Supporting Information

Induction of Antiphytopathogenic Metabolite and Squalene Production and Phytotoxin Elimination by Adjustment of the Mode of Fermentation in Cocultures of Phytopathogenic *Nigrospora oryzae* and *Irpex lacteus*

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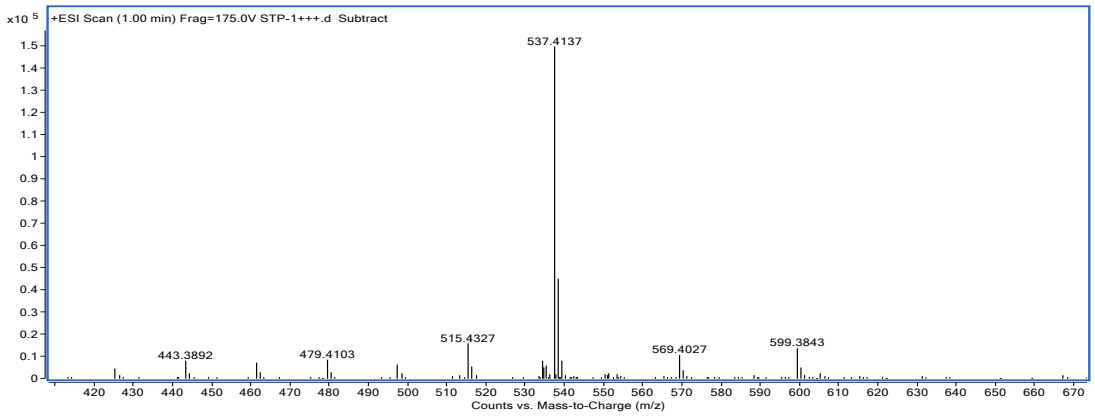


Figure S1. HRESIMS spectrum of compound **1**

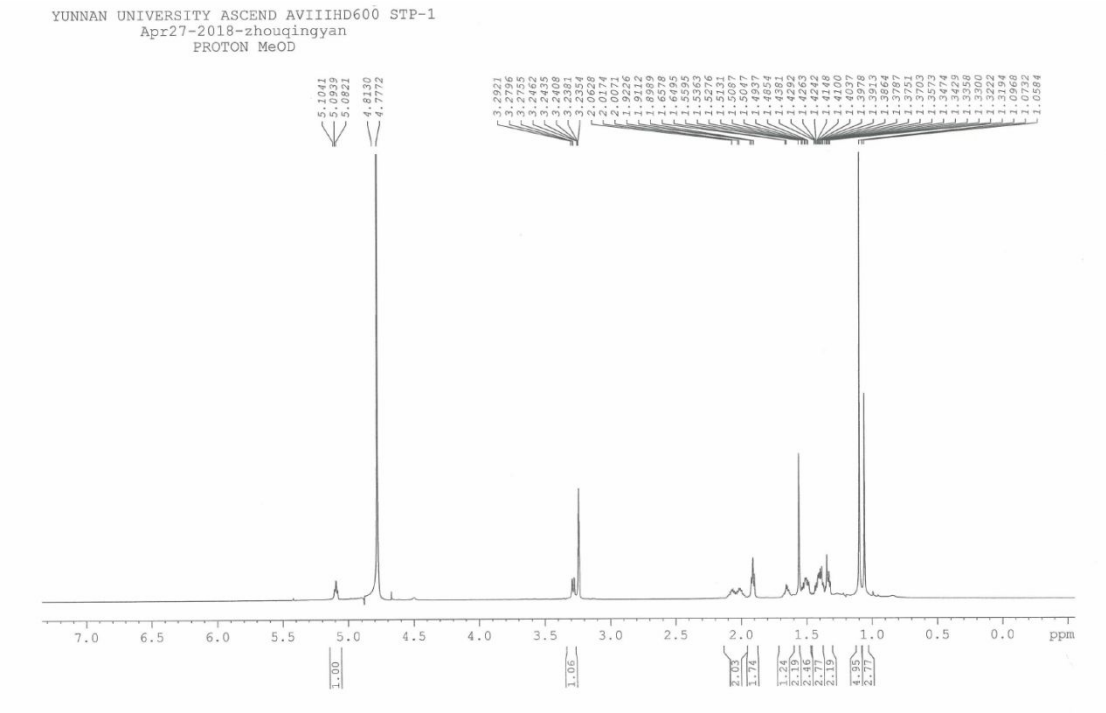


Figure S2. ^{1}H NMR spectrum of compound **1** in MeOD (600MHz)

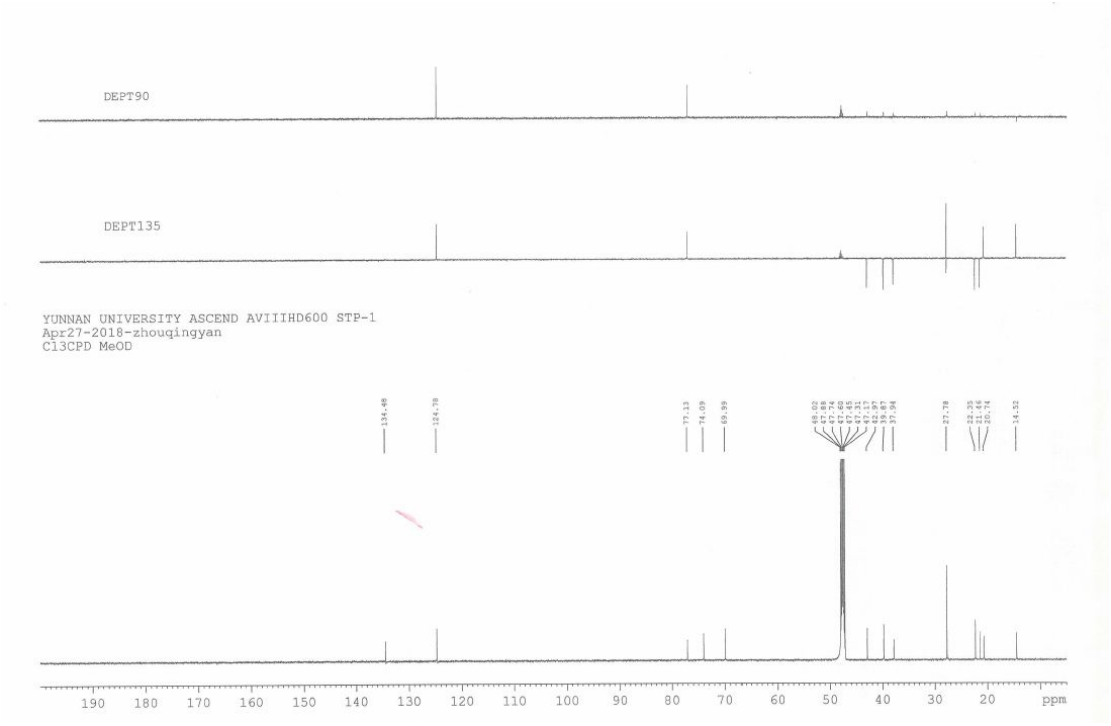


Figure S3. ^{13}C NMR spectrum of compound **1** in MeOD (150MHz)

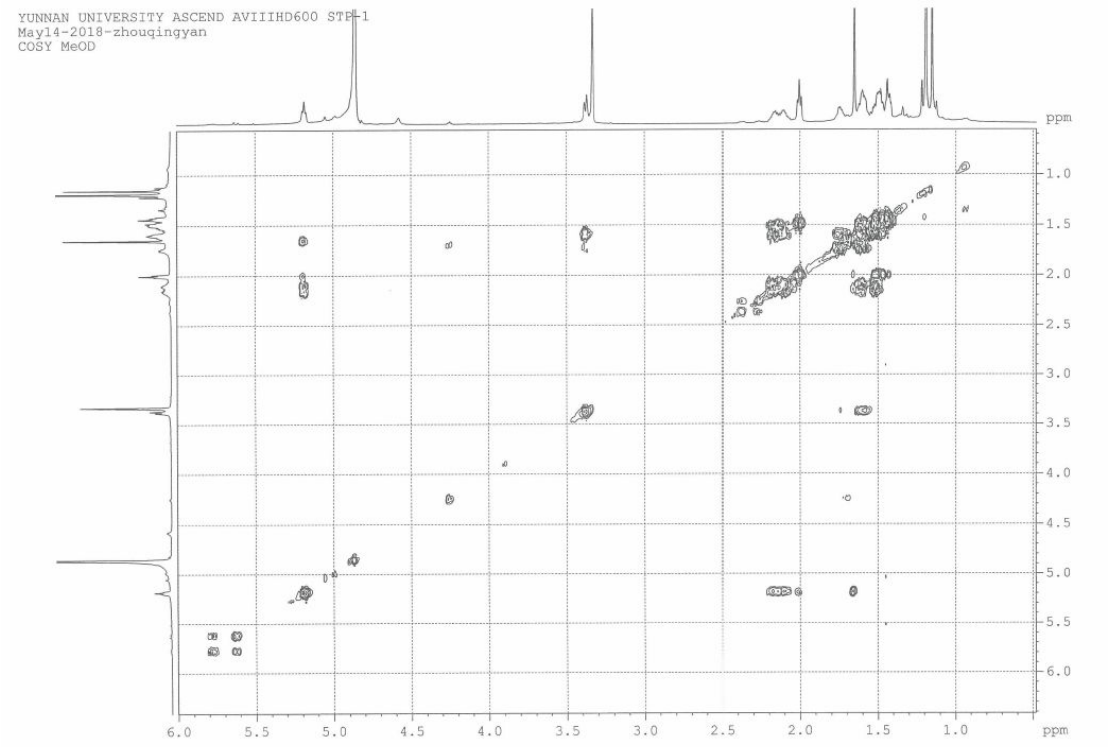


Figure S4. COSY spectrum of compound **1** in MeOD (600 MHz)

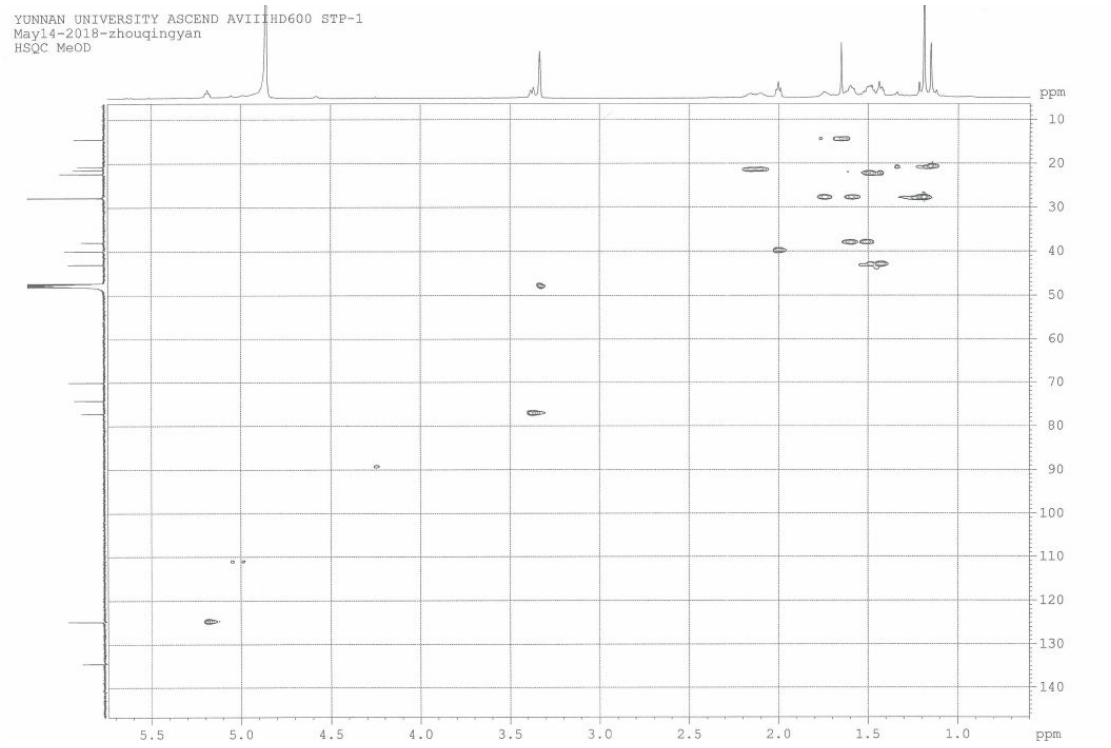


Figure S5. HSQC spectrum of compound **1** in $CDCl_3$ (500 MHz)

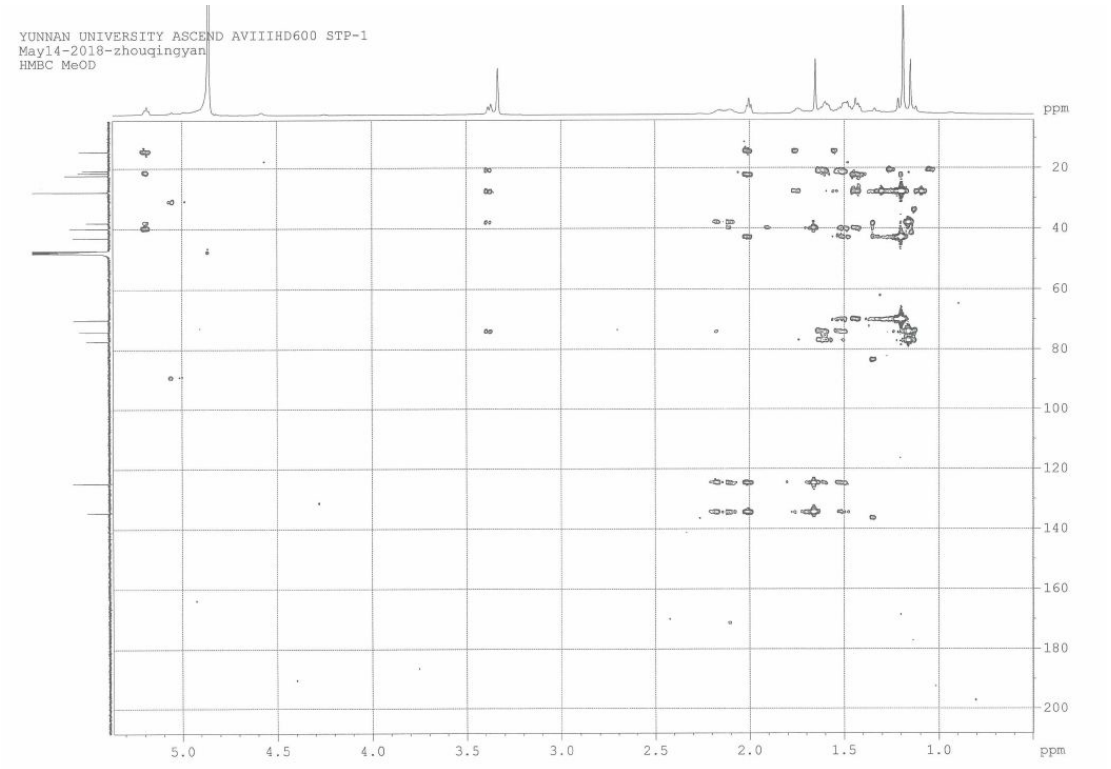


Figure S6. HMBC spectrum of compound **1** in $CDCl_3$ (500 MHz)

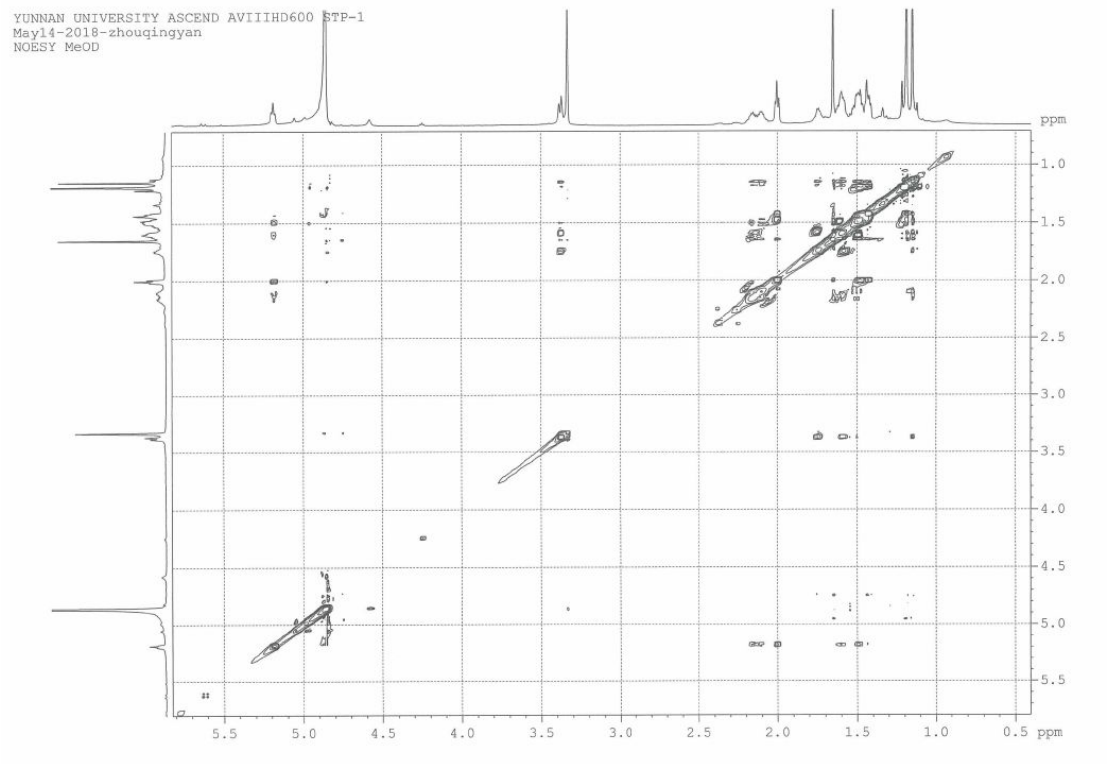


Figure S7. NOESY spectrum of compound **1** in $CDCl_3$ (500 MHz)

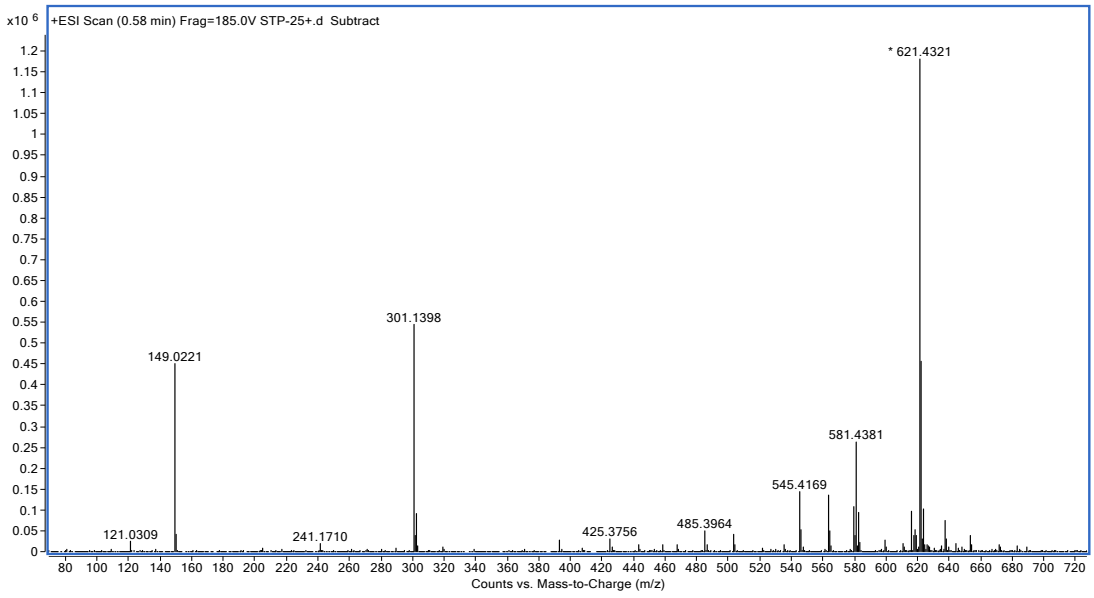


Figure S8. HRESIMS spectrum of compound **2**

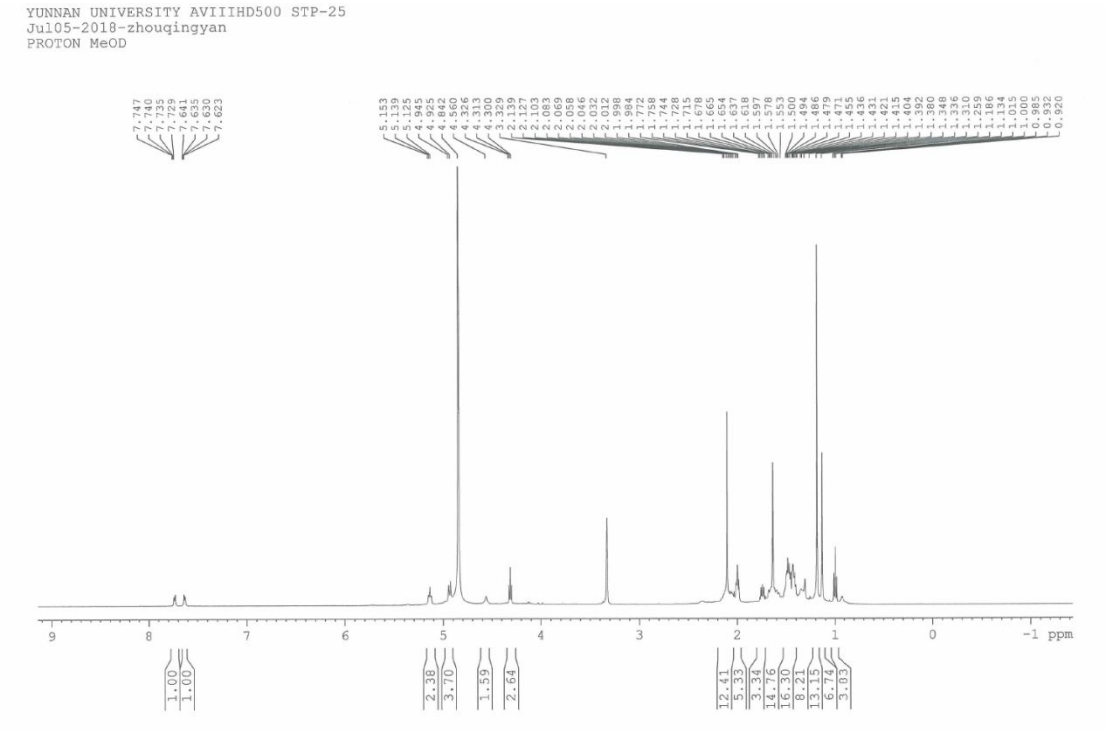


Figure S9. ^{1}H NMR spectrum of compound **2** in MeOD (500MHz)

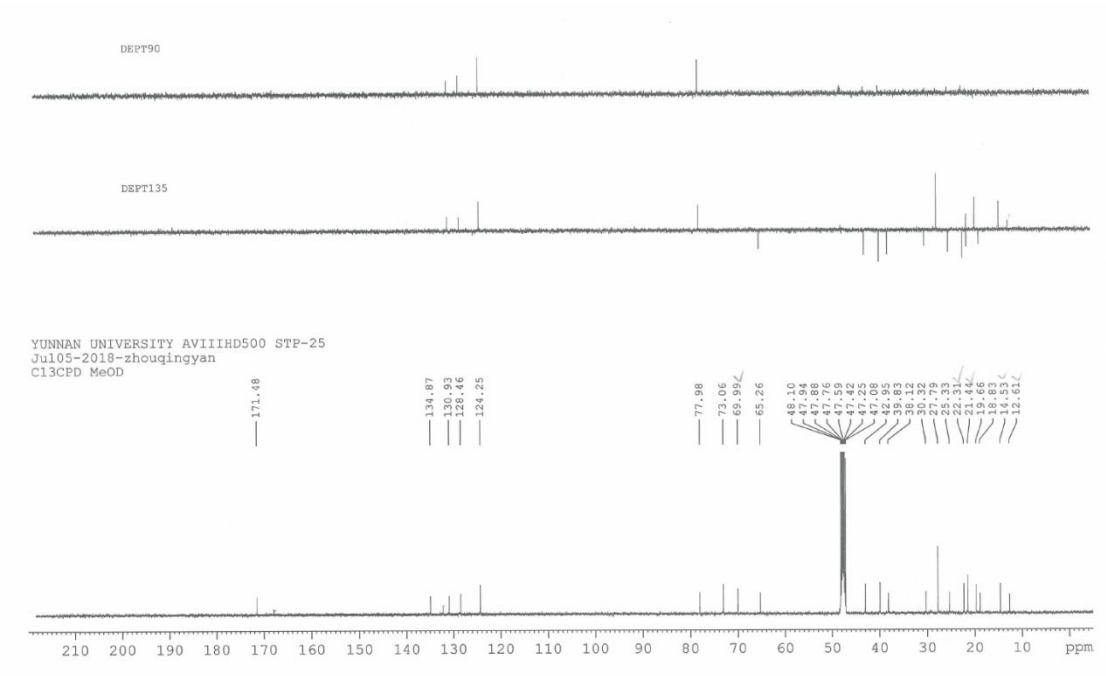


Figure S10. ^{13}C NMR spectrum of compound **2** in MeOD (125MHz)

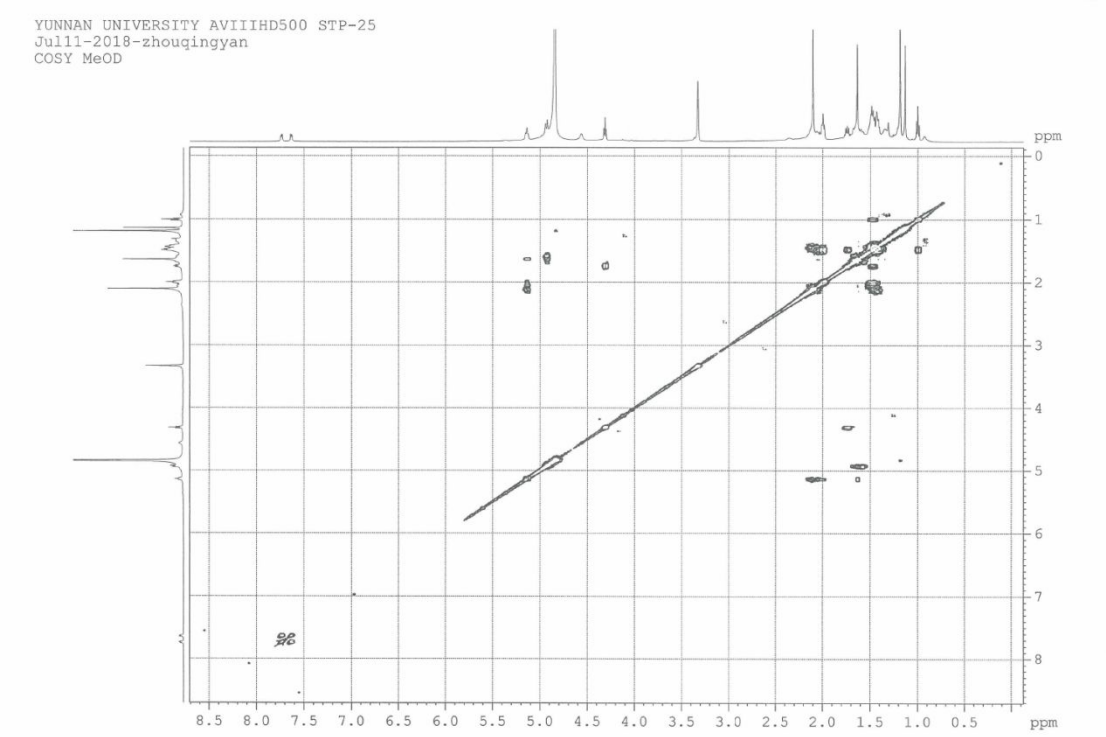


Figure S11.COSY spectrum of compound **2** in MeOD (500 MHz)

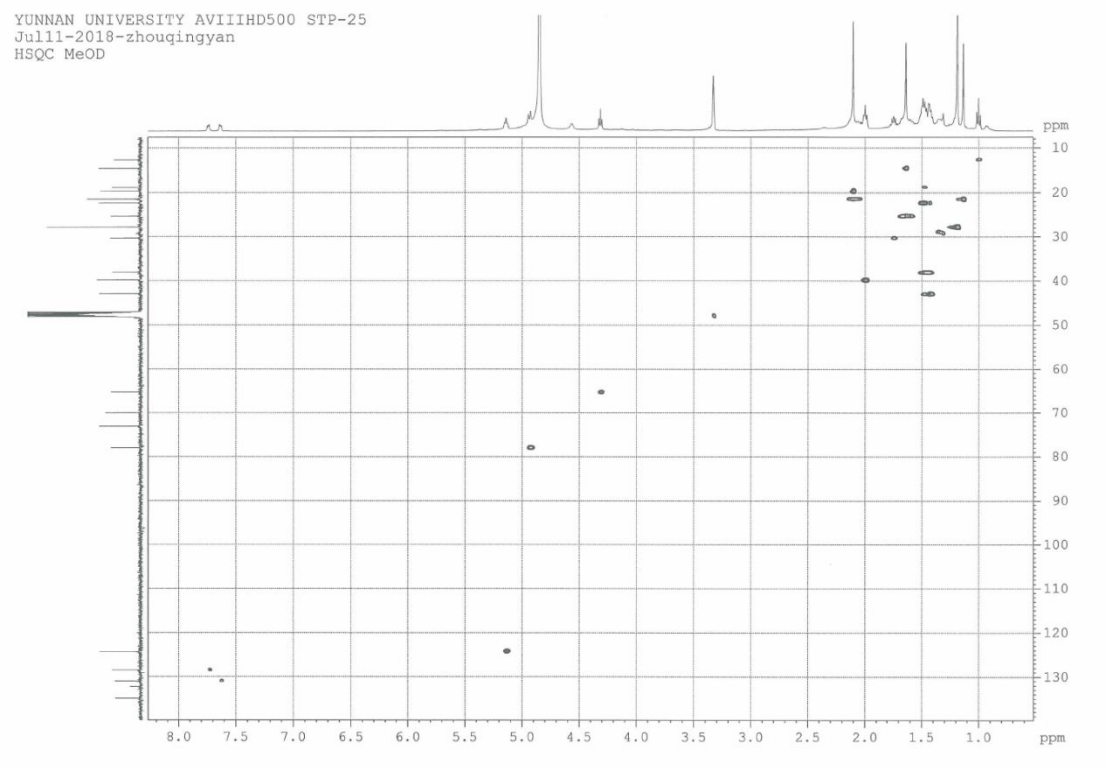


Figure S12. HSQC spectrum of compound **2** in MeOD (500 MHz)

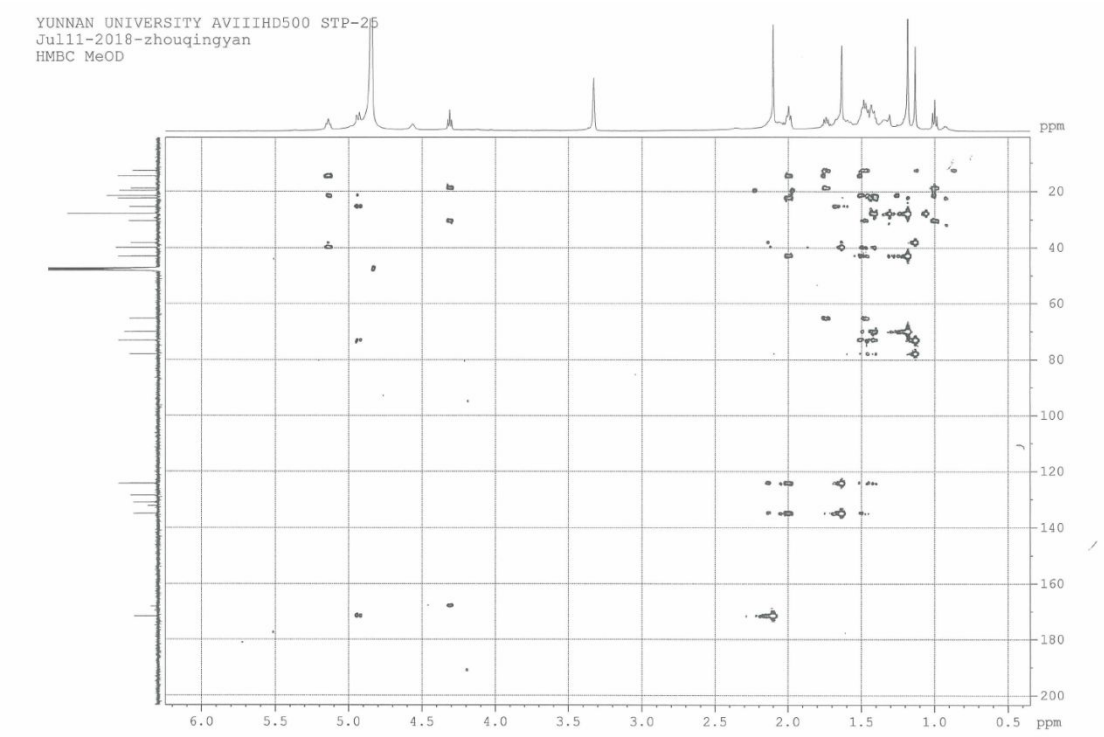


Figure S13. HMBC spectrum of compound **2** in $CDCl_3$ (500 MHz)

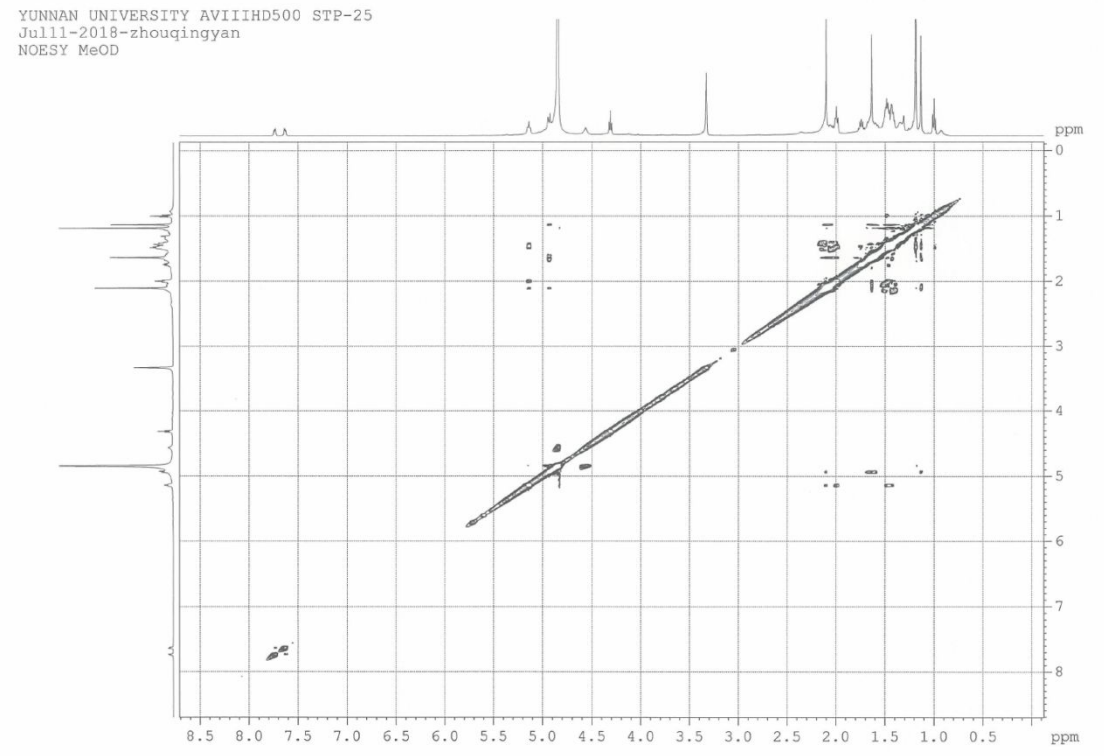


Figure S14. NOESY spectrum of compound **2** in MeOD (500 MHz)

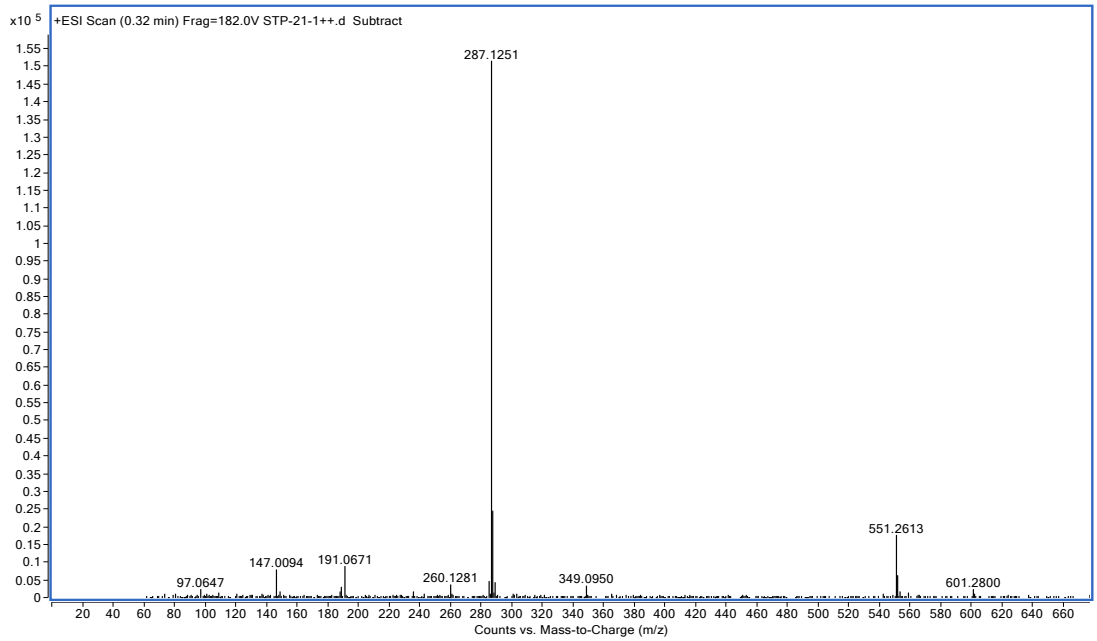


Figure S15. HRESIMS spectrum of compound **3**

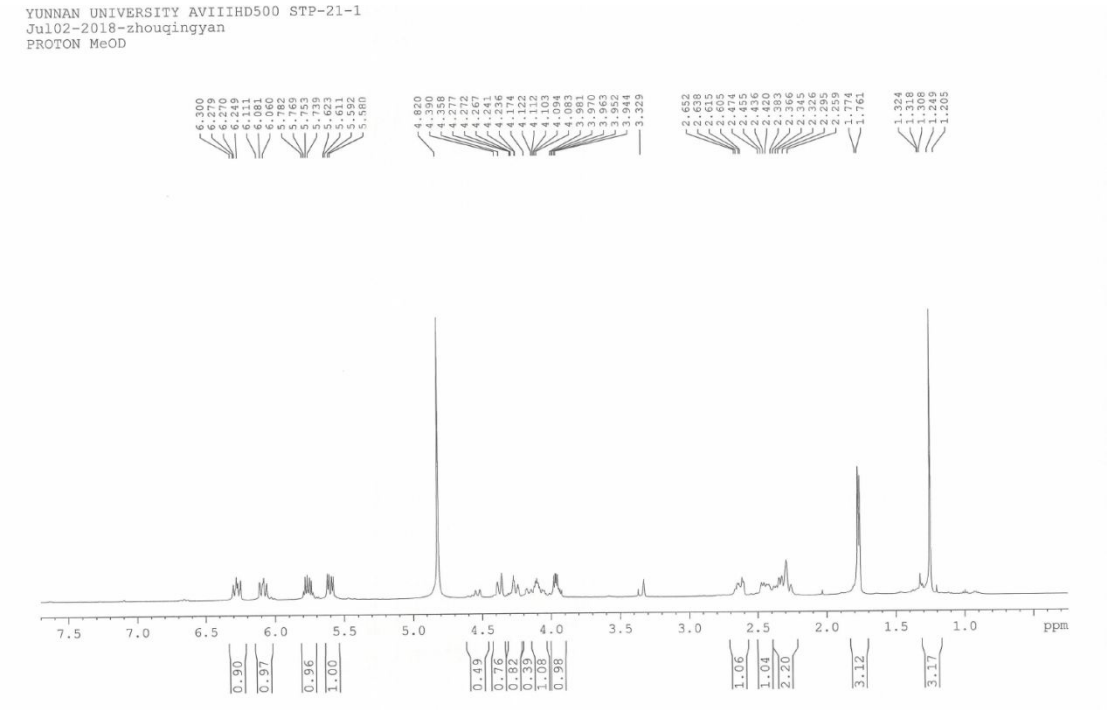


Figure S16. ^{1}H NMR spectrum of compound **3** in MeOD (500MHz)

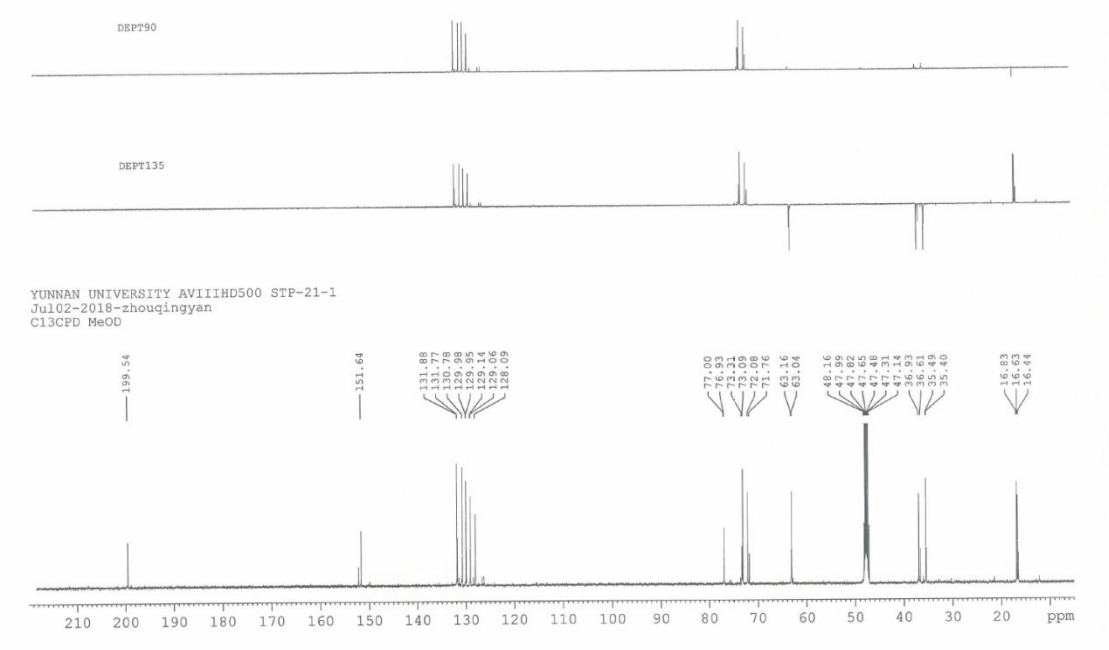


Figure S17. ^{13}C NMR spectrum of compound **3** in MeOD (125MHz)

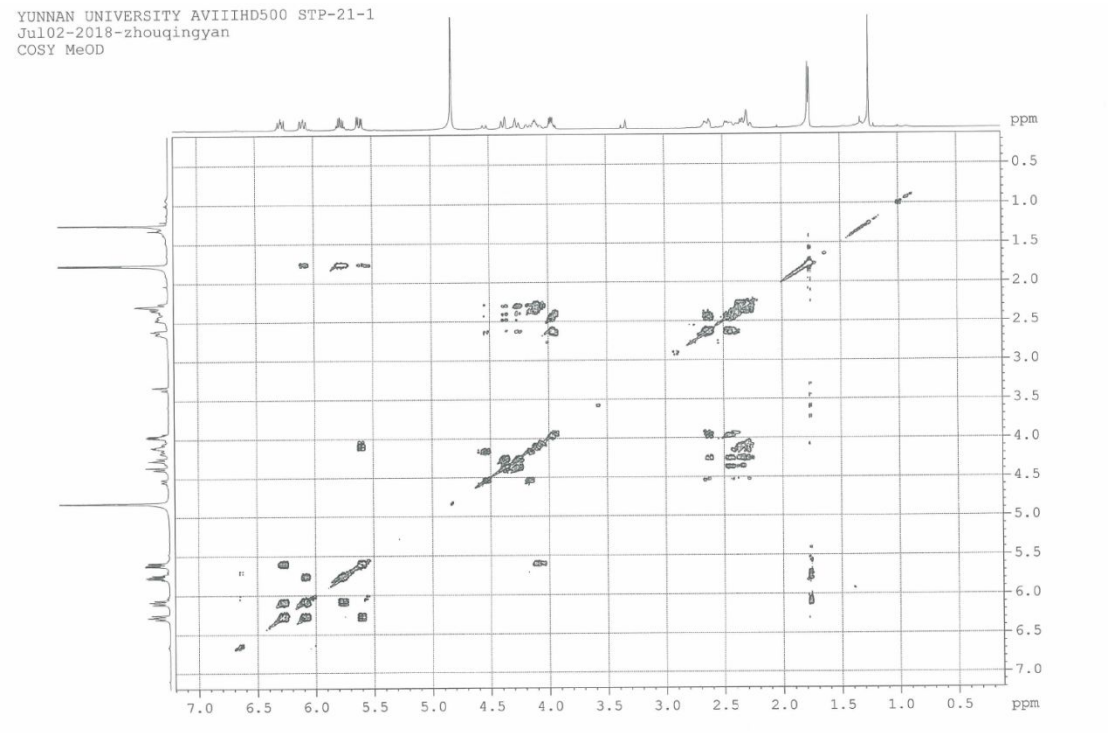


Figure S18. COSY spectrum of compound **3** in MeOD (500 MHz)

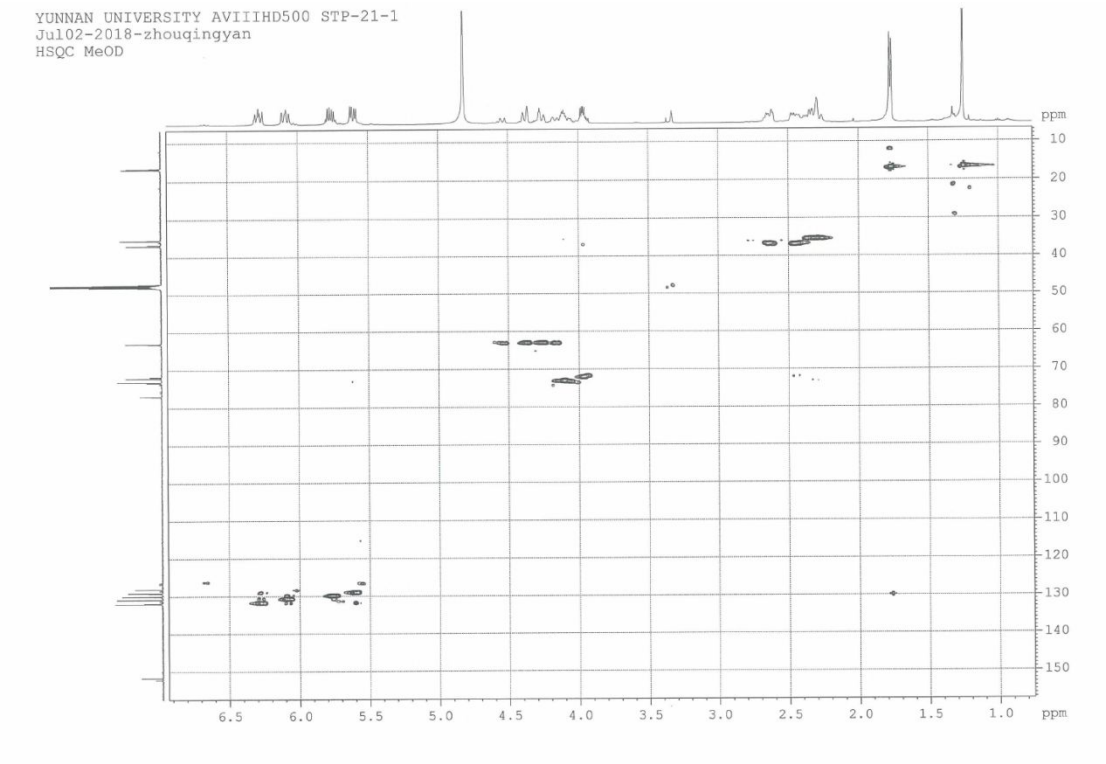


Figure S19. HSQC spectrum of compound **3** in MeOD (500 MHz)

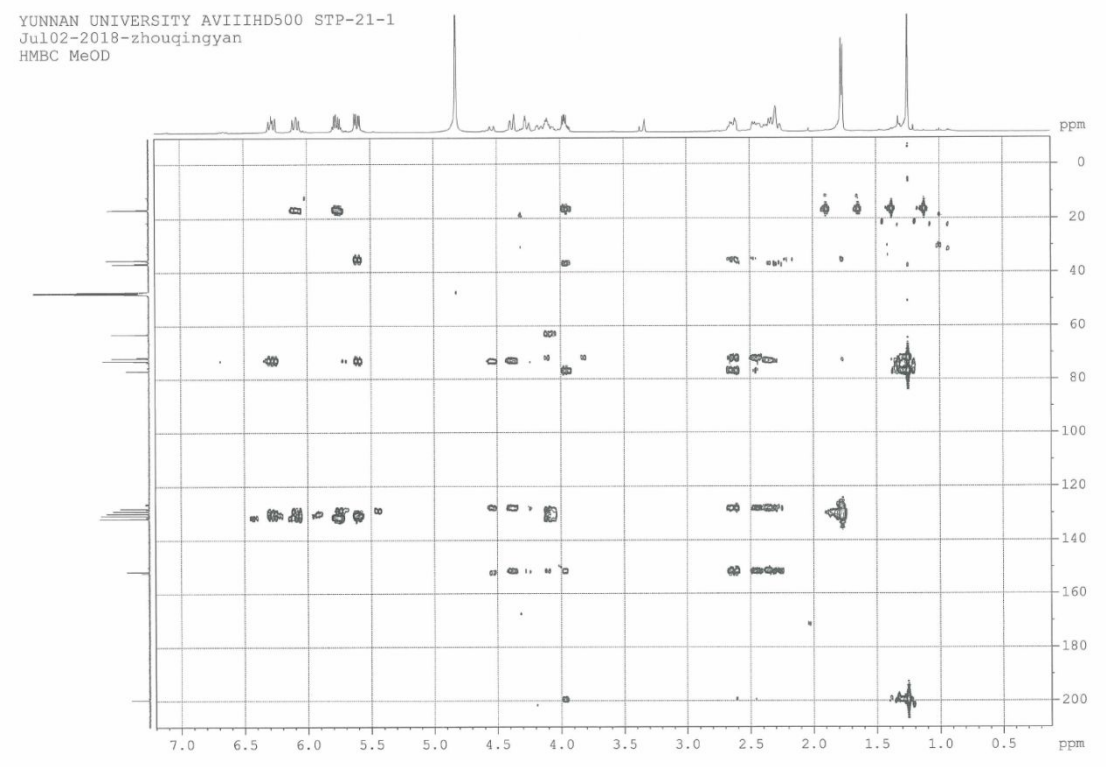


Figure S20. HMBC spectrum of compound **3** in MeOD (500 MHz)

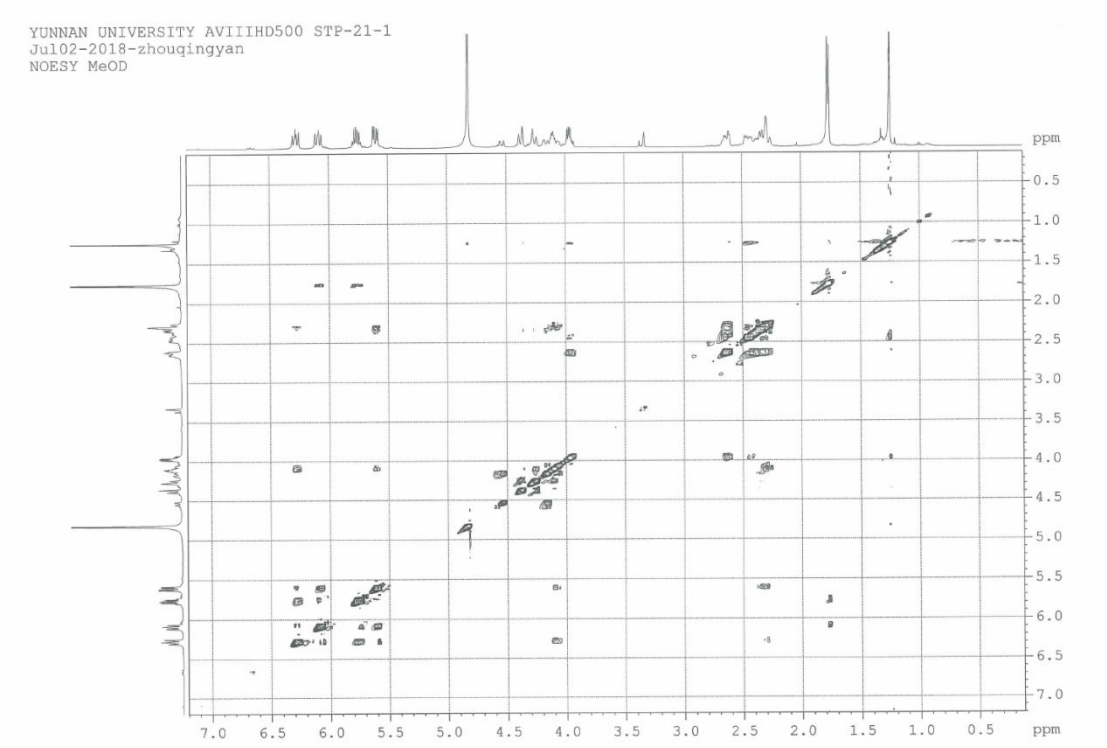


Figure S21. NOESY spectrum of compound **3** in MeOD (500 MHz)

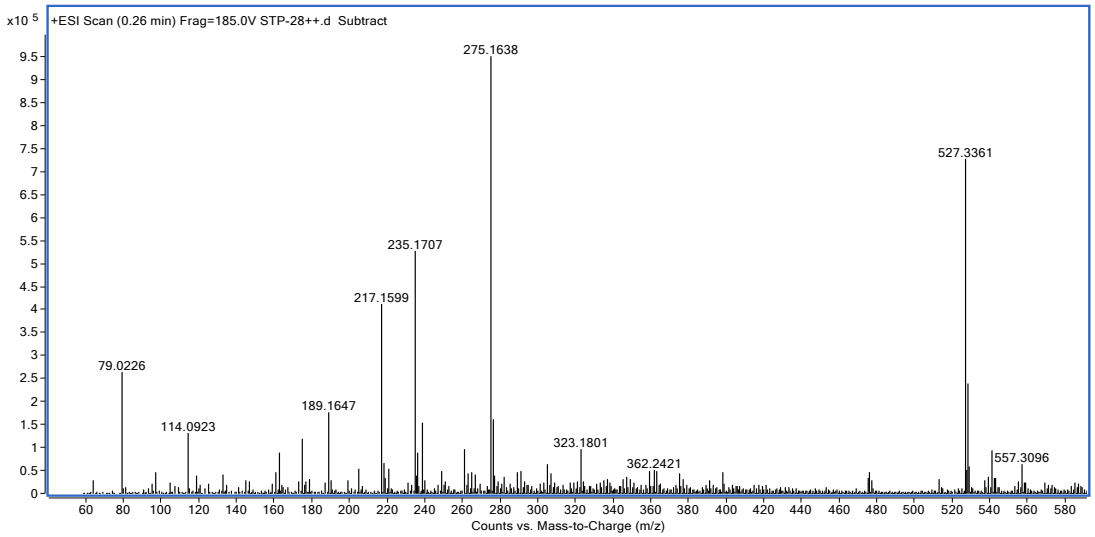


Figure S22. HRESIMS spectrum of compound **4**

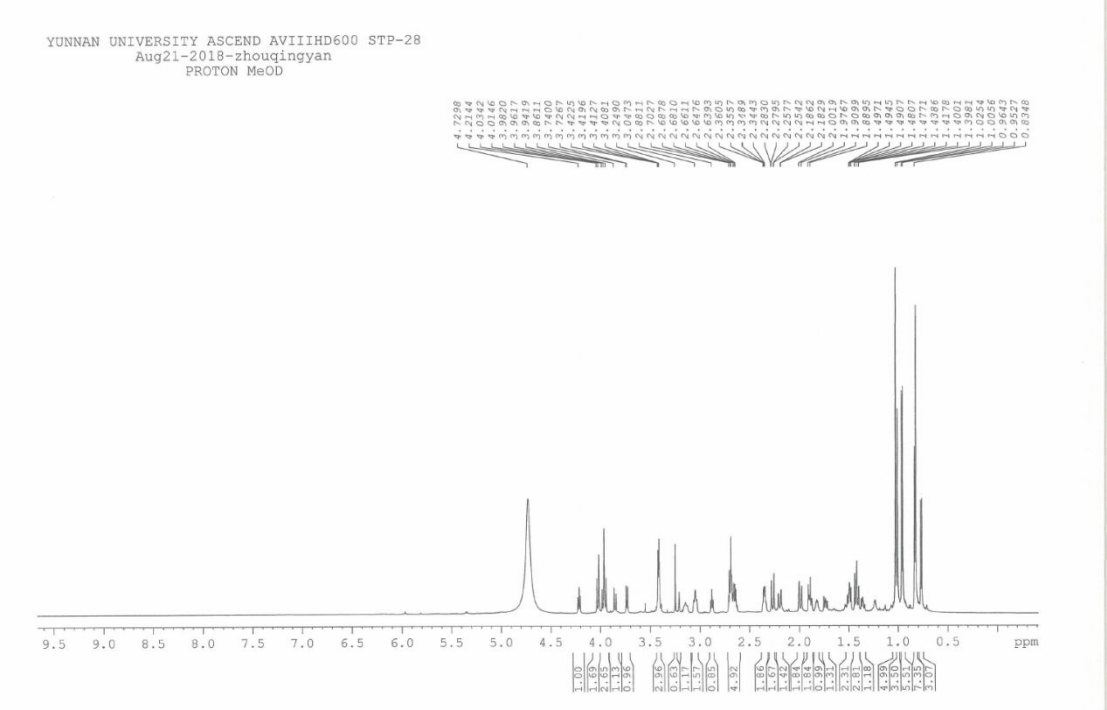


Figure S23. ^{1}H NMR spectrum of compound **4** in MeOD (600MHz)

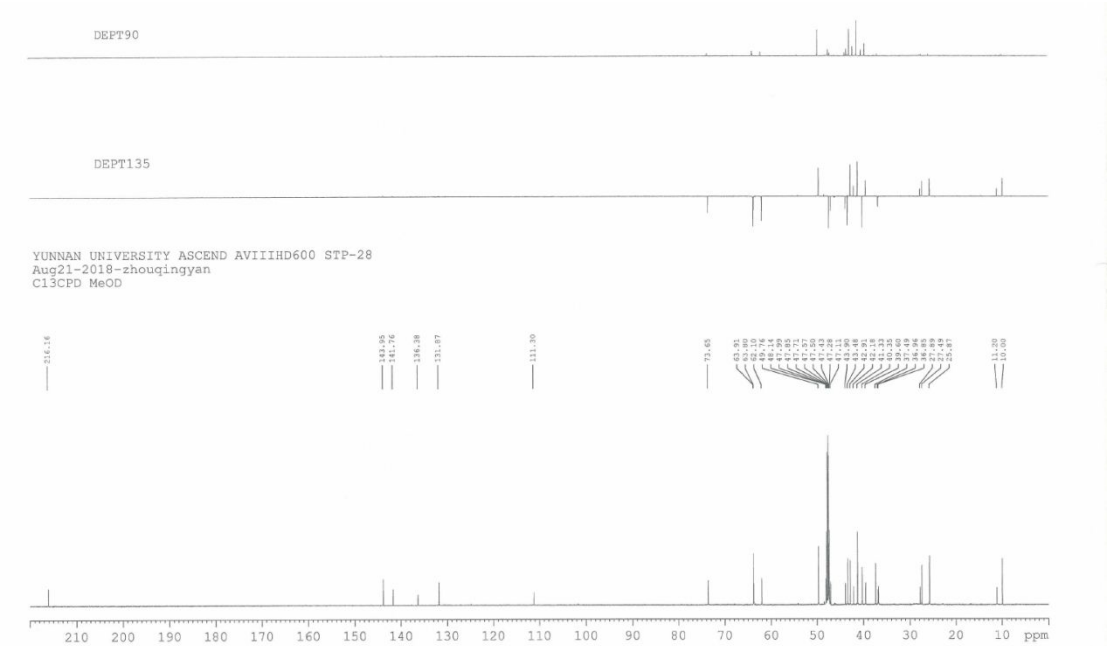


Figure S24. ^{13}C NMR spectrum of compound **4** in MeOD (150 MHz)

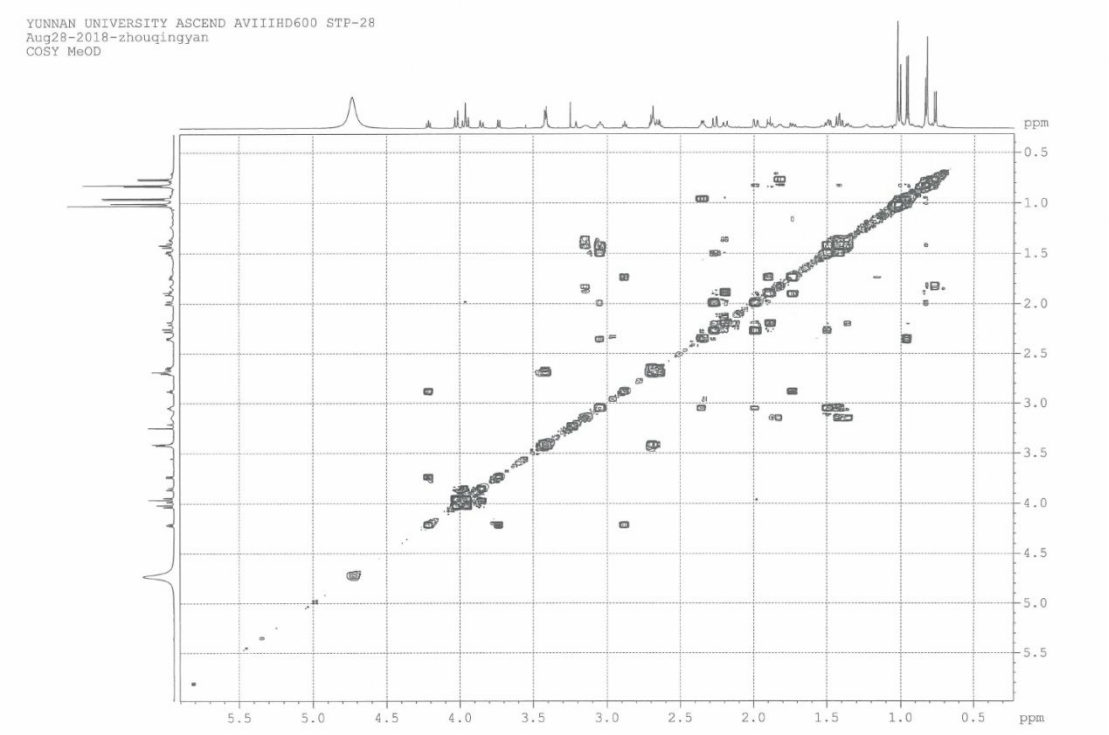


Figure S25. COSY spectrum of compound **4** in MeOD (600 MHz)

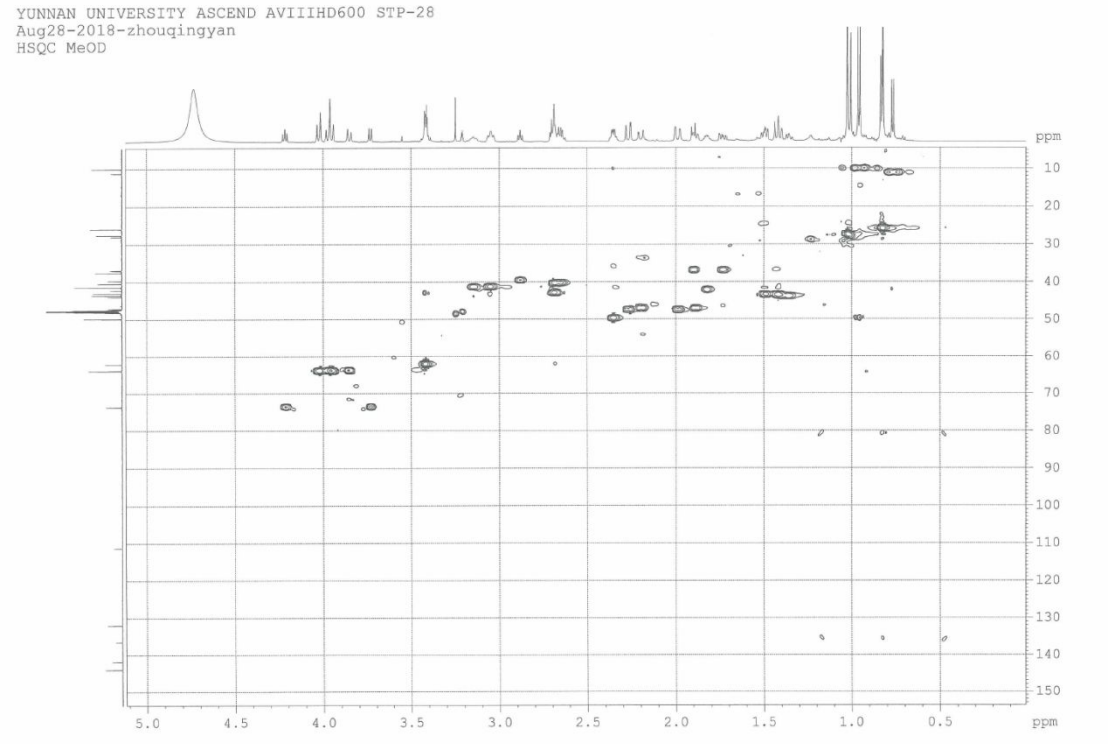


Figure S26. HSQC spectrum of compound **4** in MeOD (600 MHz)

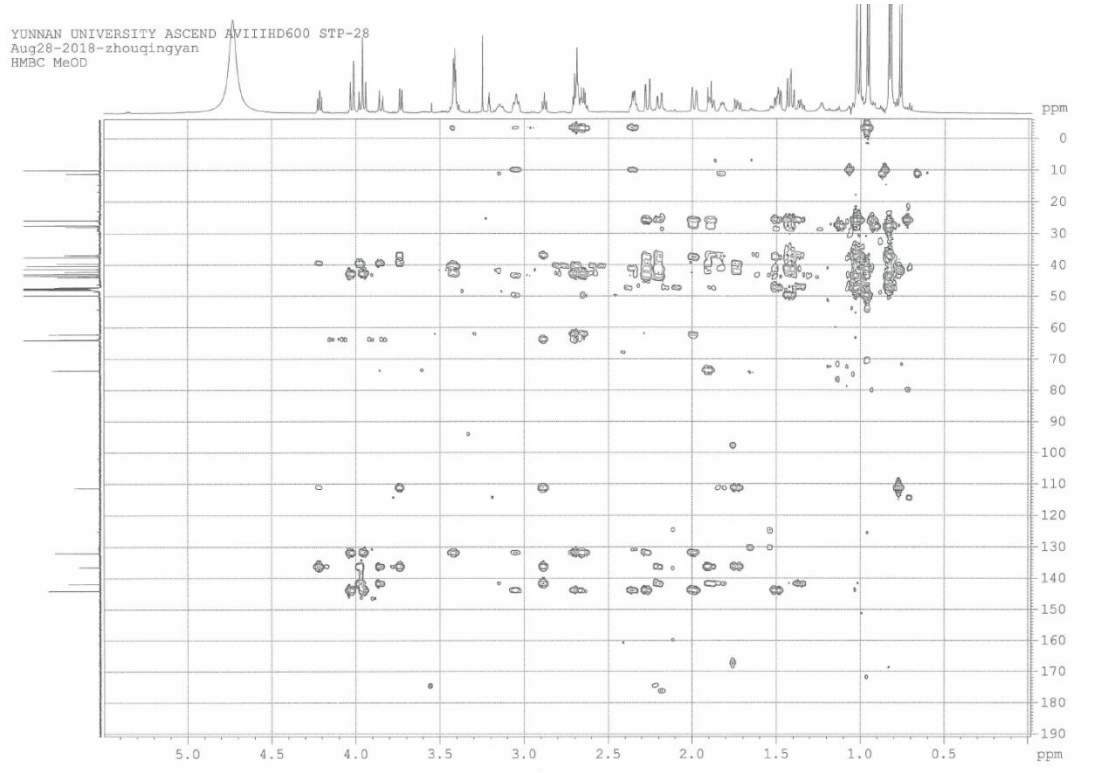


Figure S27. HMBC spectrum of compound **4** in MeOD (600 MHz)

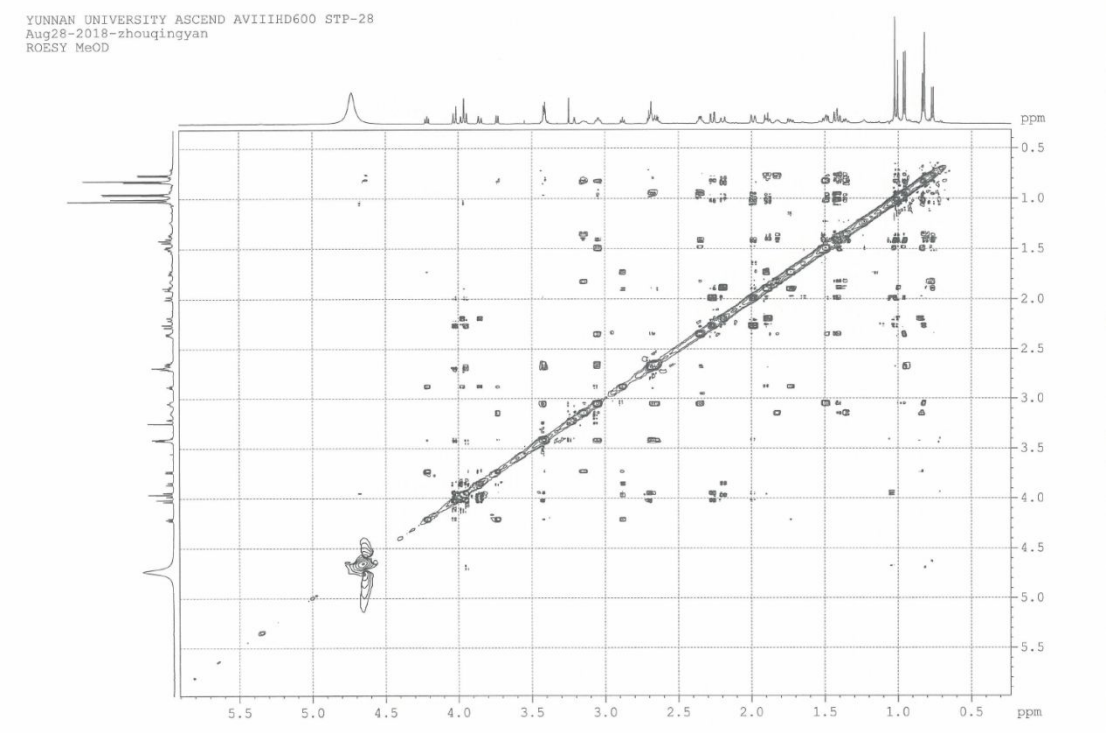


Figure S28. ROESY spectrum of compound **4** in MeOD (600 MHz)

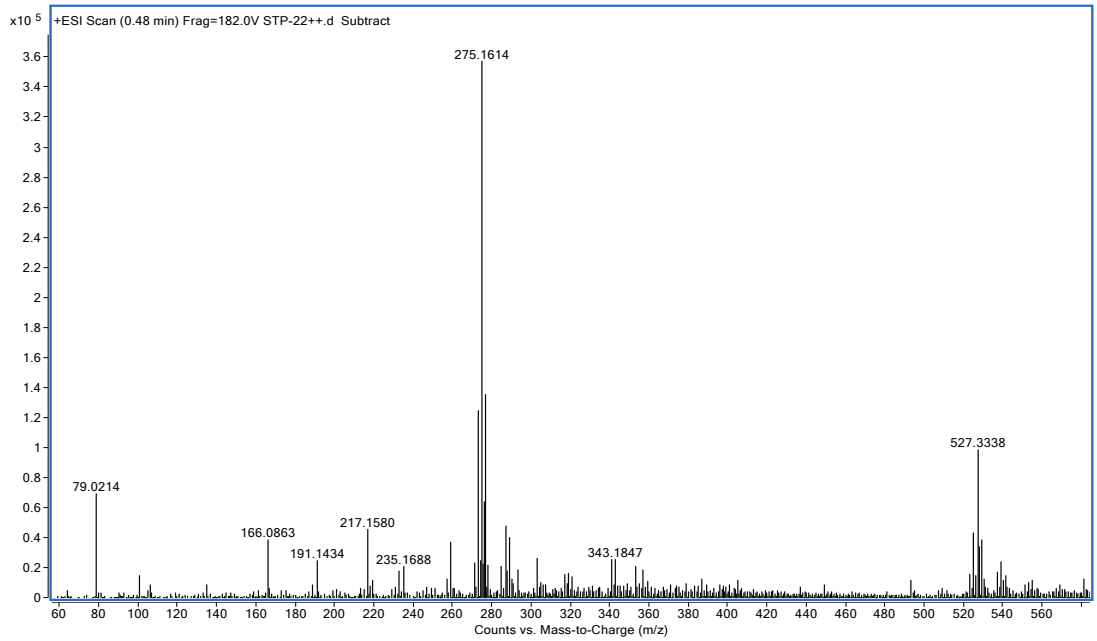


Figure S29. HRESIMS spectrum of compound **5**

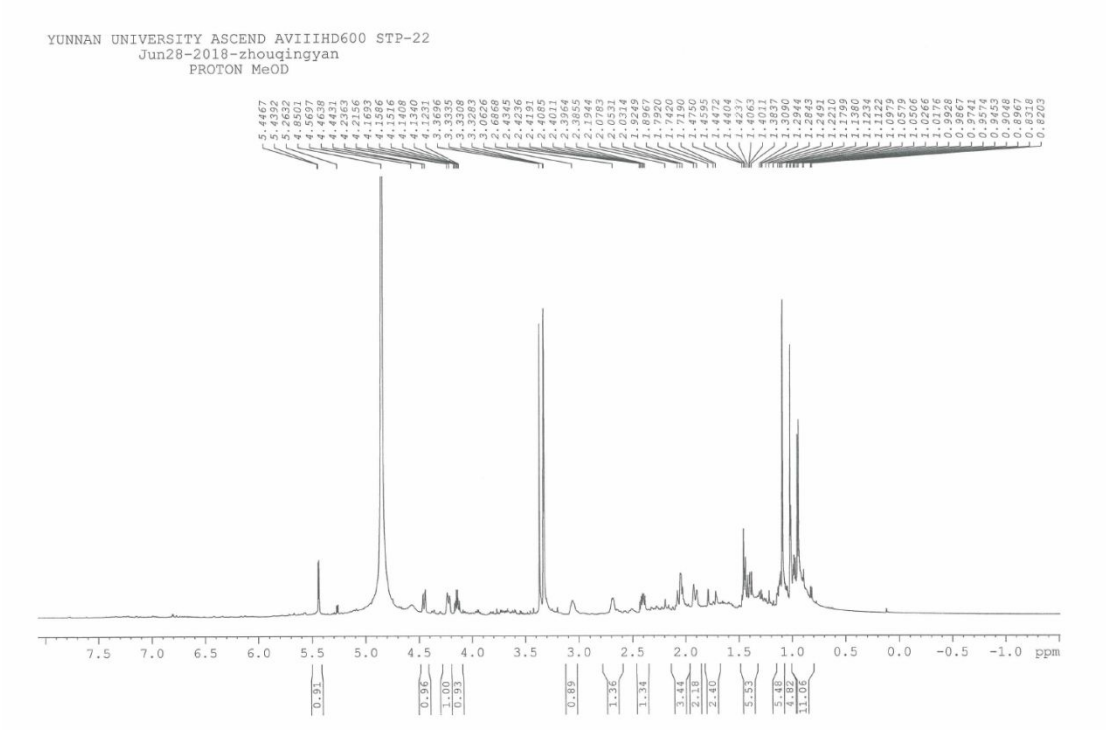


Figure S30. ^{1}H NMR spectrum of compound **5** in MeOD (600MHz)

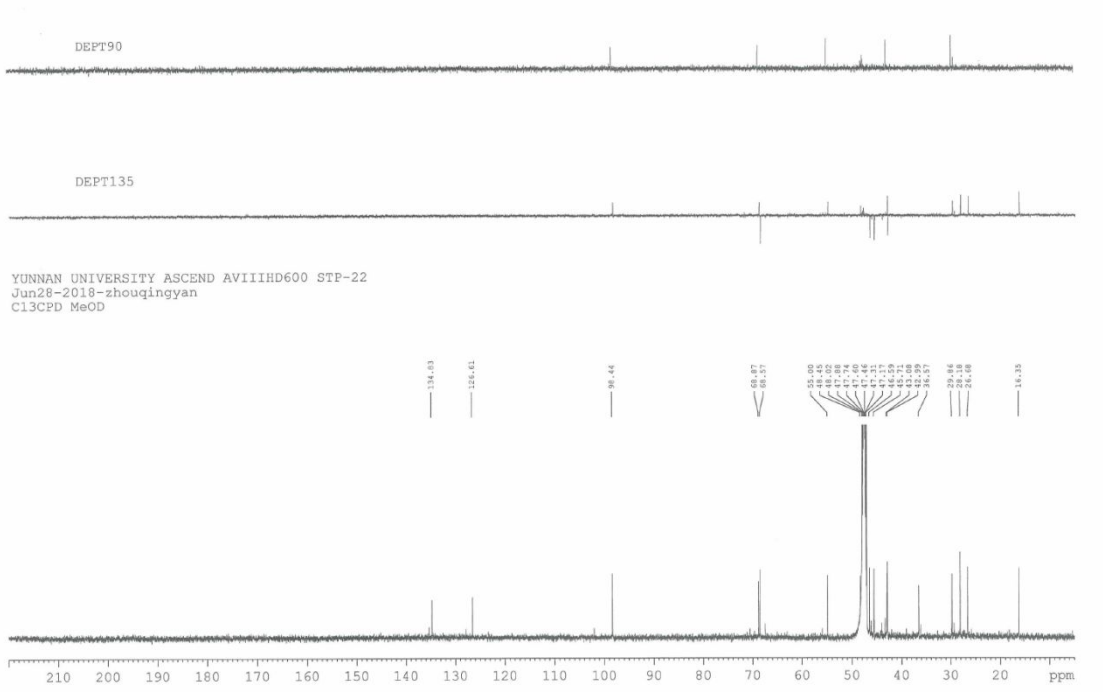


Figure S31. ^{13}C NMR spectrum of compound **5** in MeOD (150MHz)

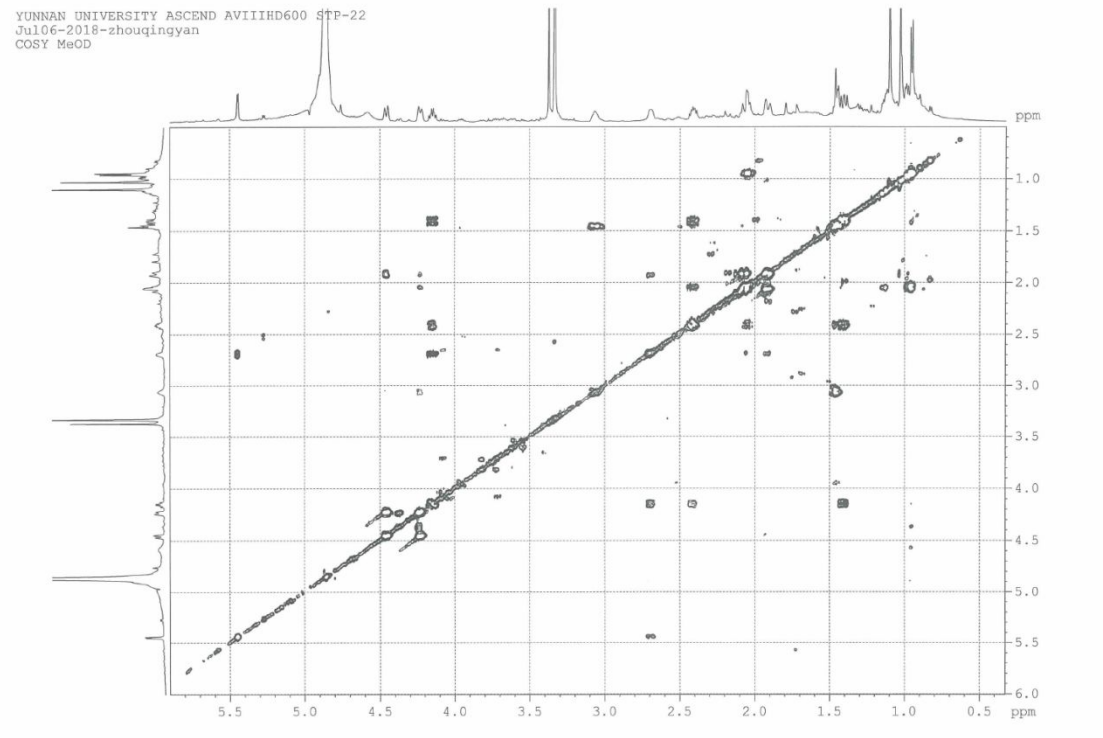


Figure S32. COSY spectrum of compound **5** in MeOD (600 MHz)

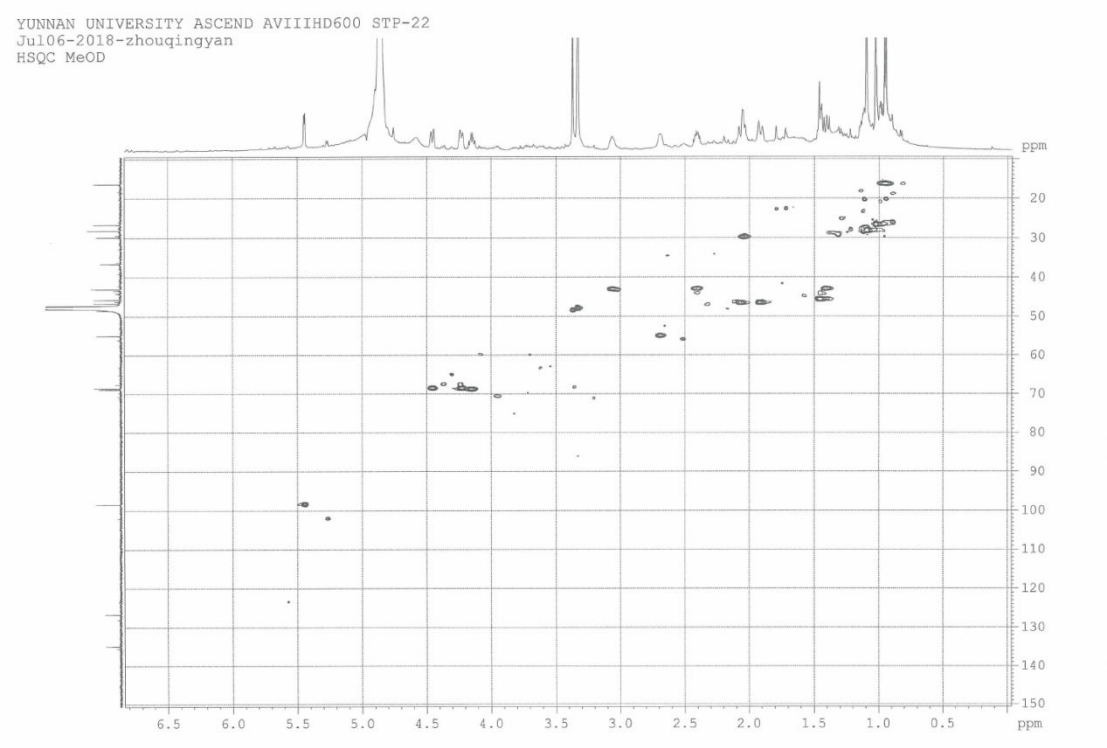


Figure S33. HSQC spectrum of compound **5** in MeOD (600 MHz)

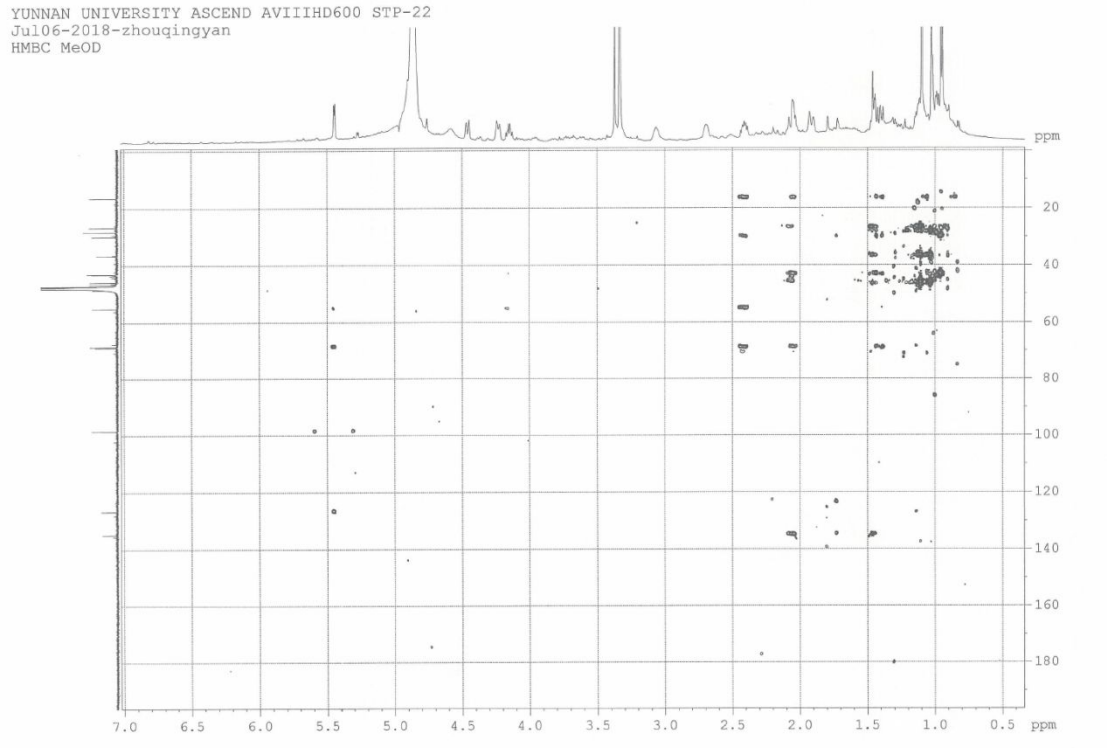


Figure S34. HMBC spectrum of compound **5** in MeOD (600 MHz)

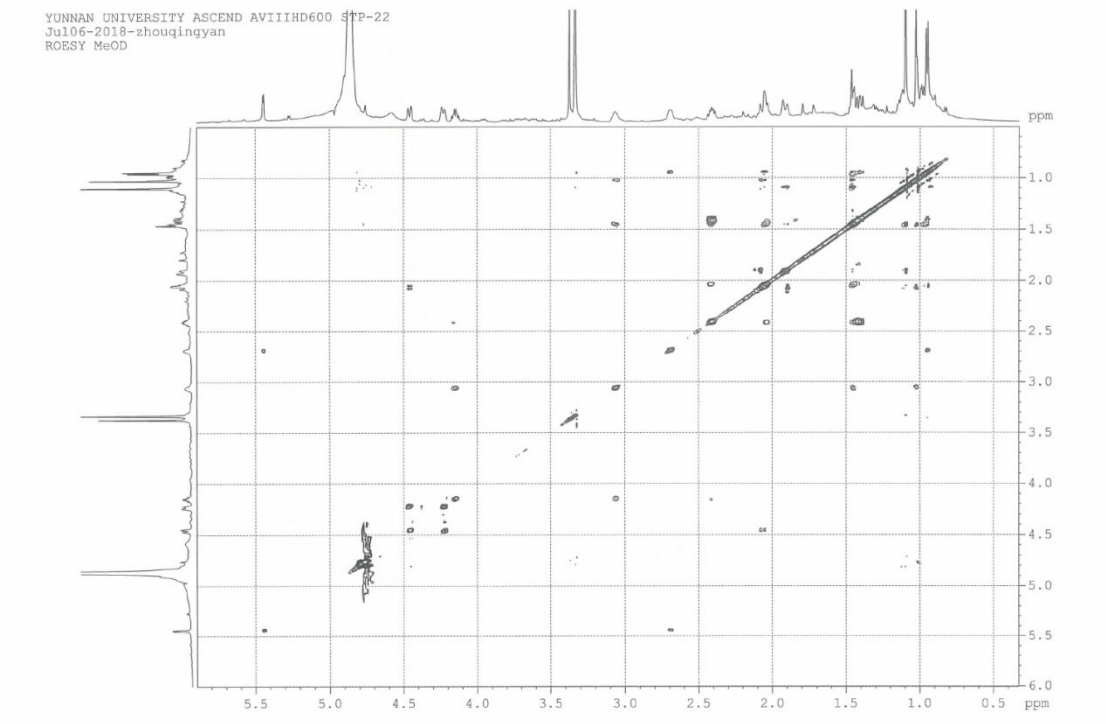


Figure S35. ROESY spectrum of compound **5** in MeOD (600 MHz)

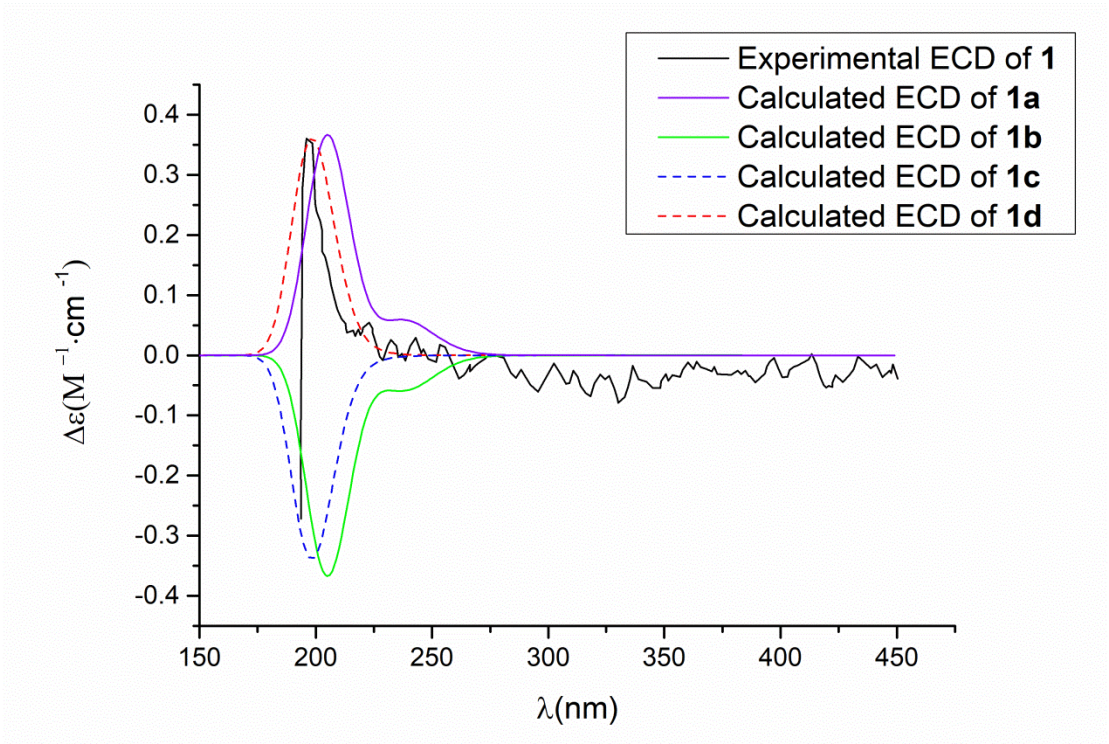


Figure S36. Experimental electronic circular dichroism (ECD) (black) and calculated ECD spectra of (10*R*,11*S*,14*S*,15*R*)-**1a**, (10*S*, 11*R*, 14*R*, 15*S*)-**1b**, (10*R*, 11*R*, 14*S*, 15*S*)-**1c**, and (10*S*, 11*S*, 14*R*, 15*R*)-**1d**.

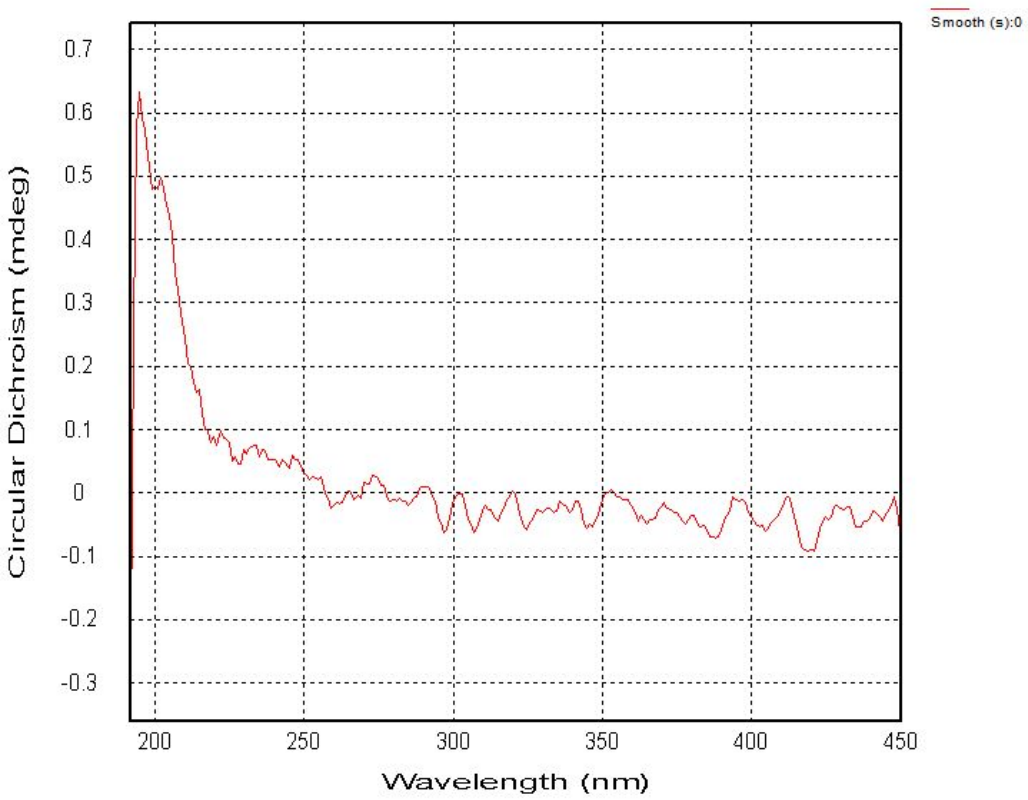


Figure S37. CD spectrum of compound **2**

Table S1 Energies of the dominative conformers of isomers **1a**-**1d**.

Isomer	B3LYP/6-31G(d)	
	Energy(A.U.)	Energy(kcal/mol)
1a	-1629.41453348	-1022473.27522339
1b	-1629.41453348	-1022473.27522339
1c	-1629.41683744	-1022474.72098042
1d	-1629.41683741	-1022474.72961600

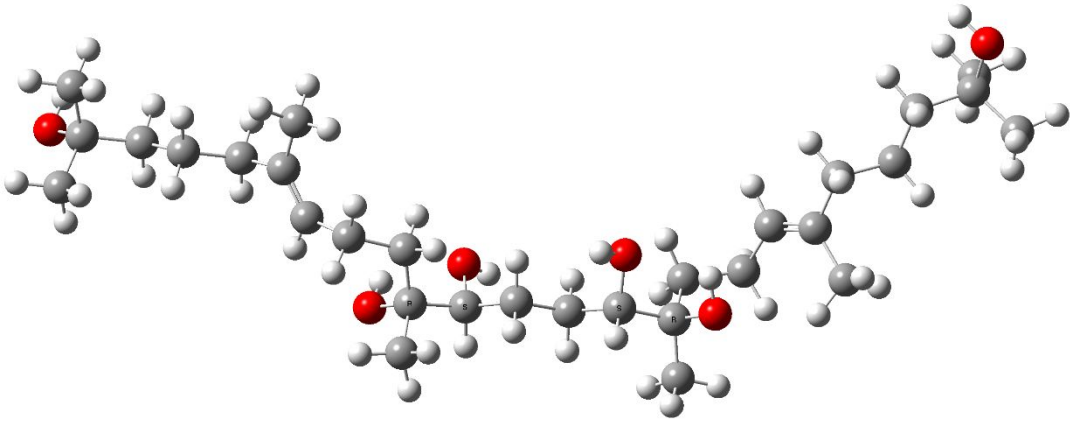


Figure S38. Optimized structure of isomer **1a**

Table S2 Standard orientation of isomer **1a**

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	-11.8795	0.6976	0.0768
2	6	0	-11.3310	1.9664	-0.5811
3	6	0	-11.5502	3.1897	0.3224
4	6	0	-9.8516	1.8096	-1.0012
5	6	0	-8.8253	1.5812	0.1176
6	8	0	-12.1215	2.1184	-1.7764
7	6	0	-7.3919	1.4169	-0.4317
8	6	0	-6.3433	1.1571	0.6346
9	6	0	-6.0347	2.3305	1.5357
10	6	0	-5.7669	-0.0533	0.7217
11	6	0	-4.7316	-0.5234	1.7121
12	6	0	-3.3416	-0.8424	1.1050
13	6	0	-3.2124	-2.1735	0.3229
14	6	0	-3.4192	-3.3977	1.2189
15	6	0	-1.8450	-2.2554	-0.4131
16	6	0	0.7126	-2.3617	-0.3317
17	6	0	1.9671	-2.2877	0.5490
18	8	0	-1.8810	-1.2083	-1.4031
19	6	0	3.3211	-2.5649	-0.1583

20	8	0	2.1038	-0.9761	1.1278
21	6	0	3.5512	-1.5734	-1.3318
22	6	0	3.4134	-4.0206	-0.6228
23	8	0	4.3357	-2.4318	0.8402
24	6	0	5.0357	-1.3739	-1.7255
25	6	0	5.7162	-0.2574	-0.9737
26	6	0	6.8074	-0.3121	-0.1936
27	6	0	7.5516	-1.5919	0.1217
28	6	0	7.3743	0.9537	0.4177
29	6	0	8.7728	1.3286	-0.1164
30	6	0	9.3214	2.6070	0.5326
31	6	0	10.7200	3.0839	0.0782
32	6	0	11.8124	2.0659	0.4161
33	6	0	10.7508	3.4447	-1.4149
34	8	0	11.0676	4.2498	0.8503
35	6	0	-0.5876	-2.1364	0.4563
36	8	0	-4.2152	-2.2772	-0.6957
37	1	0	-12.9538	0.8085	0.2563
38	1	0	-11.3880	0.4971	1.0338
39	1	0	-11.7325	-0.1661	-0.5803
40	1	0	-11.0372	3.0889	1.2851
41	1	0	-12.6200	3.3212	0.5148
42	1	0	-11.1765	4.1029	-0.1601
43	1	0	-9.5644	2.7142	-1.5622
44	1	0	-9.8044	0.9787	-1.7177
45	1	0	-8.8543	2.4185	0.8261
46	1	0	-9.0829	0.6801	0.6886
47	1	0	-11.7888	2.9028	-2.2420
48	1	0	-7.3864	0.5916	-1.1548
49	1	0	-7.1283	2.3269	-0.9944
50	1	0	-6.9144	2.6322	2.1199
51	1	0	-5.7438	3.2066	0.9392
52	1	0	-5.2263	2.1286	2.2421
53	1	0	-6.0611	-0.8071	-0.0056
54	1	0	-4.5833	0.2280	2.4951
55	1	0	-5.1141	-1.4148	2.2290
56	1	0	-3.0465	-0.0192	0.4435
57	1	0	-2.6102	-0.8605	1.9245
58	1	0	-4.4553	-3.4313	1.5671
59	1	0	-2.7644	-3.3805	2.0960

60	1	0	-3.2327	-4.3189	0.6564
61	1	0	-1.8378	-3.2296	-0.9263
62	1	0	0.6731	-3.3457	-0.8186
63	1	0	0.7959	-1.6048	-1.1210
64	1	0	1.8858	-3.0303	1.3577
65	1	0	-1.2747	-1.4459	-2.1191
66	1	0	1.5081	-0.9159	1.8881
67	1	0	3.1238	-0.5988	-1.0663
68	1	0	2.9861	-1.9335	-2.2014
69	1	0	3.2570	-4.7003	0.2217
70	1	0	4.4109	-4.2190	-1.0271
71	1	0	2.6799	-4.2488	-1.4021
72	1	0	4.2133	-1.5450	1.2214
73	1	0	5.5873	-2.3129	-1.6243
74	1	0	5.0651	-1.1187	-2.7955
75	1	0	5.2548	0.7221	-1.1226
76	1	0	6.8916	-2.4610	0.0848
77	1	0	7.9825	-1.5481	1.1300
78	1	0	8.3879	-1.7612	-0.5707
79	1	0	7.4433	0.8330	1.5106
80	1	0	6.6878	1.7916	0.2384
81	1	0	9.4641	0.4961	0.0644
82	1	0	8.7079	1.4496	-1.2056
83	1	0	8.6103	3.4288	0.3479
84	1	0	9.3616	2.4772	1.6225
85	1	0	11.6873	1.1400	-0.1538
86	1	0	11.7922	1.8257	1.4845
87	1	0	12.7956	2.4863	0.1813
88	1	0	10.5718	2.5730	-2.0537
89	1	0	11.7268	3.8676	-1.6743
90	1	0	9.9821	4.1930	-1.6509
91	1	0	10.3864	4.9204	0.6794
92	1	0	-0.6461	-2.8698	1.2725
93	1	0	-0.5684	-1.1378	0.9073
94	1	0	-3.9368	-1.6472	-1.3846

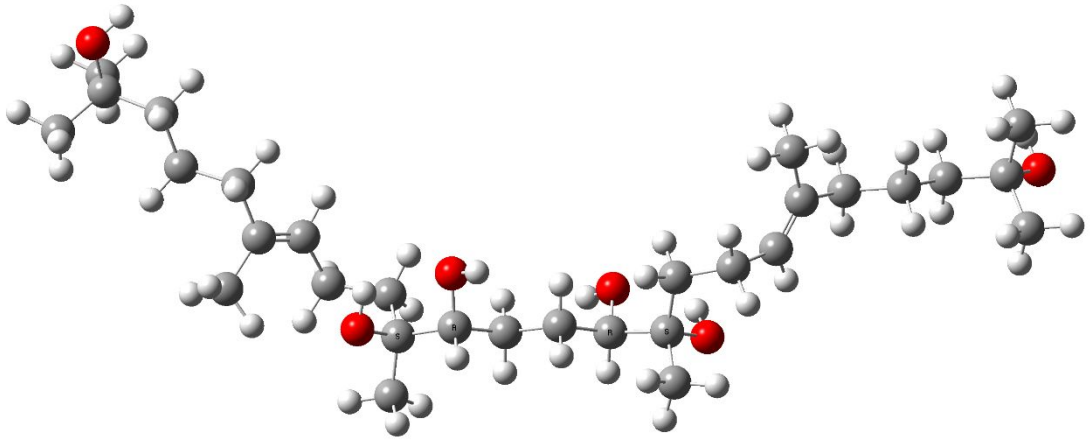


Figure S39**.** Optimized structure of isomer **1b**

Table S3 Standard orientation of isomer **1b**

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	11.8795	0.6976	0.0768
2	6	0	11.3310	1.9664	-0.5811
3	6	0	11.5502	3.1897	0.3224
4	6	0	9.8516	1.8096	-1.0012
5	6	0	8.8253	1.5812	0.1176
6	8	0	12.1215	2.1184	-1.7764
7	6	0	7.3919	1.4169	-0.4317
8	6	0	6.3433	1.1571	0.6346
9	6	0	6.0347	2.3305	1.5357
10	6	0	5.7669	-0.0533	0.7217
11	6	0	4.7316	-0.5234	1.7121
12	6	0	3.3416	-0.8424	1.1050
13	6	0	3.2124	-2.1735	0.3229
14	6	0	3.4192	-3.3977	1.2189
15	6	0	1.8450	-2.2554	-0.4131
16	6	0	-0.7126	-2.3617	-0.3317
17	6	0	-1.9671	-2.2877	0.5490
18	8	0	1.8810	-1.2083	-1.4031
19	6	0	-3.3211	-2.5649	-0.1583
20	8	0	-2.1038	-0.9761	1.1278

21	6	0	-3.5512	-1.5734	-1.3318
22	6	0	-3.4134	-4.0206	-0.6228
23	8	0	-4.3357	-2.4318	0.8402
24	6	0	-5.0357	-1.3739	-1.7255
25	6	0	-5.7162	-0.2574	-0.9737
26	6	0	-6.8074	-0.3121	-0.1936
27	6	0	-7.5516	-1.5919	0.1217
28	6	0	-7.3743	0.9537	0.4177
29	6	0	-8.7728	1.3286	-0.1164
30	6	0	-9.3214	2.6070	0.5326
31	6	0	-10.7200	3.0839	0.0782
32	6	0	-11.8124	2.0659	0.4161
33	6	0	-10.7508	3.4447	-1.4149
34	8	0	-11.0676	4.2498	0.8503
35	6	0	0.5876	-2.1364	0.4563
36	8	0	4.2152	-2.2772	-0.6957
37	1	0	12.9538	0.8085	0.2563
38	1	0	11.3880	0.4971	1.0338
39	1	0	11.7325	-0.1661	-0.5803
40	1	0	11.0372	3.0889	1.2851
41	1	0	12.6200	3.3212	0.5148
42	1	0	11.1765	4.1029	-0.1601
43	1	0	9.5644	2.7142	-1.5622
44	1	0	9.8044	0.9787	-1.7177
45	1	0	8.8543	2.4185	0.8261
46	1	0	9.0829	0.6801	0.6886
47	1	0	11.7888	2.9028	-2.2420
48	1	0	7.3864	0.5916	-1.1548
49	1	0	7.1283	2.3269	-0.9944
50	1	0	6.9144	2.6322	2.1199
51	1	0	5.7438	3.2066	0.9392
52	1	0	5.2263	2.1286	2.2421
53	1	0	6.0611	-0.8071	-0.0056
54	1	0	4.5833	0.2280	2.4951
55	1	0	5.1141	-1.4148	2.2290
56	1	0	3.0465	-0.0192	0.4435
57	1	0	2.6102	-0.8605	1.9245
58	1	0	4.4553	-3.4313	1.5671
59	1	0	2.7644	-3.3805	2.0960
60	1	0	3.2327	-4.3189	0.6564

61	1	0	1.8378	-3.2296	-0.9263
62	1	0	-0.6731	-3.3457	-0.8186
63	1	0	-0.7959	-1.6048	-1.1210
64	1	0	-1.8858	-3.0303	1.3577
65	1	0	1.2747	-1.4459	-2.1191
66	1	0	-1.5081	-0.9159	1.8881
67	1	0	-3.1238	-0.5988	-1.0663
68	1	0	-2.9861	-1.9335	-2.2014
69	1	0	-3.2570	-4.7003	0.2217
70	1	0	-4.4109	-4.2190	-1.0271
71	1	0	-2.6799	-4.2488	-1.4021
72	1	0	-4.2133	-1.5450	1.2214
73	1	0	-5.5873	-2.3129	-1.6243
74	1	0	-5.0651	-1.1187	-2.7955
75	1	0	-5.2548	0.7221	-1.1226
76	1	0	-6.8916	-2.4610	0.0848
77	1	0	-7.9825	-1.5481	1.1300
78	1	0	-8.3879	-1.7612	-0.5707
79	1	0	-7.4433	0.8330	1.5106
80	1	0	-6.6878	1.7916	0.2384
81	1	0	-9.4641	0.4961	0.0644
82	1	0	-8.7079	1.4496	-1.2056
83	1	0	-8.6103	3.4288	0.3479
84	1	0	-9.3616	2.4772	1.6225
85	1	0	-11.6873	1.1400	-0.1538
86	1	0	-11.7922	1.8257	1.4845
87	1	0	-12.7956	2.4863	0.1813
88	1	0	-10.5718	2.5730	-2.0537
89	1	0	-11.7268	3.8676	-1.6743
90	1	0	-9.9821	4.1930	-1.6509
91	1	0	-10.3864	4.9204	0.6794
92	1	0	0.6461	-2.8698	1.2725
93	1	0	0.5684	-1.1378	0.9073
94	1	0	3.9368	-1.6472	-1.3846

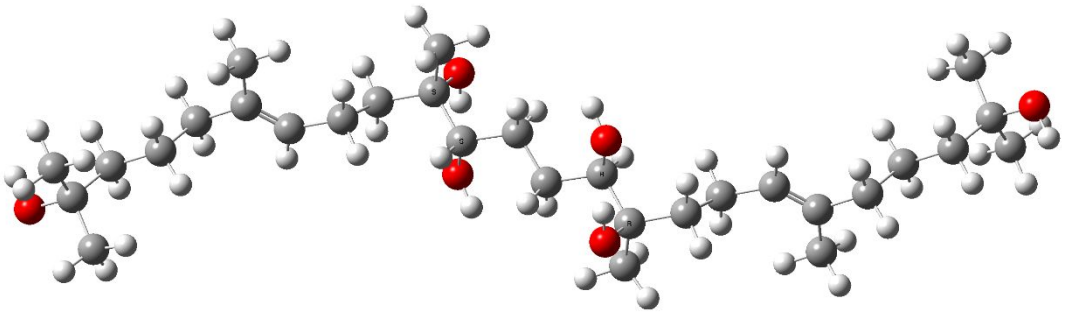


Figure S40. Optimized structure of isomer **1c**

Table S4 Standard orientation of isomer **1c**

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	11.5315	2.5593	0.0627
2	6	0	12.1008	1.1385	0.0324
3	6	0	12.5803	0.7708	-1.3804
4	6	0	11.1026	0.1018	0.5973
5	6	0	9.7840	-0.0892	-0.1656
6	8	0	13.2376	1.1913	0.9157
7	6	0	8.8592	-1.1171	0.5208
8	6	0	7.5387	-1.3413	-0.1928
9	6	0	7.6280	-2.1034	-1.4943
10	6	0	6.3994	-0.8735	0.3421
11	6	0	4.9904	-0.9814	-0.1808
12	6	0	4.0836	-1.7570	0.7979
13	6	0	2.5953	-1.9256	0.4007
14	6	0	2.4565	-2.6897	-0.9181
15	6	0	1.8589	-0.5580	0.3684
16	6	0	-0.3867	0.6604	0.0620
17	6	0	-1.8590	0.5581	-0.3680
18	8	0	1.9758	-0.0573	1.7096
19	6	0	-2.5953	1.9257	-0.4003

20	8	0	-1.9758	0.0573	-1.7092
21	6	0	-4.0836	1.7570	-0.7976
22	6	0	-2.4567	2.6898	0.9185
23	8	0	-1.9625	2.7470	-1.3923
24	6	0	-4.9905	0.9815	0.1809
25	6	0	-6.3994	0.8734	-0.3421
26	6	0	-7.5388	1.3414	0.1925
27	6	0	-7.6282	2.1038	1.4939
28	6	0	-8.8592	1.1171	-0.5212
29	6	0	-9.7839	0.0892	0.1653
30	6	0	-11.1025	-0.1020	-0.5977
31	6	0	-12.1007	-1.1387	-0.0327
32	6	0	-11.5313	-2.5594	-0.0630
33	6	0	-12.5802	-0.7709	1.3800
34	8	0	-13.2374	-1.1916	-0.9161
35	6	0	0.3866	-0.6603	-0.0615
36	8	0	1.9625	-2.7469	1.3928
37	1	0	10.6774	2.6639	-0.6135
38	1	0	11.2095	2.8184	1.0770
39	1	0	12.3030	3.2741	-0.2413
40	1	0	11.7663	0.8000	-2.1131
41	1	0	13.3576	1.4716	-1.7018
42	1	0	13.0067	-0.2413	-1.3966
43	1	0	11.6209	-0.8695	0.6505
44	1	0	10.8884	0.3903	1.6351
45	1	0	9.9923	-0.4098	-1.1941
46	1	0	9.2469	0.8650	-0.2390
47	1	0	13.6237	0.3007	0.9405
48	1	0	8.6669	-0.7835	1.5485
49	1	0	9.3989	-2.0739	0.6006
50	1	0	8.2378	-1.5663	-2.2329
51	1	0	8.1161	-3.0752	-1.3368
52	1	0	6.6532	-2.2916	-1.9501
53	1	0	6.4775	-0.3533	1.2995
54	1	0	4.9726	-1.4545	-1.1677
55	1	0	4.5921	0.0351	-0.3182
56	1	0	4.1184	-1.2655	1.7771
57	1	0	4.4863	-2.7675	0.9362
58	1	0	3.0752	-3.5927	-0.8875
59	1	0	1.4213	-3.0035	-1.0752

60	1	0	2.7738	-2.0847	-1.7742
61	1	0	2.3844	0.1175	-0.3245
62	1	0	0.0904	1.4441	-0.5399
63	1	0	-0.3730	0.9902	1.1086
64	1	0	-2.3845	-0.1175	0.3248
65	1	0	1.6088	0.8381	1.7347
66	1	0	-1.6089	-0.8381	-1.7343
67	1	0	-4.4863	2.7675	-0.9359
68	1	0	-4.1183	1.2656	-1.7768
69	1	0	-1.4215	3.0035	1.0757
70	1	0	-3.0754	3.5927	0.8879
71	1	0	-2.7741	2.0847	1.7746
72	1	0	-1.9276	2.2014	-2.1973
73	1	0	-4.9729	1.4545	1.1678
74	1	0	-4.5922	-0.0351	0.3185
75	1	0	-6.4774	0.3531	-1.2993
76	1	0	-6.6534	2.2921	1.9497
77	1	0	-8.1163	3.0756	1.3362
78	1	0	-8.2381	1.5669	2.2325
79	1	0	-9.3990	2.0739	-0.6010
80	1	0	-8.6668	0.7834	-1.5488
81	1	0	-9.9924	0.4099	1.1937
82	1	0	-9.2469	-0.8650	0.2389
83	1	0	-10.8882	-0.3906	-1.6354
84	1	0	-11.6209	0.8693	-0.6511
85	1	0	-10.6772	-2.6639	0.6133
86	1	0	-12.3027	-3.2743	0.2411
87	1	0	-11.2093	-2.8186	-1.0772
88	1	0	-11.7663	-0.8000	2.1127
89	1	0	-13.0067	0.2412	1.3962
90	1	0	-13.3575	-1.4717	1.7014
91	1	0	-13.6235	-0.3010	-0.9410
92	1	0	0.3729	-0.9902	-1.1081
93	1	0	-0.0904	-1.4441	0.5404
94	1	0	1.9276	-2.2012	2.1978

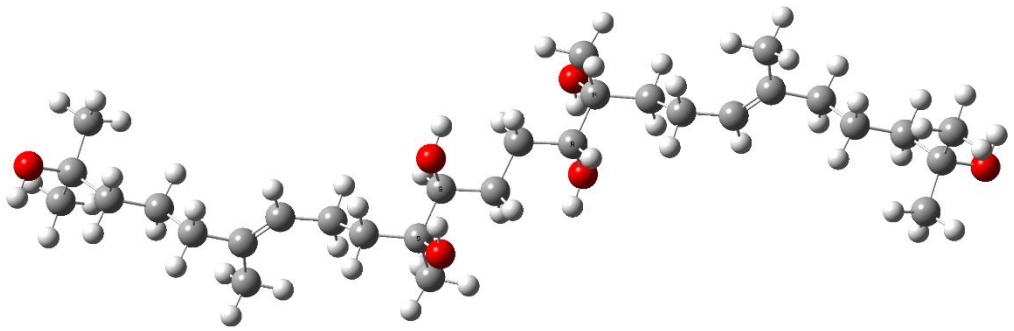


Figure S41. Optimized structure of isomer **1d**

Table S5 Standard orientation of isomer **1d**

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	-11.5313	2.5592	0.0622
2	6	0	-12.1007	1.1385	0.0316
3	6	0	-12.5799	0.7709	-1.3813
4	6	0	-11.1026	0.1017	0.5966
5	6	0	-9.7839	-0.0893	-0.1662
6	8	0	-13.2377	1.1912	0.9147
7	6	0	-8.8592	-1.1172	0.5204
8	6	0	-7.5386	-1.3414	-0.1930
9	6	0	-7.6277	-2.1036	-1.4945
10	6	0	-6.3993	-0.8737	0.3420
11	6	0	-4.9903	-0.9817	-0.1806
12	6	0	-4.0835	-1.7569	0.7985
13	6	0	-2.5952	-1.9255	0.4016
14	6	0	-2.4562	-2.6901	-0.9170
15	6	0	-1.8589	-0.5579	0.3689
16	6	0	0.3867	0.6605	0.0627
17	6	0	1.8590	0.5582	-0.3674
18	8	0	-1.9759	-0.0568	1.7100
19	6	0	2.5953	1.9258	-0.3997
20	8	0	1.9757	0.0576	-1.7086

21	6	0	4.0835	1.7573	-0.7971
22	6	0	2.4568	2.6898	0.9193
23	8	0	1.9623	2.7473	-1.3915
24	6	0	4.9906	0.9815	0.1812
25	6	0	6.3994	0.8736	-0.3420
26	6	0	7.5388	1.3416	0.1926
27	6	0	7.6282	2.1040	1.4939
28	6	0	8.8591	1.1174	-0.5213
29	6	0	9.7838	0.0892	0.1649
30	6	0	11.1023	-0.1020	-0.5982
31	6	0	12.1004	-1.1390	-0.0336
32	6	0	11.5307	-2.5596	-0.0642
33	6	0	12.5801	-0.7717	1.3792
34	8	0	13.2371	-1.1919	-0.9170
35	6	0	-0.3866	-0.6602	-0.0608
36	8	0	-1.9625	-2.7465	1.3940
37	1	0	-10.6771	2.6639	-0.6139
38	1	0	-11.2095	2.8182	1.0765
39	1	0	-12.3028	3.2740	-0.2418
40	1	0	-11.7657	0.8001	-2.1138
41	1	0	-13.3571	1.4717	-1.7028
42	1	0	-13.0063	-0.2412	-1.3977
43	1	0	-11.6210	-0.8697	0.6496
44	1	0	-10.8886	0.3901	1.6344
45	1	0	-9.9920	-0.4099	-1.1947
46	1	0	-9.2468	0.8649	-0.2394
47	1	0	-13.6238	0.3006	0.9392
48	1	0	-8.6671	-0.7836	1.5481
49	1	0	-9.3989	-2.0740	0.6001
50	1	0	-8.2376	-1.5667	-2.2331
51	1	0	-8.1157	-3.0755	-1.3371
52	1	0	-6.6528	-2.2916	-1.9503
53	1	0	-6.4776	-0.3535	1.2994
54	1	0	-4.9723	-1.4551	-1.1673
55	1	0	-4.5921	0.0348	-0.3183
56	1	0	-4.1185	-1.2651	1.7775
57	1	0	-4.4862	-2.7673	0.9370
58	1	0	-3.0748	-3.5931	-0.8861
59	1	0	-1.4209	-3.0038	-1.0738
60	1	0	-2.7734	-2.0854	-1.7733

61	1	0	-2.3844	0.1174	-0.3242
62	1	0	-0.0904	1.4442	-0.5393
63	1	0	0.3731	0.9904	1.1092
64	1	0	2.3846	-0.1174	0.3253
65	1	0	-1.6090	0.8386	1.7349
66	1	0	1.6090	-0.8379	-1.7338
67	1	0	4.4862	2.7678	-0.9353
68	1	0	4.1182	1.2660	-1.7764
69	1	0	1.4216	3.0036	1.0766
70	1	0	3.0755	3.5927	0.8888
71	1	0	2.7741	2.0845	1.7753
72	1	0	1.9275	2.2018	-2.1966
73	1	0	4.9730	1.4544	1.1682
74	1	0	4.5922	-0.0350	0.3186
75	1	0	6.4773	0.3532	-1.2992
76	1	0	6.6536	2.2920	1.9500
77	1	0	8.1160	3.0760	1.3360
78	1	0	8.2386	1.5674	2.2323
79	1	0	9.3990	2.0741	-0.6009
80	1	0	8.6667	0.7839	-1.5489
81	1	0	9.9923	0.4096	1.1934
82	1	0	9.2466	-0.8650	0.2382
83	1	0	10.8880	-0.3902	-1.6360
84	1	0	11.6208	0.8693	-0.6513
85	1	0	10.6767	-2.6642	0.6122
86	1	0	12.3021	-3.2747	0.2396
87	1	0	11.2086	-2.8185	-1.0784
88	1	0	11.7662	-0.8007	2.1119
89	1	0	13.0068	0.2403	1.3956
90	1	0	13.3573	-1.4727	1.7004
91	1	0	13.6232	-0.3013	-0.9418
92	1	0	-0.3727	-0.9903	-1.1074
93	1	0	0.0905	-1.4439	0.5413
94	1	0	-1.9277	-2.2005	2.1988

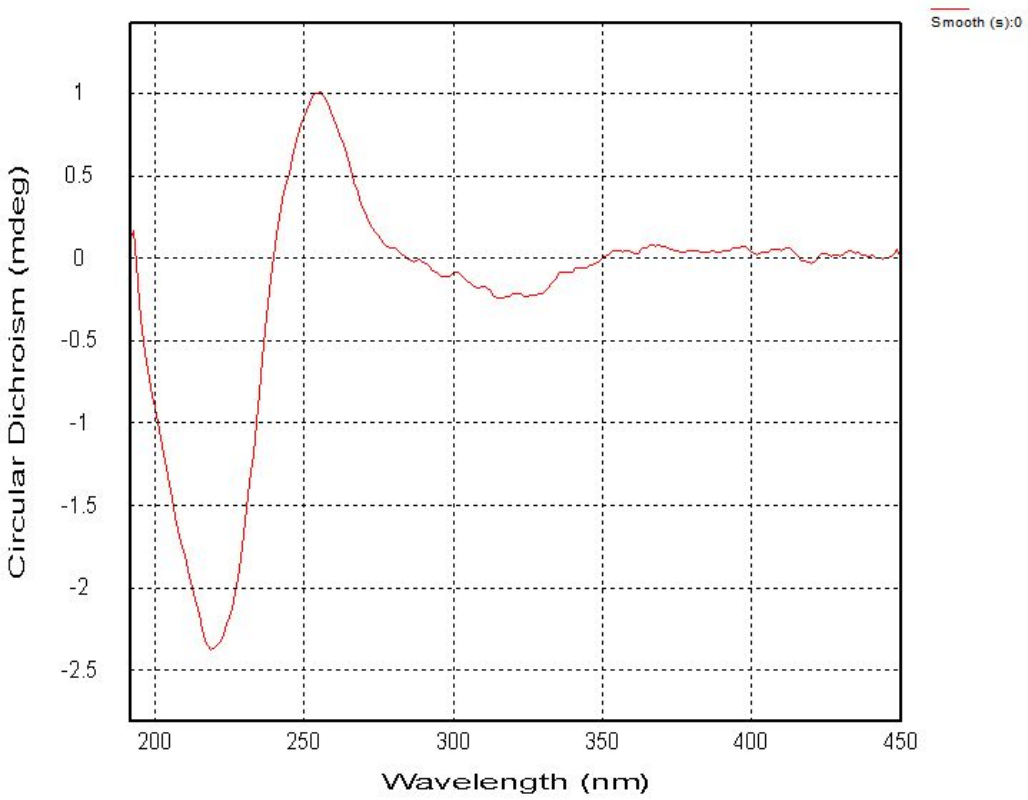


Figure S42. CD spectrum of compound **3**

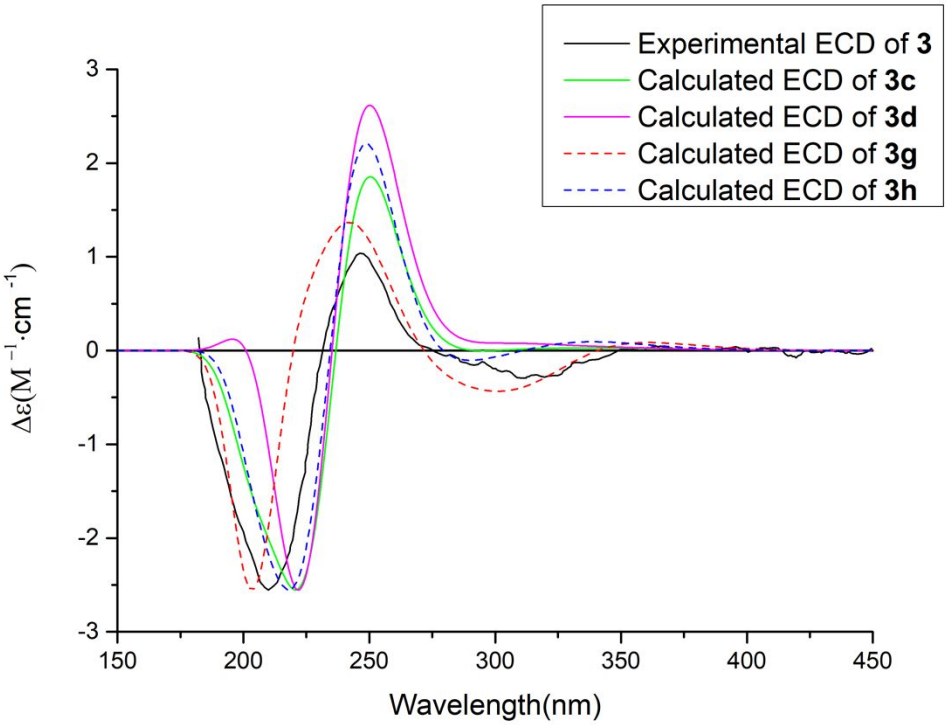
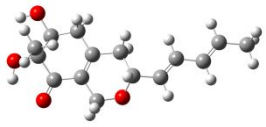
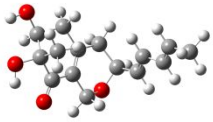
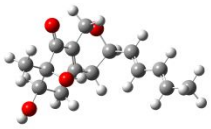
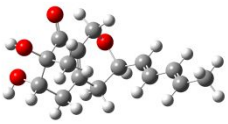
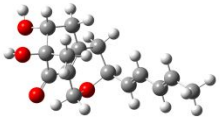
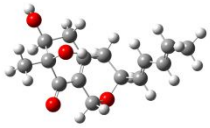
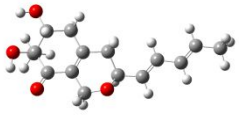
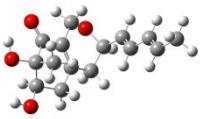


Figure S43. Experimental and some of calculated ECD spectra of compound **3**

Table S6 Energies of dominative conformers **of** isomers **3a-3h**

Compound	Structure	B3LYP/6-31G(d)	
		Energy(A.U.)	Energy(kcal/mol)
3a		-884.47801445	-555018.26816071
3b		-884.47631297	-555017.20046602
3c		-884.46017827	-555007.07579010
3d		-884.46532927	-555010.30809102
3e		-884.46532933	-555010.30812867

3f		-884.46017808	-555007.07567087
3g		-884.47801447	-555018.26817326
3h		-884.47631294	-555017.20044719

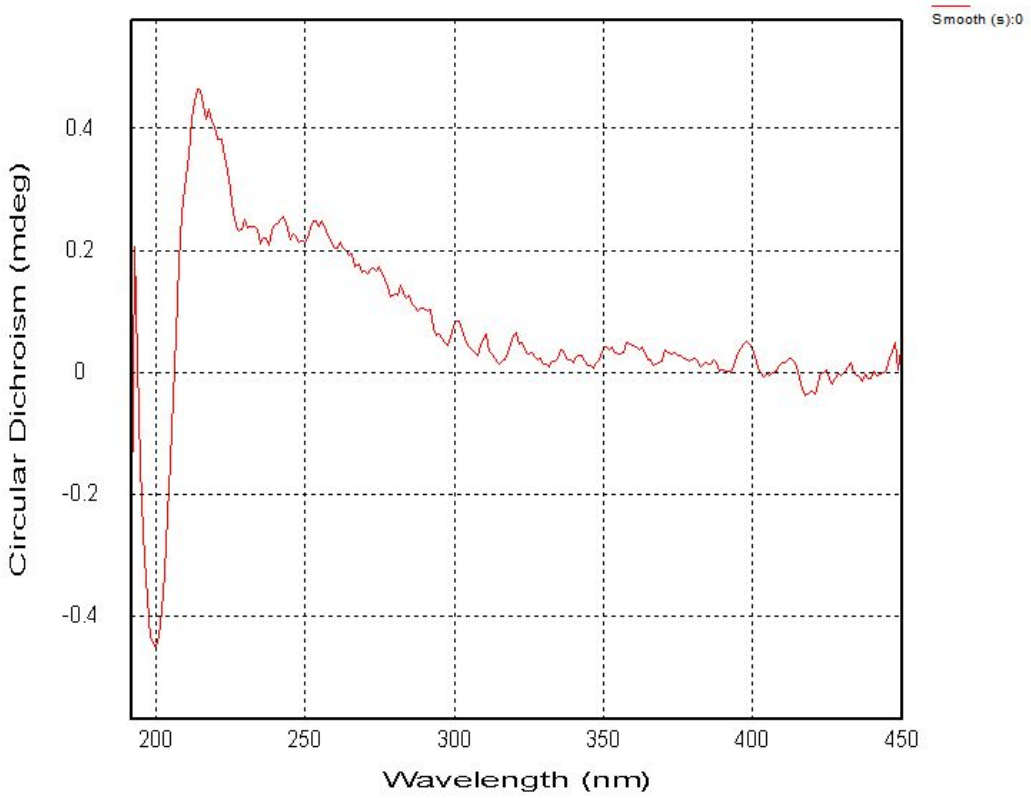
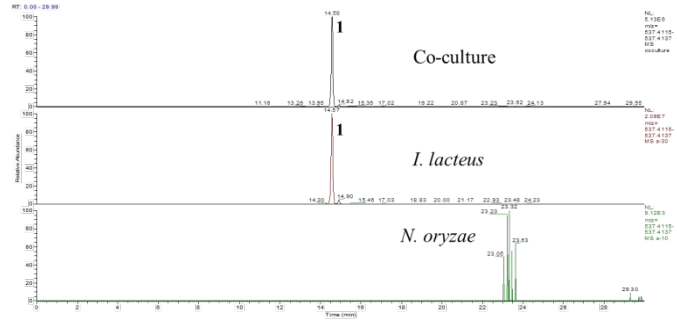
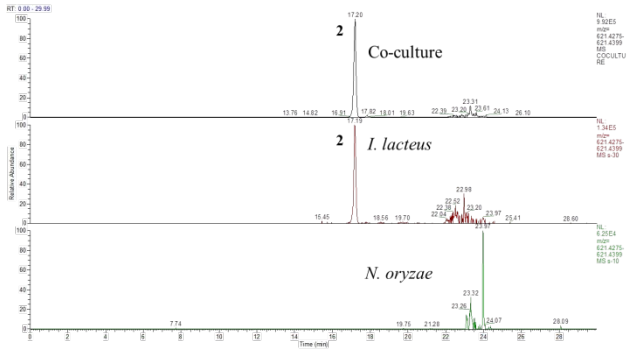
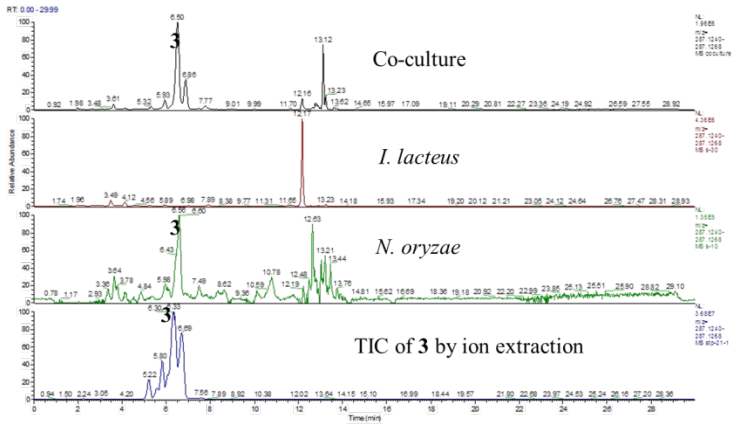
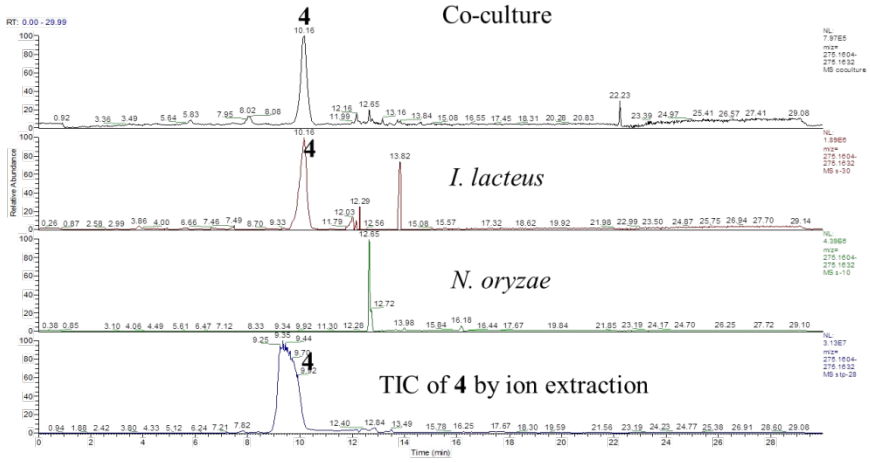


Figure S44. Experimental electronic circular dichroism (ECD) of **5**


Co-culture
I. lacteus
N. oryzae


Co-culture
I. lacteus
N. oryzae


Co-culture
I. lacteus
N. oryzae
TIC of 3 by ion extraction


Co-culture
I. lacteus
N. oryzae
TIC of 4 by ion extraction

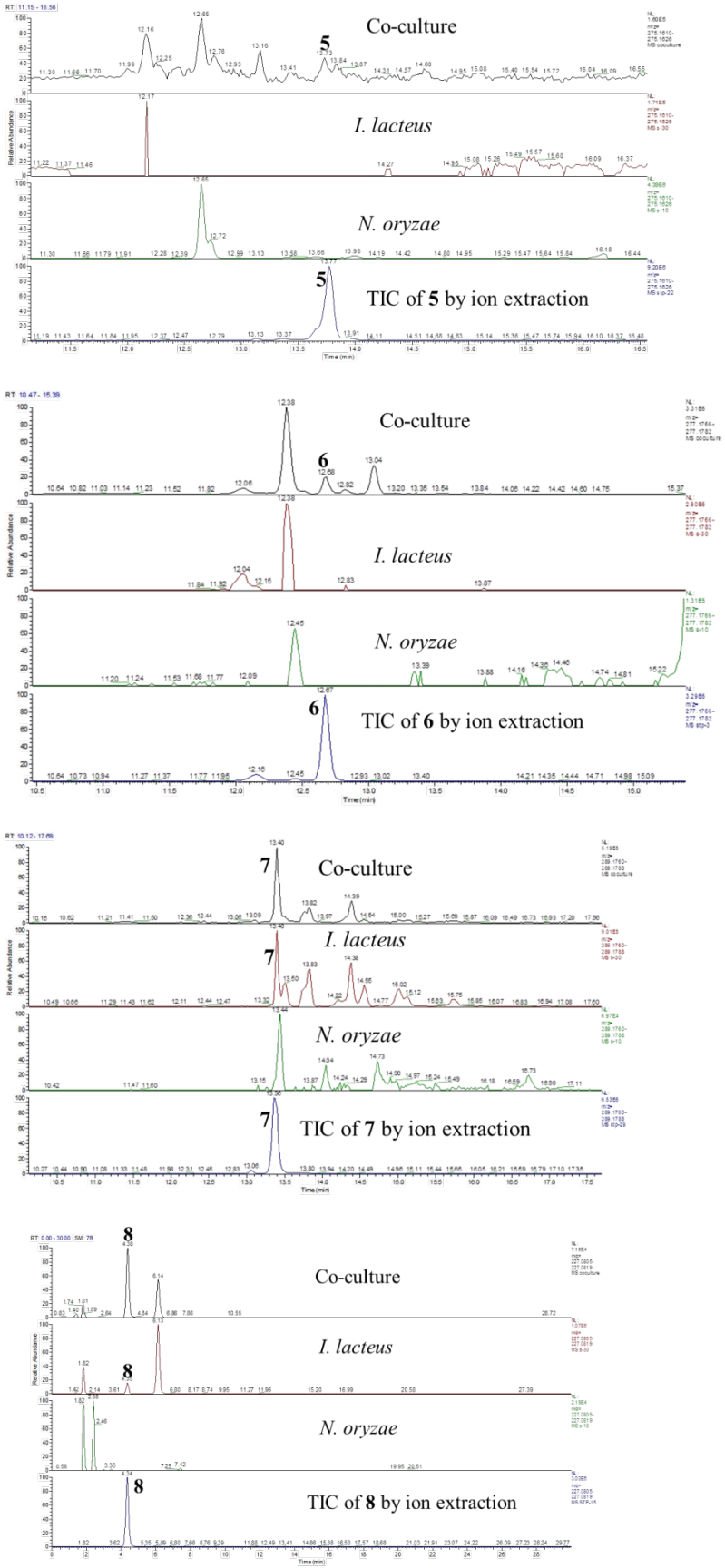


Figure S45. LC-HRMS finger-prints by ion extraction of co-culture, *Irpex lacteus*, and *Nigrospora oryzae* fermentation products and metabolites (**3**-**8**).

Leaves of *C. cerasoides* infected by *N.oryzae*

1st day (blank) | 4st day (blank) | 4st day + **6** (100 μg/mL) | 4st day + **8** (100 μg/mL) | 4st day + nystatin (100 μg/mL)

Figure S46. The in vivo antifungal activities of **6**, and **8** against leaves of *Cerasus cerasoides* infected by *Nigrospora oryzae*.

1st day 3st day 6st day

Figure S47. The phytotoxicity of nigbeauvin A against leaves of host *Dendrobium officinale* (blank (①), sample 1(②) sample 2(③) from left to the right).

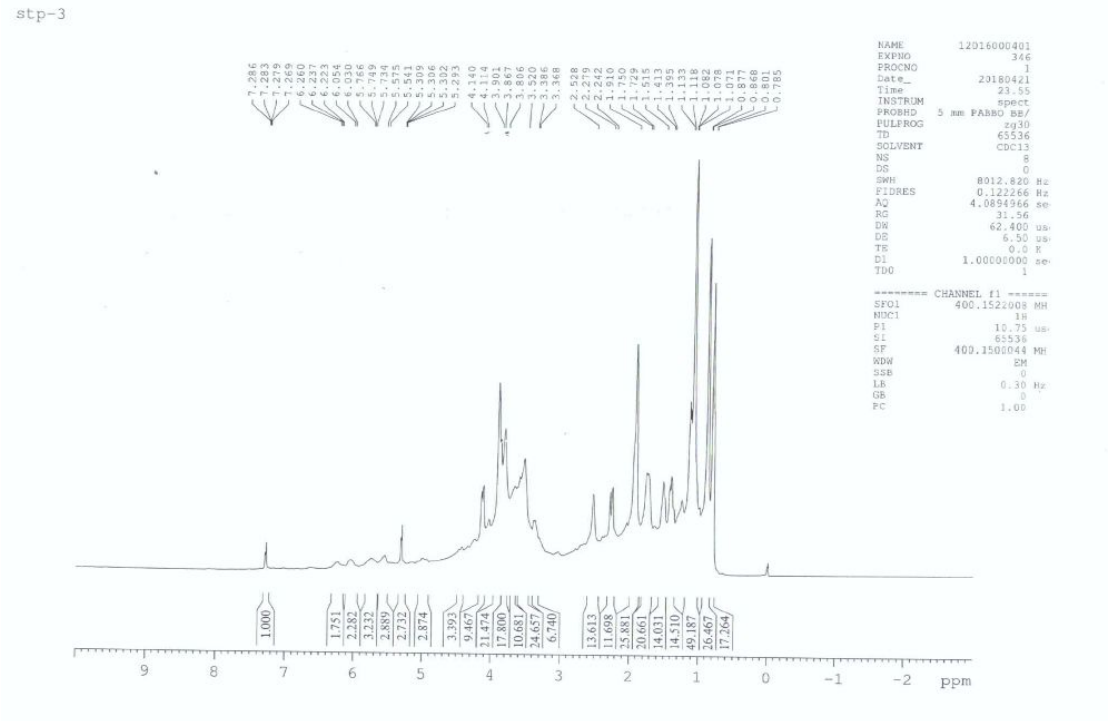


Figure S48. ^{1}H NMR spectrum of compound **6** in $CDCl_3$ (400MHz)

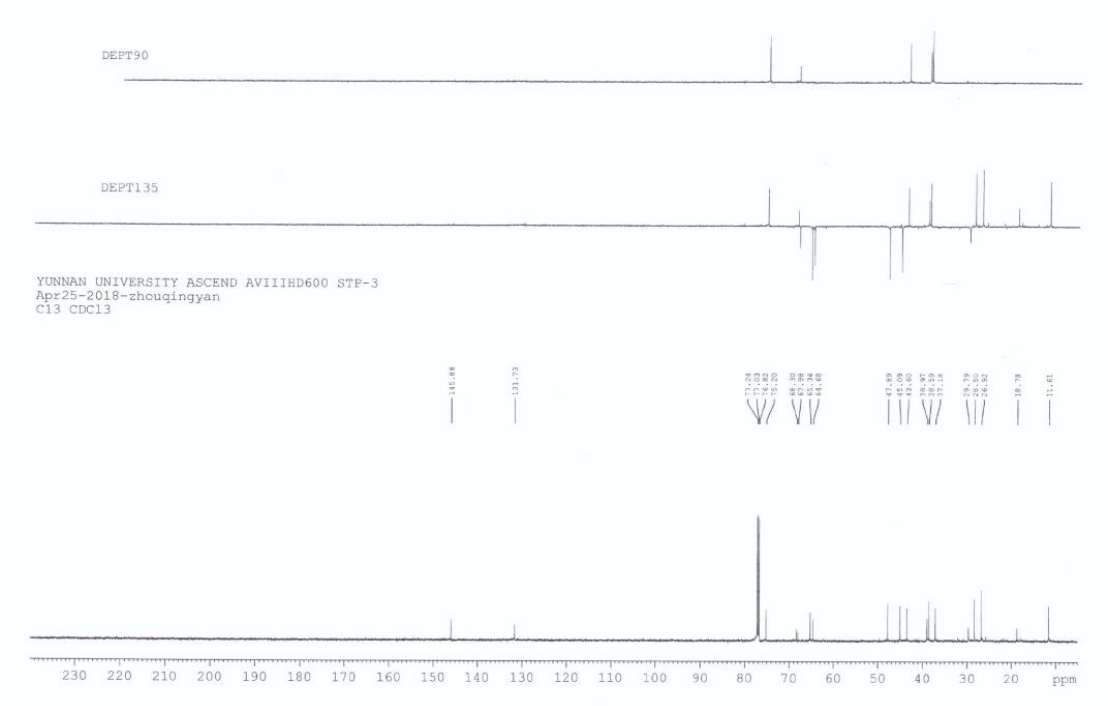


Figure S49. ^{13}C NMR spectrum of compound **6** in $CDCl_3$ (150MHz)

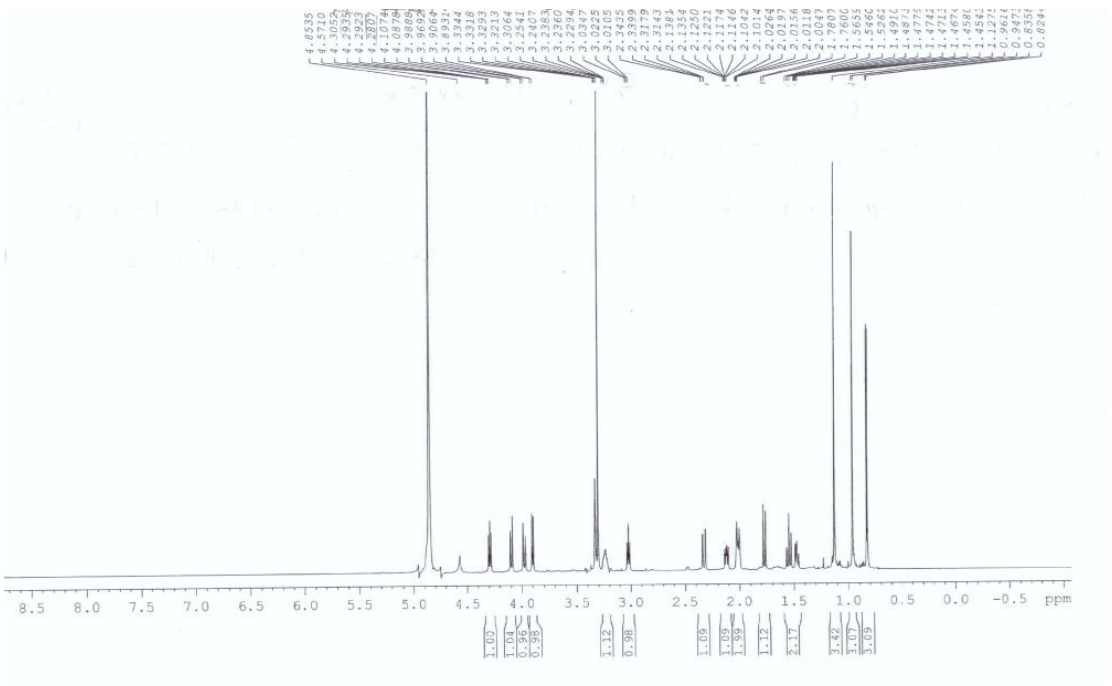


Figure S50. ^{1}H NMR spectrum of compound **7** in MeOD (600MHz)

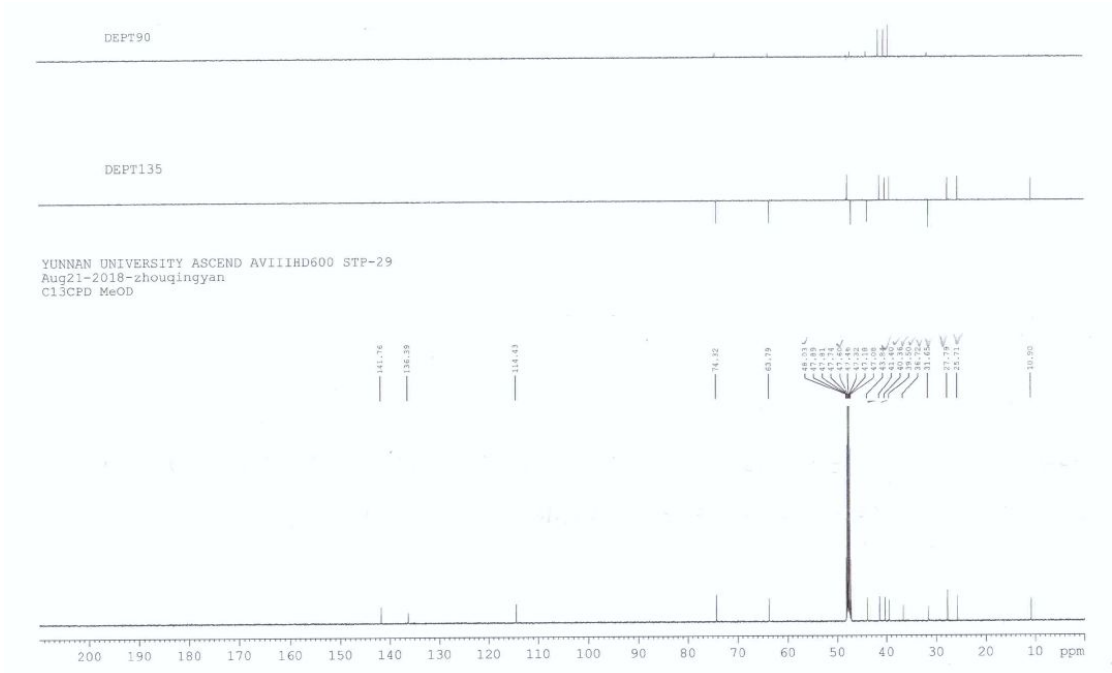


Figure S51. ^{13}C NMR spectrum of compound **7** in MeOD (150MHz)

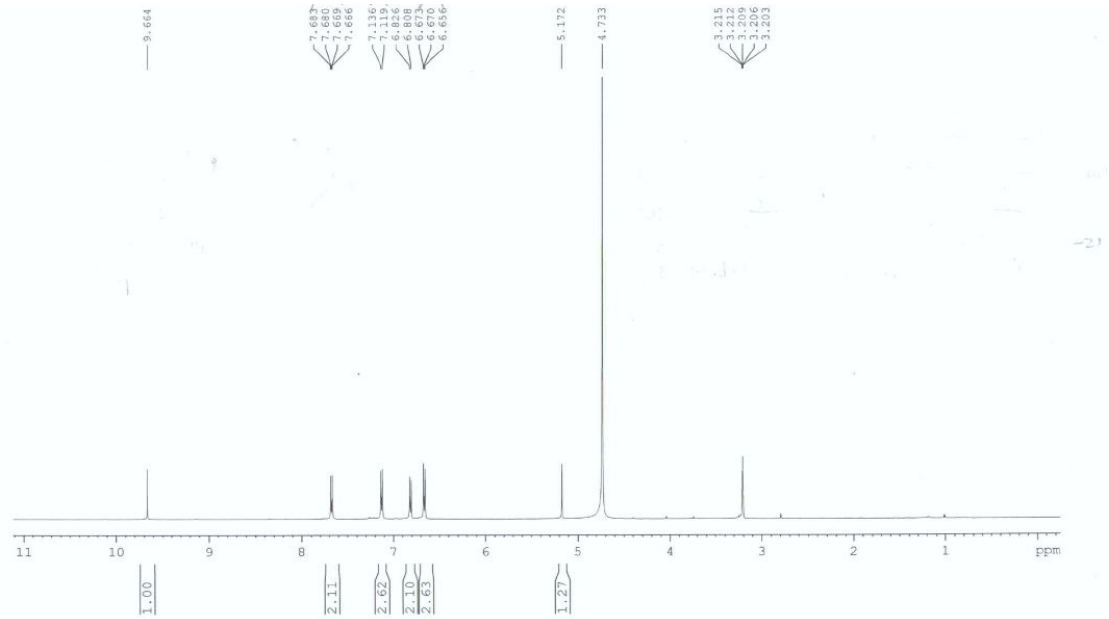


Figure S52. ^{1}H NMR spectrum of compound **8** in MeOD (500MHz)

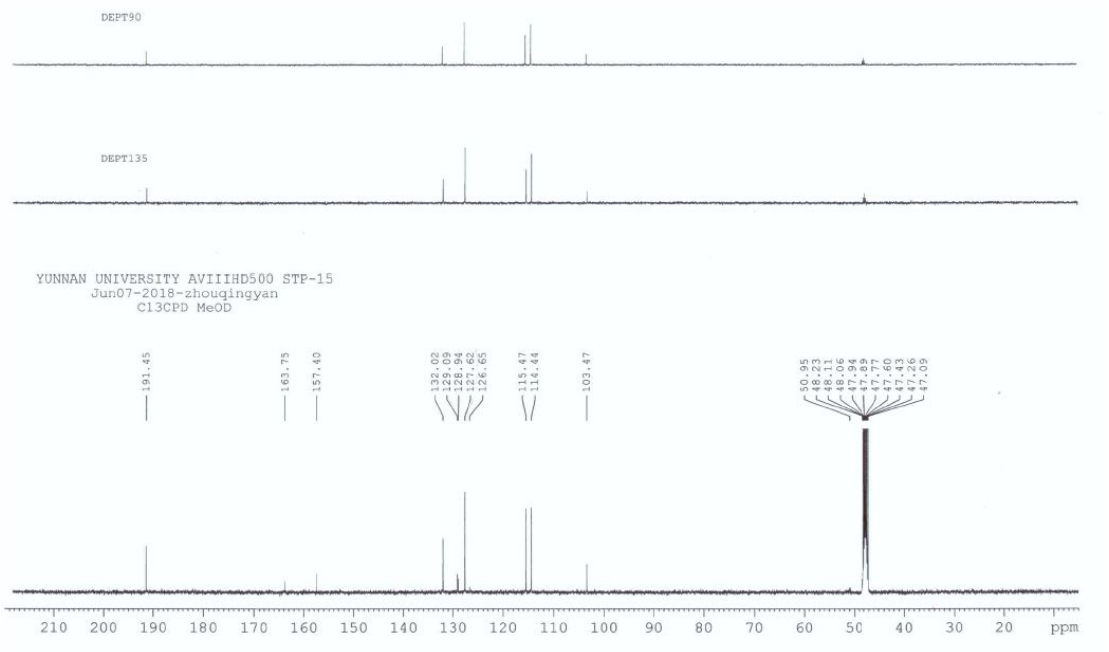


Figure S53. ^{13}C NMR spectrum of compound **8** in MeOD (125MHz)

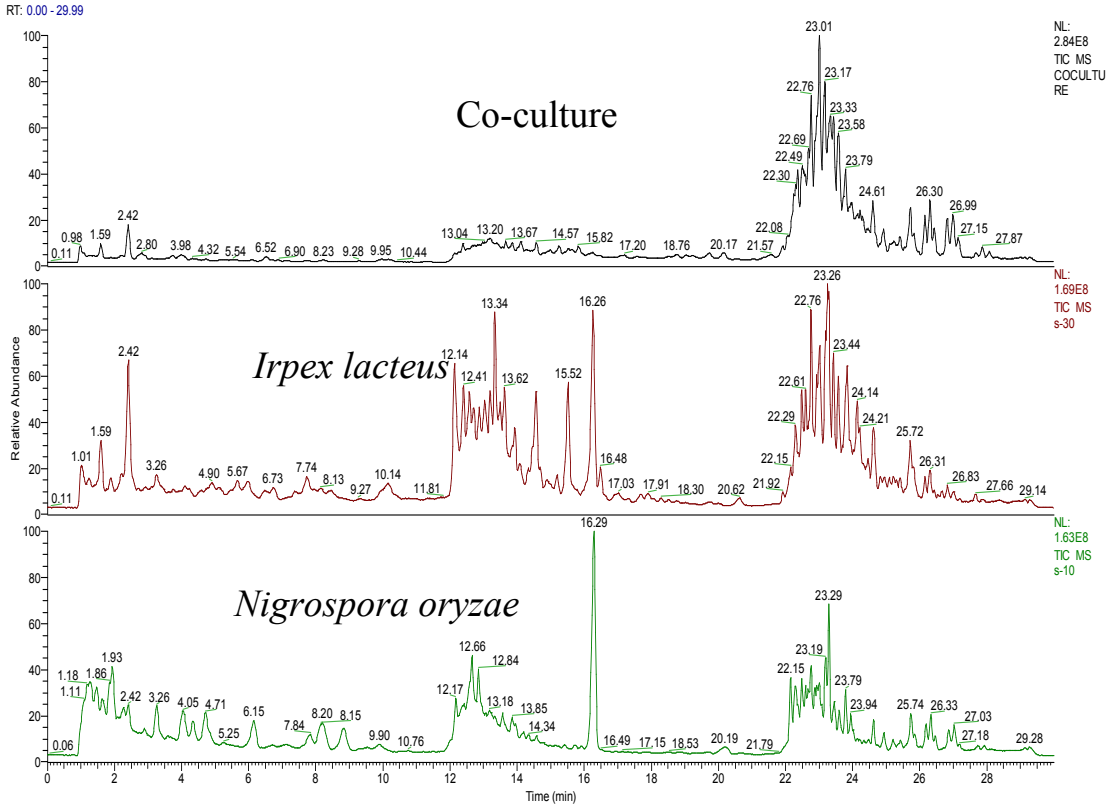


Figure S54. LC-HRMS finger-prints of co-culture, *Irpex lacteus*, and *Nigrospora oryzae* fermentation products