Supplementary Information

(−)- and (+)-Asperginulin A, a Pair of Indole Diketopiperazine Alkaloid Dimers with a 6/5/4/5/6 Pentacyclic Skeleton from the Mangrove Endophytic Fungus *Aspergillus* sp. SK-28

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EXPERIMENTAL SECTION

General Experimental Procedures. The melting points were recorded on a SGW X-4B micro melting point apparatus (Shanghai Precision Scientific Instrument Co., Ltd, Shanghai, China) and were uncorrected. Optical rotations were measured on an MCP 300 polarimeter (Anton Paar, Graz, Austria) at 25 °C. UV data were performed on a TU-1900 spectrophotometer (Persee, Beijing, China) in MeOH solution. ECD spectra were recorded on a Chirascan CD spectrometer (Applied Photophysics, London, UK). IR spectra were recorded using a Nicolet Nexus 670 spectrophotometer (Thermo Nicolet Corporation, Madison, USA) in KBr discs. All NMR experiments were measured with Bruker Avance 500 spectrometers (500 and 125 MHz) (Bruker BioSpin, Switzerland), and the residual solvent peaks of DMSO-d_6 (δ_C 39.52 / δ_H 2.50) were used as references. HRESIMS data were acquired on a Thermo Fisher LTQ Orbitrap Elite high-resolution mass spectrometer (Thermo Fisher Scientific, Waltham, MA, USA). Column chromatography (CC) was carried by silica gel (200−300 mesh, Qingdao Maine Chemical Factory) and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Stockholm, Sweden). Chiral separation was performed on a Primaide HPLC system (Hitachi Instrument Dalian Co., Ltd, Dalian, China) with a chiral INA column (5 μm, 250 × 4.6mm).

Fungal material. The fungus *Aspergillus* sp. SK-28 was isolated from the fresh leaves of the mangrove plant *Kandelia candel*, which were collected in June 2017 from the Shankou Mangrove Nature Reserve in Guangxi Province, China. The fungal strain was identified according to its morphological characteristics and a molecular biological protocol by rDNA amplification and sequencing of the internal transcribed spacer (ITS) region. A BLAST search result showed that it was most similar (99%) to the sequence of *Aspergillus* sp. (compared to MK 605973). The sequence data have been submitted to GenBank with accession number MN428770. The voucher specimen (as reference culture) is stored in our laboratory at –20 °C and its working stocks were prepared on potato dextrose agar slants stored at 4 °C.

Fermentation, extraction and isolation. The fermentation was performed on solid wheat medium (50 g of wheat, 80 mL 0.3% of saline water, in each 1L

Erlenmeyer flask) with PDB culture as seed broth. After incubation for 28 days at 25 °C, the culture (2.5 kg) was dried and soaked in EtOAc three times at room temperature to afford 126 g EtOAc extract after removing the solvent under vacuum. The EtOAc extract of *Aspergillus* sp. SK-28 was performed by UPLC-HRMS analysis (Figure S1). This extract was subjected to a silica gel (200–300 mesh) column chromatography using a petroleum ether (PE, 60–90 °C) and EtOAc gradient system (from 1:0 to 0:1) to give 10 fractions (F1 to F10). The fraction F3 was separated into two subfractions (F3a and F3b) by CC on silica gel eluting with a step gradient of PE–EtOAc (80:20 to 70:30, v/v). Compound **2** (9.8 mg) was purified from F3a by Sephadex LH-20 eluting with CH_2Cl_2–MeOH (1:1, v/v). F3b was submitted to silica gel CC (CH_2Cl_2–MeOH, 1:200, v/v) to yield **3** (11.5 mg) and **4** (20.8 mg). Fraction F6 was subjected to silica gel CC eluting with CH_2Cl_2 and MeOH (3:100, v/v) to yield two subfractions (F6a and F6b). Compound **1** (15.6 mg) was obtained from F6b by Sephadex LH-20 eluting with CH_2Cl_2–MeOH (1:1, v/v). The chiral resolution of **1** was performed on a chiral INA column (5 μm, 250 × 4.6mm) using CH_3CN–H_2O (90:10, v/v) as the eluent.

(±)-Asperginulin A (**1**): colorless needles; mp 160–162 °C; UV (MeOH) λ_{max} (log ε) 224 (4.42), 268 (2.02), and 353 (3.11) nm; IR (KBr) ν_{max} 3471, 3345, 2971, 1673, 1621, 1413, 1224, 998, 742 cm^{-1}; ^1H and ^{13}C NMR data, Table S1; HRESIMS *m*/*z* 695.3344 $[M + H]^+$ (calcd for $C_{42}H_{43}N_6O_4$, 695.3340).

(−)-Asperginulin A (**1a**): colorless needles; mp 156–158 °C; $[\alpha]_D^{25}$ −128.9 (*c* 0.5, MeOH); ECD (0.15 mM, MeOH) λ_{max} ($\Delta\varepsilon$) 211 (+37.89), 225 (+34.01), 267 (–33.26), and 382 (+38.45) nm.

(+)-Asperginulin A (**1b**): colorless needles; mp 155–157 °C; $[\alpha]_D^{25}$ +126.7 (*c* 0.5, MeOH); ECD (0.15 mM, MeOH) λ_{max} ($\Delta\varepsilon$) 211 (–43.20), 225 (–40.60), 267 (+34.56), and 382 (+38.45) nm.

UPLC-HRMS analysis. Analysis was performed by the ultraperformance liquid chromatography high-resolution mass spectrometry (UPLC-HRMS) system with an Acquity UPLC, diode array detector, and Synapt G2-Si (Waters) in the positive ion

mode. The LC column was a Waters Acquity UPLC BEH C_{18} column (1.7 μm, 2.1 × 100 mm). The mobile phase consisted of A (water with 0.05% formic acid) and B (CH_3CN with 0.05% formic acid) at a flow rate of 0.3 mL/min. The gradient elution started with 10% B for 1 min, and then it was increased linearly to 95% B in 18 min and held for 2 min.

X-ray crystallographic analysis for (±)-1, (−)-1a and (+)-1b. (±)-Asperginulin A (**1**) was obtained as colorless crystals from MeOH–CH_2Cl_2 (1:1, v/v) at room temperature, while (−)-asperginulin A (**1a**) and (+)-asperginulin A (**1b**) were obtained as colorless crystals from MeOH–CH_2Cl_2–H_2O (1:1:0.1, v/v/v) at 4 °C. Crystal X-ray diffraction data for **(±)-1**, **(−)-1a** and **(+)-1b** were collected on an Agilent Gemini Ultra diffractometer using graphite-monochromated Cu Kα radiation (λ = 1.54178 Å). Their structures were solved by direct methods (SHELXS-97), expanded using difference Fourier techniques, and refined by the program and full-matrix least-squares calculations. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were fixed at calculated positions. Crystallographic data of **(±)-1**, **(−)-1a** and **(+)-1b** have been deposited with the Cambridge Crystallographic Data Centre.

Crystal data of **(±)-1**: triclinic, 2($C_{42}H_{42}N_6O_4$), a = 14.6702(3) Å, b = 16.9058(3) Å, c = 19.4279(4) Å, α =80.2010(10)°, β = 78.740(2)°, γ =81.6490(10)°, V = 4625.27(16) Å^3, space group P-1, Z = 2, D_c = 1.328 g/cm^3, μ = 1.055 mm^{-1}, and F (000) = 1892.0. Independent reflections: 18516 (R_{int} = 0.0552). The final R_1 values were 0.0795, wR_2 = 0.2349 ($I > 2\sigma(I)$). The goodness of fit on F^2 was 1.047. CCDC number: 1952542.

Crystal data of **(−)-1a**: monoclinic, $C_{42}H_{42}N_6O_4 \cdot 4(CH_3OH) \cdot H_2O$, a = 23.9784(3) Å, b = 10.57450(10) Å, c = 17.7829(2) Å, α = γ =90°, β = 91.2630(10)°, V = 4507.93(9) Å^3, space group $C2$, Z = 4, D_c = 1.266 g/cm^3, μ = 0.732 mm^{-1}, and F (000) = 1840.0. Independent reflections: 8712 (R_{int} = 0.0499). The final R_1 values were 0.0438, wR_2 = 0.1152 ($I > 2\sigma(I)$). The goodness of fit on F^2 was 1.057. Flack parameter = −0.04(13). CCDC number: 1952543.

Crystal data of **(+)-1b**: monoclinic, 2($C_{42}H_{42}N_6O_4$)·2(CH_3OH), a = 24.0548(7) Å,

b = 10.5980(2) Å, c = 17.8698(4) Å, $\alpha = \gamma$ =90°, β = 90.958(2)°, V = 4554.96(19) Å^3, space group $C2$, Z = 2, D_c = 1.015 g/cm^3, μ = 0.543 mm^{-1}, and F (000) = 1472.0. Independent reflections: 6981 (R_{int} = 0.0579). The final R_1 values were 0.0626, wR_2 = 0.1553 ($I > 2\sigma(I)$). The goodness of fit on F^2 was 1.086. Flack parameter = 0.2(2). CCDC number: 1952544.

Antifouling assay and toxicity. The antifouling assay and toxicity were performed on barnacle *Balanus reticulatus* larvae. Adult barnacles were procured from aquaculture in Shenzhen Daya Bay, China. All of these barnacles were kept in an aquarium at 30 °C, where they were fed alga *Platymonas subcordiformis*. The barnacles were dried at room temperature overnight before being immersed in seawater, which lead to the release nauplii from the broods. These nauplii were cultured at 30 °C in 80% filtered (0.2 μm of pore filter) natural seawater, where they were fed alga *Platymonas subcordiformis* until they reached the cyprid stage within 5 days. The day that the newly transformed cyprids were collected was designated as day 0.

The test samples and compounds were dissolved in MeOH. 282.6 μg/mL of the mother liquor was prepared and the polystyrene Petri dishes (6 cm in diameter) were used as the test vessel for 3 parallels. 1 mL of the mother liquor was added and equably covered for each polystyrene Petri dish. After removing the solvent (MeOH) completely with volatilization, the 20 mL of membrane-filtered natural sea water was added for each polystyrene Petri dish. The test solution with final dose of 10 μg/cm^2 was prepared. As the control group, 1 mL of the MeOH was added and equably covered for the polystyrene Petri dish. As the blank group, only 20 mL of membrane-filtered natural sea water was added for the polystyrene Petri dish. About 30 larvae of the barnacle *Balanus reticulatus* were assed to each parallel group. The attachment and death of larvae of the barnacle *Balanus reticulatus* were observed in each group. Test dishes were incubated an aquarium (30 °C) for 120 h (5 days). The number of barnacles, as well as live and dead larvae, was assessed under a dissecting microscope at the end of the experiment.

Photochemical reaction of 4. Compound **4** (2.0 mg) was dissolved in MeOH

and EtOAc (2.0 mL), respectively. Then, these solutions and solid state of **4** were irradiated with sunlight or UV light (254 nm) at 50 °C for seven days (Table S3). After irradiation, the solvent was removed in vacuo, while the photolysis products were detected by UPLC-MS analysis (Figure S14).

Figure S1. Total ion chromatograms of the EtOAc extract of *Aspergillus* sp. SK-28 (A) and the extracted ions of **1**−**4** (B) and the UV absorptions of **1**−**4** (C).

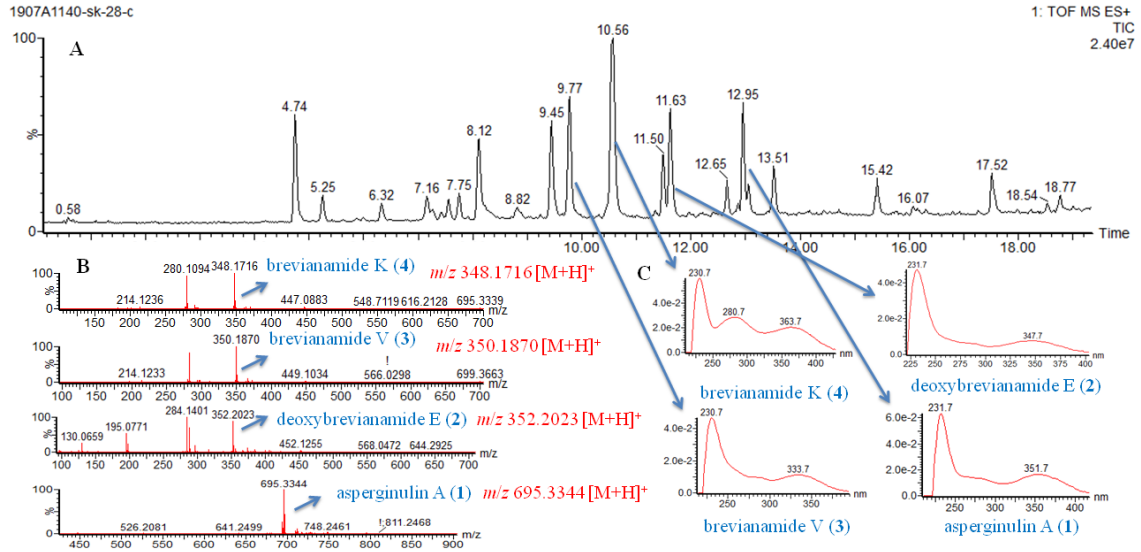
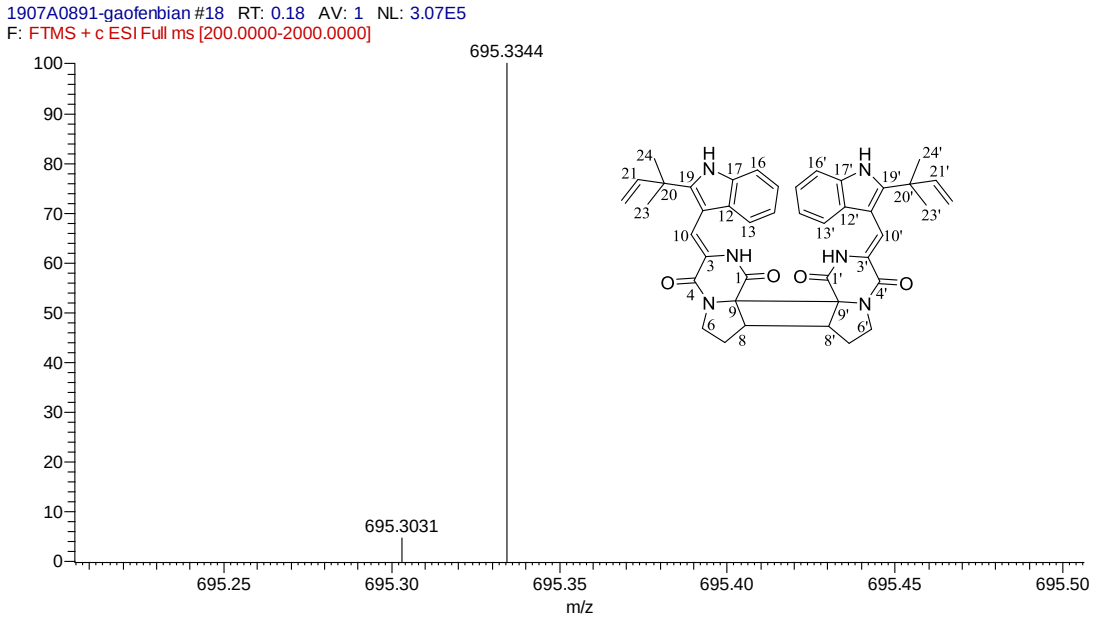


Figure S2. HRESIMS spectrum of **1**.



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
695.3344	695.3340	0.38	24.5	$C_{42}H_{43}N_6O_4$

Figure S3. ^{1}H NMR spectrum of **1** in DMSO-d_6.

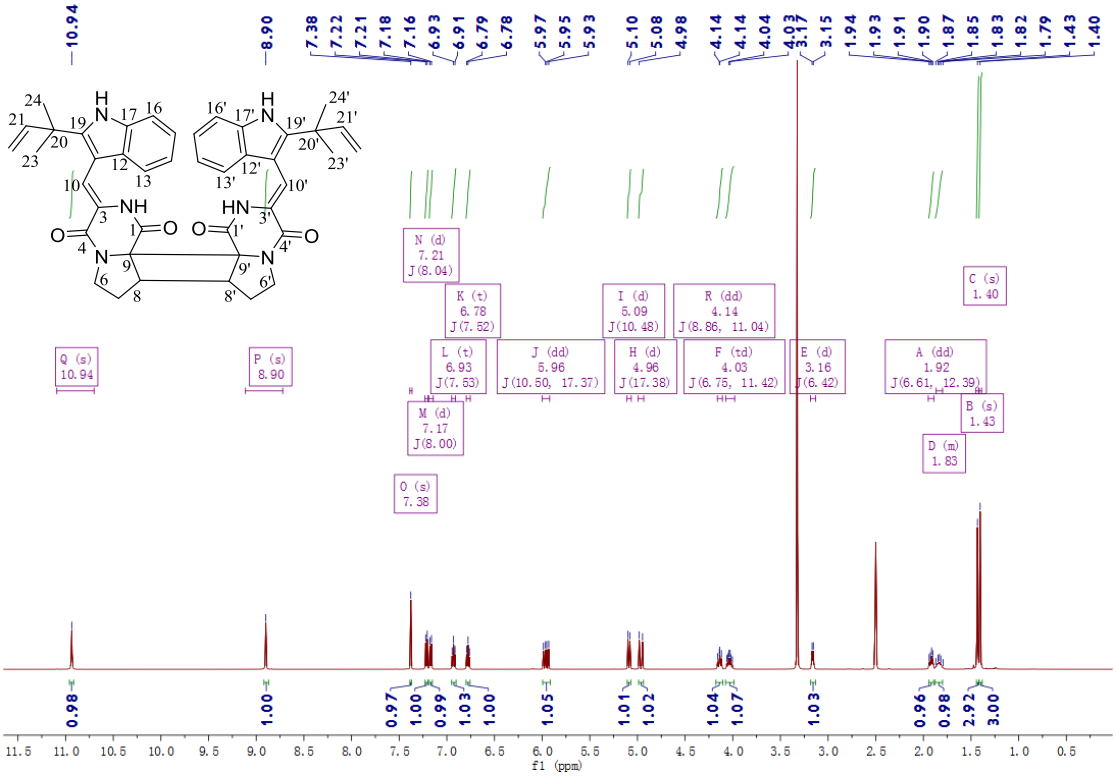


Figure S4. ^{13}C NMR spectrum of **1** in DMSO-d_6.

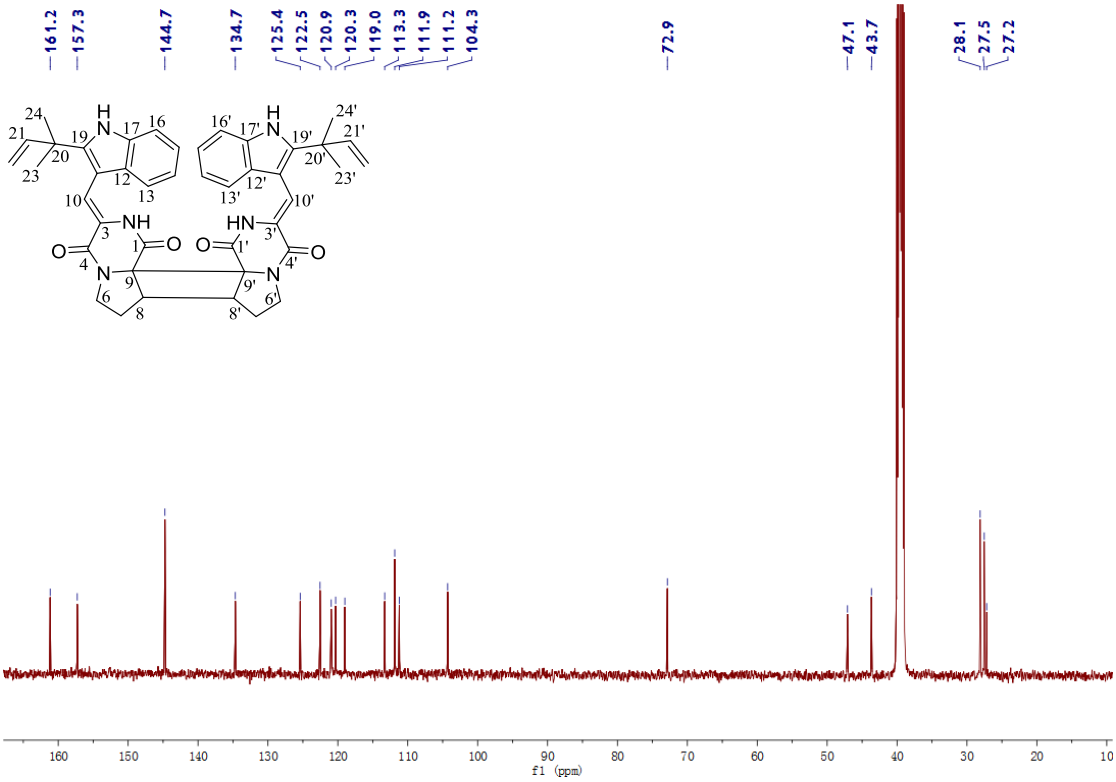


Figure S5. DEPT spectrum of **1** in DMSO-d_6.

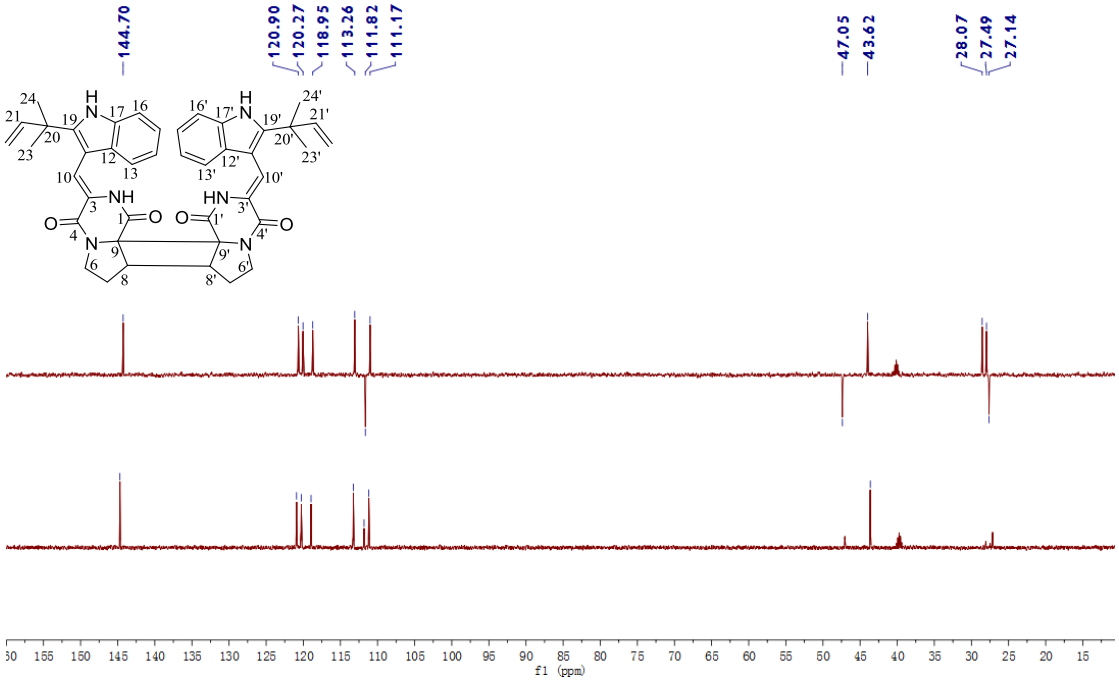


Figure S6. COSY spectrum of **1** in DMSO-d_6.

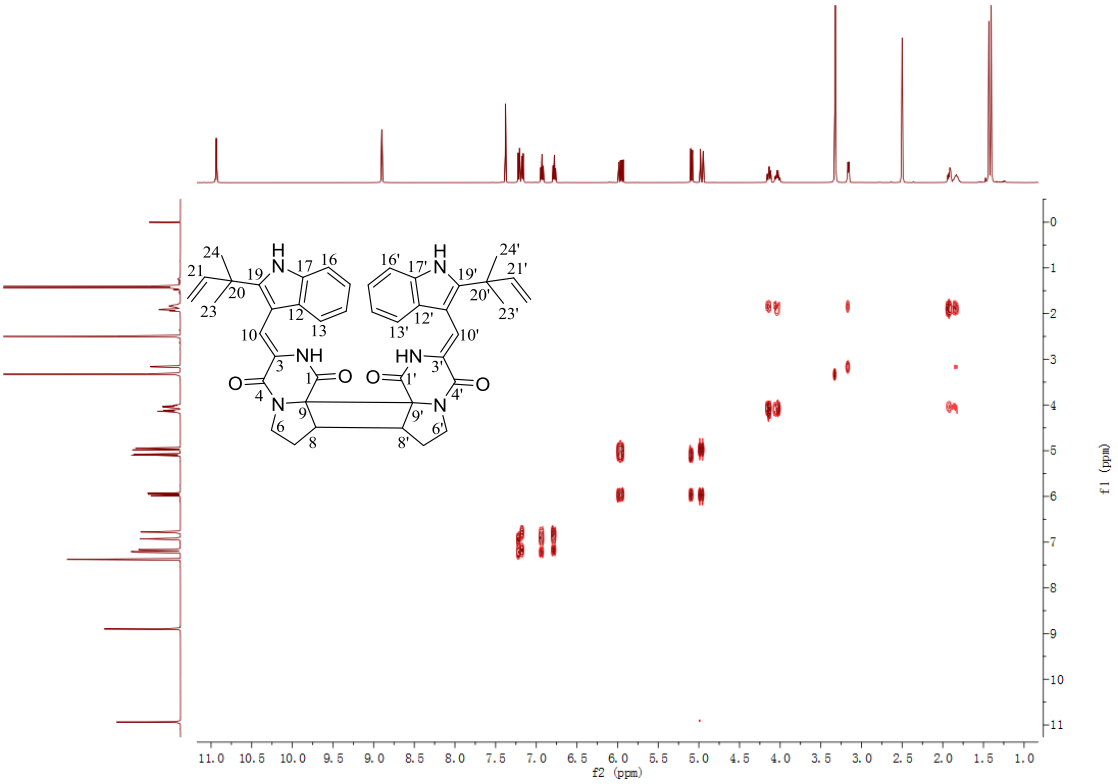


Figure S7. HSQC spectrum of **1** in DMSO-d_6.

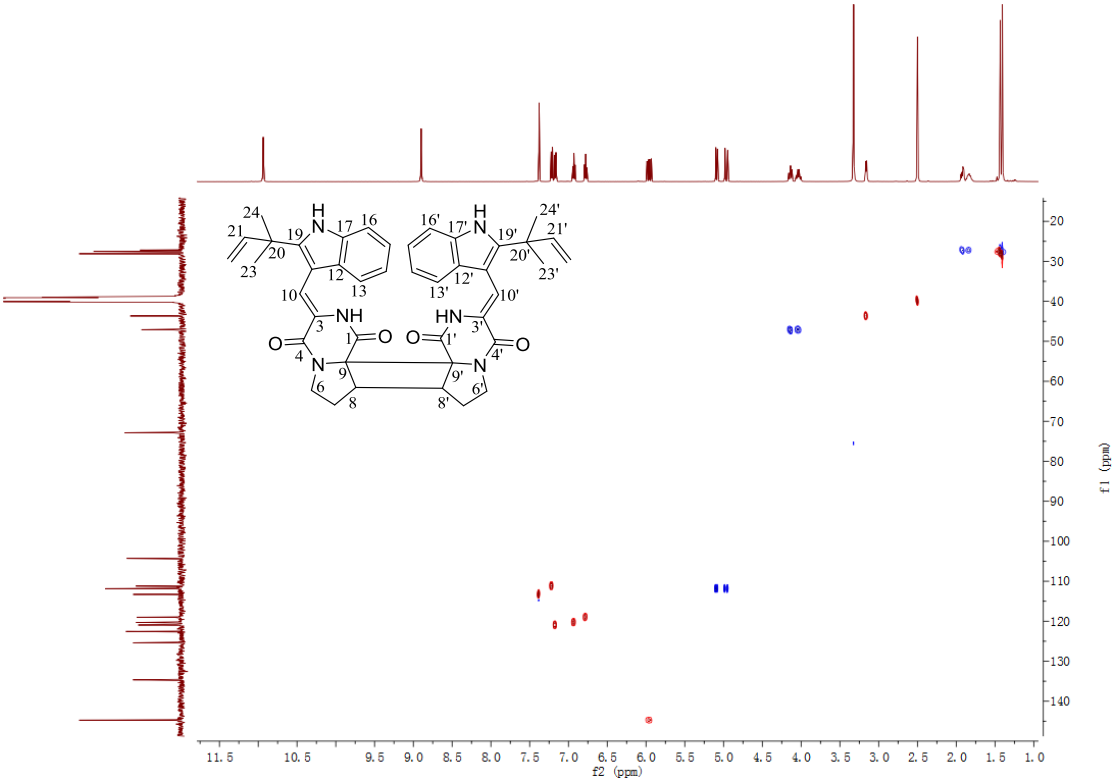


Figure S8. HMBC spectrum of **1** in DMSO-d_6.

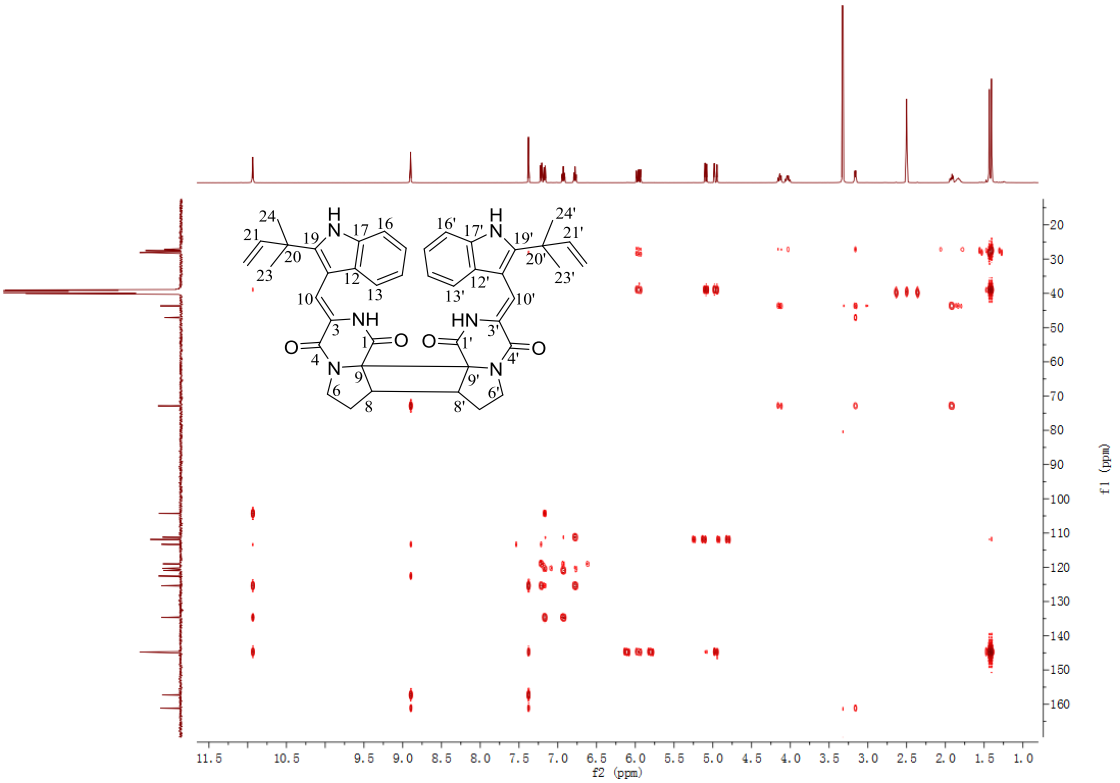


Figure S9. NOESY spectrum of **1** in DMSO-d_6.

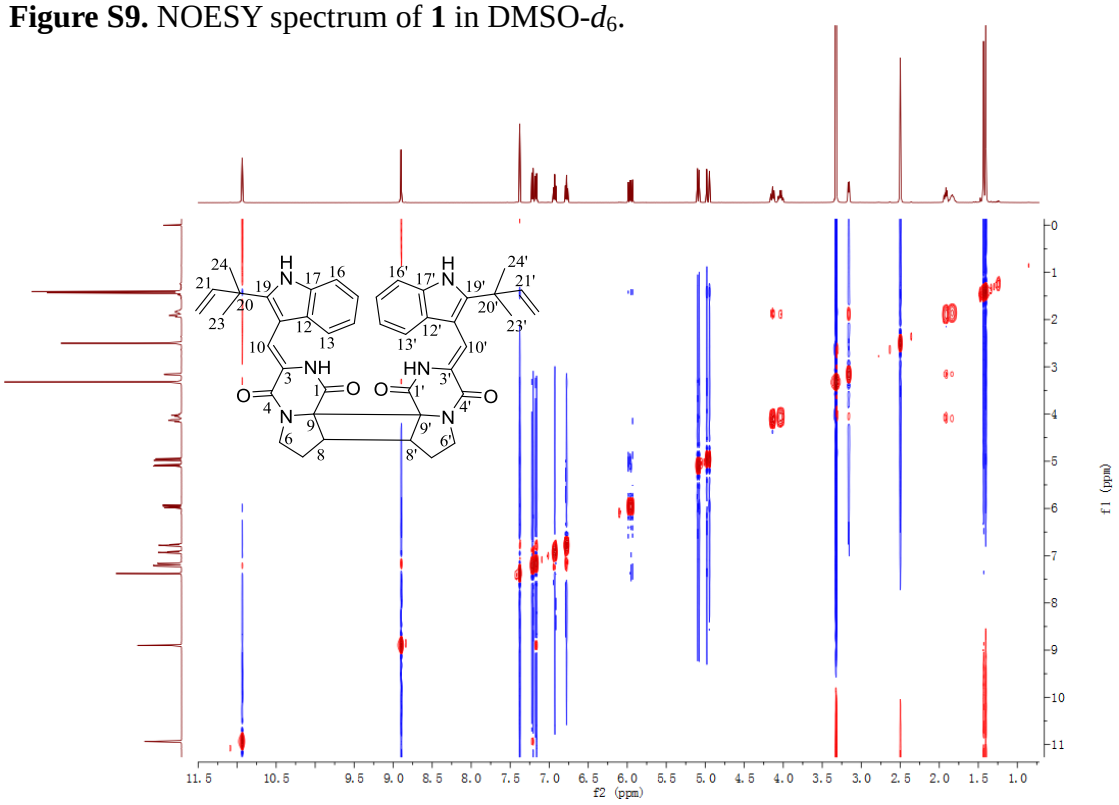


Figure S10. UV data of **1** in MeOH.

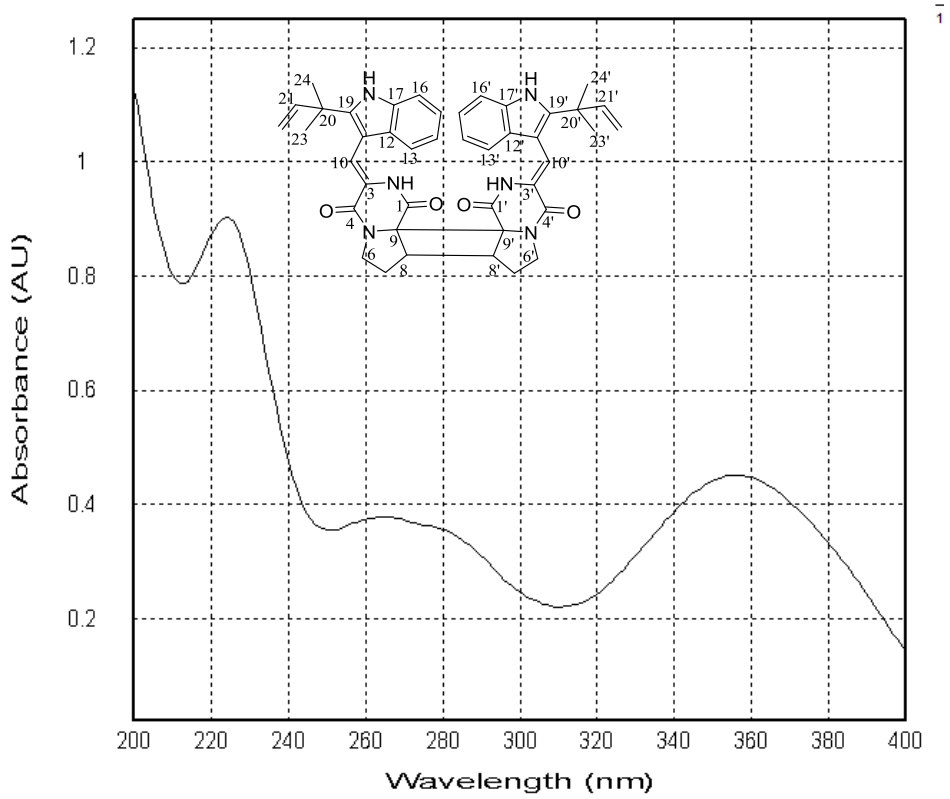


Figure S11. IR data of **1** in KBr.

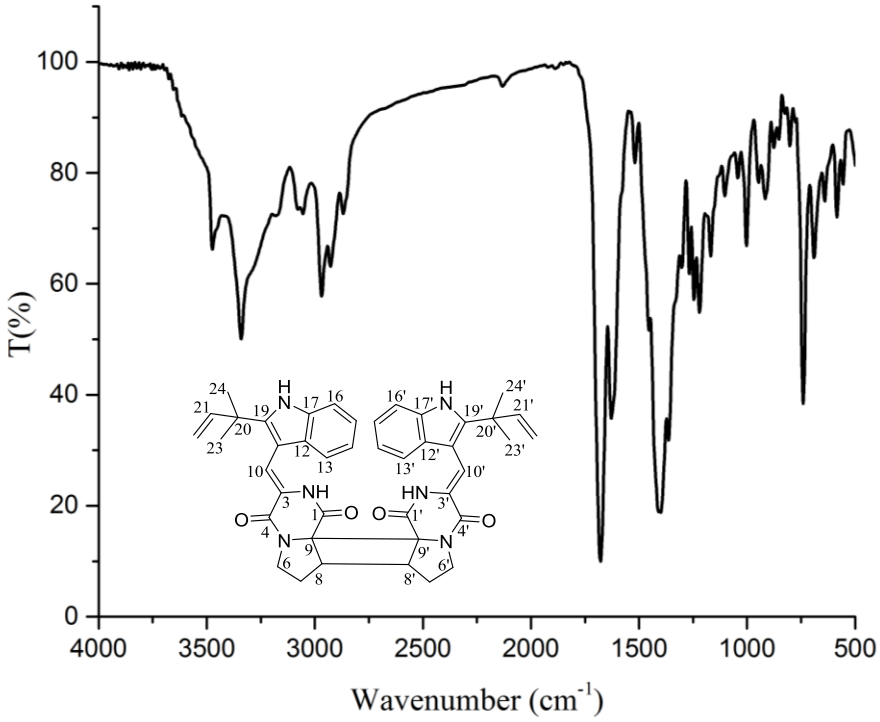


Figure S12. X-ray ORTEP drawing of (±)-asperginulin A (**1**).

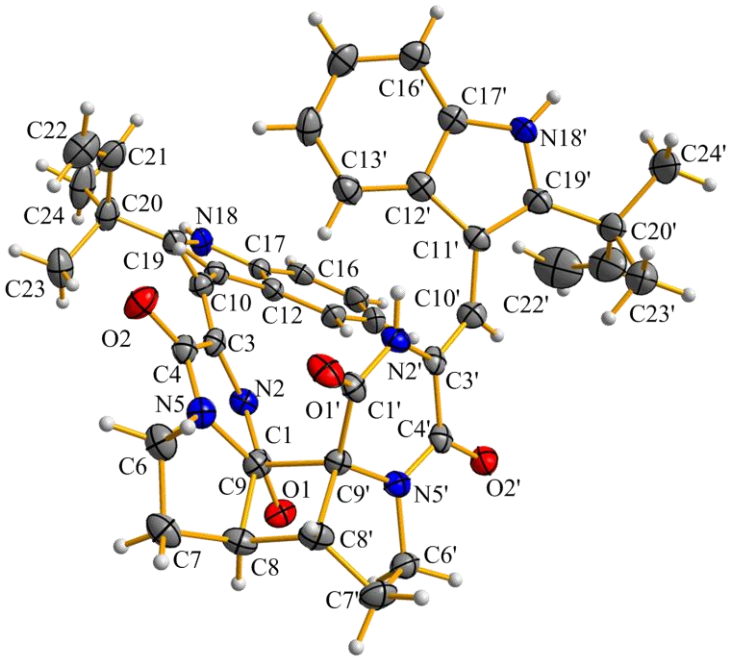
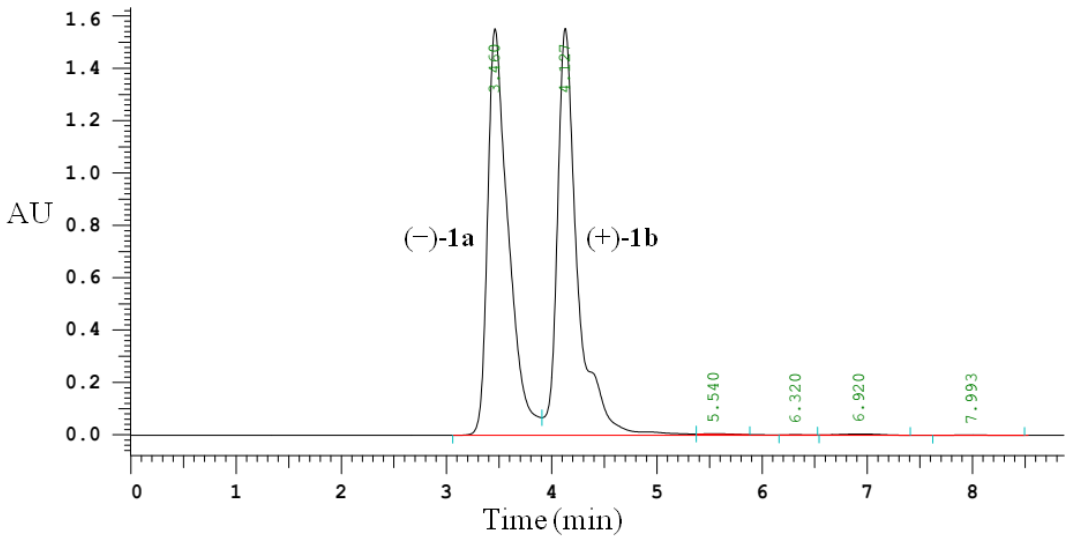


Figure S13. The chiral HPLC separation of (±)-asperginulin A (**1**).



No.	Time	Area	Concentration
1	3. 460	10615447	49. 997
2	4. 127	10535889	49. 622
3	5. 540	16878	0. 079
4	6. 320	3460	0. 016
5	6. 920	50276	0. 237
6	7. 993	10334	0. 049
		21232284	100. 000

Figure S14. UPLC-MS analyses of standard compounds (**1** and **4**) and photolysis products.

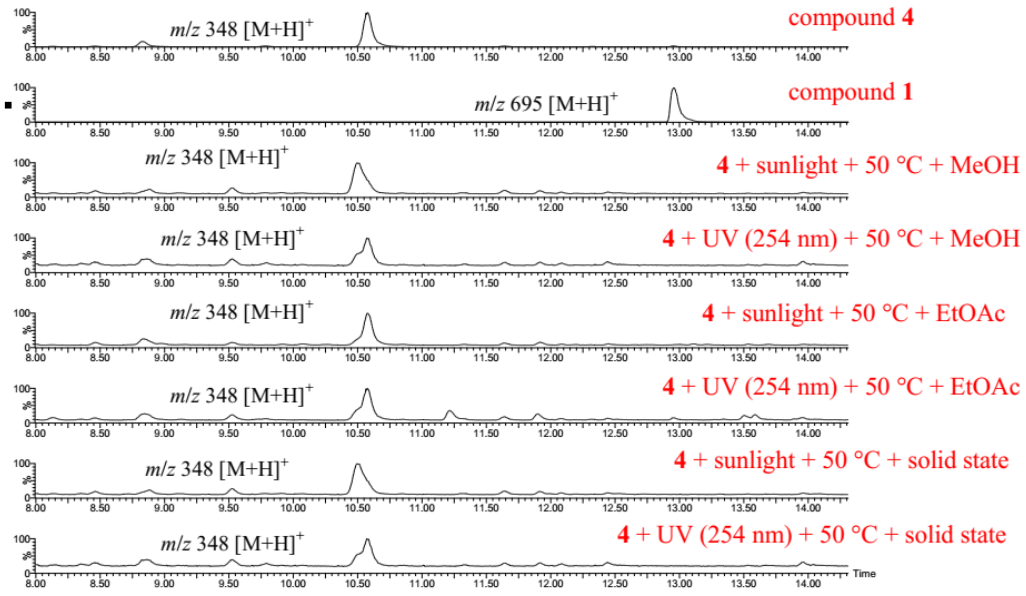


Table S1. ^{1}H (500 MHz) and ^{13}C NMR (125 MHz) Data of 1 in DMSO-d_6 (δ in ppm).

	1	
no	δ_C, type	δ_H, mult (J, Hz)
1/1'	161.2, C	
3/3'	122.5, C	
4/4'	157.3, C	
6/6'	47.1, CH_2	4.14, dd (11.4, 8.9)
		4.03, td (11.4, 6.8)
7/7'	27.2, CH_2	1.92, dd (12.4, 6.8)
		1.83, m
8/8'	43.7, CH	3.16, d (6.4)
9/9'	72.9, C	
10/10'	113.3, CH	7.38, s
11/11'	104.3, C	
12/12'	125.4, C	
13/13'	120.9, CH	7.17, d (8.0)
14/14'	119.0, CH	6.78, t (8.0)
15/15'	120.3, CH	6.93, t (8.0)
16/16'	111.2, CH	7.21, d (8.0)
17/17'	134.7, C	
19/19'	144.7, C	
20/20'	39.4, C	
21/21'	144.7, CH	5.96, dd (17.4, 10.5)
22/22'	111.9, CH_2	5.19, d (10.5)
		4.96, d (17.4)
23/23'	27.5, CH_3	1.43, s
24/24'	28.5, CH_3	1.40, s
2/2'-NH		8.90, s

18/18'-NH	10.94, s

Table S2. Effects of (−)-1a, (+)-1b, and 2−4 on the Settlement and Toxicity of *B. reticulatus* Presented as Percentages of Settled and Dead Larvae.

no.	adhesive rate (%)[a]	no.	survival rate (%)[a]
(−)-**1a**	77.2±0.5	(−)-**1a**	100
(+)-**1b**	48.4±0.6	(+)-**1b**	100
2	6.4±0.6	**2**	100
3	0	**3**	0
4	0	**4**	0
FSW[b]	78.8±0.6	**FSW**	100
MeOH[b]	81.0±0.7	**MeOH**	100

[a]The data represent the mean ± SD of three experiments. [b]Filtered seawater (FSW) and MeOH were used as the negative controls.

Table S3. Outcomes of the Photochemical Reactions of Compound 4 under a Range of Different Conditions

no	light source	solvent	time	temperature	products (compound **1**)
1	sunlight	MeOH	7 days	50 °C	not detected
2	UV (254 nm)	MeOH	7 days	50 °C	not detected
3	sunlight	EtOAc	7 days	50 °C	not detected
4	UV (254 nm)	EtOAc	7 days	50 °C	not detected
5	sunlight	solid state	7 days	50 °C	not detected
6	UV (254 nm)	solid state	7 days	50 °C	not detected

ECD calculation details

1.Method.

Conformational searches were carried out by means of the Spartan′14 software using Molecular Merck force field (MMFF). All density functional theory (DFT) and time-dependent (TD)-DFT calculations were performed with Gaussian 09 program.

Conformers within a 10 kcal/mol energy window were generated and optimized by DFT calculations at the B3LYP/6-31+G (d, p) level. Conformers with a Bolzmann distribution over 10% were chose for ECD calculations by TD-DFT method at the B3LYP/6-311+G (d, p) level. The polarizable continuum model for MeOH was used. The calculated ECD curves were generated using the SpecDis 3.0 (University of Würzburg) and Origin Pro 8.5 (Origin Lab, Ltd.) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.30 eV.

2. Results

2.1 Gibbs free energies and Boltzmann-population of low-energy conformers of 8*R*, 9*R*, 8'*R*, 9'*R*-**1**.

Conformers of 8*R*, 9*R*, 8'*R*, 9'*R*-**1**	In MeOH	
	ΔG^a	P (%)[b]
1a	0	32.2
1b	0.28	19.9
1c	0.28	19.9
1d	0.48	14.0
1e	0.48	14.0

[a]Δ*G*, B3LYP/ 6-31+G (d, p), in kcal/mol. [b]Boltzmann-population.

2.2 Gibbs free energies and Boltzmann-population of low-energy conformers of 8*S*, 9*S*, 8'*S*, 9'*S*-**1**.

Conformers of 8*S*, 9*S*, 8'*S*, 9'*S*-**1**	In MeOH	
	ΔG^a	P (%)[b]
1a	0	32.2
1b	0.28	19.9
1c	0.28	19.9
1d	0.48	14.0
1e	0.48	14.0

[a]Δ*G*, B3LYP/ 6-31+G (d, p), in kcal/mol. [b]Boltzmann-population.

2.3 Cartesian coordinates for the low-energy optimized conformers of 8*R*, 9*R*, 8'*R*, 9'*R*-**1** at B3LYP/6-31+G (d, p) level of theory in MeOH.

Conformer **1a**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	4.151461	-2.915923	-1.370034
2	6	0	4.283074	-1.970479	-0.369894

3	6	0	2.913074	-2.859567	-1.958636
4	6	0	2.191962	-1.869157	-1.298212
5	6	0	3.057976	-1.316487	-0.299336
6	6	0	2.735117	-0.295038	0.648902
7	6	0	2.243905	0.931959	0.392219
8	7	0	2.017710	1.385145	-0.889349
9	6	0	1.456919	2.595158	-1.225934
10	6	0	0.794363	3.368645	-0.027098
11	7	0	1.448155	3.052814	1.278879
12	6	0	2.079449	1.866187	1.572564
13	8	0	2.541201	1.605291	2.678170
14	8	0	1.486590	2.963600	-2.401329
15	6	0	0.769109	4.925492	-0.084613
16	6	0	1.606202	5.386212	1.114934
17	6	0	1.581078	4.235097	2.114935
18	6	0	2.383681	-3.618627	-3.008830
19	6	0	1.066359	-3.361062	-3.396775
20	6	0	0.310158	-2.385917	-2.754063
21	6	0	0.859167	-1.639246	-1.704726
22	6	0	5.598102	-1.860165	0.411928
23	6	0	5.428687	-2.625372	1.744228
24	6	0	5.939725	-0.389377	0.739469
25	6	0	6.790365	-2.372786	-0.411248
26	6	0	7.562329	-3.444586	-0.177398
27	6	0	-7.562671	-3.444451	0.177671
28	6	0	-6.790789	-2.372953	0.411441
29	6	0	-5.939095	-0.390055	-0.739458
30	6	0	-5.429619	-2.624759	-1.744060
31	6	0	-5.598450	-1.860025	-0.411851
32	6	0	-0.859395	-1.639623	1.704567
33	6	0	-0.310548	-2.385536	2.753373
34	6	0	-1.066229	-3.360340	3.397524
35	6	0	-2.383386	-3.618584	3.009142
36	6	0	-1.581057	4.235089	-2.114965
37	6	0	-1.606537	5.386923	-1.115412
38	6	0	-0.768765	4.925677	0.083703
39	8	0	-1.486750	2.964428	2.401773
40	8	0	-2.541395	1.604681	-2.678324
41	6	0	-2.078551	1.865629	-1.572406
42	7	0	-1.448538	3.052578	-1.279321
43	6	0	-0.794508	3.369488	0.027368
44	6	0	-1.456868	2.595303	1.226256
45	7	0	-2.017704	1.385436	0.889843

46	6	0	-2.242956	0.932177	-0.392281
47	6	0	-2.735222	-0.294645	-0.649160
48	6	0	-3.058181	-1.317016	0.299145
49	6	0	-2.191531	-1.868765	1.298250
50	6	0	-2.912888	-2.858844	1.958198
51	6	0	-4.283216	-1.970502	0.370492
52	7	0	-4.151197	-2.916522	1.369939
53	1	0	-1.112033	5.370983	1.024386
54	1	0	1.111169	5.371110	-1.024613
55	1	0	4.875190	-3.568402	-1.640825
56	1	0	2.947682	-0.551853	1.686159
57	1	0	2.337233	0.821758	-1.671066
58	1	0	2.639195	5.550971	0.784178
59	1	0	1.244330	6.322869	1.549661
60	1	0	2.485506	4.199586	2.729112
61	1	0	0.707834	4.290514	2.770118
62	1	0	2.967499	-4.386005	-3.506107
63	1	0	0.624853	-3.933824	-4.208879
64	1	0	-0.715523	-2.202721	-3.063649
65	1	0	0.251310	-0.889665	-1.212181
66	1	0	6.339664	-2.579991	2.352891
67	1	0	5.184272	-3.680920	1.574779
68	1	0	4.617409	-2.204704	2.348486
69	1	0	5.260324	0.039832	1.482737
70	1	0	5.896246	0.244026	-0.155112
71	1	0	6.948714	-0.300471	1.160555
72	1	0	7.024932	-1.774500	-1.293986
73	1	0	8.383630	-3.687356	-0.846322
74	1	0	7.413350	-4.100963	0.673307
75	1	0	-7.413064	-4.100658	-0.673029
76	1	0	-8.383438	-3.687413	0.845701
77	1	0	-7.024862	-1.774899	1.294353
78	1	0	-5.895888	0.244474	0.155350
79	1	0	-5.260761	0.039633	-1.482556
80	1	0	-6.948818	-0.299647	-1.160461
81	1	0	-5.183602	-3.680518	-1.575133
82	1	0	-6.339786	-2.580149	-2.352733
83	1	0	-4.616433	-2.204558	-2.348495
84	1	0	-0.251324	-0.889341	1.212388
85	1	0	0.715241	-2.202140	3.063412
86	1	0	-0.624317	-3.933232	4.209098
87	1	0	-2.968054	-4.386234	3.506284
88	1	0	-0.707006	4.290532	-2.770862

89	1	0	-2.485254	4.199269	-2.730001
90	1	0	-1.243619	6.323015	-1.550249
91	1	0	-2.639173	5.550417	-0.784342
92	1	0	-2.337442	0.821865	1.671275
93	1	0	-2.948294	-0.552656	-1.686091
94	1	0	-4.875291	-3.567140	1.640734

Conformer **1b**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	4.409498	-2.472959	-1.433699
2	6	0	4.456086	-1.508051	-0.444772
3	6	0	3.154530	-2.576511	-1.979617
4	6	0	2.338214	-1.676273	-1.301778
5	6	0	3.162030	-1.010014	-0.336195
6	6	0	2.745547	-0.027042	0.616056
7	6	0	2.101574	1.129223	0.366585
8	7	0	1.784983	1.539775	-0.910463
9	6	0	1.073882	2.670481	-1.237409
10	6	0	0.357025	3.368668	-0.024179
11	7	0	1.081279	3.146120	1.264795
12	6	0	1.858392	2.047250	1.546398
13	8	0	2.379539	1.854090	2.639686
14	8	0	1.027173	3.031246	-2.414828
15	6	0	0.139413	4.909665	-0.086720
16	6	0	0.948337	5.480260	1.084951
17	6	0	1.091616	4.342980	2.090482
18	6	0	2.688874	-3.405829	-3.007555
19	6	0	1.337229	-3.316109	-3.351012
20	6	0	0.488482	-2.436350	-2.687726
21	6	0	0.974859	-1.617526	-1.663851
22	6	0	5.771290	-1.227894	0.291883
23	6	0	5.742817	-1.994380	1.632655
24	6	0	5.937617	0.277168	0.599733
25	6	0	6.991270	-1.596739	-0.568549
26	6	0	7.897888	-2.560844	-0.355044
27	6	0	-6.137495	-0.520911	-1.596696
28	6	0	-5.877115	-1.173240	-0.454438
29	6	0	-5.036186	-3.309686	-1.619993
30	6	0	-6.412116	-3.382037	0.452474
31	6	0	-5.306998	-2.582898	-0.282095
32	6	0	-0.629375	-1.783934	1.808688
33	6	0	0.017160	-2.439211	2.862485

34	6	0	-0.607057	-3.486975	3.532062
35	6	0	-1.888188	-3.909193	3.166772
36	6	0	-2.165646	3.921887	-2.045062
37	6	0	-2.303423	5.069445	-1.049970
38	6	0	-1.381499	4.723645	0.126609
39	8	0	-1.789713	2.705446	2.470231
40	8	0	-2.797476	1.189410	-2.576806
41	6	0	-2.349554	1.512434	-1.481065
42	7	0	-1.866345	2.771762	-1.208437
43	6	0	-1.218874	3.174974	0.076692
44	6	0	-1.744897	2.334549	1.296362
45	7	0	-2.156645	1.060575	0.981015
46	6	0	-2.362437	0.573976	-0.292483
47	6	0	-2.706288	-0.706127	-0.529252
48	6	0	-2.867799	-1.755557	0.432080
49	6	0	-1.928258	-2.181866	1.424526
50	6	0	-2.518636	-3.239896	2.111061
51	6	0	-3.999016	-2.562187	0.521731
52	7	0	-3.750624	-3.455408	1.543744
53	1	0	-1.748917	5.131597	1.075614
54	1	0	0.396877	5.385851	-1.040233
55	1	0	5.198745	-3.032533	-1.725536
56	1	0	3.018533	-0.247692	1.647379
57	1	0	2.147877	1.011136	-1.697826
58	1	0	1.943892	5.765418	0.722368
59	1	0	0.486537	6.369504	1.523902
60	1	0	2.010387	4.422663	2.679232
61	1	0	0.236142	4.297112	2.770977
62	1	0	3.346466	-4.100256	-3.519182
63	1	0	0.943641	-3.947384	-4.144356
64	1	0	-0.562423	-2.384109	-2.963978
65	1	0	0.296633	-0.943425	-1.154255
66	1	0	6.660264	-1.830670	2.210281
67	1	0	5.626776	-3.074253	1.478423
68	1	0	4.905043	-1.673152	2.262579
69	1	0	5.235331	0.626026	1.363449
70	1	0	5.786601	0.891850	-0.296580
71	1	0	6.941137	0.495674	0.986002
72	1	0	7.119774	-0.982416	-1.462455
73	1	0	8.720181	-2.706207	-1.049527
74	1	0	7.859994	-3.222539	0.503578
75	1	0	-5.954474	-0.951730	-2.575483
76	1	0	-6.531724	0.490743	-1.575290

77	1	0	-6.079520	-0.644086	0.477196
78	1	0	-4.294734	-2.785537	-2.231492
79	1	0	-4.648301	-4.321168	-1.446777
80	1	0	-5.950827	-3.409132	-2.216385
81	1	0	-6.598264	-2.987101	1.458767
82	1	0	-7.361410	-3.344203	-0.096814
83	1	0	-6.147707	-4.441201	0.555738
84	1	0	-0.123977	-0.975136	1.295056
85	1	0	1.016780	-2.127932	3.155133
86	1	0	-0.089805	-3.986204	4.347489
87	1	0	-2.368377	-4.732270	3.686854
88	1	0	-1.324351	4.078999	-2.726338
89	1	0	-3.075640	3.771904	-2.632435
90	1	0	-2.071232	6.039909	-1.498061
91	1	0	-3.338395	5.108160	-0.688717
92	1	0	-2.386057	0.467843	1.772153
93	1	0	-2.930687	-0.989086	-1.556258
94	1	0	-4.381633	-4.181493	1.851904

Conformer **1c**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	-3.749997	-3.455569	1.543521
2	6	0	-3.998431	-2.562685	0.521287
3	6	0	-2.517450	-3.240174	2.110645
4	6	0	-1.928826	-2.181685	1.424484
5	6	0	-2.867332	-1.756301	0.432131
6	6	0	-2.706074	-0.706089	-0.529459
7	6	0	-2.362721	0.574142	-0.292207
8	7	0	-2.156941	1.060687	0.980112
9	6	0	-1.745575	2.334119	1.296874
10	6	0	-1.219013	3.174839	0.076925
11	7	0	-1.865993	2.772554	-1.207950
12	6	0	-2.349684	1.512199	-1.480541
13	8	0	-2.797466	1.189732	-2.576579
14	8	0	-1.789862	2.705787	2.470489
15	6	0	-1.382066	4.723355	0.126224
16	6	0	-2.303457	5.069636	-1.049865
17	6	0	-2.165949	3.921627	-2.044848
18	6	0	-1.887748	-3.909497	3.167309
19	6	0	-0.606422	-3.486434	3.531569
20	6	0	0.017468	-2.439846	2.862280
21	6	0	-0.629995	-1.784279	1.809269

22	6	0	-5.306233	-2.583337	-0.281749
23	6	0	-6.411789	-3.382126	0.451882
24	6	0	-5.035490	-3.310428	-1.619379
25	6	0	-5.876940	-1.174279	-0.455152
26	6	0	-6.137520	-0.522116	-1.597027
27	6	0	7.897957	-2.560795	-0.355243
28	6	0	6.991196	-1.595488	-0.569065
29	6	0	5.938214	0.277656	0.599060
30	6	0	5.743099	-1.994463	1.633050
31	6	0	5.771491	-1.227559	0.291237
32	6	0	0.974752	-1.617392	-1.663166
33	6	0	0.489066	-2.435909	-2.688494
34	6	0	1.337877	-3.316600	-3.351054
35	6	0	2.688854	-3.405483	-3.007371
36	6	0	1.090873	4.343019	2.090708
37	6	0	0.947576	5.480121	1.083990
38	6	0	0.138878	4.909989	-0.087291
39	8	0	1.027365	3.031399	-2.414364
40	8	0	2.379432	1.853580	2.639712
41	6	0	1.857967	2.046633	1.546336
42	7	0	1.080642	3.146553	1.265324
43	6	0	0.356419	3.369339	-0.024094
44	6	0	1.072915	2.670502	-1.236763
45	7	0	1.785029	1.539228	-0.910436
46	6	0	2.101232	1.129280	0.366878
47	6	0	2.745918	-0.026379	0.616552
48	6	0	3.161593	-1.010194	-0.336271
49	6	0	2.338474	-1.676030	-1.301024
50	6	0	3.155017	-2.575755	-1.980270
51	6	0	4.456060	-1.507598	-0.444056
52	7	0	4.409018	-2.472482	-1.433478
53	1	0	0.396158	5.385880	-1.040616
54	1	0	-1.748734	5.130968	1.075023
55	1	0	-4.381314	-4.181187	1.851793
56	1	0	-2.930959	-0.989288	-1.556526
57	1	0	-2.386167	0.467971	1.772534
58	1	0	-3.339534	5.107971	-0.688761
59	1	0	-2.071217	6.040086	-1.498566
60	1	0	-3.076130	3.770984	-2.632474
61	1	0	-1.324665	4.078554	-2.726159
62	1	0	-2.367976	-4.732022	3.686484
63	1	0	-0.089055	-3.986328	4.347186
64	1	0	1.017221	-2.127177	3.155245

65	1	0	-0.123864	-0.974664	1.295420
66	1	0	-7.360803	-3.344441	-0.096632
67	1	0	-6.597461	-2.987956	1.458351
68	1	0	-6.148127	-4.441392	0.555303
69	1	0	-4.648792	-4.321734	-1.446446
70	1	0	-4.293610	-2.785763	-2.231690
71	1	0	-5.950693	-3.409600	-2.216091
72	1	0	-6.079735	-0.644512	0.476616
73	1	0	-6.532285	0.490201	-1.574871
74	1	0	-5.954309	-0.951818	-2.575703
75	1	0	7.860556	-3.222582	0.503920
76	1	0	8.719972	-2.705439	-1.049571
77	1	0	7.119548	-0.981895	-1.462609
78	1	0	5.786051	0.891769	-0.296389
79	1	0	5.235296	0.625687	1.362644
80	1	0	6.941326	0.496051	0.985881
81	1	0	5.626836	-3.073984	1.478786
82	1	0	6.660913	-1.830956	2.210417
83	1	0	4.904874	-1.672086	2.261939
84	1	0	0.295773	-0.943452	-1.154647
85	1	0	-0.561923	-2.383854	-2.963642
86	1	0	0.943156	-3.947564	-4.144092
87	1	0	3.347189	-4.100065	-3.519605
88	1	0	0.235709	4.297327	2.770264
89	1	0	2.009568	4.423046	2.678293
90	1	0	0.486441	6.369349	1.523919
91	1	0	1.942945	5.765717	0.722045
92	1	0	2.147196	1.010963	-1.698152
93	1	0	3.018034	-0.247322	1.647729
94	1	0	5.199475	-3.031428	-1.726066

Conformer **1d**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	-4.377724	-2.638568	1.380907
2	6	0	-4.405973	-1.745817	0.325945
3	6	0	-3.191955	-2.571208	2.067645
4	6	0	-2.396123	-1.629587	1.419514
5	6	0	-3.164703	-1.116515	0.323044
6	6	0	-2.747843	-0.155361	-0.652538
7	6	0	-2.205441	1.056980	-0.431571
8	7	0	-2.014641	1.564338	0.836152
9	6	0	-1.376309	2.745861	1.138222

10	6	0	-0.601173	3.395951	-0.066276
11	7	0	-1.236252	3.075870	-1.379348
12	6	0	-1.935630	1.922039	-1.645704
13	8	0	-2.375906	1.642213	-2.755909
14	8	0	-1.431488	3.180062	2.289430
15	6	0	-0.436480	4.944188	-0.076961
16	6	0	-1.180665	5.420023	-1.332152
17	6	0	-1.235578	4.220839	-2.273079
18	6	0	-2.767988	-3.282111	3.197909
19	6	0	-1.484090	-3.025843	3.683585
20	6	0	-0.656239	-2.099954	3.058199
21	6	0	-1.097517	-1.402763	1.927344
22	6	0	-5.652071	-1.654537	-0.565132
23	6	0	-5.390746	-2.485553	-1.841584
24	6	0	-5.940067	-0.196357	-0.986801
25	6	0	-6.916463	-2.109890	0.181488
26	6	0	-7.684617	-3.181451	-0.063523
27	6	0	7.594992	-3.386554	-0.403065
28	6	0	6.452686	-3.211459	0.277019
29	6	0	6.241925	-0.723984	-0.312793
30	6	0	5.467258	-1.645656	1.876021
31	6	0	5.584051	-1.947490	0.366859
32	6	0	0.702959	-1.984958	-1.407098
33	6	0	0.125655	-2.750843	-2.425440
34	6	0	0.886464	-3.681682	-3.126189
35	6	0	2.237956	-3.872942	-2.830459
36	6	0	1.755887	4.113206	2.085364
37	6	0	1.923468	5.225219	1.053723
38	6	0	1.100695	4.799502	-0.168789
39	8	0	1.707164	2.705511	-2.397636
40	8	0	2.465471	1.431613	2.763873
41	6	0	2.079400	1.696745	1.629845
42	7	0	1.554823	2.919589	1.279336
43	6	0	0.981639	3.249256	-0.060706
44	6	0	1.615079	2.382538	-1.212170
45	7	0	2.075356	1.147896	-0.819621
46	6	0	2.233894	0.723018	0.482058
47	6	0	2.651650	-0.520421	0.784388
48	6	0	2.964432	-1.563173	-0.142862
49	6	0	2.065327	-2.157239	-1.085148
50	6	0	2.794523	-3.097473	-1.806105
51	6	0	4.211398	-2.161394	-0.285398
52	7	0	4.076257	-3.075179	-1.314659

53	1	0	1.525068	5.178259	-1.105473
54	1	0	-0.777598	5.463464	0.826129
55	1	0	-5.134826	-3.262175	1.625026
56	1	0	-2.920709	-0.450527	-1.686215
57	1	0	-2.409871	1.068210	1.628504
58	1	0	-2.202897	5.700797	-1.050767
59	1	0	-0.712415	6.292784	-1.795954
60	1	0	-2.123894	4.235684	-2.912889
61	1	0	-0.344914	4.164474	-2.905273
62	1	0	-3.409578	-4.011294	3.682243
63	1	0	-1.125513	-3.561703	4.559918
64	1	0	0.342719	-1.915727	3.446223
65	1	0	-0.432747	-0.690873	1.452891
66	1	0	-6.248997	-2.458163	-2.522779
67	1	0	-5.178475	-3.534768	-1.603223
68	1	0	-4.525552	-2.106625	-2.397981
69	1	0	-5.196608	0.188374	-1.692554
70	1	0	-5.956668	0.478365	-0.122577
71	1	0	-6.911136	-0.113300	-1.492343
72	1	0	-7.211758	-1.465006	1.011107
73	1	0	-8.562326	-3.379587	0.546871
74	1	0	-7.479029	-3.881429	-0.865552
75	1	0	8.051887	-2.602364	-0.997359
76	1	0	8.112748	-4.341259	-0.371324
77	1	0	6.077593	-4.062615	0.847713
78	1	0	6.363321	-0.877278	-1.392363
79	1	0	5.629913	0.177384	-0.187227
80	1	0	7.227954	-0.508600	0.113534
81	1	0	4.829885	-2.377973	2.387381
82	1	0	6.450083	-1.663695	2.363031
83	1	0	5.053829	-0.649164	2.066142
84	1	0	0.096917	-1.264580	-0.871604
85	1	0	-0.926192	-2.616813	-2.667775
86	1	0	0.421929	-4.268827	-3.915618
87	1	0	2.828854	-4.599505	-3.377887
88	1	0	0.865496	4.266374	2.700730
89	1	0	2.627852	4.021119	2.738861
90	1	0	1.626186	6.202510	1.444690
91	1	0	2.979559	5.288824	0.765915
92	1	0	2.371625	0.535000	-1.573789
93	1	0	2.793919	-0.776574	1.832656
94	1	0	4.825716	-3.652905	-1.668244

Conformer **1e**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	4.075477	-3.075243	-1.314832
2	6	0	4.211635	-2.160993	-0.285054
3	6	0	2.795399	-3.097546	-1.805558
4	6	0	2.065298	-2.157486	-1.085623
5	6	0	2.964958	-1.562527	-0.142760
6	6	0	2.651371	-0.520665	0.784559
7	6	0	2.233312	0.723517	0.482050
8	7	0	2.075434	1.147541	-0.819506
9	6	0	1.614891	2.382618	-1.212375
10	6	0	0.982048	3.249232	-0.061031
11	7	0	1.555261	2.919348	1.279262
12	6	0	2.079194	1.696889	1.629934
13	8	0	2.465448	1.431211	2.764457
14	8	0	1.707711	2.706377	-2.397732
15	6	0	1.100956	4.798973	-0.168301
16	6	0	1.922722	5.225137	1.054473
17	6	0	1.756005	4.113500	2.085378
18	6	0	2.238404	-3.872388	-2.829844
19	6	0	0.886484	-3.681489	-3.126424
20	6	0	0.125765	-2.750668	-2.424961
21	6	0	0.702497	-1.984695	-1.407733
22	6	0	5.583583	-1.947192	0.366465
23	6	0	5.466308	-1.645655	1.875691
24	6	0	6.241548	-0.724426	-0.313067
25	6	0	6.452945	-3.211505	0.277328
26	6	0	7.595429	-3.386572	-0.402843
27	6	0	-7.684356	-3.181918	-0.063342
28	6	0	-6.916458	-2.109813	0.181155
29	6	0	-5.939539	-0.196935	-0.987634
30	6	0	-5.390036	-2.485788	-1.840973
31	6	0	-5.651336	-1.654668	-0.565548
32	6	0	-1.097841	-1.402404	1.927948
33	6	0	-0.656724	-2.099847	3.057215
34	6	0	-1.484233	-3.025316	3.683078
35	6	0	-2.768096	-3.281754	3.197271
36	6	0	-1.235664	4.221177	-2.272944
37	6	0	-1.181227	5.419312	-1.331651
38	6	0	-0.436623	4.944248	-0.077899
39	8	0	-1.431744	3.179605	2.289402
40	8	0	-2.376504	1.641873	-2.756167
41	6	0	-1.935792	1.921697	-1.646157

42	7	0	-1.236366	3.075371	-1.379954
43	6	0	-0.601544	3.396136	-0.065924
44	6	0	-1.376057	2.745785	1.137586
45	7	0	-2.014558	1.564510	0.836277
46	6	0	-2.205445	1.056398	-0.430963
47	6	0	-2.747560	-0.154954	-0.651785
48	6	0	-3.164701	-1.116971	0.322670
49	6	0	-2.396505	-1.629922	1.420378
50	6	0	-3.191525	-2.570754	2.067418
51	6	0	-4.406012	-1.745234	0.326713
52	7	0	-4.376972	-2.638734	1.381281
53	1	0	-0.777738	5.463822	0.826131
54	1	0	1.524534	5.178865	-1.105259
55	1	0	4.825912	-3.653348	-1.668051
56	1	0	2.793684	-0.776655	1.832869
57	1	0	2.371223	0.535730	-1.573576
58	1	0	2.979013	5.288877	0.765343
59	1	0	1.625474	6.203235	1.444673
60	1	0	2.628144	4.020449	2.739278
61	1	0	0.865396	4.266489	2.700366
62	1	0	2.829033	-4.598856	-3.377770
63	1	0	0.421649	-4.269364	-3.915263
64	1	0	-0.926011	-2.616644	-2.667103
65	1	0	0.096669	-1.264845	-0.871040
66	1	0	6.449805	-1.663051	2.362817
67	1	0	4.830563	-2.377019	2.387828
68	1	0	5.054490	-0.649626	2.065375
69	1	0	5.630371	0.178147	-0.186975
70	1	0	6.363280	-0.877258	-1.392121
71	1	0	7.228037	-0.508496	0.112823
72	1	0	6.077998	-4.062722	0.847722
73	1	0	8.113120	-4.340997	-0.370992
74	1	0	8.052045	-2.601648	-0.997497
75	1	0	-7.478704	-3.881500	-0.865668
76	1	0	-8.562545	-3.379555	0.546926
77	1	0	-7.211754	-1.465181	1.011544
78	1	0	-5.956430	0.478374	-0.122577
79	1	0	-5.196954	0.187560	-1.692335
80	1	0	-6.910298	-0.113344	-1.492277
81	1	0	-5.178738	-3.535126	-1.602747
82	1	0	-6.248724	-2.457898	-2.523018
83	1	0	-4.525240	-2.107202	-2.397837
84	1	0	-0.432462	-0.690330	1.452780

85	1	0	0.342915	-1.915495	3.446350
86	1	0	-1.125834	-3.560915	4.559601
87	1	0	-3.409235	-4.011775	3.681730
88	1	0	-0.345259	4.164623	-2.905398
89	1	0	-2.123786	4.235439	-2.912918
90	1	0	-0.712482	6.291913	-1.796123
91	1	0	-2.203508	5.700565	-1.051638
92	1	0	-2.410274	1.068018	1.628149
93	1	0	-2.921205	-0.450720	-1.687076
94	1	0	-5.134253	-3.261811	1.624073

2.4 Cartesian coordinates for the low-energy optimized conformers of 8*S*, 9*S*, 8'*S*, 9'*S*-**1** at B3LYP/6-31+G (d, p) level of theory in MeOH.

Conformer **1a**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	-4.151108	-2.915795	-1.370012
2	6	0	-4.283246	-1.970880	-0.370030
3	6	0	-2.913212	-2.859164	-1.958130
4	6	0	-2.191506	-1.868999	-1.298055
5	6	0	-3.057514	-1.316314	-0.298954
6	6	0	-2.735512	-0.295320	0.649161
7	6	0	-2.243317	0.931820	0.392886
8	7	0	-2.018128	1.385652	-0.889462
9	6	0	-1.456954	2.595197	-1.225721
10	6	0	-0.794657	3.369092	-0.026945
11	7	0	-1.448148	3.052416	1.279472
12	6	0	-2.078821	1.865531	1.572714
13	8	0	-2.540734	1.604680	2.679409
14	8	0	-1.487313	2.964393	-2.401426
15	6	0	-0.768936	4.926029	-0.083797
16	6	0	-1.606111	5.386099	1.115426
17	6	0	-1.580499	4.234986	2.114706
18	6	0	-2.383460	-3.618357	-3.008819
19	6	0	-1.066052	-3.360070	-3.396864
20	6	0	-0.310388	-2.385780	-2.753871
21	6	0	-0.859003	-1.639699	-1.705487
22	6	0	-5.597718	-1.860611	0.412033
23	6	0	-5.939741	-0.390087	0.739208
24	6	0	-5.428766	-2.625205	1.743380
25	6	0	-6.790354	-2.372731	-0.411454
26	6	0	-7.561783	-3.444115	-0.177779

27	6	0	7.561824	-3.444682	0.177151
28	6	0	6.790469	-2.372825	0.411114
29	6	0	5.428780	-2.624895	-1.743742
30	6	0	5.938958	-0.389803	-0.738993
31	6	0	5.597771	-1.859921	-0.412322
32	6	0	0.859215	-1.639920	1.705290
33	6	0	0.310632	-2.385753	2.753167
34	6	0	1.066540	-3.360476	3.396943
35	6	0	2.383505	-3.618976	3.008862
36	6	0	1.580870	4.235531	-2.114681
37	6	0	1.605915	5.386793	-1.115239
38	6	0	0.769165	4.925892	0.083899
39	8	0	1.487059	2.963885	2.401442
40	8	0	2.540726	1.605471	-2.678707
41	6	0	2.078684	1.865917	-1.572559
42	7	0	1.448332	3.053588	-1.279204
43	6	0	0.794824	3.368720	0.027094
44	6	0	1.456145	2.595021	1.226230
45	7	0	2.018170	1.385787	0.889731
46	6	0	2.243313	0.932383	-0.392354
47	6	0	2.735366	-0.295168	-0.649490
48	6	0	3.057414	-1.316379	0.299221
49	6	0	2.191613	-1.869668	1.298100
50	6	0	2.913130	-2.859459	1.958466
51	6	0	4.283187	-1.970925	0.370271
52	7	0	4.151552	-2.916216	1.369351
53	1	0	1.110863	5.371633	1.024899
54	1	0	-1.111348	5.370881	-1.024393
55	1	0	-4.874740	-3.567729	-1.641143
56	1	0	-2.948202	-0.552921	1.686229
57	1	0	-2.337904	0.821973	-1.671827
58	1	0	-1.244317	6.322312	1.550028
59	1	0	-2.639793	5.550732	0.784559
60	1	0	-0.707563	4.290658	2.771112
61	1	0	-2.484757	4.199957	2.729978
62	1	0	-2.967403	-4.386312	-3.505773
63	1	0	-0.624607	-3.933874	-4.208992
64	1	0	0.715308	-2.202671	-3.063851
65	1	0	-0.251134	-0.889233	-1.212859
66	1	0	-6.948599	-0.300741	1.160321
67	1	0	-5.895759	0.244277	-0.155396
68	1	0	-5.260502	0.039765	1.482664
69	1	0	-4.616729	-2.204530	2.347816

70	1	0	-5.183925	-3.680960	1.574973
71	1	0	-6.340006	-2.580147	2.352005
72	1	0	-7.025228	-1.775024	-1.294145
73	1	0	-8.383875	-3.687836	-0.846129
74	1	0	-7.413474	-4.101279	0.672967
75	1	0	7.413137	-4.101029	-0.672939
76	1	0	8.383905	-3.686803	0.845956
77	1	0	7.024949	-1.774948	1.294320
78	1	0	5.184330	-3.680620	-1.575707
79	1	0	4.616497	-2.204732	-2.348842
80	1	0	6.339866	-2.579527	-2.352650
81	1	0	5.895359	0.243848	0.154691
82	1	0	5.260551	0.039775	-1.482734
83	1	0	6.949309	-0.299898	-1.161105
84	1	0	0.251305	-0.888996	1.212712
85	1	0	-0.715013	-2.202441	3.063531
86	1	0	0.624702	-3.934450	4.208578
87	1	0	2.967805	-4.386481	3.506093
88	1	0	2.485406	4.199653	-2.729769
89	1	0	0.707056	4.290480	-2.770560
90	1	0	2.639436	5.550361	-0.784368
91	1	0	1.243561	6.322901	-1.549993
92	1	0	2.337677	0.821206	1.671502
93	1	0	2.947822	-0.552154	-1.686936
94	1	0	4.874829	-3.567502	1.640106

Conformer **1b**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	-4.409648	-2.472161	-1.433425
2	6	0	-4.455425	-1.507820	-0.444871
3	6	0	-3.155145	-2.575228	-1.980221
4	6	0	-2.338211	-1.676426	-1.301555
5	6	0	-3.161948	-1.010783	-0.336247
6	6	0	-2.746018	-0.026419	0.616782
7	6	0	-2.101344	1.129232	0.366519
8	7	0	-1.785495	1.539977	-0.910432
9	6	0	-1.073648	2.670378	-1.237063
10	6	0	-0.355936	3.368697	-0.024012
11	7	0	-1.080924	3.146272	1.265332
12	6	0	-1.857897	2.046510	1.546050
13	8	0	-2.380528	1.854072	2.639815
14	8	0	-1.027171	3.030746	-2.414361

15	6	0	-0.138618	4.909869	-0.087543
16	6	0	-0.947760	5.480440	1.084342
17	6	0	-1.091392	4.342448	2.090572
18	6	0	-2.688759	-3.405544	-3.007015
19	6	0	-1.337491	-3.315624	-3.351449
20	6	0	-0.488472	-2.435929	-2.687832
21	6	0	-0.974735	-1.617178	-1.663083
22	6	0	-5.771454	-1.228194	0.291205
23	6	0	-5.938092	0.277107	0.599596
24	6	0	-5.742696	-1.994156	1.632932
25	6	0	-6.990802	-1.595740	-0.569538
26	6	0	-7.897538	-2.560668	-0.355381
27	6	0	6.137770	-0.521420	-1.596862
28	6	0	5.876622	-1.173460	-0.455240
29	6	0	6.411944	-3.382622	0.451577
30	6	0	5.035665	-3.309507	-1.619986
31	6	0	5.306374	-2.582673	-0.282209
32	6	0	0.629455	-1.784534	1.808513
33	6	0	-0.017136	-2.440033	2.862228
34	6	0	0.607016	-3.486725	3.532161
35	6	0	1.886880	-3.909776	3.166542
36	6	0	2.165783	3.922206	-2.044731
37	6	0	2.303992	5.069299	-1.049571
38	6	0	1.381867	4.723243	0.126877
39	8	0	1.790348	2.705393	2.470323
40	8	0	2.797453	1.190267	-2.576282
41	6	0	2.349475	1.512301	-1.481361
42	7	0	1.866204	2.772454	-1.207872
43	6	0	1.218277	3.175385	0.077153
44	6	0	1.745211	2.334702	1.297193
45	7	0	2.156774	1.060395	0.981153
46	6	0	2.362847	0.573412	-0.292842
47	6	0	2.706777	-0.706570	-0.528716
48	6	0	2.867501	-1.755882	0.431992
49	6	0	1.928272	-2.182421	1.424440
50	6	0	2.517779	-3.239929	2.110857
51	6	0	3.998437	-2.562954	0.521817
52	7	0	3.750914	-3.455954	1.544037
53	1	0	1.749178	5.131402	1.075550
54	1	0	-0.396873	5.386436	-1.039813
55	1	0	-5.198961	-3.031354	-1.725527
56	1	0	-3.018576	-0.247283	1.647537
57	1	0	-2.147322	1.010990	-1.698523

58	1	0	-0.486700	6.368899	1.524413
59	1	0	-1.942832	5.765229	0.722431
60	1	0	-0.236571	4.296875	2.770935
61	1	0	-2.009885	4.423207	2.679576
62	1	0	-3.346876	-4.099623	-3.519551
63	1	0	-0.942799	-3.947185	-4.144265
64	1	0	0.562536	-2.384285	-2.963927
65	1	0	-0.296259	-0.942697	-1.154954
66	1	0	-6.941551	0.495743	0.985298
67	1	0	-5.786502	0.891942	-0.296584
68	1	0	-5.235743	0.626189	1.362844
69	1	0	-4.905896	-1.672182	2.261739
70	1	0	-5.626438	-3.073795	1.477938
71	1	0	-6.660459	-1.830627	2.209837
72	1	0	-7.119773	-0.982000	-1.462190
73	1	0	-8.720293	-2.706276	-1.050118
74	1	0	-7.860311	-3.221898	0.503898
75	1	0	5.954158	-0.951703	-2.576053
76	1	0	6.532096	0.490945	-1.575662
77	1	0	6.080047	-0.644592	0.477041
78	1	0	6.597855	-2.987831	1.458535
79	1	0	6.147510	-4.441561	0.555000
80	1	0	7.360829	-3.344219	-0.097401
81	1	0	4.648427	-4.321963	-1.446480
82	1	0	5.950467	-3.409331	-2.215911
83	1	0	4.293900	-2.785999	-2.231597
84	1	0	0.124252	-0.975579	1.295126
85	1	0	-1.016994	-2.127392	3.154662
86	1	0	0.088970	-3.987278	4.347249
87	1	0	2.368176	-4.732023	3.686237
88	1	0	3.076276	3.771649	-2.631679
89	1	0	1.325256	4.079470	-2.725985
90	1	0	3.338936	5.108681	-0.688889
91	1	0	2.071251	6.040068	-1.497885
92	1	0	2.386126	0.468097	1.772476
93	1	0	2.930744	-0.988730	-1.556938
94	1	0	4.380489	-4.181202	1.851972

Conformer **1c**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	3.749948	-3.455790	1.543565
2	6	0	3.998856	-2.562206	0.521608

3	6	0	2.518272	-3.239612	2.110421
4	6	0	1.928444	-2.181441	1.424236
5	6	0	2.868063	-1.756187	0.431609
6	6	0	2.706459	-0.706039	-0.528950
7	6	0	2.363369	0.573814	-0.292304
8	7	0	2.156874	1.060068	0.980601
9	6	0	1.744952	2.334026	1.296980
10	6	0	1.218725	3.175741	0.077063
11	7	0	1.866737	2.771900	-1.208643
12	6	0	2.349574	1.512387	-1.480656
13	8	0	2.797121	1.190128	-2.576698
14	8	0	1.790681	2.704876	2.470677
15	6	0	1.382452	4.723197	0.126067
16	6	0	2.304350	5.068855	-1.049820
17	6	0	2.165770	3.921465	-2.044702
18	6	0	1.887331	-3.910017	3.166935
19	6	0	0.606475	-3.487022	3.532105
20	6	0	-0.017715	-2.439249	2.862080
21	6	0	0.629626	-1.784303	1.809451
22	6	0	5.305993	-2.583158	-0.281750
23	6	0	5.035992	-3.310134	-1.620014
24	6	0	6.411846	-3.382669	0.451528
25	6	0	5.876698	-1.173955	-0.454784
26	6	0	6.137685	-0.521794	-1.596498
27	6	0	-7.897607	-2.559734	-0.355186
28	6	0	-6.991315	-1.595632	-0.569187
29	6	0	-5.743618	-1.994009	1.632802
30	6	0	-5.937409	0.277137	0.599560
31	6	0	-5.772169	-1.226983	0.291553
32	6	0	-0.975680	-1.617539	-1.663004
33	6	0	-0.489302	-2.435749	-2.688368
34	6	0	-1.337785	-3.315964	-3.351586
35	6	0	-2.688770	-3.405102	-3.007460
36	6	0	-1.090411	4.342968	2.090733
37	6	0	-0.946956	5.480127	1.083892
38	6	0	-0.138371	4.910475	-0.087128
39	8	0	-1.027331	3.031220	-2.414234
40	8	0	-2.380074	1.853779	2.640328
41	6	0	-1.858663	2.046812	1.545912
42	7	0	-1.080476	3.146277	1.264814
43	6	0	-0.356305	3.368684	-0.023742
44	6	0	-1.073156	2.670366	-1.237098
45	7	0	-1.785286	1.539436	-0.910357

46	6	0	-2.101124	1.129174	0.367529
47	6	0	-2.746038	-0.027135	0.616349
48	6	0	-3.161856	-1.009923	-0.335511
49	6	0	-2.339113	-1.676059	-1.301512
50	6	0	-3.155073	-2.575818	-1.980553
51	6	0	-4.455690	-1.508260	-0.444725
52	7	0	-4.409526	-2.472351	-1.433477
53	1	0	-0.395995	5.385946	-1.039958
54	1	0	1.749207	5.130711	1.075279
55	1	0	4.380697	-4.181937	1.852201
56	1	0	2.930408	-0.989470	-1.555960
57	1	0	2.385591	0.467327	1.772068
58	1	0	2.071113	6.039594	-1.498769
59	1	0	3.339045	5.108346	-0.689416
60	1	0	1.325673	4.078884	-2.725998
61	1	0	3.076585	3.770784	-2.632548
62	1	0	2.368561	-4.732275	3.686760
63	1	0	0.089414	-3.986726	4.347174
64	1	0	-1.016776	-2.126893	3.155001
65	1	0	0.123775	-0.975234	1.295001
66	1	0	5.950305	-3.409626	-2.216368
67	1	0	4.294073	-2.786307	-2.231782
68	1	0	4.648637	-4.322136	-1.446646
69	1	0	6.148053	-4.442056	0.555159
70	1	0	6.597413	-2.988154	1.458530
71	1	0	7.361559	-3.344989	-0.096701
72	1	0	6.079700	-0.644434	0.476289
73	1	0	6.532207	0.490558	-1.575262
74	1	0	5.954206	-0.951394	-2.575847
75	1	0	-7.860583	-3.221098	0.503704
76	1	0	-8.720556	-2.705306	-1.049872
77	1	0	-7.119944	-0.981596	-1.462408
78	1	0	-5.626816	-3.073806	1.478435
79	1	0	-4.906076	-1.672190	2.262149
80	1	0	-6.660622	-1.830306	2.210297
81	1	0	-5.786795	0.892552	-0.296784
82	1	0	-5.235749	0.626848	1.362933
83	1	0	-6.941394	0.496594	0.985598
84	1	0	-0.296110	-0.942707	-1.154469
85	1	0	0.561750	-2.383920	-2.963752
86	1	0	-0.943928	-3.947315	-4.143734
87	1	0	-3.347789	-4.099738	-3.519384
88	1	0	-2.009278	4.423677	2.678934

89	1	0	-0.236274	4.296884	2.770181
90	1	0	-1.943081	5.765627	0.722541
91	1	0	-0.485960	6.368814	1.524559
92	1	0	-2.148070	1.011194	-1.697996
93	1	0	-3.018885	-0.246904	1.647524
94	1	0	-5.199218	-3.031845	-1.726030

Conformer **1d**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	4.377092	-2.638310	1.380732
2	6	0	4.406130	-1.745288	0.326160
3	6	0	3.191687	-2.571124	2.068001
4	6	0	2.396834	-1.629440	1.420246
5	6	0	3.165231	-1.116719	0.323251
6	6	0	2.748090	-0.155323	-0.652177
7	6	0	2.204804	1.056406	-0.431003
8	7	0	2.014373	1.564763	0.835830
9	6	0	1.376677	2.745441	1.137847
10	6	0	0.601619	3.396313	-0.066249
11	7	0	1.235551	3.074992	-1.379287
12	6	0	1.935811	1.921537	-1.646224
13	8	0	2.376086	1.641801	-2.756361
14	8	0	1.430700	3.180154	2.289311
15	6	0	0.436663	4.944725	-0.076927
16	6	0	1.180327	5.419343	-1.331625
17	6	0	1.236297	4.220749	-2.273604
18	6	0	2.768931	-3.281571	3.197894
19	6	0	1.483873	-3.025624	3.684055
20	6	0	0.656475	-2.099447	3.057686
21	6	0	1.098124	-1.403037	1.927569
22	6	0	5.651687	-1.655001	-0.565277
23	6	0	5.940025	-0.196251	-0.987524
24	6	0	5.390142	-2.485731	-1.841474
25	6	0	6.916834	-2.109527	0.181266
26	6	0	7.684614	-3.180941	-0.063059
27	6	0	-7.595409	-3.386533	-0.403341
28	6	0	-6.453443	-3.211353	0.276755
29	6	0	-5.466517	-1.645040	1.875616
30	6	0	-6.241453	-0.724749	-0.313020
31	6	0	-5.584191	-1.947250	0.366606
32	6	0	-0.702407	-1.985112	-1.406788
33	6	0	-0.125330	-2.750734	-2.425348

34	6	0	-0.886025	-3.681096	-3.126919
35	6	0	-2.237563	-3.873020	-2.830015
36	6	0	-1.756009	4.113416	2.085091
37	6	0	-1.923495	5.225137	1.054626
38	6	0	-1.100592	4.799657	-0.168600
39	8	0	-1.707113	2.706328	-2.398143
40	8	0	-2.466285	1.430894	2.763870
41	6	0	-2.078844	1.696831	1.629803
42	7	0	-1.555077	2.919387	1.279435
43	6	0	-0.982367	3.249489	-0.061186
44	6	0	-1.614754	2.383332	-1.212503
45	7	0	-2.074945	1.147848	-0.819511
46	6	0	-2.234012	0.723178	0.481894
47	6	0	-2.650930	-0.520874	0.785036
48	6	0	-2.964409	-1.563304	-0.142863
49	6	0	-2.065812	-2.157713	-1.084989
50	6	0	-2.795391	-3.097388	-1.806233
51	6	0	-4.211401	-2.161262	-0.284731
52	7	0	-4.076184	-3.075312	-1.314545
53	1	0	-1.525028	5.178385	-1.105584
54	1	0	0.776932	5.463422	0.826022
55	1	0	5.134624	-3.261977	1.624260
56	1	0	2.920719	-0.450700	-1.686751
57	1	0	2.409690	1.067727	1.627993
58	1	0	0.711931	6.292162	-1.795881
59	1	0	2.203310	5.700600	-1.051088
60	1	0	0.345478	4.164179	-2.904805
61	1	0	2.123852	4.235783	-2.912917
62	1	0	3.409086	-4.011441	3.682232
63	1	0	1.125640	-3.561511	4.559761
64	1	0	-0.342430	-1.915522	3.446492
65	1	0	0.432659	-0.690584	1.453481
66	1	0	6.910664	-0.112871	-1.491907
67	1	0	5.955946	0.478455	-0.122706
68	1	0	5.196823	0.187931	-1.692705
69	1	0	4.525108	-2.107257	-2.398176
70	1	0	5.177941	-3.535484	-1.603167
71	1	0	6.249001	-2.457923	-2.522815
72	1	0	7.211562	-1.465447	1.011749
73	1	0	8.561953	-3.379409	0.546374
74	1	0	7.479142	-3.881244	-0.864882
75	1	0	-8.051703	-2.601708	-0.997661
76	1	0	-8.112854	-4.341486	-0.371887

77	1	0	-6.077697	-4.063117	0.848005
78	1	0	-4.829798	-2.377768	2.387487
79	1	0	-5.054298	-0.650110	2.065998
80	1	0	-6.449774	-1.664060	2.363277
81	1	0	-6.362716	-0.877747	-1.391436
82	1	0	-5.630580	0.177318	-0.186879
83	1	0	-7.228563	-0.508313	0.113613
84	1	0	-0.096825	-1.264297	-0.870809
85	1	0	0.926044	-2.617033	-2.667336
86	1	0	-0.421824	-4.269268	-3.915373
87	1	0	-2.829200	-4.599591	-3.378218
88	1	0	-2.628706	4.020330	2.739004
89	1	0	-0.866137	4.266773	2.701052
90	1	0	-2.979477	5.289087	0.765819
91	1	0	-1.626006	6.202229	1.444364
92	1	0	-2.371482	0.534799	-1.573157
93	1	0	-2.793362	-0.777246	1.832928
94	1	0	-4.825545	-3.653667	-1.668081

Conformer **1e**		Standard Orientation (Ångstroms)			
Center Number	Atom	Type	X	Y	Z
1	7	0	-4.075666	-3.075498	-1.314777
2	6	0	-4.211122	-2.161186	-0.284864
3	6	0	-2.794869	-3.096507	-1.806239
4	6	0	-2.065126	-2.156347	-1.085655
5	6	0	-2.964892	-1.562175	-0.143037
6	6	0	-2.651180	-0.521039	0.784273
7	6	0	-2.233765	0.723836	0.481901
8	7	0	-2.075243	1.147982	-0.819297
9	6	0	-1.614661	2.382681	-1.212410
10	6	0	-0.981448	3.249999	-0.061481
11	7	0	-1.554400	2.919900	1.280000
12	6	0	-2.078806	1.696295	1.629969
13	8	0	-2.465307	1.431324	2.764156
14	8	0	-1.707780	2.705468	-2.397897
15	6	0	-1.100748	4.798843	-0.168402
16	6	0	-1.923172	5.224703	1.054035
17	6	0	-1.756169	4.113258	2.085551
18	6	0	-2.238438	-3.872134	-2.830840
19	6	0	-0.886197	-3.681178	-3.126988
20	6	0	-0.125177	-2.750427	-2.426584
21	6	0	-0.702834	-1.984496	-1.408260

22	6	0	-5.583672	-1.947327	0.367097
23	6	0	-6.241672	-0.725086	-0.312400
24	6	0	-5.466966	-1.645210	1.875902
25	6	0	-6.452043	-3.211900	0.277765
26	6	0	-7.594770	-3.387770	-0.401926
27	6	0	7.684332	-3.181429	-0.062856
28	6	0	6.916331	-2.110226	0.181879
29	6	0	5.389896	-2.486486	-1.841409
30	6	0	5.939770	-0.197673	-0.987994
31	6	0	5.651470	-1.654616	-0.565221
32	6	0	1.098094	-1.402508	1.927792
33	6	0	0.656104	-2.099052	3.057661
34	6	0	1.484063	-3.025054	3.684219
35	6	0	2.767957	-3.281198	3.197918
36	6	0	1.235649	4.220556	-2.273413
37	6	0	1.180165	5.419315	-1.332052
38	6	0	0.436792	4.944306	-0.078083
39	8	0	1.431674	3.180225	2.289354
40	8	0	2.376001	1.641661	-2.756354
41	6	0	1.935530	1.921911	-1.645988
42	7	0	1.235499	3.075221	-1.379427
43	6	0	0.601616	3.396255	-0.065793
44	6	0	1.376328	2.745425	1.138067
45	7	0	2.014635	1.564392	0.835345
46	6	0	2.205303	1.056400	-0.431638
47	6	0	2.747528	-0.155560	-0.652258
48	6	0	3.165168	-1.117061	0.322838
49	6	0	2.396452	-1.629203	1.420692
50	6	0	3.191118	-2.569976	2.067948
51	6	0	4.405832	-1.745849	0.327080
52	7	0	4.376769	-2.638016	1.381762
53	1	0	0.777179	5.463406	0.825980
54	1	0	-1.524653	5.178488	-1.104726
55	1	0	-4.825124	-3.653541	-1.668482
56	1	0	-2.793303	-0.777155	1.832887
57	1	0	-2.371440	0.535555	-1.574087
58	1	0	-1.625410	6.202982	1.445133
59	1	0	-2.979429	5.289054	0.765456
60	1	0	-0.864721	4.266297	2.700744
61	1	0	-2.627692	4.020212	2.738963
62	1	0	-2.829346	-4.599192	-3.378652
63	1	0	-0.422175	-4.268304	-3.916837
64	1	0	0.926081	-2.616289	-2.667646

65	1	0	-0.096765	-1.264162	-0.872021
66	1	0	-7.229026	-0.509636	0.113387
67	1	0	-6.362955	-0.878250	-1.392232
68	1	0	-5.630700	0.177616	-0.187890
69	1	0	-5.054607	-0.648506	2.065453
70	1	0	-4.829530	-2.377320	2.387427
71	1	0	-6.449541	-1.663514	2.362431
72	1	0	-6.075968	-4.063130	0.849010
73	1	0	-8.112444	-4.342621	-0.370102
74	1	0	-8.051795	-2.603082	-0.996503
75	1	0	7.478592	-3.881989	-0.865348
76	1	0	8.561619	-3.379967	0.547226
77	1	0	7.211605	-1.464604	1.011491
78	1	0	5.178017	-3.536034	-1.602273
79	1	0	4.525475	-2.107553	-2.397715
80	1	0	6.248259	-2.458822	-2.522645
81	1	0	5.956002	0.478074	-0.123502
82	1	0	5.196470	0.187163	-1.693125
83	1	0	6.910678	-0.114270	-1.492630
84	1	0	0.432507	-0.690593	1.452813
85	1	0	-0.342964	-1.914897	3.446186
86	1	0	1.125739	-3.560479	4.560414
87	1	0	3.409010	-4.011169	3.682437
88	1	0	2.122920	4.235445	-2.913502
89	1	0	0.344628	4.164561	-2.905193
90	1	0	2.202976	5.700626	-1.051761
91	1	0	0.711833	6.292387	-1.796804
92	1	0	2.410560	1.067873	1.628179
93	1	0	2.920854	-0.451254	-1.687065
94	1	0	5.134104	-3.261347	1.625029