Supplementary Data

Gephyyamycin and cysrabelomycin, two new angucyclinone derivatives from the *Streptomyces* sp. HN-A124

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ABSTRACT

Gephyyamycin (**1**) owned the rare 3,12a-epoxybenz[a]anthracene ring system, and cysrabelomycin (**2**) possessed an acetylated cysteine group, two new angucyclinone derivatives were isolated from the rice solid fermentation of the marine-derived *Streptomyces* sp. HN-A124, an actinobacterium isolated from the marine sediments collected from Hainan Province, China. Their structures were elucidated on the basis of MS, NMR spectroscopic, X-ray diffration data analyses and quantum chemical calculations of the electronic circular dichroism (ECD) spectra. Compound **2** was appeared to show moderate cytotoxicity against PC3 and A2780 cell lines with IC_{50} values of 19.39 and 10.23 μM, respectively; on the other hand, compound **2** have also exhibited moderate antibacterial activities against *Staphylococcus aureus* and *Candida albicans* with an MIC value of 20.0 and 20 μM, respectively.

KEYWORDS: Angucyclinones; Gephyromycins; X-ray diffraction; Cytotoxicity.

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X-ray Analysis and Crystal Data of 1.

Crystal data and details on the structure refinement are given in Table S1. The structural data has been deposited with the Cambridge Crystallographic Data Center (CCDC 1902601).

Table S1. Crystal data and structure refinement for **1**.

CCDC number	1902601
Empirical formula	$C_{25.25}H_{29.5}O_{13.25}$
Formula weight	544.99
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	12.0615(2)
b/Å	29.6569(5)
c/Å	14.0079(2)
α/°	90
β/°	96.2059(16)
γ/°	90
Volume/Å^3	4981.35(15)
Z	8
ρ_{calc}g/cm^3	1.453
μ/mm^{-1}	1.015
F(000)	2296.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	5.96 to 147.178
Index ranges	$-10 \leq h \leq 14$, $-36 \leq k \leq 32$, $-17 \leq l \leq 16$
Reflections collected	28312
Independent reflections	15553 [R_{int}= 0.0296, R_{sigma}= 0.0329]
Data/restraints/parameters	15553/19/1422
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1= 0.0699, wR_2= 0.2001
Final R indexes [all data]	R_1= 0.0711, wR_2= 0.2018
Largest diff. peak/hole / e Å^{-3}	0.74/-0.70
Flack/Hooft parameter	-0.02(5)/0.03(5)

ECD Calculation Details of 2.

1. Methods

Monte Carlo conformational searches were carried out by means of the Spartan's 10 software using Merck Molecular Force Field (MMFF). The conformers with Boltzmann-population of over 5% were chosen for ECD calculations, and then the conformers were initially optimized at B3LYP/6-31+g (d, p) level in MeOH using the CPCM polarizable conductor calculation model. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-311+g (d, p) level for all conformers of compounds **2**. Rotatory strengths for a total of 50 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

2. Results

Table S1.2.1.Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	In MeOH	
	ΔG	P (%)/100
2-1	0.00	0.473
2-2	0.63	0.162
2-3	0.64	0.160
2-4	0.93	0.099
2-5	1.33	0.051

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

Table S1.2.2**.**Cartesian coordinates for the low-energy reoptimized MMFF conformers of **2** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.

2-1		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	0.794990	5.182533	-0.312365
2.	6.	0.	-0.445716	4.930468	-0.875666
3.	6.	0.	-0.936570	3.620498	-0.976999
4.	6.	0.	-0.135840	2.566292	-0.561530
5.	6.	0.	1.141706	2.786936	-0.017713
6.	6.	0.	1.592288	4.122181	0.160799
7.	6.	0.	-0.661890	1.180410	-0.560249
8.	6.	0.	0.313886	0.042470	-0.505815
9.	6.	0.	1.656920	0.277593	-0.109039
10.	6.	0.	1.974963	1.653874	0.370022
11.	6.	0.	-0.114892	-1.277143	-0.848422

12.	6.	0.	0.792260	-2.306160	-0.748970
13.	6.	0.	2.140038	-2.126496	-0.377456
14.	6.	0.	2.632478	-0.799833	-0.093757
15.	6.	0.	2.973866	-3.269868	-0.377033
16.	6.	0.	4.326250	-3.161902	-0.139363
17.	6.	0.	4.843262	-1.872774	0.082100
18.	6.	0.	4.068122	-0.719690	0.093851
19.	8.	0.	2.751429	4.430301	0.750336
20.	8.	0.	2.965699	1.889278	1.108753
21.	8.	0.	-1.877972	1.014419	-0.594564
22.	8.	0.	4.776799	0.418166	0.210585
23.	6.	0.	5.238690	-4.360799	-0.124331
24.	16.	0.	-1.708426	-1.739488	-1.569391
25.	6.	0.	-3.321162	-1.606536	0.824203
26.	7.	0.	-4.140637	-0.582813	0.196423
27.	6.	0.	-2.351075	-1.007490	1.858002
28.	8.	0.	-2.714792	0.185589	2.361517
29.	8.	0.	-1.360905	-1.586434	2.237604
30.	6.	0.	-5.498115	-0.782273	0.015576
31.	8.	0.	-6.101580	-1.702404	0.547025
32.	6.	0.	-6.179125	0.233237	-0.884072
33.	6.	0.	-2.603742	-2.535689	-0.168433
34.	1.	0.	1.174337	6.191995	-0.197507
35.	1.	0.	-1.052920	5.761415	-1.221746
36.	1.	0.	-1.926949	3.413655	-1.364135
37.	1.	0.	0.470822	-3.308929	-1.011877
38.	1.	0.	2.523333	-4.234933	-0.588310
39.	1.	0.	5.907100	-1.729360	0.243852
40.	1.	0.	3.126859	3.582874	1.088638
41.	1.	0.	4.206792	1.094371	0.646917
42.	1.	0.	5.723912	-4.470684	0.852058
43.	1.	0.	4.691993	-5.282992	-0.335988
44.	1.	0.	6.036173	-4.257940	-0.868650
45.	1.	0.	-4.021620	-2.231107	1.395321
46.	1.	0.	-3.640679	0.031687	-0.439604
47.	1.	0.	-3.502472	0.478494	1.867148
48.	1.	0.	-6.308542	-0.204803	-1.879428
49.	1.	0.	-7.171754	0.447543	-0.484531
50.	1.	0.	-5.611649	1.161856	-0.985505
51.	1.	0.	-3.348623	-3.159495	-0.670026
52.	1.	0.	-1.915821	-3.182503	0.378562

2-2		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	0.795210	5.182655	-0.312460
2.	6.	0.	-0.445743	4.930606	-0.875208
3.	6.	0.	-0.936660	3.620638	-0.976273
4.	6.	0.	-0.135776	2.566441	-0.561092
5.	6.	0.	1.142004	2.787057	-0.017800
6.	6.	0.	1.592692	4.122310	0.160426
7.	6.	0.	-0.661798	1.180565	-0.559644
8.	6.	0.	0.314011	0.042657	-0.505697
9.	6.	0.	1.657094	0.277642	-0.108973
10.	6.	0.	1.975311	1.653981	0.369792
11.	6.	0.	-0.114878	-1.276826	-0.848597
12.	6.	0.	0.792179	-2.305939	-0.749372
13.	6.	0.	2.139932	-2.126497	-0.377674
14.	6.	0.	2.632527	-0.799932	-0.093705
15.	6.	0.	2.973558	-3.270010	-0.377318
16.	6.	0.	4.325917	-3.162326	-0.139366
17.	6.	0.	4.843094	-1.873343	0.082440
18.	6.	0.	4.068174	-0.720091	0.094235
19.	8.	0.	2.752078	4.430495	0.749438
20.	8.	0.	2.966326	1.889531	1.108135
21.	8.	0.	-1.877892	1.014517	-0.593381
22.	8.	0.	4.777022	0.417545	0.211519
23.	6.	0.	5.238131	-4.361393	-0.124273
24.	16.	0.	-1.708418	-1.738758	-1.569777
25.	6.	0.	-3.321270	-1.606670	0.823815
26.	7.	0.	-4.140819	-0.582789	0.196391
27.	6.	0.	-2.351218	-1.007927	1.857802
28.	8.	0.	-2.715130	0.184852	2.361919
29.	8.	0.	-1.360907	-1.586846	2.237071
30.	6.	0.	-5.498300	-0.782162	0.015617
31.	8.	0.	-6.101719	-1.702488	0.546799
32.	6.	0.	-6.179400	0.233703	-0.883564
33.	6.	0.	-2.603847	-2.535446	-0.169164
34.	1.	0.	1.174651	6.192107	-0.197813
35.	1.	0.	-1.053078	5.761550	-1.221067
36.	1.	0.	-1.927198	3.413782	-1.362998
37.	1.	0.	0.470669	-3.308614	-1.012556
38.	1.	0.	2.522880	-4.234954	-0.588841
39.	1.	0.	5.906922	-1.730150	0.244469

40.	1.	0.	3.127655	3.583126	1.087696
41.	1.	0.	4.206756	1.093996	0.647292
42.	1.	0.	5.722297	-4.472074	0.852554
43.	1.	0.	4.691492	-5.283339	-0.337158
44.	1.	0.	6.036413	-4.258129	-0.867670
45.	1.	0.	-4.021699	-2.231475	1.394713
46.	1.	0.	-3.640919	0.032112	-0.439281
47.	1.	0.	-3.502825	0.477909	1.867674
48.	1.	0.	-7.171970	0.447894	-0.483818
49.	1.	0.	-5.611909	1.162355	-0.984654
50.	1.	0.	-6.308891	-0.203921	-1.879089
51.	1.	0.	-3.348741	-3.159016	-0.671035
52.	1.	0.	-1.915969	-3.182512	0.377586

2-3		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	0.844152	5.060387	-0.044986
2.	6.	0.	-0.390270	4.741455	-0.584402
3.	6.	0.	-0.775073	3.403454	-0.759467
4.	6.	0.	0.108254	2.389871	-0.415496
5.	6.	0.	1.381857	2.684173	0.108924
6.	6.	0.	1.741979	4.040764	0.329925
7.	6.	0.	-0.325934	0.974091	-0.521072
8.	6.	0.	0.640712	-0.116196	-0.182668
9.	6.	0.	2.012322	0.204165	0.011203
10.	6.	0.	2.317907	1.609093	0.396624
11.	6.	0.	0.225504	-1.488679	-0.164214
12.	6.	0.	1.195845	-2.464336	-0.058083
13.	6.	0.	2.578736	-2.190706	-0.059776
14.	6.	0.	3.031289	-0.822097	-0.024496
15.	6.	0.	3.475827	-3.284298	-0.107519
16.	6.	0.	4.837042	-3.081790	-0.177015
17.	6.	0.	5.301195	-1.751720	-0.192520
18.	6.	0.	4.465091	-0.646353	-0.125491
19.	8.	0.	2.906019	4.406996	0.870887
20.	8.	0.	3.378621	1.893148	1.015075
21.	8.	0.	-1.469277	0.736547	-0.910450
22.	8.	0.	5.087242	0.541648	-0.256716

23.	6.	0.	5.815402	-4.225597	-0.244786
24.	16.	0.	-1.427654	-2.155433	-0.356017
25.	6.	0.	-3.883192	-1.348199	0.654176
26.	7.	0.	-4.093956	-0.517242	-0.534834
27.	6.	0.	-4.699322	-0.840343	1.875296
28.	8.	0.	-6.018420	-0.812310	1.697660
29.	8.	0.	-4.169149	-0.518864	2.915413
30.	6.	0.	-5.217684	-0.587095	-1.278964
31.	8.	0.	-6.220650	-1.216744	-0.900881
32.	6.	0.	-5.204746	0.142859	-2.603666
33.	6.	0.	-2.398444	-1.387672	1.013822
34.	1.	0.	1.149339	6.088621	0.115164
35.	1.	0.	-1.075257	5.537768	-0.858912
36.	1.	0.	-1.752691	3.141516	-1.144590
37.	1.	0.	0.881906	-3.501946	-0.006474
38.	1.	0.	3.064505	-4.289174	-0.115806
39.	1.	0.	6.363729	-1.543263	-0.269789
40.	1.	0.	3.379588	3.572084	1.107698
41.	1.	0.	4.588188	1.205382	0.271705
42.	1.	0.	6.517836	-4.190676	0.595474
43.	1.	0.	5.305388	-5.191623	-0.220829
44.	1.	0.	6.412023	-4.177777	-1.162687
45.	1.	0.	-4.251368	-2.358792	0.425524
46.	1.	0.	-3.278514	-0.025341	-0.885954
47.	1.	0.	-6.246354	-1.081228	0.764202
48.	1.	0.	-5.362374	-0.586892	-3.402866
49.	1.	0.	-6.043777	0.842784	-2.630885
50.	1.	0.	-4.272371	0.680382	-2.789208
51.	1.	0.	-2.265543	-1.971683	1.923814
52.	1.	0.	-2.039875	-0.377280	1.204517

2 -4		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	3.632708	-4.250002	0.051928
2.	6.	0.	2.489812	-4.769342	0.638120
3.	6.	0.	1.351902	-3.970296	0.822982
4.	6.	0.	1.408154	-2.630444	0.467284

5.	6.	0.	2.560798	-2.064211	-0.105515
6.	6.	0.	3.676015	-2.905007	-0.365769
7.	6.	0.	0.209414	-1.772128	0.569767
8.	6.	0.	0.405023	-0.287828	0.651055
9.	6.	0.	1.571002	0.299594	0.088960
10.	6.	0.	2.582617	-0.645521	-0.464518
11.	6.	0.	-0.621218	0.526965	1.216789
12.	6.	0.	-0.527564	1.890930	1.073554
13.	6.	0.	0.567194	2.526600	0.454561
14.	6.	0.	1.708934	1.748523	0.024411
15.	6.	0.	0.526784	3.939060	0.377416
16.	6.	0.	1.609981	4.655730	-0.079967
17.	6.	0.	2.761988	3.930320	-0.430472
18.	6.	0.	2.856096	2.544380	-0.369844
19.	8.	0.	4.783069	-2.485675	-0.986050
20.	8.	0.	3.500214	-0.273812	-1.241154
21.	8.	0.	-0.902922	-2.296848	0.547291
22.	8.	0.	4.086004	2.071599	-0.636001
23.	6.	0.	1.591099	6.157700	-0.194820
24.	16.	0.	-1.912315	-0.137000	2.287148
25.	6.	0.	-3.968395	0.198386	0.249821
26.	7.	0.	-3.499623	-1.119363	-0.170000
27.	6.	0.	-3.642089	1.323478	-0.773849
28.	8.	0.	-4.082348	1.095195	-2.007516
29.	8.	0.	-3.082421	2.354268	-0.464454
30.	6.	0.	-4.118698	-1.828779	-1.138145
31.	8.	0.	-5.049595	-1.349531	-1.811505
32.	6.	0.	-3.640697	-3.246762	-1.354195
33.	6.	0.	-3.499112	0.565086	1.669951
34.	1.	0.	4.509838	-4.862420	-0.126208
35.	1.	0.	2.470754	-5.812425	0.938862
36.	1.	0.	0.434761	-4.373675	1.235320
37.	1.	0.	-1.312558	2.523831	1.467739
38.	1.	0.	-0.380703	4.442762	0.694565
39.	1.	0.	3.657381	4.448889	-0.759038
40.	1.	0.	4.603330	-1.562571	-1.283663
41.	1.	0.	4.004461	1.141248	-0.955522
42.	1.	0.	1.750310	6.471584	-1.232606
43.	1.	0.	0.637759	6.572711	0.140943
44.	1.	0.	2.390857	6.608909	0.403056
45.	1.	0.	-5.066999	0.151347	0.265879
46.	1.	0.	-2.656954	-1.491633	0.269943
47.	1.	0.	-4.573660	0.225783	-2.046134

48.	1.	0.	-4.430645	-3.931490	-1.029530
49.	1.	0.	-3.490178	-3.407746	-2.424147
50.	1.	0.	-2.722832	-3.473655	-0.809377
51.	1.	0.	-4.200733	0.164299	2.407060
52.	1.	0.	-3.496269	1.651623	1.756576

2-5		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.545181	5.138571	0.205991
2.	6.	0.	0.170996	4.987703	0.269458
3.	6.	0.	-0.413425	3.713153	0.221885
4.	6.	0.	0.400218	2.594875	0.108452
5.	6.	0.	1.804058	2.712927	0.058715
6.	6.	0.	2.383964	4.010524	0.096801
7.	6.	0.	-0.209363	1.247303	0.041533
8.	6.	0.	0.662044	0.074447	-0.275639
9.	6.	0.	2.054397	0.157139	-0.030391
10.	6.	0.	2.644905	1.522239	0.000126
11.	6.	0.	0.086791	-1.141668	-0.763686
12.	6.	0.	0.911107	-2.231978	-0.933867
13.	6.	0.	2.262144	-2.250473	-0.520005
14.	6.	0.	2.869988	-1.043378	-0.018818
15.	6.	0.	2.960329	-3.479307	-0.579659
16.	6.	0.	4.248500	-3.587016	-0.099187
17.	6.	0.	4.838932	-2.434152	0.452220
18.	6.	0.	4.203554	-1.200353	0.514354
19.	8.	0.	3.699550	4.225383	0.039731
20.	8.	0.	3.889768	1.688724	-0.108872
21.	8.	0.	-1.406897	1.107842	0.283633
22.	8.	0.	4.883090	-0.244382	1.176597
23.	6.	0.	5.012498	-4.885255	-0.137760
24.	16.	0.	-1.596621	-1.326433	-1.373893
25.	6.	0.	-3.986652	-1.426353	0.047769
26.	7.	0.	-4.152973	0.025672	-0.070061
27.	6.	0.	-4.766802	-2.013442	1.257482
28.	8.	0.	-6.080490	-1.796096	1.239656
29.	8.	0.	-4.218315	-2.645482	2.132373

30.	6.	0.	-5.281465	0.593948	-0.543469
31.	8.	0.	-6.321338	-0.060138	-0.732398
32.	6.	0.	-5.228478	2.078047	-0.832025
33.	6.	0.	-2.504488	-1.770499	0.175455
34.	1.	0.	2.014583	6.115672	0.237213
35.	1.	0.	-0.460604	5.866996	0.350923
36.	1.	0.	-1.487461	3.581505	0.266774
37.	1.	0.	0.493428	-3.137180	-1.362634
38.	1.	0.	2.446683	-4.345566	-0.985674
39.	1.	0.	5.838746	-2.478255	0.872920
40.	1.	0.	4.123789	3.336186	-0.052656
41.	1.	0.	4.654079	0.623749	0.772200
42.	1.	0.	5.290958	-5.206965	0.871985
43.	1.	0.	4.424618	-5.682853	-0.598300
44.	1.	0.	5.942313	-4.775954	-0.707031
45.	1.	0.	-4.415019	-1.886626	-0.854667
46.	1.	0.	-3.311455	0.581483	0.039488
47.	1.	0.	-6.328979	-1.242356	0.448113
48.	1.	0.	-5.472918	2.234703	-1.886248
49.	1.	0.	-5.996597	2.582514	-0.240067
50.	1.	0.	-4.253298	2.521205	-0.619356
51.	1.	0.	-2.398480	-2.836123	0.373761
52.	1.	0.	-2.064188	-1.217730	1.005801

Table S1. ^{1}H (600 MHz) and ^{13}C (125 MHz) NMR Data of Compounds **1** and **2**.

	1[a]		**2**[b]	
	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)
1	206.8, qC		154.8, qC	
2	49.9, CH_2	2.50, m	114.2, CH	6.81, s
		2.53, m		
3	78.8, qC		142.1, qC	
4	48.3, CH_2	2.39, dd (14.0, 2.0)	117.4, CH	7.26, s
		1.89, d (14.0)		
4a	79.5, qC		137.6, qC	
5	30.3, CH_2	2.23, m	127.5, CH	8.05, s
		1.66, m		
6	26.4, CH_2	2.47, m	135.9, qC	
		2.19, m		
6a	81.3, qC		128.7, qC	
7	201.3, qC		187.7, qC	
7a	116.0, qC		115.4, qC	
8	159.0, qC		160.2, qC	
9	139.1, qC		123.0, CH	7.31, d (8.0)
10	134.2, CH	7.87, d (8.0)	136.8, CH	7.75, dd (8.0, 8.0)
11	120.0, CH	7.60, d (8.0)	117.6, CH	7.47, d (8.0)
11a	133.5, qC		135.6, qC	
12	193.1, qC		185.3, qC	
12a	72.6, qC		139.5, qC	
12b	77.7, qC		116.6, qC	
1'	72.5, CH	4.88, m		
2'	41.0, CH_2	2.42, m	33.4, CH_2	3.50, m
		1.38, m		3.30, m
3'	77.0, CH	3.43, m	51.0, CH	4.52, m
4'	78.4, CH	3.03, t (9.0)		
5'	73.6, CH	3.69, m	169.8, qC	8.51, d (7.8)
6'	18.6, CH_3	1.36, d (6.0)	22.4, CH_3	1.87, s
3-Me	25.3, CH_3	1.18, s	21.6, CH_3	2.43, s
1-OH				10.41, s
3'-COOH			172.0, qC	11.80, s

[a, b] Recorded in methanol-d_4 and DMSO-d_6, respectively.

Table S2. Cytotoxic activities of compounds **1** and **2** inhibiting PC-3 and A2780 cells.

Compound	IC_{50} (μM)	
	PC-3	A2780
1	>20	>20
2	19.39	10.23
adriamycin [a]	0.16	0.002

[a] was considered as a positive control.

Table S3. Antibacterial activities of compounds **1** and **2**.

Compound	MIC (μM)		
	Escherichia coli	*Staphylococcus aureus*	*Candida albicans*
1	>40	>40	20
2	>40	20	20
Vancomycin [a]		2.5	
Bacillosporin B [a]	2.5		
Amphotericin B [a]			5

[a] was considered as a positive control.

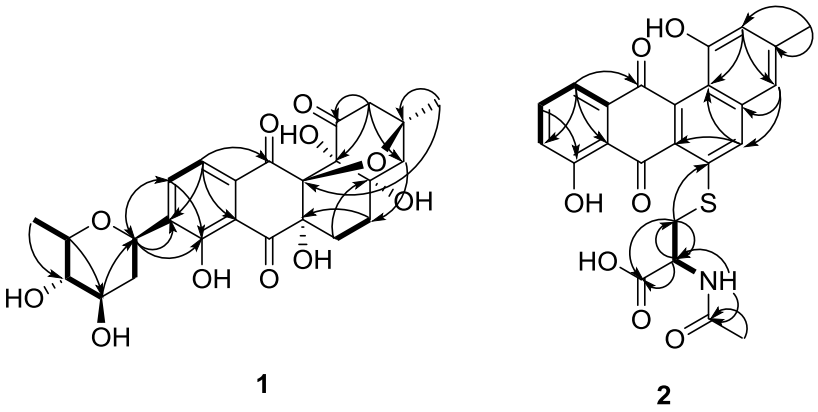

Figure S1. Key $^{1}H-^{1}H$ COSY (bold) and HMBC (arrows) correlations of **1** and **2**.

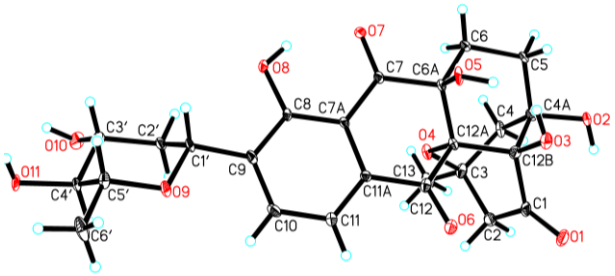

Figure S2. **ORTEP** drawing of compound **1**

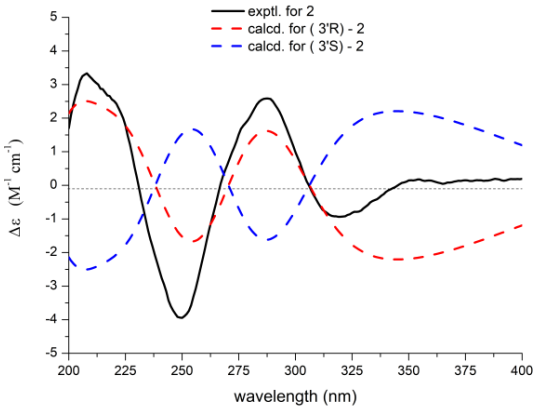

Figure S3. Experimental (black solid line) calculated ECD spectra of **2** (red dash line) and its enantiomer (blue dash line).

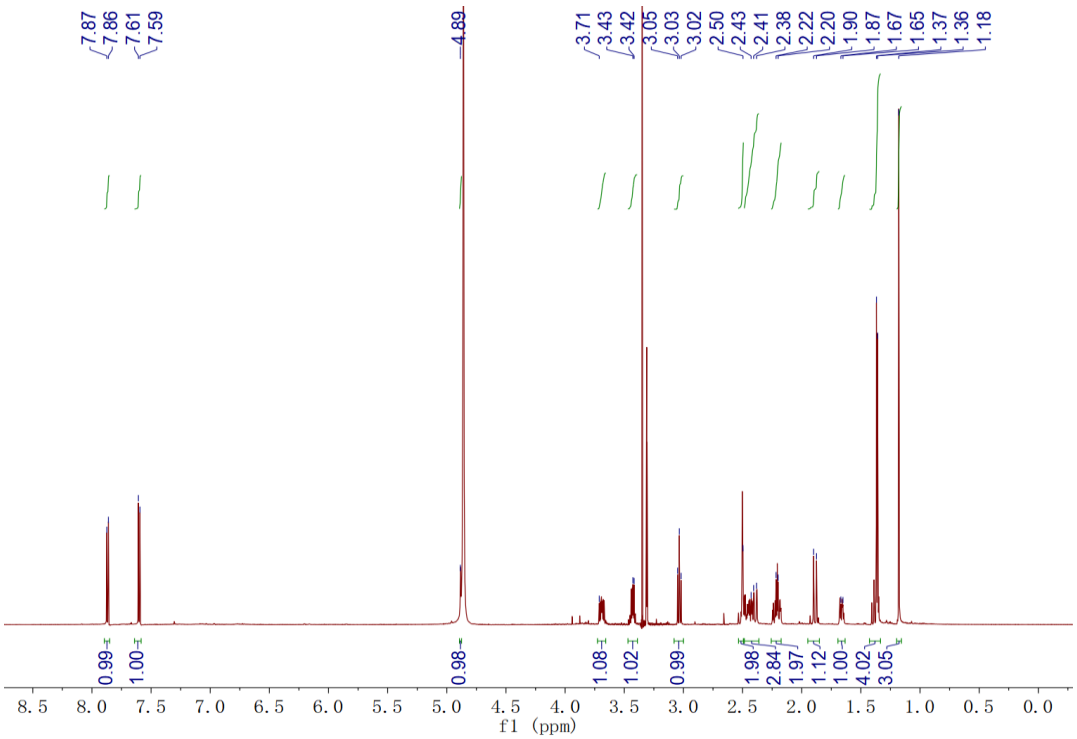

Figure S4. ^{1}H NMR spectrum (600 MHz) of **1** in methanol-d_4.

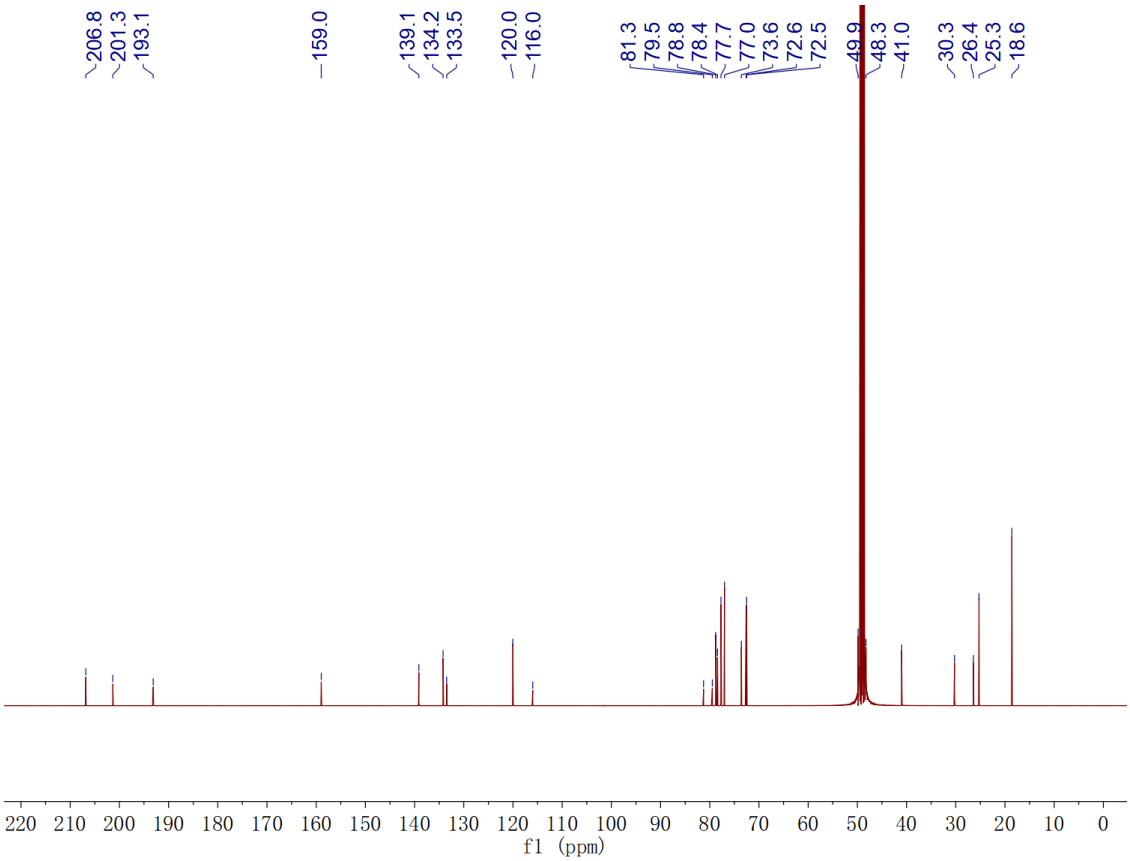

Figure S5. ^{13}C NMR spectrum (125 MHz) of **1** in methanol-d_4.

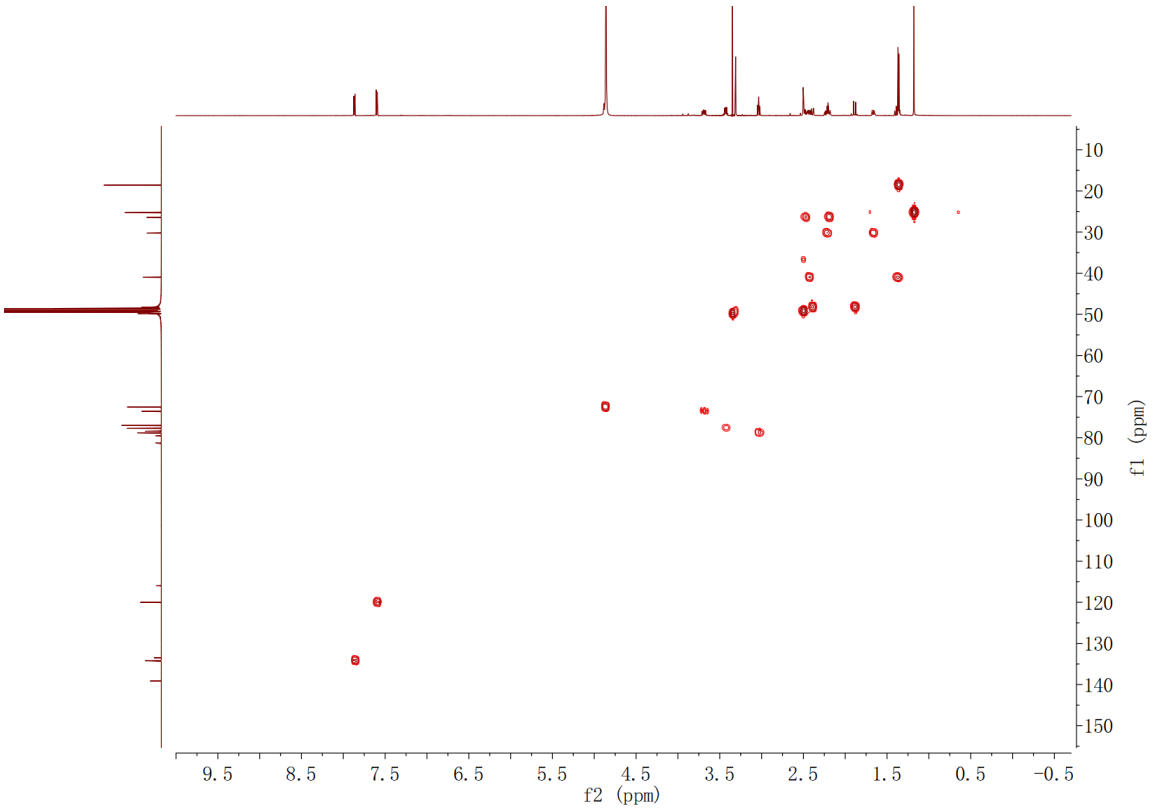

Figure S6. HSQC Spectrum of **1** in methanol-d_4.

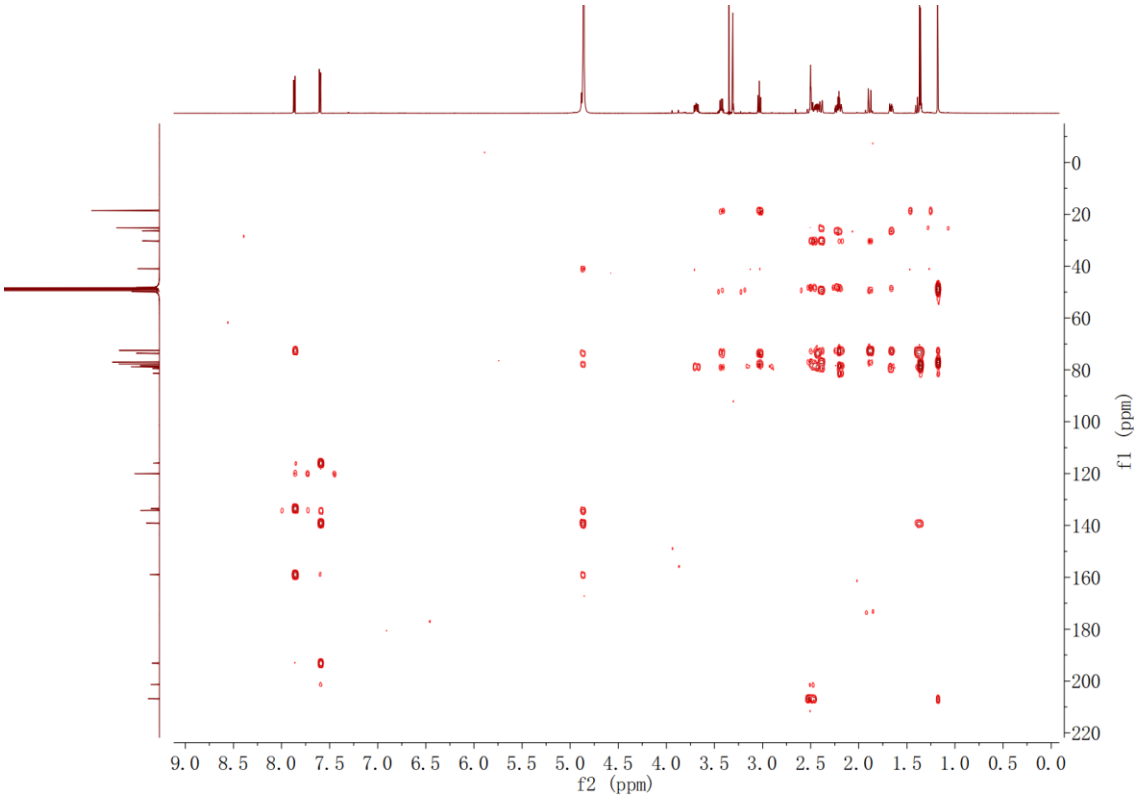

Figure S7. HMBC Spectrum of **1** in methanol-d_4.

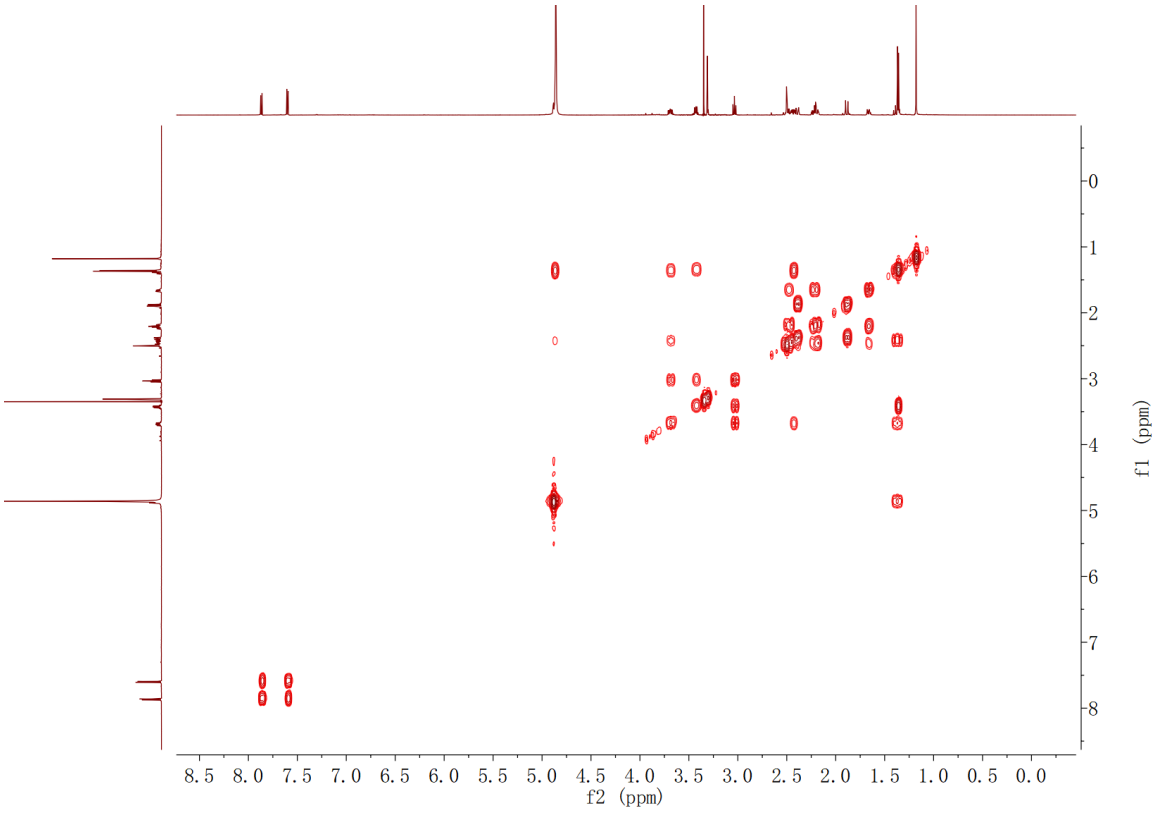

Figure S8. ^{1}H-^{1}H COSY spectrum of **1** in methanol-d_4.

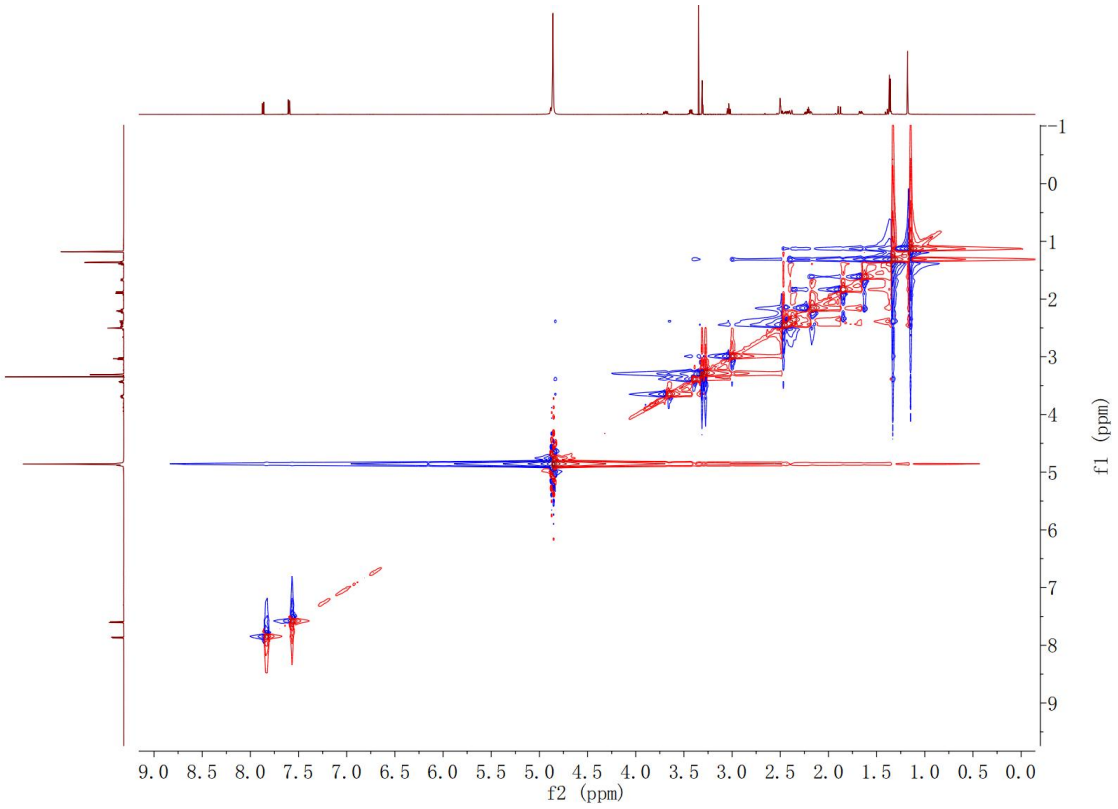

Figure S9. NOESY Spectrum of **1** in methanol-d_4.

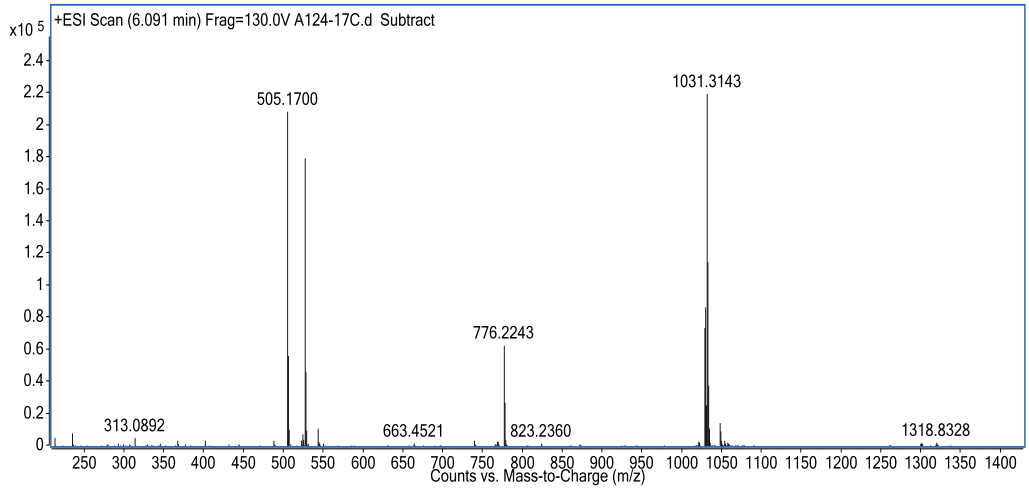

Figure S10. HRESIMS Spectrum of **1**.

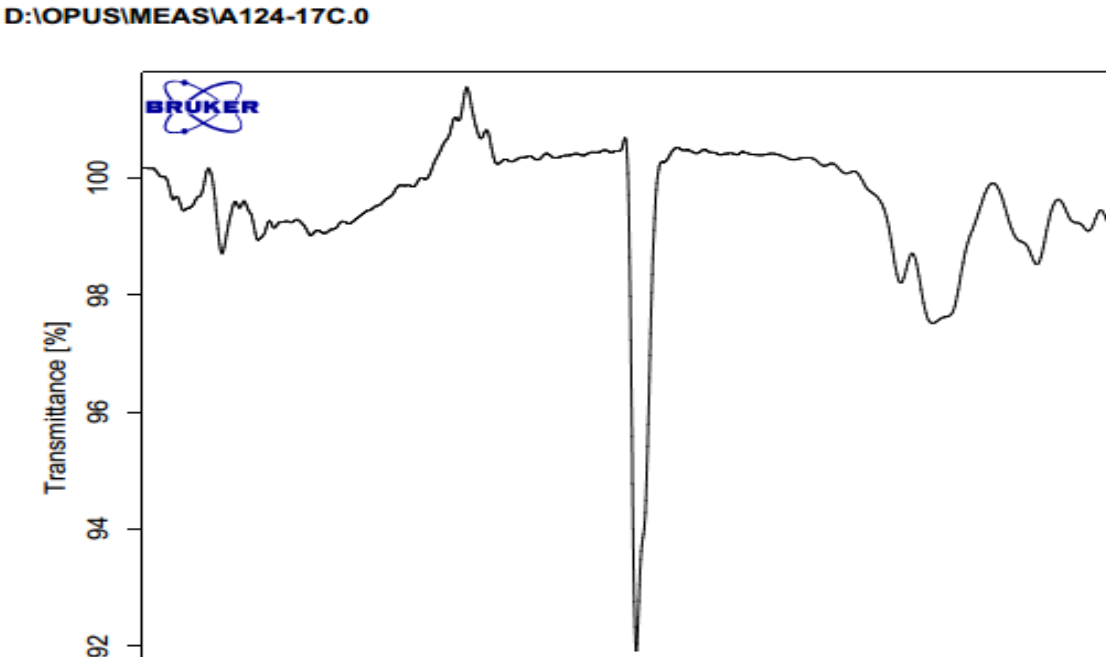

Figure S11. IR spectrum of **1**.

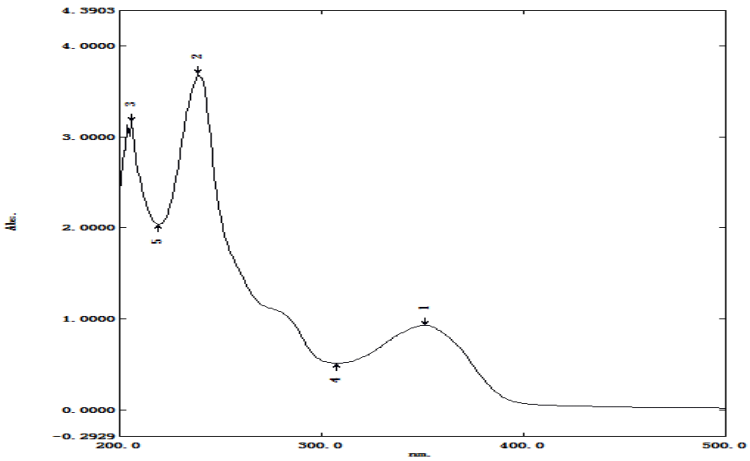

Figure S12. DAD UV-Vis spectrum of **1**.

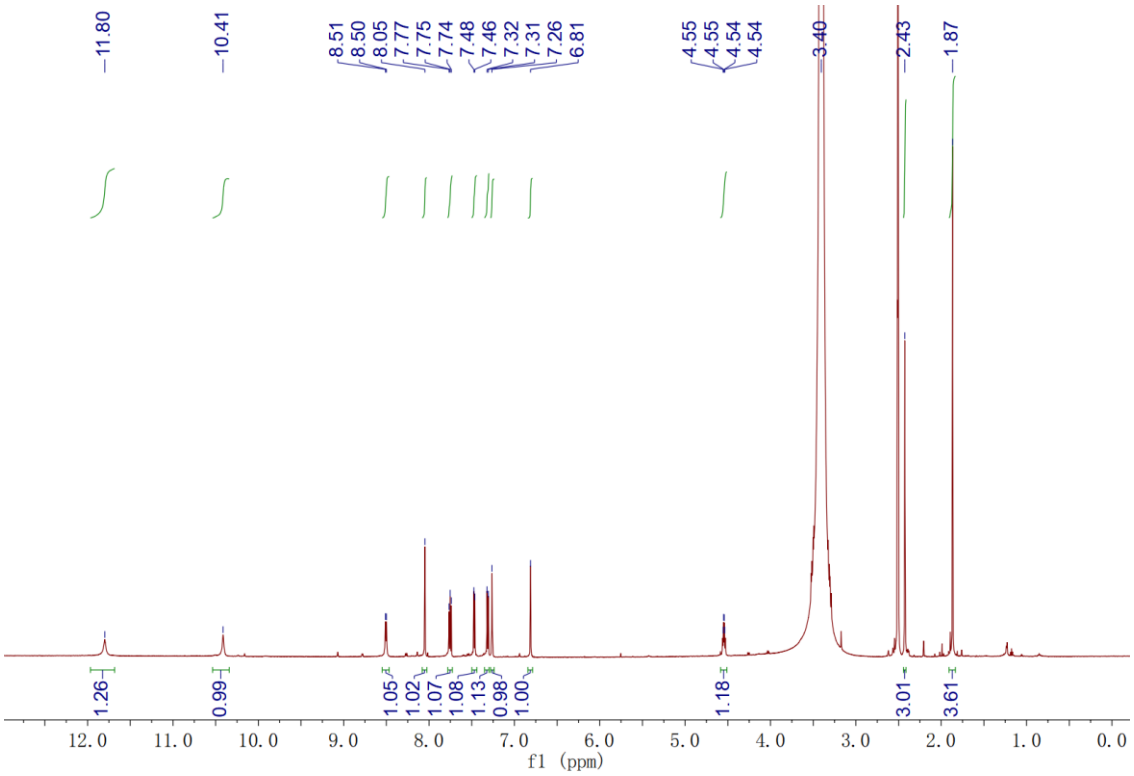

Figure S13. ^{1}H NMR spectrum (600 MHz) of **2** in DMSO-d_6.

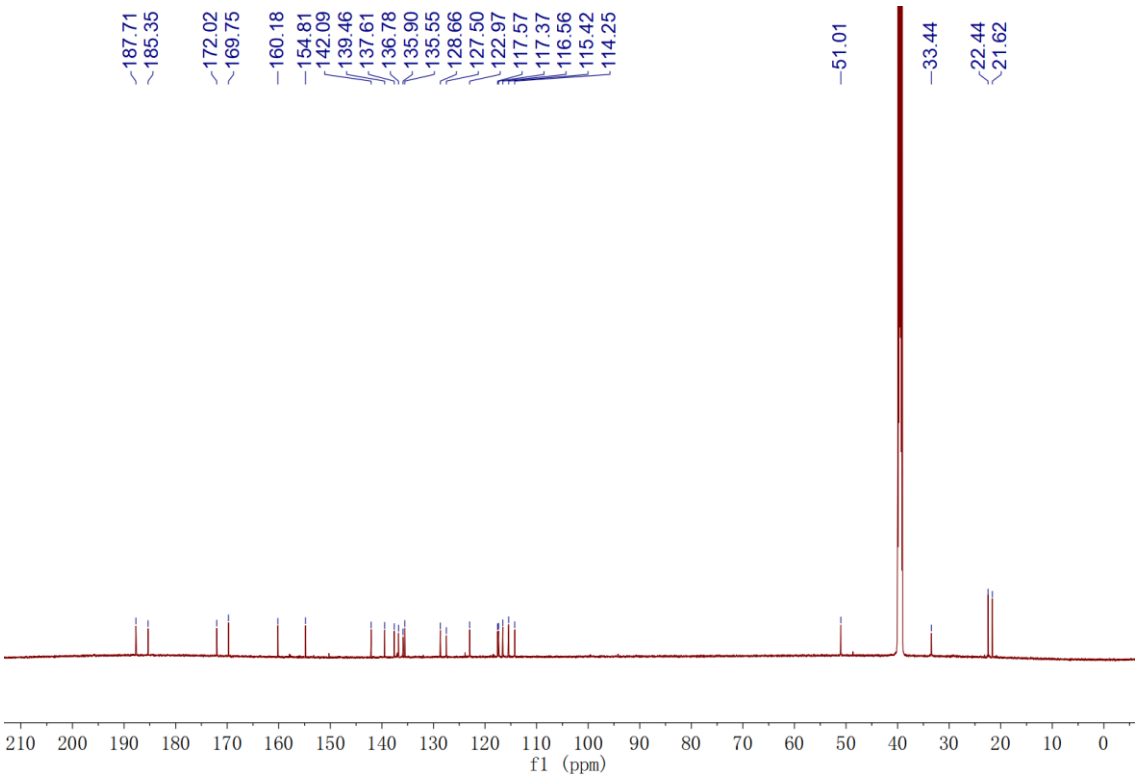

Figure S14. ^{13}C NMR spectrum (125 MHz) of **2** in DMSO-d_6.

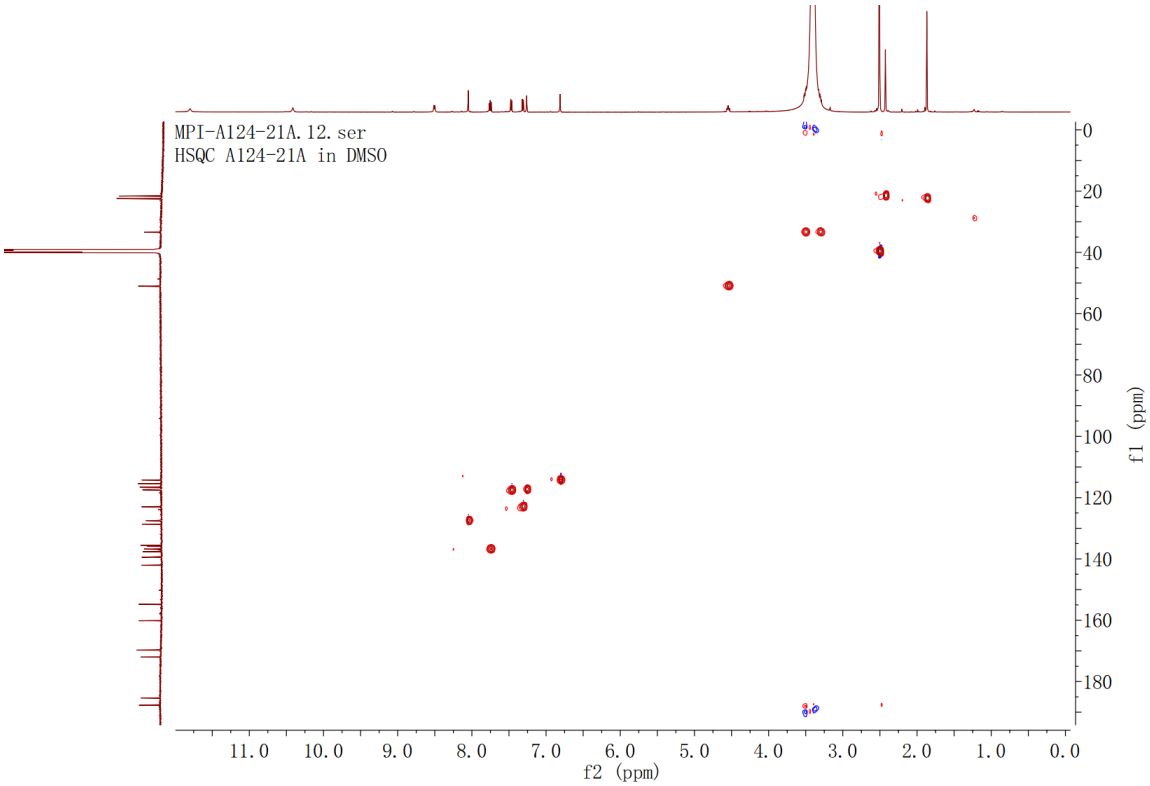

Figure S15. HSQC Spectrum of **2** in DMSO-d_6.

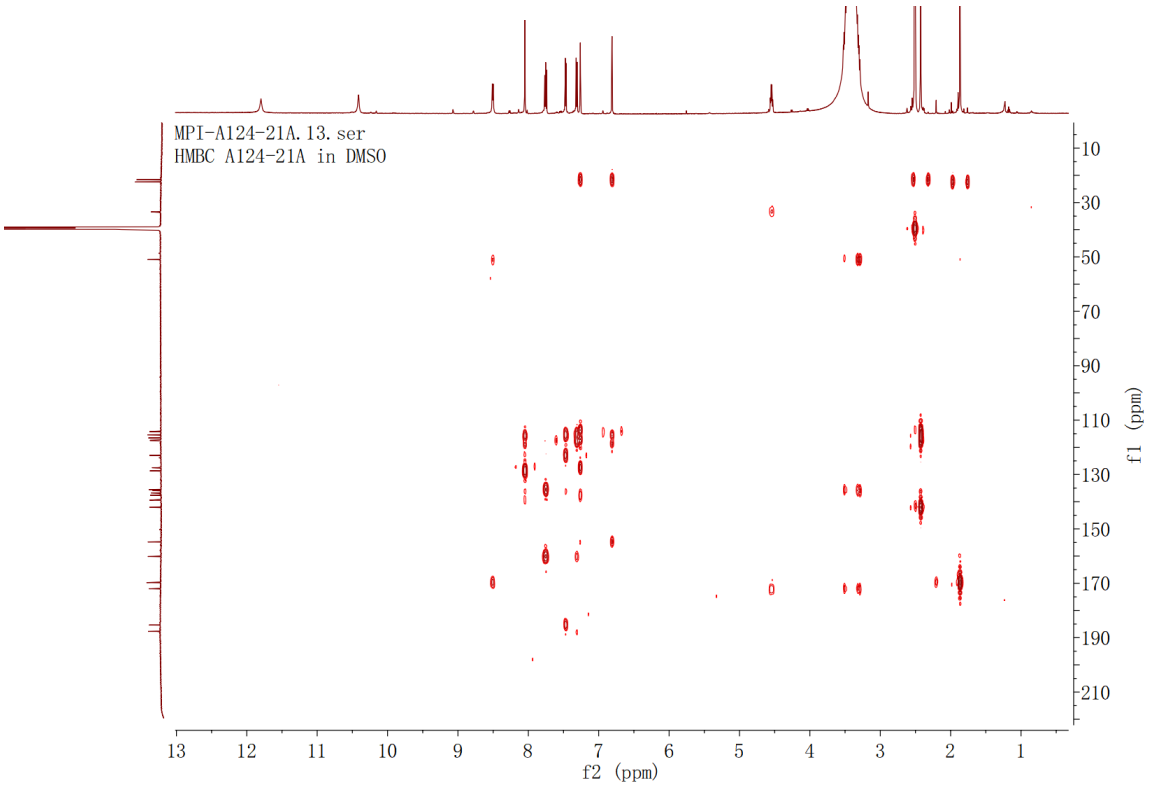

Figure S16. HMBC Spectrum of **2** in DMSO-d_6.

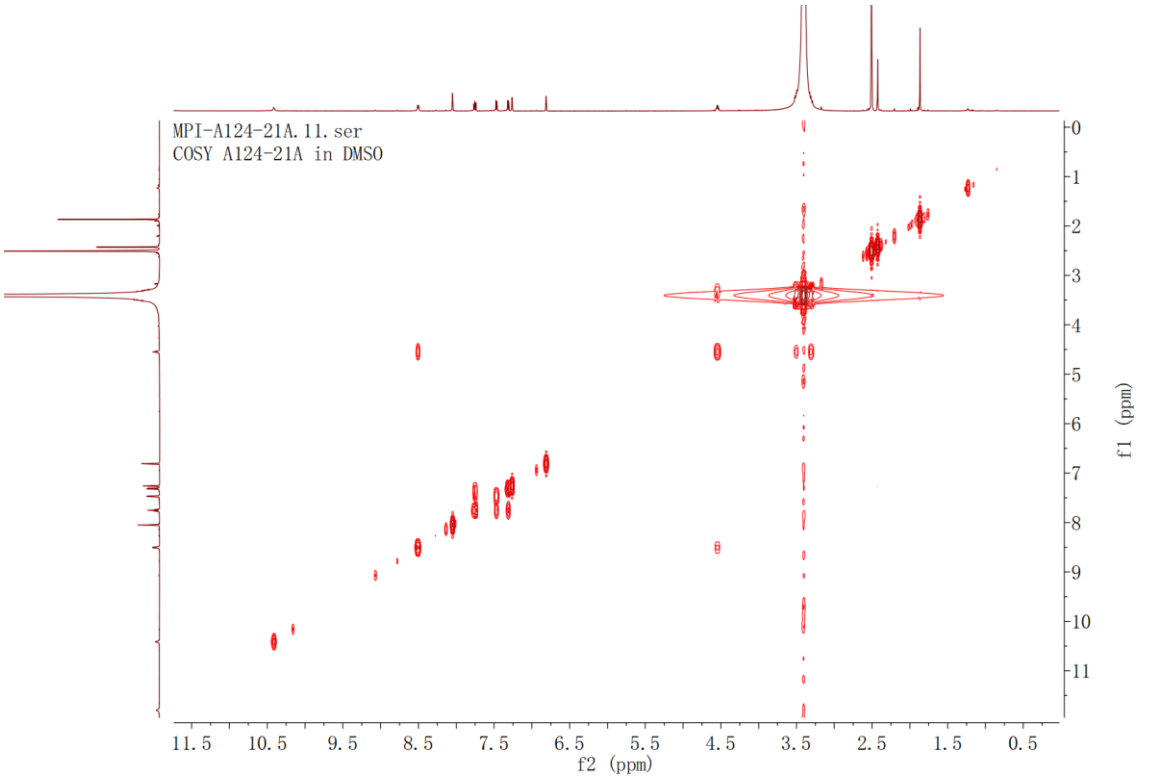

Figure S17. ^{1}H-^{1}H COSY spectrum of **2** in DMSO-d_6.

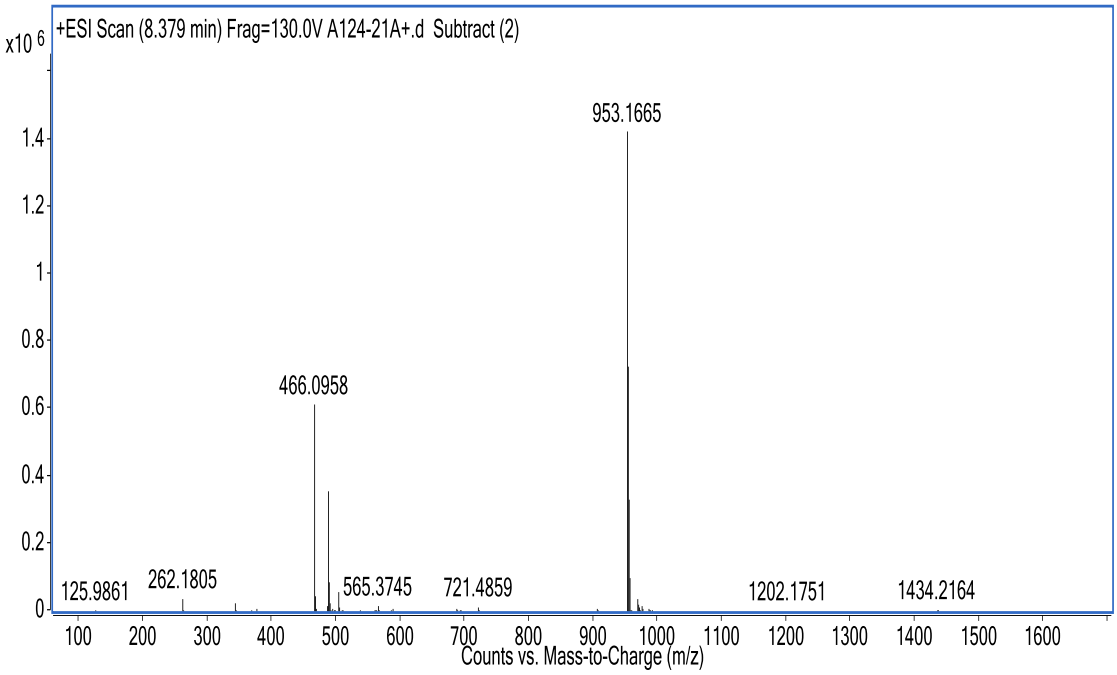

Figure S18. HRESIMS Spectrum of **2**.

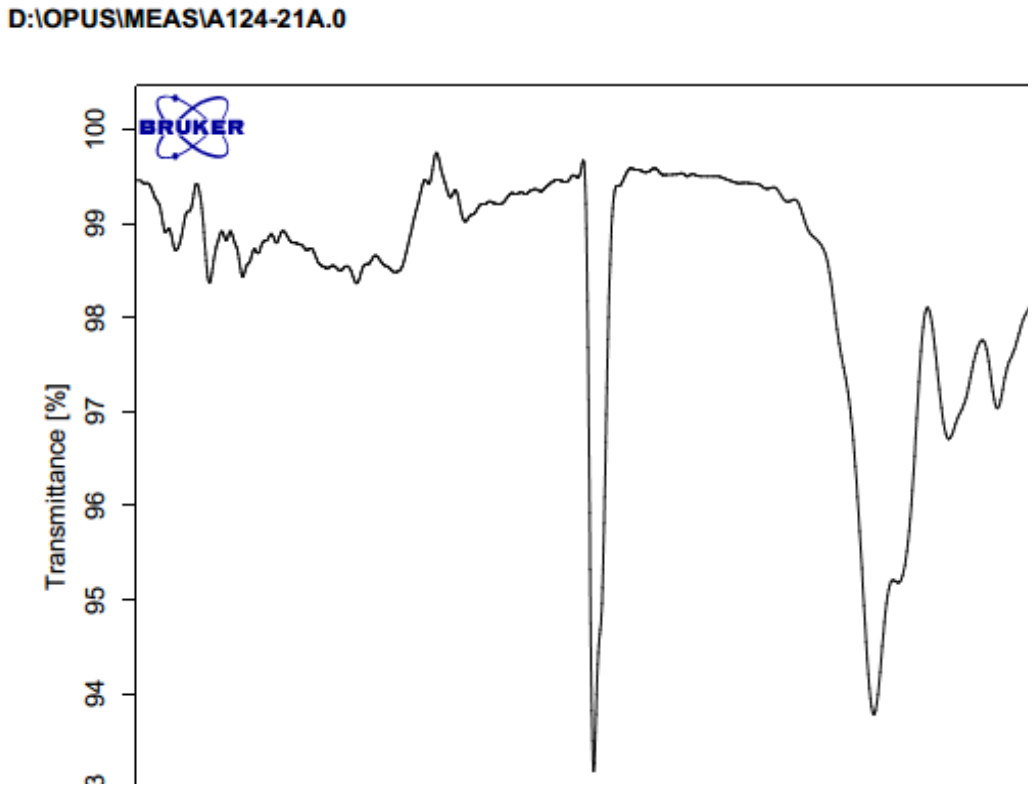

Figure S19. IR spectrum of **2**.

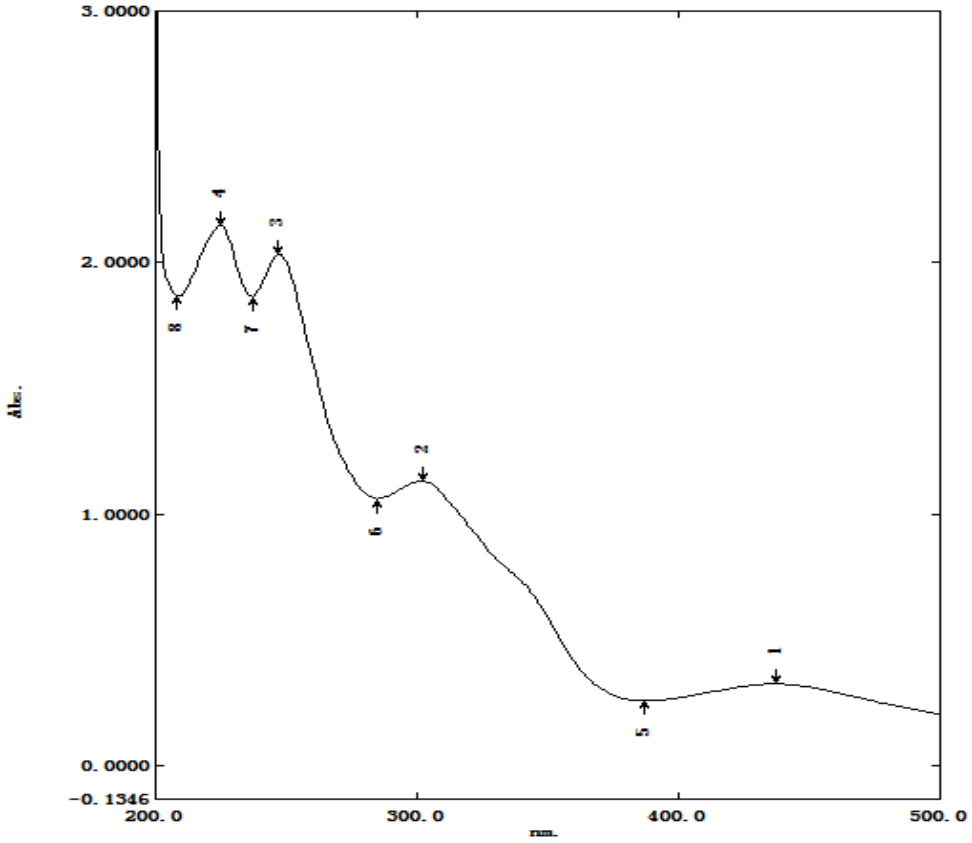

Figure S20. DAD UV-Vis spectrum of **2**.