Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Solvation of Serine-based Model Peptides and the Role of the Intramolecular OH··O Hydrogen Bond

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1. Conformational analysis of 1

Table S1. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of the computed conformers of **1** sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β).

	ϕ_{Ser} = (CC$^{\alpha}$NC)	ψ_{Ser} = (NCC$^{\alpha}$N)	α = (NC$^{\alpha}$CO)	β = (C$^{\alpha}$COH)	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
1_c1a	-83.0	73.8	58.7	61.4	0.0[a)]	0.0[a)]	56.3	30.2
1_c4b	-127.7	17.2	-171.6	-48.6	1.20	0.83	7.4	7.4
1_c9a	-151.3	-175.3	-168.7	79.2	1.30	1.03	6.3	5.3
1_c5a	-124.3	17.4	60.5	80.0	1.33	0.22	6.0	20.8
1_c2b	-84.2	63.4	-179.7	-63.7	1.44	1.39	4.9	2.9
1_c10a	-166.7	164.7	-80.7	40.8	1.46	1.09	4.8	4.8
1_c5c	-110.9	2.4	55.3	-178.3	1.56	0.70	4.0	9.3
1_c9c	-149.3	-176.5	-166.7	-174.6	1.65	1.33	3.4	3.2
1_c11b	-146.7	171.0	62.3	-59.7	2.28	1.65	1.2	1.9
1_c12a	-107.5	148.1	-60.5	55.8	2.34	1.17	1.1	4.2
1_c8b	-147.1	158.8	-173.6	-85.3	2.41	1.19	1.0	4.0
1_c6b	-85.3	-17.2	-56.4	-70.5	2.68	2.17	0.6	0.8
1_c14b	76.8	-122.2	79.9	-52.6	2.96	2.90	0.4	0.2
1_c6a	-110.1	4.9	-65.5	62.4	3.08	2.05	0.3	0.9
1_c3a	-83.6	77.3	-65.2	56.2	3.09	2.61	0.3	0.4
1_c18b	68.0	29.7	-166.5	-58.1	3.11	2.87	0.3	0.2
1_c6c	-86.2	-14.9	-58.5	179.5	3.14	2.46	0.3	0.5
1_c3c	-87.9	68.7	-60.7	178.5	3.17	2.46	0.3	0.5
1_c3b	-87.3	70.7	-55.8	-68.0	3.18	2.49	0.3	0.5
1_c11c	-147.0	167.6	67.0	-168.5	3.43	2.53	0.2	0.4
1_c1c	-84.1	48.3	49.3	179.6	3.55	3.45	0.1	0.1
1_c21b	98.0	-14.3	78.4	-63.2	3.86	3.48	0.1	0.1
1_c22b	75.5	-38.8	80.4	-52.0	3.92	4.20	0.1	0.0
1_c12c	-103.4	127.5	-67.4	172.3	3.93	2.15	0.1	0.8
1_c13c	-83.3	163.1	61.5	-171.2	4.03	2.77	0.1	0.3
1_c23a	71.2	-51.4	-61.3	69.0	4.24	3.73	0.0	0.1
1_c25c	-120.5	-89.9	58.2	-178.4	4.34	2.97	0.0	0.2
1_c25b	-135.5	-87.7	58.3	-68.8	4.39	3.75	0.0	0.1
1_c23c	76.8	-49.7	-61.9	173.1	4.62	4.21	0.0	0.0
1_c23b	76.3	-49.1	-59.4	-73.3	4.66	4.49	0.0	0.0
1_c15b	70.0	175.4	83.8	-54.2	4.68	4.78	0.0	0.0
1_c24b	70.7	-17.3	-162.3	-41.2	4.71	3.70	0.0	0.1
1_c26a	167.2	-32.8	-82.0	63.2	4.72	4.19	0.0	0.0
1_c19a	69.7	24.0	-60.6	73.8	4.91	4.16	0.0	0.0
1_c19c	71.2	26.9	-59.6	177.2	4.95	4.34	0.0	0.0
1_c16c	62.3	-164.2	-160.2	-173.4	5.27	5.01	0.0	0.0
1_c19b	72.2	23.8	-58.5	-79.7	5.42	4.84	0.0	0.0
1_c16a	61.0	-160.8	-166.0	70.7	5.52	5.54	0.0	0.0
1_c24a	73.3	-60.7	-178.2	63.1	5.53	5.26	0.0	0.0
1_c20a	50.3	51.0	67.3	59.3	5.92	5.95	0.0	0.0
1_c24c	74.1	-65.0	-168.8	-165.7	5.96	5.88	0.0	0.0
1_c17a	53.7	-143.9	-56.9	55.0	6.46	5.95	0.0	0.0
1_c7c	-78.5	-32.9	-176.6	-177.7	6.77	5.75	0.0	0.0
1_c22a	64.0	-37.8	59.7	61.5	7.23	6.90	0.0	0.0
1_c26b	-169.1	-22.3	-170.2	-42.6	7.25	7.29	0.0	0.0
1_c17c	60.1	-125.6	-62.8	174.0	7.71	6.41	0.0	0.0
1_c18a	69.4	34.3	-145.8	74.8	7.94	7.24	0.0	0.0
1_c22c	62.6	-31.1	70.2	178.0	7.97	7.83	0.0	0.0
1_c14c	41.4	-119.7	69.0	-177.6	8.34	8.41	0.0	0.0
1_c20c	57.4	35.8	55.7	173.3	9.49	9.35	0.0	0.0

[a)] referenced to E = -764.057414 hartree and G =-764.103747 hartree.

Table S2. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of the 25 lowest energy conformers of **1**··$(DMSO)_1$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β). The torsional angle definitions and conformer numbers are the same as used in Tab. S1.

	ϕ_{Ser}	ψ_{Ser}	α	β	Solvated H	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
1_c5b_$(DMSO)_1$	-91.4	-10.2	67.4	-74.5	BocNH / OH	0.0[a)]	1.27	24.5	5.8
1_c5c_$(DMSO)_1$	-103.1	-3.7	55.7	-169.6	OH	0.45	0.0[a)]	11.6	49.8
1_c9c_$(DMSO)_1$	-148.4	-174.4	-166.6	-166.7	OH	0.57	1.09	9.4	8.0
1_c6a_$(DMSO)_1$	-82.0	-20.6	-63.5	83.6	BocNH / OH	0.60	1.73	9.0	2.7
1_c9a_$(DMSO)_1$	-149.6	-174.2	-172.1	82.3	OH	0.67	1.68	7.9	2.9
1_c5a_$(DMSO)_1$	-99.9	-6.1	49.2	89.7	OH	0.70	1.54	7.5	3.7
1_c9c_$(DMSO)_1$	-148.7	-174.2	-166.4	-169.2	OH	0.90	1.59	5.4	3.4
1_c8a_$(DMSO)_1$	-138.2	146.3	177.5	47.4	OH	1.05	2.60	4.2	0.6
1_c6b_$(DMSO)_1$	-79.9	-23.2	-53.2	-73.2	OH	1.24	1.29	3.0	5.7
1_c6c_$(DMSO)_1$	-81.4	-21.7	-58.1	171.3	OH	1.47	1.22	2.1	6.4
1_c10a_$(DMSO)_1$	-166.1	160.9	-78.4	37.3	NH	1.64	3.44	1.5	0.1
1_c4b_$(DMSO)_1$	-125.3	16.7	-171.2	-48.2	BocNH	1.80	2.90	1.2	0.4
1_c5a_$(DMSO)_1$[b)]	-96.2	-8.8	49.0	89.6	OH	1.82	2.75	1.1	0.5
1_c13b_$(DMSO)_1$	-78.0	159.9	73.2	-64.5	OH	1.85	3.94	1.1	0.1
1_c13a_$(DMSO)_1$	-92.1	115.3	56.6	47.7	NHPr	2.12	3.39	0.7	0.2
1_c3a_$(DMSO)_1$	-86.5	73.1	-62.1	-68.1	BocNH	2.14	3.35	0.7	0.2
1_c13c_$(DMSO)_1$	-75.5	163.5	59.4	-170.9	OH	2.19	2.47	0.6	0.8
1_c11c_$(DMSO)_1$	-144.4	166.3	66.0	-172.2	OH	2.22	2.73	0.6	0.5
1_c25c_$(DMSO)_1$	-110.2	-91.4	57.5	-178.9	OH	2.24	2.80	0.6	0.4
1_c4Xb_$(DMSO)_1$	-125.6	-6.0	-169.9	-39.0	BocNH	2.28	3.09	0.5	0.3
1_c12a_$(DMSO)_1$	-117.1	146.8	-64.6	89.4	OH	2.29	2.25	0.5	1.1
1_c25b_$(DMSO)_1$	-108.3	-96.6	67.0	-65.5	BocNH / OH	2.30	3.93	0.5	0.1
1_c4b_$(DMSO)_1$	-127.7	-7.2	-169.8	-38.4	NPrH /BocNH	2.33	3.34	0.5	0.2
1_c25b_$(DMSO)_1$	-107.5	-99.2	67.7	-63.7	BocNH / OH	2.34	4.25	0.5	0.0
1_c12a_$(DMSO)_1$	-111.3	149.0	-59.6	58.2	NPrH	2.37	2.47	0.4	0.8
1_c11b_$(DMSO)_1$	-146.7	167.5	61.1	-60.9	NPrH	2.40	3.07	0.4	0.3
1_c6a_$(DMSO)_1$	-96.6	-30.4	-62.9	57.2	NPrH/BocNH	2.59	3.58	0.3	0.1
1_c12c_$(DMSO)_1$	-118.8	144.3	-66.7	171.5	OH	2.60	1.78	0.3	2.4
1_c13a_$(DMSO)_1$	-82.3	124.3	56.3	46.7	NPrH	2.72	4.49	0.2	0.0
1_c3b_$(DMSO)_1$	-87.0	71.7	-65.3	177.1	BocNH	2.80	3.07	0.2	0.3

[a)] referenced to E = -1317.2429 hartree and G = -1317.30348 hartree
[b)] Boc group in cis-conformation

Table S3. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of the 30 lowest energy conformers of **1**··$(DMSO)_2$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β). The torsional angle definitions are those used in Tab. S1.

	ϕ_{Ser}	ψ_{Ser}	α	β	Solvated H	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
1_c5c_$(DMSO)_2$	-100.6	-20.1	62.1	176.4	OH + NPrH/BocNH	0.0[a)]	2.80	7.8	0.3
1_c13b_$(DMSO)_2$	-77.7	159.3	73.2	-64.5	OH/BocNH + NPrH	0.01	1.95	7.6	1.1
1_c8c_$(DMSO)_2$	-143.2	132.3	-177.7	-178.5	OH + NPrH	0.07	0.0[a)]	6.9	30.0
1_c5c_$(DMSO)_2$	-104.7	-21.1	62.6	-171.2	OH + NPrH/BocNH	0.13	2.24	6.2	0.7
1_c11c_$(DMSO)_2$	-145.0	163.8	65.9	-173.3	OH + NPrH	0.19	0.18	5.7	22.3
1_c11b_$(DMSO)_2$	-147.4	164.9	66.6	-86.0	OH + NPrH	0.24	1.80	5.2	1.4
1_c8c_$(DMSO)_2$	-145.4	137.5	-175.5	-171.8	OH + NPrH	0.31	1.53	4.6	2.3
1_c5c_$(DMSO)_2$	-105.0	-16.7	63.0	-174.5	OH + NPrH/BocNH	0.44	2.58	3.7	0.4
1_c12c_$(DMSO)_2$	-120.0	145.3	-66.9	165.4	OH + NPrH	0.47	0.34	3.5	16.8
1_c8b_$(DMSO)_2$	-138.0	133.6	-172.8	-95.4	OH + NPrH	0.48	1.66	3.5	1.8
1_c6b_$(DMSO)_2$	-98.8	-8.8	-61.8	-76.0	OH + BocNH	0.51	0.93	3.3	6.2
1_c6a_$(DMSO)_2$	-78.9	-26.1	-64.2	80.9	OH/BocNH + NPrH	0.51	3.20	3.3	0.1
1_c13c_$(DMSO)_2$	-74.5	161.9	58.7	-170.8	OH + NPrH	0.52	0.88	3.2	6.8
1_c6a_$(DMSO)_2$	-92.9	-32.6	-68.1	89.7	OH + NPrH/BocNH	0.55	2.81	3.1	0.3
1_c5c_$(DMSO)_2$	-109.9	-0.5	63.5	-177.2	OH + BocNH	0.58	2.04	2.9	1.0
1_c8a_$(DMSO)_2$	-136.4	123.6	179.7	92.0	OH + NPrH	0.61	2.26	2.8	0.7
1_c9a_$(DMSO)_2$	-107.5	-165.1	-172.0	76.0	OH + BocNH	0.70	2.55	2.4	0.4
1_c5c_$(DMSO)_2$	-102.6	-2.9	64.0	-179.6	OH + BocNH	0.72	2.66	2.3	0.3
1_c5a_$(DMSO)_2$	-100.0	-20.2	56.6	94.3	OH + NPrH/BocNH	0.76	3.32	2.2	0.1
1_c9c_$(DMSO)_2$	-108.0	-166.6	-167.0	-166.9	OH + BocNH	0.77	2.55	2.1	0.4
1_c8b_$(DMSO)_2$	-139.0	133.5	-172.7	-95.5	OH + NPrH	0.83	2.72	1.9	0.3
1_c6c_$(DMSO)_2$	-102.5	-4.6	-64.1	-174.6	OH + BocNH	0.85	1.78	1.9	1.5
1_c6a_$(DMSO)_2$	-105.4	-2.8	-68.8	87.7	OH + BocNH	0.93	3.48	1.6	0.1
1_c6b_$(DMSO)_2$	-76.1	-29.6	-54.6	-76.5	OH + NPrH	0.97	2.73	1.5	0.3
1_c5a_$(DMSO)_2$	-98.1	-6.4	63.8	106.2	OH + BocNH	1.08	3.02	1.3	0.2
1_c7c_$(DMSO)_2$	-97.7	-50.9	-179.8	-174.9	OH + NPrH/BocNH	1.09	2.30	1.2	0.6
1_c12a_$(DMSO)_2$	-117.3	153.5	-67.4	86.4	OH + NPrH	1.13	2.52	1.2	0.4
1_c6c_$(DMSO)_2$	-76.5	-29.2	-58.6	170.4	OH + NPrH	1.20	2.55	1.0	0.4
1_c13c_$(DMSO)_2$	-99.7	122.2	-176.7	-165.0	OH + BocNH	1.55	1.97	0.6	1.1
1_c12a_$(DMSO)_2$	-98.4	137.1	-69.4	96.0	OH + BocNH	1.59	4.09	0.5	0.0

[a)] referenced to E = -1870.419491 hartree and G = -1870.493012 hartree

Table S4. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of the 15 lowest energy conformers of **1**··$(DMSO)_3$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β). The torsional angle definitions are those used in Tab. S1.

	ϕ_{Ser}	ψ_{Ser}	α	β	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
1_c12a_$(DMSO)_3$	-98.7	140.6	-68.9	96.8	0.0[a)]	0.73	27.4	12.1
1_c13c_$(DMSO)_3$	-102.9	123.5	-178.3	-173.2	0.37	0.62	14.7	14.5
1_c8c_$(DMSO)_3$	-98.4	124.1	-178.0	-172.8	0.52	0.0[a)]	11.5	41.6
1_c12c_$(DMSO)_3$	-98.8	140.1	-66.6	174.0	0.61	1.08	9.8	6.7
1_c8b_$(DMSO)_3$	-101.7	121.3	-175.2	-118.0	0.68	0.61	8.7	14.7
1_c8a_$(DMSO)_3$	-112.9	116.0	179.8	89.3	0.76	1.59	7.6	2.8
1_c13b_$(DMSO)_3$	-103.0	124.4	-174.9	-105.9	1.07	1.62	4.5	2.7
1_c6b_$(DMSO)_3$	-99.2	-12.3	-62.9	-76.8	1.19	2.31	3.7	0.8
1_c11c_$(DMSO)_3$	-126.1	154.6	66.5	-173.6	1.34	2.39	2.9	0.7
1_c13c_$(DMSO)_3$	-95.4	160.9	66.4	-172.0	1.41	1.86	2.5	1.8
1_c11b_$(DMSO)_3$	-130.4	160.7	64.0	-96.9	1.41	2.80	2.5	0.4
1_c5c_$(DMSO)_3$	-120.7	5.7	63.2	-179.4	1.83	3.30	1.3	0.2
1_c11b_$(DMSO)_3$	-131.7	158.3	63.5	-97.5	1.94	2.93	1.0	0.3
1_c19c_$(DMSO)_3$	62.3	40.7	-60.3	177.4	2.53	3.42	0.4	0.1
1_c19c_$(DMSO)_3$	61.4	42.3	-60.0	-177.2	2.61	3.84	0.3	0.1

[a)] referenced to E = -2423.59658 hartree and G = -2423.685341 hartree

2. Conformational analysis of 2

Table S5. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of all optmized conformers of **2** sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β/γ).

	ϕ_{Ser}	ψ_{Ser}	ϕ_{Phe}	ψ_{Phe}	α	β	γ	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2(β,pp$_{II}$)	-147.0	160.6	-69.9	151.3	-176.9	-81.6	-172.1	0.0[a)]	0.85	11.6	3.8
	-147.5	160.3	-71.0	155.0	-176.9	-80.9	-62.2	0.00	0.50	11.6	6.8
	-145.2	160.0	-78.6	165.2	-175.8	-80.2	57.9	0.90	1.82	2.5	0.7
2(δ,δ)	-75.0	-14.9	-101.6	5.7	51.9	75.6	-63.7	0.56	1.67	4.5	0.9
	-78.8	-8.3	-95.7	1.9	55.7	-178.9	56.9	0.93	2.25	2.4	0.4
	-79.6	-7.6	-93.9	1.0	53.2	80.6	57.0	0.95	1.74	2.4	0.8
	-72.0	-20.8	-88.7	-2.4	-54.0	-73.5	-64.3	0.96	2.05	2.3	0.5
	-72.6	-20.1	-91.4	1.4	-54.3	-72.8	56.4	1.12	2.86	1.8	0.1
	-79.4	-7.0	-89.8	-4.0	54.3	177.7	-65.9	1.27	1.85	1.4	0.7
	-72.8	-19.7	-88.9	-2.4	-57.1	175.8	-64.3	1.28	2.38	1.3	0.3
	-81.3	-3.4	-91.5	-4.9	-169.6	-42.7	-63.2	1.44	2.22	1.0	0.4
	-73.6	-18.7	-91.9	1.5	-57.1	176.5	56.4	1.45	3.00	1.0	0.1
	-81.6	-3.4	-98.0	1.8	-170.1	-41.6	56.3	1.55	3.27	0.8	0.1
	-79.1	-9.5	-87.8	-4.9	-72.1	73.9	-64.2	3.01	3.79	0.1	0.0
	-79.6	-10.0	-95.1	2.9	-70.8	74.0	56.0	3.06	4.32	0.1	0.0
	-67.0	-30.5	-84.7	-2.5	-169.4	-166.1	-63.5	5.17	6.21	0.0	0.0
	-66.4	-32.3	-87.2	2.1	-172.8	-176.3	56.5	5.19	6.33	0.0	0.0
2(δ,β)	-124.1	15.6	-151.7	143.5	-170.8	-48.3	-173.5	0.47	0.28	5.2	9.8
	-122.4	16.6	-150.4	141.9	59.7	81.1	-173.7	0.69	0.0[a)]	3.6	15.8
	-107.6	0.3	-151.2	141.9	56.0	-177.2	-173.2	0.83	0.61	2.9	5.6
	-106.9	-4.7	-126.1	136.6	52.9	77.7	-60.5	1.09	1.52	1.8	1.2
	-127.7	15.4	-121.1	135.9	-170.8	-49.0	-61.4	1.49	1.48	0.9	1.3
	-125.7	15.3	-152.8	162.1	-171.0	-47.9	59.1	1.71	1.98	0.7	0.6
	-83.6	-18.9	-150.9	143.9	-56.4	-69.6	-172.9	1.91	2.00	0.5	0.5
	-107.9	-0.4	-153.1	161.6	56.9	-176.4	63.9	2.07	2.57	0.4	0.2
	-124.1	17.2	-150.7	160.2	61.9	81.8	63.3	2.08	1.92	0.3	0.6
	-107.0	2.4	-150.2	143.5	-65.1	60.8	-173.8	2.13	1.84	0.3	0.7
	-111.4	0.3	-122.5	136.0	54.3	178.4	-65.6	2.26	1.66	0.3	1.0
	-82.9	-18.3	-151.1	143.3	-58.6	177.5	-173.0	2.28	2.08	0.2	0.5
	-87.2	-19.0	-120.7	130.6	-56.6	-70.2	-61.4	2.83	2.31	0.1	0.3
	-85.4	-18.3	-150.1	161.8	-57.4	-69.5	61.7	3.14	3.34	0.1	0.1
	-109.6	2.0	-119.9	133.2	-65.7	62.5	-61.1	3.37	3.02	0.0	0.1
	-86.6	-17.9	-120.2	129.1	-59.4	179.1	-61.2	3.39	2.86	0.0	0.1
	-106.3	0.0	-153.0	163.3	-65.2	60.0	59.9	3.42	3.88	0.0	0.0
	-84.9	-17.2	-150.5	161.6	-59.7	178.6	61.8	3.65	3.89	0.0	0.0
	-77.9	-32.8	-148.1	145.1	-176.4	-178.4	-172.7	5.48	4.65	0.0	0.0
	-75.3	-36.3	-149.7	162.1	180.0	176.3	59.6	6.63	6.75	0.0	0.0
	-82.3	-31.7	-108.5	125.3	-170.5	-161.5	-61.6	6.67	5.51	0.0	0.0
2(β,β)	-118.6	146.8	-151.0	163.4	-66.7	172.8	62.4	4.45	4.29	0.0	0.0
	-118.1	144.8	-118.1	139.0	-67.5	172.5	-63.6	4.28	3.20	0.0	0.1
	-145.2	168.6	-151.8	163.6	67.3	-173.0	60.4	3.48	3.21	0.0	0.1
	-143.9	166.3	-123.7	138.7	67.1	-173.4	-61.8	3.40	2.73	0.0	0.2
	-113.2	138.8	-152.6	147.6	-67.2	171.9	-172.8	3.24	2.34	0.0	0.3
	-108.7	152.2	-152.5	163.9	-60.3	55.6	62.2	2.86	2.70	0.1	0.2
	-110.5	150.4	-119.3	138.9	-60.1	55.7	-63.6	2.74	2.13	0.1	0.4
	-115.1	102.7	-151.1	163.1	55.5	52.9	66.1	2.61	2.70	0.1	0.2
	-145.4	168.9	-154.2	163.3	61.3	-60.0	60.3	2.46	2.41	0.2	0.3

Table S5 continued.

	-145.0	167.0	-125.8	138.6	61.2	-59.6	-61.8	2.40	2.23	0.2	0.4
	-147.5	169.5	-152.6	147.0	67.2	-172.1	-172.7	2.35	1.77	0.2	0.8
	-165.6	163.8	-154.9	163.5	-79.3	38.6	60.6	1.97	2.58	0.4	0.2
	-165.4	161.9	-126.5	141.6	-80.0	39.3	-62.0	1.73	2.03	0.6	0.5
	-105.9	149.4	-151.5	144.0	-60.3	55.2	-173.6	1.61	0.76	0.8	4.4
	-146.8	170.9	-153.3	146.2	61.6	-60.2	-172.9	1.30	1.37	1.3	1.6
	-166.7	164.6	-153.3	146.2	-80.0	39.9	-173.0	0.75	0.75	3.3	4.5
2(γ,β)	-85.4	76.5	-148.3	135.2	57.7	61.1	-174.3	0.21	0.72	8.1	4.7
	-87.5	69.1	-126.5	137.4	59.0	62.9	-66.2	1.22	1.14	1.5	2.3
	-86.3	66.4	-146.8	133.1	179.7	-65.0	-174.1	1.61	1.02	0.8	2.8
	-87.3	60.7	-121.9	132.6	-178.1	-63.6	-64.6	2.49	2.54	0.2	0.2
	-89.2	75.6	-146.9	131.3	-57.1	-67.4	-174.1	3.29	2.87	0.0	0.1
	-89.5	73.3	-145.2	130.1	-61.4	178.1	-174.3	3.40	2.93	0.0	0.1
	-86.9	55.5	-138.8	129.1	48.0	-178.5	-174.3	3.67	3.08	0.0	0.1
	-88.6	67.3	-124.8	136.0	-64.2	55.3	-64.9	4.08	3.60	0.0	0.0
	-89.7	63.0	-117.1	127.1	-59.9	179.4	-65.2	4.37	3.30	0.0	0.1
	-89.4	63.9	-118.4	129.7	-54.5	-68.0	-65.2	4.41	3.96	0.0	0.0
	-87.0	48.5	-105.3	126.2	49.8	-179.4	-65.9	4.56	4.11	0.0	0.0
2(δ,γ)	-114.0	3.9	-85.6	72.4	53.2	81.8	-63.3	1.19	1.20	1.6	2.1
	-126.0	14.6	-86.4	74.1	-170.2	-49.9	-61.1	1.32	2.06	1.2	0.5
	-112.3	2.7	-84.6	72.0	55.4	-178.7	-63.5	1.50	1.45	0.9	1.4
	-120.1	10.2	-85.6	83.8	57.4	83.9	-165.0	1.58	0.88	0.8	3.6
	-110.9	-0.3	-86.2	82.7	56.0	-176.8	-165.4	1.58	1.28	0.8	1.8
	-126.9	14.7	-87.3	86.8	-170.4	-49.4	-167.1	1.73	1.64	0.6	1.0
	-84.2	-20.7	-85.9	73.0	-55.5	-71.0	-62.6	2.33	2.74	0.2	0.2
	-84.4	-19.6	-85.9	72.8	-58.8	178.1	-62.6	2.73	3.05	0.1	0.1
	-109.7	3.5	-85.2	72.6	-66.1	63.6	-60.7	2.75	2.70	0.1	0.2
	-84.2	-20.6	-86.0	83.1	-55.7	-70.8	-165.4	2.85	2.69	0.1	0.2
	-109.2	-2.1	-84.6	54.2	56.3	-176.7	44.3	2.97	3.96	0.1	0.0
	-114.4	2.7	-84.1	54.5	55.0	84.7	44.2	2.98	3.82	0.1	0.0
	-109.6	1.9	-85.9	84.4	-65.5	63.6	-165.7	3.12	4.12	0.1	0.0
	-126.5	13.4	-84.4	53.8	-169.7	-48.9	44.4	3.24	4.25	0.0	0.0
	-88.7	-15.1	-85.6	81.8	-59.5	179.5	-165.2	3.30	3.16	0.0	0.1
	-83.1	-21.3	-84.1	54.6	-55.6	-71.3	44.0	4.08	5.16	0.0	0.0
	-83.7	-20.0	-84.2	54.7	-58.7	178.6	44.0	4.54	5.56	0.0	0.0
	-108.0	-1.6	-84.2	55.8	-65.7	62.9	43.2	4.55	5.09	0.0	0.0
	-79.4	-34.6	-85.0	82.8	-177.4	-179.3	-165.3	6.47	6.60	0.0	0.0
	-79.1	-34.7	-83.6	53.4	-179.9	179.3	44.5	7.53	8.33	0.0	0.0
2(γ,γ)	-84.2	69.5	-87.8	85.2	58.4	63.8	-166.4	0.64	1.24	3.9	1.9
	-89.4	60.4	-87.4	75.1	60.2	66.4	-70.1	1.38	2.24	1.1	0.4
	-85.1	60.0	-88.0	85.0	-178.1	-64.3	-166.3	2.04	2.22	0.4	0.4
	-88.4	51.9	-87.5	73.9	-174.6	-62.5	-67.9	2.55	3.56	0.2	0.0
	-84.3	48.8	-85.7	83.1	49.6	-177.7	-165.3	3.60	4.21	0.0	0.0
	-88.1	64.0	-87.0	82.1	-59.2	178.4	-165.2	3.63	4.03	0.0	0.0
	-84.2	72.5	-87.0	83.6	-65.8	56.8	-166.2	3.66	4.29	0.0	0.0
	-87.6	64.8	-87.1	82.9	-54.2	-68.8	-165.4	3.67	4.31	0.0	0.0
	-86.9	43.0	-85.2	72.5	51.0	-178.8	-66.6	3.82	4.71	0.0	0.0
	-88.1	51.5	-86.2	73.0	-56.8	178.4	-68.7	4.06	5.25	0.0	0.0
	-87.5	50.5	-86.2	73.3	-51.4	-70.2	-68.5	4.12	5.41	0.0	0.0
2(x,β)	-150.7	-176.1	-151.6	140.9	-168.5	79.4	-173.9	1.19	1.19	1.5	2.1
	-149.3	-173.2	-144.9	141.6	-165.3	-168.8	-173.7	1.40	1.43	1.1	1.4
	-149.9	-176.3	-102.4	129.0	-165.7	-165.8	-63.3	2.07	1.90	0.4	0.6
	-151.3	-174.5	-101.7	123.0	-168.0	77.9	-62.5	2.17	2.08	0.3	0.5

Table S5 continued.

	-149.9	-179.2	-154.9	163.1	-168.4	78.8	62.2	2.51	2.63	0.2	0.2
	-149.6	-175.1	-147.7	161.7	-164.8	-166.0	62.7	2.75	3.20	0.1	0.1
2(x,γ)	-151.3	-174.0	-85.4	73.3	-169.2	79.0	-61.6	1.58	2.31	0.8	0.3
	-149.8	-175.9	-85.4	76.0	-166.9	-172.2	-63.7	1.80	2.42	0.6	0.3
	-150.8	-175.2	-85.4	86.2	-169.2	79.8	-166.6	1.90	2.39	0.5	0.3
	-149.3	-177.1	-85.3	88.9	-166.6	-170.0	-167.2	1.94	2.25	0.4	0.4
	-151.3	-178.2	-84.7	56.0	-170.3	81.2	43.1	3.50	4.89	0.0	0.0
	-148.9	-177.2	-83.7	55.0	-166.5	-169.9	44.5	3.60	4.45	0.0	0.0
2(β,γ)	-166.9	164.7	-86.1	77.1	-81.2	41.4	-61.7	2.06	2.74	0.4	0.2
	-145.6	167.8	-86.8	75.4	61.0	-61.3	-60.2	2.56	2.82	0.2	0.1
	-145.1	166.4	-88.6	89.4	61.4	-61.3	-167.5	2.78	2.39	0.1	0.3
	-108.3	146.5	-85.4	76.4	-61.1	56.5	-62.6	2.99	3.23	0.1	0.1
	-102.9	143.2	-87.0	88.4	-61.5	55.5	-167.2	3.02	2.95	0.1	0.1
	-166.3	164.0	-84.3	53.6	-80.7	40.5	43.6	3.44	4.19	0.0	0.0
	-143.9	165.8	-86.2	75.6	66.5	-171.9	-60.5	3.51	3.32	0.0	0.1
	-140.7	164.2	-87.0	89.1	66.4	-173.3	-167.3	3.72	3.23	0.0	0.1
	-144.8	167.1	-85.1	53.2	60.9	-62.1	43.9	4.02	4.92	0.0	0.0
	-102.4	144.3	-83.9	55.0	-61.6	55.6	43.8	4.25	4.94	0.0	0.0
	-115.2	138.4	-84.8	75.6	-68.0	171.2	-62.5	4.39	4.13	0.0	0.0
	-101.5	128.2	-86.1	86.8	-67.6	174.5	-166.6	4.41	3.52	0.0	0.0
	-144.6	161.1	-83.5	53.2	-172.3	-95.1	44.5	4.49	5.25	0.0	0.0
	-102.4	129.3	-83.6	53.7	-67.5	173.9	44.5	5.65	5.98	0.0	0.0
2(pp$_{II}$,β)	-68.7	137.9	-155.1	146.5	-54.0	-68.7	-172.5	3.15	2.22	0.1	0.4
	-66.9	142.9	-150.6	162.4	-53.6	-69.3	64.9	4.12	4.24	0.0	0.0
	-67.0	136.7	-155.1	146.2	-57.8	172.1	-172.3	3.55	2.98	0.0	0.1
	-66.7	142.4	-150.2	162.5	-57.7	173.3	65.2	4.53	4.95	0.0	0.0
2(δ,α)	-78.7	-7.4	-75.9	-21.5	55.6	-179.5	-170.6	3.66	4.67	0.0	0.0
	-79.1	-7.3	-75.1	-21.6	52.9	79.7	-170.3	3.69	4.79	0.0	0.0
	-78.6	-7.8	-77.5	-19.8	55.7	-179.3	-169.7	3.70	4.78	0.0	0.0
	-72.5	-19.8	-75.7	-18.9	-54.3	-74.4	-168.1	3.83	4.99	0.0	0.0
	-81.9	-2.6	-78.5	-20.6	-170.0	-42.1	-169.8	4.18	5.42	0.0	0.0
	-73.8	-18.0	-76.1	-18.6	-57.3	176.7	-168.3	4.25	5.57	0.0	0.0
	-80.0	-7.0	-74.2	-22.1	-71.8	72.7	-170.3	5.66	6.57	0.0	0.0
	-67.9	-28.7	-70.5	-21.3	-170.7	-173.6	-169.6	8.07	9.28	0.0	0.0
2(pp$_{II}$,γ)	-82.1	162.9	-84.4	53.0	61.3	-172.6	44.0	5.02	5.13	0.0	0.0

[a)] referenced to E = -1242.316206 hartree and G = -1242.381459 hartree

Table S6. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of 10 conformers of each important conformer family of **2**··$(DMSO)_1$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β/γ).

	ϕ_{Ser}	ψ_{Ser}	ϕ_{Phe}	ψ_{Phe}	α	β	γ	Solvated H	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2(δ,δ)··$(DMSO)_1$	-71.6	-20.3	-84.0	-6.6	-65.8	82.8	-64.4	OH/BocNH	0.00	1.50	15.3	1.9
	-74.9	-13.2	-83.9	-7.8	62.7	-80.0	-65.0	OH/BocNH	0.04	2.13	14.3	0.6
	-74.6	-14.7	-89.8	-1.8	64.3	-79.7	57.2	OH/BocNH	0.22	2.19	10.6	0.6
	-72.4	-20.3	-88.0	-1.8	-65.3	80.8	56.9	OH/BocNH	0.57	3.16	5.8	0.1
	-77.3	-10.3	-85.3	-7.8	55.7	-168.5	-65.5	OH	0.63	0.00	5.3	23.6
	-70.9	-22.7	-85.8	-5.6	-52.5	-75.1	-64.8	OH	0.70	1.50	4.7	1.9
	-71.6	-21.4	-84.9	-6.5	-56.8	164.5	-64.6	OH	0.86	1.19	3.6	3.1
	-71.1	-23.0	-87.5	-2.7	-52.5	-76.6	57.0	OH	1.03	2.03	2.7	0.8
	-77.0	-11.9	-91.6	-1.6	56.3	-175.1	56.9	OH	1.10	1.82	2.4	1.1
	-71.7	-22.1	-88.6	-2.1	-56.6	169.0	57.3	OH	1.30	1.98	1.7	0.8
2(δ,β) ··$(DMSO)_1$	-83.1	-20.0	-146.4	136.2	-62.8	84.4	-174.5	OH/BocNH	1.31	1.27	1.7	2.8
	-83.9	-21.2	-125.3	140.1	-62.5	82.6	-64.8	OH/BocNH	1.57	2.10	1.1	0.7
	-104.4	-3.4	-151.9	161.0	56.5	-169.8	65.2	OH	1.83	0.92	0.7	5.0
	-87.8	-13.6	-152.0	159.5	64.4	-80.6	66.5	OH/BocNH	1.83	2.68	0.7	0.3
	-80.7	-22.6	-146.9	137.8	-54.1	-73.1	-174.7	OH	1.92	1.20	0.6	3.1
	-82.9	-20.8	-148.5	161.2	-63.1	84.4	64.5	OH/BocNH	1.97	2.21	0.6	0.6
	-125.0	13.1	-125.4	136.3	-170.7	-47.4	-63.7	NPrH	2.04	2.89	0.5	0.2
	-124.8	15.6	-139.7	126.1	-170.7	-48.3	-175.9	NPrH	2.15	2.59	0.4	0.3
	-81.8	-21.1	-146.7	137.6	-58.2	170.4	-174.7	OH	2.21	1.29	0.4	2.7
	-81.2	-24.1	-123.5	140.7	-54.4	-77.2	-64.3	OH	2.23	1.46	0.4	2.0
2(β,β)··$(DMSO)_1$	-148.9	-173.0	-144.2	133.5	-170.0	78.0	-175.0	OH	1.46	1.61	1.3	1.5
& **2**(x,β)··$(DMSO)_1$	-147.4	-174.3	-120.1	139.7	-166.0	-164.0	-64.1	OH	1.62	1.68	1.0	1.4
	-148.2	-172.2	-130.3	130.3	-166.0	-164.9	-175.8	OH	1.72	1.48	0.8	1.9
	-147.9	-174.1	-111.0	123.7	-165.7	-161.0	-175.4	OH	1.76	1.70	0.8	1.3
	-148.0	-178.4	-152.6	160.3	-169.7	86.2	63.3	OH	2.18	3.25	0.4	0.1
	-148.1	-174.4	-148.7	160.4	-165.0	-161.1	63.6	OH	2.38	2.84	0.3	0.2
	-144.7	167.4	-150.8	142.1	66.6	-171.7	-174.1	OH	2.72	0.89	0.2	5.2
	-165.3	163.8	-141.3	126.4	-78.5	37.9	-176.7	NPrH	2.89	3.69	0.1	0.0
	-164.9	163.8	-153.1	162.0	-78.1	37.2	63.3	NPrH	2.97	2.86	0.1	0.2
	-147.8	167.2	-152.0	143.2	65.9	-88.2	-174.4	OH	2.98	2.34	0.1	0.5
2(δ,γ) ··$(DMSO)_1$	-92.8	-9.3	-84.6	72.5	64.8	-77.0	-65.9	OH/BocNH	1.43	2.25	1.4	0.5
	-107.5	-1.3	-85.1	71.7	55.9	-172.1	-63.8	OH	1.67	1.02	0.9	4.2
	-82.9	-20.5	-85.6	71.6	-63.7	83.6	-64.3	OH/BocNH	1.76	2.42	0.8	0.4
	-105.8	-2.7	-86.1	84.1	56.0	-169.7	-167.1	OH	2.03	1.45	0.5	2.0
	-82.6	-21.4	-86.1	83.9	-63.4	84.1	-167.2	OH/BocNH	2.24	2.65	0.3	0.3
	-83.2	-21.1	-86.2	83.9	-63.1	84.6	-167.2	OH/BocNH	2.27	2.39	0.3	0.4
	-103.8	-5.5	-85.8	82.8	49.5	91.2	-166.8	OH	2.32	1.89	0.3	1.0
	-81.3	-22.3	-85.3	71.7	-54.3	-73.2	-64.2	OH	2.44	1.89	0.2	1.0
	-110.9	2.9	-83.1	72.2	51.8	101.1	-64.5	OH	2.56	2.78	0.2	0.2
	-81.8	-21.8	-85.6	72.6	-58.9	167.1	-64.2	OH	2.77	2.78	0.1	0.2

[a] referenced to E = -1795.507076 hartree and G = -1795.58426 hartree

Table S7. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of 10 conformers of each important conformer family of **2**··$(DMSO)_2$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- (α/β/γ).

	ϕ_{Ser}	ψ_{Ser}	ϕ_{Phe}	ψ_{Phe}	α	β	γ	Solvated H	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2(δ,β)··$(DMSO)_2$	-94.3	-8.9	-139.7	124.9	66.4	-74.3	-175.4	OH/BocNH + NPrH	0.0[a)]	1.30	12.0	2.4
	-100.5	-5.6	-119.8	134.0	66.4	-71.1	-66.4	OH/BocNH + NPrH	0.09	2.49	10.4	0.3
	-84.1	-18.8	-136.6	125.1	-62.7	84.6	-175.7	OH/BocNH + NPrH	0.15	1.04	9.3	3.7
	-103.8	-3.7	-152.4	160.6	56.6	-168.5	65.7	OH + NPrH	0.44	0.04	5.7	19.8
	-103.7	-2.8	-138.1	125.1	55.9	-165.2	-175.5	OH + NPrH	0.52	1.15	4.9	3.0
	-84.3	-20.7	-120.7	134.6	-62.1	83.0	-63.8	OH/BocNH + NPrH	0.55	1.93	4.8	0.8
	-81.9	-21.1	-149.3	161.0	-63.6	84.0	64.1	OH/BocNH + NPrH	0.73	1.14	3.5	3.1
	-80.3	-23.4	-139.5	125.8	-53.8	-73.6	-175.7	OH + NPrH	0.83	1.17	2.9	2.9
	-88.0	-14.3	-153.3	160.9	64.5	-78.8	66.1	OH/BocNH + NPrH	0.86	2.35	2.8	0.4
	-108.6	-0.7	-110.7	129.6	55.4	-166.5	-64.4	OH + BocNH	0.86	1.56	2.8	1.5
2(β,β)··$(DMSO)_2$	-149.4	-174.2	-120.5	131.3	-169.7	77.4	-63.6	OH + NPrH	0.41	1.53	6.0	1.6
& **2**(x,β)··$(DMSO)_2$	-148.2	-174.5	-111.4	130.2	-166.1	-164.3	-64.0	OH + NPrH	0.76	2.62	3.3	0.3
	-148.6	-179.1	-153.5	160.3	-169.3	85.7	63.1	OH + NPrH	0.81	1.45	3.0	1.8
	-148.0	-175.2	-128.5	121.9	-170.3	86.0	-175.6	OH + NPrH	0.87	2.38	2.8	0.4
	-147.7	-174.3	-150.2	161.1	-165.1	-164.2	63.7	OH + NPrH	1.00	0.0[a)]	2.2	21.2
	-148.6	-173.8	-115.9	122.6	-166.1	-163.7	-175.8	OH + NPrH	1.08	3.24	1.9	0.1
	-120.0	145.4	-141.4	126.1	-62.4	-77.9	-175.843	OH + NPrH	1.88	1.02	0.5	3.8
	-143.8	166.5	-153.7	162.3	66.3	-175.6	62.9	OH + NPrH	1.94	0.75	0.5	5.9
	-122.0	146.6	-127.3	140.8	-62.0	-77.2	-63.7	OH + NPrH	2.02	1.20	0.4	2.8
	-146.8	167.0	-152.9	161.6	66.2	-89.3	63.0	OH + NPrH	2.05	2.08	0.4	0.6
2(δ,δ)··$(DMSO)_2$	-73.9	-14.3	-81.2	-9.9	64.5	166.6	-65.3	OH + BocNH	1.29	3.37	1.4	0.1
	-73.4	-16.9	-84.4	-6.3	-65.5	-164.1	-65.2	OH + BocNH	1.50	3.30	0.9	0.1
	-73.5	-18.0	-86.6	-2.9	-63.1	-78.4	57.8	OH + BocNH	1.53	3.59	0.9	0.0
	-73.1	-16.3	-87.8	-3.1	62.7	104.5	57.8	OH + BocNH	1.59	4.18	0.8	0.0
	-73.4	-16.9	-83.9	-6.7	-65.7	-84.2	-65.2	OH + BocNH	1.67	3.26	0.7	0.1
	-72.7	-15.8	-70.9	-24.3	63.4	105.2	-170.7	OH + BocNH	2.88	5.88	0.1	0.0
	-73.5	-16.6	-70.9	-23.4	-65.1	-76.0	-169.6	OH + BocNH	3.06	6.87	0.1	0.0
	-63.8	-32.8	-78.3	-8.4	-175.3	177.6	-64.5	OH + BocNH	3.11	4.38	0.1	0.0
	-77.3	-10.0	-88.0	-3.4	-77.1	75.4	58.8	OH + BocNH	3.18	5.74	0.1	0.0
	-74.2	-13.0	-68.3	-26.6	66.4	127.5	-172.1	OH + BocNH	3.33	6.21	0.0	0.0

[a)] referenced to E = -2348.685285 hartree and G = -2348.777157 hartree

Table S8. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of 10 conformers of each important conformer family of **2**··$(DMSO)_3$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- ($\alpha/\beta/\gamma$).

	ϕ_{Ser}	ψ_{Ser}	ϕ_{Phe}	ψ_{Phe}	α	β	γ	Solvated H	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2(β,β)··$(DMSO)_3$	-141.5	164.3	-117.4	130.9	67.4	-87.9	-64.5	OH + PheNH + NPrH	0.05	0.10	13.3	14.7
& **2**(x,β)··$(DMSO)_3$	-121.5	146.4	-115.8	132.4	-66.2	168.9	-64.8	OH + PheNH + NPrH	0.45	0.0[a]	6.8	17.5
	-144.6	163.0	-121.6	118.6	65.1	-176.1	-174.9	OH + PheNH + NPrH	0.50	1.95	6.2	0.6
	-116.3	-160.8	-145.5	126.6	-169.6	68.9	-175.7	OH + BocNH + NPrH	0.73	1.34	4.2	1.8
	-146.1	163.0	-106.9	120.4	65.6	-85.4	-174.6	OH + PheNH + NPrH	0.95	1.33	2.9	1.9
	-120.6	147.1	-137.2	118.1	-65.7	171.2	-174.8	OH + PheNH + NPrH	0.96	0.71	2.9	5.3
	-116.7	-163.1	-150.5	159.3	-168.8	70.8	64.1	OH + BocNH + NPrH	1.15	1.17	2.1	2.4
	-99.5	-164.5	-123.8	138.7	-166.6	-174.1	-63.2	OH + BocNH + NPrH	1.56	0.66	1.0	5.8
	-98.3	137.2	-145.6	128.4	-66.9	175.6	-175.7	OH + BocNH + NPrH	1.62	0.58	0.9	6.6
	-98.0	-167.4	-152.1	159.8	-165.4	-171.1	63.8	OH + BocNH + NPrH	1.97	1.83	0.5	0.8
2(δ,β)··$(DMSO)_3$	-91.5	-35.2	-135.4	120.8	-68.8	89.6	-175.1	OH + PheNH/BocNH + NPrH	0.07	0.40	13.0	8.9
	-77.4	-35.9	-121.1	139.0	-173.6	175.2	-64.7	OH + PheNH/BocNH + NPrH	2.31	1.71	0.3	1.0
	-108.6	-15.8	-134.0	118.9	63.7	-174.9	-174.5	OH + BocNH + NPrH	0.0[a]	1.13	14.6	2.6
	-123.1	-15.5	-134.5	117.5	61.1	129.1	-174.0	OH + BocNH + NPrH	0.90	2.99	3.2	0.1
	-107.0	-2.9	-127.0	139.2	-69.7	86.3	-64.9	OH + BocNH + NPrH	0.51	0.68	6.1	5.6
	-99.7	-8.5	-121.3	134.5	-67.5	158.6	-65.0	OH + PheNH/BocNH + NPrH	0.51	0.31	6.1	10.4
	-91.8	-13.2	-148.4	160.7	-63.2	-73.3	64.4	OH + BocNH + NPrH	0.85	0.41	3.4	8.7
	-88.9	-11.4	-151.5	160.6	69.1	-178.0	67.3	OH + BocNH + NPrH	1.42	2.16	1.3	0.5
	-94.7	-17.1	-155.5	162.6	-72.3	84.7	64.1	OH + BocNH + NPrH	1.35	4.98	1.5	0.0
	-97.4	-1.7	-144.4	159.4	64.5	111.0	67.8	OH + BocNH + NPrH	1.77	3.62	0.7	0.0

[a] referenced to E = -2901.861463 hartree and G = -2901.966563 hartree

Table S9. Characteristic geometries parameters, relative zero-point corrected and Gibbs Free Energies (ΔE_{ZPC} and ΔG_{298K} in kcal/mol), and Boltzmann weights of the optimized conformers of **2**··$(DMSO)_4$ sorted by ΔE_{ZPC}. Color coding of the table cells refers either to secondary structure family (ϕ/ψ) or t/g+/g- ($\alpha/\beta/\gamma$).

	ϕ_{Ser}	ψ_{Ser}	ϕ_{Phe}	ψ_{Phe}	α	β	γ	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2(β,β)··$(DMSO)_4$	-89.0	147.0	-107.8	129.9	-65.7	162.9	-65.8	0.0[a]	1.14	35.3	9.5
	-84.3	161.1	-123.7	116.8	66.5	172.6	-174.6	1.04	2.97	6.0	0.4
	-99.1	159.8	-150.1	157.3	65.3	170.0	63.7	2.57	3.48	0.5	0.2
	-77.4	147.0	-136.7	117.3	-66.3	164.8	-174.1	0.06	0.0[a]	31.9	65.2
	-110.3	139.7	-112.7	134.2	-67.6	86.6	-64.8	0.63	0.78	12.1	17.4
	-100.1	145.3	-141.0	119.3	-67.8	86.7	-174.2	0.60	1.44	12.9	5.7
2(pp_{II},β)··$(DMSO)_4$	-75.8	141.9	-146.7	158.8	-62.8	-95.5	65.4	2.10	2.73	1.0	0.6
	-74.0	145.1	-146.8	157.9	-64.8	178.7	64.5	2.78	2.54	0.3	0.9

[a] referenced to E = -3455.037501 hartree and G = -3455.156565 hartree

3. Selected Cartesian coordinate

1(γ') == 1_c1a

C	1.68885100	-0.68461800	0.66796300
H	1.51476300	-0.42491200	1.71701500
C	2.43796400	0.48704800	-0.00987500
O	3.40134100	0.29733000	-0.76178700
N	1.95836700	1.70870900	0.27734300
H	1.10000000	1.75406400	0.81694800
C	2.48181900	2.91793200	-0.34099700
H	1.99967500	3.78049400	0.12092400
H	2.28754000	2.93237800	-1.41893900
H	3.56140200	2.98676000	-0.18555400
N	0.39352700	-0.91201800	0.04358200
H	0.34494200	-1.57450700	-0.71817500
C	-0.71337100	-0.19582500	0.36714700
O	-0.71524200	0.71009900	1.19558700
O	-1.77286800	-0.62690500	-0.33677500
C	-3.11288900	-0.01134000	-0.20026600
C	-3.94571500	-0.81960900	-1.19646500
H	-3.54851900	-0.71347800	-2.21038800
H	-4.97950600	-0.46213400	-1.19019700
H	-3.94468600	-1.88098800	-0.93097600
C	-3.63461100	-0.20694900	1.22468800
H	-4.67522200	0.12968900	1.27530400
H	-3.04931100	0.36273700	1.94749100
H	-3.60750400	-1.26619500	1.49953900
C	-3.05955300	1.46173000	-0.61068300
H	-2.47664200	2.05413700	0.09553800
H	-4.07814900	1.86179000	-0.64293400
H	-2.62362600	1.56523100	-1.60952000
C	2.52002500	-1.96821400	0.61260200
H	1.98847600	-2.76440400	1.14039200
H	3.47760200	-1.79489500	1.11883600
O	2.71962900	-2.41828900	-0.72145200
H	3.20749500	-1.70140800	-1.16104600

1(δ) == 1_c4b

C	-1.53118700	-0.63133300	-0.10137500
H	-1.34170200	-0.85367700	-1.15616400
C	-2.67906900	0.39170900	-0.06923600
O	-3.85108400	0.01946700	-0.21673500
N	-2.34568100	1.67890800	0.10358600
H	-1.36507600	1.89842900	0.20018500
C	-3.32850700	2.75233200	0.08698200
H	-2.82350100	3.68928200	0.32463900
H	-4.10978900	2.56723700	0.82884400
H	-3.80010700	2.83801500	-0.89695200
N	-0.29135100	-0.11276100	0.44911400
H	-0.20428000	-0.06075200	1.45581900
C	0.89227100	-0.17812500	-0.24861300
O	0.97017800	-0.42374500	-1.43837300
O	1.91409600	0.09888000	0.58044900
C	3.31625200	0.15456400	0.10302600
C	4.08308300	0.49742600	1.38094200
H	3.75087600	1.45712200	1.78820500
H	5.15268500	0.56593300	1.16268300
H	3.93441400	-0.27500800	2.14146800
C	3.74180900	-1.21427800	-0.43162000
H	4.81434700	-1.19490000	-0.65051400
H	3.20548200	-1.47344600	-1.34511800
H	3.56368700	-1.99075000	0.31916900
C	3.47051700	1.26627200	-0.93658100
H	2.92986000	1.03474100	-1.85511700
H	4.53154400	1.38598700	-1.17837400
H	3.10567400	2.21803500	-0.53701200

C	-1.94409300	-1.94428500	0.60099600
H	-2.16320100	-1.73761200	1.66117700
H	-1.09645300	-2.63409600	0.56056800
O	-3.03867900	-2.57977100	-0.03049200
H	-3.70779500	-1.88190600	-0.15832600

1(β) == 1_c9a

C	-1.42439500	-0.34155100	-0.09947500
H	-1.32405800	-0.63559600	-1.15264600
C	-2.49049900	0.76882400	-0.01204700
O	-2.19143600	1.91946900	0.31238100
N	-3.74271300	0.39034800	-0.32289300
H	-3.90891700	-0.60000200	-0.45868500
C	-4.87011100	1.30771900	-0.25094500
H	-5.75770700	0.79485400	-0.62410100
H	-4.68319900	2.19079100	-0.86743400
H	-5.05290800	1.63826200	0.77711400
N	-0.17354300	0.21072300	0.37229100
H	-0.22069000	1.16735800	0.70408700
C	1.02108200	-0.25854600	-0.08719000
O	1.14294100	-1.27991700	-0.74748000
O	2.01840800	0.55449200	0.31217100
C	3.43405900	0.26585400	0.00206900
C	4.16135700	1.43450600	0.66970500
H	3.83030100	2.38836400	0.24816200
H	5.23949400	1.34050500	0.50976800
H	3.97032400	1.44514700	1.74700700
C	3.85284000	-1.06235600	0.63700000
H	4.93369500	-1.19205800	0.51938400
H	3.34813500	-1.90756000	0.16754700
H	3.62657100	-1.06205400	1.70814900
C	3.65517000	0.28790100	-1.51230000
H	3.14293500	-0.54044800	-2.00314200
H	4.72715600	0.20902900	-1.72116500
H	3.29573600	1.23079800	-1.93686900
C	-1.80562200	-1.60658500	0.70434700
H	-2.13257900	-1.33157000	1.71089300
H	-0.92052400	-2.24314200	0.78722100
O	-2.88939600	-2.32283900	0.10579900
H	-2.54739100	-2.84440700	-0.63102600

1(δ)·(DMSO)$_1$ == 1_c5c.(DMSO)$_1$

C	1.64666200	-1.01295300	1.02620100
H	2.15316000	-0.49786500	1.84848700
C	2.77331500	-1.50460800	0.09837200
O	3.71448700	-2.15203600	0.56783600
N	2.66886000	-1.20097800	-1.20435700
H	1.86768500	-0.66217200	-1.49834200
C	3.66107600	-1.60301000	-2.18811900
H	3.34964300	-1.23526900	-3.16636400
H	3.75136000	-2.69276300	-2.22887700
H	4.64269800	-1.18421200	-1.94589600
N	0.72108000	-0.07801900	0.40746000
H	-0.20007000	-0.40147700	0.12054600
C	0.92651300	1.26869600	0.47201200
O	1.94202900	1.78582400	0.91546800
O	-0.13916000	1.92205600	-0.03220100
C	-0.17444800	3.39710400	-0.14418700
C	-1.54252900	3.64590000	-0.78184400
H	-1.61024600	3.15627800	-1.75802300
H	-1.69521200	4.71987100	-0.92218900
H	-2.34380100	3.26358300	-0.14239700
C	-0.10607300	4.03238200	1.24636500
H	-0.27587800	5.11030900	1.15745200
H	0.86608400	3.87090300	1.71353000
H	-0.88586700	3.61903800	1.89408800

C	0.94469000	3.88232200	-1.06827700
H	1.92873100	3.71921800	-0.62720800
H	0.81852200	4.95415900	-1.25200500
H	0.89558300	3.36553600	-2.03213100
C	0.90563400	-2.21929500	1.63151200
H	0.16707600	-1.84693800	2.35363500
H	1.63768800	-2.82493400	2.16999600
O	0.29867400	-3.06184800	0.66624800
H	-0.50498600	-2.62208300	0.31384300
O	-1.77722200	-1.58184000	-0.37294100
S	-3.22819400	-1.80779400	0.09594700
C	-3.83131300	-0.18352700	0.63261200
C	-4.20071400	-1.96385200	-1.42682100
H(Iso=2)	-3.27525500	0.07722500	1.53423800
H(Iso=2)	-4.89607800	-0.27209400	0.86102100
H(Iso=2)	-3.65326300	0.54500000	-0.16085700
H(Iso=2)	-3.99394400	-1.10739200	-2.07197900
H(Iso=2)	-3.89136400	-2.89537500	-1.90314300
H(Iso=2)	-5.25808700	-2.01306200	-1.15653600

1(β)·(DMSO)$_1$ == 1_c9c.(DMSO)$_1$

C	0.46939400	1.21341100	-0.26964200
H	0.58850700	1.17936300	-1.35996300
C	0.33404500	2.69169600	0.14882100
O	1.21467000	3.25535700	0.80790500
N	-0.78581900	3.30330800	-0.26445800
H	-1.49568000	2.71579500	-0.69193500
C	-1.08795000	4.68727600	0.06668800
H	-2.01356100	4.96846000	-0.43710200
H	-0.28484500	5.34720200	-0.27251900
H	-1.21406800	4.82320100	1.14622400
N	1.65667900	0.68282300	0.36711300
H	2.12080400	1.31669300	1.00711700
C	2.40679400	-0.29090000	-0.21967700
O	2.05082200	-0.93644900	-1.19548000
O	3.56956400	-0.43753000	0.44687100
C	4.56536000	-1.46536500	0.07406100
C	5.66657300	-1.24780400	1.11349500
H	6.07303800	-0.23444300	1.04115800
H	6.48003200	-1.95955300	0.94560200
H	5.27910700	-1.39738300	2.12583700
C	3.95885800	-2.86302100	0.21780400
H	4.74480500	-3.61167800	0.07512200
H	3.17489300	-3.03793200	-0.52005500
H	3.54115000	-2.99734900	1.22078400
C	5.09641400	-1.19742100	-1.33601700
H	4.32585800	-1.35650200	-2.09128500
H	5.93099100	-1.87589700	-1.54043000
H	5.46724700	-0.17049600	-1.41593400
C	-0.77390900	0.37193700	0.07825600
H	-1.05562700	0.53769100	1.12727200
H	-0.50822300	-0.68472100	-0.04507200
O	-1.83075200	0.73375300	-0.80090700
H	-2.67994500	0.36621300	-0.45560300
O	-4.19518300	-0.18386700	0.15537400
S	-4.54154000	-1.66401300	-0.07911400
C	-5.06754700	-2.30141400	1.53673700
C	-6.15935600	-1.66400400	-0.90154300
H(Iso=2)	-4.18295200	-2.30730900	2.17543500
H(Iso=2)	-5.44133800	-3.31938300	1.40356100
H(Iso=2)	-5.83875800	-1.64463200	1.94499600
H(Iso=2)	-6.85794900	-1.06098100	-0.31750800
H(Iso=2)	-6.00756400	-1.23389700	-1.89274900
H(Iso=2)	-6.50231100	-2.69763700	-0.98971900

1(δ)·(DMSO)$_2$ == 1_c5c.(DMSO)$_2$

C	-0.31483600	-0.14685100	-0.36153100
H	0.66646800	0.01250000	0.08959800

C	-1.29587000	-0.22833200	0.82650600
O	-1.17346100	0.57423600	1.76032400
N	-2.24878900	-1.17256900	0.79439600
H	-2.39640000	-1.71260000	-0.05734300
C	-3.24176700	-1.28868800	1.85098000
H	-3.86793200	-2.15772600	1.64338400
H	-3.87625100	-0.39699400	1.90700800
H	-2.75708300	-1.42477700	2.82178200
N	-0.21928500	-1.34888100	-1.16653200
H	-1.02295700	-1.64963200	-1.71107400
C	0.81021900	-2.22604000	-1.02270600
O	1.77615900	-2.05205000	-0.29069700
O	0.61322100	-3.29888600	-1.81868200
C	1.58210400	-4.41180100	-1.88882300
C	0.92695800	-5.35583600	-2.89928900
H	-0.05373300	-5.68525300	-2.54287300
H	1.55684500	-6.23834000	-3.04422500
H	0.79863100	-4.85984900	-3.86621300
C	2.92702300	-3.90932700	-2.41954500
H	3.58493900	-4.76562300	-2.60017800
H	3.41339400	-3.24044500	-1.70860100
H	2.78976700	-3.38151400	-3.36888700
C	1.70699100	-5.09158600	-0.52305300
H	2.17811700	-4.43494100	0.20926900
H	2.31653800	-5.99532000	-0.62534000
H	0.72044600	-5.38848100	-0.15269600
C	-0.62604600	1.08176800	-1.22192400
H	0.17468000	1.19176800	-1.96630200
H	-0.62376700	1.96757200	-0.57391900
O	-1.88599700	0.91005800	-1.85204000
H	-2.10278600	1.72768000	-2.35456300
O	-2.53335400	3.13459200	-3.32531600
S	-2.91460900	4.41835400	-2.57159200
C	-2.16032300	5.77699000	-3.50991900
C	-4.65047600	4.74337500	-2.99368400
H(Iso=2)	-1.08004300	5.68011800	-3.39124200
H(Iso=2)	-2.50181600	6.72318000	-3.08352100
H(Iso=2)	-2.44642000	5.68789300	-4.56025700
H(Iso=2)	-4.76396100	4.72478700	-4.07981000
H(Iso=2)	-5.24079100	3.95316700	-2.52709400
H(Iso=2)	-4.93116500	5.71524900	-2.58061700
O	-2.89581000	-2.52716900	-1.79050500
S	-4.08924500	-1.84393000	-2.47848800
C	-3.47361000	-1.27418400	-4.08762800
C	-5.14833100	-3.19740900	-3.06412000
H(Iso=2)	-2.75242600	-0.48498800	-3.86974300
H(Iso=2)	-4.31548700	-0.87562100	-4.65901800
H(Iso=2)	-3.00194300	-2.11135700	-4.60700600
H(Iso=2)	-4.54647400	-3.89420600	-3.65161000
H(Iso=2)	-5.55505300	-3.68675900	-2.17766800
H(Iso=2)	-5.95781100	-2.77019300	-3.66097500

1(β)·(DMSO)$_2$ == 1_c13b.(DMSO)$_2$

C	0.01342700	-0.23238800	-0.30152200
H	0.95040100	0.02038300	-0.80676300
C	0.30595400	-0.38317200	1.20917200
O	-0.22150800	-1.26611700	1.89155000
N	1.15314100	0.52938100	1.71408600
H	1.61727000	1.19360100	1.09074000
C	1.50454700	0.55396200	3.12481800
H	2.19558900	1.38120400	3.29421700
H	1.98783500	-0.38004000	3.43080600
H	0.61757000	0.70012800	3.74949000
N	-0.48512400	-1.46043000	-0.88376000
H	-1.47508500	-1.67740400	-0.78584400
C	0.35512900	-2.48509800	-1.18235000
O	1.57689600	-2.41108700	-1.14626700
O	-0.35640000	-3.57463100	-1.54661300

C	0.29379400	-4.82856500	-1.97698500
C	-0.90235200	-5.73025200	-2.28954300
H	-1.52407000	-5.87101500	-1.40017600
H	-0.55040100	-6.71041600	-2.62429000
H	-1.51937100	-5.29499700	-3.08155200
C	1.12647800	-4.58722900	-3.23858300
H	1.48174800	-5.54822100	-3.62462800
H	1.99040000	-3.95403700	-3.03311500
H	0.51544400	-4.11545600	-4.01495000
C	1.12199600	-5.41522100	-0.83113700
H	1.98175800	-4.78656500	-0.59665000
H	1.48285100	-6.40798100	-1.11924300
H	0.50628400	-5.52591500	0.06729400
C	-0.96105100	0.93339500	-0.56736800
H	-1.17788900	0.95321800	-1.64442000
H	-0.46145200	1.86944800	-0.30649500
O	-2.15630000	0.89477600	0.19444600
H	-2.68381600	0.10666000	-0.05182600
O	2.69941300	2.33094400	0.03592000
S	2.27510000	3.72484000	-0.44087800
C	3.33359900	4.90271600	0.44977400
C	3.00426100	3.92360100	-2.09245000
H(Iso=2)	3.04126700	4.85636500	1.50007000
H(Iso=2)	3.14996100	5.90416900	0.05325000
H(Iso=2)	4.37842600	4.61037500	0.32355200
H(Iso=2)	4.07167000	3.69757900	-2.04082000
H(Iso=2)	2.48996600	3.22104800	-2.75008000
H(Iso=2)	2.83044900	4.94865400	-2.42824600
O	-3.45757400	-1.47321100	-0.50542000
S	-4.11975500	-2.45186100	0.48520600
C	-3.69856500	-1.85637900	2.14715100
C	-5.88311800	-2.02522300	0.48234800
H(Iso=2)	-2.61034600	-1.90453100	2.22634800
H(Iso=2)	-4.16984500	-2.52368500	2.87282700
H(Iso=2)	-4.05109000	-0.82974900	2.26757000
H(Iso=2)	-5.99137700	-0.95379700	0.66371500
H(Iso=2)	-6.27350700	-2.29678100	-0.49958700
H(Iso=2)	-6.37902000	-2.61197300	1.25933100

1(β)·(DMSO)$_3$ == 1_c12a.(DMSO)$_3$

C	-0.08880000	0.35676200	-0.15587700
H	0.99464300	0.45407000	-0.06866400
C	-0.72665700	0.47471800	1.24058600
O	-1.86930000	0.05568200	1.46325300
N	0.01974300	1.09974900	2.16516400
H	0.97168700	1.39779200	1.93655500
C	-0.47583500	1.35700700	3.50785900
H	0.28677600	1.91129700	4.05709300
H	-0.68694900	0.42297900	4.03932500
H	-1.39575800	1.94972000	3.48070700
N	-0.36432300	-0.93011500	-0.76241000
H	-1.32590700	-1.15162100	-1.02959100
C	0.54167800	-1.93995600	-0.73248500
O	1.68600200	-1.84294300	-0.30428300
O	0.00122900	-3.06217800	-1.26089900
C	0.75809500	-4.32466000	-1.35888200
C	-0.25861300	-5.27049900	-2.00252900
H	-1.14810900	-5.36965400	-1.37299200
H	0.18614200	-6.26161900	-2.13125000
H	-0.56588900	-4.89894500	-2.98476500
C	1.97482600	-4.14759100	-2.27118900
H	2.43774900	-5.12402500	-2.44798500
H	2.71691400	-3.48568000	-1.82353500
H	1.66968400	-3.73714900	-3.23916500
C	1.14090700	-4.82354700	0.03709900
H	1.87132600	-4.16657900	0.51066700
H	1.57348900	-5.82612100	-0.04442500
H	0.25384200	-4.88836300	0.67555400

C	-0.59669600	1.51399800	-1.04223300
H	-0.48870800	2.44763500	-0.47866800
H	-1.66368800	1.37318800	-1.25578600
O	0.15014800	1.64026200	-2.23670600
H	-0.30971100	1.18023200	-2.97358100
O	-3.20390100	-1.45066400	-1.60105600
S	-4.10538000	-1.94980100	-0.46597500
C	-4.95904600	-0.48471800	0.18441300
C	-5.52708600	-2.73765800	-1.27949500
H(Iso=2)	-4.18741400	0.11704700	0.66649300
H(Iso=2)	-5.70234900	-0.81167700	0.91604400
H(Iso=2)	-5.42741400	0.05207500	-0.64379900
H(Iso=2)	-5.95904900	-2.04051200	-2.00104500
H(Iso=2)	-5.15016000	-3.63060500	-1.78087700
H(Iso=2)	-6.25507200	-3.01739000	-0.51417900
O	-1.13693500	0.63111200	-4.42599800
S	-0.94422300	-0.81945200	-4.89600300
C	-2.61137700	-1.52876000	-4.98776100
C	-0.59833100	-0.71090800	-6.67508900
H(Iso=2)	-2.97820900	-1.58187100	-3.96001200
H(Iso=2)	-2.53740100	-2.52997700	-5.41958000
H(Iso=2)	-3.24083000	-0.87900000	-5.60033500
H(Iso=2)	-1.37303800	-0.10739300	-7.15330500
H(Iso=2)	0.38051300	-0.23982900	-6.77842500
H(Iso=2)	-0.57288000	-1.72289100	-7.08636200
O	2.69245200	2.09343100	1.63570200
S	3.91446500	1.26166000	2.04433800
C	5.08973600	1.39793500	0.66606800
C	4.81977400	2.27069900	3.25387200
H(Iso=2)	4.64469800	0.87072000	-0.17917800
H(Iso=2)	6.02578200	0.91600400	0.95844200
H(Iso=2)	5.24234400	2.45333000	0.42962000
H(Iso=2)	5.76194400	1.77013000	3.48953600
H(Iso=2)	4.19364500	2.32913300	4.14568000
H(Iso=2)	4.99134800	3.26418300	2.83354100

2(β,pp$_{II}$)

C	-5.62117800	0.56049700	-0.50512600
C	-5.53269900	2.05281900	-0.17575300
H	-6.54112000	2.47947800	-0.16309800
H	-5.07086200	2.22050700	0.79783000
H	-4.95199900	2.57864100	-0.94055200
C	-6.28056900	0.34920100	-1.86952400
H	-5.73184500	0.88278300	-2.65154000
H	-6.30692100	-0.71403600	-2.12667300
H	-7.30740700	0.72600800	-1.84826700
C	-6.35455400	-0.23627300	0.57666600
H	-6.35323600	-1.30338900	0.33203100
H	-5.89638600	-0.09635600	1.55649900
H	-7.39589300	0.09840500	0.62735600
O	-4.26961600	0.00434400	-0.71677400
C	-3.34655600	-0.01780600	0.26771200
O	-3.48652100	0.42780100	1.39657600
N	-2.21423900	-0.62557800	-0.17768100
C	-1.00545800	-0.68874000	0.61017200
H	-0.97837400	0.15783900	1.30206100
H	-2.13777500	-0.87482900	-1.15493300
C	0.19656200	-0.65030400	-0.33021600
O	0.11181500	-0.98970900	-1.50817800
N	1.36408000	-0.28393100	0.25620500
C	2.64524000	-0.60671900	-0.34018700
H	2.59836200	-0.33732500	-1.39845600
C	2.91073100	-2.12490400	-0.22063900
O	2.41641100	-2.80055000	0.68721100
N	3.74365500	-2.64831900	-1.13432200
C	4.12087700	-4.05630200	-1.13636500
H	4.88839400	-4.20880600	-1.89593000
H	4.51971600	-4.34209900	-0.16018700

H	3.26012700	-4.69376900	-1.36113400
H	1.34287800	-0.16081100	1.26043400
H	4.05139500	-2.06835000	-1.90050600
C	-0.96151400	-2.00316400	1.44769200
H	-1.85062300	-2.01006900	2.08340800
H	-1.02016900	-2.85988000	0.76351600
O	0.16794500	-2.09107600	2.29526700
H	0.94039700	-2.39036100	1.77564400
C	3.78218800	0.18775700	0.34700000
H	3.81086800	-0.08502800	1.40818600
H	4.73027000	-0.14597100	-0.08722400
C	3.64822600	1.68851000	0.19817500
C	3.25240200	2.48724700	1.27666300
C	3.92380500	2.30922300	-1.02759100
C	3.12618400	3.87098300	1.13519700
H	3.04666600	2.02681300	2.23898700
C	3.79860400	3.69029000	-1.17439200
H	4.24412100	1.70860800	-1.87492300
C	3.39711200	4.47654200	-0.09180800
H	2.81842100	4.47269300	1.98454900
H	4.01876900	4.15276900	-2.13145300
H	3.30106600	5.55170300	-0.20391200

2(β,β)

C	-6.02371500	-1.20299700	-0.05169200
C	-6.32229400	-1.15507400	-1.55156600
H	-7.37599800	-1.40342400	-1.71542600
H	-6.12914800	-0.16563400	-1.96748000
H	-5.71360000	-1.89147500	-2.08594400
C	-6.30343800	-2.59765300	0.51049900
H	-5.71784000	-3.35397200	-0.02063900
H	-6.05137600	-2.64504000	1.57409700
H	-7.36449200	-2.83701800	0.39470000
C	-6.79014900	-0.13895200	0.73649500
H	-6.50544100	-0.16594300	1.79318300
H	-6.60762500	0.86226800	0.34434400
H	-7.86275400	-0.34783500	0.66965200
O	-4.56721800	-1.05770200	0.17944800
C	-3.90277100	0.06568500	-0.13227300
O	-4.38160700	1.03975000	-0.71277500
N	-2.61825400	-0.01164100	0.28416300
C	-1.58432300	0.95066500	-0.05624400
H	-1.58441000	1.13015400	-1.13891500
H	-2.30362800	-0.84030000	0.77451500
C	-0.24273700	0.30254400	0.33368200
O	-0.19515300	-0.67154200	1.08456000
N	0.85224900	0.88590200	-0.18903100
C	2.20638400	0.44502500	0.10455300
H	2.23261300	0.09525900	1.13950800
C	3.11611500	1.66784500	-0.07703500
O	2.86764700	2.50685100	-0.94437900
N	4.17776200	1.74787300	0.74375500
C	5.17888300	2.79904400	0.62429100
H	5.84312600	2.74514600	1.48754000
H	5.76871000	2.68459300	-0.29114000
H	4.69392500	3.77760100	0.60459000
H	0.77669400	1.66978400	-0.82685200
H	4.34242400	0.99682700	1.39694100
C	-1.76466000	2.32137900	0.64267900
H	-2.02880300	2.13902200	1.69465100
H	-0.82075300	2.87368400	0.61998200
O	-2.72563800	3.13914300	0.00064900
H	-3.46799500	2.56548800	-0.27425700
C	2.62841400	-0.72160700	-0.83672300
H	1.83488300	-1.47220200	-0.76976600
H	2.63996400	-0.34483400	-1.86438100
C	3.95912900	-1.34990600	-0.48885900
C	4.07304800	-2.20701000	0.61536700

C	5.10292000	-1.09319500	-1.25477500
C	5.29852600	-2.78425400	0.94983200
H	3.19272500	-2.43319100	1.21117700
C	6.33053400	-1.67168800	-0.92592000
H	5.03154300	-0.43868900	-2.11895900
C	6.43277000	-2.51718500	0.17965900
H	5.36531700	-3.44902700	1.80546000
H	7.20416600	-1.46410300	-1.53593500
H	7.38540000	-2.97005900	0.43528700

2(δ,δ)

C	-4.44500100	-0.67214500	-0.91678000
C	-4.16750700	0.71797200	-1.49086800
H	-5.09666200	1.13003800	-1.89734900
H	-3.79286900	1.40005200	-0.72694000
H	-3.43983400	0.65835600	-2.30654200
C	-4.97897200	-1.60924100	-2.00075100
H	-4.28070600	-1.66942400	-2.84092800
H	-5.13229600	-2.61617400	-1.60141200
H	-5.93691700	-1.23525300	-2.37334700
C	-5.39231200	-0.63582500	0.28373700
H	-5.52306100	-1.64034200	0.69840500
H	-5.02257300	0.02672000	1.06719500
H	-6.37240400	-0.27480900	-0.04420800
O	-3.17037700	-1.32713500	-0.53357400
C	-2.36123800	-0.82266100	0.41037900
O	-2.54973900	0.19335200	1.06618300
N	-1.24268300	-1.59503900	0.53576000
C	-0.32435000	-1.44612500	1.65053300
H	-0.88503000	-1.32221800	2.58334100
H	-1.16986800	-2.42491500	-0.03643600
C	0.58357200	-0.20631500	1.57652800
O	1.19729300	0.15504700	2.57525700
N	0.65546900	0.41391400	0.37696400
C	1.44234600	1.60714300	0.12819700
H	2.11495400	1.71790100	0.98393700
C	0.60474700	2.90407700	0.09419200
O	1.14616600	3.97206600	-0.19343500
N	-0.70072700	2.80614500	0.40846300
C	-1.55309500	3.98299600	0.48329800
H	-2.56261600	3.66305700	0.74428000
H	-1.19101100	4.68252900	1.24352200
H	-1.57792500	4.50551000	-0.47736600
H	0.13505200	0.00194200	-0.38586600
H	-1.08989100	1.91241400	0.68328200
C	0.52286200	-2.72344500	1.78928200
H	1.25095700	-2.57549400	2.59246200
H	-0.13338700	-3.55430800	2.06161000
O	1.14984800	-3.10757600	0.57045700
H	1.90471700	-2.53066700	0.39082200
C	2.28368500	1.46334400	-1.16054500
H	1.61182000	1.28221400	-2.00846800
H	2.76588900	2.42801900	-1.33562900
C	3.31454800	0.36003800	-1.06922500
C	3.11021900	-0.87838200	-1.69071800
C	4.49752600	0.55202100	-0.34233800
C	4.05523900	-1.90265300	-1.58209300
H	2.21005500	-1.04228500	-2.27697000
C	5.44413100	-0.46634000	-0.23082000
H	4.68036500	1.50881600	0.13931900
C	5.22493000	-1.69986700	-0.84840600
H	3.87914900	-2.85289500	-2.07673600
H	6.35447400	-0.29530700	0.33516000
H	5.96168500	-2.49223000	-0.76415800

2(γ',β)

C	4.17511300	-2.17991600	-0.20188200
C	2.92572600	-3.05818100	-0.10888400

H	3.23021200	-4.10085600	0.02845900
H	2.29291100	-2.76816600	0.73064000
H	2.34384200	-2.99484500	-1.03401400
C	5.05005200	-2.60744000	-1.38134600
H	4.48386400	-2.57265000	-2.31697300
H	5.92059900	-1.95146000	-1.47614300
H	5.40317300	-3.63137200	-1.22816600
C	4.98464200	-2.17041700	1.09650200
H	5.83673300	-1.48846300	1.01096200
H	4.37248900	-1.86992400	1.94760700
H	5.37338900	-3.17656100	1.28438900
O	3.79834500	-0.79685600	-0.57351100
C	3.00748100	-0.04021800	0.20657500
O	2.52417100	-0.36785400	1.28361900
N	2.80810100	1.17748900	-0.36384400
C	2.01418800	2.21618900	0.27254100
H	2.15023000	2.12659900	1.35467900
H	3.16849300	1.35488200	-1.29109100
C	0.51282900	2.04011300	-0.05120300
O	-0.05946600	2.75249900	-0.88429700
N	-0.10470900	1.05958700	0.63376200
C	-1.49631900	0.69549000	0.41331900
H	-2.01735600	1.59309400	0.07370300
C	-2.06274600	0.21122200	1.75415700
O	-1.42470900	-0.56978800	2.45909100
N	-3.27980400	0.67944400	2.09007100
C	-3.97446500	0.24699700	3.29441900
H	-4.89744700	0.82051100	3.38736500
H	-4.21715500	-0.81944100	3.24862500
H	-3.35253700	0.42272100	4.17589800
H	0.44906900	0.46290900	1.24332500
H	-3.76004400	1.29153100	1.44857600
C	2.50930000	3.59417700	-0.17374600
H	1.91677300	4.36767800	0.33045200
H	3.55506000	3.71170400	0.12173200
O	2.45947400	3.74993500	-1.58650600
H	1.52142400	3.65181000	-1.82130200
C	-1.62063500	-0.40614400	-0.67674700
H	-1.07767100	-0.04059000	-1.55422500
H	-1.10397100	-1.30116600	-0.31687200
C	-3.04752900	-0.73618600	-1.05361300
C	-3.77647900	0.11602500	-1.89540600
C	-3.67408800	-1.89103100	-0.56910500
C	-5.09765900	-0.17392600	-2.23762600
H	-3.30201800	1.00886400	-2.29416700
C	-4.99556400	-2.18620300	-0.91049300
H	-3.12174200	-2.56708300	0.07746700
C	-5.71255300	-1.32703700	-1.74435100
H	-5.64347700	0.49564900	-2.89515600
H	-5.46160200	-3.08898500	-0.52795500
H	-6.73864500	-1.55658500	-2.01357300

2(δ,β)

C	5.13145800	-1.43812600	-0.49318800
C	4.66926300	-2.50514300	0.50099300
H	5.45900800	-3.25476800	0.61480100
H	4.45527100	-2.07552200	1.48035700
H	3.77237000	-3.01125000	0.13010700
C	5.43065200	-2.06278000	-1.85672700
H	4.55546100	-2.59624700	-2.23952600
H	5.71597000	-1.29426200	-2.58147000
H	6.25644600	-2.77419400	-1.76406600
C	6.33569400	-0.64208900	0.01369100
H	6.60051400	0.14634900	-0.69815500
H	6.13689600	-0.19049600	0.98626800
H	7.19492600	-1.31382000	0.10978800
O	4.01208500	-0.51865200	-0.80479100
C	3.42085500	0.22666200	0.14506400

O	3.73456100	0.28677400	1.32018800
N	2.36664800	0.91430600	-0.40642600
C	1.68517000	1.97577400	0.30796600
H	2.08480600	1.97987100	1.32694800
H	2.29841400	0.88724300	-1.41509900
C	0.17010000	1.74588200	0.43945400
O	-0.57247800	2.67697700	0.77996800
N	-0.28010400	0.50625100	0.19284800
C	-1.67200300	0.11477600	0.33984900
H	-2.10352300	0.69947000	1.15631300
C	-1.67832800	-1.38216900	0.67780400
O	-0.86315900	-2.14366300	0.15507000
N	-2.61856600	-1.79383400	1.54609800
C	-2.80085200	-3.19742300	1.88936400
H	-3.54027900	-3.26610900	2.68795400
H	-3.14953100	-3.77388800	1.02643300
H	-1.85772200	-3.62731000	2.23541500
H	0.37442100	-0.21832700	-0.07771500
H	-3.27653900	-1.11907500	1.90555100
C	1.97726000	3.35448200	-0.32689000
H	3.06153600	3.46634300	-0.41339500
H	1.55013000	3.38954100	-1.34208900
O	1.50146000	4.42903000	0.46124500
H	0.58333200	4.19820500	0.69377000
C	-2.47008200	0.40114700	-0.96593800
H	-2.27736900	1.44768500	-1.22131400
H	-2.04898600	-0.21717300	-1.76509200
C	-3.95921900	0.16764500	-0.84586100
C	-4.77284200	1.09671000	-0.18145400
C	-4.55839300	-0.97539100	-1.38939000
C	-6.14622400	0.88461900	-0.05620100
H	-4.32892900	1.99849100	0.23182200
C	-5.93289400	-1.19008100	-1.26921700
H	-3.94503200	-1.70184800	-1.91515700
C	-6.73102300	-0.26156700	-0.59950500
H	-6.75998800	1.61806400	0.45743000
H	-6.37872500	-2.08019400	-1.70213000
H	-7.80002900	-0.42513600	-0.50770100

2(δ,δ)··(DMSO)$_1$

C	-2.51482000	2.97529000	-1.22405000
C	-1.31104000	3.51505000	-1.99804000
H	-1.62214900	4.38993000	-2.57774000
H	-0.50297000	3.81385000	-1.32929000
H	-0.93604000	2.76137000	-2.69772000
C	-3.63865000	2.57897000	-2.18256000
H	-3.28523000	1.84478000	-2.91270000
H	-4.48241000	2.14940000	-1.63434000
H	-3.99100000	3.46238000	-2.72265000
C	-3.02657000	3.95709000	-0.16841000
H	-3.84805000	3.51187000	0.40179000
H	-2.23538000	4.25395000	0.52091000
H	-3.40780900	4.85307000	-0.66870000
O	-2.17021000	1.68001000	-0.58850000
C	-1.19729000	1.56428000	0.32722000
O	-0.52756000	2.48324000	0.78887000
N	-1.01770000	0.25700000	0.67233000
C	-0.25931000	-0.09305000	1.86532000
H	-0.57849000	0.52603000	2.71100000
H	-1.71181000	-0.40680000	0.32796000
C	1.25266000	0.14863900	1.73890000
O	1.94677000	0.23716900	2.75086000
N	1.74963000	0.23226900	0.48557000
C	3.14497000	0.50850900	0.19683000
H	3.74005000	0.07379900	1.00456000
C	3.50292000	2.01074900	0.19726000
O	4.68627000	2.34589900	0.08135000
N	2.50027000	2.89386900	0.32106000

C	2.74525000	4.32770900	0.35692000
H	1.78682100	4.83898900	0.45306000
H	3.38072100	4.59731900	1.20658000
H	3.23855100	4.66196900	-0.56063000
H	1.09494000	0.14012900	-0.28027000
H	1.54794000	2.56983900	0.45599000
C	-0.49558000	-1.57024000	2.24319000
H	-0.20394000	-2.21774000	1.40553000
H	0.15094000	-1.79955100	3.09300000
O	-1.82971000	-1.82876000	2.63979000
H	-2.36871000	-1.96047000	1.83351000
C	3.56720000	-0.13118100	-1.14498000
H	2.93115000	0.26541900	-1.94493000
H	4.58607000	0.20838900	-1.34864000
C	3.51127000	-1.64382100	-1.14230000
C	2.52159000	-2.33156100	-1.85415000
C	4.46018000	-2.39001100	-0.42869000
C	2.47295900	-3.72813100	-1.84982000
H	1.78487000	-1.77197100	-2.42401000
C	4.41540900	-3.78409100	-0.42001000
H	5.24474000	-1.87616100	0.12042000
C	3.41906900	-4.45901100	-1.13070000
H	1.69774900	-4.24146100	-2.41019000
H	5.16113900	-4.34356100	0.13624000
H	3.38488900	-5.54380100	-1.12669000
O	-2.91891000	-1.95906000	0.10520000
S	-4.32834000	-2.00998000	-0.51209000
C	-5.48076000	-1.55844000	0.81595000
C	-4.73861100	-3.77311000	-0.63049000
H(Iso=2)	-5.29096000	-0.51121000	1.05584000
H(Iso=2)	-6.49889000	-1.67747000	0.43794000
H(Iso=2)	-5.30341000	-2.19727000	1.68370000
H(Iso=2)	-5.77589100	-3.86279000	-0.96167000
H(Iso=2)	-4.06817100	-4.20248000	-1.37651000
H(Iso=2)	-4.58950100	-4.24184000	0.34454000

2(δ,β)··(DMSO)$_2$

C	4.17357000	-2.59028100	-1.51642000
C	3.07508000	-3.06538100	-2.47009000
H	3.51613000	-3.72558100	-3.22387000
H	2.29420000	-3.61363100	-1.94189000
H	2.62409000	-2.21321100	-2.98851000
C	5.26457000	-1.84274100	-2.28509000
H	4.83971000	-1.00202100	-2.84184000
H	6.02805000	-1.45996100	-1.60119000
H	5.74577000	-2.52003100	-2.99655000
C	4.77924000	-3.73417100	-0.69998000
H	5.52209000	-3.34846100	0.00564000
H	4.01429000	-4.28072100	-0.14708000
H	5.28452000	-4.43044100	-1.37712000
O	3.64791000	-1.54401100	-0.61152000
C	2.63988000	-1.78550100	0.24938000
O	2.06218000	-2.85322000	0.39624000
N	2.33460000	-0.64973100	0.94089000
C	1.39337000	-0.67403000	2.04701000
H	1.34817000	-1.69759000	2.43192000
H	2.95008000	0.15468900	0.82679000
C	-0.05702000	-0.32412000	1.66371000
O	-0.95938000	-0.47879000	2.49111000
N	-0.25780000	0.13834000	0.41677000
C	-1.56203000	0.51635000	-0.10927000
H	-2.31726000	0.02166000	0.50309000
C	-1.63405000	0.01779000	-1.55871000
O	-0.76399000	0.35131000	-2.37317000
N	-2.67079000	-0.77374000	-1.86025000
C	-2.86538000	-1.30760000	-3.19939000
H	-3.78935000	-1.88720000	-3.20899000

H	-2.94401000	-0.49967000	-3.93308000
H	-2.03369000	-1.95694000	-3.49200000
H	0.54246000	0.23486000	-0.19512000
H	-3.31852000	-1.06015000	-1.12297000
C	1.85987000	0.22800000	3.20409000
H	1.16184000	0.09810000	4.03373000
H	2.85215000	-0.11021100	3.52973000
O	1.87061000	1.60944000	2.88234000
H	2.63338000	1.79503900	2.29589000
C	-1.75880000	2.05390000	-0.03265000
H	-1.57014000	2.34504000	1.00569000
H	-0.99019000	2.52636000	-0.65208000
C	-3.13360000	2.52030000	-0.45747000
C	-4.21980000	2.43303000	0.42471000
C	-3.35522000	3.04634000	-1.73662000
C	-5.49281000	2.85401000	0.03864000
H	-4.06576000	2.03834000	1.42538000
C	-4.62761000	3.46913000	-2.12809000
H	-2.52390000	3.12969000	-2.43084000
C	-5.70152000	3.37288000	-1.24159000
H	-6.31969000	2.78149000	0.73838000
H	-4.77722000	3.87692000	-3.12307000
H	-6.69046000	3.70382000	-1.54253000
O	-4.62252000	-1.64438000	0.11053000
S	-4.67426000	-2.82380000	1.08894000
C	-4.08638000	-2.18517000	2.68580000
C	-3.24865000	-3.88232000	0.69746000
H(Iso=2)	-4.84080000	-1.47687000	3.03308000
H(Iso=2)	-4.01542000	-3.02344000	3.38376000
H(Iso=2)	-3.11980000	-1.69306000	2.54949000
H(Iso=2)	-3.20478000	-4.68701000	1.43526000
H(Iso=2)	-3.42716000	-4.29661000	-0.29616000
H(Iso=2)	-2.33650000	-3.28241000	0.71203000
O	4.02432000	1.83666900	1.14036000
S	4.08041000	2.98126900	0.10751000
C	5.46859000	2.56781900	-0.98326000
C	4.83322000	4.38184900	0.98074000
H(Iso=2)	5.17677000	1.67595900	-1.53944000
H(Iso=2)	5.62748000	3.40301900	-1.66930000
H(Iso=2)	6.35550000	2.37667900	-0.37552000
H(Iso=2)	5.76560000	4.05350900	1.44494000
H(Iso=2)	5.00727000	5.18394900	0.25971000
H(Iso=2)	4.11443000	4.70586900	1.73493000

2(x,β)··(DMSO)$_2$

C	-4.04754000	4.00157900	-0.25051000
C	-4.47318000	3.77361000	1.20173000
H	-5.29866000	4.45058000	1.44449000
H	-4.80483000	2.74770000	1.36577000
H	-3.64387000	3.99301900	1.88182000
C	-3.59747000	5.44891900	-0.45771000
H	-2.78139000	5.70239900	0.22575000
H	-3.25427000	5.60504900	-1.48490000
H	-4.43337000	6.12764000	-0.26517000
C	-5.14487000	3.63067000	-1.25051000
H	-4.78428000	3.75367000	-2.27682000
H	-5.48194000	2.60245000	-1.11316000
H	-6.00014000	4.29931000	-1.10954000
O	-2.81379000	3.24044900	-0.54529000
C	-2.77260000	1.89438900	-0.49591000
O	-3.69597000	1.15771900	-0.17644000
N	-1.54188000	1.45374900	-0.87562000
C	-1.14036000	0.07305900	-0.70047000
H	-1.61905000	-0.33773100	0.19720000
H	-0.78434000	2.12596900	-0.90081000
C	0.38365000	0.05257900	-0.47330000
O	1.02191000	1.10147900	-0.34592000
N	0.92916900	-1.17663100	-0.41493000

C	2.35023900	-1.42145100	-0.22468000
H	2.83724000	-0.44804100	-0.16633000
C	2.88919900	-2.21554100	-1.42450000
O	2.31452900	-3.24275100	-1.80355000
N	4.01192900	-1.74299100	-1.98394000
C	4.65708900	-2.42089100	-3.09805000
H	5.57319900	-1.88285100	-3.34537000
H	4.90946900	-3.45213100	-2.83338000
H	4.00771900	-2.44220100	-3.97960000
H	0.33024900	-1.96121100	-0.66533000
H	4.40686900	-0.85550100	-1.66560000
C	-1.58701100	-0.79533100	-1.90364000
H	-2.63483000	-0.55645100	-2.11606000
H	-0.99342000	-0.53734100	-2.78674000
O	-1.41905100	-2.18382100	-1.66295000
H	-2.15180100	-2.49871100	-1.07944000
C	2.62701900	-2.21972100	1.07685000
H	2.09615900	-3.17478100	1.01154000
H	3.69875900	-2.44656100	1.10215000
C	2.23002900	-1.48250100	2.33558000
C	0.99857900	-1.72532100	2.95688000
C	3.08891000	-0.53273100	2.90635000
C	0.62979900	-1.03390100	4.11335000
H	0.32459900	-2.46583100	2.53606000
C	2.72569000	0.16035900	4.06159000
H	4.05252000	-0.33648100	2.44381000
C	1.49216000	-0.08737100	4.66904000
H	-0.32841100	-1.23888100	4.58077000
H	3.40718000	0.88892900	4.48987000
H	1.20910000	0.44838900	5.56956000
O	5.26609000	0.81808900	-1.43864000
S	5.28608000	1.70875900	-0.19001000
C	4.02752000	2.98791900	-0.46979000
C	6.76351000	2.75191900	-0.35265000
H(Iso=2)	3.06104000	2.47946900	-0.45955000
H(Iso=2)	4.08375000	3.71251900	0.34645000
H(Iso=2)	4.21326000	3.46372900	-1.43562000
H(Iso=2)	6.76199000	3.48307900	0.45937000
H(Iso=2)	7.62797000	2.09224900	-0.26130000
H(Iso=2)	6.74911000	3.24213900	-1.32863000
O	-3.37787100	-3.06927100	0.00031000
S	-4.84575100	-2.90562000	-0.43153000
C	-5.55840100	-1.68693000	0.70805000
C	-5.69768100	-4.38490000	0.18330000
H(Iso=2)	-5.05930100	-0.73930000	0.49569000
H(Iso=2)	-6.62919100	-1.60937000	0.50380000
H(Iso=2)	-5.37340100	-2.00886000	1.73539000
H(Iso=2)	-6.76930100	-4.26448000	0.00743000
H(Iso=2)	-5.31615100	-5.23093000	-0.39048000
H(Iso=2)	-5.48048100	-4.50540000	1.24693000

2(β,β)··(DMSO)$_3$

C	-5.00553000	-1.82997900	1.94513000
C	-4.46328000	-2.93810900	2.85126000
H	-5.29754100	-3.41192900	3.37868000
H	-3.93531100	-3.70128000	2.27830000
H	-3.78259000	-2.52012000	3.59991000
C	-5.75257000	-0.78059900	2.77088000
H	-5.10266000	-0.36263900	3.54569000
H	-6.10503000	0.03561100	2.13304000
H	-6.61897000	-1.23914900	3.25633000
C	-5.90106000	-2.37159900	0.82849000
H	-6.23100000	-1.55816900	0.17450000
H	-5.38399100	-3.12150900	0.22879000
H	-6.79045000	-2.83098900	1.27191000
O	-3.88952000	-1.04895000	1.37294000
C	-2.96436000	-1.60760000	0.56223000
O	-2.93753000	-2.77911000	0.20817000

N	-2.06159000	-0.67006000	0.17590000
C	-0.84159000	-1.01241000	-0.52833000
H	-0.59262000	-2.05747000	-0.31893000
H	-2.06504000	0.22702000	0.64415000
C	0.28322000	-0.10804000	0.00436000
O	0.02263000	0.91508000	0.64571000
N	1.52897000	-0.51495100	-0.29992000
C	2.72204000	0.23265900	0.06620000
H	2.39387000	1.10776900	0.62799000
C	3.46581000	0.67748900	-1.20446000
O	3.73954000	-0.13502100	-2.09623000
N	3.81569100	1.97125900	-1.25002000
C	4.56988100	2.52295900	-2.36459000
H	4.76649100	3.57655900	-2.16062000
H	5.52355100	2.00053800	-2.48965000
H	4.00964100	2.44089900	-3.30186000
H	1.65416000	-1.40171100	-0.79824000
H	3.53016100	2.60305900	-0.49638000
C	-0.98496000	-0.88100000	-2.06227000
H	-0.07772000	-1.27534000	-2.52931000
H	-1.82714000	-1.51061000	-2.37544000
O	-1.15355000	0.45338000	-2.50116000
H	-2.10542000	0.69442000	-2.49745000
C	3.68248000	-0.61243100	0.94399000
H	3.96053000	-1.51199100	0.38569000
H	4.59767000	-0.02724100	1.08732000
C	3.10114000	-0.98635100	2.28877000
C	2.48793000	-2.22924100	2.49120000
C	3.16056000	-0.08958100	3.36480000
C	1.94252000	-2.56650100	3.73220000
H	2.44083000	-2.94109100	1.67234000
C	2.61812000	-0.42178100	4.60678000
H	3.64084000	0.87597900	3.23029000
C	2.00495000	-1.66306100	4.79445000
H	1.47364900	-3.53619100	3.86863000
H	2.67888000	0.28547900	5.42824000
H	1.58508000	-1.92488100	5.76052000
O	1.70500900	-3.14944100	-1.59479000
S	3.05778900	-3.65285100	-2.11353000
C	3.21025000	-3.02629100	-3.81088000
C	2.80526900	-5.40910100	-2.50325000
H(Iso=2)	4.10350900	-3.46334100	-4.26408000
H(Iso=2)	2.31095900	-3.29238100	-4.37104000
H(Iso=2)	3.31865000	-1.94481100	-3.71905000
H(Iso=2)	3.71166900	-5.79367100	-2.97715000
H(Iso=2)	2.63263900	-5.92164100	-1.55545000
H(Iso=2)	1.93970900	-5.50945100	-3.16199000
O	-3.78068000	1.22501000	-2.79395000
S	-4.40196900	2.25406000	-1.83890000
C	-6.18455900	1.91033100	-1.84907000
C	-4.43759900	3.82340100	-2.75351000
H(Iso=2)	-6.31948000	0.93702100	-1.37520000
H(Iso=2)	-6.69175900	2.68430100	-1.26821000
H(Iso=2)	-6.53816900	1.89205100	-2.88227000
H(Iso=2)	-4.97407900	4.56315100	-2.15431000
H(Iso=2)	-3.39962900	4.13207000	-2.88774000
H(Iso=2)	-4.92407900	3.66430100	-3.71841000
O	3.10889100	3.80177900	0.87589000
S	1.84286100	4.65657900	0.72029000
C	2.24337100	6.26292900	1.46673000
C	0.68111100	4.05813900	1.98008000
H(Iso=2)	2.99767200	6.72787900	0.82984000
H(Iso=2)	1.33802200	6.87436900	1.48340000
H(Iso=2)	2.63180100	6.10059900	2.47467000
H(Iso=2)	-0.19836900	4.70686000	1.97504000
H(Iso=2)	0.40803100	3.04249900	1.68613000
H(Iso=2)	1.17546100	4.06962900	2.95423000

2(δ,β)··(DMSO)$_3$

C	-3.35971000	-4.45400100	-0.80257000
C	-2.13076000	-5.28896100	-1.17079000
H	-2.42125000	-6.34185100	-1.24721000
H	-1.70459000	-4.97527100	-2.12440000
H	-1.36488000	-5.20452100	-0.39312000
C	-3.94768000	-4.92573100	0.52899000
H	-3.19660000	-4.87691100	1.32303000
H	-4.80145000	-4.30487100	0.81708000
H	-4.28826000	-5.96117100	0.43729000
C	-4.43064000	-4.47252100	-1.89614000
H	-5.26778000	-3.82245100	-1.62182000
H	-4.02847000	-4.14739100	-2.85627000
H	-4.81512000	-5.49183100	-2.00552000
O	-2.96221000	-3.06364100	-0.50042000
C	-2.38859000	-2.26556100	-1.42664000
O	-2.13491000	-2.58711100	-2.58095000
N	-2.14372000	-1.03955100	-0.89270000
C	-1.50067000	0.00727900	-1.65944000
H	-1.41552000	-0.36195100	-2.68371000
H	-2.32427000	-0.90841100	0.10085000
C	-0.05472000	0.34041900	-1.24020000
O	0.64985000	0.98813000	-2.02145000
N	0.37604000	-0.10015000	-0.04146000
C	1.72134000	0.17489000	0.45304000
H	2.31069000	0.50765000	-0.40174000
C	2.30214000	-1.13103000	1.01683000
O	1.75245000	-1.70816000	1.96352000
N	3.41300000	-1.58424000	0.42010000
C	4.06825000	-2.80966000	0.84925000
H	4.96048000	-2.95589000	0.23872000
H	4.36310000	-2.74883000	1.90151000
H	3.40824000	-3.67510000	0.72848000
H	-0.28372000	-0.51958100	0.61204000
H	3.80487000	-1.08006000	-0.38064000
C	-2.34397000	1.28613900	-1.70976000
H	-1.84792000	2.00180900	-2.37839000
H	-3.32351000	1.03104900	-2.13647000
O	-2.47958000	1.81391900	-0.40135000
H	-3.08817000	2.58581900	-0.43292000
C	1.69702000	1.29158000	1.52741000
H	1.16959000	2.14397000	1.08686000
H	1.10397000	0.94016000	2.37676000
C	3.07165000	1.72107000	1.99180000
C	3.84041000	2.60449000	1.22058000
C	3.60935000	1.24871000	3.19597000
C	5.11188000	3.00070000	1.63688000
H	3.43644000	2.99113000	0.28875000
C	4.88158000	1.64235000	3.61743000
H	3.02545000	0.56988000	3.81065000
C	5.63807000	2.51910000	2.83816000
H	5.68880900	3.68874000	1.02662000
H	5.27808000	1.26693000	4.55583000
H	6.62556000	2.82880000	3.16541000
O	4.63750000	-0.23417000	-1.82483000
S	4.20120000	-0.64923000	-3.23694000
C	5.72998000	-0.75186000	-4.21197000
C	3.49896000	0.84113000	-3.99868000
H(Iso=2)	6.29901000	-1.59632000	-3.81966000
H(Iso=2)	5.46531000	-0.93096000	-5.25683000
H(Iso=2)	6.28827000	0.18005000	-4.09798000
H(Iso=2)	3.27557000	0.62079000	-5.04558000
H(Iso=2)	2.58004000	1.05995000	-3.45078000
H(Iso=2)	4.21885000	1.65820000	-3.91095000
O	-1.80691000	-0.74576100	2.03647000
S	-1.75555000	-1.97963100	2.95009000
C	-3.33641000	-1.99047100	3.84458000
C	-0.67459000	-1.52480100	4.33438000

H(Iso=2)	-4.11481000	-2.20713100	3.11140000
H(Iso=2)	-3.30129000	-2.78001100	4.59921000
H(Iso=2)	-3.49437000	-1.01114100	4.30190000
H(Iso=2)	-0.69795000	-2.33368100	5.06911000
H(Iso=2)	0.32433000	-1.42096000	3.90808000
H(Iso=2)	-1.02470000	-0.58541100	4.76820000
O	-4.24695100	3.91510900	-0.46001000
S	-3.67935100	5.33853900	-0.57086000
C	-4.40469100	6.26430900	0.81237000
C	-4.59793100	6.12827900	-1.92335000
H(Iso=2)	-3.97621100	5.85013900	1.72638000
H(Iso=2)	-4.12693100	7.31608900	0.71060000
H(Iso=2)	-5.48921100	6.13603900	0.79766000
H(Iso=2)	-4.31356100	7.18230900	-1.96717000
H(Iso=2)	-4.30070100	5.62134900	-2.84275000
H(Iso=2)	-5.66894100	6.01197900	-1.74337000

2(β,β)··(DMSO)$_4$

C	1.37314900	4.88969000	-1.83507000
C	-0.07452100	5.38137000	-1.75449000
H	-0.14033100	6.38229000	-2.19360000
H	-0.75211100	4.71833000	-2.29337000
H	-0.39721100	5.44740000	-0.71037000
C	2.30317900	5.84427000	-1.08249000
H	1.98942900	5.94839000	-0.03933000
H	3.33373900	5.47673000	-1.10195000
H	2.27931900	6.83240000	-1.55129000
C	1.84977900	4.70785000	-3.27869000
H	2.86894900	4.30816000	-3.29653000
H	1.19520900	4.03455000	-3.83329000
H	1.85854900	5.68056000	-3.78143000
O	1.53042900	3.63170000	-1.08262000
C	0.86414000	2.50240000	-1.42279000
O	0.07800000	2.39928000	-2.35810000
N	1.19999000	1.49520000	-0.58450000
C	0.62062000	0.17636000	-0.70603000
H	0.40138000	-0.00947000	-1.76015000
H	1.83202000	1.69012000	0.19420000
C	-0.68368000	0.03983000	0.11094000
O	-0.82468000	0.61904000	1.19051000
N	-1.60562000	-0.78183000	-0.43235000
C	-2.83910000	-1.14993100	0.24523000
H	-2.93546000	-0.49603100	1.11293000
C	-2.76783000	-2.61584100	0.70959000
O	-2.46036900	-3.51842100	-0.07887000
N	-3.09090000	-2.83471100	1.99292000
C	-3.12043900	-4.17374100	2.55983000
H	-3.43493900	-4.10037100	3.60197000
H	-3.82546900	-4.81390100	2.02006000
H	-2.13206900	-4.64332000	2.51930000
H	-1.39908000	-1.22873000	-1.33038000
H	-3.30674000	-2.04418100	2.60706000
C	1.61093000	-0.89270000	-0.22114000
H	1.91609000	-0.66173000	0.80790000
H	1.09637000	-1.86330000	-0.21506000
O	2.73307000	-0.92029000	-1.08610000
H	3.46677000	-1.39014000	-0.63117000
C	-4.07362000	-0.97416100	-0.67444000
H	-3.92865000	-1.58125100	-1.57369000
H	-4.93827000	-1.39035100	-0.14481000
C	-4.35573000	0.46330900	-1.05109000
C	-4.01091000	0.96266900	-2.31277000
C	-4.98005000	1.32758900	-0.14025000
C	-4.27839000	2.29000900	-2.65701000
H	-3.53291000	0.30691900	-3.03455000
C	-5.24811000	2.65432900	-0.47818000
H	-5.26471000	0.95628900	0.84067000
C	-4.89718000	3.14086900	-1.74019000

H	-4.00474000	2.65621900	-3.64171000
H	-5.73568100	3.30589900	0.24046000
H	-5.10858100	4.17160900	-2.00669000
O	4.82295000	-2.14129900	0.22952000
S	5.09681100	-3.62080900	-0.08382000
C	5.16818100	-4.45856900	1.52526000
C	6.86000100	-3.71431900	-0.50634000
H(Iso=2)	4.15972100	-4.42755900	1.94079000
H(Iso=2)	5.47537100	-5.49442900	1.36294000
H(Iso=2)	5.87237100	-3.93123900	2.17243000
H(Iso=2)	7.13242100	-4.76524900	-0.62903000
H(Iso=2)	6.98476100	-3.18231900	-1.45079000
H(Iso=2)	7.44378100	-3.24224900	0.28684000
O	-3.78093000	-0.67936100	3.79952000
S	-2.67763000	-0.15539100	4.73023000
C	-3.50944000	0.26112900	6.29000000
C	-2.30577000	1.52919900	4.16603000
H(Iso=2)	-3.85002000	-0.67878100	6.72752000
H(Iso=2)	-2.78537000	0.74224900	6.95201000
H(Iso=2)	-4.35427000	0.92067900	6.07932000
H(Iso=2)	-1.59942000	1.97998000	4.86776000
H(Iso=2)	-1.85005000	1.42550000	3.17916000
H(Iso=2)	-3.23483000	2.10185900	4.11698000
O	-0.87484000	-1.91373000	-3.05595000
S	-1.70499000	-3.05061000	-3.66361000
C	-1.01678900	-4.59234000	-2.99531000
C	-1.11962900	-3.22051000	-5.37474000
H(Iso=2)	-1.25167900	-4.58452000	-1.92986000
H(Iso=2)	-1.50795900	-5.43416000	-3.48986000
H(Iso=2)	0.06196100	-4.60628000	-3.16702000
H(Iso=2)	-1.60156900	-4.09328000	-5.82193000
H(Iso=2)	-1.42039000	-2.31453000	-5.90351000
H(Iso=2)	-0.03232900	-3.32527000	-5.37148000
O	3.00849000	1.84161000	1.73856000
S	4.48480000	2.14482100	1.46371000
C	5.42737000	0.78587100	2.21505000
C	4.95010900	3.45533100	2.63406000
H(Iso=2)	5.21164000	-0.11222900	1.63215000
H(Iso=2)	6.49126000	1.02869100	2.15251000
H(Iso=2)	5.11011000	0.66607100	3.25374000
H(Iso=2)	6.02582900	3.62907100	2.55342000
H(Iso=2)	4.40253900	4.35153100	2.33808000
H(Iso=2)	4.67254000	3.14658100	3.64448000