

Supporting Information

Glycosides of Indole Alkaloids from the Aerial Parts of *Strobilanthes cusia*

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ECD calculation for simplified structures **11a-11d**

The CONFLEX searches based on molecular mechanics with MMFF94S force fields were performed for **11a-11d** which gave 15, 15, 14, 14 stable conformers, respectively.^{1,2} Selected conformers (7, 7, 6, 6) with distributions higher than 1% were further optimized by the density functional theory method at the B3LYP/6-31G* level in Gaussian 09 program package,³ leading to one minimum geometry ($\Delta E > 2$ kcal/mol), respectively, which was further checked by frequency calculation and resulted in no imaginary frequencies. The ECD was calculated using TD-DFT-B3LYP/6-31G(d,p) of theory on B3LYP/6-31G(d) optimized geometry through the IEFPCM model (in MeOH). The calculated ECD curve was generated using SpecDis 1.60 with $\sigma = 0.28$ eV, and UV shift -15 nm, respectively.⁴

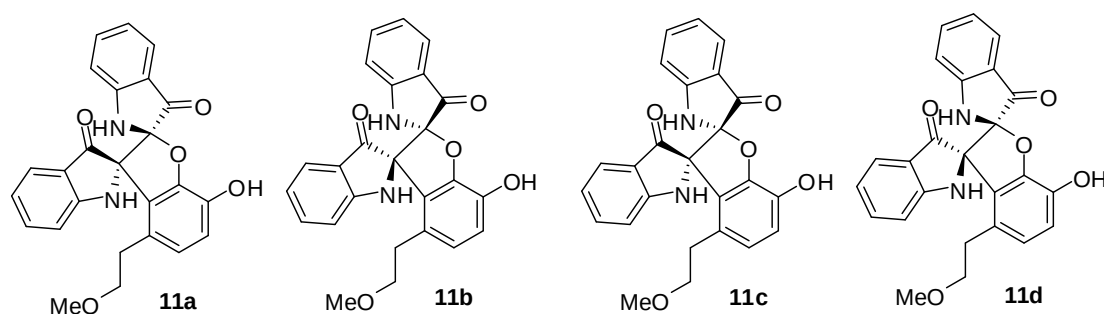
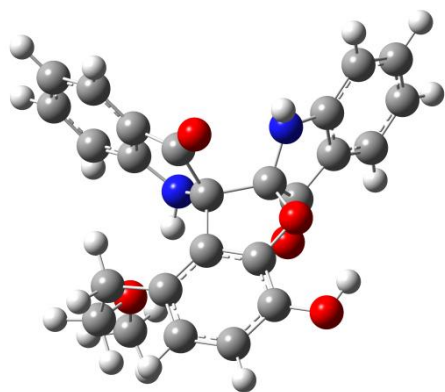
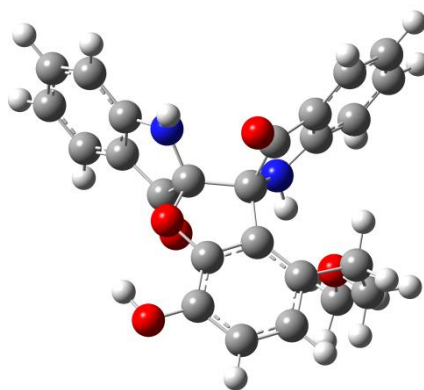


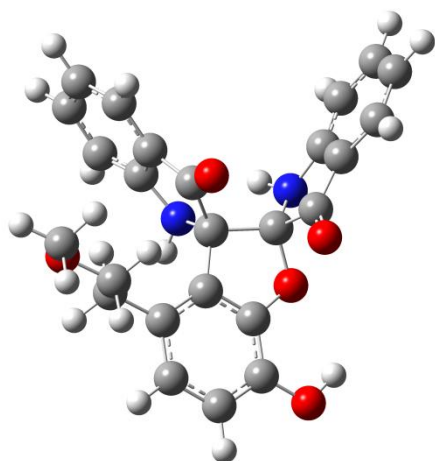
Figure S1. The simplified structures **11a-11d** in ECD calculation



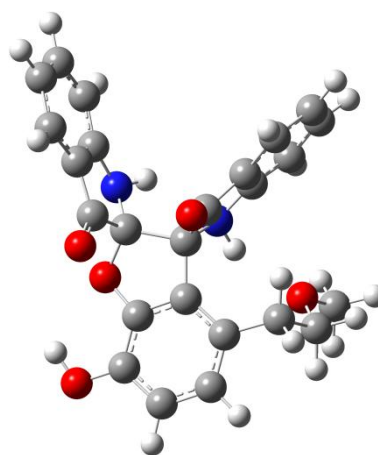
(2'''R, 2''''S)-11a



(2'''S, 2''''R)-11b



(2'''S, 2''''S)-11c



(2'''R, 2''''R)-11d

Figure S2. The most stable conformers of simplified structures **11a-11d**.

11a:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.582026	0.283002	2.333191
2	6	0	3.799528	0.249827	1.593778
3	6	0	3.495740	0.310160	0.090594
4	6	0	2.729157	-0.903642	-0.401054
5	6	0	3.416434	-2.107891	-0.644524
6	6	0	2.760891	-3.284932	-1.012090
7	6	0	1.368586	-3.306942	-1.134200
8	6	0	0.693874	-2.114700	-0.905675
9	6	0	1.340513	-0.932621	-0.564969
10	8	0	-0.679899	-2.021214	-0.970756
11	8	0	0.726634	-4.464873	-1.458691
12	7	0	-2.174263	-0.194169	-1.106445
13	8	0	-0.910631	-1.370185	1.961895
14	6	0	-1.587628	-0.968970	1.033673
15	6	0	-1.042440	-0.725635	-0.416983
16	6	0	0.271769	0.142924	-0.469398
17	7	0	0.380572	1.087445	0.633714
18	6	0	0.508388	2.376541	0.155169
19	6	0	0.721334	3.555097	0.887253
20	6	0	0.783604	4.754796	0.181308
21	6	0	0.641992	4.812558	-1.221033
22	6	0	0.445368	3.640984	-1.944606
23	6	0	0.390818	2.428430	-1.249037

24	6	0	0.229355	1.063215	-1.736932
25	8	0	0.041930	0.662109	-2.875520
26	6	0	-3.320501	-0.238417	-0.327611
27	6	0	-4.629760	0.103830	-0.676956
28	6	0	-5.612528	-0.003130	0.311047
29	6	0	-5.320406	-0.434951	1.617057
30	6	0	-4.011442	-0.775561	1.956372
31	6	0	-3.021049	-0.674922	0.978887
32	6	0	2.688444	-0.242589	3.648543
33	1	0	4.340172	-0.679207	1.824674
34	1	0	4.435038	1.098418	1.889270
35	1	0	4.459223	0.370114	-0.430330
36	1	0	2.964090	1.239135	-0.131596
37	1	0	4.498654	-2.125204	-0.539393
38	1	0	3.313115	-4.201767	-1.192710
39	1	0	-0.222936	-4.278806	-1.471557
40	1	0	-2.166663	-0.092097	-2.110668
41	1	0	0.901502	0.793917	1.456100
42	1	0	0.822796	3.531726	1.967906
43	1	0	0.942403	5.678344	0.732670
44	1	0	0.692210	5.770946	-1.728412
45	1	0	0.346454	3.647994	-3.026515
46	1	0	-4.877310	0.443578	-1.678185
47	1	0	-6.636961	0.257832	0.057717
48	1	0	-6.114471	-0.502372	2.354035
49	1	0	-3.752634	-1.116688	2.954774
50	1	0	1.676573	-0.247180	4.057372
51	1	0	3.340385	0.377742	4.279604
52	1	0	3.073464	-1.270822	3.631731

11b:

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	-2.582027	0.283002	2.333191
2	6	0	-3.799528	0.249825	1.593778
3	6	0	-3.495740	0.310159	0.090594
4	6	0	-2.729157	-0.903644	-0.401054
5	6	0	-3.416433	-2.107893	-0.644524
6	6	0	-2.760889	-3.284933	-1.012090
7	6	0	-1.368584	-3.306943	-1.134200
8	6	0	-0.693873	-2.114701	-0.905675
9	6	0	-1.340513	-0.932621	-0.564969
10	8	0	0.679900	-2.021214	-0.970756
11	8	0	-0.726632	-4.464874	-1.458690
12	7	0	2.174263	-0.194168	-1.106445
13	8	0	0.910631	-1.370184	1.961895
14	6	0	1.587628	-0.968969	1.033673
15	6	0	1.042441	-0.725635	-0.416983
16	6	0	-0.271769	0.142924	-0.469398
17	7	0	-0.380573	1.087445	0.633714
18	6	0	-0.508389	2.376541	0.155169
19	6	0	-0.721335	3.555097	0.887253
20	6	0	-0.783606	4.754796	0.181308
21	6	0	-0.641995	4.812558	-1.221033
22	6	0	-0.445369	3.640983	-1.944606

23	6	0	-0.390819	2.428429	-1.249037
24	6	0	-0.229356	1.063215	-1.736932
25	8	0	-0.041930	0.662109	-2.875519
26	6	0	3.320501	-0.238416	-0.327611
27	6	0	4.629760	0.103832	-0.676956
28	6	0	5.612528	-0.003128	0.311047
29	6	0	5.320407	-0.434949	1.617057
30	6	0	4.011443	-0.775560	1.956372
31	6	0	3.021049	-0.674922	0.978887
32	6	0	-2.688445	-0.242589	3.648543
33	1	0	-4.435039	1.098416	1.889269
34	1	0	-4.340171	-0.679208	1.824673
35	1	0	-2.964091	1.239134	-0.131597
36	1	0	-4.459223	0.370112	-0.430330
37	1	0	-4.498653	-2.125205	-0.539393
38	1	0	-3.313113	-4.201768	-1.192710
39	1	0	0.222938	-4.278806	-1.471557
40	1	0	2.166663	-0.092096	-2.110668
41	1	0	-0.901502	0.793916	1.456100
42	1	0	-0.822798	3.531726	1.967906
43	1	0	-0.942406	5.678343	0.732671
44	1	0	-0.692212	5.770945	-1.728413
45	1	0	-0.346456	3.647993	-3.026515
46	1	0	4.877310	0.443580	-1.678185
47	1	0	6.636961	0.257834	0.057717
48	1	0	6.114471	-0.502370	2.354035
49	1	0	3.752635	-1.116687	2.954774
50	1	0	-1.676574	-0.247179	4.057373
51	1	0	-3.340386	0.377741	4.279604

52	1	0	-3.073463	-1.270823	3.631731
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11c:

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	8	0	-4.536037	0.807848	1.705194
2	6	0	-3.633708	-0.262161	1.461147
3	6	0	-3.325636	-0.291302	-0.040094
4	6	0	-2.388667	-1.419231	-0.414973
5	6	0	-2.886846	-2.724778	-0.581215
6	6	0	-2.062963	-3.807833	-0.896405
7	6	0	-0.684948	-3.631852	-1.061578
8	6	0	-0.193290	-2.339225	-0.903049
9	6	0	-1.007647	-1.256196	-0.574592
10	8	0	1.135862	-2.023102	-1.070965
11	8	0	0.116103	-4.692572	-1.376789
12	7	0	2.375486	0.020279	-1.032725
13	8	0	1.278718	-1.735726	1.810447
14	6	0	1.839893	-1.007341	1.012159
15	6	0	1.313554	-0.709665	-0.447059
16	6	0	-0.107566	-0.030882	-0.580704
17	7	0	-0.195954	0.702722	-1.852264
18	6	0	-0.515908	2.028417	-1.634856
19	6	0	-0.772538	3.031226	-2.580093
20	6	0	-1.032659	4.315314	-2.105170
21	6	0	-1.042834	4.622681	-0.728820

22	6	0	-0.802204	3.622020	0.205201
23	6	0	-0.545578	2.324910	-0.256753
24	6	0	-0.315221	1.091077	0.484426
25	8	0	-0.270562	0.923018	1.695701
26	6	0	3.421062	0.232253	-0.152735
27	6	0	4.616675	0.924301	-0.363801
28	6	0	5.522196	0.986845	0.698326
29	6	0	5.265368	0.383459	1.943030
30	6	0	4.069804	-0.302322	2.145996
31	6	0	3.149628	-0.364660	1.096667
32	6	0	-4.839284	0.955086	3.081714
33	1	0	-4.081157	-1.219945	1.774890
34	1	0	-2.706534	-0.123416	2.037941
35	1	0	-2.910511	0.680073	-0.329187
36	1	0	-4.273369	-0.403323	-0.580209
37	1	0	-3.953464	-2.897265	-0.460199
38	1	0	-2.477871	-4.804569	-1.016060
39	1	0	1.042453	-4.395145	-1.361813
40	1	0	2.299038	0.432175	-1.951560
41	1	0	-0.528967	0.220497	-2.677413
42	1	0	-0.763237	2.817800	-3.644651
43	1	0	-1.231080	5.106747	-2.823553
44	1	0	-1.244748	5.639321	-0.405689
45	1	0	-0.818290	3.824436	1.272568
46	1	0	4.838883	1.391640	-1.318306
47	1	0	6.458984	1.518738	0.552313
48	1	0	5.998880	0.456161	2.740071
49	1	0	3.842237	-0.775807	3.097177
50	1	0	-5.527523	1.800036	3.175247

51	1	0	-5.322377	0.053156	3.489152
52	1	0	-3.934852	1.161103	3.674884

11d:

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	3.844696	0.908337	-0.785600
2	6	0	4.318765	0.512139	0.493811
3	6	0	3.166261	0.024961	1.381144
4	6	0	2.472949	-1.203164	0.834907
5	6	0	3.131805	-2.443365	0.834990
6	6	0	2.580987	-3.586439	0.250996
7	6	0	1.334144	-3.534012	-0.376118
8	6	0	0.679203	-2.302281	-0.366415
9	6	0	1.198219	-1.170911	0.253928
10	8	0	-0.514769	-2.111404	-1.007111
11	8	0	0.787087	-4.635437	-0.969125
12	7	0	-1.875733	-0.183795	-1.399274
13	8	0	-1.881079	-2.159105	1.503492
14	6	0	-2.119367	-1.351938	0.634218
15	6	0	-1.070082	-0.877126	-0.460031
16	6	0	0.196707	-0.052526	0.035985
17	7	0	0.627485	0.900204	-1.018447
18	6	0	0.550789	2.202952	-0.508790
19	6	0	0.939683	3.387582	-1.145127
20	6	0	0.729384	4.590139	-0.473331

21	6	0	0.148070	4.637304	0.807454
22	6	0	-0.212779	3.457263	1.447157
23	6	0	-0.000761	2.246552	0.780442
24	6	0	-0.199914	0.868921	1.245844
25	8	0	-0.627621	0.488350	2.316428
26	6	0	-3.174411	-0.017831	-0.952510
27	6	0	-4.215646	0.704817	-1.540858
28	6	0	-5.456197	0.694943	-0.899610
29	6	0	-5.675833	-0.008121	0.295718
30	6	0	-4.630318	-0.718662	0.881857
31	6	0	-3.382835	-0.707215	0.260000
32	6	0	4.890805	1.337624	-1.631630
33	1	0	5.063627	-0.294797	0.374751
34	1	0	4.829818	1.362022	0.981332
35	1	0	3.602164	-0.197952	2.365313
36	1	0	2.458881	0.847750	1.536367
37	1	0	4.108736	-2.520245	1.309686
38	1	0	3.109123	-4.536147	0.276692
39	1	0	-0.122326	-4.400213	-1.239310
40	1	0	-1.433844	0.419733	-2.079781
41	1	0	1.563703	0.678222	-1.363539
42	1	0	1.386957	3.370088	-2.136144
43	1	0	1.022211	5.520384	-0.956531
44	1	0	-0.009528	5.597296	1.292561
45	1	0	-0.642531	3.451450	2.446034
46	1	0	-4.070269	1.251219	-2.469753
47	1	0	-6.278305	1.250711	-1.346579
48	1	0	-6.658267	0.008717	0.760087
49	1	0	-4.759830	-1.268564	1.810828

50	1	0	4.453134	1.629779	-2.592457
51	1	0	5.423477	2.205686	-1.207192
52	1	0	5.626526	0.534444	-1.807163

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Figure S3. Standard orientation of **11a-11d** at B3LYP/6-31G(d) level

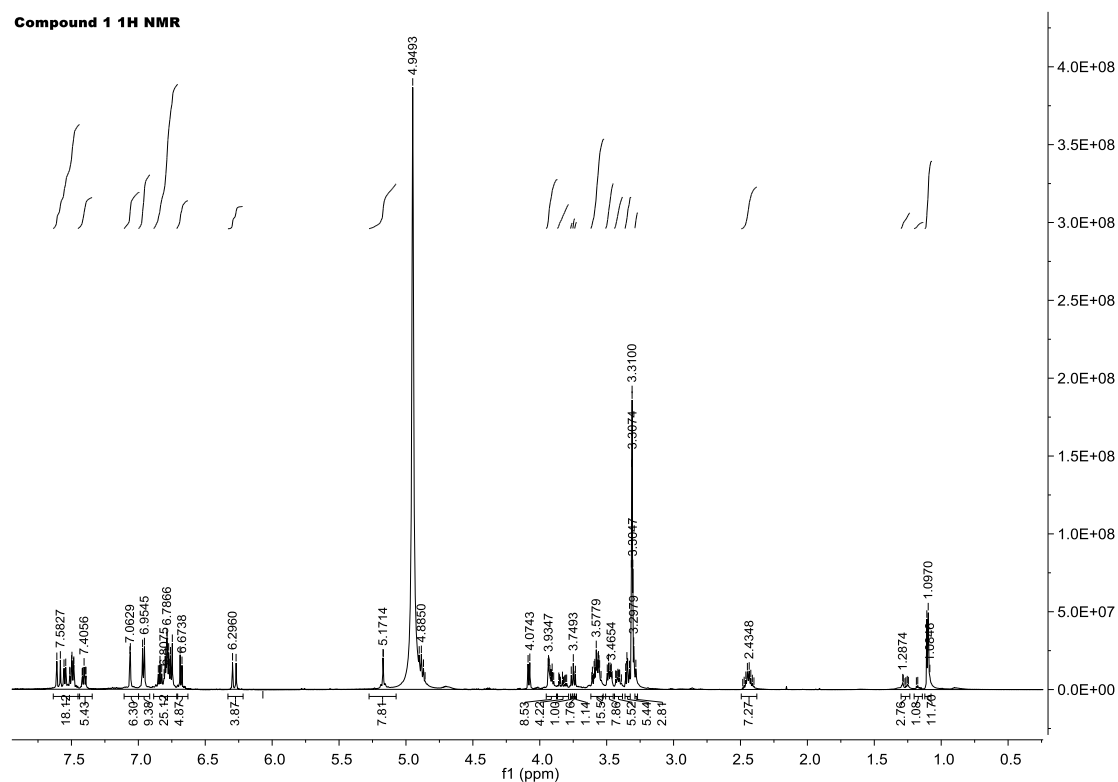


Figure S4. ^1H NMR spectrum of compound **1** (600 MHz, CD_3OD).

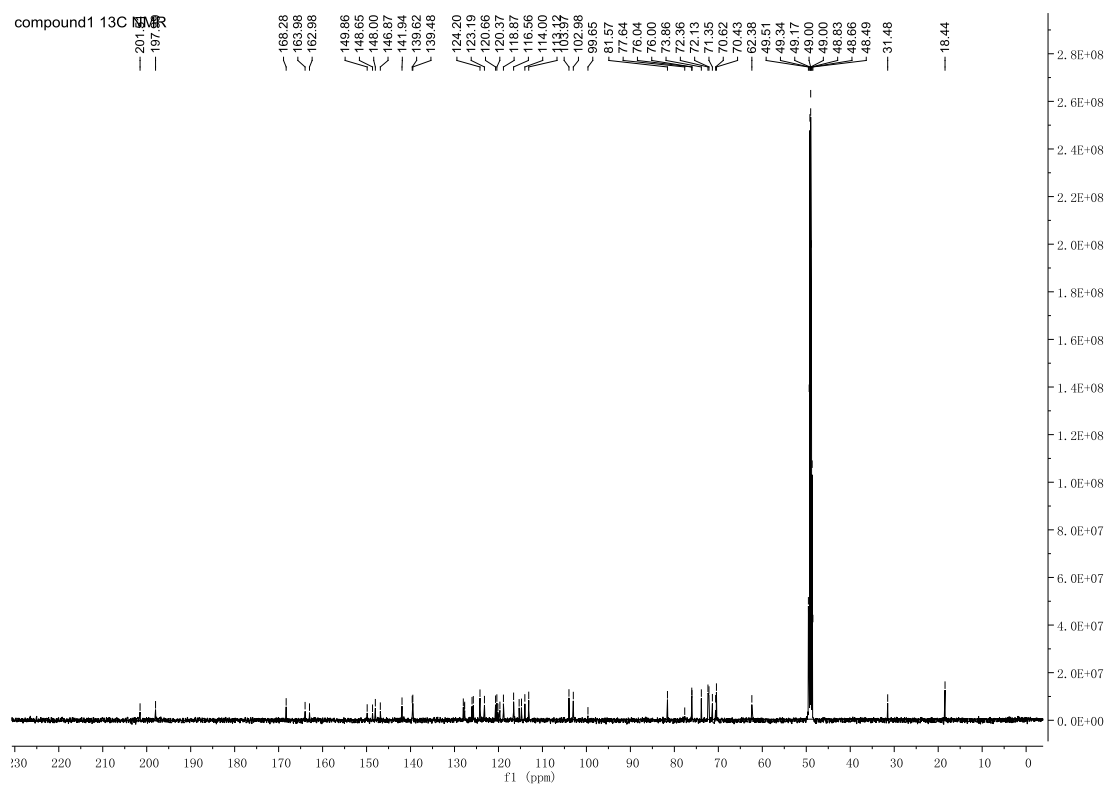


Figure S5. ^{13}C NMR spectrum of compound **1** (150 MHz, CD_3OD).

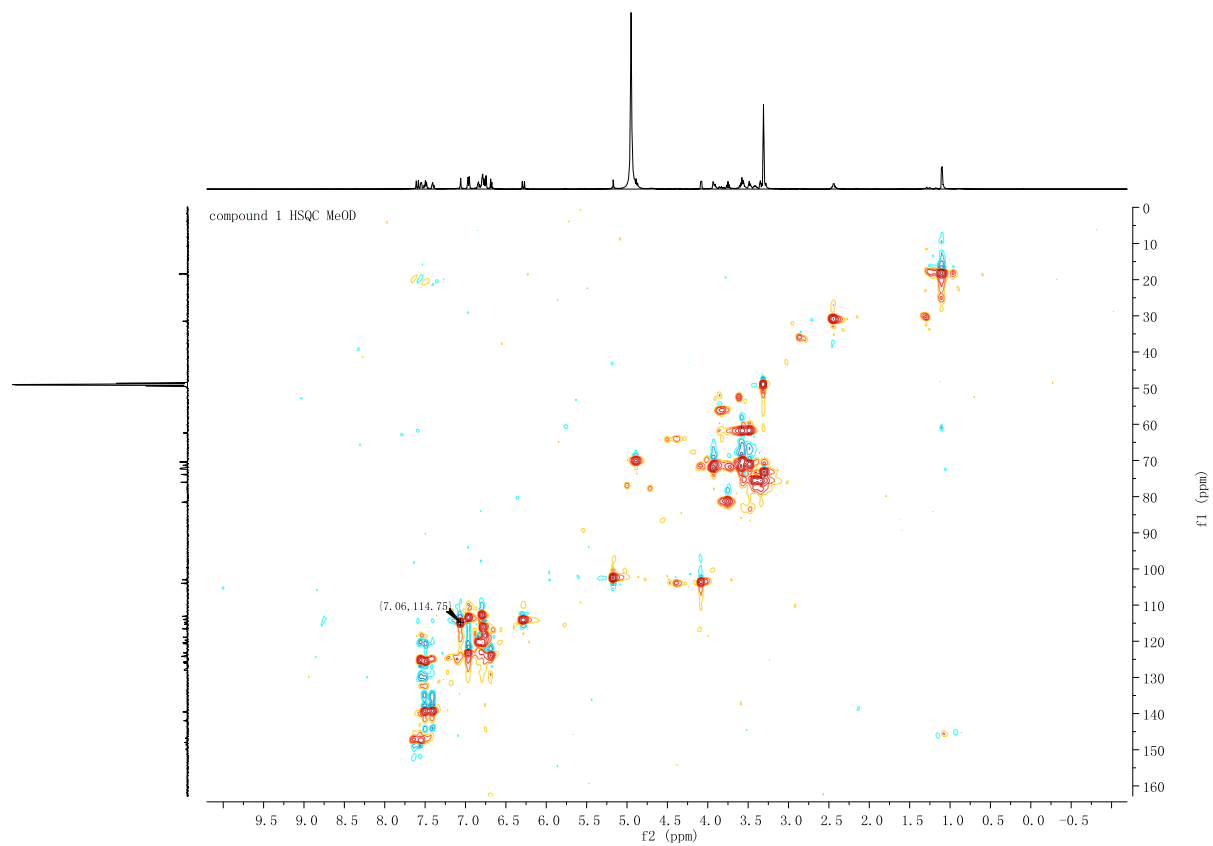


Figure S6. HSQC spectrum of compound **1** (150 MHz, CD₃OD).

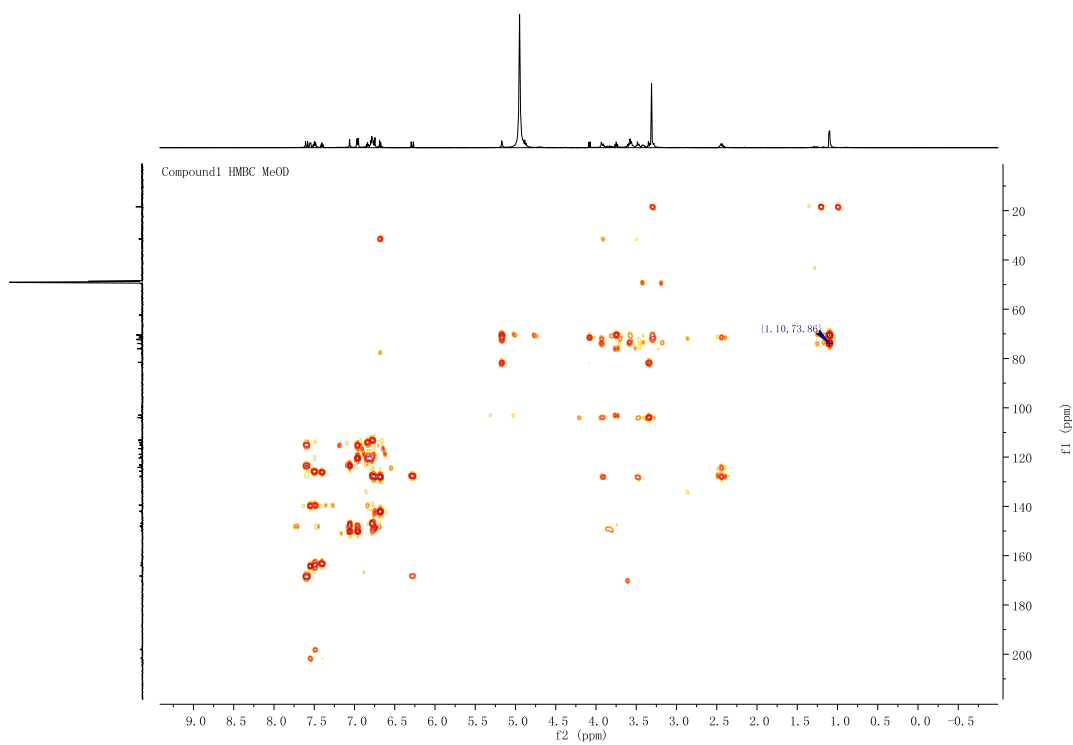


Figure S7. HMBC spectrum of compound **1** (150 MHz, CD₃OD).

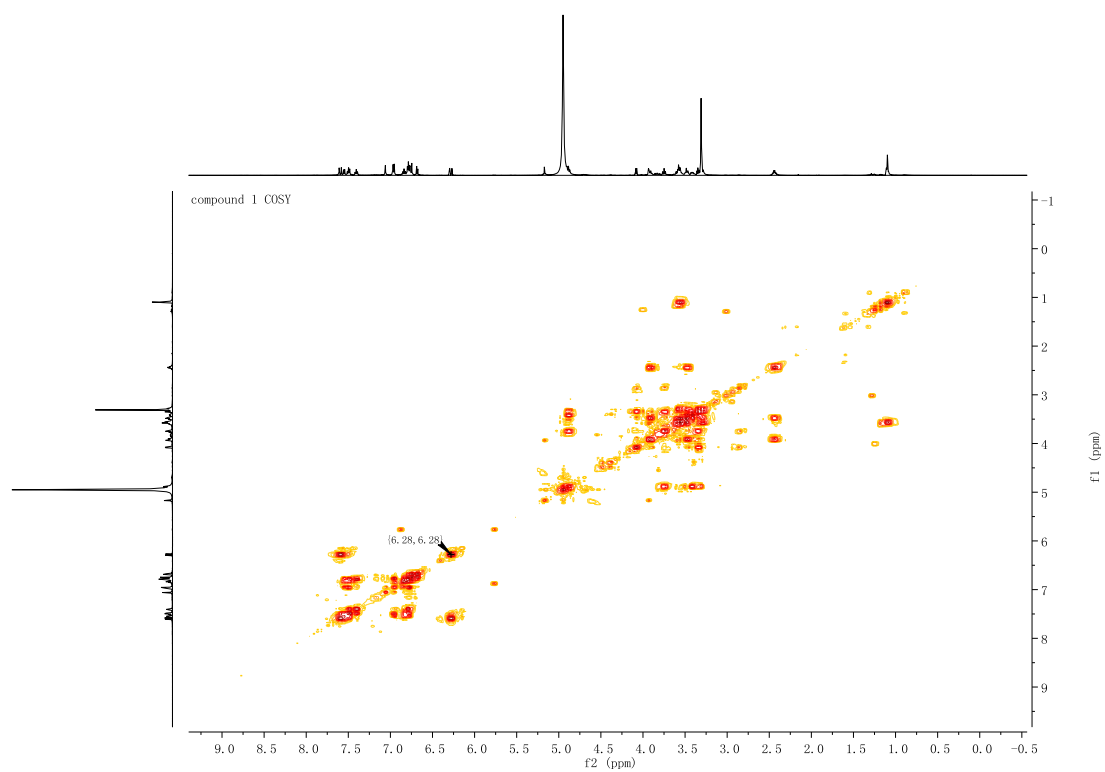


Figure S8. ^1H - ^1H COSY spectrum of compound **1** (600 MHz, CD_3OD).

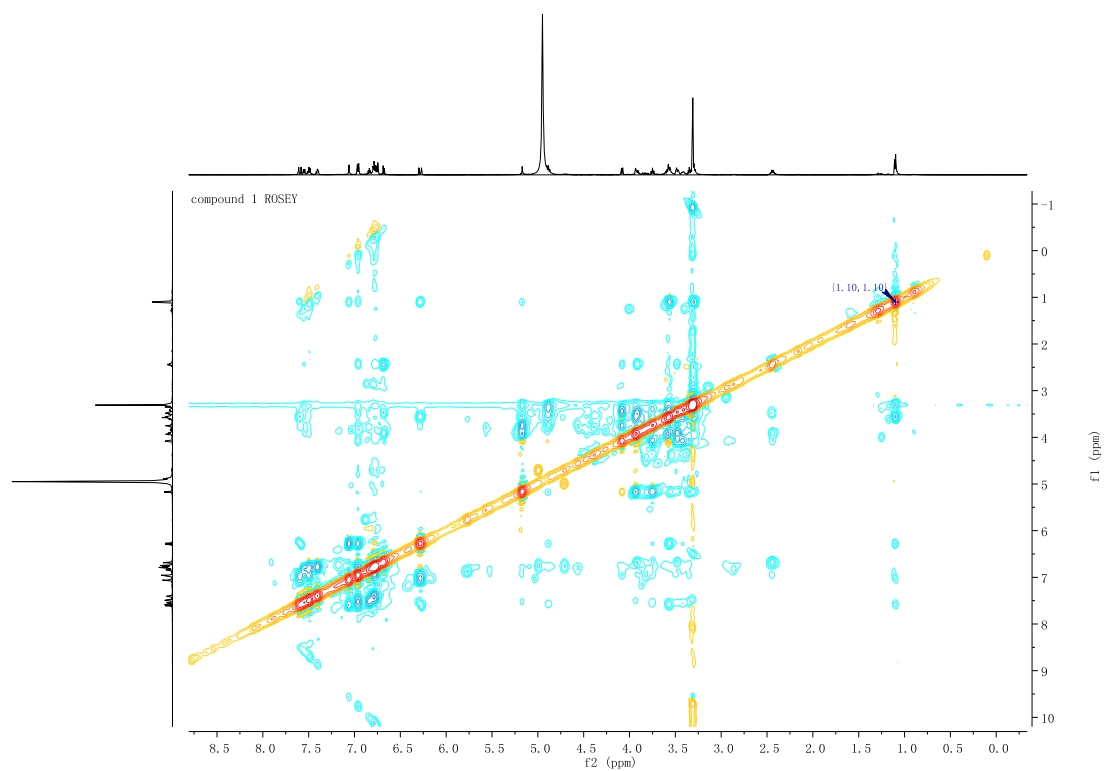


Figure S9. ROSEY spectrum of compound **1** (600 MHz, CD_3OD).

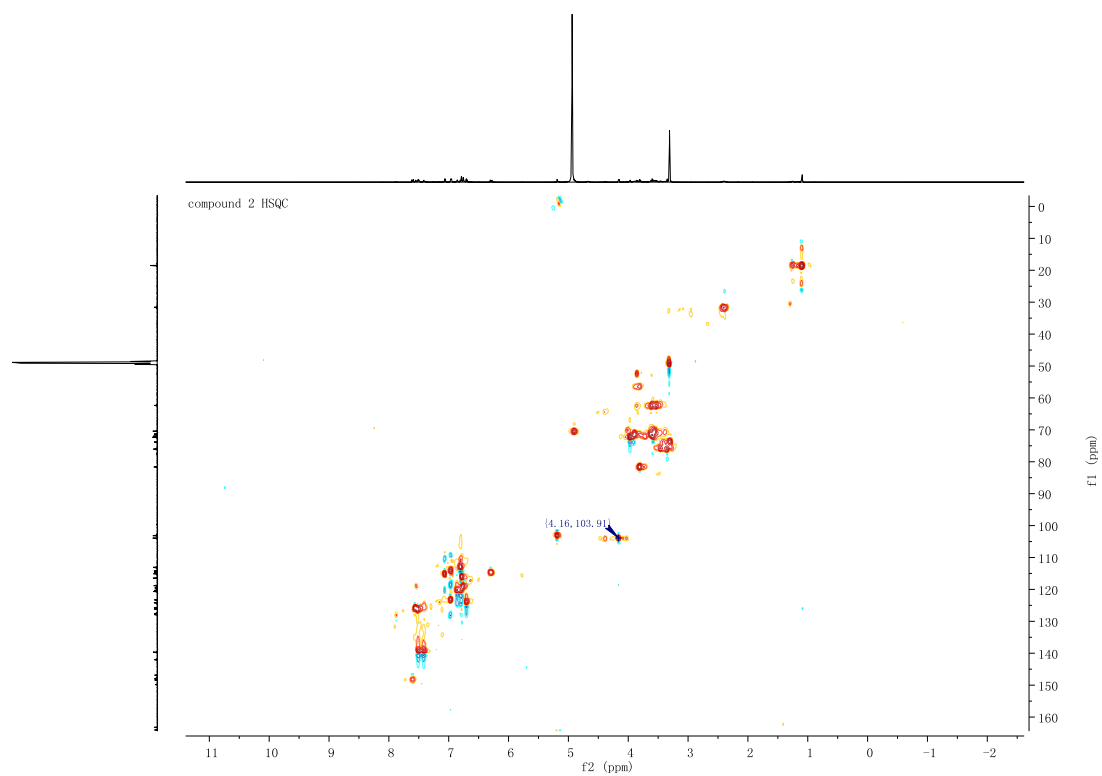


Figure S12. HSQC spectrum of compound 2 (150 MHz, CD₃OD).

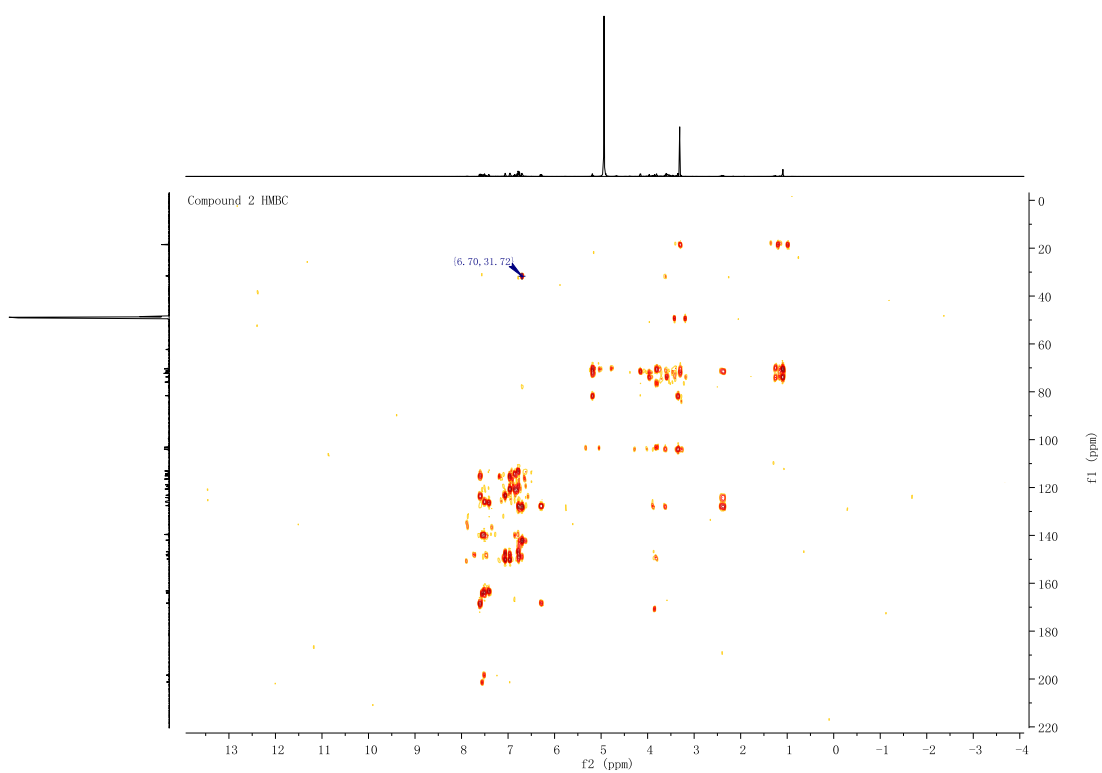


Figure S13. HMBC spectrum of compound 2 (150 MHz, CD₃OD).

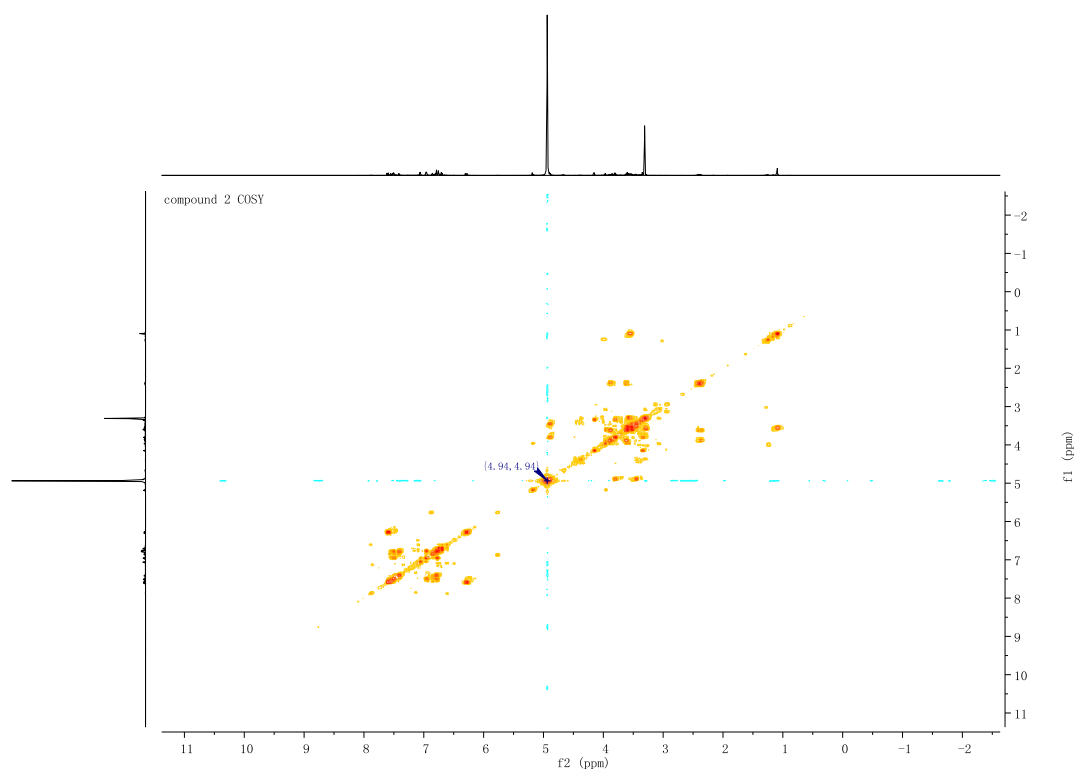


Figure S14. ^1H - ^1H COSY spectrum of compound **2** (600 MHz, CD_3OD).

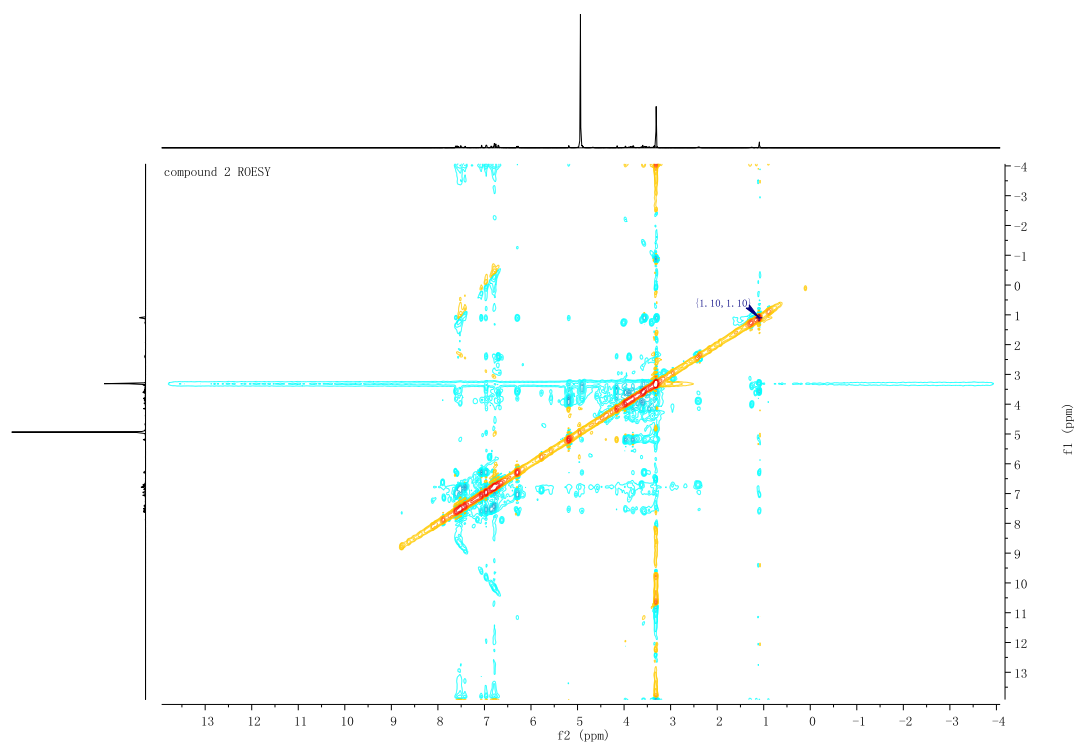


Figure S15. ROESY spectrum of compound **2** (600 MHz, CD_3OD).

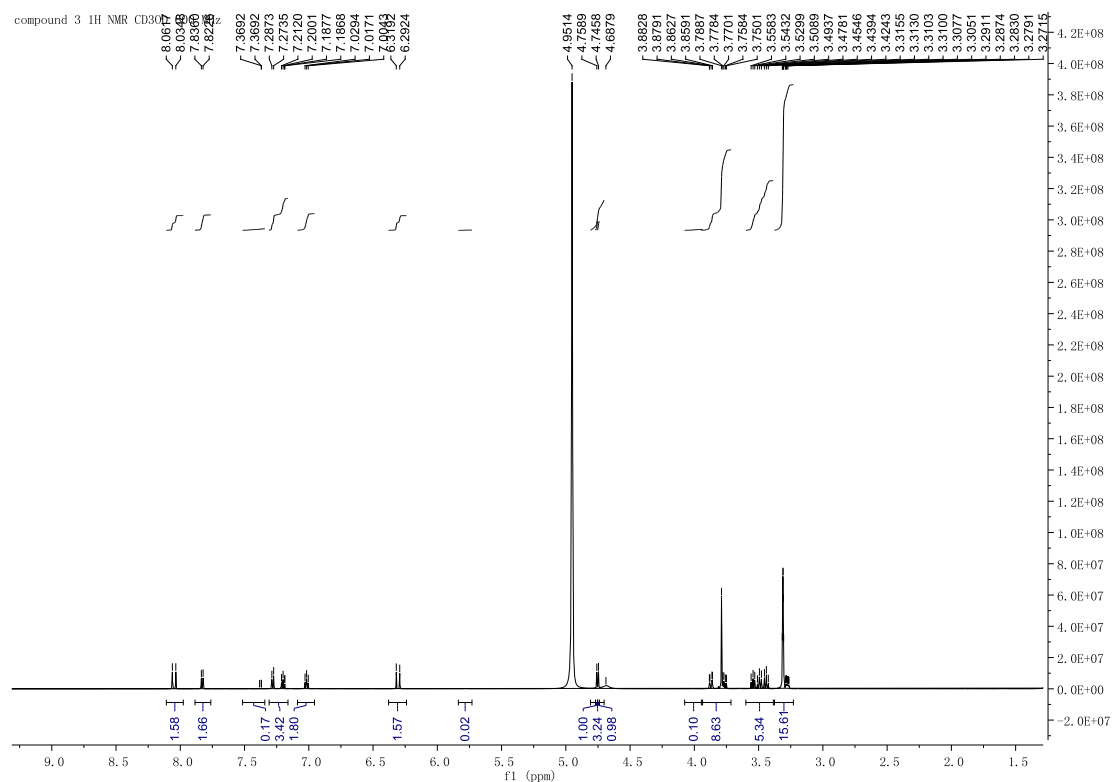


Figure S16. ¹H NMR spectrum of compound **3** (600 MHz, CD₃OD).

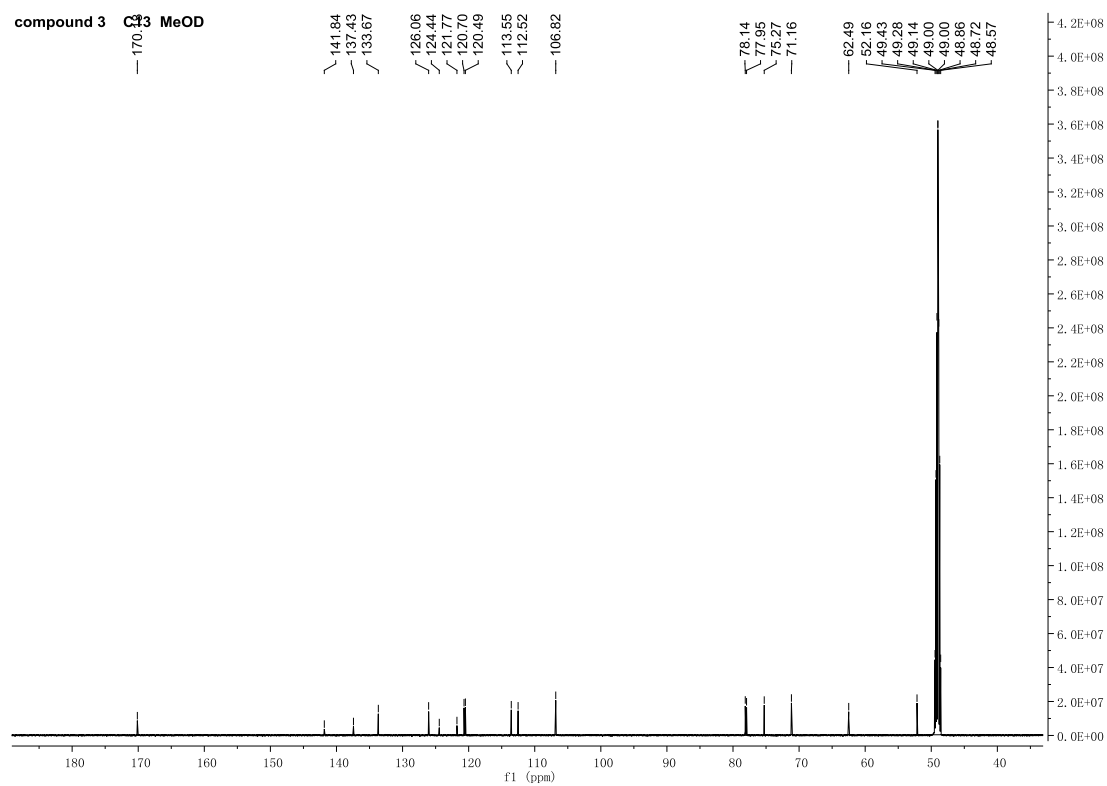


Figure S17. ¹³C NMR spectrum of compound **3** (150 MHz, CD₃OD).

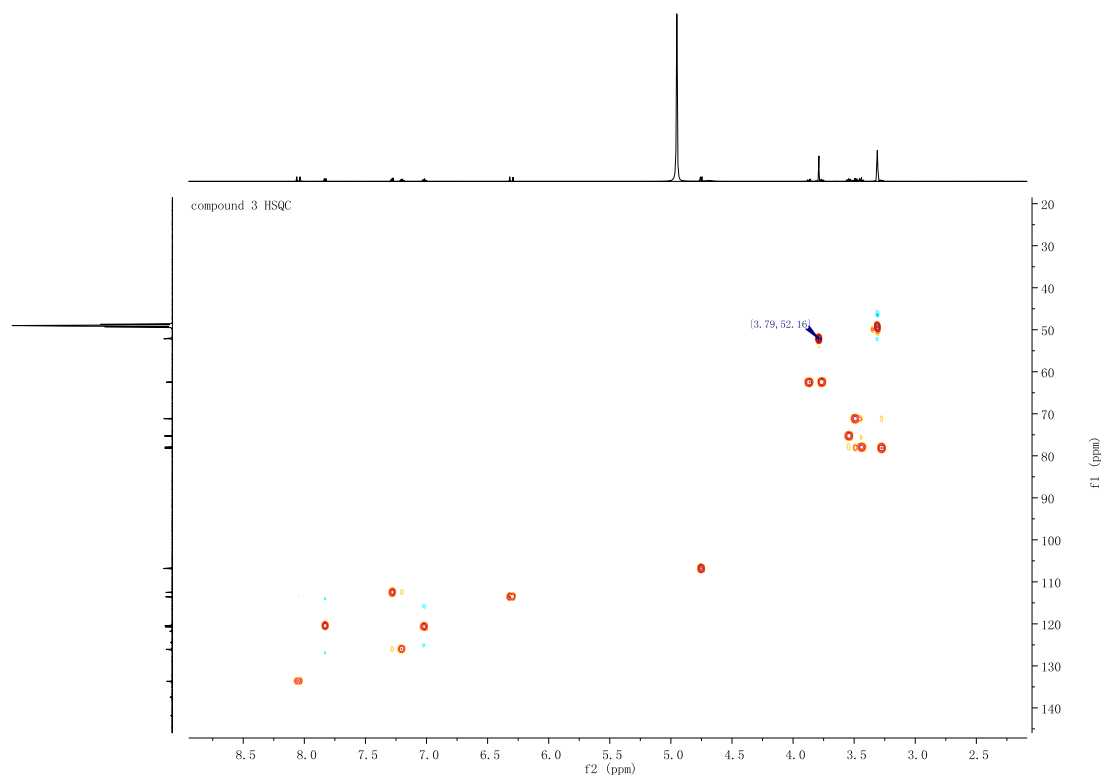


Figure S18. HSQC spectrum of compound **3** (150 MHz, CD₃OD).

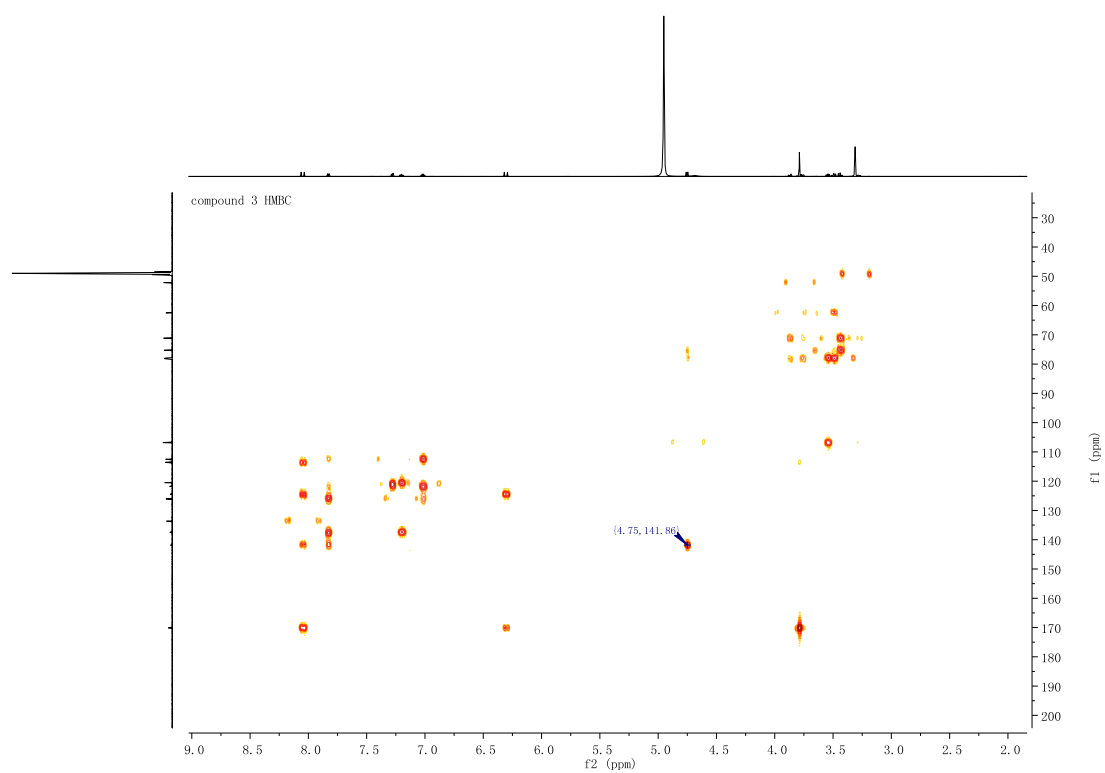


Figure S19. HMBC spectrum of compound **3** (150 MHz, CD₃OD).

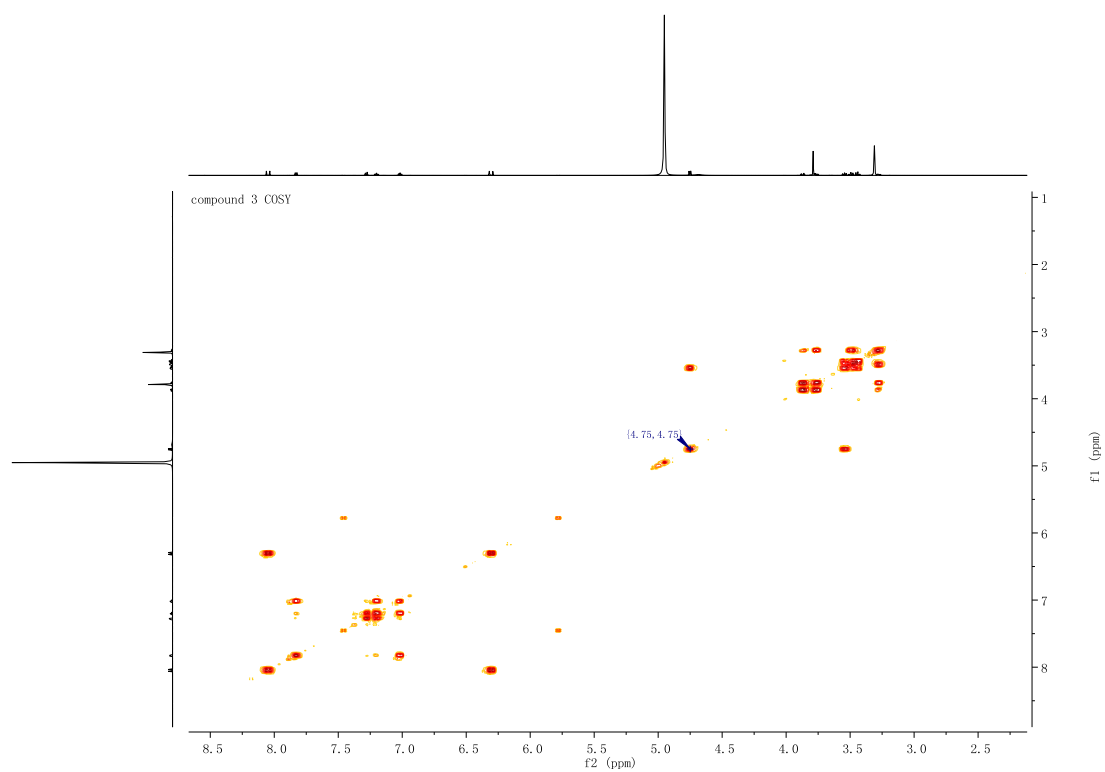


Figure S20. ^1H - ^1H COSY spectrum of compound **3** (600 MHz, CD_3OD).

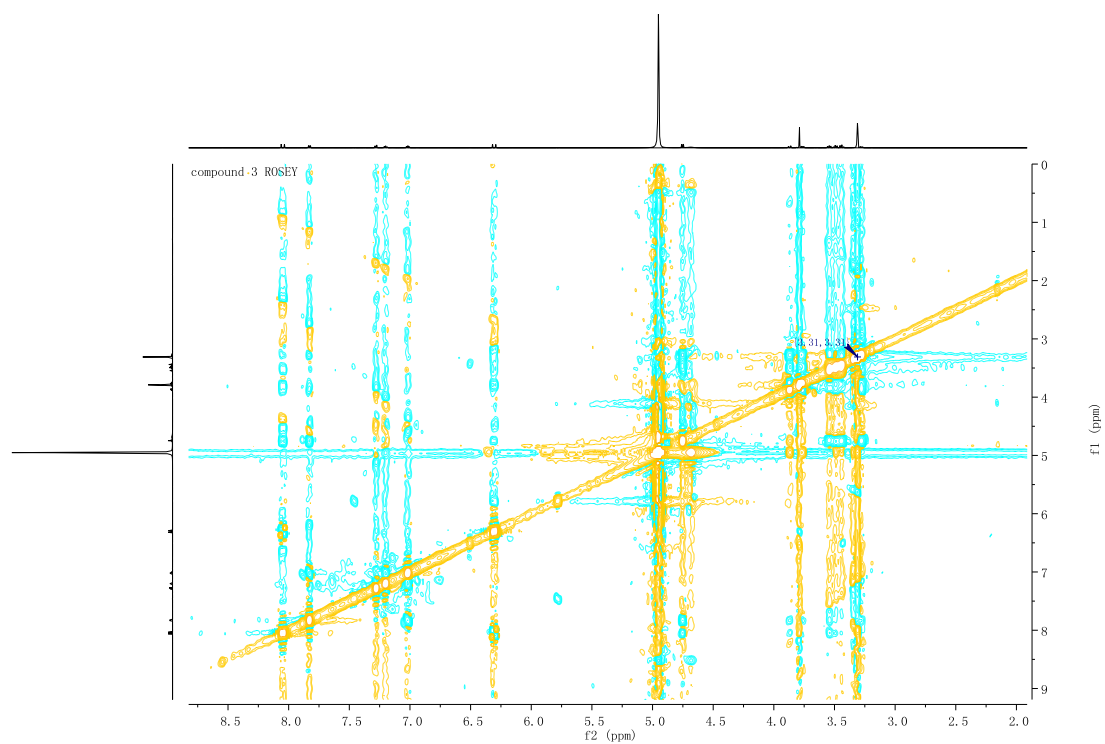


Figure S21. ROSEY spectrum of compound **3** (600 MHz, CD_3OD).

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 16-18

pcd52

14:23:43 24-Apr-2013

Voltage El+

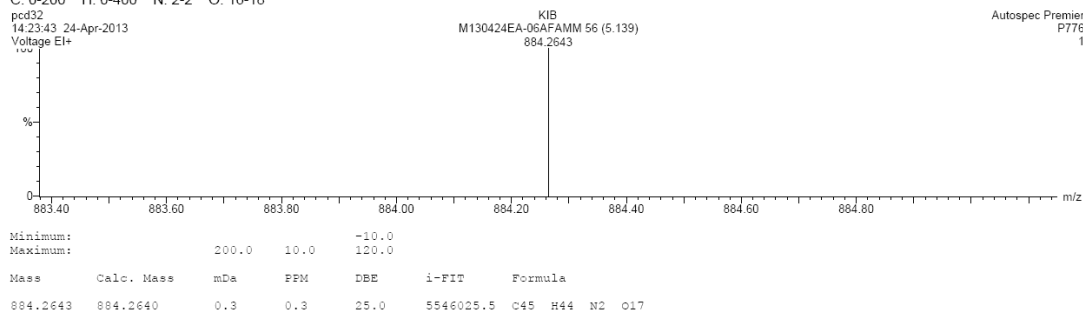


Figure S22. HREI-MS spectrum of compound 1.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 16-18

pcd33

14:23:43 24-Apr-2013

Voltage El+

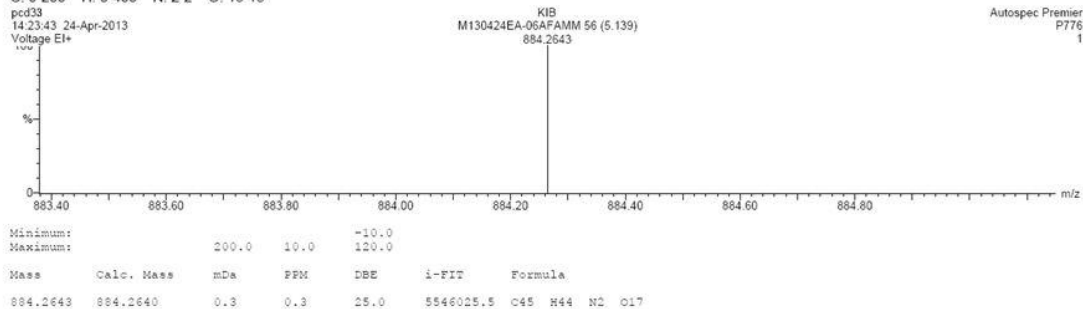


Figure S23. HREI-MS spectrum of compound 2.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 N: 1-1 O: 7-9

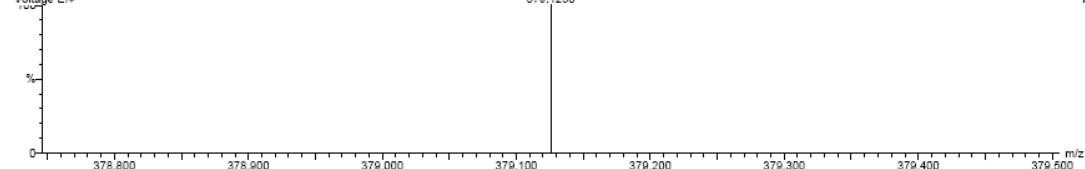
pcd23

11:11:55 02-Apr-2013

Voltage E1+

KIB
M130403EA-02AFAMM 20 (1.836)
379.1258

Autospec Premier
P776
1



Minimum:						
Maximum:	200.0	10.0	-10.0			
			120.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.1258	379.1267	-0.9	-2.4	9.0	5546026.0	C18 H21 N O8

Figure S24. HREI-MS spectrum of compound **3**.