224	-4.820676682232	2.462160376437
C	-0.921850646395	0.547258247908	-2.593672268528
C	-2.427120856897	0.562429464247	-2.940687179922
C	-0.305112836109	1.922061994951	-2.904530760125
C	-0.209477290854	-0.542224897074	-3.425932043681
H	-1.738277574248	-1.829457791837	-0.839937386993
H	-0.815210732699	-3.879757903423	3.373499258330
H	-2.355627462159	-3.065374818018	3.743764271084
H	-3.540687508406	-4.529042129444	2.051908893955
H	-1.993855517917	-5.346574237760	1.678913813663
H	-2.730233858839	-5.520272350150	3.295323401630
H	-2.561780953993	0.788702118537	-4.010596143499
H	-2.899972118344	-0.411821304679	-2.739672046666
H	-2.961238686630	1.329776459771	-2.358021034144
H	-0.793524441301	2.721372213341	-2.326773217535
H	0.769356552730	1.943579408815	-2.667488621574
H	-0.426578428107	2.147265143705	-3.975519311954
H	-0.635143217205	-1.540562432029	-3.237766523095
H	-0.321419401230	-0.324786961349	-4.500279268469
H	0.866852256740	-0.578585580858	-3.193991759514

SCF Done: E(RB3LYP) = -670.532733095

Zero-point correction= 0.239162
Thermal correction to Energy= 0.254234
Thermal correction to Enthalpy= 0.255179
Thermal correction to Gibbs Free Energy= 0.196075
Sum of electronic and zero-point Energies= -670.293571
Sum of electronic and thermal Energies= -670.278499
Sum of electronic and thermal Enthalpies= -670.277554
Sum of electronic and thermal Free Energies= -670.336658

1	O	Isotropic =	-42.4065	Anisotropy =	263.4967
2	C	Isotropic =	30.6630	Anisotropy =	106.2345
3	C	Isotropic =	84.0369	Anisotropy =	115.7285
4	C	Isotropic =	17.7944	Anisotropy =	150.8419
5	N	Isotropic =	-125.1147	Anisotropy =	259.0323
6	C	Isotropic =	37.5452	Anisotropy =	74.6879
7	O	Isotropic =	128.4782	Anisotropy =	144.2942
8	O	Isotropic =	-49.9469	Anisotropy =	573.2744
9	C	Isotropic =	127.5833	Anisotropy =	59.4910
10	C	Isotropic =	177.1666	Anisotropy =	20.0300
11	C	Isotropic =	154.0004	Anisotropy =	8.7975
12	C	Isotropic =	160.2666	Anisotropy =	41.1834
13	C	Isotropic =	164.0567	Anisotropy =	34.0453
14	C	Isotropic =	160.1854	Anisotropy =	41.3002
15	H	Isotropic =	24.4879	Anisotropy =	8.4830
16	H	Isotropic =	27.1619	Anisotropy =	6.3119
17	H	Isotropic =	27.1240	Anisotropy =	6.2101
18	H	Isotropic =	29.8967	Anisotropy =	7.4319
19	H	Isotropic =	29.8883	Anisotropy =	7.4422
20	H	Isotropic =	30.0344	Anisotropy =	9.6939

21	H	Isotropic =	30.0801	Anisotropy =	8.3571
22	H	Isotropic =	29.8944	Anisotropy =	7.7767
23	H	Isotropic =	30.2088	Anisotropy =	8.0177
24	H	Isotropic =	29.7882	Anisotropy =	8.7476
25	H	Isotropic =	29.7656	Anisotropy =	8.7467
26	H	Isotropic =	30.2697	Anisotropy =	7.8239
27	H	Isotropic =	29.8960	Anisotropy =	7.7599
28	H	Isotropic =	30.0797	Anisotropy =	8.3773
29	H	Isotropic =	30.2037	Anisotropy =	8.0187

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.930232440646	-1.431886563601	0.963627379506
C	-1.615303929262	-0.307961467389	0.282405265822
C	-0.397748826373	-0.447510437660	-0.315082233860
C	0.020332994986	-1.765230993417	0.055470439699
N	-0.891023932789	-2.345531720964	0.814043846099
C	-2.548922924002	0.842198941315	0.265050287895
O	-3.660780483080	0.594918664514	0.966773714091
O	-2.293509125895	1.872596126745	-0.327645273756
C	-4.658255855614	1.657695006690	1.018214926040
C	-5.593840524991	1.592453305619	-0.175646375925
C	1.307306801379	-2.476072307952	-0.326581348040
C	1.366392839367	-2.590328066757	-1.866313386661
C	2.502768172733	-1.637089747324	0.176958309673
C	1.361082337855	-3.880991692638	0.298185300967
H	0.116735483179	0.285171407572	-0.927620558116
H	-5.189706209687	1.472755602540	1.960697815607
H	-4.137411346821	2.623447191720	1.074308926470
H	-5.054415624147	1.792800945039	-1.113574615206
H	-6.075635350345	0.604846416695	-0.244964771419
H	-6.381676228391	2.354308302308	-0.062271540168
H	2.303746033476	-3.084329182028	-2.168626854731
H	0.524518546824	-3.186840921499	-2.252440895052
H	1.335427396053	-1.600855363943	-2.349354914203
H	3.448423617343	-2.128253320904	-0.103290992078
H	2.504790770737	-0.627128385775	-0.262606377183
H	2.481885159987	-1.533971358623	1.273542523453
H	0.518989209631	-4.503457623364	-0.040157257955
H	2.298248540419	-4.379249837196	0.004998617379
H	1.324964898074	-3.833782919721	1.397140041652

SCF Done: E(RB3LYP) = -670.532434962

Zero-point correction= 0.239543
Thermal correction to Energy= 0.254446
Thermal correction to Enthalpy= 0.255390
Thermal correction to Gibbs Free Energy= 0.196827
Sum of electronic and zero-point Energies= -670.292892
Sum of electronic and thermal Energies= -670.277989
Sum of electronic and thermal Enthalpies= -670.277045
Sum of electronic and thermal Free Energies= -670.335608

1	O	Isotropic =	-39.2750	Anisotropy =	264.0477
2	C	Isotropic =	30.0049	Anisotropy =	105.0117
3	C	Isotropic =	82.0932	Anisotropy =	119.0202
4	C	Isotropic =	18.0605	Anisotropy =	152.3827
5	N	Isotropic =	-125.6089	Anisotropy =	248.5236
6	C	Isotropic =	37.3381	Anisotropy =	74.2798
7	O	Isotropic =	125.5795	Anisotropy =	167.1657
8	O	Isotropic =	-37.7624	Anisotropy =	534.0924
9	C	Isotropic =	128.6650	Anisotropy =	66.2713
10	C	Isotropic =	176.2535	Anisotropy =	22.5848
11	C	Isotropic =	154.1977	Anisotropy =	8.6517
12	C	Isotropic =	160.1906	Anisotropy =	41.3460
13	C	Isotropic =	160.4188	Anisotropy =	41.1599
14	C	Isotropic =	164.0511	Anisotropy =	33.7985
15	H	Isotropic =	24.3016	Anisotropy =	7.7631
16	H	Isotropic =	27.3409	Anisotropy =	7.2812
17	H	Isotropic =	26.4351	Anisotropy =	5.6043
18	H	Isotropic =	29.8683	Anisotropy =	6.0870
19	H	Isotropic =	30.0503	Anisotropy =	7.6055
20	H	Isotropic =	30.2260	Anisotropy =	9.9831
21	H	Isotropic =	30.0799	Anisotropy =	8.4175
22	H	Isotropic =	30.2091	Anisotropy =	7.9908
23	H	Isotropic =	29.8880	Anisotropy =	7.7626
24	H	Isotropic =	30.0862	Anisotropy =	8.4336
25	H	Isotropic =	29.8728	Anisotropy =	7.8119
26	H	Isotropic =	30.2004	Anisotropy =	8.0571
27	H	Isotropic =	29.7678	Anisotropy =	8.6397
28	H	Isotropic =	30.2741	Anisotropy =	7.7869
29	H	Isotropic =	29.7928	Anisotropy =	8.6416

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.549850898921	-1.928122852387	-0.302870696739
C	-1.889137327354	-0.724186085513	0.208524023185
C	-0.917952232485	0.192511666098	-0.066184583811
C	0.062463408370	-0.550933757448	-0.797368762134
N	-0.315913795346	-1.808178290206	-0.935415120105
C	-3.164079836870	-0.558323220713	0.944643015008
O	-3.857879770029	-1.700688508686	1.005671671069
O	-3.502922025352	0.508945053623	1.418340009625
C	-5.133862013604	-1.661437138530	1.710658394973
C	-4.947389138395	-1.902884849615	3.197910948797
C	1.377714044522	-0.049593987221	-1.368847794302
C	2.236896264290	0.506990875191	-0.211405543158
C	2.134912062247	-1.187836395043	-2.074275409112
C	1.077442623748	1.078961517745	-2.380394203033
H	-0.910344111944	1.240014344431	0.215633919762
H	-5.613198379669	-0.692881743058	1.512783572517
H	-5.718462719458	-2.462497236070	1.240012270166
H	-5.934312516211	-1.947780975934	3.685706451050
H	-4.428175740514	-2.856541205696	3.380190165211

H	-4.371196547164	-1.088651576398	3.662609851760
H	3.191668356955	0.890311913467	-0.605746883772
H	1.731307196523	1.335205756686	0.310021238220
H	2.462312946585	-0.277207091980	0.528822446639
H	2.364862205309	-2.008786004501	-1.378429768342
H	1.547405048977	-1.605439567368	-2.905808041947
H	3.083366368859	-0.803435548951	-2.480677604350
H	0.538266468590	1.915744922379	-1.908938523664
H	2.021130555066	1.473547648918	-2.790261894477
H	0.467939503276	0.707392336778	-3.219473149036

SCF Done: E(RB3LYP) = -670.532443281

Zero-point correction= 0.239343
Thermal correction to Energy= 0.254331
Thermal correction to Enthalpy= 0.255275
Thermal correction to Gibbs Free Energy= 0.196286
Sum of electronic and zero-point Energies= -670.293100
Sum of electronic and thermal Energies= -670.278113
Sum of electronic and thermal Enthalpies= -670.277168
Sum of electronic and thermal Free Energies= -670.336158

1	O	Isotropic =	-39.5337	Anisotropy =	264.3689
2	C	Isotropic =	30.0255	Anisotropy =	105.1812
3	C	Isotropic =	82.3463	Anisotropy =	119.0306
4	C	Isotropic =	18.0755	Anisotropy =	152.2763
5	N	Isotropic =	-125.7163	Anisotropy =	248.5703
6	C	Isotropic =	37.3069	Anisotropy =	74.2551
7	O	Isotropic =	125.3195	Anisotropy =	167.4084
8	O	Isotropic =	-37.4760	Anisotropy =	533.3395
9	C	Isotropic =	128.6594	Anisotropy =	66.4234
10	C	Isotropic =	176.0684	Anisotropy =	22.8695
11	C	Isotropic =	153.8831	Anisotropy =	8.7802
12	C	Isotropic =	160.3368	Anisotropy =	41.2752
13	C	Isotropic =	163.9162	Anisotropy =	33.9069
14	C	Isotropic =	160.1835	Anisotropy =	41.5219
15	H	Isotropic =	24.3055	Anisotropy =	7.7444
16	H	Isotropic =	26.4285	Anisotropy =	5.5620
17	H	Isotropic =	27.3526	Anisotropy =	7.2945
18	H	Isotropic =	30.2209	Anisotropy =	9.9833
19	H	Isotropic =	30.0519	Anisotropy =	7.5854
20	H	Isotropic =	29.8944	Anisotropy =	6.0940
21	H	Isotropic =	30.0812	Anisotropy =	8.4293
22	H	Isotropic =	29.8752	Anisotropy =	7.7761
23	H	Isotropic =	30.2028	Anisotropy =	7.9862
24	H	Isotropic =	29.7923	Anisotropy =	8.6215
25	H	Isotropic =	29.7726	Anisotropy =	8.6215
26	H	Isotropic =	30.2635	Anisotropy =	7.7876
27	H	Isotropic =	29.8949	Anisotropy =	7.7714
28	H	Isotropic =	30.0706	Anisotropy =	8.4378
29	H	Isotropic =	30.2038	Anisotropy =	8.0339

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.991863325616	-1.783171278877	-1.010746863486
C	-1.861869592637	-1.218386580579	0.209564191173
C	-0.938253903843	-0.215775317217	0.165768087304
C	-0.503495556486	-0.206673897218	-1.198369461476
N	-1.131687903120	-1.138192505970	-1.891281631300
C	-2.704765739527	-1.774341559319	1.294083274339
O	-2.477037782395	-1.118427422006	2.441514297021
O	-3.486637159980	-2.690640681630	1.141082294422
C	-3.232230206737	-1.552287374544	3.610770261486
C	-2.533002441585	-2.695619564699	4.324097807441
C	0.523759575734	0.706920910743	-1.845017250889
C	0.046420546069	2.168622100622	-1.693834890091
C	1.873897159099	0.525373752932	-1.116367257734
C	0.690984921182	0.368921321292	-3.336512777705
H	-0.619020632702	0.418379242549	0.985803275050
H	-3.284237575943	-0.653335391423	4.238548628891
H	-4.244174498939	-1.832820586597	3.287651025768
H	-1.505646999130	-2.415576335387	4.604159119321
H	-3.086531205458	-2.944181097991	5.243770678303
H	-2.497409925811	-3.594745414926	3.690697755906
H	0.785512216712	2.851381230950	-2.142893044842
H	-0.918579844244	2.325884577073	-2.201364658621
H	-0.072717283560	2.449847009738	-0.635577531054
H	1.794341713621	0.769396852069	-0.045244488492
H	2.237458769016	-0.510670695408	-1.206288169103
H	2.629855326537	1.193767473616	-1.558863541018
H	-0.255419176300	0.491441805084	-3.884704069445
H	1.439347923321	1.040374313485	-3.785514530493
H	1.029402602723	-0.668714886363	-3.477870530675

SCF Done: E(RB3LYP) = -670.532326061

Zero-point correction= 0.239505
Thermal correction to Energy= 0.254440
Thermal correction to Enthalpy= 0.255384
Thermal correction to Gibbs Free Energy= 0.196768
Sum of electronic and zero-point Energies= -670.292822
Sum of electronic and thermal Energies= -670.277886
Sum of electronic and thermal Enthalpies= -670.276942
Sum of electronic and thermal Free Energies= -670.335558

1	O	Isotropic =	-43.0282	Anisotropy = 263.9822
2	C	Isotropic =	30.5685	Anisotropy = 105.8124
3	C	Isotropic =	83.8725	Anisotropy = 116.1902
4	C	Isotropic =	17.8631	Anisotropy = 150.7701
5	N	Isotropic =	-125.3254	Anisotropy = 259.5268
6	C	Isotropic =	37.5572	Anisotropy = 75.1597
7	O	Isotropic =	129.1739	Anisotropy = 149.7688
8	O	Isotropic =	-40.3975	Anisotropy = 570.1450
9	C	Isotropic =	128.7759	Anisotropy = 66.3435
10	C	Isotropic =	176.1442	Anisotropy = 22.7335
11	C	Isotropic =	154.0881	Anisotropy = 8.8183
12	C	Isotropic =	160.2353	Anisotropy = 41.3866
13	C	Isotropic =	160.4605	Anisotropy = 41.0783

14	C	Isotropic =	163.9745	Anisotropy =	33.9680
15	H	Isotropic =	24.4672	Anisotropy =	8.4304
16	H	Isotropic =	27.3862	Anisotropy =	7.1865
17	H	Isotropic =	26.4529	Anisotropy =	5.6454
18	H	Isotropic =	30.0501	Anisotropy =	7.4737
19	H	Isotropic =	30.2346	Anisotropy =	10.0253
20	H	Isotropic =	29.8956	Anisotropy =	6.1084
21	H	Isotropic =	30.0759	Anisotropy =	8.4070
22	H	Isotropic =	30.2040	Anisotropy =	8.0341
23	H	Isotropic =	29.8874	Anisotropy =	7.7496
24	H	Isotropic =	29.8768	Anisotropy =	7.8037
25	H	Isotropic =	30.1976	Anisotropy =	7.9845
26	H	Isotropic =	30.0800	Anisotropy =	8.3786
27	H	Isotropic =	29.7789	Anisotropy =	8.7258
28	H	Isotropic =	30.2719	Anisotropy =	7.8136
29	H	Isotropic =	29.7862	Anisotropy =	8.6972

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.384528169825	-1.820365208771	0.978903511949
C	-1.540657163791	-1.231331660997	0.602845754505
C	-1.285661876894	-0.210295686113	-0.264606261487
C	0.140064641551	-0.216642612420	-0.395288116233
N	0.669169616926	-1.173335512843	0.344541212667
C	-2.788810446112	-1.784824622612	1.178466031891
O	-3.850982944143	-1.105882771572	0.720933365830
O	-2.820186137565	-2.717256278376	1.955543308749
C	-5.161959157376	-1.529207669669	1.197989891508
C	-5.730724076699	-2.638561667655	0.331438597356
C	1.002986695996	0.705244775724	-1.239889184709
C	0.759514168760	2.161589931726	-0.785208966844
C	2.492784352886	0.355892780281	-1.080845647394
C	0.587973392120	0.548458566158	-2.719870153750
H	-2.009240526014	0.445507152424	-0.736643400210
H	-5.067468754306	-1.840712315233	2.247332975038
H	-5.770138981537	-0.617208560838	1.140047077289
H	-5.779463041672	-2.328249934863	-0.723868088180
H	-5.122025621825	-3.552258258552	0.406526329421
H	-6.752098145223	-2.876955161839	0.669101875203
H	1.364030538357	2.849875000860	-1.397452687461
H	-0.297306796285	2.451406432338	-0.896733984170
H	1.044410519885	2.301029467346	0.269801012434
H	3.099125716303	1.035338567280	-1.699951612166
H	2.820100386520	0.457972134157	-0.035085754612
H	2.698998709118	-0.677070447124	-1.399502747213
H	-0.473310854361	0.800219547968	-2.873276462501
H	1.189340670895	1.223301923454	-3.349953368612
H	0.750463284310	-0.483277910242	-3.070164508298

SCF Done: E(RB3LYP) = -670.532312029

Zero-point correction= 0.239235

Thermal correction to Energy= 0.253353
Thermal correction to Enthalpy= 0.254297
Thermal correction to Gibbs Free Energy= 0.198265
Sum of electronic and zero-point Energies= -670.293077
Sum of electronic and thermal Energies= -670.278959
Sum of electronic and thermal Enthalpies= -670.278015
Sum of electronic and thermal Free Energies= -670.334047

1	O	Isotropic =	-42.9173	Anisotropy =	264.1104
2	C	Isotropic =	30.5551	Anisotropy =	105.8956
3	C	Isotropic =	83.8793	Anisotropy =	116.2354
4	C	Isotropic =	17.8604	Anisotropy =	150.7225
5	N	Isotropic =	-125.2544	Anisotropy =	259.2945
6	C	Isotropic =	37.4726	Anisotropy =	74.7810
7	O	Isotropic =	129.1511	Anisotropy =	149.8477
8	O	Isotropic =	-39.7869	Anisotropy =	570.0404
9	C	Isotropic =	128.8884	Anisotropy =	66.2395
10	C	Isotropic =	176.0159	Anisotropy =	22.8499
11	C	Isotropic =	154.0099	Anisotropy =	8.8067
12	C	Isotropic =	160.2901	Anisotropy =	41.2421
13	C	Isotropic =	163.9670	Anisotropy =	33.9846
14	C	Isotropic =	160.1554	Anisotropy =	41.3399
15	H	Isotropic =	24.4745	Anisotropy =	8.4473
16	H	Isotropic =	26.4355	Anisotropy =	5.6293
17	H	Isotropic =	27.3900	Anisotropy =	7.1955
18	H	Isotropic =	30.0450	Anisotropy =	7.4540
19	H	Isotropic =	29.9088	Anisotropy =	6.1549
20	H	Isotropic =	30.2324	Anisotropy =	10.0172
21	H	Isotropic =	30.0809	Anisotropy =	8.4011
22	H	Isotropic =	29.8848	Anisotropy =	7.7494
23	H	Isotropic =	30.2010	Anisotropy =	8.0335
24	H	Isotropic =	30.2672	Anisotropy =	7.8172
25	H	Isotropic =	29.7870	Anisotropy =	8.7323
26	H	Isotropic =	29.7768	Anisotropy =	8.6980
27	H	Isotropic =	29.8874	Anisotropy =	7.7721
28	H	Isotropic =	30.0748	Anisotropy =	8.3891
29	H	Isotropic =	30.2016	Anisotropy =	7.9624

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.456934879536	-1.101879051667	0.150607772546
C	-0.799398592179	-1.066812099981	0.645918360610
C	-1.621869624079	-0.395712212077	-0.210328445461
C	-0.760611777573	-0.014909413900	-1.288813511404
N	0.470931788180	-0.436590511632	-1.069480859770
C	-1.020190153409	-1.730290357087	1.952387192104
O	-2.307560716511	-1.624714459615	2.313150562086
O	-0.146413878429	-2.287780385768	2.584777755994
C	-2.690819381502	-2.227307535828	3.584141432490
C	-2.491285945419	-1.256752750480	4.734414330467
C	-1.123216061865	0.763732510596	-2.541921732274
C	0.104482643790	0.931601404609	-3.453778052724

C	-2.229935115791	-0.004734439883	-3.297474068914
C	-1.652071935042	2.153369421848	-2.121366396861
H	-2.682190370988	-0.203994264350	-0.086085328397
H	-3.750043968286	-2.480689735936	3.446658191996
H	-2.108597015746	-3.148425815931	3.723597618413
H	-3.043760617505	-0.320479188764	4.559974927630
H	-2.867733794470	-1.712172028712	5.664424677107
H	-1.425512283979	-1.020990896647	4.874415274314
H	-0.179400512431	1.498626176642	-4.354068956865
H	0.912905780244	1.476790865902	-2.943660787361
H	0.504340976292	-0.043137925758	-3.772089182244
H	-1.878327894054	-1.000560687256	-3.610953323872
H	-3.129313400751	-0.138082807953	-2.675799071109
H	-2.523998010601	0.554969531252	-4.199838431757
H	-0.882418649152	2.722593940344	-1.576174922377
H	-1.936746459024	2.730810378038	-3.015508022359
H	-2.540449909255	2.071632339991	-1.475367002008

SCF Done: E(RB3LYP) = -670.532305122

Zero-point correction= 0.239255
Thermal correction to Energy= 0.254299
Thermal correction to Enthalpy= 0.255243
Thermal correction to Gibbs Free Energy= 0.195859
Sum of electronic and zero-point Energies= -670.293050
Sum of electronic and thermal Energies= -670.278006
Sum of electronic and thermal Enthalpies= -670.277062
Sum of electronic and thermal Free Energies= -670.336446

1	O	Isotropic =	-42.8089	Anisotropy =	264.0806
2	C	Isotropic =	30.5390	Anisotropy =	105.8982
3	C	Isotropic =	83.8152	Anisotropy =	116.2142
4	C	Isotropic =	17.7940	Anisotropy =	150.9302
5	N	Isotropic =	-125.3837	Anisotropy =	259.3475
6	C	Isotropic =	37.5839	Anisotropy =	74.9149
7	O	Isotropic =	129.2154	Anisotropy =	149.8679
8	O	Isotropic =	-39.4918	Anisotropy =	569.7660
9	C	Isotropic =	128.8745	Anisotropy =	66.2911
10	C	Isotropic =	176.0295	Anisotropy =	22.7868
11	C	Isotropic =	153.8804	Anisotropy =	8.8270
12	C	Isotropic =	164.0584	Anisotropy =	33.9707
13	C	Isotropic =	160.2864	Anisotropy =	41.2407
14	C	Isotropic =	160.1304	Anisotropy =	41.2749
15	H	Isotropic =	24.4744	Anisotropy =	8.4548
16	H	Isotropic =	27.3905	Anisotropy =	7.2096
17	H	Isotropic =	26.4278	Anisotropy =	5.5980
18	H	Isotropic =	30.0459	Anisotropy =	7.4592
19	H	Isotropic =	30.2258	Anisotropy =	10.0143
20	H	Isotropic =	29.9250	Anisotropy =	6.1735
21	H	Isotropic =	30.2588	Anisotropy =	7.8218
22	H	Isotropic =	29.7576	Anisotropy =	8.7174
23	H	Isotropic =	29.8059	Anisotropy =	8.7387
24	H	Isotropic =	30.2011	Anisotropy =	8.0238
25	H	Isotropic =	29.8847	Anisotropy =	7.7617
26	H	Isotropic =	30.0734	Anisotropy =	8.3986
27	H	Isotropic =	30.2057	Anisotropy =	7.9586

28 H Isotropic = 30.0721 Anisotropy = 8.4003
29 H Isotropic = 29.8940 Anisotropy = 7.7495

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-3.058048379695	-0.420182015959	0.272662540484
C	-1.852210119217	-0.876101457532	0.676459164578
C	-0.893985828478	-0.533764763036	-0.231741257301
C	-1.615352633389	0.179465035763	-1.242016640407
N	-2.898269558436	0.243315093255	-0.937699681358
C	-1.815503777579	-1.615343317091	1.960125909029
O	-0.563033309913	-2.009757542599	2.232682571910
O	-2.793781356514	-1.825506726977	2.647988058688
C	-0.359247369793	-2.752146205709	3.470855314183
C	-0.127549396888	-1.814317976613	4.642115694653
C	-1.067426185228	0.810410721911	-2.510736812514
C	-2.196326982115	1.464299270318	-3.326038598453
C	-0.024622293528	1.880181168248	-2.116134044670
C	-0.386675698632	-0.289537277912	-3.355221186786
H	0.165975352377	-0.758730561227	-0.183423510403
H	-1.230182214760	-3.401275931297	3.635603751039
H	0.524360389516	-3.369984985424	3.264741287405
H	0.720584510438	-1.140453278067	4.445024647674
H	-1.023147494602	-1.209125891828	4.848726237603
H	0.102977530218	-2.406016458245	5.542546634304
H	-1.777419130470	1.919032916315	-4.237235617533
H	-2.954497026263	0.725261748495	-3.626407140303
H	-2.704388946333	2.252188922132	-2.749700944639
H	-0.483479423361	2.677612241543	-1.510102971326
H	0.805746364050	1.444999155620	-1.537787000729
H	0.400480160392	2.340352811455	-3.022631994477
H	-1.108377103529	-1.068440666905	-3.648416606052
H	0.034472606261	0.150982275699	-4.273177763274
H	0.436267315470	-0.773736304334	-2.806040041324

SCF Done: E(RB3LYP) = -670.532320587

Zero-point correction= 0.239328
Thermal correction to Energy= 0.254322
Thermal correction to Enthalpy= 0.255267
Thermal correction to Gibbs Free Energy= 0.196394
Sum of electronic and zero-point Energies= -670.292993
Sum of electronic and thermal Energies= -670.277998
Sum of electronic and thermal Enthalpies= -670.277054
Sum of electronic and thermal Free Energies= -670.335926

1 O Isotropic = -42.9117 Anisotropy = 264.9874
2 C Isotropic = 30.5829 Anisotropy = 105.8854
3 C Isotropic = 83.9820 Anisotropy = 116.1132
4 C Isotropic = 17.9083 Anisotropy = 150.6040
5 N Isotropic = -125.2513 Anisotropy = 259.5742
6 C Isotropic = 37.5184 Anisotropy = 74.9427

7	O	Isotropic =	128.9902	Anisotropy =	149.5468
8	O	Isotropic =	-40.0100	Anisotropy =	570.5379
9	C	Isotropic =	128.8709	Anisotropy =	66.2791
10	C	Isotropic =	176.1823	Anisotropy =	22.7750
11	C	Isotropic =	153.9963	Anisotropy =	8.9229
12	C	Isotropic =	163.8834	Anisotropy =	34.0857
13	C	Isotropic =	160.0328	Anisotropy =	41.6029
14	C	Isotropic =	160.3897	Anisotropy =	41.1127
15	H	Isotropic =	24.4787	Anisotropy =	8.4123
16	H	Isotropic =	26.4285	Anisotropy =	5.6441
17	H	Isotropic =	27.3891	Anisotropy =	7.2143
18	H	Isotropic =	30.0571	Anisotropy =	7.4667
19	H	Isotropic =	29.8961	Anisotropy =	6.1508
20	H	Isotropic =	30.2263	Anisotropy =	10.0220
21	H	Isotropic =	30.2612	Anisotropy =	7.8286
22	H	Isotropic =	29.8101	Anisotropy =	8.7191
23	H	Isotropic =	29.7505	Anisotropy =	8.6883
24	H	Isotropic =	30.1977	Anisotropy =	7.9548
25	H	Isotropic =	29.8950	Anisotropy =	7.7547
26	H	Isotropic =	30.0617	Anisotropy =	8.4016
27	H	Isotropic =	30.2095	Anisotropy =	8.0183
28	H	Isotropic =	30.0766	Anisotropy =	8.3986
29	H	Isotropic =	29.8798	Anisotropy =	7.7624

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.051843369294	-0.090488860610	0.871581955472
C	-1.906407132035	-0.395228241362	-0.134135625986
C	-1.519041011174	-1.563383105425	-0.725543060589
C	-0.351335505253	-1.956169313829	-0.000073498633
N	-0.075976969612	-1.079827056065	0.947467855094
C	-3.076069367871	0.450985000734	-0.500681948609
O	-3.375711585666	1.583340832019	0.147844744711
O	-3.782036935040	0.095255622611	-1.425254253794
C	-2.631262592878	2.133941716051	1.275750691774
C	-3.334948983154	3.415023298882	1.670507805207
C	0.511431308602	-3.187673155750	-0.216908634686
C	1.683566705689	-3.214703151434	0.779280124474
C	-0.365932328913	-4.444111622004	-0.019677962361
C	1.057993691744	-3.158215694088	-1.661592507682
H	-2.004598222338	-2.061180599563	-1.557537791387
H	-2.630071060148	1.401888082037	2.095518425101
H	-1.593825891580	2.319870470333	0.964848687797
H	-4.375685926210	3.216473858992	1.969355434690
H	-2.809798726916	3.872999688487	2.523031836918
H	-3.338332891616	4.134541325257	0.837331440652
H	2.293572737097	-4.114556885168	0.604917538644
H	2.330095437436	-2.331730263041	0.663051338087
H	1.326362599605	-3.236325754704	1.819955898821
H	0.238092155083	-5.350391650698	-0.186564267155
H	-0.773194730578	-4.487340313926	1.002992795589
H	-1.210304270690	-4.467052851421	-0.726613275237

H	1.686578847857	-2.269425457440	-1.830394270068
H	1.673311583501	-4.053432744251	-1.845673481294
H	0.244822434354	-3.149703174624	-2.404455995552

SCF Done: E(RB3LYP) = -670.522266720

Zero-point correction= 0.239137
Thermal correction to Energy= 0.254150
Thermal correction to Enthalpy= 0.255094
Thermal correction to Gibbs Free Energy= 0.196347
Sum of electronic and zero-point Energies= -670.283130
Sum of electronic and thermal Energies= -670.268117
Sum of electronic and thermal Enthalpies= -670.267173
Sum of electronic and thermal Free Energies= -670.325919

1	O	Isotropic =	-37.9170	Anisotropy =	269.8524
2	C	Isotropic =	29.5471	Anisotropy =	101.6706
3	C	Isotropic =	78.4392	Anisotropy =	118.4986
4	C	Isotropic =	18.2689	Anisotropy =	154.9944
5	N	Isotropic =	-127.3106	Anisotropy =	239.6616
6	C	Isotropic =	39.2401	Anisotropy =	70.5344
7	O	Isotropic =	126.8993	Anisotropy =	135.8119
8	O	Isotropic =	-60.9826	Anisotropy =	523.6365
9	C	Isotropic =	122.7250	Anisotropy =	62.6519
10	C	Isotropic =	175.4722	Anisotropy =	22.3960
11	C	Isotropic =	154.0732	Anisotropy =	8.6356
12	C	Isotropic =	164.0129	Anisotropy =	33.7468
13	C	Isotropic =	160.2890	Anisotropy =	41.5062
14	C	Isotropic =	160.4246	Anisotropy =	41.3627
15	H	Isotropic =	24.1553	Anisotropy =	7.7199
16	H	Isotropic =	26.6161	Anisotropy =	4.1734
17	H	Isotropic =	26.5814	Anisotropy =	4.3584
18	H	Isotropic =	29.9015	Anisotropy =	7.8531
19	H	Isotropic =	30.0579	Anisotropy =	9.0632
20	H	Isotropic =	29.8993	Anisotropy =	7.8322
21	H	Isotropic =	30.2693	Anisotropy =	7.7781
22	H	Isotropic =	29.7809	Anisotropy =	8.5758
23	H	Isotropic =	29.7586	Anisotropy =	8.5800
24	H	Isotropic =	30.0734	Anisotropy =	8.4529
25	H	Isotropic =	30.2063	Anisotropy =	8.0026
26	H	Isotropic =	29.8794	Anisotropy =	7.8429
27	H	Isotropic =	30.1968	Anisotropy =	8.0175
28	H	Isotropic =	30.0733	Anisotropy =	8.4396
29	H	Isotropic =	29.8726	Anisotropy =	7.8830

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-2.209916888445	-1.180040375146	-0.364760674068
C	-1.740421489607	-0.750775417123	0.831060865542
C	-0.386562911006	-0.593367991279	0.760748998279
C	-0.057350233439	-0.956609964975	-0.583115943968
N	-1.140657419442	-1.308931012157	-1.248562667784

C	-2.608456737233	-0.547334516105	2.026266411396
O	-3.945098076580	-0.525982232508	1.953304800890
O	-2.073924635567	-0.397997982307	3.108561022609
C	-4.740056451480	-0.520976997875	0.728590542088
C	-5.214637708150	-1.919029379760	0.381131235713
C	1.314364759811	-0.971873441245	-1.236132549893
C	1.910346001870	0.451577578874	-1.162969889585
C	2.218736101613	-1.953344695417	-0.457586429540
C	1.213950371398	-1.416073855195	-2.705689069065
H	0.270750828917	-0.266867800459	1.559024274160
H	-5.586845395866	0.131951099918	0.981223494559
H	-4.173673044377	-0.056767091113	-0.087400859098
H	-5.756047189165	-2.368479709998	1.227984258831
H	-5.902853971866	-1.864824546054	-0.477834256550
H	-4.373243633221	-2.571790427617	0.106512977389
H	2.912945435937	0.459368629858	-1.619669350311
H	1.280665167421	1.174373444050	-1.705740825545
H	2.011569329933	0.797728121477	-0.122247238196
H	3.227088913395	-1.963186860477	-0.901519054491
H	2.318935372432	-1.663063036414	0.600171734961
H	1.817047640851	-2.978382455084	-0.495808861532
H	2.217762050255	-1.420359364006	-3.158317766049
H	0.792701942401	-2.429094250467	-2.791530723880
H	0.575841869212	-0.734915471396	-3.288854456863

SCF Done: E(RB3LYP) = -670.521068198

Zero-point correction= 0.239210
Thermal correction to Energy= 0.254163
Thermal correction to Enthalpy= 0.255107
Thermal correction to Gibbs Free Energy= 0.196165
Sum of electronic and zero-point Energies= -670.281859
Sum of electronic and thermal Energies= -670.266905
Sum of electronic and thermal Enthalpies= -670.265961
Sum of electronic and thermal Free Energies= -670.324903

1	O	Isotropic =	-34.5809	Anisotropy =	260.1567
2	C	Isotropic =	30.2440	Anisotropy =	103.0099
3	C	Isotropic =	78.7844	Anisotropy =	117.6778
4	C	Isotropic =	18.2514	Anisotropy =	155.5095
5	N	Isotropic =	-126.3661	Anisotropy =	236.1281
6	C	Isotropic =	38.6034	Anisotropy =	69.6607
7	O	Isotropic =	124.2030	Anisotropy =	161.1331
8	O	Isotropic =	-65.1392	Anisotropy =	525.9783
9	C	Isotropic =	123.4545	Anisotropy =	73.7085
10	C	Isotropic =	173.9673	Anisotropy =	24.7406
11	C	Isotropic =	154.0704	Anisotropy =	8.5016
12	C	Isotropic =	160.4030	Anisotropy =	41.2698
13	C	Isotropic =	160.2382	Anisotropy =	41.4931
14	C	Isotropic =	163.9483	Anisotropy =	33.7274
15	H	Isotropic =	24.2147	Anisotropy =	7.5822
16	H	Isotropic =	27.0649	Anisotropy =	6.9594
17	H	Isotropic =	26.2391	Anisotropy =	2.9142
18	H	Isotropic =	29.8076	Anisotropy =	8.1926
19	H	Isotropic =	30.0798	Anisotropy =	9.4057
20	H	Isotropic =	29.6318	Anisotropy =	5.6960

21	H	Isotropic =	30.0748	Anisotropy =	8.4687
22	H	Isotropic =	30.1989	Anisotropy =	8.0490
23	H	Isotropic =	29.8867	Anisotropy =	7.8087
24	H	Isotropic =	30.0657	Anisotropy =	8.4827
25	H	Isotropic =	29.8837	Anisotropy =	7.8828
26	H	Isotropic =	30.2043	Anisotropy =	8.0080
27	H	Isotropic =	30.2564	Anisotropy =	7.7950
28	H	Isotropic =	29.7729	Anisotropy =	8.5008
29	H	Isotropic =	29.7929	Anisotropy =	8.5553

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-2.233229807676	-1.133431543339	-0.356299702706
C	-1.679333112063	-0.018250096011	0.176994444269
C	-0.340403435847	-0.213557125538	0.355576850641
C	-0.112354651258	-1.547468665011	-0.107918639206
N	-1.236547872461	-2.090569299047	-0.534263637051
C	-2.451033330220	1.226170947149	0.458285647992
O	-3.789134333117	1.265900927140	0.442516278745
O	-1.833057223697	2.243582216618	0.708047921585
C	-4.683032524278	0.116520844276	0.332648553748
C	-5.142770858898	-0.081670882034	-1.099106987248
C	1.201582592112	-2.309123798157	-0.146306487646
C	2.200384130935	-1.522597466354	-1.024207398590
C	1.749280494985	-2.416872852960	1.294250001706
C	0.998358072221	-3.718369451000	-0.729337244367
H	0.370837340275	0.498962859455	0.758590610383
H	-4.200920595043	-0.777797663628	0.745082488525
H	-5.525079765070	0.390095052309	0.983265515881
H	-4.307765283281	-0.375564557835	-1.751662521391
H	-5.900672289100	-0.881096382346	-1.128750658324
H	-5.598939470697	0.839814668189	-1.492862765179
H	3.166079794694	-2.052051171499	-1.056278177636
H	1.829131131797	-1.423825138372	-2.056673718821
H	2.383411645841	-0.511630622849	-0.627102953827
H	2.713190766536	-2.950626304682	1.287718102439
H	1.916488086827	-1.424182342177	1.741116842187
H	1.053853505954	-2.973022567936	1.942838149598
H	0.610487387275	-3.675880164038	-1.758393050025
H	1.961097574029	-4.252391635729	-0.745798830532
H	0.289062029224	-4.304397784594	-0.125518635147

SCF Done: E(RB3LYP) = -670.521066735

Zero-point correction= 0.239266
Thermal correction to Energy= 0.254200
Thermal correction to Enthalpy= 0.255145
Thermal correction to Gibbs Free Energy= 0.196284
Sum of electronic and zero-point Energies= -670.281801
Sum of electronic and thermal Energies= -670.266866
Sum of electronic and thermal Enthalpies= -670.265922
Sum of electronic and thermal Free Energies= -670.324783

1	O	Isotropic =	-34.5948	Anisotropy =	260.0560
2	C	Isotropic =	30.2132	Anisotropy =	103.0127
3	C	Isotropic =	78.7895	Anisotropy =	117.9582
4	C	Isotropic =	18.1949	Anisotropy =	155.4821
5	N	Isotropic =	-126.4213	Anisotropy =	235.8773
6	C	Isotropic =	38.6125	Anisotropy =	69.6617
7	O	Isotropic =	124.4821	Anisotropy =	161.4702
8	O	Isotropic =	-65.0651	Anisotropy =	526.1219
9	C	Isotropic =	123.4676	Anisotropy =	73.7022
10	C	Isotropic =	173.8998	Anisotropy =	24.8588
11	C	Isotropic =	154.0416	Anisotropy =	8.5080
12	C	Isotropic =	160.4360	Anisotropy =	41.3730
13	C	Isotropic =	160.2702	Anisotropy =	41.3460
14	C	Isotropic =	163.9369	Anisotropy =	33.8223
15	H	Isotropic =	24.2040	Anisotropy =	7.6000
16	H	Isotropic =	26.2479	Anisotropy =	2.9281
17	H	Isotropic =	27.0627	Anisotropy =	6.9635
18	H	Isotropic =	29.6317	Anisotropy =	5.6942
19	H	Isotropic =	30.0739	Anisotropy =	9.4038
20	H	Isotropic =	29.8032	Anisotropy =	8.1853
21	H	Isotropic =	30.0739	Anisotropy =	8.4647
22	H	Isotropic =	30.2006	Anisotropy =	8.0200
23	H	Isotropic =	29.8767	Anisotropy =	7.9053
24	H	Isotropic =	30.0706	Anisotropy =	8.4627
25	H	Isotropic =	29.8954	Anisotropy =	7.7864
26	H	Isotropic =	30.2011	Anisotropy =	8.0344
27	H	Isotropic =	29.7777	Anisotropy =	8.5047
28	H	Isotropic =	30.2609	Anisotropy =	7.7934
29	H	Isotropic =	29.7740	Anisotropy =	8.5549

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-1.343831803345	0.243235299240	-0.091232942303
C	-2.058788395723	-0.844508949485	-0.465755255230
C	-1.297711766995	-1.966888404252	-0.312041251095
C	-0.050987557903	-1.482424837453	0.195326820554
N	-0.078669759300	-0.169410566267	0.321137628936
C	-3.444817074621	-0.764684573200	-1.009886624909
O	-4.189647699224	0.344759061474	-0.927160928108
O	-3.909199150926	-1.748888218120	-1.552982093184
C	-3.865164145102	1.543591289611	-0.159275211380
C	-3.256114799298	2.611041203465	-1.047982353381
C	1.182851411894	-2.288133456776	0.564908552355
C	1.651908019068	-3.073973100721	-0.679711858531
C	2.312956615304	-1.362978292038	1.048844271171
C	0.803657279417	-3.277027794930	1.690049726362
H	-1.593441397331	-2.986196971536	-0.534375088877
H	-4.840836947241	1.864469493194	0.231162855432
H	-3.218864647473	1.286454601712	0.688318097642
H	-3.914203819908	2.827651302968	-1.903701194327
H	-3.131157497385	3.538512668522	-0.466109449206

H	-2.268687385440	2.305301876982	-1.423442543459
H	2.538911775107	-3.676737982835	-0.427029053887
H	0.872376066492	-3.760451364246	-1.046114590950
H	1.923169583070	-2.392332571053	-1.501476598603
H	3.194917271880	-1.966570726958	1.313777947945
H	2.607581154496	-0.646496125581	0.267175289556
H	2.009629911056	-0.787584709726	1.936533246448
H	0.000337586537	-3.962369600871	1.376647575067
H	1.680173686639	-3.886936634555	1.961794737830
H	0.465853486251	-2.741631916567	2.591620288132

SCF Done: E(RB3LYP) = -670.521049822

Zero-point correction= 0.239132
Thermal correction to Energy= 0.254144
Thermal correction to Enthalpy= 0.255088
Thermal correction to Gibbs Free Energy= 0.195402
Sum of electronic and zero-point Energies= -670.281918
Sum of electronic and thermal Energies= -670.266906
Sum of electronic and thermal Enthalpies= -670.265962
Sum of electronic and thermal Free Energies= -670.325647

1	O	Isotropic =	-34.7643	Anisotropy =	259.7695
2	C	Isotropic =	30.2106	Anisotropy =	103.1880
3	C	Isotropic =	78.8601	Anisotropy =	118.0876
4	C	Isotropic =	18.2843	Anisotropy =	155.5081
5	N	Isotropic =	-126.4249	Anisotropy =	235.9615
6	C	Isotropic =	38.5248	Anisotropy =	69.4590
7	O	Isotropic =	124.2874	Anisotropy =	160.7805
8	O	Isotropic =	-65.4977	Anisotropy =	526.1486
9	C	Isotropic =	123.4562	Anisotropy =	73.8756
10	C	Isotropic =	173.9923	Anisotropy =	24.7521
11	C	Isotropic =	154.0139	Anisotropy =	8.4709
12	C	Isotropic =	160.4583	Anisotropy =	41.4035
13	C	Isotropic =	164.1317	Anisotropy =	33.6723
14	C	Isotropic =	160.1697	Anisotropy =	41.5677
15	H	Isotropic =	24.2124	Anisotropy =	7.5772
16	H	Isotropic =	27.0696	Anisotropy =	6.9524
17	H	Isotropic =	26.2591	Anisotropy =	2.8877
18	H	Isotropic =	29.8061	Anisotropy =	8.1785
19	H	Isotropic =	30.0805	Anisotropy =	9.4046
20	H	Isotropic =	29.6146	Anisotropy =	5.7204
21	H	Isotropic =	30.0766	Anisotropy =	8.4610
22	H	Isotropic =	29.8676	Anisotropy =	7.9120
23	H	Isotropic =	30.1891	Anisotropy =	8.0468
24	H	Isotropic =	30.2637	Anisotropy =	7.7938
25	H	Isotropic =	29.7898	Anisotropy =	8.5191
26	H	Isotropic =	29.7561	Anisotropy =	8.5711
27	H	Isotropic =	29.9039	Anisotropy =	7.7547
28	H	Isotropic =	30.0673	Anisotropy =	8.4808
29	H	Isotropic =	30.2119	Anisotropy =	8.0304

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

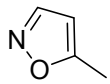
O	-1.101339139204	-1.615164964087	0.798935955249
C	-1.613586381551	-0.362925965980	0.729165213597
C	-1.472742768452	0.117854891203	-0.540466924997
C	-0.825362568988	-0.941534691815	-1.250744979505
N	-0.609059915013	-1.971187867643	-0.454755172341
C	-2.266200323957	0.324047040744	1.880636824966
O	-2.210155580764	-0.146301203868	3.132788752557
O	-2.873891716784	1.355643373065	1.665610093413
C	-1.424659605902	-1.288202912057	3.591848920313
C	-2.261051070660	-2.553476810741	3.613773707681
C	-0.413503855794	-0.968563973293	-2.712834751045
C	-1.673800575315	-0.762503651043	-3.582550415225
C	0.584081399637	0.184056208533	-2.964393531632
C	0.246801756514	-2.311728264618	-3.068736517545
H	-1.791395279292	1.088029199539	-0.905291804080
H	-0.520575242227	-1.395076889790	2.981170319472
H	-1.127127865938	-0.994297739306	4.607759833553
H	-1.675397635467	-3.366825457220	4.071906775256
H	-3.173684708914	-2.406988161733	4.211963695913
H	-2.544436001102	-2.865224912528	2.597845787351
H	-1.394578018243	-0.759801755333	-4.648372140327
H	-2.404342539939	-1.571161312678	-3.421449111998
H	-2.168976862503	0.196342122678	-3.361862341109
H	0.140835415293	1.164578272980	-2.729336607091
H	1.493129671822	0.062811150328	-2.354098110202
H	0.882073888101	0.194433618371	-4.025044917244
H	-0.438918092212	-3.155019741843	-2.896253518987
H	0.532739730411	-2.311400222883	-4.132049169188
H	1.152563886441	-2.485689378980	-2.468345866808

SCF Done: E(RB3LYP) = -670.521076971

Zero-point correction= 0.239237
Thermal correction to Energy= 0.254170
Thermal correction to Enthalpy= 0.255114
Thermal correction to Gibbs Free Energy= 0.196387
Sum of electronic and zero-point Energies= -670.281840
Sum of electronic and thermal Energies= -670.266907
Sum of electronic and thermal Enthalpies= -670.265963
Sum of electronic and thermal Free Energies= -670.324690

1	O	Isotropic =	-34.5791	Anisotropy = 260.3067
2	C	Isotropic =	29.9912	Anisotropy = 102.5271
3	C	Isotropic =	78.6940	Anisotropy = 117.6367
4	C	Isotropic =	18.3503	Anisotropy = 155.5908
5	N	Isotropic =	-126.6127	Anisotropy = 235.9739
6	C	Isotropic =	38.8417	Anisotropy = 69.8317
7	O	Isotropic =	124.0081	Anisotropy = 161.2470
8	O	Isotropic =	-64.1529	Anisotropy = 524.6474
9	C	Isotropic =	123.5451	Anisotropy = 73.7741
10	C	Isotropic =	173.9528	Anisotropy = 24.6254
11	C	Isotropic =	154.0226	Anisotropy = 8.3774
12	C	Isotropic =	160.3046	Anisotropy = 41.3720
13	C	Isotropic =	160.3281	Anisotropy = 41.3509

14	C	Isotropic =	164.0065	Anisotropy =	33.7730
15	H	Isotropic =	24.2039	Anisotropy =	7.6175
16	H	Isotropic =	26.1713	Anisotropy =	2.9379
17	H	Isotropic =	27.0599	Anisotropy =	6.9563
18	H	Isotropic =	30.0748	Anisotropy =	9.4080
19	H	Isotropic =	29.8113	Anisotropy =	8.2029
20	H	Isotropic =	29.6805	Anisotropy =	5.6164
21	H	Isotropic =	30.0779	Anisotropy =	8.4647
22	H	Isotropic =	30.2037	Anisotropy =	8.0094
23	H	Isotropic =	29.8767	Anisotropy =	7.8800
24	H	Isotropic =	29.8976	Anisotropy =	7.7993
25	H	Isotropic =	30.1997	Anisotropy =	8.0653
26	H	Isotropic =	30.0666	Anisotropy =	8.4632
27	H	Isotropic =	29.7740	Anisotropy =	8.5127
28	H	Isotropic =	30.2627	Anisotropy =	7.7907
29	H	Isotropic =	29.7782	Anisotropy =	8.5748



2k

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	-0.409620981795	0.033818299908	-0.450093442491
C	-1.533717309287	0.506003794261	0.138226026180
C	-1.250370225953	1.686208068659	0.769499044813
C	0.135831203804	1.883146727642	0.511941021968
N	0.652626153172	0.913793366370	-0.209927189886
C	-2.771249359155	-0.306368553726	-0.013083602446
H	-1.928836449269	2.318937964521	1.333227266857
H	0.778422411737	2.703902146263	0.830315227075
H	-2.632300720570	-1.314841164018	0.408389208775
H	-3.607768166467	0.179962387673	0.505530152908
H	-3.035206556215	-0.424983037554	-1.076203713753

SCF Done: E(RB3LYP) = -285.382053145

Zero-point correction= 0.085114
Thermal correction to Energy= 0.090373
Thermal correction to Enthalpy= 0.091317
Thermal correction to Gibbs Free Energy= 0.056399
Sum of electronic and zero-point Energies= -285.296939
Sum of electronic and thermal Energies= -285.291680
Sum of electronic and thermal Enthalpies= -285.290736
Sum of electronic and thermal Free Energies= -285.325654

1	O	Isotropic =	-59.9150	Anisotropy =	274.0025
2	C	Isotropic =	21.4036	Anisotropy =	136.6959
3	C	Isotropic =	91.3305	Anisotropy =	92.8572
4	C	Isotropic =	43.3284	Anisotropy =	142.2443
5	N	Isotropic =	-124.8437	Anisotropy =	264.9091

6 C Isotropic = 179.5523 Anisotropy = 22.7670
7 H Isotropic = 25.3691 Anisotropy = 3.5651
8 H Isotropic = 23.4073 Anisotropy = 2.8748
9 H Isotropic = 28.9547 Anisotropy = 8.5892
10 H Isotropic = 28.9208 Anisotropy = 7.5510
11 H Isotropic = 28.9542 Anisotropy = 8.5844

2k incorrect isomer

Conformer 1

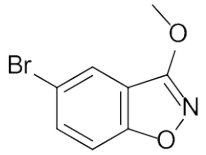
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	1.971085159972	1.126244731808	-0.325032390295
C	1.176365483265	2.181978966674	-0.062078010963
C	-0.063520233876	1.760520800371	0.306461404071
C	0.033542853261	0.332204612603	0.248170392944
N	1.238282529852	-0.049486086977	-0.125951248025
C	-1.024430834338	-0.681984559505	0.549922328444
H	1.632131960590	3.162309709415	-0.181026246784
H	-0.924418377701	2.362954080571	0.580265657910
H	-0.634036030273	-1.698908991242	0.407851038425
H	-1.376453478793	-0.579410803313	1.588623316363
H	-1.896579031958	-0.541762460404	-0.108086242090

SCF Done: E(RB3LYP) = -285.380291985

Zero-point correction= 0.085188
Thermal correction to Energy= 0.090375
Thermal correction to Enthalpy= 0.091319
Thermal correction to Gibbs Free Energy= 0.056685
Sum of electronic and zero-point Energies= -285.295104
Sum of electronic and thermal Energies= -285.289917
Sum of electronic and thermal Enthalpies= -285.288973
Sum of electronic and thermal Free Energies= -285.323607

1 O Isotropic = -49.5939 Anisotropy = 267.4907
2 C Isotropic = 34.6444 Anisotropy = 128.9540
3 C Isotropic = 88.2061 Anisotropy = 101.6823
4 C Isotropic = 31.9618 Anisotropy = 151.7385
5 N Isotropic = -116.4402 Anisotropy = 246.3887
6 C Isotropic = 179.8099 Anisotropy = 22.3650
7 H Isotropic = 23.0058 Anisotropy = 2.5521
8 H Isotropic = 25.1370 Anisotropy = 3.0667
9 H Isotropic = 29.1021 Anisotropy = 7.8408
10 H Isotropic = 29.1059 Anisotropy = 8.2407
11 H Isotropic = 29.1066 Anisotropy = 8.2355



2l

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.159267800677	-1.626393864402	0.436192728389
C	1.370694616759	-0.933775148225	0.516772334708
C	1.461409930798	0.445541384118	0.309136141405
C	0.326405903365	1.211527750544	0.005932461053
C	-0.878921859795	0.523626603780	-0.074457516488
C	-0.971837281690	-0.870404272833	0.135179167042
C	2.868954420447	0.700586156742	0.491414856288
N	3.540074692307	-0.392208600621	0.773726485288
O	2.594091460892	-1.450181273857	0.793990655988
O	3.419391024808	1.908188161799	0.384658040944
C	4.843045287084	1.981928059892	0.599459057325
Br	-2.483678825840	1.496103286235	-0.486084480996
H	0.098335982088	-2.702340626151	0.599531939371
H	0.388952852053	2.286640023230	-0.157147603752
H	-1.942610913049	-1.360702631922	0.060064520753
H	5.105648923861	3.038224452730	0.474334322096
H	5.095504588373	1.638669439548	1.614156100258
H	5.374341396863	1.361921099396	-0.138459209673

SCF Done: E(RB3LYP) = -3087.79992612

Zero-point correction= 0.127133
Thermal correction to Energy= 0.137191
Thermal correction to Enthalpy= 0.138136
Thermal correction to Gibbs Free Energy= 0.090159
Sum of electronic and zero-point Energies= -3087.672793
Sum of electronic and thermal Energies= -3087.662735
Sum of electronic and thermal Enthalpies= -3087.661791
Sum of electronic and thermal Free Energies= -3087.709767

1	C	Isotropic =	81.4731	Anisotropy = 143.8399
2	C	Isotropic =	30.1779	Anisotropy = 133.3295
3	C	Isotropic =	75.6032	Anisotropy = 122.8789
4	C	Isotropic =	69.0292	Anisotropy = 144.0470
5	C	Isotropic =	56.9269	Anisotropy = 99.9203
6	C	Isotropic =	60.1274	Anisotropy = 149.6693
7	C	Isotropic =	27.3634	Anisotropy = 102.0944
8	N	Isotropic =	-79.5290	Anisotropy = 190.6416
9	O	Isotropic =	40.4052	Anisotropy = 151.0457
10	O	Isotropic =	241.1383	Anisotropy = 114.7407
11	C	Isotropic =	135.7961	Anisotropy = 75.5508

12 Br Isotropic = 2084.9127 Anisotropy = 1328.4826
13 H Isotropic = 24.0880 Anisotropy = 4.7963
14 H Isotropic = 23.7757 Anisotropy = 10.6230
15 H Isotropic = 23.9331 Anisotropy = 9.2141
16 H Isotropic = 27.2561 Anisotropy = 8.2162
17 H Isotropic = 27.3362 Anisotropy = 8.5184
18 H Isotropic = 27.3403 Anisotropy = 8.5188

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	1.739221958903	0.218282858893	1.926345884329
C	2.072657536987	1.198618957695	0.987216687651
C	1.278556734685	1.495881649049	-0.129942369826
C	0.079375856315	0.786331527936	-0.342873855829
C	-0.252300153135	-0.187859808364	0.589995878833
C	0.554789357618	-0.477983294841	1.711677755024
C	2.036441956392	2.554189867133	-0.772006551737
N	3.136336759909	2.837797675505	-0.109631233874
O	3.173033337062	1.983732840515	1.010361409575
O	1.810705832165	3.261850984463	-1.885454277814
C	0.613446296353	3.003786169734	-2.633500804251
Br	-1.876128659263	-1.186692278923	0.351940815750
H	2.377610210999	0.010782936039	2.785181333372
H	-0.570067978004	0.978602253024	-1.193031036803
H	0.246085079213	-1.253006101455	2.413189374782
H	0.645151691680	3.697977337608	-3.481123647379
H	0.597006009300	1.969813800997	-3.010825706783
H	-0.283501827179	3.208282624992	-2.028969655022

SCF Done: E(RB3LYP) = -3087.79279688

Zero-point correction= 0.127183
Thermal correction to Energy= 0.137264
Thermal correction to Enthalpy= 0.138208
Thermal correction to Gibbs Free Energy= 0.090029
Sum of electronic and zero-point Energies= -3087.665614
Sum of electronic and thermal Energies= -3087.655533
Sum of electronic and thermal Enthalpies= -3087.654588
Sum of electronic and thermal Free Energies= -3087.702768

1 C Isotropic = 80.8832 Anisotropy = 144.5675
2 C Isotropic = 29.4476 Anisotropy = 133.4349
3 C Isotropic = 76.8041 Anisotropy = 124.0669
4 C Isotropic = 67.4659 Anisotropy = 138.8505
5 C Isotropic = 57.0891 Anisotropy = 100.5739
6 C Isotropic = 60.3825 Anisotropy = 150.1741
7 C Isotropic = 26.1921 Anisotropy = 94.4462
8 N Isotropic = -85.3954 Anisotropy = 201.2032
9 O Isotropic = 39.3333 Anisotropy = 165.1580
10 O Isotropic = 241.4050 Anisotropy = 88.7607
11 C Isotropic = 134.9808 Anisotropy = 74.9624
12 Br Isotropic = 2079.0072 Anisotropy = 1340.3621

13 H Isotropic = 24.0435 Anisotropy = 4.7823
14 H Isotropic = 23.5355 Anisotropy = 12.6019
15 H Isotropic = 23.9424 Anisotropy = 9.1725
16 H Isotropic = 27.1516 Anisotropy = 8.0074
17 H Isotropic = 27.0021 Anisotropy = 6.9814
18 H Isotropic = 27.0292 Anisotropy = 6.9634

2l incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.476295705028	-0.636681237955	0.708141751828
C	-1.607471999663	0.455860110098	-0.206907564696
C	-0.444813446819	1.221221453270	-0.554464510008
C	0.839027322978	0.931800714995	-0.020522474617
C	0.916524986328	-0.124662596861	0.852143950078
C	-0.230626799620	-0.907474685820	1.217818746593
C	-0.955229907361	2.167320446484	-1.438748013765
O	-2.263309855536	1.986167996416	-1.597700067725
N	-2.717080200677	0.881919062207	-0.810841171982
O	-0.332824237736	3.136057501973	-2.076420798445
C	-1.120273382670	3.985475770176	-2.946706450822
Br	2.608172618834	-0.598897184341	1.630236227928
H	-2.344421012142	-1.234030233507	0.989142231196
H	1.711790596013	1.523436050925	-0.294904554253
H	-0.099053951801	-1.733839823112	1.917219541345
H	-1.899638690661	4.502338831757	-2.368945898263
H	-0.408440580324	4.705628477414	-3.362763217186
H	-1.578065754113	3.387949345880	-3.747797727206

SCF Done: E(RB3LYP) = -3087.78454201

Zero-point correction= 0.126690
Thermal correction to Energy= 0.136911
Thermal correction to Enthalpy= 0.137855
Thermal correction to Gibbs Free Energy= 0.089386
Sum of electronic and zero-point Energies= -3087.657852
Sum of electronic and thermal Energies= -3087.647631
Sum of electronic and thermal Enthalpies= -3087.646687
Sum of electronic and thermal Free Energies= -3087.695156

1 C Isotropic = 78.7403 Anisotropy = 142.9775
2 C Isotropic = 35.2493 Anisotropy = 159.4281
3 C Isotropic = 91.9942 Anisotropy = 101.9807
4 C Isotropic = 68.5028 Anisotropy = 142.8716
5 C Isotropic = 60.6962 Anisotropy = 87.5476
6 C Isotropic = 57.5482 Anisotropy = 145.2780
7 C Isotropic = 25.2546 Anisotropy = 90.2714
8 O Isotropic = -27.7863 Anisotropy = 236.5710
9 N Isotropic = -92.3723 Anisotropy = 156.0519
10 O Isotropic = 210.8344 Anisotropy = 147.7138
11 C Isotropic = 134.8462 Anisotropy = 78.5509

12 Br Isotropic = 2096.4288 Anisotropy = 1313.0518
13 H Isotropic = 24.3585 Anisotropy = 5.0525
14 H Isotropic = 23.9280 Anisotropy = 10.2001
15 H Isotropic = 24.3019 Anisotropy = 8.8092
16 H Isotropic = 27.0685 Anisotropy = 8.4422
17 H Isotropic = 27.0694 Anisotropy = 8.1685
18 H Isotropic = 27.0738 Anisotropy = 8.4296

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.227889268719	0.211366191619	1.820654046755
C	-1.486551419832	1.282828726534	0.907420398499
C	-0.553689898087	1.563899023801	-0.153646465698
C	0.633337664788	0.787314521101	-0.310529732112
C	0.837666259515	-0.227106491714	0.588961284640
C	-0.082375338611	-0.521701449909	1.651930987191
C	-1.155248197410	2.646200372094	-0.797388098892
O	-2.298311917871	2.959787503075	-0.188328063190
N	-2.536177836427	2.099159252860	0.911523925124
O	-0.886174851681	3.419967992932	-1.832462933492
C	0.328024384775	3.161719805454	-2.566743887124
Br	2.413428825500	-1.317076422398	0.447951772314
H	-1.929605308055	-0.007975782922	2.626229164059
H	1.349991508360	0.983966670114	-1.104714395304
H	0.144405986792	-1.344743025780	2.330213922060
H	0.309608945614	2.148599112131	-2.994337672216
H	0.342863779793	3.905061236308	-3.370762544577
H	1.205636681555	3.295972764701	-1.917441708036

SCF Done: E(RB3LYP) = -3087.78197874

Zero-point correction= 0.127061
Thermal correction to Energy= 0.137152
Thermal correction to Enthalpy= 0.138096
Thermal correction to Gibbs Free Energy= 0.090026
Sum of electronic and zero-point Energies= -3087.654918
Sum of electronic and thermal Energies= -3087.644827
Sum of electronic and thermal Enthalpies= -3087.643882
Sum of electronic and thermal Free Energies= -3087.691953

1 C Isotropic = 77.4130 Anisotropy = 144.0877
2 C Isotropic = 35.2361 Anisotropy = 156.7362
3 C Isotropic = 91.8902 Anisotropy = 104.0293
4 C Isotropic = 68.1756 Anisotropy = 138.4267
5 C Isotropic = 59.7796 Anisotropy = 89.6709
6 C Isotropic = 58.0508 Anisotropy = 144.7113
7 C Isotropic = 23.5339 Anisotropy = 85.2793
8 O Isotropic = -30.0101 Anisotropy = 219.3709
9 N Isotropic = -85.7848 Anisotropy = 168.7533
10 O Isotropic = 208.1569 Anisotropy = 130.0382
11 C Isotropic = 134.0208 Anisotropy = 77.8247
12 Br Isotropic = 2088.9827 Anisotropy = 1321.3203

13 H Isotropic = 24.3322 Anisotropy = 4.9661
14 H Isotropic = 23.7918 Anisotropy = 12.0831
15 H Isotropic = 24.3449 Anisotropy = 8.7342
16 H Isotropic = 26.9599 Anisotropy = 6.8177
17 H Isotropic = 26.9805 Anisotropy = 8.0456
18 H Isotropic = 26.9534 Anisotropy = 6.8352

3a

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.102692492123	0.492410138386	-0.144391497962
N	-0.644169424818	1.650757775814	0.150758962395
O	0.492497984665	2.473062846915	0.423428040623
C	1.566172385135	1.684269038934	0.252522252969
N	1.273155803612	0.451178931191	-0.099549173722
C	-0.937698363577	-0.690393086694	-0.503859477820
N	2.785336709486	2.208395750192	0.507419030930
H	-0.672774928958	-1.049984673209	-1.510345850367
H	-0.750635819846	-1.515310590763	0.201209243145
H	-2.004367316008	-0.432013223143	-0.481964788758
H	3.575386585233	1.695929753030	0.130052887372
H	2.869808877198	3.219497339348	0.483860371195

SCF Done: E(RB3LYP) = -356.813287808

Zero-point correction= 0.090428
Thermal correction to Energy= 0.096833
Thermal correction to Enthalpy= 0.097777
Thermal correction to Gibbs Free Energy= 0.060430
Sum of electronic and zero-point Energies= -356.722860
Sum of electronic and thermal Energies= -356.716455
Sum of electronic and thermal Enthalpies= -356.715511
Sum of electronic and thermal Free Energies= -356.752857

1 C Isotropic = 23.3915 Anisotropy = 124.5856
2 N Isotropic = -85.9925 Anisotropy = 141.5157
3 O Isotropic = -4.6797 Anisotropy = 114.9236
4 C Isotropic = 23.4286 Anisotropy = 94.1667
5 N Isotropic = 58.4232 Anisotropy = 199.9779
6 C Isotropic = 179.6645 Anisotropy = 23.1735
7 N Isotropic = 203.5092 Anisotropy = 73.3738
8 H Isotropic = 29.3047 Anisotropy = 8.1320
9 H Isotropic = 29.3059 Anisotropy = 8.1768

10 H Isotropic = 29.3683 Anisotropy = 7.6761
11 H Isotropic = 27.0914 Anisotropy = 12.2597
12 H Isotropic = 27.1103 Anisotropy = 11.5763

3a incorrect isomer

Conformer 1

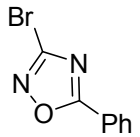
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.129311004691	0.438631362393	0.195916920966
N	0.904577683602	-0.082568336072	-0.437506802927
O	1.804563927491	1.015095745504	-0.504610664203
C	1.195676808038	2.055049413127	0.082054317726
N	0.005960107743	1.773029736258	0.536583448571
N	-1.238479898444	-0.279404662548	0.560441660733
C	1.921153803542	3.350820223573	0.143549931748
H	-2.082064569602	0.281696761438	0.640157554921
H	-1.385025983752	-1.135643690790	0.032610959894
H	2.869944794145	3.233026499887	0.689252402904
H	2.161674549208	3.704577727729	-0.870824188817
H	1.298809782720	4.096699219500	0.651684458483

SCF Done: E(RB3LYP) = -356.809628676

Zero-point correction= 0.090419
Thermal correction to Energy= 0.096948
Thermal correction to Enthalpy= 0.097892
Thermal correction to Gibbs Free Energy= 0.059642
Sum of electronic and zero-point Energies= -356.719209
Sum of electronic and thermal Energies= -356.712681
Sum of electronic and thermal Enthalpies= -356.711736
Sum of electronic and thermal Free Energies= -356.749987

1 C Isotropic = 25.1335 Anisotropy = 110.4447
2 N Isotropic = -61.6457 Anisotropy = 153.3652
3 O Isotropic = -33.1672 Anisotropy = 160.7373
4 C Isotropic = 15.8084 Anisotropy = 113.1780
5 N Isotropic = 25.3943 Anisotropy = 226.0490
6 N Isotropic = 214.2173 Anisotropy = 60.4906
7 C Isotropic = 179.8886 Anisotropy = 26.6762
8 H Isotropic = 28.0289 Anisotropy = 11.9460
9 H Isotropic = 27.9713 Anisotropy = 12.1827
10 H Isotropic = 29.0511 Anisotropy = 8.2879
11 H Isotropic = 29.0486 Anisotropy = 8.2259
12 H Isotropic = 29.0638 Anisotropy = 7.7780



3b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

O	0.126334670230	1.295071181485	0.999680862173
N	-0.974314712043	1.218700450876	1.870592526802
C	-1.844636567928	0.555121056271	1.148383630583
N	-1.443517052308	0.184233839293	-0.101327322380
C	-0.221367531275	0.665774293114	-0.140752777025
C	0.742261562390	0.590721079528	-1.234398444894
Br	-3.549127499084	0.151421183242	1.827184077126
C	2.018932986748	1.168515266031	-1.110224713200
C	2.922507196100	1.083804508418	-2.169346940633
C	2.561316258488	0.426536381200	-3.351479450450
C	1.290757181649	-0.149062364974	-3.476091230912
C	0.380710109824	-0.069414175395	-2.423048852887
H	2.297969428053	1.680003698341	-0.188385296784
H	3.913001282538	1.532150388130	-2.072407645667
H	3.272019914732	0.362611790204	-4.178103847113
H	1.009228973263	-0.661624720926	-4.397808667446
H	-0.611836201378	-0.513163854838	-2.507695907292

SCF Done: E(RB3LYP) = -3066.73990983

Zero-point correction= 0.117165
Thermal correction to Energy= 0.126456
Thermal correction to Enthalpy= 0.127400
Thermal correction to Gibbs Free Energy= 0.080227
Sum of electronic and zero-point Energies= -3066.622745
Sum of electronic and thermal Energies= -3066.613454
Sum of electronic and thermal Enthalpies= -3066.612510
Sum of electronic and thermal Free Energies= -3066.659683

1	O	Isotropic =	-62.0620	Anisotropy = 224.5454
2	N	Isotropic =	-97.9773	Anisotropy = 224.6472
3	C	Isotropic =	21.8336	Anisotropy = 70.2707
4	N	Isotropic =	15.4445	Anisotropy = 255.4312
5	C	Isotropic =	15.6458	Anisotropy = 106.7313
6	C	Isotropic =	68.9124	Anisotropy = 155.3229
7	Br	Isotropic =	2145.6401	Anisotropy = 1172.5377
8	C	Isotropic =	64.9045	Anisotropy = 178.1372
9	C	Isotropic =	63.4411	Anisotropy = 177.7568
10	C	Isotropic =	58.4084	Anisotropy = 185.5765
11	C	Isotropic =	63.4143	Anisotropy = 177.4688
12	C	Isotropic =	63.8467	Anisotropy = 175.6265
13	H	Isotropic =	23.2026	Anisotropy = 8.1493
14	H	Isotropic =	23.8098	Anisotropy = 5.1362

15 H Isotropic = 23.7019 Anisotropy = 4.9118
16 H Isotropic = 23.8160 Anisotropy = 5.2126
17 H Isotropic = 23.1734 Anisotropy = 8.2239

3b incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

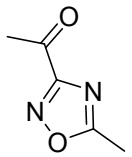
N	0.023333258808	1.716836524935	-0.605623190651
O	-0.495865426296	2.280772488399	0.574458087942
C	-1.261422203399	1.330346630930	1.122086455980
N	-1.312599789261	0.219540547285	0.457904681351
C	-0.490773870327	0.502965769014	-0.623784859308
C	-0.219579759131	-0.466578115277	-1.695002270240
Br	-2.123844064183	1.736626045993	2.725253213459
C	-0.799392341694	-1.744846310508	-1.639794495564
C	-0.547251901306	-2.671369008592	-2.653987187208
C	0.282302650537	-2.329931990408	-3.727143185837
C	0.862006416605	-1.055847489736	-3.785028327067
C	0.614589086188	-0.126166901108	-2.775667835066
H	-1.445008809803	-2.002627412651	-0.799701094863
H	-1.000550517694	-3.663534090002	-2.605527020787
H	0.478421252344	-3.055518191363	-4.519500493695
H	1.509716158827	-0.786669050760	-4.621822164181
H	1.064329859786	0.866860553847	-2.818430314266

SCF Done: E(RB3LYP) = -3066.73541848

Zero-point correction= 0.117151
Thermal correction to Energy= 0.126433
Thermal correction to Enthalpy= 0.127377
Thermal correction to Gibbs Free Energy= 0.080184
Sum of electronic and zero-point Energies= -3066.618268
Sum of electronic and thermal Energies= -3066.608985
Sum of electronic and thermal Enthalpies= -3066.608041
Sum of electronic and thermal Free Energies= -3066.655234

1 N Isotropic = -116.8203 Anisotropy = 220.1046
2 O Isotropic = -67.6529 Anisotropy = 196.0096
3 C Isotropic = 18.8093 Anisotropy = 58.0237
4 N Isotropic = 10.6654 Anisotropy = 265.7395
5 C Isotropic = 21.6733 Anisotropy = 118.9028
6 C Isotropic = 66.0119 Anisotropy = 160.1909
7 Br Isotropic = 2050.6313 Anisotropy = 1271.1916
8 C Isotropic = 64.6100 Anisotropy = 176.2684
9 C Isotropic = 63.6180 Anisotropy = 175.8811
10 C Isotropic = 60.5088 Anisotropy = 182.1717
11 C Isotropic = 63.7752 Anisotropy = 175.9927
12 C Isotropic = 66.9890 Anisotropy = 174.0784
13 H Isotropic = 23.2935 Anisotropy = 8.3995
14 H Isotropic = 23.8699 Anisotropy = 5.2225
15 H Isotropic = 23.8133 Anisotropy = 4.7955

16 H Isotropic = 23.8979 Anisotropy = 4.9938
17 H Isotropic = 23.2216 Anisotropy = 7.5610



3c

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.310074769259	-0.891223898915	0.975962319621
C	0.076031670458	-0.090694516744	-0.038966414767
N	-1.245877271343	0.268044888657	-0.194525854227
C	-1.822755033249	-0.361342546217	0.790551733324
O	-0.947604681828	-1.077849806817	1.535042335438
C	-3.254812178900	-0.387195232667	1.177911003211
C	1.175406546650	0.385148649771	-0.946672281592
C	2.570934676834	-0.088783080746	-0.636462654171
O	0.901192100618	1.120041420421	-1.876876930513
H	-3.378684996972	-0.023244203173	2.209186966123
H	-3.828441752097	0.248420187428	0.493552281395
H	-3.643691957155	-1.416072753531	1.136207185861
H	2.608986722841	-1.189790471865	-0.650511190896
H	3.271849041367	0.323705551159	-1.372482916594
H	2.859282343517	0.225005813239	0.379744417786

SCF Done: E(RB3LYP) = -454.092865282

Zero-point correction= 0.110221
Thermal correction to Energy= 0.119010
Thermal correction to Enthalpy= 0.119955
Thermal correction to Gibbs Free Energy= 0.075505
Sum of electronic and zero-point Energies= -453.982644
Sum of electronic and thermal Energies= -453.973855
Sum of electronic and thermal Enthalpies= -453.972911
Sum of electronic and thermal Free Energies= -454.017361

1 N Isotropic = -127.4286 Anisotropy = 288.6562
2 C Isotropic = 26.1302 Anisotropy = 105.0258
3 N Isotropic = 12.9207 Anisotropy = 284.0701
4 C Isotropic = 12.4249 Anisotropy = 113.0952
5 O Isotropic = -70.6061 Anisotropy = 224.9296
6 C Isotropic = 179.9670 Anisotropy = 25.9341
7 C Isotropic = 2.1022 Anisotropy = 159.1624
8 C Isotropic = 163.7122 Anisotropy = 48.3834
9 O Isotropic = -293.5909 Anisotropy = 971.7038
10 H Isotropic = 28.7988 Anisotropy = 8.1979
11 H Isotropic = 28.8183 Anisotropy = 8.1607
12 H Isotropic = 28.8013 Anisotropy = 8.2275

13 H Isotropic = 28.4954 Anisotropy = 4.6399
14 H Isotropic = 29.3957 Anisotropy = 6.5955
15 H Isotropic = 28.5152 Anisotropy = 4.6628

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.327233233902	-1.189561055247	-0.529904145157
C	-0.032963740340	0.024495112464	-0.176904857765
N	-0.894261255353	0.078010083236	0.897676121943
C	-1.051079704975	-1.182294427266	1.196538033518
O	-0.346167227575	-1.995996090949	0.379051324333
C	-1.867194663906	-1.798771607076	2.271205579712
C	0.470895060766	1.239348012592	-0.907667562605
C	-0.025290266366	2.567353468027	-0.403661677058
O	1.234206102904	1.110920464421	-1.847072189338
H	-2.380854047594	-1.011555182499	2.835052009292
H	-2.610146638861	-2.487151471632	1.840619809132
H	-1.226572011174	-2.379453925023	2.952350253289
H	0.401680171744	3.376510774577	-1.008464626108
H	-1.126149448671	2.598195290414	-0.443968819003
H	0.249884435498	2.694780553961	0.655850745814

SCF Done: E(RB3LYP) = -454.092092132

Zero-point correction= 0.110188
Thermal correction to Energy= 0.118955
Thermal correction to Enthalpy= 0.119899
Thermal correction to Gibbs Free Energy= 0.075586
Sum of electronic and zero-point Energies= -453.981904
Sum of electronic and thermal Energies= -453.973137
Sum of electronic and thermal Enthalpies= -453.972193
Sum of electronic and thermal Free Energies= -454.016506

1 N Isotropic = -124.5388 Anisotropy = 278.7426
2 C Isotropic = 26.3901 Anisotropy = 107.0264
3 N Isotropic = 11.0352 Anisotropy = 275.0916
4 C Isotropic = 12.3213 Anisotropy = 113.6026
5 O Isotropic = -72.3997 Anisotropy = 246.8497
6 C Isotropic = 180.0233 Anisotropy = 25.6904
7 C Isotropic = 0.6209 Anisotropy = 157.4330
8 C Isotropic = 162.1539 Anisotropy = 46.0659
9 O Isotropic = -277.9452 Anisotropy = 957.1808
10 H Isotropic = 28.8135 Anisotropy = 7.8618
11 H Isotropic = 28.7970 Anisotropy = 8.3122
12 H Isotropic = 28.8017 Anisotropy = 8.3263
13 H Isotropic = 29.4378 Anisotropy = 6.5011
14 H Isotropic = 28.5070 Anisotropy = 4.2591
15 H Isotropic = 28.5063 Anisotropy = 4.2751

3c incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.224512492511	-1.049807614377	1.013901269908
C	-0.561731437174	0.052288406744	0.377562957013
N	0.488843810068	0.668187992025	-0.273028517451
C	1.488692920823	-0.121224315059	0.002179383929
O	1.144420859492	-1.171259958880	0.766888212511
C	2.922409731901	0.023372848600	-0.434306752551
C	-1.955553224794	0.577338617628	0.368379446012
C	3.880366968527	-1.043022589020	0.018672610956
O	3.227233374585	0.978632687569	-1.120294064388
H	-1.978689020327	1.592918957112	0.792082227775
H	-2.328646388519	0.639041544651	-0.665328655412
H	-2.616318025779	-0.074569002809	0.953546775032
H	3.548455104261	-2.028538432624	-0.347194026855
H	4.885311888983	-0.819216099832	-0.358711258054
H	3.891305930465	-1.099973041728	1.119370391574

SCF Done: E(RB3LYP) = -454.089313672

Zero-point correction= 0.110265
Thermal correction to Energy= 0.118922
Thermal correction to Enthalpy= 0.119866
Thermal correction to Gibbs Free Energy= 0.076164
Sum of electronic and zero-point Energies= -453.979048
Sum of electronic and thermal Energies= -453.970392
Sum of electronic and thermal Enthalpies= -453.969448
Sum of electronic and thermal Free Energies= -454.013150

1	N	Isotropic =	-106.0741	Anisotropy = 222.5907
2	C	Isotropic =	21.2732	Anisotropy = 126.7642
3	N	Isotropic =	-2.1785	Anisotropy = 319.4340
4	C	Isotropic =	21.3422	Anisotropy = 96.7208
5	O	Isotropic =	-73.8894	Anisotropy = 253.4161
6	C	Isotropic =	6.7124	Anisotropy = 148.2871
7	C	Isotropic =	179.8084	Anisotropy = 22.0828
8	C	Isotropic =	162.9729	Anisotropy = 48.3971
9	O	Isotropic =	-292.6873	Anisotropy = 966.7102
10	H	Isotropic =	28.9865	Anisotropy = 8.2601
11	H	Isotropic =	28.9850	Anisotropy = 8.2585
12	H	Isotropic =	28.9125	Anisotropy = 7.7494
13	H	Isotropic =	28.4790	Anisotropy = 4.5673
14	H	Isotropic =	29.2365	Anisotropy = 6.7621
15	H	Isotropic =	28.4580	Anisotropy = 4.5385

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

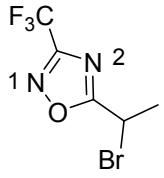
N	-0.675856282154	0.394407323627	0.380537693444
C	-0.432291490675	-0.826945847578	-0.044313440152

N	0.914166466567	-1.118549943523	-0.152303144888
C	1.473227112970	-0.005133953313	0.231100638212
O	0.590950681896	0.948722047403	0.566417810035
C	2.938967200514	0.309774953594	0.333373068728
C	-1.514422870453	-1.795414704056	-0.374212053770
C	3.875189767026	-0.799958595935	-0.054077172319
O	3.287326573509	1.411284338956	0.712396281196
H	-1.418382682591	-2.696046232914	0.251195426903
H	-2.499798922982	-1.342316794588	-0.207591034921
H	-1.432381885645	-2.109607136386	-1.425922449505
H	4.912653871640	-0.462899537211	0.059160993981
H	3.689786873304	-1.685514679702	0.574737392178
H	3.684235587074	-1.106911238375	-1.094920009121

SCF Done: E(RB3LYP) = -454.090333332

Zero-point correction= 0.110298
Thermal correction to Energy= 0.118971
Thermal correction to Enthalpy= 0.119916
Thermal correction to Gibbs Free Energy= 0.076136
Sum of electronic and zero-point Energies= -453.980035
Sum of electronic and thermal Energies= -453.971362
Sum of electronic and thermal Enthalpies= -453.970418
Sum of electronic and thermal Free Energies= -454.014198

1	N	Isotropic =	-105.8678	Anisotropy = 234.1866
2	C	Isotropic =	21.5401	Anisotropy = 124.4714
3	N	Isotropic =	-2.8533	Anisotropy = 311.4339
4	C	Isotropic =	22.3417	Anisotropy = 98.3446
5	O	Isotropic =	-68.3653	Anisotropy = 252.4767
6	C	Isotropic =	5.9629	Anisotropy = 148.1188
7	C	Isotropic =	179.8506	Anisotropy = 22.0785
8	C	Isotropic =	163.4878	Anisotropy = 47.3767
9	O	Isotropic =	-290.4424	Anisotropy = 977.7326
10	H	Isotropic =	28.9929	Anisotropy = 8.1118
11	H	Isotropic =	28.9368	Anisotropy = 8.0008
12	H	Isotropic =	28.9929	Anisotropy = 8.1158
13	H	Isotropic =	29.3478	Anisotropy = 6.8246
14	H	Isotropic =	28.4333	Anisotropy = 4.4260
15	H	Isotropic =	28.4345	Anisotropy = 4.4359



3d

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.446078453072	-1.085439739897	-0.084237260521
N	-1.340141058934	0.071737887694	0.641255506138
C	-1.602928429210	0.973936813049	-0.265275115438
O	-1.862689671960	0.442037846241	-1.475247704707
N	-1.752962207734	-0.937558158049	-1.348100293282
C	-1.654660337398	2.451446364377	-0.095994636584
C	-1.233080359226	-2.442316114673	0.532833445504
F	-0.005122781803	-2.529292917200	1.077454979982
F	-2.127636460936	-2.661995510953	1.515101124049
F	-1.360363967398	-3.419031835550	-0.377082730403
C	-2.803479338368	3.131109433932	-0.822814774318
Br	0.108677484627	3.182227752925	-0.731794094920
H	-1.648266503471	2.665333646936	0.977608854189
H	-2.766671445089	4.215135154678	-0.653842750225
H	-2.770613490359	2.932576305536	-1.903023722822
H	-3.756502979670	2.747073070955	-0.422410826642

SCF Done: E(RB3LYP) = -3251.35362678

Zero-point correction= 0.097001
Thermal correction to Energy= 0.108189
Thermal correction to Enthalpy= 0.109133
Thermal correction to Gibbs Free Energy= 0.056178
Sum of electronic and zero-point Energies= -3251.256625
Sum of electronic and thermal Energies= -3251.245438
Sum of electronic and thermal Enthalpies= -3251.244494
Sum of electronic and thermal Free Energies= -3251.297449

1	C	Isotropic =	28.3490	Anisotropy =	110.4137
2	N	Isotropic =	11.5793	Anisotropy =	288.6121
3	C	Isotropic =	10.4130	Anisotropy =	116.6610
4	O	Isotropic =	-66.9510	Anisotropy =	262.7514
5	N	Isotropic =	-117.1575	Anisotropy =	273.9757
6	C	Isotropic =	138.2490	Anisotropy =	40.4521
7	C	Isotropic =	68.4715	Anisotropy =	16.1917
8	F	Isotropic =	261.7175	Anisotropy =	117.4610
9	F	Isotropic =	260.7915	Anisotropy =	118.4382
10	F	Isotropic =	279.8940	Anisotropy =	118.6907
11	C	Isotropic =	168.5078	Anisotropy =	31.2223
12	Br	Isotropic =	1956.9050	Anisotropy =	1531.0709
13	H	Isotropic =	26.1715	Anisotropy =	8.8765
14	H	Isotropic =	29.4503	Anisotropy =	8.7670
15	H	Isotropic =	29.1370	Anisotropy =	7.0726
16	H	Isotropic =	29.5632	Anisotropy =	10.8271

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.554933162790	-0.838770063065	0.399681005522
N	-0.580052816553	0.529787415285	0.436581428297
C	-0.424756116384	0.828950530040	-0.824523403042
O	-0.302601491116	-0.258403606393	-1.610315449399

N	-0.394032767108	-1.372135104672	-0.785101716050
C	-0.365348294979	2.172326880353	-1.461505894903
C	-0.700955428847	-1.679751363822	1.640058257227
F	-1.897900708554	-1.468990993714	2.219967461978
F	-0.595017990834	-2.986713168011	1.359214121209
F	0.246382679632	-1.362952310031	2.542414096513
C	0.132422667460	3.264725139319	-0.532942242658
Br	-2.225242822295	2.591170668582	-2.110761005564
H	0.213567538383	2.108113936077	-2.389422949673
H	0.116919485655	4.233942614303	-1.048135695299
H	-0.480653655452	3.323962440647	0.376581936166
H	1.171352883782	3.038826985103	-0.241349950322

SCF Done: E(RB3LYP) = -3251.35403298

Zero-point correction= 0.097100
Thermal correction to Energy= 0.108226
Thermal correction to Enthalpy= 0.109170
Thermal correction to Gibbs Free Energy= 0.056985
Sum of electronic and zero-point Energies= -3251.256933
Sum of electronic and thermal Energies= -3251.245807
Sum of electronic and thermal Enthalpies= -3251.244863
Sum of electronic and thermal Free Energies= -3251.297048

1	C	Isotropic = 28.1072	Anisotropy =	109.3124
2	N	Isotropic = 13.5107	Anisotropy =	306.6488
3	C	Isotropic = 9.4662	Anisotropy =	113.8219
4	O	Isotropic = -70.7969	Anisotropy =	242.6593
5	N	Isotropic = -115.0331	Anisotropy =	269.3642
6	C	Isotropic = 139.6023	Anisotropy =	42.9959
7	C	Isotropic = 68.4803	Anisotropy =	16.4968
8	F	Isotropic = 260.7494	Anisotropy =	118.2825
9	F	Isotropic = 279.9734	Anisotropy =	119.1279
10	F	Isotropic = 261.8625	Anisotropy =	117.6226
11	C	Isotropic = 168.6481	Anisotropy =	31.2555
12	Br	Isotropic = 1944.4044	Anisotropy =	1553.0005
13	H	Isotropic = 26.1384	Anisotropy =	8.5340
14	H	Isotropic = 29.5166	Anisotropy =	8.7517
15	H	Isotropic = 29.1022	Anisotropy =	6.9191
16	H	Isotropic = 29.5357	Anisotropy =	10.8679

3d incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.254603045291	-0.811193445966	-0.382611877806
N	-0.749151254219	0.240899765499	0.187154670322
C	-0.646068119894	1.175820776539	-0.827383182439
N	-0.118287480985	0.714256473338	-1.937443200989
O	0.146383240091	-0.626554457612	-1.644649352835
C	-1.064596308118	2.601496447751	-0.692628357571
C	-0.058308560041	-2.179592727447	0.227282866525

F	-0.733903441028	-2.276536632082	1.376200856840
F	-0.484907934248	-3.139089126378	-0.609787186107
F	1.244182605101	-2.401791119025	0.478754631981
C	-0.560438391387	3.267327646147	0.577036312323
Br	-3.075491648301	2.649687541045	-0.745542793256
H	-0.770727021388	3.145734388336	-1.596447890646
H	-0.918320550662	4.303899065310	0.634317190270
H	-0.889598096696	2.718641492290	1.470614363294
H	0.542346007067	3.278473912254	0.558682950093

SCF Done: E(RB3LYP) = -3251.34946405

Zero-point correction= 0.096927
Thermal correction to Energy= 0.108117
Thermal correction to Enthalpy= 0.109061
Thermal correction to Gibbs Free Energy= 0.056155
Sum of electronic and zero-point Energies= -3251.252537
Sum of electronic and thermal Energies= -3251.241347
Sum of electronic and thermal Enthalpies= -3251.240403
Sum of electronic and thermal Free Energies= -3251.293309

1	C	Isotropic =	23.3318	Anisotropy =	101.6003
2	N	Isotropic =	3.9131	Anisotropy =	316.5342
3	C	Isotropic =	18.4662	Anisotropy =	124.4647
4	N	Isotropic =	-113.6651	Anisotropy =	239.6562
5	O	Isotropic =	-61.8762	Anisotropy =	242.0180
6	C	Isotropic =	136.0432	Anisotropy =	49.9864
7	C	Isotropic =	70.6881	Anisotropy =	21.9856
8	F	Isotropic =	273.5247	Anisotropy =	116.9732
9	F	Isotropic =	264.6888	Anisotropy =	119.1273
10	F	Isotropic =	256.6641	Anisotropy =	122.3340
11	C	Isotropic =	167.1145	Anisotropy =	32.2417
12	Br	Isotropic =	2004.8916	Anisotropy =	1453.0445
13	H	Isotropic =	26.1149	Anisotropy =	9.3507
14	H	Isotropic =	29.4723	Anisotropy =	8.7289
15	H	Isotropic =	29.1864	Anisotropy =	6.7028
16	H	Isotropic =	29.7120	Anisotropy =	10.7806

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

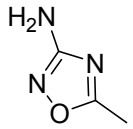
C	-0.031464893078	-0.701864073388	-0.066400876833
N	-1.207450730396	-0.291720589691	0.284947619655
C	-1.705621517513	0.178486635161	-0.918399806886
N	-0.878871834778	0.051977554502	-1.930410916461
O	0.252394110159	-0.537855340961	-1.363349457737
C	-3.071805189257	0.763589816598	-1.060896764461
C	1.014905967567	-1.351617663050	0.808488056104
F	0.685709952985	-1.224052945847	2.097293790737
F	1.125428829733	-2.661522739708	0.524228332797
F	2.216154121578	-0.784860636909	0.609467292072
C	-3.575189372492	0.879699870994	-2.487635653230
Br	-3.032289473399	2.578938925948	-0.185143080157

H	-3.762067605980	0.205013017798	-0.418015630719
H	-4.575431537144	1.331897524959	-2.501078854455
H	-2.897689995484	1.484332133511	-3.106235437941
H	-3.640780832501	-0.129311489918	-2.926888612486

SCF Done: E(RB3LYP) = -3251.34881633

Zero-point correction= 0.096939
Thermal correction to Energy= 0.108108
Thermal correction to Enthalpy= 0.109052
Thermal correction to Gibbs Free Energy= 0.056504
Sum of electronic and zero-point Energies= -3251.251877
Sum of electronic and thermal Energies= -3251.240708
Sum of electronic and thermal Enthalpies= -3251.239764
Sum of electronic and thermal Free Energies= -3251.292313

1	C	Isotropic = 23.8079	Anisotropy =	102.5240
2	N	Isotropic = -0.9873	Anisotropy =	304.1111
3	C	Isotropic = 18.1211	Anisotropy =	125.1536
4	N	Isotropic = -115.2580	Anisotropy =	249.7386
5	O	Isotropic = -62.1446	Anisotropy =	248.0882
6	C	Isotropic = 134.7901	Anisotropy =	45.2852
7	C	Isotropic = 70.6666	Anisotropy =	21.7516
8	F	Isotropic = 273.7515	Anisotropy =	117.0684
9	F	Isotropic = 257.0636	Anisotropy =	122.0493
10	F	Isotropic = 264.0964	Anisotropy =	118.8936
11	C	Isotropic = 169.3654	Anisotropy =	31.8331
12	Br	Isotropic = 1993.4784	Anisotropy =	1486.7265
13	H	Isotropic = 26.1544	Anisotropy =	8.0226
14	H	Isotropic = 29.5068	Anisotropy =	8.4759
15	H	Isotropic = 29.1269	Anisotropy =	7.4170
16	H	Isotropic = 29.4348	Anisotropy =	10.9130



3e

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.129311004691	0.438631362393	0.195916920966
N	0.904577683602	-0.082568336072	-0.437506802927
O	1.804563927491	1.015095745504	-0.504610664203
C	1.195676808038	2.055049413127	0.082054317726
N	0.005960107743	1.773029736258	0.536583448571
N	-1.238479898444	-0.279404662548	0.560441660733

C	1.921153803542	3.350820223573	0.143549931748
H	-2.082064569602	0.281696761438	0.640157554921
H	-1.385025983752	-1.135643690790	0.032610959894
H	2.869944794145	3.233026499887	0.689252402904
H	2.161674549208	3.704577727729	-0.870824188817
H	1.298809782720	4.096699219500	0.651684458483

SCF Done: E(RB3LYP) = -356.809628676

Zero-point correction= 0.090419
Thermal correction to Energy= 0.096948
Thermal correction to Enthalpy= 0.097892
Thermal correction to Gibbs Free Energy= 0.059642
Sum of electronic and zero-point Energies= -356.719209
Sum of electronic and thermal Energies= -356.712681
Sum of electronic and thermal Enthalpies= -356.711736
Sum of electronic and thermal Free Energies= -356.749987

1	C	Isotropic = 25.1335	Anisotropy =	110.4447
2	N	Isotropic = -61.6457	Anisotropy =	153.3652
3	O	Isotropic = -33.1672	Anisotropy =	160.7373
4	C	Isotropic = 15.8084	Anisotropy =	113.1780
5	N	Isotropic = 25.3943	Anisotropy =	226.0490
6	N	Isotropic = 214.2173	Anisotropy =	60.4906
7	C	Isotropic = 179.8886	Anisotropy =	26.6762
8	H	Isotropic = 28.0289	Anisotropy =	11.9460
9	H	Isotropic = 27.9713	Anisotropy =	12.1827
10	H	Isotropic = 29.0511	Anisotropy =	8.2879
11	H	Isotropic = 29.0486	Anisotropy =	8.2259
12	H	Isotropic = 29.0638	Anisotropy =	7.7780

3e incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

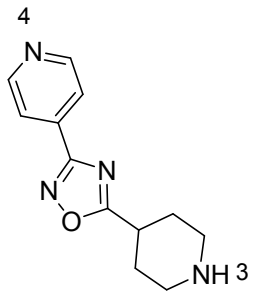
C	-0.102692492123	0.492410138386	-0.144391497962
N	-0.644169424818	1.650757775814	0.150758962395
O	0.492497984665	2.473062846915	0.423428040623
C	1.566172385135	1.684269038934	0.252522252969
N	1.273155803612	0.451178931191	-0.099549173722
C	-0.937698363577	-0.690393086694	-0.503859477820
N	2.785336709486	2.208395750192	0.507419030930
H	-0.672774928958	-1.049984673209	-1.510345850367
H	-0.750635819846	-1.515310590763	0.201209243145
H	-2.004367316008	-0.432013223143	-0.481964788758
H	3.575386585233	1.695929753030	0.130052887372
H	2.869808877198	3.219497339348	0.483860371195

SCF Done: E(RB3LYP) = -356.813287808

Zero-point correction= 0.090428
Thermal correction to Energy= 0.096833

Thermal correction to Enthalpy= 0.097777
Thermal correction to Gibbs Free Energy= 0.060430
Sum of electronic and zero-point Energies= -356.722860
Sum of electronic and thermal Energies= -356.716455
Sum of electronic and thermal Enthalpies= -356.715511
Sum of electronic and thermal Free Energies= -356.752857

1	C	Isotropic =	23.3915	Anisotropy =	124.5856
2	N	Isotropic =	-85.9925	Anisotropy =	141.5157
3	O	Isotropic =	-4.6797	Anisotropy =	114.9236
4	C	Isotropic =	23.4286	Anisotropy =	94.1667
5	N	Isotropic =	58.4232	Anisotropy =	199.9779
6	C	Isotropic =	179.6645	Anisotropy =	23.1735
7	N	Isotropic =	203.5092	Anisotropy =	73.3738
8	H	Isotropic =	29.3047	Anisotropy =	8.1320
9	H	Isotropic =	29.3059	Anisotropy =	8.1768
10	H	Isotropic =	29.3683	Anisotropy =	7.6761
11	H	Isotropic =	27.0914	Anisotropy =	12.2597
12	H	Isotropic =	27.1103	Anisotropy =	11.5763



3f

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.081343810168	1.577983145134	0.635914773011
N	0.232577532075	2.196699787883	1.753486920333
O	0.054082282892	3.544614712979	1.437634121858
C	-0.352605862370	3.601681700329	0.151859701405
N	-0.454415598698	2.420587216778	-0.393254738246
C	-0.035540959986	0.113058360751	0.500212475134
C	-0.614977172908	4.940413463496	-0.455295003769
C	0.363073519173	-0.711722067438	1.563135799930
C	0.383619485303	-2.091846075593	1.365072949743
N	0.043222709857	-2.691121710701	0.211283921665
C	-0.335711461421	-1.890691647317	-0.796804208925
C	-0.392842912411	-0.498001294700	-0.708877091901
C	-1.752502980294	5.692262440700	0.274436866708
C	-1.961531462381	7.080098841355	-0.352975917056
N	-0.749304997808	7.901768080428	-0.423532425815
C	0.348832600280	7.192996437380	-1.087879788798
C	0.662936360934	5.810957162152	-0.492612697884
H	-0.933267649233	4.733942167401	-1.490187942079
H	0.651813183228	-0.284664700325	2.523782378006

H	0.691613763844	-2.753422727748	2.180856543924
H	-0.610937370575	-2.387796403562	-1.732439918239
H	-0.708206480994	0.104709209534	-1.560330081276
H	-1.489576759008	5.804148182709	1.340910419603
H	-2.685829927555	5.106705973896	0.227370911589
H	-2.730424649474	7.632613621980	0.209960789665
H	-2.346642797171	6.957029096438	-1.382373302101
H	-0.457195562717	8.134156472279	0.529545817848
H	1.248925366581	7.827194043877	-1.056087672941
H	0.079187195866	7.074975370005	-2.153947174111
H	1.447227376216	5.308846691907	-1.083429718026
H	1.051717038923	5.930464447994	0.533843290744

SCF Done: E(RB3LYP) = -759.954573870

Zero-point correction= 0.254426
Thermal correction to Energy= 0.268109
Thermal correction to Enthalpy= 0.269053
Thermal correction to Gibbs Free Energy= 0.211708
Sum of electronic and zero-point Energies= -759.700148
Sum of electronic and thermal Energies= -759.686465
Sum of electronic and thermal Enthalpies= -759.685521
Sum of electronic and thermal Free Energies= -759.742866

1	C	Isotropic =	24.8174	Anisotropy =	114.2517
2	N	Isotropic =	-106.1866	Anisotropy =	246.3245
3	O	Isotropic =	-61.2402	Anisotropy =	236.9842
4	C	Isotropic =	8.3717	Anisotropy =	119.5202
5	N	Isotropic =	19.6810	Anisotropy =	265.6682
6	C	Isotropic =	57.3856	Anisotropy =	179.0768
7	C	Isotropic =	151.3969	Anisotropy =	24.1167
8	C	Isotropic =	72.2224	Anisotropy =	161.3900
9	C	Isotropic =	42.6628	Anisotropy =	166.8769
10	N	Isotropic =	-73.8947	Anisotropy =	554.0273
11	C	Isotropic =	41.9741	Anisotropy =	167.3299
12	C	Isotropic =	70.6944	Anisotropy =	164.5517
13	C	Isotropic =	157.9892	Anisotropy =	15.8055
14	C	Isotropic =	144.3503	Anisotropy =	28.8385
15	N	Isotropic =	217.9910	Anisotropy =	62.0647
16	C	Isotropic =	144.3236	Anisotropy =	29.0104
17	C	Isotropic =	157.7789	Anisotropy =	16.0354
18	H	Isotropic =	28.2356	Anisotropy =	7.0575
19	H	Isotropic =	23.4450	Anisotropy =	7.9059
20	H	Isotropic =	22.6428	Anisotropy =	6.6840
21	H	Isotropic =	22.5858	Anisotropy =	6.9236
22	H	Isotropic =	23.4801	Anisotropy =	8.5010
23	H	Isotropic =	29.7873	Anisotropy =	6.3756
24	H	Isotropic =	29.7651	Anisotropy =	6.6599
25	H	Isotropic =	28.3671	Anisotropy =	8.6104
26	H	Isotropic =	28.7274	Anisotropy =	8.0069
27	H	Isotropic =	31.1871	Anisotropy =	12.3342
28	H	Isotropic =	28.3844	Anisotropy =	8.6109
29	H	Isotropic =	28.7262	Anisotropy =	7.9783
30	H	Isotropic =	29.7772	Anisotropy =	6.5861
31	H	Isotropic =	29.8048	Anisotropy =	6.3344

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.458846379548	1.494968508223	-0.255380855782
N	-0.964602546619	1.568593039239	-1.468398040625
O	-1.047974928667	2.942691900813	-1.699589057718
C	-0.581866303311	3.560946798332	-0.596213410023
N	-0.203666514785	2.719333677033	0.327041041022
C	-0.193902537026	0.212009159922	0.416074395501
C	-0.563865514297	5.054323915712	-0.568236159733
C	-0.477485238197	-1.014367889267	-0.203947553474
C	-0.202752360391	-2.192123419754	0.490273253141
N	0.321787066613	-2.231174654388	1.726978021465
C	0.588295006708	-1.051354852282	2.308028122391
C	0.353204041896	0.186521120843	1.705555105219
C	-1.484078309026	5.601519515232	0.547422878391
C	-1.398484948892	7.134608533320	0.607995189995
N	-0.036098330472	7.659027512102	0.749664006024
C	0.858107159995	7.129821577558	-0.285374864474
C	0.872814927234	5.596086109342	-0.388450216499
H	-0.951164230343	5.392807058288	-1.543703227577
H	-0.903885792670	-1.048019693916	-1.206756852418
H	-0.416833933426	-3.159589380057	0.025266103274
H	1.015066321567	-1.093097533860	3.315213686998
H	0.588893862070	1.115471080627	2.224331009351
H	-1.169193032701	5.171441373348	1.514105941789
H	-2.525191850819	5.282991627425	0.371559110984
H	-2.009848965275	7.510150645147	1.443839475205
H	-1.829164780500	7.558769389122	-0.318109758642
H	0.325522598954	7.378309250850	1.665218756681
H	1.877637678000	7.500638800854	-0.094232458231
H	0.540795644679	7.555479894246	-1.255535843049
H	1.507954731662	5.275729571410	-1.231224660134
H	1.306187457588	5.164427364536	0.530476860943

SCF Done: E(RB3LYP) = -759.954792414

Zero-point correction= 0.254687
Thermal correction to Energy= 0.268302
Thermal correction to Enthalpy= 0.269246
Thermal correction to Gibbs Free Energy= 0.212133
Sum of electronic and zero-point Energies= -759.700106
Sum of electronic and thermal Energies= -759.686491
Sum of electronic and thermal Enthalpies= -759.685547
Sum of electronic and thermal Free Energies= -759.742660

1	C	Isotropic = 23.9298	Anisotropy =	112.7624
2	N	Isotropic = -101.4706	Anisotropy =	239.8850
3	O	Isotropic = -66.8014	Anisotropy =	204.0383
4	C	Isotropic = 6.9259	Anisotropy =	118.4116
5	N	Isotropic = 21.9408	Anisotropy =	292.7106
6	C	Isotropic = 57.3551	Anisotropy =	178.8332
7	C	Isotropic = 152.8649	Anisotropy =	21.3086

8	C	Isotropic =	72.3070	Anisotropy =	161.3504
9	C	Isotropic =	42.6528	Anisotropy =	166.7823
10	N	Isotropic =	-74.0067	Anisotropy =	553.5608
11	C	Isotropic =	41.9711	Anisotropy =	167.2987
12	C	Isotropic =	70.8363	Anisotropy =	164.5263
13	C	Isotropic =	156.9867	Anisotropy =	18.1029
14	C	Isotropic =	144.4480	Anisotropy =	29.0061
15	N	Isotropic =	217.7437	Anisotropy =	61.9337
16	C	Isotropic =	144.4451	Anisotropy =	29.0623
17	C	Isotropic =	156.9726	Anisotropy =	18.0979
18	H	Isotropic =	28.2874	Anisotropy =	7.0717
19	H	Isotropic =	23.4484	Anisotropy =	7.9099
20	H	Isotropic =	22.6464	Anisotropy =	6.6172
21	H	Isotropic =	22.5926	Anisotropy =	7.0263
22	H	Isotropic =	23.4937	Anisotropy =	8.3796
23	H	Isotropic =	29.8232	Anisotropy =	6.1910
24	H	Isotropic =	29.7546	Anisotropy =	6.6324
25	H	Isotropic =	28.3972	Anisotropy =	8.6057
26	H	Isotropic =	28.7167	Anisotropy =	8.1067
27	H	Isotropic =	31.1980	Anisotropy =	12.2031
28	H	Isotropic =	28.3857	Anisotropy =	8.5805
29	H	Isotropic =	28.7138	Anisotropy =	8.0960
30	H	Isotropic =	29.7383	Anisotropy =	6.6167
31	H	Isotropic =	29.7868	Anisotropy =	6.2693

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.809498170226	1.825957735142	0.299377943760
N	-1.124649458075	2.360949323809	-0.859809084793
O	-0.363413310952	3.532544414153	-0.891133677629
C	0.338907985098	3.585069522239	0.261714229934
N	0.102053211474	2.558067002118	1.032912060821
C	-1.382586215918	0.553493099625	0.767833021488
C	1.263847739552	4.731396263293	0.537185679306
C	-2.309185848198	-0.164330667842	-0.003469925965
C	-2.810440662801	-1.363569391599	0.501705936522
N	-2.461255392105	-1.882986228599	1.691030368728
C	-1.574555000815	-1.186224144886	2.418220793843
C	-1.009403825911	0.023968985216	2.010042381712
C	2.433460450074	4.822206631947	-0.478207976289
C	2.025108641521	5.481820694549	-1.798129572676
N	1.446792027478	6.801816578370	-1.526642569246
C	0.211624439991	6.692901666129	-0.743423741747
C	0.528897512797	6.094273983601	0.629564512080
H	1.679542584670	4.492193443460	1.526630133627
H	-2.631560275632	0.205386006862	-0.977150041306
H	-3.534236836333	-1.939457403401	-0.083533926730
H	-1.296185158570	-1.617207980677	3.385223588625
H	-0.292299136481	0.548676119957	2.640984864829
H	2.862060137838	3.823808954989	-0.660593235850
H	3.219201867599	5.436693584207	-0.008863560237
H	1.329130265746	4.814236128932	-2.350581371506

H	2.917881277521	5.611283945634	-2.430524290745
H	1.238647296026	7.262369684021	-2.413243357915
H	-0.563630874473	6.077734393812	-1.249107247712
H	-0.212047084253	7.701182570182	-0.610843769178
H	1.199722307438	6.785495892667	1.165764032267
H	-0.389330494078	5.995029192088	1.230207801981

SCF Done: E(RB3LYP) = -759.951627474

Zero-point correction= 0.254701
Thermal correction to Energy= 0.268235
Thermal correction to Enthalpy= 0.269179
Thermal correction to Gibbs Free Energy= 0.212403
Sum of electronic and zero-point Energies= -759.696927
Sum of electronic and thermal Energies= -759.683392
Sum of electronic and thermal Enthalpies= -759.682448
Sum of electronic and thermal Free Energies= -759.739224

1	C	Isotropic =	25.1921	Anisotropy =	116.4531
2	N	Isotropic =	-107.9744	Anisotropy =	241.4865
3	O	Isotropic =	-65.6374	Anisotropy =	229.5274
4	C	Isotropic =	6.5593	Anisotropy =	119.1841
5	N	Isotropic =	18.3879	Anisotropy =	259.7717
6	C	Isotropic =	57.4417	Anisotropy =	179.1071
7	C	Isotropic =	155.9095	Anisotropy =	20.8966
8	C	Isotropic =	72.1363	Anisotropy =	161.6501
9	C	Isotropic =	42.5543	Anisotropy =	166.7436
10	N	Isotropic =	-74.1826	Anisotropy =	553.7910
11	C	Isotropic =	42.0241	Anisotropy =	167.0849
12	C	Isotropic =	70.6998	Anisotropy =	164.7343
13	C	Isotropic =	159.7726	Anisotropy =	4.8847
14	C	Isotropic =	147.0065	Anisotropy =	32.4023
15	N	Isotropic =	213.4480	Anisotropy =	37.4744
16	C	Isotropic =	147.0213	Anisotropy =	32.1481
17	C	Isotropic =	159.9215	Anisotropy =	4.8985
18	H	Isotropic =	27.9533	Anisotropy =	8.4804
19	H	Isotropic =	23.4133	Anisotropy =	7.9806
20	H	Isotropic =	22.6322	Anisotropy =	6.7166
21	H	Isotropic =	22.5923	Anisotropy =	6.9072
22	H	Isotropic =	23.4889	Anisotropy =	8.5944
23	H	Isotropic =	29.8028	Anisotropy =	7.3788
24	H	Isotropic =	29.4720	Anisotropy =	9.0740
25	H	Isotropic =	28.1468	Anisotropy =	6.8303
26	H	Isotropic =	28.6083	Anisotropy =	8.8072
27	H	Isotropic =	30.3824	Anisotropy =	15.0548
28	H	Isotropic =	28.1290	Anisotropy =	6.8215
29	H	Isotropic =	28.5960	Anisotropy =	8.8260
30	H	Isotropic =	29.4725	Anisotropy =	9.1037
31	H	Isotropic =	29.7845	Anisotropy =	7.3847

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.714865417908	1.710739469704	0.042873020820
N	-0.334313804991	1.458375524480	-1.190599610176
O	-0.142975968487	2.729299365344	-1.735140897463
C	-0.431040026793	3.626407886288	-0.768999433843
N	-0.786699722877	3.054709020088	0.349101003197
C	-1.033934414540	0.645804766270	1.007817016759
C	-0.367435932947	5.089091668683	-1.108869947697
C	-0.940312919351	-0.710855193892	0.661817150212
C	-1.258553711037	-1.668179844190	1.624476498798
N	-1.653446149982	-1.374640987466	2.875092859737
C	-1.738746870069	-0.073676917804	3.192452391999
C	-1.444076374115	0.966638719192	2.308407081859
C	-0.259521197114	5.964083611102	0.157580739333
C	1.152738447169	5.929584237136	0.749427870006
N	2.126655601425	6.338298405164	-0.267713578919
C	2.140186384670	5.403548088230	-1.395823664328
C	0.777310269127	5.421360515734	-2.093621169951
H	-1.328345938315	5.307136479348	-1.609563403136
H	-0.625777520672	-1.012138191261	-0.337627584439
H	-1.192211427632	-2.732008755184	1.375656399168
H	-2.061248186637	0.155611443413	4.213106451325
H	-1.530450107997	2.007440338395	2.619585900423
H	-0.997376288309	5.643452239545	0.907475788231
H	-0.500206121326	6.999887442263	-0.130750920864
H	1.357068240655	4.910336367055	1.147356672799
H	1.214991121375	6.626522248156	1.600093006020
H	3.055906761310	6.366366524534	0.153312864087
H	2.379564943084	4.360722211721	-1.082924877089
H	2.924210452137	5.712780355584	-2.104804045083
H	0.593016766287	6.433173171560	-2.488631366692
H	0.770819113861	4.727079790807	-2.947032215093

SCF Done: E(RB3LYP) = -759.952755808

Zero-point correction= 0.254534
Thermal correction to Energy= 0.268025
Thermal correction to Enthalpy= 0.268969
Thermal correction to Gibbs Free Energy= 0.212241
Sum of electronic and zero-point Energies= -759.698222
Sum of electronic and thermal Energies= -759.684731
Sum of electronic and thermal Enthalpies= -759.683787
Sum of electronic and thermal Free Energies= -759.740515

1	C	Isotropic = 24.3739	Anisotropy =	113.1616
2	N	Isotropic = -105.5000	Anisotropy =	245.0568
3	O	Isotropic = -65.9280	Anisotropy =	233.8145
4	C	Isotropic = 8.4328	Anisotropy =	113.2552
5	N	Isotropic = 17.8150	Anisotropy =	287.8142
6	C	Isotropic = 57.3112	Anisotropy =	178.7990
7	C	Isotropic = 155.0634	Anisotropy =	15.9907
8	C	Isotropic = 72.1479	Anisotropy =	161.4472
9	C	Isotropic = 42.5871	Anisotropy =	166.8776
10	N	Isotropic = -73.9768	Anisotropy =	554.1368
11	C	Isotropic = 41.9402	Anisotropy =	167.1102
12	C	Isotropic = 70.6545	Anisotropy =	164.5784
13	C	Isotropic = 160.8772	Anisotropy =	7.4045

14	C	Isotropic =	145.8170	Anisotropy =	36.0996
15	N	Isotropic =	211.6577	Anisotropy =	36.1274
16	C	Isotropic =	145.3330	Anisotropy =	34.2156
17	C	Isotropic =	160.5207	Anisotropy =	5.9607
18	H	Isotropic =	28.2224	Anisotropy =	7.8287
19	H	Isotropic =	23.4064	Anisotropy =	7.9481
20	H	Isotropic =	22.6187	Anisotropy =	6.6599
21	H	Isotropic =	22.5789	Anisotropy =	7.0487
22	H	Isotropic =	23.4737	Anisotropy =	8.4761
23	H	Isotropic =	28.8981	Anisotropy =	8.2721
24	H	Isotropic =	29.5184	Anisotropy =	8.5883
25	H	Isotropic =	28.6601	Anisotropy =	6.6042
26	H	Isotropic =	28.6127	Anisotropy =	8.7469
27	H	Isotropic =	30.6191	Anisotropy =	15.0362
28	H	Isotropic =	28.9596	Anisotropy =	5.8606
29	H	Isotropic =	28.6411	Anisotropy =	8.9625
30	H	Isotropic =	29.4520	Anisotropy =	8.5498
31	H	Isotropic =	28.9709	Anisotropy =	8.4528

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	0.017847653344	1.897627150865	-0.511598018978
N	-1.031519856660	1.803214440011	-1.298741850874
O	-1.617995193300	3.066619139542	-1.207084256888
C	-0.856686637485	3.801475861157	-0.369023779705
N	0.163677723181	3.130828609699	0.091424174971
C	0.950251268688	0.779496229848	-0.294046474870
C	-1.234765987240	5.237464203905	-0.139360003542
C	2.049073108450	0.929056971974	0.562090610745
C	2.908627801371	-0.156740727437	0.743008106305
N	2.750452449266	-1.346808696327	0.143738553649
C	1.692810658322	-1.476351000551	-0.675320816263
C	0.772250313470	-0.459785742171	-0.927746358977
C	-2.763863985089	5.432937654186	-0.011257662420
C	-3.277049661392	4.961098959822	1.351826251127
N	-2.563952982688	5.670202689571	2.417748439662
C	-1.132130511741	5.352835475098	2.401581288047
C	-0.510578688356	5.831793174458	1.086009343315
H	-0.894977115168	5.770247032139	-1.045961110671
H	2.225743992596	1.874306642544	1.074775235746
H	3.772556000752	-0.060651715133	1.408350979419
H	1.572746691944	-2.450718956167	-1.159301901833
H	-0.067229547978	-0.626492276746	-1.603072856037
H	-3.291171002381	4.912058912103	-0.824375648987
H	-2.972380504961	6.509501319770	-0.117504206698
H	-3.162499678434	3.854575216360	1.424710992689
H	-4.353399270660	5.177745306514	1.438466944850
H	-2.955212857790	5.396635745832	3.319786073739
H	-0.937364049475	4.264073433347	2.523324831761
H	-0.646533459049	5.864460301432	3.247599197043
H	-0.602510154014	6.928259303553	1.027374242916
H	0.560283482477	5.582595340801	1.055549680756

SCF Done: E(RB3LYP) = -759.952748330

Zero-point correction= 0.254557
Thermal correction to Energy= 0.268054
Thermal correction to Enthalpy= 0.268998
Thermal correction to Gibbs Free Energy= 0.212230
Sum of electronic and zero-point Energies= -759.698191
Sum of electronic and thermal Energies= -759.684695
Sum of electronic and thermal Enthalpies= -759.683750
Sum of electronic and thermal Free Energies= -759.740518

1	C	Isotropic =	24.4642	Anisotropy =	112.9070
2	N	Isotropic =	-105.6067	Anisotropy =	245.2198
3	O	Isotropic =	-65.6221	Anisotropy =	233.2588
4	C	Isotropic =	8.3817	Anisotropy =	113.1983
5	N	Isotropic =	17.3227	Anisotropy =	287.5352
6	C	Isotropic =	57.3354	Anisotropy =	178.8156
7	C	Isotropic =	155.3591	Anisotropy =	16.2138
8	C	Isotropic =	70.5485	Anisotropy =	164.5592
9	C	Isotropic =	41.9849	Anisotropy =	167.1395
10	N	Isotropic =	-73.8689	Anisotropy =	554.2789
11	C	Isotropic =	42.6499	Anisotropy =	166.9213
12	C	Isotropic =	72.2061	Anisotropy =	161.4014
13	C	Isotropic =	159.7812	Anisotropy =	6.8411
14	C	Isotropic =	145.3147	Anisotropy =	34.0166
15	N	Isotropic =	212.4185	Anisotropy =	36.3806
16	C	Isotropic =	146.2488	Anisotropy =	36.3834
17	C	Isotropic =	161.3923	Anisotropy =	7.1585
18	H	Isotropic =	28.2307	Anisotropy =	7.8400
19	H	Isotropic =	23.4682	Anisotropy =	8.4640
20	H	Isotropic =	22.5766	Anisotropy =	7.0633
21	H	Isotropic =	22.6203	Anisotropy =	6.6515
22	H	Isotropic =	23.4141	Anisotropy =	7.9309
23	H	Isotropic =	29.0139	Anisotropy =	8.4687
24	H	Isotropic =	29.4316	Anisotropy =	8.5764
25	H	Isotropic =	29.0115	Anisotropy =	5.7257
26	H	Isotropic =	28.6391	Anisotropy =	8.9827
27	H	Isotropic =	30.6064	Anisotropy =	15.1073
28	H	Isotropic =	28.5768	Anisotropy =	6.8493
29	H	Isotropic =	28.6061	Anisotropy =	8.7405
30	H	Isotropic =	29.5401	Anisotropy =	8.6768
31	H	Isotropic =	28.9301	Anisotropy =	8.0953

3f incorrect isomer

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.511048282489	2.036545328344	1.181912533076
O	0.638838794330	1.934257602059	1.870733059427
N	1.607257216844	2.643021915590	1.140893254128
C	0.943770124526	3.091817604770	0.099126966664

N	-0.389724033460	2.734730614629	0.084094767548
C	-1.713288513163	1.388636755657	1.711127532732
C	1.590783386462	3.914212338238	-0.973552920230
C	-1.686729546030	0.648649697696	2.901779183821
C	-2.873685757557	0.060925607185	3.342671495062
N	-4.045412363547	0.160573571650	2.695674616810
C	-4.054665821926	0.872512807921	1.556811373246
C	-2.929898098941	1.501308989025	1.022770606498
C	1.568989901765	3.180184939636	-2.332966492672
C	2.165543771095	4.067235293343	-3.437462242132
N	1.546348611700	5.392278644747	-3.549327002306
C	1.544093416542	6.095934540471	-2.261800635407
C	0.920099951557	5.298609864608	-1.105294673203
H	2.641452528207	4.057775654009	-0.668817130559
H	-0.765303793133	0.531419397574	3.472023549526
H	-2.879459029205	-0.522273319381	4.268590572125
H	-5.016105211604	0.945984608090	1.039394652133
H	-2.990088285059	2.068132406408	0.093825984746
H	0.525515616931	2.923482146998	-2.587935788179
H	2.128545705217	2.232116853161	-2.260914941566
H	2.087487701827	3.558572849911	-4.411717545923
H	3.243828119396	4.215540266226	-3.240754141020
H	0.576040889366	5.270609120418	-3.852422615332
H	1.016565076531	7.055294575105	-2.385402475881
H	2.593278950338	6.339346090106	-2.010070718576
H	1.017055537542	5.858681608971	-0.159717717119
H	-0.159346564060	5.159541626836	-1.291743107439

SCF Done: E(RB3LYP) = -759.954291622

Zero-point correction= 0.254371
Thermal correction to Energy= 0.267996
Thermal correction to Enthalpy= 0.268941
Thermal correction to Gibbs Free Energy= 0.212252
Sum of electronic and zero-point Energies= -759.699921
Sum of electronic and thermal Energies= -759.686295
Sum of electronic and thermal Enthalpies= -759.685351
Sum of electronic and thermal Free Energies= -759.742039

1	C	Isotropic =	17.4048	Anisotropy =	103.1058
2	O	Isotropic =	-49.8058	Anisotropy =	215.8785
3	N	Isotropic =	-100.4789	Anisotropy =	211.1969
4	C	Isotropic =	15.8859	Anisotropy =	128.0903
5	N	Isotropic =	15.3528	Anisotropy =	298.5332
6	C	Isotropic =	61.0504	Anisotropy =	172.0100
7	C	Isotropic =	153.7697	Anisotropy =	18.3037
8	C	Isotropic =	71.3017	Anisotropy =	164.6444
9	C	Isotropic =	41.9280	Anisotropy =	168.9752
10	N	Isotropic =	-79.3209	Anisotropy =	562.9179
11	C	Isotropic =	41.9422	Anisotropy =	168.3156
12	C	Isotropic =	70.9709	Anisotropy =	163.0314
13	C	Isotropic =	157.2782	Anisotropy =	13.6667
14	C	Isotropic =	144.1142	Anisotropy =	29.7244
15	N	Isotropic =	216.8134	Anisotropy =	61.3243
16	C	Isotropic =	144.0335	Anisotropy =	29.8773
17	C	Isotropic =	157.6850	Anisotropy =	13.7890

18	H	Isotropic =	28.4434	Anisotropy =	7.1582
19	H	Isotropic =	23.4973	Anisotropy =	8.4774
20	H	Isotropic =	22.5230	Anisotropy =	6.8002
21	H	Isotropic =	22.5294	Anisotropy =	7.0792
22	H	Isotropic =	23.4002	Anisotropy =	8.2228
23	H	Isotropic =	29.7806	Anisotropy =	6.1033
24	H	Isotropic =	29.8789	Anisotropy =	6.8844
25	H	Isotropic =	28.3956	Anisotropy =	8.5702
26	H	Isotropic =	28.7151	Anisotropy =	8.1014
27	H	Isotropic =	31.2508	Anisotropy =	12.1464
28	H	Isotropic =	28.3919	Anisotropy =	8.5474
29	H	Isotropic =	28.7246	Anisotropy =	8.0705
30	H	Isotropic =	29.8666	Anisotropy =	6.8411
31	H	Isotropic =	29.7221	Anisotropy =	6.3581

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.163486348295	2.179349897625	0.557445965357
O	-2.297812844575	2.840688746293	0.840892711475
N	-2.059130169386	4.190498294505	0.545417210356
C	-0.814518028536	4.204839889551	0.117202218793
N	-0.215156682890	2.960003551358	0.109397174257
C	-1.117372158949	0.730834701242	0.770119266194
C	-0.171990244955	5.497052644219	-0.306306882709
C	0.051370956800	0.013796504465	0.475992260719
C	0.055664133046	-1.364455522257	0.691127606912
N	-0.995741241980	-2.052516616335	1.165455343089
C	-2.106998574656	-1.352723050407	1.442706898777
C	-2.224112790716	0.027056361089	1.266464134318
C	1.039569241811	5.887408728212	0.578143781294
C	2.321053753723	5.139614937519	0.199611646022
N	2.608715234462	5.354230875701	-1.223844203682
C	1.554740017131	4.782515123868	-2.070859191312
C	0.233987107514	5.509498735542	-1.802269470755
H	-0.958402146678	6.253508868732	-0.160423657836
H	0.932851732499	0.524184749553	0.088491533804
H	0.955259506493	-1.946674578749	0.469128941993
H	-2.956292849180	-1.924743555064	1.828657590286
H	-3.154582904105	0.539718016969	1.510078700228
H	0.802516763715	5.730828023372	1.642929732257
H	1.213422995129	6.967409279304	0.436274908799
H	2.214007797388	4.064917367397	0.456732742370
H	3.162458068534	5.535652300813	0.791034977044
H	3.496160829729	4.904909137050	-1.452862097805
H	1.420239233431	3.692721217270	-1.907575177904
H	1.839006867535	4.922249933429	-3.126473547369
H	0.351677646652	6.565111005494	-2.099891987345
H	-0.572294900691	5.083314432238	-2.420999127626

SCF Done: E(RB3LYP) = -759.950062133

Zero-point correction= 0.254573

Thermal correction to Energy= 0.268146
Thermal correction to Enthalpy= 0.269090
Thermal correction to Gibbs Free Energy= 0.212131
Sum of electronic and zero-point Energies= -759.695489
Sum of electronic and thermal Energies= -759.681916
Sum of electronic and thermal Enthalpies= -759.680972
Sum of electronic and thermal Free Energies= -759.737931

1	C	Isotropic =	18.2282	Anisotropy =	100.6979
2	O	Isotropic =	-48.4697	Anisotropy =	232.1195
3	N	Isotropic =	-101.7381	Anisotropy =	211.3084
4	C	Isotropic =	14.8955	Anisotropy =	132.0705
5	N	Isotropic =	11.9631	Anisotropy =	289.6311
6	C	Isotropic =	60.9489	Anisotropy =	171.8756
7	C	Isotropic =	159.1348	Anisotropy =	12.1503
8	C	Isotropic =	71.0264	Anisotropy =	162.6881
9	C	Isotropic =	41.8080	Anisotropy =	168.5025
10	N	Isotropic =	-79.0459	Anisotropy =	563.6931
11	C	Isotropic =	41.9712	Anisotropy =	169.0126
12	C	Isotropic =	71.2068	Anisotropy =	164.4074
13	C	Isotropic =	158.7138	Anisotropy =	5.8461
14	C	Isotropic =	147.1465	Anisotropy =	32.1818
15	N	Isotropic =	212.2795	Anisotropy =	36.2243
16	C	Isotropic =	147.3214	Anisotropy =	32.4644
17	C	Isotropic =	158.9879	Anisotropy =	5.7218
18	H	Isotropic =	28.1995	Anisotropy =	8.6243
19	H	Isotropic =	23.3188	Anisotropy =	8.1214
20	H	Isotropic =	22.4840	Anisotropy =	7.2392
21	H	Isotropic =	22.5027	Anisotropy =	6.7955
22	H	Isotropic =	23.4668	Anisotropy =	8.5099
23	H	Isotropic =	29.8041	Anisotropy =	7.2603
24	H	Isotropic =	29.4029	Anisotropy =	8.9698
25	H	Isotropic =	27.8216	Anisotropy =	6.9781
26	H	Isotropic =	28.7108	Anisotropy =	8.6431
27	H	Isotropic =	30.3835	Anisotropy =	14.6738
28	H	Isotropic =	27.8282	Anisotropy =	7.0172
29	H	Isotropic =	28.7136	Anisotropy =	8.6403
30	H	Isotropic =	29.4103	Anisotropy =	8.9841
31	H	Isotropic =	29.8118	Anisotropy =	7.2534

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.603368646001	1.795239478819	0.601870797394
O	0.710098751039	1.576866541754	0.787943802156
N	1.382906979210	2.338985162320	-0.178878565017
C	0.415003965894	2.931597324887	-0.841765167369
N	-0.849991269639	2.617584670823	-0.382056093323
C	-1.563821420650	1.118915145663	1.476681329367
C	0.636579812617	3.835973277752	-2.026909219614
C	-2.939426410156	1.323794968023	1.297152292982
C	-3.824882705101	0.663359746250	2.148876153002
N	-3.440048246562	-0.161560832054	3.136504262426

C	-2.120423572608	-0.347706270848	3.296025264603
C	-1.145500350780	0.260384875250	2.503282908327
C	-0.116251673339	5.178736718431	-1.862450772985
C	0.617048380558	6.126168947840	-0.910162963390
N	1.981601836185	6.351376886802	-1.396412843693
C	2.759125598558	5.106934592869	-1.385702547121
C	2.124269668135	4.092178514670	-2.343477378005
H	0.180225053640	3.299356157980	-2.877488789031
H	-3.302571959678	1.983874564783	0.509602521549
H	-4.903262250884	0.806142154688	2.029630343077
H	-1.820180966871	-1.021936456009	4.103961051775
H	-0.087456458246	0.069329470289	2.682240496774
H	-1.143187840796	4.996366868812	-1.511208577157
H	-0.181398876514	5.654256605742	-2.854756774203
H	0.596887539715	5.702029038221	0.120324598028
H	0.090686380590	7.093046129967	-0.869209775540
H	2.441254294656	7.034043102875	-0.792653738805
H	2.830893166265	4.660236393077	-0.370531062052
H	3.786621342057	5.330676910212	-1.714917848570
H	2.181559111663	4.495396986012	-3.367671546581
H	2.690980767043	3.148672324104	-2.326732159003

SCF Done: E(RB3LYP) = -759.951410053

Zero-point correction= 0.254504
Thermal correction to Energy= 0.267997
Thermal correction to Enthalpy= 0.268941
Thermal correction to Gibbs Free Energy= 0.212404
Sum of electronic and zero-point Energies= -759.696906
Sum of electronic and thermal Energies= -759.683413
Sum of electronic and thermal Enthalpies= -759.682469
Sum of electronic and thermal Free Energies= -759.739006

1	C	Isotropic = 17.5677	Anisotropy =	104.2208
2	O	Isotropic = -52.4803	Anisotropy =	216.8902
3	N	Isotropic = -103.7691	Anisotropy =	222.9598
4	C	Isotropic = 16.8721	Anisotropy =	125.0429
5	N	Isotropic = 12.0146	Anisotropy =	291.9720
6	C	Isotropic = 61.1348	Anisotropy =	172.2525
7	C	Isotropic = 155.5538	Anisotropy =	14.3785
8	C	Isotropic = 71.0236	Anisotropy =	162.8142
9	C	Isotropic = 41.9493	Anisotropy =	168.7782
10	N	Isotropic = -79.0673	Anisotropy =	563.8964
11	C	Isotropic = 41.8741	Anisotropy =	169.1601
12	C	Isotropic = 71.3042	Anisotropy =	164.2638
13	C	Isotropic = 159.0724	Anisotropy =	8.2403
14	C	Isotropic = 146.0450	Anisotropy =	35.6996
15	N	Isotropic = 211.8864	Anisotropy =	37.0001
16	C	Isotropic = 146.5255	Anisotropy =	36.3413
17	C	Isotropic = 162.7643	Anisotropy =	6.7988
18	H	Isotropic = 28.3498	Anisotropy =	7.6784
19	H	Isotropic = 23.4150	Anisotropy =	8.3407
20	H	Isotropic = 22.5127	Anisotropy =	7.0494
21	H	Isotropic = 22.5047	Anisotropy =	6.8655
22	H	Isotropic = 23.4744	Anisotropy =	8.4994
23	H	Isotropic = 29.1623	Anisotropy =	8.6429

24	H	Isotropic =	29.4548	Anisotropy =	8.4414
25	H	Isotropic =	28.9563	Anisotropy =	5.4207
26	H	Isotropic =	28.7352	Anisotropy =	8.7514
27	H	Isotropic =	30.6019	Anisotropy =	14.9910
28	H	Isotropic =	28.2742	Anisotropy =	7.3402
29	H	Isotropic =	28.6535	Anisotropy =	8.7991
30	H	Isotropic =	29.5530	Anisotropy =	8.6950
31	H	Isotropic =	29.0882	Anisotropy =	7.9268

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-1.117914435283	1.809753392810	0.113351756561
O	-1.949403771770	2.624319646114	-0.560228889669
N	-1.187385154414	3.731180207407	-0.962190598485
C	0.012442113890	3.470874605219	-0.493436393085
N	0.100830440056	2.273141347652	0.189988811023
C	-1.645108407389	0.555070097047	0.654655140045
C	1.185559143554	4.389064335110	-0.671712703496
C	-2.988608597787	0.190216859677	0.486994714866
C	-3.418537169980	-1.021477787857	1.030497563540
N	-2.622806189473	-1.863932098677	1.707634534811
C	-1.338794858585	-1.500407672155	1.860037375092
C	-0.800770057737	-0.314588786380	1.359795949387
C	0.902804243168	5.560537952599	-1.625879338426
C	2.132915836957	6.476635229854	-1.730408799751
N	2.637352926952	6.963456216588	-0.441228536199
C	2.885669873220	5.860803486495	0.493362307611
C	1.689163532302	4.916011469448	0.692046265200
H	1.992911467263	3.767870079960	-1.103778673394
H	-3.683685835212	0.832676290031	-0.053416045198
H	-4.462119278997	-1.329212710492	0.913105368966
H	-0.700982018274	-2.196110465266	2.413832792176
H	0.249545887506	-0.065579929497	1.510402388827
H	0.042515907231	6.140592317891	-1.247813130262
H	0.620660772861	5.184936732703	-2.623477601435
H	1.904247805549	7.345081361475	-2.368438275911
H	2.954272540794	5.925283028010	-2.225487254699
H	1.932402380399	7.582259196506	-0.031190060284
H	3.196104827276	6.283282534994	1.462427416910
H	3.744711573526	5.279644290284	0.108841955539
H	1.967553802421	4.073379528942	1.345781070742
H	0.868480699977	5.461209243503	1.192950888998

SCF Done: E(RB3LYP) = -759.953612429

Zero-point correction= 0.254201
Thermal correction to Energy= 0.267845
Thermal correction to Enthalpy= 0.268789
Thermal correction to Gibbs Free Energy= 0.211783
Sum of electronic and zero-point Energies= -759.699411
Sum of electronic and thermal Energies= -759.685767
Sum of electronic and thermal Enthalpies= -759.684823

Sum of electronic and thermal Free Energies= -759.741829

1	C	Isotropic =	17.8662	Anisotropy =	103.9213
2	O	Isotropic =	-50.3106	Anisotropy =	223.7665
3	N	Isotropic =	-100.3552	Anisotropy =	218.2464
4	C	Isotropic =	15.4929	Anisotropy =	128.2442
5	N	Isotropic =	13.5641	Anisotropy =	291.4188
6	C	Isotropic =	61.0200	Anisotropy =	172.2415
7	C	Isotropic =	152.3062	Anisotropy =	16.5618
8	C	Isotropic =	71.3294	Anisotropy =	164.5324
9	C	Isotropic =	41.9597	Anisotropy =	168.9197
10	N	Isotropic =	-79.0056	Anisotropy =	563.1069
11	C	Isotropic =	41.9154	Anisotropy =	168.4293
12	C	Isotropic =	70.9655	Anisotropy =	162.9814
13	C	Isotropic =	160.0008	Anisotropy =	10.3550
14	C	Isotropic =	144.0811	Anisotropy =	30.1708
15	N	Isotropic =	216.5811	Anisotropy =	59.2231
16	C	Isotropic =	143.7376	Anisotropy =	30.8755
17	C	Isotropic =	155.4099	Anisotropy =	12.3694
18	H	Isotropic =	28.6070	Anisotropy =	5.5626
19	H	Isotropic =	23.5061	Anisotropy =	8.4691
20	H	Isotropic =	22.5315	Anisotropy =	6.8360
21	H	Isotropic =	22.5305	Anisotropy =	7.0127
22	H	Isotropic =	23.4236	Anisotropy =	8.2511
23	H	Isotropic =	29.7652	Anisotropy =	7.2224
24	H	Isotropic =	29.5091	Anisotropy =	7.7338
25	H	Isotropic =	28.3514	Anisotropy =	8.7281
26	H	Isotropic =	28.7404	Anisotropy =	7.7844
27	H	Isotropic =	31.2702	Anisotropy =	12.1768
28	H	Isotropic =	28.3859	Anisotropy =	8.7028
29	H	Isotropic =	28.6818	Anisotropy =	7.9123
30	H	Isotropic =	29.3429	Anisotropy =	7.8989
31	H	Isotropic =	30.2803	Anisotropy =	5.5183

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

C	-0.275411082465	1.684475002277	0.452842416594
O	0.499470174405	1.494586581808	-0.629184136680
N	1.152906993104	2.712289076850	-0.871557379976
C	0.709989748962	3.502063252734	0.081168417522
N	-0.190945797659	2.895016339177	0.935281046369
C	-1.087830928861	0.570077618570	0.946203219200
C	1.167630554074	4.925982924120	0.271960613639
C	-1.062323574867	-0.688399146281	0.328434962674
C	-1.865849088029	-1.700914403943	0.855541739175
N	-2.665963208713	-1.544929827983	1.921783538261
C	-2.679275634112	-0.333889462285	2.502519109065
C	-1.918288213465	0.748927293486	2.061953066587
C	2.066924518908	5.445330833385	-0.868554792823
C	1.264394472095	5.806802607235	-2.123760760696
N	0.213503591308	6.771675125757	-1.780167127734
C	-0.743354612678	6.196629665870	-0.830366814087

C	-0.030725460024	5.881186300121	0.486668061409
H	1.755578037535	4.909774830503	1.207029801352
H	-0.432578542251	-0.876820616047	-0.540972574697
H	-1.863793104848	-2.692162897261	0.392014588880
H	-3.335902039112	-0.220156628935	3.370488525577
H	-1.964711329205	1.712692475203	2.568692471430
H	2.844596375665	4.706547721068	-1.115290244820
H	2.575537350205	6.352797445446	-0.504326566086
H	0.855823874628	4.878423865837	-2.578768993198
H	1.933758351102	6.265333745411	-2.869307628858
H	-0.281841444724	7.038609257724	-2.631757638001
H	-1.225911437691	5.270261457550	-1.219475751119
H	-1.548939273770	6.926750728474	-0.652611471949
H	0.356450184777	6.820581628946	0.914049674085
H	-0.735199454296	5.448007205186	1.212460628906

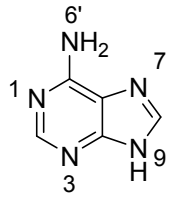
SCF Done: E(RB3LYP) = -759.951352077

Zero-point correction= 0.254434
Thermal correction to Energy= 0.267949
Thermal correction to Enthalpy= 0.268893
Thermal correction to Gibbs Free Energy= 0.212025
Sum of electronic and zero-point Energies= -759.696918
Sum of electronic and thermal Energies= -759.683403
Sum of electronic and thermal Enthalpies= -759.682459
Sum of electronic and thermal Free Energies= -759.739327

1	C	Isotropic =	17.4413	Anisotropy =	104.1315
2	O	Isotropic =	-53.0921	Anisotropy =	217.6699
3	N	Isotropic =	-104.1000	Anisotropy =	223.1607
4	C	Isotropic =	17.0274	Anisotropy =	124.7329
5	N	Isotropic =	12.1435	Anisotropy =	292.7332
6	C	Isotropic =	61.1007	Anisotropy =	172.2162
7	C	Isotropic =	155.5327	Anisotropy =	13.6452
8	C	Isotropic =	71.3107	Anisotropy =	164.5120
9	C	Isotropic =	41.8780	Anisotropy =	168.9254
10	N	Isotropic =	-79.3510	Anisotropy =	563.0341
11	C	Isotropic =	41.8809	Anisotropy =	168.5420
12	C	Isotropic =	71.0905	Anisotropy =	162.9125
13	C	Isotropic =	162.5541	Anisotropy =	6.5779
14	C	Isotropic =	146.4297	Anisotropy =	36.5595
15	N	Isotropic =	211.8701	Anisotropy =	36.7696
16	C	Isotropic =	146.0820	Anisotropy =	35.7188
17	C	Isotropic =	159.4738	Anisotropy =	7.9557
18	H	Isotropic =	28.3358	Anisotropy =	7.6490
19	H	Isotropic =	23.4694	Anisotropy =	8.5058
20	H	Isotropic =	22.5096	Anisotropy =	6.8569
21	H	Isotropic =	22.5249	Anisotropy =	7.0360
22	H	Isotropic =	23.4182	Anisotropy =	8.3217
23	H	Isotropic =	29.0574	Anisotropy =	8.1036
24	H	Isotropic =	29.5449	Anisotropy =	8.6542
25	H	Isotropic =	28.3398	Anisotropy =	7.2114
26	H	Isotropic =	28.6530	Anisotropy =	8.8297
27	H	Isotropic =	30.5998	Anisotropy =	14.9858
28	H	Isotropic =	28.9692	Anisotropy =	5.4225
29	H	Isotropic =	28.7429	Anisotropy =	8.7656

30	H	Isotropic =	29.4721	Anisotropy =	8.4236
31	H	Isotropic =	29.0979	Anisotropy =	8.7352

9. Coordinates and Shielding Constants for Compounds 4



4a

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

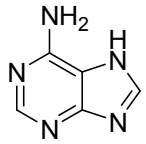
N	0.181315960998	-0.867475124613	-0.692258612144
C	-1.019189308705	-0.274407588749	-0.566006572058
C	-1.321139460061	0.846681703355	0.219747874038
C	-0.244764786290	1.404076498753	0.951739364530
N	0.974468654653	0.830841863319	0.846026685989
C	1.105715183090	-0.244601302664	0.047993485622
N	-2.660401900975	1.189332697055	0.113683245984
C	-3.150320415507	0.292963924094	-0.717733878094
N	-2.212325633162	-0.613061076204	-1.160425824689
N	-0.392244603495	2.483067787960	1.748111124468
H	2.116058138546	-0.666537640250	0.001431973339
H	-4.186042195118	0.238667857700	-1.047428382868
H	-2.372045213638	-1.383485792979	-1.800256451896
H	-1.294315454156	2.928434035181	1.845008252479
H	0.404101033820	2.846642158042	2.255197715300

SCF Done: E(RB3LYP) = -467.365655084

Zero-point correction= 0.111204
Thermal correction to Energy= 0.117954
Thermal correction to Enthalpy= 0.118898

Thermal correction to Gibbs Free Energy= 0.079842
Sum of electronic and zero-point Energies= -467.254451
Sum of electronic and thermal Energies= -467.247702
Sum of electronic and thermal Enthalpies= -467.246757
Sum of electronic and thermal Free Energies= -467.285813

1	N	Isotropic =	25.8377	Anisotropy =	365.5954
2	C	Isotropic =	44.1084	Anisotropy =	137.1756
3	C	Isotropic =	74.8264	Anisotropy =	112.7987
4	C	Isotropic =	41.4768	Anisotropy =	145.4912
5	N	Isotropic =	19.8124	Anisotropy =	344.7879
6	C	Isotropic =	40.3427	Anisotropy =	129.1039
7	N	Isotropic =	14.2272	Anisotropy =	367.5843
8	C	Isotropic =	57.7579	Anisotropy =	106.5964
9	N	Isotropic =	104.4509	Anisotropy =	104.1703
10	N	Isotropic =	185.0476	Anisotropy =	71.0613
11	H	Isotropic =	23.1221	Anisotropy =	4.4040
12	H	Isotropic =	23.8228	Anisotropy =	4.1241
13	H	Isotropic =	22.8196	Anisotropy =	7.5161
14	H	Isotropic =	26.2084	Anisotropy =	10.7802
15	H	Isotropic =	26.7361	Anisotropy =	11.7080



4b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.033631425019	-1.118881587130	-0.081853761120
C	-1.169959890119	-0.399391206318	-0.217893459850
C	-1.264430431952	0.971042799657	0.093995699592
C	-0.120251161089	1.635059700941	0.584334062312
N	1.007804921168	0.914196403595	0.717100994768
C	0.982002353420	-0.391202145406	0.378504353302
N	-2.574618365085	1.314754705049	-0.188748331295
C	-3.180893627923	0.177607036158	-0.639678877748
N	-2.384304521703	-0.875906000073	-0.674426253747
N	-0.071024716542	2.966609904031	0.882900923360

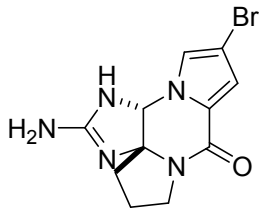
H	1.934155104898	-0.918250250700	0.508901571554
H	-3.017818468842	2.222584490637	-0.109314442383
H	-4.228717504086	0.180963642109	-0.935021206685
H	0.742387970593	3.258635214390	1.416219379424
H	-0.930240237720	3.449827293060	1.118769348516

SCF Done: E(RB3LYP) = -467.360738734

Zero-point correction= 0.112026
Thermal correction to Energy= 0.119115
Thermal correction to Enthalpy= 0.120059
Thermal correction to Gibbs Free Energy= 0.080508
Sum of electronic and zero-point Energies= -467.248713
Sum of electronic and thermal Energies= -467.241624
Sum of electronic and thermal Enthalpies= -467.240680
Sum of electronic and thermal Free Energies= -467.280231

1	N	Isotropic =	5.2717	Anisotropy =	390.7953
2	C	Isotropic =	33.9951	Anisotropy =	138.4395
3	C	Isotropic =	82.4825	Anisotropy =	116.2277
4	C	Isotropic =	44.4379	Anisotropy =	140.9578
5	N	Isotropic =	12.9562	Anisotropy =	355.1317
6	C	Isotropic =	40.8046	Anisotropy =	127.7136
7	N	Isotropic =	116.8277	Anisotropy =	109.1575
8	C	Isotropic =	53.0599	Anisotropy =	115.3856
9	N	Isotropic =	8.0533	Anisotropy =	344.9461
10	N	Isotropic =	186.8468	Anisotropy =	72.8208
11	H	Isotropic =	22.9047	Anisotropy =	4.7010
12	H	Isotropic =	22.7375	Anisotropy =	8.1002
13	H	Isotropic =	23.6183	Anisotropy =	4.4970
14	H	Isotropic =	27.0324	Anisotropy =	11.9518
15	H	Isotropic =	27.1183	Anisotropy =	10.5427

10. Coordinates and Shielding Constants for Compounds 5 and 6



5a

Conformer 1

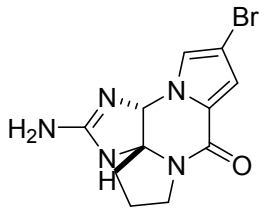
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.387071672665	-0.334302534716	2.636691196371
C	0.243414009307	-1.523448878592	1.991669081071
C	-0.038646680426	-1.413213826444	0.551812551437
N	-0.005694639788	-0.201269166955	-0.110536769999
C	0.234939303406	1.102590060137	0.541894924696
C	0.048672474642	0.981450549155	2.087214794757
N	-1.365518380665	1.330975962634	2.319194765881
C	-1.758447000047	1.941125964441	1.248077665225
N	-0.799060408091	2.072986382286	0.235058159991
C	0.872965440269	-0.254834172898	4.021902645191
C	0.903663228140	1.256844845322	4.310550421975
C	0.975732564234	1.896172595461	2.915974299945
C	-0.177809913549	-0.413452140729	-1.454110874905
C	-0.337792584646	-1.779887999080	-1.638409600329
C	-0.247455174913	-2.421669271663	-0.380656896491
N	-3.013846025604	2.440449741465	1.033934916880
O	0.399912158726	-2.613842761131	2.553092732580
Br	-0.623843048252	-2.624215831429	-3.314632739275
H	1.228069507365	1.463642720530	0.245320111330
H	-1.126007169147	2.132058788499	-0.726510107114
H	1.872247095657	-0.717216645195	4.083121315596
H	0.210964428445	-0.808321306835	4.704969921969
H	1.747639126623	1.537120463971	4.955286583977
H	-0.027990142862	1.564627638376	4.807070458443
H	0.643983033678	2.942549418306	2.892135957600
H	2.001616982415	1.838424546477	2.515942491421
H	-0.173676791049	0.395591137917	-2.178135637738
H	-0.314509379874	-3.483379310012	-0.164990208019
H	-3.555760533295	2.579146507732	1.882191889073
H	-3.081103153367	3.221556522969	0.387705948462

SCF Done: E(RB3LYP) = -3349.60731276

Zero-point correction= 0.233137
Thermal correction to Energy= 0.248026
Thermal correction to Enthalpy= 0.248970
Thermal correction to Gibbs Free Energy= 0.190253
Sum of electronic and zero-point Energies= -3349.374176
Sum of electronic and thermal Energies= -3349.359287
Sum of electronic and thermal Enthalpies= -3349.358343
Sum of electronic and thermal Free Energies= -3349.417060

1	N	Isotropic =	121.2011	Anisotropy =	104.4113
2	C	Isotropic =	41.1871	Anisotropy =	101.1464
3	C	Isotropic =	67.1419	Anisotropy =	99.5572
4	N	Isotropic =	76.6864	Anisotropy =	144.5905
5	C	Isotropic =	115.5930	Anisotropy =	16.7844
6	C	Isotropic =	98.3688	Anisotropy =	26.6167
7	N	Isotropic =	69.0114	Anisotropy =	180.8436
8	C	Isotropic =	37.4155	Anisotropy =	94.7058
9	N	Isotropic =	160.0527	Anisotropy =	73.7897
10	C	Isotropic =	145.5041	Anisotropy =	41.0520
11	C	Isotropic =	167.6897	Anisotropy =	18.6337
12	C	Isotropic =	148.1208	Anisotropy =	37.9830
13	C	Isotropic =	73.5834	Anisotropy =	94.6074
14	C	Isotropic =	74.5829	Anisotropy =	72.5269
15	C	Isotropic =	80.1739	Anisotropy =	116.1133
16	N	Isotropic =	204.1392	Anisotropy =	81.2123
17	O	Isotropic =	-11.5425	Anisotropy =	538.1385
18	Br	Isotropic =	2291.7696	Anisotropy =	1049.8494
19	H	Isotropic =	26.3867	Anisotropy =	5.9639
20	H	Isotropic =	27.3736	Anisotropy =	9.6262
21	H	Isotropic =	27.9486	Anisotropy =	9.6581
22	H	Isotropic =	27.6705	Anisotropy =	8.8328
23	H	Isotropic =	29.4630	Anisotropy =	11.0084
24	H	Isotropic =	29.2192	Anisotropy =	9.2930
25	H	Isotropic =	29.5298	Anisotropy =	7.3629
26	H	Isotropic =	29.4363	Anisotropy =	7.8608
27	H	Isotropic =	24.8339	Anisotropy =	7.4752
28	H	Isotropic =	24.8559	Anisotropy =	5.7939
29	H	Isotropic =	28.1283	Anisotropy =	13.3421
30	H	Isotropic =	28.3498	Anisotropy =	12.1353



5b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

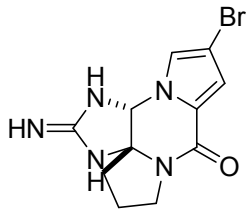
N	-1.941836742716	-1.753713562183	1.701154637037
C	-0.713084515753	-1.287514254535	2.091675864665
C	0.037743673997	-0.550918114829	1.069869790520
N	-0.524810352512	-0.183969422634	-0.134034478632
C	-1.903761707557	-0.508195875566	-0.562621875194
C	-2.540475550809	-1.577090426847	0.381718792762
N	-2.429274478568	-2.801711854501	-0.455291016714
C	-2.043961073467	-2.375594665181	-1.722719908066
N	-1.879337929788	-1.094771956131	-1.891397245372
C	-2.932367681539	-2.186884729060	2.707376479142
C	-4.245094578071	-2.275615575709	1.910897141339
C	-4.016352565601	-1.317827138412	0.733699736223
C	0.379206876802	0.535528882120	-0.862199716383
C	1.539649083968	0.627736308923	-0.101479653255
C	1.336551251978	-0.051853148257	1.121079496297
N	-1.859961422461	-3.311001512666	-2.696275331378
O	-0.288803120589	-1.453506564399	3.239032985127
Br	3.127090997533	1.519940933485	-0.642703799898
H	-2.485474991780	0.424799385817	-0.549465536645
H	-1.919832243587	-3.587244019141	-0.055064288194
H	-2.975874045443	-1.435490032674	3.512406254767
H	-2.640262509299	-3.144783515815	3.162402776352
H	-5.117221740640	-2.007416064397	2.522081561501
H	-4.394572213100	-3.298834505263	1.533681420905
H	-4.678616771609	-1.496940094054	-0.123764057621
H	-4.128665306811	-0.269909416641	1.057836889686
H	0.144136509035	0.907506655895	-1.853586944433
H	2.034654212769	-0.174915567700	1.943241132012
H	-2.436823098399	-4.144792160213	-2.641547007598
H	-1.750117965983	-2.938027989432	-3.634284098954

SCF Done: E(RB3LYP) = -3349.60713142

Zero-point correction= 0.232910
Thermal correction to Energy= 0.247837
Thermal correction to Enthalpy= 0.248781
Thermal correction to Gibbs Free Energy= 0.189892
Sum of electronic and zero-point Energies= -3349.374222
Sum of electronic and thermal Energies= -3349.359295
Sum of electronic and thermal Enthalpies= -3349.358351
Sum of electronic and thermal Free Energies= -3349.417239

1	N	Isotropic =	126.4071	Anisotropy = 111.7123
2	C	Isotropic =	40.4983	Anisotropy = 101.5297
3	C	Isotropic =	70.1743	Anisotropy = 97.5523
4	N	Isotropic =	70.0080	Anisotropy = 151.0366

5 C Isotropic = 109.8361 Anisotropy = 23.7841
6 C Isotropic = 105.7739 Anisotropy = 19.2528
7 N Isotropic = 151.3681 Anisotropy = 102.5822
8 C Isotropic = 32.1559 Anisotropy = 96.2277
9 N Isotropic = 75.6286 Anisotropy = 166.4438
10 C Isotropic = 144.4309 Anisotropy = 42.7908
11 C Isotropic = 168.6669 Anisotropy = 18.3409
12 C Isotropic = 147.2215 Anisotropy = 36.9373
13 C Isotropic = 71.6342 Anisotropy = 98.2032
14 C Isotropic = 75.6751 Anisotropy = 69.7500
15 C Isotropic = 80.0942 Anisotropy = 116.1447
16 N Isotropic = 199.7797 Anisotropy = 81.9473
17 O Isotropic = -16.3171 Anisotropy = 548.0882
18 Br Isotropic = 2299.9585 Anisotropy = 1043.3888
19 H Isotropic = 26.1324 Anisotropy = 4.5961
20 H Isotropic = 28.0129 Anisotropy = 6.4752
21 H Isotropic = 27.9311 Anisotropy = 9.1313
22 H Isotropic = 27.8756 Anisotropy = 9.2703
23 H Isotropic = 29.4269 Anisotropy = 11.2348
24 H Isotropic = 29.3366 Anisotropy = 9.3732
25 H Isotropic = 29.3045 Anisotropy = 7.6575
26 H Isotropic = 29.5991 Anisotropy = 7.8888
27 H Isotropic = 24.6317 Anisotropy = 7.5102
28 H Isotropic = 24.8602 Anisotropy = 5.7665
29 H Isotropic = 28.1238 Anisotropy = 12.3584
30 H Isotropic = 27.8814 Anisotropy = 12.6052



5c

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.890908731841	-2.440658259439	-1.116041913494
C	0.103837412037	-2.685292965127	-0.022832458875
C	-0.569834117803	-1.504432229287	0.531361948280
N	-0.555827688021	-0.282510150020	-0.114035082410
C	0.131898887316	-0.019628600537	-1.399366331795
C	1.192406746517	-1.124277107631	-1.664542373653

N	2.390738617727	-0.518196092028	-1.057644037493
C	2.212363231137	0.828859860939	-0.796683564908
N	0.964261907925	1.158709061679	-1.359247928917
C	1.411386583225	-3.536187066721	-1.955744865445
C	2.129405491112	-2.800167968125	-3.098071863227
C	1.412114428244	-1.445043648259	-3.156633244842
C	-1.341766429713	0.602920354778	0.574054544923
C	-1.848195864659	-0.067077022972	1.679894732991
C	-1.371020927199	-1.398327473733	1.661835319875
N	3.074905491804	1.573512382944	-0.210526176948
O	-0.060033173912	-3.821003684155	0.429230508234
Br	-2.989715121955	0.700940839841	2.986880149635
H	-0.622233641633	0.045679636757	-2.193677854065
H	3.002678296756	-1.063727596058	-0.463160141574
H	0.545906114993	2.041531294584	-1.083786093953
H	0.568019816720	-4.148648399664	-2.315103025573
H	2.077653352178	-4.191267306186	-1.376316397142
H	2.077813908678	-3.354505334284	-4.044384324008
H	3.191421891505	-2.651608611905	-2.848340276935
H	1.983799707801	-0.655688814435	-3.660798140118
H	0.433161929459	-1.550297085428	-3.652146554195
H	-1.490497070625	1.626856954333	0.245906941438
H	-1.575521343873	-2.192080670006	2.373519715746
H	2.704132832419	2.524895700147	-0.113971211553

SCF Done: E(RB3LYP) = -3349.60117634

Zero-point correction= 0.232767
Thermal correction to Energy= 0.247838
Thermal correction to Enthalpy= 0.248783
Thermal correction to Gibbs Free Energy= 0.189462
Sum of electronic and zero-point Energies= -3349.368409
Sum of electronic and thermal Energies= -3349.353338
Sum of electronic and thermal Enthalpies= -3349.352394
Sum of electronic and thermal Free Energies= -3349.411715

1	N	Isotropic =	125.5410	Anisotropy =	109.7279
2	C	Isotropic =	41.1434	Anisotropy =	100.6084
3	C	Isotropic =	68.4649	Anisotropy =	98.2248
4	N	Isotropic =	75.4836	Anisotropy =	142.2414
5	C	Isotropic =	117.8580	Anisotropy =	15.5884
6	C	Isotropic =	109.2579	Anisotropy =	11.9468
7	N	Isotropic =	162.7694	Anisotropy =	93.1064
8	C	Isotropic =	39.1808	Anisotropy =	90.3481
9	N	Isotropic =	162.9321	Anisotropy =	77.3281
10	C	Isotropic =	144.8059	Anisotropy =	42.2327
11	C	Isotropic =	168.7182	Anisotropy =	18.1428
12	C	Isotropic =	148.1066	Anisotropy =	37.4029
13	C	Isotropic =	72.9554	Anisotropy =	98.2544
14	C	Isotropic =	74.1948	Anisotropy =	73.1696
15	C	Isotropic =	78.8782	Anisotropy =	117.7179

16	N	Isotropic =	109.7271	Anisotropy =	198.2750
17	O	Isotropic =	-20.2500	Anisotropy =	555.2683
18	Br	Isotropic =	2288.2207	Anisotropy =	1052.6818
19	H	Isotropic =	26.4043	Anisotropy =	5.8026
20	H	Isotropic =	28.1775	Anisotropy =	7.9192
21	H	Isotropic =	27.6412	Anisotropy =	9.9808
22	H	Isotropic =	28.0128	Anisotropy =	9.6722
23	H	Isotropic =	27.7439	Anisotropy =	9.0664
24	H	Isotropic =	29.4207	Anisotropy =	11.2786
25	H	Isotropic =	29.3616	Anisotropy =	9.2838
26	H	Isotropic =	29.1716	Anisotropy =	7.6202
27	H	Isotropic =	29.4287	Anisotropy =	8.0645
28	H	Isotropic =	24.7684	Anisotropy =	7.5194
29	H	Isotropic =	24.7810	Anisotropy =	5.7744
30	H	Isotropic =	26.5750	Anisotropy =	7.2811

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

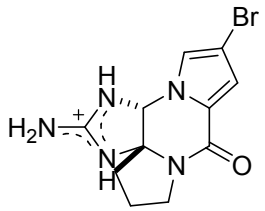
N	-1.614047653420	-2.600414877089	-0.806490283882
C	-1.170641978713	-2.552269032426	0.487979049000
C	-0.529745176700	-1.289878581474	0.876525052227
N	-0.545667187481	-0.176690163766	0.057677155517
C	-1.185173803622	-0.127847665777	-1.278065696216
C	-1.395715785105	-1.571305100920	-1.814840880002
N	-0.149374572386	-1.781349765653	-2.576507592895
C	0.534125317205	-0.592111646676	-2.774592065289
N	-0.319934526512	0.418396129511	-2.295282547445
C	-2.515029177359	-3.669845172516	-1.275312938336
C	-2.834554910953	-3.258614497780	-2.721362075996
C	-2.638169985242	-1.736695576998	-2.712677181554
C	0.037187113647	0.875734309750	0.712162662997
C	0.440698439853	0.414883381283	1.958427336622
C	0.085245608994	-0.949006848363	2.075086330500
N	1.680917208821	-0.503917368578	-3.338880664644
O	-1.339943646373	-3.485394417078	1.276408636325
Br	1.326280627572	1.461528284915	3.270378007717
H	-2.122043933098	0.437494569440	-1.197606100208
H	0.384005052781	-2.633535625668	-2.450247959048
H	0.074631197927	1.343682105900	-2.160304841874
H	-3.412886140408	-3.692768684050	-0.635882293567
H	-2.027335397638	-4.652540682770	-1.202181149265
H	-3.846336979187	-3.559357787466	-3.023679661324
H	-2.118770457353	-3.723864350743	-3.416535273097
H	-2.480604185447	-1.298934669911	-3.706485775049
H	-3.499244773278	-1.240892506618	-2.235566667574
H	0.127097773169	1.861602740666	0.267051128532
H	0.248604824655	-1.613587578054	2.917731684275

H 1.989897105649 0.474031078912 -3.347715396446

SCF Done: E(RB3LYP) = -3349.60116798

Zero-point correction= 0.232880
Thermal correction to Energy= 0.247805
Thermal correction to Enthalpy= 0.248749
Thermal correction to Gibbs Free Energy= 0.189912
Sum of electronic and zero-point Energies= -3349.368288
Sum of electronic and thermal Energies= -3349.353363
Sum of electronic and thermal Enthalpies= -3349.352418
Sum of electronic and thermal Free Energies= -3349.411256

1	N	Isotropic =	125.4830	Anisotropy =	109.5712
2	C	Isotropic =	41.2929	Anisotropy =	100.9063
3	C	Isotropic =	68.4728	Anisotropy =	98.0784
4	N	Isotropic =	75.4702	Anisotropy =	142.0240
5	C	Isotropic =	117.9404	Anisotropy =	15.8378
6	C	Isotropic =	109.1945	Anisotropy =	12.1245
7	N	Isotropic =	162.6775	Anisotropy =	92.6427
8	C	Isotropic =	38.8359	Anisotropy =	90.3344
9	N	Isotropic =	162.4593	Anisotropy =	77.9880
10	C	Isotropic =	144.8918	Anisotropy =	42.1694
11	C	Isotropic =	169.0783	Anisotropy =	17.9355
12	C	Isotropic =	148.0435	Anisotropy =	37.4647
13	C	Isotropic =	72.9807	Anisotropy =	98.1815
14	C	Isotropic =	74.1598	Anisotropy =	73.2306
15	C	Isotropic =	78.9360	Anisotropy =	117.5876
16	N	Isotropic =	108.4596	Anisotropy =	200.4011
17	O	Isotropic =	-20.1554	Anisotropy =	554.9878
18	Br	Isotropic =	2288.2682	Anisotropy =	1052.7426
19	H	Isotropic =	26.4088	Anisotropy =	5.7835
20	H	Isotropic =	28.2715	Anisotropy =	7.8449
21	H	Isotropic =	27.5790	Anisotropy =	9.9779
22	H	Isotropic =	28.0128	Anisotropy =	9.6474
23	H	Isotropic =	27.7577	Anisotropy =	9.0852
24	H	Isotropic =	29.4116	Anisotropy =	11.3061
25	H	Isotropic =	29.3416	Anisotropy =	9.3351
26	H	Isotropic =	29.1732	Anisotropy =	7.6207
27	H	Isotropic =	29.4516	Anisotropy =	8.0707
28	H	Isotropic =	24.7691	Anisotropy =	7.4978
29	H	Isotropic =	24.7863	Anisotropy =	5.7736
30	H	Isotropic =	26.5074	Anisotropy =	7.2563



5d

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

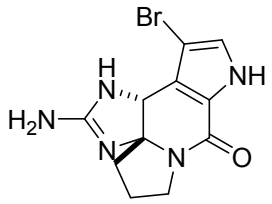
N	-2.667934219088	-0.909918558361	-0.717627994006
C	-2.289102057320	-1.230029129726	0.565160355340
C	-0.906976877470	-0.876862156381	0.904982837593
N	-0.109333892185	-0.127895669499	0.055128721894
C	-0.516772944375	0.323153532036	-1.278983754743
C	-1.776561058999	-0.458093552703	-1.756466906844
N	-1.102574928593	-1.595131958927	-2.461577285364
C	0.125144481714	-1.231418202395	-2.855511648718
N	0.455491787194	-0.047064564009	-2.295842208766
C	-4.084158567204	-0.915753908902	-1.135239867073
C	-4.024689396566	-0.472874353925	-2.605192583344
C	-2.715268174381	0.325455432543	-2.693975969828
C	1.073411171368	0.168478698162	0.684302481141
C	1.027792392482	-0.417059530386	1.940798302772
C	-0.216580626571	-1.073703819070	2.092405158508
N	0.903864569412	-1.913508276968	-3.676717292931
O	-3.076083837966	-1.716890476563	1.374700168050
Br	2.415961881633	-0.332765437453	3.227996635896
H	-0.673506302534	1.407716605100	-1.274268696044
H	-1.629512699188	-2.319067602379	-2.940041860538
H	1.397573157445	0.328319444984	-2.320290925770
H	-4.647588923965	-0.209095754858	-0.505112649392
H	-4.523774889402	-1.913712006143	-1.001652899125
H	-4.898632865519	0.125318010349	-2.893012516694
H	-3.988797996436	-1.348838191797	-3.271488781622
H	-2.310743375169	0.418312518566	-3.710040570936
H	-2.852998259623	1.335595212174	-2.277788269621
H	1.853979560685	0.757061011998	0.212866912366
H	-0.583447989078	-1.618577765179	2.956570549788
H	1.841017714975	-1.594072917222	-3.894971696401
H	0.585773164725	-2.778736633069	-4.098447745586

SCF Done: E(RB3LYP) = -3350.07014705

Zero-point correction= 0.246214
Thermal correction to Energy= 0.261562

Thermal correction to Enthalpy= 0.262506
Thermal correction to Gibbs Free Energy= 0.203095
Sum of electronic and zero-point Energies= -3349.823933
Sum of electronic and thermal Energies= -3349.808585
Sum of electronic and thermal Enthalpies= -3349.807641
Sum of electronic and thermal Free Energies= -3349.867052

1	N	Isotropic =	131.0815	Anisotropy =	117.2486
2	C	Isotropic =	41.5675	Anisotropy =	99.2587
3	C	Isotropic =	68.3334	Anisotropy =	97.9506
4	N	Isotropic =	85.0204	Anisotropy =	130.3322
5	C	Isotropic =	121.1459	Anisotropy =	16.7906
6	C	Isotropic =	104.1191	Anisotropy =	18.6969
7	N	Isotropic =	147.5854	Anisotropy =	70.7614
8	C	Isotropic =	41.8725	Anisotropy =	116.8691
9	N	Isotropic =	160.2864	Anisotropy =	64.6668
10	C	Isotropic =	144.6276	Anisotropy =	44.4344
11	C	Isotropic =	169.4494	Anisotropy =	18.9992
12	C	Isotropic =	149.7693	Anisotropy =	38.3612
13	C	Isotropic =	71.7667	Anisotropy =	97.5734
14	C	Isotropic =	72.1995	Anisotropy =	77.8593
15	C	Isotropic =	77.2358	Anisotropy =	121.3080
16	N	Isotropic =	187.4875	Anisotropy =	60.2293
17	O	Isotropic =	-34.5854	Anisotropy =	575.6748
18	Br	Isotropic =	2272.0512	Anisotropy =	1063.6761
19	H	Isotropic =	25.9895	Anisotropy =	6.1509
20	H	Isotropic =	26.2542	Anisotropy =	7.5484
21	H	Isotropic =	25.9341	Anisotropy =	10.7036
22	H	Isotropic =	27.9082	Anisotropy =	9.8364
23	H	Isotropic =	27.5470	Anisotropy =	8.9679
24	H	Isotropic =	29.2458	Anisotropy =	11.3814
25	H	Isotropic =	29.3962	Anisotropy =	9.4816
26	H	Isotropic =	29.0017	Anisotropy =	7.5352
27	H	Isotropic =	29.1220	Anisotropy =	8.2379
28	H	Isotropic =	24.6967	Anisotropy =	7.5466
29	H	Isotropic =	24.6143	Anisotropy =	5.8105
30	H	Isotropic =	26.3670	Anisotropy =	12.8623
31	H	Isotropic =	26.3786	Anisotropy =	13.0196



6a

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

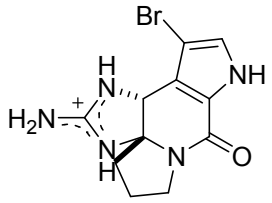
N	-0.853619608981	1.085796764352	1.935854606704
C	-1.576557115495	-0.054952295517	1.780176185531
C	-1.156843216372	-0.853121065544	0.624500795374
C	-0.045257795440	-0.616902649487	-0.169489602842
C	0.809745596970	0.607817966376	0.018229146977
C	0.109333604435	1.651262902504	0.964596147673
N	-0.559978190878	2.598724306778	0.054594849172
C	-0.044920218192	2.400945731185	-1.115952544466
N	0.941770552182	1.418709658862	-1.208608563619
C	-0.961699448080	1.902780759275	3.151594243162
C	0.091306983399	3.008484981783	2.948153826645
C	1.057620615372	2.407048681285	1.918262901485
C	0.033859577260	-1.726048104676	-1.054641757044
C	-1.021980646015	-2.587707058819	-0.778418930855
N	-1.730866084041	-2.038329260960	0.251637756277
N	-0.412300747799	3.071402159814	-2.257325670890
O	-2.457854507495	-0.423472680292	2.568731790250
Br	1.344851412511	-2.011879026668	-2.403154022920
H	1.807944658352	0.332835844530	0.391160908005
H	0.972559449420	0.896120811831	-2.082738974379
H	-0.747376598812	1.274080357781	4.032299074252
H	-1.980608477895	2.301926274903	3.274035584204
H	0.582137110490	3.288477393146	3.890370956188
H	-0.382767467992	3.905709745915	2.524777259571
H	1.739736207518	1.686800611703	2.400803675101
H	1.656690488255	3.156990232932	1.383776847467
H	-1.305737787394	-3.528048208608	-1.239743796403
H	-2.545075308216	-2.439800782228	0.703052428924
H	0.317717974059	3.171779201244	-2.957664799289
H	-0.897921011125	3.945756746599	-2.076070320256

SCF Done: E(RB3LYP) = -3349.61433084

Zero-point correction= 0.233863
Thermal correction to Energy= 0.248741
Thermal correction to Enthalpy= 0.249686
Thermal correction to Gibbs Free Energy= 0.191221
Sum of electronic and zero-point Energies= -3349.380468
Sum of electronic and thermal Energies= -3349.365589
Sum of electronic and thermal Enthalpies= -3349.364645
Sum of electronic and thermal Free Energies= -3349.423110

1 N Isotropic = 118.0411 Anisotropy = 102.6497
2 C Isotropic = 40.3751 Anisotropy = 101.7040
3 C Isotropic = 70.5747 Anisotropy = 99.3451
4 C Isotropic = 68.8506 Anisotropy = 122.7927
5 C Isotropic = 129.7002 Anisotropy = 32.0156
6 C Isotropic = 95.2183 Anisotropy = 26.6130

7 N Isotropic = 65.6954 Anisotropy = 180.4850
8 C Isotropic = 35.7311 Anisotropy = 97.9206
9 N Isotropic = 166.8701 Anisotropy = 93.7642
10 C Isotropic = 146.3090 Anisotropy = 39.6006
11 C Isotropic = 167.1349 Anisotropy = 19.4540
12 C Isotropic = 147.2172 Anisotropy = 37.5970
13 C Isotropic = 79.2491 Anisotropy = 62.2463
14 C Isotropic = 71.9695 Anisotropy = 103.4610
15 N Isotropic = 109.7582 Anisotropy = 137.7137
16 N Isotropic = 204.8728 Anisotropy = 82.4148
17 O Isotropic = 2.0778 Anisotropy = 551.0657
18 Br Isotropic = 2334.0418 Anisotropy = 932.3270
19 H Isotropic = 26.8516 Anisotropy = 3.9972
20 H Isotropic = 27.4556 Anisotropy = 13.5041
21 H Isotropic = 27.9761 Anisotropy = 9.5736
22 H Isotropic = 27.7657 Anisotropy = 9.0124
23 H Isotropic = 29.4871 Anisotropy = 10.9505
24 H Isotropic = 29.1887 Anisotropy = 9.1788
25 H Isotropic = 29.5278 Anisotropy = 7.3141
26 H Isotropic = 29.5266 Anisotropy = 6.9306
27 H Isotropic = 24.7340 Anisotropy = 5.4666
28 H Isotropic = 23.1983 Anisotropy = 9.1653
29 H Isotropic = 28.5063 Anisotropy = 11.8553
30 H Isotropic = 28.2749 Anisotropy = 13.3894



6b

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.308198498360	-2.242622719878	-1.183388447961
C	-0.717756856585	-2.363539881175	-0.276415220479
C	-1.051323232177	-1.105129955094	0.389757540716
C	-0.554836487787	0.146514959735	0.056972372886
C	0.510840586118	0.313613860742	-0.988484151963
C	1.146729583131	-1.068406317174	-1.363394422435
N	2.301815555527	-1.075383787189	-0.413746155476
C	2.620114803615	0.174803622425	-0.047107891196

N	1.691258153525	1.045352329465	-0.484924985161
C	0.589849264095	-3.304421874400	-2.168458291192
C	1.759661677973	-2.736128699423	-2.986698312024
C	1.610156210712	-1.216791977408	-2.824061967194
C	-1.270195458542	1.076336770952	0.854416565958
C	-2.167277874465	0.367066461403	1.646060699011
N	-2.021209229196	-0.955153078577	1.342115833251
N	3.698733464709	0.512336798643	0.644805084571
O	-1.332449250580	-3.415748430777	-0.100610599557
Br	-1.046383717255	2.961099263766	0.865257193446
H	0.128665691336	0.824547583307	-1.882232053556
H	2.989241141731	-1.822641999327	-0.416655736561
H	1.577280337603	1.957152058983	-0.050598486316
H	-0.308096852121	-3.473252353170	-2.785046450659
H	0.834338265230	-4.249741814358	-1.664056063712
H	1.723661884186	-3.054232103598	-4.036600552363
H	2.721670007848	-3.075899517247	-2.571062589179
H	2.526263755781	-0.647519607213	-3.029648504781
H	0.809164896962	-0.837222228874	-3.477988196474
H	-2.877720182761	0.714017540563	2.389216666466
H	-2.555634129272	-1.722103709686	1.735729091978
H	4.385854979619	-0.182348476265	0.912567792803
H	3.871104512682	1.476837280851	0.903230237151

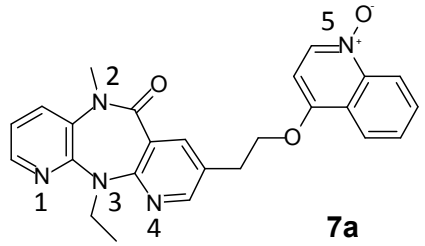
SCF Done: E(RB3LYP) = -3350.08281684

Zero-point correction= 0.246869
Thermal correction to Energy= 0.262218
Thermal correction to Enthalpy= 0.263162
Thermal correction to Gibbs Free Energy= 0.204114
Sum of electronic and zero-point Energies= -3349.835948
Sum of electronic and thermal Energies= -3349.820599
Sum of electronic and thermal Enthalpies= -3349.819655
Sum of electronic and thermal Free Energies= -3349.878703

1	N	Isotropic =	128.0227	Anisotropy =	114.9910
2	C	Isotropic =	40.5665	Anisotropy =	99.6617
3	C	Isotropic =	71.1847	Anisotropy =	99.5517
4	C	Isotropic =	71.1508	Anisotropy =	118.7581
5	C	Isotropic =	132.1612	Anisotropy =	26.5847
6	C	Isotropic =	102.8825	Anisotropy =	19.3502
7	N	Isotropic =	145.9472	Anisotropy =	74.6800
8	C	Isotropic =	41.0902	Anisotropy =	118.9132
9	N	Isotropic =	165.8370	Anisotropy =	77.1218
10	C	Isotropic =	145.4932	Anisotropy =	42.4627
11	C	Isotropic =	168.6842	Anisotropy =	19.7786
12	C	Isotropic =	149.4227	Anisotropy =	37.5993
13	C	Isotropic =	78.6687	Anisotropy =	67.3107
14	C	Isotropic =	69.6132	Anisotropy =	107.3888
15	N	Isotropic =	107.3202	Anisotropy =	141.6160
16	N	Isotropic =	189.5603	Anisotropy =	63.5220

17	O	Isotropic =	-23.4661	Anisotropy =	589.6409
18	Br	Isotropic =	2313.4333	Anisotropy =	952.7082
19	H	Isotropic =	26.4448	Anisotropy =	4.3488
20	H	Isotropic =	26.3364	Anisotropy =	7.3774
21	H	Isotropic =	25.9917	Anisotropy =	13.2975
22	H	Isotropic =	27.9503	Anisotropy =	9.9144
23	H	Isotropic =	27.6067	Anisotropy =	9.0991
24	H	Isotropic =	29.2549	Anisotropy =	11.3627
25	H	Isotropic =	29.4095	Anisotropy =	9.3765
26	H	Isotropic =	28.9878	Anisotropy =	7.2166
27	H	Isotropic =	29.2072	Anisotropy =	7.8542
28	H	Isotropic =	24.5810	Anisotropy =	5.5353
29	H	Isotropic =	22.9822	Anisotropy =	9.1790
30	H	Isotropic =	26.5490	Anisotropy =	13.2468
31	H	Isotropic =	26.5262	Anisotropy =	12.6582

11. Coordinates and Shielding Constants for Compounds 7



7a

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	3.227715149155	1.813912696654	0.097595848155
C	2.277296934917	1.380540256987	0.929594191938
C	1.520574442196	2.256726285831	1.739837939303
C	1.755985317787	3.629657889072	1.603204146848
C	2.741512665184	4.081049279940	0.724229237607
C	3.467240109917	3.129989701117	0.011243434974
N	0.625060431743	1.781038145197	2.736003233139
C	-0.407909200585	0.905446218532	2.486147771981
C	-0.401974405542	0.088487544219	1.231380376344
C	0.755159343154	-0.446912397614	0.615910058337
N	2.050374421326	-0.021166575903	0.978825048215
O	-1.326597630400	0.773630918737	3.296191673357
N	0.676969459546	-1.403967523533	-0.320114908920
C	-0.529087863279	-1.801789187554	-0.737688215406
C	-1.743146046752	-1.283282737421	-0.268991120832
C	-1.646633235806	-0.347147349089	0.763865267006
C	3.184825676321	-0.897698467565	0.618974916279
C	3.198937982267	-2.173586517211	1.456961507812
C	-3.069918092823	-1.731058316026	-0.833753252830
C	-3.619478480960	-0.843488906992	-1.955631527218
O	-3.970020582482	0.463396135822	-1.459652335696
C	-3.255659320849	1.568385762146	-1.780482595273
C	-3.820997783569	2.809710602224	-1.335041128038
C	-3.138216353286	4.027387193926	-1.608759675219
N	-1.921680468213	4.022060542719	-2.316567433607
C	-1.424268982739	2.838860282081	-2.721956556541
C	-2.056912941495	1.611062771063	-2.470795699546
C	-5.047894643761	2.879170932740	-0.622312530579
C	-5.556241620920	4.095357493090	-0.207774385283

C	-4.859800602509	5.294988609699	-0.487185932354
C	-3.663948048730	5.263816073260	-1.180148129209
O	-1.310193539382	5.132057923180	-2.561448317902
C	0.580005010115	2.490935815990	4.020335143485
H	1.185604590162	4.341148156124	2.201079907939
H	2.946789385710	5.146035945891	0.609595919350
H	4.274380397857	3.430112705521	-0.663845172747
H	-0.530681990835	-2.591516806263	-1.497683895235
H	-2.542588287342	0.036422263459	1.254060421311
H	3.163481546829	-1.139043628316	-0.454991633935
H	4.092709424890	-0.312547500710	0.804370413368
H	3.234987886834	-1.938092985062	2.532703553174
H	2.311641487924	-2.794492047240	1.264386714826
H	4.090177246205	-2.770322579131	1.203905255068
H	-2.978782756592	-2.748460927510	-1.248169052986
H	-3.824343459731	-1.777326735415	-0.032107992729
H	-2.918058762096	-0.771019027225	-2.798197775548
H	-4.560185614188	-1.271838770910	-2.332345686530
H	-0.480732735190	2.910711290996	-3.259637458408
H	-1.555521627118	0.713899121016	-2.826455142541
H	-5.577268566562	1.950941736887	-0.410586131694
H	-6.500584442502	4.131635183666	0.338857574033
H	-5.269024947324	6.250847794482	-0.154221897104
H	-3.097353267788	6.162307791392	-1.416367786276
H	1.582717466167	2.871856300086	4.249683686421
H	-0.136306064881	3.328880673290	4.006288414427
H	0.261785990022	1.787540949657	4.798681715488

SCF Done: E(RB3LYP) = -1466.00144946

Zero-point correction= 0.444680
Thermal correction to Energy= 0.472151
Thermal correction to Enthalpy= 0.473095
Thermal correction to Gibbs Free Energy= 0.382759
Sum of electronic and zero-point Energies= -1465.556769
Sum of electronic and thermal Energies= -1465.529299
Sum of electronic and thermal Enthalpies= -1465.528355
Sum of electronic and thermal Free Energies= -1465.618690

1	N	Isotropic =	-40.3526	Anisotropy =	456.1379
2	C	Isotropic =	37.0971	Anisotropy =	121.4042
3	C	Isotropic =	60.3260	Anisotropy =	123.4191
4	C	Isotropic =	63.1187	Anisotropy =	178.9356
5	C	Isotropic =	72.5879	Anisotropy =	161.4911
6	C	Isotropic =	49.0834	Anisotropy =	155.1830
7	N	Isotropic =	123.2190	Anisotropy =	92.3560
8	C	Isotropic =	27.3304	Anisotropy =	110.1502
9	C	Isotropic =	70.9827	Anisotropy =	133.9652
10	C	Isotropic =	33.6146	Anisotropy =	124.1734
11	N	Isotropic =	136.3088	Anisotropy =	66.1496
12	O	Isotropic =	-80.8734	Anisotropy =	583.1597
13	N	Isotropic =	-35.9451	Anisotropy =	455.2433
14	C	Isotropic =	41.7190	Anisotropy =	146.1407
15	C	Isotropic =	62.7570	Anisotropy =	172.7488
16	C	Isotropic =	50.2607	Anisotropy =	184.6928
17	C	Isotropic =	147.3570	Anisotropy =	36.8567

18	C	Isotropic =	177.0045	Anisotropy =	24.4255
19	C	Isotropic =	155.5268	Anisotropy =	16.0163
20	C	Isotropic =	122.8484	Anisotropy =	54.7590
21	O	Isotropic =	208.8169	Anisotropy =	127.3889
22	C	Isotropic =	42.6943	Anisotropy =	125.3331
23	C	Isotropic =	69.3171	Anisotropy =	166.6327
24	C	Isotropic =	50.3001	Anisotropy =	152.6263
25	N	Isotropic =	-21.7655	Anisotropy =	254.5110
26	C	Isotropic =	58.9027	Anisotropy =	115.5756
27	C	Isotropic =	92.6135	Anisotropy =	138.2912
28	C	Isotropic =	69.0156	Anisotropy =	177.2673
29	C	Isotropic =	65.3320	Anisotropy =	175.9111
30	C	Isotropic =	63.6792	Anisotropy =	177.2746
31	C	Isotropic =	73.4876	Anisotropy =	174.4176
32	O	Isotropic =	-25.4881	Anisotropy =	322.8846
33	C	Isotropic =	154.8258	Anisotropy =	45.8409
34	H	Isotropic =	24.3012	Anisotropy =	7.5869
35	H	Isotropic =	24.3507	Anisotropy =	4.0249
36	H	Isotropic =	23.2065	Anisotropy =	4.7145
37	H	Isotropic =	22.9780	Anisotropy =	7.9113
38	H	Isotropic =	23.7483	Anisotropy =	8.7364
39	H	Isotropic =	26.9808	Anisotropy =	7.4674
40	H	Isotropic =	27.5828	Anisotropy =	6.0081
41	H	Isotropic =	30.4347	Anisotropy =	8.2822
42	H	Isotropic =	29.8910	Anisotropy =	5.1117
43	H	Isotropic =	30.2880	Anisotropy =	11.2252
44	H	Isotropic =	28.5242	Anisotropy =	8.2101
45	H	Isotropic =	28.2666	Anisotropy =	6.9360
46	H	Isotropic =	27.0254	Anisotropy =	4.9462
47	H	Isotropic =	26.9052	Anisotropy =	8.3043
48	H	Isotropic =	24.0409	Anisotropy =	4.6312
49	H	Isotropic =	25.7473	Anisotropy =	6.4144
50	H	Isotropic =	23.1380	Anisotropy =	10.2561
51	H	Isotropic =	23.7688	Anisotropy =	5.6922
52	H	Isotropic =	23.7064	Anisotropy =	4.9091
53	H	Isotropic =	23.1406	Anisotropy =	7.8575
54	H	Isotropic =	29.0229	Anisotropy =	8.3000
55	H	Isotropic =	28.2952	Anisotropy =	9.1468
56	H	Isotropic =	27.6968	Anisotropy =	8.7391

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.568721513630	1.989955166674	4.280955301200
C	1.046298813352	2.394724625380	3.101358797341
C	1.848156928326	1.568415153474	2.282943136641
C	2.085927810428	0.260130269479	2.719752949691
C	1.572952093561	-0.165983044383	3.945531924273
C	0.837973531650	0.745521487433	4.699896594406
N	2.480740596678	2.055276596146	1.107143809833
C	1.813480423064	2.669729851669	0.070623006777
C	0.439365046211	3.221730199355	0.292123579821
C	-0.015255617099	3.821424914888	1.491622888116

N	0.719993716510	3.716081991187	2.691000304383
O	2.347159526259	2.785434730101	-1.033836410763
N	-1.143716065248	4.543877944286	1.535116938500
C	-1.885802034826	4.650868454220	0.427866695851
C	-1.580353298336	4.041551012557	-0.795497281449
C	-0.371669123195	3.343216007212	-0.841828422861
C	0.433954425705	4.696544695240	3.758725920914
C	1.674726887608	4.991983275209	4.596985556695
C	-2.495403085218	4.164933496434	-1.991396032001
C	-3.528544297828	3.046351971883	-2.102911367528
O	-2.828363664521	1.815524695780	-2.345270824104
C	-3.548312414464	0.676414782975	-2.465649480510
C	-2.798837636995	-0.519902216886	-2.717828644735
C	-3.488317220955	-1.756923001626	-2.852961370574
N	-4.891774479171	-1.811207936166	-2.743625781282
C	-5.560272969452	-0.666930099889	-2.509252200726
C	-4.925500050071	0.577989780619	-2.367099312962
C	-1.384228597048	-0.527827764671	-2.841047922456
C	-0.703003030850	-1.705565349980	-3.082875870911
C	-1.406922489726	-2.926036093503	-3.211822861509
C	-2.784535112682	-2.953862210163	-3.098678724117
O	-5.505870012166	-2.938677039232	-2.868836530265
C	3.847646847665	1.601525900497	0.821794442059
H	2.689712719473	-0.414779999627	2.112375364048
H	1.755289934851	-1.177916566714	4.309234672634
H	0.445377198486	0.471903579545	5.683927576129
H	-2.788217296632	5.266039181894	0.520882690491
H	-0.009590084449	2.917552349513	-1.778595054124
H	0.091633716155	5.607031375443	3.254352419534
H	-0.392950341830	4.347597995117	4.397322365954
H	2.016796861323	4.104325791462	5.149758368861
H	2.502569867427	5.348843489798	3.963390279932
H	1.440898776177	5.776890388134	5.334020246631
H	-3.054521177727	5.112462315559	-1.938514861021
H	-1.905234727129	4.189783864272	-2.921133234445
H	-4.117623110650	2.958850314909	-1.173561028960
H	-4.218878160990	3.246181881915	-2.939993345451
H	-6.639862628115	-0.785431936398	-2.438434050877
H	-5.558548473489	1.442702325027	-2.179642200810
H	-0.848801376893	0.415409020063	-2.741001600135
H	0.384781181862	-1.694828089871	-3.174544011891
H	-0.859691489081	-3.851392275477	-3.401988151898
H	-3.363721436119	-3.870343858239	-3.191677711468
H	4.379126277580	1.459257273936	1.770725621966
H	3.860696477999	0.659002241332	0.249928273036
H	4.353510330974	2.367397092209	0.222494564113

SCF Done: E(RB3LYP) = -1466.00571246

Zero-point correction= 0.444805
Thermal correction to Energy= 0.472249
Thermal correction to Enthalpy= 0.473193
Thermal correction to Gibbs Free Energy= 0.383694
Sum of electronic and zero-point Energies= -1465.560908
Sum of electronic and thermal Energies= -1465.533464
Sum of electronic and thermal Enthalpies= -1465.532519

Sum of electronic and thermal Free Energies= -1465.622019

1	N	Isotropic =	-42.3145	Anisotropy =	468.2243
2	C	Isotropic =	38.6766	Anisotropy =	117.7963
3	C	Isotropic =	58.5428	Anisotropy =	123.9422
4	C	Isotropic =	63.0250	Anisotropy =	177.8623
5	C	Isotropic =	72.6104	Anisotropy =	159.8950
6	C	Isotropic =	49.0853	Anisotropy =	154.5390
7	N	Isotropic =	122.9172	Anisotropy =	91.9252
8	C	Isotropic =	26.6255	Anisotropy =	109.4111
9	C	Isotropic =	71.9517	Anisotropy =	130.8966
10	C	Isotropic =	32.4459	Anisotropy =	124.1651
11	N	Isotropic =	136.8172	Anisotropy =	64.1627
12	O	Isotropic =	-81.6341	Anisotropy =	583.0236
13	N	Isotropic =	-34.7989	Anisotropy =	441.9780
14	C	Isotropic =	41.6886	Anisotropy =	145.6336
15	C	Isotropic =	61.6186	Anisotropy =	171.4223
16	C	Isotropic =	49.8802	Anisotropy =	180.4441
17	C	Isotropic =	148.6893	Anisotropy =	34.4438
18	C	Isotropic =	177.2296	Anisotropy =	23.9583
19	C	Isotropic =	157.2085	Anisotropy =	16.6018
20	C	Isotropic =	120.9391	Anisotropy =	43.7180
21	O	Isotropic =	208.9159	Anisotropy =	110.6992
22	C	Isotropic =	43.0749	Anisotropy =	123.3498
23	C	Isotropic =	69.2560	Anisotropy =	165.1854
24	C	Isotropic =	50.0947	Anisotropy =	151.2829
25	N	Isotropic =	-24.0556	Anisotropy =	254.6090
26	C	Isotropic =	57.8249	Anisotropy =	113.0532
27	C	Isotropic =	91.5784	Anisotropy =	131.4527
28	C	Isotropic =	69.3256	Anisotropy =	175.8943
29	C	Isotropic =	65.3995	Anisotropy =	175.7859
30	C	Isotropic =	63.6997	Anisotropy =	176.7278
31	C	Isotropic =	73.2851	Anisotropy =	173.6978
32	O	Isotropic =	-29.1095	Anisotropy =	326.8240
33	C	Isotropic =	154.5757	Anisotropy =	45.1616
34	H	Isotropic =	24.0489	Anisotropy =	8.3332
35	H	Isotropic =	24.3939	Anisotropy =	4.5221
36	H	Isotropic =	23.2574	Anisotropy =	4.7912
37	H	Isotropic =	23.0185	Anisotropy =	8.0080
38	H	Isotropic =	23.1090	Anisotropy =	10.2618
39	H	Isotropic =	27.4107	Anisotropy =	6.0321
40	H	Isotropic =	27.1468	Anisotropy =	8.2650
41	H	Isotropic =	30.0337	Anisotropy =	5.1840
42	H	Isotropic =	30.4111	Anisotropy =	8.0296
43	H	Isotropic =	30.2798	Anisotropy =	11.2118
44	H	Isotropic =	28.4322	Anisotropy =	8.2700
45	H	Isotropic =	28.2510	Anisotropy =	5.4868
46	H	Isotropic =	27.6042	Anisotropy =	5.5391
47	H	Isotropic =	27.2205	Anisotropy =	6.2450
48	H	Isotropic =	23.3602	Anisotropy =	5.1962
49	H	Isotropic =	25.0774	Anisotropy =	8.8135
50	H	Isotropic =	23.1902	Anisotropy =	8.9034
51	H	Isotropic =	23.7815	Anisotropy =	6.6704
52	H	Isotropic =	23.6858	Anisotropy =	5.2390
53	H	Isotropic =	23.0343	Anisotropy =	7.5204
54	H	Isotropic =	28.8162	Anisotropy =	7.7355

55 H Isotropic = 27.9035 Anisotropy = 9.8327
56 H Isotropic = 27.4000 Anisotropy = 8.1494

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.383068680542	1.862151886373	-0.307127232160
C	-3.468689599501	2.264868701853	0.578212617147
C	-2.610580253009	3.360989956038	0.339944412941
C	-2.693827890101	3.990053750074	-0.907439726428
C	-3.633589430711	3.552324714170	-1.841571918653
C	-4.473457938738	2.500350432354	-1.482572541249
N	-1.748604989541	3.873046357553	1.347424621859
C	-0.817610286972	3.109850300417	2.015003651444
C	-0.920445743442	1.616946575585	1.966399658350
C	-2.133470250939	0.888489099833	1.995519488098
N	-3.373677142497	1.533337417065	1.795479978879
O	0.091179857661	3.641771591422	2.654023623652
N	-2.160710502903	-0.430434794426	2.231737801604
C	-1.001073430647	-1.086277056829	2.350543591150
C	0.262003362305	-0.492518358331	2.232311795696
C	0.272074440719	0.897193434431	2.086903610844
C	-4.590389918798	0.829953227709	2.250224707085
C	-5.691686886661	1.811821292730	2.639697917596
C	1.531556342502	-1.308347877727	2.246588479466
C	1.996970803602	-1.767397267033	0.857662076486
O	2.340352906362	-0.647108850971	0.019345863576
C	1.500134335839	-0.187942441418	-0.939529372397
C	1.970654697788	0.958614275407	-1.662753200503
C	1.155039216095	1.527425556725	-2.680403617001
N	-0.102709549479	0.973602320347	-2.982346222594
C	-0.504081090901	-0.110629486189	-2.293425838841
C	0.262641648719	-0.706425884333	-1.279453092657
C	3.228547658776	1.564299791105	-1.400591536402
C	3.642476711367	2.671527338766	-2.116286103253
C	2.816341708046	3.221955849203	-3.124603855289
C	1.585763043784	2.658041998344	-3.405002321195
O	-0.842523770812	1.505665921802	-3.897408160481
C	-1.612412947692	5.329492806509	1.469641977118
H	-2.037538387208	4.829729761153	-1.138633753000
H	-3.717706743359	4.028615487324	-2.818900309520
H	-5.253014483819	2.147796569298	-2.164645860501
H	-1.082301906629	-2.161987126277	2.544117642336
H	1.212167061386	1.451150205262	2.087517730816
H	-4.948780386030	0.129925521617	1.478817716835
H	-4.291046500557	0.230792797372	3.117884488967
H	-6.036734122054	2.401226397318	1.777002103987
H	-6.557194705025	1.255863107745	3.034269252463
H	-5.342690004689	2.507099703873	3.420014921043
H	2.345999496153	-0.729311366856	2.709790401804
H	1.394955573374	-2.218251902883	2.854029164794
H	2.927883717545	-2.344061295394	0.955964912323
H	1.251214968266	-2.410390424610	0.369403478450

H	-1.485482898933	-0.484325658001	-2.579398648089
H	-0.170647704897	-1.565582293868	-0.772745484590
H	3.857858801074	1.134257433579	-0.622342317260
H	4.612427540471	3.124969697680	-1.903029001890
H	3.152175386927	4.096884296616	-3.684662324004
H	0.919708163289	3.050214433652	-4.170905462794
H	-2.566653044411	5.798240837482	1.199672798047
H	-1.358932184505	5.572411270384	2.508315199682
H	-0.812814066046	5.726319968975	0.822522216213

SCF Done: E(RB3LYP) = -1466.00122660

Zero-point correction= 0.444911
Thermal correction to Energy= 0.472229
Thermal correction to Enthalpy= 0.473173
Thermal correction to Gibbs Free Energy= 0.385283
Sum of electronic and zero-point Energies= -1465.556316
Sum of electronic and thermal Energies= -1465.528998
Sum of electronic and thermal Enthalpies= -1465.528053
Sum of electronic and thermal Free Energies= -1465.615943

1	N	Isotropic =	-41.4786	Anisotropy =	470.3511
2	C	Isotropic =	38.6148	Anisotropy =	119.3980
3	C	Isotropic =	59.2491	Anisotropy =	126.0584
4	C	Isotropic =	63.1163	Anisotropy =	180.4785
5	C	Isotropic =	72.3133	Anisotropy =	162.3909
6	C	Isotropic =	48.8067	Anisotropy =	156.2367
7	N	Isotropic =	123.3036	Anisotropy =	92.9495
8	C	Isotropic =	27.2414	Anisotropy =	111.1040
9	C	Isotropic =	72.1276	Anisotropy =	133.3491
10	C	Isotropic =	32.2667	Anisotropy =	125.6076
11	N	Isotropic =	138.5044	Anisotropy =	66.8624
12	O	Isotropic =	-78.9172	Anisotropy =	582.8856
13	N	Isotropic =	-35.6229	Anisotropy =	446.9100
14	C	Isotropic =	41.9521	Anisotropy =	148.4819
15	C	Isotropic =	62.7260	Anisotropy =	174.7675
16	C	Isotropic =	51.1730	Anisotropy =	182.7101
17	C	Isotropic =	148.5911	Anisotropy =	34.4259
18	C	Isotropic =	177.4250	Anisotropy =	23.8812
19	C	Isotropic =	155.3268	Anisotropy =	15.8872
20	C	Isotropic =	124.0052	Anisotropy =	53.1638
21	O	Isotropic =	208.0604	Anisotropy =	130.9248
22	C	Isotropic =	42.8649	Anisotropy =	126.6328
23	C	Isotropic =	69.5641	Anisotropy =	167.1780
24	C	Isotropic =	50.4220	Anisotropy =	153.6661
25	N	Isotropic =	-20.9829	Anisotropy =	255.2478
26	C	Isotropic =	59.1148	Anisotropy =	117.1406
27	C	Isotropic =	92.6284	Anisotropy =	140.9654
28	C	Isotropic =	68.8921	Anisotropy =	177.4640
29	C	Isotropic =	65.7081	Anisotropy =	176.3314
30	C	Isotropic =	63.8705	Anisotropy =	177.4811
31	C	Isotropic =	73.5820	Anisotropy =	174.8718
32	O	Isotropic =	-23.9282	Anisotropy =	321.9280
33	C	Isotropic =	155.2667	Anisotropy =	45.8807
34	H	Isotropic =	24.3465	Anisotropy =	6.7939
35	H	Isotropic =	24.3051	Anisotropy =	3.8283

36	H	Isotropic =	23.1341	Anisotropy =	4.7841
37	H	Isotropic =	23.0084	Anisotropy =	7.6689
38	H	Isotropic =	23.9697	Anisotropy =	7.7838
39	H	Isotropic =	27.1336	Anisotropy =	7.7040
40	H	Isotropic =	27.5201	Anisotropy =	5.9741
41	H	Isotropic =	30.0849	Anisotropy =	5.1776
42	H	Isotropic =	30.2757	Anisotropy =	11.3934
43	H	Isotropic =	30.4673	Anisotropy =	8.3969
44	H	Isotropic =	28.3381	Anisotropy =	7.0534
45	H	Isotropic =	28.5066	Anisotropy =	8.3686
46	H	Isotropic =	26.9457	Anisotropy =	8.4400
47	H	Isotropic =	26.9646	Anisotropy =	5.2465
48	H	Isotropic =	24.2128	Anisotropy =	3.9955
49	H	Isotropic =	25.7964	Anisotropy =	6.0668
50	H	Isotropic =	23.1879	Anisotropy =	10.0310
51	H	Isotropic =	23.7793	Anisotropy =	5.5236
52	H	Isotropic =	23.7023	Anisotropy =	5.0390
53	H	Isotropic =	23.1687	Anisotropy =	7.8582
54	H	Isotropic =	29.0734	Anisotropy =	8.2712
55	H	Isotropic =	27.7299	Anisotropy =	9.0764
56	H	Isotropic =	28.3907	Anisotropy =	8.9495

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.424544268177	1.947219210559	-0.319986863506
C	-3.493509591529	2.337979928451	0.553402987445
C	-2.620391419780	3.419755654497	0.301198604322
C	-2.712151102080	4.048994733218	-0.945423174519
C	-3.673010558314	3.626633992403	-1.865246663805
C	-4.524082165197	2.588543176265	-1.493193658146
N	-1.738772368220	3.922719364312	1.296463525156
C	-0.810073436300	3.148423302981	1.954044435327
C	-0.939613645000	1.657357772294	1.918338416455
C	-2.164781337963	0.951458077803	1.969415485607
N	-3.397668079991	1.612213404478	1.772594461418
O	0.116794230029	3.668526549351	2.576596482322
N	-2.212482414093	-0.364201299204	2.221105995826
C	-1.063471924059	-1.040900353519	2.322995139788
C	0.208379935348	-0.471284558232	2.180533462534
C	0.241539813632	0.917045502140	2.025802150552
C	-4.621742155803	0.932571059097	2.244269629256
C	-4.698050051635	0.905799986577	3.768509160583
C	1.463105788433	-1.309897484402	2.184306564501
C	1.909488880046	-1.775753664654	0.791445273188
O	2.269989115790	-0.660543654016	-0.046403861523
C	1.434671844706	-0.183801600264	-1.000992444570
C	1.920784037990	0.959683573013	-1.718737756592
C	1.111677261858	1.546477348160	-2.731357945403
N	-0.154737353107	1.013012590349	-3.033915093245
C	-0.570643727387	-0.069232145848	-2.350535474407
C	0.189103587254	-0.682119947419	-1.341501004301
C	3.188045938160	1.545105802408	-1.455642433460

C	3.616837069089	2.650362271177	-2.165597072918
C	2.796854933572	3.219050823477	-3.168788130992
C	1.557529455063	2.675016699987	-3.449996114765
O	-0.888516417614	1.561238838177	-3.944271492218
C	-1.579366682358	5.377418967033	1.411466563662
H	-2.046802924522	4.878687270107	-1.186537726873
H	-3.763181339841	4.103346694519	-2.841840141873
H	-5.318542235315	2.247212391767	-2.163681372490
H	-1.160997508027	-2.113144552685	2.527755271683
H	1.191359395823	1.453813478256	2.007525924820
H	-5.463744962276	1.501514818457	1.832890872706
H	-4.684323188081	-0.087583005697	1.834591446032
H	-3.879809977477	0.313704808615	4.204456208164
H	-4.651637896002	1.925382716436	4.183554062648
H	-5.650091661780	0.447929761875	4.081902724017
H	2.291613649101	-0.746349445936	2.641689022897
H	1.314513468701	-2.217665068915	2.792060076231
H	2.828950593405	-2.371684096726	0.882275855119
H	1.147219624546	-2.402061092100	0.307255938760
H	-1.557966678952	-0.426774747285	-2.636741649629
H	-0.255891269882	-1.537839442072	-0.839128330315
H	3.812515543399	1.101157978585	-0.681308672322
H	4.593804120960	3.088151137760	-1.951671659652
H	3.144410322200	4.092361251074	-3.724193629619
H	0.895652953427	3.081602703569	-4.211974539946
H	-0.784671376003	5.760660886603	0.750280257116
H	-2.530910807338	5.859189205701	1.155161965970
H	-1.305581038431	5.619772427442	2.445108942984

SCF Done: E(RB3LYP) = -1466.00119879

Zero-point correction= 0.444748
Thermal correction to Energy= 0.472155
Thermal correction to Enthalpy= 0.473099
Thermal correction to Gibbs Free Energy= 0.383409
Sum of electronic and zero-point Energies= -1465.556451
Sum of electronic and thermal Energies= -1465.529044
Sum of electronic and thermal Enthalpies= -1465.528100
Sum of electronic and thermal Free Energies= -1465.617789

1	N	Isotropic =	-40.2656	Anisotropy =	457.7774
2	C	Isotropic =	36.9106	Anisotropy =	122.4564
3	C	Isotropic =	60.6952	Anisotropy =	124.1280
4	C	Isotropic =	63.3408	Anisotropy =	180.1514
5	C	Isotropic =	72.2624	Anisotropy =	162.5374
6	C	Isotropic =	48.7775	Anisotropy =	156.4602
7	N	Isotropic =	123.1897	Anisotropy =	92.3652
8	C	Isotropic =	27.3897	Anisotropy =	111.3505
9	C	Isotropic =	70.9795	Anisotropy =	134.5145
10	C	Isotropic =	33.5622	Anisotropy =	124.6716
11	N	Isotropic =	137.9816	Anisotropy =	67.3113
12	O	Isotropic =	-79.0089	Anisotropy =	583.1770
13	N	Isotropic =	-35.9605	Anisotropy =	457.0483
14	C	Isotropic =	41.9717	Anisotropy =	147.7237
15	C	Isotropic =	62.7767	Anisotropy =	174.2444
16	C	Isotropic =	50.9213	Anisotropy =	183.5709

17	C	Isotropic =	147.5897	Anisotropy =	36.2853
18	C	Isotropic =	177.1431	Anisotropy =	24.3079
19	C	Isotropic =	155.3161	Anisotropy =	15.8875
20	C	Isotropic =	124.0605	Anisotropy =	53.1700
21	O	Isotropic =	208.1054	Anisotropy =	130.8656
22	C	Isotropic =	42.8914	Anisotropy =	126.6459
23	C	Isotropic =	69.5362	Anisotropy =	167.1768
24	C	Isotropic =	50.4282	Anisotropy =	153.7825
25	N	Isotropic =	-21.0553	Anisotropy =	255.1920
26	C	Isotropic =	59.0808	Anisotropy =	117.0940
27	C	Isotropic =	92.6612	Anisotropy =	141.1471
28	C	Isotropic =	68.9106	Anisotropy =	177.5452
29	C	Isotropic =	65.6845	Anisotropy =	176.2411
30	C	Isotropic =	63.8546	Anisotropy =	177.4272
31	C	Isotropic =	73.5496	Anisotropy =	174.8445
32	O	Isotropic =	-24.0238	Anisotropy =	321.8872
33	C	Isotropic =	155.2064	Anisotropy =	46.0297
34	H	Isotropic =	24.3635	Anisotropy =	6.8248
35	H	Isotropic =	24.3127	Anisotropy =	3.8218
36	H	Isotropic =	23.1623	Anisotropy =	4.7745
37	H	Isotropic =	22.9969	Anisotropy =	7.7532
38	H	Isotropic =	23.9477	Anisotropy =	7.7197
39	H	Isotropic =	27.7020	Anisotropy =	5.9835
40	H	Isotropic =	27.0141	Anisotropy =	7.3965
41	H	Isotropic =	29.8973	Anisotropy =	5.2183
42	H	Isotropic =	30.4388	Anisotropy =	8.3948
43	H	Isotropic =	30.2856	Anisotropy =	11.3145
44	H	Isotropic =	28.3276	Anisotropy =	7.0263
45	H	Isotropic =	28.5083	Anisotropy =	8.3499
46	H	Isotropic =	26.9457	Anisotropy =	8.4385
47	H	Isotropic =	26.9617	Anisotropy =	5.2492
48	H	Isotropic =	24.2071	Anisotropy =	4.0103
49	H	Isotropic =	25.7923	Anisotropy =	6.1082
50	H	Isotropic =	23.1807	Anisotropy =	10.0333
51	H	Isotropic =	23.7796	Anisotropy =	5.5311
52	H	Isotropic =	23.7016	Anisotropy =	5.0150
53	H	Isotropic =	23.1657	Anisotropy =	7.8335
54	H	Isotropic =	28.3915	Anisotropy =	8.9297
55	H	Isotropic =	29.0646	Anisotropy =	8.4346
56	H	Isotropic =	27.7303	Anisotropy =	9.0493

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.818877754192	-0.575715022899	0.229337249891
C	-3.542061304101	-0.951963670664	0.121575970960
C	-2.850903681595	-0.947973109239	-1.110411457562
C	-3.533448056441	-0.467358774340	-2.233879000115
C	-4.862643116159	-0.059119606677	-2.115955911425
C	-5.467986619969	-0.154478291792	-0.865131826008
N	-1.547221411216	-1.497004848359	-1.247044973696
C	-0.466841616121	-1.119180766820	-0.480899289051
C	-0.686328194315	-0.386046852495	0.806321188958

C	-1.767262552127	-0.604207717341	1.694536063640
N	-2.888381751386	-1.371569651532	1.312453779910
O	0.679442316004	-1.394028777781	-0.839333222128
N	-1.760652994180	-0.122296216478	2.945124588969
C	-0.730112429490	0.632988265701	3.340737195337
C	0.359488586456	0.978180669416	2.531886337397
C	0.368961728258	0.417014369511	1.252333142056
C	-3.742882658925	-1.916678472328	2.387448832772
C	-4.388776681293	-3.236614476734	1.975615671274
C	1.460240214744	1.883736023704	3.033306223279
C	1.303638749118	3.343648385210	2.614186642382
O	1.487688256221	3.420418483408	1.190999183185
C	1.369125187465	4.625641725593	0.587791127625
C	1.600618478009	4.647956526973	-0.827272586063
C	1.487968765783	5.879362198813	-1.530581640119
N	1.154386703983	7.066378892308	-0.849372212422
C	0.950839657614	7.006201025223	0.479609243543
C	1.050178705482	5.815740086789	1.218529699203
C	1.944916114683	3.486340803432	-1.567917181972
C	2.160577861995	3.555805328229	-2.931116119985
C	2.041290933573	4.789911575789	-3.612589026695
C	1.709104126921	5.940534807637	-2.921862875882
O	1.052492098339	8.176145310774	-1.498873559804
C	-1.245562363491	-2.263887118223	-2.462334589067
H	-3.032338199049	-0.434302123625	-3.201737234716
H	-5.415952357835	0.308736320795	-2.980845620188
H	-6.518932495305	0.117726994911	-0.728233758689
H	-0.774822509747	0.989215957632	4.376312173567
H	1.222975828166	0.555872806736	0.588902879441
H	-3.086751212703	-2.068956634040	3.251716392542
H	-4.509354912334	-1.183894216869	2.685594518464
H	-5.081281108652	-3.106886297503	1.130685109227
H	-3.624514099343	-3.977008998279	1.689604960112
H	-4.964212662059	-3.643763006461	2.822411877744
H	1.483741167990	1.865544423003	4.134138916695
H	2.441641513136	1.524965193378	2.683714802930
H	0.301925252814	3.723473465931	2.879041498768
H	2.062284302785	3.969890549949	3.113771102062
H	0.700347105551	7.961065780119	0.937871315350
H	0.866455418513	5.875217627544	2.289225023294
H	2.038408819075	2.539949078878	-1.037089849899
H	2.425182747082	2.653518834890	-3.485799589589
H	2.213523843214	4.834517564679	-4.689738369098
H	1.608925080712	6.909400804502	-3.406889685288
H	-0.458114403091	-2.990912514345	-2.231993280184
H	-2.153360877865	-2.787916854516	-2.785588697578
H	-0.883771540701	-1.618785862118	-3.279941153355

SCF Done: E(RB3LYP) = -1466.00571173

Zero-point correction= 0.444867
Thermal correction to Energy= 0.472264
Thermal correction to Enthalpy= 0.473209
Thermal correction to Gibbs Free Energy= 0.384329
Sum of electronic and zero-point Energies= -1465.560845
Sum of electronic and thermal Energies= -1465.533447

Sum of electronic and thermal Enthalpies= -1465.532503
Sum of electronic and thermal Free Energies= -1465.621383

1	N	Isotropic =	-41.8627	Anisotropy =	469.0711
2	C	Isotropic =	38.7949	Anisotropy =	117.4432
3	C	Isotropic =	58.5698	Anisotropy =	123.8404
4	C	Isotropic =	62.7142	Anisotropy =	177.8424
5	C	Isotropic =	72.5874	Anisotropy =	160.0292
6	C	Isotropic =	49.1272	Anisotropy =	154.2708
7	N	Isotropic =	122.9020	Anisotropy =	92.4439
8	C	Isotropic =	26.6795	Anisotropy =	109.4655
9	C	Isotropic =	71.9593	Anisotropy =	130.9871
10	C	Isotropic =	32.4188	Anisotropy =	124.1180
11	N	Isotropic =	137.1502	Anisotropy =	63.8208
12	O	Isotropic =	-81.2601	Anisotropy =	582.9983
13	N	Isotropic =	-35.0897	Anisotropy =	440.7254
14	C	Isotropic =	41.6077	Anisotropy =	143.2645
15	C	Isotropic =	61.3465	Anisotropy =	171.7601
16	C	Isotropic =	50.1075	Anisotropy =	181.6959
17	C	Isotropic =	148.6646	Anisotropy =	34.3784
18	C	Isotropic =	177.3077	Anisotropy =	23.7405
19	C	Isotropic =	157.3641	Anisotropy =	15.8593
20	C	Isotropic =	120.8823	Anisotropy =	44.7646
21	O	Isotropic =	208.3087	Anisotropy =	106.9878
22	C	Isotropic =	43.0018	Anisotropy =	123.1151
23	C	Isotropic =	69.1548	Anisotropy =	165.4084
24	C	Isotropic =	50.0452	Anisotropy =	151.6176
25	N	Isotropic =	-24.1391	Anisotropy =	254.2834
26	C	Isotropic =	57.8883	Anisotropy =	113.3762
27	C	Isotropic =	91.4563	Anisotropy =	131.5810
28	C	Isotropic =	69.1571	Anisotropy =	175.8234
29	C	Isotropic =	65.2959	Anisotropy =	175.8715
30	C	Isotropic =	63.7292	Anisotropy =	176.7191
31	C	Isotropic =	73.1596	Anisotropy =	173.8274
32	O	Isotropic =	-29.2276	Anisotropy =	327.8458
33	C	Isotropic =	154.5309	Anisotropy =	45.2977
34	H	Isotropic =	24.0842	Anisotropy =	8.3636
35	H	Isotropic =	24.4006	Anisotropy =	4.6177
36	H	Isotropic =	23.2639	Anisotropy =	4.7923
37	H	Isotropic =	23.0527	Anisotropy =	7.9175
38	H	Isotropic =	23.0812	Anisotropy =	10.3933
39	H	Isotropic =	27.4304	Anisotropy =	5.9633
40	H	Isotropic =	27.1433	Anisotropy =	8.3188
41	H	Isotropic =	30.0269	Anisotropy =	5.1399
42	H	Isotropic =	30.4032	Anisotropy =	8.0679
43	H	Isotropic =	30.2754	Anisotropy =	11.2130
44	H	Isotropic =	28.4922	Anisotropy =	8.3190
45	H	Isotropic =	28.2033	Anisotropy =	5.5034
46	H	Isotropic =	27.6215	Anisotropy =	5.3686
47	H	Isotropic =	27.2274	Anisotropy =	6.4056
48	H	Isotropic =	23.3610	Anisotropy =	5.2036
49	H	Isotropic =	25.0624	Anisotropy =	8.8501
50	H	Isotropic =	23.0947	Anisotropy =	8.9692
51	H	Isotropic =	23.7271	Anisotropy =	6.5916
52	H	Isotropic =	23.6579	Anisotropy =	5.1638
53	H	Isotropic =	23.0027	Anisotropy =	7.5215

54	H	Isotropic =	27.4187	Anisotropy =	8.1030
55	H	Isotropic =	28.8325	Anisotropy =	7.7459
56	H	Isotropic =	27.9355	Anisotropy =	9.7788

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.712991846595	4.456903555531	0.895979768201
C	-2.882262339173	3.136647698113	1.000450541218
C	-2.275150518353	2.371389003807	2.020319136725
C	-1.410973029412	3.032863395185	2.900304364569
C	-1.216259135301	4.408972782508	2.775108343293
C	-1.912126109179	5.080095902518	1.771857956544
N	-2.582834382503	0.997269776732	2.213869446460
C	-2.453971287705	0.041673317844	1.231666365973
C	-2.342960795498	0.467706097338	-0.199180346381
C	-3.043820616066	1.552463260692	-0.778860589699
N	-3.704598369929	2.506560947442	0.024732093107
O	-2.438577745275	-1.156302871557	1.517772078357
N	-3.130485338305	1.708120421334	-2.107202253633
C	-2.457305568561	0.866479040960	-2.899486390337
C	-1.643836932730	-0.176458380183	-2.438956523236
C	-1.645457321490	-0.386963205496	-1.057708685872
C	-4.740606805838	3.341231841064	-0.617201058155
C	-5.816875756254	3.763064153561	0.379140908522
C	-0.804261430364	-1.011311469883	-3.374654740256
C	0.616534044691	-0.469848970453	-3.585704403622
O	1.362631180583	-0.464184437795	-2.353250353023
C	1.558590344270	0.671715369330	-1.640514890239
C	2.259789013876	0.498850750927	-0.400474212300
C	2.507697281840	1.629373613979	0.427204580506
N	2.074018115485	2.910137581162	0.038109828459
C	1.432250943492	3.035737535956	-1.138200222390
C	1.161333604466	1.951295291778	-1.987575896170
C	2.717945656530	-0.768681076750	0.048212307892
C	3.384896396507	-0.893459180761	1.252049806348
C	3.621650063738	0.243450692603	2.060412148681
C	3.188153181852	1.491887571724	1.654844213842
O	2.291010873190	3.928321607556	0.802229119106
C	-2.733830387259	0.507015631972	3.589191594265
H	-0.907833843189	2.474531958788	3.690407346652
H	-0.550279853072	4.945900008499	3.451338808671
H	-1.824941763971	6.164933629940	1.658837400298
H	-2.565430834343	1.039717544359	-3.976266953738
H	-1.120937256167	-1.239442878825	-0.623443380714
H	-4.288544445841	4.222925174728	-1.098767655577
H	-5.179093828866	2.726966421640	-1.411916620108
H	-5.411409655192	4.414592612210	1.167606035847
H	-6.605533575410	4.324083058831	-0.147340483914
H	-6.278390156459	2.883731215800	0.856492707547
H	-0.728404458726	-2.041690799530	-2.992785437085
H	-1.276978844248	-1.068023065236	-4.369024441875
H	1.171750411873	-1.144910361515	-4.252657015949

H	0.606824973180	0.527526816457	-4.046444098918
H	1.126412512393	4.053115229918	-1.374704420333
H	0.619027044144	2.167532603271	-2.905048696810
H	2.531001568990	-1.638819505459	-0.579937636060
H	3.731127521062	-1.874804412777	1.582203515056
H	4.149466363845	0.134569961449	3.009890496605
H	3.347757017168	2.390963238372	2.246542259513
H	-3.414086928946	-0.352877911442	3.582745253939
H	-1.773762720080	0.177629866345	4.019776205052
H	-3.154504232873	1.309712345440	4.207192775146

SCF Done: E(RB3LYP) = -1466.00116251

Zero-point correction= 0.444724
Thermal correction to Energy= 0.472150
Thermal correction to Enthalpy= 0.473094
Thermal correction to Gibbs Free Energy= 0.384391
Sum of electronic and zero-point Energies= -1465.556439
Sum of electronic and thermal Energies= -1465.529013
Sum of electronic and thermal Enthalpies= -1465.528069
Sum of electronic and thermal Free Energies= -1465.616771

1	N	Isotropic =	-41.8150	Anisotropy =	470.3834
2	C	Isotropic =	38.3545	Anisotropy =	119.5228
3	C	Isotropic =	59.0664	Anisotropy =	126.1298
4	C	Isotropic =	63.0758	Anisotropy =	180.3726
5	C	Isotropic =	72.5187	Anisotropy =	162.1824
6	C	Isotropic =	48.8592	Anisotropy =	155.9290
7	N	Isotropic =	123.6045	Anisotropy =	93.1423
8	C	Isotropic =	27.3368	Anisotropy =	110.9323
9	C	Isotropic =	72.3171	Anisotropy =	133.3077
10	C	Isotropic =	32.4562	Anisotropy =	125.5788
11	N	Isotropic =	137.9777	Anisotropy =	66.7096
12	O	Isotropic =	-79.2472	Anisotropy =	581.9343
13	N	Isotropic =	-35.1871	Anisotropy =	446.4144
14	C	Isotropic =	42.2338	Anisotropy =	148.3271
15	C	Isotropic =	62.9796	Anisotropy =	174.3529
16	C	Isotropic =	50.8019	Anisotropy =	183.4186
17	C	Isotropic =	148.6964	Anisotropy =	34.5093
18	C	Isotropic =	177.4638	Anisotropy =	23.9666
19	C	Isotropic =	155.4843	Anisotropy =	15.9812
20	C	Isotropic =	124.3515	Anisotropy =	52.8284
21	O	Isotropic =	208.5499	Anisotropy =	130.8319
22	C	Isotropic =	43.0272	Anisotropy =	126.7264
23	C	Isotropic =	69.5179	Anisotropy =	167.3488
24	C	Isotropic =	50.3482	Anisotropy =	154.1213
25	N	Isotropic =	-21.1723	Anisotropy =	255.3910
26	C	Isotropic =	59.0190	Anisotropy =	117.2530
27	C	Isotropic =	92.8330	Anisotropy =	141.4676
28	C	Isotropic =	69.0895	Anisotropy =	177.9979
29	C	Isotropic =	65.7153	Anisotropy =	175.9150
30	C	Isotropic =	63.7271	Anisotropy =	177.4647
31	C	Isotropic =	73.4935	Anisotropy =	175.1305
32	O	Isotropic =	-24.1081	Anisotropy =	322.0520
33	C	Isotropic =	155.1556	Anisotropy =	46.1617
34	H	Isotropic =	24.3790	Anisotropy =	6.7747

35	H	Isotropic =	24.3343	Anisotropy =	3.8633
36	H	Isotropic =	23.1550	Anisotropy =	4.7556
37	H	Isotropic =	23.0291	Anisotropy =	7.6375
38	H	Isotropic =	23.9212	Anisotropy =	7.7208
39	H	Isotropic =	27.1585	Anisotropy =	7.7405
40	H	Isotropic =	27.5063	Anisotropy =	5.9530
41	H	Isotropic =	30.0622	Anisotropy =	5.2062
42	H	Isotropic =	30.2802	Anisotropy =	11.4255
43	H	Isotropic =	30.4724	Anisotropy =	8.3981
44	H	Isotropic =	28.3440	Anisotropy =	7.1251
45	H	Isotropic =	28.5309	Anisotropy =	8.3906
46	H	Isotropic =	26.9625	Anisotropy =	8.4769
47	H	Isotropic =	26.9728	Anisotropy =	5.3263
48	H	Isotropic =	24.1549	Anisotropy =	4.0244
49	H	Isotropic =	25.7316	Anisotropy =	6.2766
50	H	Isotropic =	23.1896	Anisotropy =	9.9315
51	H	Isotropic =	23.7992	Anisotropy =	5.4772
52	H	Isotropic =	23.7045	Anisotropy =	4.9743
53	H	Isotropic =	23.1849	Anisotropy =	7.6554
54	H	Isotropic =	27.7644	Anisotropy =	9.0913
55	H	Isotropic =	28.3951	Anisotropy =	8.8864
56	H	Isotropic =	29.0686	Anisotropy =	8.3094

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.097547280097	-0.370617348903	3.367999994706
C	-2.034636696773	-0.678256724533	2.069939786832
C	-0.867303441205	-1.201116809209	1.469758090843
C	0.267750119310	-1.341809568078	2.276656413430
C	0.202570796669	-1.010444659431	3.630604900023
C	-1.011825735615	-0.549858510390	4.133404635481
N	-0.851885963592	-1.668032395458	0.127315505870
C	-1.227815326269	-0.904460614155	-0.955513038305
C	-2.073445977273	0.313941800491	-0.750085426982
C	-3.088959292384	0.444854118873	0.228117322970
N	-3.208317914985	-0.466030323261	1.297826813555
O	-0.894905125156	-1.230275411681	-2.095965828898
N	-4.005404911649	1.422295872173	0.166461284360
C	-3.907005617014	2.339875788945	-0.800480534207
C	-2.897735180694	2.365818627589	-1.771742823583
C	-1.996832071260	1.298513287574	-1.741454393202
C	-4.500584679812	-0.517749488900	2.013563299372
C	-5.594642676154	-1.151580006946	1.158096724887
C	-2.816986789326	3.464295468459	-2.804395445401
C	-1.919332423845	4.642039189575	-2.413424012965
O	-0.540771619983	4.228531656104	-2.335766010700
C	0.146822600414	4.240772172300	-1.168892579270
C	1.561565688975	4.035090511782	-1.291658851731
C	2.370029759250	4.017419022061	-0.121141002258
N	1.793915347917	4.203120929832	1.149377819954
C	0.463466062296	4.393473584530	1.225310686879
C	-0.376535959424	4.414367148907	0.100566453438

C	2.200871474435	3.848551505634	-2.546309539048
C	3.566934321287	3.654320307319	-2.621107150988
C	4.353179807784	3.638354240832	-1.444693572353
C	3.763600145028	3.818354819295	-0.207388478567
O	2.535813967793	4.187247945068	2.205343868576
C	-0.092251343357	-2.888518154834	-0.170784481961
H	1.192613938985	-1.731913119938	1.850811725431
H	1.072872120118	-1.121288380169	4.278491924734
H	-1.124552057580	-0.308313103539	5.194645689321
H	-4.689340800903	3.107448229781	-0.806929376202
H	-1.240098493374	1.185699116889	-2.519099269563
H	-4.326969113401	-1.119539836931	2.912713812208
H	-4.801201429426	0.488128174272	2.344696126562
H	-6.524179494896	-1.225794314200	1.745418716633
H	-5.809409049346	-0.550186158015	0.262348726901
H	-5.306966577344	-2.165843373549	0.837846421618
H	-2.451617448436	3.055550212194	-3.760029559829
H	-3.821064997275	3.877474729449	-2.995098595503
H	-1.954819672192	5.408317936100	-3.202566227977
H	-2.246133310250	5.106503873767	-1.473368336254
H	0.087537598058	4.524985194415	2.238206615303
H	-1.439858036603	4.558030158295	0.279567942412
H	1.587956637480	3.862899333724	-3.446768974093
H	4.043313900096	3.513096684592	-3.593243556569
H	5.431772814867	3.484146910889	-1.514192503051
H	4.331129372066	3.814923629560	0.721005431240
H	0.965633510993	-2.674729553694	-0.396178085851
H	-0.152110668351	-3.562446993781	0.692630866946
H	-0.534212808578	-3.370197331676	-1.050769945176

SCF Done: E(RB3LYP) = -1466.00157017

Zero-point correction= 0.444665
Thermal correction to Energy= 0.472163
Thermal correction to Enthalpy= 0.473108
Thermal correction to Gibbs Free Energy= 0.383095
Sum of electronic and zero-point Energies= -1465.556905
Sum of electronic and thermal Energies= -1465.529407
Sum of electronic and thermal Enthalpies= -1465.528463
Sum of electronic and thermal Free Energies= -1465.618476

1	N	Isotropic =	-40.9785	Anisotropy =	455.8321
2	C	Isotropic =	37.1108	Anisotropy =	121.5704
3	C	Isotropic =	60.1162	Anisotropy =	123.0874
4	C	Isotropic =	63.2379	Anisotropy =	178.7924
5	C	Isotropic =	72.4857	Anisotropy =	161.1419
6	C	Isotropic =	49.1037	Anisotropy =	155.1874
7	N	Isotropic =	123.5920	Anisotropy =	91.8227
8	C	Isotropic =	27.2171	Anisotropy =	109.6378
9	C	Isotropic =	71.2391	Anisotropy =	133.3606
10	C	Isotropic =	33.7396	Anisotropy =	124.4633
11	N	Isotropic =	135.8440	Anisotropy =	65.5790
12	O	Isotropic =	-81.4644	Anisotropy =	583.4281
13	N	Isotropic =	-35.2167	Anisotropy =	455.6397
14	C	Isotropic =	41.5601	Anisotropy =	146.9144
15	C	Isotropic =	62.9373	Anisotropy =	172.2497

16	C	Isotropic =	50.0971	Anisotropy =	183.5475
17	C	Isotropic =	147.5010	Anisotropy =	36.8906
18	C	Isotropic =	177.1408	Anisotropy =	24.3575
19	C	Isotropic =	155.5934	Anisotropy =	16.6525
20	C	Isotropic =	122.4185	Anisotropy =	55.0914
21	O	Isotropic =	210.7762	Anisotropy =	125.4450
22	C	Isotropic =	42.9645	Anisotropy =	124.4758
23	C	Isotropic =	69.2344	Anisotropy =	166.6678
24	C	Isotropic =	50.1363	Anisotropy =	152.7267
25	N	Isotropic =	-22.2419	Anisotropy =	254.3194
26	C	Isotropic =	58.4655	Anisotropy =	115.6296
27	C	Isotropic =	92.5012	Anisotropy =	137.4393
28	C	Isotropic =	69.0396	Anisotropy =	177.3356
29	C	Isotropic =	65.5716	Anisotropy =	175.3081
30	C	Isotropic =	63.9795	Anisotropy =	176.8208
31	C	Isotropic =	73.3065	Anisotropy =	174.4984
32	O	Isotropic =	-26.0551	Anisotropy =	323.6275
33	C	Isotropic =	154.8153	Anisotropy =	45.6287
34	H	Isotropic =	24.2901	Anisotropy =	7.8296
35	H	Isotropic =	24.3971	Anisotropy =	3.9986
36	H	Isotropic =	23.2385	Anisotropy =	4.6282
37	H	Isotropic =	22.9444	Anisotropy =	7.9945
38	H	Isotropic =	23.6749	Anisotropy =	9.0253
39	H	Isotropic =	27.5759	Anisotropy =	5.9931
40	H	Isotropic =	26.9749	Anisotropy =	7.4634
41	H	Isotropic =	30.2959	Anisotropy =	11.1939
42	H	Isotropic =	29.8645	Anisotropy =	5.1066
43	H	Isotropic =	30.4184	Anisotropy =	8.3133
44	H	Isotropic =	28.2756	Anisotropy =	6.8770
45	H	Isotropic =	28.5134	Anisotropy =	8.1524
46	H	Isotropic =	26.9060	Anisotropy =	8.2246
47	H	Isotropic =	27.0118	Anisotropy =	4.7704
48	H	Isotropic =	23.9024	Anisotropy =	4.9507
49	H	Isotropic =	25.6132	Anisotropy =	6.7908
50	H	Isotropic =	23.1565	Anisotropy =	10.3110
51	H	Isotropic =	23.7945	Anisotropy =	5.7466
52	H	Isotropic =	23.7275	Anisotropy =	4.8439
53	H	Isotropic =	23.1327	Anisotropy =	7.7942
54	H	Isotropic =	28.2412	Anisotropy =	9.2812
55	H	Isotropic =	28.9983	Anisotropy =	8.2632
56	H	Isotropic =	27.6630	Anisotropy =	8.6626

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.018953280234	-2.009636682449	-1.394795626136
C	-2.529957524325	-1.101824441431	-0.559167591657
C	-2.201575042564	-1.065443834677	0.814611407156
C	-1.262889553601	-1.993440983263	1.280306899093
C	-0.723264113110	-2.935194163884	0.403304366330
C	-1.151866947505	-2.915776178492	-0.921634653471
N	-2.861295476601	-0.198834667141	1.727710905906
C	-2.938230404372	1.167363902823	1.572112420356

C	-2.696857472146	1.778243155998	0.226543696024
C	-3.065301981790	1.194998800008	-1.010161542963
N	-3.441956034216	-0.160241351174	-1.107477738552
O	-3.228211595290	1.890025518284	2.526670523261
N	-3.103265821470	1.911430297482	-2.143402560332
C	-2.705068236845	3.187021190558	-2.115383972488
C	-2.232608161771	3.846637077822	-0.973285634396
C	-2.274952037770	3.112342434642	0.214424862854
C	-4.196523625451	-0.577732626754	-2.308094793611
C	-5.619151979452	-0.024075171940	-2.302015853714
C	-1.738331466709	5.272185873358	-1.026475942730
C	-0.231462864288	5.419905708379	-1.259797011855
O	0.521524155124	4.916031115973	-0.138605818517
C	1.279609713933	3.797537020019	-0.235476815143
C	2.181883213663	3.571261684733	0.856504918601
C	3.009131401286	2.413735520515	0.851392103271
N	2.951711473710	1.497774664645	-0.215749007854
C	2.092915553734	1.743563403966	-1.222895098173
C	1.252340788669	2.867214025868	-1.259797008299
C	2.290705775405	4.463274969247	1.956733509004
C	3.172899004881	4.207492740450	2.988945489366
C	3.984812883994	3.048749349110	2.966354852212
C	3.906070540005	2.160638671819	1.909920291184
O	3.708097101680	0.452166559471	-0.212742133353
C	-3.190497056002	-0.720396542780	3.060143415653
H	-0.974125287268	-1.993501550948	2.331754716987
H	0.002103790552	-3.672990267034	0.748247833938
H	-0.784778369702	-3.653830754041	-1.641236344933
H	-2.768320828187	3.724267344695	-3.068687348947
H	-2.017775477123	3.578395607174	1.166705890367
H	-3.666392330227	-0.274587378334	-3.224070460963
H	-4.216549292384	-1.673241384526	-2.289730866929
H	-5.627105454314	1.074724925003	-2.352573387334
H	-6.166263866152	-0.406424262950	-3.178897003471
H	-6.160001287845	-0.336887049701	-1.394458692828
H	-2.241408611421	5.815203625609	-1.843444135087
H	-1.993586458232	5.793884947605	-0.090355223879
H	0.087157666254	4.936691215837	-2.194051715693
H	0.023959484127	6.488200575107	-1.325262137816
H	2.097727746039	0.990889109226	-2.009014844221
H	0.580460121448	2.957198928301	-2.110543356402
H	1.662615460691	5.353330724420	1.966278087475
H	3.245072898397	4.903458234182	3.826997354500
H	4.678140993276	2.855157836441	3.787189548606
H	4.512908261592	1.259192254930	1.852692980204
H	-2.362048107552	-0.585404508461	3.774935981741
H	-4.060632646605	-0.175519480669	3.444519081700
H	-3.427569335935	-1.787935733046	2.974263185955

SCF Done: E(RB3LYP) = -1466.00146055

Zero-point correction= 0.444771
Thermal correction to Energy= 0.472216
Thermal correction to Enthalpy= 0.473161
Thermal correction to Gibbs Free Energy= 0.383467
Sum of electronic and zero-point Energies= -1465.556689

Sum of electronic and thermal Energies= -1465.529244
Sum of electronic and thermal Enthalpies= -1465.528300
Sum of electronic and thermal Free Energies= -1465.617994

1	N	Isotropic =	-40.5824	Anisotropy =	456.4829
2	C	Isotropic =	37.2678	Anisotropy =	121.2380
3	C	Isotropic =	60.0937	Anisotropy =	122.9817
4	C	Isotropic =	63.1322	Anisotropy =	178.6189
5	C	Isotropic =	72.3594	Anisotropy =	161.2033
6	C	Isotropic =	49.0772	Anisotropy =	155.3669
7	N	Isotropic =	123.3759	Anisotropy =	91.8519
8	C	Isotropic =	27.2576	Anisotropy =	109.4175
9	C	Isotropic =	71.0588	Anisotropy =	133.5864
10	C	Isotropic =	33.7807	Anisotropy =	124.3163
11	N	Isotropic =	135.8926	Anisotropy =	65.7872
12	O	Isotropic =	-81.5321	Anisotropy =	582.9171
13	N	Isotropic =	-35.9851	Anisotropy =	454.9172
14	C	Isotropic =	41.6486	Anisotropy =	146.9943
15	C	Isotropic =	62.7678	Anisotropy =	172.8427
16	C	Isotropic =	50.2161	Anisotropy =	183.9822
17	C	Isotropic =	147.4166	Anisotropy =	36.8496
18	C	Isotropic =	177.1708	Anisotropy =	24.3334
19	C	Isotropic =	155.7118	Anisotropy =	16.0981
20	C	Isotropic =	121.7081	Anisotropy =	56.9079
21	O	Isotropic =	209.6149	Anisotropy =	126.9603
22	C	Isotropic =	42.3999	Anisotropy =	125.2284
23	C	Isotropic =	69.2954	Anisotropy =	166.3957
24	C	Isotropic =	50.2642	Anisotropy =	152.2577
25	N	Isotropic =	-22.1902	Anisotropy =	254.1721
26	C	Isotropic =	58.6389	Anisotropy =	115.5489
27	C	Isotropic =	91.8566	Anisotropy =	136.8795
28	C	Isotropic =	69.0811	Anisotropy =	176.8772
29	C	Isotropic =	65.4151	Anisotropy =	175.4974
30	C	Isotropic =	63.6939	Anisotropy =	176.8383
31	C	Isotropic =	73.4952	Anisotropy =	174.2916
32	O	Isotropic =	-25.9404	Anisotropy =	324.3843
33	C	Isotropic =	154.6782	Anisotropy =	45.8076
34	H	Isotropic =	24.2749	Anisotropy =	7.7968
35	H	Isotropic =	24.3676	Anisotropy =	3.9285
36	H	Isotropic =	23.2095	Anisotropy =	4.6453
37	H	Isotropic =	22.9314	Anisotropy =	7.9328
38	H	Isotropic =	23.6992	Anisotropy =	8.9869
39	H	Isotropic =	26.9861	Anisotropy =	7.4541
40	H	Isotropic =	27.5506	Anisotropy =	5.9908
41	H	Isotropic =	29.8459	Anisotropy =	5.1599
42	H	Isotropic =	30.2785	Anisotropy =	11.1995
43	H	Isotropic =	30.4104	Anisotropy =	8.3183
44	H	Isotropic =	28.4695	Anisotropy =	8.1488
45	H	Isotropic =	28.2750	Anisotropy =	6.9822
46	H	Isotropic =	27.0687	Anisotropy =	4.7775
47	H	Isotropic =	26.8566	Anisotropy =	8.1812
48	H	Isotropic =	24.0106	Anisotropy =	5.0278
49	H	Isotropic =	25.7694	Anisotropy =	6.2988
50	H	Isotropic =	23.1737	Anisotropy =	10.3703
51	H	Isotropic =	23.7935	Anisotropy =	5.7267
52	H	Isotropic =	23.7239	Anisotropy =	4.9151

53	H	Isotropic =	23.1522	Anisotropy =	7.9597
54	H	Isotropic =	28.2401	Anisotropy =	9.3025
55	H	Isotropic =	27.6574	Anisotropy =	8.7276
56	H	Isotropic =	28.9853	Anisotropy =	8.2842

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.559020450996	1.418462825784	2.800329493377
C	0.608096607871	2.353686113935	2.732165790361
C	-0.505924940195	2.368035114971	3.600256601080
C	-0.624795311236	1.318400776516	4.518614607929
C	0.362586598614	0.334255609263	4.578599931905
C	1.447211217832	0.441736865576	3.711247091361
N	-1.431990404405	3.445800408072	3.622952069406
C	-2.115889404155	3.894035812673	2.514837175322
C	-1.623210249784	3.545305090591	1.144497129654
C	-0.261129308967	3.430061803987	0.772329365849
N	0.762319296184	3.359837080693	1.739349653646
O	-3.119432770208	4.597159979717	2.642010055721
N	0.119224685362	3.417195708101	-0.513306398230
C	-0.818544867656	3.442345697711	-1.465813140632
C	-2.197638018864	3.464348723656	-1.221738306344
C	-2.576335918114	3.553924247481	0.120077472219
C	2.141079756304	3.661617523308	1.301656359835
C	2.966733935195	4.277804278242	2.427624803199
C	-3.204133190977	3.419703112204	-2.346487585245
C	-3.694208490567	2.015794814587	-2.716230051767
O	-2.637548504965	1.230946648293	-3.303319796973
C	-2.057577485901	0.202667728264	-2.639770559434
C	-1.168950738464	-0.606198904432	-3.423837923447
C	-0.503134458471	-1.706022612296	-2.814547910811
N	-0.713871726739	-2.006494557825	-1.455771181481
C	-1.555065985698	-1.225730494346	-0.752309426452
C	-2.230543157993	-0.126897505282	-1.306775039108
C	-0.920702935801	-0.355703735930	-4.799802393908
C	-0.055554843102	-1.157804809638	-5.519082451651
C	0.598702077393	-2.245669212388	-4.893861122886
C	0.378384770397	-2.519034558160	-3.556765671403
O	-0.106375448817	-3.007167391511	-0.912170778256
C	-1.942880280885	3.890523088225	4.925556305662
H	-1.476457804445	1.284208708679	5.198600694187
H	0.294647178482	-0.486672644444	5.293431964685
H	2.265052222175	-0.284506230451	3.743171870243
H	-0.448095991874	3.441605790830	-2.496826803085
H	-3.625062385494	3.675818947851	0.397367082641
H	2.631779546555	2.756906550260	0.909112652592
H	2.049290906804	4.367345618508	0.468649350726
H	3.114098823184	3.574314746407	3.260574862370
H	3.961181882559	4.555273946474	2.042842615915
H	2.482578481101	5.186688241097	2.819647193752
H	-4.096354058278	4.008300080065	-2.076143651575
H	-2.777721746093	3.881303292728	-3.251244475463

H	-4.138468234565	1.495723415989	-1.855676464517
H	-4.462755184952	2.093746801293	-3.499377418527
H	-1.664929346734	-1.513197258546	0.291628793214
H	-2.871096903119	0.448712428918	-0.642374291807
H	-1.428581561763	0.483866329348	-5.272913166370
H	0.124466196709	-0.951975861738	-6.576038439712
H	1.280806841347	-2.873466334414	-5.470565296563
H	0.859834883559	-3.345794789357	-3.038376795904
H	-1.153734318936	3.765290466510	5.676998542323
H	-2.221207847849	4.948252609383	4.850562284231
H	-2.837352532557	3.325209874568	5.235314728146

SCF Done: E(RB3LYP) = -1466.00156015

Zero-point correction= 0.444818
Thermal correction to Energy= 0.472235
Thermal correction to Enthalpy= 0.473179
Thermal correction to Gibbs Free Energy= 0.383985
Sum of electronic and zero-point Energies= -1465.556742
Sum of electronic and thermal Energies= -1465.529325
Sum of electronic and thermal Enthalpies= -1465.528381
Sum of electronic and thermal Free Energies= -1465.617575

1	N	Isotropic =	-42.8923	Anisotropy =	469.6888
2	C	Isotropic =	38.8629	Anisotropy =	118.2110
3	C	Isotropic =	58.6008	Anisotropy =	123.7942
4	C	Isotropic =	62.6957	Anisotropy =	177.4650
5	C	Isotropic =	72.3775	Anisotropy =	160.3483
6	C	Isotropic =	48.9121	Anisotropy =	154.9241
7	N	Isotropic =	123.1546	Anisotropy =	92.0583
8	C	Isotropic =	26.8143	Anisotropy =	107.8620
9	C	Isotropic =	71.4025	Anisotropy =	132.7223
10	C	Isotropic =	32.3856	Anisotropy =	125.9134
11	N	Isotropic =	136.5135	Anisotropy =	65.5943
12	O	Isotropic =	-81.3643	Anisotropy =	581.8707
13	N	Isotropic =	-33.5736	Anisotropy =	443.2369
14	C	Isotropic =	40.9834	Anisotropy =	149.3258
15	C	Isotropic =	62.8525	Anisotropy =	172.5400
16	C	Isotropic =	51.6810	Anisotropy =	180.8974
17	C	Isotropic =	148.7246	Anisotropy =	34.1737
18	C	Isotropic =	177.4422	Anisotropy =	24.3608
19	C	Isotropic =	155.2494	Anisotropy =	15.7335
20	C	Isotropic =	122.3758	Anisotropy =	55.5014
21	O	Isotropic =	207.6728	Anisotropy =	128.7232
22	C	Isotropic =	42.6075	Anisotropy =	124.6144
23	C	Isotropic =	69.2500	Anisotropy =	165.6962
24	C	Isotropic =	50.2450	Anisotropy =	152.0128
25	N	Isotropic =	-22.2433	Anisotropy =	253.0563
26	C	Isotropic =	58.7193	Anisotropy =	114.7488
27	C	Isotropic =	92.2027	Anisotropy =	136.8961
28	C	Isotropic =	68.9656	Anisotropy =	176.8793
29	C	Isotropic =	65.4643	Anisotropy =	174.7565
30	C	Isotropic =	63.8226	Anisotropy =	176.5461
31	C	Isotropic =	73.3948	Anisotropy =	173.7039
32	O	Isotropic =	-25.9418	Anisotropy =	322.6720
33	C	Isotropic =	154.5974	Anisotropy =	45.3654

34	H	Isotropic =	23.9022	Anisotropy =	8.5613
35	H	Isotropic =	24.2093	Anisotropy =	4.3160
36	H	Isotropic =	23.1796	Anisotropy =	4.3640
37	H	Isotropic =	23.3716	Anisotropy =	6.3173
38	H	Isotropic =	23.3600	Anisotropy =	10.0104
39	H	Isotropic =	27.3807	Anisotropy =	7.4898
40	H	Isotropic =	27.5513	Anisotropy =	5.6223
41	H	Isotropic =	30.0846	Anisotropy =	5.2561
42	H	Isotropic =	30.3602	Anisotropy =	11.1850
43	H	Isotropic =	30.4780	Anisotropy =	8.5561
44	H	Isotropic =	28.5471	Anisotropy =	7.8927
45	H	Isotropic =	28.2422	Anisotropy =	7.0745
46	H	Isotropic =	27.0531	Anisotropy =	4.4222
47	H	Isotropic =	26.8951	Anisotropy =	7.9608
48	H	Isotropic =	24.0957	Anisotropy =	5.2306
49	H	Isotropic =	25.8249	Anisotropy =	6.0670
50	H	Isotropic =	23.1458	Anisotropy =	10.5723
51	H	Isotropic =	23.7869	Anisotropy =	5.7688
52	H	Isotropic =	23.7086	Anisotropy =	5.0194
53	H	Isotropic =	23.1105	Anisotropy =	8.2045
54	H	Isotropic =	28.7955	Anisotropy =	7.8138
55	H	Isotropic =	27.4387	Anisotropy =	8.5680
56	H	Isotropic =	27.9033	Anisotropy =	9.9569

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.561841965552	1.478835936742	2.365848029977
C	-3.634417785596	2.100428505644	1.186160317001
C	-3.616348618876	3.507892098110	1.067139904943
C	-3.451196389317	4.254373177834	2.239731517705
C	-3.358874777590	3.602178826911	3.469929726469
C	-3.442940030420	2.211903898846	3.481563871813
N	-3.853294640299	4.164580805300	-0.170745246824
C	-3.141961526299	3.917851056301	-1.323769107506
C	-2.329691105240	2.665555456318	-1.444347119937
C	-2.688929794478	1.406334373627	-0.904880775661
N	-3.738568542306	1.280607650568	0.029176392229
O	-3.181065039254	4.712623732177	-2.264384372692
N	-2.074058748835	0.276267989520	-1.281121554231
C	-1.055790809241	0.350779928434	-2.144590918792
C	-0.560859341062	1.543123178076	-2.687381269326
C	-1.252829602849	2.705354914049	-2.336566057790
C	-4.338382641345	-0.057831287611	0.209251736369
C	-5.815086162318	0.035197286108	0.583115625012
C	0.631602023574	1.557908239858	-3.613619503887
C	1.970987402599	1.827822387148	-2.922256825882
O	2.317602684066	0.740632586838	-2.041806876032
C	2.361516141210	0.892393277602	-0.696788031679
C	2.913708075126	-0.218231110580	0.024987194669
C	2.996576976218	-0.158874963025	1.444068078406
N	2.547105394674	0.978729424813	2.140210342677
C	2.033417234595	2.000000149924	1.429704432953

C	1.925533797369	1.986779758831	0.029943251422
C	3.388620129921	-1.390196061535	-0.622036444425
C	3.912183594377	-2.438596257981	0.110148768968
C	3.983943866157	-2.360641174325	1.521196344647
C	3.532510093516	-1.233971290681	2.182901208540
O	2.630155999184	1.025225338945	3.427468057680
C	-4.670809574277	5.384160942488	-0.160250575465
H	-3.417830634538	5.343198407946	2.191582324458
H	-3.240252718651	4.165173684055	4.396453337934
H	-3.413655008092	1.655972615194	4.423577179357
H	-0.599665511765	-0.605228922387	-2.424101781766
H	-0.994199054830	3.666650983108	-2.784494851760
H	-4.221211598584	-0.576494881440	-0.748728523521
H	-3.781491404585	-0.636101978449	0.963350680164
H	-6.242533834222	-0.978436395007	0.645131823634
H	-5.959679962639	0.520563429469	1.559809437564
H	-6.379057035418	0.601841887971	-0.175137147342
H	0.706926717809	0.595052348048	-4.143245915869
H	0.503884211447	2.337892553161	-4.382403299661
H	2.772696360916	1.863667199274	-3.675073074646
H	1.966855806679	2.786041176276	-2.385231473280
H	1.700784510924	2.842364506147	2.033332551317
H	1.479162504627	2.860429430536	-0.439840241401
H	3.329868888412	-1.441689576191	-1.708569714259
H	4.273330015007	-3.332361897623	-0.402328763757
H	4.398812916952	-3.194427255810	2.090971029013
H	3.570540733433	-1.133084664912	3.265679606372
H	-4.063460192706	6.288463455790	0.009543103905
H	-5.162229093523	5.485339341210	-1.134950824141
H	-5.425892934088	5.297785778360	0.630554416336

SCF Done: E(RB3LYP) = -1466.00158637

Zero-point correction= 0.444841
Thermal correction to Energy= 0.472269
Thermal correction to Enthalpy= 0.473213
Thermal correction to Gibbs Free Energy= 0.383814
Sum of electronic and zero-point Energies= -1465.556746
Sum of electronic and thermal Energies= -1465.529318
Sum of electronic and thermal Enthalpies= -1465.528373
Sum of electronic and thermal Free Energies= -1465.617772

1	N	Isotropic =	-42.0494	Anisotropy =	470.2229
2	C	Isotropic =	38.5542	Anisotropy =	118.8357
3	C	Isotropic =	58.6836	Anisotropy =	124.0106
4	C	Isotropic =	62.7822	Anisotropy =	177.7624
5	C	Isotropic =	72.5968	Anisotropy =	160.6017
6	C	Isotropic =	49.1190	Anisotropy =	155.1186
7	N	Isotropic =	122.8085	Anisotropy =	91.6669
8	C	Isotropic =	26.8624	Anisotropy =	108.3413
9	C	Isotropic =	71.0726	Anisotropy =	133.3971
10	C	Isotropic =	32.3973	Anisotropy =	124.8996
11	N	Isotropic =	137.1764	Anisotropy =	65.3662
12	O	Isotropic =	-80.4150	Anisotropy =	582.4747
13	N	Isotropic =	-33.9670	Anisotropy =	442.2567
14	C	Isotropic =	40.8352	Anisotropy =	148.4237

15	C	Isotropic =	62.8851	Anisotropy =	172.7101
16	C	Isotropic =	51.5884	Anisotropy =	181.9753
17	C	Isotropic =	148.8239	Anisotropy =	34.3766
18	C	Isotropic =	177.5009	Anisotropy =	24.2368
19	C	Isotropic =	155.3742	Anisotropy =	16.1229
20	C	Isotropic =	122.7418	Anisotropy =	54.3553
21	O	Isotropic =	209.3244	Anisotropy =	126.3711
22	C	Isotropic =	42.7768	Anisotropy =	124.1866
23	C	Isotropic =	69.2579	Anisotropy =	165.9351
24	C	Isotropic =	50.2131	Anisotropy =	151.8160
25	N	Isotropic =	-21.9213	Anisotropy =	253.1868
26	C	Isotropic =	58.7329	Anisotropy =	114.6743
27	C	Isotropic =	92.6231	Anisotropy =	136.7889
28	C	Isotropic =	68.9838	Anisotropy =	176.7944
29	C	Isotropic =	65.4930	Anisotropy =	175.4446
30	C	Isotropic =	63.7857	Anisotropy =	176.6523
31	C	Isotropic =	73.5517	Anisotropy =	173.7668
32	O	Isotropic =	-25.6801	Anisotropy =	322.2480
33	C	Isotropic =	154.5812	Anisotropy =	45.6242
34	H	Isotropic =	23.9371	Anisotropy =	8.4963
35	H	Isotropic =	24.2478	Anisotropy =	4.2434
36	H	Isotropic =	23.2297	Anisotropy =	4.3618
37	H	Isotropic =	23.3375	Anisotropy =	6.4854
38	H	Isotropic =	23.3358	Anisotropy =	10.0292
39	H	Isotropic =	27.5980	Anisotropy =	5.6394
40	H	Isotropic =	27.3696	Anisotropy =	7.5258
41	H	Isotropic =	30.3640	Anisotropy =	11.1996
42	H	Isotropic =	30.1035	Anisotropy =	5.2356
43	H	Isotropic =	30.4810	Anisotropy =	8.5335
44	H	Isotropic =	28.2730	Anisotropy =	7.0747
45	H	Isotropic =	28.5365	Anisotropy =	7.9214
46	H	Isotropic =	26.9261	Anisotropy =	7.9863
47	H	Isotropic =	26.9813	Anisotropy =	4.3514
48	H	Isotropic =	23.9891	Anisotropy =	5.1519
49	H	Isotropic =	25.6549	Anisotropy =	6.5632
50	H	Isotropic =	23.1502	Anisotropy =	10.5402
51	H	Isotropic =	23.7728	Anisotropy =	5.8220
52	H	Isotropic =	23.7087	Anisotropy =	4.9839
53	H	Isotropic =	23.1203	Anisotropy =	8.0909
54	H	Isotropic =	27.9120	Anisotropy =	9.9334
55	H	Isotropic =	27.4346	Anisotropy =	8.5465
56	H	Isotropic =	28.8183	Anisotropy =	7.7721

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.127945058330	-0.507972099174	3.022103997175
C	-1.313099762976	0.069544722159	2.809507895388
C	-1.758647662017	1.184202052719	3.555100446057
C	-0.881837256445	1.718519660931	4.506289437375
C	0.360689788794	1.119984399206	4.719023788819
C	0.680847243921	-0.007436996900	3.966604048268
N	-3.079305872622	1.695970044640	3.433910877366

C	-3.641288690405	2.098145153642	2.242967091763
C	-3.043281925399	1.642742323107	0.947993780443
C	-2.458513863042	0.372569913398	0.723571223516
N	-2.131447270198	-0.489167096508	1.791297848036
O	-4.644549470894	2.812960593201	2.233548070363
N	-2.215233880297	-0.082769641486	-0.513767912878
C	-2.456396555122	0.718570970593	-1.556363557427
C	-2.949392774216	2.025693026710	-1.455620687693
C	-3.275583203390	2.455554939152	-0.166690054454
C	-1.933305886325	-1.920234560706	1.479433947360
C	-3.250581136755	-2.608125948436	1.130333750582
C	-3.139973906587	2.899065227949	-2.672410335324
C	-1.970826280245	3.841620825265	-2.975595542633
O	-0.797702611279	3.105608558785	-3.374394851251
C	0.289412522872	3.005588639400	-2.572717992593
C	1.450458328929	2.426756071388	-3.185824870102
C	2.640692518533	2.271498617389	-2.421965631326
N	2.687621685203	2.685427787978	-1.077648950625
C	1.579159194523	3.224482256209	-0.536747887947
C	0.380139328031	3.393358453667	-1.247124737760
C	1.466537369395	1.997562470199	-4.539777775292
C	2.606006642873	1.444489337185	-5.092090528564
C	3.778924538317	1.296287496173	-4.314543291791
C	3.798706717596	1.705418254387	-2.994250207096
O	3.772893715041	2.543177640290	-0.393655513113
C	-3.767181976023	2.129403990812	4.656535614546
H	-1.181287832808	2.586246194153	5.094852738088
H	1.054673685063	1.515130784397	5.461809061133
H	1.627599181730	-0.534188357004	4.119750222485
H	-2.245196782901	0.290848113320	-2.542623294282
H	-3.756573386851	3.422044421658	-0.004971375921
H	-1.204183778911	-2.042003371371	0.663701606014
H	-1.497025394652	-2.371048272273	2.377975873647
H	-3.694955642665	-2.192651827360	0.213738760271
H	-3.071464660766	-3.682280334895	0.961413574503
H	-3.979049411873	-2.504321426381	1.950455279492
H	-3.312901624885	2.271860772377	-3.561257111215
H	-4.034865190711	3.530865262136	-2.546553516246
H	-2.225312565634	4.469990174825	-3.841966785894
H	-1.747876607582	4.505901828247	-2.128835725700
H	1.686218467158	3.515604907084	0.506469775229
H	-0.460099337573	3.822094386782	-0.705694800530
H	0.559319664450	2.115466240776	-5.131149305131
H	2.602307803158	1.120161135616	-6.134540138217
H	4.674079874360	0.857571853622	-4.759762314654
H	4.679714786052	1.611663844946	-2.362566619895
H	-3.551132272682	3.182208927640	4.902343712096
H	-4.848440942032	2.033195929114	4.503537690001
H	-3.449912580906	1.488241729269	5.488051205540

SCF Done: E(RB3LYP) = -1466.00159945

Zero-point correction= 0.444805
Thermal correction to Energy= 0.472218
Thermal correction to Enthalpy= 0.473162
Thermal correction to Gibbs Free Energy= 0.383951

Sum of electronic and zero-point Energies= -1465.556794
Sum of electronic and thermal Energies= -1465.529381
Sum of electronic and thermal Enthalpies= -1465.528437
Sum of electronic and thermal Free Energies= -1465.617649

1	N	Isotropic =	-40.9789	Anisotropy =	455.7666
2	C	Isotropic =	36.8607	Anisotropy =	121.4430
3	C	Isotropic =	60.0296	Anisotropy =	122.2650
4	C	Isotropic =	62.8167	Anisotropy =	177.2388
5	C	Isotropic =	72.4994	Anisotropy =	160.5586
6	C	Isotropic =	49.0985	Anisotropy =	155.0122
7	N	Isotropic =	123.0125	Anisotropy =	91.7491
8	C	Isotropic =	26.9324	Anisotropy =	108.1792
9	C	Isotropic =	70.0265	Anisotropy =	134.4087
10	C	Isotropic =	33.5762	Anisotropy =	124.5852
11	N	Isotropic =	136.3283	Anisotropy =	65.9787
12	O	Isotropic =	-81.0332	Anisotropy =	581.8738
13	N	Isotropic =	-34.4886	Anisotropy =	454.4549
14	C	Isotropic =	41.0238	Anisotropy =	148.1597
15	C	Isotropic =	62.8212	Anisotropy =	172.6872
16	C	Isotropic =	51.2468	Anisotropy =	182.3757
17	C	Isotropic =	147.7407	Anisotropy =	36.4578
18	C	Isotropic =	177.1438	Anisotropy =	24.5954
19	C	Isotropic =	155.3009	Anisotropy =	16.0549
20	C	Isotropic =	122.3534	Anisotropy =	55.1387
21	O	Isotropic =	208.0585	Anisotropy =	128.3744
22	C	Isotropic =	42.5304	Anisotropy =	124.5187
23	C	Isotropic =	69.2522	Anisotropy =	165.7557
24	C	Isotropic =	50.2352	Anisotropy =	151.6876
25	N	Isotropic =	-22.2099	Anisotropy =	253.1355
26	C	Isotropic =	58.8232	Anisotropy =	114.5345
27	C	Isotropic =	92.2261	Anisotropy =	136.5567
28	C	Isotropic =	68.9609	Anisotropy =	176.8206
29	C	Isotropic =	65.4858	Anisotropy =	175.1990
30	C	Isotropic =	63.6737	Anisotropy =	176.4564
31	C	Isotropic =	73.3826	Anisotropy =	173.8278
32	O	Isotropic =	-25.8549	Anisotropy =	322.5460
33	C	Isotropic =	154.4757	Anisotropy =	45.7167
34	H	Isotropic =	23.9246	Anisotropy =	8.5702
35	H	Isotropic =	24.2258	Anisotropy =	4.2771
36	H	Isotropic =	23.2351	Anisotropy =	4.2993
37	H	Isotropic =	23.3419	Anisotropy =	6.5581
38	H	Isotropic =	23.3066	Anisotropy =	9.9968
39	H	Isotropic =	27.2367	Anisotropy =	7.0406
40	H	Isotropic =	27.6678	Anisotropy =	5.8235
41	H	Isotropic =	29.9937	Anisotropy =	4.9510
42	H	Isotropic =	30.3939	Anisotropy =	11.1224
43	H	Isotropic =	30.4564	Anisotropy =	8.6412
44	H	Isotropic =	28.2601	Anisotropy =	7.0708
45	H	Isotropic =	28.5190	Anisotropy =	7.8798
46	H	Isotropic =	26.8881	Anisotropy =	7.9582
47	H	Isotropic =	27.0361	Anisotropy =	4.3730
48	H	Isotropic =	24.0979	Anisotropy =	5.2403
49	H	Isotropic =	25.8033	Anisotropy =	6.1562
50	H	Isotropic =	23.1617	Anisotropy =	10.6082
51	H	Isotropic =	23.7885	Anisotropy =	5.8093

52	H	Isotropic =	23.7146	Anisotropy =	5.0070
53	H	Isotropic =	23.1202	Anisotropy =	8.2033
54	H	Isotropic =	27.8928	Anisotropy =	9.9435
55	H	Isotropic =	27.4318	Anisotropy =	8.5257
56	H	Isotropic =	28.7919	Anisotropy =	7.9565

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.573325913057	1.994747834319	3.693793993521
C	-0.693224506993	0.784087484272	3.143064074259
C	0.378447971926	-0.135256189241	3.090584719369
C	1.616504339479	0.285169950644	3.590283837680
C	1.742135877337	1.554697968373	4.155893395074
C	0.609611823282	2.363812485341	4.204955341720
N	0.204952086871	-1.474502823946	2.646931930800
C	-0.326303674454	-1.817599776016	1.423818288571
C	-1.128408489924	-0.814767739168	0.653357638305
C	-1.990436007696	0.151836705238	1.226479817726
N	-1.963256037702	0.440028313477	2.607101702996
O	-0.165689415678	-2.950465641883	0.967192545648
N	-2.893902568734	0.815274999743	0.491343626367
C	-2.927953866227	0.611382583115	-0.829612565265
C	-2.073455257380	-0.256095813653	-1.521115979848
C	-1.188780088275	-0.996632033577	-0.732448328147
C	-3.142628933225	1.115903661096	3.187797929454
C	-4.351847811377	0.186090851278	3.247656286319
C	-2.134349176749	-0.401449284560	-3.022862357109
C	-1.096563706907	0.423806242610	-3.789030386187
O	-1.357168898711	1.834870317509	-3.653422994393
C	-0.537190748752	2.649766733998	-2.948259452040
C	-0.814770720697	4.052144320552	-3.072664295935
C	-0.008323522256	4.989911542404	-2.369485216294
N	1.056290441501	4.552801434072	-1.559314250103
C	1.283509189052	3.229564631404	-1.463058121815
C	0.513704759728	2.265783418603	-2.133559770169
C	-1.872141166552	4.553827808393	-3.877515332452
C	-2.106568564237	5.912471871475	-3.969599160222
C	-1.293346374556	6.828791975215	-3.261559268119
C	-0.254691688943	6.374844981700	-2.470252472403
O	1.784832801654	5.411529461585	-0.928541333506
C	0.913064640028	-2.538182574979	3.370095538469
H	2.472926909845	-0.389061884464	3.558534614783
H	2.695386341769	1.897827163741	4.559721624149
H	0.646794100606	3.354054472820	4.668955426756
H	-3.691557951210	1.174655058865	-1.377286049444
H	-0.552531081020	-1.764547107617	-1.176547253067
H	-2.850969421619	1.423841292299	4.198302338226
H	-3.383970437267	2.029478301682	2.622819281993
H	-5.191665955969	0.705526729949	3.736853065480
H	-4.681681502541	-0.115150065621	2.242397461631
H	-4.122710095271	-0.722197964513	3.827761088270
H	-1.976666441023	-1.455354789630	-3.306649108684

H	-3.134855892696	-0.118441628786	-3.386152218614
H	-0.070980141768	0.180404445191	-3.478694298074
H	-1.184277809163	0.213656775352	-4.865397506495
H	2.116458722445	2.964411097546	-0.814665722703
H	0.774726081791	1.222513546286	-1.970968266215
H	-2.493293240884	3.841480138563	-4.419197160418
H	-2.923471594441	6.281808275696	-4.592607733980
H	-1.486609940312	7.900407364151	-3.340610095333
H	0.394464510851	7.044821346484	-1.910052647952
H	0.975033236358	-2.264554779129	4.430515982848
H	0.350257788747	-3.472266559186	3.258572474311
H	1.928687020990	-2.703936929069	2.974435320259

SCF Done: E(RB3LYP) = -1466.00160865

Zero-point correction= 0.444904
Thermal correction to Energy= 0.472290
Thermal correction to Enthalpy= 0.473234
Thermal correction to Gibbs Free Energy= 0.384389
Sum of electronic and zero-point Energies= -1465.556705
Sum of electronic and thermal Energies= -1465.529319
Sum of electronic and thermal Enthalpies= -1465.528375
Sum of electronic and thermal Free Energies= -1465.617220

1	N	Isotropic =	-40.4741	Anisotropy =	456.7713
2	C	Isotropic =	37.1191	Anisotropy =	121.5143
3	C	Isotropic =	59.9253	Anisotropy =	122.1050
4	C	Isotropic =	62.9930	Anisotropy =	177.6638
5	C	Isotropic =	72.2914	Anisotropy =	160.6230
6	C	Isotropic =	49.1090	Anisotropy =	155.5727
7	N	Isotropic =	123.0651	Anisotropy =	91.3789
8	C	Isotropic =	26.9925	Anisotropy =	108.0498
9	C	Isotropic =	70.0095	Anisotropy =	134.7354
10	C	Isotropic =	33.6177	Anisotropy =	124.6483
11	N	Isotropic =	136.3291	Anisotropy =	65.9175
12	O	Isotropic =	-81.0399	Anisotropy =	581.4975
13	N	Isotropic =	-34.7228	Anisotropy =	453.8626
14	C	Isotropic =	40.9588	Anisotropy =	147.4989
15	C	Isotropic =	62.9280	Anisotropy =	172.1792
16	C	Isotropic =	51.2941	Anisotropy =	183.7527
17	C	Isotropic =	147.6113	Anisotropy =	36.4503
18	C	Isotropic =	177.2013	Anisotropy =	24.5307
19	C	Isotropic =	155.3639	Anisotropy =	15.9650
20	C	Isotropic =	122.6280	Anisotropy =	54.5478
21	O	Isotropic =	208.3737	Anisotropy =	128.4173
22	C	Isotropic =	42.8057	Anisotropy =	124.3650
23	C	Isotropic =	69.3088	Anisotropy =	165.9129
24	C	Isotropic =	50.2054	Anisotropy =	151.9399
25	N	Isotropic =	-22.1020	Anisotropy =	253.1291
26	C	Isotropic =	58.7547	Anisotropy =	114.8058
27	C	Isotropic =	92.4469	Anisotropy =	136.3014
28	C	Isotropic =	68.9936	Anisotropy =	176.6495
29	C	Isotropic =	65.5845	Anisotropy =	175.3105
30	C	Isotropic =	63.9311	Anisotropy =	177.2977
31	C	Isotropic =	73.3238	Anisotropy =	173.9460
32	O	Isotropic =	-25.5583	Anisotropy =	322.1288

33	C	Isotropic =	154.5306	Anisotropy =	45.7927
34	H	Isotropic =	23.9463	Anisotropy =	8.5525
35	H	Isotropic =	24.2527	Anisotropy =	4.2288
36	H	Isotropic =	23.2548	Anisotropy =	4.3267
37	H	Isotropic =	23.3077	Anisotropy =	6.7057
38	H	Isotropic =	23.2880	Anisotropy =	10.0360
39	H	Isotropic =	27.6913	Anisotropy =	5.8183
40	H	Isotropic =	27.2391	Anisotropy =	7.0818
41	H	Isotropic =	30.3907	Anisotropy =	11.1533
42	H	Isotropic =	29.9906	Anisotropy =	4.9250
43	H	Isotropic =	30.4617	Anisotropy =	8.6182
44	H	Isotropic =	28.5143	Anisotropy =	7.8861
45	H	Isotropic =	28.2832	Anisotropy =	7.0171
46	H	Isotropic =	26.9745	Anisotropy =	4.2692
47	H	Isotropic =	26.9121	Anisotropy =	7.9394
48	H	Isotropic =	24.0285	Anisotropy =	5.2377
49	H	Isotropic =	25.7044	Anisotropy =	6.3530
50	H	Isotropic =	23.1723	Anisotropy =	10.6036
51	H	Isotropic =	23.7754	Anisotropy =	5.8558
52	H	Isotropic =	23.6953	Anisotropy =	5.0072
53	H	Isotropic =	23.1136	Anisotropy =	8.1664
54	H	Isotropic =	28.8118	Anisotropy =	7.9520
55	H	Isotropic =	27.4387	Anisotropy =	8.4967
56	H	Isotropic =	27.9054	Anisotropy =	9.9220

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.269331420932	-2.282127633521	-0.743377979537
C	-2.331203814882	-1.658947122711	-0.024215207790
C	-1.438854955465	-2.361157225868	0.816199422464
C	-1.516301352387	-3.759379395416	0.824447089531
C	-2.486882413720	-4.405448149894	0.059303381829
C	-3.358151277748	-3.616992720378	-0.689722722163
N	-0.559937333048	-1.694033991172	1.712112643231
C	0.346900896686	-0.733607122245	1.330250853114
C	0.194874647058	-0.040884464106	0.011371103902
C	-1.041964469928	0.304269722483	-0.588199202682
N	-2.259231511018	-0.245014805137	-0.140656386446
O	1.268799517272	-0.409723577274	2.082609315011
N	-1.108104366268	1.188902943924	-1.594976629482
C	0.019277043752	1.733726990400	-2.058831176360
C	1.300746345366	1.441119268602	-1.575079211188
C	1.356935218931	0.532574679422	-0.516971400190
C	-3.516035116498	0.498908717911	-0.374783901657
C	-4.036105039137	1.144673958405	0.910952175380
C	2.519826097148	2.183211524754	-2.071154351385
C	2.946256155337	3.348944217085	-1.164670200871
O	1.934662054009	4.373584462577	-1.100856525431
C	0.966046242933	4.345232205409	-0.151436028217
C	-0.170920714268	5.181328054812	-0.405590127939
C	-1.259317669719	5.177510473179	0.511323056334
N	-1.225155880415	4.360576899729	1.654202260197

C	-0.117204684581	3.636001529472	1.891019967657
C	0.981390349618	3.608401154651	1.020092906426
C	-0.271084572781	6.008120157086	-1.556353108535
C	-1.390396543769	6.789796886921	-1.768881297607
C	-2.460117973577	6.775346542475	-0.842426718880
C	-2.399817980458	5.975577636997	0.283407493793
O	-2.247477334537	4.307767527589	2.446572541774
C	-0.385967213917	-2.257827679592	3.056754103089
H	-0.834456049459	-4.337227323083	1.449194300288
H	-2.572330956929	-5.492694507125	0.059910966738
H	-4.161631601467	-4.071442343065	-1.277409035548
H	-0.103615080029	2.460664209709	-2.869555484984
H	2.305600885756	0.299866485968	-0.029549406281
H	-3.321569971208	1.255354299891	-1.143130365218
H	-4.250941818217	-0.206426627609	-0.780336172271
H	-5.006542816458	1.630666295591	0.712930426882
H	-4.193262350185	0.391062343849	1.700255167638
H	-3.350435875922	1.915142320145	1.300935464526
H	3.384403747724	1.502646146278	-2.145071207459
H	2.332931832041	2.579744821058	-3.081321862834
H	3.219998011446	3.003422627467	-0.157225421394
H	3.822871612310	3.850677647530	-1.596912799316
H	-0.155361522271	3.040388609125	2.801056165041
H	1.807682094038	2.955709349925	1.291508486542
H	0.555983812811	6.011453910833	-2.265378449459
H	-1.451243552059	7.421942684769	-2.656899328548
H	-3.339581251546	7.397764956677	-1.018805221166
H	-3.202172787227	5.931786953709	1.017188171513
H	-1.328135884209	-2.724085779623	3.369736355207
H	0.422467137416	-3.006589991176	3.090397883495
H	-0.124248545412	-1.446488757412	3.746035229234

SCF Done: E(RB3LYP) = -1465.99966881

Zero-point correction= 0.444833
Thermal correction to Energy= 0.472214
Thermal correction to Enthalpy= 0.473158
Thermal correction to Gibbs Free Energy= 0.384300
Sum of electronic and zero-point Energies= -1465.554835
Sum of electronic and thermal Energies= -1465.527455
Sum of electronic and thermal Enthalpies= -1465.526511
Sum of electronic and thermal Free Energies= -1465.615369

1	N	Isotropic =	-42.2224	Anisotropy = 458.6832
2	C	Isotropic =	38.3568	Anisotropy = 118.2000
3	C	Isotropic =	58.1829	Anisotropy = 121.2403
4	C	Isotropic =	62.1406	Anisotropy = 176.8869
5	C	Isotropic =	72.0112	Anisotropy = 158.5759
6	C	Isotropic =	49.4218	Anisotropy = 153.3077
7	N	Isotropic =	123.1081	Anisotropy = 91.4042
8	C	Isotropic =	26.4010	Anisotropy = 109.4663
9	C	Isotropic =	69.8056	Anisotropy = 138.5691
10	C	Isotropic =	33.9887	Anisotropy = 127.0911
11	N	Isotropic =	136.9578	Anisotropy = 63.6039
12	O	Isotropic =	-82.6321	Anisotropy = 575.8375
13	N	Isotropic =	-33.8554	Anisotropy = 444.7313

14	C	Isotropic =	41.0189	Anisotropy =	150.6100
15	C	Isotropic =	63.7465	Anisotropy =	172.4272
16	C	Isotropic =	50.1875	Anisotropy =	189.3089
17	C	Isotropic =	152.5891	Anisotropy =	46.2615
18	C	Isotropic =	176.1912	Anisotropy =	24.2930
19	C	Isotropic =	155.6688	Anisotropy =	13.3549
20	C	Isotropic =	124.3152	Anisotropy =	53.8833
21	O	Isotropic =	208.4140	Anisotropy =	139.8172
22	C	Isotropic =	42.6902	Anisotropy =	127.0174
23	C	Isotropic =	69.0134	Anisotropy =	167.7996
24	C	Isotropic =	50.4406	Anisotropy =	153.3954
25	N	Isotropic =	-20.7397	Anisotropy =	253.9106
26	C	Isotropic =	57.8954	Anisotropy =	118.6146
27	C	Isotropic =	90.1023	Anisotropy =	147.0879
28	C	Isotropic =	68.8332	Anisotropy =	177.2833
29	C	Isotropic =	65.7761	Anisotropy =	175.8807
30	C	Isotropic =	63.7785	Anisotropy =	177.4512
31	C	Isotropic =	73.4520	Anisotropy =	174.2128
32	O	Isotropic =	-13.8194	Anisotropy =	297.5621
33	C	Isotropic =	154.3692	Anisotropy =	45.6174
34	H	Isotropic =	23.9990	Anisotropy =	9.2209
35	H	Isotropic =	24.3345	Anisotropy =	4.3680
36	H	Isotropic =	23.2550	Anisotropy =	4.7915
37	H	Isotropic =	23.7512	Anisotropy =	4.5545
38	H	Isotropic =	23.2928	Anisotropy =	9.7525
39	H	Isotropic =	27.0411	Anisotropy =	5.9316
40	H	Isotropic =	26.9817	Anisotropy =	9.1873
41	H	Isotropic =	30.7167	Anisotropy =	10.4568
42	H	Isotropic =	30.4891	Anisotropy =	6.0139
43	H	Isotropic =	30.3170	Anisotropy =	9.6415
44	H	Isotropic =	28.5729	Anisotropy =	8.2602
45	H	Isotropic =	28.4998	Anisotropy =	7.2267
46	H	Isotropic =	26.5632	Anisotropy =	5.0741
47	H	Isotropic =	26.9194	Anisotropy =	7.9627
48	H	Isotropic =	23.6361	Anisotropy =	4.6672
49	H	Isotropic =	25.2946	Anisotropy =	5.8393
50	H	Isotropic =	23.1303	Anisotropy =	10.2069
51	H	Isotropic =	23.7215	Anisotropy =	5.6023
52	H	Isotropic =	23.6392	Anisotropy =	5.0478
53	H	Isotropic =	23.0198	Anisotropy =	8.1567
54	H	Isotropic =	28.8047	Anisotropy =	7.4557
55	H	Isotropic =	27.9268	Anisotropy =	10.4160
56	H	Isotropic =	27.3836	Anisotropy =	7.2629

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.171307996314	4.066987476272	0.830384372957
C	-4.257411743911	3.184545982296	1.242569222426
C	-4.083343170669	2.855135349390	2.605963330346
C	-4.872125084176	3.533909093761	3.541950694631
C	-5.818545173077	4.463348230708	3.109084921013
C	-5.945545384127	4.676844520906	1.738678976799

N	-3.222230610100	1.805628036739	3.027888531913
C	-1.890736516055	1.726787545715	2.693390576327
C	-1.362929119038	2.528772963366	1.545298293139
C	-2.066136599923	2.785935164013	0.343302197688
N	-3.455805355814	2.571086561023	0.242198491780
O	-1.129564117991	0.978859416513	3.310930549685
N	-1.440599455243	3.222068772477	-0.759323052875
C	-0.129339188244	3.479525812989	-0.699525579494
C	0.654449739313	3.343942866592	0.452340416072
C	0.000097342225	2.837048204683	1.577757793836
C	-4.035153109152	2.467274978672	-1.113781740120
C	-3.630537298011	1.166006831926	-1.801818134920
C	2.133944271497	3.648285483276	0.452838500059
C	3.038306849264	2.412133588222	0.456379560098
O	2.939345436469	1.692028270726	-0.787986248320
C	2.331344868638	0.485030748445	-0.872431355936
C	2.495925281738	-0.192269303694	-2.127012062864
C	1.893005246018	-1.466472043843	-2.319286255281
N	1.145796476339	-2.067122048668	-1.288957718414
C	1.010953505991	-1.401113796849	-0.126965833237
C	1.580524777799	-0.139577160965	0.108726117473
C	3.244045056080	0.359893061396	-3.200869270614
C	3.376300487434	-0.322999218923	-4.394745348242
C	2.765821357348	-1.587919725573	-4.567077361546
C	2.032536951697	-2.155604406423	-3.541888934866
O	0.607217403243	-3.226000367856	-1.470404510132
C	-3.675833919561	0.932317450441	4.117548860598
H	-4.761383761934	3.317513447044	4.604904902586
H	-6.449339579966	4.996184968684	3.821557912619
H	-6.696118525281	5.369258790794	1.345620565876
H	0.330378939129	3.823422993799	-1.632815198850
H	0.549195569226	2.628136211869	2.498138418622
H	-5.122646682029	2.505397326084	-0.985203193584
H	-3.745931155283	3.335811408900	-1.725341048659
H	-2.544175279159	1.115029464182	-1.966453496527
H	-3.935308062518	0.292410491721	-1.203504666941
H	-4.124588604737	1.100674845340	-2.784707535089
H	2.390493762739	4.263219373819	-0.423802615090
H	2.397952713656	4.239286309424	1.346135400162
H	4.089790134666	2.728080728647	0.524985638451
H	2.828020486577	1.751268165004	1.309315039685
H	0.414599196651	-1.920938963208	0.620487224519
H	1.384770626850	0.314778711617	1.077365290339
H	3.709826412052	1.334506875656	-3.060068272173
H	3.954969675626	0.115288409718	-5.210186982719
H	2.874703924544	-2.119152993366	-5.514669966934
H	1.547533172477	-3.125405346887	-3.632755004708
H	-3.190121703043	-0.044387043570	4.008750450249
H	-3.410207859899	1.335525153347	5.108628643142
H	-4.764634610032	0.817532333630	4.050500495044

SCF Done: E(RB3LYP) = -1466.00160686

Zero-point correction= 0.444874
Thermal correction to Energy= 0.472266
Thermal correction to Enthalpy= 0.473211

Thermal correction to Gibbs Free Energy= 0.384238
Sum of electronic and zero-point Energies= -1465.556733
Sum of electronic and thermal Energies= -1465.529340
Sum of electronic and thermal Enthalpies= -1465.528396
Sum of electronic and thermal Free Energies= -1465.617369

1	N	Isotropic =	-40.9558	Anisotropy =	455.2080
2	C	Isotropic =	37.0087	Anisotropy =	120.2128
3	C	Isotropic =	59.6400	Anisotropy =	120.5906
4	C	Isotropic =	62.6409	Anisotropy =	177.3525
5	C	Isotropic =	72.2209	Anisotropy =	159.3406
6	C	Isotropic =	48.9845	Anisotropy =	154.0649
7	N	Isotropic =	122.8741	Anisotropy =	91.3552
8	C	Isotropic =	26.4429	Anisotropy =	108.6130
9	C	Isotropic =	69.9399	Anisotropy =	136.9948
10	C	Isotropic =	33.9172	Anisotropy =	124.8030
11	N	Isotropic =	135.4561	Anisotropy =	63.8747
12	O	Isotropic =	-82.1338	Anisotropy =	575.6203
13	N	Isotropic =	-34.6459	Anisotropy =	452.8058
14	C	Isotropic =	41.1900	Anisotropy =	146.4517
15	C	Isotropic =	63.2401	Anisotropy =	171.8300
16	C	Isotropic =	51.1609	Anisotropy =	188.5015
17	C	Isotropic =	147.7160	Anisotropy =	35.3739
18	C	Isotropic =	177.5008	Anisotropy =	23.3628
19	C	Isotropic =	156.0663	Anisotropy =	14.7977
20	C	Isotropic =	122.4728	Anisotropy =	55.4837
21	O	Isotropic =	206.9688	Anisotropy =	127.9836
22	C	Isotropic =	42.5731	Anisotropy =	124.1259
23	C	Isotropic =	69.1535	Anisotropy =	166.0176
24	C	Isotropic =	50.1097	Anisotropy =	151.3706
25	N	Isotropic =	-22.0939	Anisotropy =	253.0781
26	C	Isotropic =	58.3934	Anisotropy =	114.0771
27	C	Isotropic =	91.6919	Anisotropy =	135.8654
28	C	Isotropic =	68.8277	Anisotropy =	176.8174
29	C	Isotropic =	65.5426	Anisotropy =	175.5917
30	C	Isotropic =	63.7880	Anisotropy =	176.7649
31	C	Isotropic =	73.4890	Anisotropy =	173.7601
32	O	Isotropic =	-25.7581	Anisotropy =	322.4527
33	C	Isotropic =	154.7288	Anisotropy =	45.4623
34	H	Isotropic =	23.9567	Anisotropy =	9.1479
35	H	Isotropic =	24.2819	Anisotropy =	4.5131
36	H	Isotropic =	23.2191	Anisotropy =	4.8858
37	H	Isotropic =	23.3166	Anisotropy =	6.5743
38	H	Isotropic =	23.1204	Anisotropy =	10.1709
39	H	Isotropic =	27.6237	Anisotropy =	7.0469
40	H	Isotropic =	27.1727	Anisotropy =	7.8580
41	H	Isotropic =	30.3712	Anisotropy =	7.5862
42	H	Isotropic =	30.6006	Anisotropy =	7.0609
43	H	Isotropic =	30.5592	Anisotropy =	10.3517
44	H	Isotropic =	28.4488	Anisotropy =	7.1525
45	H	Isotropic =	28.4766	Anisotropy =	7.9567
46	H	Isotropic =	26.8361	Anisotropy =	7.8540
47	H	Isotropic =	26.7186	Anisotropy =	4.1970
48	H	Isotropic =	23.6045	Anisotropy =	6.2893
49	H	Isotropic =	25.2891	Anisotropy =	5.7344
50	H	Isotropic =	23.1461	Anisotropy =	10.6788

51	H	Isotropic =	23.7639	Anisotropy =	5.8172
52	H	Isotropic =	23.6924	Anisotropy =	4.9303
53	H	Isotropic =	23.0794	Anisotropy =	8.1054
54	H	Isotropic =	27.3680	Anisotropy =	7.6261
55	H	Isotropic =	27.9030	Anisotropy =	10.1725
56	H	Isotropic =	28.7774	Anisotropy =	7.6992

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.207860785354	3.773463628104	-0.529450620596
C	-3.613643691032	3.700986157239	0.664405271283
C	-2.830640905199	4.754921563551	1.186855857572
C	-2.639410607971	5.881259082591	0.378328759359
C	-3.251902564526	5.949747737818	-0.873719306796
C	-4.047113278981	4.877940529578	-1.271788062290
N	-2.331390264878	4.738884509169	2.517603113975
C	-1.553558110531	3.726651838224	3.034170982840
C	-1.528698561845	2.389891599473	2.360113290761
C	-2.634010977908	1.780276904486	1.718202995611
N	-3.803674145864	2.506963124924	1.410482148080
O	-0.893855090724	3.905632268203	4.059119244917
N	-2.633049522320	0.478355033348	1.398708379142
C	-1.528464932206	-0.241584084345	1.622514459472
C	-0.346787761872	0.268329698430	2.173000633468
C	-0.389300855272	1.606295492233	2.572616899676
C	-5.036534071217	1.737247268488	1.142596781328
C	-5.585724889339	1.092669333131	2.412681693264
C	0.887530195278	-0.585395967427	2.349194026553
C	1.952263980403	-0.352431164851	1.280909242742
O	1.414098527301	-0.784109483423	0.020785953463
C	2.170932280035	-0.635680281827	-1.090197057798
C	1.589247809656	-1.101701274404	-2.315169939773
C	2.324518261566	-0.975200578255	-3.526280817105
N	3.610357879654	-0.400023701023	-3.527591664008
C	4.123990693609	0.022421390873	-2.357542214833
C	3.438334331419	-0.080956241913	-1.135937827151
C	0.299152283215	-1.692045515264	-2.375972679570
C	-0.221019657481	-2.128486203344	-3.579600816865
C	0.525839101649	-1.992768025614	-4.773682641002
C	1.785083286989	-1.422495142462	-4.749856616896
O	4.266804103497	-0.290000750881	-4.632590156053
C	-2.352410707215	5.994668692405	3.277932639368
H	-2.032025354673	6.711933551401	0.738858368188
H	-3.123001369786	6.822328509932	-1.515183591275
H	-4.577642650226	4.897486339547	-2.228594567922
H	-1.588506910782	-1.300531197550	1.348040135733
H	0.453124908290	2.060821575259	3.097446525094
H	-5.761035714374	2.452780032243	0.737594477326
H	-4.858164860243	0.976374141089	0.367166446604
H	-4.889476206387	0.346221264307	2.822739420183
H	-5.780927183948	1.851716240319	3.187146378605
H	-6.534261614195	0.580033352681	2.184812233687

H	1.356974576065	-0.372469941812	3.323092282466
H	0.614786655283	-1.652252915536	2.348179973023
H	2.222706250159	0.715987607034	1.220704969895
H	2.862450829241	-0.932759273394	1.509470422693
H	5.120552474532	0.453011783802	-2.435511710787
H	3.943083438682	0.289366880250	-0.246115042776
H	-0.269817802685	-1.793063417963	-1.452415228474
H	-1.214242734391	-2.580625912080	-3.610157367321
H	0.105781239020	-2.340508648930	-5.719502549820
H	2.392728734904	-1.299864643789	-5.644181396807
H	-2.404825874087	5.756517484484	4.346677467025
H	-1.444864709974	6.597218149454	3.108107454851
H	-3.235407472959	6.574051602014	2.981382947672

SCF Done: E(RB3LYP) = -1466.00582522

Zero-point correction= 0.444902
Thermal correction to Energy= 0.472294
Thermal correction to Enthalpy= 0.473238
Thermal correction to Gibbs Free Energy= 0.384133
Sum of electronic and zero-point Energies= -1465.560923
Sum of electronic and thermal Energies= -1465.533532
Sum of electronic and thermal Enthalpies= -1465.532587
Sum of electronic and thermal Free Energies= -1465.621693

1	N	Isotropic =	-40.4287	Anisotropy =	456.7933
2	C	Isotropic =	37.0771	Anisotropy =	121.0278
3	C	Isotropic =	60.2089	Anisotropy =	121.2119
4	C	Isotropic =	63.1063	Anisotropy =	177.2105
5	C	Isotropic =	72.5343	Anisotropy =	160.1144
6	C	Isotropic =	49.1963	Anisotropy =	155.0901
7	N	Isotropic =	123.0154	Anisotropy =	91.3251
8	C	Isotropic =	26.9967	Anisotropy =	108.7424
9	C	Isotropic =	70.1398	Anisotropy =	133.4337
10	C	Isotropic =	33.6072	Anisotropy =	122.9383
11	N	Isotropic =	136.1156	Anisotropy =	65.0139
12	O	Isotropic =	-80.6764	Anisotropy =	581.9370
13	N	Isotropic =	-34.2936	Anisotropy =	451.0712
14	C	Isotropic =	40.6361	Anisotropy =	145.2062
15	C	Isotropic =	61.4958	Anisotropy =	170.8584
16	C	Isotropic =	51.8680	Anisotropy =	182.5338
17	C	Isotropic =	147.3129	Anisotropy =	36.1614
18	C	Isotropic =	177.1826	Anisotropy =	23.8592
19	C	Isotropic =	156.7424	Anisotropy =	16.1851
20	C	Isotropic =	120.5951	Anisotropy =	42.4086
21	O	Isotropic =	208.5926	Anisotropy =	108.9157
22	C	Isotropic =	42.9277	Anisotropy =	123.7039
23	C	Isotropic =	69.2727	Anisotropy =	165.3748
24	C	Isotropic =	50.1215	Anisotropy =	151.4566
25	N	Isotropic =	-24.0265	Anisotropy =	253.7742
26	C	Isotropic =	57.9220	Anisotropy =	113.7361
27	C	Isotropic =	91.5634	Anisotropy =	131.5903
28	C	Isotropic =	69.3631	Anisotropy =	176.3943
29	C	Isotropic =	65.3339	Anisotropy =	175.6933
30	C	Isotropic =	63.7656	Anisotropy =	176.6247
31	C	Isotropic =	73.2205	Anisotropy =	174.0243

32	O	Isotropic =	-28.7448	Anisotropy =	325.9034
33	C	Isotropic =	154.5692	Anisotropy =	45.6466
34	H	Isotropic =	24.0811	Anisotropy =	8.4668
35	H	Isotropic =	24.4085	Anisotropy =	4.1835
36	H	Isotropic =	23.3197	Anisotropy =	4.7388
37	H	Isotropic =	22.8127	Anisotropy =	7.7223
38	H	Isotropic =	23.3703	Anisotropy =	10.3000
39	H	Isotropic =	27.5563	Anisotropy =	5.9112
40	H	Isotropic =	26.9631	Anisotropy =	7.8266
41	H	Isotropic =	29.8139	Anisotropy =	4.8049
42	H	Isotropic =	30.3632	Anisotropy =	8.4379
43	H	Isotropic =	30.2541	Anisotropy =	10.9708
44	H	Isotropic =	28.4167	Anisotropy =	7.9851
45	H	Isotropic =	28.2670	Anisotropy =	5.7412
46	H	Isotropic =	27.5033	Anisotropy =	5.3923
47	H	Isotropic =	27.2050	Anisotropy =	5.9706
48	H	Isotropic =	23.3636	Anisotropy =	5.2771
49	H	Isotropic =	25.0742	Anisotropy =	8.7135
50	H	Isotropic =	23.2072	Anisotropy =	9.6030
51	H	Isotropic =	23.7905	Anisotropy =	6.5920
52	H	Isotropic =	23.7132	Anisotropy =	5.0440
53	H	Isotropic =	23.0385	Anisotropy =	7.5529
54	H	Isotropic =	27.4890	Anisotropy =	8.3249
55	H	Isotropic =	27.9798	Anisotropy =	10.0670
56	H	Isotropic =	28.8576	Anisotropy =	7.8875

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.617018189415	2.852957947246	1.949893405300
C	-3.296208734804	1.557057166416	1.979828403596
C	-4.060171646927	0.570540331324	1.316715042447
C	-5.157033309121	1.001270306444	0.561395379376
C	-5.483812483461	2.357400762112	0.522475407514
C	-4.694925838751	3.241527332818	1.254337734434
N	-3.805716306641	-0.818604379638	1.479227055565
C	-2.586460094662	-1.409651327115	1.233763176441
C	-1.349046721661	-0.567853776567	1.184427587870
C	-1.107467404201	0.573393987291	1.987634454989
N	-2.139616753078	1.194324902535	2.721451174848
O	-2.501675525194	-2.628643424945	1.077400126822
N	0.119168649816	1.099697307176	2.113437749313
C	1.122450956893	0.579526943364	1.399275611070
C	0.989731440024	-0.491900854648	0.507060748562
C	-0.276383614673	-1.079814630523	0.446144263662
C	-1.747045032563	2.088451758195	3.831274441772
C	-1.170569083242	1.307063466196	5.009112332380
C	2.156332677290	-0.992735930028	-0.310409035020
C	2.240842951779	-0.417188531938	-1.727509054910
O	2.524156730286	0.995763187321	-1.699830237349
C	1.594211433930	1.915342930916	-2.051999382707
C	2.081831666285	3.257866438512	-2.188893407098
C	1.179144638296	4.295948980057	-2.552428274565

N	-0.181023431365	4.014578551080	-2.780009253274
C	-0.602301990214	2.743925231503	-2.639593328829
C	0.247978078720	1.686864929560	-2.278805975899
C	3.443589855979	3.602390377877	-1.976929917778
C	3.872225370058	4.908237027189	-2.119373391405
C	2.958247160749	5.926276386045	-2.480859756124
C	1.626175215812	5.625750819912	-2.696183582311
O	-0.991852236252	4.962479211716	-3.111265634788
C	-4.957008469539	-1.723170309527	1.587629436341
H	-5.767157880245	0.273936121968	0.025054694996
H	-6.339710022900	2.712514478911	-0.052708668868
H	-4.929376669063	4.309886082591	1.284792360162
H	2.102888668762	1.044909307191	1.549022915580
H	-0.447327744768	-1.978758721167	-0.149071791936
H	-1.030931332554	2.848184096127	3.481896972680
H	-2.658940705040	2.614421363407	4.135763955628
H	-0.949315818930	1.999974035918	5.836961350802
H	-1.888327727914	0.553945820923	5.372037579812
H	-0.234870813951	0.796167585745	4.738132311384
H	3.101485982030	-0.767534631211	0.208491230726
H	2.100953864986	-2.089110929150	-0.414439679275
H	3.091462496501	-0.872667729647	-2.255888045629
H	1.330910126134	-0.623743474987	-2.308235756536
H	-1.665418518823	2.602058698025	-2.824372786988
H	-0.202108119282	0.702179373002	-2.174960717558
H	4.140354990160	2.812337005124	-1.699382559611
H	4.922257839905	5.156673442116	-1.953126984114
H	3.306803160103	6.955031705982	-2.591032576259
H	0.891663602988	6.378087323615	-2.976608618379
H	-4.655266204798	-2.607839566803	2.160453772467
H	-5.769227612791	-1.201333420666	2.108424291069
H	-5.312591520663	-2.062341084891	0.600673449602

SCF Done: E(RB3LYP) = -1466.00157567

Zero-point correction= 0.444768
Thermal correction to Energy= 0.472186
Thermal correction to Enthalpy= 0.473130
Thermal correction to Gibbs Free Energy= 0.383840
Sum of electronic and zero-point Energies= -1465.556807
Sum of electronic and thermal Energies= -1465.529390
Sum of electronic and thermal Enthalpies= -1465.528446
Sum of electronic and thermal Free Energies= -1465.617736

1	N	Isotropic =	-40.4508	Anisotropy = 456.9413
2	C	Isotropic =	37.2803	Anisotropy = 121.1590
3	C	Isotropic =	59.9039	Anisotropy = 121.9436
4	C	Isotropic =	62.8146	Anisotropy = 177.8162
5	C	Isotropic =	72.1512	Anisotropy = 160.5532
6	C	Isotropic =	49.1155	Anisotropy = 155.5363
7	N	Isotropic =	123.1877	Anisotropy = 91.5129
8	C	Isotropic =	27.0266	Anisotropy = 108.3250
9	C	Isotropic =	70.1189	Anisotropy = 134.4614
10	C	Isotropic =	33.5272	Anisotropy = 124.6721
11	N	Isotropic =	135.8766	Anisotropy = 66.2614
12	O	Isotropic =	-81.0985	Anisotropy = 581.8111

13	N	Isotropic =	-34.7428	Anisotropy =	453.9968
14	C	Isotropic =	40.9723	Anisotropy =	148.0328
15	C	Isotropic =	62.9681	Anisotropy =	172.3635
16	C	Isotropic =	51.2997	Anisotropy =	182.9077
17	C	Isotropic =	147.5550	Anisotropy =	36.2247
18	C	Isotropic =	177.2971	Anisotropy =	24.5222
19	C	Isotropic =	155.2387	Anisotropy =	16.0396
20	C	Isotropic =	122.3320	Anisotropy =	55.4660
21	O	Isotropic =	208.3503	Anisotropy =	128.3379
22	C	Isotropic =	42.5201	Anisotropy =	124.2433
23	C	Isotropic =	69.2794	Anisotropy =	165.7608
24	C	Isotropic =	50.1796	Anisotropy =	151.7421
25	N	Isotropic =	-22.0965	Anisotropy =	253.1541
26	C	Isotropic =	58.7254	Anisotropy =	114.5157
27	C	Isotropic =	92.3512	Anisotropy =	136.2830
28	C	Isotropic =	69.1409	Anisotropy =	176.6656
29	C	Isotropic =	65.4416	Anisotropy =	175.0758
30	C	Isotropic =	63.6864	Anisotropy =	176.7666
31	C	Isotropic =	73.3790	Anisotropy =	173.7117
32	O	Isotropic =	-25.8024	Anisotropy =	321.8548
33	C	Isotropic =	154.5131	Anisotropy =	45.7257
34	H	Isotropic =	23.9262	Anisotropy =	8.5715
35	H	Isotropic =	24.2301	Anisotropy =	4.2671
36	H	Isotropic =	23.2300	Anisotropy =	4.3343
37	H	Isotropic =	23.3151	Anisotropy =	6.6350
38	H	Isotropic =	23.2898	Anisotropy =	10.0093
39	H	Isotropic =	27.2438	Anisotropy =	7.0306
40	H	Isotropic =	27.6755	Anisotropy =	5.8115
41	H	Isotropic =	30.3953	Anisotropy =	11.1209
42	H	Isotropic =	30.4607	Anisotropy =	8.6465
43	H	Isotropic =	29.9630	Anisotropy =	4.9671
44	H	Isotropic =	28.2593	Anisotropy =	7.0625
45	H	Isotropic =	28.5180	Anisotropy =	7.8735
46	H	Isotropic =	26.8975	Anisotropy =	7.9413
47	H	Isotropic =	27.0067	Anisotropy =	4.3056
48	H	Isotropic =	24.0706	Anisotropy =	5.2612
49	H	Isotropic =	25.7635	Anisotropy =	6.1949
50	H	Isotropic =	23.1591	Anisotropy =	10.6099
51	H	Isotropic =	23.7852	Anisotropy =	5.8172
52	H	Isotropic =	23.7086	Anisotropy =	4.9946
53	H	Isotropic =	23.1214	Anisotropy =	8.1729
54	H	Isotropic =	27.4535	Anisotropy =	8.5189
55	H	Isotropic =	28.8004	Anisotropy =	7.9486
56	H	Isotropic =	27.8957	Anisotropy =	9.9166

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.170809087222	3.234957493880	2.596866776483
C	0.706788728334	1.999336185509	2.799296703228
C	-0.367102547142	1.725094412299	3.674709297234
C	-0.990902803450	2.813997833805	4.294721251293
C	-0.514521788691	4.106176190894	4.069848188098

C	0.584624109567	4.261582184561	3.228425002587
N	-0.753454913865	0.397086212625	4.001939721936
C	-1.088458665209	-0.558645439462	3.068592291752
C	-0.683554981866	-0.376276237191	1.638469230188
C	0.526013788432	0.219116034012	1.204441467410
N	1.347273178736	0.944701639245	2.092448095697
O	-1.704134944030	-1.571538213613	3.404169420438
N	0.961391612925	0.093103330392	-0.057188022572
C	0.198710971861	-0.556735928688	-0.942419312820
C	-1.052867363433	-1.115106774507	-0.653128205938
C	-1.460518241271	-1.037861463435	0.681134436809
C	2.755417335185	1.160663319283	1.700265198440
C	3.671049183110	1.248211285440	2.918116209297
C	-1.893144177609	-1.775324625713	-1.720017477622
C	-2.899598698556	-0.845973311731	-2.405357353586
O	-2.225353651110	0.159567116741	-3.187521414513
C	-2.232575446414	1.466209907882	-2.830866096833
C	-1.722027798803	2.372564149859	-3.819185289986
C	-1.681377876638	3.766031137426	-3.535517577880
N	-2.140230716918	4.258480823991	-2.299496436460
C	-2.610729777558	3.378081089179	-1.396437444674
C	-2.666661778650	1.994465146831	-1.627413588533
C	-1.250200552558	1.936186290569	-5.085967302218
C	-0.766445159376	2.842440983780	-6.010111477039
C	-0.733532497359	4.224450881827	-5.707948774385
C	-1.186031146525	4.683568316890	-4.485054748263
O	-2.102032018787	5.524690160195	-2.052705274712
C	-1.132472396843	0.110242867841	5.391219404060
H	-1.832564999741	2.648303489629	4.967809399340
H	-0.979483139992	4.967627697049	4.550715703866
H	1.018556162368	5.249914276212	3.049020865149
H	0.610055752136	-0.637083637759	-1.954553697535
H	-2.376410861260	-1.529240182180	1.014826989611
H	3.033648799819	0.303047915241	1.077572438273
H	2.851787331725	2.062332843560	1.074899775327
H	3.585926189942	0.343607372109	3.541437150288
H	4.717053101083	1.340016851858	2.584318346631
H	3.439942019908	2.124476575889	3.541849937453
H	-1.242896524150	-2.208315627933	-2.496666015192
H	-2.470482361888	-2.607114469297	-1.284000834475
H	-3.497428281244	-1.422728789645	-3.126813355035
H	-3.588978669748	-0.386113717283	-1.683678370367
H	-2.941835722330	3.828882269869	-0.462763791010
H	-3.047268035621	1.372109285877	-0.820557054752
H	-1.279001749709	0.870510553457	-5.309992186091
H	-0.407823903348	2.491010665672	-6.979564683989
H	-0.349412834625	4.932619565616	-6.444789755610
H	-1.179683403285	5.737129015408	-4.212803050094
H	-0.533733085334	0.741243853695	6.059474903961
H	-2.203776418287	0.294647633049	5.575179584705
H	-0.931467419127	-0.947366440708	5.598290802631

SCF Done: E(RB3LYP) = -1466.00152710

Zero-point correction= 0.444783
Thermal correction to Energy= 0.472206

Thermal correction to Enthalpy= 0.473150
Thermal correction to Gibbs Free Energy= 0.383595
Sum of electronic and zero-point Energies= -1465.556745
Sum of electronic and thermal Energies= -1465.529321
Sum of electronic and thermal Enthalpies= -1465.528377
Sum of electronic and thermal Free Energies= -1465.617932

1	N	Isotropic =	-42.1570	Anisotropy =	470.4452
2	C	Isotropic =	38.8867	Anisotropy =	118.4491
3	C	Isotropic =	58.4308	Anisotropy =	123.8274
4	C	Isotropic =	62.6861	Anisotropy =	178.0142
5	C	Isotropic =	72.3127	Anisotropy =	160.3007
6	C	Isotropic =	48.9919	Anisotropy =	155.4159
7	N	Isotropic =	123.1017	Anisotropy =	91.7452
8	C	Isotropic =	26.8519	Anisotropy =	108.1182
9	C	Isotropic =	71.1806	Anisotropy =	132.9924
10	C	Isotropic =	32.3498	Anisotropy =	125.7461
11	N	Isotropic =	136.9625	Anisotropy =	65.3602
12	O	Isotropic =	-81.0758	Anisotropy =	581.3532
13	N	Isotropic =	-33.9206	Anisotropy =	443.2532
14	C	Isotropic =	40.8271	Anisotropy =	149.3655
15	C	Isotropic =	62.7944	Anisotropy =	172.8619
16	C	Isotropic =	51.6037	Anisotropy =	180.8284
17	C	Isotropic =	148.6357	Anisotropy =	34.0983
18	C	Isotropic =	177.5045	Anisotropy =	24.2327
19	C	Isotropic =	155.2301	Anisotropy =	15.9362
20	C	Isotropic =	122.2501	Anisotropy =	55.6769
21	O	Isotropic =	208.7273	Anisotropy =	127.6110
22	C	Isotropic =	42.5003	Anisotropy =	124.2603
23	C	Isotropic =	69.1895	Anisotropy =	165.7846
24	C	Isotropic =	50.3131	Anisotropy =	151.7295
25	N	Isotropic =	-22.1313	Anisotropy =	253.2628
26	C	Isotropic =	58.7989	Anisotropy =	114.3487
27	C	Isotropic =	92.2036	Anisotropy =	136.8556
28	C	Isotropic =	68.9210	Anisotropy =	176.9447
29	C	Isotropic =	65.4171	Anisotropy =	175.3453
30	C	Isotropic =	63.7166	Anisotropy =	176.4584
31	C	Isotropic =	73.4877	Anisotropy =	173.4832
32	O	Isotropic =	-26.4085	Anisotropy =	322.8392
33	C	Isotropic =	154.6127	Anisotropy =	45.6217
34	H	Isotropic =	23.9112	Anisotropy =	8.5473
35	H	Isotropic =	24.2321	Anisotropy =	4.2656
36	H	Isotropic =	23.1954	Anisotropy =	4.3534
37	H	Isotropic =	23.3291	Anisotropy =	6.3875
38	H	Isotropic =	23.3425	Anisotropy =	9.9917
39	H	Isotropic =	27.5871	Anisotropy =	5.6047
40	H	Isotropic =	27.3669	Anisotropy =	7.5211
41	H	Isotropic =	30.4829	Anisotropy =	8.5539
42	H	Isotropic =	30.3589	Anisotropy =	11.1774
43	H	Isotropic =	30.0862	Anisotropy =	5.2405
44	H	Isotropic =	28.2394	Anisotropy =	7.1040
45	H	Isotropic =	28.5458	Anisotropy =	7.8929
46	H	Isotropic =	26.8988	Anisotropy =	7.9629
47	H	Isotropic =	27.0452	Anisotropy =	4.3606
48	H	Isotropic =	24.0635	Anisotropy =	5.2398
49	H	Isotropic =	25.7753	Anisotropy =	6.2752

50	H	Isotropic =	23.1320	Anisotropy =	10.5832
51	H	Isotropic =	23.7714	Anisotropy =	5.7996
52	H	Isotropic =	23.7014	Anisotropy =	5.0110
53	H	Isotropic =	23.1194	Anisotropy =	8.1599
54	H	Isotropic =	28.8021	Anisotropy =	7.7992
55	H	Isotropic =	27.8980	Anisotropy =	9.9608
56	H	Isotropic =	27.4463	Anisotropy =	8.5345

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.735341317814	-1.294035352001	2.483632898942
C	-0.580259525741	-1.067147572715	2.451320505406
C	-1.257427968325	-0.377709803093	3.481515050051
C	-0.488161898382	0.130850201648	4.534517419841
C	0.888920889854	-0.093642022173	4.558481582220
C	1.449935842616	-0.832343261795	3.519371988111
N	-2.674451169204	-0.275376818801	3.516313616414
C	-3.434785842539	0.233312221574	2.486815551668
C	-2.848193409501	0.343885854954	1.113561075944
C	-1.939417449463	-0.578323759936	0.539518356950
N	-1.293931541385	-1.557805150944	1.323614750397
O	-4.599684873381	0.582717677011	2.683601490724
N	-1.675133241465	-0.583022238740	-0.774344509231
C	-2.236879097288	0.350581820553	-1.550132642456
C	-3.087132947719	1.361244982459	-1.086594697793
C	-3.408357126774	1.311194792097	0.272171354825
C	-0.717511155836	-2.724071436354	0.623231852363
C	-0.734868289005	-3.971486436515	1.502399310856
C	-3.638328382944	2.425601737027	-2.006792800411
C	-2.895213138741	3.756205292653	-1.920361821402
O	-1.551748243493	3.539695606553	-2.380517345365
C	-0.684979829585	4.577513563259	-2.362681466033
C	0.644188926029	4.294260749179	-2.820342267472
C	1.613329838839	5.335334090499	-2.829069432990
N	1.276216606411	6.632003049884	-2.394244842435
C	0.017918654754	6.859687116530	-1.974468419813
C	-0.974409952503	5.865697899204	-1.946944146091
C	1.042464476356	3.007789278831	-3.270600530092
C	2.335188468408	2.780214174541	-3.702753815446
C	3.284804997887	3.829081468264	-3.703386445062
C	2.930106554266	5.093710442104	-3.271747982922
O	2.164507932824	7.567422058143	-2.405170956610
C	-3.344780856355	-0.408772695790	4.815768898988
H	-0.969239233651	0.681836168438	5.343259416072
H	1.505491711475	0.284896486126	5.374602659392
H	2.518672383540	-1.066985000632	3.511317232117
H	-1.993052102610	0.290464360957	-2.616529769433
H	-4.136972485196	2.001926634751	0.700921053582
H	-1.334197315012	-2.880069462914	-0.269025633334
H	0.305371093693	-2.505424688700	0.277819629577
H	-0.365242930965	-4.833345885755	0.924024500544
H	-0.088734683074	-3.857978533980	2.385515774735

H	-1.757435418658	-4.198057677150	1.844640900709
H	-3.611838232709	2.075234951739	-3.050447816053
H	-4.692819611928	2.628928802555	-1.760342669199
H	-3.385085019854	4.513110943624	-2.556338371314
H	-2.873669822262	4.130080486370	-0.881863580153
H	-0.169033530477	7.883391929594	-1.655509552240
H	-1.961268482252	6.153617868539	-1.590508942501
H	0.305717602805	2.205366235971	-3.267291272087
H	2.626126163119	1.785462091637	-4.045801458654
H	4.303602763361	3.639274347364	-4.046813054628
H	3.628874499210	5.927691360111	-3.256561394775
H	-2.777802618579	-1.113465789988	5.436318793963
H	-3.427434307662	0.557200320559	5.340682576318
H	-4.358768988745	-0.791103477321	4.650069395286

SCF Done: E(RB3LYP) = -1466.00579094

Zero-point correction= 0.444756
Thermal correction to Energy= 0.472207
Thermal correction to Enthalpy= 0.473151
Thermal correction to Gibbs Free Energy= 0.383684
Sum of electronic and zero-point Energies= -1465.561035
Sum of electronic and thermal Energies= -1465.533584
Sum of electronic and thermal Enthalpies= -1465.532640
Sum of electronic and thermal Free Energies= -1465.622107

1	N	Isotropic =	-42.2094	Anisotropy =	469.5215
2	C	Isotropic =	38.5995	Anisotropy =	117.9210
3	C	Isotropic =	58.5243	Anisotropy =	123.8435
4	C	Isotropic =	62.7312	Anisotropy =	177.3594
5	C	Isotropic =	72.6293	Anisotropy =	159.7433
6	C	Isotropic =	49.1914	Anisotropy =	154.6455
7	N	Isotropic =	123.0990	Anisotropy =	91.8127
8	C	Isotropic =	26.8732	Anisotropy =	108.5402
9	C	Isotropic =	71.2745	Anisotropy =	132.1491
10	C	Isotropic =	32.3429	Anisotropy =	124.3041
11	N	Isotropic =	137.1312	Anisotropy =	64.2625
12	O	Isotropic =	-80.6238	Anisotropy =	581.8475
13	N	Isotropic =	-33.6657	Anisotropy =	439.6692
14	C	Isotropic =	40.6109	Anisotropy =	145.3485
15	C	Isotropic =	61.5239	Anisotropy =	171.2744
16	C	Isotropic =	52.2772	Anisotropy =	181.0978
17	C	Isotropic =	148.4393	Anisotropy =	33.8622
18	C	Isotropic =	177.4246	Anisotropy =	23.8218
19	C	Isotropic =	156.7865	Anisotropy =	16.2561
20	C	Isotropic =	120.9035	Anisotropy =	42.6839
21	O	Isotropic =	208.5470	Anisotropy =	109.8585
22	C	Isotropic =	43.0506	Anisotropy =	123.6406
23	C	Isotropic =	69.2506	Anisotropy =	165.4818
24	C	Isotropic =	50.2185	Anisotropy =	151.2788
25	N	Isotropic =	-23.8052	Anisotropy =	254.5337
26	C	Isotropic =	57.9886	Anisotropy =	113.3460
27	C	Isotropic =	91.5651	Anisotropy =	131.5085
28	C	Isotropic =	69.1906	Anisotropy =	176.0872
29	C	Isotropic =	65.2909	Anisotropy =	175.7684
30	C	Isotropic =	63.7138	Anisotropy =	176.8599

31	C	Isotropic =	73.2268	Anisotropy =	174.1541
32	O	Isotropic =	-28.6975	Anisotropy =	326.5712
33	C	Isotropic =	154.6110	Anisotropy =	45.5620
34	H	Isotropic =	24.0478	Anisotropy =	8.4140
35	H	Isotropic =	24.3967	Anisotropy =	4.1792
36	H	Isotropic =	23.2945	Anisotropy =	4.7257
37	H	Isotropic =	22.8191	Anisotropy =	7.6210
38	H	Isotropic =	23.4179	Anisotropy =	10.2671
39	H	Isotropic =	27.3911	Anisotropy =	5.7026
40	H	Isotropic =	27.1245	Anisotropy =	8.1722
41	H	Isotropic =	30.2519	Anisotropy =	11.0371
42	H	Isotropic =	30.0174	Anisotropy =	5.2186
43	H	Isotropic =	30.4056	Anisotropy =	8.3384
44	H	Isotropic =	28.2497	Anisotropy =	5.8005
45	H	Isotropic =	28.4285	Anisotropy =	8.0327
46	H	Isotropic =	27.1856	Anisotropy =	6.0111
47	H	Isotropic =	27.5572	Anisotropy =	5.4189
48	H	Isotropic =	23.3710	Anisotropy =	5.2391
49	H	Isotropic =	25.0843	Anisotropy =	8.6854
50	H	Isotropic =	23.2296	Anisotropy =	9.4982
51	H	Isotropic =	23.7956	Anisotropy =	6.5669
52	H	Isotropic =	23.7017	Anisotropy =	5.0848
53	H	Isotropic =	23.0264	Anisotropy =	7.5768
54	H	Isotropic =	28.8423	Anisotropy =	7.7585
55	H	Isotropic =	27.9716	Anisotropy =	10.0938
56	H	Isotropic =	27.4703	Anisotropy =	8.4237

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.329615843945	0.390028864858	3.909424816860
C	-1.524110099996	0.312772483877	3.317305556794
C	-2.099999351430	-0.916866646702	2.927764537161
C	-1.342403876466	-2.077407828568	3.123691800422
C	-0.087360320890	-1.992698894324	3.727831008644
C	0.364806145841	-0.736154983854	4.123720057302
N	-3.432835183211	-1.007171614161	2.443016912740
C	-3.915370755878	-0.282950071496	1.375691022030
C	-3.176374353503	0.931140045636	0.904544904828
C	-2.487012392838	1.841731047565	1.741912150479
N	-2.214299588955	1.535213900740	3.092040284750
O	-4.959893107079	-0.617897723571	0.814627712516
N	-2.093162242781	3.044937089297	1.302098725682
C	-2.304494687210	3.366121736419	0.021073018847
C	-2.905045168968	2.521873112750	-0.920178733374
C	-3.368970592096	1.297866521398	-0.431968597576
C	-1.898106508192	2.658135151558	3.998914280437
C	-2.354305640304	2.371422323381	5.426809941846
C	-3.059583731765	2.922933241721	-2.368739398479
C	-1.988238384745	2.338084133333	-3.285394631212
O	-0.724459558517	2.901650277566	-2.899349729738
C	0.390051109099	2.502078152292	-3.553055526920
C	1.618339472183	3.111226769656	-3.132746939631

C	2.833390827674	2.739625088227	-3.772279686636
N	2.835687932380	1.783385428292	-4.806596793449
C	1.662579666682	1.236428655725	-5.175462992069
C	0.436883707391	1.571091819388	-4.576423265584
C	1.678368857596	4.080875888305	-2.097043563358
C	2.884951430067	4.642721863291	-1.725336250920
C	4.082740658595	4.259839663646	-2.373846284468
C	4.059789757850	3.318894965079	-3.386547023349
O	3.944477400049	1.452012354727	-5.376760906812
C	-4.249895389059	-2.147113179548	2.877190318587
H	-1.743773258815	-3.046125438543	2.824447027329
H	0.514857732387	-2.885712213365	3.899149102860
H	1.325317628566	-0.620980854715	4.635059016120
H	-1.972641108848	4.366336131934	-0.278114567828
H	-3.930735258799	0.616091598087	-1.073324542608
H	-0.821337788789	2.889005214588	3.973135013580
H	-2.426377659595	3.531280927433	3.600022513467
H	-3.433184788478	2.149806200396	5.458638651899
H	-1.811101423014	1.522134853159	5.867365678294
H	-2.164405025051	3.254894646474	6.057211959295
H	-4.034357436904	2.581738497920	-2.752418981114
H	-3.041075099828	4.019988213636	-2.462856325615
H	-1.946800997837	1.238952447302	-3.192898957734
H	-2.198504339850	2.594927622705	-4.337652754515
H	1.741622881471	0.508670622710	-5.980900405087
H	-0.454859787446	1.071777586091	-4.949672988875
H	0.751729413422	4.371369814211	-1.603470928986
H	2.914876302625	5.386831385662	-0.927050832636
H	5.030890243553	4.710141141599	-2.073538854588
H	4.957425681749	2.997942809816	-3.911141699937
H	-4.128550067159	-3.019656683361	2.214300000242
H	-3.960372553115	-2.421910559291	3.898804179077
H	-5.305173477825	-1.850863600952	2.856281971012

SCF Done: E(RB3LYP) = -1466.00577796

Zero-point correction= 0.444630
Thermal correction to Energy= 0.472143
Thermal correction to Enthalpy= 0.473088
Thermal correction to Gibbs Free Energy= 0.382608
Sum of electronic and zero-point Energies= -1465.561148
Sum of electronic and thermal Energies= -1465.533634
Sum of electronic and thermal Enthalpies= -1465.532690
Sum of electronic and thermal Free Energies= -1465.623170

1	N	Isotropic =	-41.9099	Anisotropy = 469.2700
2	C	Isotropic =	38.7628	Anisotropy = 117.9672
3	C	Isotropic =	58.5694	Anisotropy = 123.8270
4	C	Isotropic =	62.8620	Anisotropy = 177.5128
5	C	Isotropic =	72.5958	Anisotropy = 159.8047
6	C	Isotropic =	49.1997	Anisotropy = 154.5478
7	N	Isotropic =	122.9853	Anisotropy = 91.3625
8	C	Isotropic =	26.8120	Anisotropy = 108.4965
9	C	Isotropic =	71.2642	Anisotropy = 132.1698
10	C	Isotropic =	32.4741	Anisotropy = 124.1871
11	N	Isotropic =	136.9630	Anisotropy = 64.1864

12	O	Isotropic =	-80.6951	Anisotropy =	582.1257
13	N	Isotropic =	-33.5958	Anisotropy =	439.1525
14	C	Isotropic =	40.3907	Anisotropy =	145.8363
15	C	Isotropic =	61.5218	Anisotropy =	171.2407
16	C	Isotropic =	52.2535	Anisotropy =	180.7603
17	C	Isotropic =	148.6317	Anisotropy =	33.9738
18	C	Isotropic =	177.2458	Anisotropy =	24.0818
19	C	Isotropic =	156.7454	Anisotropy =	16.2144
20	C	Isotropic =	120.8630	Anisotropy =	42.6069
21	O	Isotropic =	208.3998	Anisotropy =	109.1860
22	C	Isotropic =	42.9421	Anisotropy =	123.8894
23	C	Isotropic =	69.2750	Anisotropy =	165.5554
24	C	Isotropic =	50.2556	Anisotropy =	151.2699
25	N	Isotropic =	-23.8000	Anisotropy =	254.3336
26	C	Isotropic =	58.0294	Anisotropy =	113.3505
27	C	Isotropic =	91.5260	Anisotropy =	131.4125
28	C	Isotropic =	69.2267	Anisotropy =	175.9077
29	C	Isotropic =	65.3283	Anisotropy =	175.7967
30	C	Isotropic =	63.6736	Anisotropy =	177.0352
31	C	Isotropic =	73.3107	Anisotropy =	173.9469
32	O	Isotropic =	-28.6430	Anisotropy =	326.2789
33	C	Isotropic =	154.5667	Anisotropy =	45.5232
34	H	Isotropic =	24.0439	Anisotropy =	8.4284
35	H	Isotropic =	24.3905	Anisotropy =	4.1903
36	H	Isotropic =	23.2924	Anisotropy =	4.7650
37	H	Isotropic =	22.7956	Anisotropy =	7.6614
38	H	Isotropic =	23.4160	Anisotropy =	10.2806
39	H	Isotropic =	27.1222	Anisotropy =	8.1740
40	H	Isotropic =	27.3888	Anisotropy =	5.7574
41	H	Isotropic =	30.4119	Anisotropy =	8.2959
42	H	Isotropic =	30.0303	Anisotropy =	5.2127
43	H	Isotropic =	30.2611	Anisotropy =	11.0250
44	H	Isotropic =	28.4432	Anisotropy =	7.9795
45	H	Isotropic =	28.2427	Anisotropy =	5.7839
46	H	Isotropic =	27.5502	Anisotropy =	5.3962
47	H	Isotropic =	27.2051	Anisotropy =	6.0121
48	H	Isotropic =	23.3749	Anisotropy =	5.2475
49	H	Isotropic =	25.0874	Anisotropy =	8.7038
50	H	Isotropic =	23.1804	Anisotropy =	9.5486
51	H	Isotropic =	23.7690	Anisotropy =	6.5458
52	H	Isotropic =	23.6840	Anisotropy =	5.0885
53	H	Isotropic =	23.0274	Anisotropy =	7.5742
54	H	Isotropic =	27.9756	Anisotropy =	10.0944
55	H	Isotropic =	28.8487	Anisotropy =	7.7079
56	H	Isotropic =	27.4530	Anisotropy =	8.4140

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.693984117681	-2.137457543851	-0.134521062985
C	-1.634044044853	-1.958996964328	0.658056208483
C	-0.359230242244	-2.484693610809	0.349430893641
C	-0.216408663238	-3.163823909427	-0.866090045647

C	-1.322798093291	-3.338570370030	-1.698405000848
C	-2.546628873580	-2.826231948572	-1.275007303920
N	0.724470310364	-2.429348175831	1.267634719227
C	1.195123494142	-1.264770754088	1.832009175787
C	0.335218038349	-0.038893969144	1.833508489479
C	-1.073833080531	-0.032531547158	1.974944265331
N	-1.835807940261	-1.213774321719	1.850625019686
O	2.309690496606	-1.229195214072	2.355729284337
N	-1.748044665207	1.089864443131	2.262305900458
C	-1.077860817632	2.244211535842	2.343659699145
C	0.301320604524	2.376866402535	2.145084756095
C	1.000889215982	1.188820923978	1.919499998077
C	-3.202384721864	-1.207446838097	2.413716712978
C	-3.184342825614	-1.191044610901	3.940159126073
C	0.991320507174	3.719769520497	2.206473050960
C	1.315512144497	4.310789579451	0.837290955148
O	0.073689488662	4.575394301885	0.165585987836
C	0.111922702598	5.094487582426	-1.082626005806
C	-1.158032431216	5.335182733547	-1.703616654133
C	-1.197557512176	5.880800646547	-3.016635964176
N	-0.005396123665	6.182156778091	-3.703953747237
C	1.166957865599	5.942989012748	-3.087662469512
C	1.258466726514	5.406372857342	-1.792726122400
C	-2.392240161334	5.052400962644	-1.060700368745
C	-3.593091684740	5.301631734555	-1.697637980203
C	-3.611279064027	5.844572436659	-3.004007032420
C	-2.427774677573	6.131624683901	-3.658518689187
O	-0.054217988976	6.675586427474	-4.894882648048
C	1.599716758432	-3.603428737048	1.373409612466
H	0.753361640061	-3.575112978830	-1.147859381616
H	-1.234731061815	-3.872808963678	-2.645147834802
H	-3.451582859036	-2.967128980298	-1.873764065036
H	-1.679843707835	3.125948200678	2.589645488117
H	2.090115503124	1.185778427506	1.847033229626
H	-3.778699612387	-0.354647394311	2.023089966107
H	-3.685906931703	-2.121626576843	2.051232138581
H	-2.731196086652	-0.267989237463	4.330770682480
H	-4.217006099633	-1.247505255124	4.320707752240
H	-2.622809021560	-2.051934032035	4.337132436513
H	0.369590130597	4.439206491438	2.761918890057
H	1.944960165396	3.628776207247	2.751001232178
H	1.881373933747	5.251250407303	0.949691763454
H	1.917448348889	3.608011914840	0.235311418688
H	2.044057230722	6.200898410738	-3.678274692710
H	2.255119632562	5.253006886826	-1.384108484519
H	-2.370551167093	4.635455634871	-0.054447174165
H	-4.533659192439	5.078754905745	-1.190188132564
H	-4.565134919389	6.038082507693	-3.498621254603
H	-2.397716263944	6.549202154498	-4.662872040850
H	2.421457745123	-3.575626276675	0.638945862636
H	2.042633764414	-3.621402347667	2.376015028244
H	0.999708205109	-4.507854154638	1.214634412005

SCF Done: E(RB3LYP) = -1466.00575379

Zero-point correction= 0.444778

Thermal correction to Energy= 0.472213
Thermal correction to Enthalpy= 0.473158
Thermal correction to Gibbs Free Energy= 0.381981
Sum of electronic and zero-point Energies= -1465.560976
Sum of electronic and thermal Energies= -1465.533540
Sum of electronic and thermal Enthalpies= -1465.532596
Sum of electronic and thermal Free Energies= -1465.623773

1	N	Isotropic =	-40.4333	Anisotropy =	456.1943
2	C	Isotropic =	36.9214	Anisotropy =	121.0121
3	C	Isotropic =	60.0093	Anisotropy =	121.4722
4	C	Isotropic =	62.9949	Anisotropy =	177.3295
5	C	Isotropic =	72.4755	Anisotropy =	160.0901
6	C	Isotropic =	49.1617	Anisotropy =	154.6618
7	N	Isotropic =	123.2514	Anisotropy =	91.4709
8	C	Isotropic =	26.9832	Anisotropy =	108.5901
9	C	Isotropic =	70.0850	Anisotropy =	133.4116
10	C	Isotropic =	33.7278	Anisotropy =	123.2881
11	N	Isotropic =	136.0918	Anisotropy =	64.5813
12	O	Isotropic =	-80.8268	Anisotropy =	581.0249
13	N	Isotropic =	-34.5084	Anisotropy =	451.0898
14	C	Isotropic =	40.6752	Anisotropy =	144.9645
15	C	Isotropic =	61.6396	Anisotropy =	170.5438
16	C	Isotropic =	51.7682	Anisotropy =	182.7245
17	C	Isotropic =	147.3985	Anisotropy =	35.9494
18	C	Isotropic =	177.1506	Anisotropy =	23.9356
19	C	Isotropic =	156.7784	Anisotropy =	16.3696
20	C	Isotropic =	120.8023	Anisotropy =	42.4746
21	O	Isotropic =	209.1440	Anisotropy =	111.2808
22	C	Isotropic =	42.8426	Anisotropy =	123.9147
23	C	Isotropic =	69.3034	Anisotropy =	165.3884
24	C	Isotropic =	50.1781	Anisotropy =	151.3349
25	N	Isotropic =	-23.8726	Anisotropy =	253.5810
26	C	Isotropic =	58.0346	Anisotropy =	113.3499
27	C	Isotropic =	91.5129	Anisotropy =	131.6278
28	C	Isotropic =	69.2730	Anisotropy =	176.2923
29	C	Isotropic =	65.3690	Anisotropy =	175.5684
30	C	Isotropic =	63.7044	Anisotropy =	176.4183
31	C	Isotropic =	73.4603	Anisotropy =	173.4640
32	O	Isotropic =	-29.1165	Anisotropy =	325.7667
33	C	Isotropic =	154.5483	Anisotropy =	45.6615
34	H	Isotropic =	24.0615	Anisotropy =	8.4911
35	H	Isotropic =	24.3874	Anisotropy =	4.2025
36	H	Isotropic =	23.3071	Anisotropy =	4.7401
37	H	Isotropic =	22.7967	Anisotropy =	7.7880
38	H	Isotropic =	23.3582	Anisotropy =	10.3367
39	H	Isotropic =	26.9589	Anisotropy =	7.8120
40	H	Isotropic =	27.5380	Anisotropy =	5.9764
41	H	Isotropic =	29.8166	Anisotropy =	4.8587
42	H	Isotropic =	30.2477	Anisotropy =	10.9319
43	H	Isotropic =	30.3695	Anisotropy =	8.4216
44	H	Isotropic =	28.2720	Anisotropy =	5.7029
45	H	Isotropic =	28.4146	Anisotropy =	7.9957
46	H	Isotropic =	27.1941	Anisotropy =	5.9013
47	H	Isotropic =	27.5089	Anisotropy =	5.5066
48	H	Isotropic =	23.3801	Anisotropy =	5.2505

49	H	Isotropic =	25.0654	Anisotropy =	8.7063
50	H	Isotropic =	23.2184	Anisotropy =	9.5456
51	H	Isotropic =	23.7950	Anisotropy =	6.6370
52	H	Isotropic =	23.7091	Anisotropy =	5.0805
53	H	Isotropic =	23.0535	Anisotropy =	7.5541
54	H	Isotropic =	27.9667	Anisotropy =	10.0844
55	H	Isotropic =	27.4759	Anisotropy =	8.3460
56	H	Isotropic =	28.8377	Anisotropy =	7.9164

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.577452684636	-1.882968079401	0.198869995804
C	-3.272837294636	-1.605796408702	0.266931520560
C	-2.277625565088	-2.577460249935	0.015942100196
C	-2.701869762205	-3.853478380140	-0.372228109370
C	-4.065683192560	-4.136939336884	-0.454178025238
C	-4.964444072973	-3.122179055718	-0.134499684251
N	-0.897342243466	-2.323824969085	0.242742628552
C	-0.209072391408	-1.272808802816	-0.316835828567
C	-0.960995572964	-0.110937824507	-0.886633036698
C	-2.154537827528	0.427226566716	-0.347402781343
N	-2.912162887135	-0.275439876726	0.612548934037
O	1.023604610286	-1.264077669232	-0.331019371552
N	-2.607605792038	1.636720379604	-0.706406254495
C	-1.945246393717	2.322907360286	-1.644161945933
C	-0.800800292440	1.861594113673	-2.305421866721
C	-0.309853054028	0.624270285859	-1.881588542099
C	-3.883177065066	0.497139784117	1.415797266820
C	-3.183257653787	1.417195418070	2.412721134176
C	-0.099231103637	2.689046056965	-3.356195093637
C	1.185241723279	3.371089837461	-2.875931216280
O	0.896478263251	4.382924396266	-1.891299085428
C	1.233426164152	4.232046718985	-0.588428124797
C	1.056386026329	5.400676190780	0.225714754189
C	1.380423188364	5.345524491649	1.609929025171
N	1.876488597067	4.159147825843	2.181903655388
C	2.026479337627	3.082633151154	1.388125010456
C	1.715869859511	3.085308992666	0.018903398439
C	0.564723884482	6.627374963532	-0.295109647302
C	0.405593063240	7.729348431984	0.523206035187
C	0.731751144267	7.653107949474	1.897980684421
C	1.214986044903	6.475574339845	2.437307344689
O	2.172180805215	4.119509029047	3.437696881543
C	-0.086988523270	-3.390706388563	0.843351135603
H	-1.965716209546	-4.628907382820	-0.586346151810
H	-4.417085693084	-5.127285982004	-0.746110487895
H	-6.043515812035	-3.303011350619	-0.148630636674
H	-2.357547675564	3.307282500862	-1.892428244368
H	0.618649939465	0.220152560748	-2.290093527845
H	-4.555265095645	1.073332592428	0.761250819469
H	-4.496176124557	-0.240455342591	1.945938441095
H	-3.936676905391	1.933623968434	3.029204023183

H	-2.523430864744	0.843060729029	3.082808556656
H	-2.581520772642	2.183927136540	1.902870688703
H	0.177009296583	2.055092058836	-4.215525948033
H	-0.780900149043	3.464911111408	-3.738312180804
H	1.916154881236	2.646275894161	-2.490711007410
H	1.651565173907	3.907301844210	-3.715694445206
H	2.406547280359	2.199745577875	1.898610552469
H	1.855534583929	2.150025930863	-0.518493744048
H	0.315533109662	6.677331850419	-1.354360743053
H	0.026353197062	8.664831252076	0.107276953385
H	0.602076455354	8.529071511430	2.536596935844
H	1.478703378470	6.374600720030	3.488122821146
H	0.324757375528	-4.075070459992	0.083457513468
H	0.753716446885	-2.933068753684	1.377636334564
H	-0.711075155581	-3.957857209905	1.544820585645

SCF Done: E(RB3LYP) = -1466.00161851

Zero-point correction= 0.445024
Thermal correction to Energy= 0.472350
Thermal correction to Enthalpy= 0.473294
Thermal correction to Gibbs Free Energy= 0.384920
Sum of electronic and zero-point Energies= -1465.556595
Sum of electronic and thermal Energies= -1465.529269
Sum of electronic and thermal Enthalpies= -1465.528325
Sum of electronic and thermal Free Energies= -1465.616699

1	N	Isotropic =	-40.7523	Anisotropy =	455.0654
2	C	Isotropic =	36.9660	Anisotropy =	119.9632
3	C	Isotropic =	59.8050	Anisotropy =	120.6594
4	C	Isotropic =	62.6400	Anisotropy =	177.1522
5	C	Isotropic =	72.4244	Anisotropy =	159.7977
6	C	Isotropic =	48.9919	Anisotropy =	154.0419
7	N	Isotropic =	122.7855	Anisotropy =	91.2199
8	C	Isotropic =	26.6257	Anisotropy =	108.4956
9	C	Isotropic =	69.9520	Anisotropy =	137.0331
10	C	Isotropic =	34.0226	Anisotropy =	125.2200
11	N	Isotropic =	135.7186	Anisotropy =	63.5600
12	O	Isotropic =	-81.7265	Anisotropy =	576.8280
13	N	Isotropic =	-35.2699	Anisotropy =	452.7173
14	C	Isotropic =	40.8578	Anisotropy =	146.8391
15	C	Isotropic =	63.2280	Anisotropy =	172.0795
16	C	Isotropic =	51.3004	Anisotropy =	188.0750
17	C	Isotropic =	147.6542	Anisotropy =	35.3954
18	C	Isotropic =	177.5076	Anisotropy =	23.3761
19	C	Isotropic =	156.1706	Anisotropy =	15.1572
20	C	Isotropic =	122.7690	Anisotropy =	55.1103
21	O	Isotropic =	207.5808	Anisotropy =	128.0007
22	C	Isotropic =	42.6448	Anisotropy =	124.1526
23	C	Isotropic =	69.1162	Anisotropy =	165.7888
24	C	Isotropic =	50.2703	Anisotropy =	152.0349
25	N	Isotropic =	-22.2180	Anisotropy =	252.8331
26	C	Isotropic =	58.3883	Anisotropy =	113.9109
27	C	Isotropic =	92.0113	Anisotropy =	136.3464
28	C	Isotropic =	68.9759	Anisotropy =	177.1028
29	C	Isotropic =	65.3449	Anisotropy =	174.8042

30	C	Isotropic =	63.6095	Anisotropy =	176.8293
31	C	Isotropic =	73.3563	Anisotropy =	173.7434
32	O	Isotropic =	-25.8198	Anisotropy =	322.0622
33	C	Isotropic =	154.6548	Anisotropy =	45.4901
34	H	Isotropic =	23.9648	Anisotropy =	9.1336
35	H	Isotropic =	24.2972	Anisotropy =	4.4900
36	H	Isotropic =	23.2351	Anisotropy =	4.8830
37	H	Isotropic =	23.2917	Anisotropy =	6.5585
38	H	Isotropic =	23.1395	Anisotropy =	10.1217
39	H	Isotropic =	27.2009	Anisotropy =	7.7847
40	H	Isotropic =	27.6600	Anisotropy =	7.0276
41	H	Isotropic =	30.5700	Anisotropy =	10.2954
42	H	Isotropic =	30.6087	Anisotropy =	7.0464
43	H	Isotropic =	30.3913	Anisotropy =	7.7736
44	H	Isotropic =	28.4909	Anisotropy =	7.9154
45	H	Isotropic =	28.4267	Anisotropy =	7.1931
46	H	Isotropic =	26.7162	Anisotropy =	4.2163
47	H	Isotropic =	26.8540	Anisotropy =	7.8825
48	H	Isotropic =	23.5904	Anisotropy =	6.1613
49	H	Isotropic =	25.2693	Anisotropy =	5.9274
50	H	Isotropic =	23.1442	Anisotropy =	10.6404
51	H	Isotropic =	23.7824	Anisotropy =	5.7855
52	H	Isotropic =	23.6920	Anisotropy =	4.9055
53	H	Isotropic =	23.0736	Anisotropy =	8.0630
54	H	Isotropic =	27.9052	Anisotropy =	10.1735
55	H	Isotropic =	27.3773	Anisotropy =	7.6524
56	H	Isotropic =	28.7862	Anisotropy =	7.6953

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.576940867888	-2.696987726956	-0.334968431471
C	-3.204507915036	-1.632124892020	0.379774617593
C	-4.001590340406	-1.099294428807	1.418142095736
C	-5.247748920088	-1.693873694883	1.647547836187
C	-5.639186581870	-2.799780072201	0.891885109357
C	-4.755852127574	-3.278252047544	-0.072674470011
N	-3.534203750449	-0.068016804508	2.277741030411
C	-3.055823020736	1.143059999617	1.833974559968
C	-2.635321770709	1.298825518591	0.405708907504
C	-1.991797289419	0.300246521212	-0.364460590965
N	-1.950992206657	-1.044866899781	0.058776316661
O	-2.944844863801	2.096553883078	2.607137764447
N	-1.373541065192	0.588554977022	-1.518481546156
C	-1.422889057544	1.842049850407	-1.981947331048
C	-2.092141211479	2.896717055972	-1.349330130134
C	-2.682471968228	2.593763623509	-0.119936440376
C	-0.935757601969	-1.924765317044	-0.557449581961
C	0.473960093989	-1.573241644885	-0.089154264484
C	-2.101632326850	4.292170404313	-1.927337477903
C	-1.098736111409	5.253920069149	-1.282637914946
O	0.255584063460	4.849115651864	-1.563242544414
C	1.071773154249	4.359395124406	-0.599995402065

C	2.438906280798	4.175907962512	-0.996255699897
C	3.377971171176	3.666618058600	-0.056828052002
N	2.977614866622	3.348771402029	1.254351314793
C	1.686283271574	3.529212011444	1.588553712409
C	0.720920140584	4.022146087367	0.696024603251
C	2.903187849459	4.482743548286	-2.303181712621
C	4.227290137342	4.287362997409	-2.646646841192
C	5.145213858551	3.778062757080	-1.697833408271
C	4.727724051425	3.471401971682	-0.416154058484
O	3.837939845848	2.893102805763	2.101729781686
C	-3.854620124903	-0.159756784382	3.707651060749
H	-5.898974439685	-1.306147284370	2.431531957910
H	-6.601987163699	-3.283412309029	1.060977927171
H	-5.000260476545	-4.163312047567	-0.667872206395
H	-0.897124160991	2.019664703282	-2.926625861536
H	-3.161058287374	3.371448994853	0.478666406615
H	-1.191999799669	-2.945958957720	-0.253484884532
H	-1.001641220597	-1.882719160776	-1.655588420093
H	0.550142445201	-1.629437579611	1.008586254542
H	1.193963939413	-2.286363331152	-0.522141509568
H	0.767736075733	-0.562373823044	-0.408311429139
H	-1.894080106698	4.250529829238	-3.007995969152
H	-3.100610400456	4.744479048295	-1.810750199208
H	-1.204476990042	6.251386593897	-1.734558824974
H	-1.262871724836	5.354136202778	-0.200647534768
H	1.447134028213	3.254846439365	2.614280428144
H	-0.297556356788	4.105169953114	1.069015254870
H	2.189923187183	4.874184838780	-3.027522388659
H	4.568026638520	4.527550133161	-3.655680519372
H	6.189324477782	3.626881227461	-1.978843876315
H	5.400597810269	3.078647915300	0.343464817120
H	-4.824470834269	0.307298998139	3.945646082181
H	-3.877887999025	-1.217121795246	3.998520024913
H	-3.077858304511	0.366179442548	4.274971657895

SCF Done: E(RB3LYP) = -1466.00157131

Zero-point correction= 0.444795
Thermal correction to Energy= 0.472221
Thermal correction to Enthalpy= 0.473165
Thermal correction to Gibbs Free Energy= 0.383489
Sum of electronic and zero-point Energies= -1465.556776
Sum of electronic and thermal Energies= -1465.529350
Sum of electronic and thermal Enthalpies= -1465.528406
Sum of electronic and thermal Free Energies= -1465.618082

1 N Isotropic = -41.0321 Anisotropy = 454.1666
2 C Isotropic = 36.8534 Anisotropy = 119.7801
3 C Isotropic = 59.9987 Anisotropy = 121.3295
4 C Isotropic = 62.6016 Anisotropy = 176.7689
5 C Isotropic = 72.5411 Anisotropy = 160.1382
6 C Isotropic = 48.9593 Anisotropy = 153.8622
7 N Isotropic = 122.7639 Anisotropy = 91.1425
8 C Isotropic = 26.7245 Anisotropy = 108.5748
9 C Isotropic = 69.8656 Anisotropy = 136.9420
10 C Isotropic = 33.9287 Anisotropy = 125.3187

11	N	Isotropic =	136.0867	Anisotropy =	63.8582
12	O	Isotropic =	-82.1437	Anisotropy =	578.2815
13	N	Isotropic =	-35.0196	Anisotropy =	453.5273
14	C	Isotropic =	40.9429	Anisotropy =	147.8036
15	C	Isotropic =	63.2508	Anisotropy =	171.7402
16	C	Isotropic =	51.2269	Anisotropy =	186.6631
17	C	Isotropic =	147.6558	Anisotropy =	35.4359
18	C	Isotropic =	177.4220	Anisotropy =	23.4526
19	C	Isotropic =	155.9183	Anisotropy =	15.5751
20	C	Isotropic =	122.8191	Anisotropy =	54.6986
21	O	Isotropic =	208.1176	Anisotropy =	127.2608
22	C	Isotropic =	42.5220	Anisotropy =	124.6276
23	C	Isotropic =	69.1739	Anisotropy =	165.8336
24	C	Isotropic =	50.2923	Anisotropy =	152.1706
25	N	Isotropic =	-21.9028	Anisotropy =	252.4958
26	C	Isotropic =	58.4163	Anisotropy =	114.0935
27	C	Isotropic =	92.1865	Anisotropy =	137.0104
28	C	Isotropic =	68.9437	Anisotropy =	177.1771
29	C	Isotropic =	65.5312	Anisotropy =	175.0239
30	C	Isotropic =	63.7876	Anisotropy =	176.3872
31	C	Isotropic =	73.5188	Anisotropy =	173.5060
32	O	Isotropic =	-25.8714	Anisotropy =	321.6521
33	C	Isotropic =	154.5689	Anisotropy =	45.6230
34	H	Isotropic =	23.9628	Anisotropy =	9.1295
35	H	Isotropic =	24.2715	Anisotropy =	4.5219
36	H	Isotropic =	23.2324	Anisotropy =	4.9017
37	H	Isotropic =	23.3009	Anisotropy =	6.5113
38	H	Isotropic =	23.1697	Anisotropy =	10.0850
39	H	Isotropic =	27.6721	Anisotropy =	7.0412
40	H	Isotropic =	27.1958	Anisotropy =	7.7117
41	H	Isotropic =	30.6145	Anisotropy =	7.0038
42	H	Isotropic =	30.5728	Anisotropy =	10.2137
43	H	Isotropic =	30.4339	Anisotropy =	8.0771
44	H	Isotropic =	28.4216	Anisotropy =	7.1885
45	H	Isotropic =	28.4963	Anisotropy =	7.8718
46	H	Isotropic =	26.8816	Anisotropy =	7.8891
47	H	Isotropic =	26.7593	Anisotropy =	4.3480
48	H	Isotropic =	23.6023	Anisotropy =	6.0051
49	H	Isotropic =	25.2899	Anisotropy =	6.0543
50	H	Isotropic =	23.1194	Anisotropy =	10.5997
51	H	Isotropic =	23.7802	Anisotropy =	5.7769
52	H	Isotropic =	23.7056	Anisotropy =	4.8791
53	H	Isotropic =	23.0832	Anisotropy =	8.0169
54	H	Isotropic =	27.9022	Anisotropy =	10.1896
55	H	Isotropic =	28.7805	Anisotropy =	7.6792
56	H	Isotropic =	27.3932	Anisotropy =	7.6916

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.444401793400	-0.427334312841	4.761352156249
C	-1.395716893219	-0.304992556845	3.432472043891
C	-2.368198091183	-0.875871837154	2.581426904622

C	-3.447235630045	-1.534438756553	3.182276514805
C	-3.504747826944	-1.646977479991	4.572016492150
C	-2.464991287705	-1.095557517004	5.316756547284
N	-2.226782043855	-0.878471243867	1.167382151564
C	-2.027890636612	0.254449559880	0.410003258565
C	-1.558382882945	1.516268518723	1.065197051724
C	-0.656057823394	1.582681169394	2.153548557060
N	-0.306492391205	0.430404676187	2.889933893527
O	-2.216771140001	0.233280108009	-0.807290515531
N	-0.075358050198	2.734412378223	2.520520703783
C	-0.396901813802	3.856189953112	1.868065046341
C	-1.319833832177	3.927230759648	0.816822056186
C	-1.877767056859	2.712243908925	0.412290444166
C	0.930925062379	0.485284813507	3.695759807836
C	1.589865028824	-0.886799448807	3.807267102508
C	-1.643481378920	5.233391612039	0.130493971672
C	-0.762960159691	5.552167493607	-1.081362325012
O	-0.985335243676	4.597653007306	-2.138328973884
C	-0.025811068580	3.726666358689	-2.532958726873
C	-0.335467907139	2.972290529737	-3.713668128187
C	0.603348152184	2.021755996131	-4.202841227336
N	1.830116691665	1.822300115705	-3.542610517342
C	2.085386834302	2.547535541495	-2.437768056892
C	1.189047474420	3.492187163831	-1.912941523532
C	-1.553357119039	3.133707251507	-4.426622070967
C	-1.814305184702	2.384929343009	-5.558270686960
C	-0.868519221736	1.442493205213	-6.026760187387
C	0.328129241058	1.261932371308	-5.358659329005
O	2.677198404149	0.960598586111	-3.996345005105
C	-2.626150342378	-2.087236010855	0.435685895822
H	-4.228021262951	-1.976689675728	2.562799129459
H	-4.331454728073	-2.164934907917	5.059656155313
H	-2.444197071102	-1.189561232779	6.406726667011
H	0.107518879392	4.766003839888	2.213807582955
H	-2.551425125211	2.665719890589	-0.444359475199
H	1.599270805236	1.185598214941	3.182326475171
H	0.727915693808	0.902143613052	4.694903380310
H	1.807202365778	-1.302269945884	2.810157213269
H	2.540268660422	-0.793633724855	4.356886150446
H	0.956180142676	-1.602118188816	4.352378448112
H	-2.695217708494	5.234086105246	-0.196585639531
H	-1.528150185425	6.070193987100	0.838798075136
H	-1.051653812771	6.528287286513	-1.499305847722
H	0.299893350697	5.600320887472	-0.808683766351
H	3.048663456778	2.337403546297	-1.976808664969
H	1.491549423159	4.008686166588	-1.004749429628
H	-2.275961995607	3.861488711446	-4.059414487799
H	-2.755304642940	2.521087960381	-6.094802461786
H	-1.084243046749	0.854977874315	-6.921345266169
H	1.082990140645	0.549757281372	-5.685920878552
H	-2.419633545246	-2.964529252001	1.060802365204
H	-3.694725692154	-2.073275983828	0.164699178502
H	-2.043334171448	-2.144627710777	-0.490948228924

SCF Done: E(RB3LYP) = -1466.00128806

Zero-point correction= 0.444862
Thermal correction to Energy= 0.472307
Thermal correction to Enthalpy= 0.473251
Thermal correction to Gibbs Free Energy= 0.383463
Sum of electronic and zero-point Energies= -1465.556426
Sum of electronic and thermal Energies= -1465.528982
Sum of electronic and thermal Enthalpies= -1465.528037
Sum of electronic and thermal Free Energies= -1465.617826

1	N	Isotropic =	-41.7710	Anisotropy =	467.9473
2	C	Isotropic =	38.7441	Anisotropy =	116.5275
3	C	Isotropic =	58.6616	Anisotropy =	122.5178
4	C	Isotropic =	62.8059	Anisotropy =	176.6829
5	C	Isotropic =	72.5660	Anisotropy =	159.0306
6	C	Isotropic =	49.1551	Anisotropy =	153.9061
7	N	Isotropic =	123.3155	Anisotropy =	92.2725
8	C	Isotropic =	27.3955	Anisotropy =	107.6302
9	C	Isotropic =	72.0611	Anisotropy =	134.3921
10	C	Isotropic =	32.5619	Anisotropy =	126.7016
11	N	Isotropic =	137.3840	Anisotropy =	62.8373
12	O	Isotropic =	-81.3500	Anisotropy =	581.4340
13	N	Isotropic =	-36.2599	Anisotropy =	445.0696
14	C	Isotropic =	41.3976	Anisotropy =	149.6958
15	C	Isotropic =	62.7686	Anisotropy =	173.1145
16	C	Isotropic =	50.4325	Anisotropy =	183.0892
17	C	Isotropic =	148.5522	Anisotropy =	33.9392
18	C	Isotropic =	177.3551	Anisotropy =	23.3752
19	C	Isotropic =	156.5040	Anisotropy =	16.1316
20	C	Isotropic =	122.6756	Anisotropy =	54.7176
21	O	Isotropic =	209.5559	Anisotropy =	126.0467
22	C	Isotropic =	42.7320	Anisotropy =	124.5686
23	C	Isotropic =	69.0558	Anisotropy =	166.7446
24	C	Isotropic =	49.8296	Anisotropy =	152.2141
25	N	Isotropic =	-22.4393	Anisotropy =	253.7424
26	C	Isotropic =	58.2037	Anisotropy =	114.6217
27	C	Isotropic =	92.4092	Anisotropy =	136.9972
28	C	Isotropic =	68.8727	Anisotropy =	177.3635
29	C	Isotropic =	65.4916	Anisotropy =	175.8381
30	C	Isotropic =	63.6830	Anisotropy =	177.0242
31	C	Isotropic =	73.2325	Anisotropy =	174.4104
32	O	Isotropic =	-25.8613	Anisotropy =	322.6508
33	C	Isotropic =	154.8206	Anisotropy =	44.8334
34	H	Isotropic =	24.1059	Anisotropy =	9.4608
35	H	Isotropic =	24.3503	Anisotropy =	4.6158
36	H	Isotropic =	23.2212	Anisotropy =	4.8692
37	H	Isotropic =	22.9327	Anisotropy =	7.9396
38	H	Isotropic =	23.6967	Anisotropy =	8.7206
39	H	Isotropic =	27.4743	Anisotropy =	5.6747
40	H	Isotropic =	27.1309	Anisotropy =	8.5128
41	H	Isotropic =	30.4760	Anisotropy =	7.7124
42	H	Isotropic =	30.2802	Anisotropy =	10.9769
43	H	Isotropic =	30.0587	Anisotropy =	5.5594
44	H	Isotropic =	28.3190	Anisotropy =	6.7630
45	H	Isotropic =	28.5869	Anisotropy =	8.4163
46	H	Isotropic =	26.8594	Anisotropy =	8.2120
47	H	Isotropic =	26.8283	Anisotropy =	5.1347

48	H	Isotropic =	23.5823	Anisotropy =	5.3730
49	H	Isotropic =	25.3614	Anisotropy =	6.8466
50	H	Isotropic =	23.0153	Anisotropy =	10.3007
51	H	Isotropic =	23.6787	Anisotropy =	5.7320
52	H	Isotropic =	23.6089	Anisotropy =	4.7669
53	H	Isotropic =	22.9857	Anisotropy =	7.7495
54	H	Isotropic =	29.0126	Anisotropy =	7.4528
55	H	Isotropic =	28.1965	Anisotropy =	9.8490
56	H	Isotropic =	27.8417	Anisotropy =	7.1135

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.243051284698	0.169759616504	4.284367968071
C	-1.245836349384	-0.042375782569	2.966133253323
C	-1.981040021792	-1.088600028544	2.363746873181
C	-2.778129374259	-1.881371203710	3.197221238625
C	-2.786244188700	-1.649008093277	4.573620249725
C	-1.982524114221	-0.625770722146	5.070707878135
N	-1.851856994624	-1.404935208789	0.983904663023
C	-2.015466761651	-0.503663244544	-0.045477861457
C	-2.007788988353	0.965909168284	0.240320836859
C	-1.219259306943	1.594676138943	1.231274276694
N	-0.472388873391	0.835112688723	2.160562509277
O	-2.159377197068	-0.900423805378	-1.203569394327
N	-1.116317856784	2.927687903414	1.316529666773
C	-1.773902065707	3.681480382026	0.429275035502
C	-2.568446669690	3.179933790883	-0.608467335130
C	-2.672425933077	1.787714007465	-0.676989427158
C	0.686920191711	1.498463481414	2.791516115340
C	1.750583279395	0.488933879402	3.214994835628
C	-3.229490152545	4.091348430123	-1.621571536303
C	-2.745274549603	3.925214882461	-3.069521063878
O	-1.477729933688	4.561377089802	-3.377432565049
C	-0.367390363334	4.194702343896	-2.663995731153
C	0.245242694614	2.910540899296	-2.809125130475
C	1.344849396250	2.574456530367	-1.965882256567
N	1.840942723159	3.506414945605	-1.035203927173
C	1.322239212932	4.751042291556	-1.023854785888
C	0.224563481970	5.110446062664	-1.816664464708
C	-0.170351626535	1.945079732888	-3.766699617491
C	0.447719236067	0.712567751394	-3.845072150815
C	1.513271865806	0.387415349496	-2.972055838654
C	1.962305806242	1.308755771960	-2.045171617152
O	2.781153536027	3.167330678169	-0.222399895558
C	-1.821607748890	-2.823300867249	0.603717266923
H	-3.373021482512	-2.690970304088	2.773178520885
H	-3.392759165461	-2.260938463898	5.242393203869
H	-1.926041138966	-0.429213340985	6.145646114199
H	-1.651763739539	4.763455114746	0.544386818994
H	-3.240264584207	1.302932071653	-1.473112063828
H	1.101681085912	2.173198819224	2.031739929682
H	0.372311430378	2.116186585242	3.647929543130

H	1.386245816966	-0.185655767997	4.003763741053
H	2.078526100313	-0.120359148456	2.357434127619
H	2.627357286430	1.026327051132	3.610470228723
H	-4.313901203728	3.886250784318	-1.643269954172
H	-3.115973603218	5.144312404064	-1.319117122745
H	-2.709115141652	2.857604390388	-3.340582413550
H	-3.446242115827	4.423914381075	-3.751829329492
H	1.785972743023	5.424606598197	-0.305961328502
H	-0.191851964547	6.112945301398	-1.719360657766
H	-0.971857712852	2.202296343050	-4.458443084448
H	0.117944457534	-0.013198198138	-4.590742507014
H	1.992047406752	-0.591157080318	-3.040773709249
H	2.791265560087	1.105181508236	-1.370424028512
H	-1.348463711819	-3.396268983315	1.410399977063
H	-2.831755607587	-3.222032320941	0.413997789553
H	-1.238481784719	-2.927162605114	-0.318711863638

SCF Done: E(RB3LYP) = -1465.99358666

Zero-point correction= 0.444813
Thermal correction to Energy= 0.471969
Thermal correction to Enthalpy= 0.472914
Thermal correction to Gibbs Free Energy= 0.387043
Sum of electronic and zero-point Energies= -1465.548774
Sum of electronic and thermal Energies= -1465.521617
Sum of electronic and thermal Enthalpies= -1465.520673
Sum of electronic and thermal Free Energies= -1465.606544

1	N	Isotropic =	-41.2166	Anisotropy =	467.2325
2	C	Isotropic =	38.7615	Anisotropy =	116.3173
3	C	Isotropic =	59.0959	Anisotropy =	122.3141
4	C	Isotropic =	62.8584	Anisotropy =	176.2495
5	C	Isotropic =	72.8415	Anisotropy =	158.7550
6	C	Isotropic =	49.1326	Anisotropy =	154.0000
7	N	Isotropic =	122.3899	Anisotropy =	90.3141
8	C	Isotropic =	28.0340	Anisotropy =	109.8638
9	C	Isotropic =	72.2016	Anisotropy =	138.8397
10	C	Isotropic =	33.0819	Anisotropy =	127.9164
11	N	Isotropic =	141.3283	Anisotropy =	61.0433
12	O	Isotropic =	-77.5097	Anisotropy =	585.7138
13	N	Isotropic =	-35.7642	Anisotropy =	445.6372
14	C	Isotropic =	39.1923	Anisotropy =	152.9283
15	C	Isotropic =	62.4972	Anisotropy =	174.9118
16	C	Isotropic =	54.3326	Anisotropy =	191.8495
17	C	Isotropic =	147.8273	Anisotropy =	32.6689
18	C	Isotropic =	177.5653	Anisotropy =	22.5824
19	C	Isotropic =	155.7748	Anisotropy =	13.0438
20	C	Isotropic =	117.8176	Anisotropy =	58.9328
21	O	Isotropic =	224.9623	Anisotropy =	128.9848
22	C	Isotropic =	42.4177	Anisotropy =	126.9845
23	C	Isotropic =	67.2513	Anisotropy =	176.8176
24	C	Isotropic =	49.5219	Anisotropy =	156.4571
25	N	Isotropic =	-31.6380	Anisotropy =	269.8976
26	C	Isotropic =	57.2508	Anisotropy =	117.6446
27	C	Isotropic =	75.6287	Anisotropy =	138.2920
28	C	Isotropic =	68.7120	Anisotropy =	173.3790

29	C	Isotropic =	64.6525	Anisotropy =	179.6406
30	C	Isotropic =	63.8172	Anisotropy =	179.5684
31	C	Isotropic =	72.6002	Anisotropy =	178.2364
32	O	Isotropic =	-43.5620	Anisotropy =	354.5616
33	C	Isotropic =	154.4639	Anisotropy =	45.3517
34	H	Isotropic =	24.1310	Anisotropy =	9.4517
35	H	Isotropic =	24.3938	Anisotropy =	4.4792
36	H	Isotropic =	23.2684	Anisotropy =	4.9541
37	H	Isotropic =	23.6765	Anisotropy =	5.9958
38	H	Isotropic =	24.0306	Anisotropy =	8.5331
39	H	Isotropic =	27.9909	Anisotropy =	7.6076
40	H	Isotropic =	27.3069	Anisotropy =	8.2781
41	H	Isotropic =	30.0284	Anisotropy =	6.3325
42	H	Isotropic =	30.4893	Anisotropy =	7.0728
43	H	Isotropic =	30.2465	Anisotropy =	10.3004
44	H	Isotropic =	28.6966	Anisotropy =	9.0561
45	H	Isotropic =	28.5696	Anisotropy =	5.8484
46	H	Isotropic =	26.4738	Anisotropy =	4.5350
47	H	Isotropic =	26.8521	Anisotropy =	7.0766
48	H	Isotropic =	23.2192	Anisotropy =	4.3225
49	H	Isotropic =	24.3618	Anisotropy =	6.0513
50	H	Isotropic =	23.3724	Anisotropy =	8.4441
51	H	Isotropic =	23.7277	Anisotropy =	4.6951
52	H	Isotropic =	23.7588	Anisotropy =	4.4904
53	H	Isotropic =	23.1148	Anisotropy =	6.6622
54	H	Isotropic =	28.9621	Anisotropy =	7.3538
55	H	Isotropic =	28.1152	Anisotropy =	10.5594
56	H	Isotropic =	27.6379	Anisotropy =	6.8825

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.795701685899	-1.231165351420	1.817235148548
C	-2.644825747846	-0.555399793549	1.858010093489
C	-2.025858254486	-0.176501989686	3.070953442953
C	-2.697131707160	-0.479708449125	4.260904234296
C	-3.908483596711	-1.171990388606	4.216354004813
C	-4.404292867082	-1.546248510343	2.969734500111
N	-0.727116396817	0.400257451170	3.108740177055
C	-0.344690962471	1.517480079035	2.398207504176
C	-1.185860287849	2.003030028681	1.259098852385
C	-1.921826534587	1.174030674732	0.381630595470
N	-2.042828565272	-0.214373586215	0.617648735427
O	0.692123136566	2.116336056058	2.691167761335
N	-2.509120331497	1.654358546189	-0.722621612271
C	-2.383996863339	2.955557781629	-1.003951295857
C	-1.665142722392	3.872826422427	-0.228132215367
C	-1.067551601969	3.357036891332	0.925244286978
C	-2.348033909125	-1.070544150009	-0.546911882270
C	-1.813998316514	-2.487642598898	-0.354988697583
C	-1.506104580699	5.320875263046	-0.642779813278
C	-0.067778306628	5.760414755666	-0.953660974791
O	0.434595809248	5.363913105315	-2.256088205725

C	0.453845524229	4.033006048049	-2.579001962564
C	1.345618736985	3.105826186991	-1.954106521104
C	1.241011622280	1.722780410501	-2.284609449933
N	0.304792125190	1.286376832955	-3.240484423719
C	-0.423276759197	2.207566107264	-3.903421677567
C	-0.370526013111	3.571122658687	-3.586183306500
C	2.353452885755	3.487631528877	-1.026752752265
C	3.172339987426	2.542572439087	-0.440614636224
C	3.024500087623	1.170583238012	-0.755531451550
C	2.073034187288	0.763108643180	-1.671123482178
O	0.165623325146	0.027911131914	-3.477764472437
C	0.185175667965	-0.030218714466	4.176247621646
H	-2.262727746851	-0.194121185927	5.219438117894
H	-4.443408508190	-1.426218317973	5.132210878689
H	-5.330098606382	-2.123289227543	2.884647077462
H	-2.882849944475	3.291749170973	-1.918826056159
H	-0.457231511664	3.987211446415	1.574617203557
H	-3.430153320658	-1.086272397499	-0.753658426156
H	-1.853276506489	-0.603223407052	-1.407910255519
H	-2.315728534239	-3.006862751000	0.474894680661
H	-1.988821579503	-3.072085652350	-1.272468681065
H	-0.730409894936	-2.475063258630	-0.155317231195
H	-2.149573483327	5.543325079567	-1.508638728222
H	-1.848124994182	5.974471434129	0.178384264237
H	-0.017365829746	6.856643136890	-0.990640608482
H	0.617267632317	5.416037848615	-0.161800327866
H	-1.093108502959	1.795038136626	-4.655315663913
H	-1.028227060372	4.262113286665	-4.113340967563
H	2.487589565083	4.545318164813	-0.802472187945
H	3.944284304599	2.856186840766	0.264524906533
H	3.674859134320	0.432050446087	-0.283139773219
H	1.941727736820	-0.278861624046	-1.955929061047
H	0.077776958384	0.585047402106	5.084751493180
H	-0.023135262452	-1.079263125831	4.419163575662
H	1.216398869852	0.071979805719	3.818827644976

SCF Done: E(RB3LYP) = -1465.99355142

Zero-point correction= 0.444755
Thermal correction to Energy= 0.471915
Thermal correction to Enthalpy= 0.472859
Thermal correction to Gibbs Free Energy= 0.386911
Sum of electronic and zero-point Energies= -1465.548796
Sum of electronic and thermal Energies= -1465.521636
Sum of electronic and thermal Enthalpies= -1465.520692
Sum of electronic and thermal Free Energies= -1465.606641

1	N	Isotropic =	-41.2775	Anisotropy =	467.3898
2	C	Isotropic =	38.9823	Anisotropy =	116.3182
3	C	Isotropic =	59.1152	Anisotropy =	121.8635
4	C	Isotropic =	63.0042	Anisotropy =	176.4021
5	C	Isotropic =	72.7701	Anisotropy =	158.5176
6	C	Isotropic =	49.0680	Anisotropy =	153.7998
7	N	Isotropic =	122.4978	Anisotropy =	90.4772
8	C	Isotropic =	27.9582	Anisotropy =	109.8180
9	C	Isotropic =	72.2243	Anisotropy =	138.9253

10	C	Isotropic =	33.1740	Anisotropy =	128.1183
11	N	Isotropic =	141.2654	Anisotropy =	60.8189
12	O	Isotropic =	-77.4782	Anisotropy =	586.5826
13	N	Isotropic =	-35.8267	Anisotropy =	445.8269
14	C	Isotropic =	39.3285	Anisotropy =	153.0519
15	C	Isotropic =	62.6430	Anisotropy =	174.8556
16	C	Isotropic =	54.3056	Anisotropy =	192.1043
17	C	Isotropic =	148.0101	Anisotropy =	32.8671
18	C	Isotropic =	177.6456	Anisotropy =	22.5703
19	C	Isotropic =	155.7069	Anisotropy =	13.0233
20	C	Isotropic =	117.9179	Anisotropy =	58.8317
21	O	Isotropic =	224.5642	Anisotropy =	128.7811
22	C	Isotropic =	42.6958	Anisotropy =	127.2287
23	C	Isotropic =	67.1995	Anisotropy =	177.0502
24	C	Isotropic =	49.6126	Anisotropy =	156.7914
25	N	Isotropic =	-31.7763	Anisotropy =	269.5514
26	C	Isotropic =	57.3742	Anisotropy =	117.3957
27	C	Isotropic =	75.6832	Anisotropy =	137.7228
28	C	Isotropic =	68.7854	Anisotropy =	173.7761
29	C	Isotropic =	64.5889	Anisotropy =	179.8418
30	C	Isotropic =	63.6754	Anisotropy =	179.8025
31	C	Isotropic =	72.4520	Anisotropy =	178.2256
32	O	Isotropic =	-43.0152	Anisotropy =	354.8051
33	C	Isotropic =	154.5751	Anisotropy =	45.1618
34	H	Isotropic =	24.1412	Anisotropy =	9.4541
35	H	Isotropic =	24.4017	Anisotropy =	4.4654
36	H	Isotropic =	23.2694	Anisotropy =	4.9561
37	H	Isotropic =	23.7043	Anisotropy =	5.8971
38	H	Isotropic =	24.0207	Anisotropy =	8.5515
39	H	Isotropic =	27.3135	Anisotropy =	8.2854
40	H	Isotropic =	27.9932	Anisotropy =	7.6790
41	H	Isotropic =	30.0434	Anisotropy =	6.3429
42	H	Isotropic =	30.2609	Anisotropy =	10.3206
43	H	Isotropic =	30.4818	Anisotropy =	7.0237
44	H	Isotropic =	28.5892	Anisotropy =	5.8684
45	H	Isotropic =	28.7093	Anisotropy =	9.0906
46	H	Isotropic =	26.8487	Anisotropy =	7.1075
47	H	Isotropic =	26.4656	Anisotropy =	4.6218
48	H	Isotropic =	23.2155	Anisotropy =	4.3535
49	H	Isotropic =	24.3567	Anisotropy =	6.0680
50	H	Isotropic =	23.3936	Anisotropy =	8.4028
51	H	Isotropic =	23.7341	Anisotropy =	4.6554
52	H	Isotropic =	23.7614	Anisotropy =	4.4987
53	H	Isotropic =	23.1120	Anisotropy =	6.5632
54	H	Isotropic =	28.1043	Anisotropy =	10.5902
55	H	Isotropic =	28.9615	Anisotropy =	7.3823
56	H	Isotropic =	27.6267	Anisotropy =	6.8871

Conformer 26

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.884096622262	-1.662506703617	1.696999251180
C	-1.069171921082	-0.401995098841	2.096391418166

C	-2.335253071784	0.226072584911	2.064278084993
C	-3.401064803458	-0.494371597735	1.514104524506
C	-3.202377995623	-1.807255033192	1.084191747889
C	-1.930110789447	-2.355879108764	1.224853395176
N	-2.563759174613	1.498589628672	2.656457874068
C	-1.847155157139	2.631530359719	2.346619615500
C	-0.546080374625	2.501983675229	1.618809067017
C	0.396194376033	1.467348470746	1.819231788813
N	0.070915130217	0.307949626881	2.560015361374
O	-2.263105364966	3.746609204441	2.665397642763
N	1.644123690553	1.547352110958	1.336273581965
C	1.971387518503	2.592807317548	0.569991237885
C	1.096572932678	3.632256815410	0.222600851673
C	-0.166016634175	3.582605285766	0.815431507978
C	1.190544917217	-0.496374365957	3.092043025976
C	1.913397717945	0.225721217010	4.226108632445
C	1.533436106384	4.742912153528	-0.707708557997
C	1.676877028197	4.345205832543	-2.185843449247
O	0.447550676515	4.377977020481	-2.950586672496
C	-0.536849588625	3.460044827641	-2.695892235210
C	-0.406509414811	2.080496655362	-3.052738050252
C	-1.482154755004	1.189144060886	-2.762274635434
N	-2.669358005462	1.665711941518	-2.171708375856
C	-2.784118946934	2.987453167796	-1.925201926672
C	-1.741181480572	3.889006342595	-2.173143380427
C	0.727622755733	1.545076368893	-3.724114684130
C	0.796641577073	0.203134231609	-4.042458915936
C	-0.266293849154	-0.669524639272	-3.707882605086
C	-1.397203405476	-0.182268795569	-3.081374756907
O	-3.625210146103	0.850909091883	-1.898453305221
C	-3.811972164143	1.698044373226	3.403224546218
H	-4.386934998550	-0.034926244094	1.442170479223
H	-4.021940904753	-2.390166093979	0.662387273207
H	-1.731831190269	-3.393749904227	0.940471229680
H	3.005850171343	2.605933973713	0.207982747097
H	-0.878009442103	4.397788603825	0.682014728166
H	0.748359874039	-1.430001719573	3.458363256331
H	1.895872196343	-0.760679034982	2.288840337874
H	1.215559886380	0.479501766939	5.040123990512
H	2.699789515787	-0.428067065651	4.636575997222
H	2.394008808500	1.151488597101	3.876583916719
H	0.851935920165	5.604400625679	-0.632156081983
H	2.528965078096	5.101146500456	-0.394259628118
H	2.309876733142	5.079147743945	-2.702311521228
H	2.157181812911	3.357284215439	-2.272280653179
H	-3.739646694062	3.283022498637	-1.496542982072
H	-1.886406972243	4.941728945072	-1.931033571874
H	1.536559425974	2.217091921811	-4.008272325416
H	1.673525995057	-0.186147595395	-4.563248309631
H	-0.198861568213	-1.729585522670	-3.959457750449
H	-2.245117946919	-0.815077264775	-2.827510889424
H	-3.645994103794	2.467585495142	4.166198998303
H	-4.633804712388	2.036934180755	2.751104800717
H	-4.093507646030	0.752228354530	3.882074353611

SCF Done: E(RB3LYP) = -1465.99338132

Zero-point correction= 0.444497
Thermal correction to Energy= 0.471842
Thermal correction to Enthalpy= 0.472786
Thermal correction to Gibbs Free Energy= 0.385356
Sum of electronic and zero-point Energies= -1465.548884
Sum of electronic and thermal Energies= -1465.521539
Sum of electronic and thermal Enthalpies= -1465.520595
Sum of electronic and thermal Free Energies= -1465.608025

1	N	Isotropic =	-39.1396	Anisotropy =	456.6390
2	C	Isotropic =	37.0253	Anisotropy =	122.5461
3	C	Isotropic =	60.7517	Anisotropy =	123.5077
4	C	Isotropic =	61.8298	Anisotropy =	180.9152
5	C	Isotropic =	72.5446	Anisotropy =	161.6816
6	C	Isotropic =	49.1208	Anisotropy =	156.0914
7	N	Isotropic =	122.8159	Anisotropy =	92.6031
8	C	Isotropic =	27.3147	Anisotropy =	111.3003
9	C	Isotropic =	71.7408	Anisotropy =	134.0002
10	C	Isotropic =	34.8555	Anisotropy =	123.5625
11	N	Isotropic =	138.1943	Anisotropy =	68.3522
12	O	Isotropic =	-77.2031	Anisotropy =	580.9548
13	N	Isotropic =	-35.0805	Anisotropy =	458.7457
14	C	Isotropic =	42.1643	Anisotropy =	153.0691
15	C	Isotropic =	60.8377	Anisotropy =	175.6866
16	C	Isotropic =	50.0061	Anisotropy =	183.1660
17	C	Isotropic =	148.0332	Anisotropy =	36.2746
18	C	Isotropic =	177.3480	Anisotropy =	24.5933
19	C	Isotropic =	153.8556	Anisotropy =	15.7889
20	C	Isotropic =	115.9579	Anisotropy =	54.5238
21	O	Isotropic =	222.5033	Anisotropy =	126.4207
22	C	Isotropic =	43.4581	Anisotropy =	124.7746
23	C	Isotropic =	67.4729	Anisotropy =	174.6330
24	C	Isotropic =	49.3579	Anisotropy =	155.8206
25	N	Isotropic =	-32.3542	Anisotropy =	270.7640
26	C	Isotropic =	58.2910	Anisotropy =	116.6143
27	C	Isotropic =	76.0542	Anisotropy =	137.1758
28	C	Isotropic =	69.3132	Anisotropy =	172.4096
29	C	Isotropic =	65.1964	Anisotropy =	177.6633
30	C	Isotropic =	64.1948	Anisotropy =	177.9880
31	C	Isotropic =	72.6900	Anisotropy =	178.0368
32	O	Isotropic =	-54.0629	Anisotropy =	379.4660
33	C	Isotropic =	154.6048	Anisotropy =	46.2136
34	H	Isotropic =	23.9005	Anisotropy =	7.7108
35	H	Isotropic =	24.2198	Anisotropy =	4.3640
36	H	Isotropic =	23.2780	Anisotropy =	4.2633
37	H	Isotropic =	23.4662	Anisotropy =	7.7196
38	H	Isotropic =	23.8438	Anisotropy =	8.7531
39	H	Isotropic =	27.7976	Anisotropy =	5.9327
40	H	Isotropic =	27.3510	Anisotropy =	7.1351
41	H	Isotropic =	30.5458	Anisotropy =	8.6136
42	H	Isotropic =	30.4315	Anisotropy =	11.4289
43	H	Isotropic =	30.1130	Anisotropy =	5.0746
44	H	Isotropic =	28.4602	Anisotropy =	4.7397
45	H	Isotropic =	28.4765	Anisotropy =	8.5296
46	H	Isotropic =	26.8135	Anisotropy =	6.9162

47	H	Isotropic =	26.8581	Anisotropy =	4.4369
48	H	Isotropic =	23.4353	Anisotropy =	4.1344
49	H	Isotropic =	24.4226	Anisotropy =	5.5894
50	H	Isotropic =	23.5688	Anisotropy =	8.9791
51	H	Isotropic =	23.9489	Anisotropy =	5.2111
52	H	Isotropic =	23.9587	Anisotropy =	5.2386
53	H	Isotropic =	23.5565	Anisotropy =	6.8100
54	H	Isotropic =	27.4836	Anisotropy =	8.9058
55	H	Isotropic =	27.9265	Anisotropy =	9.1785
56	H	Isotropic =	28.8712	Anisotropy =	8.2547

Conformer 27

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.690204541822	2.951866188793	3.131326707290
C	-2.415240825110	2.554875576986	3.119056594996
C	-1.358305782434	3.407107701396	2.729385032904
C	-1.692799615020	4.691009380589	2.283808424809
C	-3.027443914245	5.098536312778	2.281863313129
C	-3.987540634981	4.197981294651	2.737199693215
N	0.004989303579	3.030130152799	2.867908172814
C	0.545514960215	1.885337654242	2.325253223290
C	-0.354816950342	0.768429225602	1.896174780267
C	-1.553865748409	0.392015910306	2.548937284767
N	-2.150034455088	1.218395252773	3.524784713367
O	1.766048849324	1.766406200063	2.206449107103
N	-2.157692207965	-0.777389175206	2.295141518615
C	-1.645431854903	-1.578192250421	1.354414449147
C	-0.512800438678	-1.279524029758	0.587032750551
C	0.143675487383	-0.089398305947	0.909519748546
C	-3.118277572279	0.596472696539	4.451584805985
C	-3.107338630915	1.280441514357	5.815887646555
C	-0.031501690094	-2.205351262365	-0.505589355563
C	-0.569661696825	-1.857274857318	-1.891607811082
O	-0.013974938238	-0.590069617880	-2.278530752518
C	-0.372765820496	-0.062689383115	-3.471484506636
C	0.235423889104	1.189722950712	-3.815199813565
C	-0.095450813972	1.806658696848	-5.053563765058
N	-1.009292676265	1.198112495967	-5.936122936265
C	-1.556341134647	0.021218703395	-5.580022567631
C	-1.261601127940	-0.627816769667	-4.369656135268
C	1.165860483174	1.849332237408	-2.969174440455
C	1.728381788364	3.055025248540	-3.342784457365
C	1.385056623694	3.653040487934	-4.578217293389
C	0.483294652899	3.037323312646	-5.426192366206
O	-1.302582517756	1.767945713512	-7.055572941966
C	0.959817040299	4.049079586426	3.321440955409
H	-0.908761529324	5.376385378593	1.960511547761
H	-3.308841482802	6.098057622841	1.948251722928
H	-5.042894367388	4.482157296903	2.790061255454
H	-2.174995485946	-2.525266955905	1.199469137734
H	1.087107219704	0.174609251311	0.430135809564
H	-4.131820214908	0.604752017586	4.020107557375

H	-2.816383477397	-0.452188678199	4.550491703525
H	-2.097132680419	1.266335087310	6.255660648508
H	-3.445003414882	2.325657122254	5.752691581872
H	-3.788696026662	0.748137312089	6.498811375742
H	1.069282827204	-2.207354497310	-0.548522538578
H	-0.348676480497	-3.237280629457	-0.287677501133
H	-0.270291914318	-2.626245842574	-2.624005518106
H	-1.671164719239	-1.790226421761	-1.879994265499
H	-2.250369948886	-0.389165721454	-6.311155180413
H	-1.757057064570	-1.577314994791	-4.178134813465
H	1.427380270668	1.382354759882	-2.020522497331
H	2.442392909447	3.549317435551	-2.681204092575
H	1.835047824887	4.605705268686	-4.864279675828
H	0.192920093455	3.462031186217	-6.384988604509
H	0.451337353126	4.724693212396	4.020101612736
H	1.793374840708	3.548463472113	3.827738430453
H	1.373077978427	4.632638474133	2.482312523995

SCF Done: E(RB3LYP) = -1466.00578069

Zero-point correction= 0.444860
Thermal correction to Energy= 0.472264
Thermal correction to Enthalpy= 0.473208
Thermal correction to Gibbs Free Energy= 0.384247
Sum of electronic and zero-point Energies= -1465.560921
Sum of electronic and thermal Energies= -1465.533517
Sum of electronic and thermal Enthalpies= -1465.532572
Sum of electronic and thermal Free Energies= -1465.621533

1	N	Isotropic =	-42.0998	Anisotropy =	469.0672
2	C	Isotropic =	38.5646	Anisotropy =	117.9290
3	C	Isotropic =	58.6943	Anisotropy =	123.5012
4	C	Isotropic =	62.8555	Anisotropy =	177.7994
5	C	Isotropic =	72.5851	Anisotropy =	159.7401
6	C	Isotropic =	49.0780	Anisotropy =	154.3716
7	N	Isotropic =	123.1006	Anisotropy =	92.3117
8	C	Isotropic =	26.5767	Anisotropy =	109.4561
9	C	Isotropic =	72.0184	Anisotropy =	130.4849
10	C	Isotropic =	32.3776	Anisotropy =	123.7818
11	N	Isotropic =	137.1636	Anisotropy =	64.4628
12	O	Isotropic =	-81.5219	Anisotropy =	582.6814
13	N	Isotropic =	-34.3137	Anisotropy =	443.2394
14	C	Isotropic =	41.7693	Anisotropy =	144.7910
15	C	Isotropic =	61.3806	Anisotropy =	171.6754
16	C	Isotropic =	50.0436	Anisotropy =	180.6838
17	C	Isotropic =	148.5569	Anisotropy =	34.4725
18	C	Isotropic =	177.3852	Anisotropy =	23.7015
19	C	Isotropic =	157.0080	Anisotropy =	16.3716
20	C	Isotropic =	120.9434	Anisotropy =	43.9782
21	O	Isotropic =	208.5684	Anisotropy =	108.9196
22	C	Isotropic =	43.0406	Anisotropy =	123.2349
23	C	Isotropic =	69.2470	Anisotropy =	165.4080
24	C	Isotropic =	49.9783	Anisotropy =	151.3011
25	N	Isotropic =	-23.8559	Anisotropy =	254.9212
26	C	Isotropic =	57.9808	Anisotropy =	113.5488
27	C	Isotropic =	91.4670	Anisotropy =	131.4376

28	C	Isotropic =	69.1911	Anisotropy =	175.8802
29	C	Isotropic =	65.3149	Anisotropy =	175.7696
30	C	Isotropic =	63.7805	Anisotropy =	176.9553
31	C	Isotropic =	73.3968	Anisotropy =	174.2762
32	O	Isotropic =	-29.0073	Anisotropy =	327.3950
33	C	Isotropic =	154.5955	Anisotropy =	45.3900
34	H	Isotropic =	24.0721	Anisotropy =	8.2937
35	H	Isotropic =	24.4169	Anisotropy =	4.5521
36	H	Isotropic =	23.2734	Anisotropy =	4.7566
37	H	Isotropic =	23.0407	Anisotropy =	7.9398
38	H	Isotropic =	23.1070	Anisotropy =	10.2234
39	H	Isotropic =	27.1346	Anisotropy =	8.3044
40	H	Isotropic =	27.3883	Anisotropy =	6.0047
41	H	Isotropic =	30.4123	Anisotropy =	8.0535
42	H	Isotropic =	30.0311	Anisotropy =	5.1895
43	H	Isotropic =	30.2669	Anisotropy =	11.2421
44	H	Isotropic =	28.2391	Anisotropy =	5.5097
45	H	Isotropic =	28.4552	Anisotropy =	8.3064
46	H	Isotropic =	27.2318	Anisotropy =	6.3399
47	H	Isotropic =	27.6324	Anisotropy =	5.4234
48	H	Isotropic =	23.3664	Anisotropy =	5.1969
49	H	Isotropic =	25.0866	Anisotropy =	8.8123
50	H	Isotropic =	23.1464	Anisotropy =	8.9165
51	H	Isotropic =	23.7573	Anisotropy =	6.6395
52	H	Isotropic =	23.6757	Anisotropy =	5.1926
53	H	Isotropic =	23.0188	Anisotropy =	7.5174
54	H	Isotropic =	28.8236	Anisotropy =	7.7516
55	H	Isotropic =	27.4249	Anisotropy =	8.1517
56	H	Isotropic =	27.9174	Anisotropy =	9.8120

Conformer 28

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.569522083477	2.541090408749	2.547271506289
C	-3.300592701364	2.477964723732	2.135475343671
C	-2.290217778666	3.310813929623	2.668224503705
C	-2.678814030739	4.287839030445	3.592622415950
C	-4.011091533980	4.369276713743	3.999832777955
C	-4.913403893934	3.450998592646	3.468703940873
N	-0.911569222513	3.110099525142	2.385330356303
C	-0.366492944683	3.039666823958	1.122267064998
C	-1.241792205190	2.785576640922	-0.066030100933
C	-2.430841252864	2.019909157830	-0.066653032598
N	-2.994668665843	1.526990349955	1.128550572636
O	0.849676710311	3.166487529241	0.966502209899
N	-3.056857663489	1.689797715719	-1.208211203089
C	-2.522020403184	2.060923158321	-2.373465340952
C	-1.328212979729	2.783551671888	-2.502370316531
C	-0.707733449613	3.151159735669	-1.308951434313
C	-3.826280537555	0.307646395198	1.066034112709
C	-3.389940904266	-0.704875914135	2.124200714997
C	-0.687563330828	3.034553206067	-3.847590302965
C	0.042540871180	1.807400597020	-4.418516389584

O	1.092424651475	1.353422758851	-3.541060118823
C	0.866362373784	0.381527230943	-2.621292874380
C	1.865090515335	0.251325893042	-1.600500258589
C	1.687510916681	-0.712222270163	-0.567776787410
N	0.543323413132	-1.529456802592	-0.541722659483
C	-0.341604229660	-1.420767593731	-1.549497761651
C	-0.209320979762	-0.488758894856	-2.589470838571
C	3.032203254554	1.060056812411	-1.564099883224
C	3.967098821585	0.906474286085	-0.558377871594
C	3.773245952344	-0.059233900878	0.457772980676
C	2.645166958789	-0.858262575869	0.457349679109
O	0.358052319132	-2.358356616211	0.433227080616
C	0.043992793548	3.279604145260	3.488396972556
H	-1.934779583773	4.964945141424	4.013204452825
H	-4.331470148050	5.115507572679	4.727830388444
H	-5.959344715348	3.441226248750	3.790259416908
H	-3.075138262825	1.751779748743	-3.268130330335
H	0.243421375055	3.684999195705	-1.316120601057
H	-4.886512723949	0.570048256300	1.190061132020
H	-3.705213767789	-0.107918287675	0.060500076601
H	-2.348668882371	-1.027508671405	1.959430389298
H	-3.469138712366	-0.287936269344	3.141096582581
H	-4.037176077848	-1.596092235797	2.077038339840
H	-1.445209897031	3.329270885569	-4.593384119356
H	0.029516105794	3.865858237878	-3.768711344995
H	-0.656712509617	0.991484102005	-4.649218403740
H	0.553884466162	2.082984549333	-5.351288344246
H	-1.189644046439	-2.099030132993	-1.477068465141
H	-0.998150620579	-0.470246712407	-3.337813453507
H	3.172126950114	1.802822336658	-2.348558749300
H	4.860089869524	1.534364058128	-0.545949649139
H	4.518252327779	-0.173438280732	1.247650408016
H	2.455779380790	-1.608946041767	1.222084080639
H	0.914646520225	2.640877537227	3.299832527413
H	0.398203062519	4.320060040718	3.573313146361
H	-0.440978870489	2.981436256981	4.425727461617

SCF Done: E(RB3LYP) = -1465.99848833

Zero-point correction= 0.444998
Thermal correction to Energy= 0.472269
Thermal correction to Enthalpy= 0.473213
Thermal correction to Gibbs Free Energy= 0.385969
Sum of electronic and zero-point Energies= -1465.553490
Sum of electronic and thermal Energies= -1465.526219
Sum of electronic and thermal Enthalpies= -1465.525275
Sum of electronic and thermal Free Energies= -1465.612520

1	N	Isotropic =	-39.0085	Anisotropy =	463.0910
2	C	Isotropic =	39.0565	Anisotropy =	115.4502
3	C	Isotropic =	59.1695	Anisotropy =	120.6415
4	C	Isotropic =	62.6476	Anisotropy =	175.7339
5	C	Isotropic =	72.6118	Anisotropy =	158.4998
6	C	Isotropic =	49.4919	Anisotropy =	153.2315
7	N	Isotropic =	123.3282	Anisotropy =	91.0555
8	C	Isotropic =	28.2273	Anisotropy =	109.1248

9 C Isotropic = 71.7581 Anisotropy = 139.0925
10 C Isotropic = 33.6343 Anisotropy = 128.2507
11 N Isotropic = 138.7155 Anisotropy = 61.3448
12 O Isotropic = -78.9815 Anisotropy = 586.9095
13 N Isotropic = -39.9889 Anisotropy = 445.1438
14 C Isotropic = 40.4042 Anisotropy = 156.3818
15 C Isotropic = 63.5839 Anisotropy = 173.9398
16 C Isotropic = 50.1064 Anisotropy = 183.4659
17 C Isotropic = 150.4121 Anisotropy = 41.0018
18 C Isotropic = 176.3093 Anisotropy = 23.3489
19 C Isotropic = 155.2805 Anisotropy = 15.7998
20 C Isotropic = 124.1925 Anisotropy = 52.7627
21 O Isotropic = 210.4026 Anisotropy = 136.1623
22 C Isotropic = 42.9850 Anisotropy = 127.8939
23 C Isotropic = 68.8753 Anisotropy = 168.9646
24 C Isotropic = 50.3102 Anisotropy = 154.2123
25 N Isotropic = -21.5369 Anisotropy = 254.6159
26 C Isotropic = 58.2600 Anisotropy = 117.3964
27 C Isotropic = 91.1181 Anisotropy = 145.8260
28 C Isotropic = 68.7835 Anisotropy = 178.9461
29 C Isotropic = 65.4332 Anisotropy = 176.4763
30 C Isotropic = 63.6171 Anisotropy = 177.9349
31 C Isotropic = 73.3850 Anisotropy = 175.2108
32 O Isotropic = -18.0218 Anisotropy = 307.6253
33 C Isotropic = 154.2882 Anisotropy = 44.8465
34 H Isotropic = 24.1962 Anisotropy = 9.7482
35 H Isotropic = 24.4007 Anisotropy = 4.5221
36 H Isotropic = 23.2571 Anisotropy = 4.7358
37 H Isotropic = 22.9367 Anisotropy = 7.3444
38 H Isotropic = 23.8640 Anisotropy = 7.1243
39 H Isotropic = 26.8626 Anisotropy = 8.9137
40 H Isotropic = 27.2276 Anisotropy = 6.0775
41 H Isotropic = 30.3615 Anisotropy = 8.1677
42 H Isotropic = 30.3888 Anisotropy = 5.6024
43 H Isotropic = 30.3826 Anisotropy = 10.7576
44 H Isotropic = 28.4725 Anisotropy = 8.6323
45 H Isotropic = 28.4595 Anisotropy = 6.7668
46 H Isotropic = 26.6068 Anisotropy = 5.5235
47 H Isotropic = 26.8928 Anisotropy = 8.1800
48 H Isotropic = 23.5459 Anisotropy = 3.8897
49 H Isotropic = 25.2056 Anisotropy = 6.4387
50 H Isotropic = 23.1032 Anisotropy = 9.8421
51 H Isotropic = 23.6728 Anisotropy = 5.3375
52 H Isotropic = 23.6295 Anisotropy = 4.6307
53 H Isotropic = 23.0566 Anisotropy = 7.6451
54 H Isotropic = 27.9730 Anisotropy = 6.6020
55 H Isotropic = 28.2326 Anisotropy = 10.2924
56 H Isotropic = 29.1001 Anisotropy = 7.0964

Conformer 29

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N 4.346227032126 2.713362371920 1.296889568987

C	3.253046148526	2.024911439923	0.958795451537
C	2.959842365387	0.753397730306	1.500541188354
C	3.829944306610	0.247361573904	2.473001920270
C	4.962729647393	0.976413540698	2.837064728410
C	5.188354214391	2.195197936937	2.201723251411
N	1.883576480423	-0.043347467026	1.022158237042
C	0.579114047784	0.387469174821	0.956518494836
C	0.273255125245	1.850361599195	1.028843659664
C	1.067757392510	2.879316724822	0.468429053650
N	2.379053570813	2.625740348547	0.012042060900
O	-0.341339592286	-0.423256019883	0.819428317319
N	0.605895423440	4.129728433947	0.325436813671
C	-0.626011616919	4.418492595857	0.760963445943
C	-1.479513125966	3.502857784439	1.387178601923
C	-0.999262359633	2.196313079796	1.493986393855
C	2.976781707685	3.599689345547	-0.924560397396
C	3.958405321929	2.928598452287	-1.881363927753
C	-2.869221234547	3.878327874615	1.846140225863
C	-3.942428023574	3.689630199793	0.773849486635
O	-3.908613579414	2.318319345736	0.347085063671
C	-4.797078395574	1.904745998196	-0.585594301907
C	-4.611066396015	0.574558704240	-1.089247533480
C	-5.533166264460	0.059014134788	-2.042753697446
N	-6.607063288373	0.847364046387	-2.501431325062
C	-6.731874635922	2.099694749025	-2.024866723076
C	-5.853197597177	2.651499027404	-1.078195855316
C	-3.531016110640	-0.257020519560	-0.688860357119
C	-3.395467720068	-1.532031676712	-1.204848045244
C	-4.331917612082	-2.032767753774	-2.139346605095
C	-5.388949399303	-1.245796767737	-2.557790671220
O	-7.437845886732	0.367496007740	-3.363901204891
C	2.103410533160	-1.488419596877	0.880918054163
H	3.632479825527	-0.724314950065	2.926732779956
H	5.659034409797	0.595879888081	3.585284203465
H	6.081420884506	2.786949565833	2.424402703971
H	-0.951023747902	5.454324949071	0.609640779526
H	-1.624936030787	1.409533261576	1.916439474419
H	2.142376065069	4.038126841708	-1.483281430250
H	3.467156539185	4.418346947402	-0.374459629741
H	4.331248589372	3.670968724472	-2.605157871441
H	4.827323470864	2.512172811218	-1.350352335061
H	3.469263947551	2.115586676543	-2.441608533923
H	-3.144717710580	3.280556584431	2.729064042423
H	-2.900275284443	4.936540059437	2.150050202679
H	-4.934885808090	3.929357020801	1.191005965192
H	-3.759101913941	4.343347296602	-0.096818433908
H	-7.577572607495	2.651155455323	-2.431464538752
H	-6.044429871768	3.671851956874	-0.752567583576
H	-2.794256444063	0.124718715164	0.016516965477
H	-2.553876165863	-2.152030377831	-0.889881806035
H	-4.216727011452	-3.042708749224	-2.537939097657
H	-6.126587983068	-1.587076938752	-3.281337633398
H	3.150425751997	-1.662341667980	0.604270372921
H	1.874585908860	-2.034018609060	1.811118368924
H	1.442024707989	-1.868817880923	0.093809661693

SCF Done: E(RB3LYP) = -1466.00697051

Zero-point correction= 0.445040
Thermal correction to Energy= 0.472364
Thermal correction to Enthalpy= 0.473308
Thermal correction to Gibbs Free Energy= 0.385841
Sum of electronic and zero-point Energies= -1465.561931
Sum of electronic and thermal Energies= -1465.534607
Sum of electronic and thermal Enthalpies= -1465.533663
Sum of electronic and thermal Free Energies= -1465.621130

1	N	Isotropic =	-41.7278	Anisotropy =	469.6776
2	C	Isotropic =	38.4115	Anisotropy =	116.5962
3	C	Isotropic =	58.4441	Anisotropy =	122.4536
4	C	Isotropic =	62.4144	Anisotropy =	177.1960
5	C	Isotropic =	72.5333	Anisotropy =	159.5768
6	C	Isotropic =	48.8986	Anisotropy =	154.1828
7	N	Isotropic =	122.0695	Anisotropy =	91.3194
8	C	Isotropic =	25.6550	Anisotropy =	108.4315
9	C	Isotropic =	71.9310	Anisotropy =	132.2053
10	C	Isotropic =	32.6814	Anisotropy =	125.0755
11	N	Isotropic =	136.9020	Anisotropy =	62.5106
12	O	Isotropic =	-77.3617	Anisotropy =	569.0036
13	N	Isotropic =	-35.1160	Anisotropy =	442.5207
14	C	Isotropic =	41.9669	Anisotropy =	148.5573
15	C	Isotropic =	62.3159	Anisotropy =	171.1223
16	C	Isotropic =	48.6646	Anisotropy =	181.3908
17	C	Isotropic =	148.5322	Anisotropy =	33.8072
18	C	Isotropic =	177.4492	Anisotropy =	23.4403
19	C	Isotropic =	157.6244	Anisotropy =	18.3336
20	C	Isotropic =	121.8183	Anisotropy =	44.3791
21	O	Isotropic =	209.2883	Anisotropy =	115.5166
22	C	Isotropic =	42.8172	Anisotropy =	122.5788
23	C	Isotropic =	69.0510	Anisotropy =	164.1847
24	C	Isotropic =	49.8170	Anisotropy =	150.9956
25	N	Isotropic =	-23.8916	Anisotropy =	255.1940
26	C	Isotropic =	57.9887	Anisotropy =	112.6087
27	C	Isotropic =	91.5954	Anisotropy =	131.6389
28	C	Isotropic =	67.5428	Anisotropy =	177.7242
29	C	Isotropic =	64.9262	Anisotropy =	175.0719
30	C	Isotropic =	63.5984	Anisotropy =	176.2287
31	C	Isotropic =	73.5394	Anisotropy =	173.2839
32	O	Isotropic =	-28.4414	Anisotropy =	325.7636
33	C	Isotropic =	154.4989	Anisotropy =	45.3482
34	H	Isotropic =	23.9057	Anisotropy =	9.1368
35	H	Isotropic =	24.2351	Anisotropy =	4.6396
36	H	Isotropic =	23.1360	Anisotropy =	4.9365
37	H	Isotropic =	22.9947	Anisotropy =	7.9086
38	H	Isotropic =	22.9691	Anisotropy =	10.3450
39	H	Isotropic =	27.4740	Anisotropy =	5.9715
40	H	Isotropic =	27.0870	Anisotropy =	8.6564
41	H	Isotropic =	30.2885	Anisotropy =	11.1015
42	H	Isotropic =	29.9967	Anisotropy =	5.3995
43	H	Isotropic =	30.4529	Anisotropy =	7.7336
44	H	Isotropic =	28.2706	Anisotropy =	5.6591
45	H	Isotropic =	28.4945	Anisotropy =	8.5642

46	H	Isotropic =	27.0063	Anisotropy =	6.2062
47	H	Isotropic =	27.6241	Anisotropy =	6.4361
48	H	Isotropic =	23.2916	Anisotropy =	5.1824
49	H	Isotropic =	24.9747	Anisotropy =	8.8559
50	H	Isotropic =	22.6140	Anisotropy =	8.8918
51	H	Isotropic =	23.5777	Anisotropy =	7.4870
52	H	Isotropic =	23.6169	Anisotropy =	5.5803
53	H	Isotropic =	22.9527	Anisotropy =	7.6992
54	H	Isotropic =	28.7458	Anisotropy =	7.4972
55	H	Isotropic =	27.8328	Anisotropy =	9.8190
56	H	Isotropic =	27.3229	Anisotropy =	7.9411

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.694858887134	4.649661808350	2.302965546009
C	-1.541462492291	3.720975949396	1.856847629030
C	-1.778741583704	2.502973167412	2.533713702346
C	-1.009770014914	2.241872122268	3.674577444978
C	-0.101511838911	3.200468099284	4.126019600862
C	-0.004228281947	4.401720938871	3.425764145808
N	-2.835384943357	1.627175648710	2.163610221813
C	-3.110394556434	1.184632120191	0.889023289655
C	-2.345736612507	1.736469020435	-0.281610979899
C	-2.005127723902	3.091168146866	-0.383795913043
N	-2.244413926572	3.992950736561	0.656153068179
O	-3.950258361746	0.306060361102	0.695433897343
N	-1.358801793278	3.534302404152	-1.532939943629
C	-1.144681550041	2.661699944947	-2.567145973064
C	-1.468419255223	1.314007591338	-2.497563537428
C	-2.082386983384	0.850389555582	-1.330396483490
C	-2.732048428363	5.371035697335	0.431357293370
C	-3.911869116664	5.404220510259	-0.532905151090
C	-1.141708021769	0.391277837708	-3.649459628470
C	0.236221044340	-0.272816164029	-3.558758930841

O	0.298997872427	-1.173325690616	-2.436198254861
C	1.064932511569	-0.919098284161	-1.350736404559
C	1.096877001417	-1.969408041165	-0.372277097877
C	1.881171797505	-1.756609096573	0.805822972324
N	2.599199334824	-0.610901608546	1.033997293050
C	2.536839595474	0.319333189111	0.098880263590
C	1.795145366312	0.231712194057	-1.104083434438
C	0.387456975762	-3.189535317780	-0.531988931390
C	0.448836731272	-4.166722904765	0.442636323659
C	1.220753059583	-3.960631220859	1.613199297980
C	1.920265259268	-2.783368004440	1.789002774633
C	-3.612116957174	0.999040023277	3.243310946682
O	-0.967320757953	4.752555193357	-1.646360077569
H	-1.139700952814	1.307679643884	4.221870859878
H	0.502923237527	3.022143410510	5.016256666423
H	0.658874398457	5.199960098290	3.772267478712
H	-0.666507454242	3.131241180152	-3.425481515754
H	-2.390689535254	-0.189365290874	-1.230792317968
H	-3.047685044068	5.728132962986	1.423053352397
H	-1.928158838628	6.024979402568	0.070745161809
H	-4.729186822225	4.746693871463	-0.195888991083
H	-4.300606094584	6.432997377339	-0.594411053019
H	-3.607981304444	5.105288606299	-1.547434806647
H	-1.904774949840	-0.399772072313	-3.713367523244
H	-1.170946700212	0.946214560182	-4.600570632110
H	1.043730480935	0.469808717888	-3.517571189387
H	0.394917711174	-0.900453030318	-4.447905949599
H	3.110315678955	1.234870166222	0.284179686925
H	1.810400772324	1.075489179959	-1.790829106226
H	-0.204011527420	-3.340194491414	-1.435011054535
H	-0.098889786761	-5.102449087533	0.312704267700
H	1.261623549089	-4.739469040315	2.377948767954
H	2.522747196689	-2.603552696841	2.681454041494
H	-3.613025294366	1.664257992361	4.114823812691
H	-4.638385936380	0.842762946349	2.892250628613
H	-3.194577246398	0.019939665523	3.528944445312

SCF Done: E(RB3LYP) = -1465.99154768

Zero-point correction= 0.444629
Thermal correction to Energy= 0.472110
Thermal correction to Enthalpy= 0.473054
Thermal correction to Gibbs Free Energy= 0.383989
Sum of electronic and zero-point Energies= -1465.546918

Sum of electronic and thermal Energies= -1465.519437
Sum of electronic and thermal Enthalpies= -1465.518493
Sum of electronic and thermal Free Energies= -1465.607559

1	N	Isotropic =	-43.3124	Anisotropy =	460.4228
2	C	Isotropic =	37.3677	Anisotropy =	117.6819
3	C	Isotropic =	59.5935	Anisotropy =	125.5554
4	C	Isotropic =	63.2775	Anisotropy =	178.1305
5	C	Isotropic =	71.7076	Anisotropy =	162.2435
6	C	Isotropic =	49.1972	Anisotropy =	155.4915
7	N	Isotropic =	118.2648	Anisotropy =	89.5529
8	C	Isotropic =	29.3109	Anisotropy =	110.4505
9	C	Isotropic =	62.2580	Anisotropy =	138.8672
10	C	Isotropic =	42.2738	Anisotropy =	111.2048
11	N	Isotropic =	163.3824	Anisotropy =	72.5868
12	O	Isotropic =	-78.7632	Anisotropy =	587.9513
13	N	Isotropic =	-45.9998	Anisotropy =	257.4137
14	C	Isotropic =	49.9903	Anisotropy =	104.9697
15	C	Isotropic =	58.2517	Anisotropy =	176.2053
16	C	Isotropic =	65.4028	Anisotropy =	159.6457
17	C	Isotropic =	144.8298	Anisotropy =	43.7846
18	C	Isotropic =	176.5633	Anisotropy =	24.3833
19	C	Isotropic =	155.4076	Anisotropy =	16.3595
20	C	Isotropic =	124.3158	Anisotropy =	52.9459
21	O	Isotropic =	203.3513	Anisotropy =	130.1815
22	C	Isotropic =	31.8916	Anisotropy =	139.8077
23	C	Isotropic =	70.5931	Anisotropy =	172.1034
24	C	Isotropic =	43.7010	Anisotropy =	183.0265
25	N	Isotropic =	-36.2639	Anisotropy =	459.2065
26	C	Isotropic =	43.3773	Anisotropy =	161.9539
27	C	Isotropic =	92.8294	Anisotropy =	140.2614
28	C	Isotropic =	69.8912	Anisotropy =	175.5263
29	C	Isotropic =	67.8266	Anisotropy =	171.2545
30	C	Isotropic =	63.5901	Anisotropy =	175.5806
31	C	Isotropic =	64.1670	Anisotropy =	151.1094
32	C	Isotropic =	154.2012	Anisotropy =	47.3529
33	O	Isotropic =	-64.3783	Anisotropy =	365.8816
34	H	Isotropic =	24.3993	Anisotropy =	7.3969
35	H	Isotropic =	24.3888	Anisotropy =	4.3190
36	H	Isotropic =	23.2614	Anisotropy =	4.7096
37	H	Isotropic =	23.2598	Anisotropy =	7.0579
38	H	Isotropic =	24.4352	Anisotropy =	7.7613
39	H	Isotropic =	28.2613	Anisotropy =	6.8935
40	H	Isotropic =	26.4138	Anisotropy =	7.7127

41	H	Isotropic =	30.4648	Anisotropy =	7.4714
42	H	Isotropic =	30.2520	Anisotropy =	11.7224
43	H	Isotropic =	30.4407	Anisotropy =	5.1130
44	H	Isotropic =	28.3309	Anisotropy =	7.0041
45	H	Isotropic =	28.6179	Anisotropy =	8.1251
46	H	Isotropic =	26.7267	Anisotropy =	4.8763
47	H	Isotropic =	26.9339	Anisotropy =	8.4411
48	H	Isotropic =	23.3636	Anisotropy =	6.3875
49	H	Isotropic =	25.3647	Anisotropy =	7.1765
50	H	Isotropic =	23.1084	Anisotropy =	10.1705
51	H	Isotropic =	23.8294	Anisotropy =	5.6991
52	H	Isotropic =	23.6599	Anisotropy =	4.8701
53	H	Isotropic =	23.6678	Anisotropy =	5.8483
54	H	Isotropic =	29.0946	Anisotropy =	8.0617
55	H	Isotropic =	27.5734	Anisotropy =	8.4810
56	H	Isotropic =	28.4466	Anisotropy =	9.0338

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.628557799937	1.793518896803	1.370771240610
C	-3.456432511058	2.418613943224	1.256561212132
C	-3.004540566952	2.996500210510	0.049107551981
C	-3.796243579189	2.805597956485	-1.090321417243
C	-5.008353673603	2.123098989074	-0.978990642231
C	-5.396677690305	1.665221862402	0.279337973944
N	-1.865893792569	3.847445673252	-0.002100985828
C	-0.624336962462	3.574057925473	0.528292586222
C	-0.422158485740	2.358783191552	1.388972599154
C	-1.381232673648	1.923738219723	2.310967134752
N	-2.641216194007	2.509541805533	2.413610390564
O	0.339279988462	4.297335648336	0.277457300767
N	-1.088985910165	0.826633610237	3.119175723010
C	0.154811260974	0.257941088943	3.058766812068
C	1.129320311019	0.666519831940	2.157475031613
C	0.827955052025	1.735508259493	1.309962820653
C	-3.277607474275	2.771605396464	3.720188937270
C	-3.804631160424	4.203560028708	3.790934274762
C	2.459936082066	-0.048872891028	2.101533677982
C	2.503074468748	-1.236653025837	1.135388133757
O	2.367449006664	-0.793275805232	-0.228404260356

C	1.274979234040	-1.077753578812	-0.973044028692
C	1.362105105140	-0.684783577073	-2.351257032745
C	0.235040463761	-0.953126230784	-3.191496221961
N	-0.907857290152	-1.564051349179	-2.743474718581
C	-0.932434526654	-1.904823340913	-1.467930339603
C	0.112846672834	-1.692271575759	-0.536703125507
C	2.510090895128	-0.051740370439	-2.897892301639
C	2.542476448716	0.306740021999	-4.231654847016
C	1.428779739833	0.045808422843	-5.068488528201
C	0.302770224875	-0.569834294803	-4.559363311758
C	-1.952243642569	5.047589958105	-0.848249890477
O	-1.967003263853	0.346852968829	3.923246412681
H	-3.480873047139	3.212569408236	-2.051588997623
H	-5.646226966199	1.970306383486	-1.850393484883
H	-6.361459352856	1.169381622633	0.421817529354
H	0.280775357096	-0.563921098780	3.762098385009
H	1.563324596650	2.119840630436	0.604528633723
H	-4.084244820881	2.046405397811	3.895987007843
H	-2.517940767842	2.599903464591	4.490413145544
H	-2.993963298122	4.935036359351	3.644341553118
H	-4.577137071049	4.386943941838	3.026945534319
H	-4.261473785129	4.383248564488	4.777725248531
H	3.247323004946	0.663455726905	1.810858722356
H	2.725060530481	-0.434505000716	3.098813660015
H	1.746420454859	-1.992256479577	1.384343091778
H	3.492745193409	-1.713350986251	1.192205381479
H	-1.848220406752	-2.390260400663	-1.111440530018
H	-0.033844013413	-2.005880955238	0.494918332333
H	3.362540552995	0.144366208593	-2.247613163912
H	3.428666487330	0.792803607499	-4.645031693779
H	1.464531932313	0.333829474784	-6.121529297640
H	-0.565907782432	-0.781574614293	-5.185784409243
H	-1.320869123647	5.830295246603	-0.412913898243
H	-1.596824780194	4.851189099581	-1.872858888203
H	-2.995090651148	5.384606528611	-0.881730023945

SCF Done: E(RB3LYP) = -1465.99205023

Zero-point correction= 0.444347
Thermal correction to Energy= 0.472004
Thermal correction to Enthalpy= 0.472948
Thermal correction to Gibbs Free Energy= 0.381826
Sum of electronic and zero-point Energies= -1465.547703
Sum of electronic and thermal Energies= -1465.520047

Sum of electronic and thermal Enthalpies= -1465.519102
Sum of electronic and thermal Free Energies= -1465.610224

1	N	Isotropic =	-42.6636	Anisotropy =	469.5686
2	C	Isotropic =	38.8730	Anisotropy =	116.4293
3	C	Isotropic =	57.7094	Anisotropy =	127.0288
4	C	Isotropic =	62.8876	Anisotropy =	178.4587
5	C	Isotropic =	71.6506	Anisotropy =	161.7468
6	C	Isotropic =	49.1055	Anisotropy =	155.4679
7	N	Isotropic =	118.7177	Anisotropy =	90.6041
8	C	Isotropic =	29.3268	Anisotropy =	110.4980
9	C	Isotropic =	63.6363	Anisotropy =	136.5980
10	C	Isotropic =	41.1369	Anisotropy =	107.7618
11	N	Isotropic =	165.6925	Anisotropy =	60.2970
12	O	Isotropic =	-79.3444	Anisotropy =	589.6271
13	N	Isotropic =	-43.3807	Anisotropy =	259.2236
14	C	Isotropic =	50.0802	Anisotropy =	105.9081
15	C	Isotropic =	58.6417	Anisotropy =	175.0327
16	C	Isotropic =	65.8480	Anisotropy =	158.6014
17	C	Isotropic =	146.6579	Anisotropy =	38.0366
18	C	Isotropic =	175.9022	Anisotropy =	25.6366
19	C	Isotropic =	155.4012	Anisotropy =	16.3313
20	C	Isotropic =	124.0701	Anisotropy =	53.0439
21	O	Isotropic =	203.2241	Anisotropy =	130.2314
22	C	Isotropic =	31.8485	Anisotropy =	139.8283
23	C	Isotropic =	70.5370	Anisotropy =	171.9199
24	C	Isotropic =	43.8190	Anisotropy =	183.3193
25	N	Isotropic =	-36.4485	Anisotropy =	458.4098
26	C	Isotropic =	43.2543	Anisotropy =	161.8646
27	C	Isotropic =	92.7236	Anisotropy =	140.1284
28	C	Isotropic =	70.0140	Anisotropy =	175.8559
29	C	Isotropic =	67.7587	Anisotropy =	170.5093
30	C	Isotropic =	63.5872	Anisotropy =	175.3680
31	C	Isotropic =	64.0130	Anisotropy =	150.8524
32	C	Isotropic =	154.2268	Anisotropy =	47.0779
33	O	Isotropic =	-70.2734	Anisotropy =	375.2011
34	H	Isotropic =	24.3702	Anisotropy =	7.5041
35	H	Isotropic =	24.3735	Anisotropy =	4.2445
36	H	Isotropic =	23.2043	Anisotropy =	4.6076
37	H	Isotropic =	23.2221	Anisotropy =	7.1473
38	H	Isotropic =	24.4309	Anisotropy =	7.8744
39	H	Isotropic =	26.8308	Anisotropy =	7.9283
40	H	Isotropic =	28.0663	Anisotropy =	6.2788
41	H	Isotropic =	30.5215	Anisotropy =	7.3421

42	H	Isotropic =	30.4183	Anisotropy =	5.0790
43	H	Isotropic =	30.4253	Anisotropy =	11.6243
44	H	Isotropic =	28.3380	Anisotropy =	6.9660
45	H	Isotropic =	28.6157	Anisotropy =	8.1873
46	H	Isotropic =	26.7473	Anisotropy =	4.8199
47	H	Isotropic =	26.9315	Anisotropy =	8.3991
48	H	Isotropic =	23.3371	Anisotropy =	6.4729
49	H	Isotropic =	25.3549	Anisotropy =	7.1798
50	H	Isotropic =	23.1031	Anisotropy =	10.2268
51	H	Isotropic =	23.8503	Anisotropy =	5.6908
52	H	Isotropic =	23.6725	Anisotropy =	4.8716
53	H	Isotropic =	23.6719	Anisotropy =	5.8783
54	H	Isotropic =	27.5568	Anisotropy =	8.3727
55	H	Isotropic =	28.4122	Anisotropy =	9.1523
56	H	Isotropic =	29.0852	Anisotropy =	7.8878

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.028396082562	1.183086030701	-2.884026429854
C	-3.052569128772	0.407909478042	-2.410566993704
C	-1.711792231381	0.502729025862	-2.846284920207
C	-1.399441246823	1.531932771065	-3.743365057176
C	-2.414454814922	2.365909290637	-4.214158686232
C	-3.718501822844	2.130073717346	-3.781195964688
N	-0.734222039869	-0.471849877585	-2.503007373866
C	-0.467402026701	-0.940809945066	-1.235563585722
C	-1.350377027372	-0.547982855975	-0.084579859772
C	-2.740178290000	-0.435828943960	-0.208529045736
N	-3.394751851063	-0.560586004778	-1.432717252253
O	0.513024295190	-1.653753176708	-1.022713312725
N	-3.493395435721	-0.127100416269	0.921831398854
C	-2.873122927992	-0.032234053708	2.138979300571
C	-1.498240543908	-0.142315382314	2.297517649910
C	-0.729286212443	-0.401484830383	1.160327777479
C	-4.669307085712	-1.294084439038	-1.566950113108
C	-4.614371813122	-2.268744846209	-2.741647739669
C	-0.878753808245	0.036736904288	3.666052657010
C	-0.509049151945	1.481733974652	3.992302032884
O	0.544903802290	1.883135263796	3.102100099095
C	1.034547520959	3.138239791575	3.199647546605

C	2.099881812890	3.467485197207	2.297086569729
C	2.644159542629	4.788866595183	2.372380879578
N	2.196828829438	5.737292567411	3.256776586637
C	1.215470394133	5.378454001512	4.063607905199
C	0.594160388638	4.105478224276	4.088172015852
C	2.623038820352	2.545229925750	1.352678124842
C	3.651472220511	2.917382120534	0.508586973454
C	4.194574102299	4.224573749727	0.577316462918
C	3.701736422921	5.137780096238	1.488126379006
C	0.203161449987	-0.894775520604	-3.554824848725
O	-4.760466059577	0.063026376485	0.839983129755
H	-0.374848439375	1.662382343640	-4.093007623655
H	-2.196613954729	3.168425731704	-4.919932281776
H	-4.552235207851	2.726518295281	-4.163426736951
H	-3.566224455623	0.171992034247	2.953771450196
H	0.349973810436	-0.529717240045	1.226389362215
H	-4.835456225540	-1.829572817839	-0.625817793701
H	-5.499714582514	-0.584075085802	-1.684616969490
H	-3.800510531565	-3.000704824296	-2.616407393791
H	-5.567631589111	-2.817074758521	-2.814790806150
H	-4.459155835608	-1.740304843937	-3.695957080304
H	-1.580846155442	-0.301429328326	4.443355882493
H	0.024861470857	-0.586168925327	3.750319523351
H	-0.157760363924	1.556429317695	5.034928349433
H	-1.376839999421	2.150546898694	3.863731966361
H	0.861853728987	6.139664256627	4.768615543867
H	-0.208468507441	3.920737752796	4.799773943171
H	2.201257364418	1.541408195073	1.305615904600
H	4.049237888353	2.202853410530	-0.215048802014
H	5.007615999779	4.508114534032	-0.094714526332
H	4.105090083761	6.149724616180	1.559094826636
H	0.493795378585	-1.934748067665	-3.368299299574
H	-0.295255071798	-0.815218608070	-4.528220896699
H	1.117195193507	-0.278977696357	-3.559008847825

SCF Done: E(RB3LYP) = -1465.99617921

Zero-point correction= 0.444574
Thermal correction to Energy= 0.472119
Thermal correction to Enthalpy= 0.473063
Thermal correction to Gibbs Free Energy= 0.382709
Sum of electronic and zero-point Energies= -1465.551605
Sum of electronic and thermal Energies= -1465.524061
Sum of electronic and thermal Enthalpies= -1465.523116

Sum of electronic and thermal Free Energies= -1465.613470

1	N	Isotropic =	-42.6590	Anisotropy =	468.2027
2	C	Isotropic =	38.6602	Anisotropy =	115.5868
3	C	Isotropic =	57.5685	Anisotropy =	125.9004
4	C	Isotropic =	62.7590	Anisotropy =	177.0519
5	C	Isotropic =	71.7783	Anisotropy =	160.8877
6	C	Isotropic =	49.2033	Anisotropy =	154.7348
7	N	Isotropic =	118.3147	Anisotropy =	90.0353
8	C	Isotropic =	28.5423	Anisotropy =	110.1524
9	C	Isotropic =	63.2685	Anisotropy =	134.8102
10	C	Isotropic =	41.0499	Anisotropy =	106.1375
11	N	Isotropic =	165.7465	Anisotropy =	59.5043
12	O	Isotropic =	-80.0206	Anisotropy =	588.6420
13	N	Isotropic =	-43.0821	Anisotropy =	257.6600
14	C	Isotropic =	50.0980	Anisotropy =	103.6914
15	C	Isotropic =	57.3320	Anisotropy =	173.3562
16	C	Isotropic =	65.1438	Anisotropy =	155.7608
17	C	Isotropic =	146.7452	Anisotropy =	37.4771
18	C	Isotropic =	175.9088	Anisotropy =	25.3802
19	C	Isotropic =	156.6000	Anisotropy =	16.5661
20	C	Isotropic =	121.4416	Anisotropy =	43.3294
21	O	Isotropic =	202.8811	Anisotropy =	109.9281
22	C	Isotropic =	32.3157	Anisotropy =	137.6326
23	C	Isotropic =	70.6366	Anisotropy =	170.8600
24	C	Isotropic =	43.9386	Anisotropy =	181.7695
25	N	Isotropic =	-38.0154	Anisotropy =	459.1201
26	C	Isotropic =	42.4786	Anisotropy =	159.4764
27	C	Isotropic =	91.2337	Anisotropy =	133.2931
28	C	Isotropic =	69.9015	Anisotropy =	173.5464
29	C	Isotropic =	67.6379	Anisotropy =	170.5960
30	C	Isotropic =	63.6417	Anisotropy =	174.8888
31	C	Isotropic =	63.8977	Anisotropy =	150.4669
32	C	Isotropic =	153.9437	Anisotropy =	46.9536
33	O	Isotropic =	-68.9479	Anisotropy =	372.3501
34	H	Isotropic =	24.0876	Anisotropy =	8.1959
35	H	Isotropic =	24.4009	Anisotropy =	4.6152
36	H	Isotropic =	23.2743	Anisotropy =	4.6113
37	H	Isotropic =	23.2701	Anisotropy =	7.3375
38	H	Isotropic =	23.7369	Anisotropy =	9.2751
39	H	Isotropic =	28.0137	Anisotropy =	6.1889
40	H	Isotropic =	26.7918	Anisotropy =	8.1374
41	H	Isotropic =	30.4131	Anisotropy =	7.2529
42	H	Isotropic =	30.3780	Anisotropy =	11.4439

43	H	Isotropic =	30.3315	Anisotropy =	4.9639
44	H	Isotropic =	28.5366	Anisotropy =	8.2769
45	H	Isotropic =	28.2771	Anisotropy =	5.4224
46	H	Isotropic =	27.1683	Anisotropy =	6.4474
47	H	Isotropic =	27.4574	Anisotropy =	5.5238
48	H	Isotropic =	22.8119	Anisotropy =	7.1746
49	H	Isotropic =	24.9720	Anisotropy =	9.5962
50	H	Isotropic =	23.1437	Anisotropy =	8.9457
51	H	Isotropic =	23.8253	Anisotropy =	6.6960
52	H	Isotropic =	23.6363	Anisotropy =	5.3631
53	H	Isotropic =	23.5571	Anisotropy =	5.6489
54	H	Isotropic =	27.2438	Anisotropy =	7.8201
55	H	Isotropic =	28.8600	Anisotropy =	7.4996
56	H	Isotropic =	27.9521	Anisotropy =	9.9382

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.235208515283	1.931976530911	-1.853633239606
C	-3.286759067701	1.005331799436	-1.711580929015
C	-2.057489764624	1.045764987202	-2.408055852151
C	-1.809366330219	2.167385964085	-3.208841680103
C	-2.789250320227	3.153101352395	-3.334867027998
C	-3.997990739603	2.973969549638	-2.664190574660
N	-1.155273028868	-0.052728480235	-2.411705251946
C	-0.712519151642	-0.739048756834	-1.303253740612
C	-1.296820570376	-0.443624432506	0.049883323532
C	-2.661857465084	-0.193679921582	0.240325966336
N	-3.548851218787	-0.075499777976	-0.832200604906
O	0.190379346049	-1.570167222002	-1.396804730441
N	-3.133257407177	-0.004099089411	1.535355132924
C	-2.276351145582	-0.146479212085	2.594628936926
C	-0.918762121665	-0.389515671801	2.440246548855
C	-0.427410914774	-0.541218135270	1.140543175176
C	-4.915024986270	-0.642090888180	-0.814843992130
C	-4.924731722893	-2.086240026545	-0.327797207770
C	-0.016348797914	-0.462706804928	3.650624231975
C	0.588177159309	0.879961849851	4.073717777897
O	1.504426223385	1.371614530562	3.076644870888
C	1.229410707619	2.459749584888	2.321842812722
C	2.307465741749	2.905425465978	1.484981333357

C	2.076683556852	4.049801567297	0.657151930622
N	0.887245544352	4.731529128682	0.631905125181
C	-0.068540673389	4.278314715131	1.422379616532
C	0.034096323020	3.158189567172	2.282335529986
C	3.572544689539	2.260382177647	1.454065751352
C	4.576521247447	2.729607529805	0.629239904836
C	4.353605407470	3.860997196406	-0.194704187899
C	3.132504238942	4.505069531652	-0.179834138128
C	-0.498563515581	-0.392377213874	-3.683261532953
O	-4.363317589535	0.292521441330	1.757198135984
H	-0.867897098313	2.256086203661	-3.751771278478
H	-2.621167601397	4.031892254791	-3.958647842499
H	-4.811771976786	3.696987006016	-2.773522682626
H	-2.767683826425	-0.013641091599	3.557364439588
H	0.622334280127	-0.766995288164	0.958404265942
H	-5.592307735983	-0.031090471549	-0.205091645853
H	-5.256255817853	-0.596655920732	-1.859847860192
H	-4.645980199643	-2.152674586074	0.734704361477
H	-5.942611524852	-2.495194161305	-0.427906242144
H	-4.240533938164	-2.717373361509	-0.917285709287
H	-0.574738425347	-0.851794066605	4.516818264120
H	0.806306947410	-1.167257807795	3.453416806024
H	1.194078029923	0.733635091371	4.979920524915
H	-0.188030188280	1.623411732913	4.299001792595
H	-1.019347281596	4.823071947569	1.398054375803
H	-0.832288940606	2.871002807455	2.874570164491
H	3.735800959567	1.391609925652	2.091718197666
H	5.546749079828	2.228820592846	0.610862972328
H	5.154200048165	4.223637203680	-0.843276384583
H	2.939134403585	5.379011363175	-0.804872982506
H	0.466494704096	0.127970140511	-3.795892195906
H	-0.308166398945	-1.471353213018	-3.702354765235
H	-1.161722637049	-0.115155138131	-4.511261990401

SCF Done: E(RB3LYP) = -1465.99151035

Zero-point correction= 0.444527
Thermal correction to Energy= 0.472051
Thermal correction to Enthalpy= 0.472995
Thermal correction to Gibbs Free Energy= 0.382917
Sum of electronic and zero-point Energies= -1465.546984
Sum of electronic and thermal Energies= -1465.519460
Sum of electronic and thermal Enthalpies= -1465.518515
Sum of electronic and thermal Free Energies= -1465.608593

1	N	Isotropic =	-43.3271	Anisotropy =	460.7062
2	C	Isotropic =	37.1898	Anisotropy =	117.8653
3	C	Isotropic =	59.6210	Anisotropy =	125.4262
4	C	Isotropic =	63.1987	Anisotropy =	178.2919
5	C	Isotropic =	71.7138	Anisotropy =	162.3353
6	C	Isotropic =	49.2192	Anisotropy =	155.4966
7	N	Isotropic =	118.3520	Anisotropy =	89.4960
8	C	Isotropic =	29.2975	Anisotropy =	110.1858
9	C	Isotropic =	62.2601	Anisotropy =	138.8522
10	C	Isotropic =	41.9665	Anisotropy =	111.1306
11	N	Isotropic =	162.8368	Anisotropy =	72.9803
12	O	Isotropic =	-78.8871	Anisotropy =	587.4461
13	N	Isotropic =	-46.1272	Anisotropy =	257.6467
14	C	Isotropic =	49.9532	Anisotropy =	105.2758
15	C	Isotropic =	58.2460	Anisotropy =	176.2452
16	C	Isotropic =	65.4639	Anisotropy =	158.9389
17	C	Isotropic =	144.6449	Anisotropy =	43.9549
18	C	Isotropic =	176.4918	Anisotropy =	24.5102
19	C	Isotropic =	155.2878	Anisotropy =	16.1872
20	C	Isotropic =	123.8802	Anisotropy =	53.4969
21	O	Isotropic =	203.1110	Anisotropy =	130.6100
22	C	Isotropic =	31.9057	Anisotropy =	139.6760
23	C	Isotropic =	70.5853	Anisotropy =	171.8692
24	C	Isotropic =	43.8177	Anisotropy =	183.3970
25	N	Isotropic =	-36.6219	Anisotropy =	458.0777
26	C	Isotropic =	43.2323	Anisotropy =	162.0147
27	C	Isotropic =	92.6639	Anisotropy =	139.9910
28	C	Isotropic =	69.9288	Anisotropy =	175.9817
29	C	Isotropic =	67.8389	Anisotropy =	170.3174
30	C	Isotropic =	63.6872	Anisotropy =	175.1031
31	C	Isotropic =	64.0090	Anisotropy =	150.8013
32	C	Isotropic =	154.3379	Anisotropy =	47.3355
33	O	Isotropic =	-64.3233	Anisotropy =	365.8285
34	H	Isotropic =	24.3829	Anisotropy =	7.4365
35	H	Isotropic =	24.3739	Anisotropy =	4.2630
36	H	Isotropic =	23.2314	Anisotropy =	4.7147
37	H	Isotropic =	23.2293	Anisotropy =	7.1026
38	H	Isotropic =	24.4299	Anisotropy =	7.8214
39	H	Isotropic =	26.3808	Anisotropy =	7.6602
40	H	Isotropic =	28.2300	Anisotropy =	6.8548
41	H	Isotropic =	30.4425	Anisotropy =	5.1668
42	H	Isotropic =	30.2462	Anisotropy =	11.6990
43	H	Isotropic =	30.4523	Anisotropy =	7.4473

44	H	Isotropic =	28.6002	Anisotropy =	8.0829
45	H	Isotropic =	28.3350	Anisotropy =	6.9821
46	H	Isotropic =	26.9133	Anisotropy =	8.4036
47	H	Isotropic =	26.7693	Anisotropy =	4.7700
48	H	Isotropic =	23.3816	Anisotropy =	6.4276
49	H	Isotropic =	25.4079	Anisotropy =	6.9573
50	H	Isotropic =	23.1098	Anisotropy =	10.2882
51	H	Isotropic =	23.8618	Anisotropy =	5.6840
52	H	Isotropic =	23.6823	Anisotropy =	4.8739
53	H	Isotropic =	23.6722	Anisotropy =	5.9380
54	H	Isotropic =	28.4233	Anisotropy =	9.1066
55	H	Isotropic =	27.5395	Anisotropy =	8.4813
56	H	Isotropic =	29.0894	Anisotropy =	8.0914

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.138806929127	2.230804287976	-1.567128540537
C	-3.912734932729	1.790082855034	-1.849299420255
C	-3.627665927921	0.957007004233	-2.954673147509
C	-4.712853196408	0.508921949091	-3.718074756103
C	-6.001190920735	0.942993221277	-3.403316745086
C	-6.159087190676	1.829769091071	-2.339232105652
N	-2.295343010459	0.679255092867	-3.368605903251
C	-1.269749631601	0.248184525450	-2.557422524676
C	-1.463105934687	0.181875791960	-1.068657204035
C	-2.168356532326	1.161992871379	-0.360227686817
N	-2.853184521691	2.195216207288	-0.997659250580
O	-0.197983814147	-0.120541729648	-3.037699211821
N	-2.250278046596	1.061418215885	1.026091705306
C	-1.557126659624	0.071708209969	1.672075336290
C	-0.842656073531	-0.910134522442	1.000538441358
C	-0.807926969470	-0.853778283007	-0.396037954964
C	-2.842837881519	3.576382984234	-0.474688827294
C	-2.566502812696	4.578331473909	-1.593892008016
C	-0.104464398039	-1.978719166252	1.773856517018
C	1.401788507528	-1.734714793900	1.908759896068
O	1.669757454017	-0.598933966364	2.752931593307
C	2.133771483260	0.570706913963	2.257636794018
C	2.495092518454	1.546308421634	3.247135997380
C	2.994788442785	2.805945072810	2.787328519796

N	3.144348782591	3.115522252543	1.459996062247
C	2.794859297280	2.181791580948	0.593991375673
C	2.285334149051	0.901640870884	0.921060165649
C	2.374865071712	1.305717510323	4.641727432179
C	2.735179858144	2.279533804284	5.552861873069
C	3.229237484032	3.529784779793	5.103989214274
C	3.356209526797	3.785327183333	3.753171986918
C	-2.015918577181	0.682800062046	-4.812855637613
O	-2.961593640393	1.884249221676	1.707064560228
H	-4.548480841809	-0.152428979302	-4.569357407746
H	-6.860724588249	0.614011055322	-3.988631396283
H	-7.144148874852	2.234663477116	-2.088934321362
H	-1.666079924594	0.113322413431	2.754493760714
H	-0.253268369880	-1.588952242790	-0.978857761319
H	-3.795874230629	3.797723471960	0.025354719098
H	-2.059249787560	3.625300967083	0.289657582603
H	-1.599516347717	4.376102219205	-2.081482062521
H	-3.354141989254	4.548853103017	-2.363614253867
H	-2.541591143056	5.599579175806	-1.180417438569
H	-0.532183500039	-2.080215807823	2.782636774025
H	-0.229409303161	-2.951224635225	1.270364716046
H	1.889310688195	-1.622846176603	0.930520934472
H	1.861620424973	-2.591617158298	2.422149136730
H	2.910784417260	2.433761433803	-0.466429348484
H	2.013446530560	0.224454391584	0.113767936643
H	1.993796482207	0.341588671413	4.978256876266
H	2.640212808657	2.087274559462	6.623606344971
H	3.510824068690	4.293062133848	5.832832508777
H	3.735171113896	4.740618623333	3.384787187140
H	-2.137871961715	-0.319569040834	-5.254457638539
H	-2.699223503935	1.384588501055	-5.305551263126
H	-0.978727142083	1.000080849194	-4.969172132238

SCF Done: E(RB3LYP) = -1465.99225645

Zero-point correction= 0.444468
Thermal correction to Energy= 0.472019
Thermal correction to Enthalpy= 0.472964
Thermal correction to Gibbs Free Energy= 0.383586
Sum of electronic and zero-point Energies= -1465.547789
Sum of electronic and thermal Energies= -1465.520237
Sum of electronic and thermal Enthalpies= -1465.519293
Sum of electronic and thermal Free Energies= -1465.608671

1	N	Isotropic =	-42.6411	Anisotropy =	468.2839
2	C	Isotropic =	38.7178	Anisotropy =	114.8559
3	C	Isotropic =	57.6235	Anisotropy =	124.9106
4	C	Isotropic =	62.4693	Anisotropy =	176.5828
5	C	Isotropic =	71.5872	Anisotropy =	160.7418
6	C	Isotropic =	49.0269	Anisotropy =	154.5126
7	N	Isotropic =	118.2105	Anisotropy =	89.2312
8	C	Isotropic =	28.6552	Anisotropy =	108.9251
9	C	Isotropic =	62.5368	Anisotropy =	138.8865
10	C	Isotropic =	41.0501	Anisotropy =	108.4080
11	N	Isotropic =	165.6046	Anisotropy =	57.7846
12	O	Isotropic =	-80.1813	Anisotropy =	585.8975
13	N	Isotropic =	-43.1208	Anisotropy =	258.2720
14	C	Isotropic =	49.5652	Anisotropy =	105.8333
15	C	Isotropic =	58.4959	Anisotropy =	175.1514
16	C	Isotropic =	66.9641	Anisotropy =	159.7338
17	C	Isotropic =	146.5157	Anisotropy =	36.1695
18	C	Isotropic =	176.1554	Anisotropy =	24.5170
19	C	Isotropic =	155.0558	Anisotropy =	15.8408
20	C	Isotropic =	123.8911	Anisotropy =	54.2932
21	O	Isotropic =	201.4205	Anisotropy =	131.6842
22	C	Isotropic =	31.7508	Anisotropy =	138.7908
23	C	Isotropic =	70.4751	Anisotropy =	170.9972
24	C	Isotropic =	43.6371	Anisotropy =	182.3240
25	N	Isotropic =	-36.9958	Anisotropy =	457.7503
26	C	Isotropic =	42.9673	Anisotropy =	160.2380
27	C	Isotropic =	92.0175	Anisotropy =	138.0424
28	C	Isotropic =	69.8563	Anisotropy =	175.0893
29	C	Isotropic =	67.6981	Anisotropy =	169.9804
30	C	Isotropic =	63.5423	Anisotropy =	175.4394
31	C	Isotropic =	63.8621	Anisotropy =	150.4046
32	C	Isotropic =	154.0799	Anisotropy =	47.0009
33	O	Isotropic =	-70.5906	Anisotropy =	377.0227
34	H	Isotropic =	23.9888	Anisotropy =	8.9509
35	H	Isotropic =	24.2819	Anisotropy =	4.4696
36	H	Isotropic =	23.2262	Anisotropy =	4.7376
37	H	Isotropic =	23.6340	Anisotropy =	6.1762
38	H	Isotropic =	23.9265	Anisotropy =	9.1804
39	H	Isotropic =	26.9688	Anisotropy =	7.9204
40	H	Isotropic =	28.5003	Anisotropy =	5.8523
41	H	Isotropic =	30.5529	Anisotropy =	6.6956
42	H	Isotropic =	30.4186	Anisotropy =	5.3237
43	H	Isotropic =	30.5174	Anisotropy =	10.9115
44	H	Isotropic =	28.5224	Anisotropy =	7.2060

45	H	Isotropic =	28.4976	Anisotropy =	7.7113
46	H	Isotropic =	26.6062	Anisotropy =	4.3725
47	H	Isotropic =	26.8685	Anisotropy =	8.0096
48	H	Isotropic =	22.9929	Anisotropy =	7.3600
49	H	Isotropic =	25.1448	Anisotropy =	6.3838
50	H	Isotropic =	23.0762	Anisotropy =	10.7154
51	H	Isotropic =	23.8173	Anisotropy =	5.8124
52	H	Isotropic =	23.6218	Anisotropy =	4.9394
53	H	Isotropic =	23.5710	Anisotropy =	6.2674
54	H	Isotropic =	27.9694	Anisotropy =	10.3077
55	H	Isotropic =	28.8430	Anisotropy =	7.3586
56	H	Isotropic =	27.2479	Anisotropy =	7.5646

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.837536191066	-1.431276356564	-2.427202837580
C	-3.225053556090	-0.254995671055	-2.289889131574
C	-3.727072585335	0.944692564302	-2.842460018152
C	-4.974957830734	0.887699083847	-3.475806572965
C	-5.632165448193	-0.337698415593	-3.592040391870
C	-5.007530400264	-1.474280114706	-3.080365869698
N	-2.958454247486	2.141077938359	-2.879321455208
C	-2.290250615759	2.706778122295	-1.816849701365
C	-2.194894610347	1.974918187143	-0.508043052036
C	-1.995862177704	0.590799531221	-0.434562562786
N	-2.007503403816	-0.227035275966	-1.562595869915
O	-1.792048362695	3.828629772902	-1.910815365566
N	-1.848751449114	-0.001058132386	0.817430859333
C	-1.794179443368	0.789739596028	1.934730436830
C	-1.979314891311	2.164336371702	1.895622562465
C	-2.194921666942	2.759468600312	0.649088553215
C	-1.046437074737	-1.335487030301	-1.733174531375
C	-0.395660974965	-1.283378941683	-3.114110309393
C	-1.908312781655	2.976429425995	3.168509452067
C	-0.577736692286	3.706538538442	3.377803671918
O	0.495715390889	2.772388689780	3.601716362259
C	1.462659133800	2.555096723629	2.681620814013
C	2.536333777008	1.708329823475	3.119738264285
C	3.594023052350	1.442449401183	2.193108819612
N	3.626533284394	1.956234252184	0.922277772760

C	2.611968852198	2.725293209193	0.571713243545
C	1.507634618506	3.060080883513	1.392458968032
C	2.582036014405	1.137050681529	4.419348104609
C	3.638428447224	0.327999626986	4.790773002470
C	4.688722838751	0.060485930088	3.877561698102
C	4.666065626861	0.605829779923	2.609433094502
C	-3.013941511543	2.948398884073	-4.107791532289
O	-1.757062150838	-1.275507690507	0.939376028372
H	-5.416237720985	1.790383236934	-3.899457646304
H	-6.600501016252	-0.408177827666	-4.088980251733
H	-5.463383028141	-2.462505203701	-3.192589098800
H	-1.636900814851	0.222527861276	2.850516010307
H	-2.333109549910	3.836177998970	0.551824841199
H	-0.292465362929	-1.234775660194	-0.945008089442
H	-1.553022106798	-2.297374595177	-1.573541426863
H	-1.143432032831	-1.391439556800	-3.916134893472
H	0.140212046188	-0.333148849197	-3.267838824727
H	0.325779674493	-2.110287097173	-3.216511750424
H	-2.699610650621	3.743649008005	3.162777656128
H	-2.091968203890	2.329858276680	4.039860811209
H	-0.636099336373	4.307664152267	4.296876867508
H	-0.344547468348	4.382818846715	2.544166146005
H	2.637439346011	3.130345968313	-0.446482171375
H	0.721454029582	3.688949437403	0.979857344907
H	1.770270695587	1.347860764933	5.115510843944
H	3.666634711491	-0.107720397293	5.791684297573
H	5.519359876955	-0.580465916495	4.181453106943
H	5.464196902840	0.413867855781	1.889706743105
H	-3.811125431849	3.708007946219	-4.060960202105
H	-2.056154348246	3.466373617235	-4.230698878287
H	-3.191843181266	2.284542143622	-4.962103941917

SCF Done: E(RB3LYP) = -1465.99226620

Zero-point correction= 0.444501
Thermal correction to Energy= 0.472052
Thermal correction to Enthalpy= 0.472997
Thermal correction to Gibbs Free Energy= 0.383419
Sum of electronic and zero-point Energies= -1465.547765
Sum of electronic and thermal Energies= -1465.520214
Sum of electronic and thermal Enthalpies= -1465.519270
Sum of electronic and thermal Free Energies= -1465.608847

1 N Isotropic = -42.5281 Anisotropy = 468.8369

2	C	Isotropic =	38.8310	Anisotropy =	114.7489
3	C	Isotropic =	57.5096	Anisotropy =	125.2173
4	C	Isotropic =	62.5110	Anisotropy =	176.4443
5	C	Isotropic =	71.5245	Anisotropy =	160.5375
6	C	Isotropic =	49.1387	Anisotropy =	154.8501
7	N	Isotropic =	118.2704	Anisotropy =	89.1636
8	C	Isotropic =	28.7001	Anisotropy =	108.7649
9	C	Isotropic =	62.5515	Anisotropy =	139.2816
10	C	Isotropic =	41.2085	Anisotropy =	108.5570
11	N	Isotropic =	165.4020	Anisotropy =	58.5284
12	O	Isotropic =	-80.4209	Anisotropy =	584.9406
13	N	Isotropic =	-42.3694	Anisotropy =	257.6829
14	C	Isotropic =	49.5018	Anisotropy =	105.5212
15	C	Isotropic =	58.6842	Anisotropy =	174.6444
16	C	Isotropic =	66.6770	Anisotropy =	160.2374
17	C	Isotropic =	146.8913	Anisotropy =	36.4483
18	C	Isotropic =	176.0749	Anisotropy =	24.5747
19	C	Isotropic =	155.0954	Anisotropy =	15.9796
20	C	Isotropic =	124.0505	Anisotropy =	54.0364
21	O	Isotropic =	201.9465	Anisotropy =	131.0259
22	C	Isotropic =	31.9479	Anisotropy =	138.7828
23	C	Isotropic =	70.4763	Anisotropy =	170.9292
24	C	Isotropic =	43.6694	Anisotropy =	182.4342
25	N	Isotropic =	-36.8475	Anisotropy =	457.6148
26	C	Isotropic =	42.9030	Anisotropy =	160.4412
27	C	Isotropic =	92.3566	Anisotropy =	138.5574
28	C	Isotropic =	69.9764	Anisotropy =	175.3223
29	C	Isotropic =	67.7564	Anisotropy =	169.6056
30	C	Isotropic =	63.5417	Anisotropy =	174.9669
31	C	Isotropic =	63.7949	Anisotropy =	150.4440
32	C	Isotropic =	154.0110	Anisotropy =	46.8769
33	O	Isotropic =	-70.3058	Anisotropy =	377.0230
34	H	Isotropic =	24.0062	Anisotropy =	8.9578
35	H	Isotropic =	24.2876	Anisotropy =	4.4533
36	H	Isotropic =	23.2097	Anisotropy =	4.7516
37	H	Isotropic =	23.6172	Anisotropy =	6.1343
38	H	Isotropic =	23.8909	Anisotropy =	9.1486
39	H	Isotropic =	28.4527	Anisotropy =	5.8204
40	H	Isotropic =	27.0013	Anisotropy =	7.9703
41	H	Isotropic =	30.4383	Anisotropy =	5.3185
42	H	Isotropic =	30.5618	Anisotropy =	6.6357
43	H	Isotropic =	30.5408	Anisotropy =	10.9109
44	H	Isotropic =	28.4809	Anisotropy =	7.7395
45	H	Isotropic =	28.5195	Anisotropy =	7.2300

46	H	Isotropic =	26.8831	Anisotropy =	8.0221
47	H	Isotropic =	26.6002	Anisotropy =	4.3426
48	H	Isotropic =	22.9773	Anisotropy =	7.3245
49	H	Isotropic =	25.1172	Anisotropy =	6.5294
50	H	Isotropic =	23.0792	Anisotropy =	10.7058
51	H	Isotropic =	23.8373	Anisotropy =	5.7936
52	H	Isotropic =	23.6419	Anisotropy =	4.9085
53	H	Isotropic =	23.5785	Anisotropy =	6.2400
54	H	Isotropic =	27.9760	Anisotropy =	10.2767
55	H	Isotropic =	27.2406	Anisotropy =	7.5175
56	H	Isotropic =	28.8457	Anisotropy =	7.3498

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.190348026283	0.639474776311	-3.727676458259
C	0.054199831411	-0.314101953324	-2.805959345111
C	1.152924072111	-0.963792890480	-2.199800424538
C	2.433408352449	-0.499554522496	-2.526416361604
C	2.575907412071	0.521559056109	-3.466825603095
C	1.426124361208	1.035740850011	-4.064460376946
N	0.994400782343	-2.123604986883	-1.391847305476
C	0.110987087783	-2.268578437283	-0.344580518852
C	-0.910653496638	-1.202140901200	-0.066543487009
C	-1.579964099977	-0.518889854521	-1.088983304825
N	-1.262047722501	-0.690262340317	-2.435289576734
O	0.171151102546	-3.248745782723	0.397258766398
N	-2.557722882232	0.411991154800	-0.747897086754
C	-2.905428972322	0.573328967092	0.566776338929
C	-2.267030044027	-0.091923107089	1.603459587266
C	-1.251126286258	-0.993617442043	1.274016797062
C	-2.303702779736	-0.774555397610	-3.478743679195
C	-2.056764829821	-1.968535073673	-4.398947045939
C	-2.656899136521	0.182951920853	3.039030278220
C	-1.748480209089	1.194323079727	3.733398348228
O	-1.908219580915	2.457444673564	3.067329884006
C	-1.183141984132	3.514611760429	3.491878478418
C	-1.388851968126	4.742035024876	2.778364752183
C	-0.637916923765	5.884631468974	3.200674086717
N	0.255402349798	5.854795267701	4.241322879505
C	0.403558090885	4.698914845243	4.861711124281

C	-0.279126480571	3.499654930511	4.541228197882
C	-2.293466057564	4.858940909253	1.690087967946
C	-2.451025434162	6.067484724757	1.039511556063
C	-1.710655462361	7.203065382240	1.452717639055
C	-0.825353625843	7.112571500574	2.508422351544
C	1.974274156552	-3.207768047598	-1.560064994343
O	-3.139381925515	1.119304476790	-1.647864918168
H	3.313976782722	-0.951886752623	-2.069155055503
H	3.563285307544	0.893499596416	-3.743186440863
H	1.493911514900	1.801562723732	-4.842855469594
H	-3.705363381151	1.297323101412	0.709989164616
H	-0.733308913301	-1.568216797494	2.041693019146
H	-3.267159223381	-0.872705306962	-2.966830354299
H	-2.337565679901	0.162762281532	-4.051244553361
H	-1.095567319526	-1.876372650156	-4.929651775639
H	-2.049454354379	-2.913986641217	-3.833413449553
H	-2.853478743320	-2.023395052607	-5.158541181083
H	-3.695024921033	0.544308108610	3.090114802177
H	-2.607853225023	-0.751126513061	3.619760735062
H	-0.692495904475	0.879403956047	3.681016470182
H	-2.033838591406	1.296629005604	4.793649765499
H	1.117987832728	4.680518642572	5.692829458937
H	-0.078090622582	2.602608340080	5.123964427910
H	-2.859398128236	3.981579199360	1.377189051108
H	-3.148158092496	6.150247731973	0.203129427091
H	-1.843349390167	8.153706535328	0.931435902466
H	-0.244881306225	7.974208362933	2.843734366483
H	2.830288598331	-3.093514343228	-0.875340745140
H	1.483940593137	-4.161849325038	-1.336702284056
H	2.332831443877	-3.205368235788	-2.596233828443

SCF Done: E(RB3LYP) = -1465.99632066

Zero-point correction= 0.444498
Thermal correction to Energy= 0.472065
Thermal correction to Enthalpy= 0.473010
Thermal correction to Gibbs Free Energy= 0.383207
Sum of electronic and zero-point Energies= -1465.551823
Sum of electronic and thermal Energies= -1465.524255
Sum of electronic and thermal Enthalpies= -1465.523311
Sum of electronic and thermal Free Energies= -1465.613114

1 N Isotropic = -42.5075 Anisotropy = 469.3355
2 C Isotropic = 38.7541 Anisotropy = 116.2271

3	C	Isotropic =	57.5698	Anisotropy =	125.6725
4	C	Isotropic =	62.7312	Anisotropy =	177.1284
5	C	Isotropic =	71.6239	Anisotropy =	160.8761
6	C	Isotropic =	49.2127	Anisotropy =	155.3439
7	N	Isotropic =	118.3549	Anisotropy =	89.5063
8	C	Isotropic =	28.7314	Anisotropy =	108.9132
9	C	Isotropic =	62.6608	Anisotropy =	136.0501
10	C	Isotropic =	41.2087	Anisotropy =	106.7393
11	N	Isotropic =	165.6494	Anisotropy =	59.1170
12	O	Isotropic =	-79.1222	Anisotropy =	586.6394
13	N	Isotropic =	-42.0207	Anisotropy =	255.8893
14	C	Isotropic =	48.6546	Anisotropy =	104.1603
15	C	Isotropic =	57.5396	Anisotropy =	173.2726
16	C	Isotropic =	67.3775	Anisotropy =	156.6579
17	C	Isotropic =	146.5468	Anisotropy =	37.4259
18	C	Isotropic =	175.8541	Anisotropy =	25.5488
19	C	Isotropic =	156.6483	Anisotropy =	16.4501
20	C	Isotropic =	121.8740	Anisotropy =	43.2692
21	O	Isotropic =	203.6277	Anisotropy =	112.3720
22	C	Isotropic =	32.4238	Anisotropy =	137.6648
23	C	Isotropic =	70.6057	Anisotropy =	171.0165
24	C	Isotropic =	44.0223	Anisotropy =	181.7990
25	N	Isotropic =	-37.9902	Anisotropy =	459.1106
26	C	Isotropic =	42.6269	Anisotropy =	159.8326
27	C	Isotropic =	91.3013	Anisotropy =	133.2197
28	C	Isotropic =	70.2168	Anisotropy =	174.3372
29	C	Isotropic =	67.7031	Anisotropy =	170.5702
30	C	Isotropic =	63.6333	Anisotropy =	174.6676
31	C	Isotropic =	63.8621	Anisotropy =	150.5920
32	C	Isotropic =	153.9667	Anisotropy =	47.1258
33	O	Isotropic =	-67.2287	Anisotropy =	369.7801
34	H	Isotropic =	24.0804	Anisotropy =	8.3178
35	H	Isotropic =	24.3870	Anisotropy =	4.1683
36	H	Isotropic =	23.2656	Anisotropy =	4.4630
37	H	Isotropic =	22.9854	Anisotropy =	7.2257
38	H	Isotropic =	24.0808	Anisotropy =	9.2998
39	H	Isotropic =	27.9828	Anisotropy =	5.7497
40	H	Isotropic =	26.7620	Anisotropy =	7.8969
41	H	Isotropic =	30.3448	Anisotropy =	5.0783
42	H	Isotropic =	30.4372	Anisotropy =	7.5131
43	H	Isotropic =	30.3643	Anisotropy =	11.3495
44	H	Isotropic =	28.3563	Anisotropy =	5.8496
45	H	Isotropic =	28.4812	Anisotropy =	8.0594
46	H	Isotropic =	27.4482	Anisotropy =	5.4473

47	H	Isotropic =	27.1556	Anisotropy =	6.2071
48	H	Isotropic =	22.8000	Anisotropy =	7.2582
49	H	Isotropic =	24.9902	Anisotropy =	9.4334
50	H	Isotropic =	23.1047	Anisotropy =	9.4993
51	H	Isotropic =	23.8386	Anisotropy =	6.6516
52	H	Isotropic =	23.6648	Anisotropy =	5.1683
53	H	Isotropic =	23.5684	Anisotropy =	5.6756
54	H	Isotropic =	28.0421	Anisotropy =	10.1681
55	H	Isotropic =	27.3014	Anisotropy =	8.0838
56	H	Isotropic =	28.8967	Anisotropy =	7.5878

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.830584260584	1.354392274716	3.768706563451
C	-2.734098070439	2.320601439531	2.855115846596
C	-3.770714151022	2.628935606684	1.945855917568
C	-4.902288035120	1.803769589935	1.958039571349
C	-4.990113216172	0.770435478780	2.891831004854
C	-3.943502640693	0.607249583600	3.798279090037
N	-3.743855570433	3.798171690388	1.136313894255
C	-2.695844775246	4.214411266888	0.344825870737
C	-1.374147598159	3.501475354632	0.407688092528
C	-0.834339237361	3.025530514362	1.608834359385
N	-1.533217275165	3.073593387758	2.813955358769
O	-2.837446550137	5.145694906175	-0.447244862276
N	0.422559130079	2.427046755577	1.590920483881
C	1.139863568847	2.399821227004	0.424097464018
C	0.639278824272	2.871467374157	-0.780497763771
C	-0.642767189449	3.429183750940	-0.782041930609
C	-0.876845621212	3.444369923849	4.083848886698
C	-1.691989426198	4.499379644924	4.829262761629
C	1.463802189029	2.766031019780	-2.044753990260
C	1.046613434064	1.613370644085	-2.953507110311
O	1.313388047203	0.385360569434	-2.256945986813
C	1.005012327184	-0.783306957188	-2.859211077741
C	1.296817906598	-1.970844306660	-2.109316302428
C	0.982578771467	-3.228282589501	-2.715879318360
N	0.423096488799	-3.342914153067	-3.963133604371
C	0.177458075522	-2.217232416917	-4.607603637745
C	0.442113849282	-0.914410647837	-4.118166461931

C	1.875614643682	-1.941017132655	-0.813024365759
C	2.135514464727	-3.117633411260	-0.137177967160
C	1.826860778078	-4.366433417615	-0.732013505094
C	1.263464906168	-4.419220128309	-1.991458336993
C	-5.001671488491	4.545451965781	0.983089538282
O	0.920687078358	1.903607752791	2.652162168431
H	-5.721163692019	1.985474591497	1.261205645062
H	-5.865323036065	0.120476620253	2.926101404969
H	-3.993104196769	-0.157021945590	4.579568614544
H	2.121485768511	1.943677801434	0.538856672967
H	-1.079158941940	3.844192390838	-1.690392465296
H	-0.731132647037	2.549396459876	4.704455677746
H	0.118363771853	3.828254859950	3.834484778775
H	-2.694501480691	4.123476919060	5.089491372536
H	-1.181718660198	4.768257749716	5.768424887121
H	-1.812277637703	5.412609410951	4.224938863459
H	1.359999943323	3.693893732537	-2.628787023406
H	2.530137379219	2.655545614840	-1.796960968564
H	1.626256174113	1.639627596915	-3.891253798292
H	-0.026719935441	1.671903808478	-3.201668166552
H	-0.268839626626	-2.314103125357	-5.604075797424
H	0.198274215507	-0.054844435178	-4.739780943316
H	2.110470800342	-0.976969893391	-0.361861554711
H	2.580397266244	-3.087632628225	0.859604114687
H	2.037049958199	-5.290407039994	-0.188741375265
H	1.017516947540	-5.369594119199	-2.468996419514
H	-4.764281189818	5.604447966531	0.832220968126
H	-5.580818496395	4.196192244129	0.112839456713
H	-5.601032061632	4.422508859165	1.893015404789

SCF Done: E(RB3LYP) = -1465.99632183

Zero-point correction= 0.444520
Thermal correction to Energy= 0.472064
Thermal correction to Enthalpy= 0.473008
Thermal correction to Gibbs Free Energy= 0.383703
Sum of electronic and zero-point Energies= -1465.551802
Sum of electronic and thermal Energies= -1465.524258
Sum of electronic and thermal Enthalpies= -1465.523314
Sum of electronic and thermal Free Energies= -1465.612618

1	N	Isotropic =	-42.2555	Anisotropy =	469.1436
2	C	Isotropic =	38.7454	Anisotropy =	116.5184
3	C	Isotropic =	57.6203	Anisotropy =	126.0189

4	C	Isotropic =	62.7016	Anisotropy =	177.2940
5	C	Isotropic =	71.6443	Anisotropy =	161.0842
6	C	Isotropic =	49.1907	Anisotropy =	155.1899
7	N	Isotropic =	118.3258	Anisotropy =	89.2649
8	C	Isotropic =	28.8213	Anisotropy =	109.0872
9	C	Isotropic =	62.5801	Anisotropy =	136.4170
10	C	Isotropic =	41.3205	Anisotropy =	106.7314
11	N	Isotropic =	165.8353	Anisotropy =	59.3221
12	O	Isotropic =	-78.9164	Anisotropy =	585.9426
13	N	Isotropic =	-42.1516	Anisotropy =	256.3060
14	C	Isotropic =	48.8360	Anisotropy =	103.2958
15	C	Isotropic =	57.4545	Anisotropy =	173.3425
16	C	Isotropic =	67.4213	Anisotropy =	157.8750
17	C	Isotropic =	146.6723	Anisotropy =	37.3596
18	C	Isotropic =	175.8115	Anisotropy =	25.5659
19	C	Isotropic =	156.5879	Anisotropy =	16.3673
20	C	Isotropic =	121.8084	Anisotropy =	43.0742
21	O	Isotropic =	203.2742	Anisotropy =	112.0666
22	C	Isotropic =	32.2725	Anisotropy =	138.0287
23	C	Isotropic =	70.6348	Anisotropy =	170.7841
24	C	Isotropic =	43.9631	Anisotropy =	182.0604
25	N	Isotropic =	-38.0324	Anisotropy =	458.4953
26	C	Isotropic =	42.5964	Anisotropy =	159.9726
27	C	Isotropic =	91.3092	Anisotropy =	133.2251
28	C	Isotropic =	70.3952	Anisotropy =	174.3918
29	C	Isotropic =	67.7849	Anisotropy =	170.4566
30	C	Isotropic =	63.6318	Anisotropy =	174.9493
31	C	Isotropic =	63.8583	Anisotropy =	150.3810
32	C	Isotropic =	154.0660	Anisotropy =	47.0565
33	O	Isotropic =	-68.1415	Anisotropy =	370.6968
34	H	Isotropic =	24.0764	Anisotropy =	8.2779
35	H	Isotropic =	24.3827	Anisotropy =	4.1738
36	H	Isotropic =	23.2651	Anisotropy =	4.4478
37	H	Isotropic =	23.0142	Anisotropy =	7.1638
38	H	Isotropic =	24.0386	Anisotropy =	9.4566
39	H	Isotropic =	26.7548	Anisotropy =	7.9179
40	H	Isotropic =	27.9962	Anisotropy =	5.7795
41	H	Isotropic =	30.3477	Anisotropy =	5.0074
42	H	Isotropic =	30.3724	Anisotropy =	11.3535
43	H	Isotropic =	30.4307	Anisotropy =	7.5154
44	H	Isotropic =	28.4344	Anisotropy =	8.0749
45	H	Isotropic =	28.3793	Anisotropy =	5.8049
46	H	Isotropic =	27.1454	Anisotropy =	6.1509
47	H	Isotropic =	27.3849	Anisotropy =	5.4946

48	H	Isotropic =	22.7989	Anisotropy =	7.2546
49	H	Isotropic =	24.9816	Anisotropy =	9.4138
50	H	Isotropic =	23.1416	Anisotropy =	9.5463
51	H	Isotropic =	23.8654	Anisotropy =	6.6423
52	H	Isotropic =	23.6769	Anisotropy =	5.1582
53	H	Isotropic =	23.5855	Anisotropy =	5.6704
54	H	Isotropic =	27.2996	Anisotropy =	8.0770
55	H	Isotropic =	28.0503	Anisotropy =	10.1310
56	H	Isotropic =	28.9183	Anisotropy =	7.5742

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.437054702619	-0.273053135253	0.170369716092
C	-4.373368711030	-0.011520948198	0.930849554279
C	-4.469579497796	0.351258296222	2.293680244705
C	-5.754193860906	0.524428235971	2.823415389731
C	-6.868620922442	0.279254872366	2.020019226723
C	-6.658603024874	-0.148985177361	0.710300564625
N	-3.329687079340	0.414788295483	3.140605807504
C	-2.150667453144	1.066062311643	2.857997860882
C	-1.933704432877	1.678097376947	1.502396343347
C	-2.336244474690	1.043739395969	0.319764572462
N	-3.092913752652	-0.130486776654	0.333693394390
O	-1.276746289506	1.191108077292	3.715901549483
N	-2.029182416315	1.640949863635	-0.897225016735
C	-1.265005541052	2.778879125121	-0.919043135307
C	-0.849366609038	3.430001300769	0.232511446407
C	-1.200800816421	2.867055672195	1.463608250951
C	-2.868556242959	-1.243776810474	-0.614303046224
C	-1.392243419726	-1.605794883383	-0.724252042096
C	-0.014137818220	4.686178849201	0.137129278127
C	1.486761304101	4.464604980020	0.348101210161
O	2.051530505199	3.689547509775	-0.726405586943
C	2.469785078103	2.415671396437	-0.548649198077
C	3.160087832374	1.841878159456	-1.669194658766
C	3.627413880170	0.495073278543	-1.543423717286
N	3.449320292538	-0.259609893036	-0.412538833063
C	2.806570499970	0.317844860715	0.586063598867
C	2.292763957744	1.637483244744	0.583719063439
C	3.391535113404	2.554934183580	-2.875580216519

C	4.060628201330	1.955145374696	-3.924855764355
C	4.524105188126	0.620964902778	-3.807335681522
C	4.312288037430	-0.090808700197	-2.643502490652
C	-3.461601545076	-0.118845067303	4.504886905846
O	-2.442426066308	1.140411164626	-2.005585716530
H	-5.881879040793	0.822157864554	3.864599785077
H	-7.878785989047	0.400398171731	2.413117606075
H	-7.502542750340	-0.398890746384	0.060493745132
H	-1.060795780212	3.133680076225	-1.927741441050
H	-0.889414227978	3.322838590822	2.403313217568
H	-3.433138282892	-2.091469282540	-0.198098773811
H	-3.278246466663	-1.011957110425	-1.605463961825
H	-0.955736668962	-1.830211678120	0.262120166605
H	-1.284937769182	-2.499046970353	-1.359757016233
H	-0.815292608283	-0.795272532796	-1.194243365302
H	-0.161254406221	5.163889463841	-0.843279609699
H	-0.343860547592	5.408330020740	0.901618696428
H	1.701115483336	4.003249876842	1.321636455042
H	2.003347187162	5.434801733743	0.310284184954
H	2.661726293587	-0.288953489559	1.487324961941
H	1.760796587398	1.992756972382	1.464122322959
H	3.032595459258	3.580830865724	-2.957593594020
H	4.234982097104	2.509668069745	-4.849291064001
H	5.051807020806	0.156269726542	-4.643211034896
H	4.660778372910	-1.119165555191	-2.530066432902
H	-4.199925313499	-0.929451419295	4.500204621867
H	-2.487106431907	-0.502792560986	4.826884172444
H	-3.776597431488	0.659950576434	5.218317483700

SCF Done: E(RB3LYP) = -1465.99168279

Zero-point correction= 0.444556
Thermal correction to Energy= 0.472066
Thermal correction to Enthalpy= 0.473010
Thermal correction to Gibbs Free Energy= 0.383594
Sum of electronic and zero-point Energies= -1465.547127
Sum of electronic and thermal Energies= -1465.519617
Sum of electronic and thermal Enthalpies= -1465.518673
Sum of electronic and thermal Free Energies= -1465.608088

1	N	Isotropic =	-43.4859	Anisotropy =	459.3700
2	C	Isotropic =	37.0747	Anisotropy =	116.2544
3	C	Isotropic =	59.2107	Anisotropy =	123.4432
4	C	Isotropic =	62.7308	Anisotropy =	176.2579

5	C	Isotropic =	71.6127	Anisotropy =	161.3854
6	C	Isotropic =	49.0984	Anisotropy =	154.4899
7	N	Isotropic =	117.8930	Anisotropy =	88.3707
8	C	Isotropic =	28.7373	Anisotropy =	108.3233
9	C	Isotropic =	61.2881	Anisotropy =	140.9421
10	C	Isotropic =	42.2941	Anisotropy =	111.6645
11	N	Isotropic =	162.9629	Anisotropy =	72.1489
12	O	Isotropic =	-79.8573	Anisotropy =	584.0117
13	N	Isotropic =	-45.2898	Anisotropy =	256.7573
14	C	Isotropic =	49.2163	Anisotropy =	105.5092
15	C	Isotropic =	58.1337	Anisotropy =	175.7901
16	C	Isotropic =	66.5602	Anisotropy =	160.0652
17	C	Isotropic =	144.9141	Anisotropy =	42.0650
18	C	Isotropic =	176.9530	Anisotropy =	24.0512
19	C	Isotropic =	155.0759	Anisotropy =	16.2286
20	C	Isotropic =	123.9412	Anisotropy =	54.5159
21	O	Isotropic =	202.2449	Anisotropy =	130.9395
22	C	Isotropic =	31.7384	Anisotropy =	138.8066
23	C	Isotropic =	70.4621	Anisotropy =	171.2550
24	C	Isotropic =	43.6390	Anisotropy =	182.3106
25	N	Isotropic =	-37.1291	Anisotropy =	458.5191
26	C	Isotropic =	43.0465	Anisotropy =	160.7245
27	C	Isotropic =	92.1150	Anisotropy =	138.7071
28	C	Isotropic =	69.7798	Anisotropy =	175.1291
29	C	Isotropic =	67.7582	Anisotropy =	170.6265
30	C	Isotropic =	63.5923	Anisotropy =	175.4268
31	C	Isotropic =	63.9297	Anisotropy =	150.4412
32	C	Isotropic =	154.1590	Anisotropy =	47.1572
33	O	Isotropic =	-64.2560	Anisotropy =	367.2226
34	H	Isotropic =	23.9980	Anisotropy =	9.0052
35	H	Isotropic =	24.2818	Anisotropy =	4.5389
36	H	Isotropic =	23.2542	Anisotropy =	4.8534
37	H	Isotropic =	23.6363	Anisotropy =	6.1051
38	H	Isotropic =	23.9157	Anisotropy =	9.0784
39	H	Isotropic =	28.3289	Anisotropy =	6.4260
40	H	Isotropic =	26.6173	Anisotropy =	7.8128
41	H	Isotropic =	30.6761	Anisotropy =	6.0506
42	H	Isotropic =	30.5661	Anisotropy =	10.3897
43	H	Isotropic =	31.1709	Anisotropy =	8.3611
44	H	Isotropic =	28.5019	Anisotropy =	7.3201
45	H	Isotropic =	28.5016	Anisotropy =	7.7580
46	H	Isotropic =	26.6110	Anisotropy =	4.4033
47	H	Isotropic =	26.8894	Anisotropy =	8.0596
48	H	Isotropic =	23.0114	Anisotropy =	7.1739

49	H	Isotropic =	25.1404	Anisotropy =	6.4694
50	H	Isotropic =	23.0792	Anisotropy =	10.6940
51	H	Isotropic =	23.8077	Anisotropy =	5.8156
52	H	Isotropic =	23.6340	Anisotropy =	4.9159
53	H	Isotropic =	23.5999	Anisotropy =	6.2461
54	H	Isotropic =	28.8293	Anisotropy =	7.6097
55	H	Isotropic =	27.2236	Anisotropy =	7.5895
56	H	Isotropic =	27.9706	Anisotropy =	10.2903

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.906238810648	4.409301282688	-2.146630840622
C	-2.610655770818	3.917486927300	-1.126763201289
C	-2.687867439177	4.550210024170	0.134711697457
C	-1.907667000554	5.696990133424	0.327261056397
C	-1.145900611884	6.196043580943	-0.730278141373
C	-1.204262923925	5.536406573050	-1.956833073989
N	-3.610093063357	4.132719320870	1.132843554339
C	-3.797223631643	2.840256929120	1.569358956410
C	-3.103203271327	1.702303991025	0.874368429987
C	-2.956132736589	1.648827773875	-0.518243282115
N	-3.328204414845	2.714083592503	-1.342208912031
O	-4.498876930416	2.602961350896	2.552291851055
N	-2.370179817077	0.523440523259	-1.085914143069
C	-2.026194202631	-0.536313247324	-0.288163057090
C	-2.156811632221	-0.515516309139	1.091895149215
C	-2.708132262998	0.628416058667	1.677302254430
C	-3.996393197445	2.527542316837	-2.648508437624
C	-5.160070648644	1.547748385587	-2.554689097296
C	-1.693019349870	-1.692431524659	1.921176915337
C	-0.289434113301	-1.517108334358	2.495549553507
O	0.633148947082	-1.472608748646	1.395022287297
C	1.947358772761	-1.299583463151	1.653256453557
C	2.810404378436	-1.254700349066	0.508142634573
C	4.210197906625	-1.072842644924	0.743436491002
N	4.751323459289	-0.942278240565	1.997197089342
C	3.910205157722	-0.992054539655	3.013458786079
C	2.507976078855	-1.167363697654	2.913028334721
C	2.332769190012	-1.381461760359	-0.823067340541
C	3.211042843319	-1.330185366527	-1.888261931443

C	4.598459050225	-1.150264787395	-1.662292517094
C	5.085352624526	-1.024747239803	-0.376371141539
C	-4.309724680831	5.178181117326	1.894902700227
O	-2.151342584053	0.454013207201	-2.350400069545
H	-1.917681213188	6.211609683342	1.288558048917
H	-0.536038973923	7.091756585750	-0.606085213109
H	-0.662082600613	5.920870935401	-2.825848693295
H	-1.614268731503	-1.373160508984	-0.848868541228
H	-2.870215862879	0.690793713877	2.753132045459
H	-4.367734508317	3.525757371554	-2.924594003837
H	-3.284586531719	2.200942243805	-3.416924809084
H	-4.807712488311	0.527820226373	-2.339214615718
H	-5.880716372101	1.849007543871	-1.777619009088
H	-5.687628301012	1.517697685719	-3.521168740905
H	-2.377164444794	-1.835834627764	2.771753749941
H	-1.718249077159	-2.615548327176	1.322658852661
H	-0.039659184017	-2.366118288686	3.153414444424
H	-0.213769680206	-0.584000039466	3.079266630688
H	4.347709671681	-0.887708464169	4.013065283285
H	1.910421988327	-1.193911969323	3.822357583603
H	1.264626578243	-1.519091037880	-0.990250744596
H	2.836705626643	-1.428216921854	-2.909363299992
H	5.283872632136	-1.111206532703	-2.511839850691
H	6.149970359441	-0.885696519844	-0.178652426124
H	-3.757462385869	5.457831385085	2.806817645326
H	-4.432031481507	6.061586069745	1.256891787759
H	-5.291534333951	4.795306957806	2.195094867329

SCF Done: E(RB3LYP) = -1465.99574932

Zero-point correction= 0.444641
Thermal correction to Energy= 0.472138
Thermal correction to Enthalpy= 0.473082
Thermal correction to Gibbs Free Energy= 0.383755
Sum of electronic and zero-point Energies= -1465.551109
Sum of electronic and thermal Energies= -1465.523611
Sum of electronic and thermal Enthalpies= -1465.522667
Sum of electronic and thermal Free Energies= -1465.611994

1	N	Isotropic =	-43.3031	Anisotropy =	460.7382
2	C	Isotropic =	37.0268	Anisotropy =	117.7542
3	C	Isotropic =	59.1928	Anisotropy =	124.1864
4	C	Isotropic =	63.1924	Anisotropy =	176.9675
5	C	Isotropic =	71.7952	Anisotropy =	161.6061

6	C	Isotropic =	49.2795	Anisotropy =	155.2376
7	N	Isotropic =	118.3656	Anisotropy =	88.1475
8	C	Isotropic =	28.8114	Anisotropy =	108.4871
9	C	Isotropic =	61.4396	Anisotropy =	138.0294
10	C	Isotropic =	42.2340	Anisotropy =	109.8306
11	N	Isotropic =	162.7840	Anisotropy =	72.2896
12	O	Isotropic =	-78.5468	Anisotropy =	584.5050
13	N	Isotropic =	-44.3437	Anisotropy =	254.3394
14	C	Isotropic =	48.4414	Anisotropy =	103.4110
15	C	Isotropic =	57.2698	Anisotropy =	174.2681
16	C	Isotropic =	66.8625	Anisotropy =	156.7679
17	C	Isotropic =	144.6290	Anisotropy =	43.0770
18	C	Isotropic =	176.4315	Anisotropy =	24.0233
19	C	Isotropic =	156.5946	Anisotropy =	16.4434
20	C	Isotropic =	121.8937	Anisotropy =	43.3745
21	O	Isotropic =	203.3607	Anisotropy =	111.6239
22	C	Isotropic =	32.3212	Anisotropy =	138.0666
23	C	Isotropic =	70.6488	Anisotropy =	170.8167
24	C	Isotropic =	43.9712	Anisotropy =	181.8941
25	N	Isotropic =	-38.0191	Anisotropy =	459.0454
26	C	Isotropic =	42.5757	Anisotropy =	159.5512
27	C	Isotropic =	91.3334	Anisotropy =	133.1838
28	C	Isotropic =	70.2191	Anisotropy =	173.9972
29	C	Isotropic =	67.6415	Anisotropy =	170.6840
30	C	Isotropic =	63.5122	Anisotropy =	175.1717
31	C	Isotropic =	63.8180	Anisotropy =	150.3553
32	C	Isotropic =	154.0875	Anisotropy =	47.2909
33	O	Isotropic =	-61.3150	Anisotropy =	359.9249
34	H	Isotropic =	24.0999	Anisotropy =	8.3225
35	H	Isotropic =	24.4002	Anisotropy =	4.2225
36	H	Isotropic =	23.3188	Anisotropy =	4.5801
37	H	Isotropic =	23.0000	Anisotropy =	7.2091
38	H	Isotropic =	24.0625	Anisotropy =	9.2882
39	H	Isotropic =	28.1668	Anisotropy =	6.5718
40	H	Isotropic =	26.3173	Anisotropy =	7.6673
41	H	Isotropic =	30.3320	Anisotropy =	4.9767
42	H	Isotropic =	30.3539	Anisotropy =	7.6351
43	H	Isotropic =	30.1751	Anisotropy =	11.4215
44	H	Isotropic =	28.4764	Anisotropy =	8.0166
45	H	Isotropic =	28.3342	Anisotropy =	5.7597
46	H	Isotropic =	27.1435	Anisotropy =	6.2220
47	H	Isotropic =	27.4688	Anisotropy =	5.4513
48	H	Isotropic =	22.8151	Anisotropy =	7.2455
49	H	Isotropic =	24.9893	Anisotropy =	9.4566

50	H	Isotropic =	23.0923	Anisotropy =	9.4896
51	H	Isotropic =	23.8175	Anisotropy =	6.6918
52	H	Isotropic =	23.6450	Anisotropy =	5.1880
53	H	Isotropic =	23.5685	Anisotropy =	5.6858
54	H	Isotropic =	28.0416	Anisotropy =	10.1471
55	H	Isotropic =	28.8981	Anisotropy =	7.7957
56	H	Isotropic =	27.2907	Anisotropy =	8.1263

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.314062353789	-1.080095459178	0.213111981042
C	-3.957836487957	-0.162140771772	1.112442166465
C	-3.433768004397	-0.489359983260	2.383804619030
C	-3.200772344350	-1.843651543872	2.653250465285
C	-3.545194924883	-2.803848977742	1.700842699692
C	-4.129546224580	-2.375039071142	0.510257195630
N	-3.267152247345	0.484860203346	3.405549221164
C	-2.650309681207	1.707920622702	3.264455454404
C	-2.206022591103	2.175422596852	1.906624224120
C	-2.972298816996	1.967154550307	0.752049511253
N	-4.140893206792	1.201070927303	0.770269724224
O	-2.416817001075	2.412048940767	4.246546535265
N	-2.522527185845	2.493011906353	-0.452969598923
C	-1.389772982209	3.265098485572	-0.474408490741
C	-0.612220860239	3.494612081439	0.649832805396
C	-1.034920276058	2.936326463238	1.860613686232
C	-5.359738856106	1.574308768862	0.020610143238
C	-5.721887375668	3.040716480430	0.224024159934
C	0.654878791104	4.315075912964	0.552415080359
C	1.927602018276	3.473502814351	0.533328705727
O	1.932826037545	2.714573560299	-0.686562643898
C	2.966492786728	1.879936540525	-0.928922009331
C	2.924762163336	1.177972850725	-2.179248389781
C	4.003734133936	0.284254988326	-2.470650414345
N	5.057801269567	0.074561918599	-1.618041077806
C	5.044475363710	0.748573277165	-0.482983754013
C	4.038482418770	1.660754806921	-0.079500541995
C	1.872623831457	1.339290187580	-3.119129733369
C	1.886342627235	0.638523432315	-4.309700324677
C	2.951237747303	-0.249068116746	-4.604152662341

C	3.984975022546	-0.421170934788	-3.705151685919
C	-3.630655599150	0.102506353043	4.778568690406
O	-3.154651673384	2.275051178423	-1.550265416266
H	-2.779182215096	-2.147378255730	3.611950358640
H	-3.379920334686	-3.864934972635	1.891764075165
H	-4.459976956916	-3.096204939238	-0.243194336233
H	-1.156618049869	3.648333050537	-1.466156406889
H	-0.485562312587	3.109344524433	2.785849711980
H	-5.253820927847	1.353437454225	-1.049005851988
H	-6.154289636815	0.931360354637	0.428022966189
H	-5.815194868754	3.289636183362	1.293272366777
H	-4.973068356401	3.704802046166	-0.233333457335
H	-6.687852259360	3.246829550593	-0.263531391428
H	0.633330546232	4.947610842391	-0.347626251251
H	0.722833584530	4.988149420579	1.421405185014
H	1.962226813667	2.788002665867	1.396972971531
H	2.816139534368	4.125780862225	0.565543597253
H	5.889231199363	0.578109052048	0.194371396533
H	4.132125188479	2.162940623469	0.881531221400
H	1.057315319242	2.024354582864	-2.886483724016
H	1.074468510911	0.767754626432	-5.028440386166
H	2.951850983766	-0.798103347789	-5.548398162550
H	4.815765796743	-1.098704082686	-3.911365881776
H	-4.434639250566	-0.642035172102	4.739786796342
H	-2.770414172445	-0.314568611671	5.326929384111
H	-3.974493654339	0.995708552119	5.312115493235

SCF Done: E(RB3LYP) = -1465.99575369

Zero-point correction= 0.444614
Thermal correction to Energy= 0.472122
Thermal correction to Enthalpy= 0.473066
Thermal correction to Gibbs Free Energy= 0.383931
Sum of electronic and zero-point Energies= -1465.551139
Sum of electronic and thermal Energies= -1465.523632
Sum of electronic and thermal Enthalpies= -1465.522688
Sum of electronic and thermal Free Energies= -1465.611823

1	N	Isotropic =	-43.3261	Anisotropy =	460.5786
2	C	Isotropic =	37.0561	Anisotropy =	117.7236
3	C	Isotropic =	59.3351	Anisotropy =	124.1914
4	C	Isotropic =	63.3594	Anisotropy =	176.5163
5	C	Isotropic =	71.6870	Anisotropy =	161.5485
6	C	Isotropic =	49.0942	Anisotropy =	155.5933

7	N	Isotropic =	117.9402	Anisotropy =	88.2054
8	C	Isotropic =	28.8673	Anisotropy =	108.7095
9	C	Isotropic =	61.1519	Anisotropy =	138.5198
10	C	Isotropic =	42.2650	Anisotropy =	109.7428
11	N	Isotropic =	163.2898	Anisotropy =	72.3994
12	O	Isotropic =	-78.3101	Anisotropy =	585.7936
13	N	Isotropic =	-44.9297	Anisotropy =	255.0082
14	C	Isotropic =	48.8453	Anisotropy =	102.4320
15	C	Isotropic =	56.9257	Anisotropy =	174.1443
16	C	Isotropic =	67.5710	Anisotropy =	157.8392
17	C	Isotropic =	144.5620	Anisotropy =	43.2607
18	C	Isotropic =	176.3630	Anisotropy =	24.0818
19	C	Isotropic =	156.4625	Anisotropy =	16.1198
20	C	Isotropic =	121.6862	Anisotropy =	43.0238
21	O	Isotropic =	203.3219	Anisotropy =	110.2687
22	C	Isotropic =	32.2761	Anisotropy =	138.0938
23	C	Isotropic =	70.5371	Anisotropy =	170.7015
24	C	Isotropic =	44.0098	Anisotropy =	182.1683
25	N	Isotropic =	-38.4030	Anisotropy =	457.0997
26	C	Isotropic =	42.5611	Anisotropy =	159.7020
27	C	Isotropic =	91.2394	Anisotropy =	133.5738
28	C	Isotropic =	70.2936	Anisotropy =	174.5851
29	C	Isotropic =	67.6316	Anisotropy =	170.5317
30	C	Isotropic =	63.6516	Anisotropy =	174.8741
31	C	Isotropic =	63.8547	Anisotropy =	149.8980
32	C	Isotropic =	154.0460	Anisotropy =	47.2991
33	O	Isotropic =	-62.5005	Anisotropy =	361.7963
34	H	Isotropic =	24.1096	Anisotropy =	8.2983
35	H	Isotropic =	24.3934	Anisotropy =	4.2497
36	H	Isotropic =	23.2935	Anisotropy =	4.5703
37	H	Isotropic =	23.0492	Anisotropy =	7.1396
38	H	Isotropic =	24.0608	Anisotropy =	9.4181
39	H	Isotropic =	26.3384	Anisotropy =	7.6875
40	H	Isotropic =	28.1654	Anisotropy =	6.6194
41	H	Isotropic =	30.3585	Anisotropy =	7.5712
42	H	Isotropic =	30.3457	Anisotropy =	5.0168
43	H	Isotropic =	30.1701	Anisotropy =	11.4391
44	H	Isotropic =	28.3886	Anisotropy =	5.6472
45	H	Isotropic =	28.4293	Anisotropy =	8.0144
46	H	Isotropic =	27.3480	Anisotropy =	5.5030
47	H	Isotropic =	27.1760	Anisotropy =	6.0920
48	H	Isotropic =	22.8208	Anisotropy =	7.2465
49	H	Isotropic =	24.9742	Anisotropy =	9.4254
50	H	Isotropic =	23.1102	Anisotropy =	9.6443

51	H	Isotropic =	23.8431	Anisotropy =	6.6561
52	H	Isotropic =	23.6721	Anisotropy =	5.1502
53	H	Isotropic =	23.6005	Anisotropy =	5.6730
54	H	Isotropic =	28.8821	Anisotropy =	7.7760
55	H	Isotropic =	28.0413	Anisotropy =	10.1214
56	H	Isotropic =	27.2796	Anisotropy =	8.1609

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.524591198229	3.695845806059	2.338083481800
C	-3.842009630346	2.692805652039	1.785324566349
C	-4.032794641481	1.339736441537	2.144239990538
C	-4.915035488473	1.073272583853	3.198911235231
C	-5.606275455825	2.125769316233	3.800209305543
C	-5.401803609839	3.415806046030	3.312564557477
N	-3.463286134419	0.271630478253	1.397358101272
C	-2.143425845466	0.160723123484	1.018090709916
C	-1.195699247837	1.306675715246	1.236100391813
C	-1.577081784057	2.641082894568	1.056697983280
N	-2.890977485262	3.014830411073	0.783619472973
O	-1.715885782922	-0.885071883886	0.530084087535
N	-0.622196802390	3.642724915505	1.225820642580
C	0.680358071308	3.297952500278	1.465808902323
C	1.094755707512	1.982859924517	1.634529564851
C	0.133188064391	0.975584253022	1.523740018378
C	-3.217161197281	4.062225520687	-0.204455175106
C	-4.276497685596	3.568721196644	-1.188141080529
C	2.550266079049	1.671341122893	1.899106285083
C	3.394898101218	1.473716364893	0.636509689746
O	2.962487150087	0.311228703659	-0.095917278057
C	2.353767884382	0.406113330815	-1.299940914798
C	2.119792666848	-0.846415220926	-1.961514280494
C	1.477560708885	-0.812591298693	-3.240159802845
N	1.083383709317	0.348960738460	-3.852924340684
C	1.322796607986	1.470805891922	-3.198816207728
C	1.946188987909	1.569652745897	-1.931296897565
C	2.500702346333	-2.094451094750	-1.400493122329
C	2.252823186018	-3.271463312269	-2.080004959023
C	1.615231292886	-3.244863836407	-3.345502507673
C	1.237689294737	-2.043385891332	-3.911097598158

C	-4.301097658744	-0.913705220638	1.158367940980
O	-0.949039844493	4.882202877673	1.160926924047
H	-5.081062346507	0.047312949808	3.528894419542
H	-6.304897117240	1.941567875663	4.617287875877
H	-5.959177355565	4.264040886077	3.720965568474
H	1.339198541442	4.160789428350	1.552775860358
H	0.401405834992	-0.074351265357	1.631945405548
H	-3.554587883192	4.970753357990	0.313558887997
H	-2.288901317801	4.316440279741	-0.727475524211
H	-3.931571696431	2.673436035453	-1.729601960006
H	-5.217996331472	3.318386043435	-0.673169237138
H	-4.497857140291	4.357985465478	-1.924924333672
H	3.016276063834	2.487617827377	2.473942921759
H	2.623492617985	0.760813554635	2.513164649937
H	4.435842893543	1.267603550927	0.926098073707
H	3.390136154633	2.367583958424	-0.001156604672
H	1.003857898392	2.397761299582	-3.689155965175
H	2.074556574648	2.554641903216	-1.486890283687
H	2.991299468969	-2.106433861443	-0.427259873492
H	2.548933766965	-4.227134972598	-1.642437096132
H	1.423650696537	-4.181284557952	-3.874195434241
H	0.746584200265	-1.998940635243	-4.885103172965
H	-4.170714808739	-1.671927451435	1.947589934250
H	-5.352233259996	-0.604208128423	1.119212501395
H	-4.008845821180	-1.363114340042	0.202623699824

SCF Done: E(RB3LYP) = -1465.99199662

Zero-point correction= 0.444370
Thermal correction to Energy= 0.471997
Thermal correction to Enthalpy= 0.472941
Thermal correction to Gibbs Free Energy= 0.382269
Sum of electronic and zero-point Energies= -1465.547626
Sum of electronic and thermal Energies= -1465.520000
Sum of electronic and thermal Enthalpies= -1465.519056
Sum of electronic and thermal Free Energies= -1465.609727

1	N	Isotropic =	-42.8526	Anisotropy =	467.7342
2	C	Isotropic =	38.8023	Anisotropy =	114.3913
3	C	Isotropic =	57.7095	Anisotropy =	124.4398
4	C	Isotropic =	62.5706	Anisotropy =	176.1361
5	C	Isotropic =	71.5545	Anisotropy =	160.6975
6	C	Isotropic =	49.1226	Anisotropy =	154.2380
7	N	Isotropic =	118.7973	Anisotropy =	89.6610

8	C	Isotropic =	29.3068	Anisotropy =	107.8274
9	C	Isotropic =	63.7115	Anisotropy =	138.1451
10	C	Isotropic =	41.0261	Anisotropy =	108.7470
11	N	Isotropic =	166.0013	Anisotropy =	59.4877
12	O	Isotropic =	-80.0514	Anisotropy =	588.0676
13	N	Isotropic =	-43.6135	Anisotropy =	259.1384
14	C	Isotropic =	50.3811	Anisotropy =	107.3896
15	C	Isotropic =	58.8193	Anisotropy =	175.2268
16	C	Isotropic =	65.5024	Anisotropy =	157.3825
17	C	Isotropic =	146.8313	Anisotropy =	37.3710
18	C	Isotropic =	175.8636	Anisotropy =	24.9805
19	C	Isotropic =	155.3377	Anisotropy =	16.8674
20	C	Isotropic =	123.9985	Anisotropy =	53.3822
21	O	Isotropic =	203.2839	Anisotropy =	130.7849
22	C	Isotropic =	31.7843	Anisotropy =	139.3832
23	C	Isotropic =	70.3565	Anisotropy =	171.7925
24	C	Isotropic =	43.5129	Anisotropy =	182.8605
25	N	Isotropic =	-36.8711	Anisotropy =	457.5941
26	C	Isotropic =	42.9503	Anisotropy =	160.6416
27	C	Isotropic =	92.5179	Anisotropy =	139.2987
28	C	Isotropic =	69.9750	Anisotropy =	175.4354
29	C	Isotropic =	67.7963	Anisotropy =	170.4435
30	C	Isotropic =	63.4482	Anisotropy =	175.3570
31	C	Isotropic =	63.7161	Anisotropy =	150.8721
32	C	Isotropic =	154.1695	Anisotropy =	46.5468
33	O	Isotropic =	-70.6467	Anisotropy =	376.8355
34	H	Isotropic =	24.1039	Anisotropy =	9.3324
35	H	Isotropic =	24.3300	Anisotropy =	4.5550
36	H	Isotropic =	23.2327	Anisotropy =	4.6719
37	H	Isotropic =	23.2129	Anisotropy =	7.1834
38	H	Isotropic =	24.4047	Anisotropy =	7.4862
39	H	Isotropic =	26.8520	Anisotropy =	8.2414
40	H	Isotropic =	28.0743	Anisotropy =	5.1368
41	H	Isotropic =	30.5920	Anisotropy =	7.0306
42	H	Isotropic =	30.4552	Anisotropy =	5.2317
43	H	Isotropic =	30.4431	Anisotropy =	11.0761
44	H	Isotropic =	28.6688	Anisotropy =	8.1579
45	H	Isotropic =	28.3226	Anisotropy =	6.7354
46	H	Isotropic =	26.8937	Anisotropy =	8.2949
47	H	Isotropic =	26.6797	Anisotropy =	4.9922
48	H	Isotropic =	22.9737	Anisotropy =	6.9480
49	H	Isotropic =	25.1533	Anisotropy =	7.2871
50	H	Isotropic =	23.0021	Anisotropy =	10.3138
51	H	Isotropic =	23.7690	Anisotropy =	5.6968

52	H	Isotropic =	23.5874	Anisotropy =	4.8279
53	H	Isotropic =	23.5408	Anisotropy =	5.9547
54	H	Isotropic =	28.2186	Anisotropy =	10.1457
55	H	Isotropic =	29.0498	Anisotropy =	7.3264
56	H	Isotropic =	27.6726	Anisotropy =	6.8913

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.497126541316	0.769910228377	2.434174241086
C	-4.293192414885	1.254898961976	2.129676746055
C	-3.469294304483	1.917164887015	3.067259932751
C	-3.916329852118	1.967142305467	4.393635736649
C	-5.161982675140	1.429660668419	4.720218939513
C	-5.929900166359	0.871908237815	3.698948389123
N	-2.295577734001	2.621886671920	2.678892833972
C	-1.285807931459	2.130806846773	1.883560775361
C	-1.442423165779	0.803451125307	1.198497473173
C	-2.654781051961	0.382054541222	0.639652463913
N	-3.839026254555	1.099554275726	0.795231181803
O	-0.231283680498	2.754494288709	1.748963076118
N	-2.695674967471	-0.834455421702	-0.038337894901
C	-1.535426829361	-1.535094817852	-0.237629025626
C	-0.316029775871	-1.138538821244	0.293211344572
C	-0.280340153462	0.044048870562	1.035459663899
C	-4.799984171360	1.271112364529	-0.312864617544
C	-5.201159794396	2.737317767611	-0.463473208234
C	0.937199403886	-1.942820988173	0.031737920150
C	1.689401038986	-1.508264871958	-1.225953545448
O	2.010200297007	-0.114277924199	-1.091820926047
C	2.728810336519	0.489140468297	-2.063115134979
C	2.905200143663	1.906737411906	-1.925272432124
C	3.696817342231	2.570385983302	-2.916596120771
N	4.268813633137	1.922083405634	-3.981762928732
C	4.052690904418	0.622797818315	-4.070003209442
C	3.296629864427	-0.148730849950	-3.153831189053
C	2.323955333656	2.660676432148	-0.870644795451
C	2.533074969158	4.024291777771	-0.791966409178
C	3.330332445419	4.684827194421	-1.759438638743
C	3.896336457038	3.973432476279	-2.798559356739
C	-2.039261370169	3.921953319939	3.317685863277

O	-3.804446773996	-1.305251989248	-0.483391603171
H	-3.306800693651	2.447265324416	5.159854012220
H	-5.534996217095	1.464132115423	5.744545702222
H	-6.933146645726	0.484634201844	3.900172673312
H	-1.683164242024	-2.447880607292	-0.812971380009
H	0.650186411158	0.404203422527	1.470655865008
H	-4.312664077090	0.906259078101	-1.223516520237
H	-5.682191066712	0.638189905490	-0.143792382260
H	-5.906545221826	2.845383168296	-1.303417425911
H	-5.701872534336	3.113048225723	0.443326025485
H	-4.323949718117	3.373571765850	-0.661945779059
H	1.613408473207	-1.857430436585	0.896008874774
H	0.693147561455	-3.009511160973	-0.087360641486
H	1.074814694740	-1.653081206738	-2.130970632363
H	2.613706616693	-2.100079870088	-1.328539324757
H	4.505719971115	0.110729839152	-4.926808204377
H	3.189074877285	-1.218561559370	-3.323324490751
H	1.695671954798	2.162707365538	-0.132630330114
H	2.076181372640	4.596085163019	0.018448664804
H	3.490927322962	5.762690100941	-1.684261597686
H	4.506761469664	4.461349625584	-3.560918278728
H	-1.425880489119	3.815640957499	4.227047399182
H	-1.494589851249	4.558483143567	2.611303024025
H	-2.998382529680	4.386348792960	3.575689201472

SCF Done: E(RB3LYP) = -1465.99729900

Zero-point correction= 0.444704
Thermal correction to Energy= 0.472169
Thermal correction to Enthalpy= 0.473113
Thermal correction to Gibbs Free Energy= 0.384968
Sum of electronic and zero-point Energies= -1465.552595
Sum of electronic and thermal Energies= -1465.525130
Sum of electronic and thermal Enthalpies= -1465.524186
Sum of electronic and thermal Free Energies= -1465.612331

1	N	Isotropic =	-42.9601	Anisotropy =	468.4343
2	C	Isotropic =	38.5083	Anisotropy =	115.3547
3	C	Isotropic =	57.4239	Anisotropy =	124.1439
4	C	Isotropic =	62.3572	Anisotropy =	176.6098
5	C	Isotropic =	71.4776	Anisotropy =	160.1946
6	C	Isotropic =	48.8918	Anisotropy =	154.6120
7	N	Isotropic =	117.9630	Anisotropy =	89.3037
8	C	Isotropic =	27.6971	Anisotropy =	108.7477

9	C	Isotropic =	63.6103	Anisotropy =	135.8208
10	C	Isotropic =	40.9800	Anisotropy =	107.4088
11	N	Isotropic =	164.9888	Anisotropy =	57.9676
12	O	Isotropic =	-76.9329	Anisotropy =	576.7776
13	N	Isotropic =	-42.8126	Anisotropy =	256.5536
14	C	Isotropic =	50.4743	Anisotropy =	104.9910
15	C	Isotropic =	58.2680	Anisotropy =	173.1914
16	C	Isotropic =	63.8165	Anisotropy =	156.5771
17	C	Isotropic =	146.7556	Anisotropy =	36.8788
18	C	Isotropic =	175.8280	Anisotropy =	25.0244
19	C	Isotropic =	156.7987	Anisotropy =	18.6535
20	C	Isotropic =	122.6263	Anisotropy =	44.1490
21	O	Isotropic =	203.6604	Anisotropy =	116.6127
22	C	Isotropic =	32.2284	Anisotropy =	136.9041
23	C	Isotropic =	70.3323	Anisotropy =	169.6565
24	C	Isotropic =	43.6767	Anisotropy =	181.5406
25	N	Isotropic =	-38.2717	Anisotropy =	458.3878
26	C	Isotropic =	42.6221	Anisotropy =	159.1186
27	C	Isotropic =	91.1798	Anisotropy =	133.1585
28	C	Isotropic =	68.8304	Anisotropy =	175.7107
29	C	Isotropic =	67.3960	Anisotropy =	170.0506
30	C	Isotropic =	63.6254	Anisotropy =	174.5593
31	C	Isotropic =	63.8985	Anisotropy =	149.4152
32	C	Isotropic =	153.8429	Anisotropy =	46.9680
33	O	Isotropic =	-68.7140	Anisotropy =	371.5373
34	H	Isotropic =	23.9128	Anisotropy =	9.0530
35	H	Isotropic =	24.2319	Anisotropy =	4.5870
36	H	Isotropic =	23.1341	Anisotropy =	4.7037
37	H	Isotropic =	23.2707	Anisotropy =	7.2325
38	H	Isotropic =	23.6135	Anisotropy =	9.3580
39	H	Isotropic =	28.0478	Anisotropy =	5.5185
40	H	Isotropic =	26.7927	Anisotropy =	8.4359
41	H	Isotropic =	30.4183	Anisotropy =	11.2388
42	H	Isotropic =	30.3356	Anisotropy =	5.0538
43	H	Isotropic =	30.4772	Anisotropy =	7.2049
44	H	Isotropic =	28.2528	Anisotropy =	5.5051
45	H	Isotropic =	28.5856	Anisotropy =	8.4390
46	H	Isotropic =	27.5449	Anisotropy =	6.3703
47	H	Isotropic =	26.9880	Anisotropy =	6.4553
48	H	Isotropic =	22.7474	Anisotropy =	7.1164
49	H	Isotropic =	24.8978	Anisotropy =	9.6117
50	H	Isotropic =	22.6369	Anisotropy =	8.8635
51	H	Isotropic =	23.6541	Anisotropy =	7.3725
52	H	Isotropic =	23.5861	Anisotropy =	5.6465

53	H	Isotropic =	23.5187	Anisotropy =	5.7760
54	H	Isotropic =	27.8703	Anisotropy =	9.9679
55	H	Isotropic =	27.1559	Anisotropy =	7.7265
56	H	Isotropic =	28.7623	Anisotropy =	7.3578

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.833168291176	3.162253984678	3.522122784657
C	-2.109672463500	1.890291083150	3.233457776909
C	-3.385639195867	1.454652911288	2.810768846044
C	-4.362162174571	2.436287669289	2.599978689345
C	-4.064188377207	3.772390892447	2.870832840179
C	-2.796210300502	4.081192538301	3.361396442168
N	-3.723351984390	0.075675067718	2.721593175596
C	-2.989917971040	-0.900992147439	2.084160591362
C	-1.625172083179	-0.585135352275	1.539526012430
C	-0.723568733000	0.248794260335	2.212067403416
N	-1.066910003228	0.939617729254	3.372939379587
O	-3.454757776470	-2.028611832201	1.919211102689
N	0.544380976417	0.443550583397	1.671268612436
C	0.913241354464	-0.251052740617	0.549759998915
C	0.048467370869	-1.091932457521	-0.135195080955
C	-1.243438476872	-1.256269227061	0.373535698743
C	-0.138942036900	1.054668386254	4.515951873987
C	-0.845931171456	0.712768820410	5.826081871893
C	0.503373426751	-1.789894684653	-1.398139721558
C	-0.008379079887	-1.135329845033	-2.678081589061
O	0.579982265281	0.172447222991	-2.768056852464
C	0.267171015875	0.955098201579	-3.823038667737
C	0.886805604356	2.248761139682	-3.848460693227
C	0.579535675791	3.106186707422	-4.952125449133
N	-0.267912114996	2.748011994991	-5.969642795661
C	-0.808519353468	1.545929977135	-5.894499191046
C	-0.585924603786	0.606898284283	-4.857331603112
C	1.776153355761	2.697082253512	-2.836393108127
C	2.343851126617	3.954337773011	-2.912588366067
C	2.043413770331	4.808904037951	-4.002535228468
C	1.181665123329	4.393581667897	-4.998177189257
C	-5.056119370345	-0.328834511670	3.195073093524
O	1.373937895711	1.262016211950	2.209899636169

H	-5.356951650942	2.154816155287	2.253128158210
H	-4.811282467524	4.553089084766	2.722593999775
H	-2.535857325666	5.108320663879	3.633829633610
H	1.936796683911	-0.046778585149	0.240753894047
H	-1.958538008608	-1.926874760595	-0.102429927018
H	0.689316792464	0.362010519880	4.330577998247
H	0.289442179111	2.065924766290	4.552519408931
H	-1.251506327425	-0.311366978764	5.805718529984
H	-0.133828864899	0.788893033455	6.663813364738
H	-1.675776485241	1.408565367680	6.028973570997
H	1.602199031736	-1.832804000366	-1.435872462933
H	0.137398182552	-2.828632713891	-1.396083189615
H	-1.107990854974	-1.045766729227	-2.666645729575
H	0.286557523969	-1.734793817587	-3.555391298886
H	-1.484322643142	1.264277238263	-6.710259950001
H	-1.086532681217	-0.358634205459	-4.899188642529
H	2.002257777668	2.034063469249	-2.001294228104
H	3.026921044121	4.293142925455	-2.130901074025
H	2.497665884252	5.800979838391	-4.052627721909
H	0.936310363943	5.034984887564	-5.846838609900
H	-5.369287650474	0.349209360957	3.997847077807
H	-5.801898420054	-0.305853343564	2.383910586547
H	-4.997535483276	-1.354958776970	3.575026317423

SCF Done: E(RB3LYP) = -1465.99635470

Zero-point correction= 0.444576
Thermal correction to Energy= 0.472113
Thermal correction to Enthalpy= 0.473057
Thermal correction to Gibbs Free Energy= 0.383754
Sum of electronic and zero-point Energies= -1465.551778
Sum of electronic and thermal Energies= -1465.524242
Sum of electronic and thermal Enthalpies= -1465.523298
Sum of electronic and thermal Free Energies= -1465.612601

1	N	Isotropic =	-42.6682	Anisotropy =	469.5607
2	C	Isotropic =	38.8810	Anisotropy =	115.9758
3	C	Isotropic =	57.5342	Anisotropy =	125.8904
4	C	Isotropic =	62.9025	Anisotropy =	176.7675
5	C	Isotropic =	71.7546	Anisotropy =	161.3933
6	C	Isotropic =	49.1385	Anisotropy =	155.2393
7	N	Isotropic =	118.2373	Anisotropy =	89.5059
8	C	Isotropic =	28.7753	Anisotropy =	108.9384
9	C	Isotropic =	62.6424	Anisotropy =	136.2842

10	C	Isotropic =	40.9987	Anisotropy =	106.0974
11	N	Isotropic =	165.9032	Anisotropy =	59.4904
12	O	Isotropic =	-78.6746	Anisotropy =	587.9526
13	N	Isotropic =	-42.2798	Anisotropy =	256.3549
14	C	Isotropic =	48.8770	Anisotropy =	103.2740
15	C	Isotropic =	57.4119	Anisotropy =	173.2488
16	C	Isotropic =	67.5615	Anisotropy =	158.0644
17	C	Isotropic =	146.5389	Anisotropy =	37.6230
18	C	Isotropic =	175.8111	Anisotropy =	25.5341
19	C	Isotropic =	156.5234	Anisotropy =	16.4018
20	C	Isotropic =	121.6951	Anisotropy =	43.1189
21	O	Isotropic =	203.3192	Anisotropy =	112.3307
22	C	Isotropic =	32.1790	Anisotropy =	137.7611
23	C	Isotropic =	70.6160	Anisotropy =	170.8318
24	C	Isotropic =	43.9936	Anisotropy =	182.1396
25	N	Isotropic =	-38.5847	Anisotropy =	456.8064
26	C	Isotropic =	42.5490	Anisotropy =	159.4977
27	C	Isotropic =	91.3177	Anisotropy =	133.1470
28	C	Isotropic =	70.3541	Anisotropy =	174.1395
29	C	Isotropic =	67.7124	Anisotropy =	170.4983
30	C	Isotropic =	63.5625	Anisotropy =	174.9081
31	C	Isotropic =	63.7760	Anisotropy =	150.3154
32	C	Isotropic =	153.9692	Anisotropy =	47.1612
33	O	Isotropic =	-67.8969	Anisotropy =	370.7569
34	H	Isotropic =	24.0952	Anisotropy =	8.2728
35	H	Isotropic =	24.3708	Anisotropy =	4.1859
36	H	Isotropic =	23.2534	Anisotropy =	4.4413
37	H	Isotropic =	23.0202	Anisotropy =	7.1708
38	H	Isotropic =	24.0670	Anisotropy =	9.4307
39	H	Isotropic =	28.0092	Anisotropy =	5.8223
40	H	Isotropic =	26.7498	Anisotropy =	7.9194
41	H	Isotropic =	30.4138	Anisotropy =	7.5030
42	H	Isotropic =	30.3636	Anisotropy =	11.3644
43	H	Isotropic =	30.3384	Anisotropy =	5.0358
44	H	Isotropic =	28.3895	Anisotropy =	5.7618
45	H	Isotropic =	28.4457	Anisotropy =	8.0713
46	H	Isotropic =	27.3845	Anisotropy =	5.4993
47	H	Isotropic =	27.1300	Anisotropy =	6.1312
48	H	Isotropic =	22.8154	Anisotropy =	7.2361
49	H	Isotropic =	24.9775	Anisotropy =	9.4288
50	H	Isotropic =	23.1550	Anisotropy =	9.5268
51	H	Isotropic =	23.8665	Anisotropy =	6.6593
52	H	Isotropic =	23.6778	Anisotropy =	5.1733
53	H	Isotropic =	23.5901	Anisotropy =	5.6634

54	H	Isotropic =	28.8865	Anisotropy =	7.5770
55	H	Isotropic =	28.0372	Anisotropy =	10.1256
56	H	Isotropic =	27.2978	Anisotropy =	8.1164

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.997610029900	-1.119377620532	-2.785443300837
C	-2.515688197266	-1.115163919455	-1.557035721646
C	-3.775923209154	-0.553685973307	-1.253215845014
C	-4.450307833447	0.108825990465	-2.286557451714
C	-3.893912209838	0.133035145112	-3.565960270261
C	-2.681403904024	-0.523556579184	-3.772898467720
N	-4.406692344641	-0.750989938273	0.006217951720
C	-3.829488100031	-0.550994402222	1.240941191125
C	-2.361001496638	-0.248894958268	1.347035969156
C	-1.406623851586	-0.871594599295	0.533330721774
N	-1.757902891482	-1.715060104427	-0.518814707806
O	-4.511228216841	-0.580496631221	2.265173194406
N	-0.058658885579	-0.589607424213	0.741562072530
C	0.307724963273	0.219602637623	1.783701717742
C	-0.611818874628	0.851519111668	2.608556390490
C	-1.969150809958	0.607802437000	2.380922150502
C	-1.026899266543	-2.967365808536	-0.797437385846
C	-1.992826254650	-4.141580516134	-0.944520578521
C	-0.141701417654	1.792978809798	3.695204380446
C	-0.152945668392	3.259926077896	3.272455839075
O	0.818464910338	3.422051568034	2.226210687375
C	0.968362789348	4.637958746774	1.658200942001
C	1.953451138963	4.726874976127	0.619045042482
C	2.138035544208	6.000004091837	-0.007820328902
N	1.425441855407	7.119577323499	0.339115648066
C	0.534076686287	6.979424607007	1.302824704192
C	0.257600384752	5.777003342415	1.999088958023
C	2.735103046100	3.617925473247	0.200003433305
C	3.669189434504	3.762563076567	-0.807623323209
C	3.856204449791	5.020259820866	-1.433420736441
C	3.107852136927	6.112481681063	-1.041765216640
C	-5.853830317717	-1.014386833608	0.009350662681
O	0.845904915926	-1.077731803248	-0.028131533052
H	-5.416179713032	0.578662213424	-2.098259622267

H	-4.404550201567	0.635408522793	-4.388469764738
H	-2.233554153229	-0.571768056089	-4.769924572806
H	1.386063753178	0.338642926513	1.870668275546
H	-2.737366894519	1.049152320618	3.015407311386
H	-0.415022342235	-2.847059599708	-1.702262045740
H	-0.336839605742	-3.133590391972	0.036608112002
H	-2.586640465355	-4.288214675287	-0.028204945709
H	-2.688261655233	-3.988613952710	-1.785517181585
H	-1.426650806129	-5.066126817284	-1.143445769981
H	-0.800130112175	1.701389380887	4.572740288403
H	0.874905416601	1.525729725935	4.020882307711
H	0.112902777398	3.905370804029	4.126164147242
H	-1.148693132882	3.556934128568	2.902088029691
H	-0.032092467759	7.877161606222	1.576757164598
H	-0.500896213572	5.778039139109	2.779792110837
H	2.586473243549	2.653209283908	0.684932654272
H	4.266663010972	2.905379337921	-1.124879717399
H	4.597212535212	5.123160606065	-2.229274449044
H	3.235324893889	7.090897652081	-1.508990314243
H	-6.124535080024	-1.524809331394	-0.922522771608
H	-6.092704716251	-1.653087375949	0.867214735941
H	-6.437756546952	-0.084205252755	0.101529228012

SCF Done: E(RB3LYP) = -1465.99634821

Zero-point correction= 0.444489
Thermal correction to Energy= 0.472083
Thermal correction to Enthalpy= 0.473027
Thermal correction to Gibbs Free Energy= 0.383060
Sum of electronic and zero-point Energies= -1465.551859
Sum of electronic and thermal Energies= -1465.524265
Sum of electronic and thermal Enthalpies= -1465.523321
Sum of electronic and thermal Free Energies= -1465.613288

1	N	Isotropic =	-42.8597	Anisotropy =	469.6054
2	C	Isotropic =	38.7077	Anisotropy =	116.0065
3	C	Isotropic =	57.6657	Anisotropy =	125.8852
4	C	Isotropic =	62.8072	Anisotropy =	176.6421
5	C	Isotropic =	71.6983	Anisotropy =	161.4068
6	C	Isotropic =	49.0344	Anisotropy =	155.5333
7	N	Isotropic =	118.4047	Anisotropy =	89.9017
8	C	Isotropic =	28.6787	Anisotropy =	109.1312
9	C	Isotropic =	62.6364	Anisotropy =	135.9634
10	C	Isotropic =	41.1735	Anisotropy =	106.5306

11	N	Isotropic =	165.8341	Anisotropy =	59.0572
12	O	Isotropic =	-79.8861	Anisotropy =	586.7757
13	N	Isotropic =	-41.7680	Anisotropy =	256.1971
14	C	Isotropic =	48.6802	Anisotropy =	104.0796
15	C	Isotropic =	57.4717	Anisotropy =	173.2280
16	C	Isotropic =	67.1941	Anisotropy =	156.1276
17	C	Isotropic =	146.8369	Anisotropy =	37.7244
18	C	Isotropic =	175.7633	Anisotropy =	25.7289
19	C	Isotropic =	156.4884	Anisotropy =	16.4342
20	C	Isotropic =	121.7846	Anisotropy =	43.2876
21	O	Isotropic =	203.5712	Anisotropy =	111.7889
22	C	Isotropic =	32.3624	Anisotropy =	137.9694
23	C	Isotropic =	70.5797	Anisotropy =	170.7419
24	C	Isotropic =	43.9142	Anisotropy =	182.0766
25	N	Isotropic =	-38.0247	Anisotropy =	458.7609
26	C	Isotropic =	42.6770	Anisotropy =	160.1419
27	C	Isotropic =	91.2918	Anisotropy =	133.0607
28	C	Isotropic =	70.2952	Anisotropy =	174.6978
29	C	Isotropic =	67.6533	Anisotropy =	170.5584
30	C	Isotropic =	63.7422	Anisotropy =	175.0186
31	C	Isotropic =	63.8504	Anisotropy =	150.0646
32	C	Isotropic =	153.9235	Anisotropy =	47.1758
33	O	Isotropic =	-67.1946	Anisotropy =	369.4134
34	H	Isotropic =	24.0888	Anisotropy =	8.2779
35	H	Isotropic =	24.3794	Anisotropy =	4.1782
36	H	Isotropic =	23.2633	Anisotropy =	4.4798
37	H	Isotropic =	22.9739	Anisotropy =	7.2167
38	H	Isotropic =	24.0809	Anisotropy =	9.2630
39	H	Isotropic =	26.7884	Anisotropy =	7.9015
40	H	Isotropic =	27.9154	Anisotropy =	5.6592
41	H	Isotropic =	30.4088	Anisotropy =	7.4632
42	H	Isotropic =	30.3471	Anisotropy =	5.1078
43	H	Isotropic =	30.3718	Anisotropy =	11.3720
44	H	Isotropic =	28.4760	Anisotropy =	8.0441
45	H	Isotropic =	28.3449	Anisotropy =	5.8418
46	H	Isotropic =	27.1567	Anisotropy =	6.2386
47	H	Isotropic =	27.4538	Anisotropy =	5.4029
48	H	Isotropic =	22.8023	Anisotropy =	7.2657
49	H	Isotropic =	24.9996	Anisotropy =	9.4233
50	H	Isotropic =	23.0698	Anisotropy =	9.5339
51	H	Isotropic =	23.8222	Anisotropy =	6.6217
52	H	Isotropic =	23.6655	Anisotropy =	5.1319
53	H	Isotropic =	23.5847	Anisotropy =	5.6545
54	H	Isotropic =	28.8876	Anisotropy =	7.5527

55 H Isotropic = 27.3339 Anisotropy = 8.1410
56 H Isotropic = 28.0313 Anisotropy = 10.1727

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.295026810223	2.170493298315	0.383084281033
C	-4.335423081980	1.726663482924	-0.429173197527
C	-3.437511338888	2.584240004621	-1.103140781719
C	-3.516042692737	3.952397259310	-0.813801475127
C	-4.499517276598	4.414937584203	0.061384361029
C	-5.386541515089	3.488928709863	0.608779576906
N	-2.571720248851	2.116274634199	-2.130232578789
C	-1.732856302559	1.026467843179	-2.049681267728
C	-1.803842695858	0.104562513818	-0.864948137911
C	-3.015375950986	-0.246227696641	-0.256836783318
N	-4.231632896928	0.325849707872	-0.624352371035
O	-0.894766753360	0.813307404937	-2.925509803450
N	-2.999865714767	-1.159731487271	0.794246818216
C	-1.820502079294	-1.758448975025	1.149412707237
C	-0.603008770727	-1.436646089427	0.565144699353
C	-0.602380580128	-0.484726238488	-0.457987171344
C	-5.466752276021	-0.473759314252	-0.750479599609
C	-6.159047609665	-0.198407082810	-2.083976923849
C	0.667000136940	-2.097780272247	1.053770884774
C	1.413684963304	-1.294368722275	2.116156335488
O	1.919832037987	-0.100454592099	1.496523865569
C	2.600630564313	0.787053509010	2.254023302932
C	3.097263090079	1.945829201645	1.569352326875
C	3.816764165510	2.911390689011	2.342720916046
N	4.050494046215	2.775016439603	3.687478462931
C	3.575225252914	1.686520334298	4.263746347945
C	2.847903423378	0.660831632216	3.611117042449
C	2.904866468807	2.162450605498	0.179270792376
C	3.404442457240	3.299008300388	-0.426789801836
C	4.114666465419	4.260840852671	0.333976908129
C	4.315943204506	4.070025641943	1.686539048689
C	-2.409688404843	2.964390439876	-3.321133575155
O	-4.075646726297	-1.453461739783	1.430865268092
H	-2.831079632618	4.653837049864	-1.291177658366
H	-4.585827258620	5.476829824490	0.294912194162

H	-6.203387333290	3.813208217136	1.260375177562
H	-1.937849928976	-2.481564573542	1.955217499693
H	0.315496486525	-0.215720609261	-0.977680947877
H	-5.180372587948	-1.527915252853	-0.671044244765
H	-6.138268219058	-0.258387845182	0.092388411646
H	-7.070929072374	-0.812358605652	-2.163410740454
H	-6.459058918051	0.858279754719	-2.171266620543
H	-5.500938057728	-0.441268363302	-2.933481037737
H	0.433192819728	-3.079164995774	1.493284206281
H	1.347019231815	-2.275274356254	0.206276683665
H	2.255369326897	-1.884669427896	2.515147938376
H	0.744462292966	-1.024322222859	2.950441818294
H	3.766169456586	1.581322524714	5.337959114822
H	2.502496087366	-0.194404078438	4.188993488784
H	2.359955976784	1.417886585176	-0.400680049492
H	3.252695403630	3.458532031647	-1.496319226252
H	4.504843404905	5.156110177456	-0.155194016212
H	4.861690215049	4.796459588625	2.291710895871
H	-1.567217324704	3.666451474077	-3.211387775453
H	-2.206567064485	2.321332156029	-4.184875458508
H	-3.335871855213	3.528053067998	-3.484810131168

SCF Done: E(RB3LYP) = -1465.99623853

Zero-point correction= 0.444607
Thermal correction to Energy= 0.472113
Thermal correction to Enthalpy= 0.473057
Thermal correction to Gibbs Free Energy= 0.384086
Sum of electronic and zero-point Energies= -1465.551631
Sum of electronic and thermal Energies= -1465.524126
Sum of electronic and thermal Enthalpies= -1465.523182
Sum of electronic and thermal Free Energies= -1465.612153

1	N	Isotropic =	-42.6027	Anisotropy =	469.2707
2	C	Isotropic =	38.8258	Anisotropy =	115.4056
3	C	Isotropic =	57.6691	Anisotropy =	125.7140
4	C	Isotropic =	62.8269	Anisotropy =	176.8620
5	C	Isotropic =	71.6517	Anisotropy =	161.2744
6	C	Isotropic =	49.1214	Anisotropy =	155.1409
7	N	Isotropic =	118.2630	Anisotropy =	90.2774
8	C	Isotropic =	28.6262	Anisotropy =	110.2055
9	C	Isotropic =	63.3292	Anisotropy =	134.5797
10	C	Isotropic =	41.0880	Anisotropy =	106.2378
11	N	Isotropic =	165.6768	Anisotropy =	59.2658

12	O	Isotropic =	-80.0864	Anisotropy =	589.0812
13	N	Isotropic =	-42.4750	Anisotropy =	257.0264
14	C	Isotropic =	50.0956	Anisotropy =	102.4333
15	C	Isotropic =	57.3553	Anisotropy =	173.3662
16	C	Isotropic =	64.9322	Anisotropy =	157.0953
17	C	Isotropic =	146.8145	Anisotropy =	37.7297
18	C	Isotropic =	175.6815	Anisotropy =	25.5983
19	C	Isotropic =	156.8810	Anisotropy =	16.2241
20	C	Isotropic =	121.4450	Anisotropy =	44.1996
21	O	Isotropic =	202.7822	Anisotropy =	109.7457
22	C	Isotropic =	32.2650	Anisotropy =	137.4903
23	C	Isotropic =	70.5791	Anisotropy =	170.9139
24	C	Isotropic =	43.8396	Anisotropy =	181.8406
25	N	Isotropic =	-38.1258	Anisotropy =	459.3925
26	C	Isotropic =	42.6509	Anisotropy =	159.7058
27	C	Isotropic =	91.2010	Anisotropy =	133.1775
28	C	Isotropic =	70.1433	Anisotropy =	173.9322
29	C	Isotropic =	67.5926	Anisotropy =	170.7233
30	C	Isotropic =	63.5520	Anisotropy =	175.2142
31	C	Isotropic =	63.7423	Anisotropy =	150.5081
32	C	Isotropic =	153.8407	Anisotropy =	46.8833
33	O	Isotropic =	-68.4677	Anisotropy =	371.6063
34	H	Isotropic =	24.1187	Anisotropy =	8.2828
35	H	Isotropic =	24.3838	Anisotropy =	4.6874
36	H	Isotropic =	23.2477	Anisotropy =	4.6277
37	H	Isotropic =	23.2983	Anisotropy =	7.2782
38	H	Isotropic =	23.6852	Anisotropy =	9.4521
39	H	Isotropic =	27.9731	Anisotropy =	6.0819
40	H	Isotropic =	26.8068	Anisotropy =	8.1704
41	H	Isotropic =	30.3866	Anisotropy =	11.4579
42	H	Isotropic =	30.3364	Anisotropy =	4.9793
43	H	Isotropic =	30.3987	Anisotropy =	7.1741
44	H	Isotropic =	28.5987	Anisotropy =	8.2404
45	H	Isotropic =	28.2232	Anisotropy =	5.4791
46	H	Isotropic =	27.1667	Anisotropy =	6.5531
47	H	Isotropic =	27.4834	Anisotropy =	5.4307
48	H	Isotropic =	22.7990	Anisotropy =	7.1934
49	H	Isotropic =	24.9844	Anisotropy =	9.5730
50	H	Isotropic =	23.0696	Anisotropy =	8.9980
51	H	Isotropic =	23.7935	Anisotropy =	6.6196
52	H	Isotropic =	23.6177	Anisotropy =	5.3197
53	H	Isotropic =	23.5435	Anisotropy =	5.6410
54	H	Isotropic =	27.9813	Anisotropy =	9.8741
55	H	Isotropic =	27.2725	Anisotropy =	7.7434

56 H Isotropic = 28.8675 Anisotropy = 7.5151

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.327054038967	0.849939760297	-0.276729048906
C	-4.263344939530	1.487144099582	-0.766540449928
C	-3.397147551361	0.917547876985	-1.726660407592
C	-3.630369656074	-0.414268829445	-2.092111598550
C	-4.724511411357	-1.093477531767	-1.554792332905
C	-5.562878454648	-0.407759899404	-0.676888059112
N	-2.406796371747	1.683740677363	-2.401549250393
C	-1.481602534165	2.515373042504	-1.809585471663
C	-1.559876216368	2.802935724287	-0.336428185584
C	-2.778050466892	2.988860628736	0.327751525028
N	-4.008386573138	2.801753962406	-0.299625469614
O	-0.561279921921	3.001043763124	-2.466811345295
N	-2.762984660642	3.313861834682	1.681881231227
C	-1.565268785698	3.533902882814	2.308120586876
C	-0.339868471403	3.363721680170	1.677939829471
C	-0.345124014270	2.988375579175	0.332005419717
C	-5.145292477112	3.717759277306	-0.079019161148
C	-5.760299724850	4.150917013110	-1.408461078607
C	0.942576456722	3.566491494918	2.454642592388
C	1.485039480925	2.291353496037	3.095625935285
O	1.899466946004	1.405263308765	2.043020958573
C	2.388077739836	0.189750381007	2.372228915305
C	2.803668563279	-0.637500774488	1.276293542778
C	3.318579487062	-1.935870461952	1.587945238381
N	3.432566160884	-2.412317261102	2.869244170078
C	3.040827752071	-1.605582580119	3.837977438041
C	2.514227409491	-0.302435739169	3.660854624903
C	2.726480191468	-0.219558942838	-0.078551556028
C	3.141151997425	-1.059824491187	-1.093796041714
C	3.648104155542	-2.348393503496	-0.792375308111
C	3.734673273964	-2.774972723669	0.517895239294
C	-2.227420323990	1.444468868285	-3.841832205952
O	-3.855186428674	3.417142742974	2.348909014153
H	-2.977527323686	-0.907676141186	-2.812833920350
H	-4.931165016458	-2.128182008639	-1.831045052551
H	-6.459879612201	-0.884936136704	-0.271134963997

H	-1.678923162633	3.820128597475	3.352706321695
H	0.583085652025	2.870992881367	-0.224634752393
H	-5.895575874962	3.235183797730	0.562655313560
H	-4.761922333274	4.583907472839	0.471325525741
H	-6.158113511866	3.289071856800	-1.968038612582
H	-6.597186677343	4.843756649071	-1.223084968584
H	-5.019314736210	4.662166656758	-2.043533287083
H	1.717303916256	3.986060994101	1.794522754422
H	0.778975287570	4.292540484103	3.265419137367
H	0.713188616267	1.799798741924	3.711515781586
H	2.350319097588	2.528030287485	3.737092941956
H	3.135942916836	-1.989999165319	4.860061220563
H	2.222906333912	0.275138398188	4.536116610885
H	2.338628771257	0.773829543852	-0.303413003809
H	3.079392711489	-0.731414518420	-2.133365601458
H	3.972355721459	-3.004848077898	-1.602912440129
H	4.123635259365	-3.762497284440	0.773474677235
H	-1.887705103700	2.374032260765	-4.312120857646
H	-1.471218171255	0.666312047162	-4.035196945841
H	-3.187009352303	1.136197307095	-4.273725168981

SCF Done: E(RB3LYP) = -1465.99612517

Zero-point correction= 0.444429
Thermal correction to Energy= 0.472033
Thermal correction to Enthalpy= 0.472977
Thermal correction to Gibbs Free Energy= 0.382916
Sum of electronic and zero-point Energies= -1465.551696
Sum of electronic and thermal Energies= -1465.524092
Sum of electronic and thermal Enthalpies= -1465.523148
Sum of electronic and thermal Free Energies= -1465.613210

1	N	Isotropic =	-42.4246	Anisotropy =	468.6897
2	C	Isotropic =	38.6557	Anisotropy =	115.6460
3	C	Isotropic =	57.5753	Anisotropy =	125.8577
4	C	Isotropic =	62.5992	Anisotropy =	177.2660
5	C	Isotropic =	71.7735	Anisotropy =	160.6493
6	C	Isotropic =	49.2434	Anisotropy =	154.5631
7	N	Isotropic =	118.3416	Anisotropy =	89.9346
8	C	Isotropic =	28.5886	Anisotropy =	110.0055
9	C	Isotropic =	63.3821	Anisotropy =	134.5621
10	C	Isotropic =	41.3077	Anisotropy =	106.2720
11	N	Isotropic =	165.8428	Anisotropy =	59.4454
12	O	Isotropic =	-79.7758	Anisotropy =	588.2922

13	N	Isotropic =	-42.9134	Anisotropy =	256.9593
14	C	Isotropic =	50.0659	Anisotropy =	103.1528
15	C	Isotropic =	57.2981	Anisotropy =	173.4791
16	C	Isotropic =	65.4556	Anisotropy =	156.5890
17	C	Isotropic =	146.6879	Anisotropy =	37.6425
18	C	Isotropic =	175.8118	Anisotropy =	25.3510
19	C	Isotropic =	156.7679	Anisotropy =	16.4867
20	C	Isotropic =	121.4027	Anisotropy =	43.7470
21	O	Isotropic =	202.5612	Anisotropy =	109.8336
22	C	Isotropic =	32.2852	Anisotropy =	137.6107
23	C	Isotropic =	70.5824	Anisotropy =	170.8176
24	C	Isotropic =	43.8635	Anisotropy =	181.8349
25	N	Isotropic =	-37.9541	Anisotropy =	459.3353
26	C	Isotropic =	42.6142	Anisotropy =	159.7653
27	C	Isotropic =	91.1963	Anisotropy =	133.2247
28	C	Isotropic =	70.2066	Anisotropy =	174.0648
29	C	Isotropic =	67.5823	Anisotropy =	170.7178
30	C	Isotropic =	63.5780	Anisotropy =	175.2547
31	C	Isotropic =	63.7920	Anisotropy =	150.2462
32	C	Isotropic =	153.9602	Anisotropy =	46.9489
33	O	Isotropic =	-68.7125	Anisotropy =	371.4416
34	H	Isotropic =	24.0876	Anisotropy =	8.2442
35	H	Isotropic =	24.4026	Anisotropy =	4.6530
36	H	Isotropic =	23.2687	Anisotropy =	4.6098
37	H	Isotropic =	23.2900	Anisotropy =	7.2894
38	H	Isotropic =	23.7337	Anisotropy =	9.3549
39	H	Isotropic =	26.7891	Anisotropy =	8.1515
40	H	Isotropic =	28.0176	Anisotropy =	6.1149
41	H	Isotropic =	30.3276	Anisotropy =	4.9890
42	H	Isotropic =	30.3779	Anisotropy =	11.4588
43	H	Isotropic =	30.4173	Anisotropy =	7.2297
44	H	Isotropic =	28.2432	Anisotropy =	5.4764
45	H	Isotropic =	28.5661	Anisotropy =	8.2514
46	H	Isotropic =	27.4765	Anisotropy =	5.4536
47	H	Isotropic =	27.1684	Anisotropy =	6.5391
48	H	Isotropic =	22.8081	Anisotropy =	7.1926
49	H	Isotropic =	24.9816	Anisotropy =	9.5828
50	H	Isotropic =	23.0927	Anisotropy =	9.0034
51	H	Isotropic =	23.8025	Anisotropy =	6.6305
52	H	Isotropic =	23.6242	Anisotropy =	5.3150
53	H	Isotropic =	23.5608	Anisotropy =	5.6289
54	H	Isotropic =	27.2273	Anisotropy =	7.7469
55	H	Isotropic =	27.9807	Anisotropy =	9.9178
56	H	Isotropic =	28.8758	Anisotropy =	7.5421

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.767859690941	2.004862595312	0.281414700028
C	-3.915057730547	2.218301966310	1.284187922190
C	-3.450404739999	3.504272214403	1.642204654872
C	-3.845723790682	4.577953263729	0.834774269133
C	-4.714602078224	4.351711701456	-0.233667150798
C	-5.173965760359	3.053580506571	-0.449623587436
N	-2.719255016958	3.736828705080	2.838873751549
C	-1.621734999784	3.023578198226	3.266806469383
C	-1.188232786933	1.789937985506	2.524939130598
C	-2.103171230229	0.864434064984	2.005050682603
N	-3.481206543540	1.093659087086	2.030353087930
O	-0.960075612768	3.405460231559	4.231763186070
N	-1.617188914149	-0.286364667560	1.395884158539
C	-0.269091964669	-0.532153729678	1.390969535515
C	0.662412935629	0.360800001411	1.897686566479
C	0.186522338888	1.542314232597	2.474829909148
C	-4.468554103900	0.033527349001	2.328186212585
C	-4.079400155353	-0.772483203180	3.561716439185
C	2.141347774364	0.057353054258	1.803807699240
C	2.832052568093	0.744091620243	0.628444524423
O	2.283098794011	0.199276289907	-0.582604675064
C	2.730966556595	0.666260309807	-1.767922671398
C	2.137414726085	0.082984578338	-2.936432687720
C	2.589183764840	0.552831976241	-4.210493986087
N	3.549588012449	1.521209821071	-4.357835852924
C	4.060652452494	2.021952967574	-3.248410600201
C	3.699640401066	1.642678656475	-1.932068613483
C	1.137859246822	-0.923639725682	-2.873117693080
C	0.601577188967	-1.449380550338	-4.032723444985
C	1.044485097492	-0.988674389766	-5.297649704433
C	2.015344024014	-0.010662574726	-5.383191116130
C	-3.043021409834	4.945614894592	3.611802834971
O	-2.411349908899	-1.131570440985	0.842440357804
H	-3.498746905650	5.587733565952	1.056231585253
H	-5.041757950627	5.173573567611	-0.871784856945
H	-5.893780194034	2.839153354098	-1.245128078665
H	-0.012570423318	-1.480103312341	0.921818668955

H	0.866565465617	2.267504990887	2.921207591150
H	-5.413753230150	0.566312930306	2.510608591441
H	-4.609799693602	-0.632218512062	1.467549957838
H	-4.889589174386	-1.478421563646	3.803673668250
H	-3.169104490410	-1.364136049658	3.382371985892
H	-3.916849565208	-0.121607262408	4.435740135601
H	2.645698885798	0.397395595867	2.721578446496
H	2.304180243521	-1.028110231289	1.725512698185
H	3.917588154908	0.552813136615	0.661405662700
H	2.665790493069	1.834498548514	0.652271675660
H	4.827847010489	2.795141627223	-3.371387239222
H	4.189959236542	2.124094671237	-1.088031142547
H	0.801528192476	-1.273319864903	-1.897110423041
H	-0.167002085102	-2.223040300079	-3.976653465579
H	0.613626000858	-1.411361507886	-6.208007517987
H	2.371552601972	0.359258696750	-6.346555492558
H	-4.102090528615	5.188831558767	3.464849908525
H	-2.849064935943	4.746539153861	4.671719915746
H	-2.423316552248	5.803990216761	3.305373416349

SCF Done: E(RB3LYP) = -1465.99575516

Zero-point correction= 0.444652
Thermal correction to Energy= 0.472139
Thermal correction to Enthalpy= 0.473084
Thermal correction to Gibbs Free Energy= 0.383365
Sum of electronic and zero-point Energies= -1465.551103
Sum of electronic and thermal Energies= -1465.523616
Sum of electronic and thermal Enthalpies= -1465.522672
Sum of electronic and thermal Free Energies= -1465.612390

1	N	Isotropic =	-43.3879	Anisotropy =	460.7069
2	C	Isotropic =	37.0969	Anisotropy =	117.3720
3	C	Isotropic =	59.5177	Anisotropy =	123.8206
4	C	Isotropic =	62.9233	Anisotropy =	176.8544
5	C	Isotropic =	71.6020	Anisotropy =	161.9014
6	C	Isotropic =	49.1985	Anisotropy =	155.4564
7	N	Isotropic =	118.2958	Anisotropy =	88.5146
8	C	Isotropic =	29.0040	Anisotropy =	108.8732
9	C	Isotropic =	61.4427	Anisotropy =	138.3170
10	C	Isotropic =	42.2465	Anisotropy =	109.9240
11	N	Isotropic =	162.9106	Anisotropy =	72.0784
12	O	Isotropic =	-78.2304	Anisotropy =	586.2376
13	N	Isotropic =	-44.5764	Anisotropy =	254.5575

14	C	Isotropic =	48.5382	Anisotropy =	103.0769
15	C	Isotropic =	57.2491	Anisotropy =	174.1392
16	C	Isotropic =	67.1436	Anisotropy =	157.3054
17	C	Isotropic =	144.7260	Anisotropy =	42.9490
18	C	Isotropic =	176.3516	Anisotropy =	24.1974
19	C	Isotropic =	156.5490	Anisotropy =	16.4966
20	C	Isotropic =	121.8617	Anisotropy =	43.3876
21	O	Isotropic =	203.4742	Anisotropy =	111.4488
22	C	Isotropic =	32.4455	Anisotropy =	138.1865
23	C	Isotropic =	70.5707	Anisotropy =	170.7482
24	C	Isotropic =	43.9428	Anisotropy =	181.9445
25	N	Isotropic =	-37.9938	Anisotropy =	458.8486
26	C	Isotropic =	42.5839	Anisotropy =	159.7036
27	C	Isotropic =	91.2321	Anisotropy =	133.2330
28	C	Isotropic =	70.1029	Anisotropy =	174.0780
29	C	Isotropic =	67.5803	Anisotropy =	170.7006
30	C	Isotropic =	63.6409	Anisotropy =	175.2110
31	C	Isotropic =	63.7901	Anisotropy =	150.2703
32	C	Isotropic =	154.0997	Anisotropy =	47.2548
33	O	Isotropic =	-61.5632	Anisotropy =	360.1431
34	H	Isotropic =	24.0930	Anisotropy =	8.3545
35	H	Isotropic =	24.3801	Anisotropy =	4.2628
36	H	Isotropic =	23.3023	Anisotropy =	4.5759
37	H	Isotropic =	23.0143	Anisotropy =	7.2111
38	H	Isotropic =	24.0707	Anisotropy =	9.3023
39	H	Isotropic =	28.1805	Anisotropy =	6.5922
40	H	Isotropic =	26.3160	Anisotropy =	7.6509
41	H	Isotropic =	30.1883	Anisotropy =	11.4224
42	H	Isotropic =	30.3352	Anisotropy =	4.9918
43	H	Isotropic =	30.3654	Anisotropy =	7.6096
44	H	Isotropic =	28.4646	Anisotropy =	8.0185
45	H	Isotropic =	28.3581	Anisotropy =	5.7232
46	H	Isotropic =	27.1472	Anisotropy =	6.1815
47	H	Isotropic =	27.4372	Anisotropy =	5.4715
48	H	Isotropic =	22.8168	Anisotropy =	7.2420
49	H	Isotropic =	24.9918	Anisotropy =	9.4550
50	H	Isotropic =	23.1116	Anisotropy =	9.5016
51	H	Isotropic =	23.8212	Anisotropy =	6.7041
52	H	Isotropic =	23.6490	Anisotropy =	5.1989
53	H	Isotropic =	23.5757	Anisotropy =	5.6805
54	H	Isotropic =	28.8817	Anisotropy =	7.8095
55	H	Isotropic =	27.2658	Anisotropy =	8.1656
56	H	Isotropic =	28.0421	Anisotropy =	10.1610

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.260786096947	-4.022241884583	-0.522881980483
C	-1.458081823068	-2.716433353857	-0.708800211448
C	-2.698634995472	-2.174244558306	-1.115073675048
C	-3.778921458545	-3.057368576310	-1.231768180492
C	-3.580767629086	-4.420501503459	-1.007598270015
C	-2.296471557864	-4.858187234981	-0.688536501974
N	-2.835280311167	-0.817505483375	-1.519304221652
C	-2.380671909835	0.278177934723	-0.823276895162
C	-1.530314387938	0.094158697372	0.401411369029
C	-0.532049456489	-0.885088420055	0.488362433972
N	-0.354531427254	-1.850079169291	-0.505977173568
O	-2.691381704566	1.419098136057	-1.171290494672
N	0.260327866493	-0.932311397416	1.630375315088
C	0.123844859393	0.036438323197	2.590554515935
C	-0.848064052209	1.023835185613	2.529811886229
C	-1.695518223447	1.036726340056	1.419191609070
C	0.979051342811	-2.306019487422	-0.955091015332
C	1.916731474140	-1.135388952471	-1.225743554727
C	-0.945728796788	2.079678950292	3.607747652854
C	-0.081190995336	3.309272574472	3.331073797772
O	-0.475215477550	3.850182494624	2.059866586623
C	0.111774818751	4.983884360647	1.619084293469
C	-0.248475783106	5.403821508888	0.295011051370
C	0.324657415736	6.624042673548	-0.186882484926
N	1.200315012087	7.385408478976	0.545204367577
C	1.513583675093	6.937432087837	1.746810569369
C	1.011565123221	5.752618665476	2.338966404128
C	-1.125170644882	4.661544737455	-0.540956576993
C	-1.435411221851	5.120369416450	-1.806809669515
C	-0.885671698007	6.336118969634	-2.283822053290
C	-0.023988910211	7.068739163123	-1.491911605656
C	-3.678436414388	-0.536157476192	-2.691356031570
O	1.129168446484	-1.864797370989	1.796997568061
H	-4.761714402097	-2.685317754102	-1.522950863285
H	-4.405573098758	-5.128140427722	-1.100026108055
H	-2.085043668580	-5.923034191673	-0.553124319605
H	0.825394995052	-0.081651402920	3.415000186392
H	-2.470861211649	1.793873182004	1.316509658472

H	1.429628986619	-2.993930462466	-0.228680924580
H	0.792895992768	-2.861230393889	-1.886461927722
H	1.477676698545	-0.421925016692	-1.941396956194
H	2.168098719243	-0.601343716379	-0.297103809217
H	2.857897991582	-1.516533526013	-1.652638512252
H	-1.993837878707	2.398706972063	3.712900207312
H	-0.629616072220	1.670857965820	4.579546649136
H	0.989970841359	3.045999837156	3.297302716659
H	-0.235423937294	4.059420666425	4.123989969791
H	2.219107784119	7.545547421088	2.324751424074
H	1.335819984680	5.482281154773	3.342256492519
H	-1.539269770433	3.717653558242	-0.187454748115
H	-2.104721061022	4.538994337120	-2.444400025961
H	-1.141335170875	6.689988825995	-3.285145594101
H	0.418449441958	8.003776638890	-1.840857110247
H	-3.638420537922	-1.394464265346	-3.372557473855
H	-4.724831393860	-0.343897052389	-2.403938262565
H	-3.292478290711	0.357683820279	-3.194069492624

SCF Done: E(RB3LYP) = -1465.99678131

Zero-point correction= 0.444894
Thermal correction to Energy= 0.472258
Thermal correction to Enthalpy= 0.473202
Thermal correction to Gibbs Free Energy= 0.385559
Sum of electronic and zero-point Energies= -1465.551887
Sum of electronic and thermal Energies= -1465.524524
Sum of electronic and thermal Enthalpies= -1465.523579
Sum of electronic and thermal Free Energies= -1465.611222

1	N	Isotropic =	-43.5460	Anisotropy =	459.4138
2	C	Isotropic =	36.7656	Anisotropy =	116.3798
3	C	Isotropic =	59.2160	Anisotropy =	122.8140
4	C	Isotropic =	62.6552	Anisotropy =	176.6283
5	C	Isotropic =	71.5101	Anisotropy =	161.2784
6	C	Isotropic =	48.9380	Anisotropy =	154.7239
7	N	Isotropic =	117.5232	Anisotropy =	88.2907
8	C	Isotropic =	27.8421	Anisotropy =	108.1614
9	C	Isotropic =	62.3697	Anisotropy =	137.8721
10	C	Isotropic =	41.9424	Anisotropy =	110.5834
11	N	Isotropic =	161.9456	Anisotropy =	70.6279
12	O	Isotropic =	-76.2615	Anisotropy =	574.6513
13	N	Isotropic =	-45.3243	Anisotropy =	254.5299
14	C	Isotropic =	50.2024	Anisotropy =	104.6085

15	C	Isotropic =	57.8099	Anisotropy =	173.9981
16	C	Isotropic =	63.4312	Anisotropy =	157.1221
17	C	Isotropic =	144.7667	Anisotropy =	42.4502
18	C	Isotropic =	176.5861	Anisotropy =	23.3807
19	C	Isotropic =	156.8689	Anisotropy =	18.4866
20	C	Isotropic =	122.6196	Anisotropy =	43.7715
21	O	Isotropic =	203.8130	Anisotropy =	117.8072
22	C	Isotropic =	32.0736	Anisotropy =	136.8721
23	C	Isotropic =	70.4440	Anisotropy =	169.8050
24	C	Isotropic =	43.6895	Anisotropy =	181.7420
25	N	Isotropic =	-38.9524	Anisotropy =	456.7592
26	C	Isotropic =	42.5738	Anisotropy =	158.6050
27	C	Isotropic =	91.1968	Anisotropy =	133.1119
28	C	Isotropic =	68.8395	Anisotropy =	175.9868
29	C	Isotropic =	67.3908	Anisotropy =	170.3110
30	C	Isotropic =	63.4239	Anisotropy =	174.7330
31	C	Isotropic =	63.8479	Anisotropy =	149.3744
32	C	Isotropic =	153.9690	Anisotropy =	46.9354
33	O	Isotropic =	-62.3908	Anisotropy =	360.5751
34	H	Isotropic =	23.9389	Anisotropy =	9.0767
35	H	Isotropic =	24.2369	Anisotropy =	4.6508
36	H	Isotropic =	23.1789	Anisotropy =	4.8107
37	H	Isotropic =	23.2837	Anisotropy =	7.1606
38	H	Isotropic =	23.6051	Anisotropy =	9.2594
39	H	Isotropic =	26.3631	Anisotropy =	8.2131
40	H	Isotropic =	28.1718	Anisotropy =	6.4439
41	H	Isotropic =	30.5027	Anisotropy =	7.0945
42	H	Isotropic =	30.5047	Anisotropy =	5.3482
43	H	Isotropic =	30.3047	Anisotropy =	11.1810
44	H	Isotropic =	28.2515	Anisotropy =	5.5727
45	H	Isotropic =	28.5588	Anisotropy =	8.5287
46	H	Isotropic =	27.5302	Anisotropy =	6.3267
47	H	Isotropic =	26.9933	Anisotropy =	6.4714
48	H	Isotropic =	22.7721	Anisotropy =	7.1071
49	H	Isotropic =	24.9192	Anisotropy =	9.6010
50	H	Isotropic =	22.6486	Anisotropy =	8.8510
51	H	Isotropic =	23.6574	Anisotropy =	7.4120
52	H	Isotropic =	23.5806	Anisotropy =	5.6283
53	H	Isotropic =	23.5279	Anisotropy =	5.7587
54	H	Isotropic =	28.7621	Anisotropy =	7.5665
55	H	Isotropic =	27.8830	Anisotropy =	9.9462
56	H	Isotropic =	27.1312	Anisotropy =	7.7515

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-6.033693100250	0.814475157043	-0.507749342248
C	-4.730801875720	0.611631903003	-0.707729191933
C	-4.201726933011	-0.621311920757	-1.152383029471
C	-5.094856689026	-1.690297508119	-1.294680823602
C	-6.454846925573	-1.487116932097	-1.056423499227
C	-6.879498067129	-0.208958576016	-0.697583443742
N	-2.848506179925	-0.757657001643	-1.567999382277
C	-1.745447712136	-0.332981249622	-0.864711071216
C	-1.915624073328	0.484609080007	0.384021891115
C	-2.884663597492	1.489680483184	0.503224057542
N	-3.853967659665	1.702039559829	-0.479891147333
O	-0.609125460720	-0.644195701354	-1.226855598866
N	-2.917366900847	2.252058881128	1.666014550335
C	-1.945292579433	2.079685692938	2.617093559989
C	-0.968748578954	1.099242079572	2.525427804615
C	-0.969848945401	0.282409653642	1.392052148652
C	-4.301149559221	3.050720030329	-0.891245946646
C	-3.124261805449	3.985746562799	-1.143406959192
C	0.089796243600	0.960192585233	3.596078738844
C	1.330386168581	1.814254106260	3.336573368689
O	1.864309403079	1.442084614734	2.055830540553
C	3.004006369430	2.025690763524	1.626116743896
C	3.419871492089	1.687367670353	0.294978275072
C	4.645708313585	2.257431884174	-0.176170250933
N	5.416225305497	3.110632985820	0.572647572040
C	4.971959598473	3.404551189232	1.780486260661
C	3.782336550468	2.902971830403	2.363292029965
C	2.668618839936	0.834788252203	-0.557743876502
C	3.124170911470	0.544593325490	-1.829527372480
C	4.345291582841	1.091246351555	-2.296212789920
C	5.086572702476	1.930062831773	-1.487982249507
C	-2.580495087030	-1.569806828101	-2.764746209381
O	-3.839484269865	3.126113291610	1.860818016012
H	-4.733165267940	-2.667481182105	-1.616230266997
H	-7.170145570657	-2.302881982545	-1.168149998664
H	-7.941622570776	0.007370593842	-0.549143866837
H	-2.052013608425	2.759885365767	3.460746270807
H	-0.221744261018	-0.497996212663	1.264299400414
H	-4.862652316421	2.893694677625	-1.824227573188

H	-4.981810034335	3.487454302879	-0.149698593581
H	-2.419075995152	3.560778166091	-1.875584031989
H	-3.500006974485	4.941554249169	-1.541604347683
H	-2.582286231196	4.206671707889	-0.211641820800
H	-0.311137964979	1.257711546180	4.576997164964
H	0.394614425395	-0.094501146069	3.674079453523
H	2.079809573923	1.632157079115	4.124271742191
H	1.081323236946	2.889280629925	3.327715921696
H	5.587494149085	4.092209460519	2.371949950658
H	3.515807248969	3.209994009520	3.372991102961
H	1.720239727644	0.424121660315	-0.212338920217
H	2.536013925683	-0.106198685201	-2.479944234766
H	4.696376939697	0.851553065249	-3.302451850423
H	6.025918181176	2.369938894103	-1.828505601497
H	-1.684151048190	-1.179264961266	-3.259372130891
H	-2.398712207470	-2.626095079882	-2.508331860309
H	-3.440690838825	-1.500941206584	-3.441279282880

SCF Done: E(RB3LYP) = -1465.99678063

Zero-point correction= 0.444874
Thermal correction to Energy= 0.472248
Thermal correction to Enthalpy= 0.473192
Thermal correction to Gibbs Free Energy= 0.385509
Sum of electronic and zero-point Energies= -1465.551907
Sum of electronic and thermal Energies= -1465.524533
Sum of electronic and thermal Enthalpies= -1465.523589
Sum of electronic and thermal Free Energies= -1465.611271

1	N	Isotropic =	-43.6868	Anisotropy =	459.2750
2	C	Isotropic =	36.6964	Anisotropy =	116.2257
3	C	Isotropic =	59.1421	Anisotropy =	122.6884
4	C	Isotropic =	62.6277	Anisotropy =	176.3269
5	C	Isotropic =	71.5213	Anisotropy =	161.3874
6	C	Isotropic =	48.8885	Anisotropy =	154.6139
7	N	Isotropic =	117.7717	Anisotropy =	88.3368
8	C	Isotropic =	27.7584	Anisotropy =	108.0107
9	C	Isotropic =	62.4366	Anisotropy =	137.9648
10	C	Isotropic =	41.9360	Anisotropy =	110.6959
11	N	Isotropic =	161.9791	Anisotropy =	70.6010
12	O	Isotropic =	-76.3526	Anisotropy =	574.9326
13	N	Isotropic =	-45.3304	Anisotropy =	254.4565
14	C	Isotropic =	50.2245	Anisotropy =	104.6244
15	C	Isotropic =	57.8488	Anisotropy =	173.8915

16	C	Isotropic =	63.3824	Anisotropy =	157.0389
17	C	Isotropic =	144.6806	Anisotropy =	42.4915
18	C	Isotropic =	176.6300	Anisotropy =	23.3955
19	C	Isotropic =	156.8948	Anisotropy =	18.4011
20	C	Isotropic =	122.5560	Anisotropy =	43.7614
21	O	Isotropic =	203.7556	Anisotropy =	117.2656
22	C	Isotropic =	32.1497	Anisotropy =	136.9125
23	C	Isotropic =	70.4286	Anisotropy =	169.8177
24	C	Isotropic =	43.7396	Anisotropy =	181.6291
25	N	Isotropic =	-38.7689	Anisotropy =	457.2526
26	C	Isotropic =	42.5499	Anisotropy =	158.7253
27	C	Isotropic =	91.1828	Anisotropy =	133.2289
28	C	Isotropic =	68.8085	Anisotropy =	175.9445
29	C	Isotropic =	67.4284	Anisotropy =	170.2928
30	C	Isotropic =	63.5357	Anisotropy =	174.5872
31	C	Isotropic =	63.8748	Anisotropy =	149.4205
32	C	Isotropic =	154.0492	Anisotropy =	46.9659
33	O	Isotropic =	-62.2743	Anisotropy =	360.4932
34	H	Isotropic =	23.9338	Anisotropy =	9.0668
35	H	Isotropic =	24.2339	Anisotropy =	4.6584
36	H	Isotropic =	23.1809	Anisotropy =	4.8098
37	H	Isotropic =	23.2850	Anisotropy =	7.1590
38	H	Isotropic =	23.6046	Anisotropy =	9.2538
39	H	Isotropic =	28.1729	Anisotropy =	6.4355
40	H	Isotropic =	26.3577	Anisotropy =	8.2216
41	H	Isotropic =	30.5008	Anisotropy =	7.0896
42	H	Isotropic =	30.2996	Anisotropy =	11.1891
43	H	Isotropic =	30.4983	Anisotropy =	5.3520
44	H	Isotropic =	28.5661	Anisotropy =	8.5220
45	H	Isotropic =	28.2574	Anisotropy =	5.5675
46	H	Isotropic =	26.9996	Anisotropy =	6.4612
47	H	Isotropic =	27.5357	Anisotropy =	6.3080
48	H	Isotropic =	22.7675	Anisotropy =	7.1076
49	H	Isotropic =	24.9189	Anisotropy =	9.5931
50	H	Isotropic =	22.6430	Anisotropy =	8.8766
51	H	Isotropic =	23.6532	Anisotropy =	7.3866
52	H	Isotropic =	23.5841	Anisotropy =	5.6185
53	H	Isotropic =	23.5280	Anisotropy =	5.7628
54	H	Isotropic =	27.1293	Anisotropy =	7.7506
55	H	Isotropic =	27.8773	Anisotropy =	9.9622
56	H	Isotropic =	28.7717	Anisotropy =	7.5574

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.950059809157	-3.346236017712	-0.507776934790
C	-1.157434170297	-2.185859394387	-1.131124460136
C	-2.363625476140	-1.456671107163	-1.024001512247
C	-3.334857333563	-1.948032379762	-0.142996816221
C	-3.106548278968	-3.146986654765	0.533975007581
C	-1.913615284141	-3.826141528693	0.292550122076
N	-2.651212959084	-0.344575593992	-1.861666936208
C	-1.815493161218	0.722516270000	-2.104716425863
C	-0.408786741726	0.714194092886	-1.574580840012
C	0.387062937086	-0.438613951252	-1.572136661747
N	-0.117098872202	-1.684979890519	-1.953330553057
O	-2.218587693428	1.710454502951	-2.718293807023
N	1.699276218059	-0.344288187443	-1.123049834932
C	2.210714083260	0.880484034528	-0.781996598209
C	1.451689494581	2.041845225334	-0.777363884499
C	0.116203346133	1.948078294762	-1.179432370087
C	0.656678767792	-2.652134980367	-2.761498273937
C	1.304393353979	-1.989404616902	-3.971556215189
C	2.070986934828	3.349286873310	-0.334876295242
C	1.907558919649	3.642342741398	1.154463208681
O	0.509696522685	3.847181813937	1.416568235706
C	0.119957691624	4.132093396613	2.678110714989
C	-1.285417632984	4.350465875977	2.866113923722
C	-1.734629373120	4.654276728293	4.190484821532
N	-0.891356199973	4.744337410263	5.268636773246
C	0.391389920307	4.535957514198	5.036261666667
C	0.959648106414	4.228561554896	3.775482753914
C	-2.225890355360	4.279556927184	1.804700584645
C	-3.568336859926	4.500816272848	2.044541152748
C	-4.020057636271	4.800749892281	3.353886733727
C	-3.123453228023	4.875632295236	4.401166461062
C	-4.018479700919	-0.225194409298	-2.390874120392
O	2.447693745252	-1.384962759107	-1.033653567142
H	-4.274573525037	-1.411436000770	-0.008665387555
H	-3.851828303245	-3.552694387900	1.219266549295
H	-1.714510398805	-4.793516190023	0.763202681227
H	3.258055687448	0.834256723372	-0.487194488101
H	-0.520848442026	2.829563702771	-1.229652417358
H	1.415874469891	-3.160683012923	-2.154222093535
H	-0.078372238470	-3.400994124121	-3.092494054060

H	1.781785989727	-2.761746685427	-4.595139354179
H	0.561600470917	-1.458827596583	-4.588545373692
H	2.088683397791	-1.279919814166	-3.667493193944
H	3.150857291885	3.342854868877	-0.547306349330
H	1.632208312795	4.181283419877	-0.906944855868
H	2.468951735446	4.552585843580	1.423329695656
H	2.280603437591	2.803927007445	1.766747835444
H	1.061112730319	4.609996739194	5.900806048300
H	2.034819194683	4.076525941459	3.701377626198
H	-1.871533227631	4.049595643647	0.800096017902
H	-4.285850312499	4.445008187005	1.223309991138
H	-5.083636941524	4.973924693256	3.532390478639
H	-3.448788892904	5.106188440327	5.417445453023
H	-4.662125431470	0.373693482510	-1.726226679070
H	-3.975372156702	0.274999566798	-3.364886014390
H	-4.444972123330	-1.228866693737	-2.504828169105

SCF Done: E(RB3LYP) = -1465.99563954

Zero-point correction= 0.444679
Thermal correction to Energy= 0.472150
Thermal correction to Enthalpy= 0.473094
Thermal correction to Gibbs Free Energy= 0.383979
Sum of electronic and zero-point Energies= -1465.550961
Sum of electronic and thermal Energies= -1465.523490
Sum of electronic and thermal Enthalpies= -1465.522545
Sum of electronic and thermal Free Energies= -1465.611660

1	N	Isotropic =	-43.0780	Anisotropy =	459.7297
2	C	Isotropic =	37.0793	Anisotropy =	117.3566
3	C	Isotropic =	59.4612	Anisotropy =	124.1921
4	C	Isotropic =	62.9949	Anisotropy =	176.9005
5	C	Isotropic =	71.6955	Anisotropy =	161.5243
6	C	Isotropic =	49.2699	Anisotropy =	154.6230
7	N	Isotropic =	117.7209	Anisotropy =	89.0941
8	C	Isotropic =	28.6325	Anisotropy =	109.6310
9	C	Isotropic =	61.9293	Anisotropy =	136.8761
10	C	Isotropic =	42.1637	Anisotropy =	109.9469
11	N	Isotropic =	162.8941	Anisotropy =	72.0648
12	O	Isotropic =	-79.2997	Anisotropy =	586.6362
13	N	Isotropic =	-45.6018	Anisotropy =	255.5634
14	C	Isotropic =	49.8823	Anisotropy =	102.7782
15	C	Isotropic =	56.9540	Anisotropy =	174.4099
16	C	Isotropic =	64.8651	Anisotropy =	156.6953

17	C	Isotropic =	144.7426	Anisotropy =	43.2578
18	C	Isotropic =	176.5700	Anisotropy =	23.9089
19	C	Isotropic =	156.7190	Anisotropy =	16.5182
20	C	Isotropic =	121.4361	Anisotropy =	43.7780
21	O	Isotropic =	203.1915	Anisotropy =	111.5339
22	C	Isotropic =	32.2628	Anisotropy =	137.6088
23	C	Isotropic =	70.5914	Anisotropy =	170.7643
24	C	Isotropic =	43.9189	Anisotropy =	181.8671
25	N	Isotropic =	-38.2536	Anisotropy =	458.8757
26	C	Isotropic =	42.6218	Anisotropy =	159.6546
27	C	Isotropic =	91.2280	Anisotropy =	133.2121
28	C	Isotropic =	70.0586	Anisotropy =	173.9553
29	C	Isotropic =	67.6699	Anisotropy =	170.5535
30	C	Isotropic =	63.6517	Anisotropy =	174.8213
31	C	Isotropic =	63.8265	Anisotropy =	150.2105
32	C	Isotropic =	153.9623	Anisotropy =	47.0872
33	O	Isotropic =	-63.2667	Anisotropy =	362.9115
34	H	Isotropic =	24.1062	Anisotropy =	8.2631
35	H	Isotropic =	24.3910	Anisotropy =	4.7112
36	H	Isotropic =	23.2959	Anisotropy =	4.7299
37	H	Isotropic =	23.3041	Anisotropy =	7.3036
38	H	Isotropic =	23.7034	Anisotropy =	9.3687
39	H	Isotropic =	26.3683	Anisotropy =	7.9080
40	H	Isotropic =	28.1797	Anisotropy =	6.6507
41	H	Isotropic =	30.1909	Anisotropy =	11.5310
42	H	Isotropic =	30.3684	Anisotropy =	7.3127
43	H	Isotropic =	30.3818	Anisotropy =	5.2981
44	H	Isotropic =	28.5530	Anisotropy =	8.1770
45	H	Isotropic =	28.2593	Anisotropy =	5.3728
46	H	Isotropic =	27.1710	Anisotropy =	6.4214
47	H	Isotropic =	27.4575	Anisotropy =	5.5736
48	H	Isotropic =	22.8018	Anisotropy =	7.2011
49	H	Isotropic =	24.9819	Anisotropy =	9.6010
50	H	Isotropic =	23.1113	Anisotropy =	8.9990
51	H	Isotropic =	23.8148	Anisotropy =	6.7089
52	H	Isotropic =	23.6354	Anisotropy =	5.3541
53	H	Isotropic =	23.5575	Anisotropy =	5.6486
54	H	Isotropic =	27.9648	Anisotropy =	9.9211
55	H	Isotropic =	27.2209	Anisotropy =	7.8459
56	H	Isotropic =	28.8573	Anisotropy =	7.7319

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.505164138735	4.243078241461	4.015796105174
C	-2.304767202562	4.203098997569	2.698059280938
C	-3.083866957990	4.938937236421	1.776218334635
C	-4.168191125168	5.663529496500	2.286185352641
C	-4.397722576659	5.681415463642	3.662645193928
C	-3.518988881709	4.983046166862	4.488916534446
N	-2.722549681995	5.056851429449	0.406459362015
C	-2.383662442310	4.018787739848	-0.432235079495
C	-2.227529683599	2.627303434053	0.114680949322
C	-1.624850438026	2.368496433716	1.352646223226
N	-1.242030757340	3.397071848760	2.217842333570
O	-2.244855213950	4.205804862531	-1.640792727657
N	-1.464946966629	1.047352531777	1.755003546087
C	-1.815829806728	0.032854726875	0.903339382038
C	-2.411074195141	0.254363854349	-0.329197208670
C	-2.620166838226	1.579495737159	-0.723350889950
C	0.013077087944	3.363760476117	2.999971477719
C	1.207753856031	2.972067726565	2.138231680460
C	-2.785009963711	-0.911657442117	-1.217724324351
C	-1.740101312283	-1.223170372000	-2.285972998325
O	-0.548092108361	-1.666154466545	-1.617262991644
C	0.536256817602	-1.979970496493	-2.358402859697
C	1.689717143847	-2.418881379656	-1.626908864177
C	2.858219167374	-2.759383203199	-2.379665816691
N	2.919616383665	-2.685097798495	-3.748037670973
C	1.828210768832	-2.276702837440	-4.368402225385
C	0.612208833736	-1.911920553638	-3.739798882445
C	1.710236565407	-2.525920059241	-0.211140161487
C	2.850364659547	-2.955225490222	0.440475362983
C	4.011236679176	-3.293271135899	-0.298812072566
C	4.013879635288	-3.197309988499	-1.676175646205
C	-2.883143822598	6.372645931071	-0.230938658093
O	-0.987042855906	0.758894121602	2.912390889798
H	-4.811903927529	6.232127331748	1.614362146182
H	-5.231825693598	6.244636814972	4.083008512742
H	-3.631816930215	5.010080926787	5.576790516989
H	-1.619685552893	-0.954536340642	1.317041855674
H	-3.065220453568	1.819125034442	-1.688728785502
H	0.142201866103	4.389442717078	3.376580758509
H	-0.072552147661	2.689334558905	3.861117290151
H	1.303658986824	3.627164419047	1.257565937483

H	2.129286572882	3.060530476301	2.735117103794
H	1.133218255868	1.927531384665	1.799957413380
H	-2.953246129824	-1.815215763626	-0.612464972552
H	-3.728253520722	-0.688676554036	-1.739703901172
H	-1.514859321663	-0.329399274182	-2.892126227841
H	-2.105712083255	-2.019837602992	-2.955170938297
H	1.881915965388	-2.220195173773	-5.461758002228
H	-0.226603133206	-1.590216157120	-4.354198834230
H	0.813579993642	-2.265522773173	0.351141506891
H	2.859231333847	-3.035259042603	1.529466745296
H	4.907103208984	-3.631573243848	0.226574196721
H	4.896354244346	-3.453105093065	-2.265793685274
H	-2.748655495499	7.154028089606	0.526456328755
H	-2.124428343012	6.477738973096	-1.014546476749
H	-3.875468324060	6.481085059531	-0.698151419891

SCF Done: E(RB3LYP) = -1465.99571793

Zero-point correction= 0.444556
Thermal correction to Energy= 0.472061
Thermal correction to Enthalpy= 0.473005
Thermal correction to Gibbs Free Energy= 0.383457
Sum of electronic and zero-point Energies= -1465.551161
Sum of electronic and thermal Energies= -1465.523657
Sum of electronic and thermal Enthalpies= -1465.522713
Sum of electronic and thermal Free Energies= -1465.612261

1	N	Isotropic =	-43.3611	Anisotropy =	459.2282
2	C	Isotropic =	37.0563	Anisotropy =	116.5723
3	C	Isotropic =	59.2143	Anisotropy =	122.8753
4	C	Isotropic =	62.7909	Anisotropy =	176.1056
5	C	Isotropic =	71.4605	Anisotropy =	160.6451
6	C	Isotropic =	49.1333	Anisotropy =	154.4953
7	N	Isotropic =	118.0579	Anisotropy =	88.3894
8	C	Isotropic =	28.9274	Anisotropy =	107.9456
9	C	Isotropic =	61.6120	Anisotropy =	139.0663
10	C	Isotropic =	42.0879	Anisotropy =	110.4480
11	N	Isotropic =	162.7275	Anisotropy =	72.3703
12	O	Isotropic =	-79.6094	Anisotropy =	585.3873
13	N	Isotropic =	-45.2976	Anisotropy =	254.7592
14	C	Isotropic =	48.5679	Anisotropy =	104.2100
15	C	Isotropic =	57.0833	Anisotropy =	174.2699
16	C	Isotropic =	66.9448	Anisotropy =	156.4612
17	C	Isotropic =	144.5803	Anisotropy =	42.4906

18	C	Isotropic =	176.6061	Anisotropy =	23.6795
19	C	Isotropic =	156.3653	Anisotropy =	16.8445
20	C	Isotropic =	121.9356	Anisotropy =	43.5478
21	O	Isotropic =	203.2432	Anisotropy =	110.7255
22	C	Isotropic =	32.2435	Anisotropy =	137.8753
23	C	Isotropic =	70.4907	Anisotropy =	170.5700
24	C	Isotropic =	43.9425	Anisotropy =	181.7883
25	N	Isotropic =	-38.0221	Anisotropy =	458.7456
26	C	Isotropic =	42.5700	Anisotropy =	159.7689
27	C	Isotropic =	91.1733	Anisotropy =	133.0766
28	C	Isotropic =	70.2288	Anisotropy =	174.0214
29	C	Isotropic =	67.6074	Anisotropy =	170.4612
30	C	Isotropic =	63.6070	Anisotropy =	174.7375
31	C	Isotropic =	63.8393	Anisotropy =	150.1489
32	C	Isotropic =	153.9853	Anisotropy =	47.2998
33	O	Isotropic =	-62.4408	Anisotropy =	360.8122
34	H	Isotropic =	23.9937	Anisotropy =	8.8680
35	H	Isotropic =	24.2648	Anisotropy =	4.5622
36	H	Isotropic =	23.1948	Anisotropy =	4.9906
37	H	Isotropic =	23.0150	Anisotropy =	7.2721
38	H	Isotropic =	24.0645	Anisotropy =	9.1491
39	H	Isotropic =	28.1877	Anisotropy =	6.3825
40	H	Isotropic =	26.3224	Anisotropy =	7.5852
41	H	Isotropic =	30.5376	Anisotropy =	6.5815
42	H	Isotropic =	30.3237	Anisotropy =	10.8319
43	H	Isotropic =	30.5210	Anisotropy =	7.5305
44	H	Isotropic =	28.3930	Anisotropy =	5.8530
45	H	Isotropic =	28.4618	Anisotropy =	7.7957
46	H	Isotropic =	27.3213	Anisotropy =	5.7108
47	H	Isotropic =	27.1253	Anisotropy =	6.1747
48	H	Isotropic =	22.7442	Anisotropy =	7.2317
49	H	Isotropic =	24.9079	Anisotropy =	9.4129
50	H	Isotropic =	23.0238	Anisotropy =	9.5845
51	H	Isotropic =	23.7786	Anisotropy =	6.6205
52	H	Isotropic =	23.6175	Anisotropy =	5.2232
53	H	Isotropic =	23.5275	Anisotropy =	5.7944
54	H	Isotropic =	28.8552	Anisotropy =	7.6311
55	H	Isotropic =	27.3169	Anisotropy =	7.7694
56	H	Isotropic =	28.0060	Anisotropy =	10.3290

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.112650904031	-0.957013610799	-1.624584528933
C	-3.985793112144	-0.364018198261	-2.020498814036
C	-3.883471480897	0.379412091370	-3.218539336084
C	-5.056106779470	0.564569592473	-3.961248780832
C	-6.243379451508	-0.030632765964	-3.532169010380
C	-6.213653726789	-0.809032788593	-2.376383858462
N	-2.631668341565	0.817904616523	-3.730354266477
C	-1.656732744664	1.485661242530	-3.022657571464
C	-1.798153432643	1.675503211985	-1.538162677692
C	-2.315618278894	0.681098620989	-0.698198945623
N	-2.839023611825	-0.513037267339	-1.201197137164
O	-0.681538483745	1.968592402281	-3.597683534145
N	-2.367601447343	0.921383151932	0.670035489793
C	-1.824738311218	2.073052235439	1.176055883587
C	-1.293304904020	3.071977750604	0.374268763890
C	-1.288674458537	2.864936286249	-1.008553432491
C	-2.609835578928	-1.823293048845	-0.554754395724
C	-1.142630746445	-2.029265548880	-0.197218329084
C	-0.710244421402	4.321264067718	0.996851939472
C	0.800382138609	4.247829084662	1.206376602540
O	1.058631845900	3.225350534562	2.182246156996
C	2.338259841881	2.947014891057	2.512738798956
C	2.522137998930	1.913039010709	3.490163043359
C	3.865156930643	1.587682070310	3.862247161468
N	4.964848996308	2.214616253331	3.333699974397
C	4.735559052650	3.160077305411	2.441306616219
C	3.457764374292	3.572853895601	1.989689253083
C	1.439345077175	1.216142499308	4.088583048902
C	1.676144750163	0.227400783909	5.023997624726
C	3.003695092966	-0.100886681063	5.395773663941
C	4.071960567855	0.564449866694	4.827911214213
C	-2.413784036386	0.711706285812	-5.181165995502
O	-2.910007163237	0.076675090351	1.471978036737
H	-5.035774053057	1.147275218794	-4.882747384371
H	-7.167336574744	0.093889333692	-4.098256229643
H	-7.109525068493	-1.333528033286	-2.031025075478
H	-1.898591976123	2.135360737678	2.260101833412
H	-0.871820784884	3.606123985401	-1.689947131904
H	-3.238589492956	-1.943213219004	0.336455353099
H	-2.922959593533	-2.569060840239	-1.300756540728
H	-0.822691244903	-1.337217720289	0.596352900483
H	-1.002440303524	-3.053820422251	0.182081664853

H	-0.489428472945	-1.894056275360	-1.074152283885
H	-0.907441214474	5.184742352871	0.343291529689
H	-1.191794893427	4.527915572276	1.964638603606
H	1.180697830946	5.214929011705	1.575350055281
H	1.319116195677	4.000495507179	0.264724967613
H	5.617379798410	3.658821580906	2.022823946017
H	3.388407815958	4.366351790072	1.248002274356
H	0.421007574878	1.474648831938	3.798904628431
H	0.838502198730	-0.304369352366	5.480012052019
H	3.179693151673	-0.884403288816	6.136173180365
H	5.102561102830	0.328758536632	5.100176535545
H	-2.990352952842	-0.137747613517	-5.566157277721
H	-2.718035829383	1.630786244823	-5.707871692447
H	-1.345398465492	0.551695129100	-5.364758566776

SCF Done: E(RB3LYP) = -1465.99569586

Zero-point correction= 0.444670
Thermal correction to Energy= 0.472147
Thermal correction to Enthalpy= 0.473091
Thermal correction to Gibbs Free Energy= 0.383645
Sum of electronic and zero-point Energies= -1465.551026
Sum of electronic and thermal Energies= -1465.523549
Sum of electronic and thermal Enthalpies= -1465.522605
Sum of electronic and thermal Free Energies= -1465.612051

1	N	Isotropic =	-43.2124	Anisotropy =	459.6627
2	C	Isotropic =	37.1632	Anisotropy =	116.4442
3	C	Isotropic =	59.1035	Anisotropy =	122.6303
4	C	Isotropic =	62.7494	Anisotropy =	176.3033
5	C	Isotropic =	71.4623	Anisotropy =	160.8161
6	C	Isotropic =	49.1388	Anisotropy =	154.6299
7	N	Isotropic =	117.9597	Anisotropy =	88.4553
8	C	Isotropic =	29.0501	Anisotropy =	107.9600
9	C	Isotropic =	61.5227	Anisotropy =	138.9401
10	C	Isotropic =	41.9443	Anisotropy =	110.5744
11	N	Isotropic =	163.2463	Anisotropy =	72.2891
12	O	Isotropic =	-79.0872	Anisotropy =	586.5401
13	N	Isotropic =	-45.4911	Anisotropy =	255.1109
14	C	Isotropic =	48.5086	Anisotropy =	104.6491
15	C	Isotropic =	57.0722	Anisotropy =	174.4775
16	C	Isotropic =	66.8168	Anisotropy =	155.8300
17	C	Isotropic =	144.9630	Anisotropy =	42.2220
18	C	Isotropic =	176.7209	Anisotropy =	23.4780

19	C	Isotropic =	156.4901	Anisotropy =	16.7842
20	C	Isotropic =	121.9893	Anisotropy =	43.5969
21	O	Isotropic =	203.1871	Anisotropy =	110.5356
22	C	Isotropic =	32.3052	Anisotropy =	137.8270
23	C	Isotropic =	70.4159	Anisotropy =	170.6168
24	C	Isotropic =	43.9187	Anisotropy =	181.8520
25	N	Isotropic =	-38.3847	Anisotropy =	458.2223
26	C	Isotropic =	42.5264	Anisotropy =	159.5698
27	C	Isotropic =	91.0520	Anisotropy =	133.2691
28	C	Isotropic =	70.3215	Anisotropy =	174.1915
29	C	Isotropic =	67.5640	Anisotropy =	170.4297
30	C	Isotropic =	63.5185	Anisotropy =	175.0920
31	C	Isotropic =	63.5997	Anisotropy =	150.0768
32	C	Isotropic =	154.1194	Anisotropy =	47.0658
33	O	Isotropic =	-62.7668	Anisotropy =	361.4604
34	H	Isotropic =	23.9988	Anisotropy =	8.8404
35	H	Isotropic =	24.2699	Anisotropy =	4.5478
36	H	Isotropic =	23.1985	Anisotropy =	4.9995
37	H	Isotropic =	22.9850	Anisotropy =	7.3078
38	H	Isotropic =	24.0552	Anisotropy =	9.0978
39	H	Isotropic =	26.3608	Anisotropy =	7.5763
40	H	Isotropic =	28.2138	Anisotropy =	6.4282
41	H	Isotropic =	30.5625	Anisotropy =	7.6717
42	H	Isotropic =	30.3485	Anisotropy =	10.7775
43	H	Isotropic =	30.5638	Anisotropy =	6.6032
44	H	Isotropic =	28.4686	Anisotropy =	7.7892
45	H	Isotropic =	28.3696	Anisotropy =	5.8841
46	H	Isotropic =	27.1185	Anisotropy =	6.2304
47	H	Isotropic =	27.3568	Anisotropy =	5.6972
48	H	Isotropic =	22.7548	Anisotropy =	7.2128
49	H	Isotropic =	24.9104	Anisotropy =	9.4228
50	H	Isotropic =	23.0087	Anisotropy =	9.5702
51	H	Isotropic =	23.7675	Anisotropy =	6.6067
52	H	Isotropic =	23.6025	Anisotropy =	5.2345
53	H	Isotropic =	23.5294	Anisotropy =	5.7873
54	H	Isotropic =	28.8589	Anisotropy =	7.6247
55	H	Isotropic =	28.0059	Anisotropy =	10.3377
56	H	Isotropic =	27.3094	Anisotropy =	7.7844

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.419923421006	0.814896302083	3.339204061069
C	-3.933477209115	1.397768951278	2.243291734177
C	-3.068950634218	2.514552133599	2.282632584458
C	-2.637994535755	2.949249313250	3.542382605668
C	-3.120291694767	2.318363831088	4.689817410607
C	-4.035448030046	1.277619471796	4.537439854074
N	-2.741790145367	3.259071710816	1.115646561309
C	-2.293048129253	2.739967823915	-0.078889449205
C	-2.268854787260	1.252708366802	-0.294083898356
C	-3.281314043232	0.409471358011	0.179190672783
N	-4.320853706202	0.867132997284	0.986616509873
O	-1.874213305053	3.480970630649	-0.967855421277
N	-3.217287667815	-0.949874748524	-0.117111508679
C	-2.223800165788	-1.414513729901	-0.936973529787
C	-1.208402499239	-0.605131221488	-1.428199634414
C	-1.236106124116	0.751615751683	-1.093647797338
C	-5.714206475823	0.414647703392	0.799924289182
C	-6.671059181809	1.604476569014	0.754183055921
C	-0.108124242398	-1.204011461728	-2.275188716081
C	1.125484674506	-1.623964700364	-1.465423189142
O	1.767766795559	-0.512235580010	-0.816377447499
C	2.675470722757	0.236029590773	-1.484930954249
C	3.265243584755	1.304816849792	-0.730576310862
C	4.241153413737	2.119381482588	-1.387766031976
N	4.629471966187	1.925276716831	-2.688723548314
C	4.053288469590	0.928866586039	-3.335073575069
C	3.076049415266	0.054783460496	-2.798517660013
C	2.921498340975	1.572818396205	0.621116959377
C	3.523122974752	2.614041947382	1.301247239549
C	4.490097161051	3.424830693299	0.656121511606
C	4.840026512052	3.182301621077	-0.657244517681
C	-2.705196118933	4.724995679086	1.232504930101
O	-4.079529438797	-1.772092578334	0.361313849700
H	-1.952440813076	3.793126870162	3.626253441103
H	-2.805865369713	2.645082033109	5.681807313143
H	-4.477621162300	0.788208775312	5.410319608291
H	-2.298179534905	-2.483717051459	-1.129573271407
H	-0.486396381733	1.443892195360	-1.473626010267
H	-5.749891773192	-0.148337451215	-0.138941211289
H	-5.991281083751	-0.281466068740	1.603738147823
H	-6.650075212762	2.174414071595	1.696986669954
H	-6.416655322812	2.290417495556	-0.069494667389
H	-7.702526686081	1.246650970606	0.603057038931

H	-0.477254720360	-2.104677513941	-2.790472360571
H	0.188481989560	-0.487674646072	-3.056487448089
H	1.844796576846	-2.161941654361	-2.101414864008
H	0.833899715489	-2.289282713912	-0.641271187611
H	4.364999488494	0.777730385363	-4.374950197375
H	2.667567823375	-0.730042488034	-3.432377250491
H	2.176826070512	0.944550710479	1.109856376609
H	3.254367902748	2.814895006544	2.340419058212
H	4.959590099569	4.245190256994	1.203529967729
H	5.582561274573	3.793558117187	-1.173771586199
H	-3.418617173800	5.038259629682	2.003970162632
H	-1.698322588337	5.088861648607	1.494264181015
H	-2.984485593538	5.160969503295	0.266697449741

SCF Done: E(RB3LYP) = -1465.99398348

Zero-point correction= 0.444588
Thermal correction to Energy= 0.472103
Thermal correction to Enthalpy= 0.473047
Thermal correction to Gibbs Free Energy= 0.383028
Sum of electronic and zero-point Energies= -1465.549395
Sum of electronic and thermal Energies= -1465.521881
Sum of electronic and thermal Enthalpies= -1465.520936
Sum of electronic and thermal Free Energies= -1465.610956

1	N	Isotropic =	-42.6094	Anisotropy =	468.6730
2	C	Isotropic =	38.7474	Anisotropy =	115.3535
3	C	Isotropic =	57.5438	Anisotropy =	125.4515
4	C	Isotropic =	62.5293	Anisotropy =	176.8824
5	C	Isotropic =	71.5127	Anisotropy =	160.4387
6	C	Isotropic =	48.9840	Anisotropy =	154.9215
7	N	Isotropic =	118.4642	Anisotropy =	90.5371
8	C	Isotropic =	28.9239	Anisotropy =	110.3651
9	C	Isotropic =	63.4625	Anisotropy =	135.1637
10	C	Isotropic =	41.1109	Anisotropy =	106.3671
11	N	Isotropic =	165.6527	Anisotropy =	59.3243
12	O	Isotropic =	-79.2108	Anisotropy =	589.3982
13	N	Isotropic =	-42.8774	Anisotropy =	257.5537
14	C	Isotropic =	50.0542	Anisotropy =	102.6546
15	C	Isotropic =	57.5314	Anisotropy =	172.8903
16	C	Isotropic =	65.7335	Anisotropy =	157.6052
17	C	Isotropic =	146.7757	Anisotropy =	37.7043
18	C	Isotropic =	175.7349	Anisotropy =	25.4192
19	C	Isotropic =	158.9246	Anisotropy =	23.0966

20	C	Isotropic =	122.7614	Anisotropy =	50.2856
21	O	Isotropic =	207.2169	Anisotropy =	136.4953
22	C	Isotropic =	33.1417	Anisotropy =	138.7755
23	C	Isotropic =	70.0944	Anisotropy =	171.9273
24	C	Isotropic =	43.5049	Anisotropy =	182.4463
25	N	Isotropic =	-38.2173	Anisotropy =	459.1182
26	C	Isotropic =	42.7156	Anisotropy =	159.5849
27	C	Isotropic =	91.7823	Anisotropy =	135.5682
28	C	Isotropic =	70.3247	Anisotropy =	175.4072
29	C	Isotropic =	67.6496	Anisotropy =	170.8158
30	C	Isotropic =	63.4235	Anisotropy =	175.6038
31	C	Isotropic =	63.6575	Anisotropy =	150.5197
32	C	Isotropic =	154.0493	Anisotropy =	46.7711
33	O	Isotropic =	-68.9524	Anisotropy =	372.4850
34	H	Isotropic =	23.9578	Anisotropy =	8.2249
35	H	Isotropic =	24.2143	Anisotropy =	4.5851
36	H	Isotropic =	23.1178	Anisotropy =	4.8400
37	H	Isotropic =	23.2872	Anisotropy =	7.6096
38	H	Isotropic =	24.5626	Anisotropy =	10.1692
39	H	Isotropic =	27.9921	Anisotropy =	6.1824
40	H	Isotropic =	26.7568	Anisotropy =	8.0810
41	H	Isotropic =	30.3365	Anisotropy =	4.9717
42	H	Isotropic =	30.4544	Anisotropy =	7.1211
43	H	Isotropic =	30.3882	Anisotropy =	11.4937
44	H	Isotropic =	28.9102	Anisotropy =	8.4427
45	H	Isotropic =	28.2976	Anisotropy =	5.8730
46	H	Isotropic =	26.6378	Anisotropy =	5.8090
47	H	Isotropic =	27.1493	Anisotropy =	6.8176
48	H	Isotropic =	22.6926	Anisotropy =	7.1401
49	H	Isotropic =	24.7276	Anisotropy =	9.0664
50	H	Isotropic =	23.3874	Anisotropy =	9.3545
51	H	Isotropic =	23.9190	Anisotropy =	6.0944
52	H	Isotropic =	23.6112	Anisotropy =	5.2214
53	H	Isotropic =	23.4990	Anisotropy =	5.7797
54	H	Isotropic =	28.9278	Anisotropy =	7.5465
55	H	Isotropic =	28.1488	Anisotropy =	9.5947
56	H	Isotropic =	27.4486	Anisotropy =	7.7723

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.935839222594	2.419373286789	4.270590218042
C	-1.783706889818	2.275034179040	3.615269891218
C	-1.246421056345	3.272640381293	2.771496344954
C	-2.024861075085	4.416101968588	2.552075418385
C	-3.246773032010	4.553551427126	3.211734815474
C	-3.643483160019	3.543059953424	4.086611186012
N	0.078043545654	3.196835135101	2.258753031958
C	0.638589319736	2.114154311931	1.617346598492
C	-0.098629900674	0.805666124861	1.558892920958
C	-0.849191259994	0.317529299878	2.635134194199
N	-1.072120525072	1.061053300621	3.792007939766
O	1.729313967972	2.212902341911	1.055804444177
N	-1.447635058610	-0.935749573152	2.523871027656
C	-1.215776512818	-1.696321064589	1.409455217826
C	-0.473914617135	-1.244256787904	0.326287388210
C	0.089084514237	0.031909832317	0.408450234500
C	-1.010397942453	0.456085010162	5.137364250610
C	-0.094459378281	1.263374796301	6.055456673451
C	-0.319262156054	-2.115647698952	-0.899787295141
C	-1.417123117870	-1.892753453510	-1.948059208094
O	-1.422777926786	-0.551696095544	-2.468302622672
C	-0.626007804539	-0.219798145728	-3.510004937016
C	-0.746493325560	1.135037800603	-3.967090397452
C	0.061960991043	1.533453503949	-5.078531283520
N	0.935767150962	0.688211570094	-5.713504288823
C	1.008793194859	-0.545100551357	-5.248284503684
C	0.264543388988	-1.059632788683	-4.158177675919
C	-1.627942727474	2.073066212443	-3.367059774489
C	-1.707429739973	3.364753298071	-3.850544805015
C	-0.909725485449	3.765920236196	-4.951188061027
C	-0.045938527764	2.870706301910	-5.550139677393
C	0.871006932344	4.435593288363	2.237542095315
O	-2.207475888547	-1.389993331640	3.453923023911
H	-1.665438494989	5.205770993604	1.891544028444
H	-3.866124834753	5.438924637774	3.062954491282
H	-4.569590649689	3.632000855572	4.662300415555
H	-1.701445428676	-2.670093456761	1.451570284398
H	0.707787266751	0.429495626213	-0.394572884342
H	-2.023254467202	0.383502567168	5.557591580320
H	-0.639073096023	-0.567268498391	5.018121595736
H	0.929569126799	1.314649264529	5.652259939397
H	-0.464038722794	2.292873380411	6.189421372920
H	-0.053469602350	0.790793979983	7.050390069848
H	0.668290008697	-1.942717721552	-1.353967222051

H	-0.358696788394	-3.178685547619	-0.613857245186
H	-2.409984791117	-2.012600766711	-1.493167079926
H	-1.326499949726	-2.620743660311	-2.768428911507
H	1.709949828169	-1.216773391864	-5.756812658422
H	0.414117155130	-2.095936054099	-3.860633208128
H	-2.237578194178	1.756249778755	-2.520857195784
H	-2.387108763284	4.081236631201	-3.384572413174
H	-0.980996189504	4.789543438115	-5.325584108276
H	0.577443732476	3.158071069217	-6.399031596030
H	0.757688608823	4.976367747728	1.283925532953
H	0.547008147275	5.079843764303	3.063470786074
H	1.928969423685	4.177341292824	2.359142041029

SCF Done: E(RB3LYP) = -1465.99396346

Zero-point correction= 0.444604
Thermal correction to Energy= 0.472119
Thermal correction to Enthalpy= 0.473063
Thermal correction to Gibbs Free Energy= 0.383616
Sum of electronic and zero-point Energies= -1465.549359
Sum of electronic and thermal Energies= -1465.521844
Sum of electronic and thermal Enthalpies= -1465.520900
Sum of electronic and thermal Free Energies= -1465.610347

1	N	Isotropic =	-42.9655	Anisotropy =	468.4533
2	C	Isotropic =	38.7082	Anisotropy =	115.3253
3	C	Isotropic =	57.4891	Anisotropy =	125.5866
4	C	Isotropic =	62.5603	Anisotropy =	176.8258
5	C	Isotropic =	71.3953	Anisotropy =	160.8553
6	C	Isotropic =	48.9911	Anisotropy =	154.7006
7	N	Isotropic =	118.4583	Anisotropy =	90.1814
8	C	Isotropic =	28.8699	Anisotropy =	110.3351
9	C	Isotropic =	63.4506	Anisotropy =	135.1698
10	C	Isotropic =	41.2532	Anisotropy =	106.6543
11	N	Isotropic =	165.8715	Anisotropy =	59.5418
12	O	Isotropic =	-79.5156	Anisotropy =	589.9715
13	N	Isotropic =	-42.8534	Anisotropy =	257.4624
14	C	Isotropic =	50.0342	Anisotropy =	103.5859
15	C	Isotropic =	57.5080	Anisotropy =	173.0767
16	C	Isotropic =	65.5659	Anisotropy =	157.4865
17	C	Isotropic =	146.9340	Anisotropy =	37.9783
18	C	Isotropic =	175.7047	Anisotropy =	25.5881
19	C	Isotropic =	158.6744	Anisotropy =	23.0561

20	C	Isotropic =	122.5676	Anisotropy =	49.9627
21	O	Isotropic =	206.9093	Anisotropy =	136.1319
22	C	Isotropic =	33.1728	Anisotropy =	138.8802
23	C	Isotropic =	70.1822	Anisotropy =	171.8378
24	C	Isotropic =	43.3595	Anisotropy =	182.3631
25	N	Isotropic =	-37.6690	Anisotropy =	460.0894
26	C	Isotropic =	42.5911	Anisotropy =	159.7990
27	C	Isotropic =	91.9615	Anisotropy =	135.1862
28	C	Isotropic =	69.9859	Anisotropy =	174.8825
29	C	Isotropic =	67.8245	Anisotropy =	170.9829
30	C	Isotropic =	63.5743	Anisotropy =	175.6777
31	C	Isotropic =	63.7960	Anisotropy =	150.6397
32	C	Isotropic =	153.9164	Anisotropy =	46.8522
33	O	Isotropic =	-69.2087	Anisotropy =	372.2286
34	H	Isotropic =	23.9719	Anisotropy =	8.2230
35	H	Isotropic =	24.2193	Anisotropy =	4.5433
36	H	Isotropic =	23.1372	Anisotropy =	4.8110
37	H	Isotropic =	23.2614	Anisotropy =	7.6524
38	H	Isotropic =	24.5581	Anisotropy =	10.0523
39	H	Isotropic =	26.7930	Anisotropy =	8.0504
40	H	Isotropic =	27.9355	Anisotropy =	6.1207
41	H	Isotropic =	30.4433	Anisotropy =	7.0774
42	H	Isotropic =	30.3367	Anisotropy =	5.0220
43	H	Isotropic =	30.3876	Anisotropy =	11.5107
44	H	Isotropic =	28.3165	Anisotropy =	5.7747
45	H	Isotropic =	28.8663	Anisotropy =	8.4290
46	H	Isotropic =	27.1302	Anisotropy =	6.8342
47	H	Isotropic =	26.6492	Anisotropy =	5.7099
48	H	Isotropic =	22.6954	Anisotropy =	7.1430
49	H	Isotropic =	24.7304	Anisotropy =	9.0635
50	H	Isotropic =	23.4406	Anisotropy =	9.3795
51	H	Isotropic =	23.9378	Anisotropy =	6.1431
52	H	Isotropic =	23.6197	Anisotropy =	5.2226
53	H	Isotropic =	23.4977	Anisotropy =	5.7862
54	H	Isotropic =	28.1572	Anisotropy =	9.5526
55	H	Isotropic =	28.9147	Anisotropy =	7.5456
56	H	Isotropic =	27.4721	Anisotropy =	7.8488

Conformer 26

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.546140974246	4.567094155430	3.802310586810
C	-2.159248196940	3.984677367727	2.771560447241
C	-3.198154621456	4.604718910271	2.041651499258
C	-3.514987571747	5.928119606218	2.372742274550
C	-2.850828140995	6.550424949313	3.430486643459
C	-1.897469299452	5.817334508237	4.135831768335
N	-3.987258976120	3.892607150516	1.096413133489
C	-3.511724703031	3.101420753593	0.073705711572
C	-2.045056008351	2.786009188941	-0.018056415893
C	-1.258388843434	2.536367691373	1.112457969389
N	-1.746581021906	2.677018443177	2.410423587833
O	-4.271757900046	2.673166780681	-0.794482205867
N	0.082584170855	2.201880216068	0.938020232930
C	0.575173041337	2.029187665955	-0.327685606046
C	-0.180463314161	2.256198487257	-1.469337831780
C	-1.511949786519	2.647527543248	-1.304050417889
C	-1.419091393494	1.708806954832	3.476198209497
C	-2.681442614211	1.259221503697	4.209372725956
C	0.427463552151	2.048161724601	-2.838986526396
C	0.152471811682	0.665018119838	-3.424481143684
O	0.824861369927	-0.301884803701	-2.601435368599
C	0.697645708445	-1.612915690666	-2.899908926087
C	1.390161456985	-2.523050882422	-2.033764851009
C	1.273930670238	-3.921070783241	-2.316548788497
N	0.542780822521	-4.417953226384	-3.365469067655
C	-0.070119521391	-3.534304492505	-4.131248370379
C	-0.034895070228	-2.128899980050	-3.956275214183
C	2.170823044398	-2.092699631650	-0.928570650419
C	2.814813218290	-3.015102839224	-0.126638368513
C	2.701989894687	-4.401136094431	-0.399635730043
C	1.949290394603	-4.842450742983	-1.469701428745
C	-5.434173339973	4.157125007367	1.083779278709
O	0.862123059454	2.051422804046	1.946965888817
H	-4.294812161312	6.458783027902	1.825535185169
H	-3.086541318677	7.577475182214	3.711981612328
H	-1.388082231247	6.248562566920	5.002750003607
H	1.625101481778	1.742613919376	-0.339746341951
H	-2.159789424900	2.827664965307	-2.161493886494
H	-0.923272841911	0.856665117616	2.998751893489
H	-0.695912459164	2.151962356240	4.174897454472
H	-3.397240671176	0.784943286141	3.519110413869
H	-2.417035711021	0.529644366335	4.992039903151
H	-3.185618536698	2.107273796477	4.700060383028
H	0.014246024272	2.787828591411	-3.541727822397

H	1.516054339680	2.205939752931	-2.802332269063
H	0.539191005542	0.604544744894	-4.455445389539
H	-0.929146652244	0.449040022676	-3.440072508496
H	-0.651888939866	-3.936246476719	-4.968785872269
H	-0.580611400225	-1.493962972157	-4.651834921708
H	2.254101655860	-1.025314438491	-0.724860313653
H	3.413643456652	-2.677055800811	0.721603900218
H	3.214807514406	-5.121767690335	0.241273395602
H	1.849208004588	-5.905025812629	-1.699267766836
H	-5.755086538830	4.425990490613	2.097218357883
H	-5.694382915809	4.971392429270	0.388078902505
H	-5.953702597567	3.249788209691	0.755932640923

SCF Done: E(RB3LYP) = -1465.99625306

Zero-point correction= 0.444400
Thermal correction to Energy= 0.472032
Thermal correction to Enthalpy= 0.472977
Thermal correction to Gibbs Free Energy= 0.382989
Sum of electronic and zero-point Energies= -1465.551853
Sum of electronic and thermal Energies= -1465.524221
Sum of electronic and thermal Enthalpies= -1465.523276
Sum of electronic and thermal Free Energies= -1465.613264

1	N	Isotropic =	-42.3029	Anisotropy =	469.0182
2	C	Isotropic =	38.7674	Anisotropy =	115.1832
3	C	Isotropic =	57.2332	Anisotropy =	124.1504
4	C	Isotropic =	62.5487	Anisotropy =	176.9180
5	C	Isotropic =	71.1561	Anisotropy =	159.4411
6	C	Isotropic =	49.2047	Anisotropy =	154.8667
7	N	Isotropic =	118.5232	Anisotropy =	89.3838
8	C	Isotropic =	28.8620	Anisotropy =	108.4101
9	C	Isotropic =	62.8563	Anisotropy =	136.8062
10	C	Isotropic =	40.6866	Anisotropy =	107.0163
11	N	Isotropic =	165.9276	Anisotropy =	58.9324
12	O	Isotropic =	-80.0862	Anisotropy =	587.1346
13	N	Isotropic =	-42.8295	Anisotropy =	256.8009
14	C	Isotropic =	48.7623	Anisotropy =	105.1926
15	C	Isotropic =	57.6219	Anisotropy =	173.4354
16	C	Isotropic =	67.1569	Anisotropy =	155.1009
17	C	Isotropic =	146.8478	Anisotropy =	36.9345
18	C	Isotropic =	175.9139	Anisotropy =	25.0438
19	C	Isotropic =	156.5653	Anisotropy =	16.5834
20	C	Isotropic =	121.9115	Anisotropy =	43.6743

21	O	Isotropic =	203.2615	Anisotropy =	110.9964
22	C	Isotropic =	32.2559	Anisotropy =	137.7192
23	C	Isotropic =	70.5217	Anisotropy =	170.7477
24	C	Isotropic =	43.8421	Anisotropy =	181.6933
25	N	Isotropic =	-37.9001	Anisotropy =	459.3753
26	C	Isotropic =	42.4710	Anisotropy =	159.7535
27	C	Isotropic =	91.0875	Anisotropy =	133.1579
28	C	Isotropic =	69.9689	Anisotropy =	173.8820
29	C	Isotropic =	67.6183	Anisotropy =	170.3759
30	C	Isotropic =	63.6165	Anisotropy =	174.8737
31	C	Isotropic =	63.8107	Anisotropy =	150.4791
32	C	Isotropic =	154.0709	Anisotropy =	46.7934
33	O	Isotropic =	-68.3372	Anisotropy =	370.7054
34	H	Isotropic =	23.9874	Anisotropy =	8.8123
35	H	Isotropic =	24.2939	Anisotropy =	4.4387
36	H	Isotropic =	23.1716	Anisotropy =	4.8787
37	H	Isotropic =	22.9755	Anisotropy =	7.3752
38	H	Isotropic =	24.0672	Anisotropy =	9.1773
39	H	Isotropic =	28.0874	Anisotropy =	6.4111
40	H	Isotropic =	26.7738	Anisotropy =	7.8588
41	H	Isotropic =	30.5187	Anisotropy =	6.8806
42	H	Isotropic =	30.4553	Anisotropy =	11.0310
43	H	Isotropic =	30.3914	Anisotropy =	5.2203
44	H	Isotropic =	28.4754	Anisotropy =	7.7221
45	H	Isotropic =	28.3842	Anisotropy =	5.8105
46	H	Isotropic =	27.1188	Anisotropy =	6.1676
47	H	Isotropic =	27.3495	Anisotropy =	5.6923
48	H	Isotropic =	22.7327	Anisotropy =	7.2431
49	H	Isotropic =	24.8943	Anisotropy =	9.4133
50	H	Isotropic =	23.0055	Anisotropy =	9.6770
51	H	Isotropic =	23.7613	Anisotropy =	6.5944
52	H	Isotropic =	23.6006	Anisotropy =	5.2233
53	H	Isotropic =	23.5045	Anisotropy =	5.8242
54	H	Isotropic =	28.8780	Anisotropy =	7.3953
55	H	Isotropic =	28.0061	Anisotropy =	10.3455
56	H	Isotropic =	27.3175	Anisotropy =	7.7139

Conformer 27

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N -1.831407754828 5.208256476342 3.025427735082

C	-2.197830156160	4.593706879533	1.900391392662
C	-3.496127368505	4.696787103833	1.352567806715
C	-4.451773354571	5.403232977195	2.093588212365
C	-4.077776317833	6.019988146846	3.288170580149
C	-2.748020768538	5.921514391327	3.695392065882
N	-3.805717763386	4.223599540778	0.047334510464
C	-3.511346412423	2.974543183030	-0.454027863982
C	-2.645089753841	2.030156908280	0.331373497483
C	-1.537616339918	2.464143629829	1.069459135496
N	-1.224432009856	3.813140998861	1.226815634951
O	-3.979609172695	2.603189867296	-1.529941788790
N	-0.756954690149	1.518447647334	1.730073642375
C	-1.028247678577	0.186445745854	1.565493709051
C	-2.111019080562	-0.278095441265	0.832557541845
C	-2.932985901171	0.666388601958	0.211198508240
C	0.166932572683	4.303669152670	1.161120256570
C	0.275574997840	5.508960125612	0.229047864300
C	-2.360231170822	-1.764323469919	0.698805070165
C	-1.793868922729	-2.365682407986	-0.584897839891
O	-0.361616958702	-2.271139270451	-0.520722100703
C	0.367501776755	-2.720963719226	-1.564797868308
C	1.791090511757	-2.602960461679	-1.432225463328
C	2.595908738110	-3.064872555057	-2.521628303747
N	2.071580574855	-3.608978156902	-3.666467925608
C	0.755909721176	-3.696362315619	-3.731732053367
C	-0.147594018549	-3.275112204266	-2.725176999650
C	2.415465998022	-2.055439002453	-0.280490600608
C	3.792181496043	-1.965229103380	-0.208372019823
C	4.595054404823	-2.418669667468	-1.284572988535
C	4.009616268364	-2.955731033246	-2.413796466152
C	-4.676218058528	5.062474118250	-0.790793102808
O	0.213609289753	1.877963227577	2.489638076190
H	-5.474027799324	5.493669071020	1.725043120279
H	-4.802398169161	6.582949277218	3.877739101686
H	-2.399753385194	6.430669627136	4.598962070168
H	-0.337421601478	-0.457797594993	2.106220560537
H	-3.789908889355	0.362764305573	-0.389654411739
H	0.523805423835	4.553556391480	2.169859705507
H	0.785528810514	3.475933876251	0.797602553126
H	-0.051298397077	5.255533737710	-0.792073943792
H	-0.336301493065	6.352068889202	0.588076747553
H	1.322301531662	5.851242604448	0.184455002481
H	-1.935103863393	-2.302862985150	1.559291088008
H	-3.444163512877	-1.956468888837	0.697534275447

H	-2.161474827913	-1.822949051658	-1.472167866889
H	-2.089692784262	-3.424470612621	-0.671740419180
H	0.341763595003	-4.133146386811	-4.647817081529
H	-1.216897455024	-3.396583097225	-2.888027778120
H	1.791667153153	-1.709577011821	0.543625460244
H	4.265656439051	-1.543217018678	0.680502403520
H	5.682571776374	-2.342298383540	-1.217262154581
H	4.608345571085	-3.312079648074	-3.254238640634
H	-5.739647831910	4.801776227710	-0.664509639701
H	-4.523275100460	6.114106211524	-0.520659746715
H	-4.409447888023	4.904500546648	-1.841822260357

SCF Done: E(RB3LYP) = -1465.99625290

Zero-point correction= 0.444556
Thermal correction to Energy= 0.472111
Thermal correction to Enthalpy= 0.473055
Thermal correction to Gibbs Free Energy= 0.383453
Sum of electronic and zero-point Energies= -1465.551697
Sum of electronic and thermal Energies= -1465.524142
Sum of electronic and thermal Enthalpies= -1465.523198
Sum of electronic and thermal Free Energies= -1465.612800

1	N	Isotropic =	-42.6210	Anisotropy =	468.2940
2	C	Isotropic =	38.5784	Anisotropy =	115.3463
3	C	Isotropic =	57.5901	Anisotropy =	124.7408
4	C	Isotropic =	62.6472	Anisotropy =	175.9742
5	C	Isotropic =	71.8755	Anisotropy =	160.3824
6	C	Isotropic =	48.9859	Anisotropy =	154.4292
7	N	Isotropic =	118.3570	Anisotropy =	89.4161
8	C	Isotropic =	28.8905	Anisotropy =	108.4330
9	C	Isotropic =	62.9195	Anisotropy =	136.8683
10	C	Isotropic =	40.8427	Anisotropy =	106.9583
11	N	Isotropic =	165.9338	Anisotropy =	58.9117
12	O	Isotropic =	-79.8024	Anisotropy =	587.9513
13	N	Isotropic =	-42.7271	Anisotropy =	256.3626
14	C	Isotropic =	48.8828	Anisotropy =	104.6889
15	C	Isotropic =	57.5031	Anisotropy =	173.2629
16	C	Isotropic =	67.0570	Anisotropy =	156.0815
17	C	Isotropic =	146.6834	Anisotropy =	36.8148
18	C	Isotropic =	176.0016	Anisotropy =	24.9346
19	C	Isotropic =	156.4887	Anisotropy =	16.6375
20	C	Isotropic =	121.8112	Anisotropy =	43.5710
21	O	Isotropic =	203.0630	Anisotropy =	110.3221

22	C	Isotropic =	32.1239	Anisotropy =	137.8753
23	C	Isotropic =	70.4752	Anisotropy =	170.5996
24	C	Isotropic =	43.8902	Anisotropy =	181.6889
25	N	Isotropic =	-38.1027	Anisotropy =	458.4991
26	C	Isotropic =	42.5703	Anisotropy =	159.7180
27	C	Isotropic =	91.0528	Anisotropy =	133.1522
28	C	Isotropic =	70.1205	Anisotropy =	173.9714
29	C	Isotropic =	67.5480	Anisotropy =	170.3995
30	C	Isotropic =	63.6211	Anisotropy =	175.0469
31	C	Isotropic =	63.8051	Anisotropy =	149.9922
32	C	Isotropic =	153.9914	Anisotropy =	46.9485
33	O	Isotropic =	-68.4781	Anisotropy =	371.1583
34	H	Isotropic =	23.9977	Anisotropy =	8.7951
35	H	Isotropic =	24.2695	Anisotropy =	4.4890
36	H	Isotropic =	23.1484	Anisotropy =	4.8947
37	H	Isotropic =	22.9959	Anisotropy =	7.3568
38	H	Isotropic =	24.0524	Anisotropy =	9.2282
39	H	Isotropic =	26.7679	Anisotropy =	7.8629
40	H	Isotropic =	28.0972	Anisotropy =	6.3510
41	H	Isotropic =	30.5227	Anisotropy =	6.8719
42	H	Isotropic =	30.3683	Anisotropy =	5.2549
43	H	Isotropic =	30.4475	Anisotropy =	11.0499
44	H	Isotropic =	28.3962	Anisotropy =	5.7811
45	H	Isotropic =	28.4643	Anisotropy =	7.7164
46	H	Isotropic =	27.3224	Anisotropy =	5.7406
47	H	Isotropic =	27.1264	Anisotropy =	6.1033
48	H	Isotropic =	22.7402	Anisotropy =	7.2400
49	H	Isotropic =	24.8936	Anisotropy =	9.4027
50	H	Isotropic =	23.0094	Anisotropy =	9.7117
51	H	Isotropic =	23.7626	Anisotropy =	6.5962
52	H	Isotropic =	23.6041	Anisotropy =	5.2216
53	H	Isotropic =	23.5247	Anisotropy =	5.8186
54	H	Isotropic =	28.0061	Anisotropy =	10.3366
55	H	Isotropic =	28.8820	Anisotropy =	7.3775
56	H	Isotropic =	27.3469	Anisotropy =	7.6986

Conformer 28

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.474724957057	-0.251800003632	-1.781042238675
C	-4.479673319556	0.532332664388	-1.365667812729

C	-4.691964498576	1.787856682552	-0.753401964986
C	-6.016503840732	2.160213583689	-0.492196312502
C	-7.058181603937	1.324548183193	-0.896811950515
C	-6.737401388758	0.145001610022	-1.567438447900
N	-3.629402519845	2.705430405231	-0.520856457504
C	-2.434943210699	2.415885784144	0.097987569036
C	-2.085054332065	0.995092250439	0.436727557933
C	-2.385709278944	-0.077302187681	-0.411691030011
N	-3.152415294640	0.074129834898	-1.565024968896
O	-1.653878293822	3.316897401364	0.409603741537
N	-1.961713591178	-1.355742915699	-0.055191451815
C	-1.172647811512	-1.520660274309	1.052352081767
C	-0.847139209836	-0.476699158629	1.907104230719
C	-1.328276054692	0.796740160273	1.595103651778
C	-2.816400665525	-0.618932234284	-2.824835005679
C	-2.798828224687	0.360896143700	-3.996548735783
C	0.044409026907	-0.709993164252	3.106143854523
C	1.532312856744	-0.551766751669	2.794180602238
O	1.734770186303	0.769469047135	2.267611530084
C	2.984966091195	1.159308837452	1.937395747228
C	3.094887978025	2.438275081498	1.295964966147
C	4.409602335735	2.895964729704	0.962059703434
N	5.546210043762	2.170326332460	1.214561647816
C	5.382234307101	0.992683166372	1.788283801557
C	4.139493828514	0.430348336009	2.170187630315
C	1.968641854955	3.242017262159	0.973709801914
C	2.139791203551	4.464416314161	0.352728749251
C	3.439107070259	4.930733874911	0.033183486785
C	4.547237667047	4.162343478214	0.329848966029
C	-3.884455546483	4.127616560256	-0.797020035253
O	-2.295211146455	-2.380743954013	-0.753348620222
H	-6.232500842429	3.109591150113	-0.001081764394
H	-8.097961166322	1.597478508579	-0.712529146744
H	-7.523205983456	-0.515036479221	-1.946689356714
H	-0.870834202333	-2.555313251508	1.208547572032
H	-1.099464341960	1.652383485658	2.227999796325
H	-1.832681718455	-1.080898110815	-2.689266561024
H	-3.532623929010	-1.432791477030	-3.004136989419
H	-2.534245787127	-0.172611289663	-4.923998079686
H	-3.786651865137	0.824992319371	-4.148309191627
H	-2.062035073683	1.163887768748	-3.834748197975
H	-0.227427920612	-0.005259112608	3.906658471045
H	-0.099339768178	-1.726609013751	3.502938082517
H	1.865772798356	-1.294577045446	2.049339213349

H	2.123566986234	-0.685762062357	3.714966012821
H	6.292947618347	0.414261728370	1.982193175496
H	4.122732803130	-0.550512915796	2.641806167070
H	0.965650399544	2.882442099457	1.201508492466
H	1.267030464042	5.071117134160	0.102331771735
H	3.561771631082	5.899987916646	-0.455406419442
H	5.557512047537	4.496774671195	0.086271292246
H	-4.252813722959	4.657061675636	0.096541958201
H	-2.945478866879	4.598576527266	-1.109405880915
H	-4.626589220832	4.205928692941	-1.600264704984

SCF Done: E(RB3LYP) = -1465.99731229

Zero-point correction= 0.444596
Thermal correction to Energy= 0.472113
Thermal correction to Enthalpy= 0.473057
Thermal correction to Gibbs Free Energy= 0.384337
Sum of electronic and zero-point Energies= -1465.552716
Sum of electronic and thermal Energies= -1465.525199
Sum of electronic and thermal Enthalpies= -1465.524255
Sum of electronic and thermal Free Energies= -1465.612975

1	N	Isotropic =	-42.8397	Anisotropy =	468.5162
2	C	Isotropic =	38.4012	Anisotropy =	114.9465
3	C	Isotropic =	57.4022	Anisotropy =	124.4647
4	C	Isotropic =	62.4256	Anisotropy =	176.2978
5	C	Isotropic =	71.5041	Anisotropy =	160.4052
6	C	Isotropic =	48.8618	Anisotropy =	155.0822
7	N	Isotropic =	117.7639	Anisotropy =	89.5325
8	C	Isotropic =	27.6579	Anisotropy =	108.6330
9	C	Isotropic =	63.6681	Anisotropy =	135.8209
10	C	Isotropic =	40.8045	Anisotropy =	107.3278
11	N	Isotropic =	165.0857	Anisotropy =	57.9242
12	O	Isotropic =	-77.4439	Anisotropy =	578.0623
13	N	Isotropic =	-42.8332	Anisotropy =	256.6619
14	C	Isotropic =	50.5461	Anisotropy =	105.4579
15	C	Isotropic =	58.2701	Anisotropy =	173.2770
16	C	Isotropic =	63.7617	Anisotropy =	156.6624
17	C	Isotropic =	146.9015	Anisotropy =	36.9510
18	C	Isotropic =	175.8540	Anisotropy =	24.9818
19	C	Isotropic =	156.7792	Anisotropy =	18.7822
20	C	Isotropic =	122.5181	Anisotropy =	43.7464
21	O	Isotropic =	203.8195	Anisotropy =	116.4934
22	C	Isotropic =	32.1967	Anisotropy =	137.0700

23	C	Isotropic =	70.4545	Anisotropy =	169.8341
24	C	Isotropic =	43.6608	Anisotropy =	181.7536
25	N	Isotropic =	-38.1459	Anisotropy =	459.0960
26	C	Isotropic =	42.5960	Anisotropy =	159.1825
27	C	Isotropic =	91.1691	Anisotropy =	133.1710
28	C	Isotropic =	68.8056	Anisotropy =	175.3844
29	C	Isotropic =	67.4578	Anisotropy =	170.0551
30	C	Isotropic =	63.5304	Anisotropy =	174.5103
31	C	Isotropic =	64.0163	Anisotropy =	149.7222
32	C	Isotropic =	153.8028	Anisotropy =	46.9558
33	O	Isotropic =	-68.5821	Anisotropy =	370.8719
34	H	Isotropic =	23.9312	Anisotropy =	9.0230
35	H	Isotropic =	24.2358	Anisotropy =	4.5859
36	H	Isotropic =	23.1303	Anisotropy =	4.7227
37	H	Isotropic =	23.2687	Anisotropy =	7.2226
38	H	Isotropic =	23.6302	Anisotropy =	9.3001
39	H	Isotropic =	28.0410	Anisotropy =	5.4725
40	H	Isotropic =	26.8025	Anisotropy =	8.4384
41	H	Isotropic =	30.4352	Anisotropy =	11.2431
42	H	Isotropic =	30.3469	Anisotropy =	5.0622
43	H	Isotropic =	30.4784	Anisotropy =	7.1927
44	H	Isotropic =	28.2578	Anisotropy =	5.5096
45	H	Isotropic =	28.5725	Anisotropy =	8.4744
46	H	Isotropic =	27.5547	Anisotropy =	6.2860
47	H	Isotropic =	26.9894	Anisotropy =	6.5005
48	H	Isotropic =	22.7515	Anisotropy =	7.1123
49	H	Isotropic =	24.9103	Anisotropy =	9.5991
50	H	Isotropic =	22.6704	Anisotropy =	8.8508
51	H	Isotropic =	23.6615	Anisotropy =	7.3553
52	H	Isotropic =	23.5843	Anisotropy =	5.6441
53	H	Isotropic =	23.5160	Anisotropy =	5.7663
54	H	Isotropic =	27.8716	Anisotropy =	9.9551
55	H	Isotropic =	27.1824	Anisotropy =	7.7463
56	H	Isotropic =	28.7651	Anisotropy =	7.3179

Conformer 29

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.560668868321	3.124739908553	1.470382510598
C	-4.618922016094	2.267718237290	1.074698618993
C	-4.644170889954	0.892544991127	1.397644398697

C	-5.661495202739	0.451006961481	2.252773527627
C	-6.629271717367	1.354149893611	2.693879466550
C	-6.554590884100	2.673240820755	2.248492818580
N	-3.761518976423	-0.043811001324	0.790567614382
C	-2.394945065436	0.082960880601	0.695225175645
C	-1.725856252571	1.366350208638	1.096516596322
C	-2.278398344335	2.622703905719	0.819601624914
N	-3.555614231464	2.775891962329	0.284961619641
O	-1.701284714562	-0.860619414399	0.311065929416
N	-1.554042269158	3.764283349697	1.156090760238
C	-0.283759840050	3.635791053476	1.652869025305
C	0.294370678564	2.405511902338	1.932917952902
C	-0.451501105680	1.256621102555	1.660068746173
C	-3.854813401337	3.777331954855	-0.758104570946
C	-4.598900089028	3.137082873648	-1.928409576780
C	1.703869322496	2.317239494079	2.473559716233
C	2.771979703105	2.217076029892	1.384678622954
O	2.471317079080	1.071743571086	0.571156064909
C	3.312696379863	0.741625724118	-0.432568993616
C	2.887909550344	-0.336001867593	-1.279705523129
C	3.774902231785	-0.736217746570	-2.329776683399
N	4.984814239980	-0.133408105954	-2.564216179916
C	5.312617237522	0.867019416903	-1.767670256705
C	4.527878949963	1.353269810200	-0.693348551484
C	1.639415932781	-0.996097027655	-1.125459917212
C	1.287443029940	-2.028001789388	-1.974260325911
C	2.167681572504	-2.440799704197	-3.005058648589
C	3.382092820708	-1.807247106920	-3.178905788494
C	-4.318885253991	-1.343971044436	0.386615760116
O	-2.059489448483	4.935287137275	1.004550994263
H	-5.711999725551	-0.597259097291	2.548852533870
H	-7.436054348855	1.031898668512	3.353296138419
H	-7.319506711183	3.403301256691	2.529365563810
H	0.196822015322	4.594211404644	1.844052320410
H	-0.044126010374	0.265963346206	1.853999943669
H	-4.438328174530	4.601719787756	-0.325159818069
H	-2.899458269927	4.199077195562	-1.088105968288
H	-5.566692674742	2.718009416260	-1.609129866139
H	-4.801881127054	3.896531737636	-2.700959324149
H	-4.005978608660	2.327526232309	-2.383129355119
H	1.941160307284	3.204144616280	3.080694706660
H	1.786432464817	1.439497374981	3.132637811485
H	3.764834446582	2.099399645601	1.848945693132
H	2.784233926835	3.119639876057	0.749745126527

H	6.277069031543	1.349804760807	-1.963536227588
H	4.900605284731	2.184380496677	-0.097445832828
H	0.949978751365	-0.673872481661	-0.345688611926
H	0.322386554465	-2.524149378915	-1.851848078005
H	1.879321724395	-3.259930822479	-3.667714491683
H	4.073212150469	-2.101827972333	-3.971013587966
H	-5.377651782365	-1.213815570807	0.133265662971
H	-3.767909429725	-1.705327161961	-0.489073668234
H	-4.222489952383	-2.095489712323	1.186906800763

SCF Done: E(RB3LYP) = -1465.99724858

Zero-point correction= 0.444548
Thermal correction to Energy= 0.472101
Thermal correction to Enthalpy= 0.473045
Thermal correction to Gibbs Free Energy= 0.384200
Sum of electronic and zero-point Energies= -1465.552700
Sum of electronic and thermal Energies= -1465.525148
Sum of electronic and thermal Enthalpies= -1465.524203
Sum of electronic and thermal Free Energies= -1465.613048

1	N	Isotropic =	-43.1458	Anisotropy =	468.3935
2	C	Isotropic =	38.5178	Anisotropy =	114.9688
3	C	Isotropic =	57.2323	Anisotropy =	124.2971
4	C	Isotropic =	62.2923	Anisotropy =	176.5797
5	C	Isotropic =	71.4122	Anisotropy =	160.7535
6	C	Isotropic =	48.8503	Anisotropy =	154.8705
7	N	Isotropic =	117.9336	Anisotropy =	89.2678
8	C	Isotropic =	27.5101	Anisotropy =	108.3983
9	C	Isotropic =	63.6754	Anisotropy =	135.8803
10	C	Isotropic =	40.9938	Anisotropy =	107.2655
11	N	Isotropic =	164.8927	Anisotropy =	57.4287
12	O	Isotropic =	-77.6006	Anisotropy =	576.6284
13	N	Isotropic =	-42.6639	Anisotropy =	256.3083
14	C	Isotropic =	50.4791	Anisotropy =	104.9911
15	C	Isotropic =	58.3802	Anisotropy =	172.8673
16	C	Isotropic =	63.7261	Anisotropy =	156.7459
17	C	Isotropic =	146.8450	Anisotropy =	37.1746
18	C	Isotropic =	175.6614	Anisotropy =	25.0250
19	C	Isotropic =	156.7932	Anisotropy =	18.8119
20	C	Isotropic =	122.6996	Anisotropy =	44.1671
21	O	Isotropic =	203.8398	Anisotropy =	117.1684
22	C	Isotropic =	32.2442	Anisotropy =	137.1776
23	C	Isotropic =	70.3986	Anisotropy =	169.7835

24	C	Isotropic =	43.6269	Anisotropy =	181.4005
25	N	Isotropic =	-37.5518	Anisotropy =	460.8259
26	C	Isotropic =	42.7649	Anisotropy =	159.5399
27	C	Isotropic =	91.1484	Anisotropy =	133.0746
28	C	Isotropic =	68.7247	Anisotropy =	175.8606
29	C	Isotropic =	67.3031	Anisotropy =	170.0698
30	C	Isotropic =	63.5868	Anisotropy =	174.4237
31	C	Isotropic =	64.0259	Anisotropy =	149.5988
32	C	Isotropic =	153.7893	Anisotropy =	47.0033
33	O	Isotropic =	-68.4052	Anisotropy =	370.3030
34	H	Isotropic =	23.9019	Anisotropy =	9.0660
35	H	Isotropic =	24.2269	Anisotropy =	4.5844
36	H	Isotropic =	23.1487	Anisotropy =	4.6970
37	H	Isotropic =	23.2692	Anisotropy =	7.2398
38	H	Isotropic =	23.6078	Anisotropy =	9.3803
39	H	Isotropic =	26.8084	Anisotropy =	8.4165
40	H	Isotropic =	27.9818	Anisotropy =	5.4659
41	H	Isotropic =	30.3543	Anisotropy =	5.0036
42	H	Isotropic =	30.4339	Anisotropy =	11.2580
43	H	Isotropic =	30.4624	Anisotropy =	7.1611
44	H	Isotropic =	28.6005	Anisotropy =	8.4258
45	H	Isotropic =	28.2468	Anisotropy =	5.5218
46	H	Isotropic =	26.9961	Anisotropy =	6.4451
47	H	Isotropic =	27.5446	Anisotropy =	6.3972
48	H	Isotropic =	22.7243	Anisotropy =	7.1431
49	H	Isotropic =	24.8961	Anisotropy =	9.6179
50	H	Isotropic =	22.6189	Anisotropy =	8.8666
51	H	Isotropic =	23.6488	Anisotropy =	7.3846
52	H	Isotropic =	23.5850	Anisotropy =	5.6546
53	H	Isotropic =	23.5046	Anisotropy =	5.7958
54	H	Isotropic =	28.7397	Anisotropy =	7.3314
55	H	Isotropic =	27.1773	Anisotropy =	7.7523
56	H	Isotropic =	27.8598	Anisotropy =	9.9560

Conformer 30

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.392432334729	0.709822186753	-2.964192208061
C	-4.102939679218	0.847003510482	-2.654314145579
C	-3.323151357932	1.948712476609	-3.072237633504
C	-3.978874098653	2.977223354297	-3.760143866167

C	-5.336409741753	2.849528472390	-4.056499169094
C	-5.991590676704	1.682299265404	-3.666104421917
N	-1.908370222317	1.971514032958	-2.925388942081
C	-1.216365656325	1.695672484624	-1.768908355265
C	-1.943440453990	1.179591960813	-0.560384190458
C	-2.967945917646	0.229554011210	-0.654839934707
N	-3.499846058588	-0.175482390771	-1.877421555870
O	-0.001878075960	1.892970907299	-1.698815334929
N	-3.522421748885	-0.275280574512	0.517262667275
C	-2.986462412883	0.085157449976	1.725969395359
C	-1.975428445301	1.027196049306	1.855244650534
C	-1.461330806557	1.594541169321	0.684132000889
C	-3.846342434815	-1.583668531957	-2.155919565504
C	-3.238519590973	-2.042798048285	-3.479952474922
C	-1.439147665704	1.375511630398	3.226821072147
C	0.037443449358	1.034353898131	3.417622317671
O	0.824090105307	2.013207748897	2.696467395942
C	2.126316647428	1.666469840898	2.426347394137
C	3.147760943575	1.895331952931	3.396877169949
C	4.486821290901	1.531576433471	3.033250891482
N	4.810729865947	1.001067803279	1.813325352995
C	3.828583215723	0.838855553257	0.944149421064
C	2.468803003802	1.151382911703	1.193088460882
C	2.902602697566	2.480979625435	4.669098630796
C	3.939546573629	2.674124764528	5.559140178235
C	5.262108651589	2.293739723036	5.213578832876
C	5.529556622768	1.739268413048	3.978744738398
C	-1.112977933532	2.491334945147	-4.048259890141
O	-4.521152975458	-1.082809818102	0.483816112346
H	-3.425161793501	3.858531758320	-4.085457590663
H	-5.866833501135	3.633424437104	-4.598511542293
H	-7.042929059048	1.518378582602	-3.920658746601
H	-3.467733221471	-0.411288212089	2.567239694903
H	-0.657947349974	2.325748343117	0.725288997144
H	-3.464442260639	-2.183390100025	-1.322966875942
H	-4.938806156541	-1.703145724512	-2.163532708071
H	-2.140464253330	-1.953915293225	-3.467874172054
H	-3.500092504122	-3.097646056500	-3.663584384372
H	-3.623007824226	-1.451200215574	-4.326344469363
H	-1.569494828606	2.452145736512	3.426865940692
H	-2.012294100930	0.835853355552	3.995494130713
H	0.265109149690	0.025523211827	3.034882193578
H	0.298926181107	1.070737280522	4.488330476878
H	4.105107256894	0.425916468020	-0.032430432643

H	1.711771826746	1.003572283884	0.421227150038
H	1.888150923054	2.789663156323	4.923921118964
H	3.744999229884	3.126731675668	6.533649722615
H	6.072251383123	2.450027208604	5.929139493739
H	6.541446245307	1.451570627320	3.687260733276
H	-1.648535307764	2.295414042179	-4.984806161577
H	-0.928035319041	3.573337590644	-3.950408341270
H	-0.144129495148	1.979266631756	-4.057999222473

SCF Done: E(RB3LYP) = -1465.98869542

Zero-point correction= 0.444158
Thermal correction to Energy= 0.471786
Thermal correction to Enthalpy= 0.472730
Thermal correction to Gibbs Free Energy= 0.383111
Sum of electronic and zero-point Energies= -1465.544538
Sum of electronic and thermal Energies= -1465.516909
Sum of electronic and thermal Enthalpies= -1465.515965
Sum of electronic and thermal Free Energies= -1465.605585

1	N	Isotropic =	-43.0122	Anisotropy =	469.1468
2	C	Isotropic =	38.3129	Anisotropy =	115.5152
3	C	Isotropic =	57.0765	Anisotropy =	125.2231
4	C	Isotropic =	62.2329	Anisotropy =	176.7765
5	C	Isotropic =	71.4644	Anisotropy =	160.8818
6	C	Isotropic =	48.9256	Anisotropy =	154.8195
7	N	Isotropic =	118.2626	Anisotropy =	89.6812
8	C	Isotropic =	27.3477	Anisotropy =	109.2172
9	C	Isotropic =	62.7449	Anisotropy =	136.1199
10	C	Isotropic =	41.1113	Anisotropy =	106.7941
11	N	Isotropic =	165.1880	Anisotropy =	58.6136
12	O	Isotropic =	-78.3555	Anisotropy =	576.7276
13	N	Isotropic =	-41.2280	Anisotropy =	254.8538
14	C	Isotropic =	50.5165	Anisotropy =	97.8653
15	C	Isotropic =	55.8579	Anisotropy =	174.5060
16	C	Isotropic =	65.8161	Anisotropy =	163.0014
17	C	Isotropic =	146.8100	Anisotropy =	37.2878
18	C	Isotropic =	175.6573	Anisotropy =	25.2947
19	C	Isotropic =	156.9927	Anisotropy =	14.9619
20	C	Isotropic =	112.8211	Anisotropy =	69.2251
21	O	Isotropic =	236.9556	Anisotropy =	100.0258
22	C	Isotropic =	28.5154	Anisotropy =	138.1227
23	C	Isotropic =	66.7298	Anisotropy =	177.2172
24	C	Isotropic =	42.6327	Anisotropy =	182.8038

25	N	Isotropic =	-54.7425	Anisotropy =	485.0540
26	C	Isotropic =	41.3528	Anisotropy =	160.9739
27	C	Isotropic =	76.7463	Anisotropy =	135.4966
28	C	Isotropic =	69.7205	Anisotropy =	168.8611
29	C	Isotropic =	66.3836	Anisotropy =	172.7686
30	C	Isotropic =	63.3650	Anisotropy =	175.4432
31	C	Isotropic =	62.7319	Anisotropy =	152.4542
32	C	Isotropic =	154.0541	Anisotropy =	47.0375
33	O	Isotropic =	-66.0083	Anisotropy =	368.6778
34	H	Isotropic =	23.9324	Anisotropy =	8.9581
35	H	Isotropic =	24.2179	Anisotropy =	4.5641
36	H	Isotropic =	23.1217	Anisotropy =	4.7052
37	H	Isotropic =	23.4246	Anisotropy =	7.3101
38	H	Isotropic =	23.1787	Anisotropy =	11.3734
39	H	Isotropic =	27.8739	Anisotropy =	5.6807
40	H	Isotropic =	26.7676	Anisotropy =	8.2716
41	H	Isotropic =	30.3744	Anisotropy =	7.2776
42	H	Isotropic =	30.3498	Anisotropy =	11.2864
43	H	Isotropic =	30.3095	Anisotropy =	4.9175
44	H	Isotropic =	28.0965	Anisotropy =	6.6050
45	H	Isotropic =	28.9647	Anisotropy =	8.1608
46	H	Isotropic =	27.8807	Anisotropy =	5.6194
47	H	Isotropic =	26.5358	Anisotropy =	5.7396
48	H	Isotropic =	22.4700	Anisotropy =	8.0406
49	H	Isotropic =	23.9132	Anisotropy =	6.7678
50	H	Isotropic =	23.1273	Anisotropy =	10.7375
51	H	Isotropic =	23.6857	Anisotropy =	6.2565
52	H	Isotropic =	23.5229	Anisotropy =	5.1816
53	H	Isotropic =	23.3274	Anisotropy =	6.2285
54	H	Isotropic =	28.8031	Anisotropy =	7.3196
55	H	Isotropic =	27.9525	Anisotropy =	9.9234
56	H	Isotropic =	27.2118	Anisotropy =	7.6380

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.529679175257	-1.450773564787	-1.818869116713
C	-1.348665607766	-2.131839733561	-1.548930033369
C	-0.503541841658	-1.678537222359	-0.527694524507
C	-0.779188823308	-0.472008261994	0.129560729809
C	-1.909650930366	0.251046975197	-0.248098399207
C	-2.767057240591	-0.246344438021	-1.211243506208
N	0.633389212859	-2.451993496893	-0.181562550685
C	0.534530526575	-3.780184652986	0.213523445669
C	-0.591428912707	-4.636505839942	-0.278533280071
C	-1.197905612191	-4.507703917396	-1.551685585032
N	-1.095556178388	-3.307675909756	-2.265963285689
O	1.405926404400	-4.274407641002	0.926082066415
N	-1.859507430617	-5.517270106766	-2.133029087448
C	-2.104091998135	-6.611532684468	-1.406113537520
C	-1.736620655482	-6.769299330969	-0.061012967038
C	-0.903705392710	-5.780014486626	0.466071509358
C	-1.209993477330	-3.311514511915	-3.739078520514
C	0.048401279599	-3.885060293762	-4.386765493200
C	-2.248525175550	-7.923586681065	0.764354445821
C	-3.657286201082	-7.693805370133	1.332551286802
O	-3.684611228845	-6.617779985227	2.291189344993
C	-4.088174620390	-5.370316451917	1.958337037898
C	-4.107587431149	-4.428486981774	3.041812979623
C	-4.502468231235	-3.084367273356	2.747388257200
N	-4.848920354383	-2.659894243317	1.490460776413
C	-4.821933649859	-3.569987906802	0.532936601936
C	-4.468213766270	-4.930536559360	0.700862350535
C	-3.750439869052	-4.779727600926	4.370919912657
C	-3.787066832501	-3.835006226198	5.378175347978
C	-4.179972502333	-2.503229002140	5.093965745424
C	-4.528544769569	-2.138153380897	3.808969840619
C	1.843710311894	-1.742672870765	0.251770234599
O	-3.386163937674	-1.930589390869	-2.645850469138
H	-0.126336059474	-0.106630566565	0.919884258389
H	-2.149907102565	1.201651778002	0.228462715272
H	-3.690504507632	0.232033283403	-1.529450252769
H	-2.648081888536	-7.411930516598	-1.920589125970
H	-0.460399576759	-5.893829896869	1.456864420702
H	-2.100997555269	-3.877290220701	-4.041255558744

H	-1.363408024924	-2.271354794928	-4.049994697041
H	0.942669632476	-3.309385764272	-4.099634438574
H	0.202891964929	-4.935514626318	-4.094642352673
H	-0.049825061633	-3.851637080376	-5.483977260339
H	-2.299655651893	-8.841836191054	0.155497150273
H	-1.563372036898	-8.126158002873	1.602083179520
H	-4.396357490971	-7.522947961642	0.536281017016
H	-3.969654709125	-8.581152584720	1.901292627648
H	-5.069158377441	-3.222320351113	-0.476858310644
H	-4.469923381596	-5.581719294529	-0.169883493517
H	-3.448812474542	-5.805993129392	4.580558380484
H	-3.512227972072	-4.113047733757	6.397828578187
H	-4.205298287550	-1.763806821839	5.897557853632
H	-4.832066827967	-1.117848495940	3.566639537681
H	1.817873111531	-1.490683217109	1.324529252311
H	2.709815017121	-2.391536719420	0.077549004675
H	1.944361371863	-0.824752048640	-0.339904042930

SCF Done: E(RB3LYP) = -1465.99493180

Zero-point correction= 0.444801
Thermal correction to Energy= 0.472082
Thermal correction to Enthalpy= 0.473026
Thermal correction to Gibbs Free Energy= 0.385630
Sum of electronic and zero-point Energies= -1465.550131
Sum of electronic and thermal Energies= -1465.522850
Sum of electronic and thermal Enthalpies= -1465.521906
Sum of electronic and thermal Free Energies= -1465.609302

1	N	Isotropic =	-45.7623	Anisotropy =	266.7867
2	C	Isotropic =	44.6230	Anisotropy =	104.8666
3	C	Isotropic =	50.8254	Anisotropy =	126.1438
4	C	Isotropic =	76.8044	Anisotropy =	159.5473
5	C	Isotropic =	69.9917	Anisotropy =	167.2499
6	C	Isotropic =	55.5802	Anisotropy =	114.0932
7	N	Isotropic =	123.9282	Anisotropy =	87.3935
8	C	Isotropic =	26.7845	Anisotropy =	104.6500
9	C	Isotropic =	73.5425	Anisotropy =	129.0410
10	C	Isotropic =	33.5310	Anisotropy =	125.2313
11	N	Isotropic =	156.7260	Anisotropy =	70.5073
12	O	Isotropic =	-92.8676	Anisotropy =	603.3824
13	N	Isotropic =	-31.0511	Anisotropy =	454.8782
14	C	Isotropic =	41.9578	Anisotropy =	150.3835
15	C	Isotropic =	61.8473	Anisotropy =	174.6530

16	C	Isotropic =	51.0771	Anisotropy =	182.1896
17	C	Isotropic =	146.8487	Anisotropy =	39.6411
18	C	Isotropic =	176.1531	Anisotropy =	25.1779
19	C	Isotropic =	154.6330	Anisotropy =	15.5287
20	C	Isotropic =	123.0052	Anisotropy =	52.2380
21	O	Isotropic =	200.9307	Anisotropy =	135.5408
22	C	Isotropic =	32.0514	Anisotropy =	140.3645
23	C	Isotropic =	70.8981	Anisotropy =	171.6635
24	C	Isotropic =	43.9496	Anisotropy =	183.0804
25	N	Isotropic =	-34.9463	Anisotropy =	457.3777
26	C	Isotropic =	43.4324	Anisotropy =	163.8225
27	C	Isotropic =	92.1577	Anisotropy =	141.8786
28	C	Isotropic =	69.9256	Anisotropy =	175.5122
29	C	Isotropic =	68.1954	Anisotropy =	170.2364
30	C	Isotropic =	63.8351	Anisotropy =	175.0190
31	C	Isotropic =	64.3505	Anisotropy =	150.4570
32	C	Isotropic =	155.3446	Anisotropy =	44.1734
33	O	Isotropic =	-73.4276	Anisotropy =	379.7736
34	H	Isotropic =	24.8657	Anisotropy =	6.6865
35	H	Isotropic =	24.3495	Anisotropy =	2.8345
36	H	Isotropic =	23.3445	Anisotropy =	5.0588
37	H	Isotropic =	22.8612	Anisotropy =	7.4357
38	H	Isotropic =	24.0290	Anisotropy =	7.4263
39	H	Isotropic =	26.6513	Anisotropy =	6.6635
40	H	Isotropic =	28.4624	Anisotropy =	6.6040
41	H	Isotropic =	30.4362	Anisotropy =	7.9666
42	H	Isotropic =	30.0281	Anisotropy =	5.4895
43	H	Isotropic =	30.3299	Anisotropy =	11.4985
44	H	Isotropic =	28.2795	Anisotropy =	8.2358
45	H	Isotropic =	28.3837	Anisotropy =	6.9639
46	H	Isotropic =	26.8664	Anisotropy =	4.8729
47	H	Isotropic =	26.8588	Anisotropy =	8.3387
48	H	Isotropic =	23.4698	Anisotropy =	5.7344
49	H	Isotropic =	25.8867	Anisotropy =	5.7919
50	H	Isotropic =	23.2391	Anisotropy =	10.3819
51	H	Isotropic =	23.9457	Anisotropy =	5.5160
52	H	Isotropic =	23.7720	Anisotropy =	5.1472
53	H	Isotropic =	23.8466	Anisotropy =	6.6787
54	H	Isotropic =	28.3499	Anisotropy =	9.4283
55	H	Isotropic =	27.9172	Anisotropy =	9.1890
56	H	Isotropic =	28.8693	Anisotropy =	8.5710

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.925609885813	-6.661861323034	0.996191744186
C	-1.651741241450	-6.126573231457	1.122970242326
C	-1.297940056699	-5.452938999021	2.300520124534
C	-2.173762393780	-5.438065770363	3.393763432564
C	-3.399215184887	-6.093010102452	3.276459331960
C	-3.758146089649	-6.691315351946	2.084244961500
N	-0.040592677848	-4.801788109831	2.369524359975
C	0.342977038191	-3.828916541852	1.454709253768
C	-0.209478433413	-3.837668572161	0.063142949298
C	-0.542736520543	-5.011796995701	-0.654684284065
N	-0.780834202684	-6.212098515241	0.025906466964
O	1.179989778541	-2.985813838410	1.770937362844
N	-0.608486428740	-5.038578132182	-1.992331976038
C	-0.523761161701	-3.877584086624	-2.649479756234
C	-0.405254818849	-2.623126392853	-2.032373471787
C	-0.172367160145	-2.637028257008	-0.655081581290
C	-0.571464093620	-7.493698458699	-0.681995488560
C	-0.361315384082	-8.649029533591	0.289311328692
C	-0.561494439946	-1.345233460440	-2.818679857056
C	-2.025231679461	-0.949670267584	-3.066109238566
O	-2.706055525778	-0.591275666342	-1.847080297702
C	-3.509843166537	-1.459573855519	-1.191726904121
C	-4.180293834328	-0.919422806902	-0.042694011813
C	-5.026394667375	-1.797854830237	0.706929699825
N	-5.215284317438	-3.117404917873	0.385211444697
C	-4.581617005099	-3.559306434814	-0.686719942436
C	-3.733604970099	-2.787339769498	-1.517001743691
C	-4.033137184093	0.432553350622	0.367273511997
C	-4.702989000891	0.903130968142	1.480058671491
C	-5.543014838908	0.039037328077	2.225992898583
C	-5.699484800923	-1.279474825941	1.847689529274
C	0.651887653943	-4.771208862126	3.663822254274
O	-3.325455883369	-7.148426448440	-0.123625060478
H	-1.905108638281	-4.925723131244	4.315487269812
H	-4.102424415222	-6.117465653297	4.109158364726
H	-4.710239915451	-7.181655319660	1.894827310652
H	-0.579337272792	-3.945288675553	-3.742003755449
H	0.069358694817	-1.716531157939	-0.120697174097
H	-1.411933281859	-7.708244576148	-1.355296483522
H	0.327742618606	-7.344382203010	-1.295938509083

H	-1.273066549834	-8.869904835626	0.865336432619
H	-0.104284027598	-9.556113645828	-0.279705417635
H	0.458978542209	-8.439863147858	0.994367325983
H	-0.057528646973	-0.514268934391	-2.301189692429
H	-0.090645227832	-1.443389521383	-3.811335817253
H	-2.056211413070	-0.037733569399	-3.679160169045
H	-2.576953453521	-1.737413892593	-3.599936237837
H	-4.709515272894	-4.621538827135	-0.926014384561
H	-3.254719119020	-3.268250967138	-2.366323887720
H	-3.384636552408	1.090048804605	-0.211809686641
H	-4.586119194661	1.944273012975	1.788063205114
H	-6.067654754521	0.420855071476	3.104709012111
H	-6.339630715436	-1.963153409082	2.408630687233
H	0.477341560278	-5.723155920724	4.179570021956
H	1.724965099922	-4.640581351518	3.482146208036
H	0.310884513012	-3.937745438230	4.299429422113

SCF Done: E(RB3LYP) = -1465.99430943

Zero-point correction= 0.444957
Thermal correction to Energy= 0.472181
Thermal correction to Enthalpy= 0.473125
Thermal correction to Gibbs Free Energy= 0.385690
Sum of electronic and zero-point Energies= -1465.549352
Sum of electronic and thermal Energies= -1465.522129
Sum of electronic and thermal Enthalpies= -1465.521184
Sum of electronic and thermal Free Energies= -1465.608620

1	N	Isotropic =	-48.3694	Anisotropy =	264.2329
2	C	Isotropic =	46.3275	Anisotropy =	108.3732
3	C	Isotropic =	49.4169	Anisotropy =	129.4540
4	C	Isotropic =	76.9463	Anisotropy =	160.4457
5	C	Isotropic =	69.8308	Anisotropy =	167.7420
6	C	Isotropic =	55.6422	Anisotropy =	113.1388
7	N	Isotropic =	123.0439	Anisotropy =	88.4605
8	C	Isotropic =	26.8958	Anisotropy =	104.3508
9	C	Isotropic =	74.6097	Anisotropy =	128.2216
10	C	Isotropic =	32.1323	Anisotropy =	126.3824
11	N	Isotropic =	154.6125	Anisotropy =	79.3862
12	O	Isotropic =	-92.0582	Anisotropy =	604.0313
13	N	Isotropic =	-32.9479	Anisotropy =	447.9567
14	C	Isotropic =	41.8454	Anisotropy =	151.5999
15	C	Isotropic =	61.6165	Anisotropy =	175.6817
16	C	Isotropic =	51.2817	Anisotropy =	181.0622

17	C	Isotropic =	147.2940	Anisotropy =	41.1250
18	C	Isotropic =	177.8162	Anisotropy =	22.3550
19	C	Isotropic =	154.5673	Anisotropy =	15.3787
20	C	Isotropic =	122.6657	Anisotropy =	52.0514
21	O	Isotropic =	200.0554	Anisotropy =	136.1577
22	C	Isotropic =	32.0150	Anisotropy =	140.3551
23	C	Isotropic =	70.8461	Anisotropy =	171.5286
24	C	Isotropic =	43.9362	Anisotropy =	183.0355
25	N	Isotropic =	-35.2007	Anisotropy =	457.2095
26	C	Isotropic =	43.1996	Anisotropy =	163.7315
27	C	Isotropic =	91.8079	Anisotropy =	141.5034
28	C	Isotropic =	69.9659	Anisotropy =	174.9598
29	C	Isotropic =	68.2777	Anisotropy =	169.7683
30	C	Isotropic =	63.9237	Anisotropy =	174.6934
31	C	Isotropic =	64.2193	Anisotropy =	150.4541
32	C	Isotropic =	155.4333	Anisotropy =	43.9683
33	O	Isotropic =	-70.0566	Anisotropy =	370.8016
34	H	Isotropic =	24.8422	Anisotropy =	6.6381
35	H	Isotropic =	24.3272	Anisotropy =	2.7793
36	H	Isotropic =	23.3618	Anisotropy =	5.0641
37	H	Isotropic =	22.8642	Anisotropy =	7.5055
38	H	Isotropic =	24.0054	Anisotropy =	7.6133
39	H	Isotropic =	26.6535	Anisotropy =	6.7354
40	H	Isotropic =	27.8341	Anisotropy =	6.8113
41	H	Isotropic =	30.6042	Anisotropy =	5.5057
42	H	Isotropic =	30.1930	Anisotropy =	11.7625
43	H	Isotropic =	30.4959	Anisotropy =	8.1017
44	H	Isotropic =	28.4196	Anisotropy =	6.9282
45	H	Isotropic =	28.3201	Anisotropy =	8.1968
46	H	Isotropic =	26.8569	Anisotropy =	8.2869
47	H	Isotropic =	26.9132	Anisotropy =	4.7253
48	H	Isotropic =	23.4629	Anisotropy =	5.6771
49	H	Isotropic =	25.9101	Anisotropy =	5.7430
50	H	Isotropic =	23.2437	Anisotropy =	10.4172
51	H	Isotropic =	23.9534	Anisotropy =	5.5042
52	H	Isotropic =	23.7742	Anisotropy =	5.1639
53	H	Isotropic =	23.8223	Anisotropy =	6.7939
54	H	Isotropic =	28.8445	Anisotropy =	8.3830
55	H	Isotropic =	27.8934	Anisotropy =	9.3092
56	H	Isotropic =	28.3191	Anisotropy =	9.4637

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.834642360673	-6.603349260439	1.367740690308
C	-1.554459976860	-6.088238412561	1.205202801638
C	-0.960413381728	-5.363425542794	2.246403020564
C	-1.595747334055	-5.273843699011	3.492250799809
C	-2.826331963201	-5.906769015763	3.661486805132
C	-3.428268310260	-6.557212573540	2.601011343436
N	0.290397620767	-4.734849136216	2.020346072645
C	0.479078032711	-3.811341443161	0.998876719320
C	-0.332140697616	-3.893589971440	-0.257269359597
C	-0.803046081641	-5.101213670546	-0.828024422593
N	-0.940322798525	-6.251217592399	-0.042724526826
O	1.357677931493	-2.957576520648	1.099332661264
N	-1.107607574898	-5.203989927999	-2.128872788906
C	-1.147336284088	-4.084241302118	-2.856585321083
C	-0.916496373804	-2.797390579951	-2.346322428147
C	-0.428252729255	-2.736320813197	-1.039596930569
C	-0.900206528657	-7.586543380344	-0.674354652453
C	0.522744550538	-7.961195547379	-1.082953798055
C	-1.220915019826	-1.565310533704	-3.161437670640
C	-2.706600239273	-1.173670086498	-3.149840074626
O	-3.145274351617	-0.737813565599	-1.847731595858
C	-3.802447523207	-1.559976284563	-0.998038711154
C	-4.237815252743	-0.946955613462	0.225022042090
C	-4.915810956191	-1.772463434787	1.177919962125
N	-5.155042263370	-3.108185819355	0.980906053064
C	-4.742762520333	-3.618231850198	-0.166287290654
C	-4.080553543739	-2.902885966931	-1.193178598313
C	-4.020917903504	0.426503307783	0.514684559589
C	-4.463482811774	0.968773919264	1.705673521609
C	-5.137124838594	0.157485716510	2.652672234736
C	-5.356609967363	-1.180816607230	2.393931175987
C	1.230326229130	-4.645085136636	3.144790530552
O	-3.454614333231	-7.137729706769	0.378224014215
H	-1.140233884190	-4.720429988949	4.311044646859
H	-3.345204451192	-5.873448050958	4.619687144412
H	-4.404843107052	-7.034542230870	2.636985400707
H	-1.401916575498	-4.214207756036	-3.914699721410
H	-0.088359774220	-1.790179930179	-0.614616723505
H	-1.290199053597	-8.299737221080	0.061120368409
H	-1.575683915247	-7.606930705313	-1.539387191478
H	1.200771571523	-7.961850309065	-0.214710215772

H	0.527547617919	-8.969305050570	-1.528387511185
H	0.919726018816	-7.260082651695	-1.833705537163
H	-0.631134393170	-0.709908556217	-2.797159049404
H	-0.946341274170	-1.723887381858	-4.217956555035
H	-2.857078446470	-0.299856156797	-3.799558431122
H	-3.345681362472	-1.988239629262	-3.521258293502
H	-4.906757569741	-4.692759976262	-0.309340454367
H	-3.776845822749	-3.437117097561	-2.090021704801
H	-3.502050828379	1.042958852030	-0.219365043810
H	-4.294837071408	2.026118342013	1.920360965428
H	-5.482821991065	0.595879875698	3.591545589072
H	-5.871582223340	-1.824644697886	3.109599818555
H	1.162841961868	-5.567277651856	3.734558431080
H	2.244774262301	-4.536327088565	2.743898664854
H	1.025569866920	-3.776024887080	3.791198564567

SCF Done: E(RB3LYP) = -1465.99499513

Zero-point correction= 0.444794
Thermal correction to Energy= 0.472067
Thermal correction to Enthalpy= 0.473011
Thermal correction to Gibbs Free Energy= 0.385371
Sum of electronic and zero-point Energies= -1465.550202
Sum of electronic and thermal Energies= -1465.522928
Sum of electronic and thermal Enthalpies= -1465.521984
Sum of electronic and thermal Free Energies= -1465.609624

1	N	Isotropic =	-45.3903	Anisotropy =	265.8903
2	C	Isotropic =	44.7653	Anisotropy =	104.9786
3	C	Isotropic =	51.1398	Anisotropy =	125.5641
4	C	Isotropic =	77.1189	Anisotropy =	158.9278
5	C	Isotropic =	69.9095	Anisotropy =	168.1502
6	C	Isotropic =	55.0675	Anisotropy =	114.4800
7	N	Isotropic =	124.1414	Anisotropy =	87.3720
8	C	Isotropic =	26.5131	Anisotropy =	103.9275
9	C	Isotropic =	73.9095	Anisotropy =	128.8355
10	C	Isotropic =	33.5265	Anisotropy =	125.8315
11	N	Isotropic =	155.7232	Anisotropy =	71.0370
12	O	Isotropic =	-94.2858	Anisotropy =	603.1586
13	N	Isotropic =	-31.0401	Anisotropy =	452.4061
14	C	Isotropic =	41.9274	Anisotropy =	150.9071
15	C	Isotropic =	61.7851	Anisotropy =	174.7946
16	C	Isotropic =	51.0844	Anisotropy =	182.1312
17	C	Isotropic =	147.0028	Anisotropy =	39.4408

18	C	Isotropic =	176.2654	Anisotropy =	25.2543
19	C	Isotropic =	154.6826	Anisotropy =	15.2996
20	C	Isotropic =	122.6183	Anisotropy =	51.8122
21	O	Isotropic =	200.0503	Anisotropy =	136.0103
22	C	Isotropic =	32.1835	Anisotropy =	140.0458
23	C	Isotropic =	70.7945	Anisotropy =	171.5624
24	C	Isotropic =	44.0003	Anisotropy =	182.8668
25	N	Isotropic =	-35.1820	Anisotropy =	457.4978
26	C	Isotropic =	43.3064	Anisotropy =	164.1522
27	C	Isotropic =	91.9561	Anisotropy =	141.3093
28	C	Isotropic =	70.1716	Anisotropy =	175.2539
29	C	Isotropic =	68.2157	Anisotropy =	169.7487
30	C	Isotropic =	63.9690	Anisotropy =	174.7347
31	C	Isotropic =	64.1740	Anisotropy =	150.5532
32	C	Isotropic =	155.3351	Anisotropy =	44.0565
33	O	Isotropic =	-72.6283	Anisotropy =	377.9063
34	H	Isotropic =	24.8413	Anisotropy =	6.7777
35	H	Isotropic =	24.3056	Anisotropy =	2.8639
36	H	Isotropic =	23.3021	Anisotropy =	5.1433
37	H	Isotropic =	22.8757	Anisotropy =	7.4777
38	H	Isotropic =	24.0251	Anisotropy =	7.4938
39	H	Isotropic =	28.4013	Anisotropy =	6.5739
40	H	Isotropic =	26.6464	Anisotropy =	6.5515
41	H	Isotropic =	30.3968	Anisotropy =	8.0468
42	H	Isotropic =	30.3226	Anisotropy =	11.4897
43	H	Isotropic =	29.9890	Anisotropy =	5.5100
44	H	Isotropic =	28.4374	Anisotropy =	6.8955
45	H	Isotropic =	28.3148	Anisotropy =	8.2050
46	H	Isotropic =	26.8567	Anisotropy =	8.2710
47	H	Isotropic =	26.9279	Anisotropy =	4.7069
48	H	Isotropic =	23.4490	Anisotropy =	5.7387
49	H	Isotropic =	25.9478	Anisotropy =	5.6383
50	H	Isotropic =	23.2509	Anisotropy =	10.4591
51	H	Isotropic =	23.9653	Anisotropy =	5.5204
52	H	Isotropic =	23.7846	Anisotropy =	5.1620
53	H	Isotropic =	23.8281	Anisotropy =	6.8050
54	H	Isotropic =	28.8365	Anisotropy =	8.5443
55	H	Isotropic =	27.8912	Anisotropy =	9.2202
56	H	Isotropic =	28.3168	Anisotropy =	9.4865

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.555066084783	-5.586787799803	2.158683375457
C	-0.708772657649	-5.777826366159	0.792717723385
C	-1.823399758150	-6.479482985283	0.312654863902
C	-2.705284288685	-7.098522354709	1.207978975426
C	-2.454179206291	-6.989793028551	2.575186401769
C	-1.388908382655	-6.237371029456	3.030330189465
N	-2.034073034596	-6.563707203773	-1.086703841636
C	-2.141687713490	-5.436901009382	-1.892200380920
C	-1.464886003445	-4.159432631788	-1.502340459828
C	-0.234271523929	-4.088855409746	-0.805682595503
N	0.226342916382	-5.189568537497	-0.072373042526
O	-2.752789072701	-5.500744147353	-2.957105054951
N	0.549087030578	-3.003010338993	-0.844305029147
C	0.065688484701	-1.898683120591	-1.422204319832
C	-1.222588614350	-1.786402849725	-1.966119882318
C	-1.954306592907	-2.972681238558	-2.059650020007
C	1.679399601644	-5.342989863747	0.156860596625
C	2.051294322128	-6.783164970313	0.488461785389
C	-1.785793615515	-0.451356526416	-2.385382370025
C	-2.365663393173	0.363712298854	-1.219209634543
O	-3.514932549576	-0.275952121936	-0.629305352195
C	-3.424873902645	-1.004889135566	0.506796413451
C	-4.672045625248	-1.515207825375	1.002125527801
C	-4.639149808986	-2.312648681951	2.190453342049
N	-3.482662334691	-2.615220415965	2.862023451791
C	-2.364981826647	-2.115016681147	2.365840402614
C	-2.269466607997	-1.301024044760	1.211337127123
C	-5.913927857189	-1.261969498252	0.361073850570
C	-7.086571560031	-1.776308380420	0.879532286227
C	-7.061341033273	-2.564030928331	2.057499082448
C	-5.865666238482	-2.825215988840	2.696358911582
C	-2.634899856253	-7.792197429093	-1.621449396751
O	0.373968158161	-4.826141835163	2.615117426186
H	-3.569049998477	-7.652329226011	0.845416139745
H	-3.107685457479	-7.469752127754	3.303921503984
H	-1.149549637401	-6.065641180624	4.077228044767
H	0.739510316923	-1.034375883076	-1.432883749586
H	-2.906400968109	-3.000604069981	-2.592513559159
H	2.157040815688	-5.033887597850	-0.783488418255
H	2.021648311453	-4.666586678748	0.951324841094
H	3.147706801498	-6.868135416121	0.546073091520
H	1.645681502989	-7.095929247959	1.462805954987

H	1.691388975541	-7.481667887635	-0.283772607218
H	-1.001321723798	0.172322820038	-2.846045268085
H	-2.574824947904	-0.591469746013	-3.140418462947
H	-1.606215209235	0.578968129912	-0.453278815821
H	-2.745261159529	1.322859010895	-1.599336147547
H	-1.438036251327	-2.383398831054	2.885752509329
H	-1.287824881988	-0.959819973744	0.891815607871
H	-5.923759875076	-0.655089046553	-0.544315918681
H	-8.037707081826	-1.576448091334	0.381648756805
H	-7.994208011046	-2.966026978566	2.459171118240
H	-5.822256292315	-3.431547936979	3.603201695835
H	-2.344255631236	-7.893702460993	-2.673485085259
H	-2.256005119955	-8.647298309889	-1.048914467496
H	-3.735905847649	-7.772877190174	-1.573047117202

SCF Done: E(RB3LYP) = -1465.99428584

Zero-point correction= 0.444844
Thermal correction to Energy= 0.472117
Thermal correction to Enthalpy= 0.473061
Thermal correction to Gibbs Free Energy= 0.385779
Sum of electronic and zero-point Energies= -1465.549442
Sum of electronic and thermal Energies= -1465.522169
Sum of electronic and thermal Enthalpies= -1465.521225
Sum of electronic and thermal Free Energies= -1465.608507

1	N	Isotropic =	-48.7754	Anisotropy =	265.2137
2	C	Isotropic =	46.0979	Anisotropy =	108.6208
3	C	Isotropic =	49.7286	Anisotropy =	129.1411
4	C	Isotropic =	77.1737	Anisotropy =	159.7498
5	C	Isotropic =	70.0144	Anisotropy =	168.1137
6	C	Isotropic =	55.6119	Anisotropy =	112.9921
7	N	Isotropic =	122.9929	Anisotropy =	87.9296
8	C	Isotropic =	26.9199	Anisotropy =	104.8138
9	C	Isotropic =	74.5982	Anisotropy =	128.4466
10	C	Isotropic =	32.3084	Anisotropy =	126.5097
11	N	Isotropic =	155.1028	Anisotropy =	79.4861
12	O	Isotropic =	-91.6673	Anisotropy =	604.6631
13	N	Isotropic =	-32.8845	Anisotropy =	449.6352
14	C	Isotropic =	42.1152	Anisotropy =	151.7297
15	C	Isotropic =	61.9137	Anisotropy =	175.5128
16	C	Isotropic =	51.3455	Anisotropy =	181.9089
17	C	Isotropic =	147.2649	Anisotropy =	41.1056
18	C	Isotropic =	177.9138	Anisotropy =	22.2322

19	C	Isotropic =	155.1173	Anisotropy =	15.6813
20	C	Isotropic =	122.9957	Anisotropy =	52.1373
21	O	Isotropic =	200.9160	Anisotropy =	135.2657
22	C	Isotropic =	32.0248	Anisotropy =	140.6872
23	C	Isotropic =	70.8534	Anisotropy =	171.7792
24	C	Isotropic =	44.0476	Anisotropy =	183.1405
25	N	Isotropic =	-35.0173	Anisotropy =	457.6759
26	C	Isotropic =	43.4205	Anisotropy =	163.8116
27	C	Isotropic =	91.8741	Anisotropy =	141.6832
28	C	Isotropic =	70.0505	Anisotropy =	175.2604
29	C	Isotropic =	68.1129	Anisotropy =	170.1662
30	C	Isotropic =	63.8719	Anisotropy =	174.8913
31	C	Isotropic =	64.2365	Anisotropy =	150.8164
32	C	Isotropic =	155.3190	Anisotropy =	43.9326
33	O	Isotropic =	-70.7262	Anisotropy =	373.4066
34	H	Isotropic =	24.8652	Anisotropy =	6.5842
35	H	Isotropic =	24.3260	Anisotropy =	2.7673
36	H	Isotropic =	23.3814	Anisotropy =	5.0228
37	H	Isotropic =	22.9025	Anisotropy =	7.4732
38	H	Isotropic =	23.9793	Anisotropy =	7.5310
39	H	Isotropic =	27.8756	Anisotropy =	6.8249
40	H	Isotropic =	26.6839	Anisotropy =	6.7554
41	H	Isotropic =	30.2146	Anisotropy =	11.7940
42	H	Isotropic =	30.6179	Anisotropy =	5.5002
43	H	Isotropic =	30.4877	Anisotropy =	8.1296
44	H	Isotropic =	28.3449	Anisotropy =	8.2143
45	H	Isotropic =	28.3827	Anisotropy =	7.0841
46	H	Isotropic =	26.9241	Anisotropy =	4.8224
47	H	Isotropic =	26.8734	Anisotropy =	8.2956
48	H	Isotropic =	23.4545	Anisotropy =	5.7120
49	H	Isotropic =	25.8808	Anisotropy =	5.8693
50	H	Isotropic =	23.2381	Anisotropy =	10.3832
51	H	Isotropic =	23.9454	Anisotropy =	5.4960
52	H	Isotropic =	23.7769	Anisotropy =	5.1389
53	H	Isotropic =	23.8320	Anisotropy =	6.6975
54	H	Isotropic =	27.8902	Anisotropy =	9.3536
55	H	Isotropic =	28.8466	Anisotropy =	8.4000
56	H	Isotropic =	28.3180	Anisotropy =	9.4258

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.105471345100	-1.230137471558	-0.030994629494
C	-0.801699951682	-1.437589046771	-1.065433440947
C	-1.766107937368	-0.461163361218	-1.349327970438
C	-1.762587990120	0.756106405666	-0.654431405773
C	-0.781320803412	0.972319672430	0.311568131984
C	0.137861909435	-0.016640159526	0.605009734104
N	-2.722582538839	-0.703958454265	-2.368560784374
C	-3.561694751858	-1.807846548169	-2.378565002940
C	-3.167146480481	-3.075056972697	-1.682363348884
C	-1.836454719646	-3.537287383343	-1.542922207238
N	-0.754499507300	-2.663413173165	-1.736836458130
O	-4.618011890056	-1.766835259881	-3.007526241796
N	-1.548106320587	-4.816249331226	-1.270426277200
C	-2.557175749757	-5.654753654401	-1.012590661088
C	-3.911083753613	-5.288866036104	-0.997399838166
C	-4.195637017526	-3.976310245220	-1.381900712732
C	0.533364737596	-3.192329671115	-2.232179395674
C	0.444138270323	-3.564873506381	-3.710725871026
C	-4.992635174412	-6.275486736150	-0.627131178422
C	-5.367489834134	-6.275271319785	0.857611807512
O	-4.266943877619	-6.756241214885	1.655118516591
C	-3.596501813437	-5.961575917288	2.518438133444
C	-2.605579167344	-6.632089734974	3.312749445849
C	-1.858932090630	-5.846713051895	4.247459235666
N	-2.048408762127	-4.499245042142	4.416834456637
C	-2.971265421675	-3.934456307958	3.659509475047
C	-3.771547755108	-4.599255317953	2.699062811853
C	-2.347689628411	-8.024373235397	3.202112954754
C	-1.381591380633	-8.621417727404	3.988612708002
C	-0.637970234723	-7.849075057891	4.915500311602
C	-0.872432026608	-6.494255125564	5.041249875489
C	-3.157371825909	0.436242169243	-3.186630253698
O	0.926182010711	-2.152433458266	0.312850775460
H	-2.508517956305	1.519223886681	-0.867566613501
H	-0.735503730404	1.912128027488	0.862166657016
H	0.914535592307	0.060060046940	1.362587759636
H	-2.272324802913	-6.691781177654	-0.804821490054
H	-5.227303870050	-3.642293934135	-1.506726008547
H	1.282541316816	-2.407876670728	-2.076446375253
H	0.836617047775	-4.056052741806	-1.626077977114
H	-0.293854058116	-4.365078307402	-3.878728453408
H	0.159777610420	-2.695813917992	-4.325224769765
H	1.422691487789	-3.932262041660	-4.060443247759

H	-5.913178837161	-6.055853129968	-1.192358609045
H	-4.681846137765	-7.295678879670	-0.903006137527
H	-5.698478251956	-5.283481177428	1.192639971991
H	-6.188841362211	-6.986431031142	1.030716373028
H	-3.118428521933	-2.856666647779	3.794429659195
H	-4.491458921245	-4.019197760225	2.125201637130
H	-2.924660775558	-8.610928256150	2.487279725498
H	-1.188707604360	-9.692415102409	3.897831430102
H	0.123773513278	-8.330852693110	5.532560338339
H	-0.312141692285	-5.880162019044	5.748925574471
H	-3.985189465766	0.992974703601	-2.717822539333
H	-2.303108934459	1.106697368861	-3.339226796288
H	-3.509081514047	0.058472729981	-4.153602804785

SCF Done: E(RB3LYP) = -1465.99506535

Zero-point correction= 0.444684
Thermal correction to Energy= 0.472104
Thermal correction to Enthalpy= 0.473048
Thermal correction to Gibbs Free Energy= 0.383825
Sum of electronic and zero-point Energies= -1465.550381
Sum of electronic and thermal Energies= -1465.522961
Sum of electronic and thermal Enthalpies= -1465.522017
Sum of electronic and thermal Free Energies= -1465.611241

1	N	Isotropic =	-45.9210	Anisotropy =	264.3009
2	C	Isotropic =	45.1023	Anisotropy =	104.1131
3	C	Isotropic =	51.6355	Anisotropy =	124.1229
4	C	Isotropic =	76.7478	Anisotropy =	157.0123
5	C	Isotropic =	70.2910	Anisotropy =	165.3091
6	C	Isotropic =	55.7685	Anisotropy =	111.2539
7	N	Isotropic =	122.9083	Anisotropy =	85.6037
8	C	Isotropic =	26.8662	Anisotropy =	104.7410
9	C	Isotropic =	70.9176	Anisotropy =	131.6466
10	C	Isotropic =	33.7706	Anisotropy =	123.5662
11	N	Isotropic =	158.8750	Anisotropy =	65.7962
12	O	Isotropic =	-91.1325	Anisotropy =	598.9053
13	N	Isotropic =	-32.2459	Anisotropy =	454.7414
14	C	Isotropic =	40.6740	Anisotropy =	149.9154
15	C	Isotropic =	62.2466	Anisotropy =	172.7787
16	C	Isotropic =	50.9540	Anisotropy =	182.6565
17	C	Isotropic =	147.0109	Anisotropy =	38.4842
18	C	Isotropic =	176.1147	Anisotropy =	25.2337
19	C	Isotropic =	155.3242	Anisotropy =	16.2827

20	C	Isotropic =	123.9389	Anisotropy =	52.6324
21	O	Isotropic =	202.9256	Anisotropy =	130.5086
22	C	Isotropic =	31.9902	Anisotropy =	139.3142
23	C	Isotropic =	70.3451	Anisotropy =	170.8444
24	C	Isotropic =	43.7239	Anisotropy =	182.5151
25	N	Isotropic =	-35.9224	Anisotropy =	457.6007
26	C	Isotropic =	43.2554	Anisotropy =	161.1800
27	C	Isotropic =	93.0949	Anisotropy =	139.3041
28	C	Isotropic =	69.8532	Anisotropy =	175.6353
29	C	Isotropic =	67.6760	Anisotropy =	169.4392
30	C	Isotropic =	63.6040	Anisotropy =	175.1232
31	C	Isotropic =	63.8887	Anisotropy =	150.4661
32	C	Isotropic =	154.5509	Anisotropy =	44.2183
33	O	Isotropic =	-80.1992	Anisotropy =	394.4509
34	H	Isotropic =	24.5193	Anisotropy =	7.7850
35	H	Isotropic =	24.2925	Anisotropy =	3.9720
36	H	Isotropic =	23.5442	Anisotropy =	4.8439
37	H	Isotropic =	23.3370	Anisotropy =	6.0843
38	H	Isotropic =	23.3618	Anisotropy =	9.8263
39	H	Isotropic =	28.5060	Anisotropy =	6.3542
40	H	Isotropic =	27.0299	Anisotropy =	6.7616
41	H	Isotropic =	30.2961	Anisotropy =	4.9453
42	H	Isotropic =	30.5149	Anisotropy =	8.1661
43	H	Isotropic =	30.4875	Anisotropy =	11.3809
44	H	Isotropic =	28.5409	Anisotropy =	7.9067
45	H	Isotropic =	28.1868	Anisotropy =	7.0328
46	H	Isotropic =	26.7913	Anisotropy =	4.5461
47	H	Isotropic =	26.9375	Anisotropy =	8.0354
48	H	Isotropic =	23.2961	Anisotropy =	6.6362
49	H	Isotropic =	25.4681	Anisotropy =	7.4080
50	H	Isotropic =	23.0451	Anisotropy =	10.5517
51	H	Isotropic =	23.8256	Anisotropy =	5.8376
52	H	Isotropic =	23.6505	Anisotropy =	4.9375
53	H	Isotropic =	23.6212	Anisotropy =	6.1000
54	H	Isotropic =	27.9769	Anisotropy =	9.8575
55	H	Isotropic =	28.6732	Anisotropy =	7.9949
56	H	Isotropic =	27.6270	Anisotropy =	8.5048

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.304752566468	-1.804758299816	-0.860890101416
C	-0.876857370910	-1.871390012080	-1.588499559948
C	-1.711173120794	-0.746150553499	-1.658795057213
C	-1.319089475255	0.461763582080	-1.067202370514
C	-0.085819403702	0.520779051039	-0.419726981876
C	0.707853607483	-0.605995535205	-0.331185403615
N	-2.937427527881	-0.831582995722	-2.366868299789
C	-3.917497865388	-1.770519234816	-2.083932648714
C	-3.560917159507	-3.072285118679	-1.434082442300
C	-2.335318901772	-3.755723783290	-1.621978501231
N	-1.227883925510	-3.093732223299	-2.176222191295
O	-5.083603452746	-1.555747390854	-2.411485875815
N	-2.189661093849	-5.056519003460	-1.340332094442
C	-3.213090111173	-5.700870646281	-0.768115786090
C	-4.435275599586	-5.106239911896	-0.424327328946
C	-4.600193786332	-3.773961824430	-0.812601631164
C	-0.257322559015	-3.875467994083	-2.973297927851
C	0.530293070788	-2.990323794854	-3.931821588098
C	-5.518972166318	-5.879681005074	0.288297239414
C	-5.517921086275	-5.725846407057	1.812404803703
O	-4.346000391815	-6.332628444655	2.392785849387
C	-3.346145217384	-5.598107892595	2.928516821507
C	-2.318733243970	-6.358241027881	3.583328697990
C	-1.231926789240	-5.637597759511	4.172897760942
N	-1.132384193572	-4.270347288141	4.142753657946
C	-2.104492070387	-3.622537718208	3.526760433577
C	-3.227189699377	-4.218163225108	2.902825448465
C	-2.346481841203	-7.776008421030	3.664111620096
C	-1.331493081984	-8.459966421300	4.304823812588
C	-0.251443360043	-7.752319502780	4.889075001930
C	-0.204336171088	-6.374012855642	4.824343267290
C	-3.384289931419	0.354209111233	-3.110014116139
O	1.037091136764	-2.845568351616	-0.702508008223
H	-1.962080183110	1.338313377091	-1.116162429697
H	0.261366946801	1.446190292554	0.040256370412
H	1.668036290140	-0.654185884397	0.177376488933
H	-3.051454684918	-6.765507723712	-0.567267314483
H	-5.559928948938	-3.269280921816	-0.686578315185
H	0.426110003281	-4.435182179248	-2.321907411563
H	-0.861215968368	-4.600260708913	-3.538021263466
H	-0.138326553112	-2.397718902370	-4.576525578616
H	1.202187601337	-2.305167601036	-3.392800147399
H	1.156755995735	-3.625981118998	-4.577063289694
H	-6.510230238930	-5.550926115395	-0.065328168543

H	-5.433356535759	-6.951933743601	0.050980360771
H	-5.609989920977	-4.674600282621	2.117493385176
H	-6.368633135765	-6.279611248431	2.235977790554
H	-2.020788997051	-2.529926784153	3.500610384690
H	-3.955274851894	-3.576761922554	2.410589543975
H	-3.180701829106	-8.312441054602	3.211978775402
H	-1.359616157946	-9.550076568037	4.362754930710
H	0.546128673399	-8.302795390950	5.393058790876
H	0.617189546885	-5.808209697989	5.267982977018
H	-2.505773922902	0.859513976668	-3.528887028785
H	-4.046251395583	0.028489062242	-3.920570694999
H	-3.946541517229	1.056774038779	-2.473464656243

SCF Done: E(RB3LYP) = -1465.99446537

Zero-point correction= 0.444808
Thermal correction to Energy= 0.472176
Thermal correction to Enthalpy= 0.473120
Thermal correction to Gibbs Free Energy= 0.384017
Sum of electronic and zero-point Energies= -1465.549657
Sum of electronic and thermal Energies= -1465.522290
Sum of electronic and thermal Enthalpies= -1465.521345
Sum of electronic and thermal Free Energies= -1465.610448

1	N	Isotropic =	-48.8420	Anisotropy =	264.1080
2	C	Isotropic =	45.9759	Anisotropy =	106.5837
3	C	Isotropic =	50.4503	Anisotropy =	126.5400
4	C	Isotropic =	76.7525	Anisotropy =	157.2279
5	C	Isotropic =	70.0064	Anisotropy =	166.0455
6	C	Isotropic =	55.6218	Anisotropy =	110.7203
7	N	Isotropic =	122.5835	Anisotropy =	86.6742
8	C	Isotropic =	26.9105	Anisotropy =	104.7867
9	C	Isotropic =	72.0466	Anisotropy =	131.0233
10	C	Isotropic =	32.4907	Anisotropy =	123.9574
11	N	Isotropic =	157.0341	Anisotropy =	77.0689
12	O	Isotropic =	-89.2284	Anisotropy =	599.8227
13	N	Isotropic =	-34.1256	Anisotropy =	446.3934
14	C	Isotropic =	40.7011	Anisotropy =	149.5953
15	C	Isotropic =	62.0744	Anisotropy =	174.0110
16	C	Isotropic =	51.1341	Anisotropy =	183.3070
17	C	Isotropic =	146.4031	Anisotropy =	41.6668
18	C	Isotropic =	177.4991	Anisotropy =	23.5404
19	C	Isotropic =	155.0559	Anisotropy =	16.0706
20	C	Isotropic =	123.4808	Anisotropy =	53.2114

21	O	Isotropic =	201.4225	Anisotropy =	133.1491
22	C	Isotropic =	31.8999	Anisotropy =	139.3261
23	C	Isotropic =	70.5242	Anisotropy =	171.2422
24	C	Isotropic =	43.6348	Anisotropy =	182.2105
25	N	Isotropic =	-35.9966	Anisotropy =	457.1606
26	C	Isotropic =	43.3429	Anisotropy =	160.8535
27	C	Isotropic =	92.5228	Anisotropy =	139.4227
28	C	Isotropic =	69.9543	Anisotropy =	175.0342
29	C	Isotropic =	67.9668	Anisotropy =	170.4410
30	C	Isotropic =	63.5386	Anisotropy =	174.9767
31	C	Isotropic =	63.8781	Anisotropy =	150.5135
32	C	Isotropic =	154.3848	Anisotropy =	44.1099
33	O	Isotropic =	-75.4681	Anisotropy =	383.5757
34	H	Isotropic =	24.5037	Anisotropy =	7.6988
35	H	Isotropic =	24.2557	Anisotropy =	3.9409
36	H	Isotropic =	23.5482	Anisotropy =	4.7124
37	H	Isotropic =	23.3551	Anisotropy =	6.0946
38	H	Isotropic =	23.3076	Anisotropy =	10.0138
39	H	Isotropic =	26.8951	Anisotropy =	6.9551
40	H	Isotropic =	28.1619	Anisotropy =	6.3413
41	H	Isotropic =	30.5132	Anisotropy =	7.9752
42	H	Isotropic =	30.6591	Anisotropy =	5.5441
43	H	Isotropic =	30.3314	Anisotropy =	11.7136
44	H	Isotropic =	28.5125	Anisotropy =	7.9047
45	H	Isotropic =	28.2266	Anisotropy =	7.0655
46	H	Isotropic =	26.8297	Anisotropy =	4.4371
47	H	Isotropic =	26.9061	Anisotropy =	7.9767
48	H	Isotropic =	23.4101	Anisotropy =	6.5067
49	H	Isotropic =	25.6151	Anisotropy =	6.9518
50	H	Isotropic =	23.0768	Anisotropy =	10.5905
51	H	Isotropic =	23.8182	Anisotropy =	5.8264
52	H	Isotropic =	23.6492	Anisotropy =	5.0057
53	H	Isotropic =	23.6261	Anisotropy =	6.2778
54	H	Isotropic =	28.6785	Anisotropy =	7.8133
55	H	Isotropic =	27.6061	Anisotropy =	8.6075
56	H	Isotropic =	27.9578	Anisotropy =	9.8123

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N 0.749219578253 -3.620445347654 -0.889536146588

C	-0.275370524092	-3.145052185573	-1.698055007917
C	-0.524417829954	-1.767834089389	-1.764392283709
C	0.342350440672	-0.865762725984	-1.132898098383
C	1.438150312086	-1.370339321890	-0.434337386170
C	1.625061592219	-2.735025951647	-0.320439932745
N	-1.656180977964	-1.308325330749	-2.483951476687
C	-2.945167587530	-1.736372948724	-2.188729660464
C	-3.177054740145	-3.090743901561	-1.592662325729
C	-2.384498220347	-4.232157569979	-1.869130396764
N	-1.079425179957	-4.084274906920	-2.355727161921
O	-3.906750012155	-1.023659422076	-2.468703656404
N	-2.843907100970	-5.478174007106	-1.700359265187
C	-4.017673245735	-5.637891515852	-1.078854706854
C	-4.794752185065	-4.589022556035	-0.569110314860
C	-4.381121089936	-3.298200450744	-0.909835151466
C	-0.452685496258	-5.172610799824	-3.133708137374
C	-1.037772470854	-5.247348330889	-4.542240902482
C	-5.968567972527	-4.857249557045	0.338004115902
C	-5.598968629586	-4.724086759874	1.821175993974
O	-4.569136648057	-5.687771592865	2.160259466502
C	-3.384825928662	-5.217463791088	2.664011718759
C	-3.306579891302	-4.609495776219	3.956765842877
C	-2.012675673334	-4.162362178722	4.391610048787
N	-0.875202604592	-4.308081944577	3.643048958524
C	-0.999188295621	-4.912692495858	2.473909632796
C	-2.220800512928	-5.388992218362	1.941288359842
C	-4.420771220148	-4.462923725387	4.828639011852
C	-4.270779175584	-3.869069990262	6.065699129827
C	-3.001010562468	-3.397280677645	6.485317790857
C	-1.899076922464	-3.544563031282	5.668450923466
C	-1.553278999737	-0.021163609143	-3.182781790077
O	0.893301714008	-4.882305358427	-0.690381498129
H	0.163968733617	0.206504315647	-1.184993653655
H	2.145144628207	-0.700891130128	0.055985151627
H	2.426210919257	-3.208046276077	0.242982657713
H	-4.353226473964	-6.672854245867	-0.953401096506
H	-5.000576289327	-2.430932141551	-0.672508458716
H	0.621883730690	-4.958373597139	-3.174259991138
H	-0.576242587578	-6.126385398251	-2.604635336177
H	-2.114932663514	-5.474537338264	-4.513915248136
H	-0.896921746821	-4.298084786530	-5.083181053438
H	-0.539067430126	-6.049392016076	-5.110223259044
H	-6.790058682871	-4.148487498659	0.141156352018
H	-6.362302569282	-5.870579594882	0.161616354496

H	-5.244340828206	-3.706428745870	2.046447429082
H	-6.482650262835	-4.933915350874	2.444367355241
H	-0.091305477798	-5.023936281708	1.869460820698
H	-2.243075437415	-5.859360216200	0.959626452118
H	-5.395213232946	-4.841170820937	4.519594245468
H	-5.132242836639	-3.766752691811	6.728809219483
H	-2.896844679735	-2.924769817914	7.464465094854
H	-0.908865058004	-3.203006031843	5.975974682926
H	-1.759120612178	0.832749332854	-2.516852106887
H	-0.543649838291	0.072621480648	-3.600648538977
H	-2.291565243509	-0.003747079214	-3.992832767107

SCF Done: E(RB3LYP) = -1465.98964596

Zero-point correction= 0.444665
Thermal correction to Energy= 0.471912
Thermal correction to Enthalpy= 0.472856
Thermal correction to Gibbs Free Energy= 0.386137
Sum of electronic and zero-point Energies= -1465.544981
Sum of electronic and thermal Energies= -1465.517734
Sum of electronic and thermal Enthalpies= -1465.516790
Sum of electronic and thermal Free Energies= -1465.603509

1	N	Isotropic =	-45.5887	Anisotropy =	263.8962
2	C	Isotropic =	44.5007	Anisotropy =	103.9465
3	C	Isotropic =	50.5695	Anisotropy =	125.2551
4	C	Isotropic =	76.4959	Anisotropy =	158.6110
5	C	Isotropic =	69.9771	Anisotropy =	166.1115
6	C	Isotropic =	55.2631	Anisotropy =	113.2624
7	N	Isotropic =	123.3901	Anisotropy =	86.2239
8	C	Isotropic =	26.2084	Anisotropy =	103.5215
9	C	Isotropic =	72.9222	Anisotropy =	128.4466
10	C	Isotropic =	33.0728	Anisotropy =	125.2597
11	N	Isotropic =	156.0583	Anisotropy =	68.3505
12	O	Isotropic =	-93.7730	Anisotropy =	603.1918
13	N	Isotropic =	-27.8710	Anisotropy =	446.2306
14	C	Isotropic =	40.1245	Anisotropy =	148.8328
15	C	Isotropic =	61.1455	Anisotropy =	173.8044
16	C	Isotropic =	52.0430	Anisotropy =	183.2395
17	C	Isotropic =	146.6579	Anisotropy =	39.2645
18	C	Isotropic =	176.0613	Anisotropy =	25.0452
19	C	Isotropic =	154.2034	Anisotropy =	16.5664
20	C	Isotropic =	111.6792	Anisotropy =	60.2016
21	O	Isotropic =	235.5876	Anisotropy =	104.7732

22	C	Isotropic =	28.0431	Anisotropy =	136.3435
23	C	Isotropic =	67.7139	Anisotropy =	174.5202
24	C	Isotropic =	42.2827	Anisotropy =	182.8201
25	N	Isotropic =	-50.9236	Anisotropy =	479.9041
26	C	Isotropic =	42.2165	Anisotropy =	162.7809
27	C	Isotropic =	78.7658	Anisotropy =	135.8402
28	C	Isotropic =	69.5247	Anisotropy =	167.0320
29	C	Isotropic =	67.3243	Anisotropy =	171.0719
30	C	Isotropic =	63.8332	Anisotropy =	174.7438
31	C	Isotropic =	62.7261	Anisotropy =	151.5517
32	C	Isotropic =	155.1141	Anisotropy =	43.9900
33	O	Isotropic =	-69.2801	Anisotropy =	367.0505
34	H	Isotropic =	24.6191	Anisotropy =	7.4547
35	H	Isotropic =	24.3125	Anisotropy =	3.4302
36	H	Isotropic =	23.3020	Anisotropy =	5.3618
37	H	Isotropic =	22.8236	Anisotropy =	7.1263
38	H	Isotropic =	23.7567	Anisotropy =	8.9255
39	H	Isotropic =	28.3328	Anisotropy =	6.2826
40	H	Isotropic =	26.4960	Anisotropy =	6.3867
41	H	Isotropic =	29.8950	Anisotropy =	5.4837
42	H	Isotropic =	30.3009	Anisotropy =	8.0019
43	H	Isotropic =	30.2381	Anisotropy =	11.3245
44	H	Isotropic =	28.6253	Anisotropy =	8.3103
45	H	Isotropic =	28.2785	Anisotropy =	6.5833
46	H	Isotropic =	27.9847	Anisotropy =	5.8223
47	H	Isotropic =	26.3422	Anisotropy =	7.0300
48	H	Isotropic =	23.0418	Anisotropy =	6.6998
49	H	Isotropic =	25.3481	Anisotropy =	5.7714
50	H	Isotropic =	23.4282	Anisotropy =	10.7099
51	H	Isotropic =	23.8475	Anisotropy =	6.0004
52	H	Isotropic =	23.6893	Anisotropy =	5.1270
53	H	Isotropic =	23.5761	Anisotropy =	6.9661
54	H	Isotropic =	28.1262	Anisotropy =	9.9254
55	H	Isotropic =	28.6974	Anisotropy =	8.2214
56	H	Isotropic =	27.7397	Anisotropy =	8.8601

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.681130117023	-6.757039846880	0.779700004739
C	-1.519737314621	-6.454840080064	0.083418444646

C	-0.295938159202	-6.411121137032	0.766125691568
C	-0.222611939478	-6.812575841642	2.106173531777
C	-1.388913584395	-7.239240773576	2.740150733620
C	-2.597687110209	-7.203958624425	2.072217835825
N	0.859525620274	-5.964435317194	0.077438848218
C	0.920300362445	-4.718920082410	-0.536898256313
C	-0.325516883227	-4.066500283000	-1.050998648886
C	-1.431881238171	-4.771491186362	-1.586145563397
N	-1.622052752028	-6.123875701817	-1.276494254397
O	2.007954279747	-4.172114085379	-0.707196542940
N	-2.312996381100	-4.197633152185	-2.414352009402
C	-2.235094569426	-2.874087707611	-2.596938265581
C	-1.312510807000	-2.037472339801	-1.954809860841
C	-0.303803526413	-2.678714302858	-1.229905926384
C	-2.390042694681	-6.977502322315	-2.208229884129
C	-2.054044897404	-8.453138454197	-2.027698917836
C	-1.455651503649	-0.537731278622	-2.002960835714
C	-2.190021026129	0.013655133300	-0.773730350476
O	-3.528637298253	-0.541658887226	-0.713430401234
C	-3.894600184323	-1.226679623851	0.415786409947
C	-4.079643442677	-0.562102036010	1.669171546264
C	-4.480813839032	-1.371679528662	2.785722901610
N	-4.704027505279	-2.719893842221	2.695867650510
C	-4.554901402483	-3.275145095498	1.505513536102
C	-4.159046612769	-2.579686576437	0.338022650502
C	-3.923496335952	0.840067791166	1.849078936838
C	-4.124476894326	1.415566584189	3.087576490132
C	-4.490542614486	0.615034978673	4.199370097077
C	-4.667654968432	-0.744952559334	4.049484994518
C	2.150847369705	-6.567106111756	0.431566054970
O	-3.833318384781	-6.642367594870	0.219350728848
H	0.723692488149	-6.790799423352	2.643014385126
H	-1.371195072986	-7.575910559237	3.776858848070
H	-3.557536171666	-7.473290044838	2.507070087632
H	-2.976670291092	-2.442933552152	-3.277799524368
H	0.531523981430	-2.113023084495	-0.812195925079
H	-3.469419760040	-6.813717699225	-2.088362687927
H	-2.104786755728	-6.641528389669	-3.214820806743
H	-2.389183971830	-8.832682313650	-1.049950007508
H	-2.571853853770	-9.039077434103	-2.803033927266
H	-0.971559235180	-8.634878519979	-2.122054763619
H	-0.468842897418	-0.047350550120	-2.042215660482
H	-2.006767985729	-0.236297174163	-2.907671156912
H	-1.644014830533	-0.230596009581	0.150703652940

H	-2.274949052019	1.109106579400	-0.852507032009
H	-4.726814200505	-4.355442987139	1.431973128050
H	-4.041851916944	-3.114546590642	-0.603010351665
H	-3.661101768042	1.462763786798	0.993829282620
H	-4.007150000897	2.493949156767	3.212652741059
H	-4.641659007989	1.082104514906	5.174993600782
H	-4.963562037039	-1.379399720441	4.887159538027
H	1.997207037521	-7.633220533539	0.637816009455
H	2.834886973427	-6.449766603327	-0.416862832195
H	2.611074683657	-6.083002962313	1.308476031830

SCF Done: E(RB3LYP) = -1465.98889345

Zero-point correction= 0.444633
Thermal correction to Energy= 0.471917
Thermal correction to Enthalpy= 0.472861
Thermal correction to Gibbs Free Energy= 0.385339
Sum of electronic and zero-point Energies= -1465.544260
Sum of electronic and thermal Energies= -1465.516977
Sum of electronic and thermal Enthalpies= -1465.516033
Sum of electronic and thermal Free Energies= -1465.603554

1	N	Isotropic =	-47.9723	Anisotropy =	262.5194
2	C	Isotropic =	45.8024	Anisotropy =	107.7330
3	C	Isotropic =	49.0174	Anisotropy =	128.0541
4	C	Isotropic =	76.1670	Anisotropy =	159.5123
5	C	Isotropic =	69.5304	Anisotropy =	166.9780
6	C	Isotropic =	55.4358	Anisotropy =	111.7028
7	N	Isotropic =	122.8243	Anisotropy =	87.2036
8	C	Isotropic =	26.4398	Anisotropy =	103.3621
9	C	Isotropic =	73.8842	Anisotropy =	127.7756
10	C	Isotropic =	31.7771	Anisotropy =	125.6939
11	N	Isotropic =	154.1607	Anisotropy =	79.2062
12	O	Isotropic =	-92.4362	Anisotropy =	603.4986
13	N	Isotropic =	-29.0272	Anisotropy =	439.7187
14	C	Isotropic =	39.9703	Anisotropy =	149.3521
15	C	Isotropic =	61.4741	Anisotropy =	174.2538
16	C	Isotropic =	52.4289	Anisotropy =	182.3842
17	C	Isotropic =	147.7447	Anisotropy =	40.7896
18	C	Isotropic =	177.7292	Anisotropy =	22.1073
19	C	Isotropic =	154.3961	Anisotropy =	16.7376
20	C	Isotropic =	111.9303	Anisotropy =	60.3857
21	O	Isotropic =	237.3158	Anisotropy =	103.5999
22	C	Isotropic =	27.7967	Anisotropy =	136.3556

23	C	Isotropic =	67.5996	Anisotropy =	174.8397
24	C	Isotropic =	42.3608	Anisotropy =	182.2169
25	N	Isotropic =	-50.7264	Anisotropy =	481.1943
26	C	Isotropic =	42.1772	Anisotropy =	162.6805
27	C	Isotropic =	78.5339	Anisotropy =	135.8814
28	C	Isotropic =	69.3007	Anisotropy =	166.6565
29	C	Isotropic =	67.0510	Anisotropy =	171.4209
30	C	Isotropic =	63.8888	Anisotropy =	174.7921
31	C	Isotropic =	62.9913	Anisotropy =	151.7908
32	C	Isotropic =	155.0042	Anisotropy =	43.8463
33	O	Isotropic =	-67.4298	Anisotropy =	366.3230
34	H	Isotropic =	24.5797	Anisotropy =	7.4048
35	H	Isotropic =	24.2733	Anisotropy =	3.4387
36	H	Isotropic =	23.3279	Anisotropy =	5.3311
37	H	Isotropic =	22.8411	Anisotropy =	7.0679
38	H	Isotropic =	23.7459	Anisotropy =	8.9939
39	H	Isotropic =	26.5559	Anisotropy =	6.5350
40	H	Isotropic =	27.6780	Anisotropy =	6.4776
41	H	Isotropic =	30.5245	Anisotropy =	5.5324
42	H	Isotropic =	30.1290	Anisotropy =	11.5876
43	H	Isotropic =	30.3672	Anisotropy =	8.1529
44	H	Isotropic =	28.6407	Anisotropy =	8.3605
45	H	Isotropic =	28.2940	Anisotropy =	6.6170
46	H	Isotropic =	28.0492	Anisotropy =	5.7247
47	H	Isotropic =	26.3521	Anisotropy =	7.0285
48	H	Isotropic =	22.9963	Anisotropy =	6.8125
49	H	Isotropic =	25.3623	Anisotropy =	5.9631
50	H	Isotropic =	23.4213	Anisotropy =	10.7274
51	H	Isotropic =	23.8351	Anisotropy =	6.0169
52	H	Isotropic =	23.6879	Anisotropy =	5.1344
53	H	Isotropic =	23.5646	Anisotropy =	6.9833
54	H	Isotropic =	28.6866	Anisotropy =	8.0817
55	H	Isotropic =	27.7206	Anisotropy =	8.9181
56	H	Isotropic =	28.1002	Anisotropy =	9.9363

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.741739538340	-3.107338006751	-2.296862616961
C	-2.516057781227	-3.749842273140	-2.423456542233
C	-2.476285492716	-5.135685464039	-2.630825588355

C	-3.665283097828	-5.851708546338	-2.824121281252
C	-4.874630538430	-5.158812855443	-2.802165399190
C	-4.896245928028	-3.801659022877	-2.541364666712
N	-1.220429982903	-5.793829220701	-2.666042684034
C	-0.302850119694	-5.725356606650	-1.625975843988
C	-0.289217543466	-4.548455126204	-0.699701408984
C	-0.620997356194	-3.226874225158	-1.082384612803
N	-1.354240118728	-2.989024893880	-2.256014359148
O	0.537245378059	-6.613048475782	-1.491275982892
N	-0.236971884325	-2.159028099475	-0.373077195297
C	0.349246858256	-2.366439568320	0.810217544829
C	0.584259863183	-3.628469074793	1.373039034862
C	0.305769362545	-4.726296916469	0.556105578194
C	-1.195201188690	-1.707511683897	-2.973837205352
C	0.147165132658	-1.648008453337	-3.699710324873
C	1.064865701409	-3.753129445506	2.799805378767
C	-0.060212506677	-4.158913733196	3.759806880334
O	-1.202730365889	-3.343111494476	3.447394463147
C	-2.377589215573	-3.569316107003	4.073740424694
C	-3.546463428566	-3.084840622285	3.398762908392
C	-4.807650762997	-3.268127040468	4.048992227235
N	-4.940105246455	-3.880754424312	5.269405333965
C	-3.832946623372	-4.331930531064	5.831012415186
C	-2.529749042210	-4.219294706734	5.286301612011
C	-3.498975761583	-2.487055231744	2.111016001941
C	-4.660694335061	-2.081992512248	1.482232853093
C	-5.910929041088	-2.239390905690	2.132695276711
C	-5.981783944517	-2.814355068494	3.386634167715
C	-1.066976506459	-6.933707551876	-3.579593502668
O	-3.798027945549	-1.862461709208	-1.978634600292
H	-3.645839898521	-6.927038257878	-2.990308941345
H	-5.819573534463	-5.677434190766	-2.964984284103
H	-5.797274324678	-3.196531656569	-2.471333983256
H	0.638046022394	-1.465214038756	1.362029724079
H	0.567855071726	-5.739846454659	0.866017874035
H	-2.022768464734	-1.637054100511	-3.689378850979
H	-1.299624944094	-0.871298954388	-2.270320646215
H	0.987762715845	-1.706286430515	-2.990498074366
H	0.246525432533	-2.472061961484	-4.424017317994
H	0.232886720396	-0.693773229503	-4.244464932701
H	1.864584843712	-4.505485538820	2.890786909592
H	1.486045017999	-2.789853698288	3.126227309616
H	-0.338001796958	-5.219169250727	3.631442936828
H	0.255545772501	-4.002925412811	4.804340707487

H	-3.947615267938	-4.829826244515	6.800828848500
H	-1.681457990064	-4.626135550249	5.834868209614
H	-2.534241272491	-2.371486407467	1.617684026938
H	-4.610531738488	-1.666728727692	0.472506076393
H	-6.825034277202	-1.911453807552	1.632330768371
H	-6.936064447477	-2.953420808153	3.898565664490
H	-1.414145964635	-7.877948592316	-3.129144877495
H	-1.636081460816	-6.731052521057	-4.494854093034
H	-0.003923214092	-7.045844567768	-3.822141340496

SCF Done: E(RB3LYP) = -1465.99820899

Zero-point correction= 0.444653
Thermal correction to Energy= 0.472051
Thermal correction to Enthalpy= 0.472995
Thermal correction to Gibbs Free Energy= 0.385372
Sum of electronic and zero-point Energies= -1465.553556
Sum of electronic and thermal Energies= -1465.526158
Sum of electronic and thermal Enthalpies= -1465.525214
Sum of electronic and thermal Free Energies= -1465.612837

1	N	Isotropic =	-44.8874	Anisotropy =	262.4016
2	C	Isotropic =	44.2076	Anisotropy =	103.6106
3	C	Isotropic =	50.9488	Anisotropy =	124.6679
4	C	Isotropic =	75.8659	Anisotropy =	158.9938
5	C	Isotropic =	70.1628	Anisotropy =	165.3758
6	C	Isotropic =	55.4541	Anisotropy =	113.0850
7	N	Isotropic =	122.7872	Anisotropy =	86.4827
8	C	Isotropic =	26.5272	Anisotropy =	104.8620
9	C	Isotropic =	71.6026	Anisotropy =	130.0724
10	C	Isotropic =	33.4879	Anisotropy =	123.5682
11	N	Isotropic =	158.4812	Anisotropy =	66.0413
12	O	Isotropic =	-91.3690	Anisotropy =	602.8122
13	N	Isotropic =	-30.5723	Anisotropy =	448.3463
14	C	Isotropic =	39.4122	Anisotropy =	146.5378
15	C	Isotropic =	61.2389	Anisotropy =	172.7659
16	C	Isotropic =	52.8310	Anisotropy =	185.8715
17	C	Isotropic =	146.4184	Anisotropy =	38.7955
18	C	Isotropic =	175.9188	Anisotropy =	25.2158
19	C	Isotropic =	157.1546	Anisotropy =	20.6504
20	C	Isotropic =	122.8754	Anisotropy =	47.8414
21	O	Isotropic =	209.0467	Anisotropy =	118.1775
22	C	Isotropic =	31.9035	Anisotropy =	137.3656
23	C	Isotropic =	70.2129	Anisotropy =	170.6923

24	C	Isotropic =	44.1131	Anisotropy =	181.4415
25	N	Isotropic =	-39.1845	Anisotropy =	460.1566
26	C	Isotropic =	42.9409	Anisotropy =	159.2642
27	C	Isotropic =	89.7833	Anisotropy =	135.9219
28	C	Isotropic =	70.1320	Anisotropy =	173.8884
29	C	Isotropic =	67.0947	Anisotropy =	173.9355
30	C	Isotropic =	63.5410	Anisotropy =	174.6520
31	C	Isotropic =	64.3636	Anisotropy =	149.7140
32	C	Isotropic =	154.7992	Anisotropy =	44.2398
33	O	Isotropic =	-65.7939	Anisotropy =	365.0003
34	H	Isotropic =	24.6068	Anisotropy =	7.4461
35	H	Isotropic =	24.4116	Anisotropy =	3.6433
36	H	Isotropic =	23.3957	Anisotropy =	5.1163
37	H	Isotropic =	22.8699	Anisotropy =	7.3954
38	H	Isotropic =	23.4111	Anisotropy =	9.4732
39	H	Isotropic =	28.2291	Anisotropy =	6.3090
40	H	Isotropic =	26.4472	Anisotropy =	6.4521
41	H	Isotropic =	29.9716	Anisotropy =	5.2739
42	H	Isotropic =	30.2945	Anisotropy =	8.0557
43	H	Isotropic =	30.2411	Anisotropy =	11.2715
44	H	Isotropic =	28.3130	Anisotropy =	8.3329
45	H	Isotropic =	28.1953	Anisotropy =	6.5662
46	H	Isotropic =	27.7513	Anisotropy =	5.6715
47	H	Isotropic =	26.7480	Anisotropy =	6.9260
48	H	Isotropic =	22.8320	Anisotropy =	6.9663
49	H	Isotropic =	24.9450	Anisotropy =	9.6631
50	H	Isotropic =	24.3583	Anisotropy =	8.1240
51	H	Isotropic =	23.8284	Anisotropy =	7.0509
52	H	Isotropic =	23.7772	Anisotropy =	6.4541
53	H	Isotropic =	23.6844	Anisotropy =	5.6646
54	H	Isotropic =	28.0543	Anisotropy =	9.9644
55	H	Isotropic =	28.6788	Anisotropy =	8.1621
56	H	Isotropic =	27.6422	Anisotropy =	8.7311

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.425573518240	-2.836205015433	-2.069640841991
C	-1.266751244955	-3.925150752388	-2.263760285265
C	-0.749624926208	-5.225441217928	-2.183684333399
C	0.627709703870	-5.425487372630	-2.020799431514

C	1.460446236127	-4.310494283037	-1.939661654333
C	0.924933237063	-3.036458806662	-1.966766575534
N	-1.634456849348	-6.328645923677	-2.293617804315
C	-2.729000893116	-6.503156916965	-1.457784305036
C	-3.381240079782	-5.323224651817	-0.804926799869
C	-3.476435182203	-4.038241501061	-1.390769868070
N	-2.630531002591	-3.677357752283	-2.452151504726
O	-3.197716267185	-7.627159623271	-1.287856596768
N	-4.373796455111	-3.132106182097	-0.985525915504
C	-5.094185599913	-3.404317405416	0.107417140534
C	-4.970937254468	-4.572149669376	0.872509440048
C	-4.136073422326	-5.562611722646	0.350393333897
C	-3.073825803863	-2.667930154079	-3.435462875249
C	-4.127175605708	-3.246501443788	-4.377931511980
C	-5.673119674250	-4.695922154260	2.204391059033
C	-4.710281731644	-4.526810854443	3.385709892984
O	-3.894352759631	-3.375013261690	3.109759210617
C	-2.872172456856	-3.065300096902	3.935961494970
C	-1.839609492001	-2.247420167270	3.369160462270
C	-0.760812334022	-1.859081770926	4.224869485448
N	-0.674482506631	-2.236704506612	5.540969032872
C	-1.638004605648	-3.014796458238	6.000394936269
C	-2.752790362581	-3.470800065363	5.254015831237
C	-1.828548910448	-1.859913868059	2.002659916580
C	-0.785321814461	-1.109840495672	1.494529781044
C	0.273310168759	-0.700402232193	2.344565252562
C	0.283090746617	-1.062944514844	3.677397774247
C	-1.147008265358	-7.536261489571	-2.972664890720
O	-0.903072848955	-1.643464662201	-2.011609220167
H	1.039855872334	-6.430890998492	-1.960826275411
H	2.538994569240	-4.424543786183	-1.829776487143
H	1.500604482686	-2.118368525989	-1.873597600621
H	-5.808065475152	-2.630873916196	0.411037576647
H	-4.072291234288	-6.547819699973	0.816481683730
H	-3.457806031169	-1.782482545186	-2.912433007957
H	-2.185028946307	-2.355545271454	-3.995931673929
H	-3.739274196538	-4.124425585131	-4.918554273256
H	-5.031991743628	-3.549769148851	-3.827936939068
H	-4.423000093316	-2.484682826234	-5.117367358257
H	-6.463181531077	-3.932331854768	2.271487169715
H	-6.159763067073	-5.678454654940	2.313084478848
H	-5.275247466299	-4.387900168893	4.322023784115
H	-4.052932289565	-5.405893741321	3.498374653226
H	-1.556621672547	-3.321677853862	7.049569316461

H	-3.494632492605	-4.108854800012	5.732255184351
H	-2.645291521850	-2.180083255118	1.356208098983
H	-0.769245710106	-0.859942956456	0.430670849955
H	1.091809082247	-0.101995118699	1.937758959789
H	1.095040617624	-0.766814338126	4.344550976374
H	-2.009238654382	-8.089690742558	-3.362354526522
H	-0.495038073283	-7.235158334656	-3.801462604809
H	-0.594552649877	-8.203422884104	-2.290991615394

SCF Done: E(RB3LYP) = -1465.99835042

Zero-point correction= 0.444847
Thermal correction to Energy= 0.472171
Thermal correction to Enthalpy= 0.473115
Thermal correction to Gibbs Free Energy= 0.386009
Sum of electronic and zero-point Energies= -1465.553503
Sum of electronic and thermal Energies= -1465.526180
Sum of electronic and thermal Enthalpies= -1465.525236
Sum of electronic and thermal Free Energies= -1465.612341

1	N	Isotropic =	-44.8060	Anisotropy =	262.6480
2	C	Isotropic =	43.9365	Anisotropy =	104.3573
3	C	Isotropic =	51.2572	Anisotropy =	124.9564
4	C	Isotropic =	76.1363	Anisotropy =	159.0697
5	C	Isotropic =	70.2332	Anisotropy =	165.6812
6	C	Isotropic =	55.2619	Anisotropy =	113.4053
7	N	Isotropic =	122.7512	Anisotropy =	86.8910
8	C	Isotropic =	26.3059	Anisotropy =	103.9371
9	C	Isotropic =	71.5769	Anisotropy =	130.3136
10	C	Isotropic =	33.0401	Anisotropy =	123.8782
11	N	Isotropic =	158.2224	Anisotropy =	65.9378
12	O	Isotropic =	-91.3035	Anisotropy =	601.7143
13	N	Isotropic =	-30.3990	Anisotropy =	449.3163
14	C	Isotropic =	39.4566	Anisotropy =	146.8925
15	C	Isotropic =	61.1031	Anisotropy =	172.9848
16	C	Isotropic =	52.7561	Anisotropy =	185.1320
17	C	Isotropic =	146.7248	Anisotropy =	38.9580
18	C	Isotropic =	175.7716	Anisotropy =	25.3725
19	C	Isotropic =	157.4371	Anisotropy =	20.3833
20	C	Isotropic =	122.6033	Anisotropy =	47.9205
21	O	Isotropic =	208.8007	Anisotropy =	117.7724
22	C	Isotropic =	31.9978	Anisotropy =	137.6316
23	C	Isotropic =	70.2638	Anisotropy =	170.7265
24	C	Isotropic =	43.9677	Anisotropy =	181.3426

25	N	Isotropic =	-38.9444	Anisotropy =	460.7429
26	C	Isotropic =	42.8842	Anisotropy =	159.2287
27	C	Isotropic =	89.7276	Anisotropy =	135.4432
28	C	Isotropic =	70.1909	Anisotropy =	173.8565
29	C	Isotropic =	67.1729	Anisotropy =	174.1641
30	C	Isotropic =	63.5568	Anisotropy =	174.9041
31	C	Isotropic =	64.3840	Anisotropy =	149.4778
32	C	Isotropic =	154.7677	Anisotropy =	44.4768
33	O	Isotropic =	-66.4441	Anisotropy =	364.5198
34	H	Isotropic =	24.6337	Anisotropy =	7.3702
35	H	Isotropic =	24.4276	Anisotropy =	3.6101
36	H	Isotropic =	23.4030	Anisotropy =	5.0752
37	H	Isotropic =	22.8627	Anisotropy =	7.3637
38	H	Isotropic =	23.4281	Anisotropy =	9.4433
39	H	Isotropic =	26.4557	Anisotropy =	6.4808
40	H	Isotropic =	28.2240	Anisotropy =	6.3147
41	H	Isotropic =	30.2766	Anisotropy =	8.0226
42	H	Isotropic =	29.9316	Anisotropy =	5.3901
43	H	Isotropic =	30.2195	Anisotropy =	11.3189
44	H	Isotropic =	28.1996	Anisotropy =	6.5856
45	H	Isotropic =	28.2906	Anisotropy =	8.3938
46	H	Isotropic =	26.7485	Anisotropy =	6.9395
47	H	Isotropic =	27.7517	Anisotropy =	5.5955
48	H	Isotropic =	22.8417	Anisotropy =	6.9560
49	H	Isotropic =	24.9403	Anisotropy =	9.6557
50	H	Isotropic =	24.3919	Anisotropy =	8.1255
51	H	Isotropic =	23.8174	Anisotropy =	6.9722
52	H	Isotropic =	23.7787	Anisotropy =	6.4398
53	H	Isotropic =	23.6997	Anisotropy =	5.6435
54	H	Isotropic =	27.6454	Anisotropy =	8.7965
55	H	Isotropic =	28.6964	Anisotropy =	8.1721
56	H	Isotropic =	28.0732	Anisotropy =	9.9655

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.542373722459	-4.366520144860	-0.927984073005
C	-0.498372128019	-4.070356126939	-1.797127488898
C	-0.619113675768	-2.772389988477	-2.315635548657
C	0.365472754608	-1.812669666749	-2.048236264629
C	1.456907332886	-2.175468744946	-1.260205361698

C	1.531382039667	-3.442688767545	-0.715354097866
N	-1.733100564068	-2.454582152959	-3.133602594658
C	-3.047531893574	-2.619128645550	-2.717898844892
C	-3.389292326202	-3.631223515676	-1.668657591173
C	-2.715263194019	-4.864439454006	-1.501583055656
N	-1.447944285334	-5.064033939218	-2.072862098982
O	-3.943940454095	-1.962132287894	-3.244155368590
N	-3.254069860766	-5.891284552884	-0.833828743114
C	-4.409195925309	-5.687021456434	-0.191168489322
C	-5.093511815645	-4.464798508361	-0.150434777642
C	-4.584488962554	-3.448148628079	-0.961991462813
C	-1.039125437996	-6.437390618200	-2.439305814624
C	0.079206603872	-6.437710402157	-3.474533766055
C	-6.275582273487	-4.277952877621	0.771955476022
C	-5.917201224646	-3.456182509528	2.015862878687
O	-4.680815072908	-3.980111346857	2.530838986286
C	-4.065269406611	-3.355222232491	3.557446868840
C	-2.661016023162	-3.613411744321	3.690320677922
C	-1.979118055450	-3.005093159563	4.790959436964
N	-2.604263254889	-2.195053269733	5.704849546893
C	-3.891944143491	-1.969169270065	5.515878725352
C	-4.675448491343	-2.505864284316	4.464269766142
C	-1.932128570583	-4.396951236060	2.756266701602
C	-0.570208862862	-4.577166500382	2.904043797241
C	0.106196968596	-3.997262523132	4.007286609780
C	-0.581961198298	-3.233307999736	4.929718221562
C	-1.525735504918	-1.516399368442	-4.244539241563
O	0.604362508109	-5.510490970037	-0.341682804308
H	0.282372844035	-0.804295107233	-2.448972894780
H	2.251846534130	-1.462011387372	-1.042498498906
H	2.327961118642	-3.793987633660	-0.063501645805
H	-4.810782635516	-6.550494681291	0.350302313268
H	-5.117358480966	-2.502724720760	-1.080852213885
H	-0.737157537596	-7.006763391544	-1.550653698862
H	-1.941365660811	-6.907796632168	-2.855669897623
H	-0.193707085393	-5.849819033581	-4.365428219066
H	1.017375098211	-6.037105629461	-3.060948251777
H	0.276016399452	-7.473591213669	-3.792288597747
H	-7.105685735267	-3.762636163457	0.262776995486
H	-6.649344376994	-5.264310505841	1.087009042142
H	-5.772878075657	-2.390930551036	1.766847114503
H	-6.717346491505	-3.535786425399	2.769965190301
H	-4.382295142145	-1.312511380781	6.243838192521
H	-5.733803962152	-2.256561629757	4.401854261218

H	-2.460169013522	-4.836600956238	1.910394387839
H	-0.016419221763	-5.145174738410	2.152291222202
H	1.182040591171	-4.149084677167	4.121416522560
H	-0.076373379953	-2.769873267108	5.779250944277
H	-1.615339371606	-0.465471207695	-3.924470337292
H	-0.529420956502	-1.687924272249	-4.669463260281
H	-2.290644782492	-1.704037900903	-5.006908875438

SCF Done: E(RB3LYP) = -1465.99775244

Zero-point correction= 0.444914
Thermal correction to Energy= 0.472198
Thermal correction to Enthalpy= 0.473143
Thermal correction to Gibbs Free Energy= 0.386295
Sum of electronic and zero-point Energies= -1465.552838
Sum of electronic and thermal Energies= -1465.525554
Sum of electronic and thermal Enthalpies= -1465.524610
Sum of electronic and thermal Free Energies= -1465.611458

1	N	Isotropic =	-47.5436	Anisotropy =	260.9939
2	C	Isotropic =	45.8406	Anisotropy =	107.8206
3	C	Isotropic =	50.0474	Anisotropy =	127.2247
4	C	Isotropic =	76.1331	Anisotropy =	159.5292
5	C	Isotropic =	70.0689	Anisotropy =	166.8877
6	C	Isotropic =	55.3466	Anisotropy =	112.1618
7	N	Isotropic =	122.3863	Anisotropy =	87.1228
8	C	Isotropic =	26.6300	Anisotropy =	104.4316
9	C	Isotropic =	72.7235	Anisotropy =	129.5716
10	C	Isotropic =	31.9630	Anisotropy =	124.6896
11	N	Isotropic =	156.4538	Anisotropy =	75.9502
12	O	Isotropic =	-90.2288	Anisotropy =	602.2793
13	N	Isotropic =	-32.6386	Anisotropy =	441.7346
14	C	Isotropic =	39.5289	Anisotropy =	146.4286
15	C	Isotropic =	61.1903	Anisotropy =	173.6905
16	C	Isotropic =	53.3973	Anisotropy =	185.0259
17	C	Isotropic =	146.6675	Anisotropy =	40.4653
18	C	Isotropic =	177.5733	Anisotropy =	22.7902
19	C	Isotropic =	157.5152	Anisotropy =	20.2392
20	C	Isotropic =	122.6967	Anisotropy =	47.5112
21	O	Isotropic =	208.8798	Anisotropy =	117.6408
22	C	Isotropic =	31.8902	Anisotropy =	138.1119
23	C	Isotropic =	70.1786	Anisotropy =	170.7899
24	C	Isotropic =	44.2012	Anisotropy =	181.3230
25	N	Isotropic =	-39.0662	Anisotropy =	460.6107

26	C	Isotropic =	42.9975	Anisotropy =	158.8927
27	C	Isotropic =	89.6349	Anisotropy =	135.9671
28	C	Isotropic =	69.8293	Anisotropy =	174.2187
29	C	Isotropic =	67.0031	Anisotropy =	174.2716
30	C	Isotropic =	63.5475	Anisotropy =	174.9736
31	C	Isotropic =	64.6104	Anisotropy =	149.1714
32	C	Isotropic =	154.7715	Anisotropy =	44.3060
33	O	Isotropic =	-62.5201	Anisotropy =	357.0060
34	H	Isotropic =	24.6168	Anisotropy =	7.3205
35	H	Isotropic =	24.3961	Anisotropy =	3.5902
36	H	Isotropic =	23.4188	Anisotropy =	5.0388
37	H	Isotropic =	22.8494	Anisotropy =	7.4161
38	H	Isotropic =	23.4699	Anisotropy =	9.4785
39	H	Isotropic =	26.4132	Anisotropy =	6.5581
40	H	Isotropic =	27.7763	Anisotropy =	6.5014
41	H	Isotropic =	30.3478	Anisotropy =	8.1139
42	H	Isotropic =	30.4567	Anisotropy =	5.5708
43	H	Isotropic =	30.1092	Anisotropy =	11.5876
44	H	Isotropic =	28.2888	Anisotropy =	8.4203
45	H	Isotropic =	28.1784	Anisotropy =	6.6278
46	H	Isotropic =	27.7564	Anisotropy =	5.5647
47	H	Isotropic =	26.7503	Anisotropy =	6.9767
48	H	Isotropic =	22.8570	Anisotropy =	6.9327
49	H	Isotropic =	24.9320	Anisotropy =	9.6352
50	H	Isotropic =	24.3450	Anisotropy =	8.1039
51	H	Isotropic =	23.7996	Anisotropy =	6.8807
52	H	Isotropic =	23.7689	Anisotropy =	6.4692
53	H	Isotropic =	23.7102	Anisotropy =	5.6462
54	H	Isotropic =	28.0641	Anisotropy =	9.9436
55	H	Isotropic =	28.7017	Anisotropy =	8.0118
56	H	Isotropic =	27.6290	Anisotropy =	8.8704

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.674688084505	-3.532506165793	0.098600327575
C	1.454969496662	-3.688697526401	-0.552960963805
C	1.305026947153	-3.219680123517	-1.865291973750
C	2.399736177340	-2.673487948868	-2.548931258565
C	3.632439682528	-2.616137027995	-1.901112746101

C	3.753529844701	-3.049109360403	-0.594460810925
N	0.044080801586	-3.334884353873	-2.505574564621
C	-1.126183974578	-2.815873389270	-1.978508610706
C	-1.266260026105	-2.588318962212	-0.504216797410
C	-0.673861617774	-3.399912443170	0.492956254541
N	0.398013072339	-4.247942799710	0.172116575665
O	-2.085970209634	-2.590674287712	-2.715976403854
N	-1.123310611043	-3.427242673301	1.753551242295
C	-2.104129369403	-2.584532680618	2.097103509017
C	-2.689746974691	-1.650926750108	1.231524345523
C	-2.261212294368	-1.693452188294	-0.097427983842
C	0.591626638811	-5.502823047367	0.928127559768
C	-0.455244962107	-6.545719656187	0.541501467443
C	-3.785322032616	-0.718017493491	1.692033404335
C	-5.191708866329	-1.103124294178	1.223586930960
O	-5.632840343174	-2.324308239986	1.849796710907
C	-5.740135222851	-3.485862895166	1.167382593039
C	-6.352475943533	-4.561923117046	1.895168597885
C	-6.495585349592	-5.819995641527	1.228126278443
N	-6.080963544414	-6.038900107254	-0.060339525325
C	-5.524099361297	-5.015017276110	-0.681545728865
C	-5.323570039303	-3.725480354567	-0.132236024784
C	-6.814383258714	-4.419810747692	3.230739177348
C	-7.396966581713	-5.486869790720	3.886840300955
C	-7.540071537802	-6.735811333109	3.232348591743
C	-7.099774793861	-6.896911357876	1.933831300623
C	0.026966302896	-3.630276009658	-3.944412769695
O	2.803179624783	-3.860544109910	1.330627202325
H	2.290296296600	-2.305488162663	-3.567187912249
H	4.511334544930	-2.213289057333	-2.404854824225
H	4.669195317015	-3.012327824637	-0.008586427834
H	-2.444822719124	-2.649353366629	3.136370102395
H	-2.731461679045	-1.066963509861	-0.857995978147
H	1.600414483823	-5.863856681714	0.698752726609
H	0.558978621726	-5.293544287843	2.005468071744
H	-0.277638496179	-7.476798484098	1.104003588958
H	-1.473271960513	-6.199013468162	0.779296977810
H	-0.410296029576	-6.776412407385	-0.534830564688
H	-3.789888782483	-0.660600655489	2.791626522532
H	-3.593308199355	0.302348467444	1.319793975355
H	-5.908439031690	-0.336468830019	1.552647906168
H	-5.256137149931	-1.178588236042	0.129022421550
H	-5.188683398236	-5.193425101180	-1.709724538946
H	-4.830006207555	-2.970702115950	-0.740879824177

H	-6.701123926099	-3.455918033113	3.726857407318
H	-7.749843637099	-5.369662231486	4.913600120166
H	-8.001982099857	-7.573152433850	3.760203028138
H	-7.200504666508	-7.849183915203	1.409521261459
H	0.104548384546	-2.717163034147	-4.556847436862
H	0.862784971056	-4.301106341975	-4.176545296866
H	-0.921904394848	-4.121836135571	-4.188207514352

SCF Done: E(RB3LYP) = -1465.99492626

Zero-point correction= 0.444732
Thermal correction to Energy= 0.472121
Thermal correction to Enthalpy= 0.473065
Thermal correction to Gibbs Free Energy= 0.384214
Sum of electronic and zero-point Energies= -1465.550194
Sum of electronic and thermal Energies= -1465.522806
Sum of electronic and thermal Enthalpies= -1465.521861
Sum of electronic and thermal Free Energies= -1465.610713

1	N	Isotropic =	-46.0689	Anisotropy =	263.4906
2	C	Isotropic =	44.7118	Anisotropy =	101.8170
3	C	Isotropic =	51.3786	Anisotropy =	123.1792
4	C	Isotropic =	76.7601	Anisotropy =	155.9730
5	C	Isotropic =	70.1897	Anisotropy =	165.0266
6	C	Isotropic =	55.6024	Anisotropy =	110.5631
7	N	Isotropic =	122.6235	Anisotropy =	85.7492
8	C	Isotropic =	26.3802	Anisotropy =	105.3398
9	C	Isotropic =	70.4444	Anisotropy =	134.5292
10	C	Isotropic =	34.0719	Anisotropy =	123.6645
11	N	Isotropic =	158.9369	Anisotropy =	64.1892
12	O	Isotropic =	-91.0800	Anisotropy =	594.4808
13	N	Isotropic =	-32.3975	Anisotropy =	453.8164
14	C	Isotropic =	40.8743	Anisotropy =	147.6467
15	C	Isotropic =	62.3201	Anisotropy =	172.1248
16	C	Isotropic =	50.4647	Anisotropy =	190.9491
17	C	Isotropic =	147.2769	Anisotropy =	37.6847
18	C	Isotropic =	176.2591	Anisotropy =	24.0584
19	C	Isotropic =	156.1421	Anisotropy =	15.1267
20	C	Isotropic =	123.2816	Anisotropy =	54.6611
21	O	Isotropic =	200.3018	Anisotropy =	132.3328
22	C	Isotropic =	31.8533	Anisotropy =	139.1044
23	C	Isotropic =	70.4019	Anisotropy =	171.1154
24	C	Isotropic =	43.7523	Anisotropy =	181.9240

25	N	Isotropic =	-36.0094	Anisotropy =	458.0891
26	C	Isotropic =	43.1469	Anisotropy =	160.4254
27	C	Isotropic =	91.4597	Anisotropy =	137.7715
28	C	Isotropic =	69.6016	Anisotropy =	174.7292
29	C	Isotropic =	67.9431	Anisotropy =	170.5249
30	C	Isotropic =	63.9042	Anisotropy =	175.7007
31	C	Isotropic =	64.1420	Anisotropy =	150.5517
32	C	Isotropic =	154.5929	Anisotropy =	44.1207
33	O	Isotropic =	-80.8235	Anisotropy =	394.6381
34	H	Isotropic =	24.5264	Anisotropy =	8.2303
35	H	Isotropic =	24.2951	Anisotropy =	4.1951
36	H	Isotropic =	23.4945	Anisotropy =	5.1959
37	H	Isotropic =	23.3579	Anisotropy =	6.4101
38	H	Isotropic =	23.0894	Anisotropy =	10.1203
39	H	Isotropic =	28.4297	Anisotropy =	6.7099
40	H	Isotropic =	26.9661	Anisotropy =	7.1852
41	H	Isotropic =	30.6443	Anisotropy =	10.5673
42	H	Isotropic =	30.7459	Anisotropy =	7.4907
43	H	Isotropic =	30.5999	Anisotropy =	6.7268
44	H	Isotropic =	28.4214	Anisotropy =	7.2252
45	H	Isotropic =	28.4653	Anisotropy =	7.8819
46	H	Isotropic =	26.8615	Anisotropy =	7.8484
47	H	Isotropic =	26.5626	Anisotropy =	4.2206
48	H	Isotropic =	23.0884	Anisotropy =	7.3867
49	H	Isotropic =	25.2243	Anisotropy =	6.4604
50	H	Isotropic =	23.1155	Anisotropy =	10.6879
51	H	Isotropic =	23.8251	Anisotropy =	5.8426
52	H	Isotropic =	23.6456	Anisotropy =	4.9823
53	H	Isotropic =	23.6177	Anisotropy =	6.3324
54	H	Isotropic =	27.9584	Anisotropy =	9.9642
55	H	Isotropic =	28.6486	Anisotropy =	7.7108
56	H	Isotropic =	27.5246	Anisotropy =	7.6825

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.097594765465	-3.340778466514	-3.987493829430
C	-0.308542250311	-2.758964565058	-2.790354503307
C	-0.637024724291	-1.396655120463	-2.757795735926
C	-0.476519612299	-0.604673304395	-3.902939864920
C	0.021709982025	-1.197244876666	-5.061948236686

C	0.305735751621	-2.549293111025	-5.086506102203
N	-1.099961310141	-0.820735214264	-1.546382306752
C	-2.191636751337	-1.301051077522	-0.843059768685
C	-2.624921748094	-2.728584042591	-0.983399395990
C	-1.746678775057	-3.816643507341	-1.203143418645
N	-0.443349847872	-3.592107478133	-1.675384464856
O	-2.782542381008	-0.568033423403	-0.049974760127
N	-2.094480100695	-5.081925746454	-0.938864495640
C	-3.348986746122	-5.326779683374	-0.543509571227
C	-4.342934920259	-4.349040107780	-0.400361493361
C	-3.937979658341	-3.027747921501	-0.605316977386
C	0.639492813745	-4.526255377267	-1.304037923356
C	1.038241691404	-4.351150660919	0.159996650734
C	-5.745239681335	-4.700860283961	0.038086429678
C	-6.054754839935	-4.380334433510	1.503522171319
O	-5.298846519335	-5.229553780230	2.390235913468
C	-4.283824177836	-4.759052771448	3.148440533242
C	-3.757811908333	-5.693986626702	4.103313009842
C	-2.678447297825	-5.258807736108	4.936171005024
N	-2.133472185199	-4.002651034009	4.864510714911
C	-2.655907268694	-3.184343982166	3.969091513909
C	-3.719806065866	-3.494893674871	3.087795623178
C	-4.267055701471	-7.012112920713	4.246537348370
C	-3.726003741491	-7.873389718326	5.181305915561
C	-2.655572138823	-7.449211694883	6.007719707689
C	-2.145229427280	-6.172055418467	5.887206646327
C	-0.692519835828	0.556971226217	-1.240166344056
O	0.302555202888	-4.603503042166	-4.062836997134
H	-0.731630269071	0.453162681690	-3.886322581042
H	0.176114311365	-0.611479724452	-5.968341634083
H	0.668617912391	-3.093832813127	-5.955332836081
H	-3.585057667039	-6.375457571827	-0.331823527277
H	-4.622185338434	-2.196295706985	-0.424314005247
H	0.322488841952	-5.558000644349	-1.505054132209
H	1.487865298920	-4.313281987902	-1.964111820274
H	1.380148529932	-3.323180929315	0.360294449077
H	0.195690615261	-4.573226866711	0.833698169743
H	1.858248169506	-5.044744889071	0.407553617290
H	-6.480915640527	-4.150346037819	-0.571952166718
H	-5.931757128434	-5.773262914951	-0.128310347177
H	-5.886236117205	-3.320113432992	1.737904654341
H	-7.109729303244	-4.610558461780	1.713137902250
H	-2.215845611475	-2.182133201330	3.910421149390
H	-4.046827793799	-2.737809064034	2.378074046619

H	-5.090465537325	-7.330086909500	3.607158720270
H	-4.123348207857	-8.885126254334	5.286106973528
H	-2.234616927935	-8.138183245719	6.743430998280
H	-1.321835259450	-5.823764148780	6.513737007321
H	0.326150440507	0.714317522258	-1.614271400626
H	-1.370534993966	1.300353105003	-1.690164422194
H	-0.713688916143	0.693861072037	-0.152835808742

SCF Done: E(RB3LYP) = -1465.99498294

Zero-point correction= 0.444714
Thermal correction to Energy= 0.472141
Thermal correction to Enthalpy= 0.473085
Thermal correction to Gibbs Free Energy= 0.383791
Sum of electronic and zero-point Energies= -1465.550269
Sum of electronic and thermal Energies= -1465.522842
Sum of electronic and thermal Enthalpies= -1465.521898
Sum of electronic and thermal Free Energies= -1465.611192

1	N	Isotropic =	-46.0272	Anisotropy =	262.7528
2	C	Isotropic =	44.6014	Anisotropy =	101.6017
3	C	Isotropic =	51.5713	Anisotropy =	123.2482
4	C	Isotropic =	76.5750	Anisotropy =	156.2963
5	C	Isotropic =	70.1940	Anisotropy =	164.4421
6	C	Isotropic =	55.6708	Anisotropy =	110.2964
7	N	Isotropic =	122.7325	Anisotropy =	86.0016
8	C	Isotropic =	26.3364	Anisotropy =	104.9591
9	C	Isotropic =	70.3622	Anisotropy =	134.5540
10	C	Isotropic =	34.0738	Anisotropy =	124.0363
11	N	Isotropic =	159.0864	Anisotropy =	63.4947
12	O	Isotropic =	-91.2355	Anisotropy =	595.0949
13	N	Isotropic =	-32.7928	Anisotropy =	454.1178
14	C	Isotropic =	40.7573	Anisotropy =	148.0303
15	C	Isotropic =	62.2108	Anisotropy =	172.2448
16	C	Isotropic =	50.5287	Anisotropy =	189.8269
17	C	Isotropic =	147.2028	Anisotropy =	37.4417
18	C	Isotropic =	176.3274	Anisotropy =	23.9901
19	C	Isotropic =	155.9209	Anisotropy =	15.5926
20	C	Isotropic =	122.9758	Anisotropy =	53.8938
21	O	Isotropic =	200.8922	Anisotropy =	133.6284
22	C	Isotropic =	31.7343	Anisotropy =	138.7620
23	C	Isotropic =	70.4073	Anisotropy =	171.2510
24	C	Isotropic =	43.4738	Anisotropy =	181.6841
25	N	Isotropic =	-36.5096	Anisotropy =	456.5910

26	C	Isotropic =	43.0078	Anisotropy =	160.3792
27	C	Isotropic =	92.0287	Anisotropy =	138.2771
28	C	Isotropic =	69.7133	Anisotropy =	174.6367
29	C	Isotropic =	68.4468	Anisotropy =	171.3055
30	C	Isotropic =	63.7313	Anisotropy =	175.0809
31	C	Isotropic =	64.0638	Anisotropy =	150.4032
32	C	Isotropic =	154.5705	Anisotropy =	44.1474
33	O	Isotropic =	-80.3622	Anisotropy =	393.1196
34	H	Isotropic =	24.5234	Anisotropy =	8.2608
35	H	Isotropic =	24.3133	Anisotropy =	4.1814
36	H	Isotropic =	23.5122	Anisotropy =	5.1985
37	H	Isotropic =	23.3231	Anisotropy =	6.4272
38	H	Isotropic =	23.0912	Anisotropy =	10.1036
39	H	Isotropic =	26.9604	Anisotropy =	7.1871
40	H	Isotropic =	28.4519	Anisotropy =	6.6798
41	H	Isotropic =	30.6278	Anisotropy =	6.7336
42	H	Isotropic =	30.7570	Anisotropy =	7.5801
43	H	Isotropic =	30.6637	Anisotropy =	10.5051
44	H	Isotropic =	28.4773	Anisotropy =	7.8364
45	H	Isotropic =	28.3826	Anisotropy =	7.2800
46	H	Isotropic =	26.5887	Anisotropy =	4.3062
47	H	Isotropic =	26.8542	Anisotropy =	7.8282
48	H	Isotropic =	23.0891	Anisotropy =	7.3654
49	H	Isotropic =	25.2393	Anisotropy =	6.5637
50	H	Isotropic =	23.0912	Anisotropy =	10.7222
51	H	Isotropic =	23.8132	Anisotropy =	5.8578
52	H	Isotropic =	23.6515	Anisotropy =	4.9560
53	H	Isotropic =	23.6339	Anisotropy =	6.2675
54	H	Isotropic =	28.6439	Anisotropy =	7.6951
55	H	Isotropic =	27.9494	Anisotropy =	9.9728
56	H	Isotropic =	27.5340	Anisotropy =	7.7227

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.554947367750	-7.449450932114	1.855165647208
C	-0.268236566066	-6.924946583425	0.863321757013
C	-0.050996048328	-7.276713640012	-0.475969489682
C	0.932932777771	-8.218049499414	-0.807475396712
C	1.678704083998	-8.796124857464	0.218389593599
C	1.476958876998	-8.409589418323	1.529591666863

N	-0.859392448479	-6.696929655151	-1.487571523945
C	-0.991799065257	-5.329776190943	-1.666168039087
C	-0.767896698088	-4.383131939644	-0.526552616116
C	-1.062049983310	-4.671143108378	0.827741698526
N	-1.242100395199	-5.998676119155	1.248760957794
O	-1.352246797590	-4.885515223347	-2.755944618353
N	-1.219025589731	-3.709976041122	1.746303829021
C	-0.994726912288	-2.441863136571	1.384344488650
C	-0.588688274208	-2.040351382451	0.104243667848
C	-0.507750806966	-3.049121357157	-0.858582382923
C	-2.143448991333	-6.289679659403	2.382908354000
C	-3.607541135517	-6.135613644711	1.975524139789
C	-0.347038285981	-0.587391948715	-0.231860713628
C	-1.501328961349	0.091901204466	-0.975020881831
O	-2.662268398672	0.208945136902	-0.128472810442
C	-3.775950686460	-0.530321913027	-0.328812725270
C	-4.892082509246	-0.183764140356	0.505701769720
C	-6.103526329536	-0.927305568867	0.339237445010
N	-6.243171602322	-1.942460247884	-0.571825525035
C	-5.184216780561	-2.220615862399	-1.310405232838
C	-3.932429984256	-1.562707072903	-1.239810258109
C	-4.833946198287	0.855351725460	1.472347963047
C	-5.937086790746	1.149490441095	2.250201854311
C	-7.139601215739	0.416652291557	2.090385426653
C	-7.219588448543	-0.597162727988	1.156631552505
C	-1.224091946225	-7.532964507114	-2.639139846442
O	0.440205373926	-7.061859784290	3.071283751301
H	1.108575846851	-8.495068258401	-1.845126892298
H	2.442207644680	-9.543765686174	0.002539716134
H	2.034399651777	-8.788165104372	2.383403588917
H	-1.141419410210	-1.690325651204	2.167904219079
H	-0.290238092942	-2.811558268553	-1.901814327357
H	-1.936744939276	-7.316899412541	2.703339211949
H	-1.898405694107	-5.631018120166	3.226378162508
H	-3.829114553981	-5.104235622918	1.658571555439
H	-3.865249689991	-6.815109965710	1.147529044353
H	-4.258801142491	-6.370651971675	2.833137800703
H	-0.144960955947	-0.018245293937	0.688945093428
H	0.546788730705	-0.490373965687	-0.870314568513
H	-1.219681062395	1.125543695419	-1.224140827855
H	-1.749427863539	-0.427740113249	-1.910713103485
H	-5.296578940843	-3.035775732912	-2.034525585791
H	-3.128028702128	-1.900136441864	-1.890225582680
H	-3.905445442351	1.414234248235	1.588969489489

H	-5.884777386667	1.949844206879	2.991281345590
H	-8.006006748133	0.657506461183	2.710441916729
H	-8.135466743535	-1.174463529600	1.016082771112
H	-2.155532109311	-7.147057904211	-3.069116123960
H	-0.452953050660	-7.514998606126	-3.426438158271
H	-1.373329975669	-8.563033599566	-2.293842247663

SCF Done: E(RB3LYP) = -1465.99496524

Zero-point correction= 0.444740
Thermal correction to Energy= 0.472145
Thermal correction to Enthalpy= 0.473089
Thermal correction to Gibbs Free Energy= 0.383947
Sum of electronic and zero-point Energies= -1465.550225
Sum of electronic and thermal Energies= -1465.522820
Sum of electronic and thermal Enthalpies= -1465.521876
Sum of electronic and thermal Free Energies= -1465.611018

1	N	Isotropic =	-45.8944	Anisotropy =	263.7607
2	C	Isotropic =	44.3734	Anisotropy =	101.8358
3	C	Isotropic =	51.4818	Anisotropy =	123.3675
4	C	Isotropic =	76.6430	Anisotropy =	156.0330
5	C	Isotropic =	70.4099	Anisotropy =	164.1745
6	C	Isotropic =	55.8564	Anisotropy =	110.0942
7	N	Isotropic =	122.7774	Anisotropy =	85.6408
8	C	Isotropic =	26.5665	Anisotropy =	105.2624
9	C	Isotropic =	70.4768	Anisotropy =	134.5117
10	C	Isotropic =	33.8246	Anisotropy =	123.4836
11	N	Isotropic =	159.2275	Anisotropy =	64.1013
12	O	Isotropic =	-91.2144	Anisotropy =	596.3996
13	N	Isotropic =	-32.9419	Anisotropy =	454.1924
14	C	Isotropic =	40.6038	Anisotropy =	148.8629
15	C	Isotropic =	62.2161	Anisotropy =	172.4530
16	C	Isotropic =	50.4846	Anisotropy =	189.4716
17	C	Isotropic =	147.3008	Anisotropy =	37.4388
18	C	Isotropic =	176.2107	Anisotropy =	24.1694
19	C	Isotropic =	156.0040	Anisotropy =	15.3660
20	C	Isotropic =	123.4427	Anisotropy =	53.7007
21	O	Isotropic =	200.8971	Anisotropy =	132.9780
22	C	Isotropic =	31.7952	Anisotropy =	139.6503
23	C	Isotropic =	70.4339	Anisotropy =	170.9145
24	C	Isotropic =	43.8268	Anisotropy =	182.4371
25	N	Isotropic =	-36.3646	Anisotropy =	456.7775
26	C	Isotropic =	43.1305	Anisotropy =	160.2983

27	C	Isotropic =	92.0470	Anisotropy =	138.7492
28	C	Isotropic =	69.8353	Anisotropy =	174.5714
29	C	Isotropic =	67.9116	Anisotropy =	170.0890
30	C	Isotropic =	63.6726	Anisotropy =	175.3769
31	C	Isotropic =	63.9704	Anisotropy =	149.9610
32	C	Isotropic =	154.5265	Anisotropy =	43.9487
33	O	Isotropic =	-80.4659	Anisotropy =	394.0666
34	H	Isotropic =	24.5266	Anisotropy =	8.2434
35	H	Isotropic =	24.3249	Anisotropy =	4.1788
36	H	Isotropic =	23.5166	Anisotropy =	5.2100
37	H	Isotropic =	23.3497	Anisotropy =	6.2842
38	H	Isotropic =	23.1037	Anisotropy =	10.0722
39	H	Isotropic =	28.4453	Anisotropy =	6.6780
40	H	Isotropic =	26.9834	Anisotropy =	7.0448
41	H	Isotropic =	30.7819	Anisotropy =	7.8284
42	H	Isotropic =	30.6079	Anisotropy =	6.7498
43	H	Isotropic =	30.6716	Anisotropy =	10.4504
44	H	Isotropic =	28.3931	Anisotropy =	7.3060
45	H	Isotropic =	28.4833	Anisotropy =	7.8298
46	H	Isotropic =	26.8598	Anisotropy =	7.8855
47	H	Isotropic =	26.5722	Anisotropy =	4.3498
48	H	Isotropic =	23.1052	Anisotropy =	7.2766
49	H	Isotropic =	25.2427	Anisotropy =	6.6393
50	H	Isotropic =	23.0922	Anisotropy =	10.6418
51	H	Isotropic =	23.8299	Anisotropy =	5.8206
52	H	Isotropic =	23.6487	Anisotropy =	4.9494
53	H	Isotropic =	23.6362	Anisotropy =	6.2466
54	H	Isotropic =	27.5346	Anisotropy =	7.6919
55	H	Isotropic =	27.9516	Anisotropy =	9.9709
56	H	Isotropic =	28.6623	Anisotropy =	7.6742

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.196919527260	-6.833510570438	-3.521873167670
C	-2.205748144298	-6.113549725934	-2.894597490854
C	-3.500917935463	-6.648512809249	-2.830226055970
C	-3.796346235142	-7.861651595804	-3.465766254755
C	-2.782736511754	-8.514761890343	-4.165475939431
C	-1.505054994238	-7.991108979269	-4.189051807978
N	-4.516914552597	-5.931657370429	-2.147337543060

C	-4.414408347307	-5.538320484661	-0.821607531229
C	-3.072400749294	-5.333266143897	-0.188323640913
C	-1.918516308259	-4.886852358033	-0.874282236283
N	-1.876819942914	-4.898404030259	-2.279371831016
O	-5.433232784462	-5.309182309817	-0.171242197581
N	-0.847229030530	-4.398822904916	-0.236169748438
C	-0.843610843074	-4.415304873611	1.101706191199
C	-1.883154339323	-4.921335433691	1.894091073365
C	-3.022128038024	-5.353683190387	1.210678154589
C	-1.063153031028	-3.875200925493	-2.971475900195
C	-1.517806252952	-3.671150870601	-4.411561256786
C	-1.799878967780	-4.929041195172	3.404033260297
C	-2.440027336055	-3.711422531738	4.066247284827
O	-1.667056302594	-2.555111009693	3.701721117448
C	-2.057147373426	-1.342666496495	4.148959004848
C	-1.229571790623	-0.235891806069	3.762978549816
C	-1.614909770869	1.066193845460	4.214365893584
N	-2.722887872313	1.296016757692	4.989773144105
C	-3.444791052144	0.240479096035	5.318206483347
C	-3.170408785733	-1.095642372520	4.935700706277
C	-0.064442771125	-0.386441367862	2.965657180468
C	0.695600378293	0.715452978463	2.623694863193
C	0.318625904821	2.008045820101	3.065760076747
C	-0.809963773166	2.178115354846	3.842752772342
C	-5.879936948042	-5.987344468479	-2.692610538935
O	0.014951517435	-6.413626806454	-3.508631672753
H	-4.798189145986	-8.283963496116	-3.418615308962
H	-2.976418471470	-9.452730310268	-4.686269507847
H	-0.652614233626	-8.448532656099	-4.686080199040
H	0.055047087824	-4.010276300053	1.579067882056
H	-3.911920234359	-5.678584388324	1.753318294225
H	-1.207469048027	-2.950168918982	-2.394649752385
H	0.003169688325	-4.133427628807	-2.940263697083
H	-0.958767285469	-2.830137452698	-4.850896998343
H	-1.316141395529	-4.559323696913	-5.029364607146
H	-2.592943468638	-3.436792026257	-4.466893708243
H	-2.310806697468	-5.819803997056	3.801964871531
H	-0.748380796698	-4.989695043276	3.725630449736
H	-3.482488346522	-3.579972446693	3.729627711850
H	-2.435385349048	-3.823514233954	5.163430100097
H	-4.328233724597	0.429055234106	5.939119700598
H	-3.837398691103	-1.889606656699	5.266620742837
H	0.219654226923	-1.383597408297	2.629851781299
H	1.590640920105	0.592225277833	2.010418555043

H	0.926484145015	2.872461385995	2.789351873826
H	-1.118430664145	3.164200510856	4.195349961721
H	-6.438294883447	-6.864706547109	-2.327516539243
H	-6.419769352479	-5.087539898145	-2.375673122831
H	-5.821081768342	-6.017758634328	-3.787149426302

SCF Done: E(RB3LYP) = -1465.99827070

Zero-point correction= 0.444875
Thermal correction to Energy= 0.472216
Thermal correction to Enthalpy= 0.473160
Thermal correction to Gibbs Free Energy= 0.384502
Sum of electronic and zero-point Energies= -1465.553395
Sum of electronic and thermal Energies= -1465.526055
Sum of electronic and thermal Enthalpies= -1465.525111
Sum of electronic and thermal Free Energies= -1465.613768

1	N	Isotropic =	-49.2590	Anisotropy =	261.4069
2	C	Isotropic =	45.8635	Anisotropy =	104.9289
3	C	Isotropic =	50.4700	Anisotropy =	125.6400
4	C	Isotropic =	76.5971	Anisotropy =	156.5027
5	C	Isotropic =	70.0879	Anisotropy =	165.3386
6	C	Isotropic =	55.6441	Anisotropy =	109.6382
7	N	Isotropic =	122.7244	Anisotropy =	86.8081
8	C	Isotropic =	27.0661	Anisotropy =	105.0118
9	C	Isotropic =	71.9461	Anisotropy =	131.1191
10	C	Isotropic =	32.2304	Anisotropy =	123.7987
11	N	Isotropic =	158.0038	Anisotropy =	73.1877
12	O	Isotropic =	-89.6527	Anisotropy =	601.5900
13	N	Isotropic =	-35.4573	Anisotropy =	445.4531
14	C	Isotropic =	39.7975	Anisotropy =	148.8532
15	C	Isotropic =	60.6811	Anisotropy =	172.0621
16	C	Isotropic =	51.7465	Anisotropy =	182.2313
17	C	Isotropic =	146.1993	Anisotropy =	40.5933
18	C	Isotropic =	177.6642	Anisotropy =	22.7475
19	C	Isotropic =	157.1961	Anisotropy =	16.1306
20	C	Isotropic =	121.0873	Anisotropy =	42.7813
21	O	Isotropic =	202.2158	Anisotropy =	111.9695
22	C	Isotropic =	32.1353	Anisotropy =	137.9487
23	C	Isotropic =	70.5470	Anisotropy =	170.7133
24	C	Isotropic =	43.8429	Anisotropy =	181.7176
25	N	Isotropic =	-37.5118	Anisotropy =	458.6633
26	C	Isotropic =	42.5087	Anisotropy =	159.5697
27	C	Isotropic =	91.0753	Anisotropy =	133.0636

28	C	Isotropic =	69.9754	Anisotropy =	173.8214
29	C	Isotropic =	67.6342	Anisotropy =	170.1409
30	C	Isotropic =	63.5415	Anisotropy =	174.7927
31	C	Isotropic =	63.9148	Anisotropy =	150.1350
32	C	Isotropic =	154.6207	Anisotropy =	43.5660
33	O	Isotropic =	-74.4320	Anisotropy =	380.0939
34	H	Isotropic =	24.5473	Anisotropy =	8.0087
35	H	Isotropic =	24.2674	Anisotropy =	4.1098
36	H	Isotropic =	23.4911	Anisotropy =	5.2536
37	H	Isotropic =	22.6773	Anisotropy =	7.8646
38	H	Isotropic =	23.3270	Anisotropy =	10.1644
39	H	Isotropic =	28.0908	Anisotropy =	6.4210
40	H	Isotropic =	26.5992	Anisotropy =	7.4159
41	H	Isotropic =	30.2560	Anisotropy =	11.2463
42	H	Isotropic =	30.5496	Anisotropy =	5.9983
43	H	Isotropic =	30.4826	Anisotropy =	7.3849
44	H	Isotropic =	28.4496	Anisotropy =	7.7220
45	H	Isotropic =	28.2654	Anisotropy =	5.9211
46	H	Isotropic =	27.3236	Anisotropy =	5.8921
47	H	Isotropic =	27.1137	Anisotropy =	5.9523
48	H	Isotropic =	22.7573	Anisotropy =	7.2428
49	H	Isotropic =	24.8920	Anisotropy =	9.4384
50	H	Isotropic =	23.0144	Anisotropy =	9.8630
51	H	Isotropic =	23.7879	Anisotropy =	6.5491
52	H	Isotropic =	23.6195	Anisotropy =	5.2306
53	H	Isotropic =	23.5373	Anisotropy =	5.8143
54	H	Isotropic =	27.9881	Anisotropy =	10.0611
55	H	Isotropic =	27.6434	Anisotropy =	8.0926
56	H	Isotropic =	28.6952	Anisotropy =	7.5643

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.844142434009	-8.592037357840	-0.963585390246
C	-1.221447495428	-7.526292092046	-0.152178046506
C	-2.362697350029	-7.638736298781	0.653587348223
C	-3.070367287521	-8.847150420871	0.709883807130
C	-2.611116622296	-9.927246167078	-0.041902785928
C	-1.506729937039	-9.787176824200	-0.860346360020
N	-2.775117095631	-6.528499532238	1.435689285974
C	-3.042958678029	-5.279274481275	0.900062785414

C	-2.396797231663	-4.838420126284	-0.377026470401
C	-1.107985038313	-5.231846743438	-0.809130332455
N	-0.474528481810	-6.347277143385	-0.235732348818
O	-3.777712554806	-4.499488700211	1.508175169094
N	-0.426614831001	-4.553781181961	-1.741697069586
C	-1.026685642648	-3.520351092921	-2.343008967295
C	-2.336206317458	-3.097649711816	-2.076154217062
C	-3.002593631739	-3.772295081409	-1.051911479162
C	1.000636985547	-6.391644025624	-0.161498785824
C	1.526965324841	-5.433760011405	0.905451255823
C	-2.957735488875	-1.917570534590	-2.786988853188
C	-2.665046717216	-0.573446474703	-2.120987601735
O	-3.150000921716	-0.630794255784	-0.768728619517
C	-3.038647535717	0.464724472331	0.012637833244
C	-3.433766700488	0.303345094274	1.382987408544
C	-3.362479378264	1.455906874104	2.229149427068
N	-2.925635610682	2.682227336598	1.796108737410
C	-2.554374600813	2.765929826576	0.532011388959
C	-2.583060104990	1.704575000361	-0.405444763694
C	-3.871339851912	-0.936422795310	1.921051930014
C	-4.240219425089	-1.028154781107	3.249484031285
C	-4.188597048562	0.112419135478	4.088583822814
C	-3.756805224279	1.325111393198	3.589209113956
C	-3.360791157487	-6.798713576381	2.755569058670
O	0.132239292620	-8.473107247530	-1.785034808770
H	-3.958878247304	-8.941994221840	1.331085078763
H	-3.124515132945	-10.888493786881	-0.011858245758
H	-1.102259220928	-10.568394432418	-1.499994388085
H	-0.426665883348	-2.996415481001	-3.095835382876
H	-3.994648029678	-3.452583661418	-0.731460514704
H	1.279496549558	-7.424695464896	0.074985530496
H	1.427684960662	-6.157524507170	-1.145516943663
H	1.119277595130	-5.679478023600	1.898995890868
H	2.626072098590	-5.500146449728	0.954777141116
H	1.264307621540	-4.389946999432	0.671465757486
H	-2.582413116188	-1.852115718707	-3.820507287208
H	-4.048998726951	-2.051437522057	-2.847703303017
H	-1.582106593947	-0.361168392586	-2.107205882609
H	-3.175938561109	0.235990145456	-2.668269274395
H	-2.199852880016	3.746102845461	0.192537149041
H	-2.256574902252	1.890154391505	-1.427022811459
H	-3.896203143100	-1.822016599862	1.286863043053
H	-4.568011384705	-1.987544822413	3.655207886745
H	-4.485903497350	0.027962786403	5.136303645071

H	-3.699980725421	2.215706701148	4.218124306913
H	-2.857210388642	-7.669127497714	3.192754619916
H	-3.204021321953	-5.921268236133	3.393591087869
H	-4.444918277143	-6.988357526848	2.698487393021

SCF Done: E(RB3LYP) = -1465.99996311

Zero-point correction= 0.444866
Thermal correction to Energy= 0.472213
Thermal correction to Enthalpy= 0.473157
Thermal correction to Gibbs Free Energy= 0.385189
Sum of electronic and zero-point Energies= -1465.555097
Sum of electronic and thermal Energies= -1465.527750
Sum of electronic and thermal Enthalpies= -1465.526806
Sum of electronic and thermal Free Energies= -1465.614774

1	N	Isotropic =	-46.2678	Anisotropy =	262.2469
2	C	Isotropic =	44.5725	Anisotropy =	101.7904
3	C	Isotropic =	51.3914	Anisotropy =	122.6985
4	C	Isotropic =	76.5532	Anisotropy =	156.1521
5	C	Isotropic =	69.9005	Anisotropy =	162.8714
6	C	Isotropic =	55.7780	Anisotropy =	110.9399
7	N	Isotropic =	122.4148	Anisotropy =	85.8587
8	C	Isotropic =	25.7508	Anisotropy =	104.2484
9	C	Isotropic =	71.4581	Anisotropy =	130.9159
10	C	Isotropic =	34.1649	Anisotropy =	123.3155
11	N	Isotropic =	159.0253	Anisotropy =	62.8217
12	O	Isotropic =	-88.6300	Anisotropy =	591.2225
13	N	Isotropic =	-34.1699	Anisotropy =	455.5907
14	C	Isotropic =	41.3868	Anisotropy =	150.3525
15	C	Isotropic =	61.5910	Anisotropy =	170.9287
16	C	Isotropic =	48.4132	Anisotropy =	183.2608
17	C	Isotropic =	146.8813	Anisotropy =	38.0461
18	C	Isotropic =	175.8908	Anisotropy =	24.1531
19	C	Isotropic =	157.5521	Anisotropy =	18.0694
20	C	Isotropic =	121.7743	Anisotropy =	43.3091
21	O	Isotropic =	202.9008	Anisotropy =	117.8960
22	C	Isotropic =	32.0890	Anisotropy =	137.3274
23	C	Isotropic =	70.3268	Anisotropy =	169.6889
24	C	Isotropic =	43.8488	Anisotropy =	181.5696
25	N	Isotropic =	-38.0372	Anisotropy =	457.7917
26	C	Isotropic =	42.7006	Anisotropy =	158.9554
27	C	Isotropic =	91.1238	Anisotropy =	133.1495
28	C	Isotropic =	68.8652	Anisotropy =	176.4270

29	C	Isotropic =	67.2657	Anisotropy =	169.6969
30	C	Isotropic =	63.6228	Anisotropy =	174.3624
31	C	Isotropic =	63.8938	Anisotropy =	149.2988
32	C	Isotropic =	154.3877	Anisotropy =	43.8885
33	O	Isotropic =	-79.9325	Anisotropy =	394.3116
34	H	Isotropic =	24.4879	Anisotropy =	8.3106
35	H	Isotropic =	24.3079	Anisotropy =	4.2553
36	H	Isotropic =	23.4558	Anisotropy =	5.0606
37	H	Isotropic =	22.9357	Anisotropy =	7.8306
38	H	Isotropic =	22.8772	Anisotropy =	10.1420
39	H	Isotropic =	28.3054	Anisotropy =	6.5280
40	H	Isotropic =	26.6922	Anisotropy =	7.7020
41	H	Isotropic =	30.4658	Anisotropy =	7.2598
42	H	Isotropic =	30.4231	Anisotropy =	11.1033
43	H	Isotropic =	30.2766	Anisotropy =	4.8909
44	H	Isotropic =	28.4426	Anisotropy =	8.6059
45	H	Isotropic =	28.2427	Anisotropy =	5.4968
46	H	Isotropic =	27.5079	Anisotropy =	6.4348
47	H	Isotropic =	26.9774	Anisotropy =	6.2877
48	H	Isotropic =	22.7605	Anisotropy =	7.1444
49	H	Isotropic =	24.8951	Anisotropy =	9.6021
50	H	Isotropic =	22.6206	Anisotropy =	9.1205
51	H	Isotropic =	23.6557	Anisotropy =	7.3508
52	H	Isotropic =	23.6004	Anisotropy =	5.6455
53	H	Isotropic =	23.5387	Anisotropy =	5.7939
54	H	Isotropic =	28.5777	Anisotropy =	7.6940
55	H	Isotropic =	27.4985	Anisotropy =	8.0311
56	H	Isotropic =	27.8323	Anisotropy =	9.6293

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.603938796526	-9.012823499897	0.847752701598
C	-3.828630398534	-8.264722713870	-0.032656803129
C	-4.298499440261	-8.011749973721	-1.328529988169
C	-5.502652123390	-8.580718729068	-1.765375178392
C	-6.210061345961	-9.403686263344	-0.890653876330
C	-5.750444879198	-9.611999310062	0.395707062192
N	-3.526746656336	-7.203745954039	-2.202925806499
C	-3.122946533432	-5.914015301489	-1.893079737743
C	-2.962494308281	-5.483083743170	-0.466400382441

C	-2.571641363823	-6.333188689962	0.594934576194
N	-2.630017334455	-7.728999851636	0.448372331682
O	-2.841889237770	-5.127728826807	-2.796328103903
N	-2.100392525792	-5.860603565921	1.756361163120
C	-2.094911681351	-4.537760694085	1.948058042911
C	-2.557157619435	-3.597031091721	1.016267704922
C	-2.960524638215	-4.104419726927	-0.220793342005
C	-1.672855781159	-8.581182398377	1.183803766347
C	-0.272853766300	-8.481807240427	0.581181355682
C	-2.540517402914	-2.115524155311	1.315473690756
C	-1.234936989281	-1.458996637129	0.871177124324
O	-1.337058665986	-0.060336363115	1.184014127945
C	-0.297932961347	0.750980538462	0.893744823970
C	-0.472555065218	2.135382782819	1.227181819481
C	0.609245803469	3.025765637587	0.936536400158
N	1.785815035383	2.617200442534	0.361582987534
C	1.890136477332	1.332638092534	0.074993308496
C	0.894566360030	0.353130393951	0.312064957579
C	-1.658285563809	2.640608301345	1.823041667375
C	-1.771329552095	3.984610067368	2.122434427895
C	-0.703571994338	4.872025859320	1.837806977933
C	0.458659179506	4.402635268681	1.258679700642
C	-3.524391542998	-7.548795507821	-3.630882751378
O	-4.241615028294	-9.167453932626	2.067302807948
H	-5.876026358293	-8.387341150637	-2.769054721513
H	-7.142086397005	-9.877926480195	-1.198746010289
H	-6.255307330265	-10.214024372542	1.147866573566
H	-1.705430049368	-4.199390214709	2.914995223554
H	-3.245562383371	-3.435134221132	-1.034494431446
H	-1.665922424664	-8.299439423277	2.244870071341
H	-2.047194895391	-9.609350840090	1.123769337379
H	0.417369378890	-9.139583615335	1.134102248354
H	-0.271055894750	-8.787467832202	-0.477245350152
H	0.118961736462	-7.454397600654	0.645748396492
H	-3.377237247400	-1.616423672798	0.802517135346
H	-2.669122878031	-1.946082916892	2.395873536718
H	-0.372003663547	-1.895996863324	1.402135789609
H	-1.076872118881	-1.584766186510	-0.213578494943
H	2.831956254383	1.011446945574	-0.384726873160
H	1.089809426266	-0.680868004566	0.033695439793
H	-2.475060680940	1.951661810438	2.039022719322
H	-2.685957527285	4.366913149025	2.580419925497
H	-0.803457927215	5.932642340059	2.079028176277
H	1.293495505391	5.068145895965	1.030649671340

H	-2.599751553509	-7.168993151854	-4.080490268504
H	-3.563411011574	-8.640305313910	-3.728865306338
H	-4.374141619120	-7.098701494511	-4.169590344936

SCF Done: E(RB3LYP) = -1465.99880498

Zero-point correction= 0.444651
Thermal correction to Energy= 0.472203
Thermal correction to Enthalpy= 0.473147
Thermal correction to Gibbs Free Energy= 0.383277
Sum of electronic and zero-point Energies= -1465.554154
Sum of electronic and thermal Energies= -1465.526602
Sum of electronic and thermal Enthalpies= -1465.525658
Sum of electronic and thermal Free Energies= -1465.615528

1	N	Isotropic =	-46.0360	Anisotropy =	263.3735
2	C	Isotropic =	44.5542	Anisotropy =	101.0283
3	C	Isotropic =	51.5004	Anisotropy =	123.6961
4	C	Isotropic =	76.7282	Anisotropy =	156.0533
5	C	Isotropic =	70.3903	Anisotropy =	164.5788
6	C	Isotropic =	55.8626	Anisotropy =	110.0182
7	N	Isotropic =	123.0064	Anisotropy =	86.3122
8	C	Isotropic =	26.9152	Anisotropy =	104.8987
9	C	Isotropic =	70.8569	Anisotropy =	131.9820
10	C	Isotropic =	33.6574	Anisotropy =	123.4316
11	N	Isotropic =	159.6615	Anisotropy =	64.2990
12	O	Isotropic =	-91.0242	Anisotropy =	601.6236
13	N	Isotropic =	-34.5102	Anisotropy =	455.7473
14	C	Isotropic =	40.5226	Anisotropy =	149.8359
15	C	Isotropic =	64.1236	Anisotropy =	166.9061
16	C	Isotropic =	50.2115	Anisotropy =	184.0884
17	C	Isotropic =	146.6807	Anisotropy =	38.2174
18	C	Isotropic =	175.9420	Anisotropy =	24.7065
19	C	Isotropic =	156.9323	Anisotropy =	32.4876
20	C	Isotropic =	121.2070	Anisotropy =	66.9012
21	O	Isotropic =	197.7857	Anisotropy =	104.2545
22	C	Isotropic =	31.9993	Anisotropy =	138.0032
23	C	Isotropic =	70.5455	Anisotropy =	170.9966
24	C	Isotropic =	43.8464	Anisotropy =	181.9417
25	N	Isotropic =	-37.8072	Anisotropy =	458.3770
26	C	Isotropic =	42.4937	Anisotropy =	159.7047
27	C	Isotropic =	91.1060	Anisotropy =	133.3772
28	C	Isotropic =	70.1380	Anisotropy =	174.2273
29	C	Isotropic =	67.5972	Anisotropy =	170.4706

30	C	Isotropic =	63.4282	Anisotropy =	174.8761
31	C	Isotropic =	63.7739	Anisotropy =	150.3832
32	C	Isotropic =	154.4567	Anisotropy =	44.0553
33	O	Isotropic =	-79.8809	Anisotropy =	391.7601
34	H	Isotropic =	24.5321	Anisotropy =	8.0305
35	H	Isotropic =	24.2987	Anisotropy =	4.1274
36	H	Isotropic =	23.4784	Anisotropy =	5.0714
37	H	Isotropic =	22.9612	Anisotropy =	8.3343
38	H	Isotropic =	23.2899	Anisotropy =	10.9065
39	H	Isotropic =	26.6649	Anisotropy =	7.3862
40	H	Isotropic =	28.2948	Anisotropy =	6.2481
41	H	Isotropic =	30.3480	Anisotropy =	11.1135
42	H	Isotropic =	30.3897	Anisotropy =	7.5979
43	H	Isotropic =	30.1586	Anisotropy =	5.1100
44	H	Isotropic =	28.2676	Anisotropy =	5.0553
45	H	Isotropic =	28.2576	Anisotropy =	5.6617
46	H	Isotropic =	27.3820	Anisotropy =	6.4060
47	H	Isotropic =	27.3752	Anisotropy =	7.3319
48	H	Isotropic =	22.7361	Anisotropy =	7.5252
49	H	Isotropic =	24.9247	Anisotropy =	8.9436
50	H	Isotropic =	23.0457	Anisotropy =	10.5467
51	H	Isotropic =	23.7940	Anisotropy =	6.1296
52	H	Isotropic =	23.5934	Anisotropy =	5.1013
53	H	Isotropic =	23.4931	Anisotropy =	5.9700
54	H	Isotropic =	27.6070	Anisotropy =	8.0594
55	H	Isotropic =	28.6563	Anisotropy =	7.6776
56	H	Isotropic =	27.9680	Anisotropy =	9.8443

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.960187515859	-1.221218315670	-0.845217584776
C	2.319469454539	-2.455011869968	-0.898649718584
C	2.189933797618	-3.117733972741	-2.126694461034
C	2.778277406430	-2.583654848427	-3.281317288641
C	3.495164064646	-1.392893528547	-3.177388553998
C	3.580529765066	-0.733914667911	-1.965837394624
N	1.487276771151	-4.348964456976	-2.181363598849
C	0.178779469281	-4.499267439971	-1.747740015985
C	-0.388767785917	-3.593278739171	-0.697047865938
C	0.358396157030	-3.003697417820	0.350267382516

N	1.760147777666	-2.950131780944	0.283420886465
O	-0.509247576864	-5.418852856466	-2.188278116451
N	-0.219173562334	-2.510525004567	1.453669144482
C	-1.554334082778	-2.489334087669	1.516391397222
C	-2.405720231742	-2.942196349180	0.498340381549
C	-1.784721045206	-3.532759073109	-0.604481210630
C	2.553430968981	-2.977155074101	1.529755705991
C	2.522530962222	-4.362854017165	2.171421597398
C	-3.909029879383	-2.867410833653	0.634831872012
C	-4.491748988514	-4.158748481371	1.205321388262
O	-5.914964179977	-3.980064904357	1.288682569177
C	-6.673430092020	-4.989513007374	1.766112980565
C	-8.084244058699	-4.736634679906	1.827823646443
C	-8.921529396448	-5.783457753914	2.328437248893
N	-8.438880770916	-6.998574981341	2.743870232882
C	-7.132885149243	-7.175259463357	2.664822336412
C	-6.200231690847	-6.220343313695	2.190222704646
C	-8.664514066809	-3.507095601689	1.418261086372
C	-10.030554602864	-3.318020332986	1.500962723409
C	-10.865847714196	-4.350446332158	1.995936400514
C	-10.323154232304	-5.554174114521	2.399770079029
C	1.972549905862	-5.373888635671	-3.115141541902
O	2.997137471613	-0.551770473554	0.246836171004
H	2.681207036020	-3.090638371166	-4.239352750215
H	3.981033733516	-0.954317630432	-4.049237331752
H	4.093833897871	0.211574088021	-1.805808606403
H	-1.980498370033	-2.073473129701	2.436443525829
H	-2.374512763227	-3.995618649811	-1.397684707244
H	3.579391286663	-2.700290374941	1.261380667316
H	2.181685981178	-2.212582957562	2.224392847166
H	2.916149055194	-5.129341674667	1.484950426425
H	3.140086489871	-4.363369927723	3.084325430669
H	1.498437827835	-4.648189754060	2.459263758267
H	-4.187281059324	-2.033156299912	1.297365729627
H	-4.370531621770	-2.676582194948	-0.346574329125
H	-4.263329287702	-5.018331479509	0.552227923666
H	-4.084407414061	-4.365940815892	2.209590235320
H	-6.752297918535	-8.147659147321	2.998229207444
H	-5.142272199592	-6.475729989715	2.170639556251
H	-8.015074094029	-2.717826224012	1.039236779045
H	-10.470770948210	-2.370168921193	1.184345312462
H	-11.944557007458	-4.190109874152	2.057122057366
H	-10.947816011449	-6.362706252246	2.784264515557
H	1.562017489235	-5.241239179438	-4.129424587918

H	3.067474178803	-5.326052551961	-3.152140026537
H	1.657079338304	-6.357552277710	-2.748646217048

SCF Done: E(RB3LYP) = -1465.99877659

Zero-point correction= 0.444587
Thermal correction to Energy= 0.472157
Thermal correction to Enthalpy= 0.473101
Thermal correction to Gibbs Free Energy= 0.383295
Sum of electronic and zero-point Energies= -1465.554189
Sum of electronic and thermal Energies= -1465.526619
Sum of electronic and thermal Enthalpies= -1465.525675
Sum of electronic and thermal Free Energies= -1465.615481

1	N	Isotropic =	-46.1100	Anisotropy =	263.0513
2	C	Isotropic =	44.9464	Anisotropy =	101.7381
3	C	Isotropic =	51.6142	Anisotropy =	123.0960
4	C	Isotropic =	76.7147	Anisotropy =	156.5943
5	C	Isotropic =	70.0664	Anisotropy =	164.4932
6	C	Isotropic =	55.7222	Anisotropy =	110.6158
7	N	Isotropic =	122.8368	Anisotropy =	85.4045
8	C	Isotropic =	27.0217	Anisotropy =	104.8584
9	C	Isotropic =	70.9706	Anisotropy =	131.8754
10	C	Isotropic =	33.5502	Anisotropy =	123.7356
11	N	Isotropic =	159.2546	Anisotropy =	63.8551
12	O	Isotropic =	-91.2941	Anisotropy =	602.5360
13	N	Isotropic =	-34.6038	Anisotropy =	455.4773
14	C	Isotropic =	40.4214	Anisotropy =	149.1796
15	C	Isotropic =	64.1617	Anisotropy =	166.8477
16	C	Isotropic =	50.2861	Anisotropy =	184.4598
17	C	Isotropic =	146.6116	Anisotropy =	38.1472
18	C	Isotropic =	175.8851	Anisotropy =	24.7528
19	C	Isotropic =	156.8352	Anisotropy =	32.3718
20	C	Isotropic =	121.2187	Anisotropy =	67.1924
21	O	Isotropic =	198.0174	Anisotropy =	104.9287
22	C	Isotropic =	31.9429	Anisotropy =	138.0843
23	C	Isotropic =	70.5472	Anisotropy =	171.0496
24	C	Isotropic =	43.8814	Anisotropy =	181.9881
25	N	Isotropic =	-38.0710	Anisotropy =	457.4101
26	C	Isotropic =	42.4494	Anisotropy =	159.5914
27	C	Isotropic =	91.0429	Anisotropy =	133.0153
28	C	Isotropic =	69.9981	Anisotropy =	173.7821
29	C	Isotropic =	67.5703	Anisotropy =	170.4328
30	C	Isotropic =	63.6062	Anisotropy =	175.1144

31	C	Isotropic =	63.7544	Anisotropy =	150.1797
32	C	Isotropic =	154.5141	Anisotropy =	43.8627
33	O	Isotropic =	-79.9328	Anisotropy =	392.2544
34	H	Isotropic =	24.5272	Anisotropy =	8.0408
35	H	Isotropic =	24.2951	Anisotropy =	4.1270
36	H	Isotropic =	23.4648	Anisotropy =	5.0810
37	H	Isotropic =	22.9731	Anisotropy =	8.2660
38	H	Isotropic =	23.3048	Anisotropy =	10.9577
39	H	Isotropic =	28.3255	Anisotropy =	6.2661
40	H	Isotropic =	26.6755	Anisotropy =	7.4305
41	H	Isotropic =	30.3860	Anisotropy =	7.6224
42	H	Isotropic =	30.3355	Anisotropy =	11.0655
43	H	Isotropic =	30.1459	Anisotropy =	5.0826
44	H	Isotropic =	28.2860	Anisotropy =	5.6672
45	H	Isotropic =	28.2453	Anisotropy =	5.0692
46	H	Isotropic =	27.3239	Anisotropy =	7.4487
47	H	Isotropic =	27.3953	Anisotropy =	6.4048
48	H	Isotropic =	22.7357	Anisotropy =	7.5264
49	H	Isotropic =	24.9167	Anisotropy =	8.9303
50	H	Isotropic =	23.0380	Anisotropy =	10.5605
51	H	Isotropic =	23.7860	Anisotropy =	6.1369
52	H	Isotropic =	23.5934	Anisotropy =	5.1081
53	H	Isotropic =	23.4943	Anisotropy =	5.9738
54	H	Isotropic =	27.9763	Anisotropy =	9.8400
55	H	Isotropic =	28.6513	Anisotropy =	7.6812
56	H	Isotropic =	27.6006	Anisotropy =	8.1221

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.244493524591	-2.834381554103	-4.092494425328
C	-0.423434580513	-3.570645537373	-3.121986950138
C	-1.590658577080	-4.269125829807	-3.465220025055
C	-2.035022869823	-4.293793400211	-4.793401901496
C	-1.290555790348	-3.620090599476	-5.760644112876
C	-0.163352592038	-2.908591946183	-5.399438571514
N	-2.297274991466	-4.981225030225	-2.461288990461
C	-2.766950341101	-4.392999933488	-1.299025529496
C	-2.121925066295	-3.155516174147	-0.757255904803
C	-0.746003595136	-2.848544164916	-0.875946559328
N	0.056304088410	-3.531593460835	-1.805929746086

O	-3.691068479911	-4.918973854704	-0.676666413414
N	-0.141871375746	-1.943311105593	-0.095868709985
C	-0.890482190944	-1.253577258808	0.773746762113
C	-2.277313031922	-1.396394241377	0.915679838087
C	-2.875796081242	-2.390912245217	0.139783064655
C	1.490719746107	-3.722410086463	-1.498336192052
C	2.087967448784	-4.885307724762	-2.281434129212
C	-3.070210421551	-0.585760013848	1.914978570271
C	-3.135078215786	-1.213235447802	3.307157746232
O	-3.703619522683	-2.527315267799	3.178114974572
C	-3.915359235701	-3.261168939626	4.291495242733
C	-4.361397003412	-4.609128525697	4.081311952365
C	-4.632502859173	-5.401541891554	5.242417774390
N	-4.473602555405	-4.938743170392	6.524133337186
C	-4.039276316735	-3.699092960066	6.656382323675
C	-3.740029673867	-2.814687257108	5.591298109461
C	-4.525650678529	-5.177481325049	2.789730780787
C	-4.956653811166	-6.483190334254	2.652731538577
C	-5.242817861855	-7.268038293265	3.797145345233
C	-5.082363034060	-6.738530834406	5.062155254282
C	-2.924723313665	-6.255750713631	-2.835955670996
O	1.256280989706	-2.108472903491	-3.785414337259
H	-2.940803769001	-4.831822838785	-5.066093537188
H	-1.594454622290	-3.628253216611	-6.807572675576
H	0.457450252283	-2.334459657694	-6.083487279795
H	-0.350222512953	-0.528621590031	1.393213215727
H	-3.937109718542	-2.616110857575	0.249545748778
H	2.058219999257	-2.802166963010	-1.687854525294
H	1.531034247681	-3.932743594742	-0.419792748171
H	2.127838977625	-4.669860387407	-3.359958560802
H	3.121371580786	-5.055940813888	-1.941136424446
H	1.516313852435	-5.814161839281	-2.125685132681
H	-2.626612369886	0.415318618631	2.034298129524
H	-4.097142166563	-0.441463597616	1.544778190487
H	-2.130360191431	-1.298078641832	3.756053266690
H	-3.765201484476	-0.594889505262	3.967421319674
H	-3.907101698829	-3.336273232229	7.682316070617
H	-3.390920858843	-1.809146071990	5.818802124883
H	-4.292098951338	-4.586936331061	1.904345141916
H	-5.071830254538	-6.912708013476	1.655386018872
H	-5.586084426460	-8.297935061568	3.675788581158
H	-5.289001544253	-7.325821671894	5.958980900019
H	-3.013029504042	-6.878244683090	-1.938045145593
H	-3.935004626326	-6.114721697150	-3.253204577492

H -2.288161940742 -6.758136326763 -3.574002546428

SCF Done: E(RB3LYP) = -1465.99940032

Zero-point correction= 0.445062
Thermal correction to Energy= 0.472330
Thermal correction to Enthalpy= 0.473274
Thermal correction to Gibbs Free Energy= 0.385778
Sum of electronic and zero-point Energies= -1465.554339
Sum of electronic and thermal Energies= -1465.527070
Sum of electronic and thermal Enthalpies= -1465.526126
Sum of electronic and thermal Free Energies= -1465.613622

1 N Isotropic = -49.1502 Anisotropy = 262.1886
2 C Isotropic = 45.6698 Anisotropy = 104.8080
3 C Isotropic = 50.5631 Anisotropy = 125.2652
4 C Isotropic = 76.6590 Anisotropy = 156.4717
5 C Isotropic = 69.8332 Anisotropy = 165.5852
6 C Isotropic = 55.3520 Anisotropy = 109.8833
7 N Isotropic = 121.6287 Anisotropy = 86.2876
8 C Isotropic = 25.7972 Anisotropy = 104.7616
9 C Isotropic = 72.4703 Anisotropy = 129.9730
10 C Isotropic = 32.3767 Anisotropy = 123.5856
11 N Isotropic = 157.3196 Anisotropy = 74.5673
12 O Isotropic = -86.4400 Anisotropy = 589.1182
13 N Isotropic = -35.6912 Anisotropy = 447.5302
14 C Isotropic = 41.6012 Anisotropy = 150.4811
15 C Isotropic = 61.3299 Anisotropy = 171.8247
16 C Isotropic = 48.3451 Anisotropy = 182.5992
17 C Isotropic = 146.3890 Anisotropy = 40.4246
18 C Isotropic = 177.5777 Anisotropy = 22.6998
19 C Isotropic = 157.6522 Anisotropy = 18.3722
20 C Isotropic = 122.0353 Anisotropy = 43.8195
21 O Isotropic = 203.0887 Anisotropy = 118.1414
22 C Isotropic = 31.9931 Anisotropy = 137.3435
23 C Isotropic = 70.3662 Anisotropy = 169.5036
24 C Isotropic = 43.6894 Anisotropy = 181.0566
25 N Isotropic = -37.7041 Anisotropy = 458.8263
26 C Isotropic = 42.7988 Anisotropy = 159.3069
27 C Isotropic = 91.2248 Anisotropy = 133.0854
28 C Isotropic = 68.7802 Anisotropy = 176.0631
29 C Isotropic = 67.3622 Anisotropy = 170.0124
30 C Isotropic = 63.6810 Anisotropy = 174.5464
31 C Isotropic = 64.2262 Anisotropy = 149.3455

32	C	Isotropic =	154.4187	Anisotropy =	43.8582
33	O	Isotropic =	-75.3882	Anisotropy =	380.8470
34	H	Isotropic =	24.4793	Anisotropy =	8.1983
35	H	Isotropic =	24.2239	Anisotropy =	4.2646
36	H	Isotropic =	23.4570	Anisotropy =	5.0830
37	H	Isotropic =	22.9578	Anisotropy =	7.9419
38	H	Isotropic =	22.9066	Anisotropy =	10.2486
39	H	Isotropic =	26.5967	Anisotropy =	7.9391
40	H	Isotropic =	28.0569	Anisotropy =	5.7703
41	H	Isotropic =	30.5243	Anisotropy =	5.9199
42	H	Isotropic =	30.2304	Anisotropy =	11.4319
43	H	Isotropic =	30.4363	Anisotropy =	7.3564
44	H	Isotropic =	28.4523	Anisotropy =	8.6151
45	H	Isotropic =	28.2426	Anisotropy =	5.4802
46	H	Isotropic =	27.5324	Anisotropy =	6.5467
47	H	Isotropic =	26.9557	Anisotropy =	6.2826
48	H	Isotropic =	22.7471	Anisotropy =	7.1716
49	H	Isotropic =	24.8992	Anisotropy =	9.6102
50	H	Isotropic =	22.6321	Anisotropy =	9.0963
51	H	Isotropic =	23.6579	Anisotropy =	7.4384
52	H	Isotropic =	23.6084	Anisotropy =	5.6710
53	H	Isotropic =	23.5487	Anisotropy =	5.8062
54	H	Isotropic =	27.4530	Anisotropy =	8.1137
55	H	Isotropic =	27.8547	Anisotropy =	9.6335
56	H	Isotropic =	28.5978	Anisotropy =	7.5001

Conformer 20----------
#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.224051391473	0.241919051617	-1.951338466091
C	-0.870105987174	-0.453901122081	-2.455772731499
C	-2.146033556192	0.122775981869	-2.399088083557
C	-2.308596959640	1.428574434200	-1.916533320629
C	-1.179644151994	2.135609481272	-1.506321958012
C	0.065647866619	1.537544280447	-1.533744375492
N	-3.263901840380	-0.616821403905	-2.864224228791
C	-3.602709908576	-1.869464620852	-2.374848554376
C	-2.557650144155	-2.770205077150	-1.788937483001
C	-1.202094484789	-2.805661038015	-2.196103679281
N	-0.652187055134	-1.748487952420	-2.937927949002
O	-4.761602624325	-2.270077393712	-2.471004136132
N	-0.404270476391	-3.849929059716	-1.938071623009

C	-0.879178056342	-4.840025992280	-1.175606053504
C	-2.163851163344	-4.864805053243	-0.614283610070
C	-3.011688934623	-3.814632875938	-0.974603306706
C	0.449630939986	-2.013767079942	-3.886340129967
C	-0.054827419990	-2.752365393661	-5.124382167818
C	-2.608610801190	-5.984182770790	0.296908969021
C	-2.442064538697	-5.613797766105	1.769136695547
O	-2.899114537876	-6.735186514405	2.542529390936
C	-2.854969888698	-6.659983042823	3.889594140783
C	-3.325128502485	-7.816443676369	4.596576255796
C	-3.292943290219	-7.774381782021	6.026435160560
N	-2.839237063579	-6.692084895981	6.736836512362
C	-2.419232038180	-5.656256443137	6.034056157831
C	-2.399861409846	-5.574448999269	4.619910013433
C	-3.811053154118	-8.976692594442	3.937882527851
C	-4.251690116011	-10.062270339581	4.670071176116
C	-4.222225922291	-10.027686115699	6.086563243121
C	-3.753687974047	-8.909873168547	6.748005812440
C	-4.343719053510	0.120619369638	-3.533608244822
O	1.380156758947	-0.308503885423	-1.899401502741
H	-3.296005225109	1.883477328818	-1.867043955476
H	-1.262737145707	3.159229635302	-1.140509173623
H	0.989694466304	2.007644602244	-1.204845253446
H	-0.193106746857	-5.676177901567	-0.999751448525
H	-4.060931396037	-3.815885430088	-0.673865592577
H	0.873862878561	-1.041967159348	-4.163081647548
H	1.242884980504	-2.582868977943	-3.384121309393
H	-0.469364832467	-3.738444163715	-4.861813802302
H	-0.836358003508	-2.174679613575	-5.643260561779
H	0.780006557762	-2.915245774657	-5.825321189950
H	-3.667639266111	-6.225489282608	0.113893301302
H	-2.022535626082	-6.893884062136	0.093710083127
H	-1.385064259616	-5.404874051869	2.007170310700
H	-3.039496080563	-4.721113912281	2.022065690538
H	-2.057856161618	-4.794139261076	6.606504371123
H	-2.030604404371	-4.667176247906	4.145120366624
H	-3.830149597257	-8.995401921487	2.848083501201
H	-4.624458718699	-10.951550452108	4.157581447800
H	-4.572682310262	-10.891666545903	6.655603885928
H	-3.721994661463	-8.861836408009	7.838195407452
H	-3.902927873022	0.940147840160	-4.113681037974
H	-4.871441641962	-0.566303714713	-4.205338144796
H	-5.077150835648	0.526598932932	-2.818039699700

SCF Done: E(RB3LYP) = -1465.99907431

Zero-point correction= 0.444604
Thermal correction to Energy= 0.472169
Thermal correction to Enthalpy= 0.473113
Thermal correction to Gibbs Free Energy= 0.383422
Sum of electronic and zero-point Energies= -1465.554471
Sum of electronic and thermal Energies= -1465.526905
Sum of electronic and thermal Enthalpies= -1465.525961
Sum of electronic and thermal Free Energies= -1465.615652

1	N	Isotropic =	-46.1611	Anisotropy =	263.5795
2	C	Isotropic =	44.6542	Anisotropy =	102.0242
3	C	Isotropic =	51.6416	Anisotropy =	123.1552
4	C	Isotropic =	76.7366	Anisotropy =	156.1204
5	C	Isotropic =	70.2490	Anisotropy =	164.8026
6	C	Isotropic =	55.7052	Anisotropy =	110.6245
7	N	Isotropic =	123.2382	Anisotropy =	85.8187
8	C	Isotropic =	26.7467	Anisotropy =	104.5379
9	C	Isotropic =	71.0637	Anisotropy =	131.0080
10	C	Isotropic =	33.3985	Anisotropy =	122.8432
11	N	Isotropic =	158.6098	Anisotropy =	65.0915
12	O	Isotropic =	-90.7117	Anisotropy =	602.2184
13	N	Isotropic =	-33.4401	Anisotropy =	454.0541
14	C	Isotropic =	40.7635	Anisotropy =	146.0367
15	C	Isotropic =	63.9544	Anisotropy =	166.4169
16	C	Isotropic =	50.0874	Anisotropy =	183.3491
17	C	Isotropic =	146.8075	Anisotropy =	38.2129
18	C	Isotropic =	175.9811	Anisotropy =	24.7956
19	C	Isotropic =	156.2588	Anisotropy =	32.9808
20	C	Isotropic =	121.2032	Anisotropy =	67.0971
21	O	Isotropic =	197.8089	Anisotropy =	104.5750
22	C	Isotropic =	31.8759	Anisotropy =	137.4974
23	C	Isotropic =	70.5885	Anisotropy =	170.9353
24	C	Isotropic =	43.7846	Anisotropy =	181.5125
25	N	Isotropic =	-37.5194	Anisotropy =	458.7671
26	C	Isotropic =	42.5617	Anisotropy =	159.6824
27	C	Isotropic =	91.1089	Anisotropy =	133.0862
28	C	Isotropic =	69.9599	Anisotropy =	173.5012
29	C	Isotropic =	67.6854	Anisotropy =	170.6194
30	C	Isotropic =	63.4977	Anisotropy =	174.7798
31	C	Isotropic =	63.9960	Anisotropy =	150.7221
32	C	Isotropic =	154.4037	Anisotropy =	43.9468
33	O	Isotropic =	-80.5102	Anisotropy =	393.1628

34	H	Isotropic =	24.5275	Anisotropy =	7.9350
35	H	Isotropic =	24.2886	Anisotropy =	4.0636
36	H	Isotropic =	23.4585	Anisotropy =	5.0418
37	H	Isotropic =	23.0076	Anisotropy =	8.0669
38	H	Isotropic =	23.3259	Anisotropy =	10.8930
39	H	Isotropic =	28.2966	Anisotropy =	6.2529
40	H	Isotropic =	26.6855	Anisotropy =	7.3753
41	H	Isotropic =	30.1333	Anisotropy =	5.0938
42	H	Isotropic =	30.3874	Anisotropy =	7.6895
43	H	Isotropic =	30.3373	Anisotropy =	11.1814
44	H	Isotropic =	28.2119	Anisotropy =	5.1730
45	H	Isotropic =	28.2092	Anisotropy =	5.3709
46	H	Isotropic =	27.5350	Anisotropy =	6.4764
47	H	Isotropic =	27.5165	Anisotropy =	7.4993
48	H	Isotropic =	22.7863	Anisotropy =	7.6502
49	H	Isotropic =	25.0242	Anisotropy =	8.9213
50	H	Isotropic =	23.0524	Anisotropy =	10.5463
51	H	Isotropic =	23.7821	Anisotropy =	6.1428
52	H	Isotropic =	23.5952	Anisotropy =	5.1086
53	H	Isotropic =	23.5041	Anisotropy =	6.0003
54	H	Isotropic =	28.6415	Anisotropy =	7.7346
55	H	Isotropic =	27.6197	Anisotropy =	8.3196
56	H	Isotropic =	27.9771	Anisotropy =	9.7993

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.348936069337	-6.092305183886	-3.551358995722
C	-0.289432739593	-6.723289463487	-2.488453360361
C	0.471896146951	-7.271484758718	-1.447519594287
C	1.871665173047	-7.263999598483	-1.518469222099
C	2.481501512132	-6.709315500224	-2.642436409168
C	1.715646444398	-6.138272292045	-3.640787945853
N	-0.189410360220	-7.861904103407	-0.339918231159
C	-1.115297805103	-7.186022726109	0.440527319267
C	-1.908191971223	-6.047363170832	-0.126816997178
C	-2.308501372177	-5.939689515990	-1.480463846769
N	-1.687835971547	-6.715471993097	-2.471965047144
O	-1.329550615233	-7.556646916471	1.593605681720
N	-3.311240733193	-5.141552641430	-1.869251325439
C	-3.873504701691	-4.338912700503	-0.960174206323

C	-3.482802902594	-4.264050833536	0.384570068099
C	-2.504371083538	-5.174439081123	0.791341451001
C	-2.449474147383	-7.111397304329	-3.674926016954
C	-3.487585975260	-8.181165700363	-3.342087589611
C	-4.113854181455	-3.275852500609	1.336578020730
C	-3.304426710559	-1.983811544151	1.427682239862
O	-3.991622780020	-1.118067292868	2.345642621703
C	-3.478927974027	0.104679046425	2.598649042376
C	-4.224563275700	0.918256532836	3.515361370708
C	-3.712048879221	2.221662920632	3.808799302254
N	-2.556608772359	2.716586559996	3.259291588663
C	-1.912199612589	1.924270536591	2.422565823178
C	-2.314565155913	0.617802196740	2.051027753276
C	-5.429361715284	0.482069384443	4.127251224154
C	-6.107042339061	1.308870892380	5.002358409123
C	-5.605217480932	2.601005139132	5.297571094896
C	-4.435441026823	3.045818591428	4.714164788550
C	0.430645758737	-9.039960517262	0.280882812272
O	-0.330119644449	-5.493322214307	-4.458174262283
H	2.470956267923	-7.686463192202	-0.714337020927
H	3.567046773893	-6.699180060496	-2.742361265222
H	2.112194737254	-5.659299192151	-4.533181991643
H	-4.695380658374	-3.711480174612	-1.323092347516
H	-2.224355535108	-5.260669360412	1.842777621436
H	-2.923469611622	-6.227563342150	-4.121467706153
H	-1.723206636425	-7.492053375562	-4.401997616994
H	-3.013224556136	-9.077039378941	-2.910720699369
H	-4.234945908692	-7.805512315103	-2.625534485102
H	-4.021754743402	-8.478141841348	-4.259282953392
H	-5.133893152634	-3.027642077143	1.004176159988
H	-4.191486648002	-3.713936328544	2.344002268696
H	-2.283670108057	-2.181522306752	1.797298472243
H	-3.229809484136	-1.494191823656	0.441651799933
H	-0.989653570072	2.324381081952	1.986232800085
H	-1.702709374782	0.053375416966	1.349550496699
H	-5.808952196765	-0.512988268887	3.894488774526
H	-7.033244074123	0.967766150451	5.469513867779
H	-6.149060532368	3.246482314307	5.990885270956
H	-4.031114318004	4.037219561598	4.927336538484
H	0.900561421244	-9.645248361177	-0.503584003875
H	1.183978513757	-8.764285926948	1.036819658282
H	-0.351437782824	-9.623491446560	0.780148799607

SCF Done: E(RB3LYP) = -1465.99906116

Zero-point correction= 0.444715
Thermal correction to Energy= 0.472225
Thermal correction to Enthalpy= 0.473169
Thermal correction to Gibbs Free Energy= 0.384048
Sum of electronic and zero-point Energies= -1465.554346
Sum of electronic and thermal Energies= -1465.526836
Sum of electronic and thermal Enthalpies= -1465.525892
Sum of electronic and thermal Free Energies= -1465.615013

1	N	Isotropic =	-46.1159	Anisotropy =	263.5468
2	C	Isotropic =	44.6907	Anisotropy =	102.2838
3	C	Isotropic =	51.2882	Anisotropy =	123.6283
4	C	Isotropic =	76.9932	Anisotropy =	156.1636
5	C	Isotropic =	70.2320	Anisotropy =	164.9973
6	C	Isotropic =	55.7210	Anisotropy =	110.6158
7	N	Isotropic =	123.2284	Anisotropy =	85.7903
8	C	Isotropic =	26.5272	Anisotropy =	104.6087
9	C	Isotropic =	71.0875	Anisotropy =	130.8148
10	C	Isotropic =	32.9550	Anisotropy =	122.7911
11	N	Isotropic =	158.4466	Anisotropy =	65.2647
12	O	Isotropic =	-90.9399	Anisotropy =	600.9110
13	N	Isotropic =	-33.3501	Anisotropy =	454.5659
14	C	Isotropic =	40.9149	Anisotropy =	146.3134
15	C	Isotropic =	64.0198	Anisotropy =	166.3468
16	C	Isotropic =	50.2395	Anisotropy =	182.6763
17	C	Isotropic =	146.4645	Anisotropy =	38.4474
18	C	Isotropic =	176.0821	Anisotropy =	24.5368
19	C	Isotropic =	156.2544	Anisotropy =	33.2041
20	C	Isotropic =	121.2189	Anisotropy =	67.0100
21	O	Isotropic =	197.8880	Anisotropy =	105.6192
22	C	Isotropic =	32.1261	Anisotropy =	138.0124
23	C	Isotropic =	70.5913	Anisotropy =	171.0558
24	C	Isotropic =	43.8740	Anisotropy =	181.8937
25	N	Isotropic =	-37.6610	Anisotropy =	458.4708
26	C	Isotropic =	42.5197	Anisotropy =	159.5533
27	C	Isotropic =	91.2873	Anisotropy =	133.3180
28	C	Isotropic =	70.0898	Anisotropy =	173.9550
29	C	Isotropic =	67.6568	Anisotropy =	170.6412
30	C	Isotropic =	63.5083	Anisotropy =	174.8336
31	C	Isotropic =	63.7991	Anisotropy =	150.2656
32	C	Isotropic =	154.7147	Anisotropy =	43.6856
33	O	Isotropic =	-80.3560	Anisotropy =	392.8252
34	H	Isotropic =	24.5404	Anisotropy =	7.8949

35	H	Isotropic =	24.2884	Anisotropy =	4.0746
36	H	Isotropic =	23.4587	Anisotropy =	5.0472
37	H	Isotropic =	23.0188	Anisotropy =	8.1043
38	H	Isotropic =	23.3257	Anisotropy =	10.7739
39	H	Isotropic =	26.6457	Anisotropy =	7.3449
40	H	Isotropic =	28.3034	Anisotropy =	6.2566
41	H	Isotropic =	30.3779	Anisotropy =	7.7286
42	H	Isotropic =	30.1082	Anisotropy =	5.0760
43	H	Isotropic =	30.3181	Anisotropy =	11.2029
44	H	Isotropic =	28.2049	Anisotropy =	5.3585
45	H	Isotropic =	28.2162	Anisotropy =	5.1606
46	H	Isotropic =	27.5311	Anisotropy =	7.3752
47	H	Isotropic =	27.5542	Anisotropy =	6.5779
48	H	Isotropic =	22.7975	Anisotropy =	7.6304
49	H	Isotropic =	25.0259	Anisotropy =	8.9321
50	H	Isotropic =	23.0449	Anisotropy =	10.5606
51	H	Isotropic =	23.7838	Anisotropy =	6.1409
52	H	Isotropic =	23.6029	Anisotropy =	5.1055
53	H	Isotropic =	23.5122	Anisotropy =	5.9915
54	H	Isotropic =	28.6802	Anisotropy =	7.7387
55	H	Isotropic =	27.9898	Anisotropy =	9.7936
56	H	Isotropic =	27.6259	Anisotropy =	8.2916

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.625246310623	-5.114080412005	-0.405021944291
C	-0.446461790132	-5.767202302939	0.191232314212
C	-0.480903897759	-5.912592545560	1.584699082063
C	0.615729788815	-5.514063754329	2.360707524521
C	1.728436011977	-4.973061071092	1.718626639782
C	1.718253409670	-4.781407752508	0.350108545916
N	-1.629754285651	-6.480728454974	2.191495030954
C	-2.902150697738	-5.948691043992	2.017487283413
C	-3.259153567271	-5.229850592419	0.754070493998
C	-2.714197280935	-5.521527691349	-0.518262467721
N	-1.491642812052	-6.194164626582	-0.635818891083
O	-3.761581907769	-6.125531717683	2.878705798199
N	-3.345643856447	-5.195645599167	-1.655218167984
C	-4.437603981256	-4.430335244663	-1.577167252409
C	-4.961358283667	-3.911186230887	-0.382374618732

C	-4.375854041953	-4.383009411277	0.792358777869
C	-1.194437595857	-6.977199049163	-1.853266076034
C	-1.998447731099	-8.275282986655	-1.883139994113
C	-6.082305113486	-2.891885371188	-0.365709442024
C	-5.826762631127	-1.701451931960	-1.304838145799
O	-4.455656426431	-1.264048952257	-1.269537501369
C	-3.973489717476	-0.567606671690	-0.214745905018
C	-2.550782985341	-0.618049488163	-0.044146996218
C	-1.982801611958	0.153938419729	1.017836898781
N	-2.734189093551	0.923438690038	1.868848525435
C	-4.041909096152	0.911870462225	1.681124984381
C	-4.722093737474	0.187419001850	0.671368958886
C	-1.710303328438	-1.426952940844	-0.854488556329
C	-0.348888839469	-1.472048463425	-0.625222491487
C	0.223001959994	-0.691234516394	0.411243395034
C	-0.574246938238	0.104183198696	1.210864545743
C	-1.438090958128	-7.296524570171	3.397348253389
O	0.608054342886	-4.839055902214	-1.660264472188
H	0.601388029259	-5.626970263975	3.442870140300
H	2.608825209237	-4.669381111998	2.285313783859
H	2.526557645330	-4.329902665046	-0.220561693208
H	-4.914816364477	-4.197418717959	-2.535009894195
H	-4.797072815261	-4.125369474902	1.765885766459
H	-1.397534014034	-6.368158664906	-2.743755210113
H	-0.119190035379	-7.190120792465	-1.842425059111
H	-1.784758382678	-8.896836909367	-0.999069889661
H	-3.080569470752	-8.073114873118	-1.912344010991
H	-1.739271143818	-8.852660337052	-2.785482182823
H	-7.041044013876	-3.344252694083	-0.674498218299
H	-6.224095450383	-2.538025986365	0.666355951922
H	-5.975969102939	-1.988730695241	-2.353931756910
H	-6.516357879682	-0.871198286041	-1.087232771071
H	-4.637399818083	1.521825845262	2.370189697787
H	-5.807343162673	0.252680678831	0.605857180300
H	-2.160948618742	-2.027365474892	-1.644423241476
H	0.278721620964	-2.131999069267	-1.228547537791
H	1.301157119108	-0.728328812893	0.582708111466
H	-0.153747825655	0.704392114432	2.020148235041
H	-2.293063122611	-7.974911366760	3.498644473190
H	-0.515334788814	-7.878683068924	3.285261543799
H	-1.380323231153	-6.683929850262	4.311862451750

SCF Done: E(RB3LYP) = -1465.99381658

Zero-point correction= 0.444798
Thermal correction to Energy= 0.472068
Thermal correction to Enthalpy= 0.473012
Thermal correction to Gibbs Free Energy= 0.385804
Sum of electronic and zero-point Energies= -1465.549018
Sum of electronic and thermal Energies= -1465.521748
Sum of electronic and thermal Enthalpies= -1465.520804
Sum of electronic and thermal Free Energies= -1465.608013

1	N	Isotropic =	-44.7828	Anisotropy =	264.8457
2	C	Isotropic =	45.1914	Anisotropy =	104.0369
3	C	Isotropic =	50.8802	Anisotropy =	125.1781
4	C	Isotropic =	76.6097	Anisotropy =	159.1398
5	C	Isotropic =	70.0305	Anisotropy =	166.9813
6	C	Isotropic =	55.1002	Anisotropy =	114.2666
7	N	Isotropic =	124.2236	Anisotropy =	86.5655
8	C	Isotropic =	26.6861	Anisotropy =	103.5508
9	C	Isotropic =	73.9656	Anisotropy =	127.9517
10	C	Isotropic =	34.5060	Anisotropy =	124.3739
11	N	Isotropic =	156.2306	Anisotropy =	69.8439
12	O	Isotropic =	-94.4007	Anisotropy =	603.5952
13	N	Isotropic =	-29.2844	Anisotropy =	455.4229
14	C	Isotropic =	41.2820	Anisotropy =	163.3377
15	C	Isotropic =	63.8192	Anisotropy =	169.2775
16	C	Isotropic =	50.6808	Anisotropy =	178.4042
17	C	Isotropic =	146.7107	Anisotropy =	39.3465
18	C	Isotropic =	176.1736	Anisotropy =	25.1690
19	C	Isotropic =	159.7219	Anisotropy =	32.0394
20	C	Isotropic =	127.5454	Anisotropy =	59.0910
21	O	Isotropic =	209.8965	Anisotropy =	148.2383
22	C	Isotropic =	34.0389	Anisotropy =	138.8313
23	C	Isotropic =	69.8898	Anisotropy =	174.1469
24	C	Isotropic =	43.7530	Anisotropy =	183.1228
25	N	Isotropic =	-38.8062	Anisotropy =	460.9210
26	C	Isotropic =	43.0759	Anisotropy =	159.7225
27	C	Isotropic =	89.8451	Anisotropy =	142.9073
28	C	Isotropic =	70.5016	Anisotropy =	177.4852
29	C	Isotropic =	67.7909	Anisotropy =	175.1298
30	C	Isotropic =	63.7173	Anisotropy =	176.5392
31	C	Isotropic =	64.4721	Anisotropy =	150.6295
32	C	Isotropic =	155.0953	Anisotropy =	44.1480
33	O	Isotropic =	-71.7212	Anisotropy =	372.8870
34	H	Isotropic =	24.7449	Anisotropy =	7.1022
35	H	Isotropic =	24.3323	Anisotropy =	3.0606

36	H	Isotropic =	23.3137	Anisotropy =	5.1381
37	H	Isotropic =	22.6224	Anisotropy =	8.3928
38	H	Isotropic =	24.1835	Anisotropy =	8.5018
39	H	Isotropic =	26.5609	Anisotropy =	6.3601
40	H	Isotropic =	28.3117	Anisotropy =	6.3459
41	H	Isotropic =	30.3916	Anisotropy =	8.0280
42	H	Isotropic =	30.0045	Anisotropy =	5.4453
43	H	Isotropic =	30.2936	Anisotropy =	11.4409
44	H	Isotropic =	28.4070	Anisotropy =	8.8829
45	H	Isotropic =	28.4355	Anisotropy =	5.0096
46	H	Isotropic =	26.5991	Anisotropy =	7.0289
47	H	Isotropic =	26.4158	Anisotropy =	6.7621
48	H	Isotropic =	22.8274	Anisotropy =	6.6996
49	H	Isotropic =	24.6960	Anisotropy =	9.1513
50	H	Isotropic =	24.1260	Anisotropy =	8.6164
51	H	Isotropic =	24.1975	Anisotropy =	4.7189
52	H	Isotropic =	23.9834	Anisotropy =	5.9517
53	H	Isotropic =	23.8129	Anisotropy =	5.6014
54	H	Isotropic =	27.8598	Anisotropy =	9.1031
55	H	Isotropic =	28.7956	Anisotropy =	8.4655
56	H	Isotropic =	28.2497	Anisotropy =	9.7540

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.137466102812	-1.764038801023	1.188683941439
C	0.159404668814	-2.486256251599	0.001882589283
C	-0.242718868132	-1.871122793551	-1.191358407712
C	-0.540854631149	-0.501908690801	-1.210635351821
C	-0.432792962325	0.222888648942	-0.024813976433
C	-0.096935089925	-0.415381102659	1.154081497631
N	-0.327706850943	-2.649224190165	-2.373672446605
C	-1.121886221643	-3.787094941226	-2.459086077658
C	-1.390550144822	-4.619921761881	-1.244891379449
C	-0.490600791066	-4.778272759029	-0.165035846774
N	0.519787769527	-3.836921784463	0.067351612575
O	-1.553927432126	-4.149813075564	-3.551500936130
N	-0.545750267590	-5.833817988935	0.659587428905
C	-1.582599486359	-6.669301433604	0.551150983291
C	-2.646242585432	-6.504203058449	-0.350366795465
C	-2.491701928674	-5.486224678726	-1.291307724854

C	1.748624351786	-4.235531375771	0.784814902036
C	2.647228034077	-5.098039459769	-0.098796782600
C	-3.891178597091	-7.366538917227	-0.300227307444
C	-4.477713562784	-7.494909386596	1.114680840022
O	-4.443254666810	-6.246150739662	1.829963748856
C	-5.322651466554	-5.256850513435	1.549529379476
C	-4.904606909418	-3.938671309171	1.928202315880
C	-5.827823608231	-2.865571721370	1.721929967259
N	-7.072925695148	-3.043802097937	1.175286549542
C	-7.392750008457	-4.274431828253	0.816475875672
C	-6.567878872095	-5.416373946334	0.966509293286
C	-3.613237685005	-3.665554591501	2.452858516221
C	-3.244280639103	-2.372393261946	2.768465382054
C	-4.164404585838	-1.308019411691	2.590660487600
C	-5.425832598208	-1.549467723054	2.082473863834
C	-0.004939507293	-1.999489834186	-3.650204839652
O	0.356222084616	-2.346663742752	2.313271992457
H	-0.848806281678	-0.012775479141	-2.132585927498
H	-0.637440628322	1.293425923929	-0.002839750995
H	-0.031834985276	0.068096646058	2.126159595100
H	-1.575455624390	-7.515438909729	1.246358804229
H	-3.212216569933	-5.364292610067	-2.102316071831
H	2.264320087042	-3.312192686701	1.073167843896
H	1.482675732557	-4.763249098669	1.709902928915
H	3.565359812612	-5.362338081023	0.450637956122
H	2.144128346005	-6.035107824600	-0.384091767299
H	2.933858191748	-4.563376712122	-1.018352959400
H	-4.641898756778	-6.944042273338	-0.984762514465
H	-3.684985689273	-8.390772952335	-0.657772964393
H	-5.496578283060	-7.910618833218	1.084804611176
H	-3.866685378299	-8.162978002906	1.735737950668
H	-8.385216156330	-4.408381804845	0.370860752999
H	-6.936128767418	-6.387647049600	0.638707197855
H	-2.912553162919	-4.490378961181	2.580649601432
H	-2.232822290459	-2.172795129332	3.130226168508
H	-3.867148192130	-0.288935845580	2.848281070923
H	-6.143832597559	-0.741684281074	1.927601699603
H	-0.864935170393	-1.453308898728	-4.070998540513
H	0.829620899069	-1.305877794289	-3.491255769936
H	0.289138115775	-2.772074818122	-4.370053209818

SCF Done: E(RB3LYP) = -1465.99380903

Zero-point correction= 0.444751

Thermal correction to Energy= 0.472035
Thermal correction to Enthalpy= 0.472979
Thermal correction to Gibbs Free Energy= 0.385678
Sum of electronic and zero-point Energies= -1465.549058
Sum of electronic and thermal Energies= -1465.521774
Sum of electronic and thermal Enthalpies= -1465.520830
Sum of electronic and thermal Free Energies= -1465.608131

1	N	Isotropic =	-44.8623	Anisotropy =	264.1808
2	C	Isotropic =	44.8787	Anisotropy =	104.9438
3	C	Isotropic =	50.6498	Anisotropy =	125.4030
4	C	Isotropic =	76.5157	Anisotropy =	159.2766
5	C	Isotropic =	70.1664	Anisotropy =	166.8496
6	C	Isotropic =	55.3215	Anisotropy =	113.8755
7	N	Isotropic =	124.1011	Anisotropy =	86.5749
8	C	Isotropic =	26.4803	Anisotropy =	103.5962
9	C	Isotropic =	74.0228	Anisotropy =	127.7861
10	C	Isotropic =	34.6681	Anisotropy =	124.5046
11	N	Isotropic =	156.0671	Anisotropy =	69.3052
12	O	Isotropic =	-94.4975	Anisotropy =	604.6798
13	N	Isotropic =	-29.3746	Anisotropy =	454.8250
14	C	Isotropic =	41.3457	Anisotropy =	164.0797
15	C	Isotropic =	63.5392	Anisotropy =	169.2929
16	C	Isotropic =	50.6173	Anisotropy =	178.4833
17	C	Isotropic =	146.8515	Anisotropy =	39.1664
18	C	Isotropic =	176.1728	Anisotropy =	25.1566
19	C	Isotropic =	159.5879	Anisotropy =	31.7020
20	C	Isotropic =	127.7110	Anisotropy =	59.7078
21	O	Isotropic =	210.0945	Anisotropy =	149.0693
22	C	Isotropic =	33.9407	Anisotropy =	138.4266
23	C	Isotropic =	69.8879	Anisotropy =	173.9836
24	C	Isotropic =	43.6846	Anisotropy =	182.6825
25	N	Isotropic =	-38.7270	Anisotropy =	461.3748
26	C	Isotropic =	42.9774	Anisotropy =	159.3554
27	C	Isotropic =	90.2725	Anisotropy =	143.1276
28	C	Isotropic =	70.0875	Anisotropy =	177.0675
29	C	Isotropic =	67.6701	Anisotropy =	174.9525
30	C	Isotropic =	63.6260	Anisotropy =	175.9989
31	C	Isotropic =	64.5279	Anisotropy =	150.3171
32	C	Isotropic =	155.0333	Anisotropy =	44.0920
33	O	Isotropic =	-70.9146	Anisotropy =	370.9882
34	H	Isotropic =	24.7292	Anisotropy =	7.1511
35	H	Isotropic =	24.3348	Anisotropy =	3.0923
36	H	Isotropic =	23.3086	Anisotropy =	5.1775

37	H	Isotropic =	22.6149	Anisotropy =	8.4980
38	H	Isotropic =	24.1639	Anisotropy =	8.5717
39	H	Isotropic =	28.3275	Anisotropy =	6.3375
40	H	Isotropic =	26.5635	Anisotropy =	6.3438
41	H	Isotropic =	30.2794	Anisotropy =	11.4008
42	H	Isotropic =	29.9662	Anisotropy =	5.4376
43	H	Isotropic =	30.3790	Anisotropy =	8.0664
44	H	Isotropic =	28.4653	Anisotropy =	4.9538
45	H	Isotropic =	28.4439	Anisotropy =	8.8545
46	H	Isotropic =	26.4385	Anisotropy =	6.6938
47	H	Isotropic =	26.6194	Anisotropy =	6.9663
48	H	Isotropic =	22.8226	Anisotropy =	6.7409
49	H	Isotropic =	24.6821	Anisotropy =	9.2038
50	H	Isotropic =	24.1006	Anisotropy =	8.6648
51	H	Isotropic =	24.1592	Anisotropy =	4.8689
52	H	Isotropic =	23.9722	Anisotropy =	6.0469
53	H	Isotropic =	23.8049	Anisotropy =	5.6110
54	H	Isotropic =	28.2271	Anisotropy =	9.7745
55	H	Isotropic =	28.7894	Anisotropy =	8.4263
56	H	Isotropic =	27.8554	Anisotropy =	9.0696

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.581520426622	-8.758219143346	-0.399896334532
C	-0.293731582925	-8.117264510063	0.467519751178
C	-1.566882189210	-8.660924764584	0.692837372533
C	-1.925960888049	-9.884171715512	0.112072771963
C	-0.991744491180	-10.547617075620	-0.682056215086
C	0.245132520791	-9.981171051406	-0.920520956788
N	-2.474489107156	-7.978045037121	1.543090827613
C	-2.871474723967	-6.665954988989	1.335997624446
C	-1.992453829506	-5.713779289572	0.584138412287
C	-0.578229686903	-5.756180904025	0.581241046758
N	0.101178027004	-6.898848137777	1.036234248194
O	-3.931110042607	-6.263781004424	1.814040414520
N	0.171264350429	-4.714969355562	0.196337898382
C	-0.448371466877	-3.631455489585	-0.284087986080
C	-1.837433176365	-3.507612335301	-0.428506381086
C	-2.603751180972	-4.570791809542	0.055004804390
C	1.433520713830	-6.727910254211	1.656568765086

C	1.803008266443	-7.912642969532	2.540713131992
C	-2.461616500386	-2.258052890172	-1.005830074617
C	-2.813979623927	-1.243297626548	0.079847721388
O	-3.399317443570	-0.107731742359	-0.577980536165
C	-3.791723586811	0.947808773170	0.166223931557
C	-4.365989940184	2.044931682366	-0.558170920092
C	-4.793795278750	3.182744991984	0.196793173185
N	-4.679434380077	3.266009913786	1.561286572851
C	-4.143887787079	2.227021441898	2.175142872926
C	-3.682721263380	1.045762839527	1.543625521685
C	-4.520440561248	2.039152788241	-1.969676964456
C	-5.080288374818	3.124780263163	-2.615212432960
C	-5.506138094324	4.255055206707	-1.873729989931
C	-5.365739028087	4.282279266572	-0.500380542173
C	-3.358436960178	-8.786919903180	2.393089966398
O	1.713040945615	-8.232832483878	-0.697783847994
H	-2.913127780298	-10.309653139092	0.281056326864
H	-1.227296113943	-11.508475573476	-1.140018054104
H	1.019977204906	-10.416374989889	-1.547551797868
H	0.205511301989	-2.806443293825	-0.588887208556
H	-3.693907521475	-4.516606378673	0.065412856741
H	2.204333364414	-6.565598141595	0.892304465263
H	1.356645655264	-5.813657768994	2.262858763456
H	2.746738415764	-7.691407566388	3.063486958046
H	1.027926778321	-8.109578052911	3.298575386120
H	1.961161906982	-8.826389342139	1.948201534566
H	-1.768028090098	-1.783607556563	-1.717427592436
H	-3.378071969565	-2.513470037618	-1.560093840403
H	-3.535160806922	-1.666425809415	0.799982040738
H	-1.912784706387	-0.928244757999	0.633036800596
H	-4.055040813949	2.298525594355	3.265338753639
H	-3.256949654666	0.249781468119	2.151860353190
H	-4.190546505527	1.165997523883	-2.532867205929
H	-5.196193196676	3.114193732600	-3.700980219803
H	-5.947543621454	5.107844745456	-2.394293770309
H	-5.686862775085	5.142243412211	0.090546335400
H	-2.812705074738	-9.680840276816	2.717906843619
H	-3.644870985131	-8.189901113554	3.266635640011
H	-4.280459073924	-9.086625362783	1.868672983790

SCF Done: E(RB3LYP) = -1465.99825890

Zero-point correction= 0.444818
Thermal correction to Energy= 0.472255

Thermal correction to Enthalpy= 0.473199
Thermal correction to Gibbs Free Energy= 0.384379
Sum of electronic and zero-point Energies= -1465.553441
Sum of electronic and thermal Energies= -1465.526004
Sum of electronic and thermal Enthalpies= -1465.525060
Sum of electronic and thermal Free Energies= -1465.613880

1	N	Isotropic =	-49.1887	Anisotropy =	262.2801
2	C	Isotropic =	45.7785	Anisotropy =	105.0024
3	C	Isotropic =	50.6567	Anisotropy =	125.5013
4	C	Isotropic =	76.5669	Anisotropy =	156.7944
5	C	Isotropic =	70.2649	Anisotropy =	166.3870
6	C	Isotropic =	55.3370	Anisotropy =	109.9146
7	N	Isotropic =	122.4927	Anisotropy =	87.2835
8	C	Isotropic =	27.1800	Anisotropy =	105.4466
9	C	Isotropic =	72.0142	Anisotropy =	130.8841
10	C	Isotropic =	32.1703	Anisotropy =	124.4786
11	N	Isotropic =	157.6484	Anisotropy =	74.3036
12	O	Isotropic =	-89.4020	Anisotropy =	602.4257
13	N	Isotropic =	-36.2615	Anisotropy =	447.6646
14	C	Isotropic =	40.5787	Anisotropy =	149.7942
15	C	Isotropic =	63.8945	Anisotropy =	167.7861
16	C	Isotropic =	50.7206	Anisotropy =	183.7892
17	C	Isotropic =	146.1738	Anisotropy =	40.7450
18	C	Isotropic =	177.6076	Anisotropy =	22.6707
19	C	Isotropic =	156.9661	Anisotropy =	32.3511
20	C	Isotropic =	121.1952	Anisotropy =	66.9450
21	O	Isotropic =	197.8025	Anisotropy =	103.8465
22	C	Isotropic =	31.9989	Anisotropy =	138.0901
23	C	Isotropic =	70.5259	Anisotropy =	171.0125
24	C	Isotropic =	43.8323	Anisotropy =	181.7906
25	N	Isotropic =	-37.5978	Anisotropy =	458.6382
26	C	Isotropic =	42.4619	Anisotropy =	159.8529
27	C	Isotropic =	91.1060	Anisotropy =	133.2531
28	C	Isotropic =	70.0557	Anisotropy =	174.0192
29	C	Isotropic =	67.6844	Anisotropy =	170.6095
30	C	Isotropic =	63.6104	Anisotropy =	174.8396
31	C	Isotropic =	63.8264	Anisotropy =	150.4453
32	C	Isotropic =	154.6688	Anisotropy =	43.5229
33	O	Isotropic =	-74.6036	Anisotropy =	378.6858
34	H	Isotropic =	24.5499	Anisotropy =	7.9245
35	H	Isotropic =	24.2392	Anisotropy =	4.1137
36	H	Isotropic =	23.4633	Anisotropy =	5.1265
37	H	Isotropic =	22.9841	Anisotropy =	8.4363

38	H	Isotropic =	23.3105	Anisotropy =	10.9732
39	H	Isotropic =	26.5993	Anisotropy =	7.5868
40	H	Isotropic =	28.0077	Anisotropy =	6.1865
41	H	Isotropic =	30.1907	Anisotropy =	11.3626
42	H	Isotropic =	30.3981	Anisotropy =	7.5834
43	H	Isotropic =	30.4852	Anisotropy =	5.7533
44	H	Isotropic =	28.2897	Anisotropy =	5.6368
45	H	Isotropic =	28.2561	Anisotropy =	5.0194
46	H	Isotropic =	27.3521	Anisotropy =	7.3481
47	H	Isotropic =	27.4089	Anisotropy =	6.3857
48	H	Isotropic =	22.7341	Anisotropy =	7.5254
49	H	Isotropic =	24.9299	Anisotropy =	8.9683
50	H	Isotropic =	23.0452	Anisotropy =	10.5378
51	H	Isotropic =	23.7889	Anisotropy =	6.1401
52	H	Isotropic =	23.5966	Anisotropy =	5.1082
53	H	Isotropic =	23.4912	Anisotropy =	5.9734
54	H	Isotropic =	28.6663	Anisotropy =	7.4992
55	H	Isotropic =	27.6011	Anisotropy =	8.2372
56	H	Isotropic =	27.9829	Anisotropy =	9.8262

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.564420569850	-8.162313874294	-1.200097832390
C	-4.480625742512	-7.849254830358	-0.389421031246
C	-3.250418998661	-8.489173573421	-0.600934394364
C	-3.135228016922	-9.496238360053	-1.568076656697
C	-4.265360398105	-9.850748736196	-2.303297326732
C	-5.459837230474	-9.186374586067	-2.105896054357
N	-2.133268083369	-8.132544716287	0.197191442935
C	-1.653250568809	-6.836228890031	0.301490810782
C	-2.556537508499	-5.665859630057	0.059061331247
C	-3.943077953448	-5.646956585501	0.341008215589
N	-4.637424910385	-6.845358422557	0.576032387823
O	-0.487657653167	-6.641075357496	0.642825862834
N	-4.640241362563	-4.507862266274	0.442118207775
C	-4.013750050478	-3.355846639965	0.177897138870
C	-2.672061851392	-3.251670002462	-0.214466415019
C	-1.941921338193	-4.442619005406	-0.232837326677
C	-5.805686906866	-6.821031998562	1.483593631721
C	-6.104916297622	-8.200788797237	2.056889569117

C	-2.040527176736	-1.914460548707	-0.525968480823
C	-1.333655896936	-1.319158574421	0.690017317403
O	-0.751459743273	-0.073978058592	0.271217207304
C	-0.040209472664	0.648242830862	1.162605900341
C	0.527662901810	1.869160003003	0.667410308587
C	1.291558716315	2.660780018114	1.582604970858
N	1.498101165475	2.307071587469	2.891905165837
C	0.950772610560	1.174397185919	3.292654191929
C	0.176291491095	0.304117716384	2.486688758554
C	0.362296448562	2.307514990110	-0.673042290780
C	0.934512031477	3.491662297386	-1.096160160639
C	1.692590443047	4.280462223773	-0.195225526961
C	1.866166477733	3.873773419806	1.112826921153
C	-1.188659441565	-9.194206444188	0.569984260927
O	-6.671320882716	-7.523524960667	-1.092255779040
H	-2.183429780120	-9.995066414437	-1.739668741593
H	-4.219968524226	-10.639706711633	-3.054297481230
H	-6.379282825854	-9.380098506388	-2.653617757307
H	-4.624169407230	-2.450478043275	0.271484116293
H	-0.869706977348	-4.439239843254	-0.437041105977
H	-5.532075694888	-6.127132940047	2.291463929975
H	-6.690290266709	-6.419179640623	0.973105766454
H	-6.907934688384	-8.113816561454	2.805532992412
H	-6.454295690872	-8.896143324733	1.278659216997
H	-5.220135259799	-8.634786556999	2.549463426611
H	-1.306113739560	-2.023088431654	-1.339292170279
H	-2.808995052859	-1.204791926189	-0.869683286752
H	-2.045705463596	-1.138516704072	1.513301205509
H	-0.540779479742	-1.993315873237	1.056610114203
H	1.118421677502	0.896537136318	4.339663706311
H	-0.226673523943	-0.607124743354	2.924872993648
H	-0.221739844007	1.694982519218	-1.360151084607
H	0.803720065947	3.823029086014	-2.128400336667
H	2.140670332283	5.214953859945	-0.540248338954
H	2.445899789875	4.465963847060	1.823452747610
H	-0.685665832808	-8.903189120555	1.499417087342
H	-1.747442747812	-10.124592816649	0.726447097495
H	-0.415411296719	-9.351855704028	-0.199458423355

SCF Done: E(RB3LYP) = -1465.99823731

Zero-point correction= 0.444633
Thermal correction to Energy= 0.472194
Thermal correction to Enthalpy= 0.473138

Thermal correction to Gibbs Free Energy= 0.383040
Sum of electronic and zero-point Energies= -1465.553605
Sum of electronic and thermal Energies= -1465.526044
Sum of electronic and thermal Enthalpies= -1465.525099
Sum of electronic and thermal Free Energies= -1465.615197

1	N	Isotropic =	-49.2165	Anisotropy =	261.2486
2	C	Isotropic =	46.1917	Anisotropy =	104.7156
3	C	Isotropic =	50.8617	Anisotropy =	125.0892
4	C	Isotropic =	76.8369	Anisotropy =	156.6100
5	C	Isotropic =	69.8601	Anisotropy =	165.5333
6	C	Isotropic =	55.5898	Anisotropy =	110.2645
7	N	Isotropic =	122.7709	Anisotropy =	86.9136
8	C	Isotropic =	27.0509	Anisotropy =	104.9413
9	C	Isotropic =	72.1604	Anisotropy =	130.8714
10	C	Isotropic =	32.1536	Anisotropy =	124.8642
11	N	Isotropic =	157.2494	Anisotropy =	74.0636
12	O	Isotropic =	-90.4145	Anisotropy =	601.8577
13	N	Isotropic =	-36.2586	Anisotropy =	446.3322
14	C	Isotropic =	40.6137	Anisotropy =	149.0207
15	C	Isotropic =	64.0537	Anisotropy =	167.8321
16	C	Isotropic =	50.6967	Anisotropy =	184.1841
17	C	Isotropic =	145.9180	Anisotropy =	41.5051
18	C	Isotropic =	177.5446	Anisotropy =	22.6770
19	C	Isotropic =	156.9325	Anisotropy =	32.4672
20	C	Isotropic =	121.3396	Anisotropy =	67.0069
21	O	Isotropic =	197.7437	Anisotropy =	104.2573
22	C	Isotropic =	32.0800	Anisotropy =	138.0164
23	C	Isotropic =	70.5070	Anisotropy =	170.9844
24	C	Isotropic =	43.8396	Anisotropy =	182.0434
25	N	Isotropic =	-37.9112	Anisotropy =	458.0722
26	C	Isotropic =	42.4266	Anisotropy =	159.6001
27	C	Isotropic =	91.1035	Anisotropy =	133.2333
28	C	Isotropic =	70.1717	Anisotropy =	174.0594
29	C	Isotropic =	67.5481	Anisotropy =	170.4977
30	C	Isotropic =	63.4754	Anisotropy =	175.0683
31	C	Isotropic =	63.7601	Anisotropy =	150.1893
32	C	Isotropic =	154.6452	Anisotropy =	43.4787
33	O	Isotropic =	-75.0568	Anisotropy =	380.7110
34	H	Isotropic =	24.5684	Anisotropy =	7.8830
35	H	Isotropic =	24.2667	Anisotropy =	4.0765
36	H	Isotropic =	23.4655	Anisotropy =	5.1129
37	H	Isotropic =	22.9614	Anisotropy =	8.3904
38	H	Isotropic =	23.3089	Anisotropy =	11.0937

39	H	Isotropic =	28.0036	Anisotropy =	6.1340
40	H	Isotropic =	26.5705	Anisotropy =	7.5441
41	H	Isotropic =	30.1806	Anisotropy =	11.3803
42	H	Isotropic =	30.4931	Anisotropy =	5.7435
43	H	Isotropic =	30.4084	Anisotropy =	7.5433
44	H	Isotropic =	28.2584	Anisotropy =	5.0386
45	H	Isotropic =	28.2835	Anisotropy =	5.6990
46	H	Isotropic =	27.3775	Anisotropy =	6.1882
47	H	Isotropic =	27.3624	Anisotropy =	7.5477
48	H	Isotropic =	22.7392	Anisotropy =	7.5064
49	H	Isotropic =	24.9242	Anisotropy =	8.9562
50	H	Isotropic =	23.0499	Anisotropy =	10.5379
51	H	Isotropic =	23.7859	Anisotropy =	6.1429
52	H	Isotropic =	23.5865	Anisotropy =	5.1112
53	H	Isotropic =	23.4969	Anisotropy =	5.9612
54	H	Isotropic =	27.6016	Anisotropy =	8.2356
55	H	Isotropic =	28.6859	Anisotropy =	7.4484
56	H	Isotropic =	27.9851	Anisotropy =	9.8464

Conformer 26

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.066465051269	-7.994526867263	2.252700224127
C	-0.107295539780	-6.646310936644	1.954822890210
C	-0.118473906711	-5.703082472129	2.991541143377
C	0.128896348843	-6.102674638989	4.311891680222
C	0.392863413273	-7.447544329480	4.565691634686
C	0.363363402391	-8.369479464107	3.536952658551
N	-0.346817417155	-4.335637823038	2.687244100938
C	-1.464297771378	-3.883020460441	2.006072397904
C	-2.209320712127	-4.785387001536	1.071207811920
C	-1.618816959745	-5.814942565165	0.301031676668
N	-0.339179992977	-6.298878045336	0.620706987818
O	-1.818766183723	-2.708960130975	2.125484917021
N	-2.221840014824	-6.343462467698	-0.771764385553
C	-3.461340925681	-5.937907726558	-1.069823798576
C	-4.190455380190	-5.000346241105	-0.325410077121
C	-3.518655461447	-4.411720446086	0.747137897381
C	0.531591786438	-6.824324846405	-0.451075124251
C	1.063443920940	-5.694558637715	-1.330766089897
C	-5.587254746406	-4.575339504464	-0.716318008338

C	-5.620892446819	-3.435492266931	-1.734387778210
O	-4.895817761941	-2.324595655411	-1.180625591222
C	-4.819713862442	-1.174800981663	-1.883712187667
C	-3.968254393819	-0.158263649848	-1.334677552218
C	-3.894090498287	1.087828680920	-2.035470696155
N	-4.579246896233	1.340542443607	-3.196981284129
C	-5.328844503862	0.360850248264	-3.667380115742
C	-5.490284912925	-0.911961892046	-3.067245413015
C	-3.201831176964	-0.346662953785	-0.153491556072
C	-2.398944306803	0.670867248096	0.325388054768
C	-2.333587140377	1.912868139864	-0.353503444874
C	-3.063130617431	2.114486031557	-1.508364839626
C	0.380029910959	-3.327905105890	3.471086402275
O	-0.022395056064	-8.882889274557	1.333344770039
H	0.120248381425	-5.376633545515	5.122531908522
H	0.606388042582	-7.794955874024	5.576734764708
H	0.528638141810	-9.438158185379	3.653730576847
H	-3.909111257463	-6.396770730134	-1.958761306955
H	-3.989477380766	-3.617191238205	1.327020383147
H	1.357383432934	-7.354183655985	0.037075877819
H	-0.020005469564	-7.561979114520	-1.048526437183
H	1.725777489873	-6.109146298947	-2.108096917229
H	0.243383587635	-5.162024409629	-1.837793435000
H	1.637350617493	-4.964091907943	-0.738536643260
H	-6.136012310032	-5.420492269654	-1.161135906118
H	-6.145210598758	-4.264294442327	0.180563251923
H	-5.150505974296	-3.734234741087	-2.687139004912
H	-6.664632747594	-3.141667959691	-1.934263793518
H	-5.868696542413	0.565230451096	-4.599299883742
H	-6.140336309068	-1.644321620362	-3.542549123637
H	-3.233552662192	-1.304047934598	0.365949605378
H	-1.807971482704	0.512888817699	1.229956050318
H	-1.697488929062	2.710625501054	0.036689595848
H	-3.022248527366	3.059449352595	-2.053573966100
H	-0.145819264594	-3.067940341598	4.404147057079
H	1.377320160049	-3.717876253008	3.707235161478
H	0.471704354072	-2.416730006880	2.868744879345

SCF Done: E(RB3LYP) = -1465.99991485

Zero-point correction= 0.444784
Thermal correction to Energy= 0.472159
Thermal correction to Enthalpy= 0.473104
Thermal correction to Gibbs Free Energy= 0.385194

Sum of electronic and zero-point Energies= -1465.555131
Sum of electronic and thermal Energies= -1465.527756
Sum of electronic and thermal Enthalpies= -1465.526811
Sum of electronic and thermal Free Energies= -1465.614721

1	N	Isotropic =	-46.2192	Anisotropy =	262.8820
2	C	Isotropic =	44.4272	Anisotropy =	102.2312
3	C	Isotropic =	51.2520	Anisotropy =	122.5926
4	C	Isotropic =	76.3732	Anisotropy =	156.4109
5	C	Isotropic =	70.2093	Anisotropy =	164.6143
6	C	Isotropic =	55.4176	Anisotropy =	110.3541
7	N	Isotropic =	122.4174	Anisotropy =	85.5506
8	C	Isotropic =	25.5127	Anisotropy =	104.5499
9	C	Isotropic =	71.2099	Anisotropy =	130.7197
10	C	Isotropic =	33.9726	Anisotropy =	122.3779
11	N	Isotropic =	159.1247	Anisotropy =	62.2600
12	O	Isotropic =	-87.7722	Anisotropy =	589.7146
13	N	Isotropic =	-35.0196	Anisotropy =	454.6510
14	C	Isotropic =	41.4944	Anisotropy =	150.7431
15	C	Isotropic =	61.6407	Anisotropy =	170.9643
16	C	Isotropic =	48.2787	Anisotropy =	183.2989
17	C	Isotropic =	146.6935	Anisotropy =	37.9854
18	C	Isotropic =	175.9199	Anisotropy =	24.2675
19	C	Isotropic =	157.3887	Anisotropy =	18.1762
20	C	Isotropic =	122.1083	Anisotropy =	43.3617
21	O	Isotropic =	203.6582	Anisotropy =	119.5011
22	C	Isotropic =	32.2295	Anisotropy =	137.7599
23	C	Isotropic =	70.3441	Anisotropy =	169.6902
24	C	Isotropic =	43.7856	Anisotropy =	181.7274
25	N	Isotropic =	-37.8492	Anisotropy =	457.8233
26	C	Isotropic =	42.6197	Anisotropy =	159.2972
27	C	Isotropic =	91.1779	Anisotropy =	133.0066
28	C	Isotropic =	68.7723	Anisotropy =	176.4840
29	C	Isotropic =	67.5662	Anisotropy =	170.0051
30	C	Isotropic =	63.7455	Anisotropy =	174.2465
31	C	Isotropic =	64.0921	Anisotropy =	149.0940
32	C	Isotropic =	154.2802	Anisotropy =	44.1213
33	O	Isotropic =	-79.7952	Anisotropy =	393.2684
34	H	Isotropic =	24.4797	Anisotropy =	8.3261
35	H	Isotropic =	24.2575	Anisotropy =	4.3002
36	H	Isotropic =	23.4303	Anisotropy =	5.0825
37	H	Isotropic =	22.9465	Anisotropy =	7.7803
38	H	Isotropic =	22.9014	Anisotropy =	10.1651
39	H	Isotropic =	28.3296	Anisotropy =	6.6010

40	H	Isotropic =	26.7241	Anisotropy =	7.7462
41	H	Isotropic =	30.4386	Anisotropy =	11.0961
42	H	Isotropic =	30.2865	Anisotropy =	4.8352
43	H	Isotropic =	30.4834	Anisotropy =	7.2104
44	H	Isotropic =	28.4251	Anisotropy =	8.6570
45	H	Isotropic =	28.2602	Anisotropy =	5.4952
46	H	Isotropic =	27.5191	Anisotropy =	6.5062
47	H	Isotropic =	26.9694	Anisotropy =	6.2911
48	H	Isotropic =	22.7614	Anisotropy =	7.1412
49	H	Isotropic =	24.9061	Anisotropy =	9.5822
50	H	Isotropic =	22.6471	Anisotropy =	9.0479
51	H	Isotropic =	23.6775	Anisotropy =	7.4512
52	H	Isotropic =	23.6167	Anisotropy =	5.6586
53	H	Isotropic =	23.5520	Anisotropy =	5.7853
54	H	Isotropic =	27.8467	Anisotropy =	9.6385
55	H	Isotropic =	28.5800	Anisotropy =	7.6775
56	H	Isotropic =	27.4725	Anisotropy =	7.9727

Conformer 27

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.496685908495	-3.306563680949	-4.852332575108
C	-2.117999180777	-3.660112787440	-3.658370322916
C	-2.462035117752	-4.998663986269	-3.425712692809
C	-2.259700590579	-5.962855359338	-4.422380135056
C	-1.722052934942	-5.560086221035	-5.643655159767
C	-1.355051991757	-4.242965064599	-5.842819552370
N	-3.048399028400	-5.361211590041	-2.185031456568
C	-2.455254607899	-5.103147555724	-0.960353429169
C	-1.491709080564	-3.967759013522	-0.800868674151
C	-1.549078142020	-2.751763225853	-1.522465156715
N	-2.307491520978	-2.658683473399	-2.701269519411
O	-2.764956665795	-5.778003070443	0.022738445189
N	-0.924948989541	-1.641759637999	-1.107267071915
C	-0.151016805559	-1.715988958721	-0.018573680996
C	0.070251338428	-2.886626836983	0.719953032743
C	-0.645585762666	-4.013610830564	0.313092789923
C	-2.906188684191	-1.363390873625	-3.085368604722
C	-4.086215258448	-1.012630368113	-2.181251634582
C	0.956124417269	-2.908084642322	1.944424551846
C	0.230571216725	-2.537417342288	3.237747373921

O	-0.865648994454	-3.451322458296	3.410556133464
C	-1.632072596945	-3.353195203119	4.517764038925
C	-2.778250467054	-4.215568342594	4.567699218974
C	-3.591100664382	-4.163128443831	5.744975596236
N	-3.333051622739	-3.327034872920	6.801725533194
C	-2.278446930175	-2.540650664572	6.690670720170
C	-1.394527602443	-2.501764277905	5.584613662528
C	-3.134928286312	-5.089925602552	3.506504945152
C	-4.251501219330	-5.896728316701	3.613878507005
C	-5.050890774463	-5.862966167344	4.783316995680
C	-4.728130027322	-5.013717608741	5.823061101114
C	-4.076685749758	-6.410470495528	-2.192480306145
O	-1.081146076814	-2.109257263632	-5.042437628023
H	-2.521611554337	-7.004654728436	-4.248237341268
H	-1.565363971843	-6.276966890361	-6.449884475820
H	-0.903275749705	-3.853028275514	-6.752177444673
H	0.334127931023	-0.780467977191	0.282717930289
H	-0.589134160851	-4.941116727690	0.883715318807
H	-2.139889038730	-0.577640100158	-3.055854552315
H	-3.233278308908	-1.458102541916	-4.126934018849
H	-3.768589735445	-0.901905883327	-1.132449060428
H	-4.527119253407	-0.054584972259	-2.501448147857
H	-4.867956047942	-1.787500456323	-2.226976156445
H	1.400794091250	-3.908380897255	2.063730048858
H	1.788718622926	-2.196481283713	1.827789295068
H	0.923048365745	-2.616287610871	4.092033361818
H	-0.161706744896	-1.506595780180	3.196574110413
H	-2.080456061841	-1.869541981880	7.534500231265
H	-0.551051377904	-1.814081882662	5.603759638486
H	-2.535696752406	-5.109163541935	2.596747154059
H	-4.521097817019	-6.559547107990	2.788978507670
H	-5.929481139748	-6.507811179575	4.857683136152
H	-5.333584831125	-4.963687288658	6.730154594103
H	-3.640952515843	-7.420556914386	-2.126002890001
H	-4.729597758288	-6.265592633759	-1.323980759624
H	-4.662661880577	-6.322369106997	-3.115143525342

SCF Done: E(RB3LYP) = -1465.99993030

Zero-point correction= 0.444827
Thermal correction to Energy= 0.472218
Thermal correction to Enthalpy= 0.473162
Thermal correction to Gibbs Free Energy= 0.384836
Sum of electronic and zero-point Energies= -1465.555103

Sum of electronic and thermal Energies= -1465.527712
Sum of electronic and thermal Enthalpies= -1465.526768
Sum of electronic and thermal Free Energies= -1465.615094

1	N	Isotropic =	-45.8831	Anisotropy =	262.7860
2	C	Isotropic =	44.5291	Anisotropy =	101.3353
3	C	Isotropic =	51.3523	Anisotropy =	122.9461
4	C	Isotropic =	76.3127	Anisotropy =	156.2803
5	C	Isotropic =	70.2376	Anisotropy =	164.2424
6	C	Isotropic =	55.6684	Anisotropy =	110.4218
7	N	Isotropic =	122.2957	Anisotropy =	85.6239
8	C	Isotropic =	25.7338	Anisotropy =	104.4592
9	C	Isotropic =	71.3237	Anisotropy =	130.8100
10	C	Isotropic =	34.1011	Anisotropy =	123.4799
11	N	Isotropic =	158.7302	Anisotropy =	63.2863
12	O	Isotropic =	-88.2007	Anisotropy =	589.7867
13	N	Isotropic =	-34.0449	Anisotropy =	455.6476
14	C	Isotropic =	41.5765	Anisotropy =	150.2531
15	C	Isotropic =	61.5734	Anisotropy =	170.7728
16	C	Isotropic =	48.0489	Anisotropy =	183.4923
17	C	Isotropic =	146.8316	Anisotropy =	37.9796
18	C	Isotropic =	175.9197	Anisotropy =	24.1624
19	C	Isotropic =	157.5464	Anisotropy =	18.2786
20	C	Isotropic =	121.9411	Anisotropy =	43.5383
21	O	Isotropic =	203.7360	Anisotropy =	119.8954
22	C	Isotropic =	31.9441	Anisotropy =	137.2153
23	C	Isotropic =	70.2948	Anisotropy =	169.5150
24	C	Isotropic =	43.9429	Anisotropy =	181.5865
25	N	Isotropic =	-38.2898	Anisotropy =	456.5548
26	C	Isotropic =	42.5825	Anisotropy =	158.9908
27	C	Isotropic =	91.0116	Anisotropy =	133.3774
28	C	Isotropic =	69.0240	Anisotropy =	177.1656
29	C	Isotropic =	67.1651	Anisotropy =	169.4885
30	C	Isotropic =	63.6625	Anisotropy =	174.0452
31	C	Isotropic =	64.0338	Anisotropy =	148.5319
32	C	Isotropic =	154.2706	Anisotropy =	44.1385
33	O	Isotropic =	-80.1744	Anisotropy =	393.2485
34	H	Isotropic =	24.4577	Anisotropy =	8.3286
35	H	Isotropic =	24.2641	Anisotropy =	4.3094
36	H	Isotropic =	23.4490	Anisotropy =	5.0671
37	H	Isotropic =	22.9598	Anisotropy =	7.8060
38	H	Isotropic =	22.8732	Anisotropy =	10.1787
39	H	Isotropic =	26.7120	Anisotropy =	7.7611
40	H	Isotropic =	28.3093	Anisotropy =	6.5657

41	H	Isotropic =	30.2711	Anisotropy =	4.8349
42	H	Isotropic =	30.4179	Anisotropy =	11.0889
43	H	Isotropic =	30.4595	Anisotropy =	7.2749
44	H	Isotropic =	28.2462	Anisotropy =	5.5163
45	H	Isotropic =	28.4509	Anisotropy =	8.6060
46	H	Isotropic =	26.9721	Anisotropy =	6.2933
47	H	Isotropic =	27.5043	Anisotropy =	6.4929
48	H	Isotropic =	22.7639	Anisotropy =	7.1447
49	H	Isotropic =	24.8917	Anisotropy =	9.5933
50	H	Isotropic =	22.5902	Anisotropy =	9.1349
51	H	Isotropic =	23.6656	Anisotropy =	7.3744
52	H	Isotropic =	23.6177	Anisotropy =	5.6333
53	H	Isotropic =	23.5755	Anisotropy =	5.7652
54	H	Isotropic =	27.8485	Anisotropy =	9.6288
55	H	Isotropic =	27.4908	Anisotropy =	8.0098
56	H	Isotropic =	28.5787	Anisotropy =	7.6895

Conformer 28

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.737506652231	-1.078779422608	-0.462563370032
C	-1.002433161453	-2.077710173105	-1.388596999804
C	-2.144695022360	-1.984859366905	-2.196959667571
C	-2.941071643335	-0.833101760481	-2.161671738785
C	-2.575444703195	0.207158320026	-1.308432186634
C	-1.483419332490	0.070744057638	-0.473775059139
N	-2.469296215761	-3.062010409265	-3.059518577410
C	-2.663583738856	-4.356717961977	-2.591707636183
C	-1.949818302324	-4.835548573843	-1.367094131842
C	-0.666689115124	-4.397082944313	-0.965111045232
N	-0.144733423207	-3.186258304489	-1.438664257813
O	-3.378742166473	-5.133221189063	-3.221983891172
N	0.112239626925	-5.121731540584	-0.149866263096
C	-0.406841079558	-6.216267988247	0.414788139027
C	-1.732867373722	-6.645227772115	0.246892503166
C	-2.477328474479	-5.956250519563	-0.711116590388
C	1.323020255517	-3.009073658599	-1.489300076856
C	1.731530776229	-1.940069292630	-2.495737257190
C	-2.329817896381	-7.773369441403	1.064110424902
C	-2.037118515058	-7.651019904429	2.567680105857
O	-2.158116638593	-6.294187838440	3.034282001311

C	-3.371655008261	-5.725878619555	3.221364011078
C	-3.390216725366	-4.292597928949	3.186324324609
C	-4.634906328789	-3.639138346865	3.451308941015
N	-5.794504900735	-4.319135570137	3.723102998178
C	-5.725059751472	-5.638454067803	3.712838973437
C	-4.556361383093	-6.399400738698	3.463622018743
C	-2.243338357287	-3.519031814553	2.864075933471
C	-2.320533043686	-2.140955284578	2.808908386290
C	-3.545395482657	-1.486354011026	3.095833528510
C	-4.673879518683	-2.217681887925	3.411158965276
C	-3.104622170849	-2.747575508424	-4.345425224771
O	0.215635216909	-1.208222202761	0.391116638429
H	-3.826157872114	-0.749291433433	-2.789143370318
H	-3.158276925919	1.127426645666	-1.266149218940
H	-1.154738316036	0.814702346333	0.248267049262
H	0.274708784337	-6.772916623929	1.066464053999
H	-3.476674169418	-6.296320759219	-0.989298126018
H	1.719299564558	-2.768940644234	-0.493738353652
H	1.724734280754	-3.986808181039	-1.789130303026
H	1.399859242864	-0.937220667565	-2.185760842694
H	2.830109416797	-1.915054558284	-2.568051917556
H	1.324873650241	-2.151541892358	-3.497588856733
H	-3.416284833276	-7.798026003211	0.891627256971
H	-1.940380896396	-8.754204587996	0.738692312817
H	-2.674815151924	-8.332977157329	3.150710280764
H	-0.992493352723	-7.905964041744	2.789186497343
H	-6.657376778927	-6.175926422194	3.921131160454
H	-4.612503411187	-7.486929523699	3.485411756622
H	-1.309015574902	-4.032597572958	2.638442018285
H	-1.440511376160	-1.562409205125	2.518225818959
H	-3.596814724364	-0.395926596894	3.056310563976
H	-5.628317987238	-1.732098099316	3.623925490757
H	-2.665745363369	-1.822421202668	-4.738131915320
H	-2.911122191911	-3.572681794235	-5.040632423681
H	-4.196735763790	-2.629930358898	-4.254302851648

SCF Done: E(RB3LYP) = -1465.99315251

Zero-point correction= 0.444955
Thermal correction to Energy= 0.472176
Thermal correction to Enthalpy= 0.473120
Thermal correction to Gibbs Free Energy= 0.386011
Sum of electronic and zero-point Energies= -1465.548198
Sum of electronic and thermal Energies= -1465.520977

Sum of electronic and thermal Enthalpies= -1465.520033
Sum of electronic and thermal Free Energies= -1465.607142

1	N	Isotropic =	-47.3239	Anisotropy =	263.1174
2	C	Isotropic =	46.2568	Anisotropy =	108.1512
3	C	Isotropic =	49.5875	Anisotropy =	127.9749
4	C	Isotropic =	76.7271	Anisotropy =	159.8610
5	C	Isotropic =	69.8666	Anisotropy =	167.5208
6	C	Isotropic =	55.3992	Anisotropy =	113.1194
7	N	Isotropic =	123.4627	Anisotropy =	86.8728
8	C	Isotropic =	26.6534	Anisotropy =	103.6983
9	C	Isotropic =	74.9898	Anisotropy =	126.7204
10	C	Isotropic =	33.3025	Anisotropy =	125.1938
11	N	Isotropic =	154.1511	Anisotropy =	78.5976
12	O	Isotropic =	-93.4258	Anisotropy =	605.5292
13	N	Isotropic =	-30.4183	Anisotropy =	449.3370
14	C	Isotropic =	41.5698	Anisotropy =	164.2006
15	C	Isotropic =	63.7331	Anisotropy =	170.1677
16	C	Isotropic =	50.9033	Anisotropy =	178.7230
17	C	Isotropic =	147.2608	Anisotropy =	40.9368
18	C	Isotropic =	177.7473	Anisotropy =	22.3952
19	C	Isotropic =	159.7451	Anisotropy =	31.3632
20	C	Isotropic =	127.9050	Anisotropy =	59.5319
21	O	Isotropic =	210.4839	Anisotropy =	147.9201
22	C	Isotropic =	34.0904	Anisotropy =	138.6542
23	C	Isotropic =	69.8434	Anisotropy =	173.7637
24	C	Isotropic =	43.8404	Anisotropy =	182.9125
25	N	Isotropic =	-38.9709	Anisotropy =	460.5505
26	C	Isotropic =	43.0358	Anisotropy =	159.4539
27	C	Isotropic =	90.0375	Anisotropy =	142.7594
28	C	Isotropic =	70.3512	Anisotropy =	176.9993
29	C	Isotropic =	67.7351	Anisotropy =	175.1541
30	C	Isotropic =	63.6810	Anisotropy =	176.3160
31	C	Isotropic =	64.4210	Anisotropy =	150.3530
32	C	Isotropic =	155.1271	Anisotropy =	43.7431
33	O	Isotropic =	-67.7160	Anisotropy =	365.4170
34	H	Isotropic =	24.7366	Anisotropy =	7.0632
35	H	Isotropic =	24.3164	Anisotropy =	3.0618
36	H	Isotropic =	23.3349	Anisotropy =	5.1434
37	H	Isotropic =	22.6013	Anisotropy =	8.3890
38	H	Isotropic =	24.1674	Anisotropy =	8.6477
39	H	Isotropic =	26.5561	Anisotropy =	6.4176
40	H	Isotropic =	27.7368	Anisotropy =	6.5876
41	H	Isotropic =	30.5525	Anisotropy =	5.4675

42	H	Isotropic =	30.1631	Anisotropy =	11.6907
43	H	Isotropic =	30.4329	Anisotropy =	8.2085
44	H	Isotropic =	28.4583	Anisotropy =	4.9705
45	H	Isotropic =	28.3924	Anisotropy =	8.9203
46	H	Isotropic =	26.3795	Anisotropy =	6.7744
47	H	Isotropic =	26.5636	Anisotropy =	7.0191
48	H	Isotropic =	22.8256	Anisotropy =	6.6963
49	H	Isotropic =	24.6642	Anisotropy =	9.2193
50	H	Isotropic =	24.1267	Anisotropy =	8.6517
51	H	Isotropic =	24.1351	Anisotropy =	4.7606
52	H	Isotropic =	23.9635	Anisotropy =	6.0859
53	H	Isotropic =	23.8016	Anisotropy =	5.6321
54	H	Isotropic =	28.7960	Anisotropy =	8.2747
55	H	Isotropic =	27.8582	Anisotropy =	9.2147
56	H	Isotropic =	28.2277	Anisotropy =	9.7781

Conformer 29

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.032989017273	-0.976819859064	-0.724699058950
C	-1.275631754336	-2.061944907742	-1.557916945684
C	-2.464559037799	-2.115282097633	-2.297940881261
C	-3.345896526123	-1.025937363817	-2.292533363509
C	-3.014726081760	0.098792091813	-1.538609065002
C	-1.867622170021	0.107979310595	-0.768146775843
N	-2.751123179145	-3.276062959866	-3.060497192263
C	-2.820281105332	-4.541284997877	-2.489400495850
C	-2.001584610835	-4.874344980118	-1.281526713230
C	-0.733552286154	-4.317687996913	-0.993121933211
N	-0.338977153455	-3.101779912611	-1.565824395714
O	-3.508145361822	-5.413597695643	-3.016187928009
N	0.147058229670	-4.930248787022	-0.189210367004
C	-0.254733099232	-6.012182464329	0.483490398545
C	-1.553943490651	-6.542372151305	0.434573748303
C	-2.403649957717	-5.978833529192	-0.517365051973
C	1.097682227853	-2.797487421920	-1.731813836725
C	1.709652154761	-3.620019856724	-2.863715330616
C	-2.014165593968	-7.646010247245	1.365587146804
C	-1.637147326744	-7.391835700368	2.833770058585
O	-1.828709801394	-6.016182463439	3.212601904790
C	-3.067794528786	-5.518866804504	3.431122590833

C	-3.189964945925	-4.096222909833	3.301056798251
C	-4.462945544128	-3.511127434410	3.590315340857
N	-5.555631912777	-4.246657402762	3.972048488917
C	-5.392840576716	-5.555574956576	4.048139688774
C	-4.187222822168	-6.251728368257	3.785632643754
C	-2.118758131580	-3.271532039201	2.865195007584
C	-2.296704872266	-1.909220309169	2.721342274339
C	-3.549392431475	-1.320377713879	3.029917173812
C	-4.605358447184	-2.102065873938	3.456046389160
C	-3.474582649148	-3.105309081639	-4.326855276576
O	-0.022131687431	-0.974042878959	0.069179155425
H	-4.269347558847	-1.054889727456	-2.867514596402
H	-3.664777874723	0.973763051445	-1.523585780364
H	-1.558494850442	0.927437408034	-0.123330922457
H	0.505070053049	-6.473079091416	1.123400773637
H	-3.389784943971	-6.407498091466	-0.705932394335
H	1.174401096577	-1.726031427502	-1.949995627431
H	1.625249393051	-2.976597849719	-0.785945062422
H	1.197148819099	-3.427787017387	-3.819726083342
H	2.773359360225	-3.356166104713	-2.980624606005
H	1.652488525726	-4.698596294797	-2.649140923545
H	-3.104450619441	-7.758304698833	1.268609915313
H	-1.574435527140	-8.619019619783	1.083791415918
H	-2.183594378776	-8.071642727620	3.505396235849
H	-0.564365992668	-7.556044553790	2.998985570722
H	-6.272448517251	-6.138453183202	4.344813341448
H	-4.164428465210	-7.336236329834	3.884329969430
H	-1.162075722706	-3.735091393265	2.625388099222
H	-1.476553247183	-1.294563600673	2.343077848594
H	-3.680706796099	-0.241634378384	2.918988772664
H	-5.580335429767	-1.668759663338	3.687784800503
H	-3.124763486872	-2.184871226546	-4.809865566816
H	-3.258524411000	-3.965623855981	-4.970884204799
H	-4.566115934574	-3.055129860227	-4.181765172693

SCF Done: E(RB3LYP) = -1465.99386965

Zero-point correction= 0.444939
Thermal correction to Energy= 0.472140
Thermal correction to Enthalpy= 0.473084
Thermal correction to Gibbs Free Energy= 0.386338
Sum of electronic and zero-point Energies= -1465.548931
Sum of electronic and thermal Energies= -1465.521730
Sum of electronic and thermal Enthalpies= -1465.520786

Sum of electronic and thermal Free Energies= -1465.607531

1	N	Isotropic =	-44.7400	Anisotropy =	264.1373
2	C	Isotropic =	44.6912	Anisotropy =	104.5621
3	C	Isotropic =	50.8055	Anisotropy =	125.2162
4	C	Isotropic =	76.4680	Anisotropy =	159.0081
5	C	Isotropic =	70.2242	Anisotropy =	166.6260
6	C	Isotropic =	55.3258	Anisotropy =	114.0455
7	N	Isotropic =	124.2449	Anisotropy =	87.1111
8	C	Isotropic =	26.5887	Anisotropy =	103.7114
9	C	Isotropic =	74.0295	Anisotropy =	127.9123
10	C	Isotropic =	34.5853	Anisotropy =	124.3533
11	N	Isotropic =	156.0648	Anisotropy =	68.8796
12	O	Isotropic =	-94.2495	Anisotropy =	604.7813
13	N	Isotropic =	-29.5878	Anisotropy =	454.4105
14	C	Isotropic =	41.2075	Anisotropy =	164.0388
15	C	Isotropic =	63.7463	Anisotropy =	169.2760
16	C	Isotropic =	50.7152	Anisotropy =	178.6052
17	C	Isotropic =	146.8202	Anisotropy =	38.9644
18	C	Isotropic =	176.1716	Anisotropy =	25.2417
19	C	Isotropic =	159.7051	Anisotropy =	31.6561
20	C	Isotropic =	127.9104	Anisotropy =	60.2156
21	O	Isotropic =	210.4628	Anisotropy =	148.2759
22	C	Isotropic =	34.1078	Anisotropy =	138.5271
23	C	Isotropic =	69.8551	Anisotropy =	173.8572
24	C	Isotropic =	43.7584	Anisotropy =	182.9246
25	N	Isotropic =	-38.8090	Anisotropy =	461.4852
26	C	Isotropic =	43.1427	Anisotropy =	159.7365
27	C	Isotropic =	90.0782	Anisotropy =	142.5199
28	C	Isotropic =	70.3208	Anisotropy =	176.9337
29	C	Isotropic =	67.6453	Anisotropy =	174.9086
30	C	Isotropic =	63.6481	Anisotropy =	176.2451
31	C	Isotropic =	64.4484	Anisotropy =	150.6074
32	C	Isotropic =	155.0753	Anisotropy =	44.0854
33	O	Isotropic =	-70.9187	Anisotropy =	370.4141
34	H	Isotropic =	24.7397	Anisotropy =	7.1323
35	H	Isotropic =	24.3558	Anisotropy =	3.0909
36	H	Isotropic =	23.3357	Anisotropy =	5.1497
37	H	Isotropic =	22.5978	Anisotropy =	8.4520
38	H	Isotropic =	24.1587	Anisotropy =	8.5564
39	H	Isotropic =	28.3264	Anisotropy =	6.2944
40	H	Isotropic =	26.5603	Anisotropy =	6.2976
41	H	Isotropic =	30.3647	Anisotropy =	8.0950
42	H	Isotropic =	30.2821	Anisotropy =	11.3829

43	H	Isotropic =	29.9623	Anisotropy =	5.5025
44	H	Isotropic =	28.4442	Anisotropy =	4.9988
45	H	Isotropic =	28.4013	Anisotropy =	8.9042
46	H	Isotropic =	26.3889	Anisotropy =	6.7971
47	H	Isotropic =	26.5648	Anisotropy =	6.9752
48	H	Isotropic =	22.8258	Anisotropy =	6.7130
49	H	Isotropic =	24.6689	Anisotropy =	9.2086
50	H	Isotropic =	24.1219	Anisotropy =	8.6123
51	H	Isotropic =	24.1532	Anisotropy =	4.8245
52	H	Isotropic =	23.9706	Anisotropy =	6.0085
53	H	Isotropic =	23.7988	Anisotropy =	5.6264
54	H	Isotropic =	28.7916	Anisotropy =	8.4195
55	H	Isotropic =	27.8500	Anisotropy =	9.0840
56	H	Isotropic =	28.2111	Anisotropy =	9.7999

Conformer 1

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.099858345853	-1.750618905765	-0.726892809133
C	0.117298064284	-2.367998502813	-1.387937721640
C	0.130152762354	-3.758012931960	-1.641458031922
C	1.196999827907	-4.500489361661	-1.122127656471
C	2.217430298032	-3.854631766758	-0.422882970751
C	2.133641561294	-2.472652568344	-0.272283411280
N	-0.836191759021	-4.383776193923	-2.475257306623
C	-2.195864189888	-4.299610278704	-2.271907221368
C	-2.754881626562	-3.203340891877	-1.419178011373
C	-2.235362062987	-1.888704030076	-1.338406680124
N	-0.960170255045	-1.562546501194	-1.844778019442
O	-2.959141533131	-5.104607408684	-2.807581935149
N	-2.943886978943	-0.882480657976	-0.804887578500
C	-4.139640838954	-1.146771461222	-0.269427458783

C	-4.721427115662	-2.419951870095	-0.213811072706
C	-4.005404829075	-3.443747113157	-0.838303856055
C	-0.670326242452	-0.135945719297	-2.101265364523
C	-1.449038263568	0.391006825212	-3.304011112745
C	-6.055193145100	-2.655699654548	0.453385531051
C	-5.960296257818	-3.045123583326	1.930614870534
O	-5.336706857347	-4.337951628165	2.068446376513
C	-4.166510623539	-4.510894309134	2.722113004642
C	-3.779844473130	-5.879658756452	2.920736523370
C	-2.546920912744	-6.130669450632	3.602564727324
N	-1.729876173994	-5.133442111067	4.069429167700
C	-2.133808650680	-3.893937592341	3.858177799662
C	-3.327666490070	-3.515999913331	3.197294053314
C	-4.569495079494	-6.972568165458	2.474280538269
C	-4.153312185383	-8.271668662239	2.692739569010
C	-2.932622289119	-8.526861460023	3.366044004379
C	-2.149314102704	-7.480305083973	3.810263048561
C	-0.379734587804	-5.440145307862	-3.386976678438
H	1.240029494794	-5.577600526939	-1.285733651002
H	3.062109196221	-4.413538605228	-0.018383671632
H	2.924525801769	-1.914525193565	0.237932767329
H	-4.675979526330	-0.283615295785	0.141251556035
H	-4.427317306120	-4.445927138089	-0.925991572592
H	-0.882084960487	0.469461020088	-1.206475546576
H	0.407036511162	-0.072932729958	-2.291204804668
H	-1.229730592282	-0.202231233400	-4.206238057814
H	-2.534399188721	0.368568503962	-3.126497711389
H	-1.160597570218	1.436474421327	-3.499675239092
H	-6.670765980270	-1.742793361055	0.401017340856
H	-6.607686691394	-3.446490754446	-0.078679865170
H	-6.971504948937	-3.154763838743	2.351006121736
H	-5.428386567568	-2.282585192606	2.513824085965
H	-1.477498240116	-3.098486542524	4.229695183509
H	-3.544315957027	-2.456791643100	3.073918690010
H	-5.507894849491	-6.767851877411	1.959023707050
H	-4.766148397372	-9.106724840532	2.346903385088
H	-2.612780679708	-9.557753305612	3.533670885007
H	-1.206095595306	-7.652981542022	4.332192007495
H	0.630878053963	-5.194471002073	-3.735768439300
H	-0.369436263045	-6.430680745235	-2.902793624476
H	-1.067119079028	-5.488403560213	-4.239507863673

SCF Done: E(RB3LYP) = -1390.83176708

Zero-point correction= 0.440767
Thermal correction to Energy= 0.467283
Thermal correction to Enthalpy= 0.468227
Thermal correction to Gibbs Free Energy= 0.380600
Sum of electronic and zero-point Energies= -1390.391000
Sum of electronic and thermal Energies= -1390.364484
Sum of electronic and thermal Enthalpies= -1390.363540
Sum of electronic and thermal Free Energies= -1390.451167

1	N	Isotropic =	-40.6703	Anisotropy =	455.8923
2	C	Isotropic =	37.2935	Anisotropy =	121.5200
3	C	Isotropic =	60.1724	Anisotropy =	122.8446
4	C	Isotropic =	63.1078	Anisotropy =	178.9016
5	C	Isotropic =	72.6126	Anisotropy =	160.8685
6	C	Isotropic =	49.2135	Anisotropy =	155.0100
7	N	Isotropic =	123.5533	Anisotropy =	91.8753
8	C	Isotropic =	27.3000	Anisotropy =	109.7283
9	C	Isotropic =	71.3469	Anisotropy =	133.1520
10	C	Isotropic =	33.8004	Anisotropy =	124.3830
11	N	Isotropic =	135.9966	Anisotropy =	65.3811
12	O	Isotropic =	-81.0266	Anisotropy =	584.0661
13	N	Isotropic =	-35.8852	Anisotropy =	454.8142
14	C	Isotropic =	41.4984	Anisotropy =	147.0508
15	C	Isotropic =	62.9375	Anisotropy =	172.2427
16	C	Isotropic =	50.3949	Anisotropy =	183.2993
17	C	Isotropic =	147.5089	Anisotropy =	36.7258
18	C	Isotropic =	177.1582	Anisotropy =	24.3699
19	C	Isotropic =	155.7982	Anisotropy =	16.7319
20	C	Isotropic =	123.5643	Anisotropy =	52.5967
21	O	Isotropic =	203.7300	Anisotropy =	129.5244
22	C	Isotropic =	31.8951	Anisotropy =	139.5634
23	C	Isotropic =	70.6042	Anisotropy =	172.0951
24	C	Isotropic =	43.5778	Anisotropy =	183.6694
25	N	Isotropic =	-36.0026	Anisotropy =	457.7887
26	C	Isotropic =	43.0988	Anisotropy =	161.5215
27	C	Isotropic =	93.0315	Anisotropy =	139.9058
28	C	Isotropic =	70.0167	Anisotropy =	175.5115
29	C	Isotropic =	68.1258	Anisotropy =	170.4056
30	C	Isotropic =	63.7151	Anisotropy =	175.6115
31	C	Isotropic =	63.9976	Anisotropy =	150.9278
32	C	Isotropic =	154.8679	Anisotropy =	45.4911
33	H	Isotropic =	24.3309	Anisotropy =	7.8573
34	H	Isotropic =	24.4501	Anisotropy =	4.0662
35	H	Isotropic =	23.2903	Anisotropy =	4.6404

36	H	Isotropic =	22.9659	Anisotropy =	7.9881
37	H	Isotropic =	23.6633	Anisotropy =	8.8822
38	H	Isotropic =	27.0088	Anisotropy =	7.4910
39	H	Isotropic =	27.6064	Anisotropy =	6.0125
40	H	Isotropic =	30.4456	Anisotropy =	8.3367
41	H	Isotropic =	29.8850	Anisotropy =	5.0743
42	H	Isotropic =	30.3093	Anisotropy =	11.1828
43	H	Isotropic =	28.4617	Anisotropy =	8.1553
44	H	Isotropic =	28.2550	Anisotropy =	6.8812
45	H	Isotropic =	26.9331	Anisotropy =	8.2244
46	H	Isotropic =	26.8003	Anisotropy =	4.8209
47	H	Isotropic =	23.3058	Anisotropy =	6.7262
48	H	Isotropic =	25.4179	Anisotropy =	7.8239
49	H	Isotropic =	23.1093	Anisotropy =	10.2776
50	H	Isotropic =	23.8539	Anisotropy =	5.7843
51	H	Isotropic =	23.6780	Anisotropy =	4.8123
52	H	Isotropic =	23.6954	Anisotropy =	5.8130
53	H	Isotropic =	29.0167	Anisotropy =	8.3299
54	H	Isotropic =	28.2610	Anisotropy =	9.3121
55	H	Isotropic =	27.6544	Anisotropy =	8.6207

Conformer 2

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.368068534420	-7.222477967192	-1.727020316367
C	-3.229531459861	-6.245153315626	-1.433485401344
C	-3.909840108443	-6.178315108887	-0.197275376752
C	-3.606448260626	-7.151384671551	0.761906806389
C	-2.694505039733	-8.163248990306	0.458831969770
C	-2.118398976392	-8.167008251193	-0.809334161319
N	-4.937284084292	-5.227588504014	0.048288188448
C	-4.776334662889	-3.867049288042	-0.093006002039
C	-3.633935449323	-3.332387928187	-0.899930125080
C	-3.109329793669	-3.935888926360	-2.068538421401
N	-3.449092526261	-5.255995651378	-2.430860879972
O	-5.577035780762	-3.086171751973	0.423523166744
N	-2.294442855682	-3.271169357867	-2.900560869067
C	-1.919085938174	-2.028538467845	-2.581565767853
C	-2.304353219368	-1.357243629889	-1.414148928720
C	-3.206943159599	-2.035716378598	-0.591696486604
C	-3.225650547415	-5.660200380654	-3.834373758988

C	-4.236003051522	-6.712076809034	-4.283934059881
C	-1.790756011697	0.024086579105	-1.085893932345
C	-0.513493168219	0.042954577922	-0.241052841424
O	-0.763395333942	-0.486829435554	1.076397306992
C	-0.215054936421	-1.646460709079	1.502055277181
C	-0.428687412059	-1.944065439463	2.890484293406
C	0.125252928790	-3.159816936242	3.403258823115
N	0.842901780390	-4.040856176112	2.635921751288
C	1.006905379971	-3.717778908126	1.365819276652
C	0.508514324381	-2.549404050494	0.740232319802
C	-1.156477711795	-1.084688484306	3.755958404843
C	-1.332503178833	-1.416691739896	5.085345008860
C	-0.787221169378	-2.619721053062	5.599189937902
C	-0.075182581336	-3.469890714598	4.776747073064
C	-6.120458373269	-5.668429999341	0.797524804074
H	-4.099688350135	-7.129520434436	1.734133463741
H	-2.451631394387	-8.937115941750	1.187979714855
H	-1.425400998678	-8.959269820258	-1.108289375206
H	-1.263624143903	-1.530939652337	-3.305590588770
H	-3.631813909410	-1.550859973920	0.288400851938
H	-3.333317923051	-4.750194450168	-4.435106889219
H	-2.195546523774	-6.023681597631	-3.976075704580
H	-4.082437451810	-6.934935600852	-5.351977901907
H	-4.123447446199	-7.653255584955	-3.725425425847
H	-5.267984330968	-6.349110644050	-4.152020332409
H	-1.567050631040	0.574377166864	-2.014622329364
H	-2.566389122455	0.596406061464	-0.552577672298
H	-0.192988681305	1.083548108541	-0.082771740182
H	0.306820170322	-0.495314332844	-0.733928317393
H	1.577652700194	-4.425648901202	0.753692155557
H	0.697369285969	-2.401956426853	-0.321324151184
H	-1.571414585681	-0.160877325922	3.352942670632
H	-1.892960599630	-0.750742315386	5.744814274148
H	-0.932040564200	-2.872668132610	6.651896144725
H	0.354420857850	-4.401211074956	5.150867075597
H	-6.973613053374	-5.045586643640	0.504250483498
H	-6.323514324272	-6.718202707048	0.552584059250
H	-5.983600068214	-5.566031908210	1.886732455042

SCF Done: E(RB3LYP) = -1390.83171512

Zero-point correction= 0.440782
Thermal correction to Energy= 0.467274
Thermal correction to Enthalpy= 0.468218

Thermal correction to Gibbs Free Energy= 0.381025
Sum of electronic and zero-point Energies= -1390.390933
Sum of electronic and thermal Energies= -1390.364441
Sum of electronic and thermal Enthalpies= -1390.363497
Sum of electronic and thermal Free Energies= -1390.450690

1	N	Isotropic =	-42.0113	Anisotropy =	469.5924
2	C	Isotropic =	39.0739	Anisotropy =	118.0862
3	C	Isotropic =	58.8288	Anisotropy =	125.1342
4	C	Isotropic =	62.9460	Anisotropy =	179.4480
5	C	Isotropic =	72.4325	Anisotropy =	161.0801
6	C	Isotropic =	49.4866	Anisotropy =	154.8328
7	N	Isotropic =	123.5962	Anisotropy =	92.0079
8	C	Isotropic =	27.1179	Anisotropy =	109.8513
9	C	Isotropic =	72.3068	Anisotropy =	132.5072
10	C	Isotropic =	32.6155	Anisotropy =	125.6567
11	N	Isotropic =	136.7509	Anisotropy =	66.0459
12	O	Isotropic =	-81.0782	Anisotropy =	582.7846
13	N	Isotropic =	-35.1702	Anisotropy =	444.2799
14	C	Isotropic =	41.5889	Anisotropy =	147.5871
15	C	Isotropic =	62.6865	Anisotropy =	173.2075
16	C	Isotropic =	50.6305	Anisotropy =	182.7815
17	C	Isotropic =	148.6366	Anisotropy =	34.4620
18	C	Isotropic =	177.3950	Anisotropy =	24.0170
19	C	Isotropic =	155.5799	Anisotropy =	16.6412
20	C	Isotropic =	123.3344	Anisotropy =	53.3426
21	O	Isotropic =	203.4008	Anisotropy =	131.1636
22	C	Isotropic =	31.7621	Anisotropy =	139.9172
23	C	Isotropic =	70.5274	Anisotropy =	171.9536
24	C	Isotropic =	43.8107	Anisotropy =	183.2929
25	N	Isotropic =	-36.1823	Anisotropy =	457.4484
26	C	Isotropic =	43.3272	Anisotropy =	161.4729
27	C	Isotropic =	92.6652	Anisotropy =	139.7081
28	C	Isotropic =	70.0162	Anisotropy =	175.9157
29	C	Isotropic =	67.8628	Anisotropy =	170.2557
30	C	Isotropic =	63.6041	Anisotropy =	175.4330
31	C	Isotropic =	63.9599	Anisotropy =	150.7528
32	C	Isotropic =	154.9734	Anisotropy =	45.4456
33	H	Isotropic =	24.3198	Anisotropy =	7.6640
34	H	Isotropic =	24.4221	Anisotropy =	4.0345
35	H	Isotropic =	23.2513	Anisotropy =	4.6687
36	H	Isotropic =	22.9555	Anisotropy =	7.9213
37	H	Isotropic =	23.7136	Anisotropy =	8.8478
38	H	Isotropic =	27.4383	Anisotropy =	5.8133

39	H	Isotropic =	27.1700	Anisotropy =	7.9241
40	H	Isotropic =	30.2992	Anisotropy =	11.2569
41	H	Isotropic =	30.0946	Anisotropy =	5.1448
42	H	Isotropic =	30.4814	Anisotropy =	8.3063
43	H	Isotropic =	28.4687	Anisotropy =	8.1649
44	H	Isotropic =	28.2663	Anisotropy =	6.9456
45	H	Isotropic =	26.9222	Anisotropy =	8.2334
46	H	Isotropic =	26.8175	Anisotropy =	4.8447
47	H	Isotropic =	23.3755	Anisotropy =	6.6042
48	H	Isotropic =	25.4914	Anisotropy =	7.4120
49	H	Isotropic =	23.1039	Anisotropy =	10.2996
50	H	Isotropic =	23.8633	Anisotropy =	5.7194
51	H	Isotropic =	23.6822	Anisotropy =	4.8573
52	H	Isotropic =	23.6990	Anisotropy =	5.9125
53	H	Isotropic =	27.6707	Anisotropy =	8.7172
54	H	Isotropic =	29.0628	Anisotropy =	8.0781
55	H	Isotropic =	28.2853	Anisotropy =	9.2625

Conformer 3

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-4.168502160204	-5.382801171774	-4.130193522676
C	-4.150325616543	-5.428071042224	-2.795547586009
C	-4.570192907741	-6.565812690743	-2.069786351207
C	-4.960520526058	-7.692973907500	-2.802105117750
C	-4.967925781310	-7.646708800356	-4.196707568473
C	-4.585028160911	-6.458074109928	-4.813364024387
N	-4.698851139662	-6.555374642418	-0.654112926609
C	-3.681147721754	-6.212442170162	0.205446787471
C	-2.500473615664	-5.448396481985	-0.307059773367
C	-2.554552686153	-4.439099200669	-1.298982232430
N	-3.691406884492	-4.267633113507	-2.115790958600
O	-3.743903588204	-6.503454956339	1.401610623725
N	-1.538867840029	-3.585954274289	-1.492115408871
C	-0.422071277199	-3.736467810369	-0.771423722289
C	-0.220820828251	-4.743798739394	0.179491016423
C	-1.309081384105	-5.588856036476	0.410848140881
C	-3.841355695354	-2.974606608591	-2.815845538770
C	-4.180234190060	-1.844902378209	-1.846683691450
C	1.065818488745	-4.855578621769	0.963078258675
C	0.979169150902	-4.338783859537	2.401626188459

O	0.785645572790	-2.910275468233	2.424658124864
C	-0.372273089245	-2.346923579763	2.834786138722
C	-0.336304674081	-0.917358894451	2.968543049781
C	-1.531098017566	-0.258970259635	3.401203144652
N	-2.693342797587	-0.925823005772	3.691833513309
C	-2.670525189661	-2.238530381611	3.548673481891
C	-1.556721575404	-3.004197472306	3.126793774213
C	0.826480081573	-0.149996672252	2.691932104266
C	0.808888147565	1.223754241077	2.836644666377
C	-0.371482931474	1.881800208458	3.263752711054
C	-1.513329912127	1.156412568402	3.539605145921
C	-5.855566894464	-7.235718415114	-0.058409125952
H	-5.280284725178	-8.595863363413	-2.280994465050
H	-5.277267337651	-8.510824501325	-4.785858473426
H	-4.606600972232	-6.358647122306	-5.902837300892
H	0.371410578133	-3.006806301775	-0.967871029174
H	-1.268523970522	-6.355084530354	1.187691860010
H	-2.931112070497	-2.735434457645	-3.387152165307
H	-4.654426426082	-3.110930653770	-3.537802473411
H	-3.365883935414	-1.667601727752	-1.128642967315
H	-4.341593708765	-0.912125234477	-2.410884425244
H	-5.099838268996	-2.071237901239	-1.283543804680
H	1.383402000066	-5.910278050283	1.020700237095
H	1.868738116834	-4.308205175979	0.445085327624
H	1.938518970032	-4.510348097677	2.911970352176
H	0.193733260526	-4.850527826748	2.974467557389
H	-3.602367095725	-2.768969993996	3.776319926184
H	-1.672000690936	-4.081605197747	3.027375815228
H	1.730123052405	-0.663807683819	2.364181997125
H	1.706955000585	1.806860480582	2.622223922256
H	-0.374770626850	2.968434165659	3.374850444039
H	-2.433516771852	1.641812640361	3.870500798441
H	-6.084948618319	-6.760265866163	0.902418652477
H	-6.711969513602	-7.138469158026	-0.736861003545
H	-5.656340602233	-8.303506694667	0.129981896155

SCF Done: E(RB3LYP) = -1390.83181324

Zero-point correction= 0.440998
Thermal correction to Energy= 0.467384
Thermal correction to Enthalpy= 0.468328
Thermal correction to Gibbs Free Energy= 0.382027
Sum of electronic and zero-point Energies= -1390.390815
Sum of electronic and thermal Energies= -1390.364429

Sum of electronic and thermal Enthalpies= -1390.363485
Sum of electronic and thermal Free Energies= -1390.449786

1	N	Isotropic =	-40.6783	Anisotropy =	455.0681
2	C	Isotropic =	37.1116	Anisotropy =	120.0456
3	C	Isotropic =	59.8452	Anisotropy =	120.8215
4	C	Isotropic =	62.5787	Anisotropy =	176.6050
5	C	Isotropic =	72.2740	Anisotropy =	158.7043
6	C	Isotropic =	49.1325	Anisotropy =	154.2436
7	N	Isotropic =	122.8955	Anisotropy =	91.5662
8	C	Isotropic =	26.5216	Anisotropy =	108.2254
9	C	Isotropic =	70.1873	Anisotropy =	136.6622
10	C	Isotropic =	33.7981	Anisotropy =	124.0362
11	N	Isotropic =	136.0432	Anisotropy =	64.3449
12	O	Isotropic =	-82.3800	Anisotropy =	577.6661
13	N	Isotropic =	-34.8329	Anisotropy =	452.3656
14	C	Isotropic =	40.9288	Anisotropy =	147.0400
15	C	Isotropic =	63.2039	Anisotropy =	172.2105
16	C	Isotropic =	51.2251	Anisotropy =	187.1388
17	C	Isotropic =	147.7852	Anisotropy =	35.5143
18	C	Isotropic =	177.3431	Anisotropy =	23.5282
19	C	Isotropic =	156.1056	Anisotropy =	15.3241
20	C	Isotropic =	123.3501	Anisotropy =	54.1839
21	O	Isotropic =	201.4635	Anisotropy =	132.4785
22	C	Isotropic =	31.6131	Anisotropy =	139.1681
23	C	Isotropic =	70.4056	Anisotropy =	171.0979
24	C	Isotropic =	43.7838	Anisotropy =	182.0291
25	N	Isotropic =	-36.2021	Anisotropy =	456.8096
26	C	Isotropic =	42.9676	Anisotropy =	160.1771
27	C	Isotropic =	92.0181	Anisotropy =	138.2111
28	C	Isotropic =	69.8415	Anisotropy =	175.1937
29	C	Isotropic =	67.8840	Anisotropy =	170.1086
30	C	Isotropic =	63.7321	Anisotropy =	174.9199
31	C	Isotropic =	64.0857	Anisotropy =	150.0552
32	C	Isotropic =	154.7621	Anisotropy =	45.5108
33	H	Isotropic =	23.9716	Anisotropy =	9.1012
34	H	Isotropic =	24.3084	Anisotropy =	4.4947
35	H	Isotropic =	23.2380	Anisotropy =	4.8885
36	H	Isotropic =	23.3271	Anisotropy =	6.4792
37	H	Isotropic =	23.1155	Anisotropy =	10.1691
38	H	Isotropic =	27.2079	Anisotropy =	7.8204
39	H	Isotropic =	27.6762	Anisotropy =	7.0378
40	H	Isotropic =	30.5237	Anisotropy =	7.8094
41	H	Isotropic =	30.6066	Anisotropy =	10.3010

42	H	Isotropic =	30.6573	Anisotropy =	7.0414
43	H	Isotropic =	28.4724	Anisotropy =	7.9149
44	H	Isotropic =	28.4000	Anisotropy =	7.1901
45	H	Isotropic =	26.8609	Anisotropy =	7.8777
46	H	Isotropic =	26.5422	Anisotropy =	4.3353
47	H	Isotropic =	23.0417	Anisotropy =	7.4361
48	H	Isotropic =	25.1562	Anisotropy =	6.7451
49	H	Isotropic =	23.0918	Anisotropy =	10.6750
50	H	Isotropic =	23.8458	Anisotropy =	5.8144
51	H	Isotropic =	23.6750	Anisotropy =	4.9083
52	H	Isotropic =	23.6379	Anisotropy =	6.1955
53	H	Isotropic =	27.3803	Anisotropy =	7.7524
54	H	Isotropic =	28.7849	Anisotropy =	7.7008
55	H	Isotropic =	27.8912	Anisotropy =	10.1575

Conformer 4

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.609141335829	-1.283109386770	3.817283883604
C	-2.081923894070	-2.465710475839	3.490496658075
C	-0.798299819422	-2.591360706014	2.913918592971
C	-0.099970697780	-1.412887305904	2.626510891037
C	-0.659967857235	-0.177220487560	2.953480698825
C	-1.909136137224	-0.167259636589	3.569477233093
N	-0.179731427458	-3.855518409592	2.716120098700
C	-0.750445748578	-4.891630215418	2.010779990372
C	-2.223196054214	-4.886243966859	1.740342552462
C	-3.212535133850	-4.395335001705	2.626485350933
N	-2.869661821970	-3.619256552401	3.754109372925
O	-0.060280899922	-5.832526633586	1.615228530973
N	-4.512665809909	-4.672582384920	2.454990411484
C	-4.886284336830	-5.381701109421	1.384388483435
C	-4.010804355579	-5.855360975308	0.399399057381
C	-2.653606448935	-5.613526687056	0.625104988952
C	-3.864408446168	-3.515573566128	4.841660227079
C	-3.193469446332	-3.350222043235	6.202424721409
C	-4.515511826996	-6.597201874108	-0.816318651832
C	-4.748117877092	-5.705125371700	-2.033515232107
O	-3.470857552607	-5.212479201416	-2.473975731935
C	-3.426558136411	-4.366389532725	-3.524967486254
C	-2.119784848071	-3.925611666774	-3.921061490422

C	-2.034641404101	-3.022799218985	-5.028038525147
N	-3.131808579230	-2.571635989934	-5.716847877959
C	-4.307976006200	-3.014173972856	-5.312069260304
C	-4.524796625269	-3.905800655669	-4.232846666878
C	-0.932563413584	-4.347565814975	-3.266380585075
C	0.299988649614	-3.889591484917	-3.690427299630
C	0.391130781331	-2.992845522027	-4.783963821785
C	-0.749853245173	-2.570724371452	-5.436916930682
C	1.257535977227	-3.971508082857	2.992841621646
H	0.888642615183	-1.463829692544	2.169247284911
H	-0.128161730197	0.752418110415	2.747394600854
H	-2.374413561602	0.773287108248	3.879648258889
H	-5.959866488820	-5.587448656688	1.304233745779
H	-1.895174193963	-6.027433729492	-0.040233888645
H	-4.566490489103	-2.688483022919	4.650781742497
H	-4.444062940137	-4.445086416320	4.814892593965
H	-2.493902910172	-4.178284496565	6.400010956631
H	-2.640061674955	-2.402027741901	6.273511666520
H	-3.961341402518	-3.350883447458	6.992588757665
H	-3.810571452399	-7.395655179569	-1.097710342430
H	-5.477200372614	-7.081626012351	-0.585036679043
H	-5.403630033314	-4.855165883863	-1.778815149820
H	-5.217144486819	-6.281746950803	-2.848407931644
H	-5.181419973924	-2.652392524137	-5.866845889927
H	-5.542367868247	-4.204347801653	-3.987879362743
H	-1.009740547289	-5.038608131226	-2.427176523939
H	1.208790114190	-4.218653992728	-3.182304211212
H	1.370592028617	-2.636363821277	-5.110569799536
H	-0.703345268508	-1.882051878439	-6.282728436586
H	1.513711935601	-3.302190087007	3.823228656458
H	1.478772482231	-5.009170422572	3.268608409014
H	1.870909996624	-3.715727024448	2.113117736997

SCF Done: E(RB3LYP) = -1390.83585095

Zero-point correction= 0.440814
Thermal correction to Energy= 0.467299
Thermal correction to Enthalpy= 0.468243
Thermal correction to Gibbs Free Energy= 0.381316
Sum of electronic and zero-point Energies= -1390.395037
Sum of electronic and thermal Energies= -1390.368552
Sum of electronic and thermal Enthalpies= -1390.367608
Sum of electronic and thermal Free Energies= -1390.454535

1	N	Isotropic =	-41.9863	Anisotropy =	468.4887
2	C	Isotropic =	38.7965	Anisotropy =	117.3681
3	C	Isotropic =	58.7034	Anisotropy =	124.1707
4	C	Isotropic =	62.7352	Anisotropy =	177.7555
5	C	Isotropic =	72.7495	Anisotropy =	160.0446
6	C	Isotropic =	49.2546	Anisotropy =	154.2955
7	N	Isotropic =	122.9753	Anisotropy =	91.8948
8	C	Isotropic =	26.6329	Anisotropy =	109.4134
9	C	Isotropic =	72.0880	Anisotropy =	130.9320
10	C	Isotropic =	32.3588	Anisotropy =	123.9336
11	N	Isotropic =	137.0405	Anisotropy =	64.4129
12	O	Isotropic =	-81.4048	Anisotropy =	582.9558
13	N	Isotropic =	-34.9383	Anisotropy =	441.5671
14	C	Isotropic =	41.5229	Anisotropy =	144.4782
15	C	Isotropic =	61.3796	Anisotropy =	171.9134
16	C	Isotropic =	50.3136	Anisotropy =	180.6776
17	C	Isotropic =	148.5296	Anisotropy =	34.4893
18	C	Isotropic =	177.4385	Anisotropy =	23.7686
19	C	Isotropic =	157.1180	Anisotropy =	16.2672
20	C	Isotropic =	120.8689	Anisotropy =	43.2913
21	O	Isotropic =	202.4994	Anisotropy =	111.9819
22	C	Isotropic =	32.0396	Anisotropy =	138.2043
23	C	Isotropic =	70.5298	Anisotropy =	170.9505
24	C	Isotropic =	44.0211	Anisotropy =	181.8356
25	N	Isotropic =	-37.5955	Anisotropy =	458.3264
26	C	Isotropic =	42.6428	Anisotropy =	159.6877
27	C	Isotropic =	91.0858	Anisotropy =	133.3975
28	C	Isotropic =	70.2120	Anisotropy =	174.1287
29	C	Isotropic =	67.6561	Anisotropy =	170.5332
30	C	Isotropic =	63.6310	Anisotropy =	174.9985
31	C	Isotropic =	63.7519	Anisotropy =	150.3138
32	C	Isotropic =	154.4003	Anisotropy =	45.4142
33	H	Isotropic =	24.0549	Anisotropy =	8.3022
34	H	Isotropic =	24.4132	Anisotropy =	4.5638
35	H	Isotropic =	23.2834	Anisotropy =	4.7835
36	H	Isotropic =	23.0215	Anisotropy =	7.9204
37	H	Isotropic =	23.0648	Anisotropy =	10.2543
38	H	Isotropic =	27.1563	Anisotropy =	8.2900
39	H	Isotropic =	27.4079	Anisotropy =	5.9673
40	H	Isotropic =	30.4134	Anisotropy =	8.0734
41	H	Isotropic =	30.0318	Anisotropy =	5.1834
42	H	Isotropic =	30.2669	Anisotropy =	11.2482
43	H	Isotropic =	28.1768	Anisotropy =	5.4604
44	H	Isotropic =	28.4210	Anisotropy =	8.3244

45	H	Isotropic =	27.5561	Anisotropy =	5.4750
46	H	Isotropic =	27.1495	Anisotropy =	6.4351
47	H	Isotropic =	22.8218	Anisotropy =	7.1988
48	H	Isotropic =	24.9856	Anisotropy =	9.5850
49	H	Isotropic =	23.0831	Anisotropy =	9.0497
50	H	Isotropic =	23.8231	Anisotropy =	6.6241
51	H	Isotropic =	23.6489	Anisotropy =	5.2943
52	H	Isotropic =	23.5751	Anisotropy =	5.6422
53	H	Isotropic =	28.8233	Anisotropy =	7.7433
54	H	Isotropic =	27.4005	Anisotropy =	8.1137
55	H	Isotropic =	27.9135	Anisotropy =	9.8014

Conformer 5

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.976893055524	-7.297134443144	-1.397431224738
C	-2.192766962545	-6.253850796320	-1.680984089732
C	-0.909250375378	-6.093055468211	-1.112572400380
C	-0.490666347982	-7.048214020942	-0.179049750122
C	-1.315933053421	-8.132046800834	0.123327153367
C	-2.541796941204	-8.223067020909	-0.531407861614
N	-0.019555506189	-5.066820135266	-1.531905530472
C	-0.336653531315	-3.726641147798	-1.521858468535
C	-1.771627709981	-3.302149021361	-1.475785291843
C	-2.842039534897	-3.981265324135	-2.106380131263
N	-2.699775488273	-5.294753804188	-2.598634614940
O	0.550281994704	-2.873494537579	-1.576521838784
N	-4.034831870666	-3.396217492832	-2.293429612920
C	-4.239295024737	-2.172832176015	-1.795964738933
C	-3.289825357723	-1.440900519342	-1.070704971525
C	-2.027736604017	-2.027964320170	-0.956562001851
C	-3.694406725599	-5.768469995013	-3.584023533284
C	-3.518751865320	-5.083181678618	-4.936873971154
C	-3.610013234509	-0.088515366008	-0.480577402480
C	-4.195148959416	-0.128692153959	0.934824595025
O	-3.230164408752	-0.624544209357	1.884476217270
C	-3.353308408170	-1.839761333232	2.463133510748
C	-2.402681517380	-2.116320152116	3.503131130751
C	-2.480553281983	-3.388438529800	4.154233896132
N	-3.412681135020	-4.341337908789	3.832929561484
C	-4.261303359935	-4.033668940908	2.868816513776

C	-4.286396001087	-2.814509371895	2.149553460071
C	-1.407721608851	-1.184104536335	3.901061625849
C	-0.517777857319	-1.498870010162	4.909725747136
C	-0.588932647086	-2.757309330621	5.557803587348
C	-1.547969572594	-3.679035912280	5.187920458679
C	1.405537709630	-5.396600367035	-1.657580259016
H	0.488539139613	-6.955843205709	0.291582243363
H	-1.004605291075	-8.892089376888	0.840902224221
H	-3.210783200729	-9.070813676031	-0.355005601219
H	-5.228423494978	-1.742211017311	-1.989824516705
H	-1.200428646532	-1.485835562693	-0.496062747712
H	-3.535681418224	-6.848166038043	-3.683080723884
H	-4.716844799422	-5.620516407505	-3.203822226896
H	-2.501044806926	-5.240257300383	-5.328766213793
H	-4.235934139445	-5.505417887850	-5.659260632375
H	-3.704671558905	-4.001016515663	-4.870500294929
H	-2.702734579283	0.535782115276	-0.460942907069
H	-4.346184075378	0.434835110809	-1.113016731891
H	-5.124004160074	-0.713706706736	0.977234396537
H	-4.422956390179	0.895895424187	1.264084518823
H	-5.002604575193	-4.798805871338	2.610912353640
H	-5.025897922592	-2.684840872302	1.362093959904
H	-1.360127797199	-0.218821934758	3.397029397592
H	0.244053396259	-0.776715375011	5.210713239892
H	0.119452620707	-2.996194695364	6.354199772406
H	-1.622030936410	-4.653774383136	5.674044364435
H	1.856476148263	-4.726254339265	-2.398557305052
H	1.947466227039	-5.265116540038	-0.706485327424
H	1.500298503204	-6.437578119075	-1.990201005916

SCF Done: E(RB3LYP) = -1390.83169842

Zero-point correction= 0.440888
Thermal correction to Energy= 0.467319
Thermal correction to Enthalpy= 0.468263
Thermal correction to Gibbs Free Energy= 0.381600
Sum of electronic and zero-point Energies= -1390.390811
Sum of electronic and thermal Energies= -1390.364380
Sum of electronic and thermal Enthalpies= -1390.363435
Sum of electronic and thermal Free Energies= -1390.450098

1	N	Isotropic =	-40.6430	Anisotropy =	456.1312
2	C	Isotropic =	37.3322	Anisotropy =	121.4871
3	C	Isotropic =	60.2733	Anisotropy =	122.8983

4	C	Isotropic =	63.3687	Anisotropy =	178.7989
5	C	Isotropic =	72.3512	Anisotropy =	161.1528
6	C	Isotropic =	49.1130	Anisotropy =	155.6039
7	N	Isotropic =	123.7647	Anisotropy =	91.9240
8	C	Isotropic =	27.2048	Anisotropy =	109.5187
9	C	Isotropic =	71.3779	Anisotropy =	133.1140
10	C	Isotropic =	33.6217	Anisotropy =	123.8863
11	N	Isotropic =	135.8759	Anisotropy =	66.5583
12	O	Isotropic =	-81.9326	Anisotropy =	583.0829
13	N	Isotropic =	-35.0975	Anisotropy =	457.3095
14	C	Isotropic =	41.5563	Anisotropy =	148.5051
15	C	Isotropic =	62.7523	Anisotropy =	172.7928
16	C	Isotropic =	50.0091	Anisotropy =	182.4982
17	C	Isotropic =	147.3420	Anisotropy =	36.9950
18	C	Isotropic =	176.9777	Anisotropy =	24.5674
19	C	Isotropic =	155.2174	Anisotropy =	16.8553
20	C	Isotropic =	123.1569	Anisotropy =	53.8762
21	O	Isotropic =	202.2314	Anisotropy =	132.8162
22	C	Isotropic =	31.9012	Anisotropy =	139.8138
23	C	Isotropic =	70.5519	Anisotropy =	171.6803
24	C	Isotropic =	43.8271	Anisotropy =	183.4221
25	N	Isotropic =	-36.7088	Anisotropy =	455.4525
26	C	Isotropic =	43.2092	Anisotropy =	161.5017
27	C	Isotropic =	92.5160	Anisotropy =	139.5187
28	C	Isotropic =	70.0759	Anisotropy =	175.7348
29	C	Isotropic =	68.0802	Anisotropy =	170.1821
30	C	Isotropic =	63.6868	Anisotropy =	175.1715
31	C	Isotropic =	63.8183	Anisotropy =	150.5449
32	C	Isotropic =	154.8970	Anisotropy =	45.7581
33	H	Isotropic =	24.3356	Anisotropy =	7.7533
34	H	Isotropic =	24.4106	Anisotropy =	3.9219
35	H	Isotropic =	23.2458	Anisotropy =	4.6427
36	H	Isotropic =	22.8943	Anisotropy =	8.0429
37	H	Isotropic =	23.7635	Anisotropy =	8.6705
38	H	Isotropic =	27.5702	Anisotropy =	5.9777
39	H	Isotropic =	26.9804	Anisotropy =	7.3951
40	H	Isotropic =	30.4257	Anisotropy =	8.3256
41	H	Isotropic =	30.2911	Anisotropy =	11.1822
42	H	Isotropic =	29.8522	Anisotropy =	5.0985
43	H	Isotropic =	28.3136	Anisotropy =	6.8666
44	H	Isotropic =	28.4162	Anisotropy =	8.0846
45	H	Isotropic =	26.8100	Anisotropy =	4.7904
46	H	Isotropic =	26.9018	Anisotropy =	8.1602
47	H	Isotropic =	23.4401	Anisotropy =	6.6139

48	H	Isotropic =	25.5723	Anisotropy =	7.0433
49	H	Isotropic =	23.1401	Anisotropy =	10.3602
50	H	Isotropic =	23.8872	Anisotropy =	5.7147
51	H	Isotropic =	23.7086	Anisotropy =	4.8861
52	H	Isotropic =	23.7342	Anisotropy =	6.0017
53	H	Isotropic =	27.6850	Anisotropy =	8.7971
54	H	Isotropic =	28.2587	Anisotropy =	9.3499
55	H	Isotropic =	29.0130	Anisotropy =	8.2981

Conformer 6

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.924770167236	-6.754336338963	1.264832342041
C	-5.030124761576	-6.341577354943	0.363463284823
C	-4.580838780121	-7.166138513368	-0.692187449946
C	-5.061875804430	-8.479737171556	-0.737310860097
C	-5.984883373198	-8.913747269640	0.214936023951
C	-6.402008989007	-8.004212085771	1.183906399795
N	-3.749394034212	-6.674071978939	-1.734467242888
C	-2.544973900458	-6.041424554327	-1.524740155435
C	-2.218685774360	-5.487607803692	-0.172611077589
C	-3.151324826566	-4.892793445222	0.711698861305
N	-4.540822832585	-5.013594996788	0.500975465453
O	-1.738748703195	-5.907847874275	-2.447240693008
N	-2.758745762014	-4.169096099079	1.769219059695
C	-1.450454918451	-4.047173213931	2.019375769666
C	-0.437979425501	-4.644369772501	1.259031106661
C	-0.860220301997	-5.354213426951	0.132299454223
C	-5.423128198887	-4.043460368330	1.182393518591
C	-6.686098145171	-3.767551923484	0.371318799379
C	1.022401897277	-4.466522033645	1.602059321007
C	1.737112008825	-3.385340192656	0.786099920072
O	1.208850557217	-2.080312963131	1.096423211274
C	0.479538039735	-1.367829601642	0.209492553834
C	0.125820870883	-0.044453658155	0.641000325196
C	-0.644433920253	0.764129281285	-0.253810520581
N	-1.051454010304	0.336891996121	-1.491422689314
C	-0.699701994801	-0.888590714728	-1.835997395693
C	0.054791509883	-1.785485001315	-1.041483980827
C	0.508839965683	0.477779541377	1.904972599587
C	0.140730076729	1.757205950655	2.273925560242

C	-0.623228356170	2.562576649257	1.392813572400
C	-1.005515829350	2.076532140659	0.158436047772
C	-4.015291528185	-7.130388873034	-3.104530224009
H	-4.731283914836	-9.153049220316	-1.528700615188
H	-6.379645666395	-9.930174010367	0.191873769511
H	-7.151182096959	-8.284195054609	1.930664262210
H	-1.188497783040	-3.439093754650	2.892299348312
H	-0.136207748055	-5.789639698919	-0.559127562714
H	-5.679032631194	-4.393784173435	2.194904476073
H	-4.837047709288	-3.124573505256	1.295857196743
H	-6.434801706292	-3.409148447850	-0.639849666590
H	-7.315774845138	-4.664704826434	0.276635569147
H	-7.282585396916	-2.990033181809	0.874888297323
H	1.128439899269	-4.220595183656	2.670307925185
H	1.569004283073	-5.409479570738	1.435061103425
H	1.685133377460	-3.586425801902	-0.292306245898
H	2.798034750669	-3.346818618999	1.074277203507
H	-1.029604879161	-1.229799989630	-2.824069229421
H	0.264666903210	-2.779092612005	-1.432268973974
H	1.096194448967	-0.148270462584	2.576567925819
H	0.438644542050	2.151660902414	3.247661633544
H	-0.909247403623	3.572736742004	1.694360078980
H	-1.593360290774	2.679035211653	-0.536768887933
H	-3.479925684033	-8.064788785357	-3.340748172712
H	-5.094244426216	-7.288522997236	-3.222591931232
H	-3.672846610981	-6.358761289604	-3.803848411698

SCF Done: E(RB3LYP) = -1390.83173120

Zero-point correction= 0.440826
Thermal correction to Energy= 0.467312
Thermal correction to Enthalpy= 0.468256
Thermal correction to Gibbs Free Energy= 0.381131
Sum of electronic and zero-point Energies= -1390.390905
Sum of electronic and thermal Energies= -1390.364419
Sum of electronic and thermal Enthalpies= -1390.363475
Sum of electronic and thermal Free Energies= -1390.450601

1	N	Isotropic =	-42.1671	Anisotropy =	468.8585
2	C	Isotropic =	38.9542	Anisotropy =	116.7324
3	C	Isotropic =	58.4417	Anisotropy =	123.0329
4	C	Isotropic =	62.5855	Anisotropy =	176.7881
5	C	Isotropic =	72.5820	Anisotropy =	159.3780
6	C	Isotropic =	49.1202	Anisotropy =	153.8324

7	N	Isotropic =	122.9022	Anisotropy =	91.4279
8	C	Isotropic =	26.7052	Anisotropy =	108.1238
9	C	Isotropic =	71.2004	Anisotropy =	135.3543
10	C	Isotropic =	32.7724	Anisotropy =	126.6621
11	N	Isotropic =	137.2295	Anisotropy =	62.7520
12	O	Isotropic =	-81.7835	Anisotropy =	579.5075
13	N	Isotropic =	-33.9808	Anisotropy =	442.1329
14	C	Isotropic =	40.7316	Anisotropy =	149.1028
15	C	Isotropic =	63.2752	Anisotropy =	172.3961
16	C	Isotropic =	51.3504	Anisotropy =	185.7490
17	C	Isotropic =	148.9075	Anisotropy =	33.3024
18	C	Isotropic =	177.4633	Anisotropy =	23.3172
19	C	Isotropic =	156.2064	Anisotropy =	15.7020
20	C	Isotropic =	123.9614	Anisotropy =	52.8014
21	O	Isotropic =	201.6863	Anisotropy =	132.3223
22	C	Isotropic =	31.8599	Anisotropy =	139.2515
23	C	Isotropic =	70.4136	Anisotropy =	171.0800
24	C	Isotropic =	43.6669	Anisotropy =	182.4065
25	N	Isotropic =	-36.1110	Anisotropy =	456.1814
26	C	Isotropic =	43.0409	Anisotropy =	160.3599
27	C	Isotropic =	92.4185	Anisotropy =	139.3284
28	C	Isotropic =	69.9482	Anisotropy =	175.4087
29	C	Isotropic =	67.8668	Anisotropy =	170.0617
30	C	Isotropic =	63.6097	Anisotropy =	175.1595
31	C	Isotropic =	63.9869	Anisotropy =	150.1200
32	C	Isotropic =	154.7361	Anisotropy =	45.4449
33	H	Isotropic =	23.9781	Anisotropy =	9.0711
34	H	Isotropic =	24.2932	Anisotropy =	4.5034
35	H	Isotropic =	23.2092	Anisotropy =	4.9515
36	H	Isotropic =	23.3520	Anisotropy =	6.4052
37	H	Isotropic =	23.2160	Anisotropy =	10.1172
38	H	Isotropic =	27.3385	Anisotropy =	8.2701
39	H	Isotropic =	27.8938	Anisotropy =	7.0276
40	H	Isotropic =	30.5947	Anisotropy =	7.3928
41	H	Isotropic =	30.1255	Anisotropy =	5.8421
42	H	Isotropic =	30.4495	Anisotropy =	10.6903
43	H	Isotropic =	28.3814	Anisotropy =	7.2756
44	H	Isotropic =	28.4901	Anisotropy =	7.8175
45	H	Isotropic =	26.5619	Anisotropy =	4.5597
46	H	Isotropic =	26.9010	Anisotropy =	7.8986
47	H	Isotropic =	23.0456	Anisotropy =	7.3381
48	H	Isotropic =	25.1687	Anisotropy =	7.1019
49	H	Isotropic =	23.0761	Anisotropy =	10.6033
50	H	Isotropic =	23.8316	Anisotropy =	5.8220

51	H	Isotropic =	23.6481	Anisotropy =	4.9025
52	H	Isotropic =	23.6176	Anisotropy =	6.1092
53	H	Isotropic =	27.9060	Anisotropy =	10.1804
54	H	Isotropic =	28.8136	Anisotropy =	7.5275
55	H	Isotropic =	27.3999	Anisotropy =	7.7767

Conformer 7

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-6.765012325399	-3.212282510279	-1.678884986672
C	-5.914161463481	-3.086579452780	-0.657236540542
C	-6.345194380399	-3.048365592944	0.687571891094
C	-7.713277023571	-3.211634702987	0.934389222382
C	-8.598350790542	-3.359112784034	-0.134109999094
C	-8.075584384214	-3.330399424307	-1.424928829973
N	-5.457026356293	-2.759603036630	1.758954808711
C	-4.294235106102	-3.454141644452	1.999910651897
C	-3.699880468798	-4.308734731018	0.924038176698
C	-3.702906180425	-3.997427709339	-0.457829083802
N	-4.532549914023	-2.982952216194	-0.978298752106
O	-3.721304076754	-3.361553965374	3.087619927517
N	-2.901635443787	-4.631841571243	-1.324784718367
C	-2.114181084127	-5.616325901023	-0.876713202486
C	-2.078804936212	-6.063122724991	0.449110043707
C	-2.885944054022	-5.362802147863	1.349070641514
C	-4.194476463822	-2.435711018814	-2.308672147747
C	-4.598354346177	-0.969216042682	-2.432124575680
C	-1.165570135694	-7.182730458791	0.889953308625
C	0.068250466543	-6.725924648297	1.673717425679
O	0.966279668673	-5.974351247548	0.832533862969
C	1.146372250225	-4.643117263469	0.980060092954
C	2.189397464470	-4.079881923977	0.168990263079
C	2.433783022676	-2.674153586476	0.280433947729
N	1.725351488153	-1.852415564693	1.118882041370
C	0.776672302462	-2.423006701187	1.838912087058
C	0.437153491004	-3.797325220025	1.817827446007
C	2.972234440637	-4.859375563535	-0.723791751828
C	3.963965674647	-4.268845598436	-1.482842067575
C	4.210391241244	-2.877131328419	-1.377619875418
C	3.462783463864	-2.099724247681	-0.515731204964
C	-5.938546252931	-1.894766089579	2.843428014797

H	-8.085522245325	-3.200642389813	1.959184144639
H	-9.669166473061	-3.477408046816	0.035639496541
H	-8.731391188593	-3.404816982758	-2.297665598135
H	-1.472785892906	-6.090255603804	-1.628146009901
H	-2.866951437239	-5.594028355649	2.416019638411
H	-3.109128125582	-2.541150008067	-2.415207869528
H	-4.660048123414	-3.036427576326	-3.106023203472
H	-4.126140395083	-0.362236847639	-1.643063434551
H	-4.271205167449	-0.579854943050	-3.409537555594
H	-5.688759184018	-0.838747714734	-2.366797629791
H	-1.714343079918	-7.885813002080	1.539084509236
H	-0.826892821373	-7.756249096993	0.013073597080
H	0.643599991383	-7.605734688610	1.997466947895
H	-0.203392891192	-6.150509937718	2.569454627443
H	0.207463138487	-1.763361550929	2.504048804951
H	-0.382818582770	-4.140799268162	2.444932668955
H	2.775587462031	-5.928827866404	-0.798840309347
H	4.561742683955	-4.874794057400	-2.166945369337
H	4.996643947036	-2.419966966485	-1.982546004815
H	3.635614736803	-1.026163022310	-0.418161123355
H	-5.077625073342	-1.390036981935	3.296953760259
H	-6.629022201047	-1.151990789202	2.425411349352
H	-6.451308865207	-2.468457684051	3.632978445533

SCF Done: E(RB3LYP) = -1390.83168233

Zero-point correction= 0.440804
Thermal correction to Energy= 0.467288
Thermal correction to Enthalpy= 0.468232
Thermal correction to Gibbs Free Energy= 0.380920
Sum of electronic and zero-point Energies= -1390.390878
Sum of electronic and thermal Energies= -1390.364394
Sum of electronic and thermal Enthalpies= -1390.363450
Sum of electronic and thermal Free Energies= -1390.450763

1	N	Isotropic =	-42.4151	Anisotropy =	468.7410
2	C	Isotropic =	38.6857	Anisotropy =	116.4116
3	C	Isotropic =	58.4175	Anisotropy =	122.8955
4	C	Isotropic =	62.5552	Anisotropy =	177.2317
5	C	Isotropic =	72.5391	Anisotropy =	159.3975
6	C	Isotropic =	49.0675	Anisotropy =	153.9110
7	N	Isotropic =	122.9374	Anisotropy =	92.0088
8	C	Isotropic =	26.4401	Anisotropy =	108.2443
9	C	Isotropic =	71.1993	Anisotropy =	135.5682

10	C	Isotropic =	32.7595	Anisotropy =	126.4423
11	N	Isotropic =	136.5593	Anisotropy =	62.8765
12	O	Isotropic =	-81.7159	Anisotropy =	576.8077
13	N	Isotropic =	-33.6852	Anisotropy =	440.8679
14	C	Isotropic =	40.9673	Anisotropy =	146.9952
15	C	Isotropic =	62.9758	Anisotropy =	172.2857
16	C	Isotropic =	51.3049	Anisotropy =	188.1957
17	C	Isotropic =	148.8658	Anisotropy =	33.2680
18	C	Isotropic =	177.5736	Anisotropy =	23.2031
19	C	Isotropic =	155.7707	Anisotropy =	15.6475
20	C	Isotropic =	123.4024	Anisotropy =	53.8733
21	O	Isotropic =	200.7047	Anisotropy =	132.5955
22	C	Isotropic =	31.8748	Anisotropy =	139.3287
23	C	Isotropic =	70.3407	Anisotropy =	171.0478
24	C	Isotropic =	43.6936	Anisotropy =	181.9127
25	N	Isotropic =	-36.1012	Anisotropy =	456.8142
26	C	Isotropic =	42.9566	Anisotropy =	160.0247
27	C	Isotropic =	92.0615	Anisotropy =	138.5543
28	C	Isotropic =	69.8669	Anisotropy =	174.8297
29	C	Isotropic =	67.9552	Anisotropy =	170.0874
30	C	Isotropic =	63.6654	Anisotropy =	174.8338
31	C	Isotropic =	64.0527	Anisotropy =	150.3471
32	C	Isotropic =	154.7429	Anisotropy =	45.2086
33	H	Isotropic =	23.9599	Anisotropy =	9.1181
34	H	Isotropic =	24.2799	Anisotropy =	4.5256
35	H	Isotropic =	23.2048	Anisotropy =	4.9003
36	H	Isotropic =	23.3304	Anisotropy =	6.5506
37	H	Isotropic =	23.1281	Anisotropy =	10.2887
38	H	Isotropic =	27.7700	Anisotropy =	6.6108
39	H	Isotropic =	27.3095	Anisotropy =	8.4399
40	H	Isotropic =	30.5859	Anisotropy =	7.4590
41	H	Isotropic =	30.4393	Anisotropy =	10.7939
42	H	Isotropic =	30.1196	Anisotropy =	5.7379
43	H	Isotropic =	28.4589	Anisotropy =	7.8354
44	H	Isotropic =	28.4155	Anisotropy =	7.2010
45	H	Isotropic =	26.8500	Anisotropy =	7.8524
46	H	Isotropic =	26.5218	Anisotropy =	4.2552
47	H	Isotropic =	23.0396	Anisotropy =	7.4821
48	H	Isotropic =	25.1467	Anisotropy =	6.6801
49	H	Isotropic =	23.1049	Anisotropy =	10.6992
50	H	Isotropic =	23.8374	Anisotropy =	5.8378
51	H	Isotropic =	23.6628	Anisotropy =	4.9228
52	H	Isotropic =	23.6230	Anisotropy =	6.2190
53	H	Isotropic =	27.3630	Anisotropy =	7.6783

54 H Isotropic = 28.7922 Anisotropy = 7.5426
55 H Isotropic = 27.9145 Anisotropy = 10.1426

Conformer 8

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.750905037564	-3.691278188217	-0.283574709775
C	1.039935970478	-2.580457626160	-0.074318290571
C	0.807053858406	-1.625670643085	-1.089112977973
C	1.296892187738	-1.908922586045	-2.369261245908
C	2.025592408092	-3.078409823797	-2.589783498115
C	2.245051474920	-3.926817367115	-1.507083745193
N	0.186889907721	-0.375334047304	-0.821347911507
C	-1.044232745507	-0.239831921024	-0.219257602525
C	-1.628304825333	-1.386367343125	0.546256579261
C	-0.887085983338	-2.307501516655	1.325598106869
N	0.518847970146	-2.383082445586	1.233596010810
O	-1.661395499632	0.824015674056	-0.291544183498
N	-1.481373702951	-3.124377904569	2.206612717050
C	-2.815118080818	-3.110359398942	2.303981187269
C	-3.658656405674	-2.302041094861	1.532492122749
C	-3.022128957856	-1.408682277042	0.667696534090
C	1.244928862946	-3.028390202760	2.346909024613
C	2.634935968868	-2.426318394720	2.533023541006
C	-5.163421563321	-2.381187883950	1.644582632228
C	-5.811659701905	-3.269801127487	0.586013393113
O	-5.384255241577	-4.621756595298	0.825949732668
C	-5.807444714486	-5.596551427983	-0.006155533328
C	-5.363661877783	-6.924620663403	0.307028465782
C	-5.789842417265	-7.984201533235	-0.555145676346
N	-6.592472458773	-7.786180208430	-1.649938482577
C	-6.972789981689	-6.544498406405	-1.888209185100
C	-6.620856529670	-5.412622557899	-1.112440600759
C	-4.534961385768	-7.217143639006	1.422323738483
C	-4.138976009495	-8.515979819742	1.677154639141
C	-4.556113851717	-9.569848141636	0.826428280718
C	-5.362475394169	-9.308813388123	-0.263581724643
C	0.714502894723	0.816586473706	-1.497128637479
H	1.127410574515	-1.205102335873	-3.184702985152
H	2.425133023465	-3.313326712613	-3.577063121408
H	2.841975108696	-4.836932373402	-1.619668512645

H	-3.243890672113	-3.790056311864	3.048359741661
H	-3.597258012359	-0.677213850805	0.096831614900
H	0.637358665097	-2.865044384691	3.244025623110
H	1.309597493825	-4.116887736409	2.190862838065
H	3.116417884831	-2.879572845119	3.414327163861
H	3.281951358381	-2.614560736373	1.663334075115
H	2.574359826087	-1.337957223084	2.693872964989
H	-5.452368095635	-2.754359782391	2.639670505723
H	-5.601937194777	-1.376514845935	1.535544402101
H	-5.508228264566	-2.960589004490	-0.428777294469
H	-6.910965927405	-3.215300020084	0.657199884678
H	-7.614919886375	-6.391638244190	-2.763351603216
H	-6.995447834653	-4.432901833543	-1.402978041857
H	-4.218478838531	-6.401921589804	2.072904955062
H	-3.502016419266	-8.733680640961	2.537000615583
H	-4.236859928581	-10.593016382725	1.036853287541
H	-5.696514582010	-10.104933838708	-0.931727340671
H	1.796264259574	0.697115772155	-1.633170559606
H	0.237558446867	0.982593942207	-2.477169380764
H	0.512579802058	1.693387004541	-0.870731533153

SCF Done: E(RB3LYP) = -1390.83584690

Zero-point correction= 0.440797
Thermal correction to Energy= 0.467281
Thermal correction to Enthalpy= 0.468225
Thermal correction to Gibbs Free Energy= 0.380933
Sum of electronic and zero-point Energies= -1390.395050
Sum of electronic and thermal Energies= -1390.368566
Sum of electronic and thermal Enthalpies= -1390.367622
Sum of electronic and thermal Free Energies= -1390.454914

1	N	Isotropic =	-41.9685	Anisotropy =	469.5600
2	C	Isotropic =	38.6509	Anisotropy =	117.9058
3	C	Isotropic =	58.4834	Anisotropy =	123.7605
4	C	Isotropic =	62.7700	Anisotropy =	177.4771
5	C	Isotropic =	72.6717	Anisotropy =	159.9660
6	C	Isotropic =	49.1570	Anisotropy =	154.5802
7	N	Isotropic =	123.1486	Anisotropy =	91.9804
8	C	Isotropic =	26.7559	Anisotropy =	108.4301
9	C	Isotropic =	71.2889	Anisotropy =	132.1055
10	C	Isotropic =	32.4246	Anisotropy =	124.3197
11	N	Isotropic =	136.8999	Anisotropy =	64.2208
12	O	Isotropic =	-81.0050	Anisotropy =	581.1534

13	N	Isotropic =	-33.5863	Anisotropy =	439.1334
14	C	Isotropic =	40.3980	Anisotropy =	146.0346
15	C	Isotropic =	61.2711	Anisotropy =	171.2866
16	C	Isotropic =	51.8316	Anisotropy =	179.9587
17	C	Isotropic =	148.5938	Anisotropy =	33.8465
18	C	Isotropic =	177.3543	Anisotropy =	23.9764
19	C	Isotropic =	156.6959	Anisotropy =	16.0231
20	C	Isotropic =	120.9238	Anisotropy =	42.3927
21	O	Isotropic =	202.6816	Anisotropy =	113.6754
22	C	Isotropic =	32.1384	Anisotropy =	138.0778
23	C	Isotropic =	70.6321	Anisotropy =	171.0532
24	C	Isotropic =	43.9302	Anisotropy =	181.8747
25	N	Isotropic =	-37.6348	Anisotropy =	458.1397
26	C	Isotropic =	42.5530	Anisotropy =	159.8401
27	C	Isotropic =	91.3085	Anisotropy =	133.1777
28	C	Isotropic =	70.2063	Anisotropy =	174.4934
29	C	Isotropic =	67.8250	Anisotropy =	170.3756
30	C	Isotropic =	63.6307	Anisotropy =	174.4409
31	C	Isotropic =	63.8322	Anisotropy =	150.5145
32	C	Isotropic =	154.5293	Anisotropy =	45.7236
33	H	Isotropic =	24.0388	Anisotropy =	8.4395
34	H	Isotropic =	24.3838	Anisotropy =	4.1984
35	H	Isotropic =	23.2848	Anisotropy =	4.7845
36	H	Isotropic =	22.7440	Anisotropy =	7.6967
37	H	Isotropic =	23.4058	Anisotropy =	10.2200
38	H	Isotropic =	27.3707	Anisotropy =	5.7739
39	H	Isotropic =	27.1185	Anisotropy =	8.1878
40	H	Isotropic =	30.2546	Anisotropy =	11.0349
41	H	Isotropic =	30.0148	Anisotropy =	5.2260
42	H	Isotropic =	30.4012	Anisotropy =	8.2799
43	H	Isotropic =	28.1843	Anisotropy =	5.7017
44	H	Isotropic =	28.4238	Anisotropy =	7.9595
45	H	Isotropic =	27.4855	Anisotropy =	5.4504
46	H	Isotropic =	27.1707	Anisotropy =	6.0194
47	H	Isotropic =	22.8134	Anisotropy =	7.2688
48	H	Isotropic =	25.0168	Anisotropy =	9.4371
49	H	Isotropic =	23.0869	Anisotropy =	9.7552
50	H	Isotropic =	23.8407	Anisotropy =	6.5154
51	H	Isotropic =	23.6649	Anisotropy =	5.1402
52	H	Isotropic =	23.5678	Anisotropy =	5.7024
53	H	Isotropic =	28.8304	Anisotropy =	7.7186
54	H	Isotropic =	27.9533	Anisotropy =	10.1047
55	H	Isotropic =	27.4760	Anisotropy =	8.3866

Conformer 9

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.029965960902	-6.561047464971	-0.878084066455
C	-4.923350435259	-6.108428535427	0.373744786909
C	-5.869021536918	-5.228934956288	0.946431825331
C	-6.913855881837	-4.781176520003	0.129875397190
C	-7.014176675622	-5.242301110298	-1.183369747358
C	-6.058330669265	-6.150017120773	-1.633264714850
N	-5.836477282765	-4.878113089800	2.323251289638
C	-4.740905069863	-4.331645235931	2.953884365573
C	-3.388232731466	-4.436815674666	2.320356452971
C	-2.924066769187	-5.544994114818	1.570801264584
N	-3.805565586455	-6.555107546033	1.130126744869
O	-4.862790442442	-3.771434107753	4.044396510184
N	-1.626312484591	-5.702268872569	1.274682881761
C	-0.758599750308	-4.755369651705	1.647367991903
C	-1.107458470056	-3.581311993842	2.325219907134
C	-2.452484744549	-3.461943042024	2.683543322147
C	-3.219054614659	-7.857080400491	0.750602428411
C	-4.182969915649	-9.008491790423	1.023409233472
C	-0.084079730369	-2.523899743449	2.668466263790
C	-0.060836989567	-1.346399691076	1.697414547789
O	0.364787917785	-1.840779739984	0.416009833287
C	0.472426541362	-0.974750945350	-0.613395273226
C	0.909139676339	-1.534262386041	-1.860480609266
C	1.039451016331	-0.644665330837	-2.973804946151
N	0.767883386404	0.697960140283	-2.899645314264
C	0.368453729181	1.157260603613	-1.728063882170
C	0.200767268527	0.382537959967	-0.554100662833
C	1.211010493072	-2.912243301693	-2.023271737245
C	1.628521036843	-3.395915432014	-3.248260225340
C	1.759937607100	-2.520366626313	-4.354853562909
C	1.472236168211	-1.176728943076	-4.219535393845
C	-7.112905543457	-4.788396553487	3.043178218570
H	-7.658904352502	-4.091853757521	0.528428568757
H	-7.826189003578	-4.913957940503	-1.833244481588
H	-6.114256364576	-6.569527753329	-2.642316007522
H	0.289229381434	-4.944202002983	1.389254745909
H	-2.797155045652	-2.624512143538	3.293122373926
H	-2.908856075408	-7.851156409114	-0.306291938853

H	-2.311719736672	-7.971046935566	1.354179992116
H	-3.687472033237	-9.964636485774	0.790420940281
H	-4.486545072512	-9.026331118374	2.082488706793
H	-5.088574716234	-8.940160450320	0.402404086102
H	-0.290588644358	-2.111744427110	3.669179512218
H	0.922815603900	-2.968537664226	2.703758759010
H	0.646092928423	-0.575544926387	2.047046028609
H	-1.061161062928	-0.890433088873	1.601938683756
H	0.152338765626	2.230553692813	-1.674126951151
H	-0.133988791189	0.869603137602	0.359851792719
H	1.108087711900	-3.579670261617	-1.167644896958
H	1.858982799662	-4.456728905266	-3.366489638477
H	2.090958777702	-2.913384684211	-5.318738479198
H	1.566604972547	-0.484190995462	-5.058200456187
H	-7.806562199344	-5.529770369878	2.628101639445
H	-6.933080573614	-4.999715164413	4.103763587396
H	-7.561600825359	-3.784130128675	2.968090303293

SCF Done: E(RB3LYP) = -1390.83585583

Zero-point correction= 0.440824
Thermal correction to Energy= 0.467298
Thermal correction to Enthalpy= 0.468242
Thermal correction to Gibbs Free Energy= 0.380908
Sum of electronic and zero-point Energies= -1390.395032
Sum of electronic and thermal Energies= -1390.368558
Sum of electronic and thermal Enthalpies= -1390.367614
Sum of electronic and thermal Free Energies= -1390.454948

1	N	Isotropic =	-41.8429	Anisotropy =	469.3972
2	C	Isotropic =	38.9848	Anisotropy =	117.3210
3	C	Isotropic =	58.2949	Anisotropy =	123.9168
4	C	Isotropic =	62.5743	Anisotropy =	177.7256
5	C	Isotropic =	72.4587	Anisotropy =	159.7006
6	C	Isotropic =	49.5048	Anisotropy =	154.1875
7	N	Isotropic =	123.0569	Anisotropy =	92.0279
8	C	Isotropic =	26.8943	Anisotropy =	108.4734
9	C	Isotropic =	71.2570	Anisotropy =	132.3220
10	C	Isotropic =	32.3622	Anisotropy =	124.1544
11	N	Isotropic =	136.9934	Anisotropy =	64.1289
12	O	Isotropic =	-80.5241	Anisotropy =	581.3328
13	N	Isotropic =	-33.8587	Anisotropy =	439.1461
14	C	Isotropic =	40.5561	Anisotropy =	145.5435
15	C	Isotropic =	61.4847	Anisotropy =	171.2215

16	C	Isotropic =	51.9664	Anisotropy =	181.0766
17	C	Isotropic =	148.2021	Anisotropy =	34.0519
18	C	Isotropic =	177.4669	Anisotropy =	23.7989
19	C	Isotropic =	156.6955	Anisotropy =	16.1891
20	C	Isotropic =	121.0852	Anisotropy =	42.3428
21	O	Isotropic =	202.3146	Anisotropy =	113.5717
22	C	Isotropic =	32.2062	Anisotropy =	138.4999
23	C	Isotropic =	70.5333	Anisotropy =	170.7604
24	C	Isotropic =	44.0281	Anisotropy =	182.0278
25	N	Isotropic =	-37.5642	Anisotropy =	457.9908
26	C	Isotropic =	42.6533	Anisotropy =	159.5536
27	C	Isotropic =	91.2963	Anisotropy =	133.3251
28	C	Isotropic =	70.1704	Anisotropy =	174.4255
29	C	Isotropic =	67.6804	Anisotropy =	170.2688
30	C	Isotropic =	63.6240	Anisotropy =	174.8649
31	C	Isotropic =	63.8302	Anisotropy =	150.1991
32	C	Isotropic =	154.6309	Anisotropy =	45.6385
33	H	Isotropic =	24.0133	Anisotropy =	8.4249
34	H	Isotropic =	24.3814	Anisotropy =	4.2168
35	H	Isotropic =	23.2811	Anisotropy =	4.7360
36	H	Isotropic =	22.7478	Anisotropy =	7.7412
37	H	Isotropic =	23.3790	Anisotropy =	10.3038
38	H	Isotropic =	27.0832	Anisotropy =	8.1696
39	H	Isotropic =	27.3568	Anisotropy =	5.7102
40	H	Isotropic =	30.2375	Anisotropy =	11.0490
41	H	Isotropic =	30.3912	Anisotropy =	8.3265
42	H	Isotropic =	30.0055	Anisotropy =	5.2347
43	H	Isotropic =	28.4078	Anisotropy =	8.0043
44	H	Isotropic =	28.2104	Anisotropy =	5.6214
45	H	Isotropic =	27.1376	Anisotropy =	5.9493
46	H	Isotropic =	27.4883	Anisotropy =	5.5726
47	H	Isotropic =	22.8279	Anisotropy =	7.2338
48	H	Isotropic =	24.9876	Anisotropy =	9.4546
49	H	Isotropic =	23.1257	Anisotropy =	9.7058
50	H	Isotropic =	23.8488	Anisotropy =	6.5997
51	H	Isotropic =	23.6683	Anisotropy =	5.1916
52	H	Isotropic =	23.5902	Anisotropy =	5.6958
53	H	Isotropic =	28.8411	Anisotropy =	7.7323
54	H	Isotropic =	27.4673	Anisotropy =	8.3931
55	H	Isotropic =	27.9653	Anisotropy =	10.0862

Conformer 10

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.061929091323	-0.384538493469	0.495602212900
C	0.575172508056	-1.616111115454	0.552294258833
C	1.051286830032	-2.185253683315	1.754791487241
C	0.918465149298	-1.429495185007	2.925472516338
C	0.372083475219	-0.146812944238	2.865497566249
C	-0.020333561570	0.339368824830	1.620791248176
N	1.734213589651	-3.431565087122	1.782536167891
C	1.216469321941	-4.603161077940	1.276219002748
C	0.084811057177	-4.554896500898	0.297214576951
C	-0.095403225904	-3.556091148108	-0.690347515199
N	0.634566166602	-2.349086602440	-0.663245503709
O	1.692490821396	-5.690675751584	1.605518106720
N	-0.945932117254	-3.721462629866	-1.713271144228
C	-1.695363777097	-4.827911399498	-1.758201160110
C	-1.664405848343	-5.847381464154	-0.799412684880
C	-0.721284249193	-5.696051148330	0.219986828815
C	0.710680449071	-1.567957434094	-1.915712269293
C	1.593490787287	-2.255160999604	-2.954368474950
C	-2.572505145226	-7.051815828007	-0.887473186030
C	-3.785548429565	-6.982466079044	0.036226507722
O	-4.612189437829	-5.890700486259	-0.402346398979
C	-5.751670672294	-5.626643970822	0.271030709478
C	-6.534053974334	-4.531027515523	-0.225292387028
C	-7.750502482454	-4.223364647659	0.462750104041
N	-8.191694411496	-4.920164251889	1.558969614556
C	-7.431705012440	-5.917825184646	1.971409041679
C	-6.210276671682	-6.321531071794	1.378446488746
C	-6.150193544489	-3.758573295498	-1.353290651280
C	-6.943969567553	-2.714498392411	-1.787763312335
C	-8.149983970116	-2.404498514378	-1.111047816656
C	-8.542806340671	-3.142139080154	-0.011942126758
C	2.889322916456	-3.566443240339	2.678631429700
H	1.263723629888	-1.835112108048	3.876959382402
H	0.268158478758	0.461967742187	3.764419349314
H	-0.422600329305	1.351436559180	1.514922565932
H	-2.365332537103	-4.913042108481	-2.620791382203
H	-0.561876338628	-6.485372212101	0.957265932500
H	-0.296527449503	-1.386863246428	-2.321511579284
H	1.133474439990	-0.594293850699	-1.643220527898
H	2.608326804363	-2.423411658252	-2.559585420369
H	1.174576765254	-3.223718740178	-3.265093997583

H	1.672436100782	-1.618368568713	-3.850283698706
H	-2.926367131853	-7.183376664767	-1.921999740906
H	-2.015239843218	-7.963641148844	-0.618508826870
H	-3.478629256242	-6.814591645097	1.082806494018
H	-4.360665269389	-7.922085390153	-0.015213362446
H	-7.788843186863	-6.471549915071	2.847423333443
H	-5.665994186771	-7.162632089709	1.803699577784
H	-5.221075257858	-4.002552166130	-1.868506669280
H	-6.642748016777	-2.124311977956	-2.655760164241
H	-8.770028242982	-1.577059966805	-1.463162397024
H	-9.467662134898	-2.921126918560	0.524414560395
H	3.564166673662	-4.327169528714	2.269141494039
H	3.407190711368	-2.601256792539	2.736580130324
H	2.593265853324	-3.885322205406	3.691661709310

SCF Done: E(RB3LYP) = -1390.83586341

Zero-point correction= 0.440883
Thermal correction to Energy= 0.467335
Thermal correction to Enthalpy= 0.468279
Thermal correction to Gibbs Free Energy= 0.381269
Sum of electronic and zero-point Energies= -1390.394981
Sum of electronic and thermal Energies= -1390.368529
Sum of electronic and thermal Enthalpies= -1390.367585
Sum of electronic and thermal Free Energies= -1390.454595

1	N	Isotropic =	-40.4202	Anisotropy =	456.6648
2	C	Isotropic =	37.1246	Anisotropy =	121.1339
3	C	Isotropic =	59.9496	Anisotropy =	121.7421
4	C	Isotropic =	62.9314	Anisotropy =	177.2502
5	C	Isotropic =	72.5233	Anisotropy =	160.1260
6	C	Isotropic =	49.1979	Anisotropy =	154.8752
7	N	Isotropic =	123.0382	Anisotropy =	91.1832
8	C	Isotropic =	26.9758	Anisotropy =	108.6197
9	C	Isotropic =	70.1872	Anisotropy =	133.3419
10	C	Isotropic =	33.7544	Anisotropy =	123.5064
11	N	Isotropic =	136.3743	Anisotropy =	64.5419
12	O	Isotropic =	-81.3395	Anisotropy =	581.9355
13	N	Isotropic =	-34.5791	Anisotropy =	450.2042
14	C	Isotropic =	40.3881	Anisotropy =	144.4460
15	C	Isotropic =	61.4366	Anisotropy =	170.5705
16	C	Isotropic =	51.6326	Anisotropy =	182.0702
17	C	Isotropic =	147.4785	Anisotropy =	36.2868
18	C	Isotropic =	177.0688	Anisotropy =	23.9508

19	C	Isotropic =	156.7483	Anisotropy =	16.1622
20	C	Isotropic =	120.9321	Anisotropy =	42.1756
21	O	Isotropic =	201.9620	Anisotropy =	111.4633
22	C	Isotropic =	32.3310	Anisotropy =	138.7311
23	C	Isotropic =	70.6949	Anisotropy =	171.0438
24	C	Isotropic =	43.9373	Anisotropy =	181.6859
25	N	Isotropic =	-36.2114	Anisotropy =	462.3269
26	C	Isotropic =	42.7536	Anisotropy =	159.8350
27	C	Isotropic =	91.3781	Anisotropy =	132.9604
28	C	Isotropic =	70.1289	Anisotropy =	172.5313
29	C	Isotropic =	67.5441	Anisotropy =	170.0265
30	C	Isotropic =	63.4207	Anisotropy =	175.4524
31	C	Isotropic =	63.9121	Anisotropy =	151.3792
32	C	Isotropic =	154.4695	Anisotropy =	45.6001
33	H	Isotropic =	24.0690	Anisotropy =	8.5035
34	H	Isotropic =	24.4055	Anisotropy =	4.2057
35	H	Isotropic =	23.3163	Anisotropy =	4.7535
36	H	Isotropic =	22.7517	Anisotropy =	7.8034
37	H	Isotropic =	23.3363	Anisotropy =	10.2493
38	H	Isotropic =	26.9287	Anisotropy =	7.8255
39	H	Isotropic =	27.5606	Anisotropy =	5.9599
40	H	Isotropic =	30.3677	Anisotropy =	8.4054
41	H	Isotropic =	29.8259	Anisotropy =	4.8127
42	H	Isotropic =	30.2535	Anisotropy =	10.9387
43	H	Isotropic =	28.1983	Anisotropy =	5.6310
44	H	Isotropic =	28.3619	Anisotropy =	8.0236
45	H	Isotropic =	27.4620	Anisotropy =	5.4885
46	H	Isotropic =	27.1242	Anisotropy =	5.9823
47	H	Isotropic =	22.8089	Anisotropy =	7.2736
48	H	Isotropic =	24.9818	Anisotropy =	9.4785
49	H	Isotropic =	23.2061	Anisotropy =	9.6420
50	H	Isotropic =	23.8650	Anisotropy =	6.6502
51	H	Isotropic =	23.6455	Anisotropy =	5.2321
52	H	Isotropic =	23.5411	Anisotropy =	5.7613
53	H	Isotropic =	27.4813	Anisotropy =	8.3645
54	H	Isotropic =	28.8334	Anisotropy =	7.8937
55	H	Isotropic =	27.9705	Anisotropy =	10.0694

Conformer 11

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.106964320693	-2.027118554736	-2.193591446106
C	-3.807986892215	-2.000548958345	-2.502763262784
C	-3.269013365447	-2.741287246415	-3.578547726471
C	-4.140716738065	-3.568591713994	-4.295983270704
C	-5.495806083053	-3.602779728615	-3.964374235899
C	-5.933508449515	-2.794259627829	-2.918221312064
N	-1.919589886724	-2.590036982843	-3.999002418081
C	-0.834080466770	-2.757485668389	-3.168107336784
C	-1.016466900103	-2.688768207233	-1.683810754095
C	-1.931374406087	-1.840454970292	-1.014138009231
N	-2.969256645611	-1.178908154053	-1.703028028017
O	0.290519587398	-2.938369904548	-3.637445355291
N	-1.837439186390	-1.602542511390	0.302179286050
C	-0.903597494732	-2.245451897812	1.010619985245
C	-0.000083446362	-3.172409938237	0.476655253144
C	-0.059424900248	-3.351841818230	-0.907205350008
C	-3.601002258481	-0.019026781831	-1.039606894071
C	-2.661843070766	1.183476126862	-0.990667953791
C	0.992205939374	-3.911908126072	1.343479033423
C	0.517374607732	-5.297660579483	1.773765758137
O	-0.623186777182	-5.123789582615	2.631934209929
C	-1.243969326259	-6.217048951948	3.122450838776
C	-2.363712593870	-5.967959246813	3.984447810626
C	-3.049285723058	-7.103534106264	4.521196172232
N	-2.685771277929	-8.398445774797	4.251298966402
C	-1.646553863314	-8.567786864364	3.454694062046
C	-0.886590758687	-7.529932289614	2.861480878051
C	-2.804159503697	-4.659600156760	4.317017100408
C	-3.889352470850	-4.479214286762	5.152851309362
C	-4.573690538940	-5.599432915886	5.686818479899
C	-4.162408080122	-6.880737329792	5.377704190323
C	-1.641127111081	-2.589532223751	-5.440358538174
H	-3.763084495617	-4.165166777651	-5.126941456584
H	-6.193607311185	-4.233181352684	-4.516786832381
H	-6.991494253969	-2.758681867474	-2.641236368834
H	-0.867354496131	-2.003047091703	2.078267829067
H	0.668396834909	-3.982859775397	-1.420773545461
H	-4.492956814226	0.220730115170	-1.629478402017
H	-3.939157723782	-0.287942380252	-0.026996783296
H	-3.189106582232	2.044360355028	-0.548707986009
H	-1.773742576431	0.979668733967	-0.374351514567
H	-2.328802820734	1.464979161025	-2.002516695612
H	1.938941402471	-4.049883673367	0.797441867880
H	1.221747763822	-3.324255185003	2.246228418483

H	1.313860423745	-5.824380145187	2.325694484590
H	0.232244250803	-5.906444249179	0.898808284172
H	-1.359367826300	-9.604308415221	3.243157335488
H	-0.046432737423	-7.787794365163	2.219270671516
H	-2.272556012947	-3.802557658006	3.903541015027
H	-4.222701910825	-3.470261897898	5.404517247044
H	-5.430473273004	-5.445312890765	6.346559836750
H	-4.674017098464	-7.757999095676	5.778302618181
H	-1.488326276637	-3.607865571020	-5.834298450827
H	-2.482604037231	-2.118564055017	-5.963206255156
H	-0.723632026869	-2.016962945672	-5.619746759939

SCF Done: E(RB3LYP) = -1390.83590875

Zero-point correction= 0.440889
Thermal correction to Energy= 0.467329
Thermal correction to Enthalpy= 0.468273
Thermal correction to Gibbs Free Energy= 0.381531
Sum of electronic and zero-point Energies= -1390.395020
Sum of electronic and thermal Energies= -1390.368580
Sum of electronic and thermal Enthalpies= -1390.367636
Sum of electronic and thermal Free Energies= -1390.454377

1	N	Isotropic =	-40.6051	Anisotropy =	455.8673
2	C	Isotropic =	36.9192	Anisotropy =	120.7332
3	C	Isotropic =	59.9397	Anisotropy =	121.9467
4	C	Isotropic =	62.9658	Anisotropy =	177.1609
5	C	Isotropic =	72.4769	Anisotropy =	160.1982
6	C	Isotropic =	49.2308	Anisotropy =	154.8713
7	N	Isotropic =	123.3845	Anisotropy =	91.7882
8	C	Isotropic =	26.8996	Anisotropy =	108.4583
9	C	Isotropic =	70.3584	Anisotropy =	132.9535
10	C	Isotropic =	33.7015	Anisotropy =	123.5711
11	N	Isotropic =	135.8495	Anisotropy =	64.5381
12	O	Isotropic =	-81.2467	Anisotropy =	581.9163
13	N	Isotropic =	-33.9776	Anisotropy =	450.6944
14	C	Isotropic =	40.3714	Anisotropy =	145.9233
15	C	Isotropic =	61.4763	Anisotropy =	170.9958
16	C	Isotropic =	51.4860	Anisotropy =	180.5717
17	C	Isotropic =	147.1470	Anisotropy =	36.2485
18	C	Isotropic =	177.0542	Anisotropy =	24.0754
19	C	Isotropic =	156.5359	Anisotropy =	16.2010
20	C	Isotropic =	121.0016	Anisotropy =	42.5130
21	O	Isotropic =	202.5683	Anisotropy =	113.4523

22	C	Isotropic =	32.2294	Anisotropy =	138.1932
23	C	Isotropic =	70.5409	Anisotropy =	170.9130
24	C	Isotropic =	44.0258	Anisotropy =	181.9498
25	N	Isotropic =	-37.8516	Anisotropy =	457.3502
26	C	Isotropic =	42.5585	Anisotropy =	159.3208
27	C	Isotropic =	91.1967	Anisotropy =	133.1950
28	C	Isotropic =	70.0910	Anisotropy =	174.1032
29	C	Isotropic =	67.6744	Anisotropy =	170.5636
30	C	Isotropic =	63.6524	Anisotropy =	175.0953
31	C	Isotropic =	63.7967	Anisotropy =	150.2945
32	C	Isotropic =	154.6579	Anisotropy =	45.5937
33	H	Isotropic =	24.0747	Anisotropy =	8.4759
34	H	Isotropic =	24.3811	Anisotropy =	4.2227
35	H	Isotropic =	23.3099	Anisotropy =	4.8181
36	H	Isotropic =	22.7029	Anisotropy =	7.8341
37	H	Isotropic =	23.3700	Anisotropy =	10.1675
38	H	Isotropic =	27.5436	Anisotropy =	5.9417
39	H	Isotropic =	26.9492	Anisotropy =	7.8171
40	H	Isotropic =	30.2459	Anisotropy =	10.9341
41	H	Isotropic =	29.7818	Anisotropy =	4.8265
42	H	Isotropic =	30.3586	Anisotropy =	8.3964
43	H	Isotropic =	28.4300	Anisotropy =	7.9514
44	H	Isotropic =	28.1599	Anisotropy =	5.6457
45	H	Isotropic =	27.1644	Anisotropy =	6.0574
46	H	Isotropic =	27.5030	Anisotropy =	5.4665
47	H	Isotropic =	22.8448	Anisotropy =	7.2301
48	H	Isotropic =	25.0197	Anisotropy =	9.4266
49	H	Isotropic =	23.0702	Anisotropy =	9.7383
50	H	Isotropic =	23.8090	Anisotropy =	6.6119
51	H	Isotropic =	23.6384	Anisotropy =	5.1844
52	H	Isotropic =	23.5729	Anisotropy =	5.6976
53	H	Isotropic =	27.9706	Anisotropy =	10.0942
54	H	Isotropic =	28.8374	Anisotropy =	7.8793
55	H	Isotropic =	27.4759	Anisotropy =	8.3431

Conformer 12

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.563764063877	-6.786612258562	-2.308123789523
C	-3.495650923187	-5.832680970820	-2.239194735166
C	-4.768822330269	-6.054114279127	-1.668558204536

C	-5.015853506829	-7.311370075839	-1.105385179752
C	-4.034458143084	-8.301802411068	-1.163099216537
C	-2.831920335719	-7.995962125920	-1.796006896407
N	-5.805657553393	-5.084439777668	-1.737723498712
C	-5.677930991373	-3.787343725480	-1.292565836360
C	-4.315187767550	-3.210577255976	-1.064031847155
C	-3.170467656564	-3.492169826779	-1.848562249898
N	-3.159082061227	-4.558562547739	-2.773168051944
O	-6.676236586766	-3.092686377283	-1.095708566737
N	-2.061509550205	-2.743683460423	-1.773212400852
C	-2.017115911411	-1.741969448328	-0.887944227304
C	-3.054604870966	-1.414124032369	-0.007356515809
C	-4.227889666118	-2.160456384741	-0.143444226950
C	-2.133537973008	-4.528434370892	-3.836283820070
C	-2.619040602183	-5.224130758259	-5.104807602434
C	-2.916946990163	-0.305164630515	1.009879980082
C	-2.591110592037	-0.796902069780	2.417663467329
O	-1.292995851575	-1.413877372126	2.378845032669
C	-0.787559384703	-1.940386606674	3.514080126121
C	0.508984145151	-2.544802129583	3.401314703920
C	1.078250153410	-3.112978687906	4.584858725966
N	0.446237385135	-3.104005167111	5.802407161314
C	-0.744164888591	-2.534800004350	5.847148634806
C	-1.413525339751	-1.938938970868	4.750031934661
C	1.230362944458	-2.597695836579	2.179411909087
C	2.475775671636	-3.193696041172	2.128683442983
C	3.045664805063	-3.757983251982	3.297133751126
C	2.362303674470	-3.717655827918	4.496251051955
C	-7.173294987429	-5.552823641118	-1.994355925552
H	-5.980777315628	-7.520303420949	-0.642528475825
H	-4.209565840530	-9.291242577018	-0.738973118882
H	-2.045253833932	-8.749434465494	-1.899826335469
H	-1.090423149451	-1.157826331661	-0.878886765157
H	-5.118455886149	-1.914252196261	0.437916377093
H	-1.934275115023	-3.469778360999	-4.037529702281
H	-1.190844729459	-4.975127413043	-3.482169504129
H	-1.859196038719	-5.117467616562	-5.895502369546
H	-2.786712607016	-6.299309473309	-4.943142062190
H	-3.558297554051	-4.774837982558	-5.465524757425
H	-2.134144600417	0.402441290743	0.694811494019
H	-3.858566446201	0.263017531069	1.077449492338
H	-3.337631171279	-1.532514059081	2.763103238789
H	-2.575758448842	0.048572752047	3.125705592604
H	-1.245114804785	-2.530317771815	6.822145630211

H	-2.396198469017	-1.497266760419	4.904386748946
H	0.785013715377	-2.161896903269	1.285048888694
H	3.025034841467	-3.231217051626	1.185639276952
H	4.031018079428	-4.226516801442	3.245800408172
H	2.782264051720	-4.145639377695	5.408552299512
H	-7.733163662998	-4.748234908923	-2.485247507250
H	-7.130014179135	-6.430842330731	-2.650397139594
H	-7.702817086704	-5.815985446048	-1.063838839900

SCF Done: E(RB3LYP) = -1390.83588946

Zero-point correction= 0.440831
Thermal correction to Energy= 0.467305
Thermal correction to Enthalpy= 0.468249
Thermal correction to Gibbs Free Energy= 0.381245
Sum of electronic and zero-point Energies= -1390.395059
Sum of electronic and thermal Energies= -1390.368584
Sum of electronic and thermal Enthalpies= -1390.367640
Sum of electronic and thermal Free Energies= -1390.454644

1	N	Isotropic =	-42.5073	Anisotropy =	469.2599
2	C	Isotropic =	38.7432	Anisotropy =	117.7081
3	C	Isotropic =	59.0416	Anisotropy =	123.7523
4	C	Isotropic =	62.7919	Anisotropy =	177.4253
5	C	Isotropic =	72.6682	Anisotropy =	160.4637
6	C	Isotropic =	49.1171	Anisotropy =	154.3373
7	N	Isotropic =	123.0499	Anisotropy =	92.3038
8	C	Isotropic =	26.7509	Anisotropy =	108.3085
9	C	Isotropic =	71.1160	Anisotropy =	132.1932
10	C	Isotropic =	32.2430	Anisotropy =	123.6600
11	N	Isotropic =	137.3154	Anisotropy =	64.1540
12	O	Isotropic =	-80.4556	Anisotropy =	581.3357
13	N	Isotropic =	-33.8809	Anisotropy =	439.8141
14	C	Isotropic =	40.5550	Anisotropy =	145.9212
15	C	Isotropic =	61.4352	Anisotropy =	171.6005
16	C	Isotropic =	51.9881	Anisotropy =	181.0154
17	C	Isotropic =	148.3034	Anisotropy =	33.7509
18	C	Isotropic =	177.4555	Anisotropy =	23.8197
19	C	Isotropic =	156.9421	Anisotropy =	16.0831
20	C	Isotropic =	121.1016	Anisotropy =	42.2475
21	O	Isotropic =	202.6520	Anisotropy =	114.4369
22	C	Isotropic =	32.2258	Anisotropy =	138.3428
23	C	Isotropic =	70.4661	Anisotropy =	170.6314
24	C	Isotropic =	43.9424	Anisotropy =	182.0384

25	N	Isotropic =	-37.9037	Anisotropy =	456.9592
26	C	Isotropic =	42.6185	Anisotropy =	159.7262
27	C	Isotropic =	91.2690	Anisotropy =	133.1297
28	C	Isotropic =	70.3858	Anisotropy =	174.6751
29	C	Isotropic =	67.7526	Anisotropy =	170.4431
30	C	Isotropic =	63.6343	Anisotropy =	175.1186
31	C	Isotropic =	63.7650	Anisotropy =	149.8291
32	C	Isotropic =	154.6915	Anisotropy =	45.6152
33	H	Isotropic =	24.0400	Anisotropy =	8.3913
34	H	Isotropic =	24.3637	Anisotropy =	4.2299
35	H	Isotropic =	23.2761	Anisotropy =	4.7266
36	H	Isotropic =	22.7607	Anisotropy =	7.7366
37	H	Isotropic =	23.3918	Anisotropy =	10.2776
38	H	Isotropic =	27.4090	Anisotropy =	5.6000
39	H	Isotropic =	27.1172	Anisotropy =	8.1781
40	H	Isotropic =	30.2434	Anisotropy =	11.0259
41	H	Isotropic =	29.9766	Anisotropy =	5.2580
42	H	Isotropic =	30.4043	Anisotropy =	8.3569
43	H	Isotropic =	28.2221	Anisotropy =	5.7016
44	H	Isotropic =	28.4090	Anisotropy =	8.0279
45	H	Isotropic =	27.4886	Anisotropy =	5.4897
46	H	Isotropic =	27.1254	Anisotropy =	6.0054
47	H	Isotropic =	22.8316	Anisotropy =	7.2341
48	H	Isotropic =	25.0065	Anisotropy =	9.4440
49	H	Isotropic =	23.1457	Anisotropy =	9.6864
50	H	Isotropic =	23.8606	Anisotropy =	6.5975
51	H	Isotropic =	23.6755	Anisotropy =	5.1850
52	H	Isotropic =	23.6105	Anisotropy =	5.6568
53	H	Isotropic =	27.4350	Anisotropy =	8.4051
54	H	Isotropic =	28.8356	Anisotropy =	7.7747
55	H	Isotropic =	27.9618	Anisotropy =	10.1125

Conformer 13

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.753325362066	-6.110828361757	3.376641877493
C	-1.954177468404	-6.455323088878	2.363661310239
C	-0.546468027405	-6.474364245479	2.480198506894
C	0.008584754053	-6.049255315115	3.692784062553
C	-0.827983769849	-5.673148688649	4.744418663624
C	-2.204379189948	-5.743962525766	4.543109662097

N	0.289131558828	-6.993493199964	1.454587852187
C	0.265436329155	-6.558485186014	0.148213147604
C	-0.914210763928	-5.787623795521	-0.357869472900
C	-2.258663414039	-6.009695936060	0.027435663336
N	-2.580772411103	-6.816258059034	1.139591604286
O	1.200607000840	-6.813335967527	-0.612319153472
N	-3.284528078693	-5.492592783560	-0.663045044438
C	-3.026398038070	-4.694961026825	-1.704983004698
C	-1.741865870875	-4.338525324490	-2.132508019863
C	-0.683550259421	-4.938784695592	-1.446150257262
C	-3.957045346321	-7.347497935679	1.224589850166
C	-3.993843989943	-8.699604569772	1.931343943040
C	-1.518386187151	-3.380008769471	-3.278958803245
C	-1.256177872557	-1.942488645472	-2.836784591685
O	-2.454487780507	-1.448821676001	-2.213849490018
C	-2.461959429043	-0.193700857490	-1.717871181831
C	-3.694643805281	0.238865127644	-1.124401857848
C	-3.739593486367	1.564598207761	-0.587516789107
N	-2.671061493440	2.424438120485	-0.616213996135
C	-1.563231943597	1.973478857094	-1.175306074410
C	-1.392211626927	0.686356309302	-1.741500873048
C	-4.847677727454	-0.586874869152	-1.054395761916
C	-6.009178150414	-0.117065387496	-0.472178883679
C	-6.060453412695	1.194612546158	0.061842047878
C	-4.951374648638	2.015057305441	0.004934682222
C	1.453178465159	-7.795311924507	1.851695906580
H	1.091479282494	-6.034801091638	3.819975874309
H	-0.416462249181	-5.348586418384	5.700897664191
H	-2.902599243058	-5.496495535672	5.348430172901
H	-3.903458753066	-4.312022452157	-2.237965390370
H	0.348374546300	-4.791918848643	-1.770506970218
H	-4.622134751967	-6.627534122266	1.727193238540
H	-4.309974330352	-7.448446546893	0.192248220168
H	-5.023127054482	-9.092592685923	1.918705868893
H	-3.340110401548	-9.427523598322	1.424557128704
H	-3.678097430341	-8.620243217659	2.982259853642
H	-0.646197680042	-3.699276889544	-3.871500435932
H	-2.388119072748	-3.385541132920	-3.954623820373
H	-1.008438527616	-1.311253583916	-3.706686085250
H	-0.420552039333	-1.895989680094	-2.117703535080
H	-0.712503156513	2.664417439809	-1.196138070041
H	-0.430931666644	0.421587754361	-2.177967978885
H	-4.801078162193	-1.594675478557	-1.466977684941
H	-6.892344705792	-0.757318338466	-0.422003417229

H	-6.983755099081	1.555892557831	0.520209570851
H	-4.968590309320	3.028826041450	0.409632987893
H	2.343538768075	-7.171125861122	2.033784441032
H	1.205516351530	-8.352251733288	2.763592069643
H	1.690467130978	-8.494420216599	1.041290772909

SCF Done: E(RB3LYP) = -1390.83589956

Zero-point correction= 0.440965
Thermal correction to Energy= 0.467399
Thermal correction to Enthalpy= 0.468343
Thermal correction to Gibbs Free Energy= 0.381145
Sum of electronic and zero-point Energies= -1390.394934
Sum of electronic and thermal Energies= -1390.368500
Sum of electronic and thermal Enthalpies= -1390.367556
Sum of electronic and thermal Free Energies= -1390.454754

1	N	Isotropic =	-42.0956	Anisotropy =	469.1143
2	C	Isotropic =	38.5554	Anisotropy =	117.9182
3	C	Isotropic =	58.6021	Anisotropy =	123.5531
4	C	Isotropic =	63.0770	Anisotropy =	177.1545
5	C	Isotropic =	72.6882	Anisotropy =	159.7566
6	C	Isotropic =	49.1804	Anisotropy =	154.5273
7	N	Isotropic =	122.8407	Anisotropy =	92.3418
8	C	Isotropic =	26.8689	Anisotropy =	108.6584
9	C	Isotropic =	71.3302	Anisotropy =	132.2836
10	C	Isotropic =	32.5383	Anisotropy =	123.6476
11	N	Isotropic =	136.8694	Anisotropy =	64.2406
12	O	Isotropic =	-80.8998	Anisotropy =	580.5912
13	N	Isotropic =	-33.7723	Anisotropy =	439.0788
14	C	Isotropic =	40.5557	Anisotropy =	145.8527
15	C	Isotropic =	61.3714	Anisotropy =	171.2819
16	C	Isotropic =	52.2176	Anisotropy =	179.8613
17	C	Isotropic =	148.5878	Anisotropy =	33.9940
18	C	Isotropic =	177.2952	Anisotropy =	24.0132
19	C	Isotropic =	156.6998	Anisotropy =	16.1658
20	C	Isotropic =	120.8718	Anisotropy =	42.0218
21	O	Isotropic =	202.2815	Anisotropy =	112.0985
22	C	Isotropic =	32.2212	Anisotropy =	138.4676
23	C	Isotropic =	70.5370	Anisotropy =	170.8379
24	C	Isotropic =	43.9754	Anisotropy =	181.8778
25	N	Isotropic =	-37.5332	Anisotropy =	458.2334
26	C	Isotropic =	42.5767	Anisotropy =	159.6969
27	C	Isotropic =	91.2269	Anisotropy =	133.4819

28	C	Isotropic =	70.1541	Anisotropy =	174.5719
29	C	Isotropic =	67.6662	Anisotropy =	170.2835
30	C	Isotropic =	63.5654	Anisotropy =	174.4337
31	C	Isotropic =	63.8368	Anisotropy =	150.3379
32	C	Isotropic =	154.5787	Anisotropy =	45.5938
33	H	Isotropic =	24.0478	Anisotropy =	8.4164
34	H	Isotropic =	24.3865	Anisotropy =	4.1912
35	H	Isotropic =	23.2841	Anisotropy =	4.7617
36	H	Isotropic =	22.7413	Anisotropy =	7.7106
37	H	Isotropic =	23.3818	Anisotropy =	10.2439
38	H	Isotropic =	27.1206	Anisotropy =	8.1919
39	H	Isotropic =	27.3522	Anisotropy =	5.7725
40	H	Isotropic =	30.2532	Anisotropy =	11.0289
41	H	Isotropic =	30.4027	Anisotropy =	8.2947
42	H	Isotropic =	30.0437	Anisotropy =	5.1800
43	H	Isotropic =	28.4130	Anisotropy =	7.9891
44	H	Isotropic =	28.1915	Anisotropy =	5.6307
45	H	Isotropic =	27.1500	Anisotropy =	6.0223
46	H	Isotropic =	27.4851	Anisotropy =	5.4748
47	H	Isotropic =	22.8231	Anisotropy =	7.2479
48	H	Isotropic =	24.9808	Anisotropy =	9.4780
49	H	Isotropic =	23.0860	Anisotropy =	9.7361
50	H	Isotropic =	23.8358	Anisotropy =	6.5392
51	H	Isotropic =	23.6716	Anisotropy =	5.1489
52	H	Isotropic =	23.5876	Anisotropy =	5.6803
53	H	Isotropic =	27.9640	Anisotropy =	10.0972
54	H	Isotropic =	28.8597	Anisotropy =	7.6868
55	H	Isotropic =	27.4809	Anisotropy =	8.3444

Conformer 14

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-0.247163983055	-0.783527189095	1.962860352513
C	0.093862155135	-1.247055778045	0.757705937647
C	1.279164318005	-1.983381854225	0.535936078172
C	2.079916868680	-2.271247604079	1.647274882173
C	1.716223264358	-1.794599418906	2.907357688185
C	0.553449393219	-1.034660377783	3.008180663327
N	1.713549542826	-2.341728404529	-0.769137449161
C	0.946269387918	-3.053780159480	-1.664146868756
C	-0.537187598885	-3.128700696872	-1.476629599162

C	-1.347535225509	-2.084064368196	-0.969417458223
N	-0.790093036584	-0.963572365049	-0.318214376052
O	1.468385485759	-3.609890728393	-2.631540207553
N	-2.681100137639	-2.096252624159	-1.108190331172
C	-3.263269330219	-3.160700273787	-1.669670553544
C	-2.576369587449	-4.290991356359	-2.129160031376
C	-1.183210450819	-4.230155660998	-2.049460496359
C	-1.633473264055	0.243856325575	-0.191496535103
C	-1.835581702389	0.936133164151	-1.536898640688
C	-3.300478484391	-5.489084038265	-2.697836209884
C	-3.524558782677	-6.609055420668	-1.684960851617
O	-4.413137820596	-6.111732489014	-0.669674922789
C	-4.749714690651	-6.922459497045	0.355544911982
C	-5.644738668151	-6.364878886972	1.328563551314
C	-6.023656959475	-7.196079835628	2.430174778248
N	-5.573904144192	-8.481958283370	2.591899414566
C	-4.753190684162	-8.942823964932	1.666018694862
C	-4.304971631787	-8.222760485962	0.531524954322
C	-6.157004689212	-5.043814434141	1.236396222320
C	-7.016853881326	-4.558850683050	2.202936315426
C	-7.396141745770	-5.376541374883	3.296550116633
C	-6.910374167903	-6.664316205148	3.406506944461
C	3.148439245098	-2.255655081494	-1.067899960250
H	2.997204817246	-2.847112159437	1.521485399573
H	2.331000606245	-1.999747054764	3.784547397278
H	0.242420165123	-0.609214798923	3.967125301051
H	-4.353294842051	-3.109550742667	-1.765816538280
H	-0.564136083835	-5.024438808699	-2.470941907175
H	-2.603325714521	-0.007119684826	0.265032356755
H	-1.108915124464	0.910523414261	0.502263714773
H	-2.419375389091	1.859371220873	-1.391094046259
H	-0.868764958746	1.207450293882	-1.990425838605
H	-2.386151794205	0.297224555443	-2.242982557564
H	-4.277357233209	-5.184995687008	-3.105484894333
H	-2.721394339265	-5.918456319988	-3.530776341456
H	-2.572822220833	-6.920145884669	-1.221399894974
H	-3.981219378391	-7.485432817945	-2.174678291491
H	-4.396980525378	-9.970868746023	1.799479961673
H	-3.626631317810	-8.705519460904	-0.169524570684
H	-5.860891968647	-4.420850355483	0.392423352067
H	-7.406840467084	-3.541785863502	2.126124772785
H	-8.076532532727	-4.983205056942	4.055145518151
H	-7.189235241419	-7.311473571146	4.240314317422
H	3.683392860936	-3.183416302723	-0.805946053089

H	3.273113832071	-2.086740814285	-2.143889751540
H	3.577357855955	-1.416475303727	-0.506708420538

SCF Done: E(RB3LYP) = -1390.83591438

Zero-point correction= 0.440933
Thermal correction to Energy= 0.467364
Thermal correction to Enthalpy= 0.468308
Thermal correction to Gibbs Free Energy= 0.381573
Sum of electronic and zero-point Energies= -1390.394981
Sum of electronic and thermal Energies= -1390.368550
Sum of electronic and thermal Enthalpies= -1390.367606
Sum of electronic and thermal Free Energies= -1390.454342

1	N	Isotropic =	-40.6957	Anisotropy =	456.0428
2	C	Isotropic =	36.9682	Anisotropy =	121.0077
3	C	Isotropic =	59.9616	Anisotropy =	121.5552
4	C	Isotropic =	62.8038	Anisotropy =	177.3441
5	C	Isotropic =	72.4328	Anisotropy =	160.1051
6	C	Isotropic =	49.2012	Anisotropy =	154.7634
7	N	Isotropic =	123.3855	Anisotropy =	91.5475
8	C	Isotropic =	26.8984	Anisotropy =	108.5244
9	C	Isotropic =	70.2990	Anisotropy =	132.6489
10	C	Isotropic =	33.7072	Anisotropy =	123.4256
11	N	Isotropic =	135.9315	Anisotropy =	64.5879
12	O	Isotropic =	-81.6507	Anisotropy =	581.6121
13	N	Isotropic =	-33.9695	Anisotropy =	450.6853
14	C	Isotropic =	40.4170	Anisotropy =	145.8698
15	C	Isotropic =	61.4474	Anisotropy =	170.6487
16	C	Isotropic =	51.5556	Anisotropy =	180.5005
17	C	Isotropic =	147.3997	Anisotropy =	36.0769
18	C	Isotropic =	177.0896	Anisotropy =	23.9304
19	C	Isotropic =	156.6342	Anisotropy =	16.4245
20	C	Isotropic =	121.1681	Anisotropy =	42.2294
21	O	Isotropic =	202.6791	Anisotropy =	112.7120
22	C	Isotropic =	32.2820	Anisotropy =	138.9292
23	C	Isotropic =	70.5413	Anisotropy =	170.8098
24	C	Isotropic =	43.9085	Anisotropy =	181.9198
25	N	Isotropic =	-36.7604	Anisotropy =	460.0349
26	C	Isotropic =	42.5726	Anisotropy =	160.2886
27	C	Isotropic =	91.1993	Anisotropy =	133.3955
28	C	Isotropic =	69.9821	Anisotropy =	174.2439
29	C	Isotropic =	67.8804	Anisotropy =	170.0239
30	C	Isotropic =	63.9036	Anisotropy =	174.6258

31	C	Isotropic =	64.1657	Anisotropy =	150.1297
32	C	Isotropic =	154.5810	Anisotropy =	45.6066
33	H	Isotropic =	24.0570	Anisotropy =	8.5209
34	H	Isotropic =	24.3845	Anisotropy =	4.2223
35	H	Isotropic =	23.3184	Anisotropy =	4.7874
36	H	Isotropic =	22.7091	Anisotropy =	7.8432
37	H	Isotropic =	23.3873	Anisotropy =	10.1421
38	H	Isotropic =	26.9581	Anisotropy =	7.8600
39	H	Isotropic =	27.5493	Anisotropy =	5.9376
40	H	Isotropic =	30.2453	Anisotropy =	10.9161
41	H	Isotropic =	30.3632	Anisotropy =	8.4408
42	H	Isotropic =	29.7852	Anisotropy =	4.8000
43	H	Isotropic =	28.1752	Anisotropy =	5.6589
44	H	Isotropic =	28.4190	Anisotropy =	7.9679
45	H	Isotropic =	27.5200	Anisotropy =	5.4999
46	H	Isotropic =	27.1540	Anisotropy =	6.0417
47	H	Isotropic =	22.8096	Anisotropy =	7.2580
48	H	Isotropic =	25.0079	Anisotropy =	9.4575
49	H	Isotropic =	23.0846	Anisotropy =	9.7056
50	H	Isotropic =	23.8321	Anisotropy =	6.6119
51	H	Isotropic =	23.6632	Anisotropy =	5.1585
52	H	Isotropic =	23.5831	Anisotropy =	5.6788
53	H	Isotropic =	27.9636	Anisotropy =	10.1019
54	H	Isotropic =	27.4863	Anisotropy =	8.3593
55	H	Isotropic =	28.8319	Anisotropy =	7.8974

Conformer 15

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.980613750470	-5.165479251862	3.896887607481
C	-1.814155875144	-5.346917457023	3.272349430388
C	-0.640753923721	-4.649970711548	3.638908543599
C	-0.746122856965	-3.697070592318	4.658706108544
C	-1.968798021031	-3.500954532995	5.302197967974
C	-3.051628239680	-4.278837652529	4.899745785781
N	0.628930477918	-4.960810453184	3.080394538408
C	0.894367298222	-4.965273777248	1.729204864379
C	-0.235914772544	-5.041669750714	0.750202215039
C	-1.431210099175	-5.775900354786	0.943146899154
N	-1.788303385014	-6.288350181330	2.208710124707
O	2.055640012824	-4.928005146238	1.319503331448

N	-2.265411503729	-6.043587544485	-0.071305699214
C	-1.996850522259	-5.537725182730	-1.279707058351
C	-0.891238943668	-4.731833720305	-1.575193897677
C	0.008519630259	-4.524638878202	-0.526687345860
C	-2.790591043065	-7.373913987501	2.248609907067
C	-2.224496488443	-8.683978615719	1.706672283417
C	-0.672471699026	-4.150023530121	-2.952564459544
C	-1.054446129950	-2.676778587835	-3.066496534896
O	-2.471892115174	-2.571716830724	-2.849043517813
C	-3.046317435568	-1.350834340709	-2.876796767095
C	-4.462133543601	-1.318982916229	-2.645930649929
C	-5.106171931294	-0.041223306894	-2.666646293218
N	-4.437421407939	1.134590847688	-2.895181060672
C	-3.136603783712	1.044908223081	-3.102673910986
C	-2.384650231830	-0.155569463819	-3.107170053655
C	-5.229259067131	-2.488699529957	-2.401878726223
C	-6.590673312753	-2.398519147629	-2.184456747036
C	-7.234795817887	-1.136292188317	-2.203015155526
C	-6.508785384118	0.014265424397	-2.438852174624
C	1.795408871123	-4.956203120608	3.971909905608
H	0.132453482313	-3.127743915214	4.963597570275
H	-2.069898487246	-2.770328909285	6.105601036494
H	-4.022698963543	-4.188675245458	5.395941287897
H	-2.709516321412	-5.795380898537	-2.070934209074
H	0.945030454702	-3.988159170582	-0.690269812178
H	-3.072203364678	-7.490160593326	3.301289255660
H	-3.697723216327	-7.085140833681	1.695717271834
H	-1.964619918541	-8.603778135044	0.640780603758
H	-1.323393328311	-8.984500583878	2.264960497383
H	-2.977686734875	-9.481609595005	1.811236716587
H	0.390806704313	-4.229154652558	-3.230867659806
H	-1.245052344190	-4.721404479735	-3.699796771301
H	-0.806652043865	-2.291454938669	-4.069739331468
H	-0.520889379384	-2.069958392221	-2.315031712464
H	-2.606877006233	1.987034117438	-3.285368242618
H	-1.312872475142	-0.109542673209	-3.291093561063
H	-4.726914400524	-3.455941381017	-2.388625087131
H	-7.174640452885	-3.302015994048	-1.997132095919
H	-8.311582858680	-1.076368717775	-2.029718611346
H	-6.984463291735	0.996689986586	-2.457735148691
H	1.481731855117	-5.293585306259	4.967365267744
H	2.549164448087	-5.641398562512	3.566704582245
H	2.253022637584	-3.956264867622	4.051098692507

SCF Done: E(RB3LYP) = -1390.83589881

Zero-point correction= 0.440894
Thermal correction to Energy= 0.467332
Thermal correction to Enthalpy= 0.468276
Thermal correction to Gibbs Free Energy= 0.381475
Sum of electronic and zero-point Energies= -1390.395005
Sum of electronic and thermal Energies= -1390.368567
Sum of electronic and thermal Enthalpies= -1390.367623
Sum of electronic and thermal Free Energies= -1390.454424

1	N	Isotropic =	-40.4219	Anisotropy =	456.0478
2	C	Isotropic =	37.1575	Anisotropy =	121.0700
3	C	Isotropic =	60.1717	Anisotropy =	121.3708
4	C	Isotropic =	62.8997	Anisotropy =	177.4574
5	C	Isotropic =	72.4663	Anisotropy =	160.2478
6	C	Isotropic =	49.1448	Anisotropy =	154.8246
7	N	Isotropic =	123.1622	Anisotropy =	91.0886
8	C	Isotropic =	26.9505	Anisotropy =	108.5617
9	C	Isotropic =	70.1285	Anisotropy =	133.2770
10	C	Isotropic =	33.6806	Anisotropy =	123.1154
11	N	Isotropic =	136.3246	Anisotropy =	65.0196
12	O	Isotropic =	-81.0088	Anisotropy =	581.8922
13	N	Isotropic =	-34.4246	Anisotropy =	451.6539
14	C	Isotropic =	40.5550	Anisotropy =	144.9848
15	C	Isotropic =	61.4743	Anisotropy =	170.7533
16	C	Isotropic =	52.0479	Anisotropy =	182.8761
17	C	Isotropic =	147.2581	Anisotropy =	36.3065
18	C	Isotropic =	177.0549	Anisotropy =	23.9507
19	C	Isotropic =	156.8570	Anisotropy =	15.9832
20	C	Isotropic =	121.0159	Anisotropy =	42.1657
21	O	Isotropic =	202.4913	Anisotropy =	113.6445
22	C	Isotropic =	32.2677	Anisotropy =	138.4508
23	C	Isotropic =	70.5908	Anisotropy =	170.8058
24	C	Isotropic =	43.9900	Anisotropy =	181.5830
25	N	Isotropic =	-37.4958	Anisotropy =	458.0425
26	C	Isotropic =	42.6759	Anisotropy =	159.6312
27	C	Isotropic =	91.3107	Anisotropy =	133.3758
28	C	Isotropic =	70.1702	Anisotropy =	174.0906
29	C	Isotropic =	67.7750	Anisotropy =	171.0105
30	C	Isotropic =	63.6642	Anisotropy =	174.8859
31	C	Isotropic =	64.0615	Anisotropy =	150.0685
32	C	Isotropic =	154.4320	Anisotropy =	45.9190
33	H	Isotropic =	24.0694	Anisotropy =	8.4430

34	H	Isotropic =	24.4067	Anisotropy =	4.1959
35	H	Isotropic =	23.3146	Anisotropy =	4.7073
36	H	Isotropic =	22.7490	Anisotropy =	7.7778
37	H	Isotropic =	23.3686	Anisotropy =	10.3129
38	H	Isotropic =	27.5251	Anisotropy =	5.9786
39	H	Isotropic =	26.9230	Anisotropy =	7.8435
40	H	Isotropic =	29.8111	Anisotropy =	4.8193
41	H	Isotropic =	30.3509	Anisotropy =	8.4195
42	H	Isotropic =	30.2142	Anisotropy =	10.9746
43	H	Isotropic =	28.3998	Anisotropy =	8.0156
44	H	Isotropic =	28.2017	Anisotropy =	5.7347
45	H	Isotropic =	27.1284	Anisotropy =	6.0136
46	H	Isotropic =	27.4565	Anisotropy =	5.4779
47	H	Isotropic =	22.8359	Anisotropy =	7.2254
48	H	Isotropic =	24.9837	Anisotropy =	9.4378
49	H	Isotropic =	23.1740	Anisotropy =	9.6858
50	H	Isotropic =	23.8494	Anisotropy =	6.6701
51	H	Isotropic =	23.6753	Anisotropy =	5.1817
52	H	Isotropic =	23.6079	Anisotropy =	5.6726
53	H	Isotropic =	28.8435	Anisotropy =	7.8969
54	H	Isotropic =	27.4751	Anisotropy =	8.3572
55	H	Isotropic =	27.9832	Anisotropy =	10.0619

Conformer 16

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-5.161294223456	-2.533851891543	-2.387504089085
C	-3.855376011056	-2.393433648076	-2.629834002639
C	-3.169037467061	-3.189848338400	-3.573887785077
C	-3.896523911940	-4.192335901402	-4.225702793188
C	-5.258646470697	-4.344170876190	-3.963054429873
C	-5.849796685745	-3.473051650988	-3.051354266595
N	-1.819736602140	-2.934222733568	-3.940433998577
C	-0.778393366120	-2.866512041220	-3.041671386320
C	-1.062702042909	-2.643701660237	-1.588572297948
C	-2.109755170065	-1.838439352979	-1.077964605926
N	-3.165479633923	-1.389451376155	-1.899016679756
O	0.387593544530	-2.964588608064	-3.427130556209
N	-2.132469112110	-1.440336136976	0.201944483027
C	-1.181159523533	-1.879874424668	1.032548937014
C	-0.143003843096	-2.744023150392	0.664744409982

C	-0.088867086501	-3.089064869144	-0.687915044049
C	-3.961407141538	-0.238650172077	-1.422991155094
C	-3.161659604527	1.060517486413	-1.477641224505
C	0.872588396412	-3.243473222734	1.665979839417
C	0.611860437431	-4.666357004321	2.152537854603
O	-0.629438262411	-4.663016712424	2.878089800644
C	-1.088259864200	-5.825185181511	3.388284255087
C	-2.332803728079	-5.750212396492	4.098270740884
C	-2.851105705611	-6.963227523218	4.652885840000
N	-2.217613649762	-8.174424941381	4.536439195965
C	-1.075660247068	-8.183786878455	3.873896290697
C	-0.459577420065	-7.055065314794	3.279682003853
C	-3.052382578055	-4.537515139303	4.264955512013
C	-4.247707632385	-4.524339868586	4.957695262544
C	-4.767135063157	-5.722178618278	5.508994481068
C	-4.084140730978	-6.912836078327	5.359468755594
C	-1.449627952318	-3.078007703443	-5.353931573577
H	-3.402898942282	-4.835539180411	-4.954816972865
H	-5.845592655751	-5.112895900676	-4.467085100728
H	-6.921257451678	-3.527974680939	-2.836241186288
H	-1.246003099448	-1.514763133951	2.063482331341
H	0.739727589718	-3.680624220993	-1.082059709865
H	-4.832090671472	-0.175187848302	-2.085395420112
H	-4.336465835300	-0.420802169035	-0.404080514504
H	-2.797083367824	1.255985724853	-2.498867156533
H	-3.804951261359	1.902031766187	-1.173533200030
H	-2.297536187853	1.034005000768	-0.797438429913
H	1.878894259303	-3.236601755883	1.217135227681
H	0.904092239739	-2.573352057725	2.539262575204
H	1.425604859399	-5.000336995867	2.817935581400
H	0.540634150571	-5.368406107816	1.304244935277
H	-0.573063026606	-9.153797739305	3.784096492455
H	0.486513134042	-7.180751214679	2.756445579037
H	-2.646676313968	-3.620376854498	3.837803868505
H	-4.796264426710	-3.588372395092	5.082150953556
H	-5.713050062764	-5.700218689441	6.054758127937
H	-4.465401534217	-7.847387446167	5.775541677089
H	-1.157679513140	-4.111474487328	-5.603404325332
H	-2.302944744885	-2.779968429209	-5.975389394531
H	-0.592808785381	-2.426015255560	-5.560167712756

SCF Done: E(RB3LYP) = -1390.83595392

Zero-point correction= 0.440944

Thermal correction to Energy= 0.467375
Thermal correction to Enthalpy= 0.468319
Thermal correction to Gibbs Free Energy= 0.381734
Sum of electronic and zero-point Energies= -1390.395010
Sum of electronic and thermal Energies= -1390.368579
Sum of electronic and thermal Enthalpies= -1390.367635
Sum of electronic and thermal Free Energies= -1390.454219

1	N	Isotropic =	-40.5134	Anisotropy =	456.1252
2	C	Isotropic =	36.9666	Anisotropy =	120.4406
3	C	Isotropic =	60.1310	Anisotropy =	122.0239
4	C	Isotropic =	63.0104	Anisotropy =	177.4611
5	C	Isotropic =	72.5578	Anisotropy =	160.3750
6	C	Isotropic =	49.1529	Anisotropy =	154.6011
7	N	Isotropic =	123.2309	Anisotropy =	91.7366
8	C	Isotropic =	26.9018	Anisotropy =	108.4135
9	C	Isotropic =	70.2557	Anisotropy =	133.2371
10	C	Isotropic =	33.6721	Anisotropy =	123.1034
11	N	Isotropic =	136.3308	Anisotropy =	65.0967
12	O	Isotropic =	-81.3814	Anisotropy =	582.0780
13	N	Isotropic =	-34.2758	Anisotropy =	451.1236
14	C	Isotropic =	40.5708	Anisotropy =	144.9917
15	C	Isotropic =	61.5638	Anisotropy =	170.7342
16	C	Isotropic =	51.6978	Anisotropy =	182.4901
17	C	Isotropic =	147.4034	Anisotropy =	36.4057
18	C	Isotropic =	177.0095	Anisotropy =	24.0338
19	C	Isotropic =	156.7721	Anisotropy =	16.2306
20	C	Isotropic =	121.0266	Anisotropy =	42.3626
21	O	Isotropic =	202.5373	Anisotropy =	114.1914
22	C	Isotropic =	32.3351	Anisotropy =	138.7028
23	C	Isotropic =	70.4859	Anisotropy =	170.5155
24	C	Isotropic =	44.0144	Anisotropy =	182.2419
25	N	Isotropic =	-38.1004	Anisotropy =	456.3079
26	C	Isotropic =	42.4779	Anisotropy =	159.4826
27	C	Isotropic =	91.2836	Anisotropy =	133.2993
28	C	Isotropic =	70.2567	Anisotropy =	174.4125
29	C	Isotropic =	67.7560	Anisotropy =	170.2931
30	C	Isotropic =	63.6553	Anisotropy =	174.9973
31	C	Isotropic =	63.7331	Anisotropy =	149.6861
32	C	Isotropic =	154.6341	Anisotropy =	45.6453
33	H	Isotropic =	24.0887	Anisotropy =	8.4432
34	H	Isotropic =	24.3987	Anisotropy =	4.1960
35	H	Isotropic =	23.3201	Anisotropy =	4.7224
36	H	Isotropic =	22.7492	Anisotropy =	7.8035

37	H	Isotropic =	23.3480	Anisotropy =	10.2968
38	H	Isotropic =	27.5480	Anisotropy =	5.9407
39	H	Isotropic =	26.9244	Anisotropy =	7.8454
40	H	Isotropic =	30.3648	Anisotropy =	8.4140
41	H	Isotropic =	30.2445	Anisotropy =	10.9404
42	H	Isotropic =	29.8247	Anisotropy =	4.7948
43	H	Isotropic =	28.4005	Anisotropy =	7.9924
44	H	Isotropic =	28.2177	Anisotropy =	5.6612
45	H	Isotropic =	27.1200	Anisotropy =	6.0058
46	H	Isotropic =	27.4440	Anisotropy =	5.4639
47	H	Isotropic =	22.8452	Anisotropy =	7.2135
48	H	Isotropic =	24.9925	Anisotropy =	9.4437
49	H	Isotropic =	23.1432	Anisotropy =	9.7272
50	H	Isotropic =	23.8499	Anisotropy =	6.6551
51	H	Isotropic =	23.6668	Anisotropy =	5.1837
52	H	Isotropic =	23.6108	Anisotropy =	5.6511
53	H	Isotropic =	27.9638	Anisotropy =	10.0815
54	H	Isotropic =	28.8435	Anisotropy =	7.8745
55	H	Isotropic =	27.4663	Anisotropy =	8.3825

Conformer 17

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.251624806372	-0.364752016483	-1.957848146218
C	-3.357748927389	-0.873273829355	-1.408677842595
C	-3.968218672178	-0.307380440507	-0.267256907242
C	-3.335760216672	0.790330279582	0.327593550346
C	-2.171308429819	1.310641987118	-0.238550804057
C	-1.681126929784	0.710164125863	-1.395785359015
N	-5.226251594923	-0.756730085058	0.217390815076
C	-5.503393865423	-2.065029832117	0.546713185001
C	-4.620562725070	-3.163617948318	0.041095308824
C	-3.984631564387	-3.180689831112	-1.224298790919
N	-3.917641020833	-2.023431150351	-2.028681290346
O	-6.484032010821	-2.340014587609	1.239979880909
N	-3.449601034794	-4.300845770420	-1.729657754276
C	-3.467370172874	-5.416191310345	-0.991786805595
C	-3.999404309924	-5.504991924541	0.299805634407
C	-4.609101901685	-4.346714049204	0.788138627228
C	-3.643642131816	-2.206808537303	-3.468902013293
C	-4.300883941448	-1.115316562419	-4.309005703076

C	-3.942673646623	-6.785080729216	1.100671236972
C	-2.829267822135	-6.813471299615	2.144133561337
O	-1.571836652489	-6.774661288621	1.448105300478
C	-0.429836039266	-6.776154849362	2.167381683420
C	0.788057515334	-6.737393782395	1.409792097015
C	2.019610375681	-6.739803033675	2.138377442195
N	2.083013815469	-6.776537200190	3.508253939136
C	0.931587397024	-6.810972985292	4.153379762294
C	-0.350176390570	-6.813195478999	3.550092098734
C	0.811061073313	-6.697709466312	-0.009343199997
C	2.014128457781	-6.661875075823	-0.687694169042
C	3.237600746108	-6.664342596757	0.027551780296
C	3.239055853236	-6.702417875462	1.407777766957
C	-6.179425773612	0.250468147863	0.700054191463
H	-3.765997181442	1.250190526368	1.217805888781
H	-1.668749043963	2.171912561182	0.203212542392
H	-0.792409882314	1.103334584521	-1.898692978551
H	-3.027977346205	-6.302892150429	-1.461853610828
H	-5.130286061291	-4.351079965047	1.747316090752
H	-2.559024959307	-2.244305105277	-3.657493296459
H	-4.052774375020	-3.187859658658	-3.734897951091
H	-3.880656308734	-0.122239689557	-4.091031577462
H	-4.133190346094	-1.323981541808	-5.377789665573
H	-5.387623766321	-1.081323724359	-4.130244547621
H	-4.892132010646	-6.933959601699	1.639637134992
H	-3.815226781940	-7.647047888908	0.427206318962
H	-2.888695787444	-7.736965066311	2.744162582864
H	-2.900112122758	-5.947104422805	2.823936628800
H	0.987606073564	-6.840285297672	5.247735486662
H	-1.234705110550	-6.844763228820	4.183681156472
H	-0.134120452468	-6.695672635320	-0.552265437974
H	2.024788622137	-6.631420798343	-1.779196554203
H	4.183046060563	-6.635819673385	-0.518726294746
H	4.169477376002	-6.704905807519	1.978867263966
H	-6.031953295238	0.482453954205	1.767732298274
H	-6.058001065085	1.165730015154	0.107888748812
H	-7.195826888482	-0.141286389076	0.576830696359

SCF Done: E(RB3LYP) = -1390.83592577

Zero-point correction= 0.440790
Thermal correction to Energy= 0.467275
Thermal correction to Enthalpy= 0.468219
Thermal correction to Gibbs Free Energy= 0.381331

Sum of electronic and zero-point Energies= -1390.395136
Sum of electronic and thermal Energies= -1390.368651
Sum of electronic and thermal Enthalpies= -1390.367706
Sum of electronic and thermal Free Energies= -1390.454594

1	N	Isotropic =	-41.9527	Anisotropy =	470.1083
2	C	Isotropic =	38.9670	Anisotropy =	118.3425
3	C	Isotropic =	58.7304	Anisotropy =	123.7785
4	C	Isotropic =	62.9209	Anisotropy =	178.1638
5	C	Isotropic =	72.6792	Anisotropy =	160.1177
6	C	Isotropic =	49.1844	Anisotropy =	154.6960
7	N	Isotropic =	122.8932	Anisotropy =	91.1431
8	C	Isotropic =	26.8365	Anisotropy =	108.2870
9	C	Isotropic =	71.1330	Anisotropy =	132.4772
10	C	Isotropic =	32.3162	Anisotropy =	124.4901
11	N	Isotropic =	136.6509	Anisotropy =	64.0231
12	O	Isotropic =	-81.0254	Anisotropy =	581.1044
13	N	Isotropic =	-33.6956	Anisotropy =	439.9005
14	C	Isotropic =	40.6968	Anisotropy =	144.9308
15	C	Isotropic =	61.5295	Anisotropy =	170.9268
16	C	Isotropic =	51.8183	Anisotropy =	181.9016
17	C	Isotropic =	148.4720	Anisotropy =	33.8940
18	C	Isotropic =	177.3637	Anisotropy =	23.9743
19	C	Isotropic =	156.8944	Anisotropy =	15.8572
20	C	Isotropic =	121.1908	Anisotropy =	42.2196
21	O	Isotropic =	202.3613	Anisotropy =	114.2286
22	C	Isotropic =	32.2657	Anisotropy =	138.4445
23	C	Isotropic =	70.5585	Anisotropy =	170.7451
24	C	Isotropic =	43.8760	Anisotropy =	181.9131
25	N	Isotropic =	-37.5419	Anisotropy =	458.1467
26	C	Isotropic =	42.4307	Anisotropy =	159.6447
27	C	Isotropic =	91.2065	Anisotropy =	133.3605
28	C	Isotropic =	70.0562	Anisotropy =	174.2596
29	C	Isotropic =	67.8041	Anisotropy =	170.4031
30	C	Isotropic =	63.6314	Anisotropy =	174.8164
31	C	Isotropic =	63.8305	Anisotropy =	150.3458
32	C	Isotropic =	154.5536	Anisotropy =	45.4922
33	H	Isotropic =	24.0328	Anisotropy =	8.4691
34	H	Isotropic =	24.3720	Anisotropy =	4.2336
35	H	Isotropic =	23.2601	Anisotropy =	4.7590
36	H	Isotropic =	22.7649	Anisotropy =	7.7108
37	H	Isotropic =	23.3650	Anisotropy =	10.3703
38	H	Isotropic =	27.1178	Anisotropy =	8.2394
39	H	Isotropic =	27.3839	Anisotropy =	5.6910

40	H	Isotropic =	30.0164	Anisotropy =	5.1964
41	H	Isotropic =	30.2540	Anisotropy =	11.0250
42	H	Isotropic =	30.4172	Anisotropy =	8.3021
43	H	Isotropic =	28.4079	Anisotropy =	8.0214
44	H	Isotropic =	28.2378	Anisotropy =	5.6445
45	H	Isotropic =	27.1389	Anisotropy =	5.9656
46	H	Isotropic =	27.4610	Anisotropy =	5.5268
47	H	Isotropic =	22.8242	Anisotropy =	7.2339
48	H	Isotropic =	24.9781	Anisotropy =	9.4543
49	H	Isotropic =	23.1341	Anisotropy =	9.7131
50	H	Isotropic =	23.8528	Anisotropy =	6.6098
51	H	Isotropic =	23.6670	Anisotropy =	5.1940
52	H	Isotropic =	23.5868	Anisotropy =	5.6851
53	H	Isotropic =	27.9774	Anisotropy =	10.0814
54	H	Isotropic =	28.8508	Anisotropy =	7.7346
55	H	Isotropic =	27.4696	Anisotropy =	8.3384

Conformer 18

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.543113031725	-5.647540557609	-4.818804622039
C	0.489504103911	-5.743178258422	-3.487950354518
C	1.605552246575	-5.482683386790	-2.662312417632
C	2.782919552642	-5.049467536115	-3.283078837424
C	2.832154682032	-4.934501481661	-4.672895652838
C	1.690542517322	-5.267583091106	-5.398124616742
N	1.586415185601	-5.736876084053	-1.264237619320
C	0.650067714318	-5.216619582347	-0.398924071347
C	-0.637857655764	-4.670966078747	-0.934314168966
C	-1.343971437447	-5.189579420322	-2.046532297816
N	-0.753999022559	-6.130123019466	-2.917025630949
O	0.855496402376	-5.212522947584	0.815799171630
N	-2.609068687543	-4.831524766050	-2.309797750655
C	-3.198122933499	-3.920454096667	-1.528587450267
C	-2.580746384370	-3.287352463406	-0.442830168977
C	-1.283606937151	-3.712252804540	-0.145602053933
C	-1.655490649011	-6.937536837833	-3.764683252533
C	-1.071527839594	-8.319138640560	-4.046411191933
C	-3.305295084452	-2.254399993159	0.388629074589
C	-3.958122361443	-2.871716004052	1.623697999940
O	-4.608858644665	-1.805625457378	2.334499098415

C	-5.257604172173	-2.087033745930	3.484176969181
C	-5.887758339202	-0.974633333633	4.135138425512
C	-6.583439807943	-1.233230922580	5.358538644194
N	-6.671632900844	-2.479734627988	5.924395684255
C	-6.074164908622	-3.465787012143	5.280945041125
C	-5.356361200764	-3.340156073620	4.066121956840
C	-5.844936053819	0.346305771877	3.616134025063
C	-6.470556116888	1.380193692453	4.285769046729
C	-7.161132417608	1.131357607462	5.498146676654
C	-7.215529219184	-0.145315911086	6.021245917559
C	2.790657197142	-6.311173538175	-0.651195374756
H	3.664160641378	-4.824479846039	-2.681548734328
H	3.742493852463	-4.608634598007	-5.177458997554
H	1.689812026790	-5.229823003238	-6.491675497834
H	-4.230881756963	-3.665396939782	-1.792430792529
H	-0.754096704407	-3.327083050008	0.727699341679
H	-2.596102018616	-7.029564004111	-3.210190672864
H	-1.880984082873	-6.410637869918	-4.705297193284
H	-0.144546349429	-8.259311856101	-4.635947833354
H	-0.853923476852	-8.853757720507	-3.107848398090
H	-1.798080062130	-8.914289201633	-4.622498786563
H	-2.604240109137	-1.471035063768	0.716924203694
H	-4.086243727332	-1.765335282019	-0.214089722960
H	-3.204440270363	-3.345434192854	2.275544270765
H	-4.701973184229	-3.635233520296	1.338553634770
H	-6.148092248683	-4.459834644141	5.736973214431
H	-4.902467938379	-4.224802010203	3.623134899719
H	-5.311491028172	0.529352036877	2.683247687385
H	-6.434064873154	2.393878788825	3.881384197256
H	-7.652257938560	1.956123607761	6.019363204238
H	-7.742108935661	-0.359531017002	6.953263809218
H	3.272537002593	-6.978990287194	-1.375703486704
H	3.506560119420	-5.534010801434	-0.336629043486
H	2.494981203198	-6.878718923978	0.238840497356

SCF Done: E(RB3LYP) = -1390.83564755

Zero-point correction= 0.440648
Thermal correction to Energy= 0.467298
Thermal correction to Enthalpy= 0.468242
Thermal correction to Gibbs Free Energy= 0.380673
Sum of electronic and zero-point Energies= -1390.395000
Sum of electronic and thermal Energies= -1390.368349
Sum of electronic and thermal Enthalpies= -1390.367405

Sum of electronic and thermal Free Energies= -1390.454974

1	N	Isotropic =	-42.1391	Anisotropy =	468.2019
2	C	Isotropic =	38.8878	Anisotropy =	116.7610
3	C	Isotropic =	58.5669	Anisotropy =	122.8542
4	C	Isotropic =	62.7034	Anisotropy =	177.1654
5	C	Isotropic =	72.3545	Anisotropy =	159.5103
6	C	Isotropic =	49.1231	Anisotropy =	153.9966
7	N	Isotropic =	122.8968	Anisotropy =	91.6730
8	C	Isotropic =	27.0748	Anisotropy =	108.1530
9	C	Isotropic =	71.6040	Anisotropy =	133.0420
10	C	Isotropic =	32.2241	Anisotropy =	125.8454
11	N	Isotropic =	137.1841	Anisotropy =	63.5502
12	O	Isotropic =	-81.8332	Anisotropy =	582.7576
13	N	Isotropic =	-35.9908	Anisotropy =	442.0396
14	C	Isotropic =	40.7604	Anisotropy =	147.4088
15	C	Isotropic =	64.8602	Anisotropy =	166.9035
16	C	Isotropic =	51.1496	Anisotropy =	182.3708
17	C	Isotropic =	148.5888	Anisotropy =	33.9356
18	C	Isotropic =	177.2516	Anisotropy =	23.7165
19	C	Isotropic =	156.5705	Anisotropy =	32.6250
20	C	Isotropic =	121.2963	Anisotropy =	66.9612
21	O	Isotropic =	197.6009	Anisotropy =	103.4146
22	C	Isotropic =	31.9960	Anisotropy =	138.0829
23	C	Isotropic =	70.5380	Anisotropy =	171.0310
24	C	Isotropic =	43.7261	Anisotropy =	182.0098
25	N	Isotropic =	-37.7399	Anisotropy =	458.1745
26	C	Isotropic =	42.4499	Anisotropy =	159.9680
27	C	Isotropic =	91.1092	Anisotropy =	132.9902
28	C	Isotropic =	70.2013	Anisotropy =	173.9027
29	C	Isotropic =	67.7212	Anisotropy =	170.2291
30	C	Isotropic =	63.6254	Anisotropy =	175.2288
31	C	Isotropic =	63.6796	Anisotropy =	150.5280
32	C	Isotropic =	154.5201	Anisotropy =	45.3647
33	H	Isotropic =	23.9506	Anisotropy =	8.8640
34	H	Isotropic =	24.2718	Anisotropy =	4.4730
35	H	Isotropic =	23.1672	Anisotropy =	4.9216
36	H	Isotropic =	22.9712	Anisotropy =	8.4017
37	H	Isotropic =	23.3695	Anisotropy =	11.1361
38	H	Isotropic =	27.4063	Anisotropy =	6.0520
39	H	Isotropic =	27.0716	Anisotropy =	8.2931
40	H	Isotropic =	30.0054	Anisotropy =	5.1888
41	H	Isotropic =	30.3789	Anisotropy =	8.0557
42	H	Isotropic =	30.2382	Anisotropy =	10.9731

43	H	Isotropic =	28.2636	Anisotropy =	4.9994
44	H	Isotropic =	28.2863	Anisotropy =	5.5977
45	H	Isotropic =	27.3184	Anisotropy =	7.4676
46	H	Isotropic =	27.3906	Anisotropy =	6.2297
47	H	Isotropic =	22.7118	Anisotropy =	7.5261
48	H	Isotropic =	24.9065	Anisotropy =	8.9712
49	H	Isotropic =	23.0625	Anisotropy =	10.5283
50	H	Isotropic =	23.8017	Anisotropy =	6.1251
51	H	Isotropic =	23.5955	Anisotropy =	5.0994
52	H	Isotropic =	23.4799	Anisotropy =	5.9692
53	H	Isotropic =	28.8180	Anisotropy =	7.4463
54	H	Isotropic =	27.9348	Anisotropy =	9.9871
55	H	Isotropic =	27.4445	Anisotropy =	8.0653

Conformer 19

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.191865574546	-6.847781187849	-4.397146013220
C	0.301363639791	-5.780138983599	-3.602805367109
C	1.459773912688	-5.518616688355	-2.837790537898
C	2.492012284817	-6.462822547580	-2.883423848566
C	2.368660926087	-7.586525203529	-3.701533136552
C	1.206367981229	-7.721656916835	-4.457083001542
N	1.631742674447	-4.305128093624	-2.118509929904
C	0.738156553646	-3.828619005251	-1.185330427107
C	-0.661871171472	-4.359142202474	-1.154118786492
C	-1.414907843899	-4.743154732521	-2.289808314373
N	-0.809250051674	-4.893250508862	-3.555311170727
O	1.076841751731	-2.955110201056	-0.385224351199
N	-2.736951821111	-4.956768110444	-2.221973131368
C	-3.348744855149	-4.849806516978	-1.037953816516
C	-2.701516548483	-4.539204688187	0.164456226568
C	-1.334795214958	-4.266992322989	0.069250427482
C	-1.688463663756	-4.859083038351	-4.742315256941
C	-0.966766842792	-4.286395439678	-5.959007361349
C	-3.456095016122	-4.439978502712	1.469858154935
C	-3.896291508997	-3.007194070550	1.762636075727
O	-4.592655018705	-3.025826975657	3.019473144860
C	-5.085091737385	-1.868642070301	3.509933234486
C	-5.770118171500	-1.962731862712	4.766963458074
C	-6.306407962196	-0.756222813371	5.318528861710

N	-6.193821507868	0.465868875766	4.705574909123
C	-5.553287605554	0.492607800008	3.551427778034
C	-4.979310569514	-0.628216858799	2.902483343936
C	-5.930117260580	-3.187783816069	5.466854158614
C	-6.599866292935	-3.219304624325	6.674850306513
C	-7.133656114548	-2.028128895709	7.226965194907
C	-6.989581352993	-0.825643504382	6.563771972417
C	2.962850348487	-3.685287104123	-2.117454691205
H	3.397965238531	-6.307393709712	-2.296935882273
H	3.165310803467	-8.329167780213	-3.759327613860
H	1.077099375212	-8.565250198286	-5.141872243733
H	-4.428805551321	-5.036416521563	-1.043355558551
H	-0.765871128277	-3.946111689703	0.943738746717
H	-2.086139887690	-5.862400789069	-4.962230715850
H	-2.540427451691	-4.224340789092	-4.473574388784
H	-0.131132434253	-4.926722773294	-6.278879126405
H	-1.672514578363	-4.209904096929	-6.801660279308
H	-0.573070400939	-3.279547859939	-5.746110751239
H	-4.349191258897	-5.083427520054	1.440714597148
H	-2.824587098553	-4.790546863589	2.301098652110
H	-4.567785604061	-2.631073230197	0.971971053807
H	-3.026244392660	-2.332003338808	1.831345216912
H	-5.466042864650	1.471445812037	3.065822603443
H	-4.472944962510	-0.488299532519	1.949202908848
H	-5.516590677951	-4.099579308308	5.035501303382
H	-6.719697998144	-4.164626957408	7.208194054265
H	-7.661347126852	-2.064686786948	8.182621497417
H	-7.392162604061	0.103992495046	6.970651071037
H	3.596013666802	-4.065720276056	-1.299048519570
H	3.449141256264	-3.887587991555	-3.079563607130
H	2.846138165318	-2.604029482743	-1.979241123703

SCF Done: E(RB3LYP) = -1390.83566342

Zero-point correction= 0.440761
Thermal correction to Energy= 0.467357
Thermal correction to Enthalpy= 0.468302
Thermal correction to Gibbs Free Energy= 0.381393
Sum of electronic and zero-point Energies= -1390.394903
Sum of electronic and thermal Energies= -1390.368306
Sum of electronic and thermal Enthalpies= -1390.367362
Sum of electronic and thermal Free Energies= -1390.454271

1 N Isotropic = -41.4275 Anisotropy = 470.1748

2	C	Isotropic =	38.7290	Anisotropy =	116.8374
3	C	Isotropic =	58.4140	Anisotropy =	122.8114
4	C	Isotropic =	62.6315	Anisotropy =	177.2706
5	C	Isotropic =	72.4357	Anisotropy =	159.4587
6	C	Isotropic =	49.0475	Anisotropy =	154.0945
7	N	Isotropic =	123.0135	Anisotropy =	92.0198
8	C	Isotropic =	26.9366	Anisotropy =	108.1306
9	C	Isotropic =	71.3696	Anisotropy =	133.1968
10	C	Isotropic =	32.2368	Anisotropy =	126.0638
11	N	Isotropic =	137.0524	Anisotropy =	63.1742
12	O	Isotropic =	-81.7493	Anisotropy =	582.3407
13	N	Isotropic =	-35.5012	Anisotropy =	443.6525
14	C	Isotropic =	40.9447	Anisotropy =	147.8274
15	C	Isotropic =	64.7166	Anisotropy =	166.9486
16	C	Isotropic =	50.7233	Anisotropy =	182.0751
17	C	Isotropic =	148.3455	Anisotropy =	34.2363
18	C	Isotropic =	177.2314	Anisotropy =	23.7964
19	C	Isotropic =	156.7814	Anisotropy =	32.5679
20	C	Isotropic =	121.2161	Anisotropy =	67.0215
21	O	Isotropic =	197.7362	Anisotropy =	104.2262
22	C	Isotropic =	32.1432	Anisotropy =	138.0920
23	C	Isotropic =	70.5494	Anisotropy =	171.0617
24	C	Isotropic =	43.8328	Anisotropy =	182.4623
25	N	Isotropic =	-37.8961	Anisotropy =	457.9035
26	C	Isotropic =	42.3607	Anisotropy =	159.7024
27	C	Isotropic =	91.2041	Anisotropy =	133.4161
28	C	Isotropic =	70.1754	Anisotropy =	174.4048
29	C	Isotropic =	67.6127	Anisotropy =	170.1446
30	C	Isotropic =	63.5502	Anisotropy =	175.0355
31	C	Isotropic =	63.6536	Anisotropy =	149.9498
32	C	Isotropic =	154.5917	Anisotropy =	45.2318
33	H	Isotropic =	23.9668	Anisotropy =	8.8577
34	H	Isotropic =	24.2552	Anisotropy =	4.4966
35	H	Isotropic =	23.1361	Anisotropy =	4.9698
36	H	Isotropic =	22.9759	Anisotropy =	8.3878
37	H	Isotropic =	23.3211	Anisotropy =	11.1196
38	H	Isotropic =	27.0511	Anisotropy =	8.2862
39	H	Isotropic =	27.4214	Anisotropy =	6.0552
40	H	Isotropic =	29.9771	Anisotropy =	5.2548
41	H	Isotropic =	30.2307	Anisotropy =	10.9352
42	H	Isotropic =	30.3847	Anisotropy =	8.0515
43	H	Isotropic =	28.2861	Anisotropy =	5.6472
44	H	Isotropic =	28.2548	Anisotropy =	5.0006
45	H	Isotropic =	27.4229	Anisotropy =	6.3286

46	H	Isotropic =	27.3369	Anisotropy =	7.4057
47	H	Isotropic =	22.7362	Anisotropy =	7.5028
48	H	Isotropic =	24.9125	Anisotropy =	8.9773
49	H	Isotropic =	23.0434	Anisotropy =	10.5387
50	H	Isotropic =	23.7937	Anisotropy =	6.1313
51	H	Isotropic =	23.5845	Anisotropy =	5.1125
52	H	Isotropic =	23.4904	Anisotropy =	5.9585
53	H	Isotropic =	27.9358	Anisotropy =	10.0003
54	H	Isotropic =	28.7996	Anisotropy =	7.4914
55	H	Isotropic =	27.4542	Anisotropy =	8.0705

Conformer 20

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.420538164971	-5.614709190419	-3.232884244340
C	-2.616840290025	-5.686463549521	-2.643766144620
C	-3.060131933820	-6.842272197228	-1.963243363184
C	-2.167991697736	-7.916019705150	-1.861952222016
C	-0.911826958664	-7.832912886642	-2.464175244754
C	-0.594633756302	-6.667802573637	-3.158535767888
N	-4.389684573699	-6.969177115643	-1.477043846144
C	-4.987337746087	-6.069519545413	-0.622577515333
C	-4.407654200096	-4.698196883585	-0.462344323751
C	-3.797708779256	-3.945719031671	-1.495405636460
N	-3.449980288345	-4.537717968387	-2.728523171271
O	-6.004952664346	-6.379117437231	-0.000926634548
N	-3.553303765255	-2.634808125596	-1.363342791520
C	-3.840214821037	-2.037270257558	-0.201591489766
C	-4.376069312594	-2.689164927116	0.914951338927
C	-4.685640993383	-4.040554532217	0.740911918838
C	-3.234178040241	-3.638132778257	-3.880628582405
C	-3.598188338094	-4.315983786147	-5.198682470822
C	-4.626500598772	-1.966224157622	2.218123830662
C	-3.564786803217	-2.228726499005	3.282774986375
O	-2.320302542413	-1.689138936093	2.805927982862
C	-1.215243877638	-1.829661415598	3.567776122099
C	-0.005994340818	-1.279956242749	3.025420305884
C	1.187181558330	-1.411868595332	3.804294837922
N	1.221839363676	-2.030758468510	5.028154422140
C	0.079641495812	-2.516381595934	5.478436190057
C	-1.165025953659	-2.450606788559	4.805293455788

C	0.045276731118	-0.623885602598	1.767114536589
C	1.238971936620	-0.114933415213	1.292861800951
C	2.424537849152	-0.242664663251	2.058756860347
C	2.397932887379	-0.876164320471	3.285353130722
C	-5.056505255569	-8.269107877871	-1.623542986105
H	-2.465109826481	-8.821855095558	-1.332588363327
H	-0.205288645252	-8.661743870488	-2.406216054461
H	0.362468916677	-6.568214647159	-3.679443867202
H	-3.629178199503	-0.963169515029	-0.155853936460
H	-5.190299043965	-4.605100734545	1.527328359227
H	-3.877158258716	-2.766935927308	-3.712428595701
H	-2.194188566422	-3.275784802817	-3.902755616611
H	-4.640811831005	-4.672201548046	-5.183954027881
H	-3.491774975499	-3.593925704836	-6.024091006019
H	-2.940696337743	-5.171243177084	-5.414478737392
H	-4.688273813962	-0.880858453467	2.042561565580
H	-5.593251846073	-2.280401547599	2.643378426710
H	-3.449033432246	-3.310154325942	3.468703396342
H	-3.839962360946	-1.736308182318	4.230508723836
H	0.112451059210	-3.009374607494	6.456928927009
H	-2.045540701415	-2.885983446045	5.274066476245
H	-0.870661618143	-0.529481044985	1.183703770829
H	1.271421055338	0.388144090855	0.324206194214
H	3.362902892413	0.163141491090	1.674178746049
H	3.298803942911	-0.985587943423	3.892207536312
H	-6.138849939644	-8.104211208201	-1.679677335438
H	-4.703825850789	-8.745706009507	-2.546288482303
H	-4.857908744798	-8.935232719865	-0.767781384795

SCF Done: E(RB3LYP) = -1390.83584896

Zero-point correction= 0.440727
Thermal correction to Energy= 0.467237
Thermal correction to Enthalpy= 0.468181
Thermal correction to Gibbs Free Energy= 0.381030
Sum of electronic and zero-point Energies= -1390.395122
Sum of electronic and thermal Energies= -1390.368612
Sum of electronic and thermal Enthalpies= -1390.367668
Sum of electronic and thermal Free Energies= -1390.454818

1	N	Isotropic =	-41.5605	Anisotropy =	470.3757
2	C	Isotropic =	38.6618	Anisotropy =	118.2682
3	C	Isotropic =	58.7616	Anisotropy =	123.5988
4	C	Isotropic =	62.8759	Anisotropy =	177.4740

5	C	Isotropic =	72.7105	Anisotropy =	159.6965
6	C	Isotropic =	49.2563	Anisotropy =	154.7546
7	N	Isotropic =	122.8958	Anisotropy =	91.5751
8	C	Isotropic =	26.8815	Anisotropy =	108.6397
9	C	Isotropic =	71.0616	Anisotropy =	132.3545
10	C	Isotropic =	32.3199	Anisotropy =	123.6806
11	N	Isotropic =	137.2028	Anisotropy =	64.7993
12	O	Isotropic =	-79.8320	Anisotropy =	583.5420
13	N	Isotropic =	-34.2018	Anisotropy =	438.7078
14	C	Isotropic =	40.3815	Anisotropy =	145.2085
15	C	Isotropic =	61.3644	Anisotropy =	171.4858
16	C	Isotropic =	52.1851	Anisotropy =	181.6932
17	C	Isotropic =	148.7503	Anisotropy =	33.9387
18	C	Isotropic =	177.3777	Anisotropy =	23.9086
19	C	Isotropic =	156.9426	Anisotropy =	16.1413
20	C	Isotropic =	120.9752	Anisotropy =	42.1839
21	O	Isotropic =	202.3477	Anisotropy =	113.2247
22	C	Isotropic =	32.1538	Anisotropy =	138.4992
23	C	Isotropic =	70.5229	Anisotropy =	170.7660
24	C	Isotropic =	44.0386	Anisotropy =	181.9930
25	N	Isotropic =	-37.7046	Anisotropy =	457.5918
26	C	Isotropic =	42.6408	Anisotropy =	159.9735
27	C	Isotropic =	91.2308	Anisotropy =	133.1486
28	C	Isotropic =	70.2740	Anisotropy =	174.5524
29	C	Isotropic =	67.6644	Anisotropy =	170.5107
30	C	Isotropic =	63.7258	Anisotropy =	175.0313
31	C	Isotropic =	63.8767	Anisotropy =	150.2460
32	C	Isotropic =	154.5890	Anisotropy =	45.5736
33	H	Isotropic =	24.0728	Anisotropy =	8.3698
34	H	Isotropic =	24.4146	Anisotropy =	4.1766
35	H	Isotropic =	23.2901	Anisotropy =	4.7098
36	H	Isotropic =	22.7891	Anisotropy =	7.6749
37	H	Isotropic =	23.3648	Anisotropy =	10.3451
38	H	Isotropic =	27.4003	Anisotropy =	5.6945
39	H	Isotropic =	27.0947	Anisotropy =	8.2465
40	H	Isotropic =	30.3991	Anisotropy =	8.3477
41	H	Isotropic =	30.2417	Anisotropy =	11.0254
42	H	Isotropic =	30.0299	Anisotropy =	5.2242
43	H	Isotropic =	28.2303	Anisotropy =	5.7608
44	H	Isotropic =	28.3918	Anisotropy =	8.0455
45	H	Isotropic =	27.4677	Anisotropy =	5.4399
46	H	Isotropic =	27.1261	Anisotropy =	6.0270
47	H	Isotropic =	22.8199	Anisotropy =	7.2365
48	H	Isotropic =	25.0010	Anisotropy =	9.4254

49	H	Isotropic =	23.1839	Anisotropy =	9.6645
50	H	Isotropic =	23.8710	Anisotropy =	6.5863
51	H	Isotropic =	23.6872	Anisotropy =	5.1660
52	H	Isotropic =	23.6042	Anisotropy =	5.6663
53	H	Isotropic =	27.4567	Anisotropy =	8.4255
54	H	Isotropic =	28.8598	Anisotropy =	7.7235
55	H	Isotropic =	27.9758	Anisotropy =	10.0828

Conformer 21

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.123586236889	-5.874166313562	2.875686016734
C	-0.441576834317	-5.695227214461	1.741519071827
C	0.779102837121	-4.986199877352	1.693780125019
C	1.239476835334	-4.408624839737	2.882798997305
C	0.517683847001	-4.584368628154	4.063963590788
C	-0.648241798376	-5.344707092485	4.011510222971
N	1.573426881882	-4.929100145738	0.516776133475
C	1.109725697807	-4.488724984811	-0.703137712602
C	-0.363909934877	-4.424938502945	-0.961037283376
C	-1.319033293869	-5.344706496356	-0.462633418983
N	-0.994475327951	-6.260369720772	0.559688384937
O	1.899400288231	-4.164887731803	-1.591584102918
N	-2.561895420751	-5.409846388149	-0.960780346538
C	-2.925680156814	-4.539190055250	-1.907863500646
C	-2.098162215319	-3.532477939624	-2.420895895683
C	-0.785771498859	-3.520479904220	-1.942067731186
C	-1.873399089760	-7.436155472229	0.729688609495
C	-1.103089973483	-8.643486596967	1.256986573904
C	-2.599094882624	-2.542935389777	-3.445883099629
C	-3.155734519239	-1.244384549750	-2.854531411168
O	-4.348879690614	-1.506395136155	-2.088880448146
C	-4.388831230356	-1.371863252089	-0.744823487278
C	-5.682922578356	-1.571608445892	-0.154790524974
C	-5.793634437258	-1.443144653301	1.266109266154
N	-4.731628997237	-1.138135586821	2.078053438582
C	-3.565642801681	-0.965983733017	1.482383165936
C	-3.325985077219	-1.069190514022	0.090705444712
C	-6.835275039734	-1.887375479711	-0.922628263536
C	-8.057560470896	-2.072716220262	-0.305971195793
C	-8.173541923172	-1.948444111101	1.101011157802

C	-7.067247113679	-1.640425551056	1.867482302964
C	3.031350944534	-5.023494847425	0.662053425696
H	2.170924148256	-3.841776593741	2.887226657710
H	0.863769848572	-4.151531362752	5.003326098631
H	-1.230798241453	-5.541320273255	4.916656193230
H	-3.948450238744	-4.647733865339	-2.284788720024
H	-0.046902944858	-2.831308502221	-2.355310445959
H	-2.721076897898	-7.195748802875	1.390944944126
H	-2.287428357450	-7.653698418465	-0.261142964892
H	-1.776305398841	-9.514333840377	1.306212549146
H	-0.261216072064	-8.895664261994	0.592304366489
H	-0.708016424826	-8.467724073432	2.268606407211
H	-1.782299434163	-2.261142305951	-4.130571739510
H	-3.387410016636	-3.006808474075	-4.059740971216
H	-3.471331335183	-0.574597240326	-3.668159139318
H	-2.404953557701	-0.717060878479	-2.251430743092
H	-2.717552677957	-0.725541065704	2.133899810450
H	-2.313477724861	-0.919260536673	-0.278381087363
H	-6.737002722709	-1.980499314701	-2.004142058906
H	-8.939115491230	-2.315436862190	-0.903009124281
H	-9.144509218015	-2.097211390961	1.578749794817
H	-7.133421698616	-1.539254244408	2.952517817562
H	3.261042552352	-5.681701501778	1.508874820826
H	3.449374091792	-5.443596897790	-0.260186632645
H	3.495891023654	-4.037443917519	0.827506661162

SCF Done: E(RB3LYP) = -1390.83178025

Zero-point correction= 0.440785
Thermal correction to Energy= 0.467273
Thermal correction to Enthalpy= 0.468217
Thermal correction to Gibbs Free Energy= 0.380987
Sum of electronic and zero-point Energies= -1390.390995
Sum of electronic and thermal Energies= -1390.364508
Sum of electronic and thermal Enthalpies= -1390.363563
Sum of electronic and thermal Free Energies= -1390.450793

1	N	Isotropic =	-42.4734	Anisotropy =	470.3142
2	C	Isotropic =	38.6788	Anisotropy =	118.8506
3	C	Isotropic =	58.3199	Anisotropy =	124.2550
4	C	Isotropic =	62.7709	Anisotropy =	177.5681
5	C	Isotropic =	72.4175	Anisotropy =	160.4885
6	C	Isotropic =	49.3479	Anisotropy =	154.7297
7	N	Isotropic =	123.1089	Anisotropy =	91.7996

8	C	Isotropic =	26.8114	Anisotropy =	108.1179
9	C	Isotropic =	71.4511	Anisotropy =	132.8041
10	C	Isotropic =	32.3268	Anisotropy =	125.2904
11	N	Isotropic =	136.6632	Anisotropy =	65.4933
12	O	Isotropic =	-81.6621	Anisotropy =	581.5143
13	N	Isotropic =	-33.1447	Anisotropy =	443.1332
14	C	Isotropic =	41.0846	Anisotropy =	149.1755
15	C	Isotropic =	63.1025	Anisotropy =	172.2186
16	C	Isotropic =	51.5866	Anisotropy =	181.0402
17	C	Isotropic =	148.9240	Anisotropy =	33.9145
18	C	Isotropic =	177.4438	Anisotropy =	24.5058
19	C	Isotropic =	155.6442	Anisotropy =	16.0094
20	C	Isotropic =	124.0320	Anisotropy =	52.6948
21	O	Isotropic =	202.2225	Anisotropy =	131.2174
22	C	Isotropic =	31.8707	Anisotropy =	139.2993
23	C	Isotropic =	70.5180	Anisotropy =	171.3214
24	C	Isotropic =	43.7601	Anisotropy =	182.4594
25	N	Isotropic =	-35.8565	Anisotropy =	456.9205
26	C	Isotropic =	43.3917	Anisotropy =	161.0996
27	C	Isotropic =	92.9996	Anisotropy =	139.9893
28	C	Isotropic =	69.9082	Anisotropy =	175.1790
29	C	Isotropic =	68.1217	Anisotropy =	170.8229
30	C	Isotropic =	63.5930	Anisotropy =	174.9085
31	C	Isotropic =	64.0373	Anisotropy =	150.5255
32	C	Isotropic =	154.6041	Anisotropy =	45.4995
33	H	Isotropic =	23.9442	Anisotropy =	8.5221
34	H	Isotropic =	24.2752	Anisotropy =	4.2860
35	H	Isotropic =	23.2707	Anisotropy =	4.4231
36	H	Isotropic =	23.3495	Anisotropy =	6.1935
37	H	Isotropic =	23.3594	Anisotropy =	9.9944
38	H	Isotropic =	27.4623	Anisotropy =	7.5199
39	H	Isotropic =	27.6259	Anisotropy =	5.6243
40	H	Isotropic =	30.4008	Anisotropy =	11.1733
41	H	Isotropic =	30.5149	Anisotropy =	8.5726
42	H	Isotropic =	30.1362	Anisotropy =	5.2400
43	H	Isotropic =	28.5297	Anisotropy =	7.9263
44	H	Isotropic =	28.2179	Anisotropy =	7.1485
45	H	Isotropic =	26.9477	Anisotropy =	8.0320
46	H	Isotropic =	26.7874	Anisotropy =	4.5398
47	H	Isotropic =	23.4391	Anisotropy =	6.4732
48	H	Isotropic =	25.5306	Anisotropy =	7.3563
49	H	Isotropic =	23.0722	Anisotropy =	10.5341
50	H	Isotropic =	23.8229	Anisotropy =	5.8277
51	H	Isotropic =	23.6630	Anisotropy =	4.9778

52	H	Isotropic =	23.6657	Anisotropy =	6.1561
53	H	Isotropic =	28.8362	Anisotropy =	7.7739
54	H	Isotropic =	27.4873	Anisotropy =	8.5325
55	H	Isotropic =	27.9184	Anisotropy =	9.9442

Conformer 22

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-7.484441698110	-1.649023811399	-2.187099477242
C	-6.707926996114	-1.675766794940	-1.100960409061
C	-7.183111965625	-2.097495814527	0.161166390039
C	-8.504303865696	-2.553251375234	0.235777507704
C	-9.310573422792	-2.535105233893	-0.903083709303
C	-8.759446900567	-2.050335491078	-2.086640592425
N	-6.402034759997	-1.975611819652	1.342508267530
C	-5.142961906271	-2.513508466700	1.489856985188
C	-4.350703628356	-2.896888803174	0.278618451397
C	-4.373668729042	-2.214012443109	-0.961341753521
N	-5.361120930486	-1.250672312332	-1.257488191482
O	-4.652307429486	-2.660221093151	2.610253158057
N	-3.446708934428	-2.433372446619	-1.905563127039
C	-2.518167824657	-3.371029959852	-1.693394556195
C	-2.437177021939	-4.161444937317	-0.539960765641
C	-3.366995117486	-3.875389142919	0.462110228999
C	-5.081495802675	-0.300743650582	-2.354968166629
C	-3.992099357002	0.697839495483	-1.972589711834
C	-1.363938743389	-5.211725655934	-0.372619695749
C	-0.129521487375	-4.659628223864	0.337500488069
O	0.811898272529	-5.739882443615	0.446631317133
C	1.998915948099	-5.515135919188	1.048459774181
C	2.887881170441	-6.639107890825	1.116788456020
C	4.156466681296	-6.440365905111	1.748156919165
N	4.550742979411	-5.239614178861	2.281699537976
C	3.692522301324	-4.240463358660	2.189960738461
C	2.410634236182	-4.308867615435	1.590696258243
C	2.557109238145	-7.915324903474	0.589592708695
C	3.452937953356	-8.962923318038	0.682932269486
C	4.711195933331	-8.773213115309	1.307007756279
C	5.053817850184	-7.540733381415	1.826795608141
C	-7.077907439590	-1.556472285849	2.576642419751
H	-8.907229593510	-2.898599060836	1.188303947463

H	-10.345427474411	-2.877202292537	-0.864104001813
H	-9.359813633605	-1.982284045323	-2.998897121398
H	-1.791008295383	-3.510580877838	-2.501568943532
H	-3.329330241147	-4.390135579513	1.423928412341
H	-4.807985292014	-0.840085817089	-3.274963462100
H	-6.023562605253	0.223573733141	-2.551413009629
H	-4.267601394218	1.252388976674	-1.061194569597
H	-3.026986939826	0.199121596576	-1.799650716074
H	-3.854812539274	1.423820793962	-2.790226063399
H	-1.753022756472	-6.061413506225	0.209698563378
H	-1.058222805896	-5.599678767152	-1.356818484912
H	-0.384139591140	-4.287186760306	1.344449481513
H	0.320422411355	-3.831981269430	-0.237143182351
H	4.012491508855	-3.283298699998	2.617735980363
H	1.784868050346	-3.418457376390	1.571422293902
H	1.587269721714	-8.053214125326	0.111309829890
H	3.192604536017	-9.941942575135	0.275256321220
H	5.411814238370	-9.608387701228	1.375540003533
H	6.017380364116	-7.372160537011	2.311491743028
H	-6.345994998084	-1.064069501595	3.227420601471
H	-7.880333567921	-0.854070998148	2.319883067133
H	-7.501787705829	-2.411623312698	3.128544225177

SCF Done: E(RB3LYP) = -1390.83564295

Zero-point correction= 0.440706
Thermal correction to Energy= 0.467328
Thermal correction to Enthalpy= 0.468272
Thermal correction to Gibbs Free Energy= 0.380819
Sum of electronic and zero-point Energies= -1390.394937
Sum of electronic and thermal Energies= -1390.368315
Sum of electronic and thermal Enthalpies= -1390.367371
Sum of electronic and thermal Free Energies= -1390.454824

1	N	Isotropic =	-40.4023	Anisotropy =	455.8345
2	C	Isotropic =	37.0016	Anisotropy =	119.8973
3	C	Isotropic =	59.8615	Anisotropy =	120.6764
4	C	Isotropic =	62.7351	Anisotropy =	176.9301
5	C	Isotropic =	72.2569	Anisotropy =	159.5797
6	C	Isotropic =	49.1417	Anisotropy =	154.5019
7	N	Isotropic =	123.0639	Anisotropy =	91.2560
8	C	Isotropic =	27.1194	Anisotropy =	108.2262
9	C	Isotropic =	70.4443	Anisotropy =	134.1539
10	C	Isotropic =	33.9687	Anisotropy =	125.1959

11	N	Isotropic =	136.2751	Anisotropy =	64.7177
12	O	Isotropic =	-81.6667	Anisotropy =	582.6568
13	N	Isotropic =	-36.1945	Anisotropy =	455.0241
14	C	Isotropic =	40.8062	Anisotropy =	147.9286
15	C	Isotropic =	64.7890	Anisotropy =	166.7841
16	C	Isotropic =	50.5791	Anisotropy =	182.6628
17	C	Isotropic =	147.2525	Anisotropy =	36.2578
18	C	Isotropic =	176.9372	Anisotropy =	24.1044
19	C	Isotropic =	156.8978	Anisotropy =	32.6478
20	C	Isotropic =	121.1746	Anisotropy =	66.8355
21	O	Isotropic =	197.7862	Anisotropy =	104.5247
22	C	Isotropic =	31.9454	Anisotropy =	138.2046
23	C	Isotropic =	70.5556	Anisotropy =	171.1235
24	C	Isotropic =	43.8104	Anisotropy =	181.5131
25	N	Isotropic =	-37.6467	Anisotropy =	458.7350
26	C	Isotropic =	42.5301	Anisotropy =	159.7442
27	C	Isotropic =	91.1439	Anisotropy =	133.5666
28	C	Isotropic =	69.9088	Anisotropy =	173.6875
29	C	Isotropic =	67.8937	Anisotropy =	171.3223
30	C	Isotropic =	63.4992	Anisotropy =	174.7786
31	C	Isotropic =	63.8914	Anisotropy =	150.6299
32	C	Isotropic =	154.6157	Anisotropy =	45.3861
33	H	Isotropic =	23.9802	Anisotropy =	8.9194
34	H	Isotropic =	24.2912	Anisotropy =	4.4561
35	H	Isotropic =	23.1993	Anisotropy =	4.9197
36	H	Isotropic =	22.9505	Anisotropy =	8.4319
37	H	Isotropic =	23.2934	Anisotropy =	11.0255
38	H	Isotropic =	26.9764	Anisotropy =	7.8046
39	H	Isotropic =	27.5537	Anisotropy =	6.1515
40	H	Isotropic =	30.3512	Anisotropy =	8.0681
41	H	Isotropic =	29.8320	Anisotropy =	5.4231
42	H	Isotropic =	30.2467	Anisotropy =	10.8524
43	H	Isotropic =	28.2426	Anisotropy =	5.0603
44	H	Isotropic =	28.2653	Anisotropy =	5.5869
45	H	Isotropic =	27.3342	Anisotropy =	7.3062
46	H	Isotropic =	27.4009	Anisotropy =	6.3776
47	H	Isotropic =	22.7291	Anisotropy =	7.5144
48	H	Isotropic =	24.9214	Anisotropy =	8.9321
49	H	Isotropic =	23.0423	Anisotropy =	10.5340
50	H	Isotropic =	23.7730	Anisotropy =	6.1605
51	H	Isotropic =	23.5864	Anisotropy =	5.1161
52	H	Isotropic =	23.4826	Anisotropy =	5.9776
53	H	Isotropic =	27.4699	Anisotropy =	8.0505
54	H	Isotropic =	28.8086	Anisotropy =	7.6539

55 H Isotropic = 27.9293 Anisotropy = 10.0081

Conformer 23

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	0.197364238735	-2.287989455110	5.606104947371
C	0.023009923895	-3.259526252344	4.706615428782
C	1.103539065432	-3.972174287736	4.140196330164
C	2.397344795467	-3.588977282016	4.512216541785
C	2.577493435607	-2.566292391001	5.444450799080
C	1.442705200465	-1.962061755363	5.979869269748
N	0.906811925599	-5.103249625234	3.302050432843
C	0.145097675616	-5.085766392513	2.154790354388
C	-0.865221899057	-4.000281784886	1.947489316774
C	-1.629568811349	-3.389998517219	2.971208596829
N	-1.314237885793	-3.564919414875	4.334996316269
O	0.269799617869	-5.971737993588	1.307957043882
N	-2.703242363630	-2.634950289128	2.695563165799
C	-3.018697693842	-2.402327223171	1.417815677334
C	-2.298248656621	-2.890556591443	0.320650899173
C	-1.220973854450	-3.726979034003	0.621798112366
C	-2.370097736160	-3.262574106656	5.324309223485
C	-3.492886273895	-4.296177520977	5.285140797220
C	-2.714873345076	-2.585881913781	-1.099441147726
C	-3.597365832425	-3.689498675177	-1.679023532473
O	-3.938852109084	-3.301025757896	-3.019638476682
C	-4.720211952385	-4.118783546578	-3.756490176703
C	-5.033977404151	-3.660309281027	-5.079119020887
C	-5.860750112383	-4.500480604749	-5.890370304093
N	-6.356080093326	-5.706304131966	-5.463182649269
C	-6.034719564450	-6.077730466972	-4.237611586184
C	-5.228271069046	-5.337704572196	-3.338257336707
C	-4.562429470922	-2.425681119171	-5.598206366621
C	-4.898464341508	-2.033069879543	-6.879466898150
C	-5.717284268940	-2.860052192238	-7.688343812391
C	-6.186489226411	-4.065080211200	-7.204328081837
C	1.813699022707	-6.246756634718	3.461932970455
H	3.259734809882	-4.106038950040	4.090465660721
H	3.576858463071	-2.258696256994	5.754565896444
H	1.529092527422	-1.178985279815	6.739225971943
H	-3.903531292633	-1.776717781832	1.253396016521

H	-0.650168315440	-4.212500320664	-0.171794515758
H	-1.880800975650	-3.272717494445	6.304858229989
H	-2.770414313201	-2.249089656195	5.167271529264
H	-4.022018146897	-4.284312627741	4.320833424204
H	-3.100393518004	-5.311329582413	5.456633419574
H	-4.227118972629	-4.071630155837	6.075622135520
H	-3.270981716551	-1.636154806930	-1.134220708201
H	-1.826951508375	-2.471544340214	-1.740740311115
H	-4.518048174985	-3.812250464781	-1.083390571657
H	-3.062983041396	-4.654681813947	-1.697860053083
H	-6.432931599967	-7.041963198746	-3.901047002430
H	-5.028555365282	-5.742404685693	-2.347750531878
H	-3.933255757416	-1.794984688116	-4.969888490140
H	-4.532960853468	-1.082126297824	-7.272656502947
H	-5.976838746987	-2.539823501706	-8.699868066967
H	-6.818370144102	-4.717786806070	-7.809779512541
H	2.723827479966	-6.143495000507	2.848386241797
H	2.094089976893	-6.330778192200	4.519029389437
H	1.291578249259	-7.155899192819	3.141561517277

SCF Done: E(RB3LYP) = -1390.83566720

Zero-point correction= 0.440719
Thermal correction to Energy= 0.467320
Thermal correction to Enthalpy= 0.468264
Thermal correction to Gibbs Free Energy= 0.380863
Sum of electronic and zero-point Energies= -1390.394948
Sum of electronic and thermal Energies= -1390.368347
Sum of electronic and thermal Enthalpies= -1390.367403
Sum of electronic and thermal Free Energies= -1390.454805

1	N	Isotropic =	-40.6183	Anisotropy =	455.2493
2	C	Isotropic =	37.0989	Anisotropy =	119.8343
3	C	Isotropic =	60.0101	Anisotropy =	120.7949
4	C	Isotropic =	62.9443	Anisotropy =	176.9175
5	C	Isotropic =	72.1419	Anisotropy =	159.7479
6	C	Isotropic =	48.9772	Anisotropy =	154.5151
7	N	Isotropic =	123.1840	Anisotropy =	90.9160
8	C	Isotropic =	27.1188	Anisotropy =	108.3460
9	C	Isotropic =	70.6149	Anisotropy =	134.1901
10	C	Isotropic =	33.5083	Anisotropy =	125.1061
11	N	Isotropic =	136.0114	Anisotropy =	64.6597
12	O	Isotropic =	-82.1839	Anisotropy =	583.3175
13	N	Isotropic =	-36.2215	Anisotropy =	453.7452

14	C	Isotropic =	40.6167	Anisotropy =	147.4184
15	C	Isotropic =	65.0810	Anisotropy =	166.5834
16	C	Isotropic =	50.5064	Anisotropy =	183.5870
17	C	Isotropic =	147.5355	Anisotropy =	35.8846
18	C	Isotropic =	176.8843	Anisotropy =	24.1459
19	C	Isotropic =	157.1068	Anisotropy =	32.3236
20	C	Isotropic =	121.1151	Anisotropy =	67.1984
21	O	Isotropic =	198.3645	Anisotropy =	106.7528
22	C	Isotropic =	31.8553	Anisotropy =	137.6025
23	C	Isotropic =	70.3974	Anisotropy =	170.6305
24	C	Isotropic =	43.8415	Anisotropy =	182.1565
25	N	Isotropic =	-38.9061	Anisotropy =	454.7104
26	C	Isotropic =	42.3414	Anisotropy =	159.2793
27	C	Isotropic =	90.9549	Anisotropy =	132.9730
28	C	Isotropic =	70.4642	Anisotropy =	175.1337
29	C	Isotropic =	67.5177	Anisotropy =	170.2867
30	C	Isotropic =	63.5129	Anisotropy =	175.1296
31	C	Isotropic =	63.4721	Anisotropy =	149.2941
32	C	Isotropic =	154.5140	Anisotropy =	45.1697
33	H	Isotropic =	23.9754	Anisotropy =	8.9420
34	H	Isotropic =	24.2713	Anisotropy =	4.4831
35	H	Isotropic =	23.1803	Anisotropy =	4.9317
36	H	Isotropic =	22.9529	Anisotropy =	8.4082
37	H	Isotropic =	23.2930	Anisotropy =	11.1065
38	H	Isotropic =	27.5526	Anisotropy =	6.1726
39	H	Isotropic =	26.9527	Anisotropy =	7.8509
40	H	Isotropic =	29.8333	Anisotropy =	5.3845
41	H	Isotropic =	30.3643	Anisotropy =	8.0436
42	H	Isotropic =	30.2626	Anisotropy =	10.8262
43	H	Isotropic =	28.2859	Anisotropy =	5.6515
44	H	Isotropic =	28.2284	Anisotropy =	5.1239
45	H	Isotropic =	27.4062	Anisotropy =	6.4580
46	H	Isotropic =	27.2790	Anisotropy =	7.4859
47	H	Isotropic =	22.7483	Anisotropy =	7.5020
48	H	Isotropic =	24.9118	Anisotropy =	8.9330
49	H	Isotropic =	22.9983	Anisotropy =	10.6168
50	H	Isotropic =	23.7884	Anisotropy =	6.1304
51	H	Isotropic =	23.5956	Anisotropy =	5.0928
52	H	Isotropic =	23.5267	Anisotropy =	5.9165
53	H	Isotropic =	27.9311	Anisotropy =	9.9920
54	H	Isotropic =	28.7931	Anisotropy =	7.6339
55	H	Isotropic =	27.4464	Anisotropy =	8.0675

Conformer 24

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc) #symmetry=(none) scrf=(cpcm,solvent=dmso)

N	1.301338677789	-4.441484334766	0.610119678546
C	0.359359109040	-4.950834014574	1.408025688434
C	0.223025459926	-4.567416339769	2.761134632377
C	1.085702684892	-3.575942023164	3.242856001798
C	2.063055368850	-3.038348496114	2.404370923288
C	2.144488207429	-3.522398817675	1.101042791915
N	-0.676587388174	-5.221567412491	3.645961261027
C	-2.026575954586	-5.354975623024	3.408984566902
C	-2.557685567578	-5.193063478645	2.018376933606
C	-1.884118109065	-5.590661643579	0.837460979004
N	-0.512816458937	-5.918567276473	0.841284618622
O	-2.798855946979	-5.631072718992	4.328210194719
N	-2.525243044253	-5.705025573451	-0.334566293357
C	-3.813331110460	-5.354361586913	-0.403999549921
C	-4.560585126547	-4.859736900223	0.672484216057
C	-3.902655356198	-4.824281302760	1.904509457519
C	0.005817710570	-6.706566505016	-0.296940188947
C	-0.487505199890	-8.150574013928	-0.253705625509
C	-5.996246523164	-4.422006336250	0.508099367333
C	-6.179624370898	-2.926434184982	0.232101212733
O	-5.647742228115	-2.571103331909	-1.060135646642
C	-4.520483473315	-1.838783985822	-1.198462408026
C	-4.197799900023	-1.470515610122	-2.548435841260
C	-3.015132462089	-0.693413250856	-2.761349849153
N	-2.188873333880	-0.288207660213	-1.744807364196
C	-2.533215563197	-0.656074346713	-0.523971890918
C	-3.672267748560	-1.425222563880	-0.184100028183
C	-5.000343101228	-1.845288646763	-3.658753996203
C	-4.644493357923	-1.466211288505	-4.938684424727
C	-3.473689672138	-0.697893907617	-5.156422999401
C	-2.679135339356	-0.320802206186	-4.092130801128
C	-0.230087098629	-5.475281181092	5.021397449330
H	1.007648466639	-3.244241504539	4.278616199778
H	2.751361937754	-2.272158573990	2.763070754807
H	2.914603503037	-3.158533134090	0.414151435209
H	-4.286298108792	-5.477572594535	-1.384452523592
H	-4.436510400403	-4.546575148961	2.815306896074
H	-0.266705586299	-6.232295476172	-1.252215385698
H	1.098231935508	-6.676443413028	-0.216543248777

H	-0.037472815861	-8.718333479369	-1.084133675236
H	-0.200792436357	-8.637154430259	0.692343670295
H	-1.580964972951	-8.208800326850	-0.359273654747
H	-6.468871494405	-4.982641690041	-0.313918271051
H	-6.567399570114	-4.650967120351	1.422945145569
H	-5.738546779186	-2.306445445364	1.024400657010
H	-7.253187030670	-2.693869900347	0.175134799065
H	-1.868896079092	-0.334476560090	0.286463953942
H	-3.840001490001	-1.680752603636	0.860135046582
H	-5.899369205304	-2.435917642793	-3.482680388886
H	-5.266550837611	-1.758203501441	-5.787385425282
H	-3.201275926079	-0.403426295162	-6.172412270697
H	-1.773455812954	0.271563305376	-4.235977639806
H	-0.772863648306	-6.344442782596	5.410786116519
H	0.847162807343	-5.681998093500	5.011748709790
H	-0.433390239211	-4.621117025796	5.688216033494

SCF Done: E(RB3LYP) = -1390.83178026

Zero-point correction= 0.440774
Thermal correction to Energy= 0.467262
Thermal correction to Enthalpy= 0.468206
Thermal correction to Gibbs Free Energy= 0.380915
Sum of electronic and zero-point Energies= -1390.391006
Sum of electronic and thermal Energies= -1390.364519
Sum of electronic and thermal Enthalpies= -1390.363574
Sum of electronic and thermal Free Energies= -1390.450865

1	N	Isotropic =	-40.6077	Anisotropy =	456.3132
2	C	Isotropic =	37.2286	Anisotropy =	121.1742
3	C	Isotropic =	59.8186	Anisotropy =	121.9276
4	C	Isotropic =	62.9000	Anisotropy =	177.3592
5	C	Isotropic =	72.2841	Anisotropy =	160.3611
6	C	Isotropic =	49.1165	Anisotropy =	155.2277
7	N	Isotropic =	123.1327	Anisotropy =	91.1880
8	C	Isotropic =	26.7953	Anisotropy =	108.0898
9	C	Isotropic =	70.2337	Anisotropy =	133.9306
10	C	Isotropic =	33.8881	Anisotropy =	124.5583
11	N	Isotropic =	135.8519	Anisotropy =	65.7442
12	O	Isotropic =	-81.7071	Anisotropy =	579.8277
13	N	Isotropic =	-33.8692	Anisotropy =	453.7065
14	C	Isotropic =	41.1885	Anisotropy =	148.6904
15	C	Isotropic =	62.9235	Anisotropy =	172.3526
16	C	Isotropic =	50.8790	Anisotropy =	182.6041

17	C	Isotropic =	147.7909	Anisotropy =	36.6830
18	C	Isotropic =	177.2329	Anisotropy =	24.5221
19	C	Isotropic =	155.5851	Anisotropy =	15.8882
20	C	Isotropic =	123.4914	Anisotropy =	53.3345
21	O	Isotropic =	201.3941	Anisotropy =	132.8409
22	C	Isotropic =	31.7573	Anisotropy =	139.4690
23	C	Isotropic =	70.5680	Anisotropy =	171.1314
24	C	Isotropic =	43.7444	Anisotropy =	182.2262
25	N	Isotropic =	-35.8112	Anisotropy =	456.9987
26	C	Isotropic =	43.3537	Anisotropy =	160.9578
27	C	Isotropic =	92.7319	Anisotropy =	139.5981
28	C	Isotropic =	69.9217	Anisotropy =	175.0191
29	C	Isotropic =	67.9161	Anisotropy =	170.1848
30	C	Isotropic =	63.7252	Anisotropy =	174.9223
31	C	Isotropic =	64.0605	Anisotropy =	150.4231
32	C	Isotropic =	154.4204	Anisotropy =	45.6155
33	H	Isotropic =	23.9421	Anisotropy =	8.6101
34	H	Isotropic =	24.2684	Anisotropy =	4.3185
35	H	Isotropic =	23.2766	Anisotropy =	4.4208
36	H	Isotropic =	23.3641	Anisotropy =	6.3273
37	H	Isotropic =	23.2861	Anisotropy =	9.9986
38	H	Isotropic =	27.3308	Anisotropy =	7.0470
39	H	Isotropic =	27.6980	Anisotropy =	5.8231
40	H	Isotropic =	30.4148	Anisotropy =	11.1372
41	H	Isotropic =	30.4679	Anisotropy =	8.7001
42	H	Isotropic =	30.0018	Anisotropy =	4.9251
43	H	Isotropic =	28.2052	Anisotropy =	7.1006
44	H	Isotropic =	28.4897	Anisotropy =	7.9525
45	H	Isotropic =	26.8368	Anisotropy =	4.5121
46	H	Isotropic =	26.9337	Anisotropy =	7.9706
47	H	Isotropic =	23.5223	Anisotropy =	6.4780
48	H	Isotropic =	25.6417	Anisotropy =	7.0170
49	H	Isotropic =	23.0826	Anisotropy =	10.5913
50	H	Isotropic =	23.8303	Anisotropy =	5.8400
51	H	Isotropic =	23.6756	Anisotropy =	4.9941
52	H	Isotropic =	23.6789	Anisotropy =	6.2461
53	H	Isotropic =	27.4513	Anisotropy =	8.4853
54	H	Isotropic =	28.8151	Anisotropy =	7.9682
55	H	Isotropic =	27.9117	Anisotropy =	9.9201

Conformer 25

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)

#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-1.327920207978	-7.055230729242	-1.201857054806
C	-0.833505636262	-5.893563120516	-1.636991563635
C	0.509189232600	-5.511045319156	-1.418982822487
C	1.313774254428	-6.374495246184	-0.666402647078
C	0.791708665640	-7.582926436895	-0.203206988745
C	-0.530011292400	-7.888028628077	-0.518872048348
N	1.071331095356	-4.350620064247	-2.017328067431
C	0.547786914722	-3.084575115396	-1.879209437761
C	-0.870818440592	-2.911381454320	-1.432657788559
C	-1.943190109799	-3.770307287940	-1.776486330897
N	-1.718988800898	-5.040062948231	-2.348443099672
O	1.230110285396	-2.092961124868	-2.141384242346
N	-3.221670548288	-3.405832670769	-1.603212381272
C	-3.485966350635	-2.232628592420	-1.018628556499
C	-2.511901768451	-1.337879750638	-0.558525817308
C	-1.186045663135	-1.695908796360	-0.816091851320
C	-2.848467506433	-5.682515713346	-3.052927456813
C	-3.167067120126	-4.976728273679	-4.368503091965
C	-2.879902569757	-0.051439136230	0.141129701168
C	-2.870463815400	-0.127886932333	1.670710476032
O	-3.931186740864	-0.977264723716	2.153036918913
C	-3.689278624034	-2.185944803462	2.707049248136
C	-4.836697177439	-2.832730517312	3.279127590140
C	-4.644216528542	-4.115391913900	3.884011019790
N	-3.427302785635	-4.744463369637	3.941576598286
C	-2.407566283282	-4.105205326382	3.397662959512
C	-2.468638657938	-2.838061877938	2.769075288423
C	-6.131885163105	-2.250024427862	3.266318528291
C	-7.203150216767	-2.914052574678	3.832020798639
C	-7.019432081268	-4.185038430238	4.431696296367
C	-5.769308024573	-4.770375347329	4.456703075478
C	2.444906436065	-4.433863293369	-2.529344662535
H	2.352704961138	-6.112007522308	-0.464750659806
H	1.404607800206	-8.274100267595	0.376561785899
H	-0.975970994244	-8.838186229553	-0.209606645393
H	-4.547523231515	-1.984009611396	-0.911669080853
H	-0.366879530372	-1.014296933317	-0.579306847503
H	-2.540641841579	-6.716994973798	-3.242660078003
H	-3.738839451462	-5.718398833859	-2.406408625647
H	-3.972085699224	-5.518188081826	-4.891216396178
H	-3.508200008625	-3.944145637308	-4.202625164959
H	-2.283815952672	-4.951929710624	-5.026744710617

H	-2.173301809410	0.745976062305	-0.142857732308
H	-3.880790881831	0.277996679779	-0.179813699721
H	-3.086728487315	0.866868622115	2.087408423033
H	-1.896032270899	-0.455169018317	2.058547798940
H	-1.436676937160	-4.612199136070	3.440548252160
H	-1.560302336703	-2.419926428986	2.340374247831
H	-6.263803936334	-1.272298053477	2.802982766539
H	-8.196054029920	-2.459692362016	3.818559996622
H	-7.873160805472	-4.701645641872	4.876002718483
H	-5.604520688885	-5.748073559322	4.913690155540
H	2.619421944145	-5.447016936009	-2.911712534185
H	2.562166489608	-3.704590336209	-3.339426872401
H	3.192002927921	-4.201488143662	-1.752559687177

SCF Done: E(RB3LYP) = -1390.83184468

Zero-point correction= 0.440843
Thermal correction to Energy= 0.467292
Thermal correction to Enthalpy= 0.468236
Thermal correction to Gibbs Free Energy= 0.381400
Sum of electronic and zero-point Energies= -1390.391001
Sum of electronic and thermal Energies= -1390.364553
Sum of electronic and thermal Enthalpies= -1390.363609
Sum of electronic and thermal Free Energies= -1390.450444

1	N	Isotropic =	-40.8283	Anisotropy =	455.8826
2	C	Isotropic =	37.2477	Anisotropy =	121.6546
3	C	Isotropic =	60.0217	Anisotropy =	121.3926
4	C	Isotropic =	62.8732	Anisotropy =	177.3978
5	C	Isotropic =	72.3581	Anisotropy =	160.0445
6	C	Isotropic =	49.0907	Anisotropy =	155.4347
7	N	Isotropic =	123.2140	Anisotropy =	91.3677
8	C	Isotropic =	26.8812	Anisotropy =	107.9732
9	C	Isotropic =	70.0812	Anisotropy =	134.3395
10	C	Isotropic =	33.5715	Anisotropy =	124.1412
11	N	Isotropic =	136.1204	Anisotropy =	66.4198
12	O	Isotropic =	-81.5085	Anisotropy =	581.2051
13	N	Isotropic =	-34.3358	Anisotropy =	454.0568
14	C	Isotropic =	41.1327	Anisotropy =	148.0692
15	C	Isotropic =	62.7668	Anisotropy =	172.5921
16	C	Isotropic =	51.0474	Anisotropy =	182.2322
17	C	Isotropic =	147.6136	Anisotropy =	36.2496
18	C	Isotropic =	177.1874	Anisotropy =	24.4899
19	C	Isotropic =	155.2303	Anisotropy =	16.0149

20	C	Isotropic =	123.1157	Anisotropy =	53.5067
21	O	Isotropic =	201.2754	Anisotropy =	133.4270
22	C	Isotropic =	31.6619	Anisotropy =	139.3187
23	C	Isotropic =	70.5342	Anisotropy =	171.1628
24	C	Isotropic =	43.6604	Anisotropy =	181.8224
25	N	Isotropic =	-36.0145	Anisotropy =	456.8662
26	C	Isotropic =	43.3396	Anisotropy =	160.7252
27	C	Isotropic =	92.4148	Anisotropy =	138.7212
28	C	Isotropic =	69.8341	Anisotropy =	174.5876
29	C	Isotropic =	68.0300	Anisotropy =	170.4575
30	C	Isotropic =	63.7452	Anisotropy =	175.1715
31	C	Isotropic =	64.0966	Anisotropy =	150.5131
32	C	Isotropic =	154.4711	Anisotropy =	45.8061
33	H	Isotropic =	23.9608	Anisotropy =	8.5977
34	H	Isotropic =	24.2772	Anisotropy =	4.3116
35	H	Isotropic =	23.2628	Anisotropy =	4.3909
36	H	Isotropic =	23.3452	Anisotropy =	6.5165
37	H	Isotropic =	23.2838	Anisotropy =	10.0698
38	H	Isotropic =	27.7189	Anisotropy =	5.7940
39	H	Isotropic =	27.2870	Anisotropy =	7.0747
40	H	Isotropic =	30.4198	Anisotropy =	11.1325
41	H	Isotropic =	29.9879	Anisotropy =	4.9149
42	H	Isotropic =	30.4776	Anisotropy =	8.6180
43	H	Isotropic =	28.4919	Anisotropy =	7.8602
44	H	Isotropic =	28.2353	Anisotropy =	7.0114
45	H	Isotropic =	26.8957	Anisotropy =	7.9319
46	H	Isotropic =	26.7980	Anisotropy =	4.3960
47	H	Isotropic =	23.4939	Anisotropy =	6.5866
48	H	Isotropic =	25.6135	Anisotropy =	6.9631
49	H	Isotropic =	23.0935	Anisotropy =	10.6209
50	H	Isotropic =	23.8303	Anisotropy =	5.8557
51	H	Isotropic =	23.6731	Anisotropy =	5.0032
52	H	Isotropic =	23.6733	Anisotropy =	6.2869
53	H	Isotropic =	28.8111	Anisotropy =	7.8882
54	H	Isotropic =	27.4539	Anisotropy =	8.4826
55	H	Isotropic =	27.9047	Anisotropy =	9.9361

Conformer 26

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N 2.058412655775 -4.404181129361 -3.076345150456

C	1.447062887054	-5.230826874754	-2.224279489774
C	1.978510897041	-5.539358036744	-0.952500180392
C	3.159835647720	-4.892860809309	-0.570506057196
C	3.788375799178	-4.016520632404	-1.455985007376
C	3.208483753491	-3.823059318855	-2.707560521937
N	1.406473556134	-6.535832039487	-0.116269599918
C	0.087288009565	-6.544918917025	0.278852082269
C	-0.919532232229	-5.725478474422	-0.467919638002
C	-0.908894977001	-5.494953138241	-1.865361004228
N	0.219214469461	-5.806536806600	-2.652413424759
O	-0.274797009319	-7.236132818234	1.232092145563
N	-1.977837438127	-5.001943487719	-2.507070507220
C	-3.058670480710	-4.661961279329	-1.797163969612
C	-3.159946249745	-4.771654111638	-0.404854673795
C	-2.063675457978	-5.346899401650	0.242660346846
C	0.020356381593	-5.948585695599	-4.109786701606
C	0.995008589071	-6.955641303264	-4.713986765814
C	-4.388259265975	-4.311228874378	0.343953602394
C	-4.223151877640	-2.890394503517	0.879383378978
O	-5.428297944944	-2.561578460416	1.589431904140
C	-5.527311488195	-1.353328302087	2.183177812226
C	-6.753945156808	-1.099060362168	2.882495144839
C	-6.895297722023	0.170030307565	3.528142304221
N	-5.923115193915	1.137588206476	3.505168341445
C	-4.816280253952	0.849376409144	2.845561178544
C	-4.555081627612	-0.366717589567	2.167389776992
C	-7.809687689800	-2.045803996901	2.954141845808
C	-8.969398422630	-1.747670966755	3.643315911427
C	-9.115821656738	-0.492963887729	4.285954531895
C	-8.102235807715	0.442945068421	4.228926324163
C	2.314934592232	-7.413831431359	0.631931404454
H	3.597023383567	-5.092725456154	0.408128149071
H	4.714648233452	-3.509983487736	-1.182238545002
H	3.681949294474	-3.174915963720	-3.451206151328
H	-3.904514889369	-4.275045682480	-2.376729096705
H	-2.094157405147	-5.554524910780	1.313812942444
H	-1.011467024045	-6.291114708431	-4.245764026208
H	0.108603331028	-4.972047763450	-4.611639192843
H	2.038817025381	-6.619677308055	-4.624385978180
H	0.901210310984	-7.938094655301	-4.224000601267
H	0.773844511137	-7.082172564593	-5.785930476663
H	-5.269155191276	-4.339875204087	-0.316094924375
H	-4.589311404142	-4.983777838279	1.192759904281
H	-4.070510096019	-2.172459584643	0.055422440984

H	-3.360482759496	-2.824690379638	1.564216779057
H	-4.042867122630	1.625983352281	2.829847994946
H	-3.603564064732	-0.494892265282	1.654566460867
H	-7.689112625243	-3.008634406591	2.457387924109
H	-9.777614606765	-2.480191920302	3.694656419698
H	-10.036690605706	-0.267821661959	4.828529053438
H	-8.193637423735	1.415641973542	4.716167126549
H	1.806315561502	-8.366655429982	0.819164225337
H	3.217305732125	-7.584101659201	0.032035211255
H	2.598438549395	-6.982789817251	1.606319016418

SCF Done: E(RB3LYP) = -1390.83586777

Zero-point correction= 0.440736
Thermal correction to Energy= 0.467325
Thermal correction to Enthalpy= 0.468269
Thermal correction to Gibbs Free Energy= 0.381424
Sum of electronic and zero-point Energies= -1390.395132
Sum of electronic and thermal Energies= -1390.368543
Sum of electronic and thermal Enthalpies= -1390.367599
Sum of electronic and thermal Free Energies= -1390.454444

1	N	Isotropic =	-42.3105	Anisotropy =	468.8620
2	C	Isotropic =	38.5785	Anisotropy =	117.4721
3	C	Isotropic =	58.8768	Anisotropy =	122.6061
4	C	Isotropic =	62.9242	Anisotropy =	176.8610
5	C	Isotropic =	72.4641	Anisotropy =	159.5203
6	C	Isotropic =	48.7718	Anisotropy =	154.5574
7	N	Isotropic =	122.9182	Anisotropy =	91.3674
8	C	Isotropic =	26.7884	Anisotropy =	108.3274
9	C	Isotropic =	71.5822	Anisotropy =	131.9345
10	C	Isotropic =	32.0161	Anisotropy =	125.0506
11	N	Isotropic =	136.8351	Anisotropy =	63.8176
12	O	Isotropic =	-80.8725	Anisotropy =	583.3653
13	N	Isotropic =	-34.7507	Anisotropy =	442.1639
14	C	Isotropic =	40.9003	Anisotropy =	146.2491
15	C	Isotropic =	64.7313	Anisotropy =	166.8152
16	C	Isotropic =	50.9459	Anisotropy =	180.8373
17	C	Isotropic =	148.6000	Anisotropy =	34.0014
18	C	Isotropic =	177.3599	Anisotropy =	23.6451
19	C	Isotropic =	156.5138	Anisotropy =	32.5093
20	C	Isotropic =	121.1268	Anisotropy =	67.0404
21	O	Isotropic =	197.5105	Anisotropy =	104.2213
22	C	Isotropic =	31.9179	Anisotropy =	137.6903

23	C	Isotropic =	70.5373	Anisotropy =	170.7952
24	C	Isotropic =	43.8118	Anisotropy =	181.5229
25	N	Isotropic =	-37.6136	Anisotropy =	458.6925
26	C	Isotropic =	42.5572	Anisotropy =	159.5091
27	C	Isotropic =	91.0128	Anisotropy =	132.7562
28	C	Isotropic =	70.0201	Anisotropy =	173.8240
29	C	Isotropic =	67.7180	Anisotropy =	170.5950
30	C	Isotropic =	63.6511	Anisotropy =	175.2810
31	C	Isotropic =	63.9417	Anisotropy =	150.5554
32	C	Isotropic =	154.5272	Anisotropy =	45.1335
33	H	Isotropic =	23.9640	Anisotropy =	8.7196
34	H	Isotropic =	24.2656	Anisotropy =	4.4192
35	H	Isotropic =	23.1565	Anisotropy =	4.9116
36	H	Isotropic =	22.9973	Anisotropy =	8.2506
37	H	Isotropic =	23.4066	Anisotropy =	11.0154
38	H	Isotropic =	27.3653	Anisotropy =	6.1387
39	H	Isotropic =	27.0834	Anisotropy =	8.1557
40	H	Isotropic =	29.9916	Anisotropy =	5.1266
41	H	Isotropic =	30.3798	Anisotropy =	8.1430
42	H	Isotropic =	30.2383	Anisotropy =	11.0328
43	H	Isotropic =	28.2028	Anisotropy =	5.4940
44	H	Isotropic =	28.2289	Anisotropy =	5.2034
45	H	Isotropic =	27.5447	Anisotropy =	6.4013
46	H	Isotropic =	27.5518	Anisotropy =	7.5792
47	H	Isotropic =	22.8036	Anisotropy =	7.6307
48	H	Isotropic =	25.0584	Anisotropy =	8.8748
49	H	Isotropic =	23.0503	Anisotropy =	10.5573
50	H	Isotropic =	23.7851	Anisotropy =	6.1333
51	H	Isotropic =	23.5916	Anisotropy =	5.1173
52	H	Isotropic =	23.5094	Anisotropy =	6.0037
53	H	Isotropic =	27.4106	Anisotropy =	8.2473
54	H	Isotropic =	28.8132	Anisotropy =	7.5544
55	H	Isotropic =	27.9474	Anisotropy =	9.9210

Conformer 27

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.747086033885	-5.136897574916	-1.508403367338
C	1.585217439132	-4.988341696834	-2.149754618762
C	1.291774711195	-3.852594326610	-2.936667189317
C	2.246626959460	-2.829993902341	-2.978710346701

C	3.453502920973	-2.979889732864	-2.294380082623
C	3.664853971993	-4.163642591457	-1.591285537313
N	0.122638080660	-3.772967721700	-3.740896698554
C	-1.156547344672	-3.941925968457	-3.260049798866
C	-1.371990586297	-4.607426777976	-1.935840837632
C	-0.594027718611	-5.674868751185	-1.424728727368
N	0.634134272269	-6.036708382386	-2.015989525397
O	-2.126971182603	-3.565163853802	-3.918845982254
N	-1.002605972128	-6.409430246979	-0.380498842153
C	-2.146652704435	-6.084190416111	0.230337852268
C	-2.963202801010	-5.007314614294	-0.135752408828
C	-2.557749989804	-4.290379152412	-1.264488757982
C	1.161332120672	-7.386888605597	-1.728985461203
C	1.977473754919	-7.930300472048	-2.898422546444
C	-4.214716603548	-4.660565410947	0.635358542439
C	-3.963811729169	-3.549681540667	1.652942498450
O	-5.210807635222	-3.298894670420	2.321570230460
C	-5.258923789964	-2.348397109925	3.278709220200
C	-6.533840210498	-2.158262459526	3.908504014983
C	-6.623800935147	-1.158629369415	4.928475762562
N	-5.559449734399	-0.387612968680	5.321759722746
C	-4.411125387124	-0.606166684493	4.707950867993
C	-4.193070384509	-1.563198351284	3.686493173157
C	-7.684724152010	-2.913830313438	3.561025124247
C	-8.887599401444	-2.688646063401	4.202258710672
C	-8.983937371226	-1.700236316977	5.213407802734
C	-7.877677441173	-0.953529855413	5.567206000200
C	0.241657866073	-3.171779979273	-5.075236098831
H	2.054794772344	-1.930152142356	-3.563966571799
H	4.215385496519	-2.199981399548	-2.322186947180
H	4.609325038931	-4.345095296208	-1.069423394903
H	-2.435314719134	-6.725979756574	1.070500633114
H	-3.181392187501	-3.493829416562	-1.674355364565
H	1.759729213909	-7.383906040259	-0.804242053403
H	0.288061579100	-8.023487555669	-1.547780134616
H	1.380005892070	-7.941422035047	-3.824174781165
H	2.884767232038	-7.334065202008	-3.076569500562
H	2.292065229780	-8.962941746911	-2.677886137638
H	-5.007821270490	-4.331131020541	-0.054553732062
H	-4.588766225144	-5.548343199575	1.168483464409
H	-3.618347185882	-2.627548913770	1.155043769286
H	-3.202073841482	-3.853933435382	2.390908763558
H	-3.563867958020	0.012398824775	5.025889679051
H	-3.200294186628	-1.657445173400	3.250263746286

H	-7.602454474153	-3.672253229340	2.782255198437
H	-9.769010279451	-3.273243546265	3.930558242540
H	-9.939889776901	-1.530364205173	5.713784045907
H	-7.929194669109	-0.187233580898	6.343054969876
H	0.092502508584	-2.079711564915	-5.052349666377
H	1.237315297247	-3.395972102014	-5.476943608574
H	-0.527910542870	-3.604562380529	-5.725143315166

SCF Done: E(RB3LYP) = -1390.83591039

Zero-point correction= 0.440682
Thermal correction to Energy= 0.467312
Thermal correction to Enthalpy= 0.468256
Thermal correction to Gibbs Free Energy= 0.381122
Sum of electronic and zero-point Energies= -1390.395229
Sum of electronic and thermal Energies= -1390.368598
Sum of electronic and thermal Enthalpies= -1390.367654
Sum of electronic and thermal Free Energies= -1390.454788

1	N	Isotropic =	-41.9647	Anisotropy =	469.5749
2	C	Isotropic =	38.5444	Anisotropy =	117.4678
3	C	Isotropic =	58.5521	Anisotropy =	122.8103
4	C	Isotropic =	62.8784	Anisotropy =	176.9047
5	C	Isotropic =	72.3730	Anisotropy =	159.5975
6	C	Isotropic =	48.9440	Anisotropy =	154.6081
7	N	Isotropic =	122.7181	Anisotropy =	91.5367
8	C	Isotropic =	26.8900	Anisotropy =	108.3070
9	C	Isotropic =	71.4917	Anisotropy =	132.1468
10	C	Isotropic =	32.3642	Anisotropy =	124.7092
11	N	Isotropic =	136.9298	Anisotropy =	63.9926
12	O	Isotropic =	-81.4831	Anisotropy =	582.1450
13	N	Isotropic =	-34.0781	Anisotropy =	444.6027
14	C	Isotropic =	41.0973	Anisotropy =	145.8845
15	C	Isotropic =	64.5548	Anisotropy =	166.6399
16	C	Isotropic =	50.9293	Anisotropy =	181.1961
17	C	Isotropic =	148.5857	Anisotropy =	34.0832
18	C	Isotropic =	177.3414	Anisotropy =	23.7833
19	C	Isotropic =	156.5495	Anisotropy =	32.8599
20	C	Isotropic =	121.1719	Anisotropy =	67.0022
21	O	Isotropic =	197.7766	Anisotropy =	105.6705
22	C	Isotropic =	32.1752	Anisotropy =	137.9854
23	C	Isotropic =	70.6060	Anisotropy =	170.9235
24	C	Isotropic =	43.6736	Anisotropy =	181.7436
25	N	Isotropic =	-37.6455	Anisotropy =	458.3010

26	C	Isotropic =	42.4893	Anisotropy =	159.5185
27	C	Isotropic =	91.3734	Anisotropy =	133.1263
28	C	Isotropic =	70.1839	Anisotropy =	173.6792
29	C	Isotropic =	67.8082	Anisotropy =	170.6447
30	C	Isotropic =	63.5468	Anisotropy =	174.8902
31	C	Isotropic =	63.8423	Anisotropy =	150.4472
32	C	Isotropic =	154.3918	Anisotropy =	45.5746
33	H	Isotropic =	23.9681	Anisotropy =	8.7011
34	H	Isotropic =	24.2682	Anisotropy =	4.4110
35	H	Isotropic =	23.1430	Anisotropy =	4.9102
36	H	Isotropic =	22.9843	Anisotropy =	8.2496
37	H	Isotropic =	23.3823	Anisotropy =	10.9843
38	H	Isotropic =	27.0869	Anisotropy =	8.1734
39	H	Isotropic =	27.3765	Anisotropy =	6.1974
40	H	Isotropic =	30.3659	Anisotropy =	8.0840
41	H	Isotropic =	29.9725	Anisotropy =	5.1869
42	H	Isotropic =	30.2369	Anisotropy =	11.0313
43	H	Isotropic =	28.1919	Anisotropy =	5.2749
44	H	Isotropic =	28.2022	Anisotropy =	5.5186
45	H	Isotropic =	27.5216	Anisotropy =	7.5623
46	H	Isotropic =	27.5649	Anisotropy =	6.4303
47	H	Isotropic =	22.8123	Anisotropy =	7.6219
48	H	Isotropic =	25.0500	Anisotropy =	8.8836
49	H	Isotropic =	23.0381	Anisotropy =	10.5881
50	H	Isotropic =	23.7752	Anisotropy =	6.1468
51	H	Isotropic =	23.5977	Anisotropy =	5.1022
52	H	Isotropic =	23.5179	Anisotropy =	5.9890
53	H	Isotropic =	27.9321	Anisotropy =	9.9244
54	H	Isotropic =	28.8094	Anisotropy =	7.5046
55	H	Isotropic =	27.4609	Anisotropy =	8.2741

Conformer 28

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-2.274311699391	-1.867647663363	-4.967681850290
C	-2.805425204359	-2.961086094268	-4.414893234410
C	-4.186904266257	-3.079530763908	-4.142947294999
C	-4.998470829513	-1.973981139961	-4.423023947682
C	-4.439561835612	-0.828572505410	-4.991297712500
C	-3.074225215770	-0.834267776511	-5.266081233672
N	-4.768056099420	-4.297806953127	-3.697156237035

C	-4.351258205008	-4.982714921066	-2.577651327269
C	-2.998362747735	-4.707845639422	-1.997883829930
C	-1.839857854742	-4.391337277340	-2.748274812544
N	-1.917277930960	-4.027354049251	-4.108524140787
O	-5.073728492996	-5.836600438024	-2.061438980958
N	-0.612988670697	-4.450588245258	-2.210430572301
C	-0.490574047535	-4.740549646083	-0.911145629877
C	-1.565416153165	-4.991714117100	-0.049345544566
C	-2.831477101680	-5.000764446260	-0.640107954179
C	-0.681899183650	-4.124428156053	-4.914255777805
C	-0.286155386871	-5.577081365357	-5.166233092096
C	-1.358851408974	-5.255946747640	1.423253258460
C	-1.581634538657	-3.996733316298	2.258193687599
O	-1.359875078118	-4.353135715621	3.632498060089
C	-1.498291542985	-3.404707116235	4.583007936056
C	-1.250701102221	-3.828827807657	5.931034222938
C	-1.388174298650	-2.851050285473	6.966631738875
N	-1.741257110727	-1.547190463908	6.727709365928
C	-1.956191135498	-1.213208838230	5.468578115005
C	-1.852689511941	-2.084853530967	4.356646689367
C	-0.879938931129	-5.158407981237	6.264042498898
C	-0.651723768871	-5.510694974731	7.580316953718
C	-0.786218047995	-4.547384943744	8.611138429591
C	-1.146221189794	-3.248770377979	8.310320900684
C	-6.076510118632	-4.680010136459	-4.242429407174
H	-6.068531855856	-2.019219893775	-4.218383733281
H	-5.055901045003	0.040163332219	-5.225678678038
H	-2.593846683504	0.025783321014	-5.742357810011
H	0.535402111889	-4.780808226801	-0.528059037924
H	-3.715387015140	-5.279523353337	-0.063484120370
H	-0.896264816266	-3.620514278998	-5.863484567016
H	0.141014543044	-3.576497070309	-4.429944493144
H	0.601614656369	-5.608838925033	-5.818374528735
H	-0.035325503365	-6.097655131662	-4.230179400224
H	-1.100664325168	-6.126626817179	-5.664809851887
H	-2.054415653156	-6.035697631759	1.772190336794
H	-0.335857699630	-5.621465393665	1.602458228321
H	-2.610712407979	-3.618067467836	2.134898349790
H	-0.878873612695	-3.198439386111	1.964244535530
H	-2.237642247006	-0.170172932839	5.283036075555
H	-2.053019481159	-1.698802144149	3.358858945308
H	-0.778149625616	-5.893286845923	5.465289663668
H	-0.366468104906	-6.534809133926	7.829905272030
H	-0.603311274947	-4.836765339390	9.648394336948

H	-1.255553308525	-2.490566756478	9.088142967609
H	-6.145131625087	-4.326897756914	-5.278589183359
H	-6.162512861205	-5.772574024964	-4.215005828651
H	-6.909263455537	-4.258864708240	-3.655386756047

SCF Done: E(RB3LYP) = -1390.83587496

Zero-point correction= 0.440615
Thermal correction to Energy= 0.467270
Thermal correction to Enthalpy= 0.468214
Thermal correction to Gibbs Free Energy= 0.380496
Sum of electronic and zero-point Energies= -1390.395260
Sum of electronic and thermal Energies= -1390.368605
Sum of electronic and thermal Enthalpies= -1390.367661
Sum of electronic and thermal Free Energies= -1390.455379

1	N	Isotropic =	-40.7618	Anisotropy =	456.3995
2	C	Isotropic =	36.9043	Anisotropy =	120.5041
3	C	Isotropic =	59.6736	Anisotropy =	121.4866
4	C	Isotropic =	62.7564	Anisotropy =	177.2517
5	C	Isotropic =	72.2914	Anisotropy =	159.9987
6	C	Isotropic =	49.1557	Anisotropy =	154.3497
7	N	Isotropic =	122.7486	Anisotropy =	91.1326
8	C	Isotropic =	27.2521	Anisotropy =	109.0710
9	C	Isotropic =	70.4471	Anisotropy =	133.2562
10	C	Isotropic =	33.2289	Anisotropy =	124.0934
11	N	Isotropic =	135.9733	Anisotropy =	65.1136
12	O	Isotropic =	-81.6525	Anisotropy =	583.7654
13	N	Isotropic =	-35.6694	Anisotropy =	453.0123
14	C	Isotropic =	40.9413	Anisotropy =	144.7908
15	C	Isotropic =	64.8660	Anisotropy =	166.1183
16	C	Isotropic =	51.2469	Anisotropy =	182.1052
17	C	Isotropic =	147.3705	Anisotropy =	35.9476
18	C	Isotropic =	177.0263	Anisotropy =	24.2268
19	C	Isotropic =	156.3695	Anisotropy =	32.7923
20	C	Isotropic =	121.1490	Anisotropy =	67.1755
21	O	Isotropic =	197.8076	Anisotropy =	104.7820
22	C	Isotropic =	31.9346	Anisotropy =	137.9934
23	C	Isotropic =	70.5636	Anisotropy =	170.9036
24	C	Isotropic =	43.8629	Anisotropy =	181.6662
25	N	Isotropic =	-37.6047	Anisotropy =	458.6726
26	C	Isotropic =	42.6458	Anisotropy =	159.5005
27	C	Isotropic =	90.9610	Anisotropy =	132.8505
28	C	Isotropic =	69.9831	Anisotropy =	173.8956

29	C	Isotropic =	67.6106	Anisotropy =	170.7001
30	C	Isotropic =	63.5382	Anisotropy =	175.5558
31	C	Isotropic =	63.8655	Anisotropy =	150.5570
32	C	Isotropic =	154.4269	Anisotropy =	45.3877
33	H	Isotropic =	23.9767	Anisotropy =	8.8084
34	H	Isotropic =	24.2762	Anisotropy =	4.4086
35	H	Isotropic =	23.1954	Anisotropy =	4.8682
36	H	Isotropic =	22.9933	Anisotropy =	8.2993
37	H	Isotropic =	23.3531	Anisotropy =	10.9646
38	H	Isotropic =	27.5513	Anisotropy =	6.0498
39	H	Isotropic =	26.9401	Anisotropy =	7.7035
40	H	Isotropic =	30.2538	Anisotropy =	10.9336
41	H	Isotropic =	29.8260	Anisotropy =	5.3265
42	H	Isotropic =	30.3518	Anisotropy =	8.1399
43	H	Isotropic =	28.1894	Anisotropy =	5.2159
44	H	Isotropic =	28.2424	Anisotropy =	5.4528
45	H	Isotropic =	27.4969	Anisotropy =	7.5874
46	H	Isotropic =	27.5817	Anisotropy =	6.4881
47	H	Isotropic =	22.8109	Anisotropy =	7.6331
48	H	Isotropic =	25.0475	Anisotropy =	8.8927
49	H	Isotropic =	23.0503	Anisotropy =	10.5483
50	H	Isotropic =	23.7760	Anisotropy =	6.1497
51	H	Isotropic =	23.5800	Anisotropy =	5.1358
52	H	Isotropic =	23.4993	Anisotropy =	6.0256
53	H	Isotropic =	28.7859	Anisotropy =	7.6733
54	H	Isotropic =	27.4666	Anisotropy =	8.2432
55	H	Isotropic =	27.9258	Anisotropy =	9.9155

Conformer 29

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	2.805180047898	-4.709778583150	2.110184713148
C	1.603089589380	-5.074005834115	2.563685267311
C	0.993934553174	-4.456328671220	3.678925007084
C	1.672178984720	-3.388488171187	4.277817411491
C	2.923590538958	-3.002790243092	3.795658616132
C	3.457818391520	-3.711862130175	2.722640422017
N	-0.210959074866	-4.948003976591	4.250523375506
C	-1.379240917040	-5.122392564507	3.542741907874
C	-1.337308532672	-5.209193962744	2.048549129677
C	-0.298104914774	-5.809125882924	1.296309986722

N	0.945746310449	-6.130496553557	1.877183316559
O	-2.456450015394	-5.232306478149	4.130053425947
N	-0.456875034277	-6.125905026918	0.002836653798
C	-1.597399243170	-5.792083200549	-0.608948372449
C	-2.661020290166	-5.119870092622	0.006254642959
C	-2.512907633037	-4.865876330857	1.371826306197
C	1.801546050145	-7.105083387517	1.167938286894
C	1.230413403912	-8.518670737354	1.245602203431
C	-3.897191409131	-4.717295344513	-0.762396909820
C	-3.799189867733	-3.282009815283	-1.275363769986
O	-5.020597749789	-2.997522305406	-1.976696614668
C	-5.175623877397	-1.786663663188	-2.552819869191
C	-6.420985894468	-1.571983702857	-3.232077041480
C	-6.620217639777	-0.301812237021	-3.860171849800
N	-5.685957773442	0.702453050230	-3.838499930738
C	-4.560084424558	0.450068247105	-3.196662265056
C	-4.242801762344	-0.762720567754	-2.536782465562
C	-7.440772994832	-2.557609869092	-3.299815603633
C	-8.621118467216	-2.296317660013	-3.968612373462
C	-8.824607904775	-1.041030043124	-4.594293595145
C	-7.846760407710	-0.067652003137	-4.540672754937
C	-0.330956855561	-4.951096848978	5.713671412663
H	1.232204856190	-2.876202847322	5.133971526507
H	3.472681226652	-2.179539878326	4.254199005529
H	4.450243961074	-3.471633994010	2.329326028252
H	-1.673915545872	-6.083445480467	-1.662675879043
H	-3.330265513720	-4.432433680651	1.950981697708
H	1.946422158039	-6.802459102245	0.119426599016
H	2.780700439422	-7.064646247398	1.658348309252
H	0.260643701168	-8.593080111757	0.731769040695
H	1.924744874788	-9.223170853537	0.759771049129
H	1.096734790233	-8.832847773857	2.293194840237
H	-4.044432295445	-5.388703067276	-1.622620533232
H	-4.788516293631	-4.801089097634	-0.120819766046
H	-2.941607688814	-3.166226691817	-1.959952406686
H	-3.678193460021	-2.570349376641	-0.440657760903
H	-3.817334806106	1.256083111147	-3.181442048553
H	-3.280283911971	-0.859815002365	-2.037853119926
H	-7.276310339194	-3.520592195779	-2.816112133467
H	-9.401645598370	-3.058480022897	-4.016753108424
H	-9.761344474094	-0.845154565531	-5.120840550581
H	-7.982568067551	0.906292500261	-5.014860911341
H	-1.028974159153	-5.744069312760	6.006563469411
H	0.656886541064	-5.144405373466	6.149527823627

H -0.721735580714 -3.995276345414 6.099780159358

SCF Done: E(RB3LYP) = -1390.83587024

Zero-point correction= 0.440650
Thermal correction to Energy= 0.467283
Thermal correction to Enthalpy= 0.468228
Thermal correction to Gibbs Free Energy= 0.381098
Sum of electronic and zero-point Energies= -1390.395220
Sum of electronic and thermal Energies= -1390.368587
Sum of electronic and thermal Enthalpies= -1390.367643
Sum of electronic and thermal Free Energies= -1390.454772

1 N Isotropic = -40.8324 Anisotropy = 455.3446
2 C Isotropic = 37.2737 Anisotropy = 120.8117
3 C Isotropic = 59.7492 Anisotropy = 121.8689
4 C Isotropic = 62.7595 Anisotropy = 177.6512
5 C Isotropic = 72.3390 Anisotropy = 160.0448
6 C Isotropic = 49.2803 Anisotropy = 153.9903
7 N Isotropic = 123.1882 Anisotropy = 90.5841
8 C Isotropic = 27.0286 Anisotropy = 108.5061
9 C Isotropic = 70.5214 Anisotropy = 132.9309
10 C Isotropic = 33.2636 Anisotropy = 124.0635
11 N Isotropic = 135.5091 Anisotropy = 65.3523
12 O Isotropic = -81.9334 Anisotropy = 582.5552
13 N Isotropic = -35.1258 Anisotropy = 453.6266
14 C Isotropic = 41.1183 Anisotropy = 145.7714
15 C Isotropic = 64.9692 Anisotropy = 165.9536
16 C Isotropic = 50.7189 Anisotropy = 181.1337
17 C Isotropic = 147.5035 Anisotropy = 36.2363
18 C Isotropic = 177.0496 Anisotropy = 24.1227
19 C Isotropic = 156.5569 Anisotropy = 32.6403
20 C Isotropic = 121.1394 Anisotropy = 67.1373
21 O Isotropic = 197.6021 Anisotropy = 104.8222
22 C Isotropic = 31.9678 Anisotropy = 137.8774
23 C Isotropic = 70.5379 Anisotropy = 170.7789
24 C Isotropic = 43.8604 Anisotropy = 181.6623
25 N Isotropic = -37.6114 Anisotropy = 458.6673
26 C Isotropic = 42.5918 Anisotropy = 159.5797
27 C Isotropic = 90.9847 Anisotropy = 132.8310
28 C Isotropic = 69.9457 Anisotropy = 173.6598
29 C Isotropic = 67.7959 Anisotropy = 170.8056
30 C Isotropic = 63.7315 Anisotropy = 175.4967
31 C Isotropic = 63.9599 Anisotropy = 150.5412

32	C	Isotropic =	154.6207	Anisotropy =	45.2682
33	H	Isotropic =	23.9553	Anisotropy =	8.7961
34	H	Isotropic =	24.2736	Anisotropy =	4.4242
35	H	Isotropic =	23.2042	Anisotropy =	4.8724
36	H	Isotropic =	22.9827	Anisotropy =	8.3694
37	H	Isotropic =	23.3445	Anisotropy =	10.8735
38	H	Isotropic =	26.9528	Anisotropy =	7.7056
39	H	Isotropic =	27.5510	Anisotropy =	6.0460
40	H	Isotropic =	29.8107	Anisotropy =	5.3451
41	H	Isotropic =	30.2609	Anisotropy =	10.9267
42	H	Isotropic =	30.3555	Anisotropy =	8.1117
43	H	Isotropic =	28.2133	Anisotropy =	5.3590
44	H	Isotropic =	28.2002	Anisotropy =	5.2652
45	H	Isotropic =	27.5360	Anisotropy =	6.5398
46	H	Isotropic =	27.5593	Anisotropy =	7.4878
47	H	Isotropic =	22.8038	Anisotropy =	7.6382
48	H	Isotropic =	25.0625	Anisotropy =	8.8929
49	H	Isotropic =	23.0491	Anisotropy =	10.5462
50	H	Isotropic =	23.7729	Anisotropy =	6.1570
51	H	Isotropic =	23.5829	Anisotropy =	5.1288
52	H	Isotropic =	23.5058	Anisotropy =	6.0030
53	H	Isotropic =	27.4744	Anisotropy =	8.2248
54	H	Isotropic =	28.8107	Anisotropy =	7.6668
55	H	Isotropic =	27.9409	Anisotropy =	9.9130

Conformer 30

#B3LYP/cc-pVDZ freq=(noraman) nmr=(giao) opt=(maxcycle=250,noeigen,calcfc)
#symmetry=(none) scrf=(cpcm,solvent=dmso)

N	-3.474862525282	-4.294100966260	5.408775784008
C	-3.493420509744	-3.848369214839	4.149930130764
C	-3.523713123824	-2.471214054408	3.834086932444
C	-3.474041229243	-1.561701158232	4.896540139552
C	-3.443547505961	-2.030052051899	6.210689514917
C	-3.469661641855	-3.407561264305	6.414164626523
N	-3.701771748810	-2.003300814178	2.503066738649
C	-2.891703708014	-2.362078472734	1.450854710975
C	-2.035571539846	-3.584527632149	1.554887068481
C	-2.392421487410	-4.776635006451	2.229864730880
N	-3.488377995752	-4.824395282093	3.117616263868
O	-2.886041211856	-1.697898382041	0.411114358392
N	-1.718373094958	-5.921023090963	2.044815272235

C	-0.647760455124	-5.919350176852	1.242885737352
C	-0.158307640334	-4.789302878903	0.577153603084
C	-0.898995902505	-3.617491443784	0.740512516781
C	-4.041206202284	-6.154345044717	3.449947213380
C	-4.769444635967	-6.776536419671	2.261255018153
C	1.049677620284	-4.846954394543	-0.328668486826
C	0.718454444808	-5.193491643659	-1.779959351608
O	-0.211691489180	-4.213515998108	-2.271782160164
C	-0.605855792774	-4.275489509228	-3.561631212031
C	-1.619052963304	-3.338340670928	-3.955606493746
C	-2.029509375609	-3.350044087044	-5.327013952092
N	-1.516347011552	-4.215786164009	-6.259435716017
C	-0.605261866223	-5.071526047689	-5.834529028462
C	-0.110767593230	-5.156003935088	-4.509951095692
C	-2.225051511120	-2.427849417334	-3.049055125993
C	-3.194412987584	-1.547263151201	-3.489906678208
C	-3.592392472083	-1.540476773982	-4.849797329990
C	-3.024007175282	-2.423827208626	-5.745951854963
C	-4.573678506514	-0.841270012692	2.289769207361
H	-3.483615358461	-0.490067664229	4.695329212816
H	-3.414266395695	-1.338179603877	7.053251888754
H	-3.482570837345	-3.825324925727	7.425398343557
H	-0.140143264356	-6.884130018409	1.128586250589
H	-0.620026571312	-2.707513344010	0.208400474986
H	-3.246813808613	-6.825451833623	3.811607633183
H	-4.738466634463	-5.995960208572	4.280498930018
H	-4.083805737193	-6.974926477795	1.424284036178
H	-5.216764791725	-7.736530014373	2.565792632871
H	-5.576968726693	-6.117500749420	1.904004550453
H	1.576135641071	-3.879901333208	-0.308991378984
H	1.760177457977	-5.608853823543	0.029048075199
H	0.262192342618	-6.195363092609	-1.858903274515
H	1.637458655264	-5.176060547767	-2.388666302044
H	-0.203784983762	-5.766150344277	-6.581510682927
H	0.647981104360	-5.899655811149	-4.273181020851
H	-1.937889933200	-2.438874820573	-1.998040958016
H	-3.659422551612	-0.856616618703	-2.783285403802
H	-4.357119767805	-0.837028369398	-5.186875405186
H	-3.320480873634	-2.443887931915	-6.796482062587
H	-4.991730457131	-0.897497825999	1.277852374214
H	-5.383359122197	-0.866230841740	3.029244504371
H	-4.024816547961	0.110618569524	2.378546499715

SCF Done: E(RB3LYP) = -1390.83679904

Zero-point correction= 0.440970
Thermal correction to Energy= 0.467368
Thermal correction to Enthalpy= 0.468312
Thermal correction to Gibbs Free Energy= 0.382574
Sum of electronic and zero-point Energies= -1390.395829
Sum of electronic and thermal Energies= -1390.369431
Sum of electronic and thermal Enthalpies= -1390.368487
Sum of electronic and thermal Free Energies= -1390.454225

1	N	Isotropic =	-40.8027	Anisotropy =	454.6721
2	C	Isotropic =	36.9038	Anisotropy =	119.9033
3	C	Isotropic =	59.8584	Anisotropy =	120.1282
4	C	Isotropic =	62.5756	Anisotropy =	176.7859
5	C	Isotropic =	72.4211	Anisotropy =	159.4513
6	C	Isotropic =	48.9421	Anisotropy =	154.2388
7	N	Isotropic =	122.4423	Anisotropy =	91.1984
8	C	Isotropic =	25.9322	Anisotropy =	108.0747
9	C	Isotropic =	70.9751	Anisotropy =	133.1152
10	C	Isotropic =	33.9581	Anisotropy =	123.8970
11	N	Isotropic =	135.9687	Anisotropy =	63.3329
12	O	Isotropic =	-78.4664	Anisotropy =	572.4226
13	N	Isotropic =	-36.0511	Anisotropy =	454.0432
14	C	Isotropic =	41.8922	Anisotropy =	148.1141
15	C	Isotropic =	62.3674	Anisotropy =	170.7398
16	C	Isotropic =	48.4913	Anisotropy =	181.7434
17	C	Isotropic =	147.5142	Anisotropy =	35.8177
18	C	Isotropic =	177.0686	Anisotropy =	23.4034
19	C	Isotropic =	157.2155	Anisotropy =	18.1707
20	C	Isotropic =	121.8552	Anisotropy =	43.4204
21	O	Isotropic =	202.9869	Anisotropy =	118.6641
22	C	Isotropic =	32.0308	Anisotropy =	137.4578
23	C	Isotropic =	70.4387	Anisotropy =	169.8514
24	C	Isotropic =	43.7078	Anisotropy =	181.3608
25	N	Isotropic =	-37.4460	Anisotropy =	459.1189
26	C	Isotropic =	42.5725	Anisotropy =	159.0897
27	C	Isotropic =	91.1166	Anisotropy =	133.2792
28	C	Isotropic =	68.3859	Anisotropy =	175.5375
29	C	Isotropic =	67.3256	Anisotropy =	169.8634
30	C	Isotropic =	63.6512	Anisotropy =	174.1041
31	C	Isotropic =	64.1885	Anisotropy =	149.6527
32	C	Isotropic =	154.3148	Anisotropy =	45.7139
33	H	Isotropic =	23.9224	Anisotropy =	9.1714
34	H	Isotropic =	24.2701	Anisotropy =	4.6163

35	H	Isotropic =	23.1703	Anisotropy =	4.9181
36	H	Isotropic =	22.9380	Anisotropy =	7.9393
37	H	Isotropic =	22.8843	Anisotropy =	10.3345
38	H	Isotropic =	26.9687	Anisotropy =	8.2231
39	H	Isotropic =	27.5407	Anisotropy =	6.4825
40	H	Isotropic =	29.9214	Anisotropy =	5.3137
41	H	Isotropic =	30.3242	Anisotropy =	10.9918
42	H	Isotropic =	30.4287	Anisotropy =	7.5646
43	H	Isotropic =	28.2612	Anisotropy =	5.5257
44	H	Isotropic =	28.4436	Anisotropy =	8.5150
45	H	Isotropic =	27.5093	Anisotropy =	6.5097
46	H	Isotropic =	26.9666	Anisotropy =	6.2398
47	H	Isotropic =	22.7558	Anisotropy =	7.1432
48	H	Isotropic =	24.8807	Anisotropy =	9.5925
49	H	Isotropic =	22.5897	Anisotropy =	9.0831
50	H	Isotropic =	23.6413	Anisotropy =	7.4081
51	H	Isotropic =	23.5879	Anisotropy =	5.6379
52	H	Isotropic =	23.5146	Anisotropy =	5.8287
53	H	Isotropic =	27.3487	Anisotropy =	7.9439
54	H	Isotropic =	28.7246	Anisotropy =	7.6334
55	H	Isotropic =	27.8150	Anisotropy =	9.7992