SUPPLWMENTARY INFORMATION

Beshanzuamide A, an unprecedented prenylated indole alkaloid produced by *Aspergillus* sp. Y-2 from the critically endangered conifer *Abies beshanzuensis*

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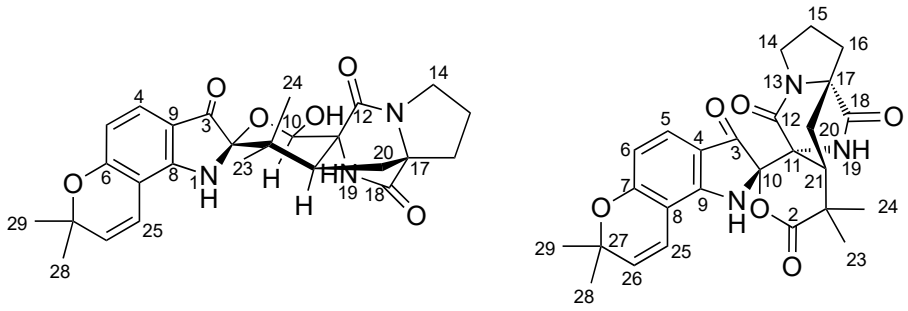
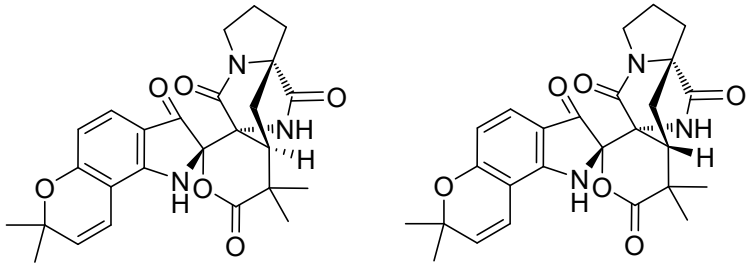
The structures of notoamide O and compound 1



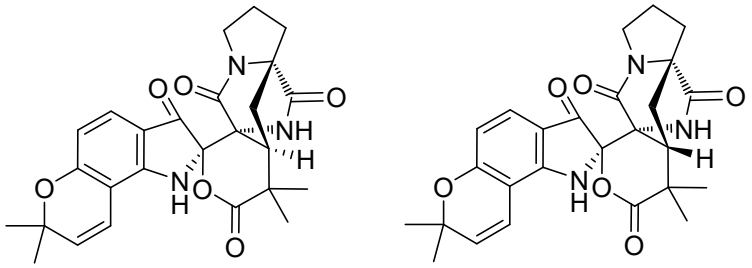
Notoamide O **1**

Fig. S1. Four possible relative configurations of compound **1** for quantum calculations

GIAO ^{13}NMR data computational details for 1.



(10*S**,11*R**,17*S**,21*S**)-**1**a (10*S**,11*R**,17*S**,21*R**)-**1**b

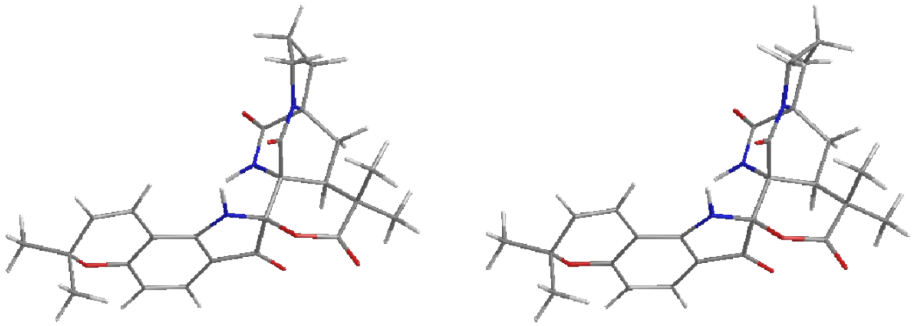


(10*R**,11*R**,17*S**,21*S**)-**1**c (10*R**,11*R**,17*S**,21*R**)-**1**d

Fig. S2. Four possible relative configurations of compound **1** for quantum calculations

Table S1. ^{13}C NMR calculation of **1**a-**1**d, fitting to the experimental data of compound **1**.

no.	Exptl.	Calcd. of **1**a	Abs dev	Calcd. of **1**b	Abs dev	Calcd. of **1**c	Abs dev	Calcd. of **1**d	Abs dev
2	178.4	177.81	0.59	178.34	0.06	177.52	0.88	178.61	0.21
3	193.3	193.75	0.45	194.04	0.74	191.64	1.66	194.21	0.91
4	127.9	130.34	2.44	129.63	1.73	130.58	2.68	129.36	1.46
5	111.9	112.26	0.36	112.74	0.84	113.29	1.39	112.53	0.63
6	164	164.59	0.59	163.49	0.51	164.46	0.46	162.43	1.57
7	106.2	105.07	1.13	106.90	0.70	106.88	0.68	106.92	0.72
8	158.8	157.89	0.91	159.40	0.60	157.56	1.24	157.06	1.74
9	112.3	110.29	2.01	113.32	1.02	113.13	0.83	113.87	1.57
10	90.5	92.56	2.06	89.71	0.79	91.19	0.69	92.55	2.05
11	61.7	61.72	0.02	62.85	1.15	62.41	0.71	66.17	4.47
12	168.2	169.17	0.97	166.68	1.52	166.14	2.06	167.47	0.73
14	45.3	45.29	0.01	44.20	1.10	43.81	1.49	44.25	1.05
15	25.4	26.16	0.76	25.28	0.12	24.02	1.38	25.53	0.13
16	30	30.72	0.72	29.75	0.25	28.79	1.21	30.00	0.00
17	68.2	68.35	0.15	67.53	0.67	67.68	0.52	68.00	0.20
18	175	171.92	3.08	172.30	2.70	174.52	0.48	171.84	3.16
20	31.6	32.70	1.10	32.52	0.92	32.99	1.39	32.87	1.27
21	42.3	41.38	0.92	42.50	0.20	44.25	1.95	40.59	1.71
22	43.4	43.41	0.01	43.69	0.29	42.68	0.72	42.52	0.88
23	26.5	25.39	1.11	24.85	1.65	28.64	2.14	23.30	3.20
24	22.5	21.84	0.66	25.63	3.13	23.47	0.97	24.83	2.33
25	116.3	119.14	2.84	118.73	2.43	118.98	2.68	118.98	2.68
26	129.9	128.77	1.13	129.00	0.90	130.12	0.22	129.20	0.70
27	79.4	80.26	0.86	79.36	0.04	79.55	0.15	79.05	0.35
28	28.5	27.55	0.95	27.04	1.46	26.05	2.45	27.11	1.39
29	28.6	27.78	0.82	26.62	1.98	25.75	2.85	26.84	1.76
		MAE	1.02	MAE	1.06	MAE	1.30	MAE	1.42
		RMS	1.31	RMS	1.33	RMS	1.52	RMS	1.77
		P_{mean}	40.82%	P_{mean}	34.04%	P_{mean}	25.16%	P_{mean}	18.50%
		Prel	99.12%	Prel	0.88%	Prel	0.00%	Prel	0.00%

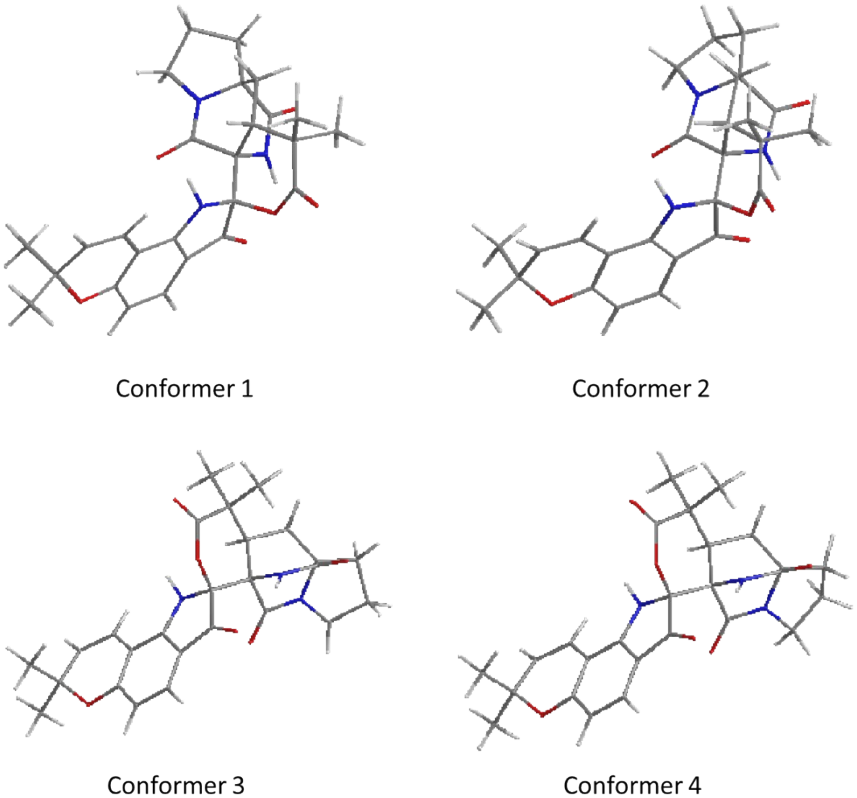


Conformer 1 Conformer 2

Fig. S3. Conformers of **1**a optimized on B3LYP-D3(BJ)/TZVP (IEFPCM, CH_3OH) level of theory for NMR calculation.

Table S2. Gibbs free energy and Boltzmann distribution of conformers of **1**a calculated on B3LYP-D3(BJ)/TZVP level with IEFPCM solvation model (CH_3OH).

Conformers	Gibbs free energy (a.u.)	ΔG (kcal/mol)	Population
1	-1622.945662	0	58.31%
2	-1622.945273	0.244101157	39.83%



Conformer 1 Conformer 2

Conformer 3 Conformer 4

Fig. S4. Conformers of structure **1**b optimized on B3LYP-D3(BJ)/TZVP (IEFPCM, CH_3OH) level of theory for NMR calculation.

Table S3. Gibbs free energy and Boltzmann distribution of conformers of **1**b calculated on B3LYP-D3(BJ)/TZVP level with IEFPCM solvation model (CH_3OH)

Conformers	Gibbs free energy (a.u.)	ΔG (kcal/mol)	Population
1	-1622.940707	0	48.16%
2	-1622.940253	0.284889268	29.76%
3	-1622.939741	0.60617408	17.29%
4	-1622.938532	1.364832945	4.80%

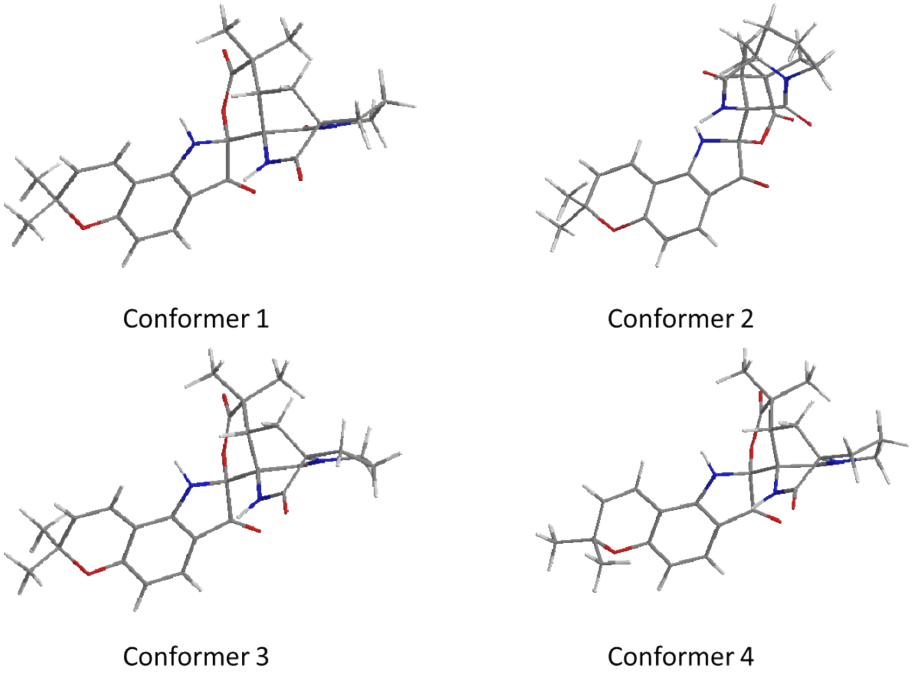
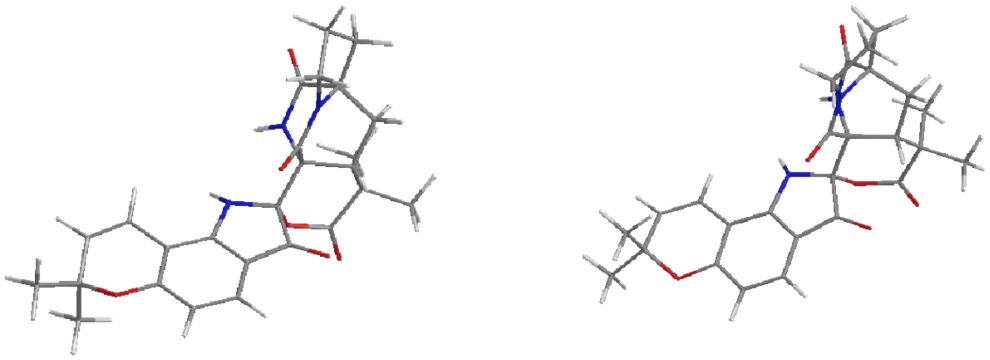


Fig. S5. Conformers of **1**c optimized on B3LYP-D3(BJ)/TZVP (IEFPCM, CH_3OH) level of theory for NMR calculation

Table S4. Gibbs free energy and Boltzmann distribution of conformers of **1**c calculated on B3LYP-D3(BJ)/TZVP level with IEFPCM solvation model (CH_3OH)

Conformers	Gibbs free energy (a.u.)	ΔG (kcal/mol)	Population
1	-1622.932835	0	40.61%
2	-1622.932265	0.357680358	22.19%
3	-1622.932213	0.390310847	21.00%
4	-1622.931968	0.54405065	16.20%



Conformer 1 Conformer 2

Fig. S6. Conformers of **1**d optimized on B3LYP-D3(BJ)/TZVP (IEFPCM, CH_3OH) level of theory for NMR calculation

Table S5. Gibbs free energy and Boltzmann distribution of conformers of **1**d calculated on B3LYP-D3(BJ)/TZVP level with IEFPCM solvation model (CH_3OH)

Conformers	Gibbs free energy (a.u.)	ΔG (kcal/mol)	Population
1	-1622.941767	0	66.84%
2	-1622.941106	0.414783713	33.16%

ECD computational details for 1.

Table S6. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of (*10S*)-**1**.

Conformers	In MeOH	
	Δ*G*	*P* (%)/100
1	0.00	0.629
2	0.33	0.362
3	2.86	0.005

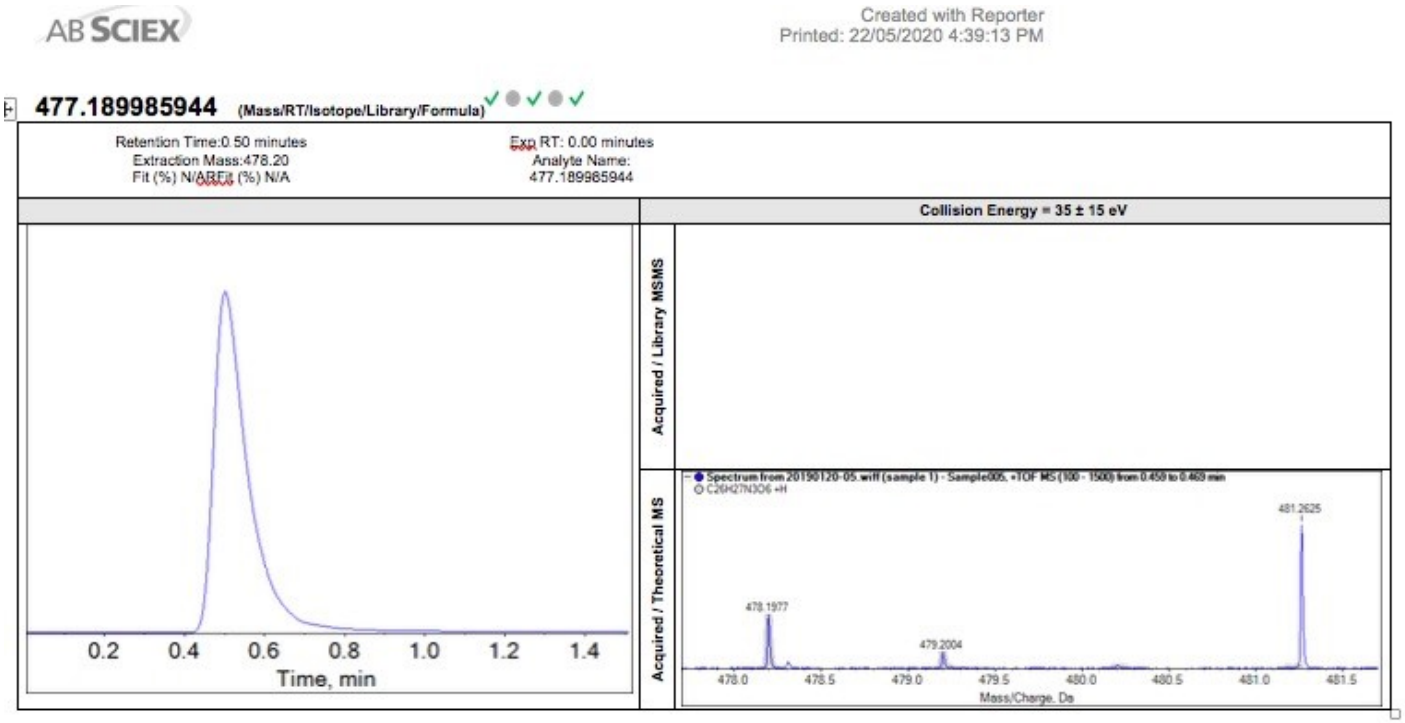
[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Table S7. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of (*10R*)-**1**.

Conformers	In MeOH	
	Δ*G*	*P* (%)/100
1	0.00	0.712
2	0.54	0.288
3	5.41	0.000

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Fig. S7. The HR-ESIMS of compound **1**



	Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
✓●✓●✓	477.189985944(Y2G7B)	96%	C26H27N3O6	3228465	5	478.1973	478.1977	0.9	0.00	0.50	0.50	1.1%	N/A

Fig. S8. The ^{1}H-NMR spectrum of compound **1** (600 MHz) in CD_3OD

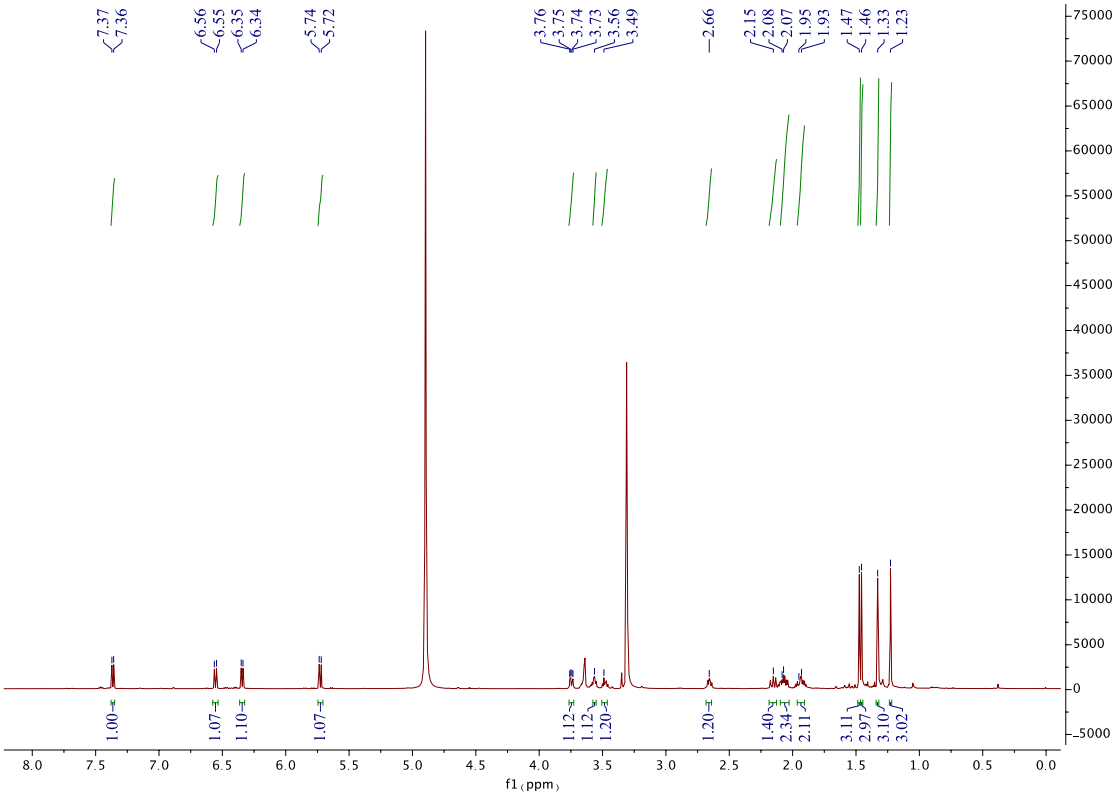


Fig. S9. The ^{13}C -NMR spectrum of compound **1** (150 MHz) in CD_3OD

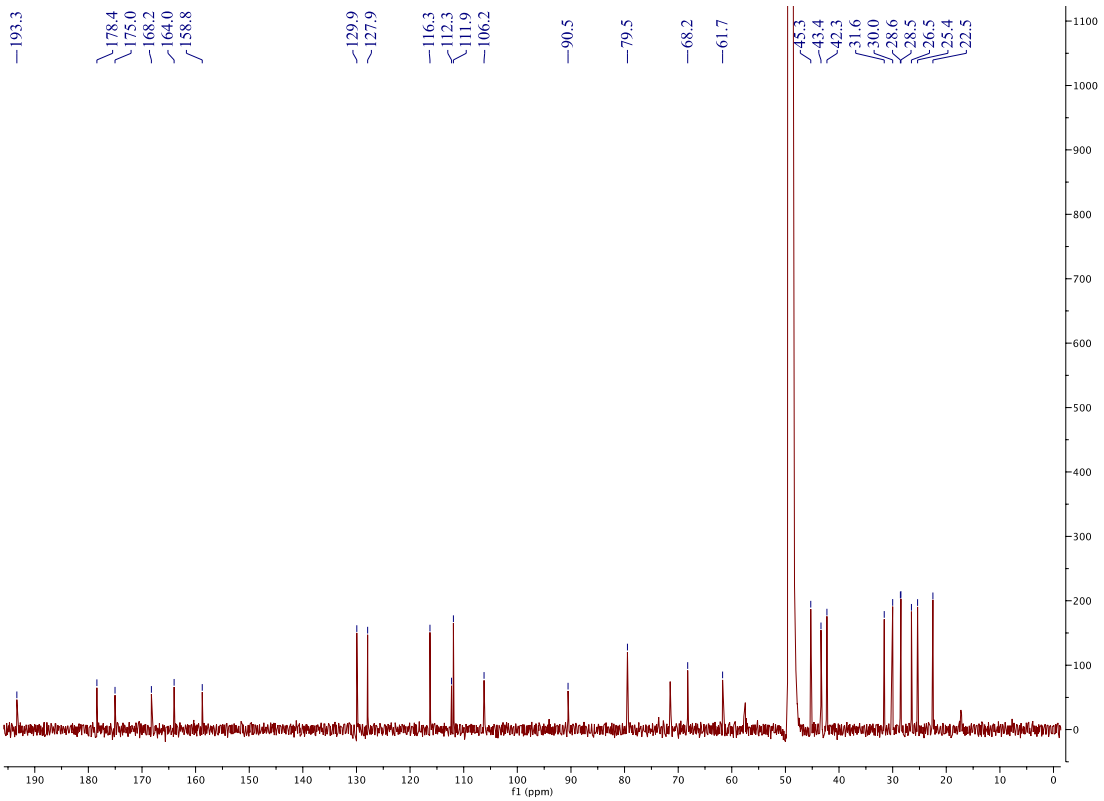


Fig. S10. The DEPT 135 spectrum of compound **1** (150 MHz) in CD_3OD

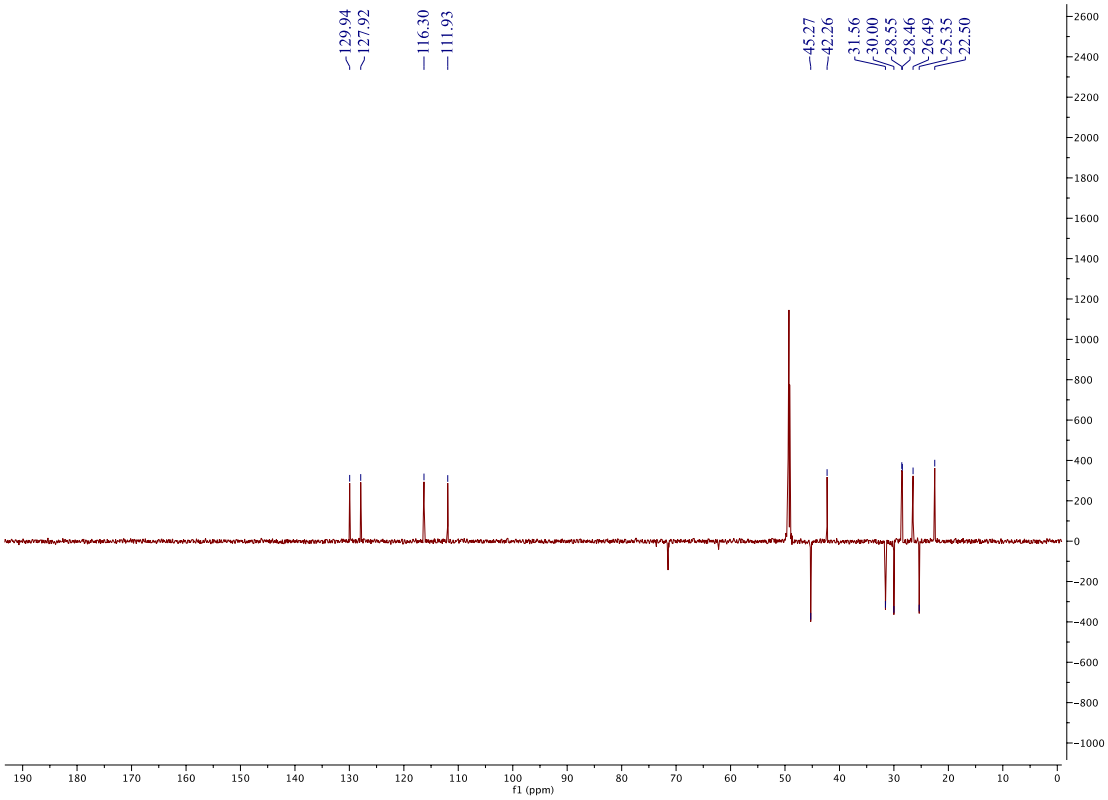


Fig. S11. The HSQC spectrum of compound **1** (600 MHz) in CD_3OD

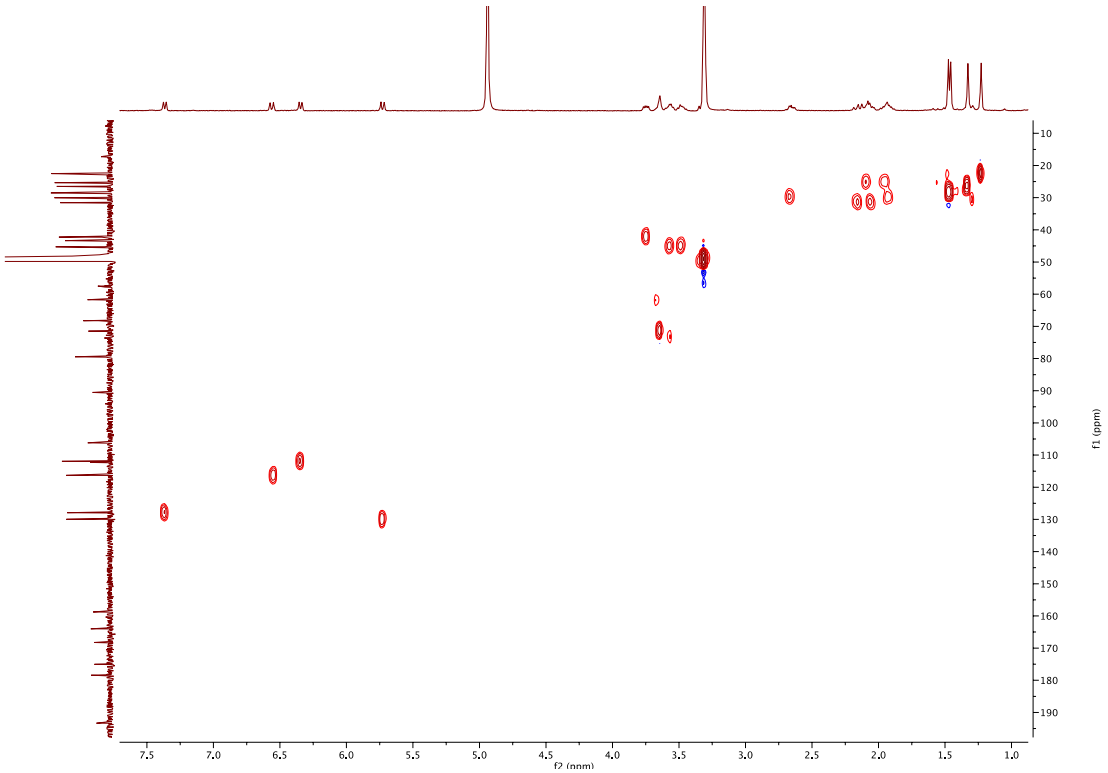


Fig. S12. The HMBC spectrum of compound **1** (600 MHz) in CD_3OD

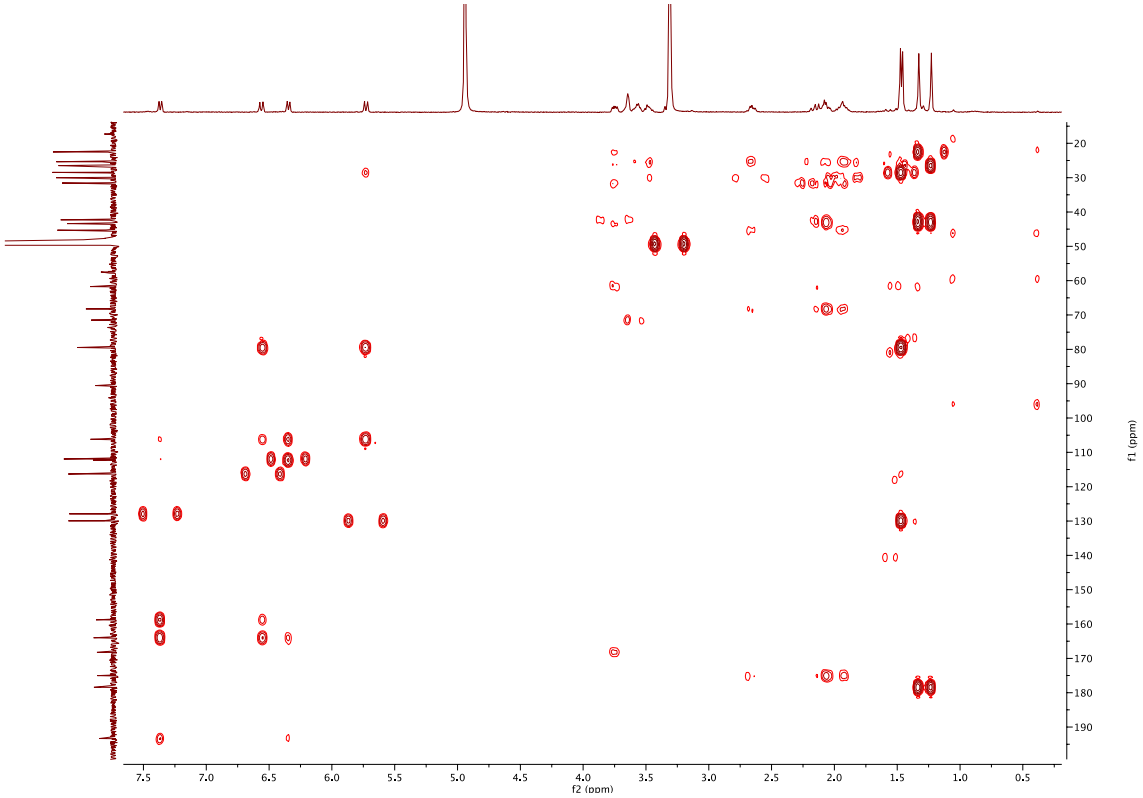


Fig. S13. The ^1H-^1H COSY spectrum of compound **1** (600 MHz) in CD_3OD

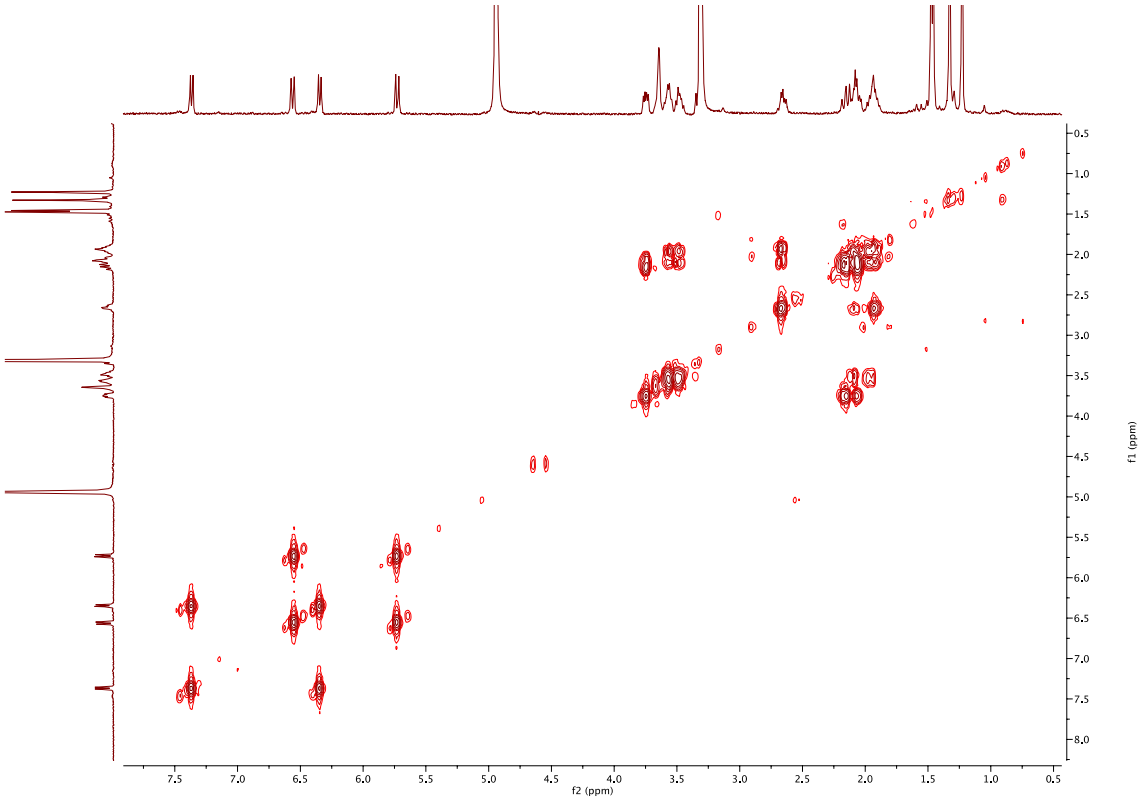


Fig. S14. The ROESY spectrum of compound **1** in CD_3OD

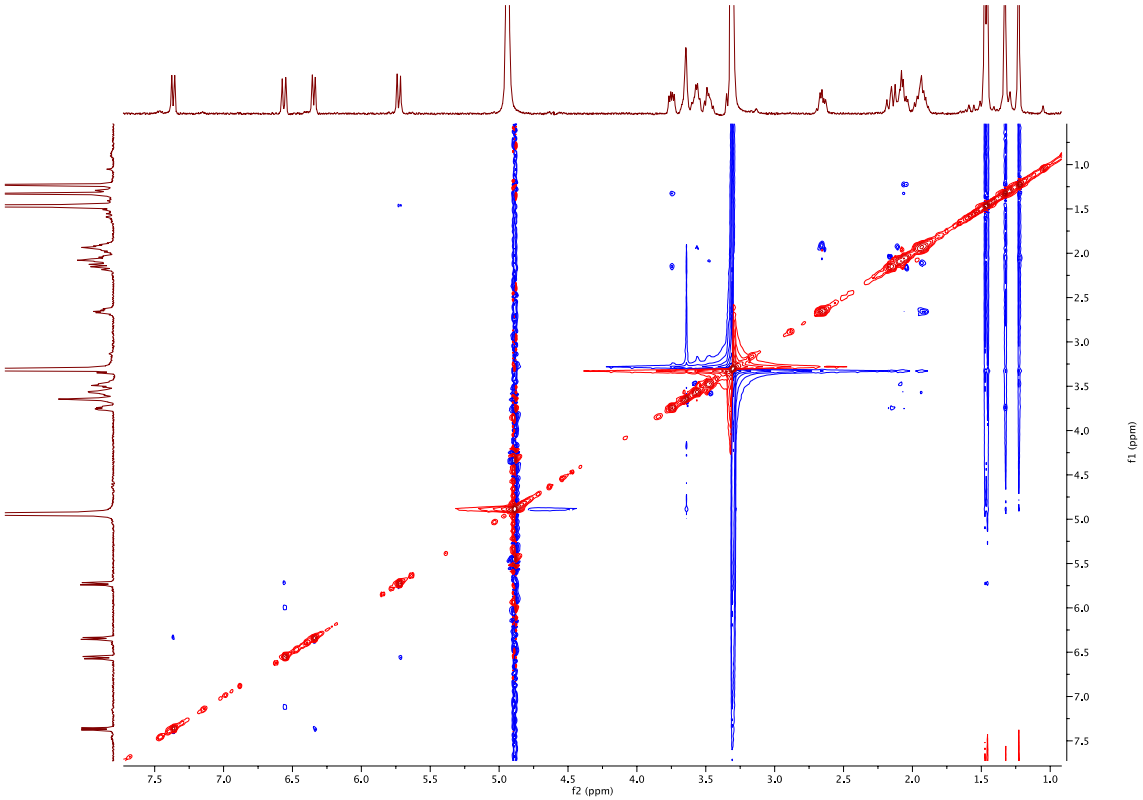


Fig. S15. The ^{1}H-NMR spectrum of compound **1** (400 MHz) in **DMSO-*d*$_6$**

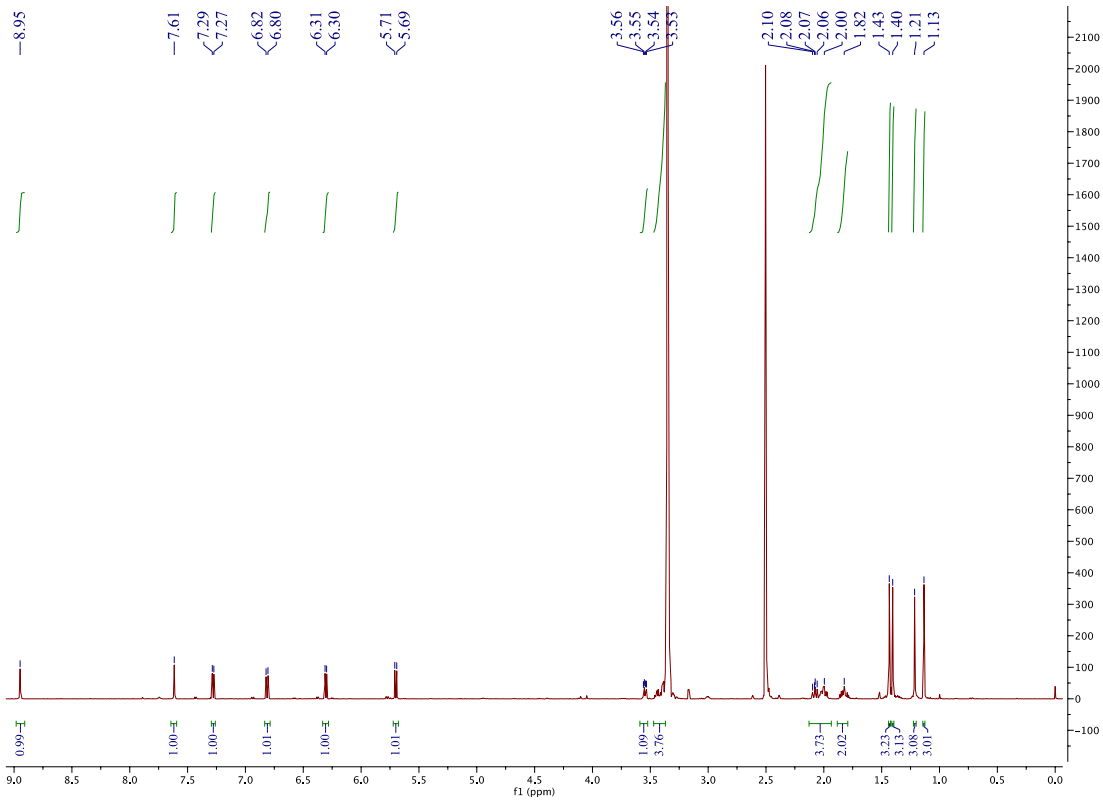


Fig. S16. The ^{13}C -NMR spectrum of compound **1** (150 MHz) in DMSO-d_6

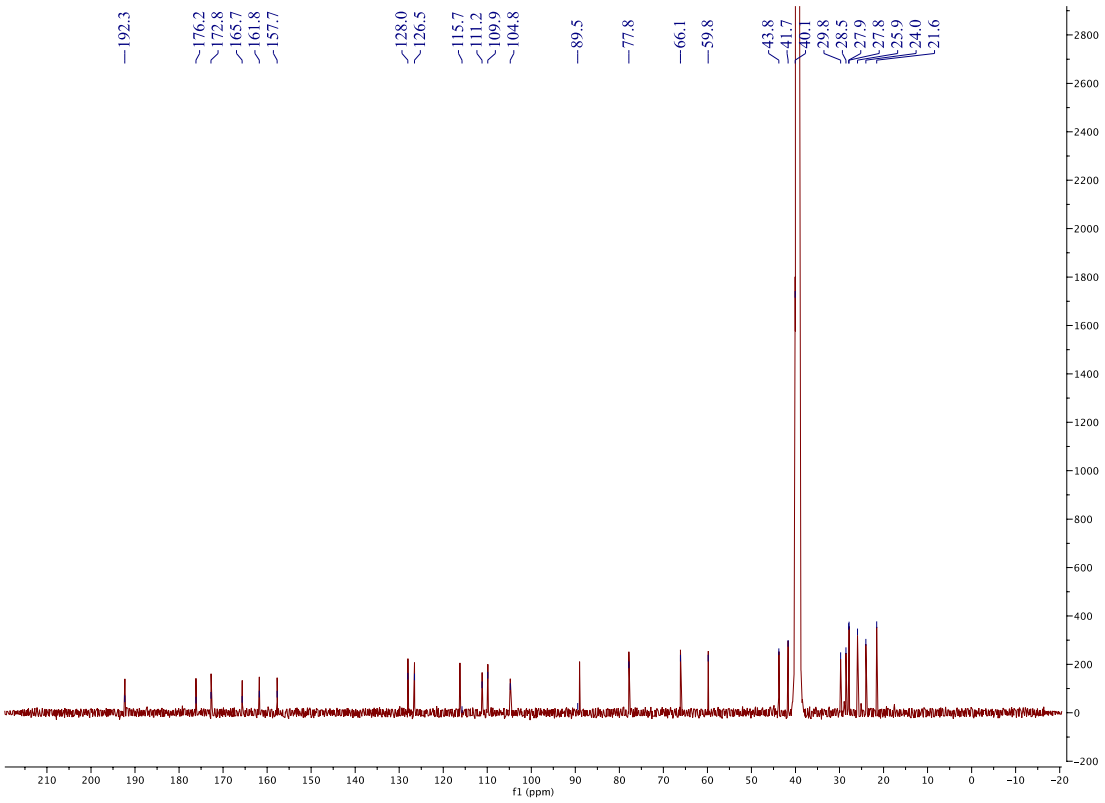


Fig. S17. The HMBC spectrum of compound **1** (600 MHz) in DMSO-d_6

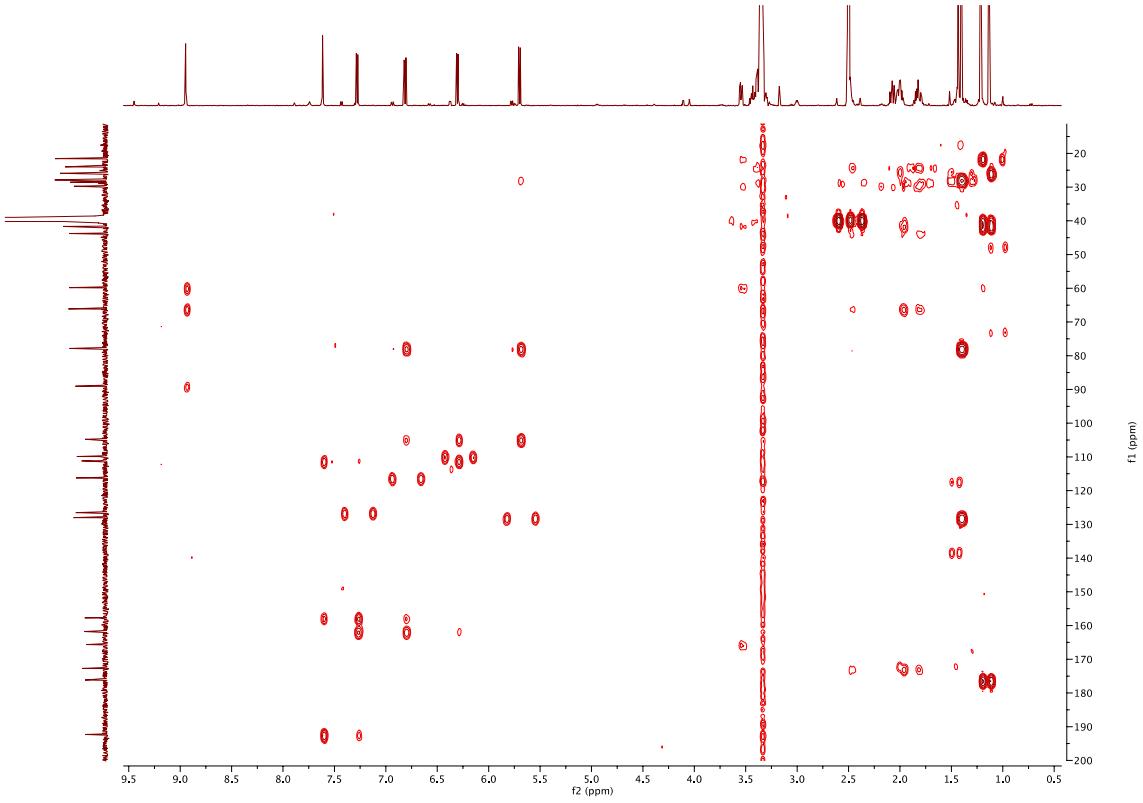


Fig. S18. The ROESY spectrum of compound **1** in DMSO-d_6