Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Ugi 4-CR/Pictet-Spengler Reaction as a Short Route to Tryptophan-derived Peptidomimetics

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Supporting Information

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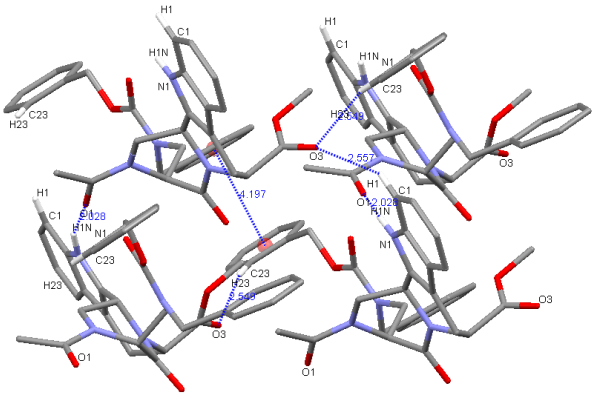
Crystallography. Crystals of **7** suitable for X-ray crystallography were grown by slow evaporation from methanolic solutions. They were mounted on a CAD-4 diffractometer using Mo-Kα (λ= 0.71073 Å) radiation at 293(2)K. The lattice parameters were determined by least-squares refinements of 25 high angle reflections. The structures were solved by direct methods[1] and the refinements were carried out by full-matrix least-squares with SHELX-97 package.[2] All non-H-atoms were refined anisotropically. Hydrogen atoms were detected in a difference Fourier synthesis and refined with isotropic thermal factors or were introduced at calculated positions, in their described geometries and allowed to ride on the attached carbon atom with fixed isotropic thermal parameters (1.2Ueq of the parent carbon atom). Geometrical calculations were carried out using the program PARST.[3] The supplementary crystallographic data were deposited with the Cambridge Crystallographic Data Centre (CCDC deposition number 881658). Copies can be obtained, free of charge, from CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(1223) 336033; e-mail: deposit@ccdc.cam.ac.uk).

Crystal data for 7: $C_{34}H_{34}N_4O_6$, M_r = 594.65 g/mol, Monoclinic, Space group $P2_1/c$, a = 8.740(4) Å, b = 34.939(6) Å, c = 10.664(4) Å, β = 112.69(1)°, V = 3004(4) Å^3, Z = 4, D_{calc} = 1.315 Mg/m^3, R = 0.071 (4688 reflections), *wR2* = 0.171, T = 293(2)K, *GOF* = 0.951. The reflections were collected in the range $2.33° \leq \theta \leq 23.98°$ employing a 0.50 x 0.40 x 0.30 crystal.

For compound **7**, the overall molecular conformation is determined by the 1,2,3,4-tetrahydro-β-carboline-based tetracyclic framework, having its side chains axially oriented. The indole ring system is planar, whereas the piperidine adopts a half-chair and the piperazine a boat conformation, as described by the puckering parameters Q= 0.456(5) Å, φ=-6.2(6)°, θ=119.9(5)° and Q=0.604(4) Å, φ=-4.9(3)°, θ=83.4(3)°. In the piperidine, C10 is out of the best mean plane of the remaining five atoms by 0.607(5)Å, while in the piperazine moiety C11 and C13 are apart from the best mean plane calculated over the other four atoms by 0.592(4)Å and 0.427(4)Å, respectively. The C18-C23

and C25-C30 benzene rings are perpendicularly oriented with respect to the indole moiety forming dihedral angles of 85(1)° and 89(1)°, while between each other they are slightly inclined, with a dihedral angle of 13(1)°. The crystal packing is characterized by intermolecular N1-H1···O1^{I} (^{I} at x, 3/2-y, z-1/2) hydrogen bonds at a distance of 2.03(1)Å and angle of 153(1)°, leading to the formation of *zig-zag* chains running parallel to the *c* axis. Bifurcated weak intermolecular O···H-Cπ contacts involving O3 and C1-H1^{II} (^{II} at x+1, y, z) and C23-H23^{III} (^{III} at x+1, 3/2-y, z+1/2) together with stacking interactions between phenyl rings at 4.197(1)Å, contribute to stabilize the crystal.



Crystal packing: intermolecular interactions viewed about along the *b* axis. For the sake of clarity, only the hydrogen atoms involved in intermolecular contacts were represented.

[1] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Gagliardi, A.; Polidori, G. *J. Appl. Cryst.*, **1994**, *27*, 435 [Links].

[2] Sheldrick, G. M. SHELX-97, Program for the Refinement of Crystal Structure, University of Göttingen, Germany, 1997.

[3] Nardelli, M.; *J. Appl. Crystallogr.*, **1995**, *28*, 659 [Links]

Conformational analysis

Results from conformational analysis of compounds **a-c** and **10-12**

Table 1. MC/EM Conformational Analysis

	a	**b**	**c**	**10**	**11**	**12**
Conf. within 6 kcal/mol	32	10	10	11	41	20
$d\alpha < 7$Å	25%	0%	0%	54%	2%	//
$\lvert\beta\rvert < 60°$	84%	10%	0%	72%	0%	//
7-membered H bond	0%	40%	60%	27%	76%	0%
11-membered H bond	19%	0%	0%	18%	0%	//

Computational data from conformational analysis for model **a**

SPARTAN '10 CONFORMATION SEARCH: PC/x86 1.1.0
Using systematic algorithm.
Using rotatable bonds from rule normal set.
Adjusted 7 (out of 165) low frequency modes

Conf Energy
(216) kJ/mol Remark
---
1 262.137
2 274.873
3 274.489
4 287.041
5 269.246
6 278.609
7 273.580
8 286.021
9 269.246 Prev. Min.
10 278.609 Prev. Min.
11 273.580 Prev. Min.
12 286.021 Prev. Min.
13 249.396 !New Best!
14 262.062
15 279.388
16 292.186
17 249.396 Prev. Min.
18 262.062 Prev. Min.
19 269.256
20 281.992
21 245.636 !New Best!
22 258.298
23 269.256 Prev. Min.
24 281.992 Prev. Min.
25 278.697
26 288.141
27 295.833
28 308.593
29 275.134
30 287.689
31 291.677
32 304.363
33 275.134 Prev. Min.
34 287.689
35 290.667
36 303.418
37 254.917
38 267.155
39 269.625
40 281.725
41 262.043
42 274.355
43 268.160
44 280.176
45 260.116
46 269.567
47 268.160 Prev. Min.
48 280.176 Prev. Min.
49 238.076 !New Best!
50 250.495
51 255.111
52 267.339
53 246.125
54 258.323
55 256.619
56 268.866
57 246.125 Prev. Min.
58 258.323 Prev. Min.
59 260.385
60 272.623
61 268.595
62 277.827
63 279.717
64 292.029
65 255.293
66 267.359
67 273.767
68 285.988
69 247.758
70 259.959
71 275.384
72 287.690
73 269.331
74 274.873 Prev. Min.
75 283.821
76 287.041
77 269.246 Prev. Min.
78 278.609 Prev. Min.
79 282.258
80 320.196
81 254.591
82 258.298 Prev. Min.
83 282.258
84 320.196
85 249.396 Prev. Min.
86 262.062 Prev. Min.
87 279.388 Prev. Min.
88 292.186
89 254.591 Prev. Min.
90 262.062 Prev. Min.
91 269.256 Prev. Min.
92 281.992
93 254.591 Prev. Min.
94 258.298 Prev. Min.
95 269.256 Prev. Min.
96 281.992
97 297.485
98 287.689
99 269.256 Prev. Min.
100 281.992
101 275.134 Prev. Min.
102 287.689
103 291.677
104 304.363
105 275.134 Prev. Min.
106 287.689
107 290.667
108 303.418
109 259.904
110 297.302
111 275.181
112 312.672
113 272.220
114 310.651
115 273.121
116 310.192
117 274.540
118 269.567 Prev. Min.
119 273.121 Prev. Min.
120 310.192
121 246.215
122 284.426
123 261.852
124 299.535
125 250.002
126 288.015
127 263.125
128 300.763
129 250.002 Prev. Min.
130 288.015
131 267.414
132 305.137
133 282.540
134 298.958
135 287.250
136 324.769
137 261.326
138 298.958
139 282.490
140 320.389
141 253.254
142 290.954
143 283.332
144 321.221
145 258.008
146 273.280
147 266.876
148 280.916
149 235.616 !New Best!
150 265.284
151 256.242
152 277.091
153 236.488
154 265.284 Prev. Min.
155 256.510 Prev. Min.
156 277.091 Prev. Min.
157 243.248
158 256.917
159 277.050
160 292.857
161 236.631
162 256.917 Prev. Min.
163 266.545
164 282.319
165 236.631 Prev. Min.
166 251.756
167 266.545 Prev. Min.
168 282.319
169 246.555
170 275.931
171 266.545 Prev. Min.
172 282.319
173 270.186
174 283.892
175 288.434
176 303.445
177 270.186 Prev. Min.
178 283.892
179 288.132
180 303.572
181 251.025
182 267.134
183 258.910
184 274.181
185 252.541
186 258.150
187 250.292
188 269.175
189 230.379 !New Best!
190 258.150 Prev. Min.
191 250.292 Prev. Min.
192 269.175 Prev. Min.
193 234.476
194 250.717
195 252.661
196 267.461
197 234.838
198 251.318
199 252.557
200 268.903
201 234.838 Prev. Min.
202 251.318 Prev. Min.
203 258.076
204 272.804
205 235.475
206 264.574
207 279.371
208 293.098
209 248.924
210 264.043
211 271.136
212 284.999
213 243.673
214 259.202
215 273.687
216 287.882

Partition function correction to the energy
2.455929 kJ/mol
45.598% not in most favorable conformer.
Pruning list starting with 75 molecules out of 75
Keeping 75 conformations. (75 original) Lowest energy conformation 230.3793 kJ/mol

Cartesian coordinates for **a** (Å) and geometry optimization results

Atom	X	Y	Z
C0	4.2802501	2.6571632	-3.3657405
C1	4.9420230	2.8279803	-2.1517979
C2	4.4498913	2.2542157	-0.9756922
C3	3.2743243	1.4990453	-1.0638057
C4	2.5893138	1.3111581	-2.2673194
C5	3.1019995	1.9049120	-3.4369958
N6	2.5707818	0.8409885	-0.0765933
C7	1.4761153	0.2272023	-0.6228679
C8	1.4443714	0.5221634	-1.9739591
C9	0.4643767	-0.6128928	0.0885865
N10	-0.7950824	-0.3641930	-0.6368644
C11	-0.7729719	-0.7061134	-2.0853781
C12	0.3120224	0.0916378	-2.8625517
C13	-0.6724474	-2.2339061	-2.2660701
C14	0.3411343	-0.4022712	1.5978983
N15	-0.2735497	0.8831195	1.9099986
C16	-1.5694188	1.1309284	1.2408707
C17	-1.6893465	0.6086061	-0.2113598
C18	0.5319699	1.8766523	2.4435828
O19	1.7279048	1.6923504	2.6804187
C20	-0.1014435	3.2119941	2.7390828
O21	-2.6050130	1.0187394	-0.9304580
O22	-0.0103255	-2.7767609	-3.1457468
H24	0.7380856	-1.6638712	-0.0685013
C25	-2.8031533	0.7084649	2.0738295
N26	-2.7249895	-0.5680734	2.7732845
C27	-2.8739451	-1.7789710	2.1407581
O31	-2.9389520	-1.9092925	0.9229532
H1	4.6797790	3.1131417	-4.2680275
H2	5.8548215	3.4180602	-2.1164818
H3	4.9640631	2.3929791	-0.0302357
H4	2.5908700	1.7798522	-4.3866934
H5	2.8101660	0.8716824	0.9091854
H6	-1.7427306	-0.4531462	-2.5347540
H7	0.6951573	-0.4651114	-3.7238590
H8	-0.1536242	1.0058674	-3.2543306
H9	-0.2934317	-1.1827192	2.0235846
H10	1.3141118	-0.5122344	2.0887218
H11	-1.6567034	2.2151408	1.0999366
H12	-0.1719328	3.8001988	1.8207651
H13	-1.0879098	3.0859296	3.1916068
H14	0.5233898	3.7538167	3.4558550
H18	-2.9627658	1.4541209	2.8614101
H19	-3.7071000	0.6936378	1.4540645
N1	-1.5106559	-2.9384686	-1.4189627
H16	-2.0114531	-2.4219262	-0.6901180
C6	-1.5787653	-4.3740416	-1.4271236
H15	-2.5270864	-4.6801391	-0.9795693
H17	-0.7479521	-4.7641883	-0.8336111
H31	-1.5072340	-4.7556003	-2.4489329
H46	-2.6498330	-0.5468153	3.7829026
C10	-2.8811750	-2.9625667	3.0702280
H20	-3.6226982	-3.6869937	2.7220916
H21	-3.1439425	-2.6695585	4.0904460
H22	-1.8892903	-3.4218941	3.0723399

Method : MMFF94
Stoichiometry : C21 H25 N5 O4
Number of Atoms : 55
Point Group : C1
Degrees of Freedom : 159
E 230.37926
Performing final solvation calculation
E 98.75434
Solvation energy -131.62493
Combined energy 98.75434
Net Charge : 0.000
Dipole Moment : 9.413 Debye
components : -2.8288 0.3407 8.9719

Computational data from conformational analysis for model **b**

SPARTAN '10 CONFORMATION SEARCH: PC/x86 1.1.0
Using systematic algorithm.
Using rotatable bonds from rule normal set.
Adjusted 7 (out of 165) low frequency modes

Conf	Energy	Remark
(216)	kJ/mol	
1	251.588	
2	281.299	
3	269.256	
4	281.299	Prev. Min.
5	239.694	!New Best!
6	300.054	
7	275.889	
8	289.602	
9	275.571	
10	281.798	
11	267.191	
12	281.798	
13	293.223	
14	303.709	
15	294.314	
16	303.441	
17	294.314	
18	293.613	
19	234.139	!New Best!
20	265.115	
21	252.964	
22	265.115	Prev. Min.
23	259.209	
24	283.857	
25	257.252	
26	272.969	
27	259.676	
28	266.679	
29	251.656	
30	265.117	
31	276.825	
32	287.817	
33	277.240	
34	287.545	
35	277.240	
36	277.611	
37	270.373	
38	296.732	
39	267.899	
40	293.821	
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42	277.452	
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44	293.821	
45	267.899	Prev. Min.
46	300.186	
47	267.899	Prev. Min.
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50	296.819	
51	276.686	
52	296.819	
53	301.208	
54	296.377	
55	252.727	
56	281.434	
57	231.574	!New Best!
58	278.026	
59	222.535	!New Best!
60	243.088	
61	266.234	
62	276.979	
63	251.411	
64	284.782	
65	252.894	
66	278.049	
67	261.048	
68	280.245	
69	259.854	
70	281.600	
71	285.457	
72	281.172	
73	255.353	
74	285.006	
75	271.174	
76	285.006	
77	278.607	
78	304.103	
79	277.260	
80	290.841	
81	279.865	
82	284.676	
83	272.527	
84	284.676	
85	296.090	
86	306.972	
87	292.677	
88	305.898	
89	295.304	
90	294.756	
91	243.584	
92	272.890	
93	258.780	
94	272.890	
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98	278.946	
99	267.519	
100	272.585	
101	260.231	
102	272.585	
103	283.913	
104	294.656	
105	282.802	
106	293.621	
107	282.802	
108	284.981	
109	278.298	
110	303.487	
111	274.295	
112	300.243	
113	243.263	
114	260.471	
115	274.295	
116	300.243	
117	274.295	
118	304.262	
119	274.295	
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122	303.276	
123	284.315	
124	303.276	
125	304.391	
126	302.827	
127	266.504	
128	291.211	
129	262.099	
130	288.306	
131	234.220	
132	290.702	
133	262.099	Prev. Min.
134	288.306	
135	262.099	Prev. Min.
136	289.478	
137	262.099	Prev. Min.
138	289.478	
139	272.292	
140	291.104	
141	272.292	
142	291.104	
143	292.079	
144	290.702	
145	291.164	
146	323.597	
147	271.174	
148	323.597	
149	239.694	Prev. Min.
150	304.103	
151	277.260	
152	327.424	
153	277.931	
154	320.495	
155	307.723	
156	320.495	
157	296.090	
158	306.972	
159	296.090	
160	305.898	
161	295.304	
162	297.180	
163	253.831	
164	285.913	
165	258.780	Prev. Min.
166	285.913	
167	234.715	
168	304.885	
169	264.461	
170	290.348	
171	281.500	
172	283.009	
173	269.724	
174	283.009	
175	294.979	
176	294.656	
177	298.927	
178	Rejected	No Minima
179	298.927	
180	298.148	
181	308.939	
182	338.826	
183	252.408	
184	333.563	
185	243.263	Prev. Min.
186	263.191	
187	309.881	
188	333.563	
189	309.881	
190	337.615	
191	309.881	
192	331.988	
193	317.921	
194	338.485	
195	317.921	
196	338.485	
197	342.645	
198	337.953	
199	271.592	
200	300.756	
201	240.090	
202	296.042	
203	249.622	
204	265.110	
205	272.274	
206	296.042	
207	272.274	
208	294.289	
209	272.274	
210	294.289	
211	280.255	
212	300.571	
213	280.255	
214	300.571	
215	305.154	
216	300.165	

Partition function correction to the energy
0.555724 kJ/mol
5.148% not in most favorable conformer.
Pruning list starting with 31 molecules out of 31
Keeping 31 conformations. (31 original)
Lowest energy conformation 222.5353 kJ/mol

Cartesian coordinates for **b** (Å) and geometry optimization results

Atom	X	Y	Z
C0	4.0804290	2.0545301	-4.5801813
C1	3.5476049	3.3186059	-4.3377252
C2	2.6129369	3.5235456	-3.3183175
C3	2.2299139	2.4131671	-2.5564083
C4	2.7448740	1.1342224	-2.7788436
C5	3.6899572	0.9548874	-3.8073182
N6	1.3543378	2.3263616	-1.4954191
C7	1.2579145	1.0254427	-1.0736979
C8	2.1396051	0.2750373	-1.8236416
C9	0.4013996	0.5519821	0.0527872
N10	0.5036911	-0.9286580	0.1449732
C11	1.8239491	-1.5587329	-0.1627359
C12	2.3354760	-1.1793225	-1.5717841
C13	2.8813044	-1.2816346	0.9364712
C14	-1.0674354	0.9675577	-0.1206741
N15	-1.8430792	0.4380255	0.9991952
C16	-1.8275800	-1.0398287	1.1068489
C17	-0.3977449	-1.6219616	0.9527373
C18	-2.0055656	1.2716885	2.0996637
O19	-1.5902300	2.4314101	2.1016351
C20	-2.7244737	0.7206679	3.3039663
O21	-0.1170280	-2.7313169	1.4135563
O22	4.0515487	-0.9960685	0.6961444
N23	2.4298077	-1.5173082	2.2249152
H24	0.7941531	0.9488693	0.9981901
C25	-2.7177140	-1.7112179	0.0404470
N26	-4.0815890	-1.2015128	0.0191177
C27	-4.9762261	-1.5267065	1.0110054
O31	-4.7013041	-2.2737862	1.9437139
C34	3.3392209	-1.4747227	3.3407347
H1	4.8114028	1.9190877	-5.3734234
H2	3.8680799	4.1611668	-4.9462895
H3	2.2077206	4.5117317	-3.1273690
H4	4.1171038	-0.0248296	-3.9984343
H5	0.8679448	3.1191760	-1.0975058
H6	1.6927278	-2.6494432	-0.1592535
H7	3.3851923	-1.4616561	-1.7065760
H8	1.7511538	-1.7297891	-2.3204423
H9	-1.1675005	2.0572683	-0.1773562
H10	-1.4873159	0.5662587	-1.0505876
H11	-2.1700401	-1.3366411	2.1010712
H12	-3.6242221	0.1794578	3.0046707
H13	-2.0543658	0.0733309	3.8750112
H14	-3.0369013	1.5506861	3.9453234
H15	1.6087153	-2.1141262	2.3075773
H16	-2.3128042	-1.5696340	-0.9675733
H17	-2.7583197	-2.7926373	0.2198731
H22	3.9672851	-2.3692591	3.3178294
H23	3.9708611	-0.5845242	3.2775643
H25	2.7556337	-1.4541488	4.2638031
H36	-4.2891879	-0.4169352	-0.5860220
C6	-6.3171371	-0.8579593	0.8807074
H18	-6.3739873	-0.0290123	1.5909064
H19	-7.1033841	-1.5861251	1.0981380
H20	-6.4768084	-0.4746664	-0.1309983

Method : MMFF94
Stoichiometry : C21 H25 N5 O4
Number of Atoms : 55
Point Group : C1
Degrees of Freedom : 159
E 222.53535
Performing final solvation calculation
E 78.54438 0.0
Solvation energy -143.99097
Combined energy 78.54438
Net Charge : 0.000
Dipole Moment : 5.350 Debye
components : -4.2787 1.5375 -2.8206

Computational data from conformational analysis for model **c**

SPARTAN '10 CONFORMATION SEARCH: PC/x86 1.1.0
Using systematic algorithm.
Using rotatable bonds from rule normal set.
Adjusted 6 (out of 165) low frequency modes

Conf (216)	Energy kJ/mol	Remark
1	242.028	
2	273.461	
3	249.547	
4	273.461	Prev. Min.
5	249.547	Prev. Min.
6	287.858	
7	265.589	
8	272.597	
9	267.905	
10	274.302	
11	267.905	Prev. Min.
12	274.302	Prev. Min.
13	279.302	
14	293.064	
15	279.018	
16	294.262	
17	274.231	
18	285.459	
19	232.962	!New Best!
20	264.497	
21	240.514	
22	264.497	Prev. Min.
23	240.514	Prev. Min.
24	278.936	
25	256.392	
26	263.447	
27	258.930	
28	265.152	
29	258.930	Prev. Min.
30	265.152	Prev. Min.
31	270.249	
32	284.196	
33	269.967	
34	285.350	
35	265.113	
36	276.533	
37	268.781	
38	292.379	
39	276.759	
40	291.479	
41	275.437	
42	290.690	
43	277.556	
44	288.179	
45	278.549	
46	293.110	
47	278.549	
48	293.110	
49	275.084	
50	299.385	
51	280.975	
52	299.385	
53	287.374	
54	290.690	
55	259.418	
56	283.195	
57	267.627	
58	282.248	
59	266.449	
60	281.481	
61	268.307	
62	278.683	
63	269.408	
64	283.586	
65	269.408	Prev. Min.
66	283.586	
67	266.017	
68	290.275	
69	271.629	
70	290.275	
71	278.112	
72	281.481	
73	277.640	
74	313.055	
75	290.188	
76	313.055	
77	290.188	
78	325.979	
79	297.594	
80	307.801	
81	296.938	
82	310.912	
83	296.938	
84	310.912	
85	315.661	
86	335.343	
87	315.661	
88	335.827	
89	307.991	
90	325.754	
91	230.745	!New Best!
92	264.456	
93	256.150	
94	264.456	Prev. Min.
95	250.745	
96	278.033	
97	264.310	
98	275.146	
99	255.729	
100	266.634	
101	255.729	Prev. Min.
102	266.634	Prev. Min.
103	282.472	
104	283.614	
105	262.148	
106	286.045	
107	262.148	Prev. Min.
108	292.131	
109	292.871	
110	321.951	
111	308.368	
112	320.666	
113	305.006	
114	319.226	
115	306.272	
116	316.404	
117	305.535	
118	320.815	
119	305.535	
120	320.815	
121	302.616	
122	332.258	
123	308.971	
124	332.258	
125	312.178	
126	319.226	
127	257.839	
128	287.541	
129	273.952	
130	286.417	
131	261.832	
132	286.040	
133	272.717	
134	284.092	
135	272.200	
136	288.529	
137	272.200	Prev. Min.
138	288.529	
139	269.177	
140	297.621	
141	276.337	
142	289.262	
143	278.787	
144	285.218	
145	242.028	Prev. Min.
146	273.461	
147	249.547	Prev. Min.
148	273.461	
149	249.547	Prev. Min.
150	287.858	
151	265.589	Prev. Min.
152	272.597	
153	267.905	Prev. Min.
154	274.302	
155	267.905	Prev. Min.
156	274.302	
157	279.302	
158	293.064	
159	274.231	
160	294.262	
161	249.547	Prev. Min.
162	285.459	
163	230.745	Prev. Min.
164	264.456	Prev. Min.
165	240.612	
166	264.456	Prev. Min.
167	250.745	Prev. Min.
168	278.033	
169	253.290	
170	264.805	
171	255.729	Prev. Min.
172	266.634	Prev. Min.
173	255.729	Prev. Min.
174	266.634	Prev. Min.
175	270.822	
176	283.614	
177	262.148	Prev. Min.
178	286.045	
179	262.148	Prev. Min.
180	264.456	Prev. Min.
181	268.781	Prev. Min.
182	292.379	
183	276.759	
184	291.479	
185	275.437	
186	290.690	
187	277.556	
188	288.179	
189	278.549	
190	293.110	
191	278.549	
192	293.110	
193	275.084	
194	299.385	
195	280.975	
196	299.385	
197	275.437	
198	290.690	
199	254.939	
200	281.071	
201	265.344	
202	280.349	
203	261.832	Prev. Min.
204	279.522	
205	264.468	
206	279.123	
207	266.222	
208	283.860	
209	266.222	Prev. Min.
210	283.860	
211	261.890	
212	289.262	
213	270.658	
214	289.262	
215	273.033	
216	279.522	

Partition function correction to the energy
0.976299 kJ/mol
31.447% not in most favorable conformer.
Pruning list starting with 44 molecules out of 44
Keeping 44 conformations. (44 original)
Lowest energy conformation 230.7449 kJ/mol

Cartesian coordinates for **c** (Å) and geometry optimization results

Atom	X	Y	Z
C0	5.0070508	2.1791118	-2.6096460
C1	4.2580200	3.3518226	-2.6749417
C2	2.9261290	3.3810298	-2.2508330
C3	2.3763744	2.1922677	-1.7561990
C4	3.1035685	1.0024715	-1.6778097
C5	4.4421608	0.9975778	-2.1155408
N6	1.1065598	1.9316447	-1.2863062
C7	1.0155460	0.6250162	-0.8844969
C8	2.2277133	0.0223007	-1.1418392
C9	-0.2117871	-0.0256560	-0.3424852
N10	0.0821972	-1.4012529	0.1096443
C11	1.4756241	-1.9046467	0.2375729
C12	2.4352523	-1.4225815	-0.8689694
C13	2.0449173	-1.5271535	1.6290268
C14	-0.9234426	0.7652045	0.7648897
N15	-2.1076424	0.0659315	1.2889580
C16	-2.2630317	-1.3766096	0.9769301
C17	-0.9157474	-2.1030523	0.7831913
C18	-3.0590240	0.6740286	2.0914822
O19	-4.0877524	0.0965320	2.4491067
C20	-2.8114660	2.1076000	2.4881854
O21	-0.7672217	-3.2762759	1.1304075
O22	1.6209834	-0.5827956	2.2992446
N23	3.1005071	-2.2464030	2.1299911
H24	-0.9033708	-0.1382228	-1.1857006
C25	-3.1612839	-1.6679017	-0.2474107
N26	-4.3582931	-0.8425574	-0.3223226
C27	-4.3365344	0.3771570	-0.9627561
O31	-3.3729555	0.8034672	-1.5936386
C34	3.4683361	-3.5865409	1.7410362
H1	6.0406676	2.1792455	-2.9465170
H2	4.7147744	4.2592312	-3.0634679
H3	2.3452834	4.2956993	-2.3070192
H4	5.0341115	0.0888161	-2.0709547
H5	0.3607589	2.6139941	-1.2633901
H6	1.4262638	-2.9986440	0.1946572
H7	3.4809326	-1.6137768	-0.6061021
H8	2.2219764	-1.9763098	-1.7920586
H9	-0.2557547	0.9449991	1.6141642
H10	-1.2366111	1.7462137	0.3909490
H11	-2.7331337	-1.8341634	1.8577814
H12	-1.8077635	2.2281963	2.9029154
H13	-2.9501186	2.7620866	1.6239931
H14	-3.5293795	2.3957383	3.2622413
H15	3.3372875	-1.9524421	3.0712022
H16	-2.6066651	-1.5590666	-1.1853452
H17	-3.4978421	-2.7104333	-0.2062987
H22	3.6629991	-3.6301875	0.6675584
H23	4.3696455	-3.8707187	2.2890267
H25	2.6498194	-4.2659465	1.9929049
H36	-5.0004514	-0.9248028	0.4615952
C6	-5.6007083	1.1763911	-0.7954264
H18	-5.4284222	1.9691201	-0.0628214
H19	-6.4295680	0.5488830	-0.4558800
H20	-5.8767370	1.6156830	-1.7579647

Method : MMFF94
Stoichiometry : C21 H25 N5 O4
Number of Atoms : 55
Point Group : C1
Degrees of Freedom : 159
E 242.02842
Performing final solvation calculation
E 78.54438 0.0
Solvation energy -141.80747
Combined energy 100.22096
Net Charge : 0.000
Dipole Moment : 2.395 Debye
components : 2.1914 0.2554 -0.9317

Computational data from conformational analysis for **10**

SPARTAN '10 CONFORMATION SEARCH: PC/x86 1.1.0
Initializing 4 threads
Using systematic algorithm.
Using rotatable bonds from rule normal set.
Adjusted 12 (out of 237) low frequency modes

Conf	Energy (1944) kJ/mol	Remark
1	260.972	
2	273.895	
3	270.357	
4	283.023	
5	268.786	
6	281.442	
7	265.077	
8	274.817	
9	276.954	
10	286.584	
11	272.266	
12	281.849	
13	275.242	
14	288.312	
15	284.968	
16	297.932	
17	277.438	
18	290.407	
19	270.259	
20	282.880	
21	263.451	
22	276.149	
23	259.965	!New Best!
24	272.592	
25	274.115	
26	283.433	
27	270.272	
28	279.593	
29	265.838	
30	275.273	
31	274.115	Prev. Min.
32	283.433	Prev. Min.
33	270.272	Prev. Min.
34	279.593	Prev. Min.
35	265.838	Prev. Min.
36	275.273	Prev. Min.
37	304.698	
38	317.518	
39	299.294	
40	309.202	
41	297.691	
42	310.710	
43	278.384	
44	319.504	
45	277.261	
46	323.685	
47	304.464	
48	316.988	
49	274.584	
50	287.939	
51	263.914	
52	273.859	
53	269.602	
54	280.237	
55	255.935	!New Best!
56	307.997	
57	302.528	
58	315.122	
59	296.422	
60	308.937	
61	250.930	!New Best!
62	322.511	
63	266.656	
64	287.017	
65	250.930	Prev. Min.
66	265.177	
67	250.930	Prev. Min.
68	282.200	
69	266.656	Prev. Min.
70	265.177	Prev. Min.
71	250.930	Prev. Min.
72	264.781	Duplicate
73	279.600	
74	289.929	
75	263.900	
76	273.847	
77	269.703	
78	283.376	
79	274.584	Prev. Min.
80	287.939	Prev. Min.
81	263.914	Prev. Min.
82	273.859	Prev. Min.
83	269.602	Prev. Min.
84	283.314	
85	285.535	
86	298.686	
87	263.914	Prev. Min.
88	273.859	Prev. Min.
89	269.602	Prev. Min.
90	280.237	Prev. Min.
91	271.205	
92	281.039	
93	268.023	
94	280.943	
95	4331.835	Bond Strain
96	4379.981	Bond Strain
97	265.218	
98	275.108	
99	266.656	Prev. Min.
100	265.177	Prev. Min.
101	4329.163	Bond Strain
102	4380.706	Bond Strain
103	265.218	Prev. Min.
104	275.108	Prev. Min.
105	266.656	Prev. Min.
106	265.177	Prev. Min.
107	4330.449	Bond Strain
108	4377.463	Bond Strain
109	277.299	
110	290.237	
111	279.372	
112	292.284	
113	277.299	Prev. Min.
114	290.237	Prev. Min.
115	275.398	
116	288.604	
117	279.607	
118	292.644	
119	273.548	
120	286.570	
121	275.398	Prev. Min.
122	288.604	Prev. Min.
123	279.607	Prev. Min.
124	292.644	Prev. Min.
125	273.548	Prev. Min.
126	286.570	Prev. Min.
127	275.886	
128	288.721	
129	284.380	
130	297.250	
131	270.480	
132	283.398	
133	270.871	
134	283.866	
135	278.634	
136	291.839	
137	265.552	
138	278.597	
139	270.871	Prev. Min.
140	283.866	Prev. Min.
141	278.634	Prev. Min.
142	290.160	
143	265.552	Prev. Min.
144	278.597	Prev. Min.
145	284.234	
146	297.172	
147	278.132	
148	291.087	
149	274.305	
150	292.051	
151	258.452	
152	271.158	
153	254.927	
154	267.639	
155	255.777	
156	268.463	
157	265.551	
158	278.256	
159	254.927	Prev. Min.
160	267.639	Prev. Min.
161	255.777	Prev. Min.
162	268.463	Prev. Min.
163	226.094	!New Best!
164	259.423	
165	284.813	
166	297.939	
167	226.094	Prev. Min.
168	235.682	
169	250.899	
170	Rejected	Chirality Different
171	268.658	
172	281.396	
173	250.899	Prev. Min.
174	263.773	
175	250.899	Prev. Min.
176	263.773	Prev. Min.
177	268.659	
178	281.397	
179	250.899	Prev. Min.
180	263.773	Prev. Min.
181	272.698	
182	285.565	
183	269.621	
184	282.513	
185	267.285	
186	280.145	
187	258.452	Prev. Min.
188	271.158	
189	254.927	Prev. Min.
190	267.639	Prev. Min.
191	255.777	Prev. Min.
192	268.463	
193	265.551	Prev. Min.
194	278.256	
195	254.927	Prev. Min.
196	267.640	Prev. Min.
197	255.777	Prev. Min.
198	268.463	
199	264.024	
200	277.052	
201	281.066	
202	293.928	
203	264.024	Prev. Min.
204	274.594	
205	270.871	
206	263.773	Prev. Min.
207	268.658	
208	281.396	
209	250.899	Prev. Min.
210	291.839	
211	270.871	
212	263.773	Prev. Min.
213	268.658	
214	281.396	
215	255.777	Prev. Min.
216	263.773	Prev. Min.
217	277.333	
218	290.913	
219	280.017	
220	292.869	
221	278.470	
222	291.289	
223	284.821	
224	294.035	
225	289.742	
226	302.637	
227	284.690	
228	297.543	
229	284.821	
230	297.024	
231	301.685	
232	311.506	
233	293.792	
234	306.644	
235	264.900	
236	273.869	
237	269.097	
238	288.105	
239	264.900	Prev. Min.
240	273.869	
241	280.671	
242	293.698	
243	276.200	
244	295.412	
245	274.240	
246	281.924	
247	280.671	
248	293.698	
249	276.200	
250	295.412	
251	274.240	
252	281.924	
253	272.698	
254	285.565	
255	269.621	
256	282.513	
257	267.285	Prev. Min.
258	280.145	
259	258.452	Prev. Min.
260	271.158	

261 254.927 Prev. Min.
262 268.463
263 255.777 Prev. Min.
264 302.713
265 265.551 Prev. Min.
266 276.058
267 254.927 Prev. Min.
268 267.639 Prev. Min.
269 255.777 Prev. Min.
270 268.463
271 264.024 Prev. Min.
272 277.052
273 281.066
274 293.928
275 264.024 Prev. Min.
276 277.052
277 286.157
278 299.284
279 250.899 Prev. Min.
280 281.396
281 250.899 Prev. Min.
282 263.773 Prev. Min.
283 286.144
284 Rejected No Minima
285 285.621
286 298.542
287 250.899 Prev. Min.
288 263.773 Prev. Min.
289 298.821
290 311.708
291 294.705
292 307.558
293 293.415
294 306.427
295 292.136
296 305.653
297 294.188
298 307.311
299 291.114
300 304.666
301 301.930
302 305.653
303 296.896
304 268.463
305 291.114
306 304.666
307 290.469
308 303.701
309 288.626
310 301.735
311 288.020
312 300.764
313 286.144
314 299.179
315 285.621
316 298.542
317 250.899 Prev. Min.
318 301.179
319 293.430
320 306.172
321 285.621
322 298.542
323 288.076
324 301.179
325 250.266
326 262.435
327 256.117
328 268.252
329 254.760
330 266.867
331 251.686
332 260.860
333 262.963
334 272.171
335 257.705
336 266.855
337 251.686 Prev. Min.
338 260.860 Prev. Min.
339 262.963 Prev. Min.
340 272.171
341 257.705 Prev. Min.
342 266.855 Prev. Min.
343 243.827
344 255.933
345 251.150
346 263.269
347 243.827 Prev. Min.
348 255.933 Prev. Min.
349 248.491
350 257.591
351 256.690
352 265.835
353 248.491 Prev. Min.
354 257.591 Prev. Min.
355 248.491 Prev. Min.
356 257.591 Prev. Min.
357 256.690 Prev. Min.
358 265.835 Prev. Min.
359 248.491 Prev. Min.
360 257.591 Prev. Min.
361 300.365
362 274.249
363 296.440
364 306.195
365 293.499
366 306.131
367 265.883
368 275.600
369 257.582
370 267.309
371 262.437
372 275.488
373 265.883 Prev. Min.
374 278.501
375 257.582 Prev. Min.
376 267.309 Prev. Min.
377 262.437 Prev. Min.
378 Rejected No Minima
379 290.564
380 306.352
381 301.099
382 313.559
383 296.600
384 308.959
385 244.571
386 273.372
387 258.520
388 270.923
389 244.571 Prev. Min.
390 257.527
391 244.571 Prev. Min.
392 273.375
393 258.520 Prev. Min.
394 270.923
395 244.571 Prev. Min.
396 257.527 Prev. Min.
397 272.096
398 281.547
399 256.195
400 265.862
401 256.195 Prev. Min.
402 265.862 Prev. Min.
403 265.883 Prev. Min.
404 278.501
405 257.582 Prev. Min.
406 267.309 Prev. Min.
407 262.437 Prev. Min.
408 275.488
409 265.883 Prev. Min.
410 275.600
411 257.582 Prev. Min.
412 Rejected No Minima
413 262.437 Prev. Min.
414 Rejected No Minima
415 266.129
416 275.622
417 259.194
418 271.437
419 4318.262 Bond Strain
420 4366.649 Bond Strain
421 263.005
422 272.544
423 258.520 Prev. Min.
424 270.923
425 4318.920 Bond Strain
426 4368.521 Bond Strain
427 263.005 Prev. Min.
428 272.544
429 244.571 Prev. Min.
430 270.923
431 4318.920 Bond Strain
432 4368.521 Bond Strain
433 245.925
434 258.315
435 247.437
436 259.838
437 246.273
438 258.691
439 243.073
440 255.541
441 249.159
442 261.629
443 245.439
444 257.908
445 258.402
446 270.826
447 249.159 Prev. Min.
448 261.629 Prev. Min.
449 245.439 Prev. Min.
450 257.908 Prev. Min.
451 248.570
452 260.857
453 238.664
454 250.962
455 238.664 Prev. Min.
456 250.962 Prev. Min.
457 248.930
458 261.276
459 240.458
460 252.809
461 240.996
462 253.366
463 248.930 Prev. Min.
464 261.276 Prev. Min.
465 240.458 Prev. Min.
466 252.809 Prev. Min.
467 240.996 Prev. Min.
468 253.366 Prev. Min.
469 251.439
470 263.711
471 240.560
472 252.862
473 262.063
474 274.393
475 250.545
476 262.762
477 260.952
478 273.278
479 248.699
480 260.907
481 250.545 Prev. Min.
482 262.762 Prev. Min.
483 246.544
484 258.753
485 248.699 Prev. Min.
486 260.901 Prev. Min.
487 229.302
488 244.106
489 245.350
490 257.620
491 231.783
492 244.106 Prev. Min.
493 237.347
494 249.605
495 251.342
496 263.560
497 237.347 Prev. Min.
498 249.605 Prev. Min.
499 237.347 Prev. Min.
500 249.605 Prev. Min.
501 251.342 Prev. Min.
502 263.560 Prev. Min.
503 237.347 Prev. Min.
504 249.605 Prev. Min.
505 251.439 Prev. Min.
506 263.711 Prev. Min.
507 240.560 Prev. Min.
508 252.862 Prev. Min.
509 244.458
510 256.725
511 250.545 Prev. Min.
512 262.762 Prev. Min.
513 246.544 Prev. Min.
514 258.753 Prev. Min.
515 248.699 Prev. Min.
516 260.901 Prev. Min.
517 250.545 Prev. Min.
518 262.762 Prev. Min.
519 246.544 Prev. Min.
520 258.753 Prev. Min.
521 248.699 Prev. Min.
522 Rejected No Minima
523 242.690
524 254.958
525 245.350 Prev. Min.
526 257.620 Prev. Min.
527 231.783 Prev. Min.
528 244.106 Prev. Min.
529 249.800
530 261.969
531 251.342 Prev. Min.
532 263.560 Prev. Min.
533 237.347 Prev. Min.
534 249.605 Prev. Min.
535 249.800 Prev. Min.
536 261.969 Prev. Min.
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538 263.560 Prev. Min.
539 237.347 Prev. Min.
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555 269.510
556 278.909
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562 277.697
563 255.219
564 264.375

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567 255.610
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570 261.820
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572 271.025
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578 263.711 Prev. Min.
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581 244.458 Prev. Min.
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583 250.545 Prev. Min.
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586 272.176
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588 270.600
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591 262.161
592 258.753 Prev. Min.
593 257.003
594 269.390
595 242.690 Prev. Min.
596 254.958 Prev. Min.
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598 257.620 Prev. Min.
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625 266.898 Prev. Min.
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636 268.697
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663 296.406
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704 293.109
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709 271.818
710 312.980
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712 304.043
713 250.930 Prev. Min.
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720 264.781 Prev. Min.
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744 4329.809 Bond Strain
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748 Rejected No Minima
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805 274.769
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818 263.773 Prev. Min.
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1560 263.052
1561 258.010
1562 272.889
1563 Rejected No Minima
1564 261.417
1565 248.326
1566 263.052
1567 221.566 Prev. Min.
1568 274.967
1569 221.566 Prev. Min.
1570 274.967
1571 221.566 Prev. Min.
1572 274.967
1573 278.477
1574 303.907
1575 271.114
1576 291.460
1577 263.150
1578 259.516
1579 278.477
1580 301.519
1581 271.114
1582 291.460
1583 243.562 Prev. Min.
1584 259.516
1585 286.964
1586 318.227
1587 284.916
1588 316.169
1589 283.158
1590 314.382
1591 278.792
1592 265.439
1593 278.341
1594 263.052
1595 275.394
1596 263.052
1597 278.792
1598 265.439
1599 Rejected No Minima
1600 316.559
1601 293.924
1602 308.339
1603 276.876
1604 305.031
1605 278.489
1606 311.797
1607 276.894
1608 305.031
1609 261.139
1610 301.306
1611 271.114
1612 291.460
1613 290.847
1614 306.129
1615 288.274
1616 304.476
1617 271.114
1618 291.460
1619 290.147
1620 306.129
1621 243.268
1622 259.527
1623 251.284
1624 266.855
1625 249.283
1626 264.758
1627 238.247
1628 279.101
1629 250.348
1630 289.005
1631 244.282
1632 283.668
1633 264.787
1634 279.754
1635 272.615
1636 288.326
1637 266.113
1638 276.346
1639 236.912
1640 252.742
1641 240.980
1642 257.558
1643 236.912 Prev. Min.
1644 252.742
1645 235.469
1646 277.533
1647 240.739
1648 280.357
1649 235.469 Prev. Min.
1650 277.533
1651 235.469 Prev. Min.
1652 257.591
1653 240.739 Prev. Min.
1654 283.204
1655 235.469 Prev. Min.
1656 257.591
1657 285.195
1658 309.875
1659 282.236
1660 299.068
1661 280.014
1662 302.049
1663 240.096
1664 267.357
1665 236.882
1666 259.501
1667 Rejected No Minima
1668 267.310
1669 240.861
1670 267.357
1671 236.882 Prev. Min.
1672 259.501
1673 240.301
1674 267.167
1675 251.927
1676 282.675
1677 287.175
1678 280.649
1679 281.693
1680 282.506
1681 239.695
1682 269.301
1683 249.598
1684 269.961
1685 235.185
1686 264.790
1687 239.699 Prev. Min.
1688 269.301
1689 249.242
1690 269.961
1691 235.185 Prev. Min.
1692 269.961
1693 240.831
1694 271.800
1695 231.009
1696 259.317
1697 238.741
1698 269.006
1699 240.861 Prev. Min.
1700 267.357
1701 236.882 Prev. Min.
1702 259.501
1703 240.301 Prev. Min.
1704 267.167
1705 240.861 Prev. Min.
1706 267.357
1707 236.882 Prev. Min.
1708 259.501
1709 240.301 Prev. Min.
1710 267.167
1711 247.598
1712 278.173
1713 243.525
1714 278.937
1715 4323.216 Bond Strain
1716 4331.371 Bond Strain
1717 247.219
1718 273.951
1719 249.598
1720 264.790
1721 4325.567 Bond Strain
1722 4332.197 Bond Strain
1723 247.219
1724 273.951
1725 249.598
1726 264.790
1727 4325.567 Bond Strain
1728 4332.197 Bond Strain
1729 239.619
1730 254.400
1731 243.416
1732 257.399
1733 242.733
1734 257.034
1735 239.071
1736 254.505
1737 244.336
1738 259.766
1739 241.162
1740 256.563
1741 256.047
1742 270.944
1743 244.336 Prev. Min.
1744 259.766
1745 239.938
1746 256.563
1747 243.500
1748 257.731
1749 231.332
1750 246.364
1751 231.332 Prev. Min.
1752 246.364 Prev. Min.
1753 243.610
1754 258.991
1755 235.909
1756 251.484
1757 235.953
1758 251.573
1759 243.610 Prev. Min.
1760 258.991
1761 235.909 Prev. Min.
1762 251.484
1763 Rejected No Minima
1764 251.573
1765 256.027
1766 272.475
1767 251.463
1768 268.167
1769 251.513
1770 268.018
1771 240.432
1772 256.256
1773 247.558
1774 263.905
1775 238.831
1776 254.748
1777 240.432 Prev. Min.
1778 256.256
1779 236.993

1780 252.845
1781 238.826 Prev. Min.
1782 254.748
1783 224.939
1784 240.931
1785 224.939 Prev. Min.
1786 240.931 Prev. Min.
1787 224.127
1788 240.931 Prev. Min.
1789 228.591
1790 244.336
1791 Rejected No Minima
1792 Rejected No Minima
1793 228.591 Prev. Min.
1794 244.336 Prev. Min.
1795 228.591 Prev. Min.
1796 244.336 Prev. Min.
1797 Rejected No Minima
1798 244.336 Prev. Min.
1799 228.591 Prev. Min.
1800 244.336 Prev. Min.
1801 243.583
1802 259.770
1803 232.867
1804 249.128
1805 236.932
1806 253.130
1807 240.432 Prev. Min.
1808 256.256
1809 236.993 Prev. Min.
1810 252.845
1811 238.826 Prev. Min.
1812 254.748
1813 240.432 Prev. Min.
1814 256.256
1815 236.993 Prev. Min.
1816 252.845
1817 238.826 Prev. Min.
1818 254.748
1819 239.021
1820 254.309
1821 224.939 Prev. Min.
1822 240.931 Prev. Min.
1823 224.939 Prev. Min.
1824 240.931 Prev. Min.
1825 244.915
1826 259.647
1827 228.591 Prev. Min.
1828 Rejected No Minima
1829 228.591 Prev. Min.
1830 244.336 Prev. Min.
1831 243.513
1832 259.647
1833 228.591 Prev. Min.
1834 244.336 Prev. Min.
1835 227.784
1836 244.336 Prev. Min.
1837 233.404
1838 264.905
1839 242.213
1840 269.395
1841 241.931
1842 268.994
1843 234.386 Prev. Min.
1844 265.349
1845 238.475
1846 268.836
1847 235.792
1848 264.866
1849 256.869
1850 265.349
1851 238.475 Prev. Min.
1852 268.836
1853 255.502
1854 264.866
1855 241.914
1856 265.357
1857 241.914 Prev. Min.
1858 286.262
1859 241.914 Prev. Min.
1860 265.357
1861 242.893
1862 280.367
1863 242.893 Prev. Min.
1864 279.712
1865 242.893 Prev. Min.
1866 268.147
1867 242.893 Prev. Min.
1868 280.367
1869 Rejected No Minima
1870 279.712
1871 242.893 Prev. Min.
1872 268.147
1873 243.583 Prev. Min.
1874 259.770
1875 232.142
1876 249.128
1877 236.173
1878 253.130
1879 245.713
1880 267.642
1881 243.089
1882 264.639
1883 242.308
1884 265.423
1885 245.713 Prev. Min.
1886 267.642
1887 243.089 Prev. Min.
1888 264.639
1889 242.308 Prev. Min.
1890 269.774
1891 242.960
1892 254.309
1893 224.939 Prev. Min.
1894 240.931 Prev. Min.
1895 224.939 Prev. Min.
1896 240.931 Prev. Min.
1897 242.963
1898 259.647
1899 247.560
1900 267.906
1901 239.155
1902 260.517
1903 242.963 Prev. Min.
1904 268.652
1905 247.560
1906 244.336 Prev. Min.
1907 239.155 Prev. Min.
1908 268.652
1909 250.503
1910 279.909
1911 Rejected No Minima
1912 281.332
1913 248.181
1914 277.368
1915 245.713 Prev. Min.
1916 267.642
1917 243.089 Prev. Min.
1918 264.639
1919 242.308 Prev. Min.
1920 265.423
1921 245.713 Prev. Min.
1922 267.642
1923 243.089 Prev. Min.
1924 264.639
1925 242.308 Prev. Min.
1926 269.774
1927 244.120
1928 273.568
1929 254.885
1930 273.568
1931 244.120 Prev. Min.
1932 273.568
1933 239.155 Prev. Min.
1934 268.652
1935 247.560
1936 267.906
1937 239.155 Prev. Min.
1938 268.652
1939 239.155 Prev. Min.
1940 268.652
1941 247.560
1942 267.906
1943 239.155 Prev. Min.
1944 268.652

Partition function correction to the energy
0.183194 kJ/mol
1.271% not in most favorable conformer.
Pruning list starting with 108 molecules out of 205
Filtering using default clustering measure.
... Filtering 0.93% complete
Keeping 100 conformations. (108 original)
Lowest energy conformation 205.0111 kJ/mol

Cartesian coordinates for **10** (Å) and geometry optimization results

Atom	X	Y	Z
C0	5.9986579	-1.6957887	-3.7173266
C1	6.5060856	-1.0629299	-2.5847265
C2	5.6540645	-0.4733723	-1.6462354
C3	4.2769319	-0.5389295	-1.8891564
C4	3.7401756	-1.1630201	-3.0171112
C5	4.6187929	-1.7547221	-3.9448142
N6	3.2219408	-0.0664324	-1.1389406
C7	2.0383593	-0.3288437	-1.7772038
C8	2.3290750	-1.0362806	-2.9240671
C9	0.6902253	0.0557655	-1.2655560
N10	-0.3483575	-0.4221460	-2.2012431
C11	-0.0824721	-1.6273865	-3.0436612
C12	1.2499792	-1.5324157	-3.8187612
C13	-0.1779230	-2.9335781	-2.2111364
C14	0.5764532	1.5816402	-1.0953519
N15	-0.7834476	2.0599779	-0.8342880
C16	-1.9013253	1.0997494	-0.9534067
C17	-1.6625689	-0.0249527	-1.9826428
C18	-1.0802801	3.3967358	-0.6053389
O19	-2.2336309	3.8119128	-0.4990166
C20	0.0851793	4.3459638	-0.4774995
O21	-2.6098842	-0.6487851	-2.4689947
O22	0.6254063	-3.8585403	-2.2986714
H24	0.5120734	-0.4486998	-0.3098117
C25	-2.2736403	0.4177108	0.3866486
N26	-2.5009387	1.3393128	1.5040692
C27	-1.5097685	1.6945757	2.3985150
C28	-3.8116575	1.9716989	1.6150681
O30	-0.3189916	1.0920025	2.1236840
O31	-1.6657448	2.4628111	3.3401352
C32	0.7146830	1.4194580	3.0571226
H1	6.6788059	-2.1529570	-4.4317060
H2	7.5814675	-1.0307711	-2.4255588
H3	6.0522642	0.0133020	-0.7624724
H4	4.2325221	-2.2559954	-4.8270588
H5	3.3250133	0.3881801	-0.2408320
H6	-0.8831268	-1.7064562	-3.7915633
H7	1.5216261	-2.4953483	-4.2646709
H8	1.1343923	-0.8126979	-4.6392417
H9	1.2321010	1.9256515	-0.2878411

Atom	X	Y	Z
H10	0.9085437	2.0842926	-2.0135639
H11	-2.7751255	1.6544818	-1.3173593
H12	0.7019283	4.0712258	0.3820608
H13	0.6807818	4.3483006	-1.3934314
H14	-0.2922423	5.3603719	-0.3154776
H18	-3.1762632	-0.1905636	0.2531014
H19	-1.4941604	-0.2952180	0.6754273
H20	-3.7567839	2.8766897	2.2315915
H21	-4.1264435	2.2994230	0.6180745
H26	0.8953196	2.5006987	3.0249178
H27	0.4215721	1.1243232	4.0719696
N1	-1.3283705	-3.0285484	-1.4426560
H16	-2.1048646	-2.4391173	-1.7392915
C6	-1.6486818	-4.2510012	-0.7517375
H15	-1.9731420	-4.9955025	-1.4835849
H17	-2.4559865	-4.0483585	-0.0444291
H31	-0.7691954	-4.6227410	-0.2190725
C10	-4.8383782	1.0377953	2.2138327
C15	-6.7256615	-0.7133354	3.3290619
C19	-5.8516695	0.4823736	1.4190723
C21	-4.7848567	0.7040309	3.5751287
C22	-5.7240422	-0.1669218	4.1290849
C23	-6.7900185	-0.3888743	1.9751804
H22	-5.9175723	0.7257193	0.3608529
H23	-4.0087320	1.1271935	4.2106224
H25	-5.6742659	-0.4163040	5.1857351
H32	-7.5732057	-0.8128913	1.3520842
H33	-7.4579595	-1.3897860	3.7617147
C24	1.9739371	0.6743434	2.6809452
C26	4.3351041	-0.7334950	2.1104323
C29	1.9380555	-0.7017074	2.4099028
C30	3.2120563	1.3330340	2.6683919
C31	4.3860282	0.6321958	2.3834887
C33	3.1112496	-1.3995835	2.1194544
H28	0.9928743	-1.2415699	2.4351641
H29	3.2744802	2.3944500	2.9015998
H30	5.3431284	1.1485860	2.3900860
H34	3.0716283	-2.4661977	1.9080764
H35	5.2484170	-1.2832117	1.8942135

Method : MMFF94
Stoichiometry : C34 H35 N5 O5
Number of Atoms : 79
Point Group : C1
Degrees of Freedom : 231
Performing final solvation calculation
Cycle E Gmax maxDist MaxTors
0 58.63872 0.0
Solvation energy -146.37237
Combined energy 58.63872

Net Charge : 0.000
Dipole Moment : 3.212 Debye
components : 3.1644 0.1986 0.5107

Computational data from conformational analysis for **11**

Using Monte-Carlo algorithm.
Using rotatable bonds from rule normal set.

Conf Energy (1944) kJ/mol Remark

1 265.246
2 277.436
3 Rejected No Minima
4 281.959
5 271.502
6 Rejected No Minima
7 267.586
8 Rejected No Minima
9 234.639 !New Best!
10 218.292 !New Best!
11 Rejected No Minima
12 217.409 !New Best!
13 212.111 !New Best!
14 217.409 Prev. Min.
15 238.962
16 252.222
17 Rejected No Minima
18 Rejected No Minima
19 247.236
20 256.997
21 261.529
22 Rejected No Minima
23 265.992
Increasing initial
24 264.138
25 282.015
26 264.138 Prev. Min.
27 282.015 Prev. Min.
28 250.329
29 247.667
30 238.665
31 244.051
32 256.288
33 253.007
34 263.157
35 284.212
36 Rejected No Minima
37 278.155
38 295.516
39 Rejected No Minima
40 296.122
41 278.674
42 242.942
43 278.674 Prev. Min.
44 296.122 Prev. Min.
45 278.201
46 247.643
47 246.979
48 259.088
49 279.093
50 Rejected No Minima
51 270.493
52 233.755
53 273.570
54 282.081
55 234.671
56 236.105
57 253.575
58 267.635
59 Rejected No Minima
60 Rejected No Minima
61 258.158
62 270.438
63 Rejected No Minima
64 233.614
65 Rejected No Minima
66 250.154
67 257.008
68 259.882
69 247.191
70 257.008 Prev. Min.
71 247.191 Prev. Min.
72 257.008 Prev. Min.
73 247.684
74 235.785
75 225.152
76 241.625
77 243.443
78 272.215
79 297.885
80 292.254
81 265.340
82 271.299
83 296.751
84 292.371
85 268.132
86 277.405
87 291.524
88 260.702
89 Rejected No Minima
90 255.462
91 257.147
92 264.415
93 Rejected No Minima
94 255.885
95 248.566
96 255.885 Prev. Min.
97 271.254
98 Rejected No Minima
99 Rejected No Minima
100 Rejected No Minima
101 269.677
102 Rejected No Minima
103 269.677 Same Min.
104 261.670
105 275.925
106 277.504
107 312.092
108 294.515
109 282.359
110 Rejected No Minima
111 Rejected No Minima
112 297.776
113 312.092 Prev. Min.
114 Rejected No Minima
115 296.843
116 258.980
117 261.670 Prev. Min.
118 271.371
119 249.091
120 247.436
121 259.470
122 261.275
123 285.410
124 276.039
125 265.179
126 270.592
127 265.179 Prev. Min.
128 270.592 Prev. Min.
129 268.813
130 267.111
131 246.439
132 251.527
133 253.575 Duplicate
134 255.345
135 247.791
136 253.563
137 247.791 Prev. Min.
138 255.345 Prev. Min.
139 250.329 Prev. Min.
140 234.671 Duplicate
141 289.531
142 241.342
143 250.269
144 233.755 Duplicate
145 238.752
146 227.534
147 257.025
148 227.534 Prev. Min.
149 250.151
150 231.847
151 240.564
152 271.502 Prev. Min.
153 272.759
154 260.803
155 266.552
156 Rejected No Minima
157 283.053
158 264.072
159 264.072 Same Min.
160 278.493
161 264.072 Prev. Min.
162 Rejected No Minima
163 253.807
164 275.476
165 280.035
166 280.011
167 241.766
168 Rejected No Minima
169 238.752 Prev. Min.
170 235.681
171 256.840
172 270.970
173 252.222 Prev. Min.
174 260.449
175 Rejected No Minima
176 Rejected No Minima
177 Rejected No Minima
178 260.509
179 266.194
180 274.975
181 257.054
182 247.568
183 Rejected No Minima
184 Rejected No Minima
185 259.864
186 243.374
187 234.556
188 Rejected No Minima
189 233.418
190 242.265
191 260.235
192 252.153
193 265.234
194 258.197
195 279.093 Prev. Min.
196 279.522
197 261.062
198 274.974
199 Rejected No Minima
200 Rejected No Minima
201 278.155 Prev. Min.
202 Rejected No Minima
203 Rejected No Minima
204 278.674 Prev. Min.
205 271.747
206 278.674 Prev. Min.
207 268.109
208 Rejected No Minima
209 Rejected No Minima
210 269.395
211 260.509 Prev. Min.
212 272.690
213 282.060
214 284.262
215 248.283
216 246.298
217 247.099
218 240.717
219 249.789
220 255.332
221 270.493 Prev. Min.
222 260.449 Prev. Min.
223 272.606
224 279.093 Prev. Min.
225 281.415
226 261.310
227 252.846
228 256.874
229 Rejected No Minima
230 259.412
231 259.412 Same Min.
232 253.752
233 250.329
234 Rejected No Minima
235 243.601
236 279.755
237 290.132
238 282.180
239 260.950
240 246.364
241 266.428
242 263.317
243 238.221
244 229.233
245 224.787
246 232.649
247 236.805
248 271.747 Prev. Min.
249 269.896
250 278.155 Prev. Min.
251 242.368
252 255.069
253 244.051 Prev. Min.
254 240.888
255 Rejected No Minima
256 Rejected No Minima
257 255.360
258 Rejected No Minima
259 251.744
260 Rejected No Minima
261 243.282
262 244.057
263 235.587
264 277.456
265 287.309
266 303.143
267 Rejected No Minima
268 Rejected No Minima
269 Rejected No Minima
270 Rejected No Minima
271 297.987
272 310.618
273 310.618 Prev. Min.

274 312.092 Duplicate
275 Rejected No Minima
276 Rejected No Minima
277 Rejected No Minima
278 Rejected No Minima
279 316.153
280 294.024
281 Rejected No Minima
282 280.188
283 276.039 Duplicate
284 282.059
285 280.188 Prev. Min.
286 280.188 Same Min.
287 257.897
288 280.188 Prev. Min.
289 282.059 Prev. Min.
290 Rejected No Minima
291 Rejected No Minima
292 248.689
293 239.876
294 239.876 Same Min.
295 251.146
296 240.820
297 224.459
298 235.513
299 250.917
300 269.295
301 270.851
302 Rejected No Minima
303 283.904
304 258.015
305 242.595
306 258.015 Prev. Min.
307 266.678
308 264.735
309 265.703
310 256.810
311 222.645
312 Rejected No Minima
313 230.957
314 223.549
315 234.556 Prev. Min.
316 243.374 Duplicate
317 267.300
318 277.713
319 257.867
320 248.717
321 257.867 Prev. Min.
322 277.713 Prev. Min.
323 263.372
324 273.801
325 265.703 Prev. Min.
326 264.735 Prev. Min.
327 288.266
328 272.616
329 269.276
330 254.451
331 259.413
332 251.216
333 249.238
334 242.595 Duplicate
335 263.481
336 261.275 Prev. Min.
337 251.464
338 Rejected No Minima
339 245.821
340 236.421
341 250.929
342 Rejected No Minima
343 Rejected No Minima
344 Rejected No Minima
345 Rejected No Minima
346 236.421 Prev. Min.
347 250.929 Prev. Min.
348 247.236 Duplicate
349 247.236 Prev. Min.
350 253.055
351 247.236 Prev. Min.
352 256.997 Duplicate
353 248.717 Duplicate
354 253.055 Prev. Min.
355 Rejected No Minima
356 260.189
357 272.979
358 280.084
359 287.651
360 Rejected No Minima
361 Rejected No Minima
362 282.060 Duplicate
363 283.387
364 278.568
365 241.623
366 241.309
367 Rejected No Minima
368 246.298 Duplicate
369 266.354
370 Rejected No Minima
371 Rejected No Minima
372 Rejected No Minima
373 Rejected No Minima
374 265.334
375 Rejected No Minima
376 Rejected No Minima
377 5859.630 Bond Strain
378 308.782
379 Rejected No Minima
380 265.514
381 Rejected No Minima
382 274.237
383 239.851
384 243.179
385 256.440
386 247.684 Duplicate
387 265.300
388 250.329 Duplicate
389 278.493 Duplicate
390 250.329 Prev. Min.
391 270.244
392 250.154 Duplicate
393 280.049
394 Rejected No Minima
395 Rejected No Minima
396 270.244 Prev. Min.
397 Rejected No Minima
398 280.049 Prev. Min.
399 257.449
400 249.754
401 264.980
402 247.667 Duplicate
403 267.586 Duplicate
404 269.896 Duplicate
405 269.896 Prev. Min.
406 256.288 Duplicate
407 235.312
408 244.051 Duplicate
409 228.987
410 Rejected No Minima
411 258.339
412 279.823
413 256.255
414 Rejected No Minima
415 253.339
416 240.888 Duplicate
417 270.667
418 Rejected No Minima
419 273.812
420 280.624
421 267.112
422 270.659
423 266.684
424 5681.014 Bond Strain
425 4049.725 Bond Strain
426 269.742
427 235.685
428 240.891
429 227.546
430 234.669
431 227.546 Prev. Min.
432 243.248
433 260.193
434 241.513
435 269.399
436 Rejected No Minima
437 Rejected No Minima
438 Rejected No Minima
439 241.625 Duplicate
440 262.344
441 268.834
442 235.513 Prev. Min.
443 259.190
444 292.254 Duplicate
445 275.029
446 275.035
447 266.234
448 256.136
449 Rejected No Minima
450 261.711
451 259.044
452 259.044 Same Min.
453 224.629
454 242.199
455 Rejected No Minima
456 283.347
457 291.584
458 296.627
459 287.651 Duplicate
460 281.863
461 293.520
462 Rejected No Minima
463 Rejected No Minima
464 270.892
465 258.305
466 265.334
467 256.946
468 Rejected No Minima
469 251.653
470 242.595 Prev. Min.
471 251.653 Prev. Min.
472 250.759
473 267.961
474 257.897 Prev. Min.
475 249.771
476 240.887
477 Rejected No Minima
478 232.131
479 252.484
480 248.719
481 242.095
482 270.895 Duplicate
483 224.127
484 Rejected No Minima
485 Rejected No Minima
486 Rejected No Minima
487 231.285
488 265.334 Duplicate
489 250.327
490 243.374 Prev. Min.
491 259.415
492 249.599
493 Rejected No Minima
494 252.920
495 256.874 Duplicate
496 Rejected No Minima
497 244.517
498 Rejected No Minima
499 252.022
500 271.818
501 Rejected No Minima
502 241.766 Duplicate
503 252.022 Prev. Min.
504 261.207
505 Rejected No Minima
506 265.112
507 278.674 Duplicate
508 268.109 Duplicate
509 269.395 Duplicate
510 255.345 Duplicate
511 Rejected No Minima
512 261.062 Duplicate
513 289.531 Duplicate
514 261.207 Prev. Min.
515 257.816
516 261.207 Prev. Min.
517 Rejected No Minima
518 Rejected No Minima
519 265.112 Prev. Min.
520 268.813 Duplicate
521 Rejected No Minima
522 255.345 Prev. Min.
523 250.329 Duplicate
524 264.924
525 268.813 Prev. Min.
526 265.407
527 285.389
528 278.532
529 282.081 Duplicate
530 Rejected No Minima
531 285.389 Prev. Min.
532 345.548
533 285.389 Prev. Min.
534 345.548 Prev. Min.
535 305.036
536 Rejected No Minima
537 285.389 Prev. Min.
538 Rejected No Minima
539 Rejected No Minima
540 277.512
541 282.180 Duplicate
542 257.634
543 260.950 Duplicate
544 Rejected No Minima
545 260.950 Prev. Min.
546 Rejected No Minima
547 268.813 Prev. Min.
548 260.950 Prev. Min.
549 268.813 Prev. Min.
550 260.950 Prev. Min.
551 247.684 Duplicate
552 261.137
553 273.831
554 Rejected No Minima
555 261.208 Prev. Min.
556 252.022 Prev. Min.
557 238.192
558 233.770
559 240.736
560 233.886
561 227.685
562 215.073
563 260.090
564 226.289
565 233.886 Prev. Min.
566 227.546 Duplicate
567 265.340 Duplicate
568 227.685 Prev. Min.
569 233.755 Duplicate
570 233.886 Prev. Min.
571 232.131 Duplicate
572 240.818
573 239.131
574 248.265
575 247.643 Duplicate
576 248.265 Same Min.
577 248.266 Same Min.

578 Rejected No Minima
579 254.404
580 258.518
581 272.636
582 275.159
583 275.159 Prev. Min.
584 249.238 Duplicate
585 251.653 Duplicate
586 249.238 Prev. Min.
587 237.871
588 252.874
589 Rejected No Minima
590 256.411
591 Rejected No Minima
592 262.523
593 267.978
594 262.523 Prev. Min.
595 264.068
596 259.571
597 245.837
598 253.008
599 292.708
600 266.678 Duplicate
601 291.144
602 247.893
603 282.678
604 270.010
605 253.285
606 245.256
607 253.285 Prev. Min.
608 247.893 Prev. Min.
609 253.008 Prev. Min.
610 270.010 Prev. Min.
611 247.893 Prev. Min.
612 Rejected No Minima
613 245.828
614 244.906
615 246.364 Duplicate
616 245.828 Prev. Min.
617 Rejected No Minima
618 249.339
619 253.045
620 244.063
621 233.377
622 267.961
623 269.753
624 264.735 Duplicate
625 283.053 Duplicate
626 259.110
627 269.753 Prev. Min.
628 255.913
629 Rejected No Minima
630 243.643
631 241.049
632 254.899
633 244.300
634 256.570
635 267.348
636 275.326
637 270.576
638 Rejected No Minima
639 263.253
640 271.077
641 Rejected No Minima
642 260.702 Prev. Min.
643 260.702 Same Min.
644 255.219
645 265.992 Duplicate
646 260.702 Prev. Min.
647 255.219 Prev. Min.
648 272.979 Duplicate
649 265.992 Prev. Min.
650 251.842
651 252.264
652 264.648
653 271.502 Duplicate
654 Rejected No Minima
655 268.669
656 255.889
657 238.772
658 247.791 Duplicate
659 255.889 Prev. Min.
660 244.519
661 261.529 Duplicate
662 236.543
663 224.127 Prev. Min.
664 231.285 Prev. Min.
665 244.519 Prev. Min.
666 227.716
667 240.888 Duplicate
668 224.629 Duplicate
669 230.203
670 Rejected No Minima
671 Rejected No Minima
672 223.549 Duplicate
673 241.707
674 259.175
675 249.091 Duplicate
676 Rejected No Minima
677 257.544
678 Rejected No Minima
679 259.413 Duplicate
680 262.837
681 257.944
682 262.837 Prev. Min.
683 Rejected No Minima
684 262.523 Duplicate
685 Rejected No Minima
686 260.768
687 250.929 Duplicate
688 250.929 Prev. Min.
689 251.359 Same Min.
690 259.571
691 253.412
692 270.576 Duplicate
693 244.693
694 271.395
695 262.244
696 240.887 Duplicate
697 Rejected No Minima
698 271.395 Prev. Min.
699 253.464
700 257.634 Prev. Min.
701 277.512 Prev. Min.
702 Rejected No Minima
703 251.146 Duplicate
704 285.389 Prev. Min.
705 278.532 Prev. Min.
706 270.591
707 253.464 Prev. Min.
708 257.634 Prev. Min.
709 253.464 Prev. Min.
710 241.513 Duplicate
711 248.717 Duplicate
712 269.399 Duplicate
713 Rejected No Minima
714 269.399 Prev. Min.
715 Rejected No Minima
716 Rejected No Minima
717 282.065
718 274.974 Duplicate
719 Rejected No Minima
720 241.625 Duplicate
721 284.212 Duplicate
722 Rejected No Minima
723 244.772
724 Rejected No Minima
725 259.110 Duplicate
726 250.890
727 269.896 Duplicate
728 269.896 Prev. Min.
729 256.288 Duplicate
730 261.711 Duplicate
731 Rejected No Minima
732 261.711 Prev. Min.
733 253.293
734 240.888 Prev. Min.
735 243.282 Duplicate
736 Rejected No Minima
737 244.519 Prev. Min.
738 256.946 Duplicate
739 236.543 Prev. Min.
740 244.300 Duplicate
741 246.615
742 255.462 Duplicate
743 225.746
744 246.615 Prev. Min.
745 233.755 Prev. Min.
746 238.665 Duplicate
747 273.570 Duplicate
748 238.665 Prev. Min.
749 261.404
750 Rejected No Minima
751 279.823 Duplicate
752 Rejected No Minima
753 240.820 Duplicate
754 Rejected No Minima
755 Rejected No Minima
756 270.244 Duplicate
757 269.343
758 256.561
759 235.785 Duplicate
760 Rejected No Minima
761 235.785 Prev. Min.
762 247.684 Prev. Min.
763 238.034
764 250.184
765 268.687
766 261.426
767 279.483
768 Rejected No Minima
769 285.389 Prev. Min.
770 278.532 Prev. Min.
771 261.426 Prev. Min.
772 279.483 Prev. Min.
773 282.065 Prev. Min.
774 Rejected No Minima
775 244.772 Prev. Min.
776 257.449 Duplicate
777 250.890 Prev. Min.
778 269.936
779 249.754 Duplicate
780 271.747 Duplicate
781 250.890 Prev. Min.
782 256.136 Duplicate
783 274.974 Prev. Min.
784 Rejected No Minima
785 Rejected No Minima
786 238.962 Duplicate
787 Rejected No Minima
788 278.155 Duplicate
789 Rejected No Minima
790 Rejected No Minima
791 Rejected No Minima
792 Rejected No Minima
Restarting from minima
252.153
793 263.253 Duplicate
794 261.149
795 274.298
796 284.765
797 Rejected No Minima
798 283.053 Prev. Min.
799 Rejected No Minima
800 275.035 Prev. Min.
801 266.684 Duplicate
802 Rejected No Minima
803 283.282
804 Rejected No Minima
805 Rejected No Minima
806 Rejected No Minima
807 275.035 Prev. Min.
808 257.449 Duplicate
809 240.547
810 247.056
811 238.221 Prev. Min.
812 Rejected No Minima
813 228.987 Duplicate
814 251.146 Prev. Min.
815 256.440 Duplicate
816 Rejected No Minima
817 240.820 Prev. Min.
818 244.051 Prev. Min.
819 245.852
820 Rejected No Minima
821 247.684 Duplicate
822 241.342 Prev. Min.
823 250.329 Prev. Min.
824 234.671 Prev. Min.
825 236.105 Duplicate
826 248.689 Prev. Min.
827 233.614 Duplicate
828 234.671 Prev. Min.
829 236.105 Prev. Min.
830 245.949
831 255.219 Duplicate
832 252.071
833 236.773
834 233.332
835 222.645 Prev. Min.
836 230.957 Prev. Min.
837 248.722
838 Rejected No Minima
839 285.257
840 240.891 Prev. Min.
841 235.664
842 232.131 Prev. Min.
843 266.684 Prev. Min.
844 257.147 Duplicate
845 296.843 Duplicate
846 253.412 Duplicate
847 Rejected No Minima
848 232.131 Prev. Min.
849 230.156
850 Rejected No Minima
851 234.556 Prev. Min.
852 241.732
853 243.374 Prev. Min.
854 249.599 Duplicate
855 258.404
856 Rejected No Minima
857 Rejected No Minima
858 260.235 Prev. Min.
859 252.153 Prev. Min.
860 261.149 Prev. Min.
861 Rejected No Minima
862 267.957 Prev. Min.
863 261.149 Prev. Min.
864 252.329
865 240.547 Prev. Min.
866 252.329 Prev. Min.
867 Rejected No Minima
868 275.029 Prev. Min.
869 268.132 Duplicate
870 267.339
871 Rejected No Minima
872 Rejected No Minima
873 247.383
874 256.136 Prev. Min.
875 5352.232 Bond Strain
876 266.234 Prev. Min.
877 Rejected No Minima
878 Rejected No Minima
879 275.035 Prev. Min.

880 256.810 Prev. Min.
881 244.771 Duplicate
882 245.596
883 233.614 Prev. Min.
884 244.771 Prev. Min.
885 Rejected No Minima
886 254.590
887 224.459 Prev. Min.
888 241.399
889 230.641
890 235.513 Prev. Min.
891 259.190 Prev. Min.
892 275.029 Prev. Min.
893 282.059
894 268.132 Prev. Min.
895 280.624 Duplicate
896 277.405 Duplicate
897 Rejected No Minima
898 275.029 Prev. Min.
899 273.473
900 Rejected No Minima
901 239.072
902 248.230
903 262.837 Duplicate
904 262.837 Prev. Min.
905 284.123
906 242.228
907 Rejected No Minima
908 Rejected No Minima
909 Rejected No Minima
910 271.502 Prev. Min.
911 240.564 Prev. Min.
912 271.502 Prev. Min.
913 248.193
914 231.285 Duplicate
915 242.228 Prev. Min.
916 Rejected No Minima
917 248.193 Prev. Min.
918 250.151 Prev. Min.
919 269.227
920 253.285 Duplicate
921 248.193 Prev. Min.
922 281.863 Prev. Min.
923 242.228 Prev. Min.
924 271.502 Prev. Min.
925 Rejected No Minima
926 227.716 Duplicate
927 234.054
928 242.228 Prev. Min.
929 248.230 Prev. Min.
930 291.519
931 246.269
932 289.588
933 252.548
934 238.198
935 234.154
936 249.339 Duplicate
937 246.269 Prev. Min.
938 280.624 Prev. Min.
939 267.112 Duplicate
940 Rejected No Minima
941 289.588 Prev. Min.
942 246.269 Prev. Min.
943 257.544 Duplicate
944 262.360
945 248.043
946 262.887
947 242.199 Duplicate
948 283.758
949 251.247
950 266.782
951 Rejected No Minima
952 266.428 Duplicate
953 266.428 Prev. Min.
954 243.179 Duplicate
955 255.693
956 262.111
957 Rejected No Minima
958 241.625 Prev. Min.
959 253.464 Prev. Min.
960 248.717 Prev. Min.
961 Rejected No Minima
962 263.007
963 Rejected No Minima
964 Rejected No Minima
965 264.598
966 253.464 Prev. Min.
967 257.634 Prev. Min.
968 253.622 Same Min.
969 261.426 Prev. Min.
970 224.459 Duplicate
971 Rejected No Minima
972 252.517
973 Rejected No Minima
974 261.286
975 Rejected No Minima
976 255.335
977 Rejected No Minima
978 252.517 Prev. Min.
979 255.335 Prev. Min.
980 264.193
981 253.639
982 247.643 Prev. Min.
983 238.508
984 Rejected No Minima
985 247.643 Prev. Min.
986 Rejected No Minima
987 Rejected No Minima
988 244.517 Prev. Min.
989 227.534 Duplicate
990 250.269 Duplicate
991 250.269 Prev. Min.
992 233.755 Prev. Min.
993 240.818 Prev. Min.
994 239.876 Duplicate
995 Rejected No Minima
996 Rejected No Minima
997 252.846 Duplicate
998 253.494
999 240.887 Prev. Min.
1000 249.771 Duplicate
1001 249.091 Prev. Min.
1002 267.112 Duplicate
1003 257.897 Duplicate
1004 247.437 Duplicate
1005 267.112 Prev. Min.
1006 Rejected No Minima
1007 Rejected No Minima
1008 261.670 Duplicate
1009 251.920
1010 224.471
1011 228.912
1012 241.732 Duplicate
1013 224.471 Prev. Min.
1014 240.891 Duplicate
1015 239.005
1016 232.131 Prev. Min.
1017 240.700
1018 246.991
1019 245.155
1020 237.783
1021 Rejected No Minima
1022 230.156 Duplicate
1023 Rejected No Minima
1024 245.155 Prev. Min.
1025 Rejected No Minima
1026 235.724
1027 231.847 Duplicate
1028 250.327 Prev. Min.
1029 241.732 Prev. Min.
1030 265.396
1031 276.963
1032 235.785 Prev. Min.
1033 269.807
1034 235.785 Prev. Min.
1035 247.684 Prev. Min.
1036 237.153
1037 244.913
1038 Rejected No Minima
1039 Rejected No Minima
1040 Rejected No Minima
1041 256.874 Prev. Min.
1042 268.755
1043 282.043
1044 254.404 Prev. Min.
1045 246.439 Duplicate
1046 258.518 Prev. Min.
1047 248.265 Prev. Min.
1048 264.489
1049 239.131 Prev. Min.
1050 248.265 Prev. Min.
1051 238.508 Prev. Min.
1052 247.643 Prev. Min.
1053 269.227 Duplicate
1054 238.508 Prev. Min.
1055 Rejected No Minima
1056 247.643 Prev. Min.
1057 238.508 Prev. Min.
1058 Rejected No Minima
1059 260.787
1060 Rejected No Minima
1061 244.517 Prev. Min.
1062 238.508 Prev. Min.
1063 247.643 Prev. Min.
1064 Rejected No Minima
1065 239.131 Duplicate
1066 237.978
1067 Rejected No Minima
1068 242.073
1069 244.519 Prev. Min.
1070 237.153 Prev. Min.
1071 249.367
1072 251.527 Duplicate
1073 253.571
1074 Rejected No Minima
1075 244.771 Prev. Min.
1076 257.449 Prev. Min.
1077 236.678
1078 248.689 Duplicate
1079 247.191 Duplicate
1080 236.105 Duplicate
1081 248.689 Prev. Min.
1082 257.449 Prev. Min.
1083 248.416
1084 Rejected No Minima
1085 Rejected No Minima
1086 278.532 Prev. Min.
1087 248.689 Prev. Min.
1088 248.689 Same Min.
1089 278.532 Prev. Min.
1090 248.689 Same Min.
1091 248.689 Same Min.
1092 248.770 Same Min.
1093 233.614 Duplicate
1094 239.876 Prev. Min.
1095 Rejected No Minima
1096 224.459 Prev. Min.
Restarting from minima
224.471
1097 242.086
1098 251.920 Prev. Min.
1099 267.368
1100 242.086 Prev. Min.
1101 248.621
1102 240.409
1103 233.377 Duplicate
1104 233.377 Prev. Min.
1105 237.783 Prev. Min.
1106 252.071 Duplicate
1107 230.156 Prev. Min.
1108 234.556 Duplicate
1109 236.421 Duplicate
1110 237.783 Prev. Min.
1111 223.788
1112 237.783 Prev. Min.
1113 236.773 Duplicate
1114 236.773 Prev. Min.
1115 244.300 Prev. Min.
1116 244.963
1117 257.118
1118 225.746 Prev. Min.
1119 215.073 Prev. Min.
1120 245.585
1121 260.090 Prev. Min.
1122 226.289 Prev. Min.
1123 212.111 Duplicate
1124 256.826
1125 234.154 Duplicate
1126 256.774
1127 262.288
1128 257.853
1129 Rejected No Minima
1130 Rejected No Minima
1131 247.032
1132 240.409 Prev. Min.
1133 Rejected No Minima
1134 272.759 Duplicate
1135 Rejected No Minima
1136 242.095 Prev. Min.
1137 240.409 Prev. Min.
1138 251.937
1139 251.937 Prev. Min.
1140 272.759 Prev. Min.
1141 272.759 Prev. Min.
1142 272.759 Prev. Min.
1143 Rejected No Minima
1144 240.564 Duplicate
1145 242.095 Prev. Min.
1146 240.409 Prev. Min.
1147 247.032 Prev. Min.
1148 240.564 Prev. Min.
1149 248.193 Duplicate
1150 271.502 Prev. Min.
1151 9460.359 Bond Strain
1152 231.319
1153 228.987 Duplicate
1154 215.073 Prev. Min.
1155 225.746 Prev. Min.
1156 217.409 Duplicate
1157 234.054 Duplicate
1158 226.289 Prev. Min.
1159 245.526
1160 226.289 Prev. Min.
1161 255.693 Prev. Min.
1162 Rejected No Minima
1163 233.886 Prev. Min.
1164 248.416 Prev. Min.
1165 249.771 Prev. Min.
1166 254.590 Duplicate
1167 248.416 Same Min.
1168 248.689 Prev. Min.
1169 Rejected No Minima
1170 Rejected No Minima
1171 Rejected No Minima
1172 Rejected No Minima
1173 Rejected No Minima
1174 Rejected No Minima
Restarting from minima
228.987
1175 215.073 Duplicate
1176 242.228 Duplicate
1177 215.073 Prev. Min.
1178 217.409 Duplicate
1179 234.054 Duplicate

1180 245.585 Duplicate
1181 Rejected No Minima
1182 228.987 Prev. Min.
1183 235.312 Prev. Min.
1184 217.409 Prev. Min.
1185 250.890 Duplicate
1186 233.770 Duplicate
1187 234.718
1188 233.770 Prev. Min.
1189 240.736 Duplicate
1190 237.783 Duplicate
1191 238.192 Duplicate
1192 272.092
1193 217.409 Prev. Min.
1194 235.312 Prev. Min.
1195 257.072
1196 227.716 Duplicate
1197 256.255 Prev. Min.
1198 217.409 Prev. Min.
1199 235.312 Prev. Min.
1200 212.111 Duplicate
1201 250.890 Prev. Min.
1202 239.470
1203 Rejected No Minima
1204 261.718
1205 Rejected No Minima
1206 255.198
1207 261.718 Prev. Min.
1208 255.198 Prev. Min.
1209 Rejected No Minima
1210 261.718 Prev. Min.
1211 261.718 Prev. Min.
1212 259.098
1213 Rejected No Minima
1214 254.090
1215 242.073 Duplicate
1216 258.203
1217 268.013
1218 242.942 Duplicate
1219 Rejected No Minima
1220 258.203 Prev. Min.
1221 271.747 Duplicate
1222 245.852 Duplicate
1223 Rejected No Minima
1224 256.255 Prev. Min.
1225 235.312 Prev. Min.
1226 269.896 Prev. Min.
1227 Rejected No Minima
1228 269.896 Prev. Min.
1229 228.987 Prev. Min.
1230 235.312 Prev. Min.
1231 Rejected No Minima
1232 217.409 Prev. Min.
1233 223.788 Duplicate
1234 239.470 Prev. Min.
Restarting from minima
244.906
1235 242.199 Duplicate
1236 273.592
1237 250.720
1238 237.871 Duplicate
1239 251.920 Duplicate
1240 237.871 Prev. Min.
1241 252.874 Duplicate
1242 235.587 Duplicate
1243 249.238 Duplicate
1244 247.437 Duplicate
1245 235.587 Prev. Min.
1246 251.216 Duplicate
1247 244.394
1248 269.276 Duplicate
1249 260.018
1250 252.153 Duplicate
1251 251.216 Prev. Min.
1252 249.238 Prev. Min.
1253 Rejected No Minima
1254 257.064
1255 249.238 Prev. Min.
1256 261.275 Duplicate
1257 257.064 Prev. Min.
1258 249.599 Duplicate
1259 244.519 Duplicate
1260 249.599 Prev. Min.
1261 242.124
1262 254.385
1263 256.874 Duplicate
1264 234.556 Duplicate
1265 249.599 Duplicate
1266 236.421 Duplicate
1267 236.421 Prev. Min.
1268 240.887 Duplicate
1269 248.446
1270 247.436 Prev. Min.
1271 247.436 Prev. Min.
1272 243.064
1273 236.421 Prev. Min.
1274 243.064 Prev. Min.
1275 236.421 Same Min.
1276 240.887 Prev. Min.
1277 Rejected No Minima
1278 248.446 Prev. Min.
1279 248.446 Same Min.
1280 291.597
1281 259.571 Duplicate
1282 249.771 Duplicate
1283 252.071 Duplicate
1284 251.464 Duplicate
1285 259.571 Prev. Min.
Restarting from minima
251.464
1286 266.130
1287 267.300 Duplicate
1288 267.300 Prev. Min.
1289 242.124 Duplicate
1290 266.130 Prev. Min.
1291 242.124 Prev. Min.
1292 249.599 Prev. Min.
1293 236.543 Duplicate
1294 249.789 Duplicate
1295 242.124 Prev. Min.
1296 288.725
1297 249.599 Prev. Min.
1298 257.064 Prev. Min.
1299 258.404 Duplicate
1300 242.124 Prev. Min.
Restarting from minima
223.788
1301 Rejected No Minima
1302 224.127 Prev. Min.
1303 240.717 Duplicate
1304 240.717 Prev. Min.
1305 Rejected No Minima
1306 223.549 Prev. Min.
1307 240.547 Duplicate
1308 233.970
1309 Rejected No Minima
1310 240.547 Prev. Min.
1311 230.957 Duplicate
1312 246.671
1313 Rejected No Minima
1314 233.970 Prev. Min.
1315 230.957 Prev. Min.
1316 266.678 Duplicate
1317 266.678 Prev. Min.
1318 Rejected No Minima
1319 266.678 Prev. Min.
1320 231.285 Prev. Min.
1321 224.127 Prev. Min.
1322 243.374 Prev. Min.
1323 Rejected No Minima
1324 237.907
1325 236.543 Prev. Min.
1326 243.374 Prev. Min.
1327 258.404 Duplicate
1328 244.889
1329 241.844
1330 237.783 Duplicate
1331 Rejected No Minima
1332 238.962 Duplicate
1333 Rejected No Minima
1334 280.035
1335 280.035
1336 235.681 Duplicate
1337 244.889 Duplicate
1338 217.409 Duplicate
1339 235.681 Prev. Min.
1340 238.752 Duplicate
1341 241.844 Prev. Min.
1342 Rejected No Minima
1343 241.766 Duplicate
Restarting from minima
257.544
1344 273.210
1345 277.512
1346 280.624
1347 244.693 Prev. Min.
1348 253.412 Prev. Min.
1349 249.771 Prev. Min.
1350 266.684 Duplicate
1351 240.887 Prev. Min.
1352 244.693 Prev. Min.
1353 259.831
1354 249.771 Prev. Min.
1355 253.412 Prev. Min.
1356 315.756
1357 260.702 Duplicate
1358 266.418
1359 270.576 Prev. Min.
1360 266.418 Prev. Min.
1361 257.867 Duplicate
1362 270.576 Prev. Min.
1363 Rejected No Minima
1364 249.771 Prev. Min.
1365 266.684 Prev. Min.
1366 245.821 Duplicate
1367 245.821 Prev. Min.
1368 Rejected No Minima
1369 248.446 Duplicate
1370 236.421 Prev. Min.
1371 250.230
1372 282.359
1373 240.887 Prev. Min.
1374 244.693 Prev. Min.
1375 253.055 Duplicate
1376 240.887 Prev. Min.
1377 232.131 Prev. Min.
1378 230.156 Prev. Min.
1379 4093.673 Bond Strain
1380 232.131 Prev. Min.
1381 237.783 Prev. Min.
1382 Rejected No Minima
1383 243.374 Prev. Min.
1384 250.327 Prev. Min.
1385 234.556 Prev. Min.
1386 241.732 Prev. Min.
1387 233.418 Duplicate
Restarting from minima
240.409
1388 215.073 Prev. Min.
1389 Rejected No Minima
1390 Rejected No Minima
1391 228.987 Prev. Min.
1392 234.054 Prev. Min.
1393 226.289 Prev. Min.
1394 Rejected No Minima
1395 Rejected No Minima
1396 233.886 Prev. Min.
1397 233.886 Prev. Min.
1398 215.073 Prev. Min.
1399 Rejected No Minima
1400 249.754 Prev. Min.
1401 Rejected No Minima
1402 260.090 Prev. Min.
1403 246.119
1404 227.685 Prev. Min.
1405 225.746 Prev. Min.
1406 234.054 Prev. Min.
1407 234.054 Prev. Min.
1408 Rejected No Minima
1409 227.685 Prev. Min.
1410 249.754 Prev. Min.
1411 Rejected No Minima
1412 Rejected No Minima
1413 227.685 Prev. Min.
1414 217.409 Prev. Min.
1415 239.470 Duplicate
1416 212.111 Prev. Min.
Restarting from minima
227.685
1417 259.008
1418 Rejected No Minima
1419 215.073 Prev. Min.
1420 226.289 Prev. Min.
1421 217.409 Prev. Min.
1422 237.906 Prev. Min.
1423 237.906 Prev. Min.
1424 235.312 Duplicate
1425 238.962 Prev. Min.
1426 Rejected No Minima
1427 250.890 Prev. Min.
1428 212.111 Prev. Min.
1429 226.289 Prev. Min.
1430 217.409 Prev. Min.
1431 244.771 Prev. Min.
Restarting from minima
215.073
1432 215.073 Same Min.
1433 225.746 Prev. Min.
1434 273.570
1435 234.671 Duplicate
1436 233.755 Prev. Min.
1437 245.585 Prev. Min.
1438 226.784
1439 252.222 Duplicate
1440 225.746 Prev. Min.
1441 226.784 Prev. Min.
1442 244.051 Duplicate
1443 244.963 Prev. Min.
1444 236.773 Prev. Min.
1445 224.459 Prev. Min.
1446 238.034 Prev. Min.
1447 247.684 Prev. Min.
1448 247.684 Prev. Min.
1449 239.876 Prev. Min.
1450 270.591
1451 239.876 Same Min.
1452 240.818 Prev. Min.
1453 248.416 Prev. Min.
Restarting from minima
225.152
1454 Rejected No Minima
1455 233.970 Duplicate
1456 Rejected No Minima
1457 253.752 Duplicate
1458 232.794
1459 Rejected No Minima
1460 Rejected No Minima
1461 212.111 Duplicate
1462 215.073 Duplicate
1463 215.073 Prev. Min.
1464 Rejected No Minima
1465 234.054 Duplicate
1466 260.090 Duplicate
1467 260.090 Prev. Min.

1468 228.987 Duplicate
1469 228.987 Prev. Min.
1470 246.119 Duplicate
1471 Rejected No Minima
1472 227.685 Duplicate
Restarting from minima
238.221
1473 Rejected No Minima
1474 256.774 Duplicate
1475 273.168
1476 269.295
1477 229.233 Prev. Min.
1478 212.111 Prev. Min.
1479 217.409 Prev. Min.
1480 217.409 Prev. Min.
1481 240.730
1482 217.409 Prev. Min.
1483 212.111 Prev. Min.
1484 230.641 Prev. Min.
1485 229.233 Prev. Min.
1486 243.443 Duplicate
1487 235.312 Duplicate
1488 Rejected No Minima
1489 212.111 Prev. Min.
1490 223.549 Prev. Min.
1491 256.810 Prev. Min.
1492 230.641 Prev. Min.
1493 233.332 Prev. Min.
1494 234.556 Prev. Min.
1495 230.156 Prev. Min.
1496 4093.673 Bond Strain
1497 236.421 Duplicate
Restarting from minima
227.716
1498 Rejected No Minima
1499 224.629 Prev. Min.
1500 228.986
1501 Rejected No Minima
1502 264.762
1503 Rejected No Minima
1504 230.203 Prev. Min.
1505 223.549 Prev. Min.
1506 230.957 Prev. Min.
1507 240.547 Prev. Min.
1508 256.810 Duplicate
1509 230.957 Prev. Min.
1510 234.556 Prev. Min.
1511 Rejected No Minima
1512 224.127 Prev. Min.
1513 224.127 Prev. Min.
1514 Rejected No Minima
1515 231.285 Prev. Min.
1516 240.717 Prev. Min.
Restarting from minima
215.073
1517 227.685 Prev. Min.
1518 246.119 Prev. Min.
1519 226.289 Prev. Min.
1520 246.119 Prev. Min.
1521 225.746 Prev. Min.
1522 225.746 Prev. Min.
1523 Rejected No Minima
1524 215.073 Same Min.
1525 227.685 Prev. Min.
1526 Rejected No Minima
1527 Rejected No Minima
1528 225.746 Prev. Min.
Restarting from minima
212.111
1529 230.641 Prev. Min.
1530 223.549 Prev. Min.
1531 244.771 Prev. Min.
1532 229.233 Prev. Min.
1533 Rejected No Minima
1534 217.409 Prev. Min.
1535 Rejected No Minima
1536 226.289 Duplicate
1537 224.459 Prev. Min.
1538 234.494
1539 234.494 Prev. Min.
1540 244.771 Prev. Min.
1541 226.289 Prev. Min.
1542 222.645 Prev. Min.
1543 217.409 Prev. Min.
1544 234.718 Duplicate
1545 212.111 Prev. Min.
1546 224.459 Prev. Min.
1547 226.289 Prev. Min.
1548 226.289 Prev. Min.
1549 234.494 Prev. Min.
1550 226.289 Prev. Min.
1551 217.409 Prev. Min.
Restarting from minima
212.111
1552 229.233 Prev. Min.
1553 222.645 Prev. Min.
1554 244.771 Prev. Min.
1555 234.494 Prev. Min.
1556 212.111 Prev. Min.
1557 230.641 Prev. Min.
1558 229.233 Prev. Min.
1559 224.459 Prev. Min.
1560 234.494 Prev. Min.
1561 226.289 Prev. Min.
1562 225.152 Duplicate
1563 225.152 Prev. Min.
1564 229.233 Prev. Min.
Restarting from minima
215.073
1565 234.054 Prev. Min.
1566 249.754 Prev. Min.
1567 260.090 Prev. Min.
1568 228.987 Prev. Min.
1569 Rejected No Minima
1570 249.754 Prev. Min.
1571 246.119 Prev. Min.
1572 Rejected No Minima
1573 Rejected No Minima
1574 217.409 Prev. Min.
1575 226.289 Prev. Min.
1576 215.073 Same Min.
1577 217.409 Prev. Min.
Restarting from minima
218.292
1578 225.746 Duplicate
1579 Rejected No Minima
1580 234.671 Prev. Min.
1581 Rejected No Minima
1582 217.409 Prev. Min.
1583 233.770 Duplicate
1584 250.890 Duplicate
1585 250.890 Prev. Min.
1586 233.770 Prev. Min.
1587 215.073 Duplicate
1588 212.111 Prev. Min.
1589 241.625 Prev. Min.
1590 223.549 Prev. Min.
1591 217.409 Prev. Min.
Restarting from minima
228.987
1592 230.613
1593 231.314 Duplicate
1594 230.613 Prev. Min.
1595 227.534 Duplicate
1596 234.610
1597 240.085
1598 235.724 Duplicate
1599 231.847 Duplicate
1600 278.915
1601 235.724 Prev. Min.
1602 Rejected No Minima
1603 242.199 Duplicate
1604 245.155 Duplicate
1605 242.199 Prev. Min.
1606 231.847 Prev. Min.
1607 250.151 Duplicate
1608 252.264 Duplicate
1609 240.564 Duplicate
1610 259.944
1611 252.264 Prev. Min.
1612 249.483
1613 224.471 Duplicate
1614 250.151 Prev. Min.
1615 248.621 Duplicate
1616 244.057 Duplicate
1617 235.724 Prev. Min.
1618 271.892
1619 224.471 Prev. Min.
1620 228.912 Duplicate
1621 240.891 Duplicate
1622 267.368
1623 240.391
1624 240.391 Prev. Min.
1625 239.006 Duplicate
1626 231.847 Prev. Min.
1627 235.587 Duplicate
1628 267.368
1629 267.368
1630 240.891 Prev. Min.
1631 240.391 Prev. Min.
1632 245.828 Duplicate
1633 243.601 Duplicate
1634 245.828 Prev. Min.
1635 228.912 Prev. Min.
1636 245.374
1637 Rejected No Minima
1638 281.289
1639 261.396
1640 237.871 Duplicate
1641 250.329 Duplicate
1642 250.329 Prev. Min.
1643 Rejected No Minima
1644 Rejected No Minima
1645 Rejected No Minima
1646 228.962
1647 224.629 Duplicate
1648 235.785 Duplicate
1649 Rejected No Minima
1650 255.938
1651 224.629 Prev. Min.
1652 228.962 Prev. Min.
1653 238.772 Duplicate
1654 259.044 Duplicate
1655 238.772 Prev. Min.
1656 Rejected No Minima
1657 236.805 Duplicate
1658 233.377 Duplicate
1659 235.724 Prev. Min.
1660 228.986 Duplicate
1661 231.285 Duplicate
1662 236.805 Prev. Min.
1663 240.564 Prev. Min.
Restarting from minima
215.073
1664 Rejected No Minima
1665 Rejected No Minima
1666 226.289 Prev. Min.
1667 Rejected No Minima
1668 249.754 Prev. Min.
1669 246.119 Prev. Min.
1670 Rejected No Minima
1671 228.987 Prev. Min.
1672 228.987 Prev. Min.
1673 249.754 Prev. Min.
1674 Rejected No Minima
1675 260.090 Prev. Min.
1676 217.409 Prev. Min.
1677 235.312 Prev. Min.
1678 212.111 Prev. Min.
Restarting from minima
212.111
1679 226.289 Prev. Min.
1680 Rejected No Minima
1681 230.641 Prev. Min.
1682 230.641 Prev. Min.
1683 229.233 Prev. Min.
1684 226.289 Prev. Min.
1685 234.494 Prev. Min.
1686 234.494 Prev. Min.
1687 223.549 Prev. Min.
1688 244.771 Prev. Min.
1689 229.233 Prev. Min.
1690 226.289 Prev. Min.
1691 224.459 Prev. Min.
Restarting from minima
215.073
1692 225.746 Prev. Min.
1693 228.987 Prev. Min.
1694 Rejected No Minima
1695 225.746 Prev. Min.
1696 249.754 Prev. Min.
1697 234.054 Prev. Min.
1698 246.119 Prev. Min.
1699 Rejected No Minima
1700 217.409 Prev. Min.
1701 Rejected No Minima
1702 Rejected No Minima
1703 249.754 Prev. Min.
1704 Rejected No Minima
1705 Rejected No Minima
Restarting from minima
212.111
1706 225.152 Prev. Min.
1707 217.409 Prev. Min.
1708 244.771 Prev. Min.
1709 234.494 Prev. Min.
1710 234.494 Prev. Min.
1711 241.625 Prev. Min.
1712 225.152 Prev. Min.
1713 Rejected No Minima
1714 217.409 Prev. Min.
1715 239.470 Duplicate
1716 226.784 Duplicate
1717 237.906 Duplicate
1718 237.907 Prev. Min.
Restarting from minima
215.073
1719 228.987 Prev. Min.
1720 217.409 Prev. Min.
1721 245.585 Prev. Min.
1722 249.754 Prev. Min.
1723 Rejected No Minima
1724 215.073 Same Min.
1725 Rejected No Minima
1726 Rejected No Minima
1727 Rejected No Minima
1728 246.119 Prev. Min.
1729 249.754 Prev. Min.
1730 Rejected No Minima
Restarting from minima
212.111
1731 244.771 Prev. Min.
1732 229.233 Prev. Min.
1733 229.233 Prev. Min.
1734 244.771 Prev. Min.
1735 244.771 Prev. Min.
1736 229.233 Prev. Min.
1737 226.289 Prev. Min.
1738 244.771 Prev. Min.
1739 234.494 Prev. Min.
1740 230.641 Prev. Min.
1741 244.771 Prev. Min.
1742 Rejected No Minima
1743 229.233 Prev. Min.

Restarting from minima
212.111
1744 226.289 Prev. Min.
1745 223.549 Prev. Min.
1746 229.233 Prev. Min.
1747 241.625 Prev. Min.
1748 241.625 Prev. Min.
1749 226.289 Prev. Min.
1750 230.641 Prev. Min.
1751 244.771 Prev. Min.
1752 244.771 Prev. Min.
1753 225.152 Prev. Min.
1754 229.233 Prev. Min.
1755 Rejected No Minima
1756 224.459 Prev. Min.
Restarting from minima
217.409
1757 235.312 Prev. Min.
1758 238.962 Prev. Min.
1759 233.770 Prev. Min.
1760 239.470 Prev. Min.
1761 Rejected No Minima
1762 226.784 Prev. Min.
1763 235.312 Prev. Min.
1764 250.890 Prev. Min.
1765 235.312 Prev. Min.
1766 250.890 Prev. Min.
1767 250.890 Prev. Min.
1768 237.906 Prev. Min.
1769 215.073 Prev. Min.
No improvements found, exiting search early
Partition function correction to the energy
1.545134 kJ/mol
32.840% not in most favorable conformer.
Pruning list starting with 373 molecules out of 520
Removed 124 molecules outside of energy window.
Filtering using default clustering measure.
... Filtering 0.80% complete
Keeping 100 conformations. (373 original)
Lowest energy conformation 212.1108 kJ/mol

Cartesian coordinates for **11** (Å) and geometry optimization results

Atom	X	Y	Z
C0	6.6941012	1.0812454	2.4047034
C1	5.9982559	1.3316562	3.5853357
C2	4.6341622	1.0449697	3.6925020
C3	3.9958048	0.5006007	2.5717859
C4	4.6669214	0.2407750	1.3748196
C5	6.0414803	0.5359727	1.2929129
N6	2.6824269	0.1207452	2.3988363
C7	2.4934256	-0.3405370	1.1215749
C8	3.7098282	-0.2973002	0.4730604
C9	1.1932631	-0.8271372	0.5707463
N10	1.3473755	-1.0144002	-0.8968874
C11	2.6397936	-1.5847374	-1.3850437
C12	3.8592722	-0.7436328	-0.9398038
C13	2.7977561	-3.0817938	-1.0164729
C14	0.0472550	0.1427519	0.8751127
N15	-1.1724025	-0.3186782	0.2187954
C16	-1.0801950	-0.4021265	-1.2507415
C17	0.2110453	-1.1413025	-1.6930057
C18	-2.0425211	-1.0914244	0.9759932
O19	-1.8178686	-1.3715962	2.1541554
C20	-3.3063880	-1.5690519	0.3131582
O21	0.2600445	-1.7012195	-2.7926676
O22	3.8488866	-3.5761084	-0.6171417
N23	1.6851187	-3.8540859	-1.3088356
H24	0.9649203	-1.8163592	0.9881464
C25	-1.0879412	0.9707979	-1.9706467
N26	-2.3944855	1.6482817	-1.9911731
C27	-2.8776403	2.3799945	-0.9198516
C28	-3.2166145	1.5348817	-3.1922403
C29	-3.8959221	0.1954047	-3.3242434
O30	-1.9647556	2.4994226	0.0747485
O31	-3.9942732	2.8818774	-0.8758941
C32	-2.4168394	3.2219114	1.2233652
C33	-1.3331323	3.1367008	2.2700141
C34	1.7313024	-5.2876633	-1.1810811
C35	-5.1062704	-0.0492764	-2.6598850
C36	-5.7327378	-1.2919731	-2.7630981
C37	-5.1551084	-2.3026847	-3.5288185
C38	-3.9532431	-2.0711364	-4.1951534
C39	-3.3267163	-0.8278047	-4.0965039
C40	-0.1019162	3.7792557	2.0700771
C41	0.9176692	3.6711762	3.0176771
C42	0.7160202	2.9257677	4.1775476
C43	-0.5021646	2.2823037	4.3872980
C44	-1.5214027	2.3844120	3.4377527
H1	7.7558466	1.3069645	2.3448093
H2	6.5248221	1.7520353	4.4390556
H3	4.0969038	1.2351907	4.6154552
H4	6.5932844	0.3397041	0.3787535
H5	1.9710897	0.1973625	3.1146717
H6	2.6308194	-1.5665168	-2.4834390
H7	4.7986172	-1.2893364	-1.0793986
H8	3.9115053	0.1561137	-1.5667831
H9	-0.1078576	0.2284488	1.9548196
H10	0.2854715	1.1451910	0.5062197
H11	-1.9038456	-1.0122437	-1.6235299
H12	-4.0108348	-1.9047660	1.0804070
H13	-3.7762808	-0.7474593	-0.2292593
H14	-3.0917898	-2.4082298	-0.3525743
H15	1.0284842	-3.4584367	-1.9777643
H16	-0.3574005	1.6503176	-1.5181604
H17	-0.7625995	0.8521345	-3.0118291
H18	-3.9797503	2.3226993	-3.2080833
H19	-2.5796073	1.7302753	-4.0638131
H20	-2.5924683	4.2723432	0.9623948
H21	-3.3494209	2.7862208	1.6016997
H22	2.1986357	-5.5663763	-0.2327571
H23	0.7100698	-5.6730017	-1.2219187
H25	2.3161480	-5.6964040	-2.0093586
H26	-5.5640655	0.7308822	-2.0528759
H27	-6.6715759	-1.4704307	-2.2448875
H28	-5.6440834	-3.2701534	-3.6093709
H29	-3.5039976	-2.8591503	-4.7946080
H30	-2.3883290	-0.6673275	-4.6236449
H31	0.0706606	4.3586876	1.1654024
H32	1.8696722	4.1693845	2.8501527
H33	1.5072818	2.8506291	4.9188186
H34	-0.6621125	1.6972834	5.2897642
H35	-2.4588833	1.8590896	3.6107018

Method : MMFF94
Stoichiometry : C34 H35 N5 O5
Number of Atoms : 79
Point Group : C1
Energy: 212.11079
Degrees of Freedom : 231
Solvation energy -144.66482
Combined energy 67.44597
Net Charge : 0.000
Dipole Moment : 3.149 Debye
components : -1.5259 1.3432 -2.4045

Computational data from conformational analysis for **12**

Using Monte-Carlo algorithm.
Using rotatable bonds from rule normal set.

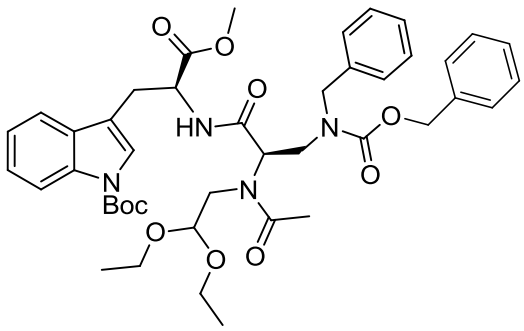
Conf	Energy (108) kJ/mol	Remark
1	415.367	
2	428.114	
3	425.387	
4	438.095	
5	416.515	
6	429.229	
7	417.928	
8	431.015	
9	404.824	!New Best!
10	417.609	
11	402.406	!New Best!
12	415.164	
13	435.693	
14	448.624	
15	426.445	
16	439.137	
17	432.949	
18	445.772	
19	405.955	
20	418.213	
21	408.863	
22	421.125	
23	405.561	
24	417.852	
25	381.291	!New Best!
26	393.633	
27	386.799	
28	399.075	
29	389.692	
30	401.969	
31	417.237	
32	429.724	
33	409.400	
34	421.614	
35	404.230	
36	416.533	
37	423.257	
38	428.114	
39	425.387	
40	438.095	
41	429.281	
42	467.564	
43	417.928	Prev. Min.
44	431.015	
45	404.824	Prev. Min.
46	417.609	Prev. Min.
47	402.406	Prev. Min.
48	415.164	Prev. Min.
49	404.824	Prev. Min.
50	417.609	Prev. Min.
51	426.445	
52	439.137	
53	432.949	
54	445.772	
55	410.103	
56	447.945	
57	417.033	
58	455.087	
59	412.691	
60	451.372	
61	388.417	
62	426.583	
63	393.979	
64	432.131	
65	395.061	
66	433.186	
67	388.417	Prev. Min.
68	426.583	
69	416.771	
70	454.930	
71	410.922	
72	449.028	
73	408.054	
74	424.505	
75	420.887	
76	436.319	
77	403.961	
78	419.649	
79	415.237	
80	415.035	
81	399.129	
82	415.035	Prev. Min.
83	396.743	
84	411.688	
85	428.709	
86	444.608	
87	419.577	
88	435.273	
89	428.647	
90	444.778	
91	395.884	
92	413.305	
93	403.421	
94	418.089	
95	391.035	
96	407.569	
97	377.203	!New Best!
98	392.372	
99	380.448	
100	395.584	
101	382.867	
102	398.895	
103	411.387	
104	426.243	
105	402.368	
106	417.269	
107	399.368	
108	414.766	

Partition function correction to the energy
1.752985 kJ/mol
38.036% not in most favorable conformer.
Pruning list starting with 54 molecules out of 54
Keeping 54 conformations. (54 original)
Lowest energy conformation 377.2034 kJ/mol

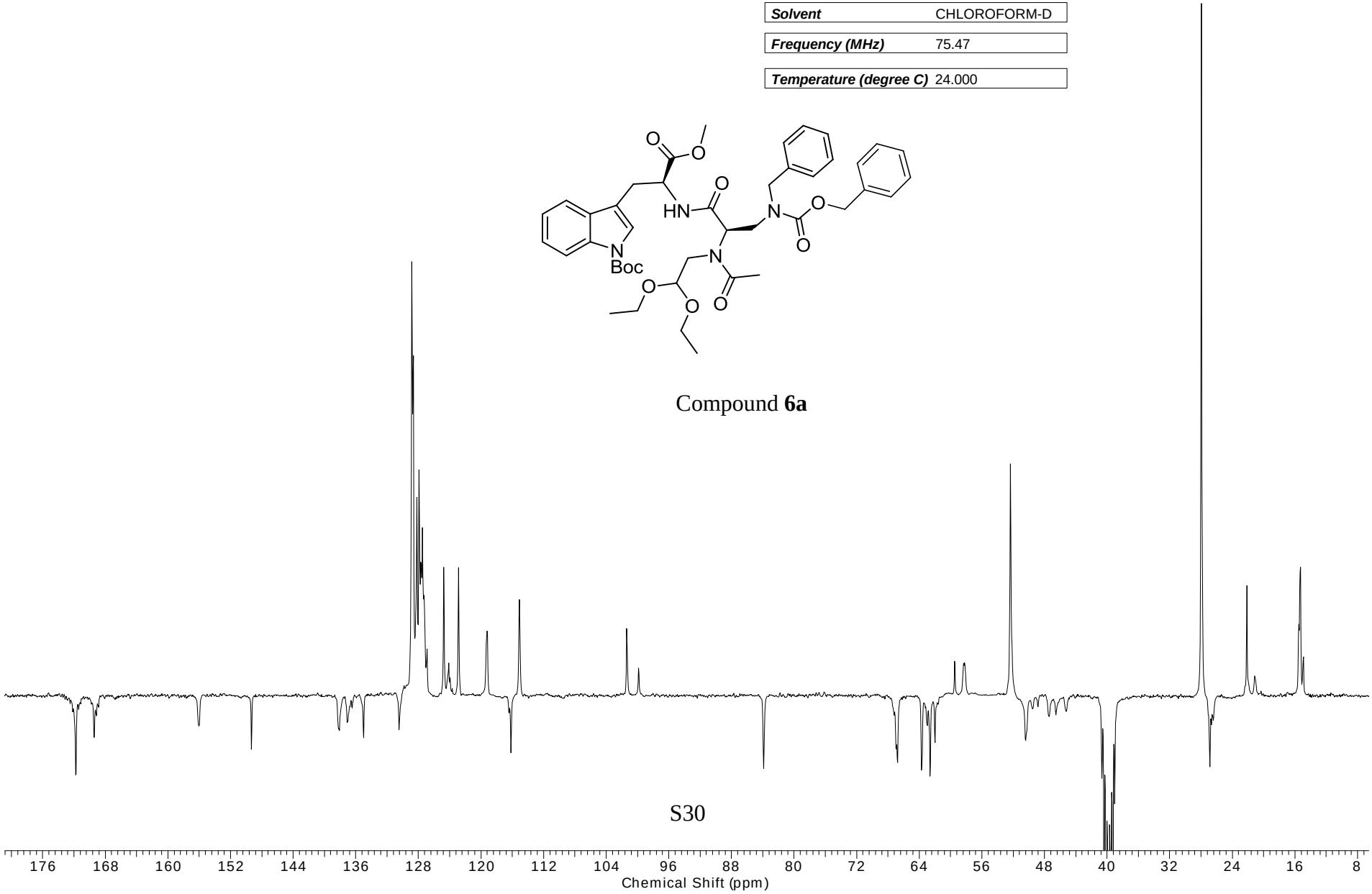
Cartesian coordinates for **12** (Å) and geometry optimization results

Atom	X	Y	Z
C0	-3.7712527	-2.1416502	-3.1330895
C1	-4.5903474	-2.1562219	-2.0065430
C2	-4.1651281	-1.5946601	-0.7988763
C3	-2.8892001	-1.0191974	-0.7639647
C4	-2.0477372	-0.9882154	-1.8779115
C5	-2.4985540	-1.5614392	-3.0828165
N6	-2.2237037	-0.4047152	0.2756431
C7	-0.9840817	0.0030182	-0.1373940
C8	-0.8535376	-0.3327434	-1.4746867
C9	0.0327538	0.7529821	0.6816966
N10	1.3216539	0.5478699	-0.0105277
C11	1.3438963	0.9002748	-1.4573555
C12	0.3912785	-0.0362478	-2.2548910
C13	1.0771979	2.3986355	-1.7531398
C14	0.0648759	0.4064410	2.1763772
N15	0.6912450	-0.8837084	2.4354992
C16	1.9937861	-1.1028277	1.7851251
C17	2.1619460	-0.4976967	0.3752528
C18	0.3357295	-1.7399061	3.4645018
O19	0.9905340	-2.7440195	3.7462485
C20	-0.9165290	-1.4151807	4.2374093
O21	3.0918180	-0.8711540	-0.3485633
O22	0.8155008	3.2317840	-0.8877202
H24	-0.2290269	1.8132738	0.6194868
C25	3.1945729	-0.6663295	2.6699503
N26	3.2114370	0.7560254	3.0561310
H1	-4.1216116	-2.5862871	-4.0612605
H2	-5.5756727	-2.6130719	-2.0657413
H3	-4.8062631	-1.6106748	0.0762432
H4	-1.8673641	-1.5573469	-3.9659897
H5	-2.6171965	-0.2836311	1.1980308
H6	2.3618048	0.7377335	-1.8370612
H7	0.1299308	0.3788482	-3.2335691
H8	0.9036675	-0.9906018	-2.4332685
H9	0.6468574	1.1606185	2.7165879
H10	-0.9434935	0.4472555	2.5954276
H11	2.0815373	-2.1878133	1.6327642
H12	-0.8178132	-0.4440072	4.7291898
H13	-1.7839945	-1.4272535	3.5724066
H14	-1.0705105	-2.1732143	5.0116617
H18	3.1943315	-1.2546163	3.5941643
H19	4.1358998	-0.8906595	2.1544853
N1	1.2089816	2.7493694	-3.0870426
H16	1.6933024	2.1141271	-3.7085442
C6	1.0937007	4.1265894	-3.4984711
H15	0.9646185	4.1555291	-4.5827781
H17	2.0096913	4.6540348	-3.2194141
H31	0.2375539	4.5976915	-3.0080902
H36	4.0181130	0.9170295	3.6601659
H47	3.3748021	1.3259595	2.2242616

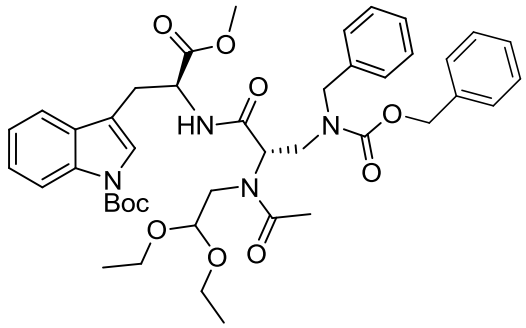
Method : MMFF94
Stoichiometry : C19 H23 N5 O3
Number of Atoms : 50
Point Group : C1
Degrees of Freedom : 144
Solvation energy -131.22486
Combined energy 284.14251
Net Charge : 0.000
Dipole Moment : 5.187 Debye
components : -2.2957 3.4984 -3.0647



Compound **6a**



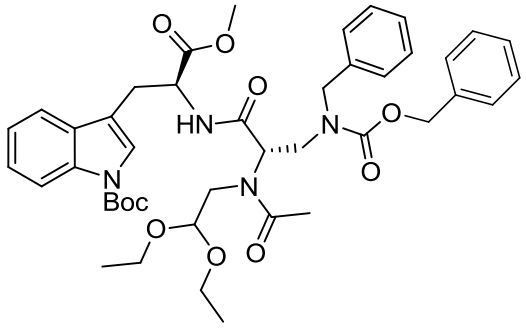
Compound **6a**



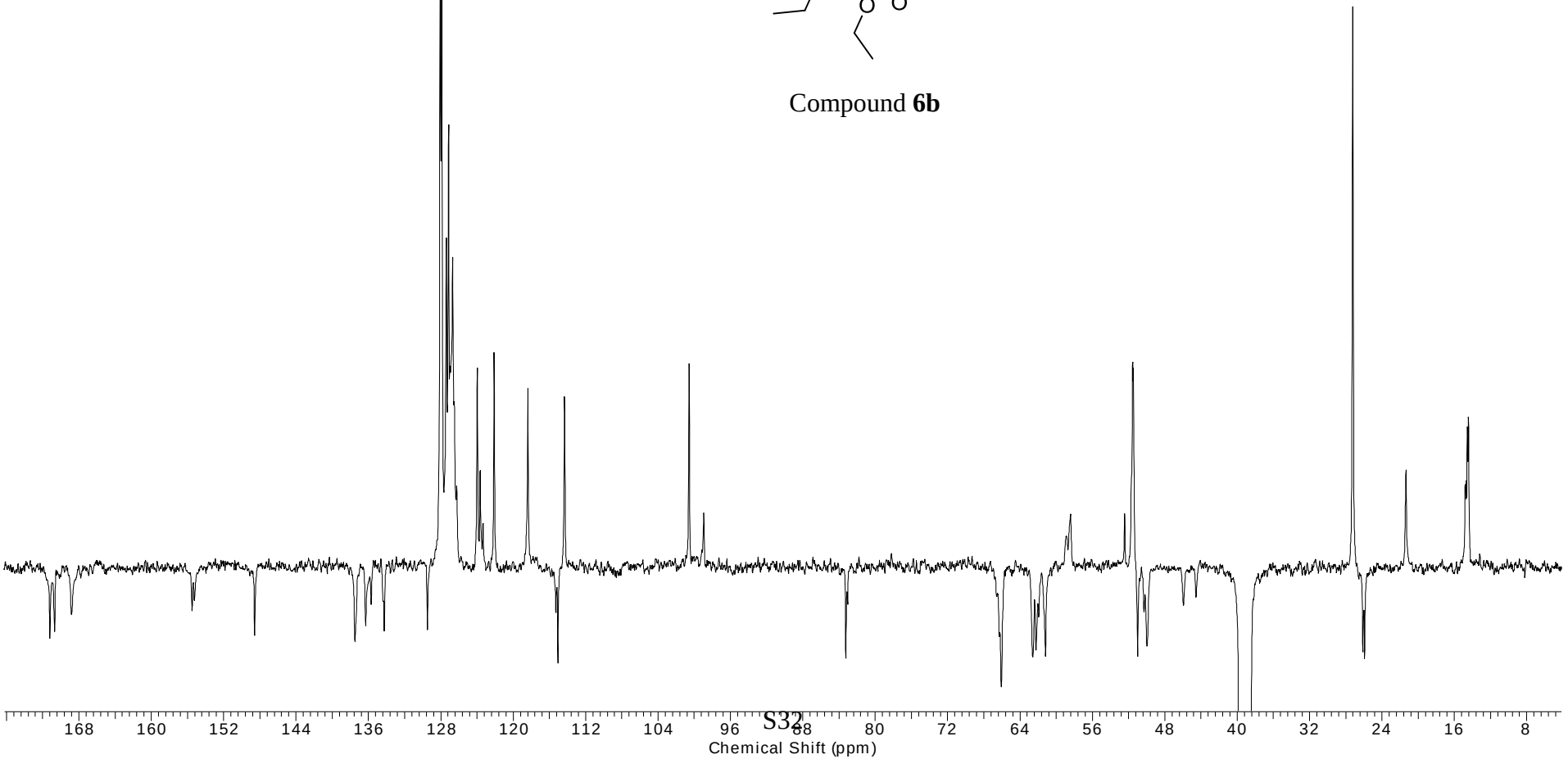
Compound **6b**

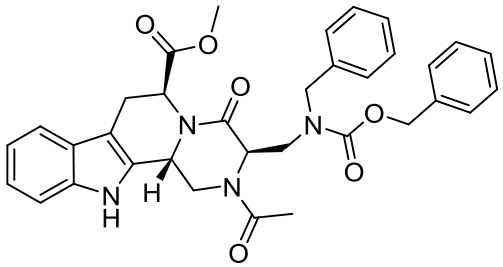
Frequency (MHz)	400.10
Temperature (degree C)	100.400
Solvent	DMSO-D6

Frequency (MHz)	100.62
Temperature (degree C)	30.400
Solvent	DMSO-D6

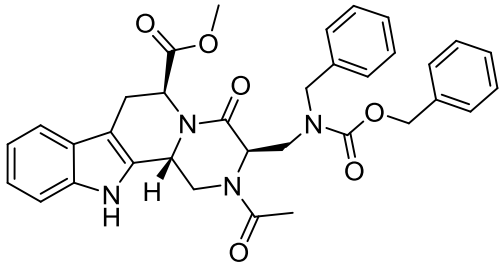


Compound **6b**



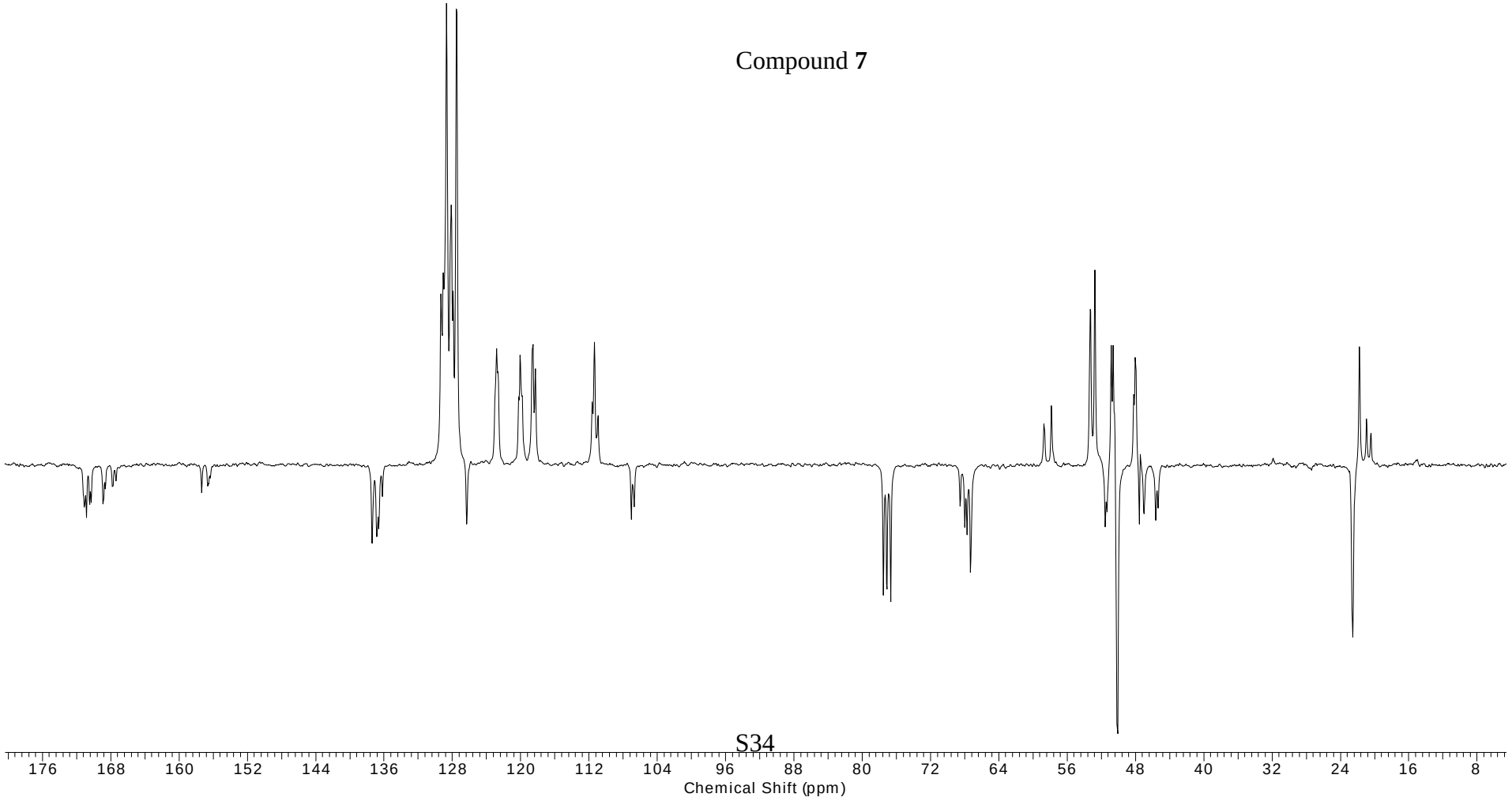


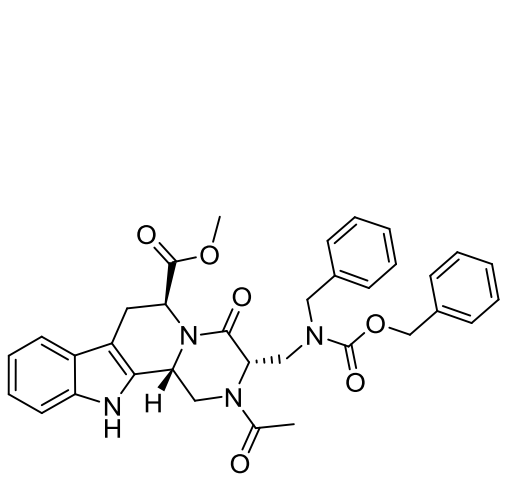
Compound **7**



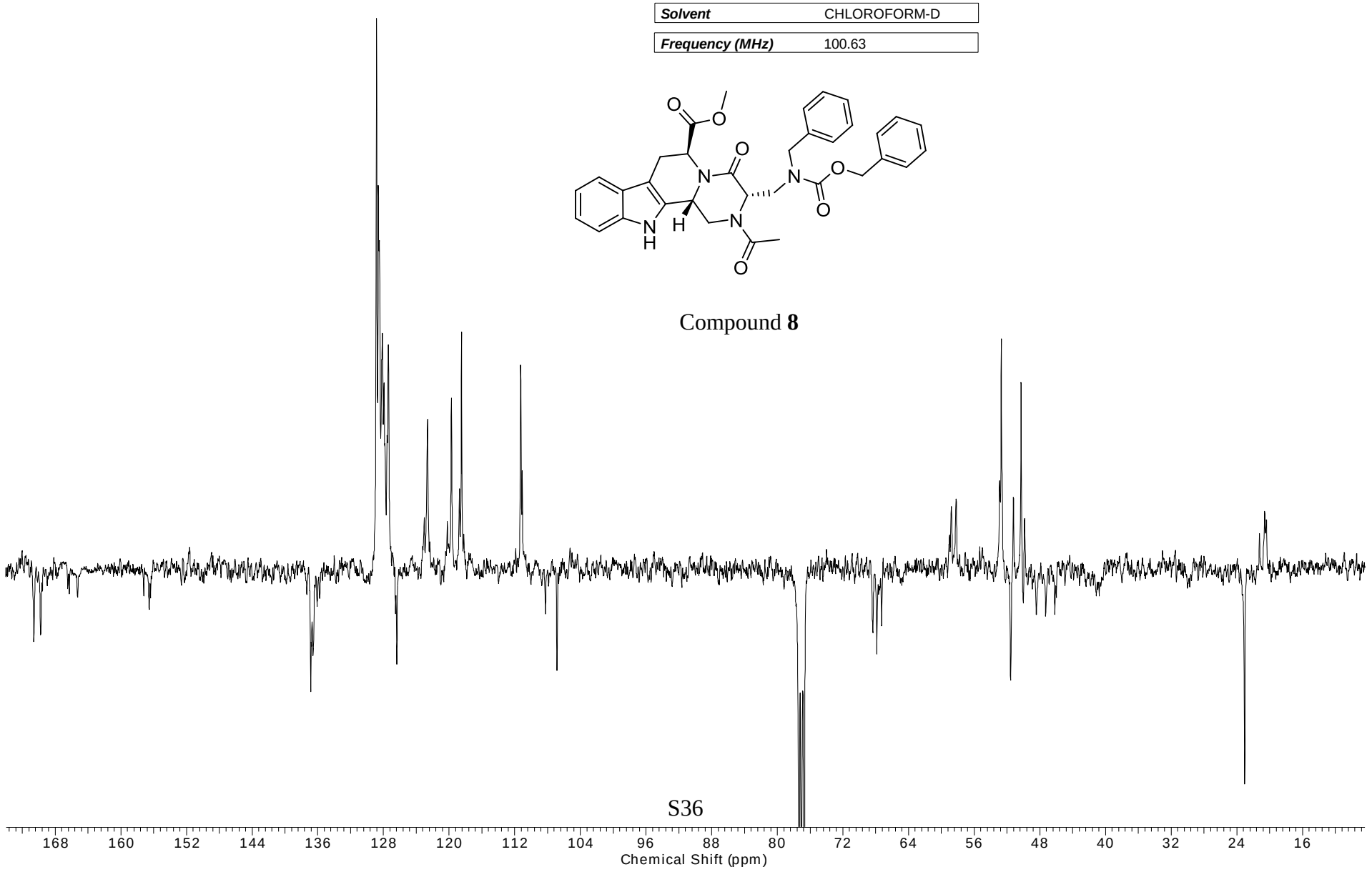
Frequency (MHz)	75.47
Temperature (degree C)	24.000

Compound **7**

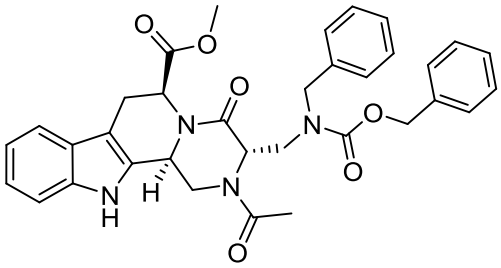




Compound **8**

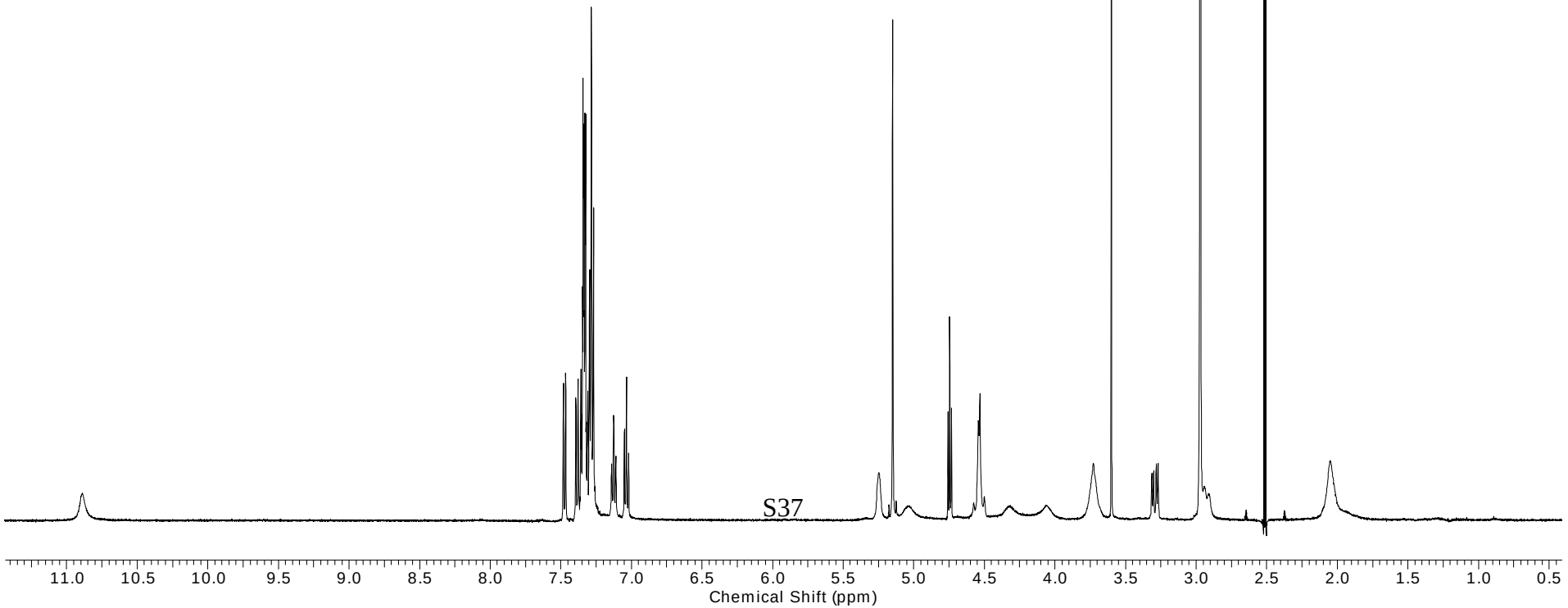


Compound **8**

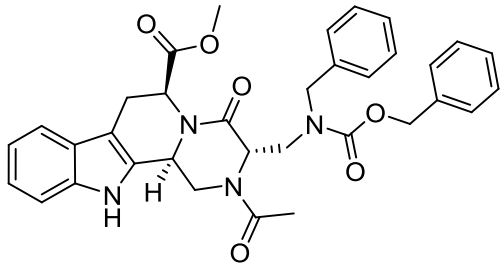


Compound **9**

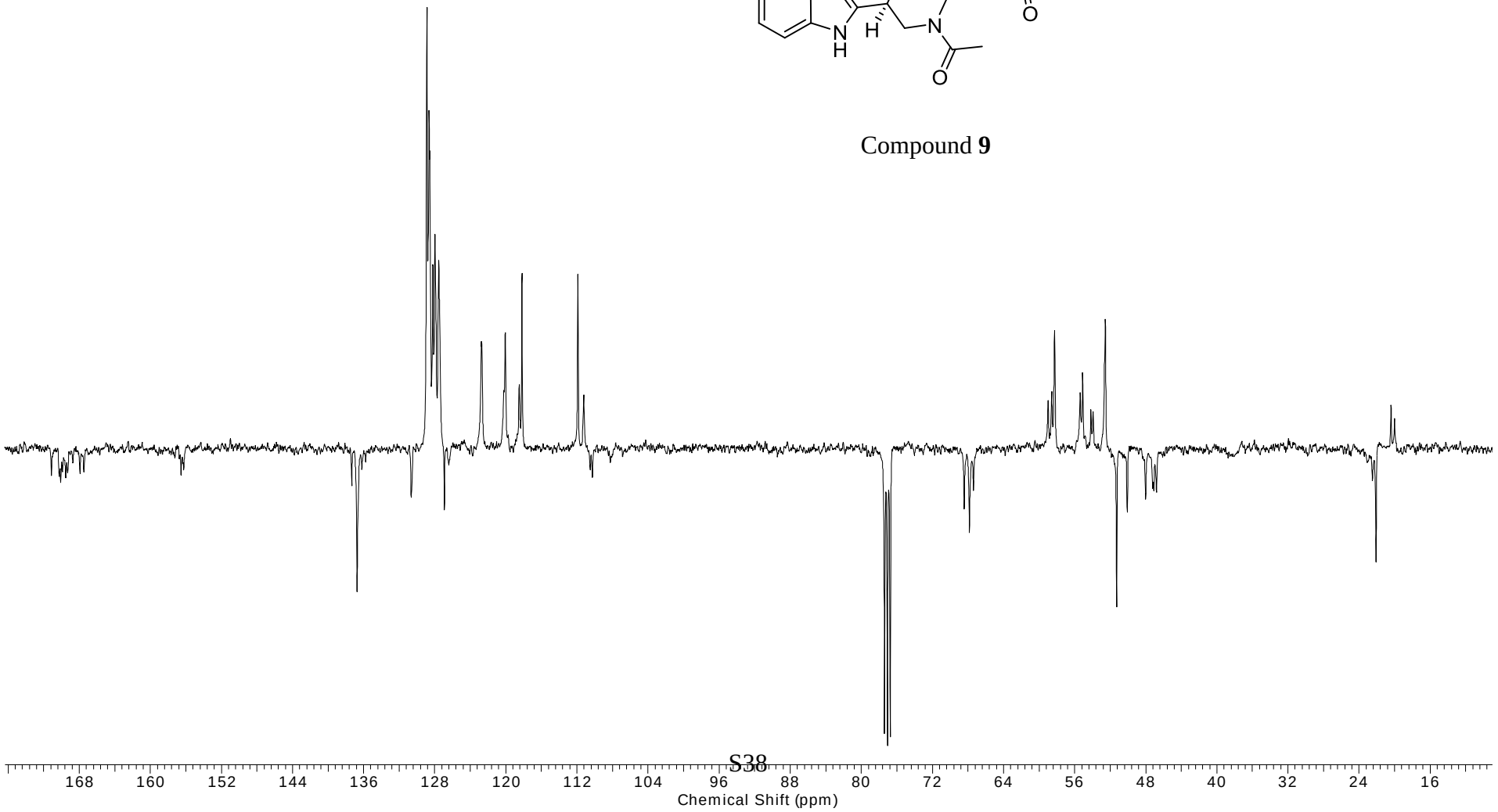
Frequency (MHz)	500.13
Temperature (degree C)	100.100
Solvent	DMSO-D6

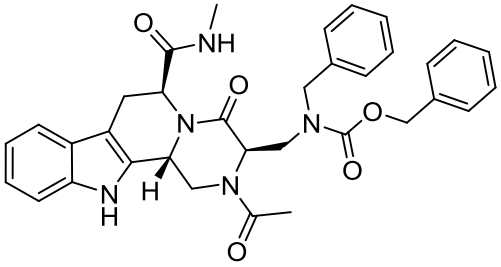


Frequency (MHz)	100.63
Temperature (degree C)	30.000
Solvent	CHLOROFORM-D

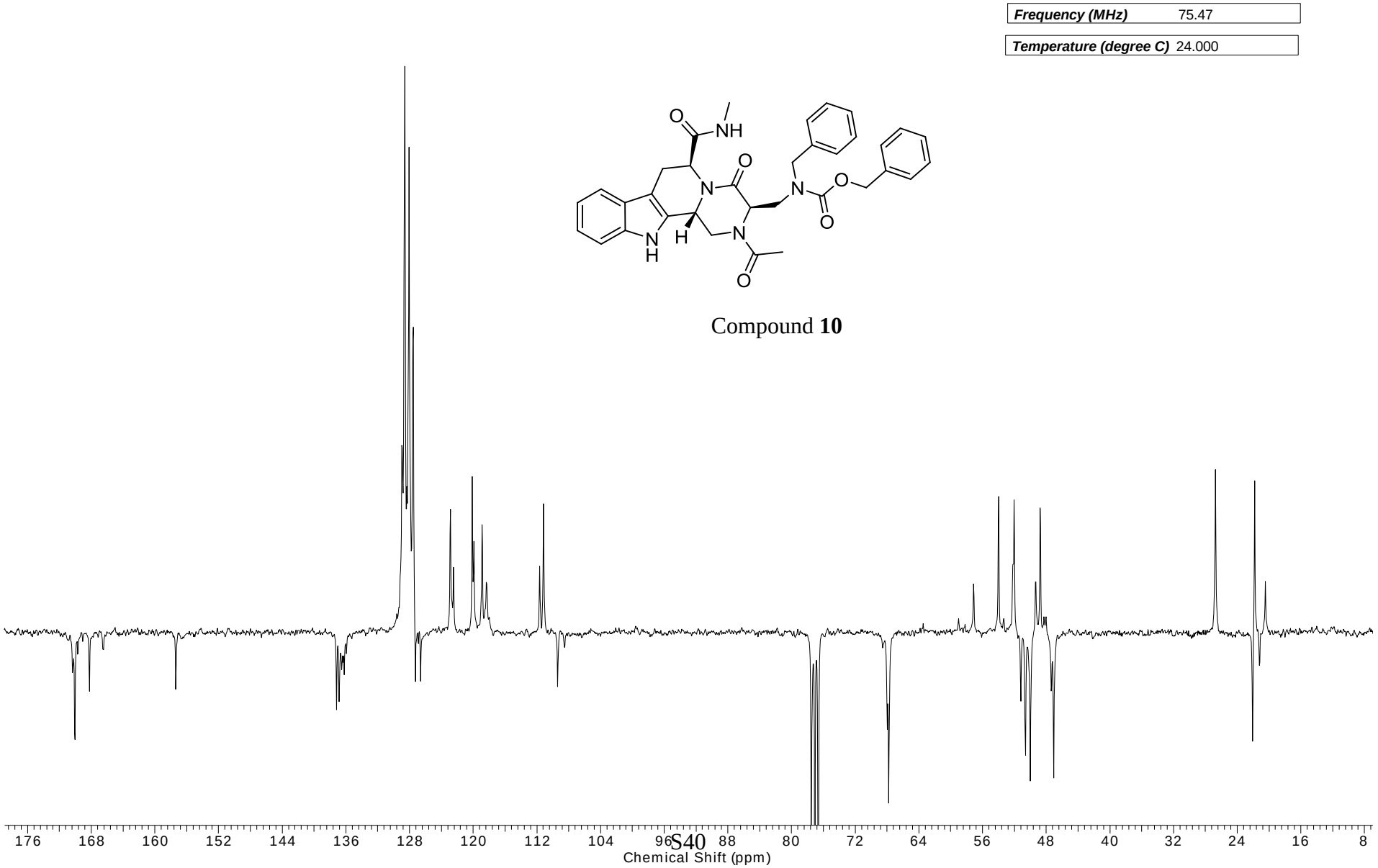


Compound **9**

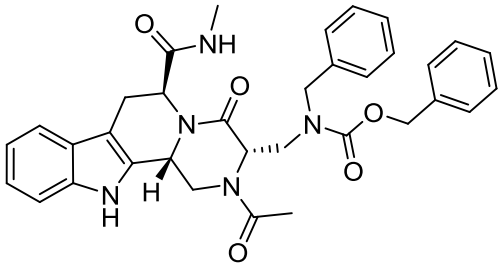




Compound **10**



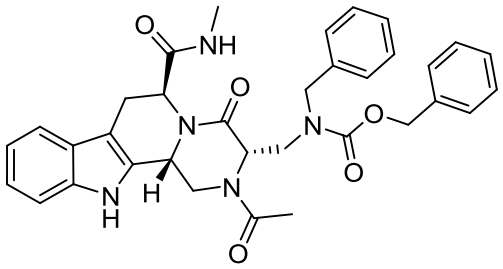
Compound **10**



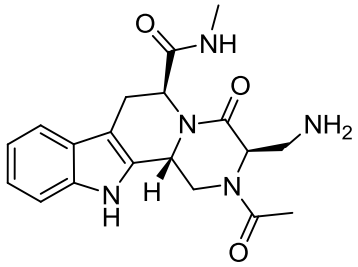
Compound **11**

Frequency (MHz)	400.10
Temperature (degree C)	100.000
Solvent	DMSO-D6

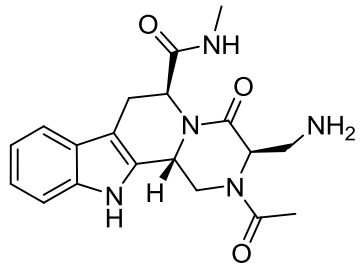
Frequency (MHz)	100.62
Temperature (degree C)	24.300
Solvent	MeOD + CDCl3



Compound **11**



Compound **12**



Frequency (MHz)	125.77
Temperature (degree C)	31.700
Solvent	MeOD

Compound **12**