Curdepsidones B-G, Six Depsidones with Anti-inflammatory Activities from the Marine-Derived Fungus *Curvularia* sp. IFB-Z10

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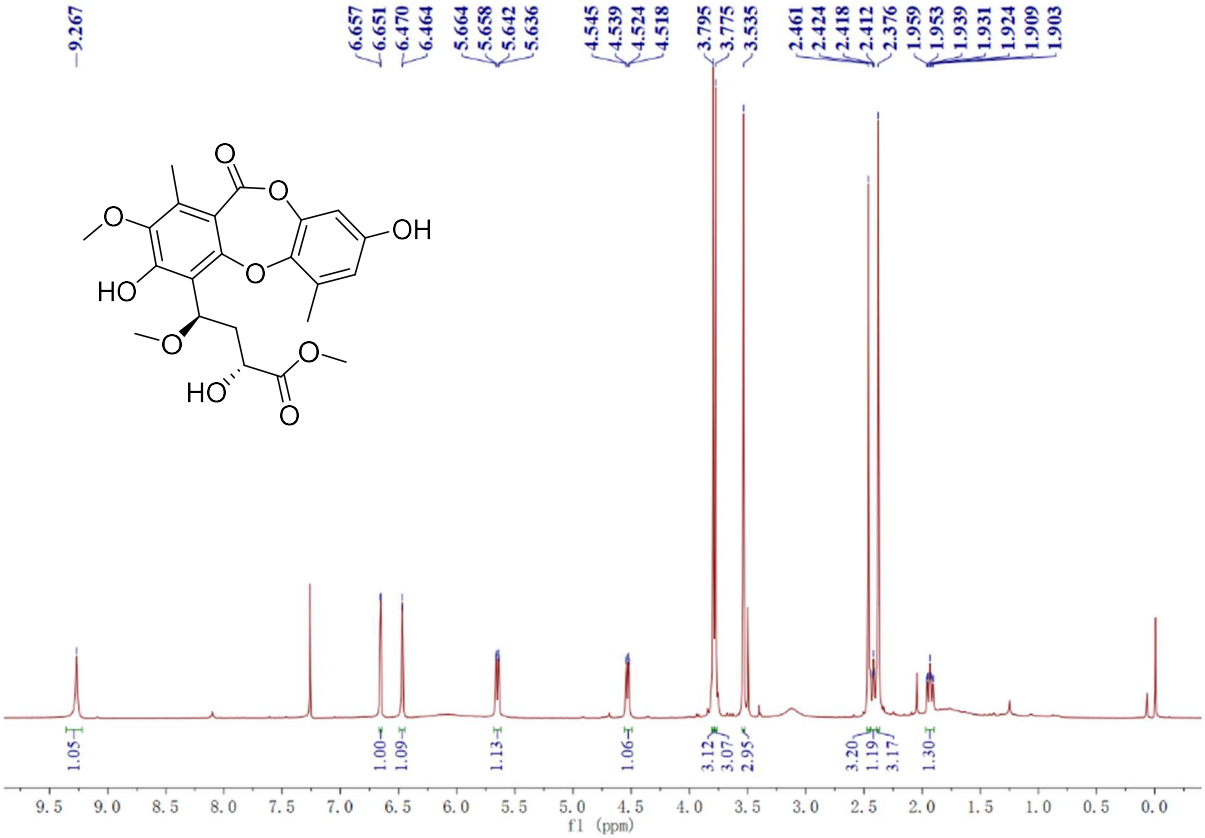
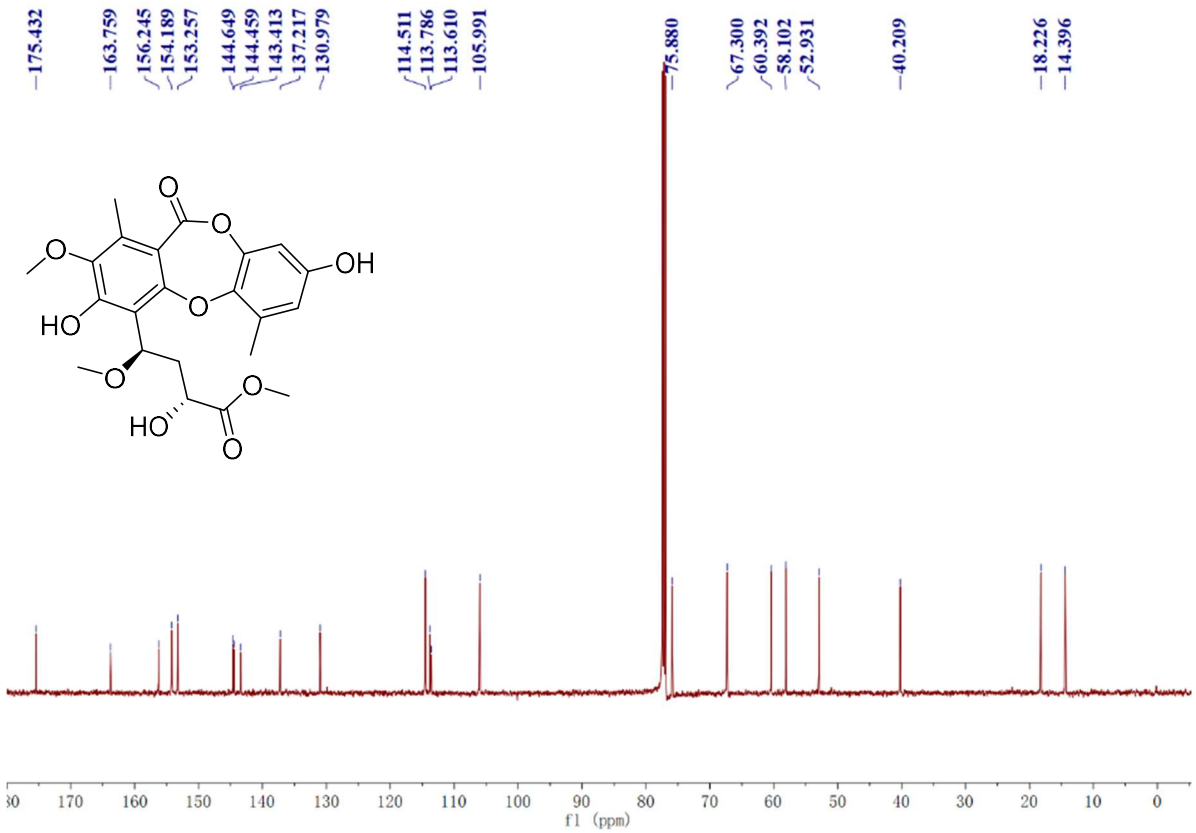


Figure S1. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **1**.



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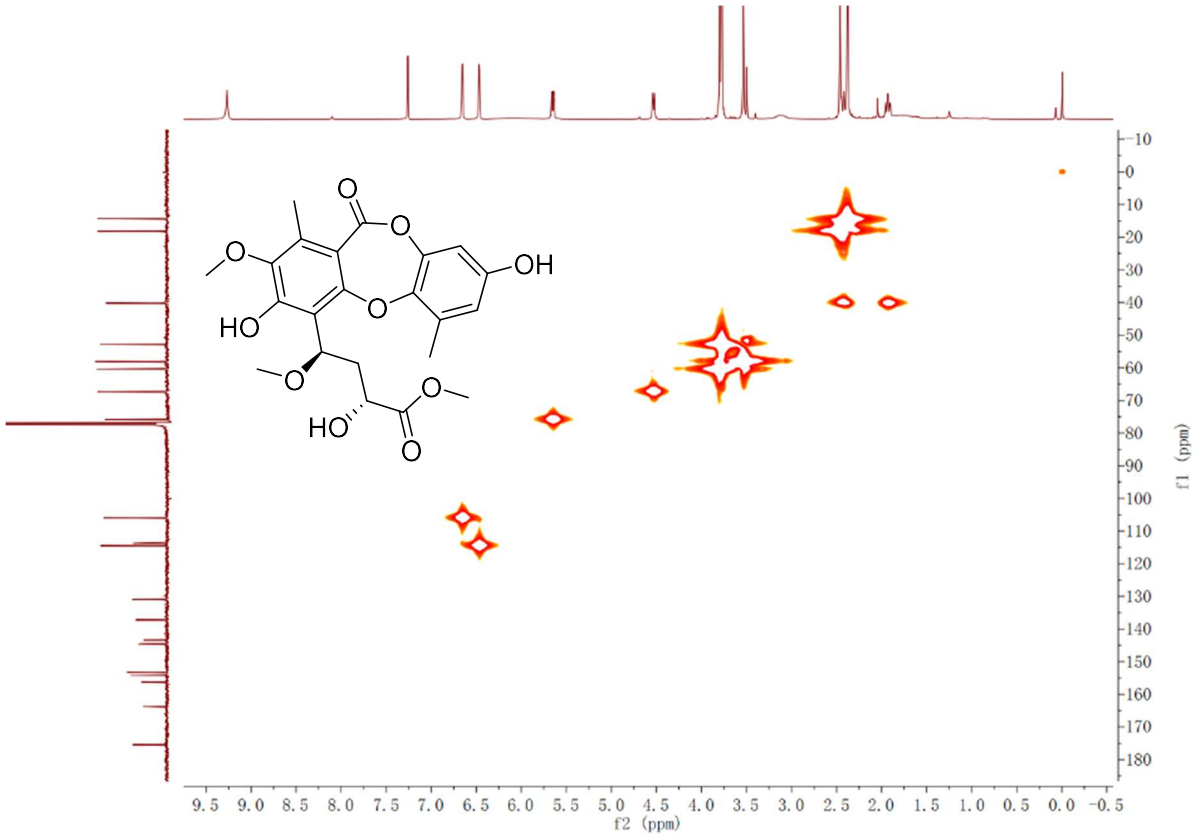

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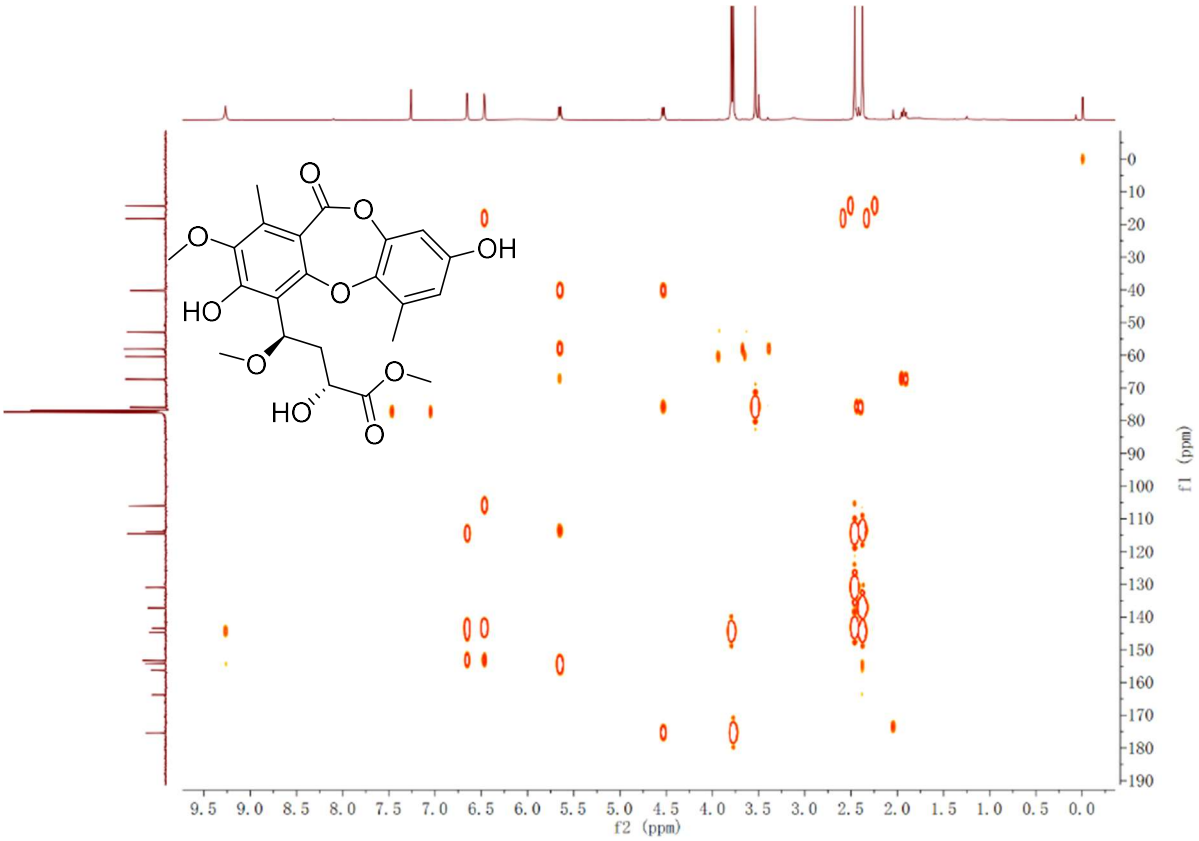
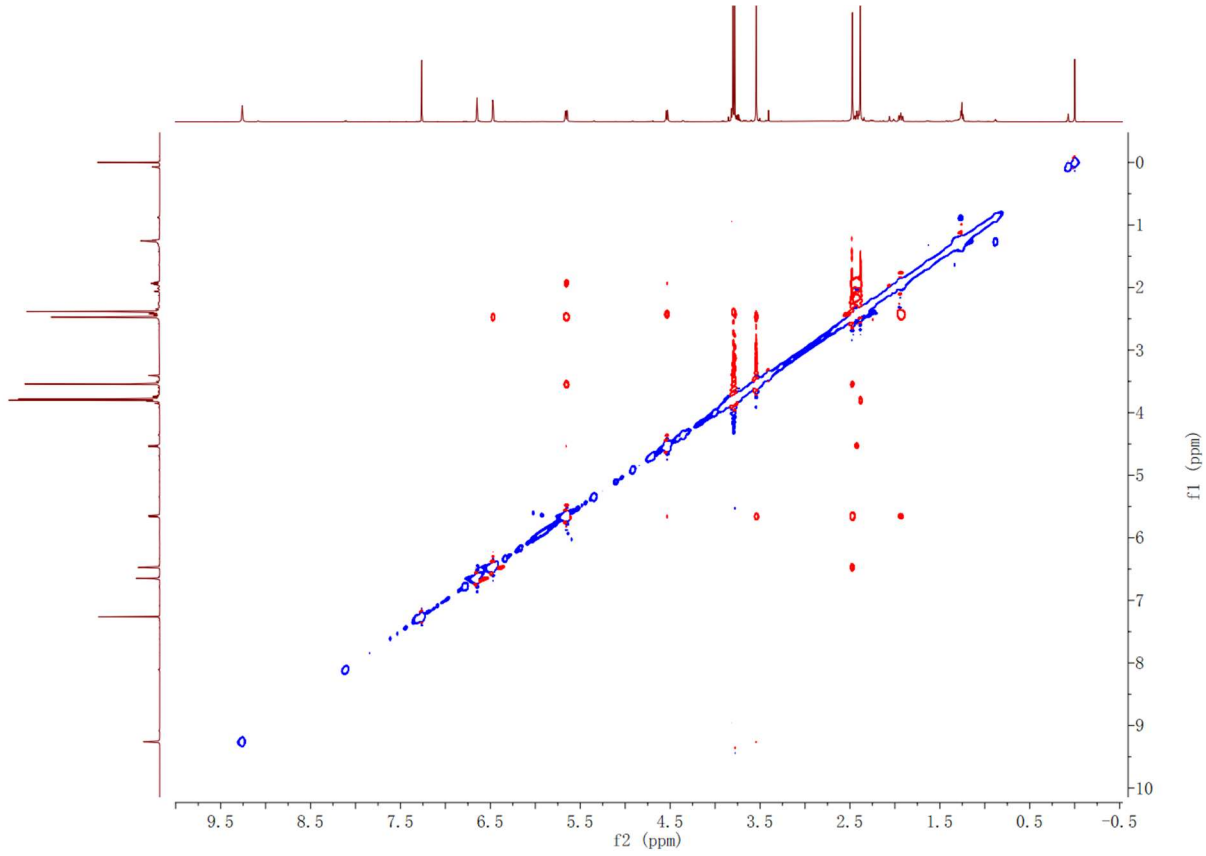


Figure S4. HMBC spectra ($CDCl_3$) of **1**.



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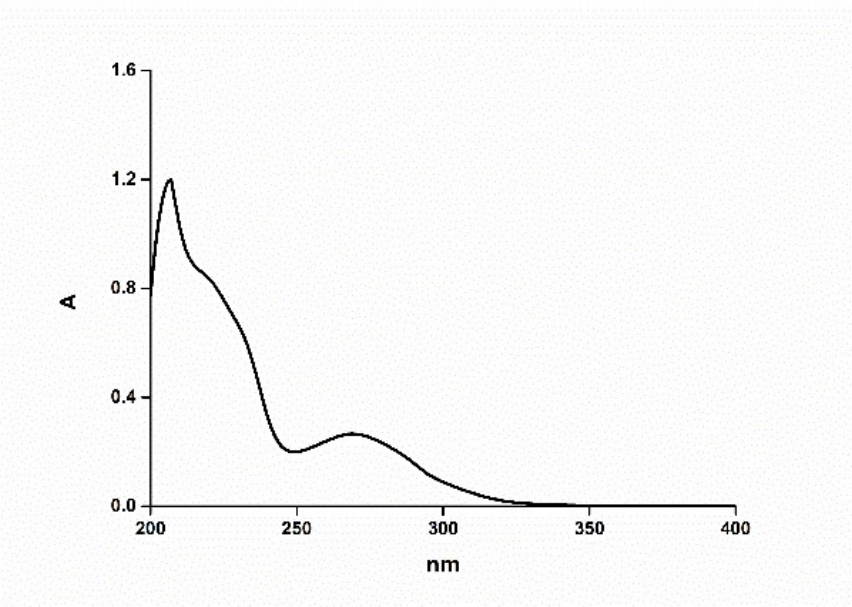


Figure S6. UV spectra (MeOH) of **1**.

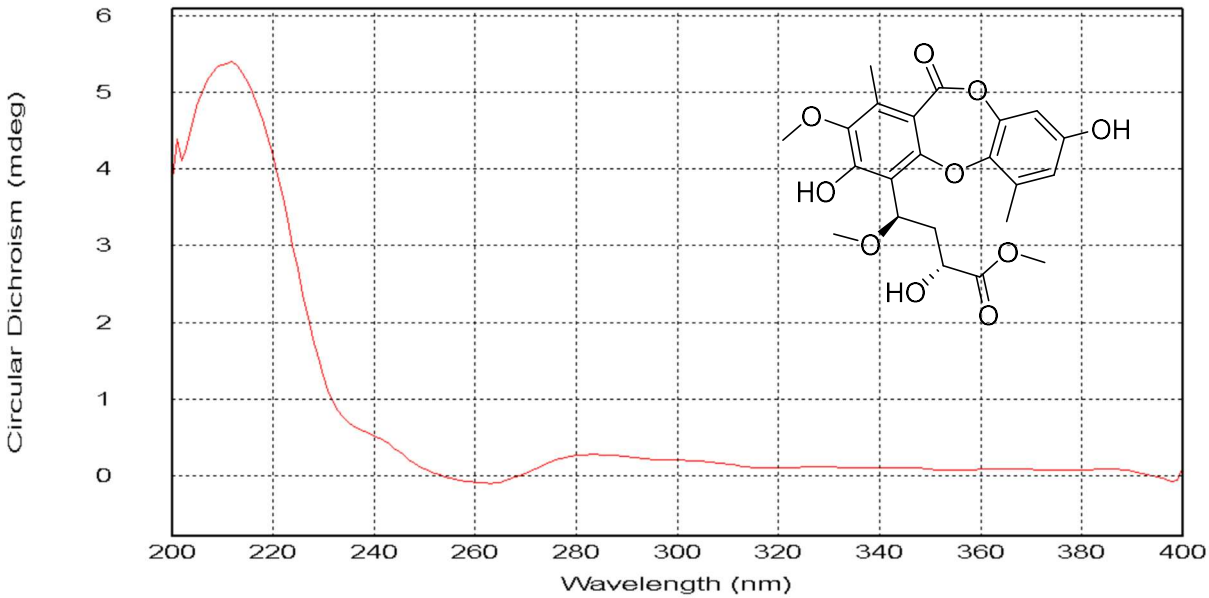


Figure S7. ECD spectra (MeOH) of **1**.

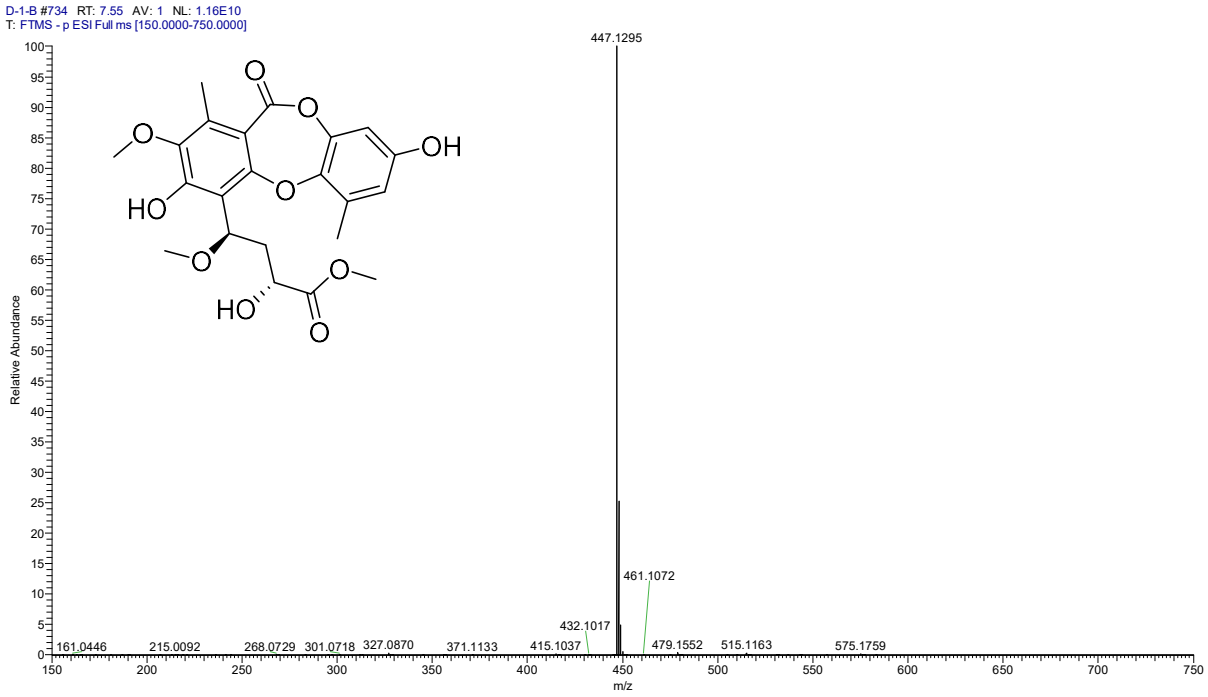


Figure S8. HRESIMS spectra of **1**.

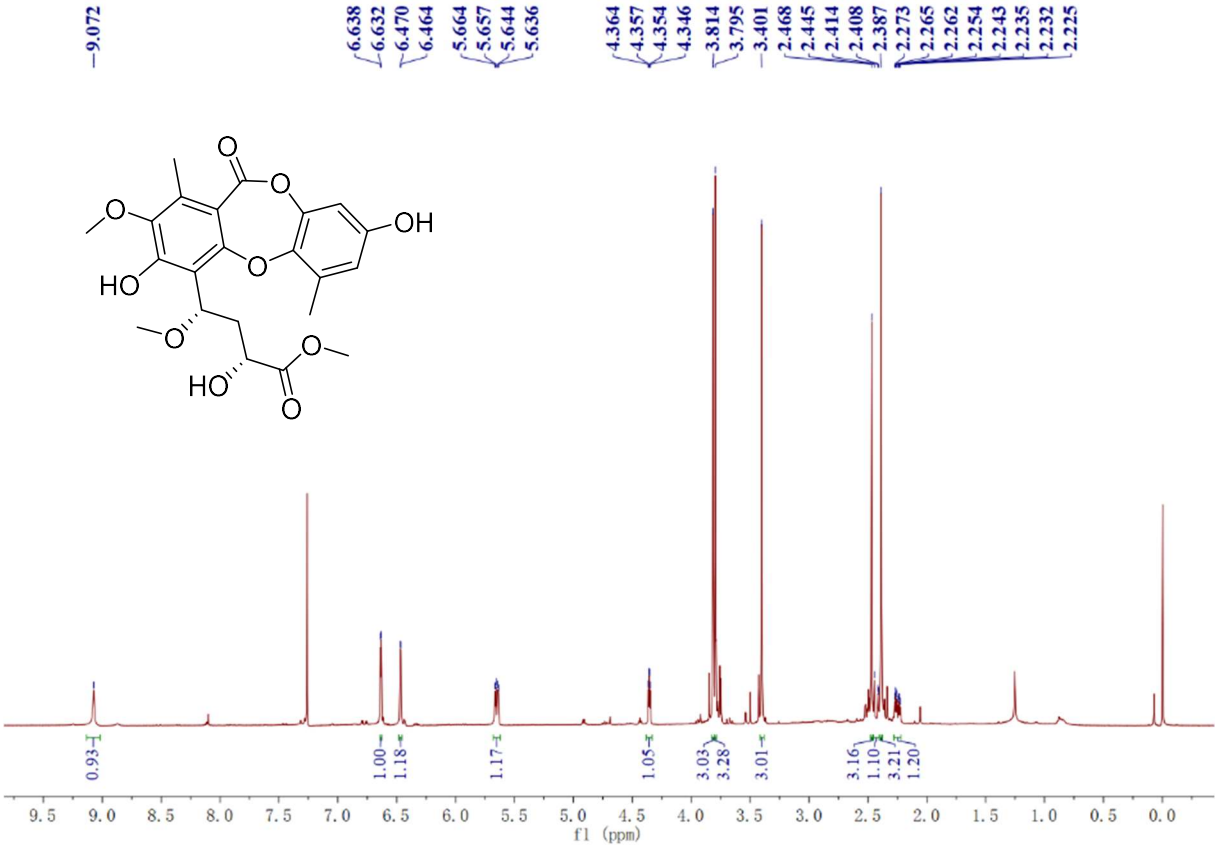


Figure S9. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **2**.

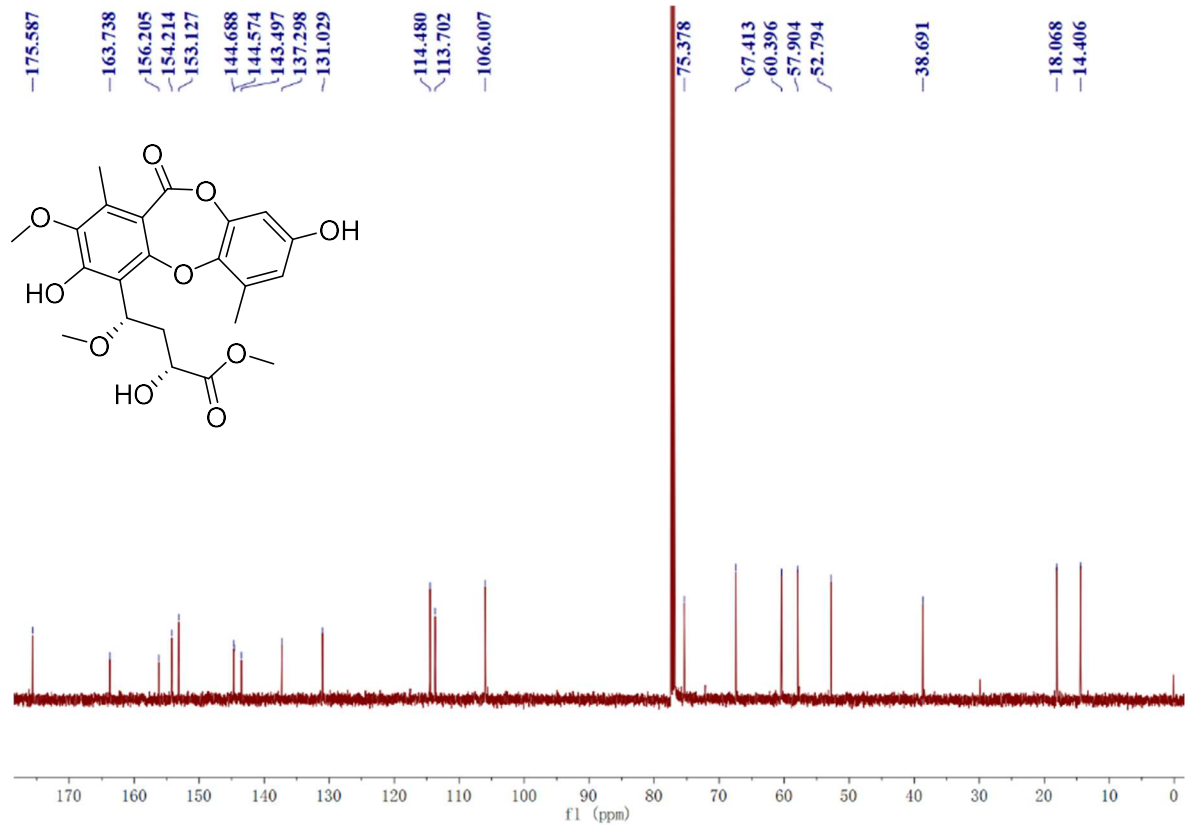


Figure S10. ^{13}C NMR spectra (125 MHz, $CDCl_3$) of **2**.

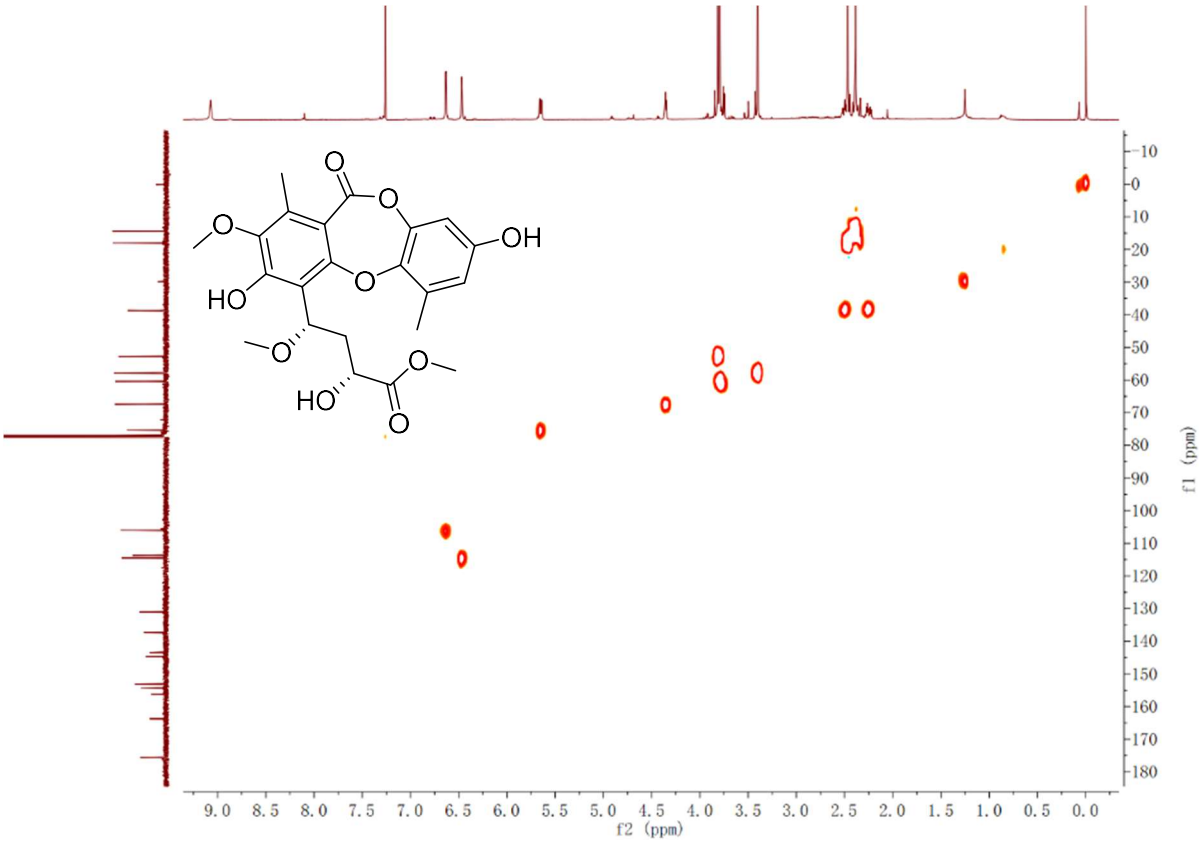


Figure S11. HMQC spectra ($CDCl_3$) of **2**.

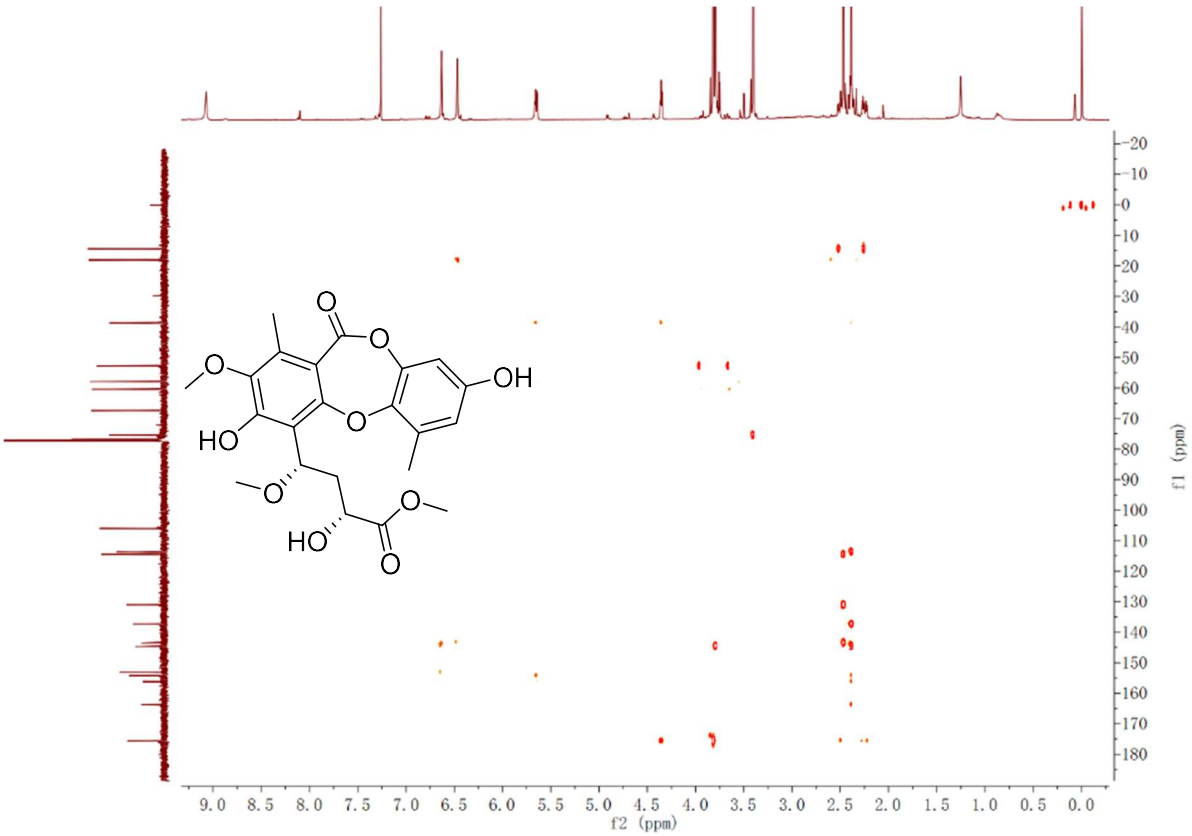


Figure S12. HMBC spectra ($CDCl_3$) of **2**.

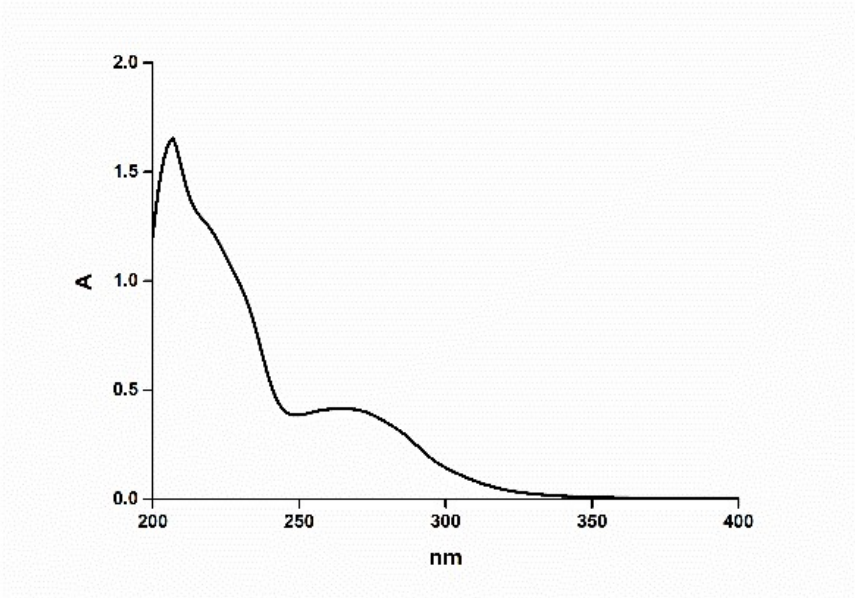


Figure S13. UV spectra (MeOH) of **2**.

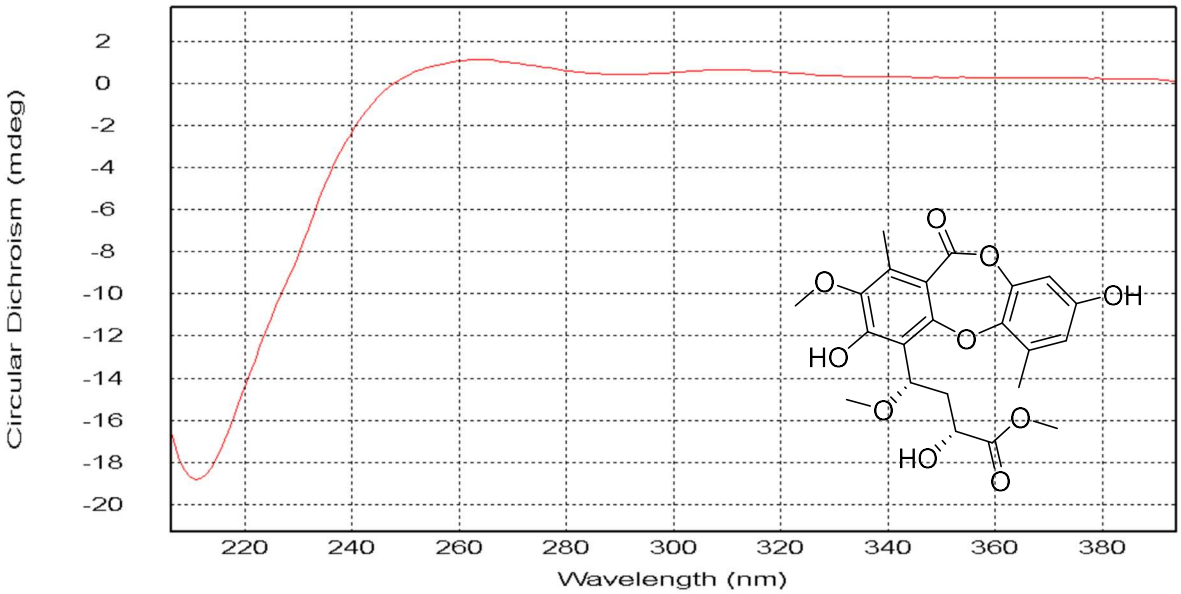


Figure S14. ECD spectra (MeOH) of **2**.

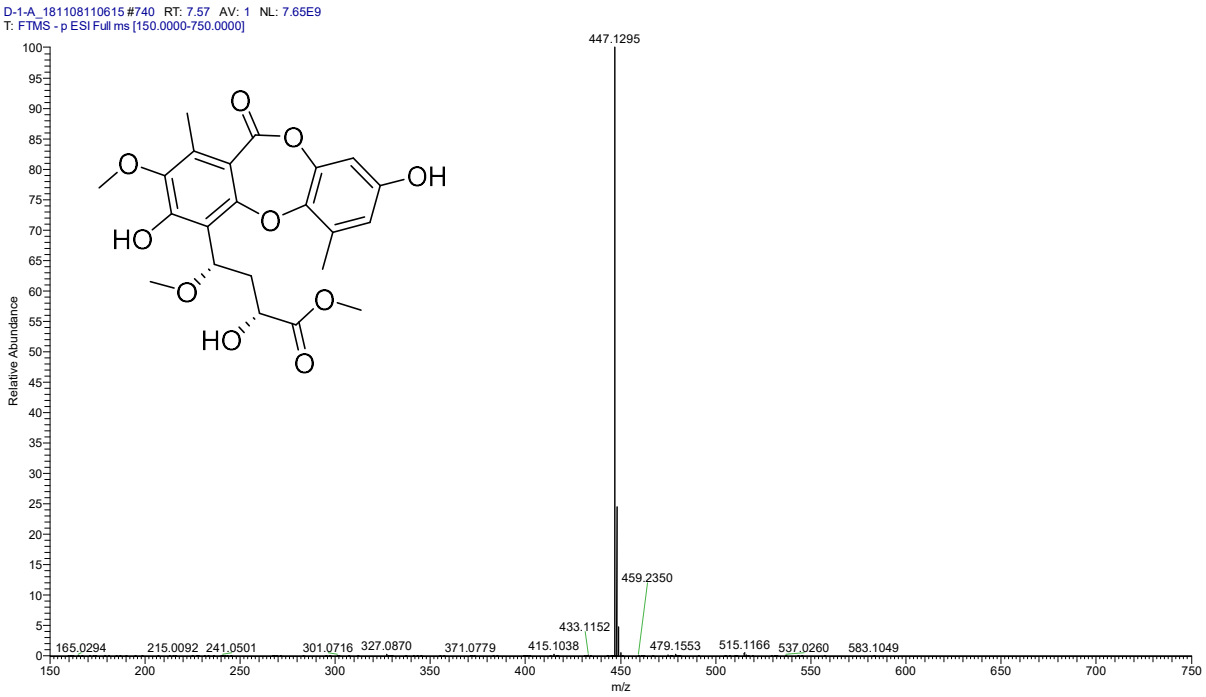


Figure S15. HRESIMS spectra of **2**.

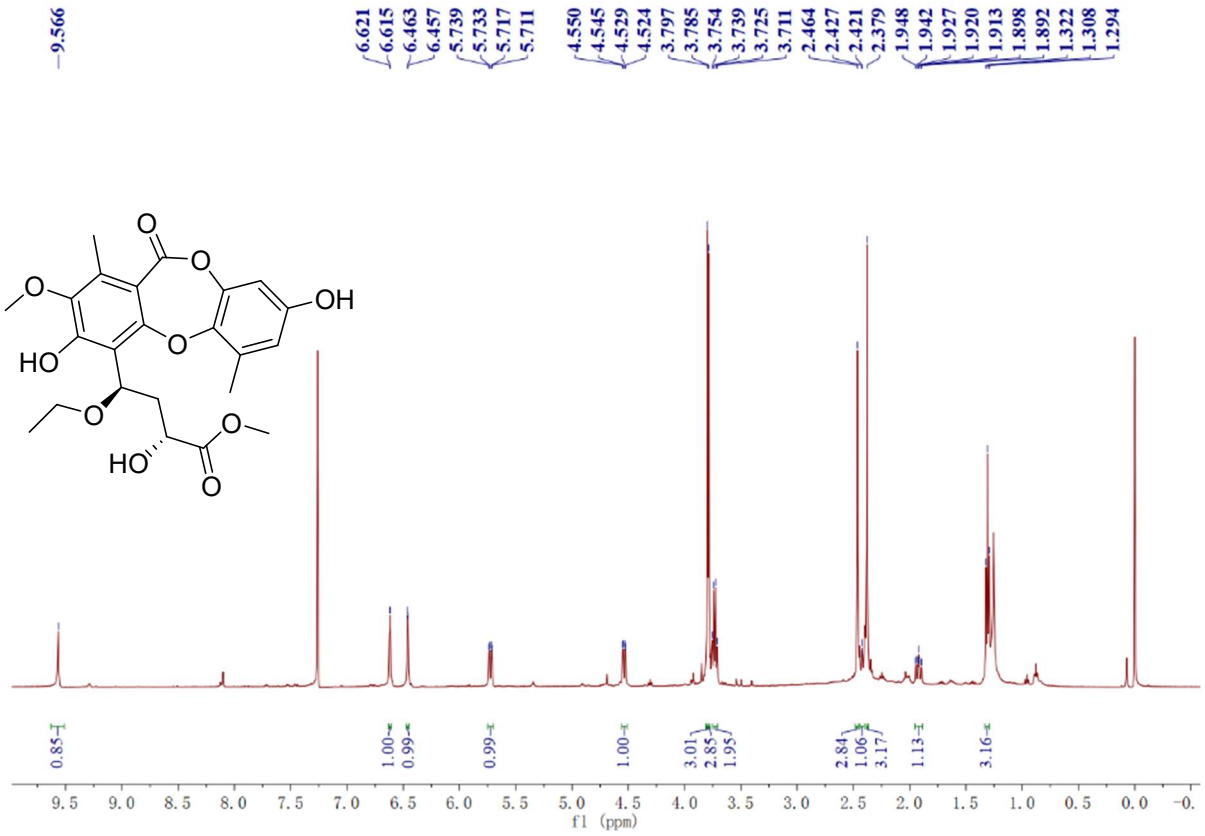


Figure S16. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **3**.

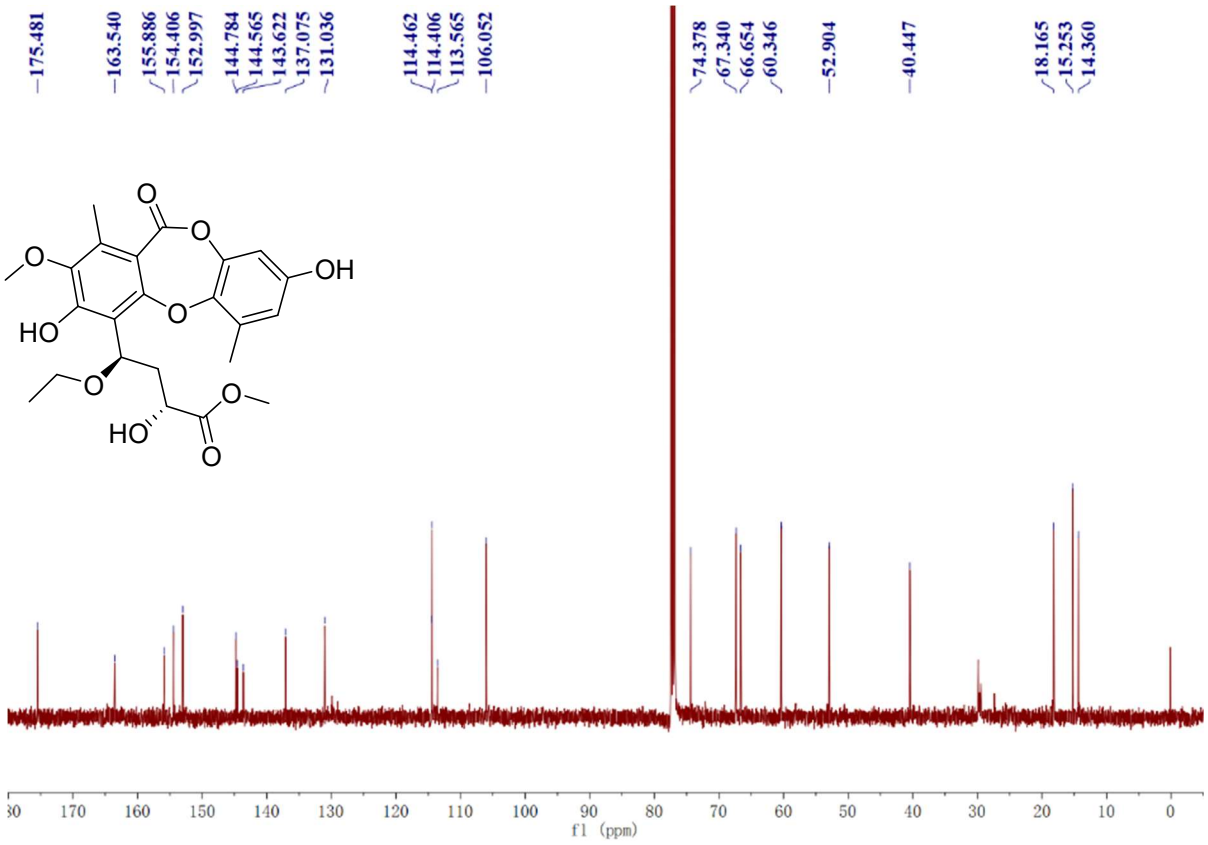


Figure S17. ^{13}C NMR spectra (125 MHz, $CDCl_3$) of **3**.

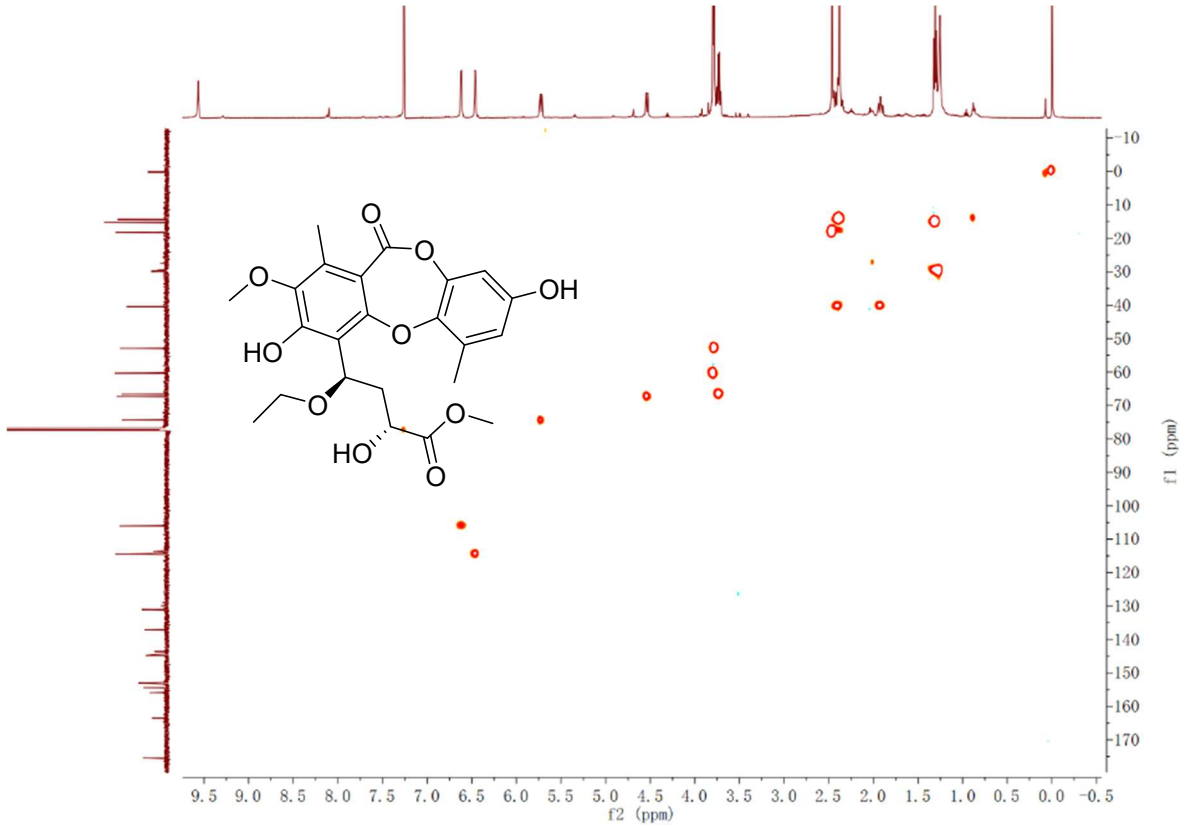


Figure S18. HSQC spectra ($CDCl_3$) of **3**.

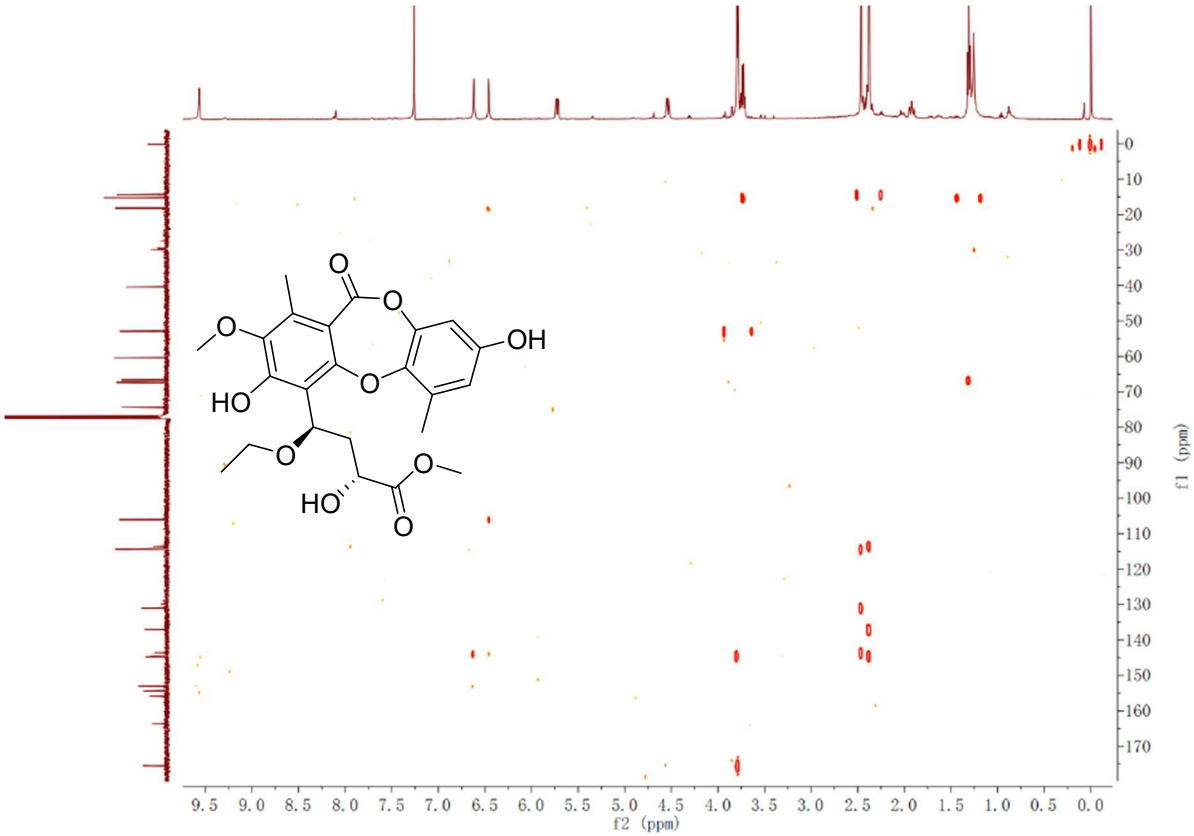


Figure S19. HMBC spectra ($CDCl_3$) of **3**.

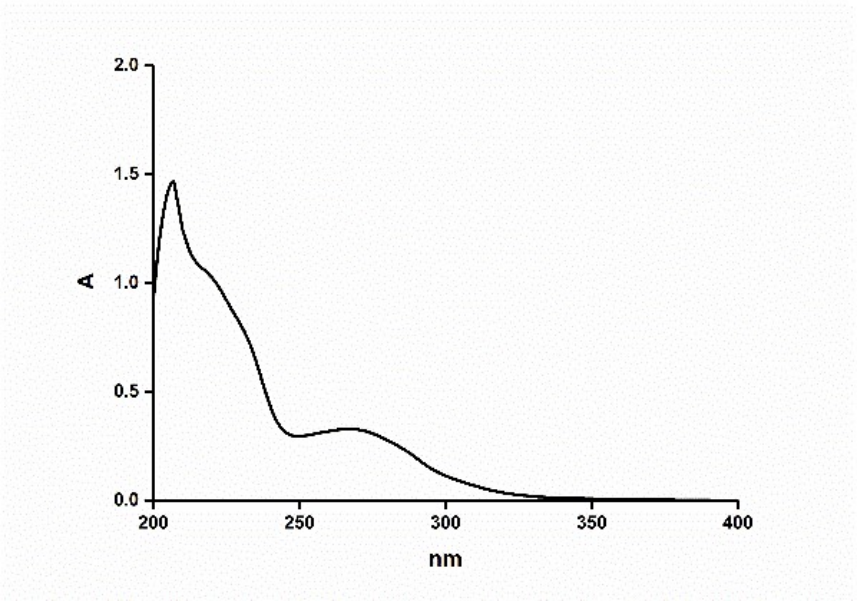


Figure S20. UV spectra (MeOH) of **3**.

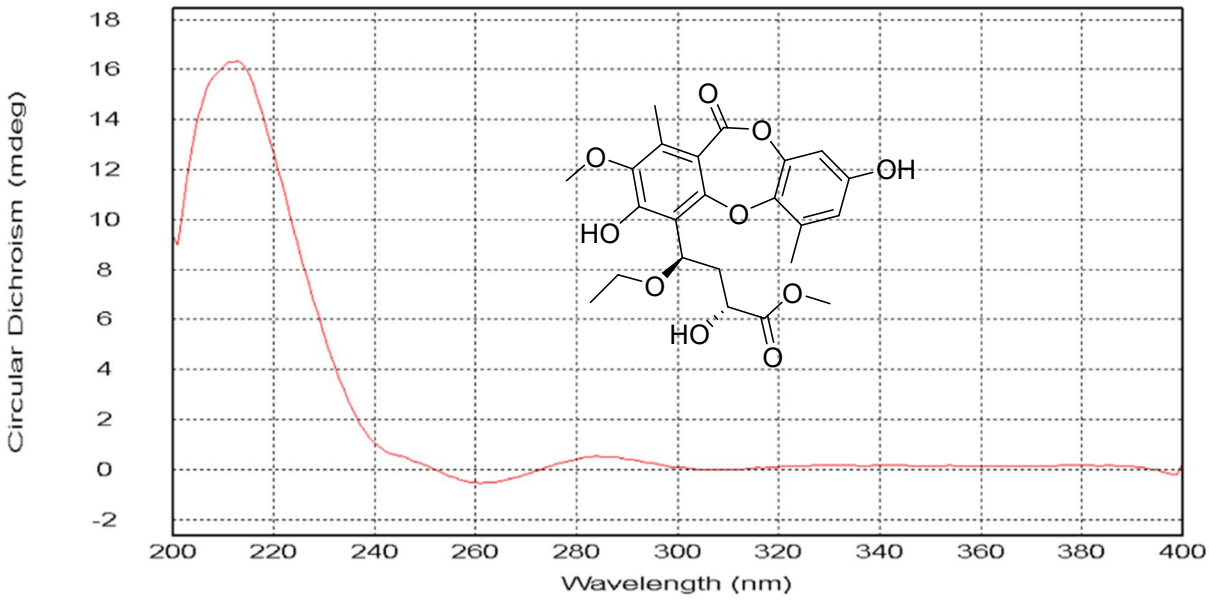


Figure S21. ECD spectra (MeOH) of **3**.

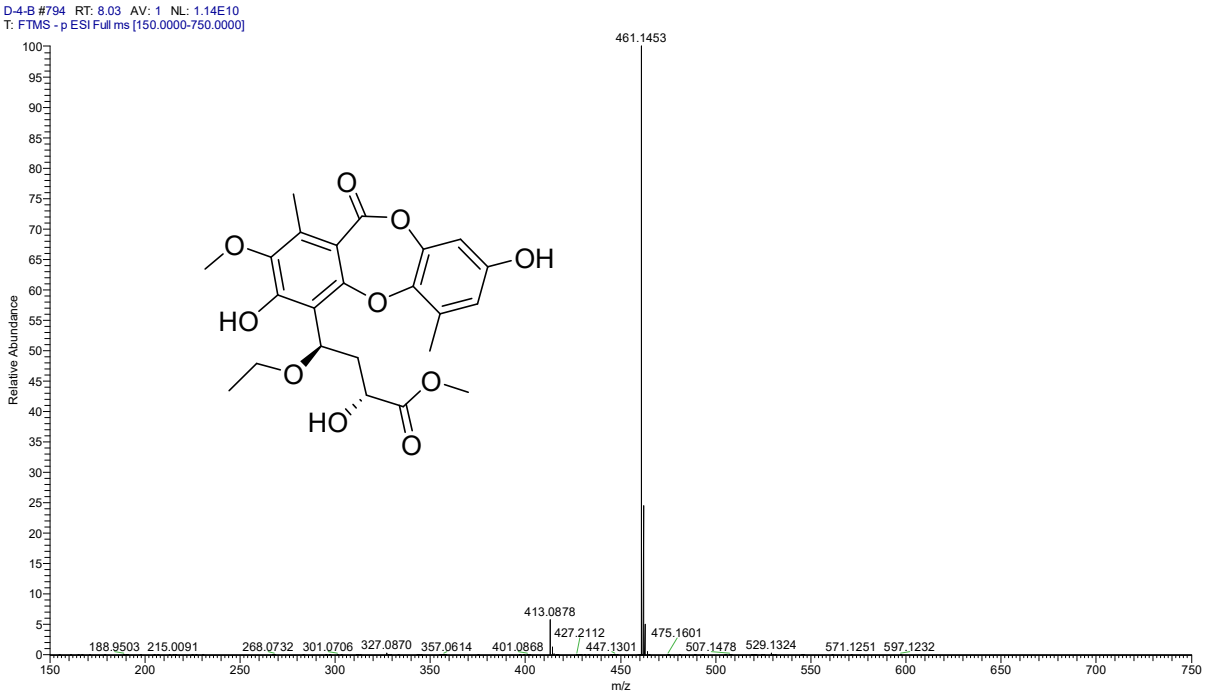


Figure S22. HRESIMS spectra of **3**.

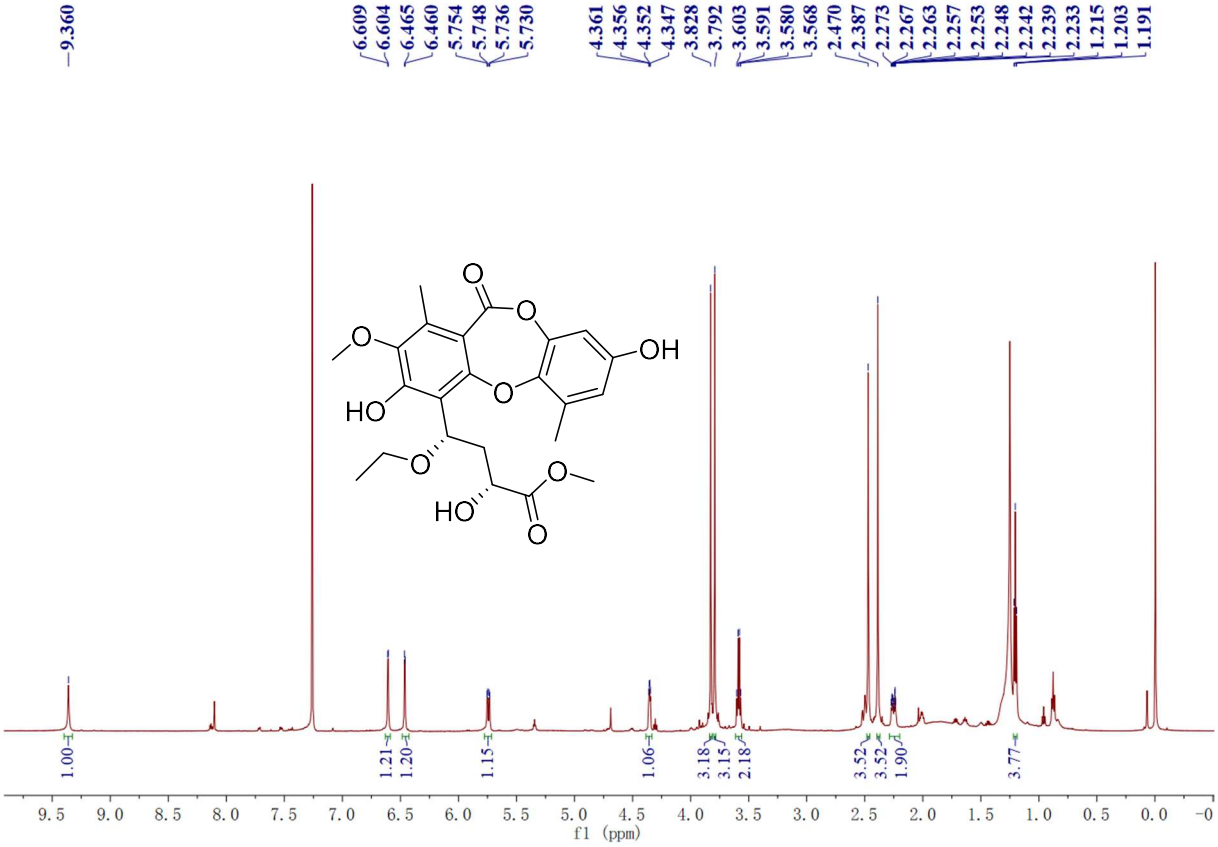


Figure S23. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **4**.

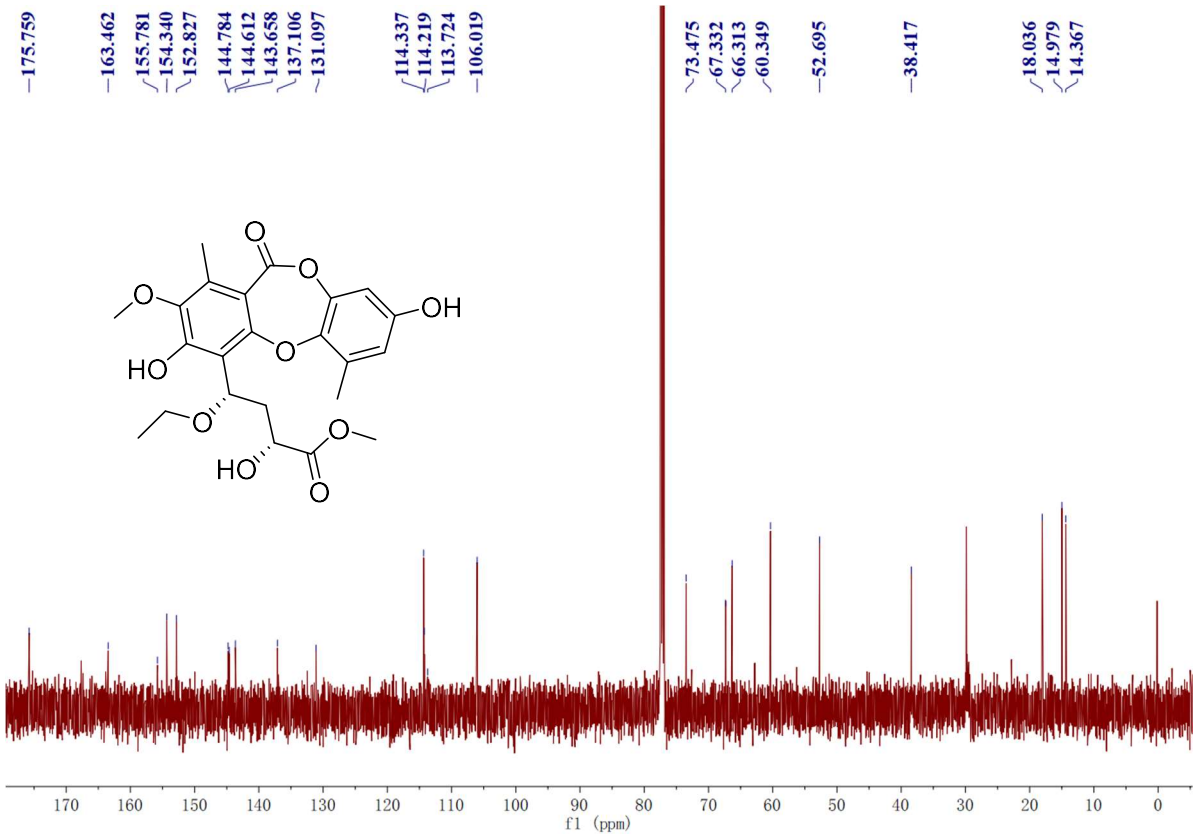


Figure S24. ^{13}C NMR spectra (125 MHz, $CDCl_3$) of **4**.

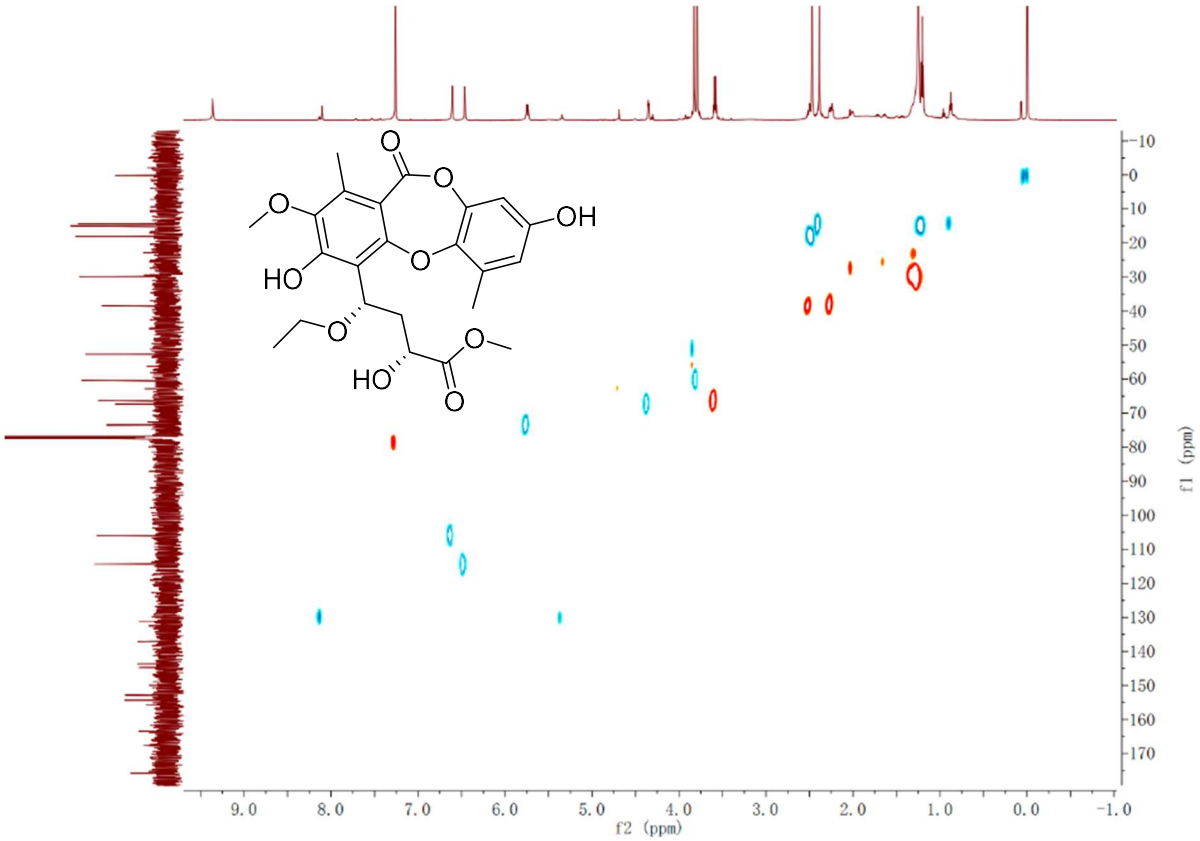


Figure S25. HSQC spectra ($CDCl_3$) of **4**.

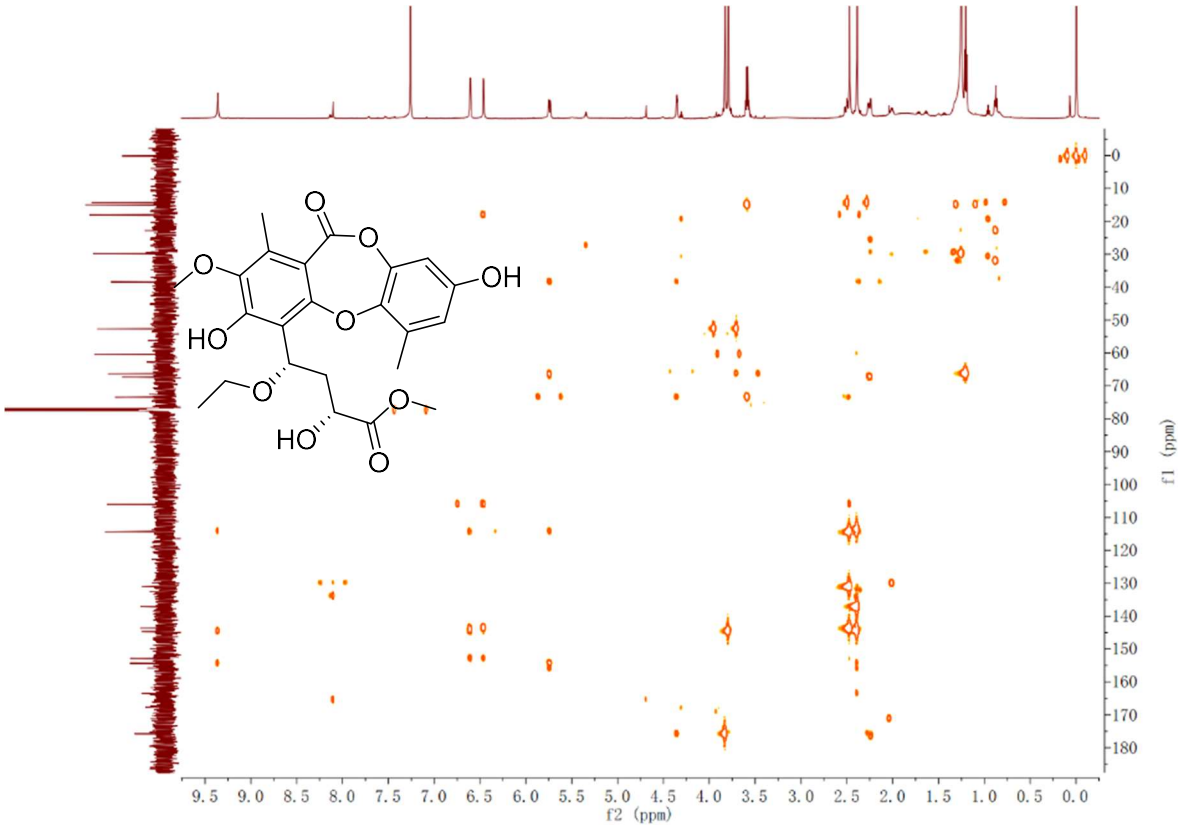


Figure S26. HMBC spectra ($CDCl_3$) of **4**.

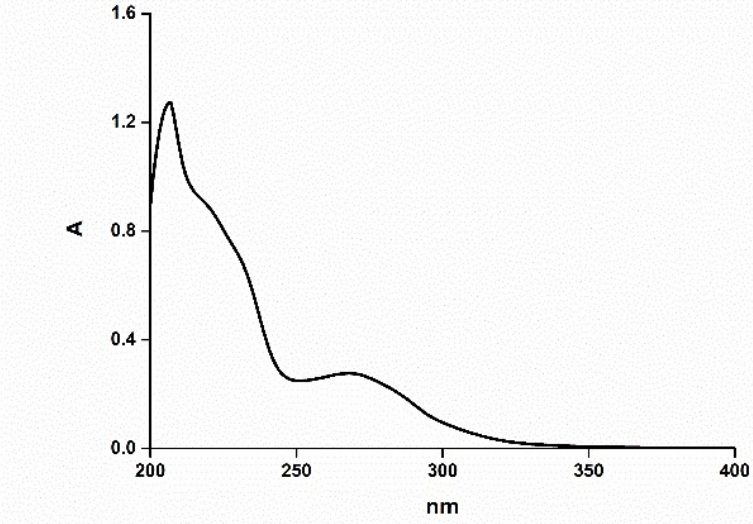


Figure S27. UV spectra (MeOH) of **4**.

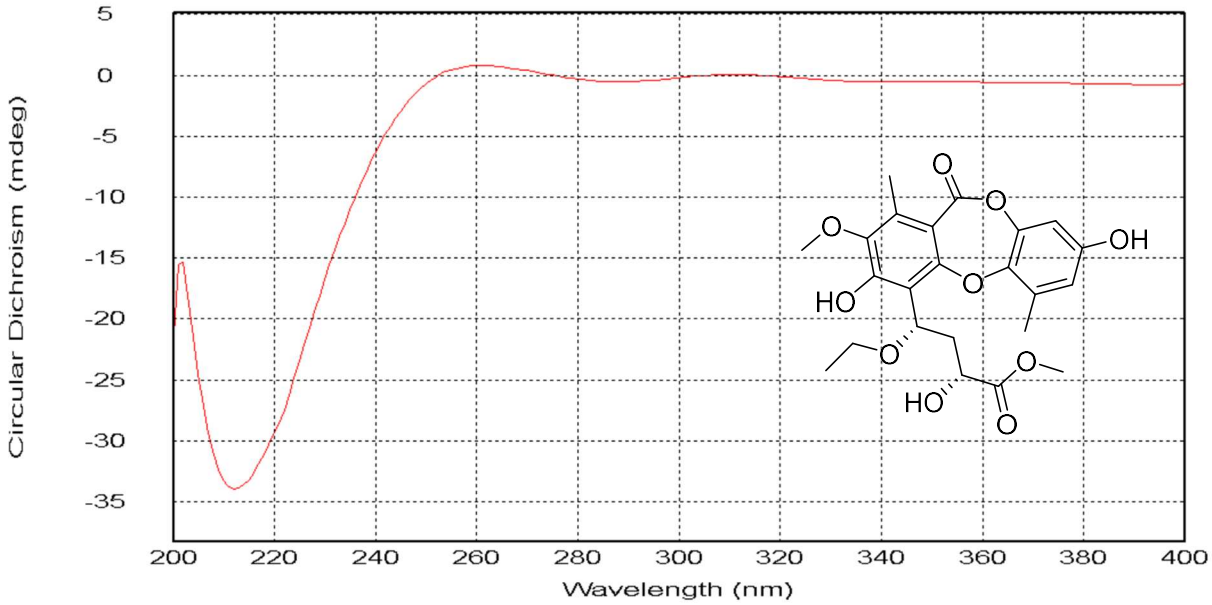


Figure S28. ECD spectra (MeOH) of **4**.

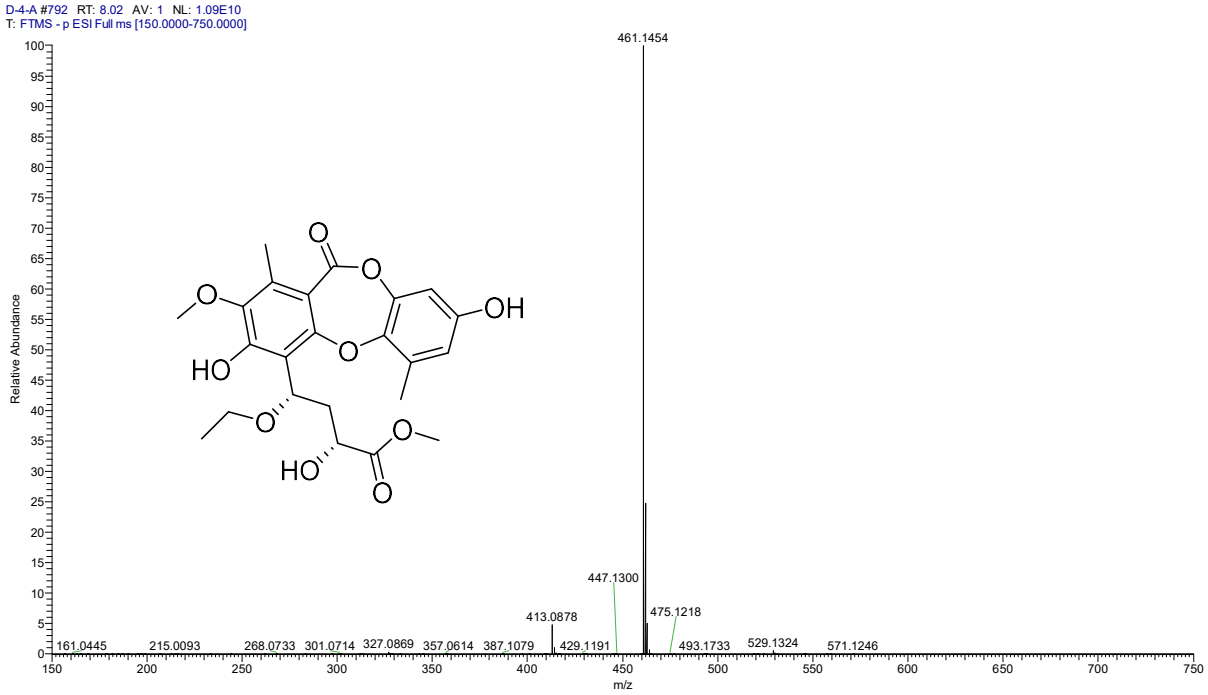


Figure S29. HRESIMS spectra of **4**.

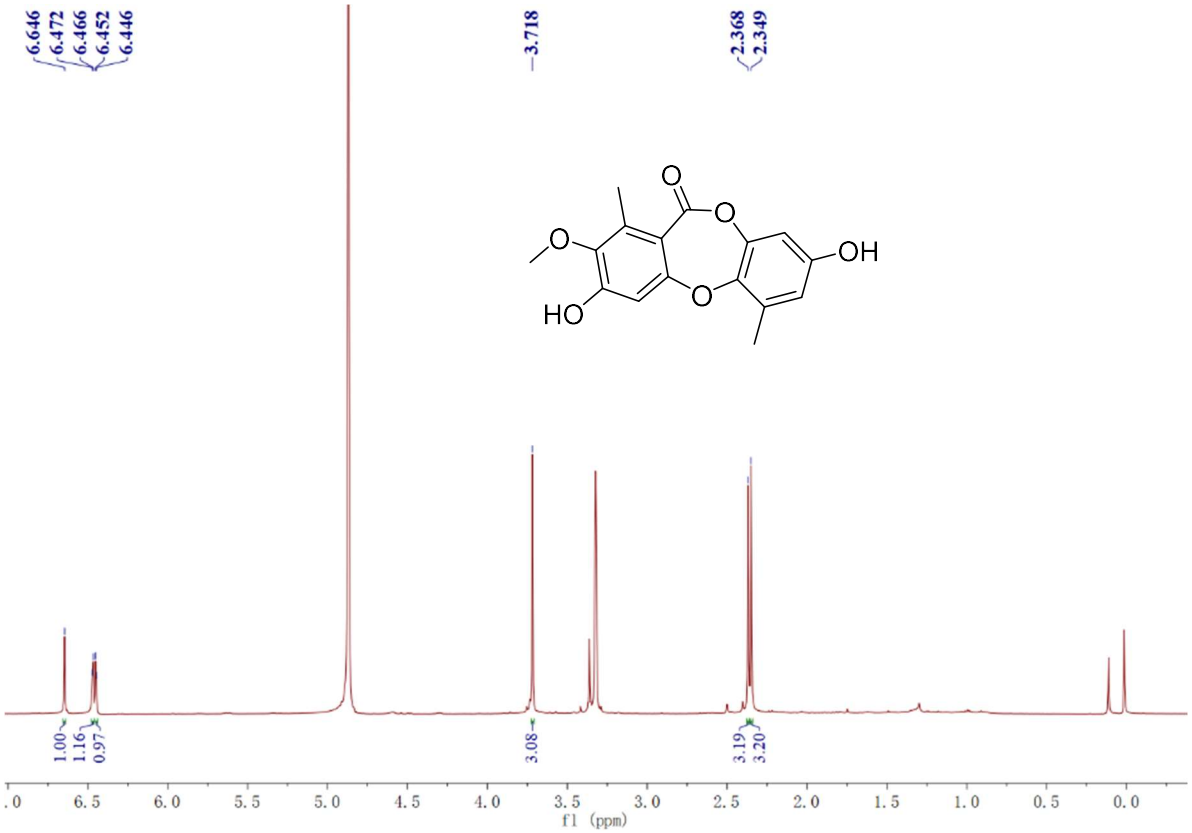


Figure S30. ^{1}H NMR spectra (500 MHz, CD_3OD) of **5**.

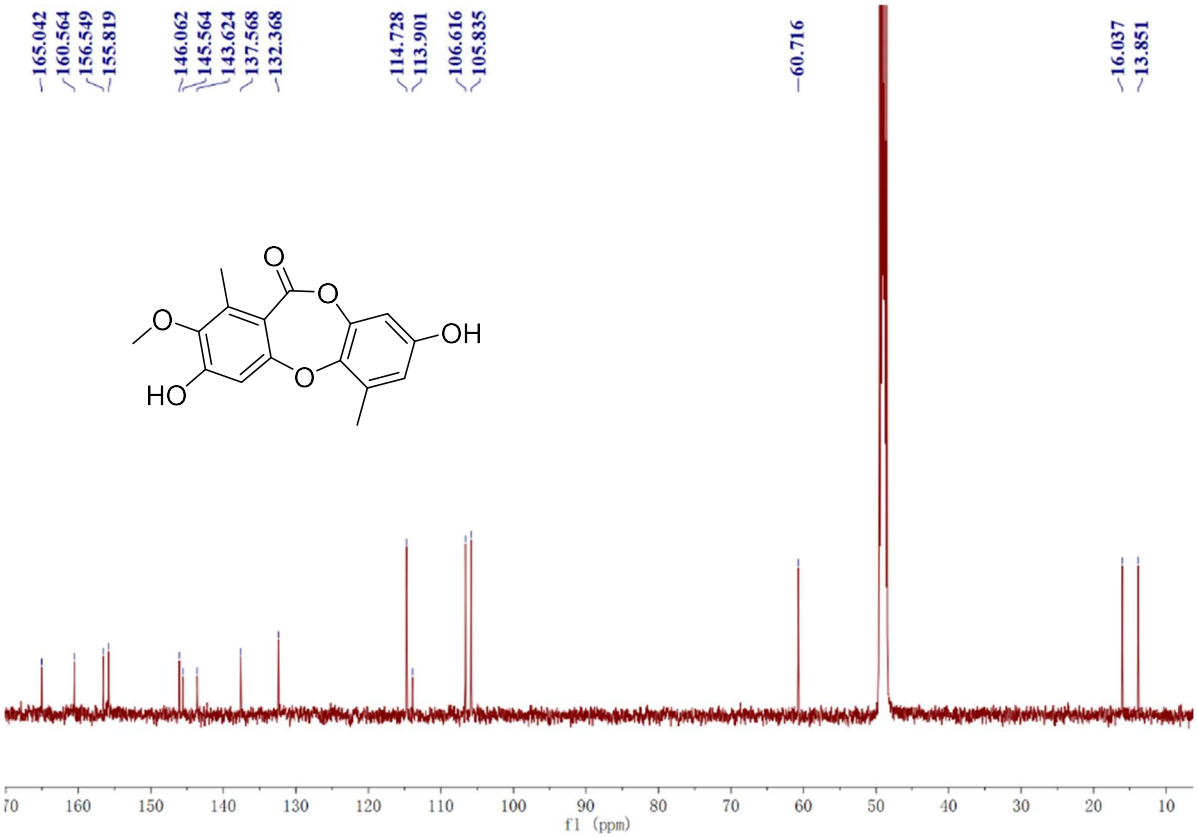


Figure S31. ^{13}C NMR spectra (125 MHz, CD_3OD) of **5**.

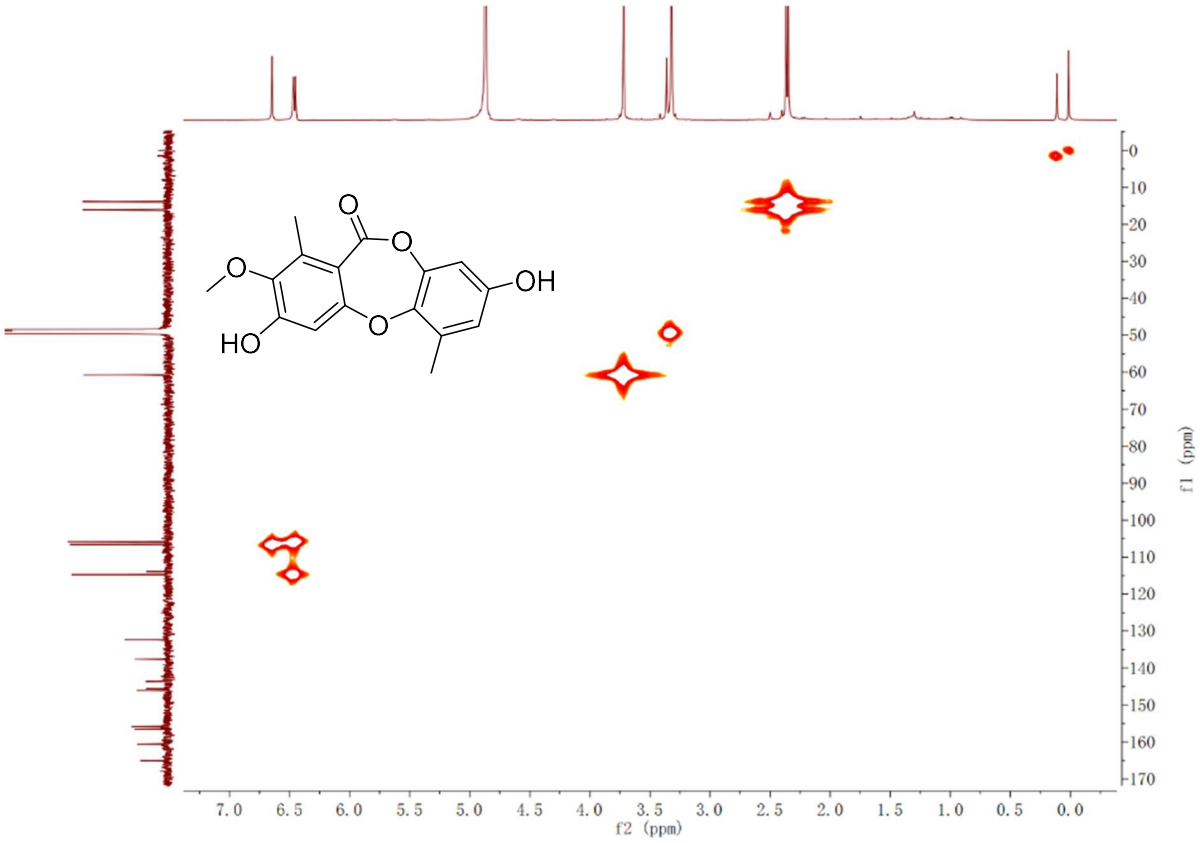


Figure S32. HSQC spectra (CD_3OD) of **5**.

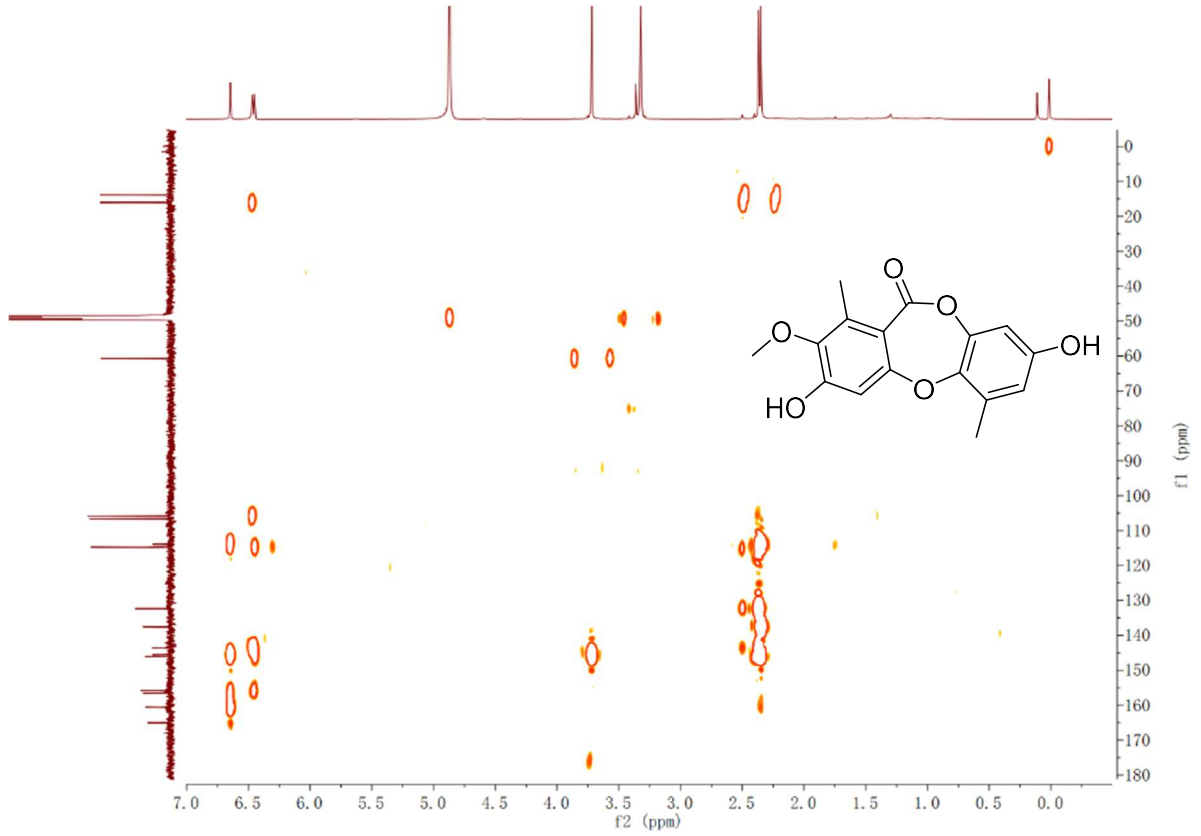


Figure S33. HMBC spectra (CD_3OD) of **5**.

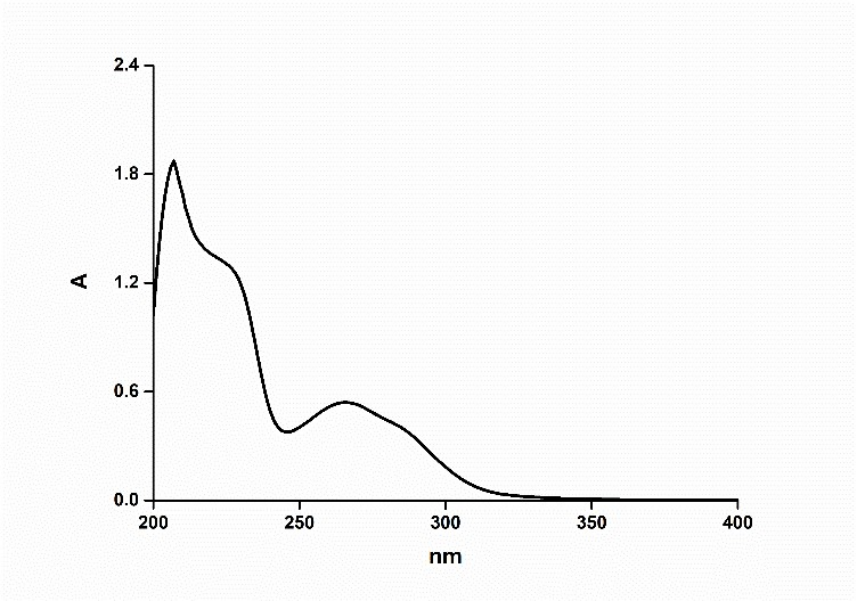


Figure S34. UV spectra (MeOH) of **5**.

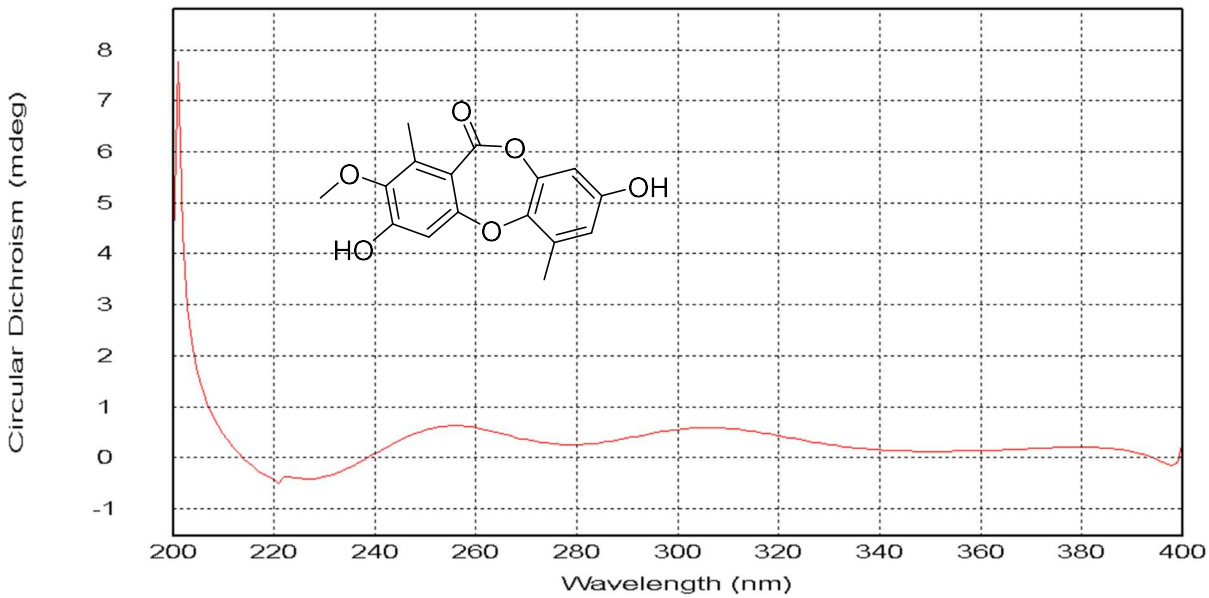


Figure S35. ECD spectra (MeOH) of **5**.

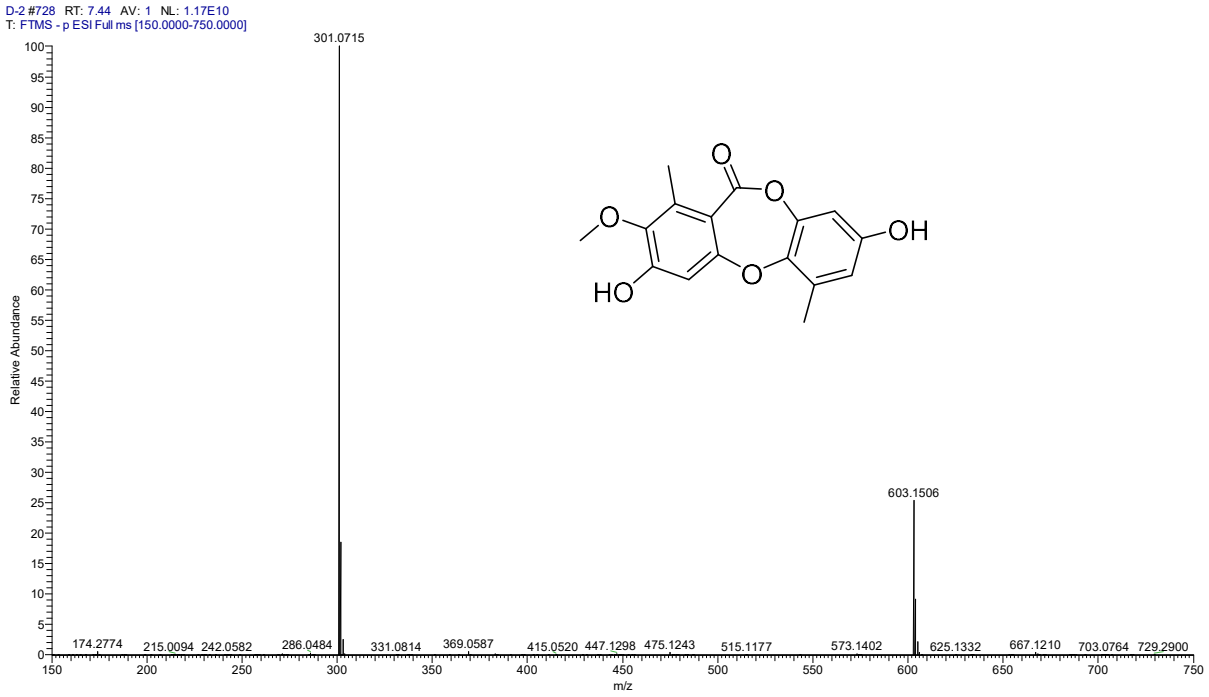


Figure S36. HRESIMS spectra of **5**.

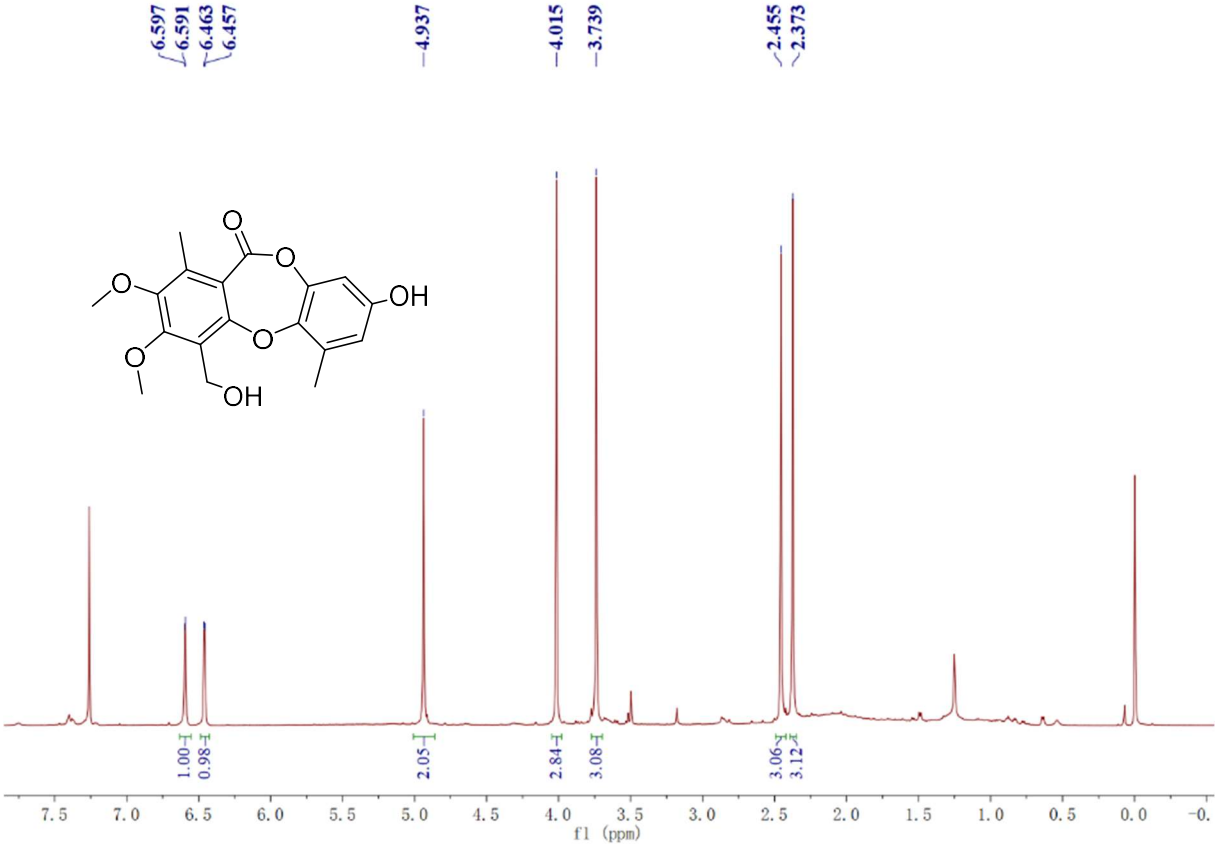


Figure S37. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **6**.

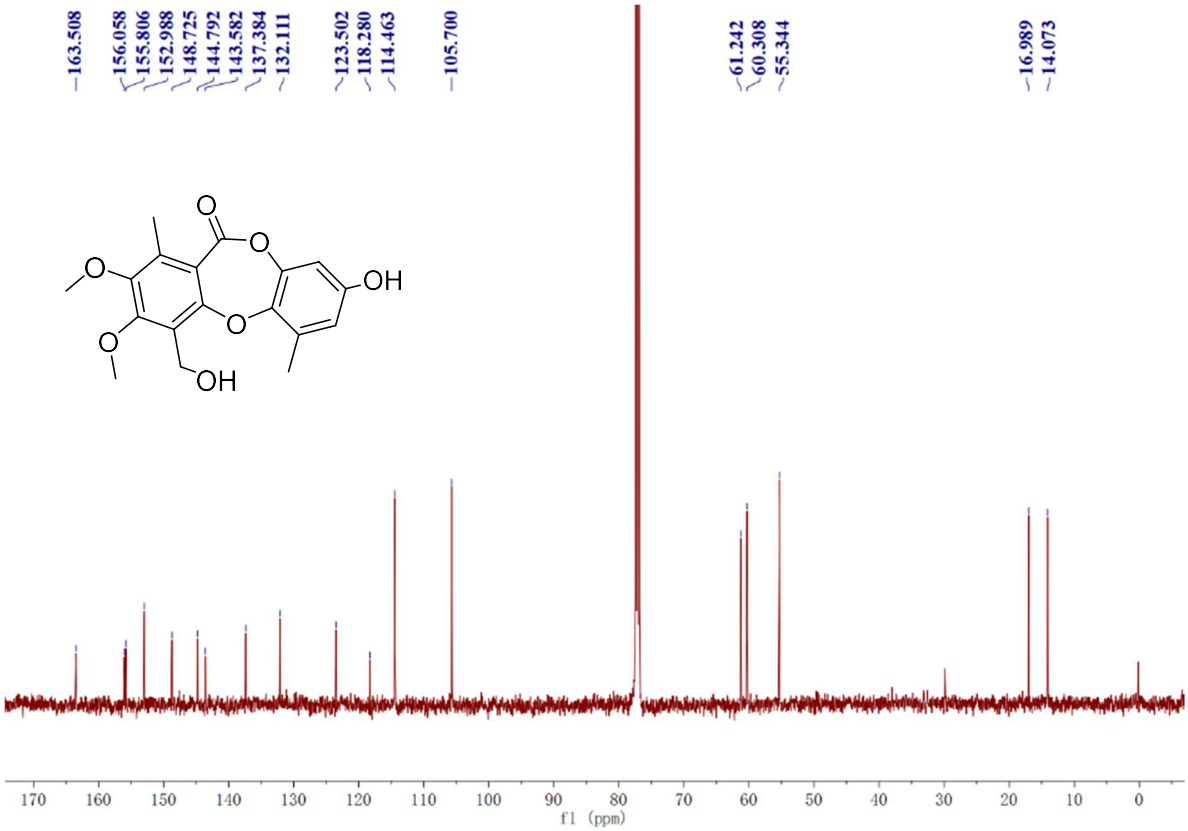


Figure S38. ^{13}C NMR spectra (125 MHz, $CDCl_3$) of **6**.

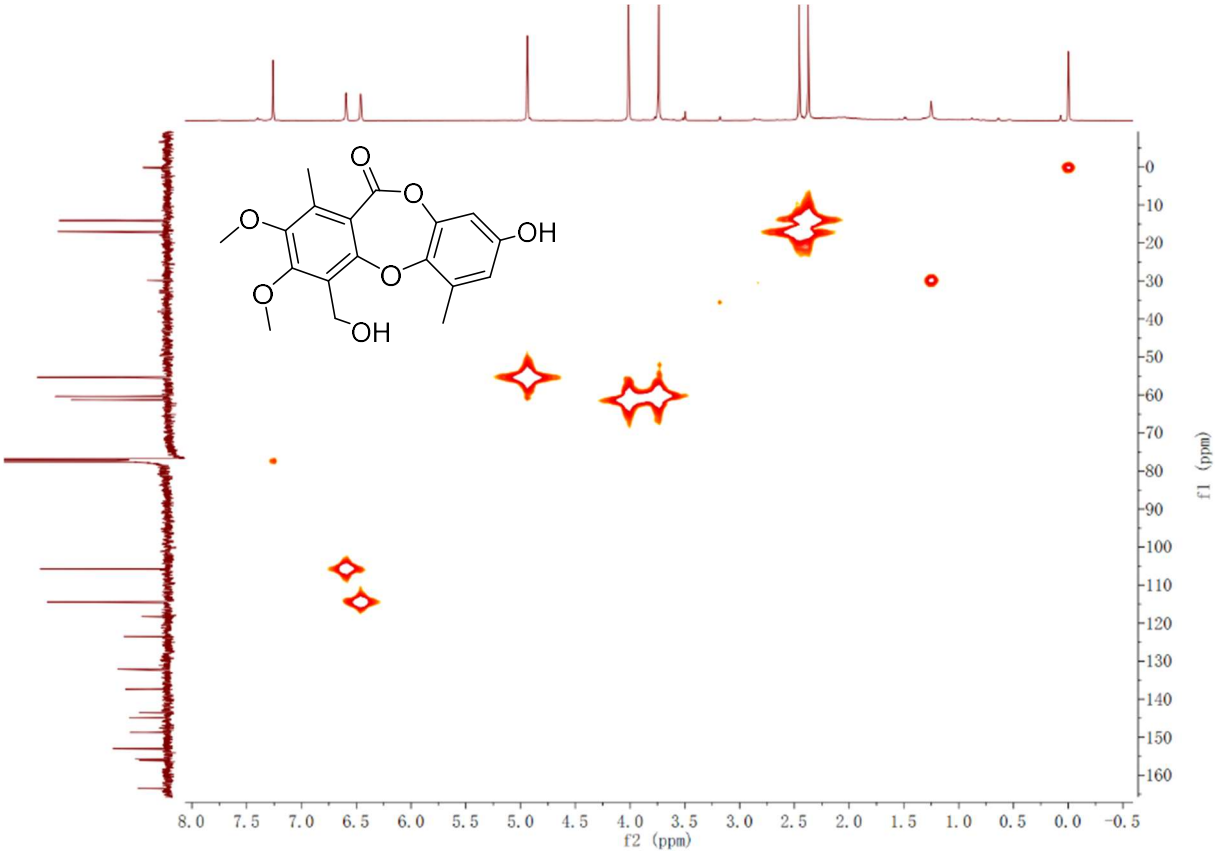


Figure S39. HSQC spectra ($CDCl_3$) of **6**.

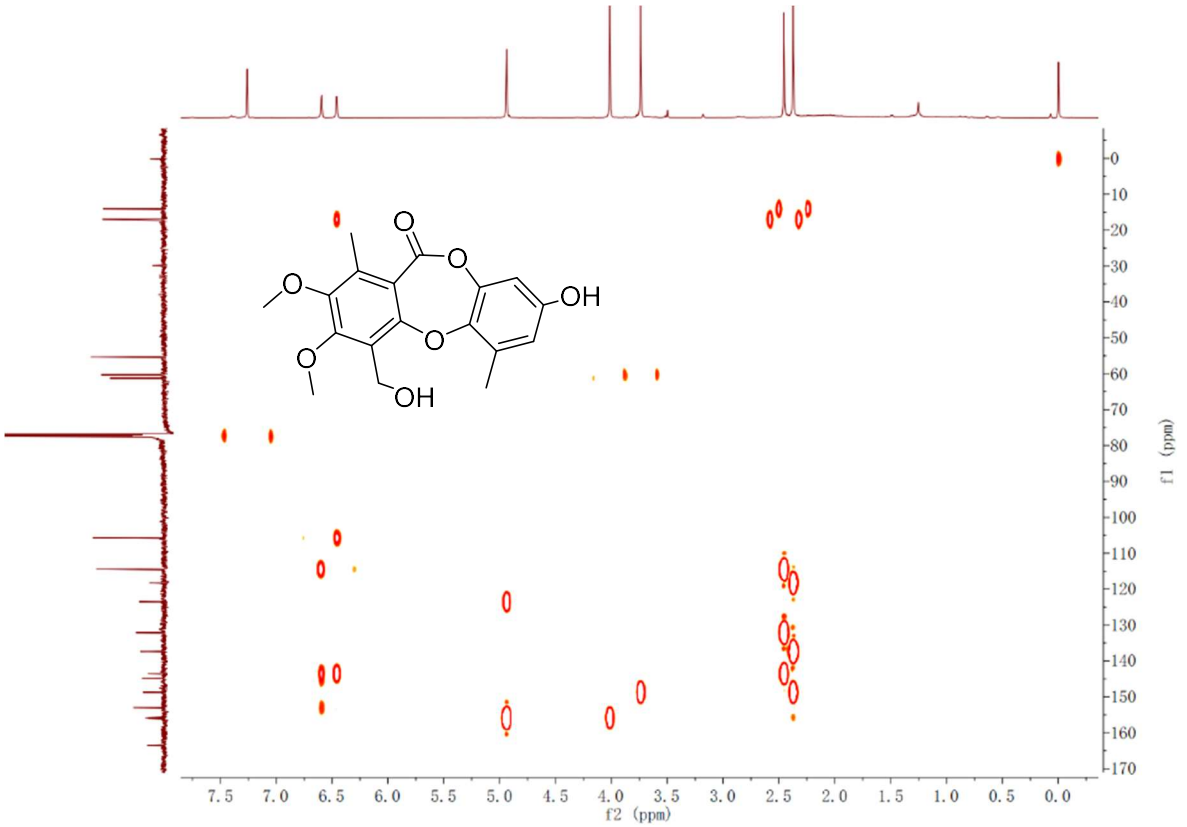


Figure S40. HMBC spectra ($CDCl_3$) of **6**.

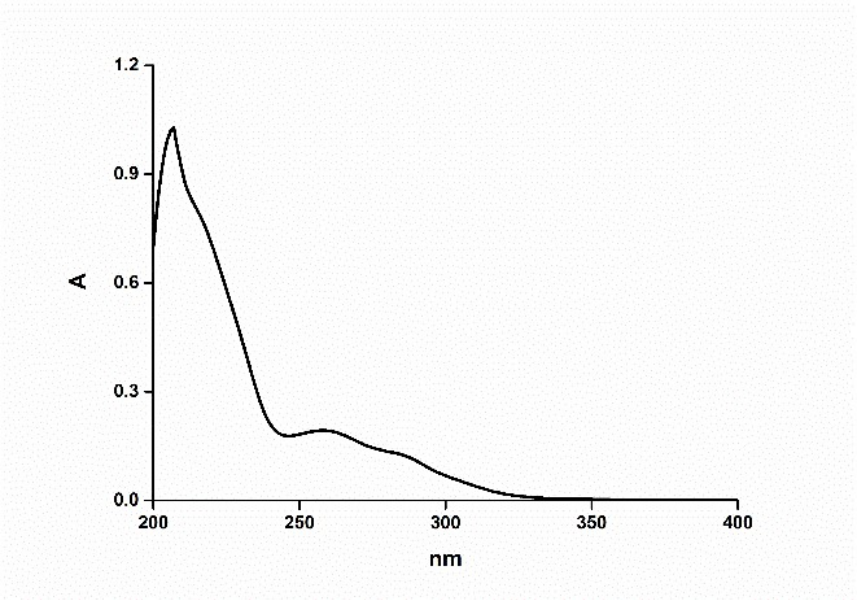


Figure S41. UV spectra (MeOH) of **6**.

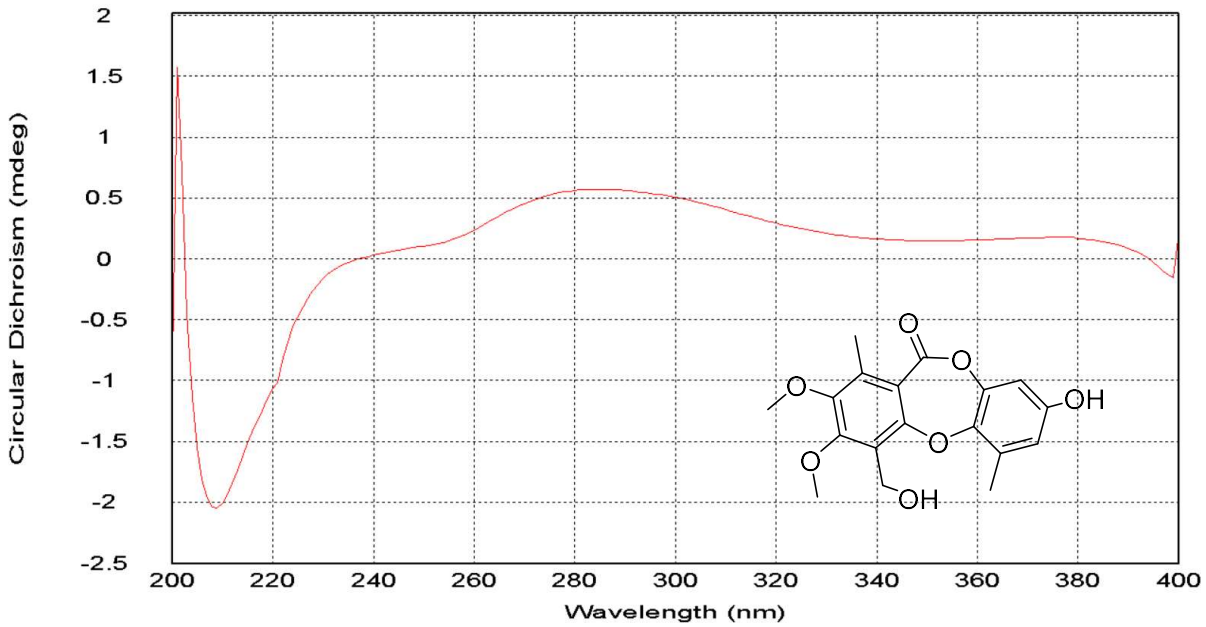


Figure S42. ECD spectra (MeOH) of **6**.

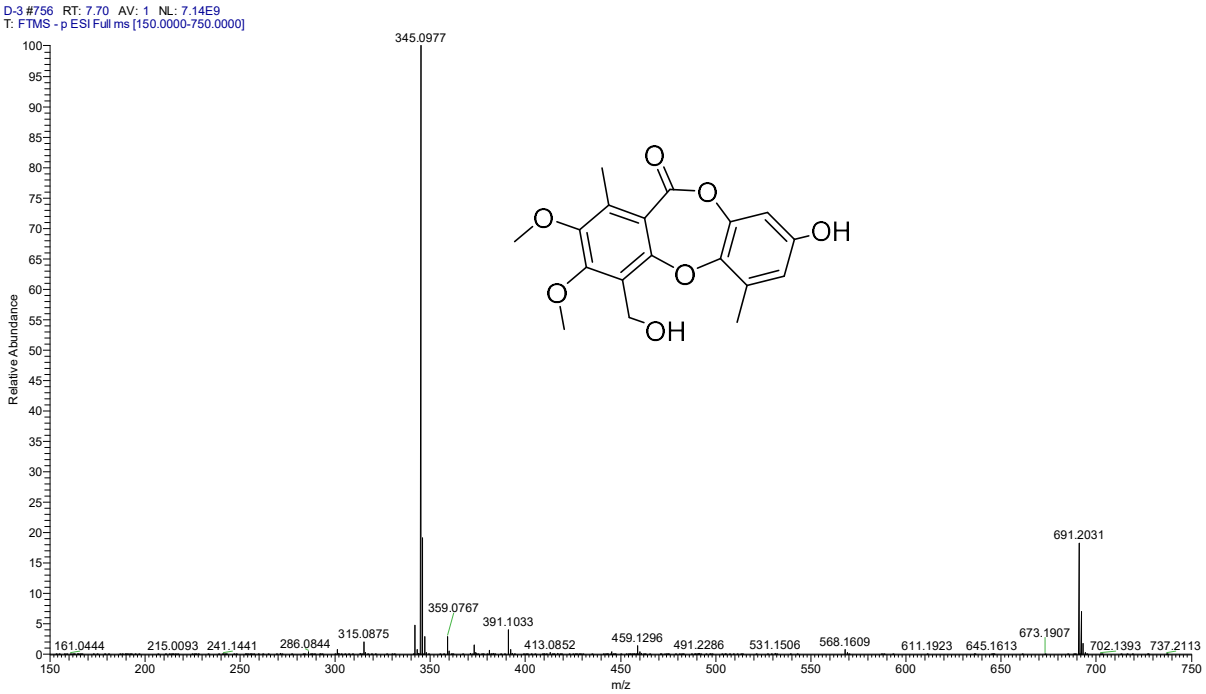


Figure S43. HRESIMS spectra of **6**.

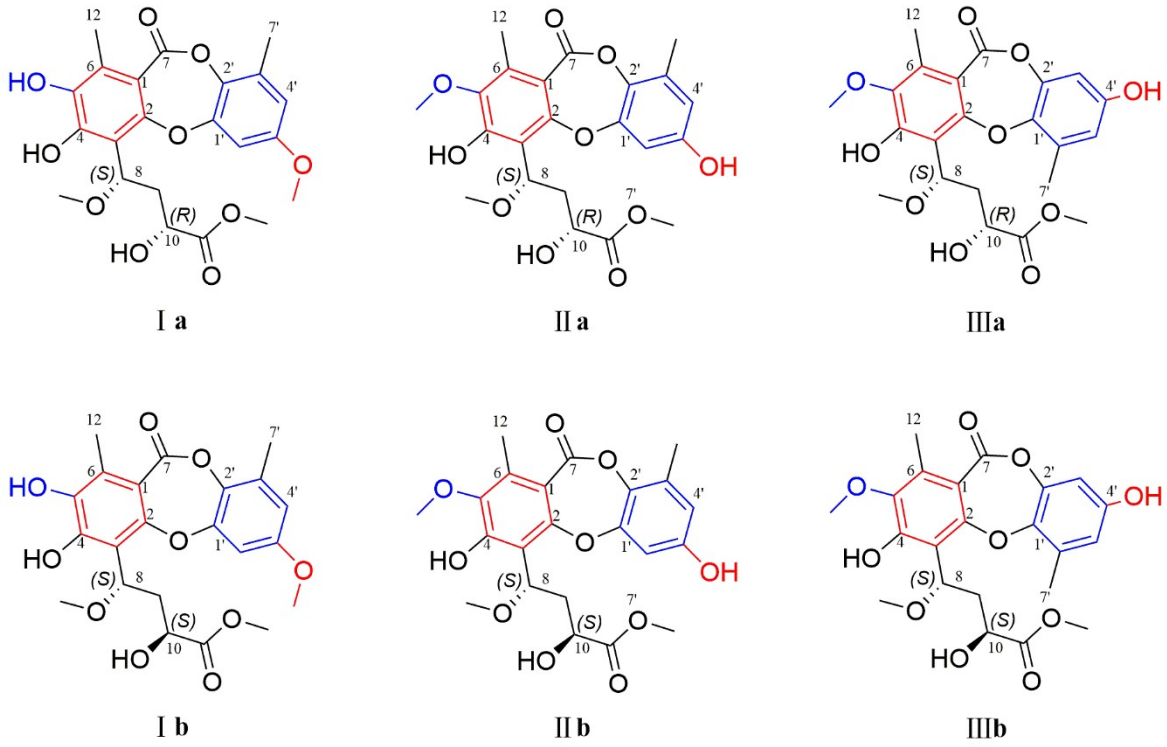


Figure S44. Chemical structure of undetermined relative configurations of compounds **I**, **II** and **III** (enantiomers not shown).

Table S1. Energies of conformers at MMFF94x force field.

Configuration	Conformer	E (kcal/mol)	ΔE (kcal/mol)
Ia	1	100.26	0.00
Ia	2	102.31	2.05
Ia	3	102.31	2.05
Ia	4	102.31	2.05
Ia	5	102.31	2.05
Ia	6	102.31	2.05
Ia	7	102.31	2.05
Ia	8	102.31	2.05
Ia	9	102.31	2.05
Ia	10	102.31	2.05
Ia	11	102.31	2.05
Ia	12	102.31	2.05
Ia	13	102.31	2.05
Ia	14	102.72	2.46
Ia	15	102.85	2.58
Ia	16	102.88	2.62
Ia	17	102.92	2.66

Ia	18	103.59	3.33
Ia	19	103.63	3.36
Ia	20	104.22	3.96
Ia	21	104.53	4.27
Ia	22	104.62	4.36
Ia	23	104.64	4.38
Ia	24	104.72	4.45
Ia	25	104.72	4.45
Ia	26	104.72	4.45
Ia	27	104.72	4.45
Ia	28	104.72	4.45
Ia	29	104.72	4.45
Ia	30	104.72	4.45
Ia	31	104.72	4.45
Ia	32	104.72	4.45
Ia	33	104.72	4.45
Ia	34	104.72	4.45
Ia	35	104.72	4.45
Ia	36	104.72	4.45
Ia	37	104.72	4.45
Ia	38	104.72	4.45
Ia	39	104.72	4.45
Ia	40	104.91	4.64
Ia	41	105.05	4.79
Ia	42	105.20	4.94
Ib	1	101.09	0.00
Ib	2	101.22	0.13
Ib	3	102.39	1.30
Ib	4	102.60	1.51
Ib	5	102.98	1.88
Ib	6	103.01	1.92
Ib	7	103.62	2.52
Ib	8	103.62	2.52
Ib	9	103.62	2.52
Ib	10	103.62	2.52
Ib	11	103.62	2.52
Ib	12	103.62	2.52
Ib	13	103.62	2.52
Ib	14	103.62	2.52
Ib	15	103.62	2.52
Ib	16	103.62	2.52
Ib	17	103.62	2.52
Ib	18	103.62	2.52

Ib	19	103.62	2.52
Ib	20	103.62	2.52
Ib	21	103.62	2.52
Ib	22	103.62	2.52
Ib	23	103.62	2.52
Ib	24	103.91	2.81
Ib	25	104.10	3.01
Ib	26	104.46	3.37
Ib	27	104.46	3.37
Ib	28	104.46	3.37
Ib	29	104.46	3.37
Ib	30	104.46	3.37
Ib	31	104.46	3.37
Ib	32	104.46	3.37
Ib	33	104.46	3.37
Ib	34	104.46	3.37
Ib	35	104.46	3.37
Ib	36	104.46	3.37
Ib	37	104.46	3.37
Ib	38	104.46	3.37
Ib	39	104.46	3.37
Ib	40	104.63	3.53
Ib	41	104.73	3.64
Ib	42	104.84	3.74
Ib	43	104.85	3.76
Ib	44	104.94	3.85
Ib	45	105.15	4.06
Ib	46	105.32	4.22
Ib	47	105.41	4.31
Ib	48	105.45	4.36
Ib	49	105.51	4.41
Ib	50	105.64	4.55
Ib	51	105.68	4.58
Ib	52	105.77	4.67
Ib	53	105.83	4.73
IIa	1	108.61	0.00
IIa	2	108.65	0.04
IIa	3	108.72	0.11
IIa	4	109.24	0.63
IIa	5	110.39	1.77
IIa	6	110.94	2.33
IIa	7	111.02	2.41
IIa	8	111.10	2.48

IIa	9	111.16	2.54
IIa	10	111.97	3.36
IIa	11	112.30	3.69
IIa	12	112.46	3.85
IIa	13	112.53	3.92
IIa	14	112.95	4.34
IIa	15	113.07	4.46
IIa	16	113.10	4.49
IIa	17	113.12	4.51
IIa	18	113.20	4.58
IIa	19	113.25	4.64
IIa	20	113.48	4.86
IIa	21	113.60	4.99
IIb	1	106.87	0.00
IIb	2	109.51	2.64
IIb	3	109.89	3.02
IIb	4	110.25	3.38
IIb	5	110.47	3.60
IIb	6	110.48	3.61
IIb	7	110.69	3.82
IIb	8	111.13	4.26
IIb	9	111.16	4.28
IIb	10	111.16	4.28
IIb	11	111.47	4.60
IIb	12	111.50	4.63
IIb	13	111.71	4.84
IIb	14	111.82	4.95
IIIa	1	110.80	0.00
IIIa	2	111.52	0.72
IIIa	3	112.91	2.12
IIIa	4	112.99	2.19
IIIa	5	113.23	2.43
IIIa	6	113.27	2.48
IIIa	7	113.58	2.78
IIIa	8	113.72	2.93
IIIa	9	113.77	2.97
IIIa	10	113.95	3.16
IIIa	11	114.26	3.46
IIIa	12	114.36	3.56
IIIa	13	114.38	3.58
IIIa	14	114.52	3.72
IIIa	15	114.55	3.75
IIIa	16	114.57	3.77

IIIa	17	114.62	3.83
IIIa	18	115.00	4.20
IIIa	19	115.03	4.23
IIIa	20	115.04	4.24
IIIa	21	115.19	4.39
IIIa	22	115.23	4.44
IIIa	23	115.45	4.65
IIIa	24	115.46	4.66
IIIa	25	115.49	4.69
IIIa	26	115.49	4.69
IIIa	27	115.52	4.72
IIIa	28	115.53	4.73
IIIa	29	115.56	4.76
IIIa	30	115.63	4.83
IIIa	31	115.75	4.95
IIIb	1	111.67	0.00
IIIb	2	111.67	0.00
IIIb	3	112.02	0.36
IIIb	4	112.19	0.53
IIIb	5	112.28	0.62
IIIb	6	112.83	1.16
IIIb	7	113.24	1.58
IIIb	8	113.37	1.71
IIIb	9	113.47	1.81
IIIb	10	113.47	1.81
IIIb	11	113.72	2.05
IIIb	12	113.79	2.12
IIIb	13	113.79	2.12
IIIb	14	113.80	2.13
IIIb	15	113.86	2.20
IIIb	16	113.88	2.22
IIIb	17	113.90	2.23
IIIb	18	113.94	2.28
IIIb	19	114.15	2.49
IIIb	20	114.17	2.50
IIIb	21	114.21	2.55
IIIb	22	114.22	2.55
IIIb	23	114.22	2.55
IIIb	24	114.22	2.55
IIIb	25	114.26	2.59
IIIb	26	114.39	2.73
IIIb	27	114.44	2.77
IIIb	28	114.45	2.78

IIIb	29	114.52	2.86
IIIb	30	114.55	2.88
IIIb	31	114.68	3.01
IIIb	32	114.72	3.06
IIIb	33	114.75	3.08
IIIb	34	114.75	3.08
IIIb	35	114.79	3.12
IIIb	36	114.89	3.23
IIIb	37	115.04	3.38
IIIb	38	115.09	3.42
IIIb	39	115.16	3.49
IIIb	40	115.24	3.57
IIIb	41	115.37	3.71
IIIb	42	115.38	3.71
IIIb	43	115.47	3.81
IIIb	44	115.61	3.95
IIIb	45	115.64	3.97
IIIb	46	115.65	3.99
IIIb	47	115.71	4.04
IIIb	48	115.89	4.23
IIIb	49	115.92	4.25
IIIb	50	115.93	4.27
IIIb	51	115.99	4.33
IIIb	52	115.99	4.33
IIIb	53	116.00	4.34
IIIb	54	116.12	4.46
IIIb	55	116.31	4.64
IIIb	56	116.32	4.65
IIIb	57	116.40	4.74
IIIb	58	116.51	4.84
IIIb	59	116.51	4.85
IIIb	60	116.52	4.85
IIIb	61	116.52	4.85
IIIb	62	116.53	4.87
IIIb	63	116.54	4.88
IIIb	64	116.56	4.89
IIIb	65	116.64	4.98
IIIb	66	116.64	4.98

Table S2. Energies of compounds I, II and III at B3LYP/6-311G (d, p) in gas phase.

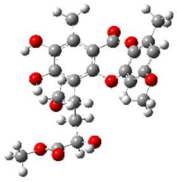
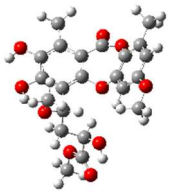
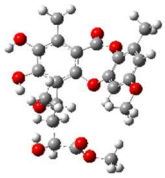
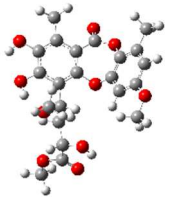
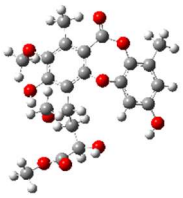
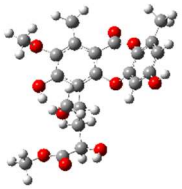
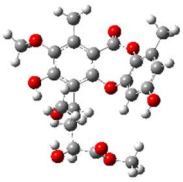
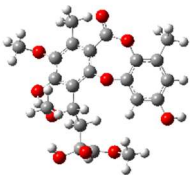
Configuration	Conformer	Structure	E (Hartree)	E (kcal/mol)	Population (%)
Ia	1		-1605.12910673	-1007233.71	95.47
Ia	2		-1605.12622941	-1007231.91	4.53
Ib	1		-1605.12656489	-1007232.12	4.85
Ib	2		-1605.12937477	-1007233.88	95.15
IIa	2		-1605.12216137	-1007229.36	72.45
IIa	18		-1605.12124832	-1007228.78	27.55
IIb	3		-1605.11814092	-1007226.83	50.11
IIb	6		-1605.11813694	-1007226.83	49.89

Table S3. Standard orientations of compounds I, II and III at B3LYP/6-311G (d, p) level in gas phase.

Conformer **Ia**-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.046049	3.349012	-0.727929
2	8	0	0.309909	4.525420	-1.321784
3	1	0	1.227024	4.430017	-1.612412
4	6	0	0.917032	2.334209	-0.617620
5	6	0	0.600659	1.096952	-0.053142
6	6	0	1.631060	-0.012427	0.071685
7	6	0	2.389152	0.023509	1.398091
8	1	0	2.939915	0.961410	1.501739
9	6	0	3.355327	-1.160683	1.561086
10	8	0	2.677572	-2.383403	1.347541
11	1	0	3.264388	-2.914575	0.788078
12	1	0	3.755187	-1.125243	2.585134
13	6	0	4.567791	-1.102546	0.635632
14	8	0	5.259761	0.031391	0.762496
15	6	0	6.438313	0.149442	-0.060309
16	1	0	6.878441	1.108622	0.200474
17	1	0	6.162930	0.125857	-1.115278
18	1	0	7.131446	-0.665486	0.150354
19	1	0	1.650550	-0.022186	2.201418
20	8	0	2.612790	0.066052	-0.991339
21	6	0	2.227451	-0.612881	-2.187999
22	1	0	2.133128	-1.686346	-1.998140
23	1	0	3.021374	-0.447341	-2.915726
24	1	0	1.282631	-0.223492	-2.582036
25	1	0	1.134099	-0.979470	0.001613
26	6	0	-0.697243	0.928439	0.436514
27	6	0	-1.663250	1.937606	0.367074
28	6	0	-1.337470	3.178450	-0.238396
29	6	0	-2.314269	4.317798	-0.387736
30	1	0	-3.325063	3.961437	-0.583885
31	1	0	-1.997994	4.972219	-1.198953
32	1	0	-2.362446	4.908131	0.530684
33	8	0	-0.960779	-0.277579	1.079790
34	6	0	-1.956034	-1.049301	0.496501
35	6	0	-3.254520	-0.570079	0.436252
36	8	0	-3.643282	0.602977	1.058952
37	6	0	-2.975510	1.806086	1.061830
38	6	0	-1.623653	-2.314185	0.015855
39	1	0	-0.602330	-2.651130	0.121399

40	6	0	-2.628598	-3.104938	-0.540595
41	8	0	-2.435814	-4.360917	-1.033388
42	6	0	-1.138408	-4.931446	-0.937674
43	1	0	-0.809645	-5.010129	0.104335
44	1	0	-0.402411	-4.352655	-1.507601
45	1	0	-1.219754	-5.928707	-1.366608
46	6	0	-3.936570	-2.611549	-0.623365
47	1	0	-4.694856	-3.246706	-1.064902
48	6	0	-4.269226	-1.353746	-0.135486
49	6	0	-5.683758	-0.838013	-0.177918
50	1	0	-5.746815	0.096618	-0.741881
51	1	0	-6.050142	-0.620774	0.828707
52	1	0	-6.347891	-1.568139	-0.642184
53	8	0	-3.516676	2.714729	1.630440
54	8	0	2.149208	2.646897	-1.113278
55	1	0	2.659678	1.813404	-1.170698
56	8	0	4.885459	-2.027266	-0.077899

Conformer **Ia**-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.640144	3.307276	0.936507
2	8	0	-1.051106	4.491461	1.475938
3	1	0	-1.724856	4.282159	2.137280
4	6	0	-1.256308	2.123153	1.366575
5	6	0	-0.859166	0.876139	0.874880
6	6	0	-1.530826	-0.397694	1.369316
7	6	0	-2.827369	-0.747679	0.624230
8	1	0	-3.421774	-1.386540	1.283763
9	6	0	-2.539906	-1.532057	-0.668103
10	8	0	-1.882768	-2.748977	-0.366613
11	1	0	-2.490687	-3.453847	-0.636368
12	1	0	-1.903033	-0.936776	-1.330404
13	6	0	-3.831683	-1.836926	-1.415065
14	8	0	-4.455655	-0.734398	-1.835914
15	6	0	-5.690482	-0.937649	-2.556554
16	1	0	-6.036196	0.058155	-2.821549
17	1	0	-6.418770	-1.444760	-1.922801
18	1	0	-5.510681	-1.535695	-3.450324
19	1	0	-3.402414	0.153693	0.401329
20	8	0	-1.884288	-0.271883	2.768220
21	6	0	-0.781311	-0.435959	3.659691
22	1	0	-0.349100	-1.436410	3.550495
23	1	0	-1.174353	-0.321789	4.669661

24	1	0	-0.001875	0.313592	3.483884
25	1	0	-0.845485	-1.240321	1.268445
26	6	0	0.150646	0.864658	-0.090548
27	6	0	0.765822	2.035022	-0.548023
28	6	0	0.370282	3.290126	-0.021231
29	6	0	0.987300	4.602731	-0.434281
30	1	0	2.056987	4.507035	-0.619098
31	1	0	0.820127	5.350177	0.340023
32	1	0	0.539744	4.963552	-1.363651
33	8	0	0.460297	-0.368160	-0.658269
34	6	0	1.759444	-0.807198	-0.447237
35	6	0	2.825370	-0.078271	-0.949803
36	8	0	2.656536	1.007044	-1.792132
37	6	0	1.721569	2.011547	-1.691920
38	6	0	1.952567	-2.004933	0.236921
39	1	0	1.078701	-2.553896	0.557046
40	6	0	3.255068	-2.464737	0.427271
41	8	0	3.575697	-3.624421	1.067513
42	6	0	2.517978	-4.452541	1.530098
43	1	0	1.873027	-4.778208	0.706800
44	1	0	1.909963	-3.942179	2.285987
45	1	0	2.995534	-5.321030	1.980485
46	6	0	4.335222	-1.712844	-0.051802
47	1	0	5.335946	-2.092408	0.115215
48	6	0	4.140636	-0.526318	-0.748441
49	6	0	5.296246	0.257012	-1.313980
50	1	0	5.319264	1.273519	-0.911644
51	1	0	5.208805	0.352326	-2.399372
52	1	0	6.244275	-0.229275	-1.080653
53	8	0	1.751432	2.854808	-2.546312
54	8	0	-2.241311	2.285699	2.296794
55	1	0	-2.408731	1.409670	2.702711
56	8	0	-4.231353	-2.964659	-1.594006

Conformer **Ib**-1

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.683515	-3.284213	0.508280
2	8	0	-2.066853	-4.503945	0.983914
3	1	0	-1.284918	-4.918513	1.372985
4	6	0	-0.335490	-2.910936	0.615172
5	6	0	0.103614	-1.662891	0.172277
6	6	0	1.561149	-1.255024	0.258466
7	6	0	2.382887	-1.735403	-0.944834

8	1	0	2.404725	-2.829124	-0.962346
9	6	0	3.841879	-1.228086	-0.969112
10	8	0	4.624393	-1.746094	0.082336
11	1	0	4.073500	-1.728923	0.876345
12	1	0	4.304335	-1.555917	-1.901806
13	6	0	3.853758	0.305350	-0.962783
14	8	0	3.951716	0.793740	-2.209374
15	6	0	3.896998	2.228390	-2.342851
16	1	0	4.098686	2.429844	-3.392010
17	1	0	4.647286	2.697446	-1.706120
18	1	0	2.905899	2.594114	-2.069474
19	1	0	1.868910	-1.402725	-1.850709
20	8	0	2.183258	-1.793906	1.460102
21	6	0	1.897786	-1.033123	2.642322
22	1	0	2.321572	-0.029392	2.548352
23	1	0	2.371687	-1.555422	3.472861
24	1	0	0.819798	-0.967681	2.818476
25	1	0	1.618168	-0.169770	0.318796
26	6	0	-0.843161	-0.811880	-0.402340
27	6	0	-2.185585	-1.175424	-0.549729
28	6	0	-2.623097	-2.439795	-0.078784
29	6	0	-4.051184	-2.915901	-0.168434
30	1	0	-4.759917	-2.098003	-0.044476
31	1	0	-4.236527	-3.674383	0.591001
32	1	0	-4.248984	-3.357585	-1.148480
33	8	0	-0.367745	0.400874	-0.894980
34	6	0	-0.916029	1.525063	-0.289198
35	6	0	-2.268817	1.786266	-0.430564
36	8	0	-3.085307	1.032950	-1.256012
37	6	0	-3.130742	-0.340218	-1.345581
38	6	0	-0.077986	2.379890	0.424471
39	1	0	0.973314	2.138480	0.495054
40	6	0	-0.626267	3.526203	1.000799
41	8	0	0.084950	4.442575	1.713887
42	6	0	1.479993	4.229706	1.887838
43	1	0	1.679203	3.301175	2.434050
44	1	0	1.838331	5.075208	2.472268
45	1	0	2.007014	4.201975	0.928282
46	6	0	-1.995975	3.786211	0.865438
47	1	0	-2.392530	4.683395	1.324967
48	6	0	-2.829847	2.933761	0.151988
49	6	0	-4.295630	3.228853	-0.029011
50	1	0	-4.913732	2.430444	0.390794

51	1	0	-4.551620	3.297458	-1.089303
52	1	0	-4.564585	4.166940	0.458009
53	8	0	-3.963244	-0.800971	-2.077374
54	8	0	0.485360	-3.837734	1.189743
55	1	0	1.321880	-3.392178	1.425105
56	8	0	3.749732	0.992805	0.027056

Conformer **Ib**-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.449419	3.471274	0.788576
2	8	0	0.340508	4.718286	1.332778
3	1	0	-0.461532	4.723433	1.872650
4	6	0	-0.560026	2.532656	1.054475
5	6	0	-0.483613	1.231393	0.555169
6	6	0	-1.554159	0.192137	0.844965
7	6	0	-2.640905	0.137168	-0.229026
8	1	0	-3.190441	1.081913	-0.259346
9	6	0	-3.614339	-1.029188	0.024809
10	8	0	-2.925065	-2.262159	0.120778
11	1	0	-3.141107	-2.752630	-0.686733
12	1	0	-4.140166	-0.846705	0.966743
13	6	0	-4.642784	-1.118897	-1.093006
14	8	0	-5.459548	-0.062548	-1.126408
15	6	0	-6.442038	-0.052739	-2.185201
16	1	0	-7.004008	0.867484	-2.048050
17	1	0	-7.095280	-0.921758	-2.101514
18	1	0	-5.949037	-0.063635	-3.157699
19	1	0	-2.149213	-0.004512	-1.195377
20	8	0	-2.208503	0.450211	2.109296
21	6	0	-1.517466	-0.090252	3.237214
22	1	0	-2.092703	0.185584	4.120859
23	1	0	-0.503786	0.316842	3.320871
24	1	0	-1.466842	-1.181166	3.163698
25	1	0	-1.091173	-0.793513	0.896887
26	6	0	0.608216	0.920079	-0.259386
27	6	0	1.610694	1.846921	-0.560688
28	6	0	1.539265	3.155483	-0.017042
29	6	0	2.580656	4.219373	-0.259157
30	1	0	3.584736	3.799120	-0.309164
31	1	0	2.539895	4.964330	0.534315
32	1	0	2.403722	4.722901	-1.212816
33	8	0	0.605768	-0.349412	-0.831449
34	6	0	1.674909	-1.158027	-0.471995

35	6	0	2.965155	-0.788231	-0.815412
36	8	0	3.235860	0.297935	-1.629297
37	6	0	2.665612	1.549554	-1.570661
38	6	0	1.412419	-2.349200	0.201337
39	1	0	0.383588	-2.602348	0.414595
40	6	0	2.482102	-3.178753	0.536961
41	8	0	2.356874	-4.371220	1.184526
42	6	0	1.051215	-4.829233	1.507777
43	1	0	0.542355	-4.142120	2.193256
44	1	0	1.186841	-5.791337	1.998715
45	1	0	0.438551	-4.963248	0.609639
46	6	0	3.788727	-2.795300	0.209915
47	1	0	4.599592	-3.458176	0.486478
48	6	0	4.048683	-1.611541	-0.470092
49	6	0	5.447713	-1.217688	-0.865521
50	1	0	5.726746	-0.256717	-0.424676
51	1	0	5.528340	-1.099506	-1.949101
52	1	0	6.167686	-1.969808	-0.540637
53	8	0	3.079946	2.360502	-2.353343
54	8	0	-1.581173	2.984958	1.837525
55	1	0	-2.109901	2.205671	2.106783
56	8	0	-4.685117	-2.046802	-1.867461

Conformer **IIa**-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.476520	3.120910	-0.416441
2	8	0	0.280410	4.388540	-0.906041
3	6	0	-0.183180	4.480090	-2.259381
4	1	0	-0.220620	5.544140	-2.491071
5	1	0	-1.179100	4.047211	-2.367641
6	1	0	0.515170	3.984050	-2.942901
7	6	0	-0.632660	2.286820	-0.183451
8	6	0	-0.457620	0.998320	0.341579
9	6	0	-1.632681	0.045441	0.476109
10	6	0	-2.015291	-0.590919	-0.865011
11	1	0	-2.477381	0.158281	-1.512601
12	6	0	-2.951601	-1.803729	-0.727271
13	8	0	-2.337901	-2.823439	0.042779
14	1	0	-2.934131	-2.990489	0.789629
15	1	0	-3.160291	-2.184949	-1.734511
16	6	0	-4.294981	-1.453049	-0.095911
17	8	0	-5.010491	-0.620989	-0.850941
18	6	0	-6.278391	-0.200779	-0.305211

19	1	0	-6.118070	0.366001	0.612369
20	1	0	-6.906201	-1.066468	-0.093471
21	1	0	-6.728580	0.426671	-1.070181
22	1	0	-1.103931	-0.934230	-1.359021
23	8	0	-2.812230	0.728581	0.963289
24	6	0	-2.811900	0.939431	2.377279
25	1	0	-2.843241	-0.019839	2.903449
26	1	0	-3.710980	1.508561	2.611659
27	1	0	-1.929650	1.504331	2.695599
28	1	0	-1.370531	-0.745349	1.180579
29	6	0	0.834920	0.601210	0.682659
30	6	0	1.947650	1.429290	0.505289
31	6	0	1.767360	2.713370	-0.067321
32	6	0	2.914470	3.666510	-0.294171
33	1	0	3.792830	3.150900	-0.684571
34	1	0	3.218320	4.127660	0.647839
35	1	0	2.615960	4.453540	-0.982761
36	8	0	0.974319	-0.655520	1.256999
37	6	0	1.734779	-1.547070	0.511069
38	6	0	3.085999	-1.297900	0.318859
39	8	0	3.735469	-0.244570	0.941519
40	6	0	3.287080	1.052750	1.045329
41	6	0	1.125319	-2.682900	-0.006981
42	1	0	0.064979	-2.843400	0.157069
43	6	0	1.902659	-3.590170	-0.724601
44	8	0	1.377859	-4.730750	-1.262141
45	1	0	0.441259	-4.779660	-1.041871
46	6	0	3.262779	-3.344570	-0.925041
47	1	0	3.842789	-4.066120	-1.487561
48	6	0	3.872289	-2.203620	-0.406411
49	6	0	5.345459	-1.945771	-0.586471
50	1	0	5.849339	-1.866261	0.380249
51	1	0	5.520479	-1.001241	-1.108901
52	1	0	5.811819	-2.748831	-1.158571
53	8	0	4.031900	1.835200	1.569799
54	8	0	-1.862910	2.766961	-0.493231
55	1	0	-2.520140	2.186831	-0.061911
56	8	0	-4.659421	-1.925679	0.956979

Conformer **IIa**-18

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.089100	3.028971	0.319230
2	8	0	-0.268940	4.295831	0.711810

3	6	0	-0.528090	4.472811	2.109730
4	1	0	-1.386390	3.880301	2.431040
5	1	0	-0.746570	5.532141	2.242110
6	1	0	0.353080	4.207341	2.705080
7	6	0	-0.877970	2.005081	0.329430
8	6	0	-0.548980	0.709191	-0.098290
9	6	0	-1.594970	-0.393389	-0.152750
10	6	0	-2.402420	-0.364939	-1.451640
11	1	0	-2.925090	0.588321	-1.559560
12	6	0	-3.412560	-1.518749	-1.552260
13	8	0	-2.767660	-2.757369	-1.341060
14	1	0	-3.338380	-3.254459	-0.735790
15	1	0	-3.849650	-1.488499	-2.561480
16	6	0	-4.588620	-1.400489	-0.586220
17	8	0	-5.241750	-0.242229	-0.709290
18	6	0	-6.388410	-0.068319	0.147410
19	1	0	-6.799580	0.903791	-0.112930
20	1	0	-6.082270	-0.089229	1.193970
21	1	0	-7.118370	-0.858639	-0.030570
22	1	0	-1.697150	-0.454159	-2.281180
23	8	0	-2.539310	-0.274599	0.937370
24	6	0	-2.095650	-0.863449	2.159690
25	1	0	-1.158430	-0.412669	2.503910
26	1	0	-1.957590	-1.941669	2.032740
27	1	0	-2.877430	-0.686799	2.897770
28	1	0	-1.111080	-1.366979	-0.083370
29	6	0	0.750120	0.484891	-0.553660
30	6	0	1.711890	1.499491	-0.625160
31	6	0	1.374910	2.801061	-0.173500
32	6	0	2.350250	3.951591	-0.212420
33	1	0	2.445950	4.335121	-1.230220
34	1	0	3.349300	3.643581	0.098690
35	1	0	2.000650	4.758681	0.427300
36	8	0	1.030130	-0.795569	-1.018340
37	6	0	2.039240	-1.453979	-0.331500
38	6	0	3.338690	-0.960729	-0.384920
39	8	0	3.687630	0.101371	-1.198510
40	6	0	3.008840	1.293741	-1.329540
41	6	0	1.736440	-2.610189	0.371980
42	1	0	0.725650	-2.994469	0.390010
43	6	0	2.762550	-3.286419	1.029340
44	8	0	2.426800	-4.424299	1.706800
45	1	0	3.218240	-4.803509	2.102300

46	6	0	4.066460	-2.790058	0.986160
47	1	0	4.862040	-3.320638	1.501250
48	6	0	4.374430	-1.627588	0.276770
49	6	0	5.784860	-1.106488	0.189690
50	1	0	6.115230	-1.046908	-0.850370
51	1	0	6.472870	-1.751388	0.738360
52	1	0	5.858050	-0.095238	0.599030
53	8	0	3.527860	2.125241	-2.022790
54	8	0	-2.119480	2.324191	0.764690
55	1	0	-2.602230	1.484901	0.905430
56	8	0	-4.916720	-2.300229	0.153190

Conformer **IIb**-3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.466309	-2.347301	0.326950
2	8	0	-3.260069	-3.379581	0.762320
3	6	0	-3.236358	-4.567151	-0.040620
4	1	0	-3.951068	-5.251811	0.414900
5	1	0	-2.244098	-5.022711	-0.040400
6	1	0	-3.546738	-4.347701	-1.068030
7	6	0	-1.070969	-2.442970	0.494590
8	6	0	-0.239689	-1.370870	0.140410
9	6	0	1.269721	-1.434410	0.290910
10	6	0	1.970011	-2.051200	-0.927270
11	1	0	1.687821	-3.104230	-1.020800
12	6	0	3.512041	-1.970499	-0.883670
13	8	0	4.076691	-2.735879	0.156460
14	1	0	3.499521	-2.635619	0.925680
15	1	0	3.904991	-2.366359	-1.821980
16	6	0	3.947741	-0.502499	-0.787820
17	8	0	4.263681	-0.011399	-1.995930
18	6	0	4.622410	1.384581	-2.048110
19	1	0	3.757600	2.004881	-1.807150
20	1	0	4.943230	1.563181	-3.071380
21	1	0	5.429130	1.594881	-1.345790
22	1	0	1.606081	-1.532680	-1.818370
23	8	0	1.653481	-2.215020	1.457430
24	6	0	1.530621	-1.497590	2.693980
25	1	0	2.218851	-0.647700	2.700270
26	1	0	1.798871	-2.194490	3.487120
27	1	0	0.505271	-1.147980	2.846370
28	1	0	1.646461	-0.424770	0.439040
29	6	0	-0.837719	-0.227630	-0.390270

30	6	0	-2.217789	-0.113881	-0.579350
31	6	0	-3.052549	-1.201181	-0.212460
32	6	0	-4.554219	-1.155281	-0.353410
33	1	0	-4.849629	-1.312301	-1.393020
34	1	0	-4.952919	-0.182291	-0.064090
35	1	0	-5.004729	-1.927381	0.266520
36	8	0	0.025040	0.785890	-0.799090
37	6	0	-0.131950	1.990190	-0.124970
38	6	0	-1.319940	2.696000	-0.246620
39	8	0	-2.320700	2.310699	-1.121430
40	6	0	-2.810730	1.038449	-1.315350
41	6	0	0.924590	2.479100	0.636500
42	1	0	1.847990	1.912860	0.696960
43	6	0	0.776210	3.705660	1.282030
44	8	0	1.767210	4.259220	2.040760
45	1	0	2.539260	3.683890	2.027860
46	6	0	-0.422891	4.413100	1.173450
47	1	0	-0.512041	5.361790	1.688490
48	6	0	-1.479560	3.925849	0.408020
49	6	0	-2.761251	4.700459	0.249390
50	1	0	-2.715711	5.641849	0.798210
51	1	0	-3.616920	4.126729	0.615830
52	1	0	-2.958331	4.917109	-0.803590
53	8	0	-3.726680	0.932869	-2.084560
54	8	0	-0.585369	-3.591380	1.021820
55	1	0	0.347411	-3.436370	1.263740
56	8	0	3.970611	0.147291	0.232950

Conformer **IIb**-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.364201	-2.316779	-0.643600
2	8	0	-3.035287	-3.328192	-1.285890
3	6	0	-3.262493	-4.513873	-0.513140
4	1	0	-2.319171	-4.990709	-0.239380
5	1	0	-3.836250	-5.184165	-1.152390
6	1	0	-3.842314	-4.285855	0.388070
7	6	0	-0.976141	-2.437314	-0.443320
8	6	0	-0.242765	-1.379961	0.116680
9	6	0	1.270736	-1.464056	0.235700
10	6	0	1.970644	-1.161573	-1.097160
11	1	0	1.611337	-1.848234	-1.868390
12	6	0	3.511985	-1.282337	-1.059880
13	8	0	3.953090	-2.616575	-1.000300

14	1	0	3.534971	-3.004737	-0.220430
15	1	0	3.906693	-0.863356	-1.987790
16	6	0	4.088642	-0.464805	0.101020
17	8	0	4.164287	0.843515	-0.216980
18	6	0	4.686843	1.721227	0.803410
19	1	0	4.117974	1.615505	1.727660
20	1	0	4.584720	2.725177	0.398500
21	1	0	5.734004	1.485681	0.997400
22	1	0	1.686011	-0.151714	-1.402020
23	8	0	1.686511	-2.791204	0.652480
24	6	0	1.553391	-3.022565	2.060310
25	1	0	2.225569	-2.358742	2.611020
26	1	0	1.840265	-4.058933	2.235280
27	1	0	0.520971	-2.868308	2.389710
28	1	0	1.603013	-0.754524	0.995850
29	6	0	-0.936959	-0.229064	0.491670
30	6	0	-2.324960	-0.106959	0.351700
31	6	0	-3.051846	-1.171262	-0.242270
32	6	0	-4.541386	-1.106188	-0.477450
33	1	0	-4.852200	-0.111569	-0.798350
34	1	0	-5.088975	-1.319230	0.443190
35	1	0	-4.824053	-1.833509	-1.235750
36	8	0	-0.180003	0.789829	1.058470
37	6	0	-0.230388	2.011109	0.401770
38	6	0	-1.429660	2.712314	0.345690
39	8	0	-2.562099	2.281450	1.011720
40	6	0	-3.081424	1.005758	0.993310
41	6	0	0.931580	2.527873	-0.151810
42	1	0	1.858763	1.972777	-0.113870
43	6	0	0.888236	3.782323	-0.757620
44	8	0	2.058694	4.265617	-1.272430
45	1	0	1.897931	5.123657	-1.678270
46	6	0	-0.314387	4.487378	-0.822310
47	1	0	-0.343071	5.463508	-1.297710
48	6	0	-1.486995	3.965744	-0.272230
49	6	0	-2.782928	4.732539	-0.304740
50	1	0	-3.553526	4.181076	-0.850340
51	1	0	-2.649172	5.703120	-0.784490
52	1	0	-3.168088	4.891018	0.705530
53	8	0	-4.149233	0.859644	1.522470
54	8	0	-0.388136	-3.592152	-0.832460
55	1	0	0.504274	-3.617908	-0.436970
56	8	0	4.401823	-0.917834	1.172870

Conformer **IIIa**-9					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.435483	3.258198	0.495900
2	8	0	0.385676	4.547098	0.967600
3	6	0	-0.476028	5.441893	0.251100
4	1	0	-0.176929	5.512095	-0.800400
5	1	0	-0.359533	6.415594	0.726000
6	1	0	-1.518127	5.124088	0.321200
7	6	0	-0.646913	2.394693	0.750400
8	6	0	-0.582306	1.037493	0.392200
9	6	0	-1.805102	0.141587	0.549000
10	6	0	-2.771803	0.343882	-0.625300
11	1	0	-3.081708	1.391281	-0.658100
12	6	0	-4.084199	-0.473024	-0.574200
13	8	0	-5.047902	0.116271	-1.423200
14	1	0	-5.087699	-0.436929	-2.216500
15	1	0	-4.464499	-0.459826	0.450000
16	6	0	-3.880692	-1.920723	-1.002500
17	8	0	-3.248388	-2.665020	-0.082200
18	6	0	-3.042181	-4.051119	-0.438300
19	1	0	-2.379981	-4.126216	-1.301400
20	1	0	-3.995979	-4.522924	-0.674100
21	1	0	-2.590079	-4.511517	0.436500
22	1	0	-2.240402	0.140985	-1.559500
23	8	0	-2.548604	0.463083	1.748800
24	6	0	-1.999401	-0.075514	2.949500
25	1	0	-0.964503	0.251491	3.101400
26	1	0	-2.039695	-1.169314	2.929400
27	1	0	-2.616403	0.291383	3.769400
28	1	0	-1.496197	-0.901212	0.601300
29	6	0	0.587696	0.578199	-0.221700
30	6	0	1.627792	1.448904	-0.589700
31	6	0	1.556485	2.812803	-0.198400
32	6	0	2.665580	3.799209	-0.475200
33	1	0	2.606576	4.619509	0.237800
34	1	0	2.582178	4.203109	-1.486400
35	1	0	3.647082	3.330414	-0.407300
36	8	0	0.633703	-0.775801	-0.528600
37	6	0	1.776106	-1.467395	-0.123600
38	6	0	3.007704	-1.150589	-0.681400
39	8	0	3.138300	-0.210289	-1.676800
40	6	0	2.640493	1.075409	-1.615000

41	6	0	1.674311	-2.526596	0.787700
42	6	0	0.348713	-2.912603	1.389600
43	1	0	0.418718	-3.888302	1.872700
44	1	0	-0.435087	-2.954906	0.632300
45	1	0	0.033910	-2.188204	2.145900
46	6	0	2.826515	-3.235390	1.123100
47	1	0	2.775819	-4.063991	1.818800
48	6	0	4.065113	-2.900984	0.574500
49	8	0	5.143517	-3.641279	0.961700
50	1	0	5.930515	-3.324075	0.506900
51	6	0	4.158208	-1.853084	-0.335900
52	1	0	5.094907	-1.575879	-0.805800
53	8	0	3.046290	1.836511	-2.449400
54	8	0	-1.727516	2.929987	1.359900
55	1	0	-2.317012	2.193984	1.622000
56	8	0	-4.251990	-2.343325	-2.071900

Conformer **IIIa**-14

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.685863	3.287587	0.346000
2	8	0	0.757290	4.604685	0.730200
3	6	0	-0.038491	5.521102	-0.032600
4	1	0	0.174929	6.511297	0.369100
5	1	0	-1.102796	5.304024	0.078400
6	1	0	0.240008	5.491296	-1.091800
7	6	0	-0.461252	2.540310	0.676400
8	6	0	-0.516881	1.162411	0.412300
9	6	0	-1.793097	0.369338	0.658200
10	6	0	-2.753495	0.487157	-0.532200
11	1	0	-3.074873	1.526364	-0.641300
12	6	0	-4.041212	-0.359916	-0.410600
13	8	0	-5.009604	0.041604	-1.360600
14	1	0	-4.776812	-0.362101	-2.204200
15	1	0	-4.476109	-0.192407	0.575100
16	6	0	-3.692043	-1.841523	-0.500700
17	8	0	-3.908952	-2.325219	-1.738000
18	6	0	-3.556281	-3.707426	-1.956700
19	1	0	-3.876786	-3.932019	-2.970900
20	1	0	-4.069494	-4.344915	-1.236900
21	1	0	-2.478484	-3.840448	-1.855900
22	1	0	-2.216000	0.215646	-1.446000
23	8	0	-2.515587	0.856253	1.813300
24	6	0	-2.044598	0.342043	3.059700

25	1	0	-2.637988	0.818455	3.839600
26	1	0	-0.985793	0.577821	3.216100
27	1	0	-2.192620	-0.741154	3.100900
28	1	0	-1.545219	-0.677167	0.824000
29	6	0	0.593107	0.563789	-0.192700
30	6	0	1.694922	1.314366	-0.637600
31	6	0	1.749251	2.702065	-0.334500
32	6	0	2.932969	3.568341	-0.691800
33	1	0	2.850376	3.935942	-1.717100
34	1	0	3.869157	3.013921	-0.634500
35	1	0	2.974686	4.421340	-0.016500
36	8	0	0.505679	-0.803810	-0.413500
37	6	0	1.591563	-1.577532	0.001200
38	6	0	2.824966	-1.408857	-0.612900
39	8	0	3.002784	-0.541061	-1.667100
40	6	0	2.640712	0.790047	-1.660200
41	6	0	1.424643	-2.565828	0.981600
42	6	0	0.097338	-2.789701	1.657600
43	1	0	-0.144845	-1.959296	2.326900
44	1	0	0.126819	-3.699302	2.259100
45	1	0	-0.723064	-2.880684	0.944400
46	6	0	2.521626	-3.356751	1.320700
47	1	0	2.423010	-4.132649	2.069900
48	6	0	3.763830	-3.173377	0.712400
49	8	0	4.784413	-3.987498	1.110400
50	1	0	5.580918	-3.767214	0.616600
51	6	0	3.919550	-2.193480	-0.262800
52	1	0	4.859854	-2.031599	-0.777400
53	8	0	3.097325	1.463737	-2.543100
54	8	0	-1.480839	3.203631	1.264300
55	1	0	-2.125253	2.535945	1.578100
56	8	0	-3.223956	-2.491833	0.402800

Conformer **IIIa**-26

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.832814	2.979488	0.501404
2	8	0	-1.357816	4.196287	0.864704
3	6	0	-2.666616	4.486485	0.358504
4	1	0	-3.405215	3.786984	0.755404
5	1	0	-2.676316	4.457985	-0.736796
6	1	0	-2.902918	5.495385	0.695604
7	6	0	-1.319113	1.812787	1.119304
8	6	0	-0.729211	0.562188	0.862304

9	6	0	-1.300709	-0.695813	1.505604
10	6	0	-2.513008	-1.261814	0.748404
11	1	0	-3.060508	-1.909015	1.439604
12	6	0	-2.088107	-2.109714	-0.462696
13	8	0	-1.356106	-3.244713	-0.041296
14	1	0	-1.907705	-4.013414	-0.251096
15	1	0	-1.463208	-1.512813	-1.135096
16	6	0	-3.307207	-2.571916	-1.251096
17	8	0	-3.973708	-1.558516	-1.809496
18	6	0	-5.145608	-1.914018	-2.574996
19	1	0	-4.872907	-2.582218	-3.392196
20	1	0	-5.535009	-0.974419	-2.958196
21	1	0	-5.879707	-2.405619	-1.935796
22	1	0	-3.176710	-0.454515	0.430504
23	8	0	-1.765610	-0.427913	2.851104
24	6	0	-0.725410	-0.320412	3.822604
25	1	0	-1.204910	-0.066013	4.767404
26	1	0	-0.003911	0.460789	3.559404
27	1	0	-0.203408	-1.276911	3.930104
28	1	0	-0.536908	-1.469712	1.554804
29	6	0	0.338489	0.517589	-0.040396
30	6	0	0.780788	1.658590	-0.728696
31	6	0	0.195986	2.917889	-0.434696
32	6	0	0.662784	4.204190	-1.072396
33	1	0	1.741084	4.205891	-1.231196
34	1	0	0.389883	5.044490	-0.436696
35	1	0	0.203684	4.340089	-2.054096
36	8	0	0.873191	-0.735410	-0.309096
37	6	0	2.252591	-0.884408	-0.162296
38	6	0	3.119590	-0.145507	-0.958696
39	8	0	2.681389	0.656993	-1.988796
40	6	0	1.646288	1.561991	-1.935696
41	6	0	2.761692	-1.843607	0.724104
42	6	0	1.846694	-2.728909	1.531004
43	1	0	1.474493	-2.203709	2.416404
44	1	0	2.386695	-3.610808	1.879104
45	1	0	0.983894	-3.054610	0.947804
46	6	0	4.144393	-1.993205	0.823304
47	1	0	4.566194	-2.731405	1.494504
48	6	0	5.012691	-1.213004	0.060204
49	8	0	6.352492	-1.413602	0.228504
50	1	0	6.839191	-0.836702	-0.368996
51	6	0	4.499090	-0.289505	-0.844796

52	1	0	5.136289	0.301496	-1.492796
53	8	0	1.492987	2.243891	-2.912296
54	8	0	-2.356813	1.957886	1.973304
55	1	0	-2.440512	1.122286	2.478704
56	8	0	-3.621405	-3.736116	-1.343896

Conformer **IIIb**-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.201324	3.162592	0.540205
2	8	0	-0.006165	4.441794	0.997805
3	6	0	-1.059858	5.169103	0.354505
4	1	0	-1.050750	6.165803	0.794905
5	1	0	-2.028962	4.699411	0.535805
6	1	0	-0.878958	5.247001	-0.723395
7	6	0	-0.697784	2.147900	0.920605
8	6	0	-0.450496	0.808998	0.577505
9	6	0	-1.442505	-0.290894	0.927005
10	6	0	-2.508707	-0.464985	-0.157795
11	1	0	-3.107399	0.445920	-0.243295
12	6	0	-3.424617	-1.666377	0.136905
13	8	0	-2.676228	-2.860683	0.266805
14	1	0	-2.898632	-3.402081	-0.505595
15	1	0	-3.955716	-1.477372	1.075005
16	6	0	-4.454019	-1.842168	-0.969895
17	8	0	-5.312910	-0.821461	-1.042795
18	6	0	-6.305311	-0.901252	-2.089095
19	1	0	-6.917618	-1.794147	-1.960395
20	1	0	-5.822311	-0.932356	-3.066195
21	1	0	-6.906803	-0.001947	-1.984695
22	1	0	-1.996908	-0.627489	-1.110495
23	8	0	-2.141503	-0.011788	2.162805
24	6	0	-1.413206	-0.367894	3.338205
25	1	0	-0.444402	0.142197	3.380105
26	1	0	-1.259815	-1.450996	3.376205
27	1	0	-2.019703	-0.060089	4.189605
28	1	0	-0.916614	-1.236498	1.036205
29	6	0	0.692402	0.525188	-0.177995
30	6	0	1.546010	1.534880	-0.647595
31	6	0	1.306222	2.879282	-0.257295
32	6	0	2.219332	4.016575	-0.647295
33	1	0	1.973435	4.388077	-1.644595
34	1	0	3.261729	3.700866	-0.682095
35	1	0	2.111539	4.830475	0.067505

36	8	0	0.882590	-0.806114	-0.524995
37	6	0	2.128385	-1.364525	-0.239595
38	6	0	3.272690	-0.861135	-0.855295
39	8	0	3.214598	0.111766	-1.828295
40	6	0	2.514308	1.294072	-1.752095
41	6	0	2.219076	-2.481325	0.596605
42	6	0	0.997770	-3.099415	1.228105
43	1	0	0.149570	-3.124608	0.543305
44	1	0	0.686675	-2.539012	2.115305
45	1	0	1.210662	-4.121217	1.547105
46	6	0	3.479671	-3.040936	0.823805
47	1	0	3.559263	-3.913937	1.465305
48	6	0	4.627075	-2.506346	0.239005
49	8	0	5.873071	-3.022557	0.448905
50	1	0	5.808565	-3.774956	1.045805
51	6	0	4.523585	-1.411845	-0.614295
52	1	0	5.394888	-1.009553	-1.112695
53	8	0	2.719215	2.085970	-2.630995
54	8	0	-1.782081	2.524909	1.635005
55	1	0	-2.214688	1.709813	1.962905
56	8	0	-4.466227	-2.804368	-1.702595

Conformer **IIIb**-15

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.194607	3.159899	0.538705
2	8	0	-0.015990	4.439100	0.994805
3	6	0	-1.072188	5.163002	0.351505
4	1	0	-2.039689	4.690204	0.533105
5	1	0	-0.891588	5.241302	-0.726395
6	1	0	-1.066086	6.159802	0.791905
7	6	0	-0.702895	2.143601	0.918605
8	6	0	-0.452498	0.804901	0.576605
9	6	0	-1.444301	-0.295697	0.924705
10	6	0	-2.510502	-0.467594	-0.160695
11	1	0	-3.107699	0.444407	-0.246195
12	6	0	-3.428604	-1.667592	0.133505
13	8	0	-2.682307	-2.862794	0.263805
14	1	0	-2.902609	-3.403293	-0.509895
15	1	0	-3.959804	-1.477591	1.071305
16	6	0	-4.457905	-1.840790	-0.973895
17	8	0	-5.316402	-0.819488	-1.044695
18	6	0	-6.309103	-0.897085	-2.090795
19	1	0	-6.921705	-1.790084	-1.963395

20	1	0	-5.826503	-0.926786	-3.068095
21	1	0	-6.910300	0.002216	-1.984695
22	1	0	-1.998702	-0.630896	-1.113295
23	8	0	-2.143500	-0.017195	2.160505
24	6	0	-1.417601	-0.378497	3.336205
25	1	0	-0.447400	0.128601	3.380505
26	1	0	-1.267604	-1.462097	3.371605
27	1	0	-2.024401	-0.070896	4.187505
28	1	0	-0.918803	-1.241598	1.032605
29	6	0	0.692901	0.522098	-0.175395
30	6	0	1.545703	1.533496	-0.644595
31	6	0	1.301606	2.878096	-0.256195
32	6	0	2.213009	4.017594	-0.644195
33	1	0	2.100411	4.831595	0.069805
34	1	0	1.969310	4.387995	-1.642495
35	1	0	3.256408	3.704892	-0.675395
36	8	0	0.885698	-0.809103	-0.518495
37	6	0	2.132896	-1.365006	-0.233295
38	6	0	3.272098	-0.862308	-0.850095
39	8	0	3.218400	0.111492	-1.822195
40	6	0	2.518403	1.295394	-1.744995
41	6	0	2.227194	-2.483106	0.607005
42	6	0	1.005492	-3.097303	1.241205
43	1	0	0.686194	-2.522802	2.116405
44	1	0	1.223990	-4.111403	1.579005
45	1	0	0.161492	-3.138801	0.551705
46	6	0	3.483792	-3.042909	0.834005
47	1	0	3.586290	-3.911709	1.472705
48	6	0	4.630394	-2.509912	0.245305
49	8	0	5.822092	-3.111314	0.530705
50	1	0	6.528193	-2.664116	0.053105
51	6	0	4.525296	-1.416811	-0.608795
52	1	0	5.384097	-0.997313	-1.120395
53	8	0	2.730905	2.089193	-2.620595
54	8	0	-1.788594	2.518404	1.631305
55	1	0	-2.218596	1.702305	1.960905
56	8	0	-4.470507	-2.801390	-1.708695

Table S4. Experimental (**1** and **2**) and computed (a and b) ^{13}C-NMR chemical shifts.

Position	**1**	**Ia**	**Ib**	**2**	**Ia**	**Ib**
1	113.6	116.4	116.3	113.7	116.3	116.2
2	156.2	153.7	153.6	156.2	153.8	153.7
3	113.8	114.1	114.0	113.7	114.0	113.9
4	154.2	148.1	147.8	154.2	148.1	147.9
5	144.5	142.1	142.2	144.6	142.1	142.2
6	137.2	130.3	130.5	137.3	130.3	130.4
7	163.8	163.2	163.3	163.7	163.3	163.3
8	75.9	78.9	80.1	75.4	78.7	79.9
9	40.2	40.3	42.3	38.7	40.0	42.0
10	67.3	69.3	68.4	67.4	69.0	68.2
11	175.4	179.0	179.0	175.6	179.1	179.1
12	14.4	16.4	15.6	14.4	16.0	15.3
1′	153.3	153.1	152.9	153.1	153.1	152.9
2′	143.4	138.3	138.4	143.5	138.3	138.4
3′	131.0	134.2	134.4	131.0	134.2	134.4
4′	114.5	116.0	115.9	114.5	116.0	115.8
5′	144.6	157.6	157.5	144.7	157.6	157.6
6′	106.0	101.3	101.0	106.0	101.2	100.9
7′	18.2	19.9	19.3	18.1	19.6	19.0
8-OCH_3	58.1	58.0	58.0	57.9	57.8	57.8
11-OCH_3	60.4	54.2	54.1	60.4	54.0	53.9
5′-OCH_3	52.9	54.8	54.4	52.8	54.5	54.2

Position	**1**	**IIa**	**IIb**	**2**	**IIa**	**IIb**
1	113.6	114.2	113.7	113.7	114.1	113.6
2	156.2	155.3	155.0	156.2	155.3	155.1
3	113.8	114.5	113.0	113.7	114.4	112.9
4	154.2	155.3	155.2	154.2	155.4	155.3
5	144.5	142.9	143.3	144.6	142.9	143.3
6	137.2	139.3	140.9	137.3	139.3	140.9
7	163.8	161.7	161.3	163.7	161.8	161.3
8	75.9	75.3	80.0	75.4	75.1	79.9
9	40.2	40.5	38.5	38.7	40.2	38.2
10	67.3	68.5	71.9	67.4	68.3	71.7
11	175.4	176.7	175.8	175.6	176.8	175.9
12	14.4	16.3	15.5	14.4	15.9	15.1
1′	144.6	150.9	150.6	144.7	150.9	150.6
2′	143.4	136.9	136.7	143.5	136.9	136.7
3′	131.0	133.0	133.2	131.0	133.0	133.2
4′	114.5	112.2	112.1	114.5	112.1	112.0

5′	153.3	153.1	152.8	153.1	153.2	152.9
6′	106.0	105.2	104.2	106.0	105.1	104.1
7′	18.2	19.4	18.9	18.1	19.1	18.6
5-OCH_3	52.9	57.7	57.7	52.8	57.5	57.5
8-OCH_3	58.1	56.7	56.6	57.9	56.5	56.3
11-OCH_3	60.4	53.4	52.4	60.4	53.2	52.1

Position	**1**	**IIIa**	**IIIb**	**2**	**IIIa**	**IIIb**
1	113.8	113.32	113.1	113.7	113.24	113.02
2	156.2	157.69	156.76	156.2	157.73	156.8
3	113.8	112.23	112.74	113.7	112.15	112.66
4	154.2	155.87	155.91	154.2	155.91	155.95
5	144.5	142.66	142.43	144.6	142.66	142.43
6	137.2	141.61	141.34	137.3	141.61	141.34
7	163.8	161.45	161.43	163.7	161.5	161.48
8	75.9	77.36	77.49	75.4	77.18	77.31
9	40.2	44.28	42.09	38.7	44.01	41.81
10	67.3	67.06	67.19	67.4	66.85	66.98
11	175.4	176.48	177.03	175.6	176.57	177.12
12	14.4	15.72	15.79	14.4	15.37	15.44
1′	143.4	142.55	142.79	143.5	142.55	142.8
2′	144.6	144.66	145.19	144.7	144.67	145.2
3′	106.0	102.64	103.67	106.0	102.53	103.56
4′	153.3	152.96	153	153.1	152.99	153.03
5′	114.5	112.26	111.75	114.5	112.17	111.67
6′	131.0	133.17	132.66	131.0	133.15	132.63
7′	18.2	19.5	19.93	18.1	19.16	19.59
5-OCH_3	52.9	57.44	57.56	52.8	57.21	57.32
8-OCH_3	58.1	55.19	56.15	57.9	54.95	55.91
11-OCH_3	60.4	52.99	53.1	60.4	52.74	52.85

Table S5. Experimental (**1** and **2**) and computed (a and b) ^{1}H-NMR chemical shifts.

Position	**1**	**Ia**	**Ib**	**2**	**Ia**	**Ib**
8	5.65	5.58	5.48	5.65	5.55	5.45
9a	1.93	2.43	2.34	2.25	2.48	2.39
9b	2.41	2.43	2.04	2.45	2.47	2.09
10	4.53	4.42	4.60	4.36	4.41	4.59
12	2.38	2.37	2.47	2.39	2.41	2.51
4′	6.47	6.64	6.59	6.47	6.59	6.53
6′	6.65	6.67	6.61	6.63	6.61	6.54
7′	2.46	2.31	2.42	2.47	2.35	2.46
8-OCH_3	3.54	3.28	3.53	3.40	3.31	3.55

11-OCH_3	3.79	3.75	3.76	3.79	3.76	3.77
5′-OCH_3	3.78	3.71	3.76	3.81	3.72	3.78
4-OH	9.07	9.17	9.09	9.27	9.34	9.28

Position	**1**	**IIa**	**IIb**	**2**	**IIa**	**IIb**
8	5.65	5.51	5.53	5.65	5.48	5.49
9a	1.93	2.15	2.01	2.25	2.20	2.08
9b	2.41	2.60	2.53	2.45	2.65	2.58
10	4.53	4.39	4.43	4.36	4.39	4.43
12	2.38	2.43	2.43	2.39	2.48	2.48
4′	6.47	6.39	6.57	6.47	6.34	6.51
6′	6.65	6.94	6.67	6.63	6.87	6.60
7′	2.46	2.35	2.28	2.47	2.40	2.34
5-OCH_3	3.78	3.78	3.83	3.81	3.79	3.84
8-OCH_3	3.54	3.29	3.48	3.40	3.32	3.50
11-OCH_3	3.79	3.75	3.83	3.79	3.76	3.84
4-OH	9.07	9.17	9.09	9.27	9.34	9.28

Position	II	3a	3b	I	3a	3b
8	5.65	5.66	5.74	5.65	5.61	5.68
9a	1.93	2.18	1.78	2.25	2.24	1.87
9b	2.41	2.15	2.27	2.45	2.21	2.33
10	4.53	4.35	4.63	4.36	4.34	4.61
12	2.38	2.46	2.48	2.39	2.51	2.53
3′	6.65	6.41	6.46	6.63	6.34	6.38
5′	6.47	6.66	6.47	6.47	6.57	6.39
7′	2.46	2.64	2.62	2.47	2.69	2.68
5-OCH_3	3.78	3.84	3.84	3.81	3.85	3.85
8-OCH_3	3.54	3.46	3.55	3.40	3.48	3.57
11-OCH_3	3.79	3.71	3.73	3.79	3.72	3.75
4-OH	9.27	9.34	9.28	9.07	9.17	9.09

Table S6. Statistics of Ordinary Least Squares Linear Regression (OLS-LR) of experimental and computed ^{13}C- and ^{1}H-NMR chemical shifts.

Type	Experimental	Compound	CMAD[a]	CLAD[b]	R^2	*RMSE*	*F*	*p* value
C	**2**	**Ia**	3.2	12.9	0.9920	4.6	2482.05	< 0.01
C	**2**	**Ib**	3.2	12.9	0.9917	4.6	2399.26	< 0.01
C	**2**	**IIa**	2.1	7.2	0.9963	3.1	5439.24	< 0.01
C	**2**	**IIb**	2.5	8.3	0.9951	3.6	4095.03	< 0.01
C	**2**	**IIIa**	**2.2**	**7.7**	**0.9965**	3.0	5744.66	< 0.01
C	**2**	**IIIb**	**2.0**	**7.6**	**0.9971**	2.7	6931.61	< 0.01
C	**1**	**Ia**	3.2	13.0	0.9921	4.5	2497.03	< 0.01

C	**1**	**Ib**	3.2	12.9	0.9919	4.6	2454.72	< 0.01
C	**1**	**IIa**	2.1	7.0	0.9964	3.1	5462.78	< 0.01
C	**1**	**IIb**	2.6	8.0	0.9951	3.6	4061.24	< 0.01
C	**1**	**IIIa**	**2.1**	**7.4**	**0.9968**	2.9	6199.11	< 0.01
C	**2**	**IIIb**	**2.0**	**7.3**	**0.9973**	2.7	7277.87	< 0.01
H	**2**	**Ia**	0.08	0.23	0.9959	0.11	2162.44	< 0.01
H	**2**	**Ib**	0.13	0.36	0.9892	0.18	821.91	< 0.01
H	**2**	**IIa**	0.10	0.24	0.9938	0.14	1432.35	< 0.01
H	**2**	**IIb**	0.09	0.17	0.9956	0.11	2051.67	< 0.01
H	**2**	**IIIa**	**0.11**	**0.29**	**0.9952**	0.16	2079.63	< 0.01
H	**2**	**IIIb**	**0.15**	**0.38**	**0.9923**	0.20	1283.78	< 0.01
H	**1**	**Ia**	0.13	0.50	0.9859	0.21	629.48	< 0.01
H	**1**	**Ib**	0.13	0.41	0.9869	0.20	675.50	< 0.01
H	**1**	**IIa**	0.14	0.29	0.9898	0.18	869.99	< 0.01
H	**1**	**IIb**	0.08	0.18	0.9966	0.10	2599.94	< 0.01
H	**1**	**IIIa**	**0.14**	**0.26**	**0.9942**	0.18	1708.42	< 0.01
H	**1**	**IIIb**	**0.09**	**0.19**	**0.9975**	0.12	3932.50	< 0.01

[a] CMAD = corrected mean absolute deviation, computed as $(1/n)\sum_{i}^{n}|\delta_{calc}-\delta_{exp}|$, where δ_{calc} and δ_{exp} refer to the calculated and experimental chemical shifts. [b] CLAD = corrected largest absolute deviation, computed as $\max(|\delta_{calc}-\delta_{exp}|)$.