

Supporting Information

Didymorenoids A-B, two polycyclic cyclopenta[b]fluorene-type alkaloids with anti-hepatoma activity from the mangrove endophytic fungus *Didymella* sp. CYSK-4

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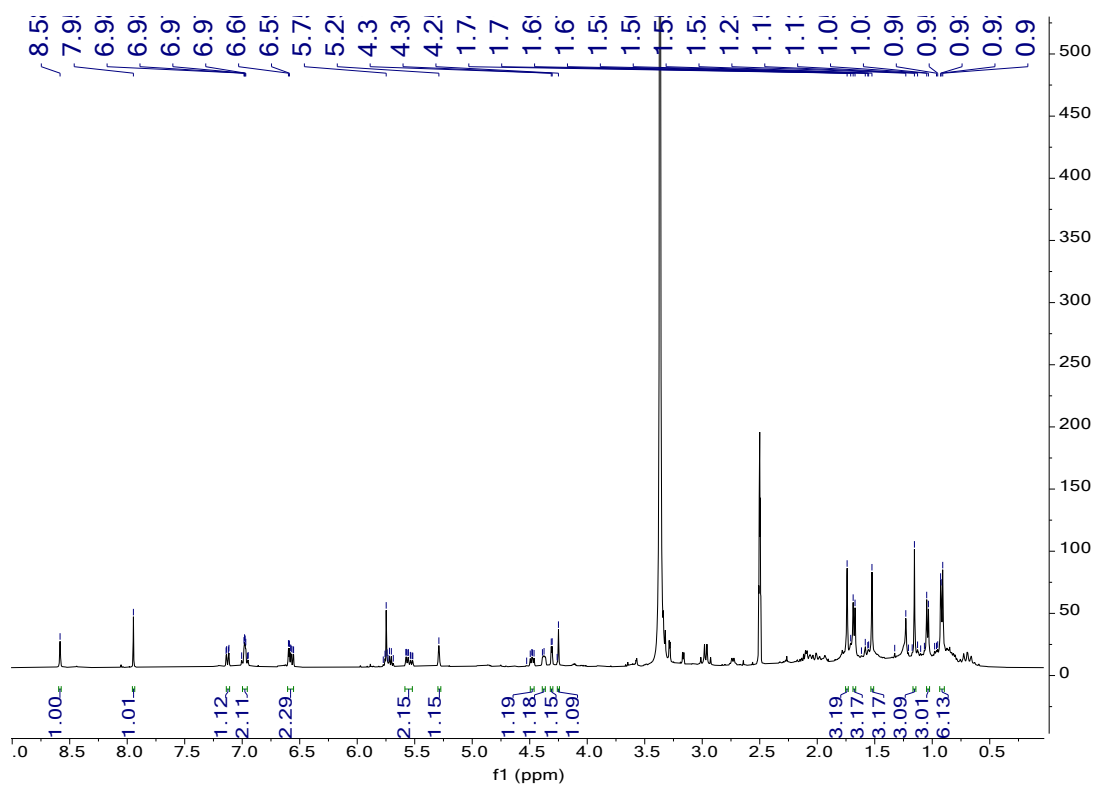


Figure S1 ^1H NMR of 1 in $\text{DMSO-}d_6$ (400 MHz)

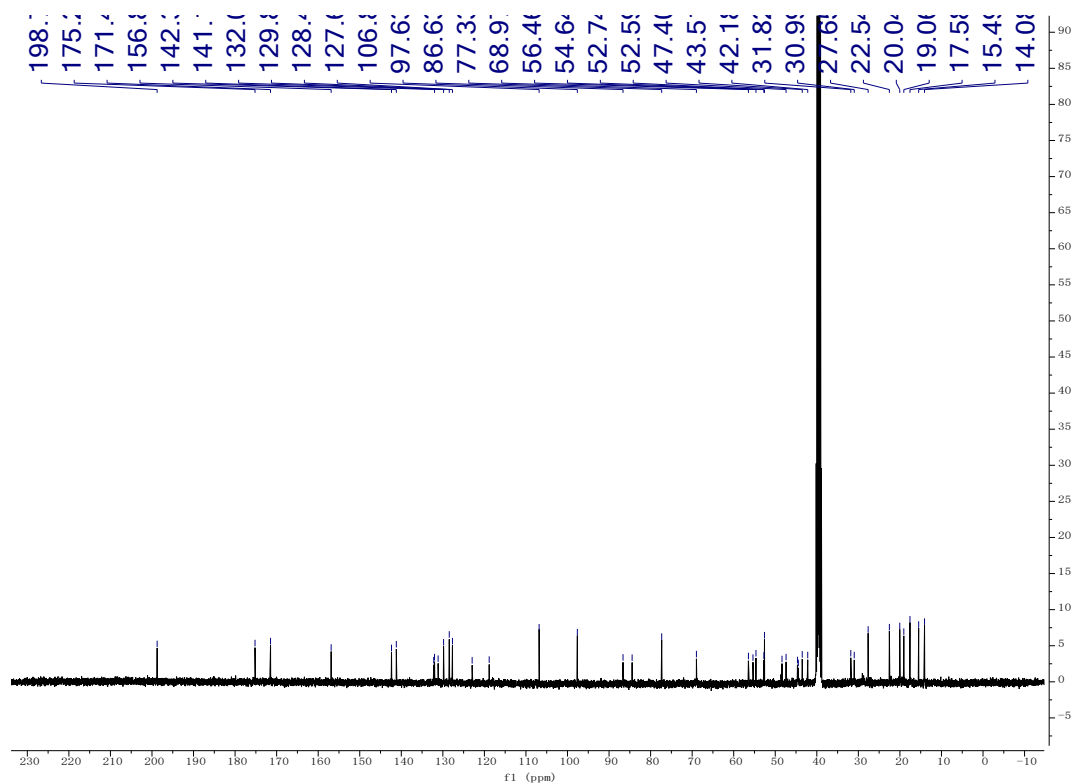


Figure S2 ^{13}C NMR of 1 in $\text{DMSO-}d_6$ (100 MHz)

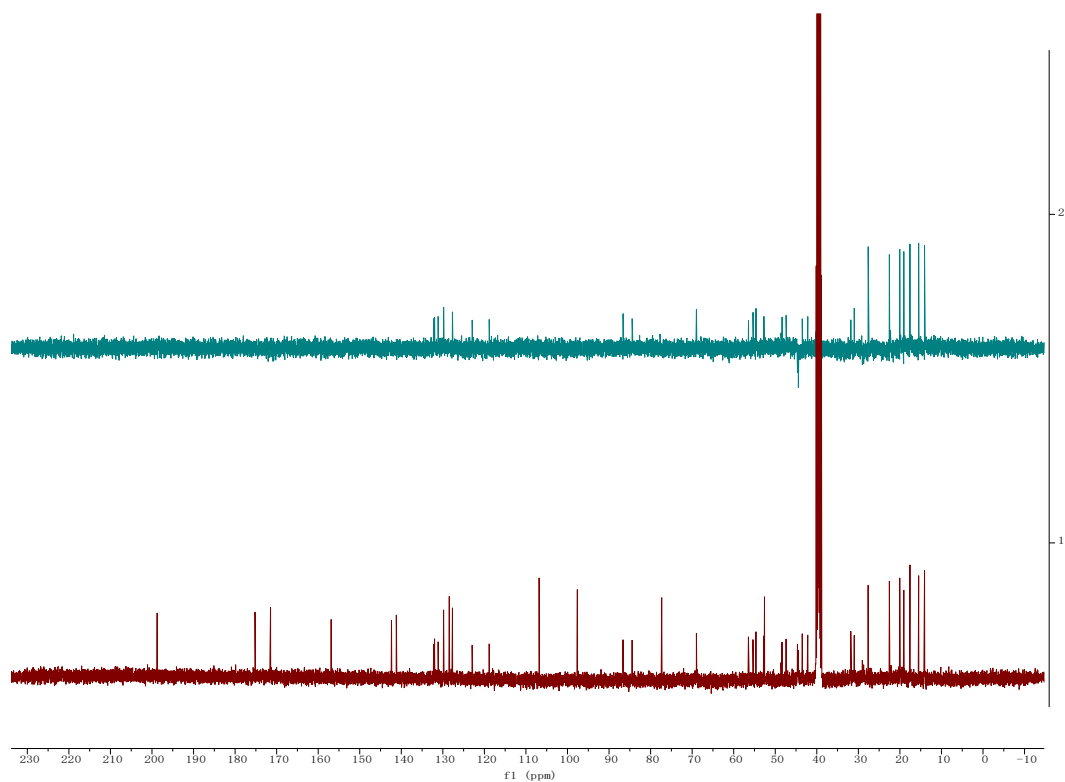


Figure S3 DEPT135 of **1** in DMSO- d_6 (100 MHz)

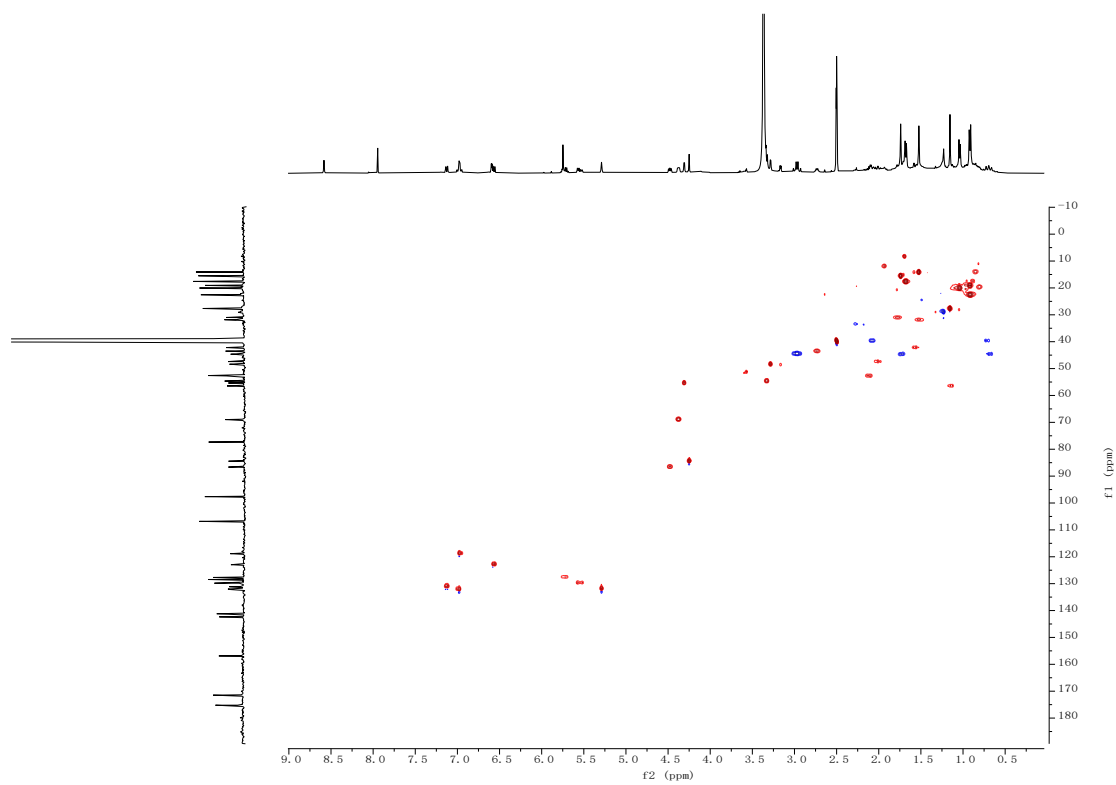


Figure S4 HSQC spectrum of **1** in DMSO- d_6

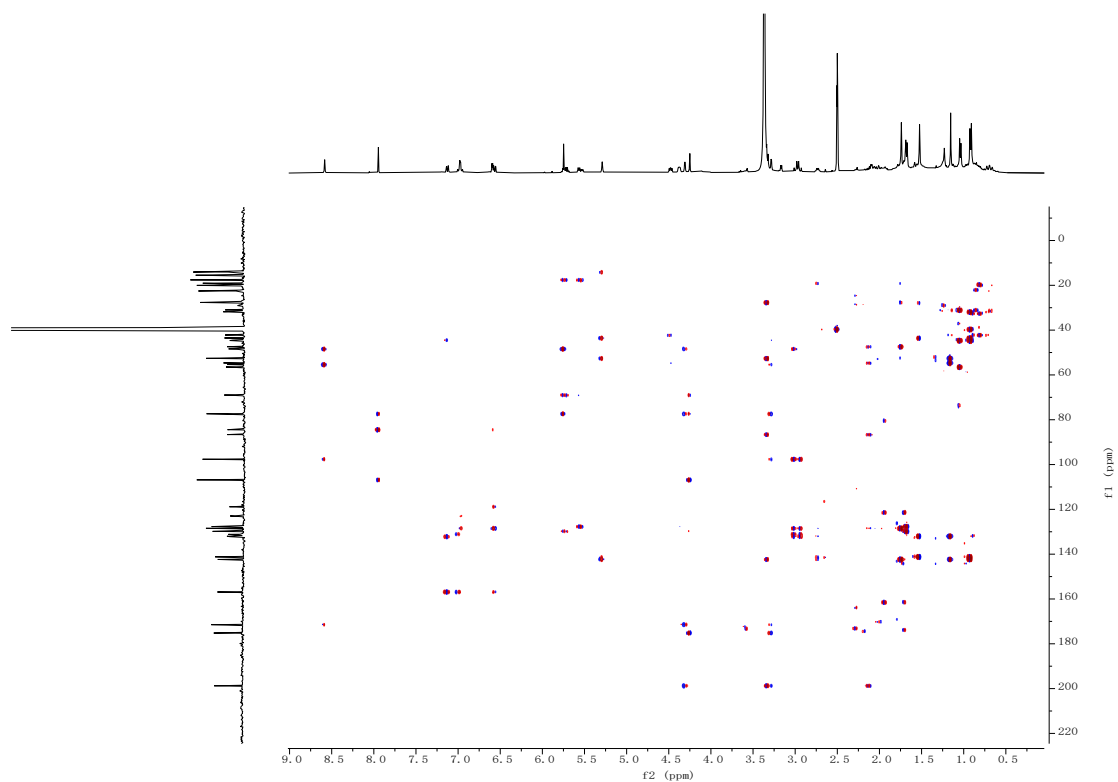


Figure S5 HMBC spectrum of **1** in DMSO- d_6

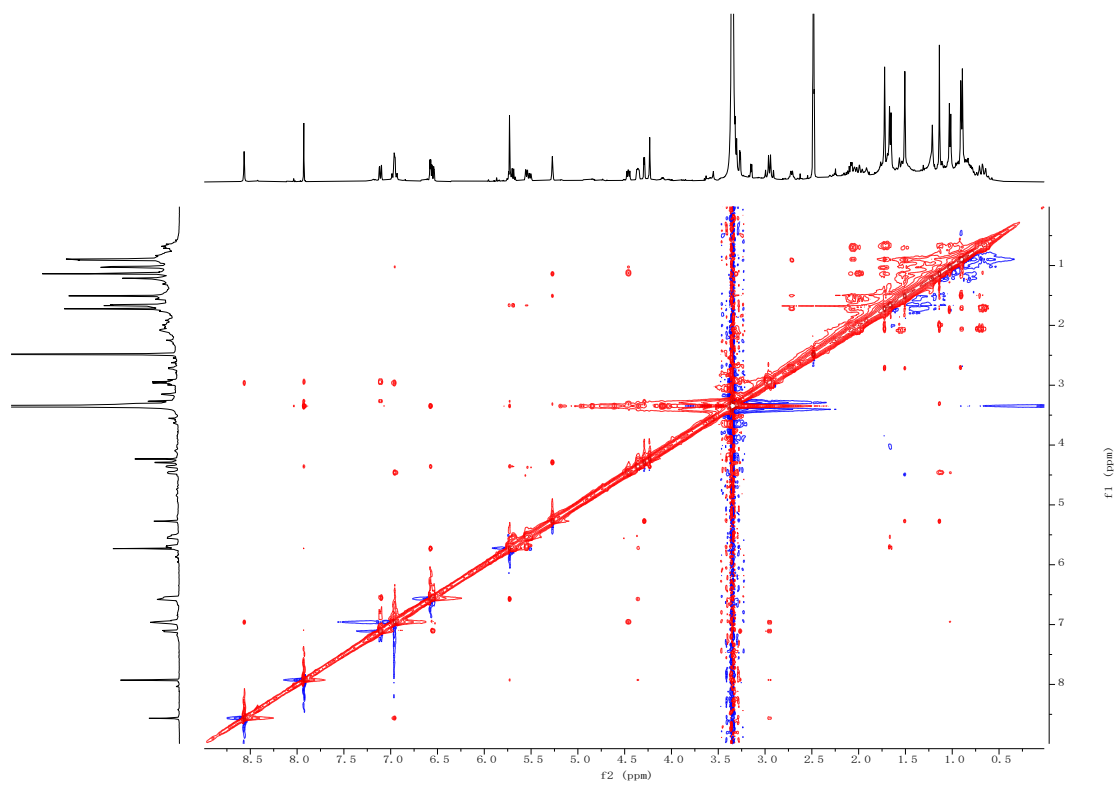


Figure S6 COSY spectrum of **1** in DMSO- d_6

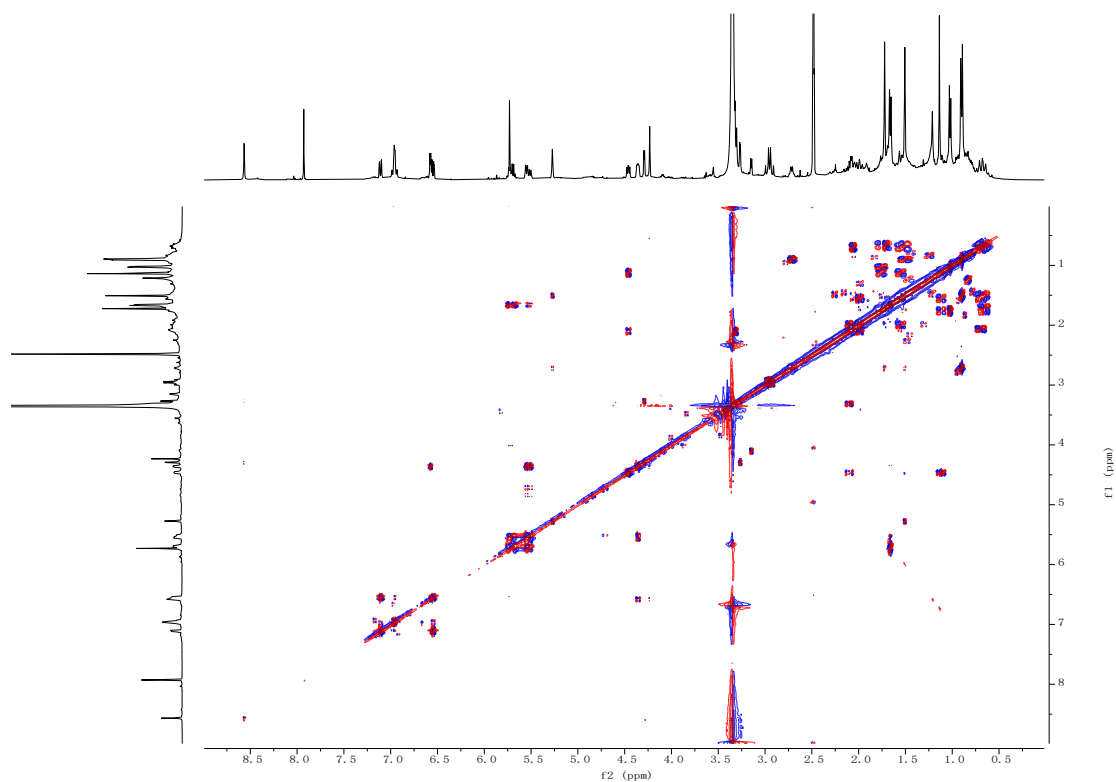


Figure S7 NOESY spectrum of **1** in DMSO- d_6

2SK4-8POS #11 RT: 0.04769 AV: 1 NL: 4.60E7
T: FTMS + p ESI Full ms [100.0000-1050.0000]

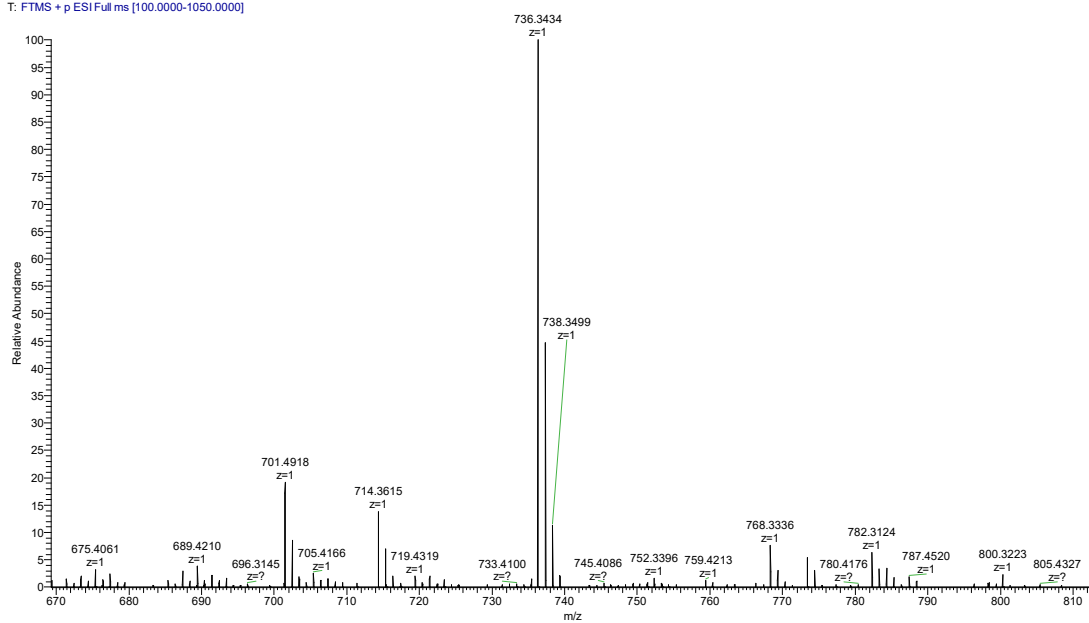


Figure S8 HR-ESI-MS spectrum of **1**

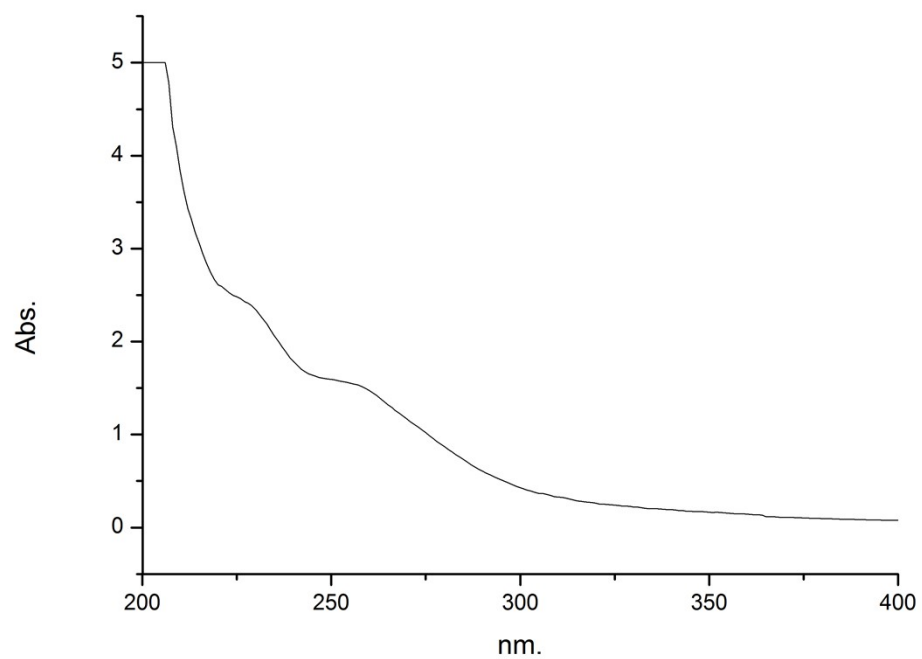


Figure S9 UV spectrum of compound **1** in MeOH

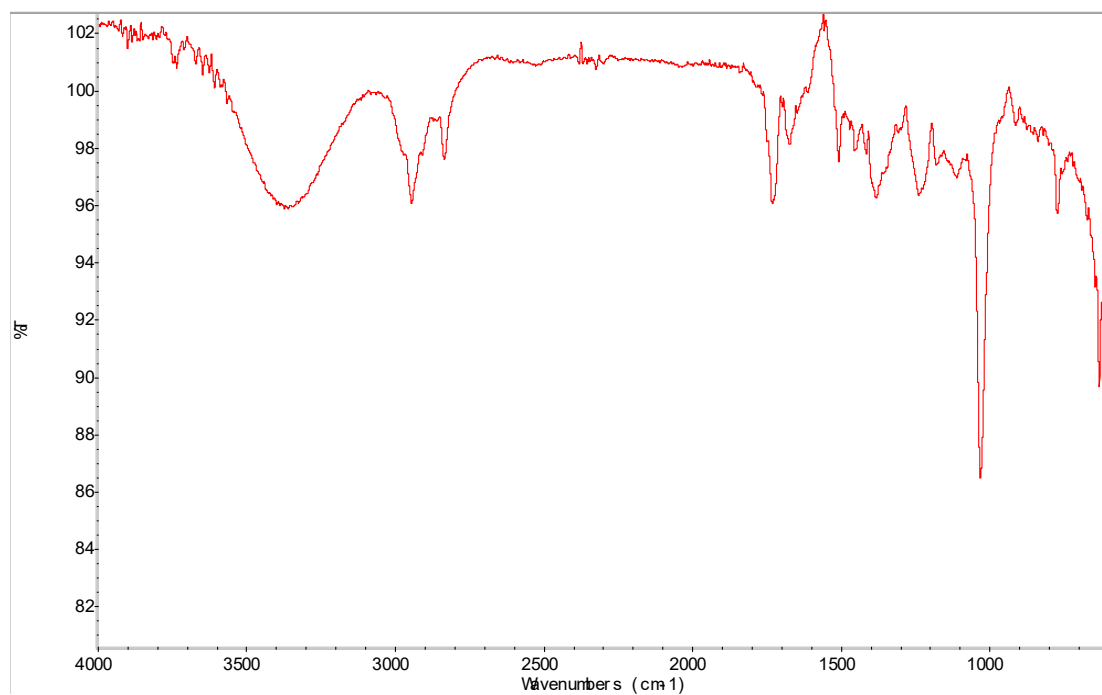


Figure S10 IR spectrum of compound **1**

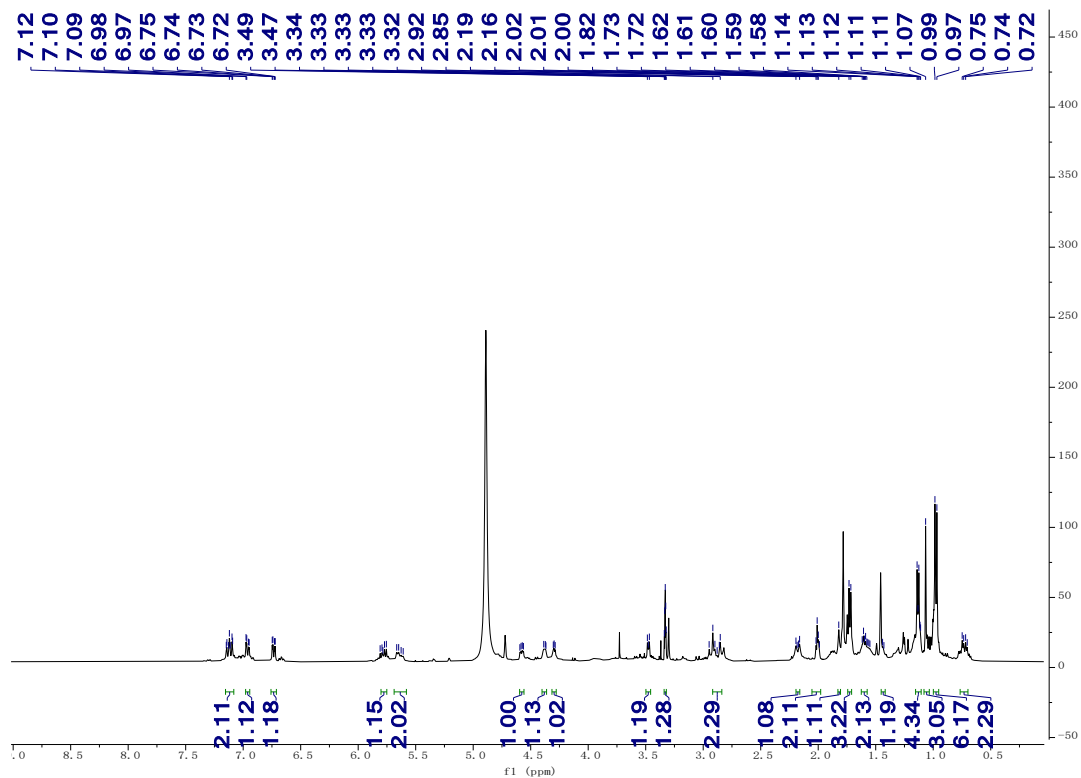


Figure S11 ^1H NMR of **2** in CD_3OD (400 MHz)

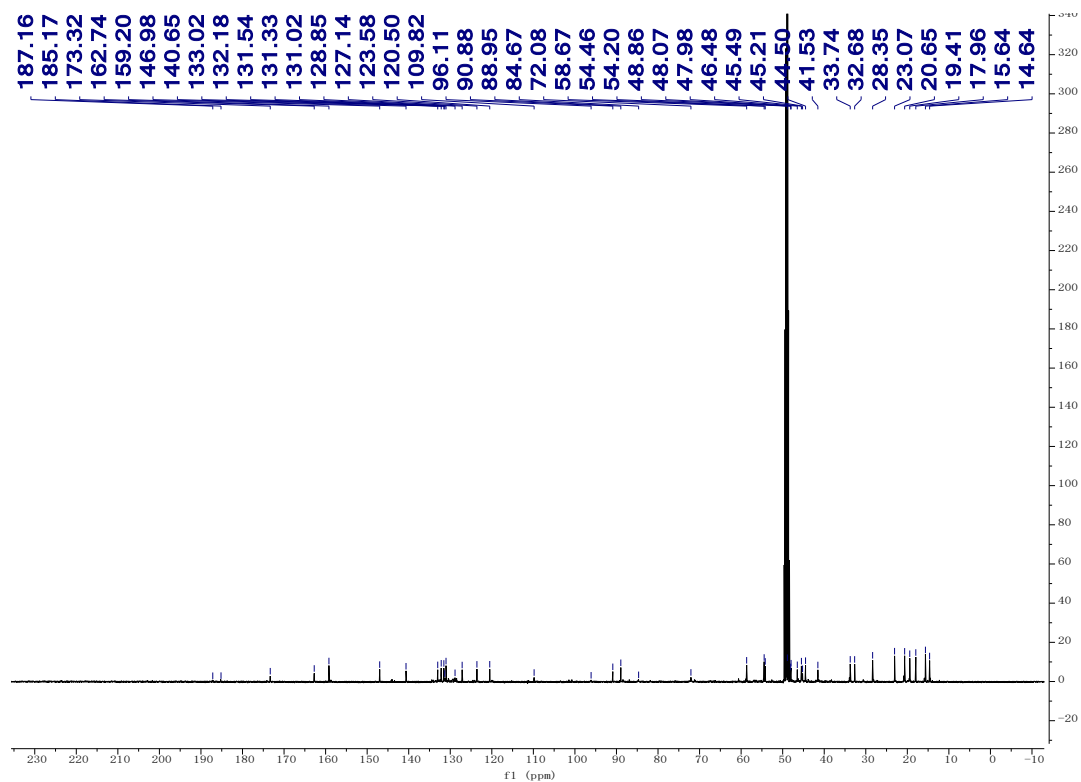


Figure S12 ^{13}C NMR of **2** in CD_3OD (400 MHz)

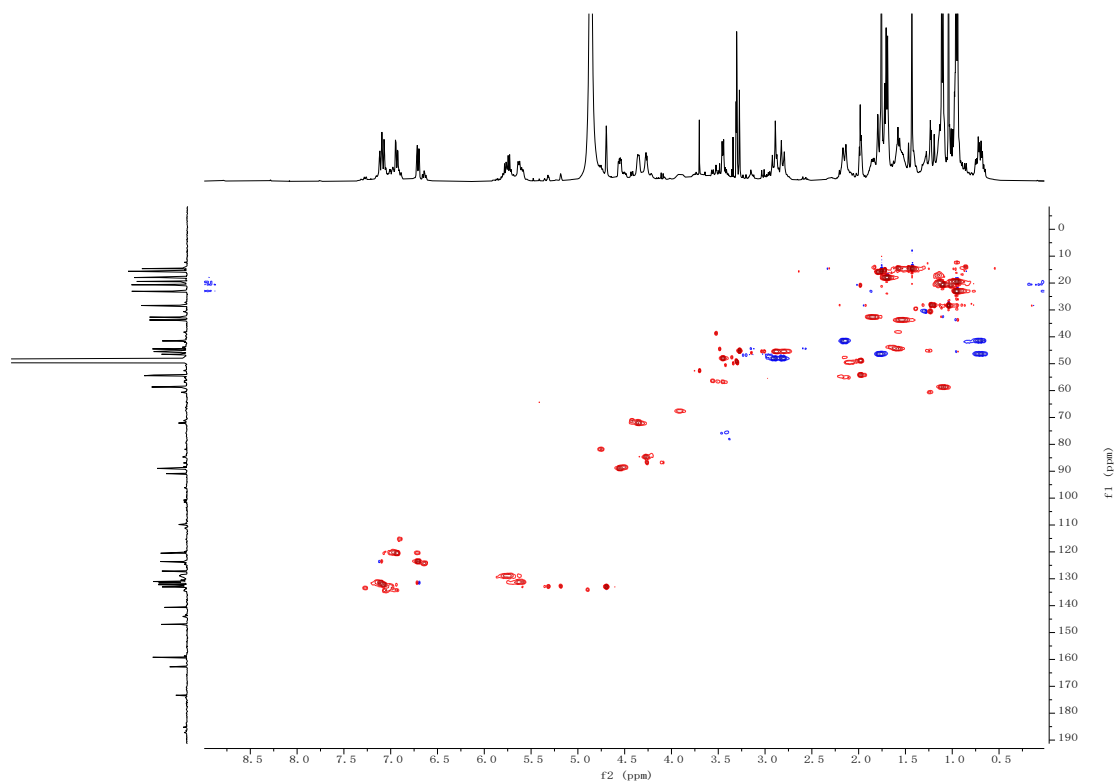


Figure S13 HSQC spectrum of **2** in CD₃OD

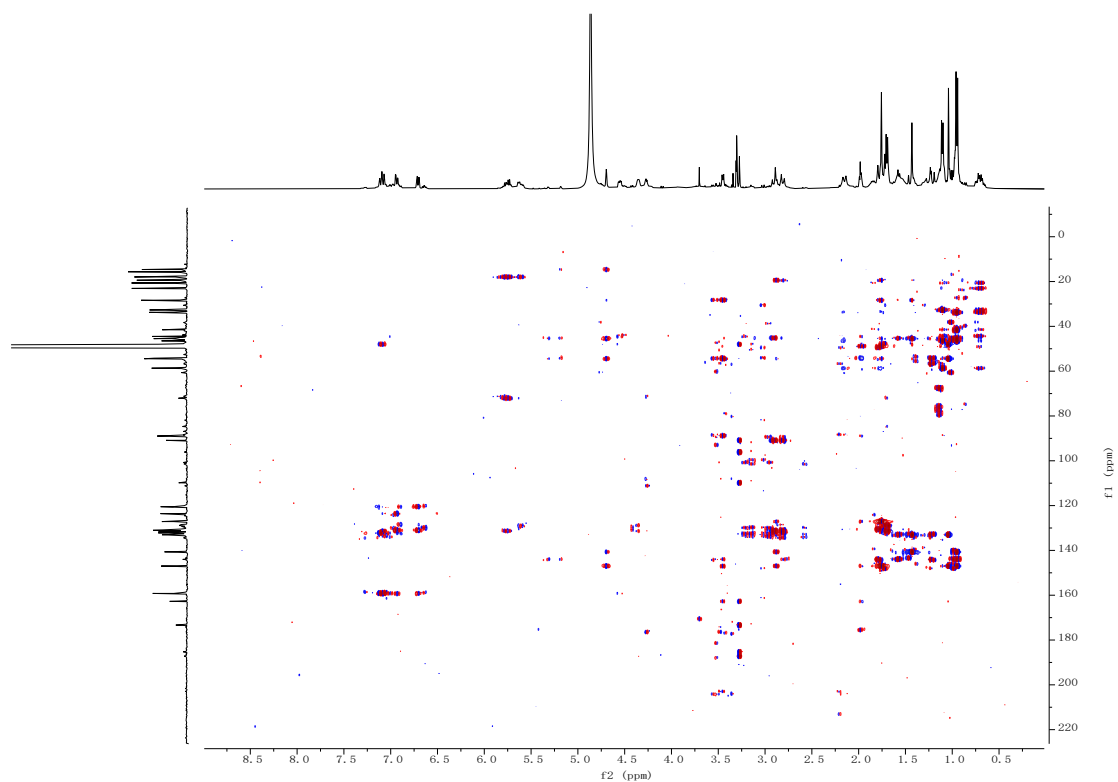


Figure S14 HMBC spectrum of **2** in CD₃OD

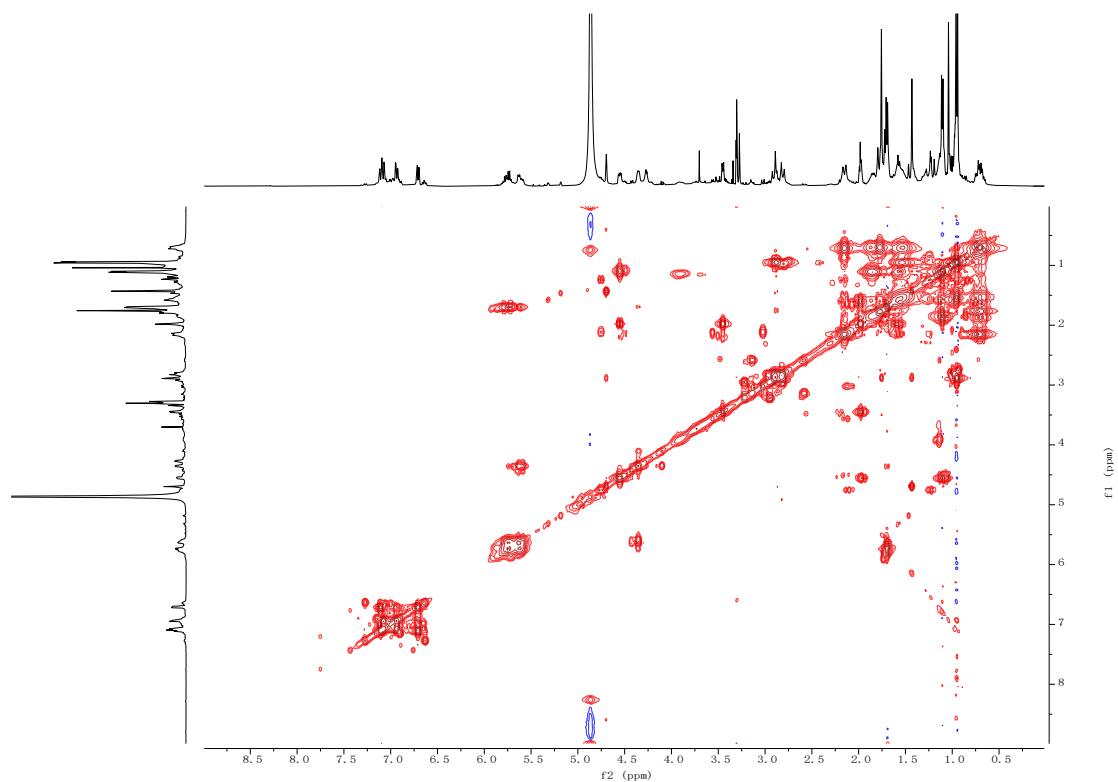


Figure S15 COSY spectrum of **2** in CD₃OD

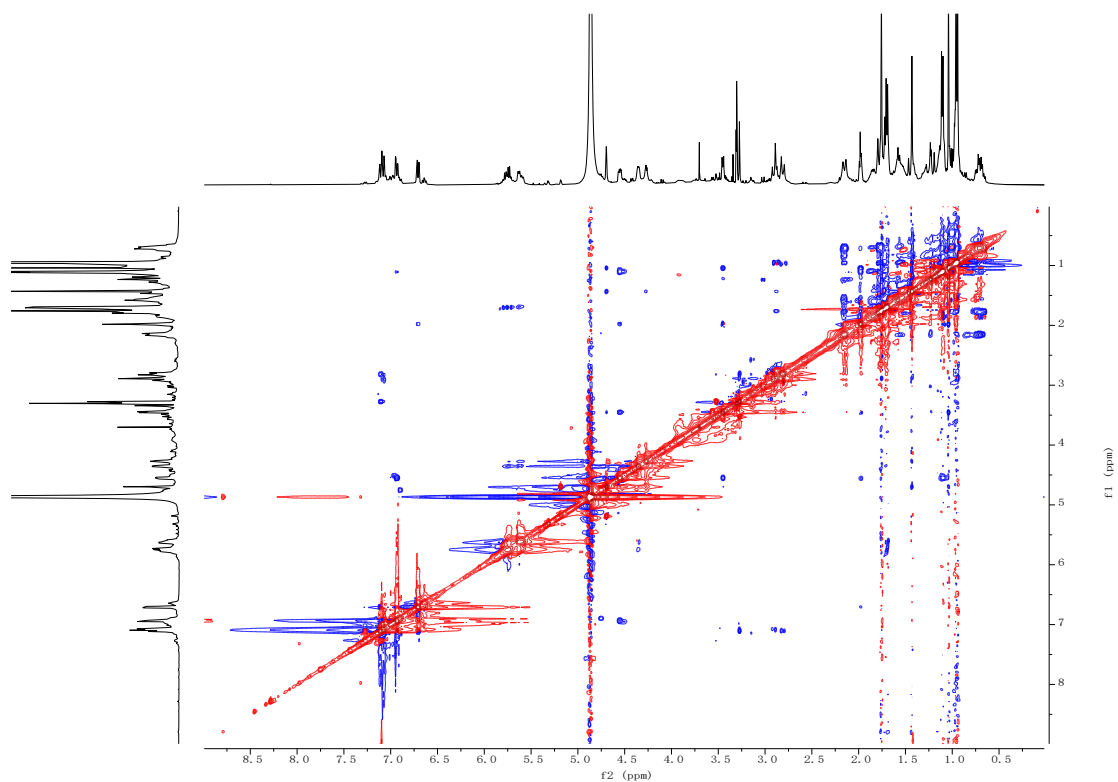


Figure S16 NOESY spectrum of **2** in CD₃OD

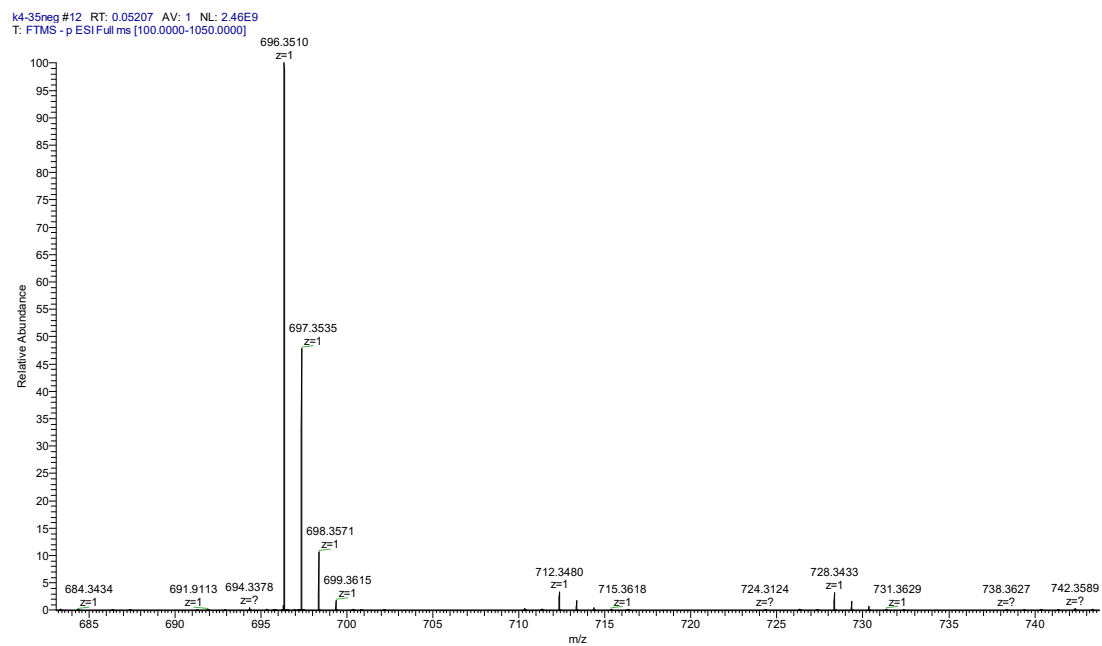


Figure S17 HR-ESI-MS spectrum of **2**

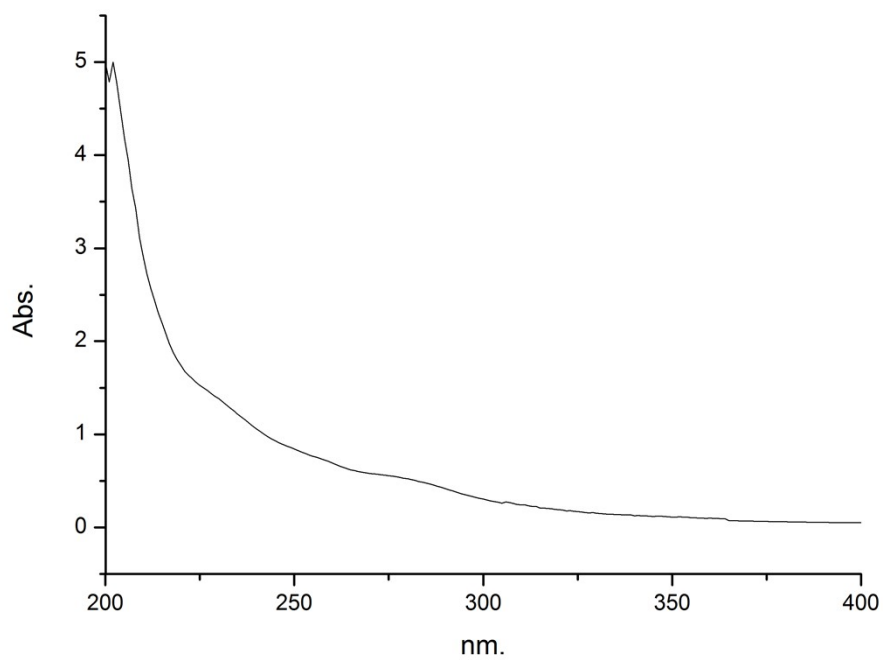


Figure S18 UV spectrum of compound **2** in MeOH

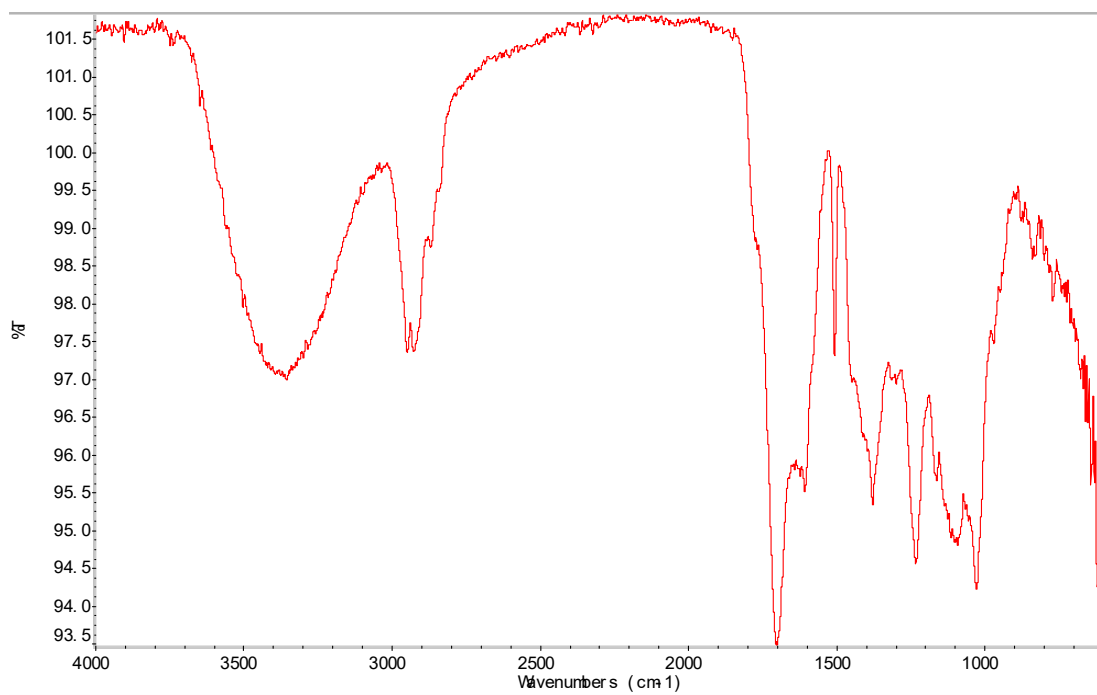


Figure S19 IR spectrum of compound **2**

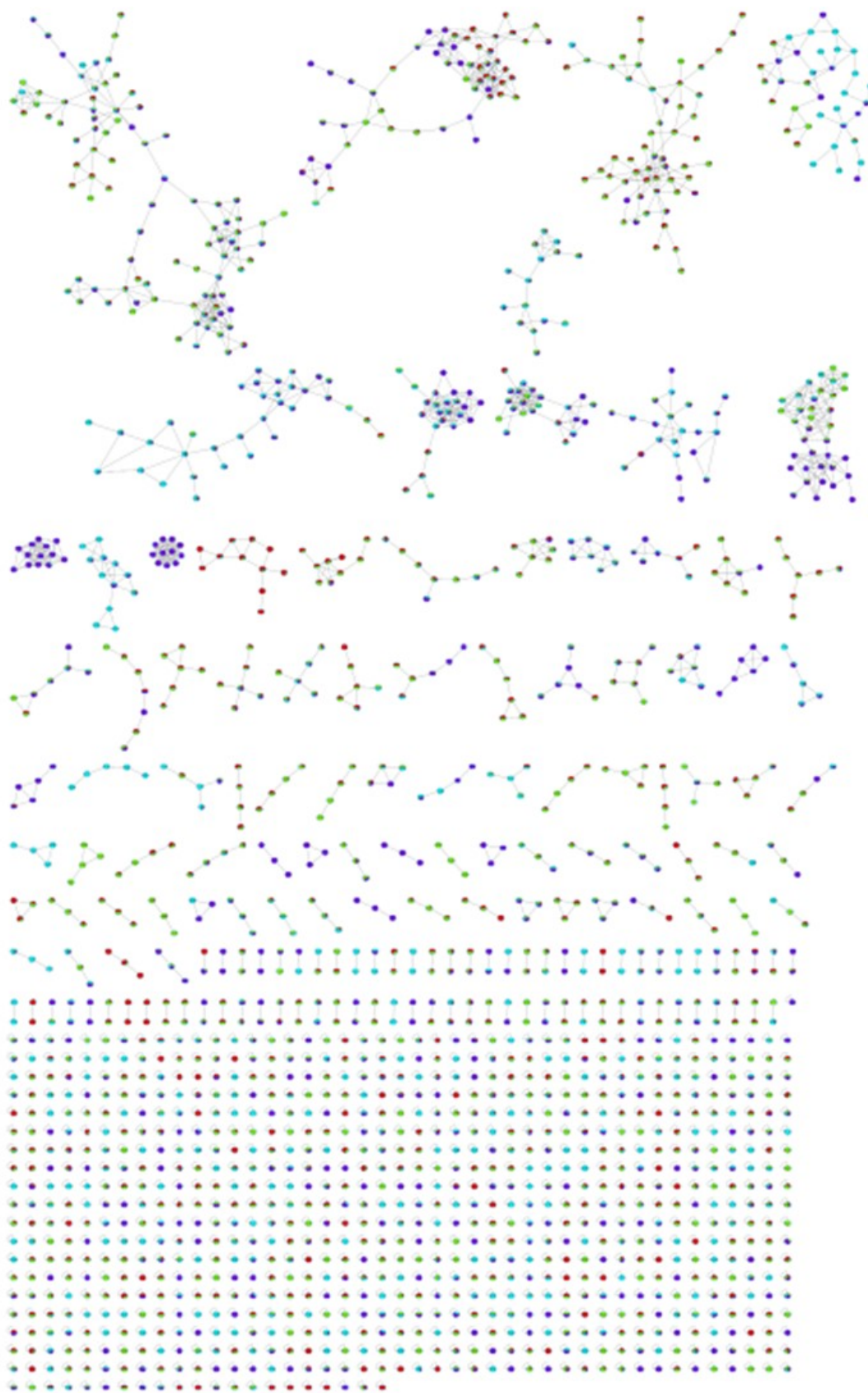


Figure S20. The total clusters of extracts from the strain *Didymella* sp. CYSK-4 generated by GNPS

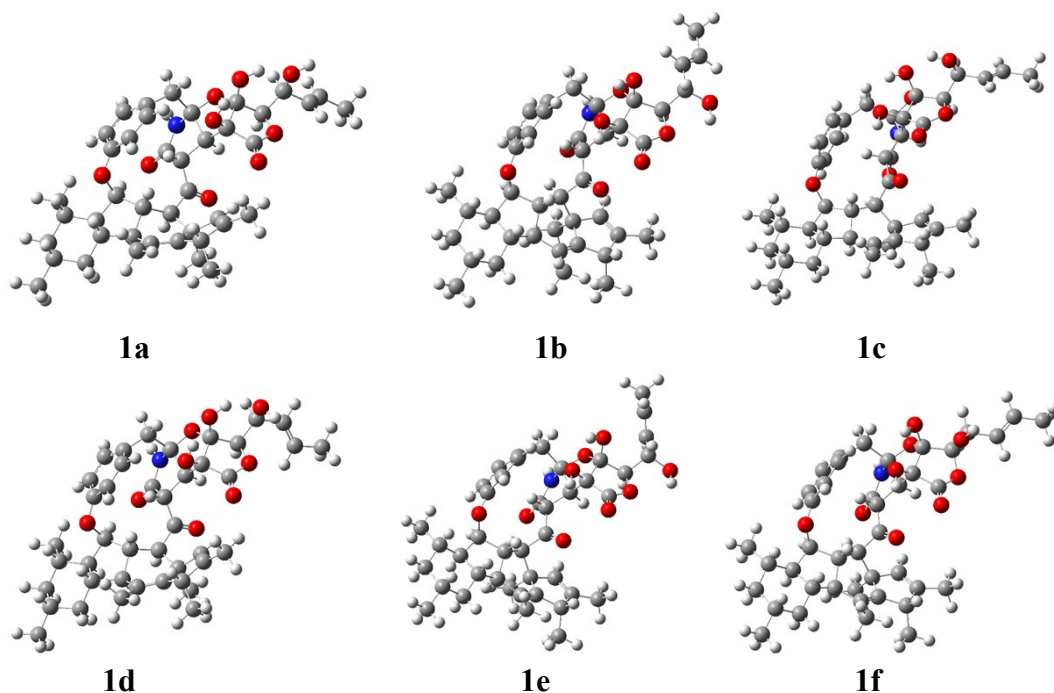


Figure S21. Optimized low-energy conformers of **1a-1f** at the B3LYP/6-31G(d) level.

Table S1. Energy analysis for the conformers of **1a-1f**.

Conformation	E(Hartree)	E(kcal/mol)	rel.E(kcal/mol)	Q (i)	Boltzmann Dist
1a	-2362.84936	-1482694.82	1.522824	0.0763886	3.18%
1b	-2362.85178	-1482696.34	0	1	41.61%
1c	-2362.85088	-1482695.78	0.565317	0.3848994	16.01%
1d	-2362.85060	-1482695.61	0.739010	0.2870422	11.94%
1e	-2362.85046	-1482695.51	0.830311	0.2460239	10.24%
1f	-2362.85094	-1482695.82	0.529173	0.4091273	17.02%

Table S2. Cartesian coordinates of conformer **1b**.

Center Number	Standard Orientation (Ångstroms)				
	Atom	Type	X	Y	Z
1	6	0	-2.652789	0.044222	0.152282
2	6	0	-3.89223	0.991374	0.04885
3	6	0	-3.45526	2.348991	-0.46191
4	6	0	-2.46195	2.91342	0.245344
5	6	0	-1.78682	2.173817	1.408363
6	6	0	-1.48581	0.666	1.001372
7	6	0	-3.2835	-1.34381	0.544989
8	6	0	-4.80716	-1.16567	0.289102
9	6	0	-4.91842	0.074246	-0.63153
10	6	0	-1.74999	4.236315	-0.01483
11	6	0	-0.52474	4.137851	0.882777
12	6	0	-0.54756	3.024145	1.620843

13	6	0	-5.63913	-2.36322	-0.19496
14	6	0	-7.09632	-1.88876	-0.39706
15	6	0	-7.24991	-0.63411	-1.27834
16	6	0	-6.37524	0.522497	-0.75079
17	6	0	-5.59222	-3.55446	0.771648
18	6	0	-8.72046	-0.21817	-1.40423
19	6	0	-4.07037	2.94686	-1.70053
20	6	0	0.543215	5.189847	0.883008
21	6	0	-2.61349	5.479481	0.293713
22	6	0	-2.57398	2.179852	2.748991
23	1	0	-5.23665	-0.85884	1.257071
24	1	0	-4.55569	-0.20046	-1.63498
25	1	0	-4.28657	1.140941	1.060979
26	6	0	2.258685	-0.46073	0.060575
27	6	0	0.826731	-0.48147	0.597303
28	6	0	-1.07755	-3.2989	1.180314
29	6	0	-1.57861	-2.94648	-0.08189
30	6	0	-0.76783	-3.13169	-1.20901
31	6	0	0.587875	-3.39672	-1.04596
32	6	0	1.161601	-3.47538	0.234653
33	6	0	0.285811	-3.56311	1.328281
34	6	0	-0.16155	0.611369	0.223168
35	8	0	-2.83149	-2.43847	-0.29222
36	1	0	-2.30031	-0.0752	-0.87997
37	8	0	0.072101	1.30984	-0.74585
38	6	0	2.92096	-1.6486	0.80328
39	7	0	2.428672	-1.34453	2.132696
40	6	0	1.158866	-0.77653	2.095298
41	6	0	2.987621	-0.46689	-1.28114
42	6	0	4.434304	-0.80291	-0.73998
43	8	0	4.31058	-1.41027	0.563815
44	6	0	2.629911	-3.15249	0.409818
45	6	0	3.214652	0.882083	-1.95835
46	8	0	4.304905	1.490714	-1.44751
47	6	0	5.098663	0.593151	-0.59562
48	8	0	5.126919	-1.6062	-1.63044
49	8	0	2.568996	-1.39542	-2.25418
50	8	0	2.577477	1.299571	-2.89148
51	6	0	6.563537	0.735958	-1.04296
52	6	0	7.470369	-0.08882	-0.16793
53	6	0	8.391242	0.421481	0.651693
54	8	0	6.929895	2.104867	-0.96906
55	6	0	9.30232	-0.39387	1.522828

56	8	0	0.460717	-0.59037	3.073492
57	1	0	0.306129	-1.37265	0.245938
58	1	0	2.711559	0.407536	0.558314
59	1	0	5.003835	0.951498	0.430963
60	1	0	-1.35661	0.094086	1.92341
61	1	0	-3.08545	-1.5957	1.591745
62	1	0	-1.43182	4.299763	-1.06765
63	1	0	0.211438	2.746316	2.350303
64	1	0	-5.24028	-2.69111	-1.16422
65	1	0	-7.6871	-2.71068	-0.82465
66	1	0	-7.53729	-1.67879	0.590988
67	1	0	-6.88271	-0.88714	-2.28599
68	1	0	-6.47122	1.389199	-1.41588
69	1	0	-6.74595	0.84087	0.23646
70	1	0	-4.57728	-3.95067	0.868266
71	1	0	-5.94591	-3.26512	1.770455
72	1	0	-6.23717	-4.36813	0.418183
73	1	0	-9.33046	-1.02902	-1.82018
74	1	0	-9.14017	0.044186	-0.42441
75	1	0	-8.83226	0.654965	-2.05835
76	1	0	-3.48233	3.787126	-2.08068
77	1	0	-5.09114	3.311742	-1.5199
78	1	0	-4.14166	2.202019	-2.50371
79	1	0	0.980289	5.303841	-0.11869
80	1	0	0.148026	6.174095	1.167548
81	1	0	1.351495	4.939905	1.578029
82	1	0	-2.05274	6.405245	0.117996
83	1	0	-2.94251	5.475674	1.339252
84	1	0	-3.50633	5.506381	-0.33942
85	1	0	-3.46774	1.549607	2.740738
86	1	0	-2.88032	3.199608	3.003141
87	1	0	-1.92578	1.810754	3.553032
88	1	0	-1.72062	-3.27727	2.053971
89	1	0	-1.19364	-2.95948	-2.19277
90	1	0	1.231191	-3.40551	-1.91806
91	1	0	0.679738	-3.72578	2.328443
92	1	0	2.696109	-1.86742	2.958679
93	1	0	3.181286	-3.37033	-0.5079
94	1	0	3.099015	-3.74877	1.204325
95	1	0	4.45479	-2.04228	-2.19168
96	1	0	2.14261	-0.86621	-2.95773
97	1	0	6.628622	0.37109	-2.07964
98	1	0	7.328639	-1.16525	-0.24598

99	1	0	8.507395	1.502592	0.693216
100	1	0	6.293631	2.594482	-1.51482
101	1	0	9.173038	-0.13353	2.582241
102	1	0	9.117882	-1.46778	1.411693
103	1	0	10.35664	-0.202	1.281547