Supporting Information

Cytochathiazines A–C: Three Merocytochalasans with a 2*H*-1,4-Thiazine Functionality from Coculture of *Chaetomium globosum* and *Aspergillus flavipes*

Wenjing Wang, Fanrong Zeng, Qiong Bie, Chong Dai,Chunmei Chen, Qingyi Tong, Junjun Liu, Jianping Wang, Yuan Zhou, Hucheng Zhu,* Yonghui Zhang*

Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, People's Republic of China.

Content

Table S1. Natural Products containing thiazine rings.

Origins		Compounds (Figure S1)	References
Fungi (3 compounds)	*Cephalosporium acremonium*	**1, 2**	*Tetrahedron Lett*. **1988**, *29*, 2101–2102
	Paraphaeosphaeria neglecta	**3**	*Org. Lett.* **2015**, *17*, 3556–3559
***Streptomyces* sp. (10 compounds)**	*Streptomyces* sp. MJ672-m3	**4**–**8**	*J. Antibiot.* **1995**, *48*, 471–478
	Streptomyces sp.	**9**, **10**	*J. Antibiot.* **2000**, *53*, 724–727
	Streptomyces hygroscopicus 17997	**11**	*Biosci. Biotechnol. Biochem.* **2011**, *75*, 2042–2045
	Streptomyces hygroscopicus	**12**, **13**	*J. Microbiol. Biotechnol.* **2012**, *22*, 1478–1481
marine organisms (16 compounds)	*Aplidium conicum*	**14**, **15**	*Eur. J. Org. Chem.***2010**, *2003*, 898–900
	Aplidium sp.	**16**, **17**	*J. Nat. Prod.* **2007,** *70,* 936–940
	Adocia sp.	**18**–**20**	*J. Org. Chem.* **1988**, *53*, 3922–3925
	Plakortis lita	**21**–**24**	*J. Org. Chem.* **2013**, *78*, 9608–9613
	Neamphius huxleyi	**25**	*Tetrahedron Lett.* **1991**, *32*, 2707–2710
	Aplidium conicum	**26**, **27**	*J. Med. Chem.* **2005,** *48*, 3410–3416
	Codakia orbicularis	**28**	*J. Nat. Prod.* **2017**, *80,* 1693–1696
	Actinomycetospora chlora	**29**	*J. Nat. Prod.* **2015**, *78*, 548–551
Plants (7 compounds)	*Xanthium strumarium*	**30**	*J. Asian Nat. Prod. Res.* **2016**, *18*, 354–359
	Xanthium strumarium	**31**	*Phytochemistry* **1998**, *48*, 1083–1085
	Xanthium strumarium	**32**	*Fitoterapia* **2006**, *77*, 245–246
	Xanthium sibiricum Patr	**33, 34**	*Molecules* **2013**, *18*, 12464–12473
	Xanthium strumarium	**35**	*J. Asian Nat. Prod. Res.* **2008**, *10*, 303–305
	Raphanus sativus L	**36**	*J. Asian Nat. Prod. Res.* **2010**, *12*, 113–118

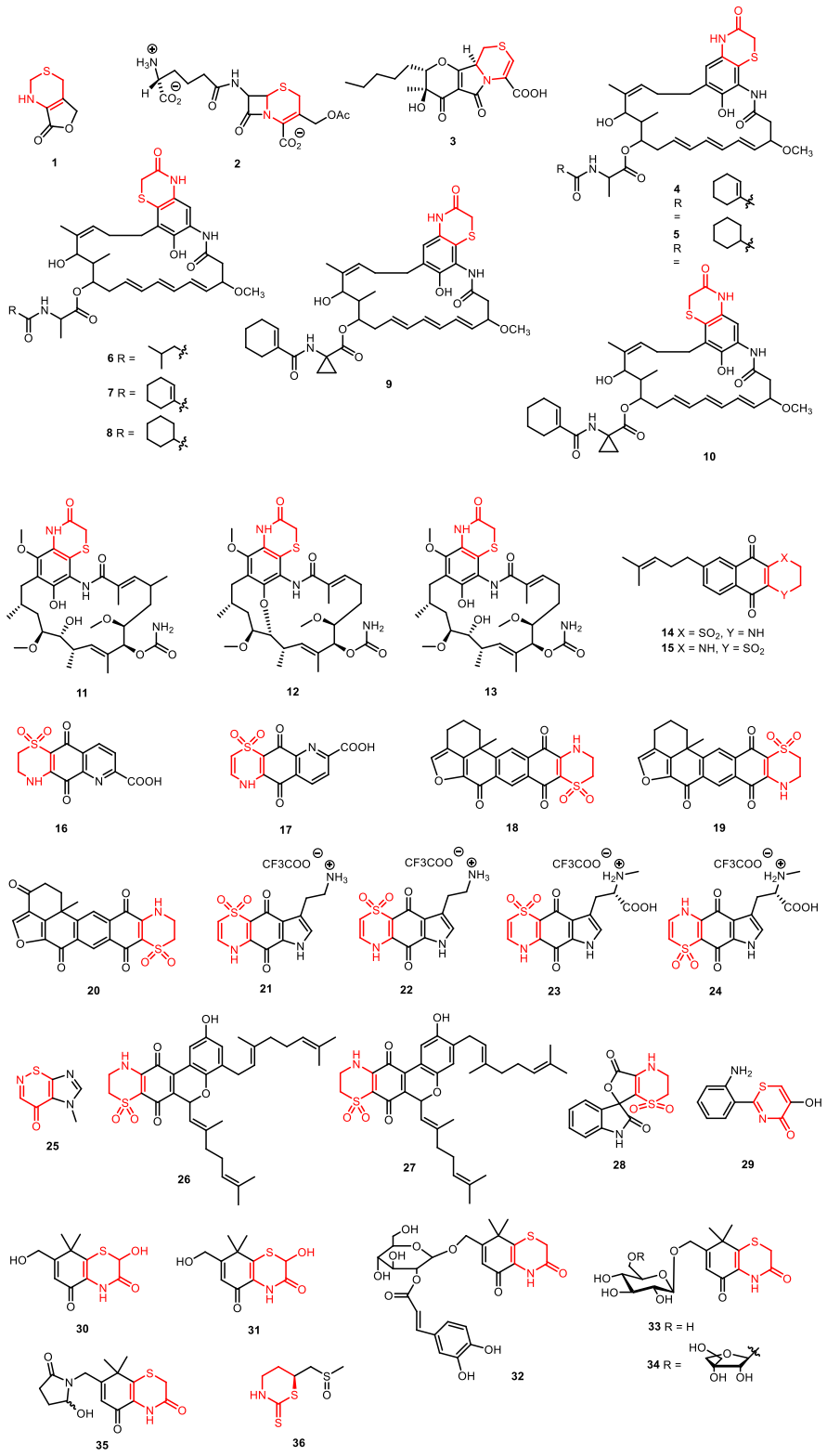

Figure S1. The structures of natural products containing thiazine rings.

Table S2. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) data of **1**–**3** in DMSO-d_6.

no.	**1**		**2**		**3**	
	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1		173.8		174.1		174.0
3	3.26 dd (9.6, 4.2)	52.5	3.37 (overlap)	57.5	3.68 m	52.6
4	2.17 t (4.2)	46.4	2.71 brs	50.6	2.20 dd (5.4, 2.0)	49.1
5	2.62 m	31.9		125.5	1.54 m	36.1
6		150.9		133.7		56.7
7	3.54 dd (11.2, 6.8)	68.4	3.59 t (8.7)	67.5	2.63 d (6.0)	60.2
8	2.65 m	48.2	2.05 d (11.0)	52.2	2.24 dd (9.9, 6.0)	48.0
9		61.2		61.4		62.5
10a	2.80 dd (14.6, 5.4)	31.2	2.82 dd (14.2, 5.8)	32.3	2.87 dd (14.3, 4.2)	32.6
10b	2.74 dd (14.6, 4.3)		2.50 (overlap)		2.70 (overlap)	
11	0.81 d (6.7)	13.6	1.06 s	16.8	0.65 d (7.2)	12.3
12a	4.90 brs	112.6	1.50 s	14.6	1.10 s	19.4
12b	5.17 brs					
13	5.69 dd (14.9, 9.5)	126.8	6.04 dd (15.0, 10.0)	128.0	5.99 dd (15.1, 9.8)	126.6
14	4.90 overlap	134.1	4.96 ddd (15.0, 11.0, 3.0)	134.1	5.00 ddd (15.1, 11.2, 2.9)	134.5
15a	2.28 brd (13.0)	39.8	2.33 m	40.3	2.33 m	39.6
15b	1.75 brd (13.0)		1.98 d (13.3)		1.84 m	
16	2.68 overlap	32.9	2.75 m	33.1	2.70 (overlap)	32.8
17	6.35 dd (9.8, 1.5)	157.1	6.44 d (9.3)	156.4	6.41 d (9.8)	156.9
18		132.0		133.6		132.4
19		194.3		194.5		194.5
20		151.5		151.5		151.5
21	3.79 dt (11.3, 2.2)	26.1	4.49 (overlap)	25.8	4.04 (overlap)	26.2
22a	2.88 dd (19.7, 11.3)	43.2	3.17 dd (20.5, 7.2)	46.2	3.03 dd (19.8, 10.9)	44.4
22b	1.23 dd (19.7, 2.1)		2.95 dd (20.5, 3.9)		1.74 dd (19.8, 2.1)	
23		206.6		206.9		207.0
24	1.04 d (6.7)	19.3	1.05 d (7.2)	19.4	1.06 d (6.7)	19.2
25	1.79 s	10.6	1.86 s	10.9	1.80 s	10.7
1'a		135.8		136.2		136.0
2'	7.19 brs	124.8	7.14 s	124.0	7.21 s	124.8
3'		108.6		109.7		108.6
3'a		127.6		127.0		127.5
4'	7.47 d (7.9)	118.1	7.47 d (7.8)	118.1	7.50 d (7.9)	118.1
5'	7.00 t (7.0)	118.7	7.01 t (7.4)	118.6	7.01 t (7.3)	118.8
6'	7.09 t (7.3)	120.9	7.07 t (7.3)	121.1	7.09 t (7.2)	121.0
7'	7.38 d (8.0)	112.1	7.36 d (8.0)	111.6	7.36 d (8.1)	112.0
2"	7.27 d (2.2)	119.5	7.41 d (2.2)	118.6	7.32 d (2.2)	119.6
3"		133.9		135.9		134.1
5"		161.8		162.0		161.9
7"a	4.06 dd (17.6, 6.1)	40.9	4.02 d (6.1)	41.0	4.06 dd (17.7, 6.3)	40.9
7"b	3.99 dd (17.6. 5.7)				4.01 dd (17.7, 5.6)	
8"		170.1		170.3		170.2
9"	3.64 s	51.9	3.65 s	51.9	3.65	52.0
NH-2	8.22 s		8.34 s		8.43 s	
NH-1'	11.0 s		10.9 s		10.99 s	
NH-6"	7.68 t (5.9)		8.07 t (6.0)		7.74 t (5.9)	
7-OH	4.71 d (7.0)		4.49 overlap			

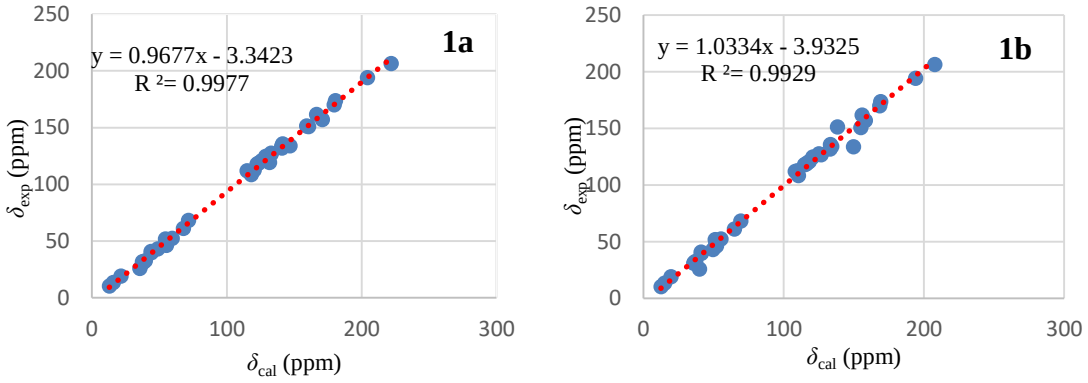

Figure S2. The ^{13}C NMR correlation of experimental data and calculated dada about **1a** and **1b**.

Table S3. The Computed ^{13}C NMR Data for **1a** and **1b**.

no	**1a**			**1b**		
	Expt	Calc	Δδ	Expt	Calc	Δδ
1	173.8	180.5	-2.5	173.8	169.2	-2.9
3	52.5	59.5	1.7	52.5	55.2	0.6
4	46.4	55.3	3.8	46.4	51.9	3.3
5	31.9	37.5	1.0	31.9	36.3	1.7
6	150.9	160.6	1.2	150.9	154.9	5.2
7	68.4	71.7	-2.4	68.4	69.3	-0.8
8	48.2	55.0	1.7	48.2	51.5	1.1
9	61.2	67.7	1.0	61.2	64.9	1.9
10	31.2	38.0	2.2	31.2	35.8	1.9
11	13.6	15.8	-1.6	13.6	14.9	-2.1
12	112.6	120.2	0.4	112.6	109.7	-3.1
13	126.8	132.8	-1.7	126.8	126.6	0.1
14	134.1	146.7	4.5	134.1	134.2	0.7
15	39.8	44.1	-0.4	39.8	41.3	-1.1
16	32.9	39.5	2.0	32.9	37.1	1.5
17	157.1	170.9	4.9	157.1	158.1	2.4
18	132	140.8	0.9	132	133.1	1.6
19	194.3	204.2	-0.1	194.3	193.9	2.2
20	151.5	159.1	-0.9	151.5	138.2	-12.6
21	26.1	35.5	5.0	26.1	39.9	11.2
22	43.2	48.7	0.6	43.2	49.6	4.1
23	206.6	221.9	4.7	206.6	207.6	4.0
24	19.3	21.6	-1.7	19.3	19.6	-2.9
25	10.6	13.0	-1.4	10.6	12.5	-1.6
1'a	135.8	141.4	-2.3	135.8	133.3	-2.0
2'	124.8	128.9	-3.4	124.8	120.7	-4.0
3'	108.6	118.0	2.2	108.6	110.4	1.5
3'a	127.6	132.7	-2.5	127.6	125.1	-2.3
4'	118.1	122.4	-3.0	118.1	114.7	-3.5
5'	118.7	123.5	-2.5	118.7	115.8	-2.9
6'	120.9	125.6	-2.7	120.9	118.2	-2.7
7'	112.1	115.0	-4.2	112.1	108.2	-4.2
2"	119.5	131.7	4.6	133.9	149.6	16.8
3"	133.9	140.7	-1.1	119.5	116.5	-3.0
5"	161.8	166.5	-4.0	161.8	155.8	-4.7
7"	40.9	43.8	-1.8	40.9	41.1	-2.4
8"	170.1	179.5	0.3	170.1	168.5	0.1
9"	51.9	54.4	-2.6	51.9	51.2	-3.0
		AveDev	2.25		AveDev	3.26
		MaxDev	5.0		MaxDev	16.8

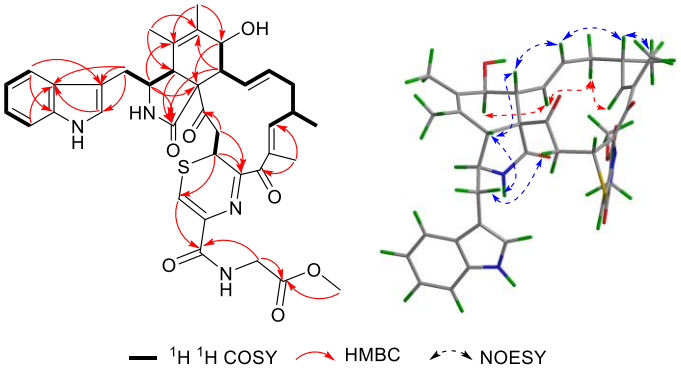

Figure S3. Key 2D correlations of **2**

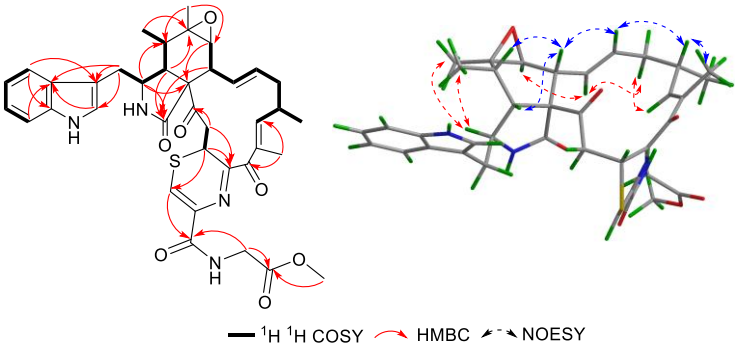

Figure S4. Key 2D correlations of **3**

EXPERIMENTAL SECTION

General experimental procedures. NMR spectra were obtained on a Bruker AM-400 NMR spectrometer (Bruker, Karlsruhe, Germany). HRESIMS data were measured on a Bruker micrOTOF Ⅱ spectrometer. Optical rotations were recorded in a 0.7 mL cell on a Rudolph Autopol IV automatic polarimeter (Rudolph Research Analytical, Hackettstown, NJ, U.S.A.). UV spectra were acquired with a PerkinElmer Lambda 35 spectrophotometer (PerkinElmer, Inc., U.S.A.). ECD data were recorded with a JASCO-810 instrument (JASCO Co., Ltd., Tokyo. Japan) IR spectra were measured by a Bruker Vertex 70 FT-IR spectrophotometer (Bruker, Karlsruhe, Germany). Compounds were purified by an Agilent 1220 HPLC system semi-preparative HPLC equipped with a UV detector. Chemical shifts are expressed in ppm with reference to the DMSO-d_6 (δ_H 2.50/δ_C 39.52) signals. The crystallographic data were obtained on a Bruker APEX DUO diffractometer equipped with graphite-monochromatized Cu Kα radiation (λ = 1.54178 Å). Packing materials for column chromatography were silica gel (80–120 mesh, 100–200 mesh, and 200–300 mesh, Qingdao Marine Chemical Inc., Qingdao, People's Republic of China), ODS (50 μm, YMC, Japan), and Sephadex LH-20 (Pharmacia Biotech AB, Uppsala, Sweden).

Fungal Material. The fungus *Chaetomium globosum* TW1-1 was isolated from *Armadillidium vulgare* in November 2012 at Tongji Medical College, Hubei Province, China and *Aspergillus flavipes* (507) was derived from the intertidal zone of the Yangtze River, Wuhan, Hubei Province, China. The sequence data for these strains have been submitted to the DDBJ/EMBL/GenBank under accession no. KF993614 and KP339510. Two voucher samples, CCM20121113 and QM507, were preserved in the culture collection center of Tongji Medical College, Huazhong University of Science and Technology.

Fermentation and Isolation. Each fungus was cultured on potato dextrose agar at 28 ℃ for 7 d to prepare the seed culture, and then inoculated into Erlenmeyer flasks (1 L) contained 200 g of rice and 200 mL of distilled water as previously described. At the time of harvest, CH_3CH_2OH was added, and then extracted with an equal volume of EtOAc. The separation of the EtOAc extract (100 g) was carried out by silica gel column chromatography (CC, 80–120 mesh) eluting with CH_2Cl_2–MeOH (100:1–0:1, v/v) to afford seven fractions (Fr. A–Fr. G) as previously described.[1]

Fr. F (6.0 g) was subjected to silica gel CC [CH_2Cl_2–MeOH (70:1–5:1, v/v)] to yield five fractions (F1–F5). Of these, Fr. F4 was subjected to MPLC (MeOH–H_2O, 20:80–100:0) to give seven fractions (F4.1–F4.6). Fr. F4.3 was purified by repeated CC on Sephadex LH-20 (CH_2Cl_2–MeOH 1:1), and then purified by silica gel CC to get four fractions (F4.3.1–F4.3.4), F4.3.2 was purified by semi-preparative HPLC (MeCN–H_2O, 53:47, v/v) to yield **1** (5.1 mg), F4.3.3 was purified by semi-preparative HPLC (MeCN–H_2O, 62:38, v/v) to yield **2** (7.3 mg), F4.3.4 was purified by semi-preparative HPLC (MeCN–H_2O, 62:38, v/v) to yield **3** (4.5 mg).

Cytochathiazine A (1): pale yellow crystals. (MeOH), $[\alpha]^{25}_D$ +216.7 (*c* 0.12, MeOH); IR ν_{max} = 3403, 1688, 1649, 1539, 1220, 1024 cm^{-1}; UV (MeOH) λ_{max} (log ε) = 220 (4.45), 262 (3.75) and 360 (3.20) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 216 (–3.72), 264 (+6.19) nm; for ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data see Table S2; HRESIMS $[M + Na]^+$ *m/z* 721.2689 (calcd for $C_{38}H_{42}N_4O_7SNa$, 721.2672).

Cytochathiazine B (2): pale yellow power. (MeOH), $[\alpha]^{25}_D$ +143.1 (*c* 0.13, MeOH); IR ν_{max} = 3404, 1693, 1659, 1541, 1221, 1030 cm^{-1}; UV (MeOH) λ_{max} (log ε) = 221 (4.38), 260 (3.74) and 338 (3.19) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 218 (–6.20), 260 (+4.64) nm; for ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data see Table S2; HRESIMS $[M + Na]^+$ *m/z* 721.2672 (calcd for $C_{38}H_{42}N_4O_7SNa$, 721.2672).

Cytochathiazine C (3): pale yellow power. (MeOH), $[\alpha]^{25}_D$ +162.0 (*c* 0.10, MeOH); IR ν_{max} = 3408, 1693, 1654, 1540, 1435, 1218, 1027 cm^{-1}; UV (MeOH) λ_{max} (log ε) = 207 (4.49), 262 (3.75) and 359 (3.24) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 219 (–4.73), 264 (+5.63) nm; For ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data see Table S2; HRESIMS $[M + Na]^+$ *m/z* 721.2666 (calcd for $C_{38}H_{42}N_4O_7SNa$, 721.2672).

X-ray Crystal Structure Analysis. Crystals of **1** was obtained from CH_3CH_2OH- H_2O. The intensity data was collected at 100 K on a Bruker APEX DUO diffractometer outfitted with an APEX Ⅱ CCD using Cu Kα radiation. Cell refinement and data reduction were performed with Bruker SAINT. The structures were determined by direct methods using SHELXS-97. Crystallographic data for the reported structure have been deposited with the Cambridge Crystallographic Data Center (CCDC) as supplementary publications no. CCDC 1827757.

Crystal Data for Cytochathiazine A (1): $C_{38}H_{42}N_4O_7S$, M = 698.81, a = 11.9204(3) Å, b = 10.2457(2) Å, c = 15.0219(3) Å, α = 90 °, β = 95.8030(10) °, γ = 90 °, V = 1825.27(7) Å^3, T = 296(2) K, space group $P21$, Z = 2, μ(CuKα) = 1.231 mm^{-1}, 20076 reflections measured, 6268 independent reflections (R_{int} = 0.0259). The final R_1 values were 0.0453 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1216 ($I > 2\sigma(I)$). The final R_1 values were 0.0459 (all data). The final $wR(F^2)$ values were 0.1223 (all data). The goodness of fit on F^2 was 1.018. Flack parameter = 0.073(4).

BIOLOGICAL ASSAYS

Cytotoxicity against Cancer Cell Lines. Cytotoxicity of the isolated compounds against the six cancer cell lines (SW480, HL-60, A549, MCF-7, NB4, and SMMC-7721), was evaluated using the MTT method as previously described.[1]

Table S4. Cytotoxic activities of compounds **1**–**3** against six tumor cell lines (IC_{50} in μM)

Compounds	**MCF-7**	**SMMC-7721**	**A-549**	**SW480**	**HL-60**	**NB4**
1	39.01	>40	>40	>40	>40	>40
2	19.24	>40	>40	23.02	12.52	9.63
3	15.46	>40	18.69	26.79	17.58	24.71
Doxorubicin	0.85	0.20	0.15	1.30	0.05	0.08

(1) Wang, W.; Gong, J.; Liu, X.; Dai, C.; Wang, Y.; Li, X. N.; Wang, J.; Luo, Z.; Zhou, Y.; Xue, Y.; Zhu, H.; Chen, C.; Zhang, Y. *J. Nat. Prod.* **2018**, *81*, 1578–1587.

NMR calculations

The conformations of **1** generated by BALLOON were subjected to semiempirical PM3 quantum mechanical geometry optimizations using the Gaussian 09 program. Duplicate conformations were identified and removed when the root-mean-square (RMS) distance was less than 0.5 Å for any two geometry-optimized conformations. The remaining conformations were further optimized at the B3LYP/6-31G(d) level in dimethylsulfoxide with the IEFPCM solvation model using Gaussian 09, and the duplicate conformations emerging after these calculations were removed according to the same RMS criteria above. The harmonic vibrational frequencies were calculated to confirm the stability of the final conformers. The NMR chemical shifts were calculated for each conformer at the B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) level with dimethylsulfoxide as solvent by the IEFPCM solvation model implemented in Gaussian 09 program, which were then combined using Boltzmann weighting according to their population contributions.

Table S5. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **1a** at B3LYP/6-31G(d) level in dimethylsulfoxide

Conformation	**Internal Energy**	**%**
1	-2616.95	35.98%
2	-2616.95	24.31%
3	-2616.95	15.09%
4	-2616.94	7.04%
5	-2616.94	6.47%
6	-2616.94	5.94%
7	-2616.94	3.22%
8	-2616.94	1.36%

Table S6. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **1b** at B3LYP/6-31G(d) level in dimethylsulfoxide

Conformation	**Internal Energy**	**%**
1	-2616.93	13.57%
2	-2616.93	13.15%
3	-2616.93	12.34%
4	-2616.93	11.10%
5	-2616.93	10.64%
6	-2616.93	5.82%
7	-2616.93	5.07%
8	-2616.93	4.96%
9	-2616.93	3.28%
10	-2616.93	3.15%
11	-2616.93	3.05%
12	-2616.93	3.02%
13	-2616.93	1.51%
14	-2616.93	1.44%
15	-2616.93	1.23%

Table S7. Compound **1a** structure optimized at B3LYP/6-31G*

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.156	-3.273	1.709	O	6.807	-0.72	-1.345
C	2.973	-2.477	0.971	O	-1.395	4.356	-1.97
C	-8.719	-0.651	-0.904	O	7.495	-2.156	-2.952
C	-9.063	-1.892	-1.482	S	1.198	-2.665	3.023

C	-7.485	-0.462	-0.291	H	2.128	-4.342	1.533
C	-8.183	-2.968	-1.454	H	-9.431	0.168	-0.941
C	1.566	3.165	-1.002	H	-10.034	-2.01	-1.955
C	0.552	2.31	-1.193	H	-7.239	0.499	0.153
C	3.623	1.836	0.532	H	-8.447	-3.926	-1.896
C	-4.875	-2.996	0.022	H	1.422	4.015	-0.331
C	-6.569	-1.53	-0.249	H	0.682	1.45	-1.847
C	3.664	1.888	1.881	H	3.229	0.934	0.071
C	-5.24	-1.697	0.295	H	-3.963	-3.521	0.271
C	-6.942	-2.774	-0.835	H	-5.204	3.928	-1.132
C	3.043	0.815	2.694	H	-4.094	4.045	-2.603
C	2.521	-0.469	2.084	H	3.21	3.859	-2.209
C	-3.204	3.26	-0.856	H	2.993	2.106	-2.199
C	-0.363	0.756	1.244	H	0.491	-1.02	0.394
C	-1.541	0.032	-0.931	H	-0.791	-1.308	1.546
C	-4.221	3.763	-1.562	H	-0.683	3.186	0.279
C	3.752	-3.098	-0.149	H	4.069	3.874	0.057
C	6.685	-1.759	-1.968	H	0.817	-0.348	3.382
C	2.951	3.004	-1.569	H	-2.572	3.444	1.163
C	0.1	-0.69	1.362	H	-1.944	2.401	-2.383
C	-0.801	2.47	-0.54	H	-2.755	1.132	1.8
C	4.026	2.904	-0.451	H	-4.498	0.86	-0.542
C	1.119	-0.904	2.495	H	4.665	3.806	2.063
C	-3.287	2.83	0.596	H	4.937	2.696	3.417
C	-1.839	3.075	-1.517	H	3.393	3.52	3.269
C	-2.785	1.365	0.731	H	5.454	1.623	-1.514
C	-3.72	0.335	0.024	H	6.19	2.647	-0.273
C	-1.345	1.153	0.111	H	5.666	3.362	-1.811
C	4.195	3.047	2.691	H	-4.932	4.094	1.244
C	5.418	2.614	-1.049	H	-4.617	2.715	2.307
C	-4.652	3.036	1.26	H	-5.451	2.476	0.761
C	8.588	-1.268	-3.276	H	8.204	-0.297	-3.593
C	-4.399	-0.663	0.99	H	9.123	-1.754	-4.091
C	5.589	-2.779	-1.726	H	9.241	-1.142	-2.409
N	3.291	-1.166	1.322	H	-3.622	-1.157	1.586
N	-2.838	-0.339	-0.918	H	-5.011	-0.082	1.692
N	-5.889	-3.644	-0.653	H	5.043	-2.943	-2.664
N	4.717	-2.31	-0.676	H	6.047	-3.741	-1.462
O	2.888	0.944	3.908	H	-3.169	-1.085	-1.519
O	-0.02	1.6	2.054	H	-5.864	-4.608	-0.952

O	-0.67	-0.451	-1.656	H	4.911	-1.408	-0.257
O	3.522	-4.243	-0.553	H	-0.485	4.228	-2.295
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.156	2.599	1.659	O	-7.056	2.549	0.012
C	-2.894	1.762	0.884	O	2.107	-4.482	-2.333
C	3.653	4.847	-0.569	O	-7.693	2.772	-2.147
C	4.792	5.525	-1.053	S	-1.146	2.029	2.95
C	3.749	3.563	-0.045	H	-2.23	3.673	1.531
C	6.051	4.934	-1.017	H	2.685	5.34	-0.608
C	-0.96	-3.586	-1.366	H	4.685	6.528	-1.458
C	-0.013	-2.645	-1.48	H	2.863	3.055	0.325
C	-3.128	-2.518	0.199	H	6.93	5.455	-1.386
C	6.837	1.638	0.261	H	-0.764	-4.464	-0.746
C	5.008	2.933	0.003	H	-0.197	-1.759	-2.084
C	-3.178	-2.669	1.541	H	-2.797	-1.56	-0.192
C	5.477	1.651	0.476	H	7.561	0.866	0.484
C	6.144	3.642	-0.487	H	5.86	-3.762	-1.406
C	-2.656	-1.606	2.434	H	4.789	-3.861	-2.907
C	-2.254	-0.243	1.91	H	-2.523	-4.326	-2.653
C	3.801	-3.306	-1.124	H	-2.433	-2.566	-2.538
C	0.729	-1.173	1.061	H	-0.258	0.564	0.277
C	1.91	-0.237	-1.028	H	0.981	0.901	1.461
C	4.872	-3.654	-1.843	H	1.262	-3.515	-0.038
C	-3.735	2.345	-0.21	H	-3.459	-4.537	-0.433
C	-6.833	2.433	-1.174	H	-0.564	-0.258	3.231
C	-2.34	-3.494	-1.959	H	3.147	-3.696	0.858
C	0.146	0.222	1.236	H	2.495	-2.467	-2.621
C	1.336	-2.74	-0.807	H	3.122	-1.436	1.671
C	-3.448	-3.531	-0.867	H	4.907	-0.848	-0.581
C	-0.903	0.302	2.359	H	-2.799	-4.343	2.849
C	3.821	-2.986	0.358	H	-3.989	-4.682	1.575
C	2.435	-3.197	-1.798	H	-4.423	-3.685	2.973
C	3.2	-1.579	0.588	H	-4.883	-2.246	-1.906
C	4.072	-0.43	-0.007	H	-5.626	-3.355	-0.738
C	1.767	-1.431	-0.062	H	-5.036	-3.97	-2.296
C	-3.622	-3.918	2.262	H	5.552	-4.161	0.947
C	-4.833	-3.258	-1.487	H	5.099	-2.907	2.11
C	5.185	-3.134	1.042	H	5.944	-2.471	0.614

C	-8.959	3.315	-1.715	H	-9.493	2.587	-1.1
C	4.657	0.53	1.054	H	-9.513	3.524	-2.628
C	-5.544	1.884	-1.787	H	-8.802	4.232	-1.142
N	-3.083	0.412	1.175	H	3.836	0.932	1.661
N	3.169	0.242	-0.931	H	5.279	-0.073	1.728
N	7.239	2.823	-0.317	H	-5.796	1.048	-2.446
N	-4.584	1.461	-0.802	H	-5.1	2.67	-2.406
O	-2.497	-1.802	3.638	H	3.459	1.037	-1.487
O	0.439	-2.083	1.819	H	8.192	3.059	-0.554
O	1.032	0.215	-1.764	H	-4.68	0.554	-0.363
O	-3.638	3.527	-0.554	H	1.195	-4.411	-2.67
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-1.65	3.07	1.925	O	-6.532	1.024	-1.152
C	-2.537	2.377	1.162	O	1.274	-4.552	-2.282
C	4.383	4.446	-0.735	O	-7.156	2.596	-2.655
C	5.598	4.917	-1.278	S	-0.708	2.322	3.175
C	4.282	3.167	-0.201	H	-1.554	4.144	1.811
C	6.737	4.118	-1.294	H	3.513	5.098	-0.735
C	-1.574	-3.214	-1.173	H	5.646	5.921	-1.689
C	-0.508	-2.421	-1.346	H	3.34	2.82	0.217
C	-3.499	-1.846	0.49	H	7.674	4.478	-1.709
C	7.004	0.739	-0.017	H	-1.474	-4.107	-0.553
C	5.415	2.329	-0.204	H	-0.592	-1.52	-1.949
C	-3.508	-1.979	1.835	H	-3.06	-0.943	0.073
C	5.679	0.987	0.262	H	7.595	-0.145	0.181
C	6.631	2.83	-0.755	H	5.129	-4.408	-1.53
C	-2.798	-1	2.692	H	3.984	-4.353	-2.978
C	-2.201	0.28	2.144	H	-3.289	-3.727	-2.372
C	3.179	-3.641	-1.16	H	-2.953	-1.995	-2.271
C	0.562	-1.089	1.158	H	-0.164	0.8	0.446
C	1.751	-0.315	-0.994	H	1.156	0.909	1.585
C	4.149	-4.154	-1.923	H	0.691	-3.468	0.039
C	-3.298	3.118	0.104	H	-4.096	-3.816	-0.091
C	-6.354	2.088	-1.714	H	-0.485	-0.033	3.394
C	-2.958	-2.929	-1.693	H	2.571	-3.916	0.856
C	0.216	0.376	1.38	H	1.946	-2.618	-2.605
C	0.844	-2.713	-0.738	H	2.933	-1.667	1.636
C	-3.998	-2.823	-0.542	H	4.644	-1.378	-0.732

C	-0.764	0.593	2.547	H	-4.624	-3.838	1.932
C	3.318	-3.318	0.315	H	-4.792	-2.798	3.355
C	1.815	-3.329	-1.774	H	-3.307	-3.706	3.116
C	2.925	-1.833	0.553	H	-5.357	-1.386	-1.49
C	3.921	-0.833	-0.113	H	-6.134	-2.432	-0.294
C	1.493	-1.482	-0.019	H	-5.694	-3.085	-1.884
C	-4.091	-3.149	2.589	H	4.885	-4.732	0.832
C	-5.379	-2.404	-1.086	H	4.679	-3.42	2.002
C	4.677	-3.662	0.933	H	5.503	-3.118	0.462
C	-8.31	1.8	-3.005	H	-7.995	0.828	-3.392
C	4.712	0.028	0.899	H	-8.829	2.369	-3.775
C	-5.191	3.02	-1.437	H	-8.951	1.659	-2.132
N	-2.937	1.071	1.443	H	4	0.57	1.535
N	3.072	-0.035	-0.986	H	5.256	-0.662	1.556
N	7.576	1.835	-0.628	H	-4.656	3.212	-2.375
N	-4.327	2.43	-0.443	H	-5.58	3.989	-1.1
O	-2.628	-1.209	3.893	H	3.441	0.71	-1.565
O	0.168	-1.957	1.917	H	8.541	1.901	-0.917
O	0.905	0.271	-1.671	H	-4.571	1.518	-0.073
O	-3.001	4.268	-0.236	H	0.367	-4.346	-2.573
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.699	-2.527	1.965	O	7.423	-2.442	-0.161
C	3.32	-1.771	1.021	O	-2.382	3.735	-2.539
C	-8.634	-1.325	-0.767	O	7.866	-2.959	-2.32
C	-8.902	-2.602	-1.303	S	1.797	-1.832	3.273
C	-7.417	-1.044	-0.157	H	2.809	-3.606	1.963
C	-7.962	-3.624	-1.236	H	-9.393	-0.55	-0.833
C	0.959	3.268	-1.548	H	-9.863	-2.792	-1.775
C	-0.022	2.363	-1.63	H	-7.228	-0.055	0.255
C	3.322	2.423	-0.172	H	-8.167	-4.609	-1.646
C	-4.667	-3.41	0.253	H	0.852	4.103	-0.853
C	-6.44	-2.055	-0.076	H	0.075	1.524	-2.316
C	3.511	2.712	1.135	H	2.977	1.425	-0.427
C	-5.107	-2.126	0.479	H	-3.728	-3.873	0.525
C	-6.738	-3.337	-0.62	H	-5.626	3.919	-0.4
C	3.103	1.748	2.184	H	-4.834	4.048	-2.065
C	2.701	0.324	1.86	H	2.328	4.007	-3.046
C	-3.72	3	-0.614	H	2.323	2.254	-2.85

C	-0.348	1.044	1.146	H	0.605	-0.779	0.552
C	-1.527	-0.152	-0.81	H	-0.52	-0.947	1.88
C	-4.784	3.686	-1.042	H	-1.123	3.221	-0.052
C	4.077	-2.463	-0.072	H	3.54	4.375	-1.016
C	7.081	-2.522	-1.321	H	1.14	0.453	3.327
C	2.263	3.202	-2.3	H	-2.818	3.172	1.303
C	0.277	-0.304	1.48	H	-2.805	1.823	-2.179
C	-1.263	2.41	-0.776	H	-2.713	0.828	1.87
C	3.493	3.335	-1.358	H	-4.532	0.437	-0.441
C	1.422	-0.201	2.502	H	3.217	4.533	2.258
C	-3.54	2.501	0.815	H	4.32	4.71	0.877
C	-2.56	2.705	-1.572	H	4.846	3.882	2.351
C	-2.867	1.108	0.822	H	5.675	3.195	-1.484
C	-3.721	-0.01	0.148	H	4.884	3.653	-3.007
C	-1.469	1.107	0.083	H	4.819	1.972	-2.442
C	3.999	4.036	1.673	H	-5.178	3.563	1.781
C	4.798	3.019	-2.116	H	-4.608	2.149	2.673
C	-4.813	2.538	1.67	H	-5.622	1.944	1.23
C	9.201	-3.359	-1.947	H	9.743	-2.516	-1.513
C	-4.334	-1.021	1.144	H	9.676	-3.683	-2.872
C	5.703	-2.146	-1.869	H	9.164	-4.179	-1.227
N	3.48	-0.391	1.126	H	-3.523	-1.447	1.747
N	-2.778	-0.659	-0.751	H	-4.983	-0.465	1.833
N	-5.637	-4.138	-0.404	H	5.831	-1.407	-2.666
N	4.816	-1.633	-0.858	H	5.257	-3.039	-2.314
O	3.046	2.078	3.369	H	-3.021	-1.5	-1.262
O	-0.03	2.057	1.747	H	-5.555	-5.109	-0.669
O	-0.603	-0.618	-1.477	H	4.907	-0.672	-0.549
O	4.008	-3.682	-0.249	H	-2.27	4.57	-2.054
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-1.553	3.121	2.207	O	-4.448	1.161	-2.469
C	-2.493	2.494	1.452	O	0.698	-4.455	-2.387
C	4.42	4.233	-0.46	O	-5.705	2.766	-3.451
C	5.635	4.673	-1.026	S	-0.625	2.291	3.417
C	4.271	2.928	-0.004	H	-1.396	4.19	2.115
C	6.726	3.819	-1.145	H	3.588	4.927	-0.379
C	-2.001	-3.001	-1.109	H	5.721	5.699	-1.375
C	-0.893	-2.264	-1.271	H	3.329	2.604	0.432

C	-3.756	-1.594	0.692	H	7.664	4.156	-1.578
C	6.86	0.355	-0.096	H	-1.937	-3.937	-0.55
C	5.355	2.034	-0.112	H	-0.941	-1.322	-1.814
C	-3.719	-1.79	2.028	H	-3.269	-0.709	0.294
C	5.564	0.652	0.256	H	7.41	-0.57	0.02
C	6.573	2.506	-0.684	H	4.578	-4.62	-1.793
C	-2.908	-0.904	2.897	H	3.382	-4.416	-3.186
C	-2.251	0.359	2.378	H	-3.79	-3.335	-2.263
C	2.705	-3.738	-1.304	H	-3.334	-1.636	-2.086
C	0.369	-1.125	1.242	H	-0.224	0.849	0.646
C	1.524	-0.334	-0.919	H	1.125	0.798	1.756
C	3.604	-4.279	-2.131	H	0.286	-3.455	0.013
C	-3.225	3.28	0.405	H	-4.53	-3.482	0.044
C	-5.014	2.236	-2.433	H	-0.523	-0.08	3.572
C	-3.38	-2.598	-1.559	H	2.166	-4.073	0.723
C	0.143	0.349	1.548	H	1.491	-2.557	-2.64
C	0.459	-2.675	-0.735	H	2.703	-1.897	1.593
C	-4.368	-2.477	-0.363	H	4.34	-1.593	-0.827
C	-0.79	0.583	2.749	H	-3.593	-3.576	3.235
C	2.927	-3.497	0.177	H	-4.95	-3.577	2.089
C	1.343	-3.301	-1.841	H	-5.009	-2.587	3.556
C	2.645	-2.004	0.505	H	-6.447	-1.89	-0.011
C	3.683	-1.037	-0.146	H	-6.141	-2.558	-1.627
C	1.221	-1.528	0.01	H	-5.616	-0.908	-1.237
C	-4.355	-2.95	2.755	H	4.417	-5.034	0.558
C	-5.727	-1.922	-0.835	H	4.349	-3.771	1.794
C	4.285	-3.959	0.717	H	5.125	-3.448	0.234
C	-5.762	1.979	-4.66	H	-6.359	2.564	-5.358
C	4.572	-0.294	0.876	H	-6.236	1.015	-4.462
C	-5.06	3.165	-1.224	H	-4.757	1.819	-5.055
N	-2.957	1.208	1.716	H	3.925	0.242	1.583
N	2.859	-0.132	-0.936	H	5.105	-1.056	1.457
N	7.466	1.457	-0.662	H	-4.637	4.136	-1.494
N	-4.308	2.643	-0.114	H	-6.112	3.33	-0.96
O	-2.703	-1.181	4.079	H	3.258	0.613	-1.495
O	-0.062	-1.999	1.976	H	8.422	1.492	-0.984
O	0.697	0.334	-1.542	H	-4.496	1.707	0.224
O	-2.86	4.408	0.062	H	-0.201	-4.17	-2.634
Conformation 6							

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.242	2.614	1.499	O	-7.329	3.296	-2.48
C	-2.948	1.76	0.712	O	2.137	-4.538	-2.221
C	3.662	4.818	-0.639	O	-6.956	2.541	-0.383
C	4.823	5.478	-1.097	S	-1.282	2.07	2.838
C	3.732	3.549	-0.076	H	-2.313	3.686	1.349
C	6.076	4.883	-0.996	H	2.699	5.313	-0.729
C	-0.957	-3.628	-1.369	H	4.737	6.469	-1.533
C	-0.008	-2.687	-1.469	H	2.829	3.055	0.274
C	-3.172	-2.531	0.107	H	6.972	5.389	-1.345
C	6.795	1.618	0.398	H	-0.779	-4.494	-0.727
C	4.985	2.914	0.036	H	-0.174	-1.812	-2.094
C	-3.262	-2.656	1.45	H	-2.829	-1.58	-0.292
C	5.429	1.643	0.561	H	7.507	0.85	0.668
C	6.142	3.605	-0.429	H	5.857	-3.813	-1.179
C	-2.768	-1.575	2.337	H	4.836	-3.943	-2.713
C	-2.347	-0.223	1.801	H	-2.479	-4.396	-2.687
C	3.792	-3.343	-0.977	H	-2.392	-2.633	-2.606
C	0.654	-1.166	1.066	H	-0.293	0.569	0.229
C	1.898	-0.27	-1.005	H	0.904	0.912	1.454
C	4.885	-3.711	-1.652	H	1.22	-3.527	0.03
C	-3.743	2.318	-0.428	H	-3.484	-4.562	-0.495
C	-6.673	2.651	-1.686	H	-0.706	-0.211	3.182
C	-2.318	-3.549	-2.005	H	3.073	-3.687	0.991
C	0.074	0.235	1.204	H	2.538	-2.529	-2.532
C	1.319	-2.768	-0.753	H	3.029	-1.409	1.753
C	-3.459	-3.565	-0.948	H	4.882	-0.874	-0.458
C	-1.014	0.332	2.288	H	-4.073	-4.669	1.499
C	3.765	-2.989	0.498	H	-4.549	-3.645	2.864
C	2.449	-3.244	-1.698	H	-2.922	-4.304	2.801
C	3.139	-1.578	0.676	H	-5.64	-3.39	-0.891
C	4.03	-0.443	0.081	H	-5	-4.03	-2.419
C	1.726	-1.444	-0.02	H	-4.861	-2.3	-2.054
C	-3.727	-3.892	2.182	H	5.476	-4.152	1.166
C	-4.824	-3.305	-1.616	H	4.985	-2.875	2.288
C	5.105	-3.124	1.228	H	5.878	-2.468	0.813
C	-8.118	3.266	0.072	H	-8.184	3.068	1.141
C	4.583	0.54	1.138	H	-9.013	2.909	-0.442
C	-5.447	1.836	-2.103	H	-7.993	4.336	-0.114
N	-3.148	0.417	1.021	H	3.743	0.961	1.705

N	3.155	0.208	-0.885	H	5.177	-0.048	1.847
N	7.226	2.786	-0.196	H	-5.81	0.945	-2.626
N	-4.565	1.425	-1.04	H	-4.9	2.444	-2.828
O	-2.65	-1.746	3.55	H	3.462	0.992	-1.448
O	0.335	-2.064	1.826	H	8.188	3.011	-0.403
O	1.041	0.169	-1.774	H	-4.683	0.521	-0.598
O	-3.644	3.494	-0.79	H	1.237	-4.471	-2.591
Conformation 7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.981	-3.508	1.315	O	6.545	-2.066	-3.748
C	2.946	-2.688	0.822	O	-0.859	4.784	-1.421
C	-8.503	-0.634	-0.517	O	4.802	-0.994	-2.785
C	-8.844	-1.884	-1.077	S	0.885	-3.015	2.567
C	-7.232	-0.399	-0.004	H	1.91	-4.537	0.978
C	-7.922	-2.924	-1.132	H	-9.248	0.156	-0.487
C	2.019	3.189	-0.532	H	-9.845	-2.037	-1.471
C	0.966	2.48	-0.95	H	-6.988	0.568	0.428
C	3.831	1.544	0.994	H	-8.183	-3.888	-1.561
C	-4.507	-2.827	0.071	H	1.874	3.954	0.234
C	-6.274	-1.43	-0.047	H	1.093	1.712	-1.711
C	3.748	1.452	2.339	H	3.41	0.734	0.404
C	-4.9	-1.547	0.387	H	-3.557	-3.316	0.24
C	-6.644	-2.684	-0.614	H	-4.813	3.605	-1.727
C	2.975	0.35	2.96	H	-3.504	3.717	-3.024
C	2.458	-0.817	2.145	H	3.809	3.886	-1.508
C	-2.806	3.381	-1.055	H	3.463	2.17	-1.736
C	-0.223	0.753	1.185	H	0.617	-0.939	0.17
C	-1.367	0.35	-1.072	H	-0.808	-1.292	1.112
C	-3.757	3.572	-1.975	H	-0.366	3.319	0.459
C	3.847	-3.198	-0.262	H	4.528	3.557	0.775
C	5.791	-1.898	-2.81	H	0.62	-0.751	3.245
C	3.434	2.985	-1.001	H	-2.378	3.732	0.987
C	0.134	-0.726	1.13	H	-1.198	3	-2.442
C	-0.436	2.676	-0.425	H	-2.543	1.477	1.753
C	4.412	2.655	0.163	H	-4.334	1.031	-0.485
C	0.992	-1.192	2.319	H	4.855	3.254	2.825
C	-3.046	3.082	0.407	H	4.926	1.985	4.06
C	-1.332	3.427	-1.437	H	3.461	2.937	3.878
C	-2.561	1.622	0.668	H	6.513	2.092	0.421

C	-3.49	0.549	0.02	H	6.189	3.049	-1.039
C	-1.12	1.357	0.07	H	5.729	1.336	-0.98
C	4.279	2.469	3.319	H	-4.723	4.4	0.794
C	5.796	2.258	-0.39	H	-4.522	3.117	1.998
C	-4.462	3.345	0.928	H	-5.225	2.75	0.417
C	4.645	-0.207	-3.986	H	5.553	0.365	-4.187
C	-4.052	-0.483	1.025	H	3.807	0.46	-3.788
C	5.897	-2.718	-1.525	H	4.426	-0.857	-4.836
N	3.283	-1.465	1.398	H	-3.216	-0.948	1.561
N	-2.648	-0.069	-0.994	H	-4.635	0.069	1.774
N	-5.545	-3.511	-0.528	H	5.78	-3.769	-1.804
N	4.939	-2.421	-0.492	H	6.918	-2.591	-1.15
O	2.695	0.355	4.158	H	-3.007	-0.759	-1.642
O	0.134	1.461	2.11	H	-5.506	-4.471	-0.836
O	-0.539	-0.032	-1.9	H	5.026	-1.575	0.057
O	3.61	-4.245	-0.871	H	-1.438	5.287	-2.016
Conformation 8							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.953	-3.421	1.01	O	7.835	-2.3	-2.74
C	2.826	-2.555	0.432	O	-1.277	4.77	-1.466
C	-8.698	-0.769	-0.391	O	7.02	-1.076	-1.023
C	-9.047	-2.011	-0.964	S	0.964	-2.981	2.367
C	-7.416	-0.536	0.093	H	1.893	-4.449	0.671
C	-8.121	-3.044	-1.061	H	-9.447	0.016	-0.328
C	1.68	3.285	-0.793	H	-10.057	-2.164	-1.334
C	0.639	2.519	-1.136	H	-7.166	0.425	0.536
C	3.626	1.707	0.637	H	-8.387	-4.002	-1.499
C	-4.675	-2.948	0.053	H	1.542	4.058	-0.035
C	-6.453	-1.559	0.007	H	0.755	1.743	-1.888
C	3.636	1.582	1.982	H	3.195	0.897	0.057
C	-5.068	-1.675	0.401	H	-3.718	-3.433	0.187
C	-6.831	-2.805	-0.572	H	-5.21	3.501	-1.551
C	2.946	0.441	2.627	H	-3.983	3.673	-2.921
C	2.4	-0.723	1.825	H	3.392	4.048	-1.857
C	-3.162	3.311	-1.004	H	3.113	2.316	-2.059
C	-0.38	0.743	1.061	H	0.409	-0.95	0.006
C	-1.61	0.309	-1.147	H	-0.925	-1.314	1.071
C	-4.169	3.499	-1.862	H	-0.635	3.299	0.359
C	3.624	-3.014	-0.752	H	4.182	3.763	0.419

C	6.912	-1.952	-2.033	H	0.654	-0.731	3.071
C	3.079	3.136	-1.329	H	-2.627	3.631	1.019
C	0.003	-0.729	0.999	H	-1.631	2.991	-2.49
C	-0.737	2.665	-0.527	H	-2.694	1.35	1.738
C	4.111	2.86	-0.2	H	-4.563	0.915	-0.445
C	0.969	-1.156	2.118	H	4.691	3.423	2.432
C	-3.308	2.973	0.461	H	4.93	2.125	3.614
C	-1.714	3.401	-1.473	H	3.41	3.004	3.589
C	-2.766	1.523	0.659	H	6.256	2.482	0.01
C	-3.695	0.441	0.027	H	5.816	3.377	-1.458
C	-1.347	1.318	-0.01	H	5.512	1.631	-1.354
C	4.199	2.596	2.948	H	-5.003	4.225	0.971
C	5.508	2.568	-0.785	H	-4.689	2.926	2.134
C	-4.699	3.177	1.068	H	-5.47	2.566	0.588
C	8.341	-0.545	-0.779	H	9.028	-1.353	-0.519
C	-4.208	-0.616	1.031	H	8.226	0.145	0.055
C	5.485	-2.432	-2.242	H	8.706	-0.022	-1.665
N	3.172	-1.327	0.991	H	-3.347	-1.082	1.527
N	-2.874	-0.148	-1.022	H	-4.768	-0.085	1.812
N	-5.725	-3.627	-0.529	H	5.134	-1.971	-3.178
N	4.593	-2.147	-1.142	H	5.503	-3.511	-2.411
O	2.756	0.408	3.842	H	-3.24	-0.842	-1.662
O	0.007	1.465	1.963	H	-5.689	-4.582	-0.855
O	-0.804	-0.046	-2.008	H	4.738	-1.317	-0.58
O	3.399	-4.089	-1.317	H	-1.904	5.265	-2.019

Table S8. Compound **1b** structure optimized at B3LYP/6-31G*

Conformation 1						
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-8.023	-2.526	-0.378	O	5.331	-5.249	0.217
C	-8.066	-3.836	-0.903	O	-3.195	3.616	-2.438
C	-6.853	-2.011	0.169	O	6.7	-5.5	-1.567
C	-6.943	-4.655	-0.889	S	2.575	-0.877	2.927
C	-5.697	-2.813	0.197	H	-8.92	-1.913	-0.403
C	-5.768	-4.132	-0.337	H	-8.995	-4.211	-1.325
C	3.816	0.784	0.723	H	-6.838	-1.001	0.572
C	0.257	3.887	-1.8	H	-6.975	-5.664	-1.291
C	-0.516	2.796	-1.779	H	4.536	1.335	0.128
C	2.843	3.537	-0.64	H	0.048	4.701	-1.102
C	-3.679	-3.796	0.425	H	-0.309	1.98	-2.467

C	-4.349	-2.621	0.681	H	2.613	2.492	-0.839
C	2.907	1.427	1.489	H	-2.655	-4.066	0.645
C	3.128	3.893	0.632	H	-6.149	3.216	0.055
C	2.986	2.91	1.737	H	-5.575	3.491	-1.68
C	3.999	-0.659	0.756	H	1.315	4.855	-3.417
C	-4.138	2.67	-0.375	H	1.659	3.134	-3.23
C	-0.284	1.496	1.029	H	0.962	-0.12	0.377
C	-1.333	0.041	-0.826	H	0.012	-0.459	1.808
C	-5.351	3.145	-0.676	H	-1.608	3.431	-0.091
C	4.901	-1.263	-0.302	H	2.627	5.472	-1.519
C	5.937	-4.79	-0.732	H	1.497	1.239	3.093
C	1.472	4.061	-2.672	H	-3.104	3.018	1.45
C	0.629	0.313	1.324	H	-3.17	1.668	-2.027
C	-1.646	2.597	-0.801	H	-2.466	0.737	1.945
C	2.738	4.433	-1.848	H	-4.348	0.005	-0.242
C	1.826	0.659	2.227	H	3.617	5.973	0.249
C	-3.717	2.213	1.017	H	4.348	5.297	1.714
C	-3.052	2.597	-1.454	H	2.639	5.7	1.706
C	-2.772	0.992	0.923	H	3.892	4.959	-3.621
C	-3.43	-0.274	0.292	H	4.889	4.688	-2.177
C	-1.479	1.294	0.066	H	4.188	3.308	-3.042
C	3.449	5.296	1.088	H	-4.5	1.634	2.959
C	4.005	4.341	-2.722	H	-5.429	2.911	2.169
C	-4.878	1.982	1.992	H	-5.592	1.241	1.616
C	6.794	-6.916	-1.295	H	7.449	-7.315	-2.068
C	-3.769	-1.385	1.311	H	7.222	-7.083	-0.305
C	5.925	-3.324	-1.126	H	5.806	-7.378	-1.352
N	3.577	-1.448	1.697	H	-4.47	-0.968	2.045
N	-2.435	-0.723	-0.671	H	-2.854	-1.643	1.859
N	-4.522	-4.703	-0.183	H	5.564	-3.233	-2.158
N	5.085	-2.595	-0.207	H	6.954	-2.944	-1.121
O	2.918	3.288	2.907	H	-2.536	-1.596	-1.176
O	-0.14	2.567	1.593	H	-4.267	-5.64	-0.456
O	-0.386	-0.221	-1.569	H	4.647	-3.108	0.551
O	5.412	-0.561	-1.179	H	-3.198	4.469	-1.971
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.191	5.292	-0.656	O	-7.812	3.897	-1.871
C	3.149	6.255	-1.039	O	3.516	-4.19	-2.039

C	2.573	4.092	-0.067	O	-7.104	3.031	0.095
C	4.508	6.038	-0.837	S	-1.94	1.382	2.435
C	3.942	3.839	0.15	H	1.136	5.495	-0.825
C	4.889	4.829	-0.243	H	2.82	7.183	-1.498
C	-3.294	-0.699	0.704	H	1.823	3.362	0.225
C	0.212	-4.142	-1.46	H	5.247	6.779	-1.128
C	0.884	-2.985	-1.536	H	-4.038	-1.363	0.278
C	-2.311	-3.628	-0.182	H	0.557	-4.913	-0.768
C	6.011	3.109	0.671	H	0.542	-2.204	-2.211
C	4.686	2.745	0.733	H	-2.141	-2.63	-0.577
C	-2.323	-1.17	1.517	H	6.888	2.573	1.01
C	-2.503	-3.757	1.15	H	6.786	-2.356	-0.828
C	-2.345	-2.581	2.045	H	5.956	-2.805	-2.416
C	-3.502	0.72	0.458	H	-0.952	-5.314	-2.845
C	4.666	-2.524	-0.767	H	-1.325	-3.588	-2.842
C	0.895	-1.297	0.98	H	-0.435	0.066	-0.001
C	1.995	-0.127	-1.035	H	0.534	0.775	1.267
C	5.862	-2.556	-1.362	H	2.176	-3.425	0.078
C	-4.488	1.094	-0.63	H	-2.059	-5.68	-0.733
C	-6.96	3.352	-1.196	H	-0.835	-0.654	2.969
C	-1.068	-4.436	-2.195	H	3.936	-3.034	1.161
C	-0.061	-0.114	1.012	H	3.35	-2.163	-2.437
C	2.122	-2.682	-0.725	H	3.183	-0.857	1.839
C	-2.248	-4.717	-1.221	H	4.972	0.168	-0.243
C	-1.214	-0.265	2.02	H	-2.88	-5.894	1.181
C	4.433	-2.174	0.69	H	-3.616	-4.992	2.516
C	3.407	-2.843	-1.571	H	-1.887	-5.297	2.528
C	3.419	-0.999	0.779	H	-4.402	-5.095	-1.327
C	3.99	0.339	0.213	H	-3.831	-3.869	-2.474
C	2.083	-1.284	-0.019	H	-3.504	-5.586	-2.778
C	-2.733	-5.062	1.872	H	6.284	-1.066	1.119
C	-3.578	-4.823	-1.995	H	5.439	-1.682	2.549
C	5.7	-1.907	1.509	H	6.35	-2.788	1.511
C	-8.375	3.37	0.689	H	-8.303	3.05	1.728
C	4.143	1.451	1.275	H	-8.545	4.448	0.629
C	-5.599	2.956	-1.768	H	-9.184	2.843	0.179
N	-3.031	1.686	1.186	H	4.815	1.066	2.052
N	3.048	0.695	-0.839	H	3.171	1.617	1.756
N	6.139	4.35	0.086	H	-5.189	3.841	-2.265
N	-4.641	2.424	-0.831	H	-5.781	2.201	-2.538

O	-2.214	-2.729	3.26	H	3.166	1.523	-1.412
O	0.786	-2.229	1.758	H	7.011	4.839	-0.056
O	1.117	0.035	-1.884	H	-4.168	3.044	-0.184
O	-5.072	0.224	-1.279	H	2.664	-4.398	-2.466
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-8.328	-2.44	-0.412	O	7.511	-3.216	0.315
C	-8.406	-3.727	-0.988	O	-3.202	3.674	-2.362
C	-7.138	-1.966	0.128	O	7.892	-4.416	-1.566
C	-7.297	-4.565	-1.031	S	2.32	-1.3	2.826
C	-5.995	-2.787	0.098	H	-9.214	-1.812	-0.392
C	-6.1	-4.083	-0.485	H	-9.35	-4.07	-1.402
C	3.66	0.434	0.738	H	-7.096	-0.973	0.57
C	0.243	3.776	-1.671	H	-7.355	-5.557	-1.471
C	-0.571	2.714	-1.702	H	4.409	0.99	0.186
C	2.798	3.278	-0.495	H	0.052	4.569	-0.945
C	-3.99	-3.813	0.243	H	-0.386	1.917	-2.418
C	-4.633	-2.638	0.559	H	2.536	2.252	-0.746
C	2.761	1.067	1.523	H	-2.967	-4.109	0.431
C	3.076	3.563	0.796	H	-6.21	3.295	0.072
C	2.885	2.531	1.849	H	-5.602	3.607	-1.646
C	3.791	-1.014	0.693	H	1.359	4.768	-3.231
C	-4.215	2.689	-0.351	H	1.638	3.03	-3.11
C	-0.426	1.284	1.041	H	0.771	-0.327	0.297
C	-1.537	-0.041	-0.872	H	-0.203	-0.727	1.695
C	-5.405	3.219	-0.651	H	-1.66	3.327	-0.004
C	4.693	-1.594	-0.377	H	2.659	5.258	-1.285
C	7.122	-3.715	-0.719	H	1.323	0.843	3.096
C	1.477	3.94	-2.518	H	-3.187	2.934	1.495
C	0.444	0.055	1.269	H	-3.268	1.712	-2.03
C	-1.722	2.524	-0.747	H	-2.652	0.618	1.925
C	2.741	4.232	-1.661	H	-4.556	0.023	-0.28
C	1.641	0.301	2.202	H	3.638	5.641	0.523
C	-3.83	2.171	1.03	H	4.324	4.871	1.963
C	-3.117	2.612	-1.418	H	2.629	5.331	1.951
C	-2.939	0.913	0.908	H	4.904	4.427	-1.946
C	-3.646	-0.306	0.238	H	4.17	3.115	-2.887
C	-1.626	1.181	0.068	H	3.94	4.801	-3.39
C	3.435	4.93	1.325	H	-5.753	1.266	1.577

C	4.018	4.137	-2.521	H	-4.661	1.565	2.944
C	-5.012	1.961	1.985	H	-5.522	2.908	2.187
C	9.278	-4.561	-1.191	H	9.735	-5.148	-1.987
C	-4.017	-1.438	1.224	H	9.755	-3.58	-1.116
C	5.693	-3.639	-1.259	H	9.361	-5.082	-0.235
N	3.323	-1.838	1.583	H	-4.704	-1.023	1.972
N	-2.674	-0.759	-0.746	H	-3.109	-1.738	1.761
N	-4.862	-4.68	-0.381	H	5.328	-4.654	-1.439
N	4.793	-2.945	-0.375	H	5.72	-3.123	-2.223
O	2.812	2.852	3.036	H	-2.812	-1.607	-1.283
O	-0.24	2.318	1.659	H	-4.63	-5.61	-0.697
O	-0.603	-0.318	-1.625	H	4.365	-3.437	0.4
O	5.257	-0.863	-1.193	H	-3.167	4.507	-1.863
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-8.2	-1.609	-0.404	O	3.573	-4.462	-1.5
C	-8.389	-2.973	-0.718	O	-2.384	3.515	-2.973
C	-7.005	-1.157	0.143	O	5.417	-5.707	-1.914
C	-7.387	-3.91	-0.489	S	2.279	-0.931	3.401
C	-5.969	-2.079	0.386	H	-9.005	-0.904	-0.594
C	-6.185	-3.45	0.063	H	-9.334	-3.296	-1.145
C	3.908	0.254	1.14	H	-6.878	-0.104	0.381
C	1.012	3.41	-2.062	H	-7.53	-4.96	-0.728
C	0.091	2.446	-1.963	H	4.739	0.624	0.551
C	3.431	2.892	-0.636	H	0.871	4.339	-1.505
C	-4.117	-3.251	0.922	H	0.229	1.515	-2.509
C	-4.636	-1.976	0.937	H	3.078	1.867	-0.719
C	3.042	1.104	1.735	H	-3.152	-3.604	1.261
C	3.662	3.383	0.601	H	-5.539	3.884	-0.731
C	3.305	2.585	1.804	H	-4.813	3.812	-2.43
C	3.885	-1.184	1.363	H	2.311	3.986	-3.689
C	-3.602	3.021	-0.896	H	2.392	2.28	-3.243
C	-0.066	1.538	0.99	H	0.977	-0.302	0.646
C	-1.215	-0.002	-0.731	H	-0.109	-0.322	2.019
C	-4.71	3.598	-1.37	H	-1.014	3.464	-0.487
C	4.767	-2.033	0.471	H	3.558	4.694	-1.778
C	4.699	-4.811	-1.218	H	1.509	1.313	3.218
C	2.3	3.295	-2.834	H	-2.653	3.507	0.943
C	0.644	0.292	1.503	H	-2.676	1.664	-2.302

C	-1.124	2.548	-1.077	H	-2.388	1.272	1.821
C	3.544	3.613	-1.955	H	-4.233	0.463	-0.364
C	1.813	0.588	2.459	H	4.428	5.326	0.006
C	-3.348	2.735	0.579	H	4.991	4.759	1.587
C	-2.464	2.642	-1.851	H	3.348	5.357	1.416
C	-2.591	1.398	0.751	H	4.888	3.725	-3.667
C	-3.391	0.148	0.266	H	5.726	3.529	-2.114
C	-1.217	1.375	-0.031	H	4.897	2.147	-2.855
C	4.132	4.785	0.907	H	-4.338	2.583	2.508
C	4.844	3.23	-2.69	H	-5.012	3.833	1.459
C	-4.594	2.822	1.47	H	-5.383	2.135	1.144
C	4.774	-6.269	-3.077	H	5.5	-6.959	-3.506
C	-3.931	-0.737	1.413	H	3.864	-6.801	-2.789
C	5.516	-4.303	-0.029	H	4.526	-5.481	-3.792
N	3.283	-1.782	2.347	H	-4.606	-0.123	2.023
N	-2.426	-0.573	-0.55	H	-3.089	-1.016	2.057
N	-5.038	-4.135	0.4	H	6.427	-3.837	-0.415
N	4.8	-3.351	0.779	H	5.817	-5.158	0.583
O	3.206	3.122	2.907	H	-2.628	-1.489	-0.932
O	0.204	2.646	1.422	H	-4.895	-5.129	0.298
O	-0.282	-0.5	-1.361	H	4.177	-3.673	1.509
O	5.409	-1.525	-0.45	H	-2.292	4.42	-2.628
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	8.179	1.631	0.163	O	-5.47	5.668	-2.574
C	8.329	3.012	-0.09	O	1.647	-4.565	-2.483
C	6.946	1.095	0.516	O	-3.756	4.259	-2.139
C	7.249	3.883	0.009	S	-1.639	1.739	2.894
C	5.831	1.948	0.621	H	9.044	0.979	0.08
C	6.009	3.339	0.365	H	9.305	3.402	-0.364
C	-3.755	0.192	1.378	H	6.85	0.03	0.712
C	-1.503	-3.702	-1.541	H	7.362	4.946	-0.182
C	-0.575	-2.75	-1.685	H	-4.7	-0.242	1.073
C	-3.636	-2.779	0.161	H	-1.259	-4.597	-0.965
C	3.853	2.995	0.901	H	-0.801	-1.851	-2.256
C	4.441	1.753	0.964	H	-3.323	-1.8	-0.191
C	-2.8	-0.564	1.964	H	2.828	3.281	1.098
C	-3.626	-3.002	1.494	H	5.343	-2.731	-2.196
C	-3.072	-1.976	2.414	H	4.133	-2.757	-3.591

C	-3.652	1.637	1.243	H	-3.097	-4.421	-2.799
C	3.299	-2.988	-1.659	H	-3.049	-2.668	-2.6
C	0.192	-1.405	0.879	H	-0.947	0.263	0.162
C	1.336	-0.303	-1.137	H	0.351	0.679	1.251
C	4.309	-2.813	-2.518	H	0.814	-3.666	-0.382
C	-4.69	2.323	0.378	H	-3.946	-4.768	-0.563
C	-4.904	4.878	-1.844	H	-1.009	-0.54	3.134
C	-2.909	-3.62	-2.071	H	2.848	-3.853	0.218
C	-0.46	-0.046	1.094	H	1.716	-2.566	-3.062
C	0.813	-2.836	-1.096	H	2.576	-1.832	1.457
C	-3.975	-3.742	-0.945	H	4.349	-0.608	-0.49
C	-1.432	0.005	2.287	H	-4.437	-5.014	1.459
C	3.415	-2.988	-0.153	H	-4.744	-4.118	2.956
C	1.874	-3.183	-2.166	H	-3.139	-4.76	2.644
C	2.666	-1.725	0.372	H	-6.151	-3.626	-0.728
C	3.417	-0.396	0.046	H	-5.478	-2.444	-1.866
C	1.228	-1.573	-0.269	H	-5.605	-4.15	-2.335
C	-4.009	-4.299	2.163	H	5.498	-2.314	0.108
C	-5.389	-3.473	-1.5	H	4.8	-3.135	1.512
C	4.831	-3.125	0.416	H	5.282	-4.066	0.083
C	-3.184	4.573	-3.426	H	-2.266	3.99	-3.486
C	3.756	0.456	1.291	H	-3.872	4.29	-4.225
C	-5.469	4.482	-0.48	H	-2.966	5.642	-3.493
N	-2.832	2.397	1.901	H	4.391	-0.155	1.947
N	2.516	0.293	-0.866	H	2.832	0.655	1.848
N	4.785	3.946	0.543	H	-6.393	3.926	-0.665
N	-4.615	3.675	0.354	H	-5.739	5.406	0.039
O	-2.796	-2.256	3.581	H	2.774	1.162	-1.319
O	-0.033	-2.348	1.616	H	4.599	4.934	0.448
O	0.488	0.12	-1.925	H	-3.845	4.102	0.854
O	-5.533	1.666	-0.237	H	2.33	-4.821	-3.124
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.385	5.505	-0.497	O	-5.897	4.122	0.272
C	2.21	6.555	-0.956	O	4.053	-3.152	-2.558
C	1.931	4.356	0.064	O	-7.375	4.061	-1.441
C	3.595	6.477	-0.861	S	-2.234	0.411	2.906
C	3.331	4.242	0.172	H	0.306	5.6	-0.583
C	4.141	5.318	-0.295	H	1.755	7.44	-1.391

C	-3.259	-1.512	0.804	H	1.282	3.558	0.418
C	0.723	-3.983	-1.793	H	4.232	7.284	-1.211
C	1.297	-2.776	-1.81	H	-3.894	-2.198	0.255
C	-1.847	-4.074	-0.549	H	1.096	-4.738	-1.097
C	5.497	3.725	0.528	H	0.931	-2.015	-2.495
C	4.224	3.233	0.696	H	-1.82	-3.01	-0.77
C	-2.218	-1.962	1.54	H	6.447	3.282	0.796
C	-2.016	-4.448	0.739	H	6.997	-2.117	-0.232
C	-2.023	-3.429	1.82	H	6.409	-2.499	-1.942
C	-3.696	-0.125	0.816	H	-0.202	-5.144	-3.363
C	4.898	-1.996	-0.561	H	-0.838	-3.509	-3.177
C	0.932	-1.493	0.973	H	-0.599	-0.155	0.304
C	1.709	0.1	-0.903	H	0.31	0.408	1.688
C	6.167	-2.209	-0.924	H	2.546	-3.196	-0.165
C	-4.743	0.276	-0.204	H	-1.316	-5.956	-1.411
C	-6.447	3.532	-0.637	H	-0.806	-1.483	3.078
C	-0.471	-4.38	-2.619	H	4.021	-2.552	1.294
C	-0.17	-0.482	1.256	H	3.701	-1.227	-2.188
C	2.414	-2.376	-0.879	H	2.992	-0.445	1.862
C	-1.623	-4.959	-1.748	H	4.675	0.683	-0.308
C	-1.261	-0.996	2.212	H	-2.095	-6.593	0.412
C	4.459	-1.643	0.855	H	-2.933	-6.034	1.869
C	3.771	-2.146	-1.59	H	-1.178	-6.096	1.849
C	3.308	-0.61	0.825	H	-2.724	-5.714	-3.472
C	3.718	0.77	0.224	H	-3.703	-5.595	-1.995
C	2.064	-1.11	-0.012	H	-3.286	-4.13	-2.904
C	-2.056	-5.874	1.232	H	6.139	-0.343	1.405
C	-2.914	-5.109	-2.578	H	5.206	-0.968	2.781
C	5.599	-1.216	1.789	H	6.324	-2.026	1.915
C	-7.73	5.437	-1.183	H	-8.485	5.684	-1.928
C	3.854	1.895	1.276	H	-8.136	5.54	-0.175
C	-6.17	2.088	-1.012	H	-6.854	6.08	-1.295
N	-3.378	0.756	1.716	H	4.618	1.581	1.996
N	2.66	1.046	-0.739	H	2.909	1.969	1.831
N	5.454	4.969	-0.066	H	-5.848	2.045	-2.06
N	-5.163	1.554	-0.127	H	-7.104	1.515	-0.949
O	-1.856	-3.758	2.995	H	2.609	1.92	-1.249
O	0.982	-2.561	1.558	H	6.259	5.539	-0.278
O	0.735	0.197	-1.65	H	-4.791	2.16	0.596
O	-5.161	-0.534	-1.037	H	4.227	-3.977	-2.074

Conformation 7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.982	5.02	0.044	O	-3.667	4.146	-1.573
C	4.067	5.81	-0.393	O	2.648	-3.734	-3.039
C	3.169	3.703	0.447	O	-5.582	5.315	-1.871
C	5.36	5.3	-0.432	S	-1.852	0.859	3.326
C	4.465	3.152	0.415	H	1.985	5.452	0.066
C	5.545	3.973	-0.026	H	3.89	6.837	-0.703
C	-3.588	-0.488	1.24	H	2.324	3.109	0.786
C	-0.699	-3.662	-1.985	H	6.198	5.907	-0.764
C	0.199	-2.672	-1.951	H	-4.439	-0.916	0.723
C	-3.076	-3.164	-0.475	H	-0.508	-4.572	-1.412
C	6.375	1.956	0.521	H	0.015	-1.758	-2.51
C	5.023	1.863	0.759	H	-2.782	-2.126	-0.611
C	-2.649	-1.278	1.807	H	7.15	1.214	0.658
C	-3.22	-3.623	0.788	H	5.933	-3.91	-0.961
C	-2.846	-2.766	1.943	H	5.126	-3.895	-2.624
C	-3.614	0.957	1.407	H	-2.048	-4.314	-3.539
C	3.955	-3.132	-1.046	H	-2.162	-2.601	-3.132
C	0.461	-1.658	0.945	H	-0.701	0.086	0.5
C	1.549	-0.165	-0.858	H	0.445	0.284	1.806
C	5.064	-3.668	-1.564	H	1.394	-3.624	-0.499
C	-4.598	1.732	0.555	H	-3.182	-5.009	-1.55
C	-4.782	4.461	-1.215	H	-1.023	-1.366	3.199
C	-2.022	-3.602	-2.702	H	3.098	-3.62	0.836
C	-0.296	-0.413	1.386	H	2.925	-1.852	-2.452
C	1.457	-2.724	-1.121	H	2.802	-1.39	1.7
C	-3.216	-3.935	-1.762	H	4.584	-0.555	-0.52
C	-1.397	-0.689	2.426	H	-3.937	-5.612	0.298
C	3.756	-2.835	0.435	H	-4.41	-5.028	1.903
C	2.76	-2.817	-1.955	H	-2.759	-5.558	1.625
C	2.975	-1.513	0.625	H	-4.623	-4.153	-3.412
C	3.74	-0.254	0.114	H	-5.405	-3.934	-1.833
C	1.579	-1.519	-0.116	H	-4.658	-2.55	-2.653
C	-3.603	-5.034	1.162	H	4.819	-2.645	2.32
C	-4.558	-3.623	-2.455	H	5.491	-3.874	1.245
C	5.04	-2.877	1.273	H	5.79	-2.163	0.914
C	-5.048	5.875	-3.09	H	-5.831	6.526	-3.478
C	4.286	0.646	1.246	H	-4.142	6.448	-2.879

C	-5.489	3.948	0.04	H	-4.821	5.08	-3.804
N	-2.968	1.62	2.317	H	4.955	0.032	1.861
N	2.751	0.434	-0.704	H	3.447	0.94	1.89
N	6.691	3.212	0.049	H	-6.398	3.425	-0.27
N	-4.672	3.057	0.823	H	-5.793	4.804	0.649
O	-2.673	-3.255	3.059	H	2.935	1.333	-1.132
O	0.258	-2.744	1.46	H	7.621	3.527	-0.186
O	0.605	0.299	-1.497	H	-4.014	3.432	1.494
O	-5.28	1.162	-0.299	H	2.602	-4.627	-2.657
Conformation 8							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.414	5.415	-0.632	O	-7.315	2.679	0.466
C	3.398	6.292	-1.136	O	3.723	-3.576	-2.452
C	2.765	4.207	-0.038	O	-7.759	3.942	-1.359
C	4.752	5.981	-1.053	S	-2.052	0.924	2.897
C	4.126	3.859	0.058	H	1.366	5.691	-0.709
C	5.101	4.764	-0.455	H	3.094	7.229	-1.595
C	-3.298	-0.813	0.755	H	1.996	3.544	0.349
C	0.288	-3.907	-1.744	H	5.511	6.656	-1.438
C	1.039	-2.801	-1.761	H	-4.017	-1.392	0.187
C	-2.288	-3.58	-0.555	H	0.526	-4.7	-1.031
C	6.178	2.988	0.406	H	0.805	-2.005	-2.464
C	4.841	2.728	0.605	H	-2.084	-2.537	-0.782
C	-2.365	-1.42	1.522	H	7.042	2.397	0.678
C	-2.549	-3.911	0.729	H	6.717	-3.043	-0.032
C	-2.412	-2.898	1.808	H	6.117	-3.364	-1.751
C	-3.505	0.626	0.755	H	-0.773	-4.936	-3.32
C	4.683	-2.563	-0.429	H	-1.149	-3.218	-3.17
C	0.822	-1.443	1.016	H	-0.466	0.129	0.339
C	1.826	-0.008	-0.877	H	0.498	0.526	1.745
C	5.903	-3.007	-0.748	H	2.174	-3.377	-0.08
C	-4.438	1.191	-0.298	H	-2.045	-5.532	-1.388
C	-6.957	3.229	-0.554	H	-0.934	-1.167	3.097
C	-0.936	-4.127	-2.592	H	3.696	-2.912	1.421
C	-0.111	-0.271	1.293	H	3.659	-1.62	-2.082
C	2.181	-2.557	-0.807	H	3.001	-0.646	1.897
C	-2.182	-4.504	-1.741	H	4.843	0.113	-0.312
C	-1.287	-0.615	2.222	H	-3.011	-6.006	0.405
C	4.278	-2.097	0.964	H	-3.717	-5.31	1.873

C	3.574	-2.539	-1.487	H	-2.001	-5.686	1.83
C	3.299	-0.902	0.874	H	-4.332	-4.81	-2.033
C	3.921	0.373	0.225	H	-3.67	-3.439	-2.943
C	2.003	-1.24	0.036	H	-3.349	-5.097	-3.484
C	-2.834	-5.308	1.225	H	5.085	-1.468	2.881
C	-3.463	-4.459	-2.6	H	6.032	-2.73	2.089
C	5.452	-1.82	1.911	H	6.136	-1.064	1.508
C	-9.142	4.033	-0.958	H	-9.629	4.633	-1.727
C	4.257	1.494	1.235	H	-9.589	3.038	-0.908
C	-5.536	3.212	-1.119	H	-9.223	4.52	0.016
N	-3.083	1.445	1.67	H	4.965	1.081	1.964
N	2.908	0.788	-0.736	H	3.345	1.746	1.791
N	6.338	4.202	-0.229	H	-5.209	4.241	-1.291
N	-4.597	2.535	-0.262	H	-5.562	2.707	-2.089
O	-2.321	-3.244	2.986	H	2.988	1.644	-1.272
O	0.702	-2.504	1.605	H	7.226	4.619	-0.469
O	0.872	0.218	-1.623	H	-4.188	3.026	0.524
O	-4.973	0.455	-1.129	H	3.757	-4.418	-1.967
Conformation 9							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-8.275	-1.23	-0.22	O	5.127	-6.018	-2.145
C	-8.552	-2.56	-0.603	O	-2.189	3.689	-2.861
C	-7.031	-0.872	0.286	O	3.491	-4.544	-1.632
C	-7.591	-3.559	-0.484	S	2.307	-1.228	3.264
C	-6.034	-1.858	0.416	H	-9.05	-0.475	-0.324
C	-6.339	-3.194	0.027	H	-9.534	-2.809	-0.996
C	4	0.031	1.093	H	-6.835	0.156	0.58
C	1.188	3.422	-1.954	H	-7.803	-4.584	-0.776
C	0.24	2.482	-1.89	H	4.848	0.41	0.534
C	3.592	2.764	-0.555	H	1.072	4.335	-1.365
C	-4.222	-3.151	0.784	H	0.35	1.567	-2.467
C	-4.673	-1.855	0.9	H	3.22	1.751	-0.689
C	3.15	0.873	1.723	H	-3.262	-3.571	1.05
C	3.826	3.19	0.706	H	-5.364	4.027	-0.639
C	3.451	2.341	1.867	H	-4.631	3.993	-2.335
C	3.935	-1.415	1.237	H	2.506	4.022	-3.556
C	-3.441	3.135	-0.821	H	2.535	2.298	-3.179
C	0.042	1.445	1.007	H	1.055	-0.378	0.522
C	-1.188	0.035	-0.769	H	-0.036	-0.487	1.885

C	-4.538	3.745	-1.282	H	-0.837	3.476	-0.376
C	4.805	-2.24	0.311	H	3.765	4.614	-1.609
C	4.687	-5.118	-1.458	H	1.608	1.044	3.201
C	2.473	3.298	-2.729	H	-2.48	3.538	1.032
C	0.731	0.153	1.423	H	-2.546	1.818	-2.282
C	-0.976	2.59	-1.005	H	-2.285	1.277	1.847
C	3.724	3.543	-1.837	H	-4.184	0.589	-0.328
C	1.898	0.354	2.404	H	4.628	5.145	0.206
C	-3.2	2.8	0.646	H	5.179	4.492	1.759
C	-2.306	2.766	-1.783	H	3.547	5.127	1.615
C	-2.489	1.433	0.781	H	5.073	3.702	-3.541
C	-3.339	0.228	0.273	H	5.903	3.409	-1.999
C	-1.122	1.379	-0.012	H	5.039	2.088	-2.808
C	4.322	4.566	1.08	H	-5.252	2.247	1.194
C	5.015	3.162	-2.589	H	-4.197	2.629	2.569
C	-4.444	2.902	1.538	H	-4.831	3.925	1.551
C	2.703	-5.054	-2.728	H	1.777	-4.481	-2.711
C	-3.885	-0.677	1.402	H	3.23	-4.907	-3.673
C	5.483	-4.513	-0.3	H	2.5	-6.118	-2.585
N	3.302	-2.048	2.178	H	-4.507	-0.056	2.059
N	-2.417	-0.496	-0.589	H	-3.037	-1.026	2.004
N	-5.214	-3.955	0.263	H	6.346	-4.005	-0.739
N	4.779	-3.575	0.537	H	5.86	-5.345	0.302
O	3.363	2.824	2.996	H	-2.662	-1.386	-1.006
O	0.337	2.515	1.512	H	-5.13	-4.947	0.097
O	-0.288	-0.473	-1.438	H	4.141	-3.91	1.248
O	5.483	-1.7	-0.565	H	-2.088	4.575	-2.473
Conformation 10							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-7.667	-3.466	-0.919	O	6.42	-4.585	-0.698
C	-8.44	-3.456	0.263	O	-2.72	3.943	-2.725
C	-6.321	-3.121	-0.9	O	8.287	-3.992	-1.831
C	-7.88	-3.104	1.487	S	2.093	-1.905	2.14
C	-5.724	-2.757	0.323	H	-8.136	-3.748	-1.858
C	-6.523	-2.758	1.502	H	-9.49	-3.73	0.216
C	3.583	0.595	1.306	H	-5.738	-3.136	-1.817
C	0.285	4.101	-1.074	H	-8.472	-3.099	2.398
C	-0.21	2.954	-1.549	H	4.32	1.388	1.242
C	2.465	3.551	0.73	H	-0.316	4.693	-0.38

C	-4.435	-2.149	2.07	H	0.378	2.353	-2.24
C	-4.39	-2.362	0.712	H	2.539	2.643	0.136
C	2.382	0.809	1.886	H	-3.643	-1.859	2.748
C	2.295	3.418	2.064	H	-5.924	1.53	-2.655
C	2.087	2.071	2.655	H	-4.778	2.299	-3.883
C	4.032	-0.717	0.867	H	1.604	5.605	-1.878
C	-3.958	1.966	-1.965	H	2.182	3.946	-2.053
C	-0.601	0.834	0.537	H	1.101	-0.158	-0.308
C	-1.114	-0.025	-1.838	H	-0.048	-1.215	0.472
C	-4.936	1.921	-2.876	H	-1.93	2.998	-0.325
C	5.313	-0.773	0.059	H	2.081	5.642	0.493
C	7.165	-3.738	-1.152	H	0.649	-0.115	2.74
C	1.662	4.632	-1.37	H	-3.835	2.304	0.123
C	0.467	-0.249	0.581	H	-2.204	2.077	-3.224
C	-1.571	2.414	-1.18	H	-2.993	0.186	0.797
C	2.514	4.817	-0.084	H	-4.128	-0.894	-1.624
C	1.302	-0.256	1.875	H	2.328	5.527	2.572
C	-4.079	1.463	-0.541	H	2.858	4.444	3.87
C	-2.599	2.573	-2.33	H	1.148	4.563	3.486
C	-2.976	0.399	-0.276	H	4.557	5.387	0.464
C	-3.191	-0.933	-1.058	H	4.458	4.379	-0.992
C	-1.539	0.919	-0.695	H	3.989	6.088	-1.066
C	2.15	4.558	3.041	H	-5.839	0.149	-0.715
C	3.968	5.189	-0.439	H	-5.473	0.686	0.927
C	-5.477	0.995	-0.123	H	-6.197	1.813	-0.234
C	8.613	-5.387	-2.022	H	7.821	-5.887	-2.582
C	-3.193	-2.212	-0.181	H	9.544	-5.39	-2.587
C	6.939	-2.243	-1.023	H	8.748	-5.878	-1.056
N	3.509	-1.849	1.227	H	-2.276	-2.224	0.422
N	-2.078	-0.957	-1.998	H	-3.126	-3.075	-0.858
N	-5.708	-2.38	2.547	H	6.89	-1.801	-2.026
N	5.724	-2.011	-0.28	H	7.806	-1.79	-0.525
O	1.649	1.943	3.799	H	-1.97	-1.686	-2.694
O	-0.779	1.596	1.471	H	-5.987	-2.309	3.515
O	-0.082	0.051	-2.506	H	5.195	-2.817	0.035
O	5.913	0.26	-0.254	H	-3.197	4.408	-2.017
Conformation 11							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-8.346	-2.337	-0.321	O	7.796	-4.715	-1.792

C	-8.456	-3.595	-0.952	O	-3.227	3.826	-2.132
C	-7.135	-1.899	0.201	O	7.313	-3.504	0.055
C	-7.358	-4.44	-1.069	S	2.406	-1.447	2.624
C	-6.002	-2.728	0.096	H	-9.225	-1.703	-0.244
C	-6.14	-3.995	-0.541	H	-9.416	-3.911	-1.351
C	3.709	0.347	0.562	H	-7.068	-0.928	0.686
C	0.25	3.833	-1.58	H	-7.44	-5.411	-1.551
C	-0.589	2.794	-1.633	H	4.448	0.913	0.007
C	2.842	3.251	-0.534	H	0.11	4.589	-0.804
C	-4.005	-3.777	0.13	H	-0.454	2.034	-2.4
C	-4.625	-2.612	0.519	H	2.56	2.239	-0.815
C	2.844	0.962	1.398	H	-2.979	-4.09	0.271
C	3.169	3.481	0.757	H	-6.143	3.36	0.4
C	3.001	2.411	1.775	H	-5.601	3.752	-1.323
C	3.819	-1.1	0.461	H	1.316	4.882	-3.139
C	-4.176	2.752	-0.134	H	1.571	3.136	-3.111
C	-0.359	1.243	1.04	H	0.792	-0.345	0.184
C	-1.551	0.017	-0.892	H	-0.138	-0.798	1.594
C	-5.369	3.311	-0.359	H	-1.597	3.34	0.136
C	4.685	-1.651	-0.654	H	2.706	5.264	-1.235
C	7.029	-4.034	-1.14	H	1.455	0.699	3.008
C	1.45	4.019	-2.47	H	-3.073	2.89	1.679
C	0.503	-0.004	1.183	H	-3.313	1.85	-1.898
C	-1.703	2.575	-0.641	H	-2.555	0.546	1.968
C	2.755	4.253	-1.656	H	-4.548	0.09	-0.192
C	1.735	0.187	2.084	H	3.768	5.556	0.545
C	-3.744	2.159	1.202	H	4.459	4.724	1.948
C	-3.123	2.715	-1.248	H	2.774	5.218	1.977
C	-2.876	0.899	0.981	H	4.907	4.425	-2.025
C	-3.624	-0.276	0.276	H	4.11	3.165	-2.986
C	-1.593	1.194	0.106	H	3.89	4.873	-3.41
C	3.563	4.822	1.327	H	-5.655	1.247	1.783
C	3.992	4.173	-2.572	H	-4.505	1.471	3.117
C	-4.889	1.915	2.193	H	-5.381	2.856	2.46
C	8.634	-3.778	0.567	H	8.679	-3.281	1.536
C	-3.976	-1.45	1.219	H	8.781	-4.854	0.679
C	5.624	-3.688	-1.635	H	9.392	-3.374	-0.107
N	3.365	-1.95	1.332	H	-4.634	-1.064	2.007
N	-2.694	-0.691	-0.763	H	-3.054	-1.782	1.711
N	-4.905	-4.607	-0.505	H	5.157	-4.623	-1.958

N	4.768	-3.002	-0.701	H	5.744	-3.056	-2.52
O	2.975	2.685	2.975	H	-2.861	-1.512	-1.332
O	-0.14	2.247	1.696	H	-4.692	-5.524	-0.87
O	-0.645	-0.238	-1.686	H	4.334	-3.515	0.058
O	5.242	-0.896	-1.453	H	-3.152	4.631	-1.593
Conformation 12							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-7.878	-2.886	-0.92	O	5.376	-3.131	-2.183
C	-8.723	-2.636	0.183	O	-1.985	3.769	-3.108
C	-6.506	-2.678	-0.835	O	7.496	-3.924	-2.21
C	-8.212	-2.177	1.393	S	1.717	-2.049	2.659
C	-5.957	-2.211	0.374	H	-8.311	-3.247	-1.849
C	-6.829	-1.97	1.474	H	-9.791	-2.807	0.087
C	3.568	0.157	1.724	H	-5.868	-2.878	-1.693
C	0.894	3.74	-1.241	H	-8.86	-1.987	2.244
C	0.3	2.612	-1.644	H	4.402	0.847	1.649
C	2.872	3.149	0.775	H	0.321	4.466	-0.66
C	-4.729	-1.502	2.127	H	0.86	1.879	-2.22
C	-4.617	-1.902	0.816	H	2.891	2.181	0.281
C	2.363	0.571	2.174	H	-3.958	-1.201	2.824
C	2.585	3.177	2.095	H	-5.401	1.637	-3.183
C	2.171	1.932	2.792	H	-4.066	2.14	-4.357
C	3.878	-1.237	1.451	H	2.433	4.992	-2.082
C	-3.484	1.99	-2.331	H	2.823	3.27	-2.042
C	-0.511	0.786	0.588	H	1.137	-0.439	-0.023
C	-0.948	-0.259	-1.727	H	-0.171	-1.303	0.743
C	-4.362	1.91	-3.336	H	-1.496	2.983	-0.594
C	5.193	-1.528	0.756	H	2.747	5.232	0.305
C	6.402	-3.427	-1.61	H	0.469	-0.047	2.958
C	2.342	4.079	-1.476	H	-3.515	2.567	-0.294
C	0.433	-0.386	0.814	H	-1.622	1.826	-3.417
C	-1.142	2.273	-1.351	H	-2.985	0.48	0.7
C	3.122	4.309	-0.151	H	-4.05	-0.79	-1.653
C	1.162	-0.355	2.17	H	2.854	5.308	2.405
C	-3.796	1.681	-0.881	H	3.102	4.312	3.849
C	-2.042	2.43	-2.605	H	1.47	4.604	3.268
C	-2.854	0.546	-0.384	H	5.174	4.718	0.493
C	-3.161	-0.846	-1.017	H	5.059	3.571	-0.855
C	-1.336	0.847	-0.723	H	4.792	5.301	-1.14

C	2.501	4.424	2.94	H	-5.672	0.546	-1.089
C	4.629	4.484	-0.427	H	-5.407	1.253	0.507
C	-5.273	1.42	-0.567	H	-5.877	2.287	-0.854
C	7.412	-4.095	-3.64	H	8.379	-4.495	-3.943
C	-3.354	-1.993	0.009	H	6.611	-4.794	-3.893
C	6.654	-3.286	-0.108	H	7.225	-3.134	-4.127
N	3.191	-2.256	1.869	H	-2.485	-2.015	0.679
N	-1.999	-1.097	-1.86	H	-3.337	-2.94	-0.548
N	-6.05	-1.536	2.525	H	7.463	-2.564	0.035
N	5.492	-2.841	0.616	H	6.995	-4.247	0.287
O	1.636	1.976	3.899	H	-1.929	-1.909	-2.462
O	-0.678	1.648	1.433	H	-6.384	-1.302	3.448
O	0.126	-0.367	-2.318	H	4.788	-3.51	0.903
O	5.922	-0.61	0.375	H	-2.464	4.336	-2.481
Conformation 13							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.362	4.632	-0.074	O	4.445	6.095	2.151
C	-4.516	5.312	0.372	O	-2.131	-4.114	2.908
C	-3.423	3.304	-0.481	O	2.902	4.517	1.657
C	-5.753	4.678	0.417	S	1.837	1.181	-3.267
C	-4.66	2.631	-0.445	H	-2.411	5.158	-0.1
C	-5.811	3.341	0.005	H	-4.436	6.349	0.685
C	3.668	0.031	-1.149	H	-2.527	2.794	-0.826
C	1.187	-3.588	1.921	H	-6.643	5.201	0.757
C	0.174	-2.716	1.891	H	4.556	-0.289	-0.614
C	3.504	-2.742	0.474	H	1.121	-4.502	1.327
C	-6.446	1.257	-0.55	H	0.233	-1.802	2.476
C	-5.092	1.297	-0.795	H	3.064	-1.76	0.63
C	2.869	-0.866	-1.768	H	-7.147	0.445	-0.689
C	3.74	-3.137	-0.797	H	-5.372	-4.585	0.806
C	3.274	-2.306	-1.938	H	-4.587	-4.516	2.478
C	3.492	1.469	-1.274	H	2.585	-4.108	3.484
C	-3.49	-3.599	0.928	H	2.481	-2.383	3.126
C	-0.174	-1.671	-0.988	H	0.713	0.217	-0.509
C	-1.455	-0.365	0.832	H	-0.411	0.257	-1.848
C	-4.54	-4.263	1.423	H	-0.875	-3.771	0.397
C	4.321	2.347	-0.359	H	3.831	-4.589	1.498
C	4.048	5.179	1.458	H	1.31	-1.138	-3.213
C	2.479	-3.38	2.666	H	-2.56	-3.943	-0.951

C	0.409	-0.329	-1.407	H	-2.625	-2.257	2.385
C	-1.057	-2.902	1.039	H	-2.526	-1.677	-1.768
C	3.721	-3.527	1.742	H	-4.421	-1.104	0.441
C	1.566	-0.436	-2.416	H	4.695	-5.032	-0.341
C	-3.312	-3.251	-0.544	H	5.157	-4.325	-1.898
C	-2.345	-3.178	1.856	H	3.581	-5.08	-1.722
C	-2.693	-1.842	-0.697	H	5.121	-3.615	3.411
C	-3.609	-0.693	-0.173	H	5.89	-3.242	1.854
C	-1.314	-1.696	0.061	H	4.956	-1.997	2.704
C	4.325	-4.469	-1.199	H	-5.407	-2.818	-1.034
C	5.001	-3.067	2.469	H	-4.371	-3.144	-2.438
C	-4.573	-3.427	-1.399	H	-4.901	-4.472	-1.4
C	2.115	4.948	2.788	H	1.238	4.303	2.793
C	-4.241	0.162	-1.295	H	2.685	4.83	3.712
C	4.846	4.657	0.263	H	1.824	5.994	2.669
N	2.792	2.062	-2.193	H	-4.845	-0.507	-1.919
N	-2.719	0.087	0.676	H	-3.435	0.546	-1.934
N	-6.879	2.474	-0.068	H	5.763	4.214	0.662
N	4.189	3.679	-0.567	H	5.134	5.525	-0.337
O	3.194	-2.782	-3.071	H	-3.012	0.951	1.116
O	0.183	-2.713	-1.51	H	-7.835	2.697	0.168
O	-0.578	0.196	1.489	H	3.512	3.974	-1.259
O	5.058	1.85	0.495	H	-2.001	-4.985	2.495
Conformation 14							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	5.009	-1.683	-3.189	O	-7.935	-3.048	2.479
C	6.395	-1.942	-3.26	O	2.134	4.194	2.547
C	4.317	-1.793	-1.988	O	-5.769	-2.404	2.395
C	7.114	-2.32	-2.131	S	-1.587	-2.618	-1.914
C	5.015	-2.171	-0.824	H	4.476	-1.392	-4.09
C	6.413	-2.432	-0.924	H	6.909	-1.846	-4.212
C	-3.261	-0.096	-1.823	H	3.249	-1.592	-1.955
C	-0.565	3.898	0.531	H	8.18	-2.524	-2.183
C	-0.16	2.828	1.229	H	-4.01	0.658	-2.037
C	-2.337	2.968	-1.541	H	0.156	4.426	-0.098
C	5.786	-2.775	1.207	H	-0.867	2.285	1.852
C	4.637	-2.394	0.552	H	-2.527	2.163	-0.836
C	-1.972	0.083	-2.185	H	5.929	-3.045	2.245
C	-1.891	2.633	-2.772	H	5.048	1.802	3.923

C	-1.551	1.22	-3.081	H	3.598	2.645	4.696
C	-3.764	-1.341	-1.263	H	-2.044	5.437	0.819
C	3.382	2.159	2.651	H	-2.615	3.797	1.138
C	0.745	0.438	-0.341	H	-1.113	-0.396	0.335
C	0.829	-0.016	2.19	H	0.137	-1.566	0.004
C	4.043	2.197	3.811	H	1.787	2.81	0.405
C	-5.174	-1.329	-0.71	H	-2.038	5.087	-1.577
C	-6.942	-2.744	1.848	H	-0.092	-0.878	-2.528
C	-1.983	4.397	0.47	H	3.79	2.274	0.58
C	-0.324	-0.646	-0.383	H	1.385	2.459	3.404
C	1.265	2.33	1.238	H	3.21	0.074	-0.05
C	-2.565	4.342	-0.971	H	3.846	-0.757	2.631
C	-0.896	-0.909	-1.789	H	-1.853	4.63	-3.62
C	3.892	1.524	1.376	H	-2.067	3.327	-4.802
C	1.989	2.769	2.539	H	-0.485	3.6	-4.09
C	2.938	0.357	0.969	H	-4.466	4.727	-1.985
C	3.042	-0.892	1.899	H	-4.642	3.96	-0.396
C	1.417	0.789	1.014	H	-4.223	5.68	-0.507
C	-1.559	3.61	-3.873	H	5.606	0.372	2.146
C	-4.066	4.697	-0.966	H	5.654	0.703	0.412
C	5.37	1.12	1.384	H	5.996	1.998	1.574
C	-5.724	-2.405	3.837	H	-4.706	-2.119	4.096
C	3.274	-2.241	1.171	H	-6.44	-1.684	4.239
C	-6.931	-2.693	0.32	H	-5.954	-3.401	4.223
N	-3.158	-2.488	-1.317	H	2.496	-2.371	0.408
N	1.767	-0.894	2.606	H	3.114	-3.039	1.908
N	6.85	-2.793	0.332	H	-7.56	-1.849	0.023
N	-5.641	-2.532	-0.302	H	-7.415	-3.606	-0.037
O	-0.888	0.934	-4.078	H	1.568	-1.53	3.369
O	1.121	1.007	-1.35	H	7.795	-3.055	0.573
O	-0.297	0.108	2.671	H	-4.998	-3.314	-0.343
O	-5.822	-0.281	-0.661	H	1.245	4.556	2.378
Conformation 15							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-5.034	4.988	-0.183	O	-4.976	-1.942	-0.664
C	-6.067	4.231	-0.778	O	4.656	4.073	-0.956
C	-3.89	4.374	0.314	O	-6.687	-3.416	-0.788
C	-5.977	2.847	-0.884	S	0.205	-2.108	2.435
C	-3.766	2.974	0.222	H	-5.137	6.068	-0.115

C	-4.825	2.23	-0.38	H	-6.949	4.739	-1.159
C	0.253	-3.924	-0.002	H	-3.104	4.969	0.773
C	5.13	0.485	-0.418	H	-6.773	2.264	-1.339
C	4.092	1.169	-0.913	H	0.227	-4.747	-0.708
C	4.725	-2.603	-0.88	H	5.413	0.633	0.627
C	-3.237	0.784	0.263	H	3.797	1.022	-1.95
C	-2.758	2.022	0.627	H	4.32	-2.536	-1.891
C	1.434	-3.333	0.285	H	-2.794	-0.193	0.4
C	4.002	-3.272	0.035	H	2.44	5.891	-1.916
C	2.678	-3.811	-0.426	H	1.393	6.464	-0.507
C	-1.002	-3.558	0.63	H	5.683	-0.464	-2.26
C	2.356	4.583	-0.259	H	7.031	-0.07	-1.196
C	1.858	0.447	0.926	H	0.366	-0.69	-0.14
C	0.961	1.687	-1.12	H	2.007	-0.938	-0.671
C	2.04	5.698	-0.924	H	3.772	2.326	0.838
C	-2.271	-4.141	0.042	H	6.296	-1.89	0.387
C	-5.449	-3.043	-0.454	H	2.433	-2.006	1.678
C	6.001	-0.456	-1.208	H	2.712	3.996	1.741
C	1.39	-0.82	0.23	H	3.04	3.399	-1.923
C	3.295	2.199	-0.143	H	0.975	2.495	2.06
C	6.05	-1.917	-0.682	H	-0.656	3.998	0.235
C	1.503	-2.067	1.113	H	3.601	-3.924	2.07
C	1.834	4.212	1.113	H	4.783	-2.606	1.965
C	3.319	3.566	-0.878	H	5.233	-4.252	1.507
C	1.06	2.864	1.035	H	6.964	-2.758	-2.486
C	-0.368	2.957	0.41	H	7.225	-3.733	-1.029
C	1.81	1.791	0.163	H	8.132	-2.224	-1.263
C	4.421	-3.515	1.472	H	0.167	5.639	1.299
C	7.159	-2.708	-1.408	H	1.689	6.185	2.008
C	1.054	5.307	1.848	H	0.725	4.946	2.828
C	-7.501	-2.428	-1.457	H	-8.449	-2.924	-1.66
C	-1.441	2.28	1.3	H	-7.025	-2.114	-2.389
C	-4.714	-4.195	0.228	H	-7.652	-1.562	-0.809
N	-1.121	-2.844	1.708	H	-1.569	2.915	2.188
N	-0.216	2.302	-0.883	H	-1.04	1.324	1.66
N	-4.468	0.901	-0.34	H	-4.597	-5.008	-0.495
N	-3.409	-3.821	0.706	H	-5.337	-4.568	1.047
O	2.583	-4.552	-1.399	H	-0.952	2.302	-1.578
O	2.305	0.422	2.06	H	-5.009	0.105	-0.657
O	1.284	1.126	-2.167	H	-3.322	-3.19	1.493

O	-2.231	-4.849	-0.965	H	4.924	4.339	-0.061

Figure S5. (+)-HR-ESI-MS Spectrum of **1**

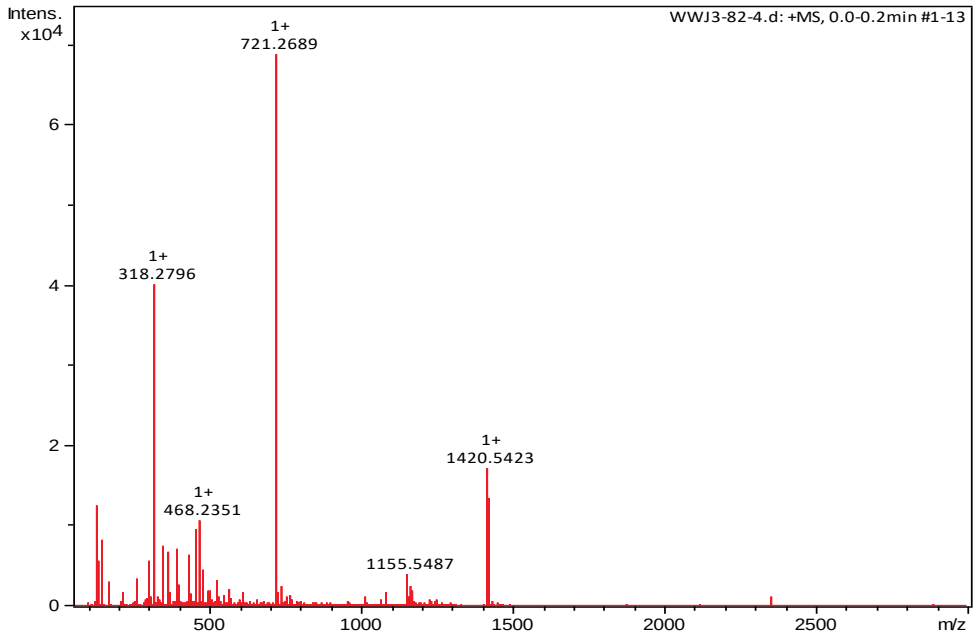

Figure S6. IR Spectrum of **1**

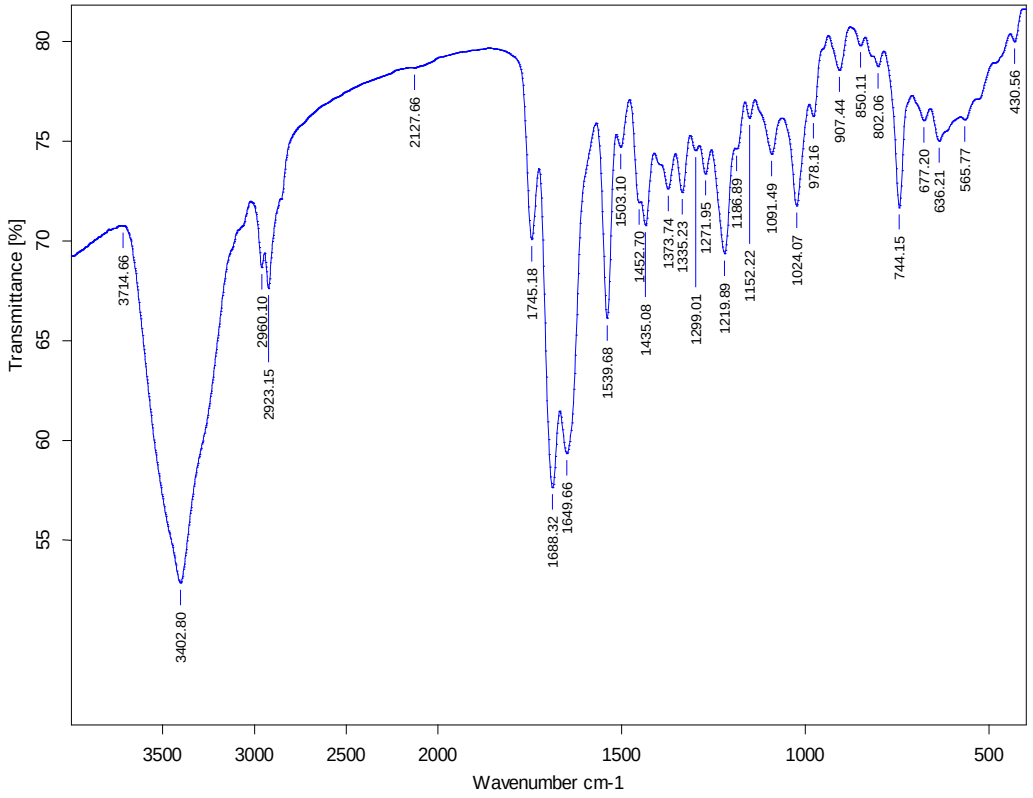

Figure S7. UV Spectrum of **1**

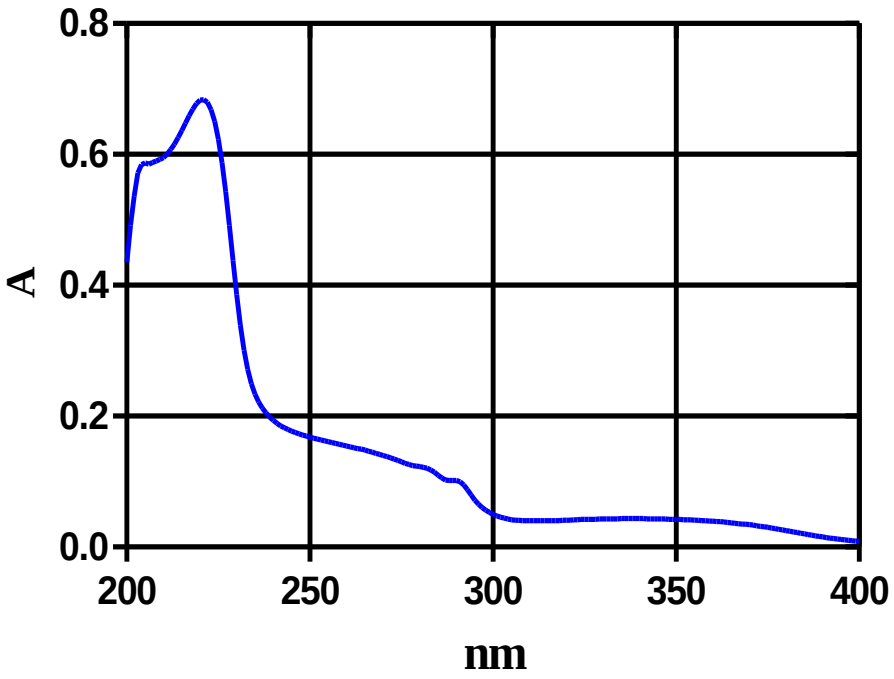

Figure S8. ^{1}H NMR Spectrum of **1** in DMSO-d_6

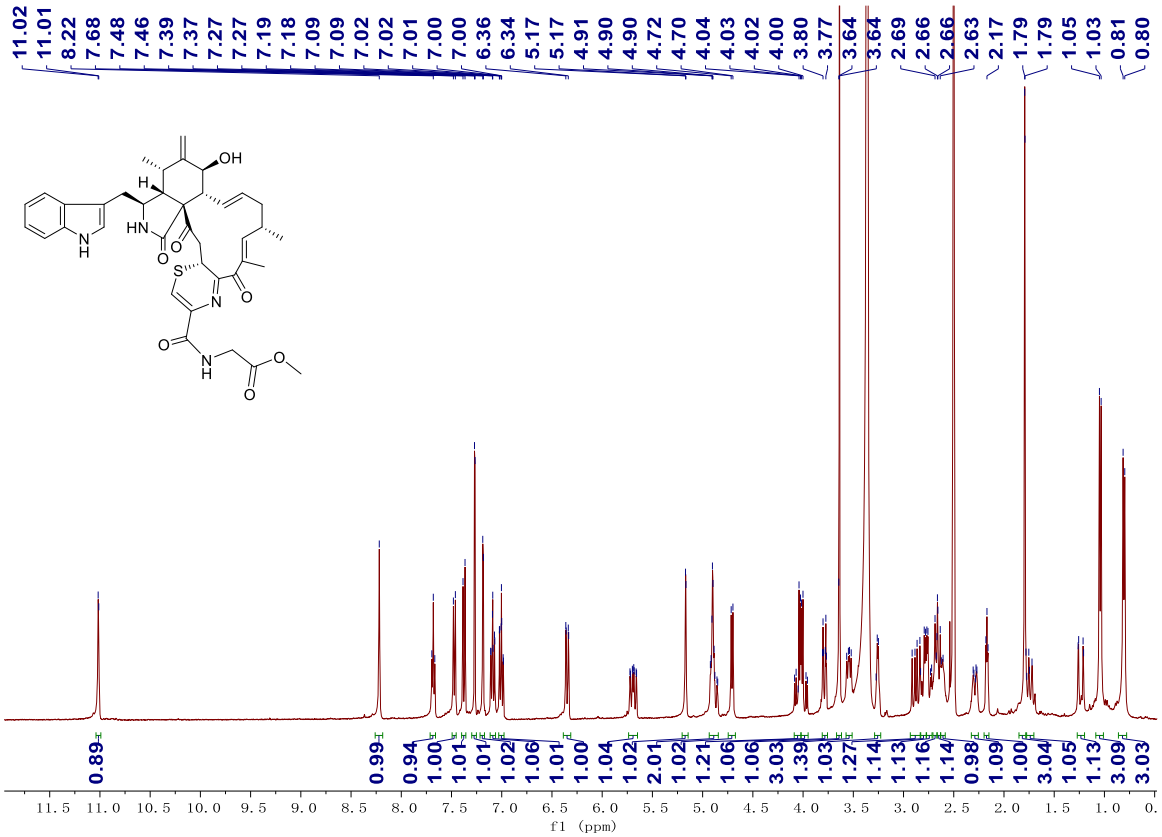

Figure S9. ^{13}C NMR Spectrum of **1** in DMSO-d_6

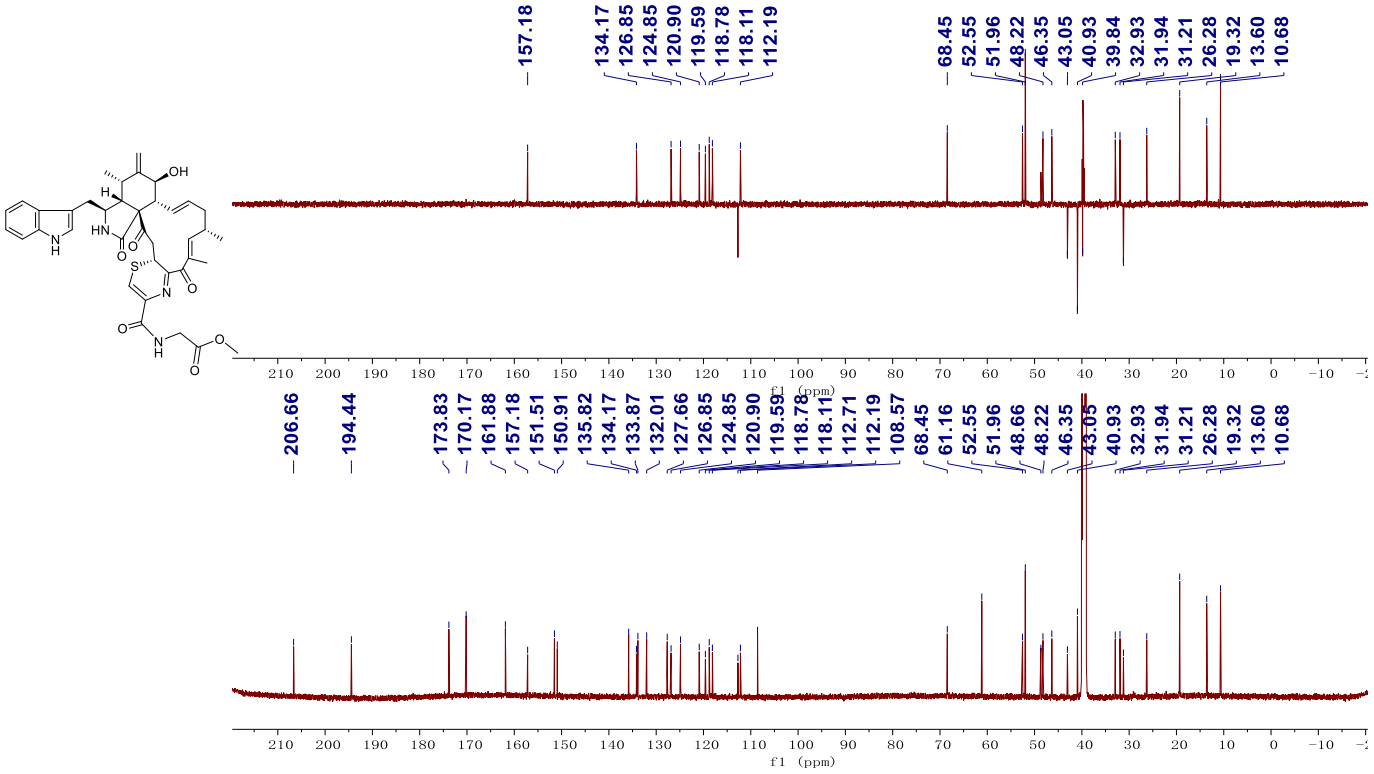

Figure S10. HSQC Spectrum of **1** in DMSO-d_6

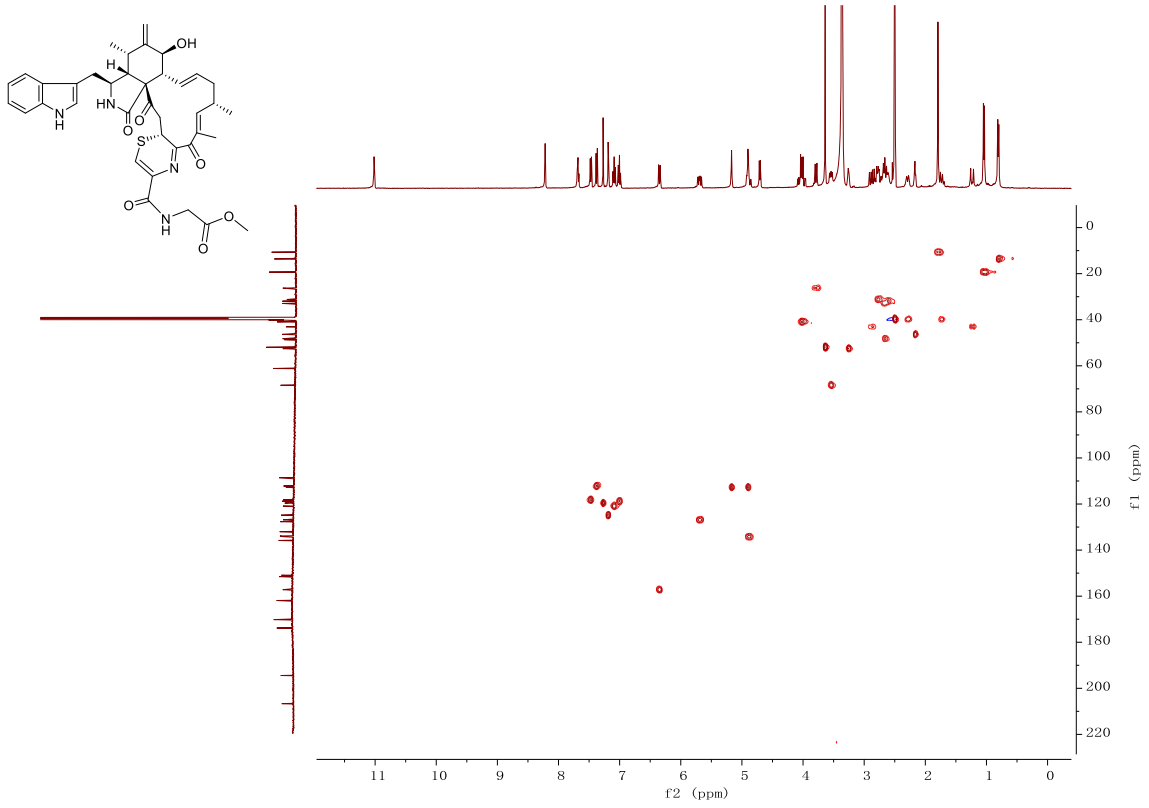

Figure S11. HMBC Spectrum of **1** in DMSO-d_6

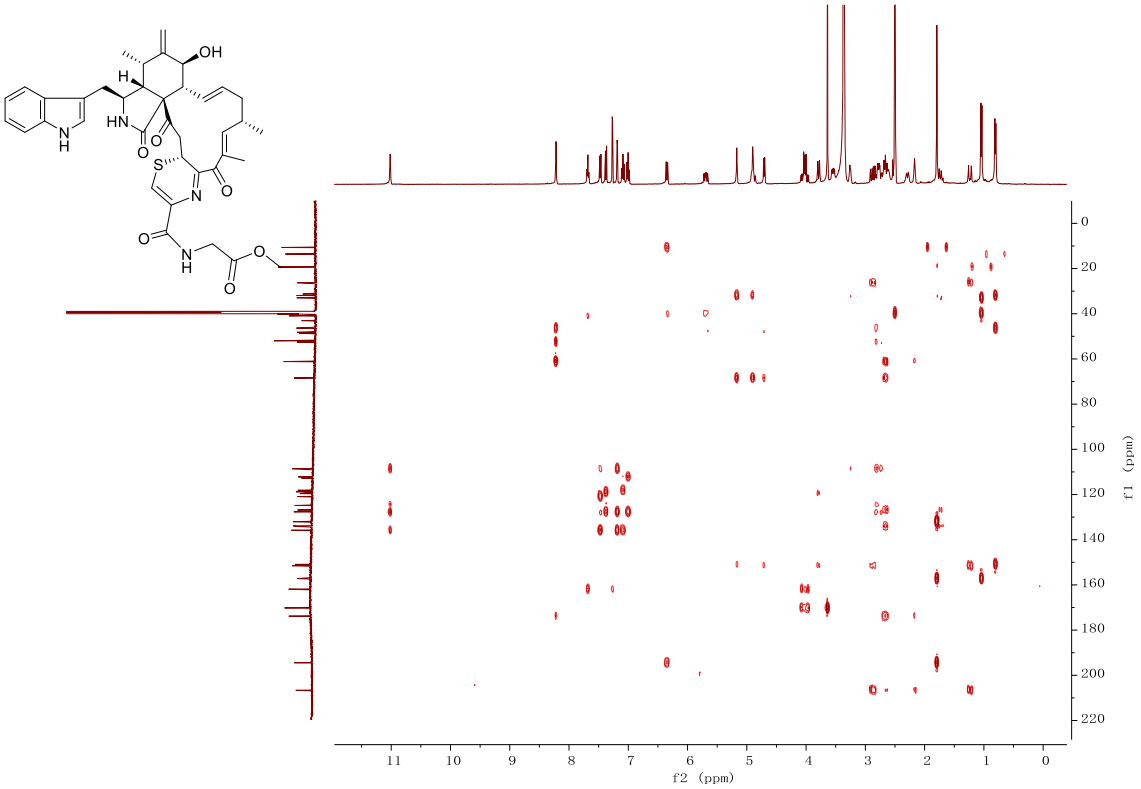

Figure S12. ^{1}H–^{1}H COSY Spectrum of **1** in DMSO-d_6

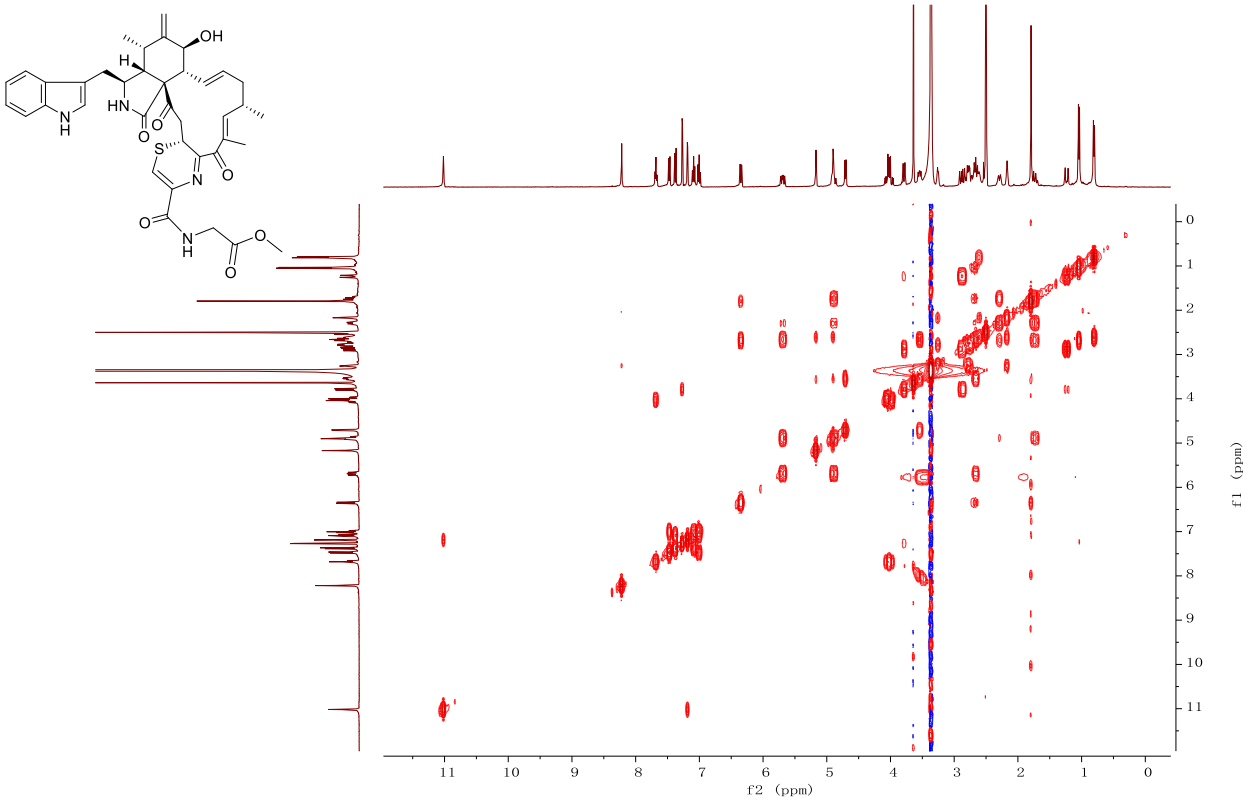

Figure S13. NOESY Spectrum of **1** in DMSO-d_6

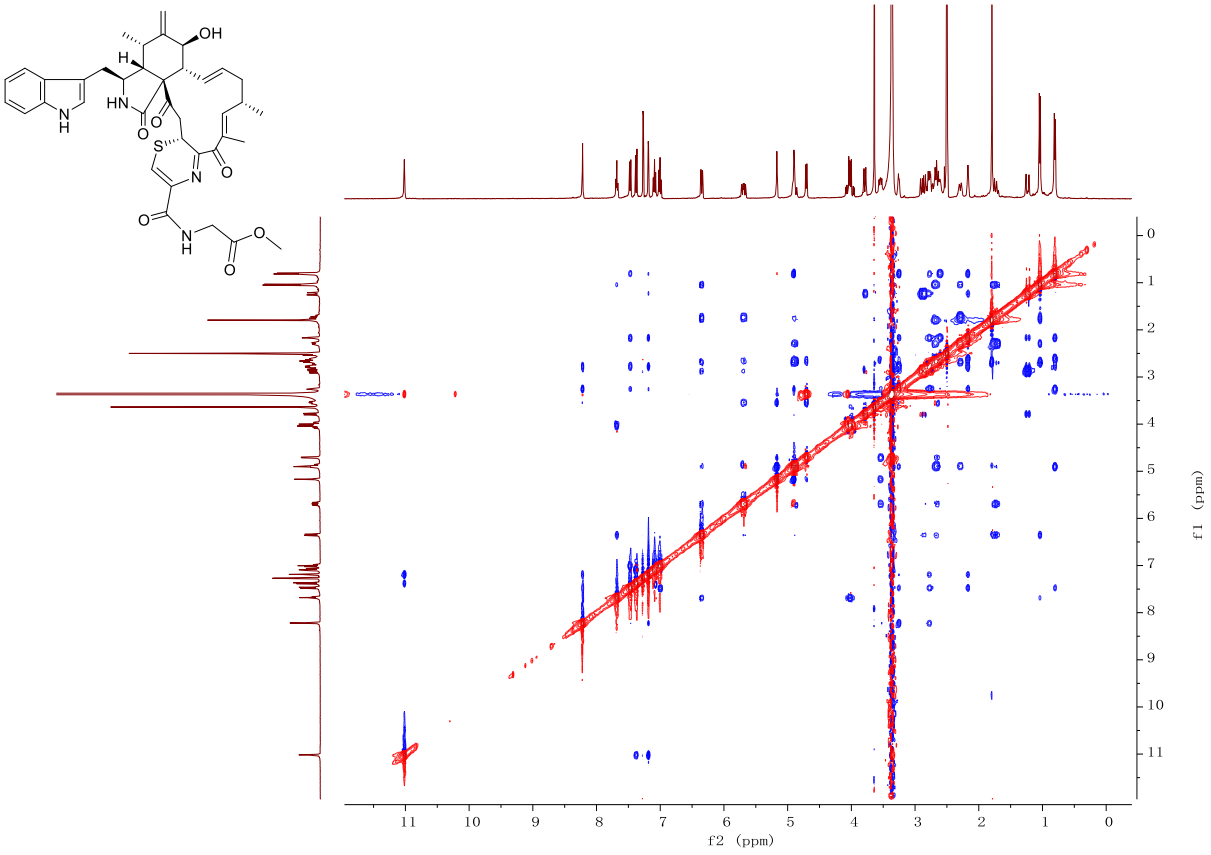

Figure S14. (+)-HR-ESI-MS Spectrum of **2**

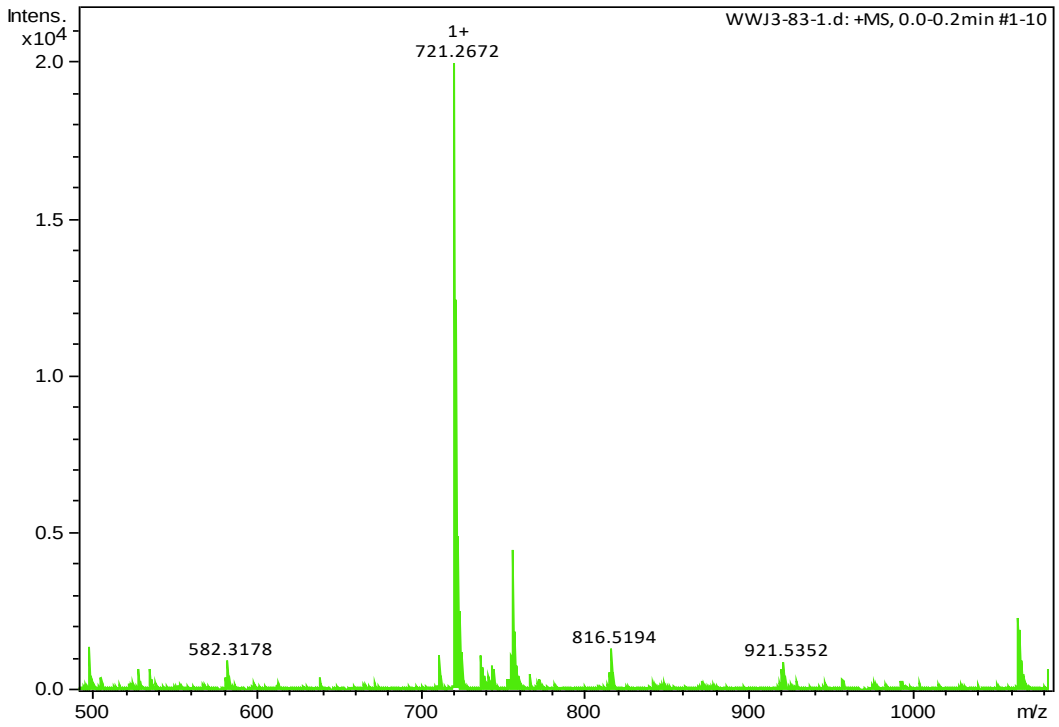

Figure S15. IR Spectrum of **2**

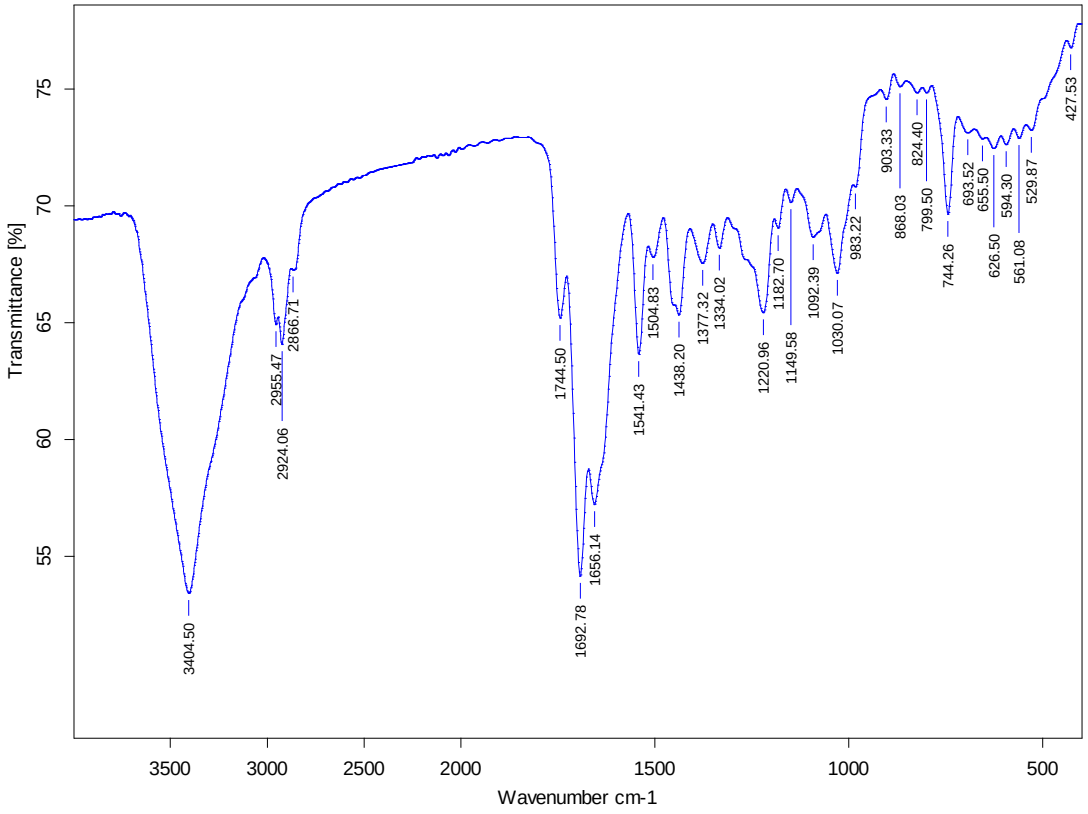

Figure S16. UV Spectrum of **2**

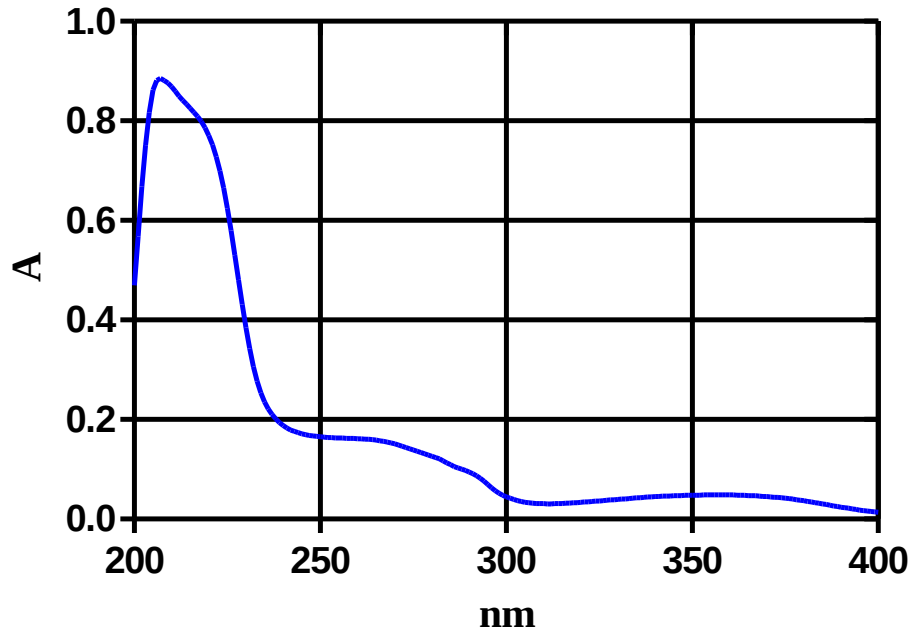

Figure S17. ^{1}H NMR Spectrum of **2** in DMSO-d_6

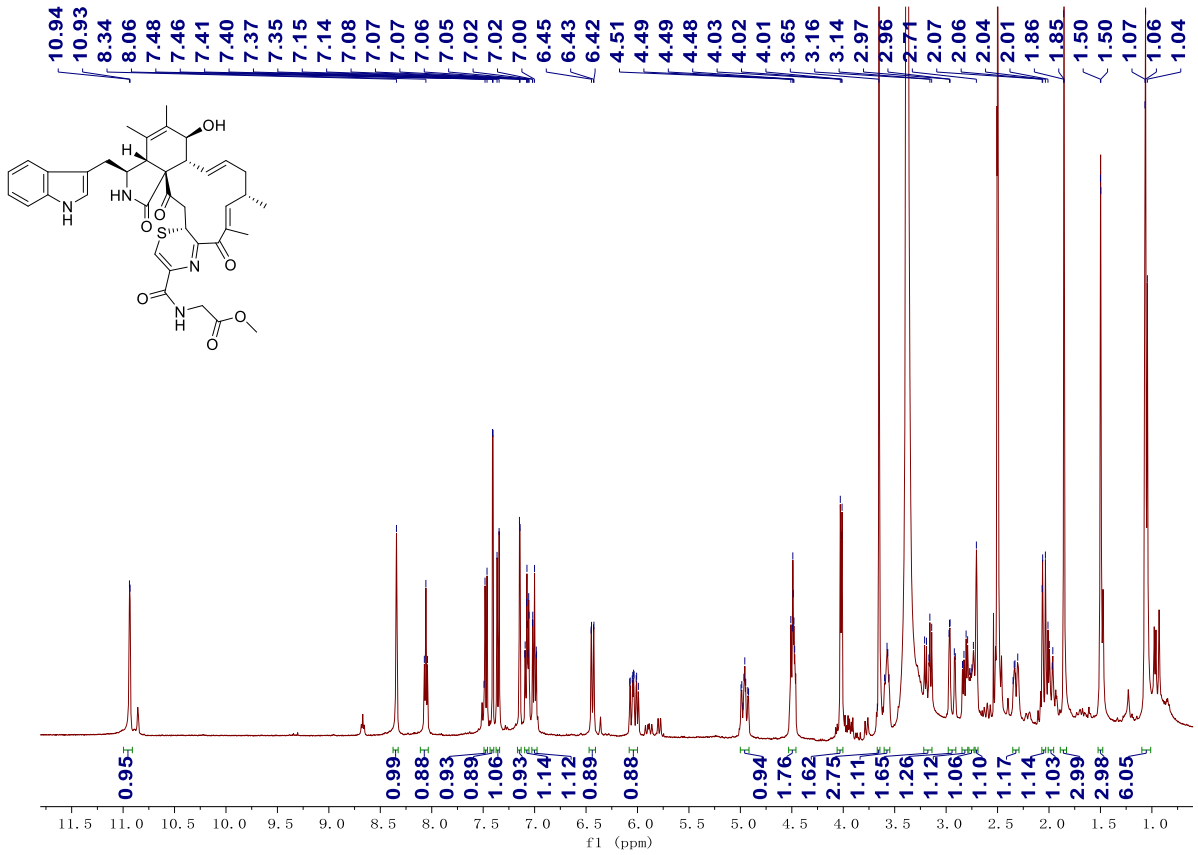

Figure S18. ^{13}C NMR Spectrum of **2** in DMSO-d_6

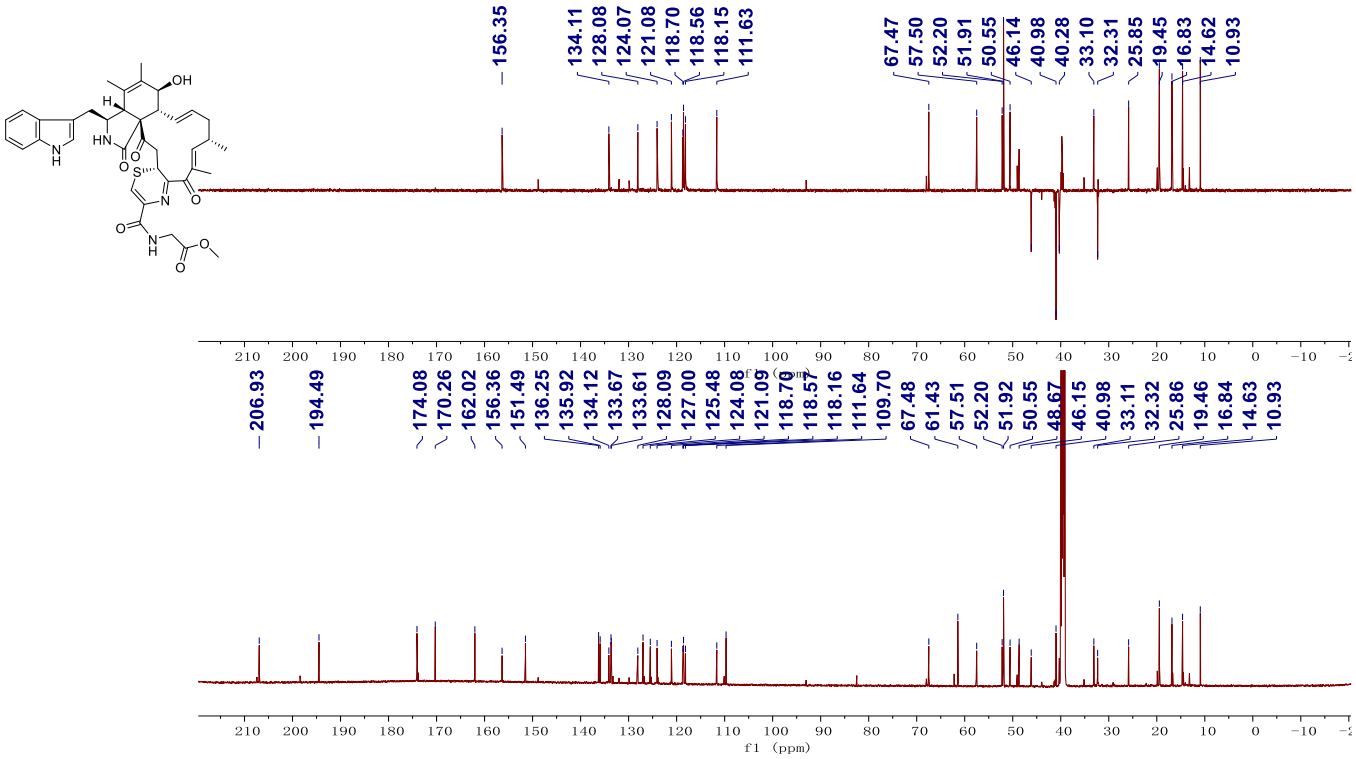

Figure S19. HSQC Spectrum of **2** in DMSO-d_6

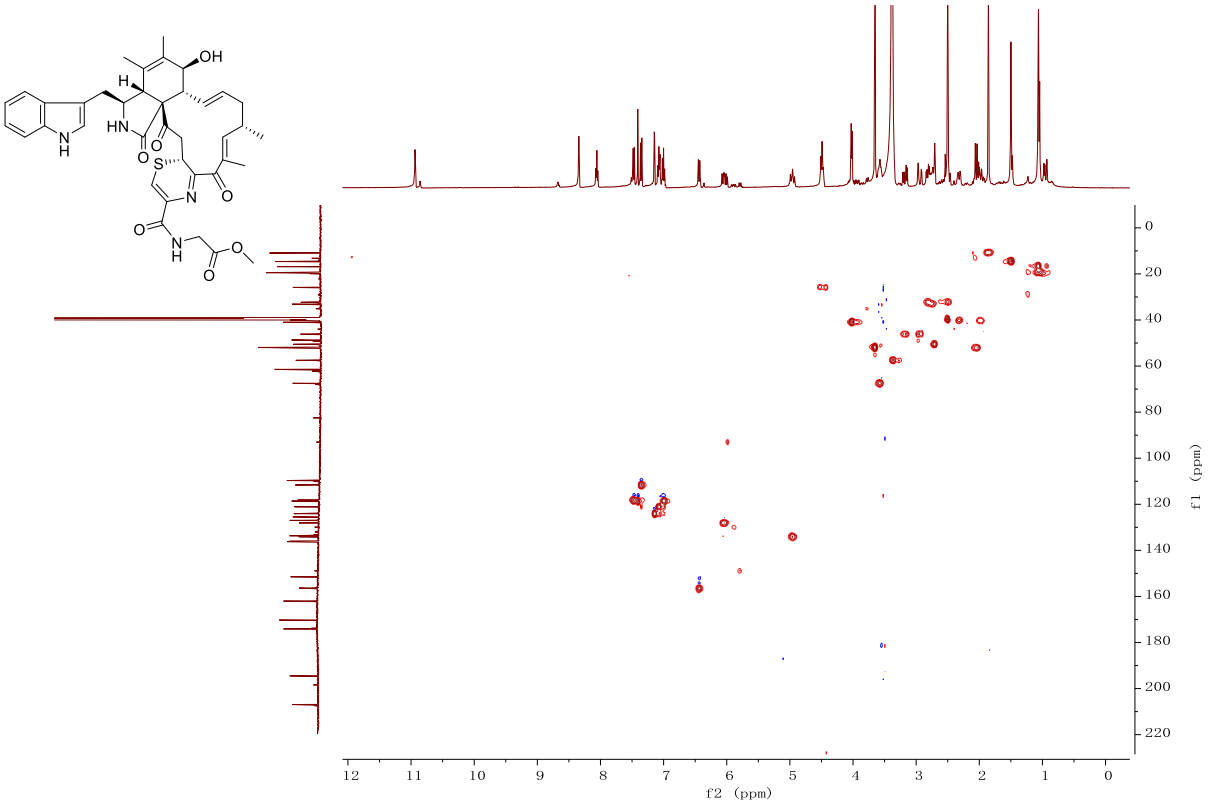

Figure S20. HMBC Spectrum of **2** in DMSO-d_6

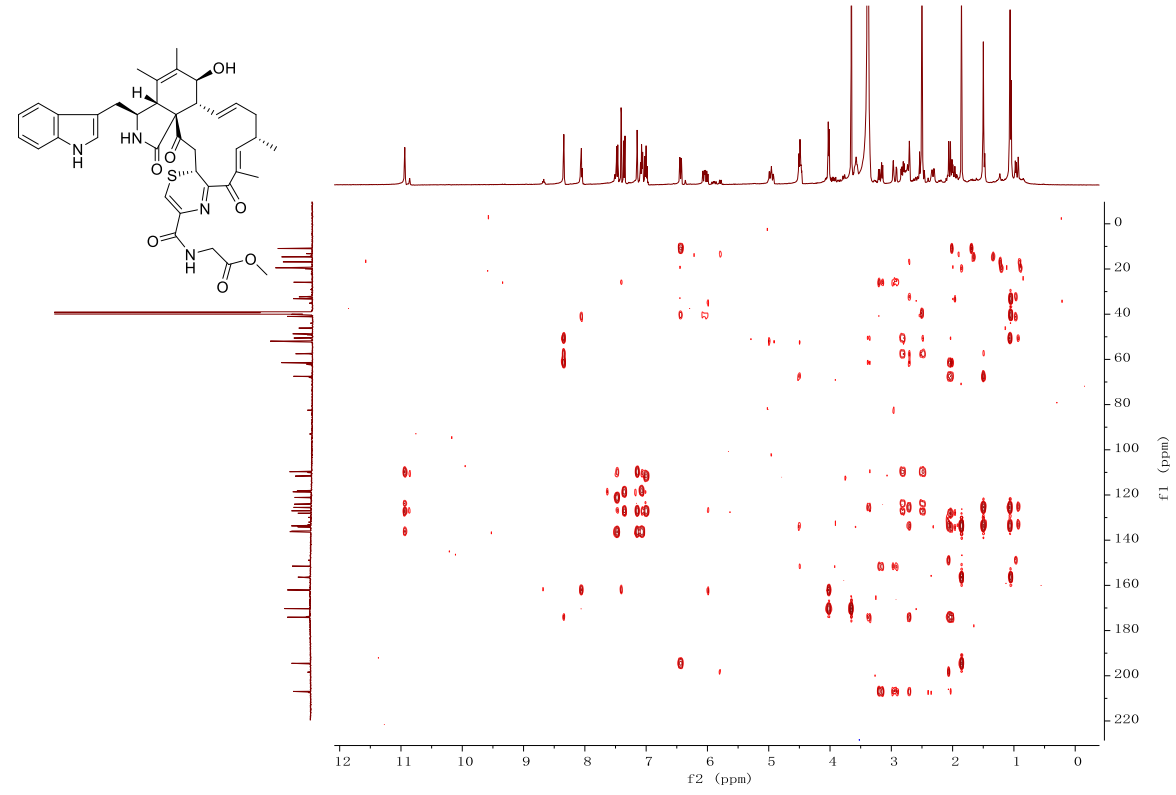

Figure S21. $^{1}H–^{1}H$ COSY Spectrum of **2** in DMSO-d_6

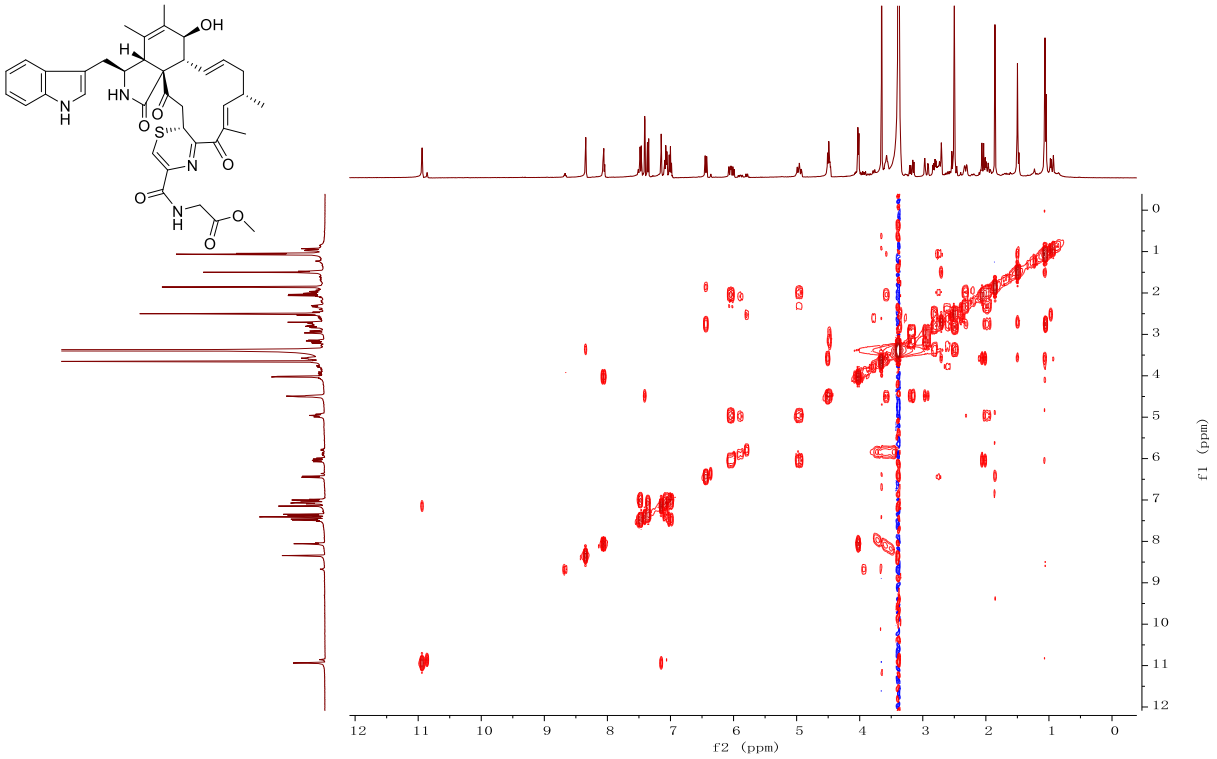

Figure S22. NOESY Spectrum of **2** in DMSO-d_6

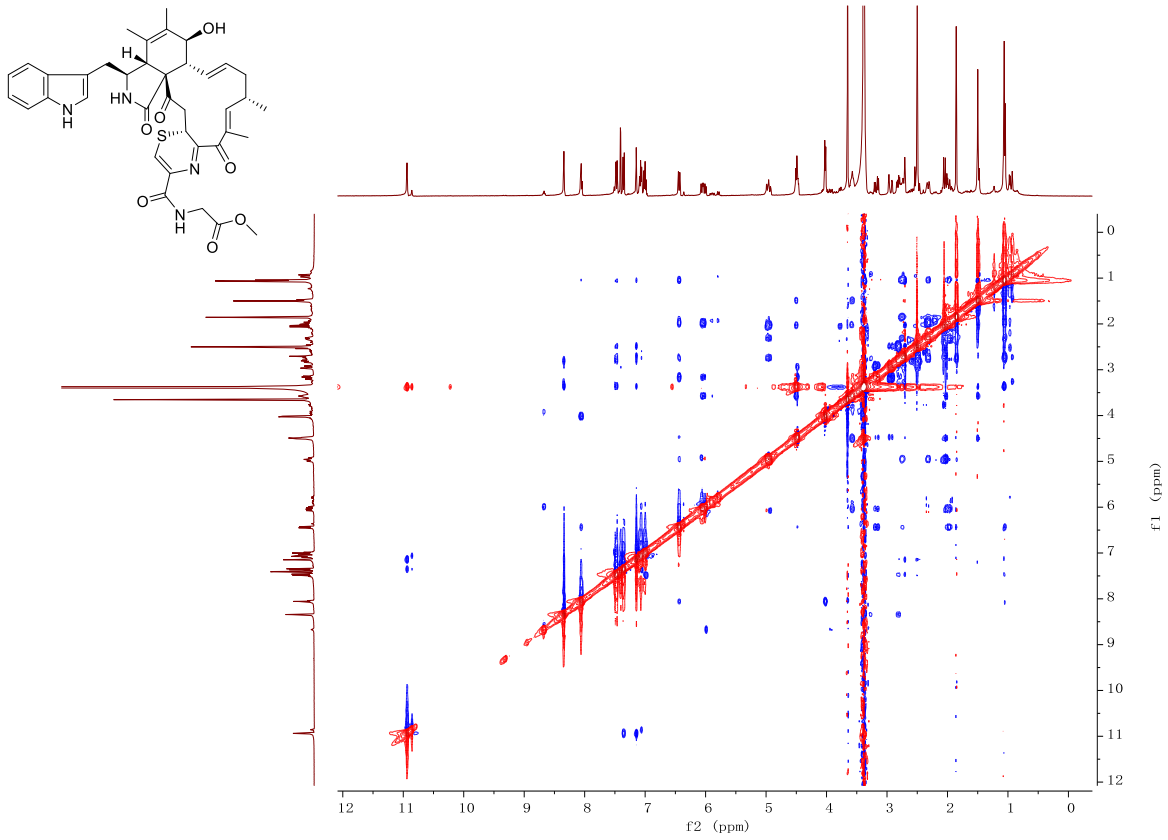

Figure S23. (+)-HR-ESI-MS Spectrum of **3**

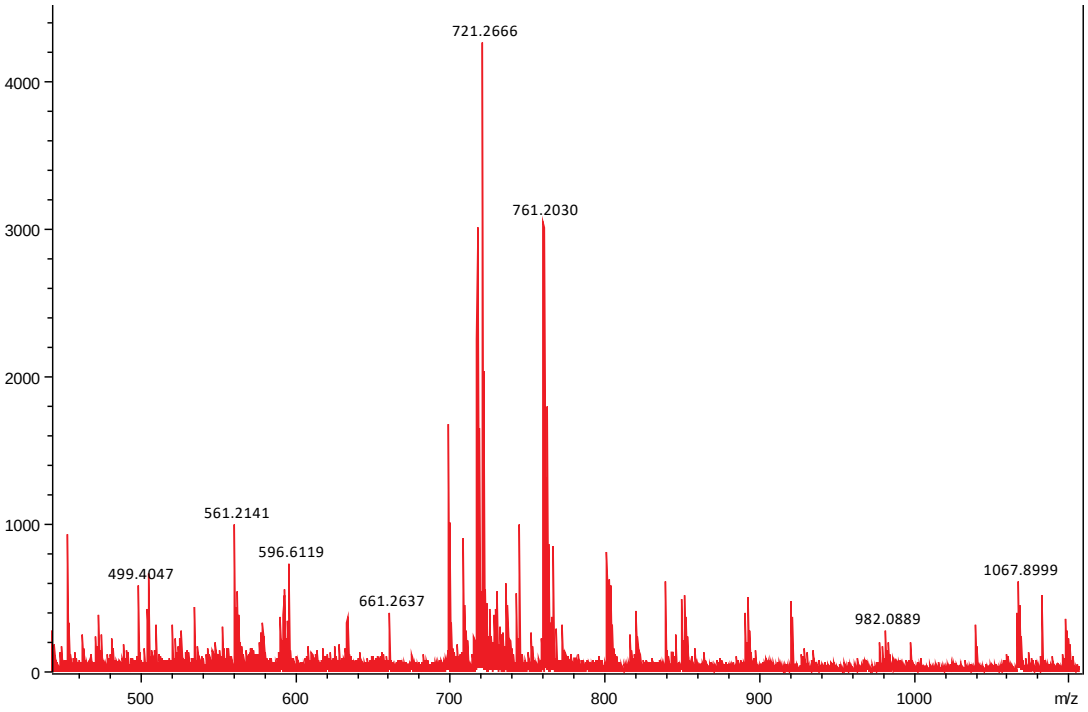

Figure S24. IR Spectrum of **3**

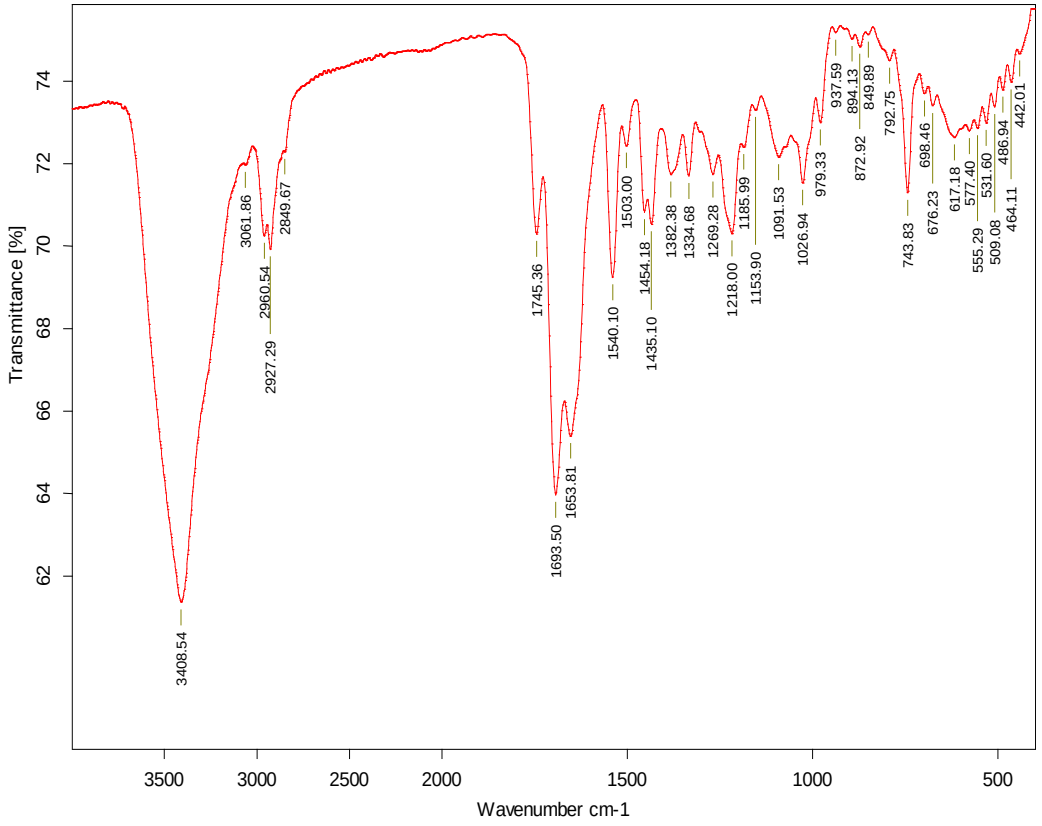

Figure S25. UV Spectrum of **3**

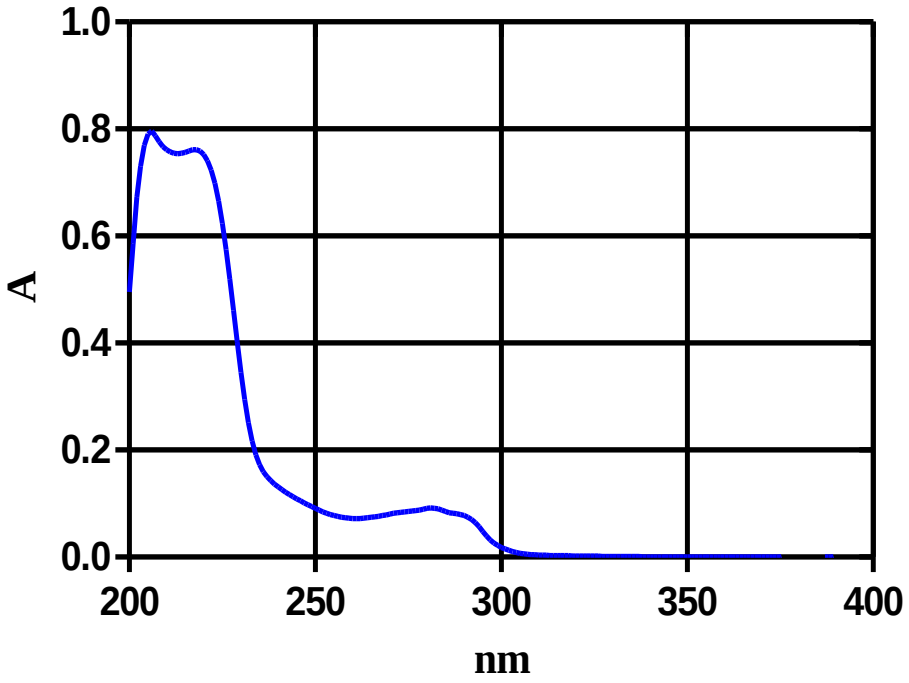

Figure S26. ^{1}H NMR Spectrum of **3** in DMSO-d_6

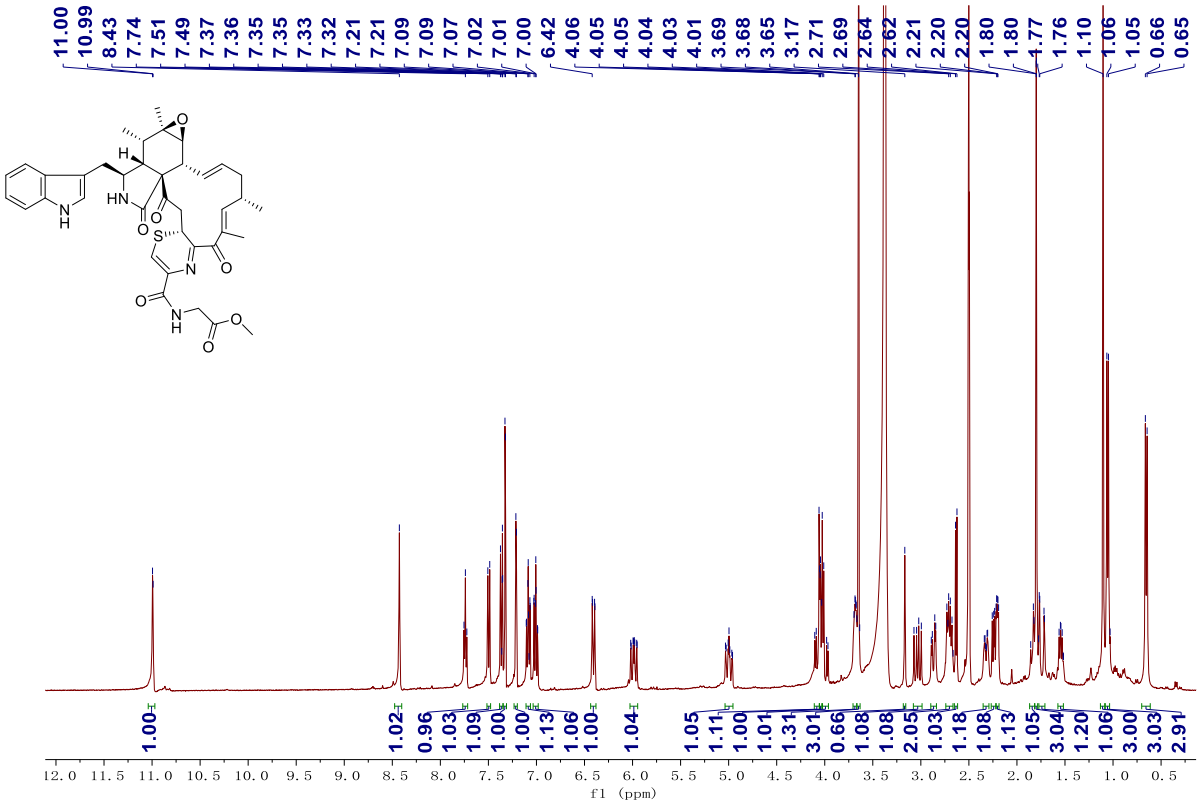

Figure S27. ^{13}C NMR Spectrum of **3** in DMSO-d_6

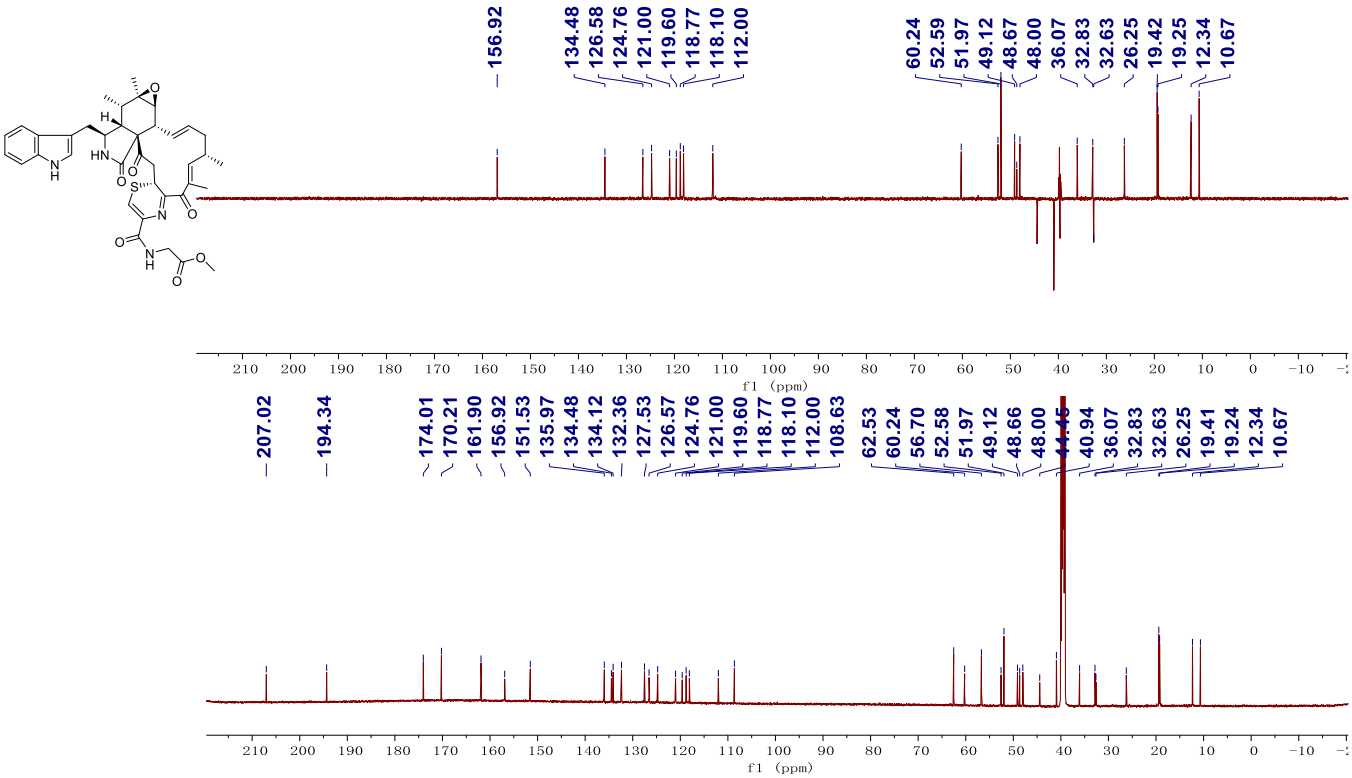

Figure S28. HSQC Spectrum of **3** in DMSO-d_6

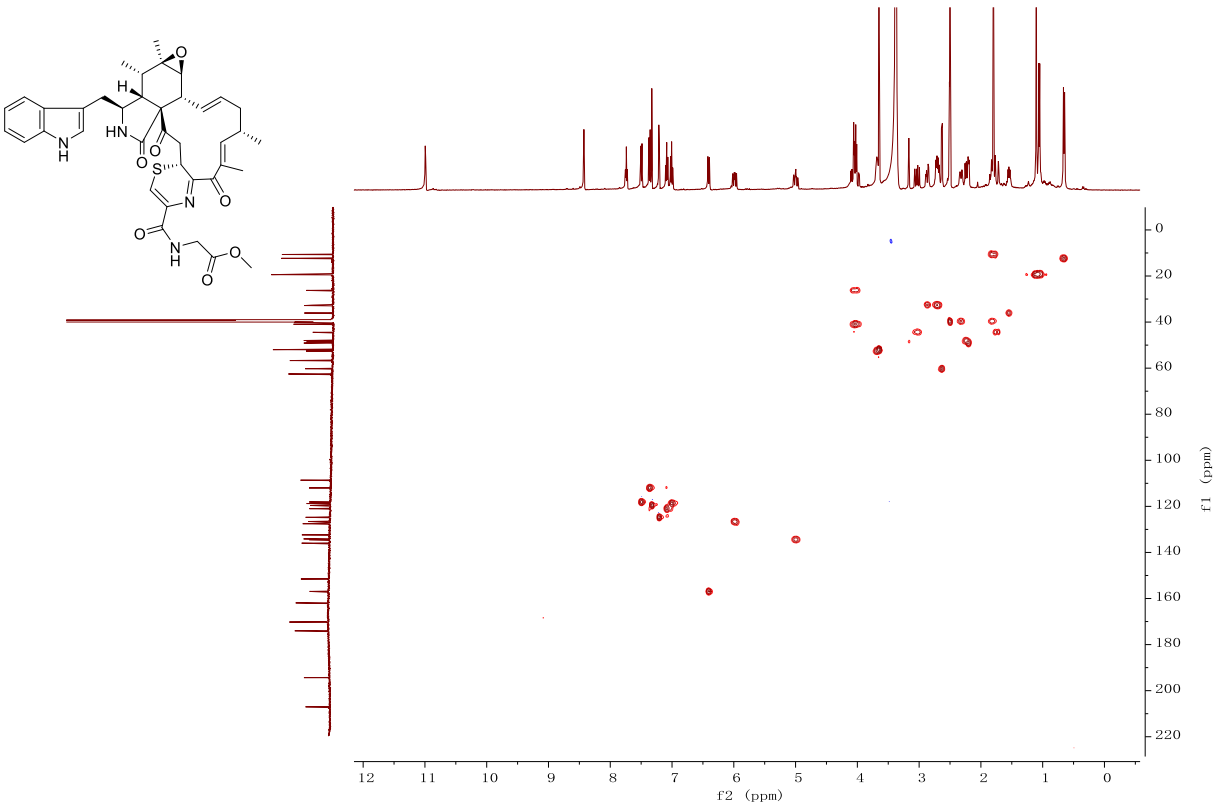

Figure S29. HMBC Spectrum of **3** in DMSO-d_6

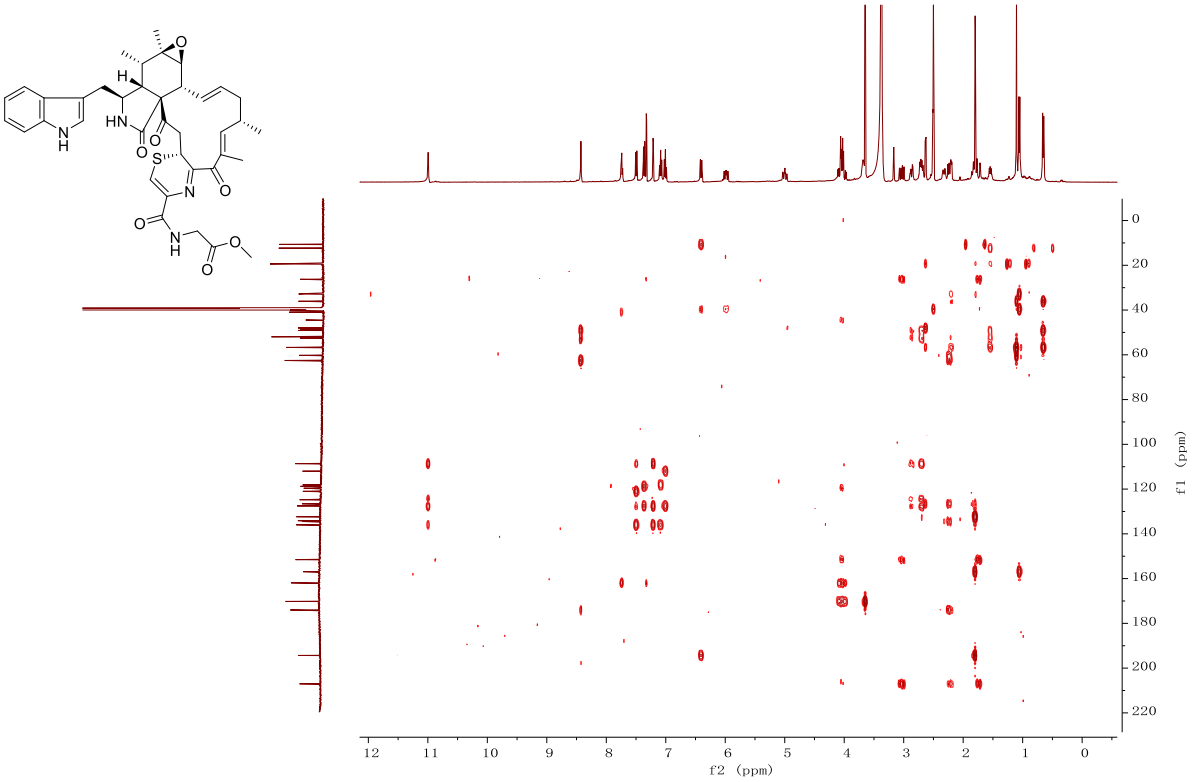

Figure S30. ^{1}H–^{1}H COSY Spectrum of **3** in DMSO-d_6

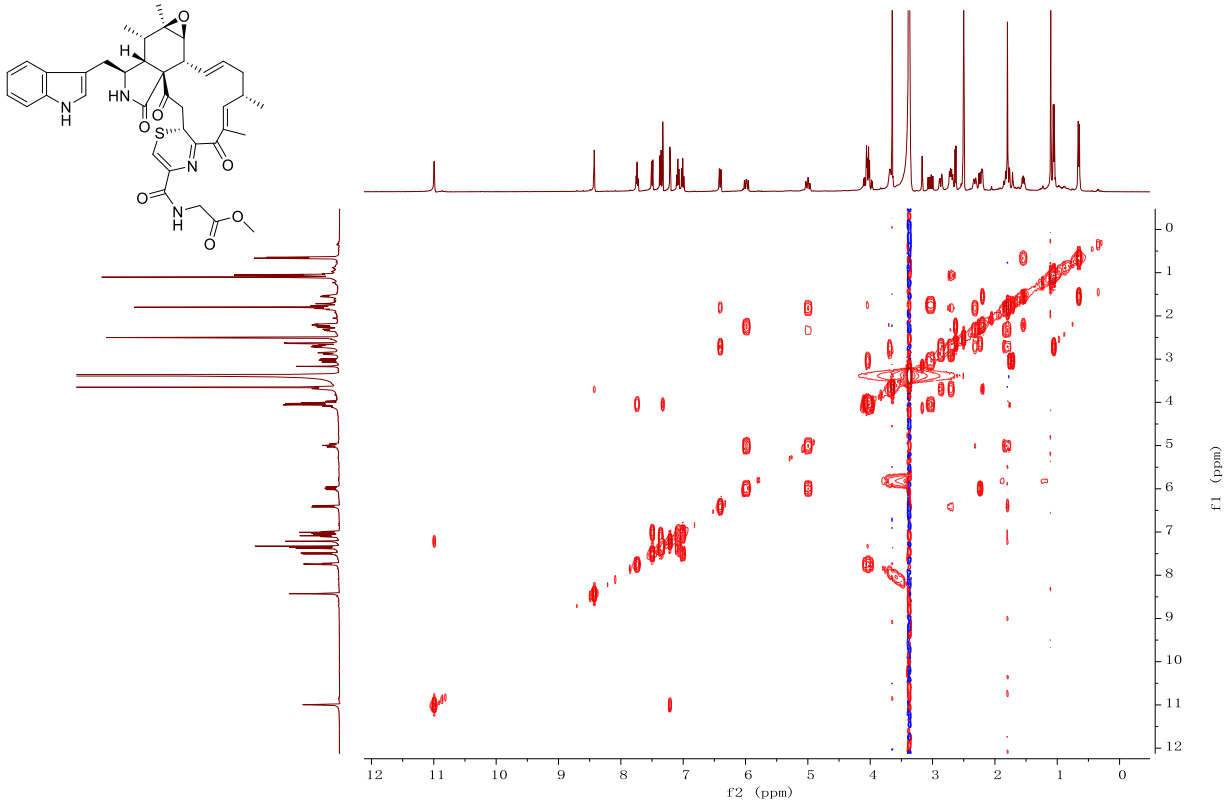

Figure S31. NOESY Spectrum of **3** in DMSO-d_6