Supporting Information

The Solution Structure of (+)-Spongistatin 1 in DMSO

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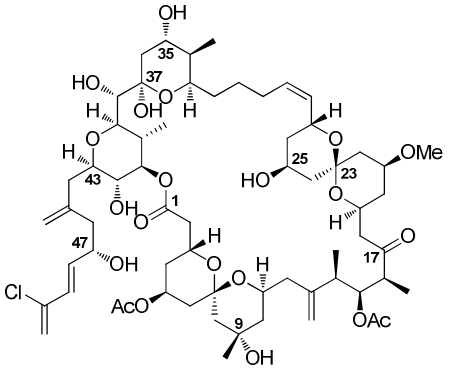


(+)-Spongistatin 1 (**1**)

A . $^{1}H/^{13}C$ signals of (+)Spongistatin 1 in MeCN

From published NMR spectra of Kitagawa, Pettit ,Paterson and Smith

$^{1}H/^{13}C$ No.	Natural	Synthetic	Natural	Synthetic
	^{13}C (100 MHz)	^{13}C (125 MHz)	^{1}H (400 MHz)	^{1}H (500 MHz)
1	173.07	173.07		
2	40.86	40.86	2.44 dd (10, 18)	2.45 dd (10.5, 16.2)
			2.53 dd (2, 18)	2.52 dd (1.8, 16.2)
3	63.59	63.59	4.25 brt (10)	4.24 brt (10.7)
4	34.65	34.65	1.55*, 1.68*	1.55*, 1.68*
5	67.06	67.06	4.92 brs	4.92 brs
6	38.17	38.16	1.67 dd (5, 14); 1.78 brd	1.66 dd (4.4, 15.2); 1.78 d
7	99.26	99.25		
8	46.76	46.75	1.47 d (14), 1.60*	1.46 d (14.0), 1.60*
9	69.64	69.63		
9a	30.21	30.21	1.06 s	1.06 s
10	44.96	44.95	1.28*, 1.55*	1.28*, 1.55*
11	64.701	64.70	4.25 brt (10)	4.24 bit (10.7)
12	44.24	44.24	1.99*; 2.27 brd (14)	1.99*; 2.26 brd (14.0)
13	148.03	148.03		
13a	114.86	114.86	4.83 brs; 4.83 brs	4.83 brs; 4.83 brs
14	36.60	36.59	2.78*	2.78*
14a	12.09	12.09	1.04 d (6.9)	1.04 d (6.9)
15	75.34	75.34	5.12 dd (1.7, 11)	5.11 dd (1.8, 10.7)
16	47.62	47.61	3.04 dq (7, 11)	3.04 dq (6.9, 10.7)
16a	13.73	13.73	1.15 d (7)	1.15 d (6.9)
17	213.52	213.52		
18	51.94	51.95	2.62 brd (18); 2.86 dd (11, 18)	2.61 brd (18.2); 2.86 dd (10.1, 19.4)
19	66.16	66.15	4.00 bit (11)	3.99 bit (11.1)
20	37.70	37.70	0.97 ddd (12, 12, 12);	0.96 ddd (12, 12, 12); 1.98*
21	73.98	73.98	3.46 tt (4, 4, 12, 12)	3.46 tt (4.2, 4.2, 11.6, 11.6)
22	44.18	44.18	1.08 t (12); 1.99*	1.08 t (12.1), 1.99*
23	99.91	99.91		
24	34.91	34.90	1.55*; 2.28*	1.55*; 2.27*
25	64.41	64.41	3.93 brm	3.94 brm

26	39.11	39.11	1.57*; 1.57*	1.57*; 1.57*
27	61.22	61.21	5.00 ddd (4.3, 10, 10)	5.00 ddd (3.8, 9.9, 9.9)
28	131.22	131.21	15.32 brd (10)	5.32 brd (10.8)
29	133.42	133.41	5.48 ddd (10, 10, 10)	5.48 ddd (9.9, 9.9, 10.6)
30	28.07	28.08	2.00*;2.19*	2.00*;2.18*
31	27.04	27.04	1.23*;1.60*	1.23*;1.60*
32	32.82	32.83	1.30 m;1.42 m	1.30m; 1.42 m
33	67.15	67.15	4.13 dt(3.4, 3.4, 8)	4.12 dt (3.0, 3.0, 9.0)
34	39.32	39.32	1.57 m	1.57 m
34a	11.55	11.55	0.81 d(7)	0.81 d (7.2)
35	71.47	71.47	3.65 brs	3.65 m
36	33.79	33.78	1.61*;1.89*	1.61*;1.89*
37	99.41	99.41		
38	73.11	73.09	3.34 brs	3.34 d (10.7)
39	81.30	81.30	3.72 brd (10)	3.72 brd (10.2)
40	37.26	37.26	1.91*	1.91*
40a	12.69	12.69	0.74 d(7)	0.74 d(6.6)
41	80.60	80.60	4.75 dd (9,11)	4.75 dd (9.2,11)
42	73.11	73.09	3.12t (9)	3.11 dt (5.4, 9.1)
43	78.72	78.70	3.39 brt (9)	3.38 dt (2.2, 8.6)
44	40.24	40.23	2.08*; 2.76 brd (13)	2.08*; 2.75 brd (13.9)
45	144.00	143.98		
45a	116.61	116.63	4.86 brs; 4.89 brs	4.86 brs; 4.89 brs
46	43.93	43.92	2.33 brdd (7, 14); 2.19*	2.33 brdd (6.3, 13.6); 2.18*
47	70.13	70.12	4.36 ddd (6, 7, 11)	4.36*
48	139.21	139.20	6.11 dd (6, 15)	6.11 dd (5.7, 15.0)
49	126.99	126.98	6.41 brd (15)	6.41 dd (1.1, 15.0)
50	139.21	139.20		
51	116.48	116.49	5.35 brs; 5.45 brs	5.35 brs; 5.45 brs
OMe	55.72	55.71	3.24s	3.24s
OAc	21.78	27.78	1.94s	1.94s
	171.61	171.61		
OAc	21.00	21.00	1.84s	1.84s
	170.21	170.19		
OH(C9)			4.32 brs	4.31 brs
OH(C25)			4.39 d (9.9)	4.39d (10.0)
OH(C35)			3.83 brm	3.82 d (9.4)
OH(C37)			4.73 d (2)	4.72 d (2.5)
OH(C38)				2.86 brd (10.1)
OH(C42)				4.35 brd (5.3)
OH(C47)				3.51 brd (2.5)

* coupling constants for these signals were not measured due to overlapping.

B. ^{1}H signals of (+)Spongistatin 1 in DMSO

^{1}H	**Synthetic**
	^{1}H (500 MHz)
1	
2	2.47*
	2.70*
3	4.15 brt (11.3)
4	1.52*, 1.65*
5	4.88 brs
6	1.65*, 1.76*
7	
8	1.63* , 1.65*
9	
9a	1.00 s
10	1.23*, 1.54*
11	4.13 bd (10.7)
12	2.01*; 2.28*
13	
13a	4.71 brs; 4.73 brs
14	2.82dq (6.8, 1.5)
14a	0.9 (6.7)
15	5.17 dd (1.5, 10.8)
16	3.04 dq (6.9, 10.4)
16a	1.07 d (6.9)
17	
18	2.61 brd (18.2); 2.86 dd (10.1, 19.4)
19	3.99 bit (11.1)
20	0.96*; 1.98*
21	3.46 tt (4.2, 4.2, 11.6, 11.6)
22	1.23*, 1.99*
23	
24	1.52*; 2.24*
25	3.84 brm
26	1.55*; 1.55*
27	4.88*
28	5.33 brd (10.1)
29	5.35 ddd (9.7, 9.7, 10.2)
30	2.00*;2.10*
31	1.11 m;1.24 m
32	1.11 m;1.24 m
33	3.58 dt (3.3, 2.9, 9.3)
34	1.40 m
34a	0.79 d (7.1)
35	3.58 m
36	1.52*;2.24*
37	
38	3.27 d (10.2)
39	3.65 brd (10.0)
40	1.83*
40a	0.71 d(6.5)

41	4.67 dd (9.7,11)
42	3.11 dt (6.4, 9.7)
43	3.36 dt (1.9, 9.1)
44	2.05*; 2.71*
45	
45a	4.80 brs; 4.83 brs
46	2.05*, 2.23*
47	4.24 brd (5.9)
48	6.11 dd (5.4, 15.1)
49	6.40 dd (1.1, 15.1)
50	
51	5.36 brs; 5.55 brs
OMe	3.19s
OAc	1.93s
OAc	1.80s
OH(C9)	3.91 brs
OH(C25)	4.32d (10.0)
OH(C35)	4.56 d (9.3)
OH(C37)	4.78 brs
OH(C38)	4.02 d (9.7)
OH(C42)	4.15 brd (5.1)
OH(C47)	5.05 brd (2.5)

C. Buildup curves for determination optimum mixing time for NOESY experiments

Mixing time ms	**43/40Me**	**39/40Me**	**38/40Me**	**15/16Me**	**19/21**
30	45.05	44.27	51.48	38.09	135.37
50	101.78	95.41	53.64	118.06	285.69
80	132.23	110.96	146.02	136.13	299.68
100	250.47	187	202.06	234.05	550.54
200	264.12	246.6	336.07	299.77	565.96
400	359.33	358.44	456.23	395.16	713.12
600	390.44	384.42	466.57	422.19	657.55
800	369.56	360.21	425.01	385.5	536.64

NOESY integrations between two protons with different mixing time

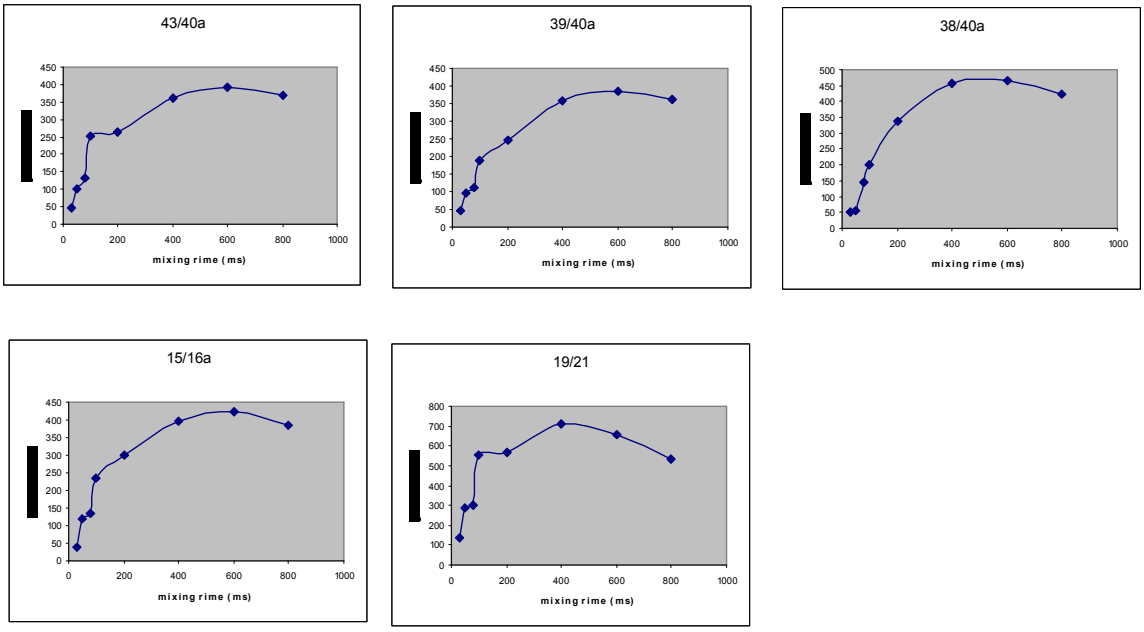


Figure 1: Buildup curves for NOESY at different mixing times

D.NOESY derived interproton distances used in calculations

H1	H2	NOE distance in angstroms
40Me	38	2.82
40Me	42	4.8
40Me	16	4.08
40Me	14	4.94
40Me	16Me	4.06
34Me	21	5.11
34Me	38	5.56
14Me	35OH	4.23
9Me	21	3.82
9Me	21OMe	6.08
16Me	39	3.46
16Me	43	4.75
16Me	38	6.3
16Me	41	3.25
34Me	21OMe	6.79

E. 1H NMR Coupling constants used in calculations

H1	**H2**	***J(Hz)***
2proR	3	1.8
5	6proS	4.4
15	14	1.8
15	16	10.7
27	28	9.9
29	30proR	9.9
29	30proS	9.9
33	32proR	9.0
33	33proS	3.0
38	39	10.2
43	44proS	2.2

II. Computational Studies

A. Conformational Searches

Energy calculations were performed with MMFF94 force field in Macromodel 7.2 by utilizing the GB/SA solvation in water, chloroform, DMSO or acetonitrile with constant dielectric constant. For the later the dielectric constants were adjusted to the experimental value. MMFF was chosen as the force field as it is better parameterized for our system (185 high, 1 medium quality stretch parameters ; 351 high, 1 medium quality bending parameters; 533 high, 10 low quality torsion parameters). Constant dielectic constants with extended cutoffs were utilized. Custom choice of longer VDW, electrostatic and H-bond cutoffs did not change the energy ordering of the lowest energy conformers. (Our observations showed the extended VDW and electrostatic cutoffs may change energy ordering of conformations in older versions of Macromodel). Atomic charges were calculated by Gaussian software package with CHELPG keyword. The MMFF values were in acceptable limits with the extracted atomic charges so they are utilized for all calculations.

Conformational searches were performed without any constraints. MCMM torsional sampling was used where intermediate torsional sampling options was chosen. A 100 kJ/mol energy window was chosen for keeping the conformations. Consecutive conformational searches of 30,000 steps were utilized. Final conformers were saved and minimized for complete convergence (with Polak-Ribiere *conjugate gradient* algorithm) with the default gradient convergence threshold of 0.05. The final compounds were clustered according to their backbone dihedral angles with Xcluster. These calculations were repeated starting from different geometries until not new low energy families were detected after clustering.

Solvation energy of conformations in water vary -30 to -90 kj/mol where the total energy is in the order of ~430 kj/mol.

PM3 level relative energies of the gas phase/PM3 minimized conformers are as follows

	$CHCl_3$	water	DMSO	Kitagawa structure
PM3 energy (kcal/mol)	0	0.2	6.6	50.4

B. MD Simulations

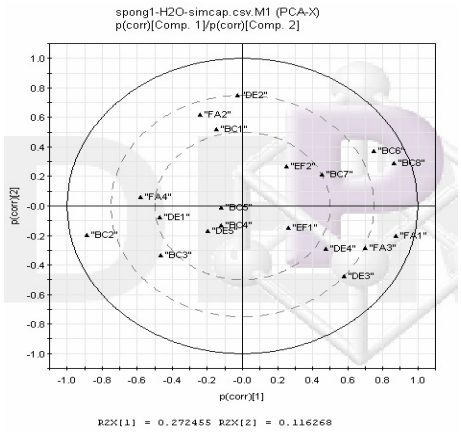
MD simulations in water were performed with Macromodel 7.2 with the same options for the force field and solvation. SHAKE algorithm was used for bonds to hydrogen. Structures at every 150fs were extracted from five nanosecond simulation (1.5fs timestep, 300K). The structures were minimized first and clustered by Xcluster according to their backbone torsional angles eliminated the redundant structures and yielded 2921 disctinct structures. The dihedral angles extracted from these were given into PCA. During the simulation western perimeter was observed to have a preferred conformation where the CD ring moved up and down generating a variety of conformers. The potential energy surface was flat allowing the molecule to have large amount of conformations.

C. Principal Component Analysis

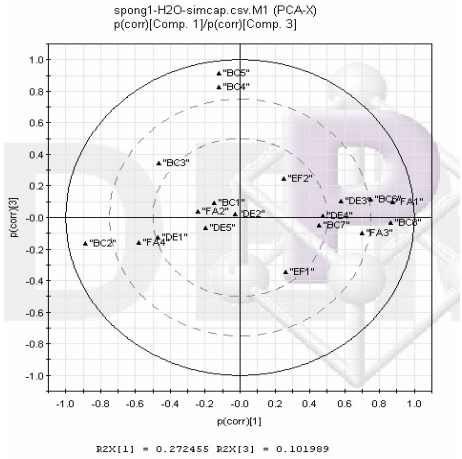
Principal component analysis (PCA) is a very useful method for identifying the correlated torsional angles responsible for the twisting and bending of the macrocycles during a molecular dynamics simulations. Backbone dihedral angles of the conformations obtained in water were converted into 0-360 º scale are given into PCA analysis utilizing SIMCA-P software[1] by the default settings. Only 40% of the variation could be expressed by 2 principal components while the 4 principal components generated 60% of the variation.

Figure 2 a) Loadings PCA 1 vs 2 (38%) **b)** Loadings PCA 1 vs 3 (37%) **c)** Loadings PCA 1 vs 4 (35%) **d)** Component contributions

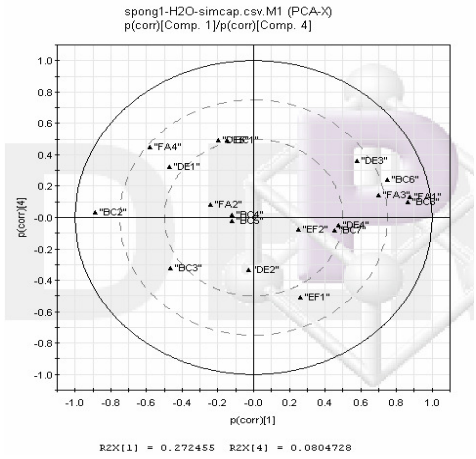
a.



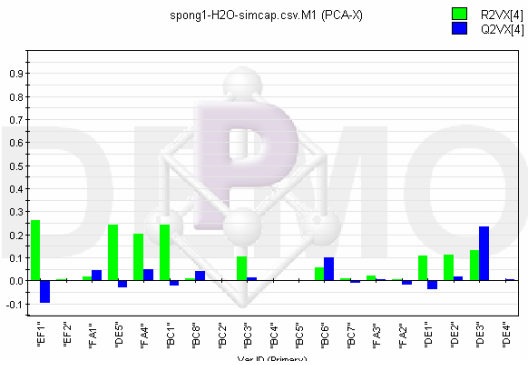
b.



c.



d.



The most important correlations are seen among the following long range (non-adjacent) torsional angles (See Figure 3 for the names)

[1] Simca-P, Umetrics http://www.umetrics.com

1. FA2, DE2, BC1
2. FA1, BC8, FA3 and BC8

Rest of the changes seen in the torsional angles during the simulations are not correlated. Changes around EF1, DE5, FA4, BC1 have the highest component contributions in the PCA model.

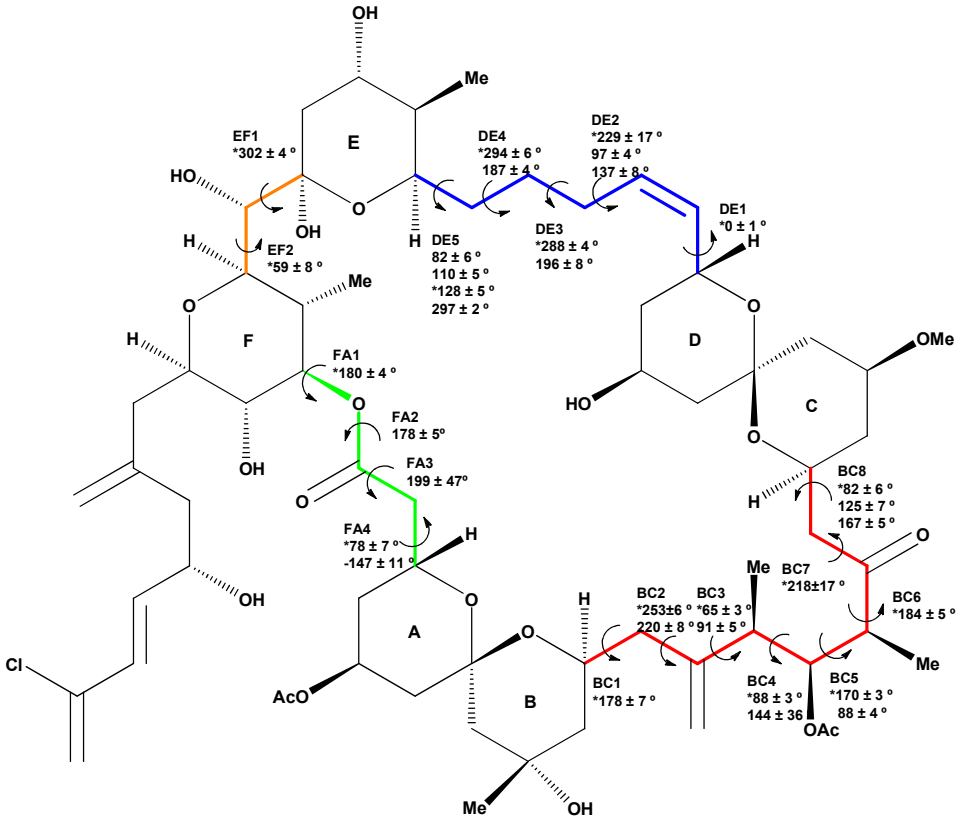


Figure 3: Summary of preferred angles for each backbone torsional angle. Most accessed values are highlighted with a * sign. See Figure 4 for more details.

D.Polar Maps

Backbone dihedral angles of the conformations obtained in water were converted into 0-360 ° scale and plotted onto polar coordinate graphs by using OriginPro 7.5[2] software. Conformations within 20 kJ/mol energy to the global minimum were taken.

[2] OriginLab http://www.originlab.com/

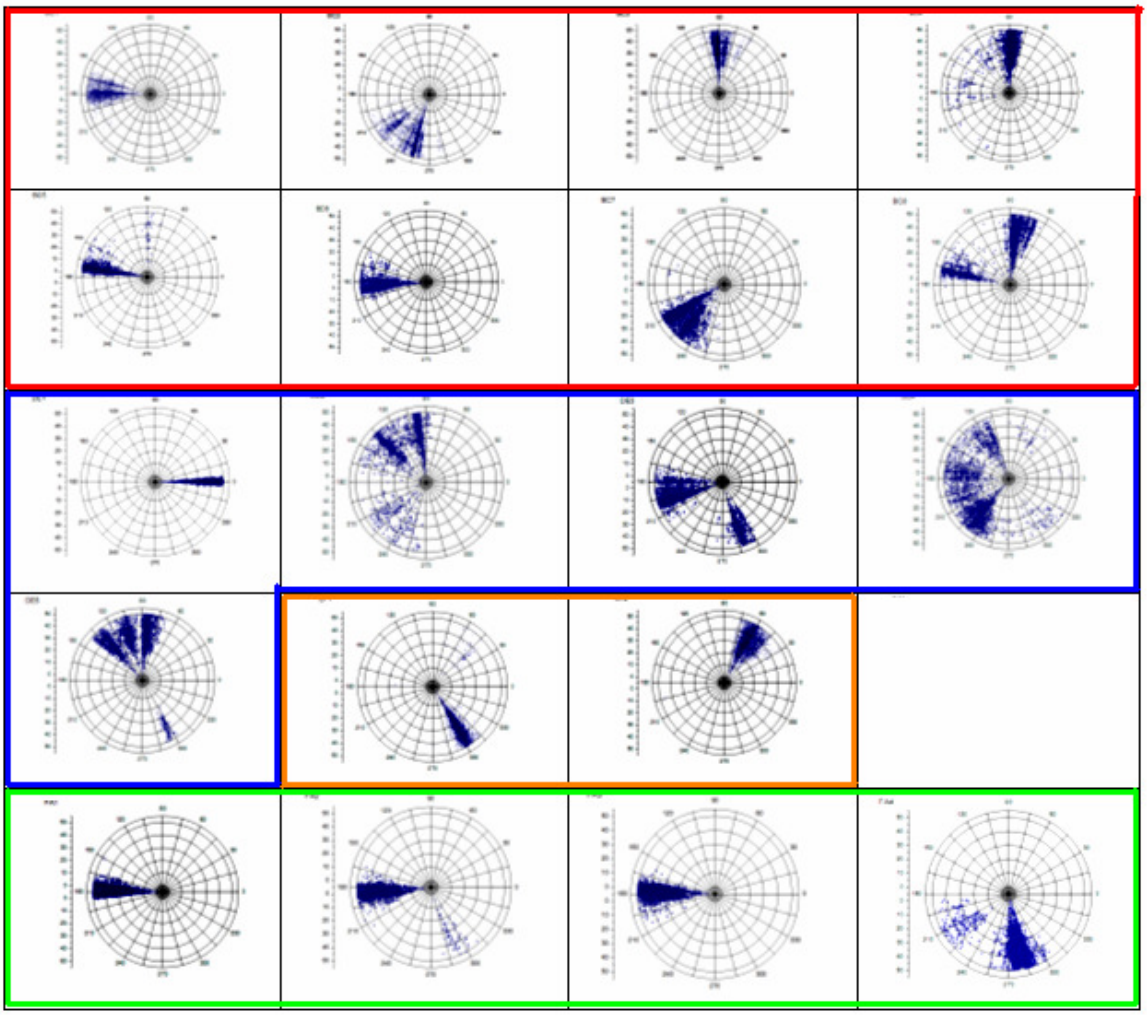


Figure 4: Polar maps drawn for each backbone dihedral angle. Each dot is a conformer.Center represents the lowest energy. **Raw 1** BC1-BC4; **Raw 2** BC5-BC8; **Raw 3** DE1-DE4 **Raw 4** DE5, EF1, EF2 **Raw 5** FA1-FA4 (The dihedral angle names are given according to their position between the rings. Color codes are matching to Figure 3).

E. DISCO (Distribution of Conformations)

Disco (Distribution of conformations) is a Windows(XP/NT/2000/98) application for calculating the solution conformation distributions of organic molecules from NOEs, coupling constants and a set of precalculated conformations. It is a new implementation

of NAMFIS[3] methodology with two differences **1**) A clustering routine clusters conformations according to the given NOEs and coupling constants prior to deconvolution at the desired level. **2**) A general genetic algorithm solver is utilized for deconvolution which is advantageous for finding the global minimum.

Disco takes and generates NAMFIS type input and output files which makes it possible to use it with Janocchio.[4]

The test files are included in the distribution package which includes NAMFIS test files for a peptide[3], (+)-discodermolide.[5] The results of former two can be compared to the original articles which give very similar distributions but small changes are result of input conformers, deconvolution algorithm and clustering scheme. Results also can differ slightly according to random number generator.

Fitting Spongistatin Data with DISCO

Spongistatin conformers obtained from conformational searches with different solvent models were combined and subjected to DISCO. Hierarchical clustering followed by selection of representative structures from the clusters gradually decreased the set to 220 conformers. The clustering level than gradually lowered to 25 where RMS deviation of 3.08 was observed (Discrimination and clustering analysis were repeated lowered the number of independent variables). The separate calculation with NOE and torsional constraints are calculated and similar results were obtained. Overall the consistency of the distributions for two independent observations shows the success of the current distribution. RMS deviations calculated for NOE constrained calculations were is 3.1 angstroms where in *J* constrained calculations it was 0.7 Hz.

Calculated distribution of conformations under NOE and/or *J* coupling constraints obtained from NMR studies

	NOE+*J*	**NOE**	**J**
Conformation 1 %	57	66	53
Conformation 2 %	13	7	11
Conformation 3 %	8	10	9
Conformation 4 %	4	6	4

F. Coordinates for solution conformations

Minimum energy conformer in WATER

spg h2o minimum

-
180186 0 0 0 0 0 0 0 0 0 0 0
1.9606 3.5730 0.8964 C 0 0 0 0 0 0 0 0 0 0 0 0

[3] Cicero, D.O.; Barbato, G.; Bazzo R. *J. Am. Chem. Soc.*, **1995**, 117 , 1027.
[4] a) Evans, D. A.; Bodkin, M. J.; Baker, S. R.; Sharman, G. J. *Magn. Reson. Chem.*, **2007**, 45, 595. b) http://janocchio.sourceforge.net/
[5] Monteagudo, E .; Cicero, D. O.; Cornett, B.; Myles, D. C. and Snyder, J. P. *J. Am. Chem. Soc.*, **2001**, 123, 6929.

1.6267	4.7363	0.1384	O	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2334	4.4508	-1.2046	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.4082	3.8538	-2.0009	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.7792	2.5203	-1.3185	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0612	2.7178	0.2012	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.4370	4.1287	2.2523	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.7012	5.7932	-1.7875	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0026	3.6381	-3.4494	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0411	1.4322	0.7941	O	0	0	0	0	0	0	0	0	0	0	0	0	0
1.6489	6.8260	-1.7636	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2128	7.5256	-1.6443	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.6426	6.2113	-1.0740	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.5167	5.1056	-1.2523	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.8754	5.2839	-0.8390	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.5155	6.5713	-1.4003	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.6136	7.7890	-1.0727	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.4965	6.3678	0.3191	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.5851	3.9956	-1.2835	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.7594	6.5280	-2.9001	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.5913	8.0836	0.3027	O	0	0	0	0	0	0	0	0	0	0	0	0	0
0.1234	5.7043	0.6302	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.8137	7.0525	-0.8560	H	0	0	0	0	0	0	0	0	0	0	0	0	0
4.0003	0.9361	-2.6909	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.9485	0.4573	-3.0667	O	0	0	0	0	0	0	0	0	0	0	0	0	0
2.5404	3.0750	3.3102	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.7288	2.6467	3.7409	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2624	2.5663	3.9022	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.9615	7.4825	0.7048	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.8761	3.7603	-0.5166	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.4916	2.4226	-0.9046	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.9044	2.3091	-0.4588	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.4586	1.2027	0.0378	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.7187	-0.0869	0.2714	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.0209	-2.9608	0.6285	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.1186	-0.6657	1.6314	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.0738	-0.9218	-0.8362	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.6080	-2.0959	1.8246	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.2296	-2.1536	2.1000	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.7714	-2.2944	-0.7447	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.6063	-2.9768	-1.8619	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.9968	-4.3289	-2.2601	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.5023	-4.1625	-2.5627	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.8198	-3.5242	-1.3467	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.3866	-2.2372	-1.0729	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.5956	-4.8273	-3.4590	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.3216	-3.3066	-1.5862	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.7607	-1.8262	1.3397	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.4660	-3.6044	-0.3699	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.6872	-4.5430	0.3717	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3120	-2.6362	-0.1278	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.0824	1.0473	3.6996	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8567	0.7322	2.3409	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0930	0.5414	4.4898	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.6589	-0.6435	4.2464	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.8214	-1.1370	4.9718	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.7430	-1.9198	4.4105	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0745	-3.3028	0.5211	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.1022	-2.2886	0.5664	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.2814	-4.4241	-0.2921	O	0	0	0	0	0	0	0	0	0	0	0	0	0
1.6157	-1.9651	-0.8254	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.1797	-2.7553	1.5083	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.9548	-2.7808	2.8247	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.5014	-3.1789	0.9529	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.8334	-1.5156	0.7613	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.6016	-5.6222	0.2783	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.9576	-6.3677	-0.6129	O	0	0	0	0	0	0	0	0	0	0	0	0	0
0.5140	-5.9341	1.7418	C	0	0	0	0	0	0	0	0	0	0	0	0	0
4.4380	-1.9700	0.7501	C	0	0	0	0	0	0	0	0	0	0	0	0	0
4.9219	-1.3433	2.0594	C	0	0	0	0	0	0	0	0	0	0	0	0	0
5.5125	-2.5203	-0.0124	O	0	0	0	0	0	0	0	0	0	0	0	0	0

6.0931	-0.3608	1.8349	C	0	0	0	0	0	0	0	0	0	0	0	0	0
6.6394	0.1115	3.1851	C	0	0	0	0	0	0	0	0	0	0	0	0	0
7.1999	-1.0664	1.0213	C	0	0	0	0	0	0	0	0	0	0	0	0	0
5.6457	0.8163	1.1621	O	0	0	0	0	0	0	0	0	0	0	0	0	0
5.6761	0.6259	0.2218	H	0	0	0	0	0	0	0	0	0	0	0	0	0
6.6199	-1.6825	-0.2737	C	0	0	0	0	0	0	0	0	0	0	0	0	0
6.1826	-0.5759	-1.0676	O	0	0	0	0	0	0	0	0	0	0	0	0	0
5.6793	-0.9010	-2.3682	C	0	0	0	0	0	0	0	0	0	0	0	0	0
6.6898	-1.7214	-3.1767	C	0	0	0	0	0	0	0	0	0	0	0	0	0
7.1346	-2.9757	-2.4125	C	0	0	0	0	0	0	0	0	0	0	0	0	0
7.6537	-2.5577	-1.0241	C	0	0	0	0	0	0	0	0	0	0	0	0	0
5.3897	0.4477	-3.0485	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-8.8107	-5.5004	-3.2659	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.6379	1.0061	1.8554	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.9746	-0.6572	6.5927	Cl	0	0	0	0	0	0	0	0	0	0	0	0	0
1.0245	2.9725	1.0272	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.3981	3.7030	-1.1964	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.2785	4.5542	-1.9643	H	0	0	0	0	0	0	0	0	0	0	0	0	0
4.0595	3.1985	0.3481	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.4115	4.6451	2.1260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.7309	4.9111	2.6044	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.5339	5.6550	-2.8865	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2522	2.8418	-3.5521	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.5644	4.5581	-3.8713	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.8642	3.3637	-4.0702	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.5287	8.3689	-1.4332	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2922	7.4364	-2.7503	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.8826	5.3391	0.2787	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.4983	6.6951	-0.8829	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.0541	8.7128	-1.5117	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.7989	4.0439	-2.3757	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.9122	3.1238	-1.1476	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.4515	7.3192	-3.2138	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.8187	6.6697	-3.4591	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.1869	5.5608	-3.2087	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.8382	1.9063	4.5299	H	0	0	0	0	0	0	0	0	0	0	0	0	0
4.6722	3.0004	3.3315	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.3925	3.1047	3.4743	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2574	2.7953	4.9866	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.6911	3.7883	0.5755	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.5876	4.5873	-0.7190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.4751	2.2963	-2.0071	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.8872	1.5787	-0.4981	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.5170	3.2124	-0.5786	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-8.5251	1.1933	0.2959	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.6096	0.0935	0.2222	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-8.0962	-3.2054	0.7229	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.4719	-3.9303	0.6503	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.7343	-0.0040	2.4316	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-8.2217	-0.6683	1.7409	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.0265	-2.5274	2.7639	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-8.6529	-3.1038	-1.5218	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.6604	-2.3175	-2.7537	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-7.1341	-5.0664	-1.4289	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.0405	-5.1442	-2.7839	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.3527	-3.5410	-3.4682	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.0005	-4.1715	-0.4437	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.9677	-3.9661	-2.4055	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.1321	-2.2703	-1.9391	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.9695	-2.2050	-1.1100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0012	0.5099	4.0527	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.4677	1.1898	5.2929	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.2809	-1.3043	3.4443	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.6826	-2.2274	3.3633	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.6176	-2.2820	4.9424	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3355	-3.6115	1.5651	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.6702	-1.3416	1.0016	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.3344	-1.1280	-0.7955	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.1427	-2.8226	-1.2762	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.7774	-1.6921	-1.4861	H	0	0	0	0	0	0	0	0	0	0	0	0	0

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  2.7009   -3.1081    3.5436 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.0126   -2.4471    3.2673 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.9770   -3.9301    1.6146 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.3468   -3.6923   -0.0356 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.0269   -0.7999    0.9989 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.6460   -0.9626    0.2711 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.2214   -1.8963    1.7244 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.8867   -6.9454    1.9492 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.1120   -5.2248    2.3356 H   0  0  0  0  0  0  0  0  0  0  0  0
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  3.8986   -1.2029    0.1245 H   0  0  0  0  0  0  0  0  0  0  0  0
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  5.2461   -2.1342    2.7656 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.5096    0.7687    3.0578 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.8792    0.6769    3.7447 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.9506   -0.7388    3.8053 H   0  0  0  0  0  0  0  0  0  0  0  0
  8.0190   -0.3595    0.7822 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.6536   -1.8723    1.6301 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.7319   -1.4856   -2.2442 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.2467   -1.9922   -4.1556 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.5877   -1.1138   -3.4066 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.9239   -3.5147   -2.9868 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.9069   -3.4462   -0.4128 H   0  0  0  0  0  0  0  0  0  0  0  0
  8.5930   -1.9843   -1.1460 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.4406    0.3250   -4.1494 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.1638    1.2000   -2.7904 H   0  0  0  0  0  0  0  0  0  0  0  0
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 -8.6935   -6.3944   -2.6411 H   0  0  0  0  0  0  0  0  0  0  0  0
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  4.0115    2.0269   -1.8715 O   0  0  0  0  0  0  0  0  0  0  0  0
  5.3294   -4.4821   -3.1026 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.0689   -3.8850   -2.1259 O   0  0  0  0  0  0  0  0  0  0  0  0
  5.7396   -4.5015   -4.2457 O   0  0  0  0  0  0  0  0  0  0  0  0
  4.0644   -5.0700   -2.5383 C   0  0  0  0  0  0  0  0  0  0  0  0
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  4.2096   -6.1324   -2.3028 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.7397   -4.5622   -1.6073 H   0  0  0  0  0  0  0  0  0  0  0  0
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77 78 1 0 0 0 0
77 82 1 0 0 0 0
78 79 1 0 0 0 0
79 80 1 0 0 0 0
79 83 1 0 0 0 0
79160 1 0 0 0 0
80 81 1 0 0 0 0
80161 1 0 0 0 0
80162 1 0 0 0 0
81 82 1 0 0 0 0

```
 81163  1  0  0  0  0
 81175  1  0  0  0  0
 82164  1  0  0  0  0
 82165  1  0  0  0  0
 83166  1  0  0  0  0
 83167  1  0  0  0  0
 84168  1  0  0  0  0
 84169  1  0  0  0  0
 84170  1  0  0  0  0
174175  1  0  0  0  0
174176  2  0  0  0  0
174177  1  0  0  0  0
177178  1  0  0  0  0
177179  1  0  0  0  0
177180  1  0  0  0  0
```

Minimum energy conformer in chloroform
spg chcl3 minimum

```
-
180186  0  0  0  0  0  0  0  0  0  0    0
   2.4176   -1.1042   -0.4668 C   0  0  0  0  0  0
   3.7684   -0.8941   -0.9141 O   0  0  0  0  0  0
   3.8521   -0.7103   -2.3414 C   0  0  0  0  0  0
   3.4133   -2.0226   -3.0301 C   0  0  0  0  0  0
   1.9956   -2.4157   -2.5615 C   0  0  0  0  0  0
   1.8978   -2.4372   -1.0259 C   0  0  0  0  0  0
   2.4077   -1.0967    1.0769 C   0  0  0  0  0  0
   5.3081   -0.2856   -2.6791 C   0  0  0  0  0  0
   3.4675   -1.9230   -4.5589 C   0  0  0  0  0  0
   0.5373   -2.6290   -0.6281 O   0  0  0  0  0  0
   6.1944   -1.3886   -2.4188 O   0  0  0  0  0  0
   7.1938    1.3843   -2.3420 C   0  0  0  0  0  0
   5.7844    0.9758   -1.8859 C   0  0  0  0  0  0
   4.8656    2.0462   -2.1083 O   0  0  0  0  0  0
   5.1881    3.2543   -1.3965 C   0  0  0  0  0  0
   6.5612    3.7987   -1.8441 C   0  0  0  0  0  0
   7.6243    2.6980   -1.6887 C   0  0  0  0  0  0
   5.8648    0.6683   -0.4881 O   0  0  0  0  0  0
   4.0067    4.2181   -1.6037 C   0  0  0  0  0  0
   6.5525    4.3232   -3.2862 C   0  0  0  0  0  0
   7.9001    2.4936   -0.2988 O   0  0  0  0  0  0
   5.0424    0.1746   -0.2801 H   0  0  0  0  0  0
   6.2290   -1.4771   -1.4457 H   0  0  0  0  0  0
   0.5311   -3.9223   -3.7278 C   0  0  0  0  0  0
  -0.3464   -3.0817   -3.8683 O   0  0  0  0  0  0
   2.6542    0.2399    1.7652 C   0  0  0  0  0  0
   2.9165    1.3952    1.1295 C   0  0  0  0  0  0
   2.5859    0.2207    3.2871 C   0  0  0  0  0  0
   7.2367    1.8536    0.0393 H   0  0  0  0  0  0
   4.0850    5.4776   -0.7361 C   0  0  0  0  0  0
   2.8632    6.3735   -0.9569 C   0  0  0  0  0  0
   2.7727    7.4777    0.0625 C   0  0  0  0  0  0
   2.0624    7.4396    1.2056 C   0  0  0  0  0  0
   1.2961    6.2552    1.7333 C   0  0  0  0  0  0
  -0.6784    4.9318    3.3208 C   0  0  0  0  0  0
   1.6237    5.9622    3.1961 C   0  0  0  0  0  0
  -0.0979    6.5606    1.6235 O   0  0  0  0  0  0
   0.8013    4.7675    3.6700 C   0  0  0  0  0  0
   1.3399    3.5894    3.0843 O   0  0  0  0  0  0
  -0.9142    5.4008    1.8656 C   0  0  0  0  0  0
  -2.3664    5.8582    1.6613 C   0  0  0  0  0  0
  -3.3408    4.6809    1.6463 C   0  0  0  0  0  0
  -2.8833    3.6524    0.6129 C   0  0  0  0  0  0
  -1.4285    3.2598    0.8480 C   0  0  0  0  0  0
  -0.6033    4.4208    0.8756 O   0  0  0  0  0  0
  -4.6574    5.1007    1.2677 O   0  0  0  0  0  0
  -0.8907    2.3784   -0.2794 C   0  0  0  0  0  0
```

0.8325	2.8109	3.4042	H	0	0	0	0	0	0
-1.1842	0.9219	-0.0068	C	0	0	0	0	0	0
-0.6207	0.3464	0.9273	O	0	0	0	0	0	0
-2.1891	0.2228	-0.9192	C	0	0	0	0	0	0
1.1618	0.0305	3.8489	C	0	0	0	0	0	0
0.3048	1.0862	3.4069	O	0	0	0	0	0	0
1.1541	0.0887	5.3482	C	0	0	0	0	0	0
0.7992	-0.9389	6.1387	C	0	0	0	0	0	0
0.7857	-0.9133	7.5853	C	0	0	0	0	0	0
0.3820	0.1270	8.3251	C	0	0	0	0	0	0
-2.8650	-0.9608	-0.1744	C	0	0	0	0	0	0
-3.8037	-1.8143	-1.0902	C	0	0	0	0	0	0
-3.6611	-0.3311	0.8747	O	0	0	0	0	0	0
-4.9599	-0.9969	-1.6904	C	0	0	0	0	0	0
-4.3654	-3.0789	-0.4309	C	0	0	0	0	0	0
-5.1889	-3.0561	0.6335	C	0	0	0	0	0	0
-4.0959	-4.3958	-1.1378	C	0	0	0	0	0	0
-1.4760	-0.1656	-2.2093	C	0	0	0	0	0	0
-3.3946	-0.4088	2.1999	C	0	0	0	0	0	0
-3.8748	0.4177	2.9721	O	0	0	0	0	0	0
-2.5517	-1.5480	2.6874	C	0	0	0	0	0	0
-2.6725	-4.9834	-1.0430	C	0	0	0	0	0	0
-2.1985	-5.1400	0.4037	C	0	0	0	0	0	0
-2.7471	-6.2613	-1.6939	O	0	0	0	0	0	0
-0.9107	-5.9644	0.4908	C	0	0	0	0	0	0
-0.5441	-6.2281	1.9515	C	0	0	0	0	0	0
-1.0887	-7.2853	-0.2709	C	0	0	0	0	0	0
0.1732	-5.2026	-0.0680	O	0	0	0	0	0	0
0.2959	-5.5241	-0.9889	H	0	0	0	0	0	0
-1.5470	-7.0233	-1.7153	C	0	0	0	0	0	0
-0.4733	-6.3479	-2.3840	O	0	0	0	0	0	0
-0.7345	-6.0690	-3.7659	C	0	0	0	0	0	0
-0.9176	-7.3845	-4.5257	C	0	0	0	0	0	0
-2.0440	-8.2178	-3.9167	C	0	0	0	0	0	0
-1.8335	-8.3665	-2.4074	C	0	0	0	0	0	0
0.4711	-5.3111	-4.3117	C	0	0	0	0	0	0
-3.2886	-7.5411	-4.2106	O	0	0	0	0	0	0
-5.3736	5.7378	2.3186	C	0	0	0	0	0	0
0.1009	0.8575	2.4706	H	0	0	0	0	0	0
1.2450	-2.3846	8.3805	Cl	0	0	0	0	0	0
1.7751	-0.2887	-0.8258	H	0	0	0	0	0	0
3.1771	0.1078	-2.6258	H	0	0	0	0	0	0
4.0883	-2.8355	-2.7285	H	0	0	0	0	0	0
2.4925	-3.2724	-0.6334	H	0	0	0	0	0	0
1.4392	-1.4730	1.4229	H	0	0	0	0	0	0
3.1756	-1.7954	1.4344	H	0	0	0	0	0	0
5.3640	-0.0615	-3.7500	H	0	0	0	0	0	0
2.8478	-1.0960	-4.9213	H	0	0	0	0	0	0
4.4905	-1.7644	-4.9123	H	0	0	0	0	0	0
3.1110	-2.8439	-5.0315	H	0	0	0	0	0	0
7.9159	0.6030	-2.0756	H	0	0	0	0	0	0
7.2092	1.5089	-3.4311	H	0	0	0	0	0	0
5.2238	3.0214	-0.3248	H	0	0	0	0	0	0
6.8341	4.6322	-1.1846	H	0	0	0	0	0	0
8.5706	3.0273	-2.1323	H	0	0	0	0	0	0
3.9050	4.4836	-2.6625	H	0	0	0	0	0	0
3.0801	3.6790	-1.3626	H	0	0	0	0	0	0
7.5645	4.5913	-3.6085	H	0	0	0	0	0	0
6.1574	3.5843	-3.9904	H	0	0	0	0	0	0
5.9431	5.2285	-3.3706	H	0	0	0	0	0	0
3.0804	2.3194	1.6793	H	0	0	0	0	0	0
2.9675	1.4830	0.0512	H	0	0	0	0	0	0
3.0001	1.1606	3.6779	H	0	0	0	0	0	0
3.2436	-0.5761	3.6581	H	0	0	0	0	0	0
4.1471	5.1792	0.3180	H	0	0	0	0	0	0
4.9935	6.0461	-0.9643	H	0	0	0	0	0	0
2.9154	6.8257	-1.9552	H	0	0	0	0	0	0
1.9441	5.7763	-0.9566	H	0	0	0	0	0	0
3.3022	8.3964	-0.1846	H	0	0	0	0	0	0
2.0379	8.3333	1.8256	H	0	0	0	0	0	0

```
 1.5381   5.3731   1.1317 H   0  0  0  0  0  0  0
-1.0832   5.6952   3.9986 H   0  0  0  0  0  0  0
-1.2041   3.9958   3.5309 H   0  0  0  0  0  0  0
 2.6951   5.7582   3.3095 H   0  0  0  0  0  0  0
 1.3711   6.8308   3.8177 H   0  0  0  0  0  0  0
 0.9135   4.6598   4.7547 H   0  0  0  0  0  0  0
-2.6460   6.5983   2.4204 H   0  0  0  0  0  0  0
-2.4511   6.3970   0.7065 H   0  0  0  0  0  0  0
-3.3859   4.1986   2.6306 H   0  0  0  0  0  0  0
-3.5386   2.7740   0.6424 H   0  0  0  0  0  0  0
-3.0023   4.0873  -0.3890 H   0  0  0  0  0  0  0
-1.3364   2.7330   1.8027 H   0  0  0  0  0  0  0
-1.2920   2.6798  -1.2528 H   0  0  0  0  0  0  0
 0.1991   2.4735  -0.3665 H   0  0  0  0  0  0  0
-2.9567   0.9744  -1.1448 H   0  0  0  0  0  0  0
 0.7321  -0.9175   3.5064 H   0  0  0  0  0  0  0
 1.4603   1.0362   5.7859 H   0  0  0  0  0  0  0
 0.5103  -1.8863   5.6870 H   0  0  0  0  0  0  0
 0.0453   1.0532   7.8719 H   0  0  0  0  0  0  0
 0.3675   0.0777   9.4091 H   0  0  0  0  0  0  0
-2.1001  -1.6196   0.2476 H   0  0  0  0  0  0  0
-3.1942  -2.1611  -1.9341 H   0  0  0  0  0  0  0
-5.6012  -1.6290  -2.3158 H   0  0  0  0  0  0  0
-5.5897  -0.5459  -0.9163 H   0  0  0  0  0  0  0
-4.5874  -0.1907  -2.3293 H   0  0  0  0  0  0  0
-5.6207  -3.9667   1.0406 H   0  0  0  0  0  0  0
-5.4904  -2.1306   1.1135 H   0  0  0  0  0  0  0
-4.8027  -5.1589  -0.7798 H   0  0  0  0  0  0  0
-4.3568  -4.2819  -2.1996 H   0  0  0  0  0  0  0
-2.1884  -0.4252  -2.9978 H   0  0  0  0  0  0  0
-0.8548   0.6511  -2.5918 H   0  0  0  0  0  0  0
-0.8215  -1.0232  -2.0480 H   0  0  0  0  0  0  0
-2.5726  -1.5564   3.7822 H   0  0  0  0  0  0  0
-2.9631  -2.5001   2.3511 H   0  0  0  0  0  0  0
-1.5126  -1.4403   2.3790 H   0  0  0  0  0  0  0
-1.9811  -4.3400  -1.5997 H   0  0  0  0  0  0  0
-2.0371  -4.1493   0.8422 H   0  0  0  0  0  0  0
-2.9817  -5.6430   0.9860 H   0  0  0  0  0  0  0
 0.3991  -6.7821   2.0216 H   0  0  0  0  0  0  0
-0.3914  -5.2861   2.4910 H   0  0  0  0  0  0  0
-1.3208  -6.8009   2.4683 H   0  0  0  0  0  0  0
-0.1351  -7.8287  -0.2822 H   0  0  0  0  0  0  0
-1.8337  -7.9025   0.2476 H   0  0  0  0  0  0  0
-1.6333  -5.4464  -3.8502 H   0  0  0  0  0  0  0
-1.1314  -7.1740  -5.5802 H   0  0  0  0  0  0  0
 0.0104  -7.9685  -4.4772 H   0  0  0  0  0  0  0
-2.0346  -9.2007  -4.3980 H   0  0  0  0  0  0  0
-2.7161  -8.8279  -1.9511 H   0  0  0  0  0  0  0
-0.9792  -9.0391  -2.2580 H   0  0  0  0  0  0  0
 0.4246  -5.2041  -5.4011 H   0  0  0  0  0  0  0
 1.3991  -5.8442  -4.0709 H   0  0  0  0  0  0  0
-6.3821   5.9582   1.9581 H   0  0  0  0  0  0  0
-5.4529   5.0769   3.1870 H   0  0  0  0  0  0  0
-4.8980   6.6802   2.6018 H   0  0  0  0  0  0  0
 1.2776  -1.6888  -2.9611 H   0  0  0  0  0  0  0
 0.4599  -3.5594  -0.3180 H   0  0  0  0  0  0  0
 1.7085  -3.7419  -3.0684 O   0  0  0  0  0  0  0
-4.4861  -8.1590  -4.3379 C   0  0  0  0  0  0  0
-5.5116  -7.5088  -4.5235 O   0  0  0  0  0  0  0
-4.5064  -9.6575  -4.2835 C   0  0  0  0  0  0  0
-3.9654 -10.0741  -5.1362 H   0  0  0  0  0  0  0
-4.1030 -10.0223  -3.3378 H   0  0  0  0  0  0  0
-5.5447  -9.9991  -4.3483 H   0  0  0  0  0  0  0
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1  6  1  0  0  0
1  7  1  0  0  0
1 88  1  0  0  0
2  3  1  0  0  0
3  4  1  0  0  0
3  8  1  0  0  0
```

3 89 1 0 0 0
4 5 1 0 0 0
4 9 1 0 0 0
4 90 1 0 0 0
5 6 1 0 0 0
5172 1 0 0 0
5174 1 0 0 0
6 10 1 0 0 0
6 91 1 0 0 0
7 26 1 0 0 0
7 92 1 0 0 0
7 93 1 0 0 0
8 11 1 0 0 0
8 13 1 0 0 0
8 94 1 0 0 0
9 95 1 0 0 0
9 96 1 0 0 0
9 97 1 0 0 0
10173 1 0 0 0
11 23 1 0 0 0
12 13 1 0 0 0
12 17 1 0 0 0
12 98 1 0 0 0
12 99 1 0 0 0
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15 16 1 0 0 0
15 19 1 0 0 0
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20107 1 0 0 0
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24 25 2 0 0 0
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26 27 2 0 0 0
26 28 1 0 0 0
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49 51 1 0 0 0
51 58 1 0 0 0
51 65 1 0 0 0
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52 54 1 0 0 0
52 53 1 0 0 0
52133 1 0 0 0
53 86 1 0 0 0
54 55 2 0 0 0
54134 1 0 0 0
55 56 1 0 0 0
55135 1 0 0 0
56 57 2 0 0 0
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58 60 1 0 0 0
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59 61 1 0 0 0
59 62 1 0 0 0
59139 1 0 0 0
60 66 1 0 0 0
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61141 1 0 0 0
61142 1 0 0 0
62 63 2 0 0 0
62 64 1 0 0 0
63143 1 0 0 0
63144 1 0 0 0
64 69 1 0 0 0
64145 1 0 0 0
64146 1 0 0 0
65147 1 0 0 0
65148 1 0 0 0
65149 1 0 0 0
66 67 2 0 0 0
66 68 1 0 0 0
68150 1 0 0 0
68151 1 0 0 0
68152 1 0 0 0
69 70 1 0 0 0
69 71 1 0 0 0
69153 1 0 0 0

```
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 70154  1  0  0  0
 70155  1  0  0  0
 71 77  1  0  0  0
 72 73  1  0  0  0
 72 74  1  0  0  0
 72 75  1  0  0  0
 73156  1  0  0  0
 73157  1  0  0  0
 73158  1  0  0  0
 74 77  1  0  0  0
 74159  1  0  0  0
 74160  1  0  0  0
 75 76  1  0  0  0
 77 78  1  0  0  0
 77 82  1  0  0  0
 78 79  1  0  0  0
 79 80  1  0  0  0
 79 83  1  0  0  0
 79161  1  0  0  0
 80 81  1  0  0  0
 80162  1  0  0  0
 80163  1  0  0  0
 81 82  1  0  0  0
 81 84  1  0  0  0
 81164  1  0  0  0
 82165  1  0  0  0
 82166  1  0  0  0
 83167  1  0  0  0
 83168  1  0  0  0
 84175  1  0  0  0
 85169  1  0  0  0
 85170  1  0  0  0
 85171  1  0  0  0
175176  2  0  0  0
175177  1  0  0  0
177178  1  0  0  0
177179  1  0  0  0
177180  1  0  0  0
```

Minimum energy conformer in DMSO
spg dmso minimum

```
-
180186  0  0  0  0  0  0  0  0  0  0    0
   -2.0310    2.3440   -3.6770 C   0  0  0  0  0  0  0
   -2.2730    3.0140   -2.4470 O   0  0  0  0  0  0  0
   -1.6330    2.4110   -1.3310 C   0  0  0  0  0  0  0
   -2.2330    1.0060   -1.1110 C   0  0  0  0  0  0  0
   -2.0620    0.1590   -2.3880 C   0  0  0  0  0  0  0
   -2.6140    0.9150   -3.6130 C   0  0  0  0  0  0  0
   -2.6790    3.1950   -4.7870 C   0  0  0  0  0  0  0
   -1.7380    3.3440   -0.0960 C   0  0  0  0  0  0  0
   -1.6090    0.3030    0.1050 C   0  0  0  0  0  0  0
   -2.1980    0.2450   -4.7870 O   0  0  0  0  0  0  0
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   -0.0330    6.6700    1.0620 C   0  0  0  0  0  0  0
   -1.5840    5.4480   -1.3010 O   0  0  0  0  0  0  0
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   -2.3270   -2.2330   -2.5590 C   0  0  0  0  0  0  0
   -1.4070   -2.4250   -3.3540 O   0  0  0  0  0  0  0
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6.6960	-0.4550	1.8940	H	0	0	0	0	0	0
3.1020	1.1250	3.7240	H	0	0	0	0	0	0
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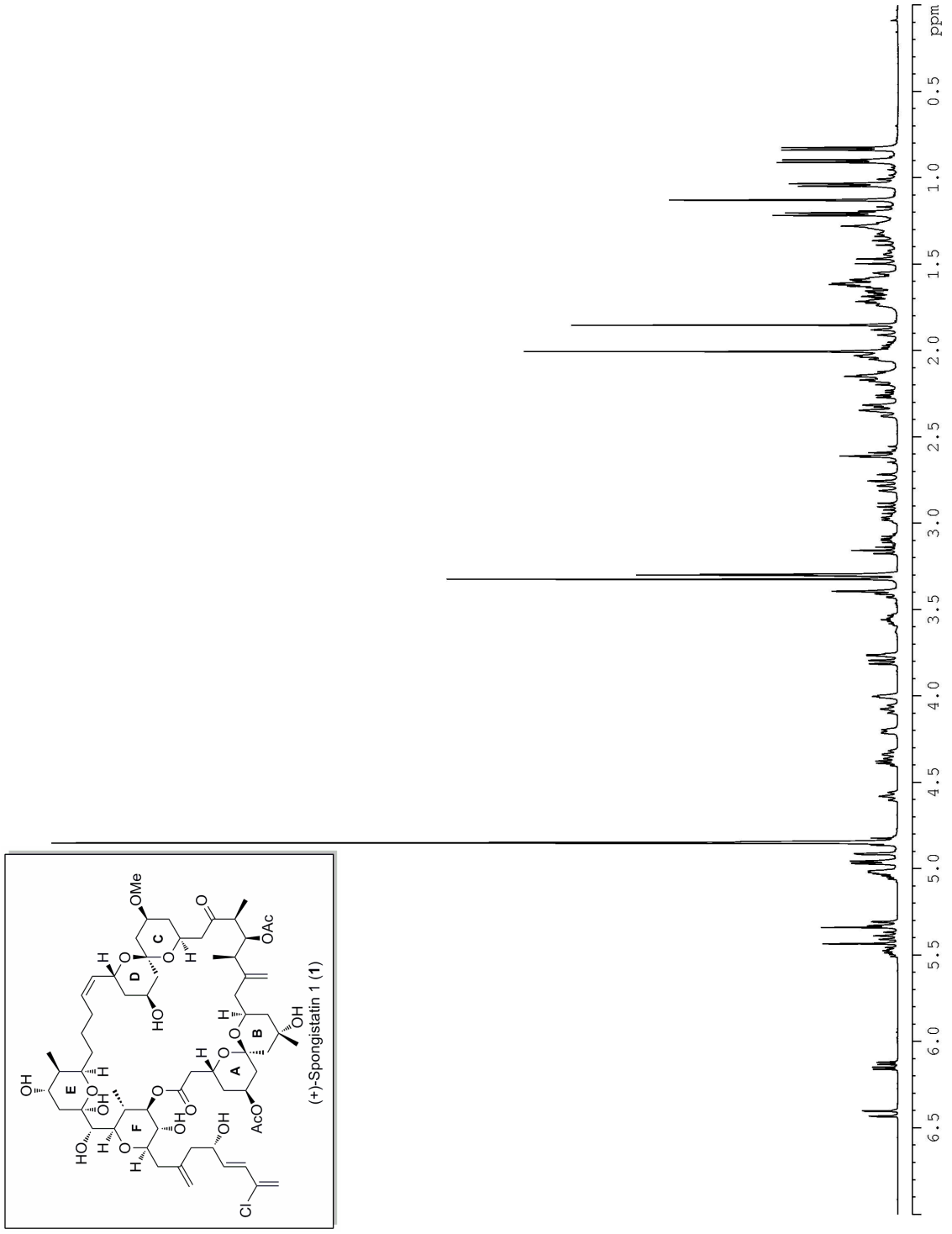
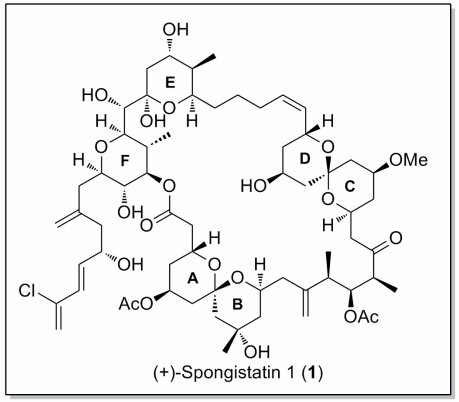
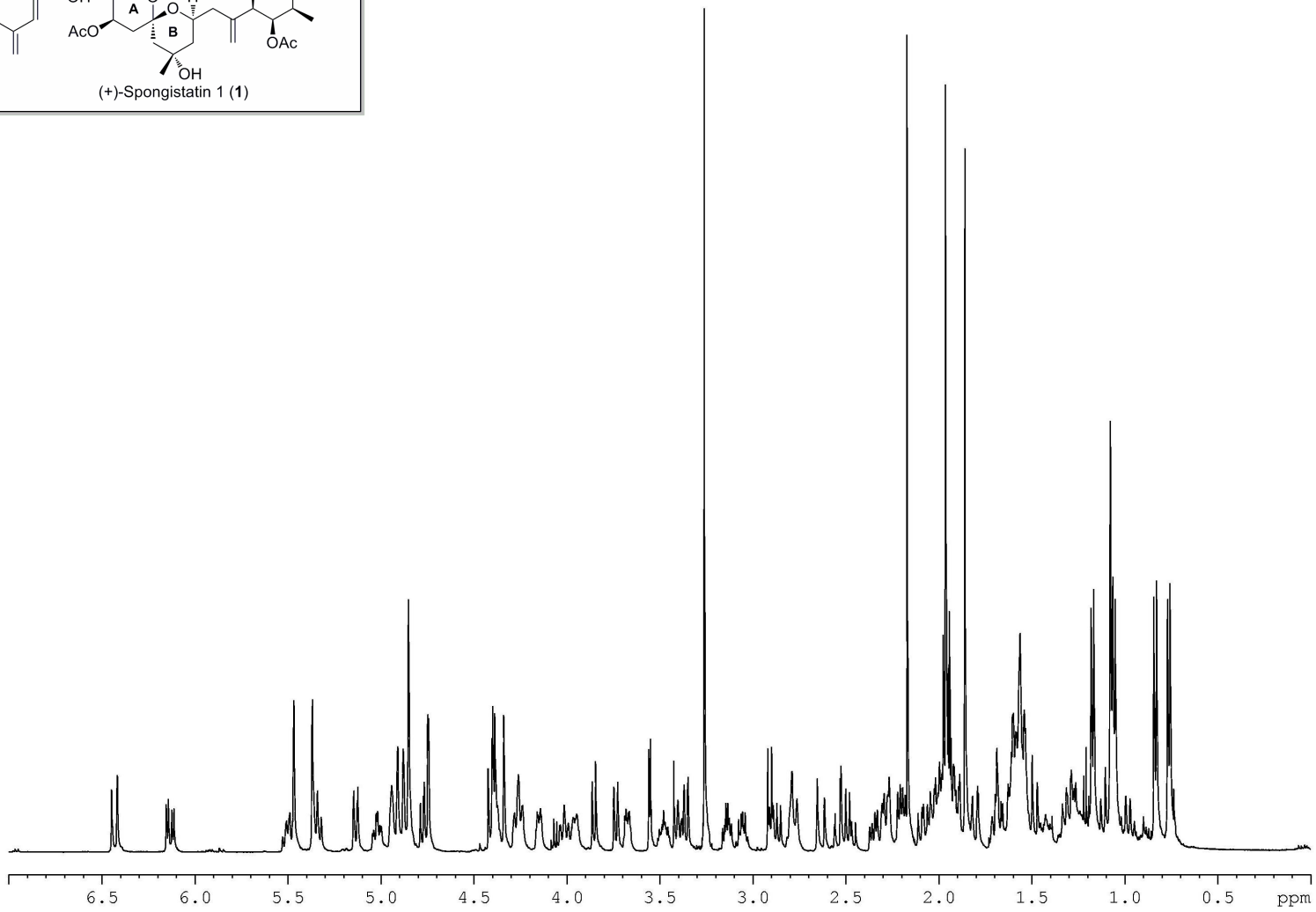
III.SPECTRA

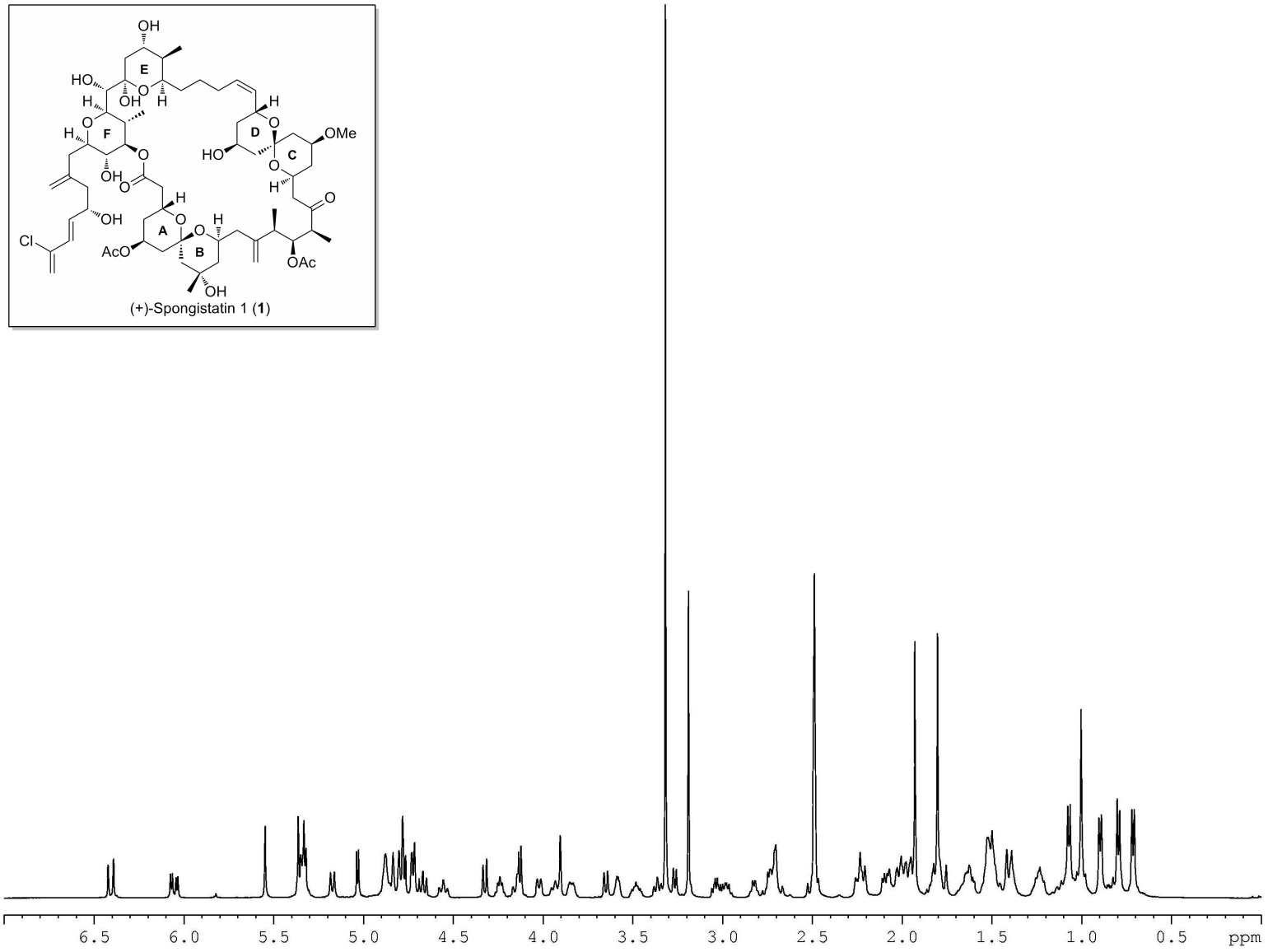


^{1}H NMR spectrum of (+)-Spongistatin 1 in methanol-D4

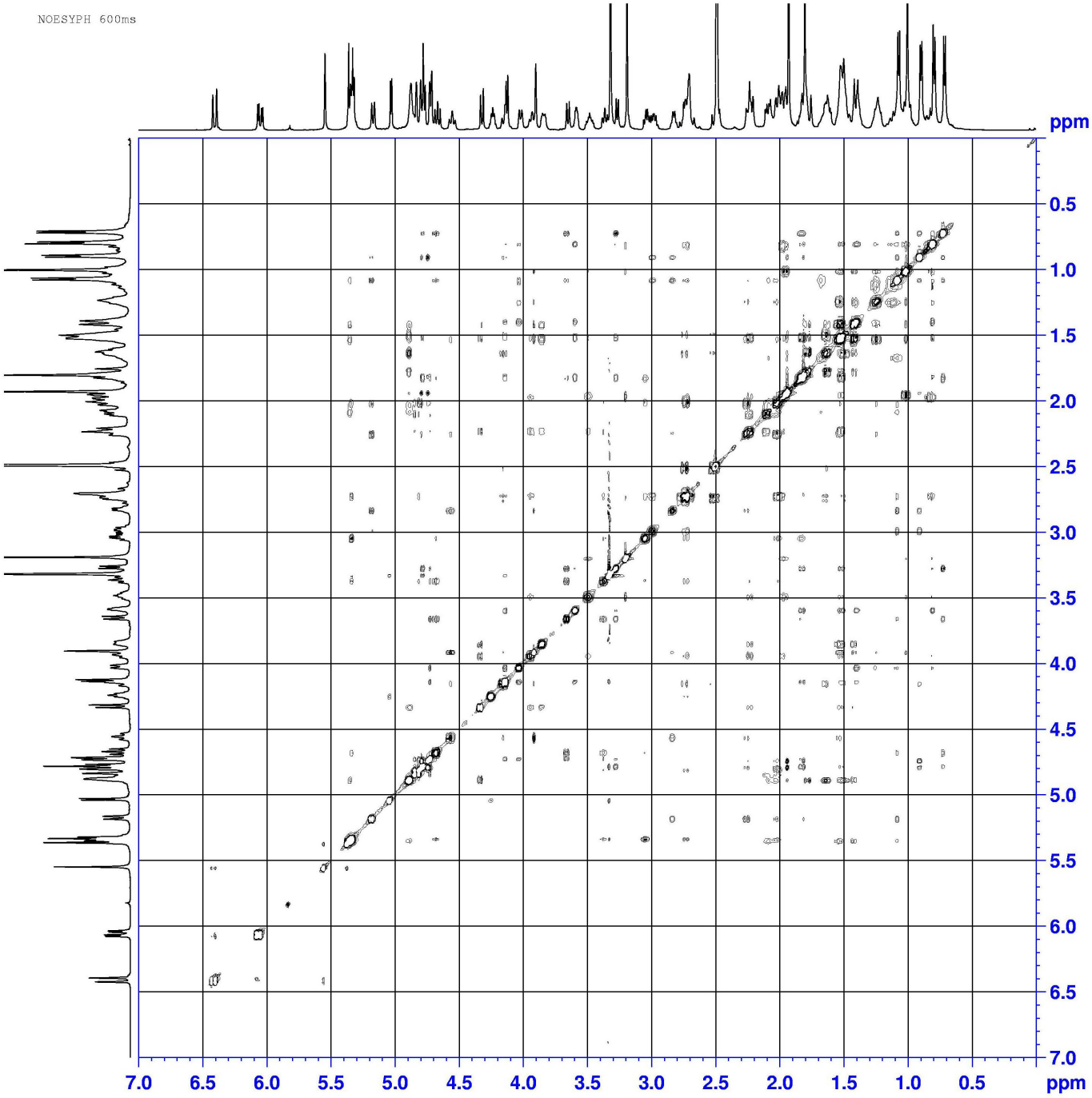




^{1}H NMR spectrum of (+)-Spongistatin 1 in acetonitrile-D3



^{1}H NMR spectrum of (+)-Spongistatin 1 in DMSO-D6



NOESY NMR spectrum of (+)-Spongistatin 1 in DMSO-D6 (mixing time of 600 ms)