Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Applanmerotic acids A and B, two meroterpenoid dimers with an unprecedented polycyclic skeleton from *Ganoderma applanatum* that inhibit formyl peptide receptor 2

Xingrong Peng,[a,‡] Haiguo Su,[a,b,‡], Huirong Wang,[c] Guilin Hu,[a,b], Kun Hu,[a] Lin Zhou,[a] Minghua Qiu[*,a]

[a]*State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Science, Kunming 650201, People's Republic of China*

[b]*University of the Chinese Academy of Science, Beijing 100049, People's Republic of China*

[c]*Department of Biology, Southern University of Science and Technology, Shenzhen, China*

Contents

1D and 2D NMR spectra of compound 1

Figure S1. ^{1}H NMR (600 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).

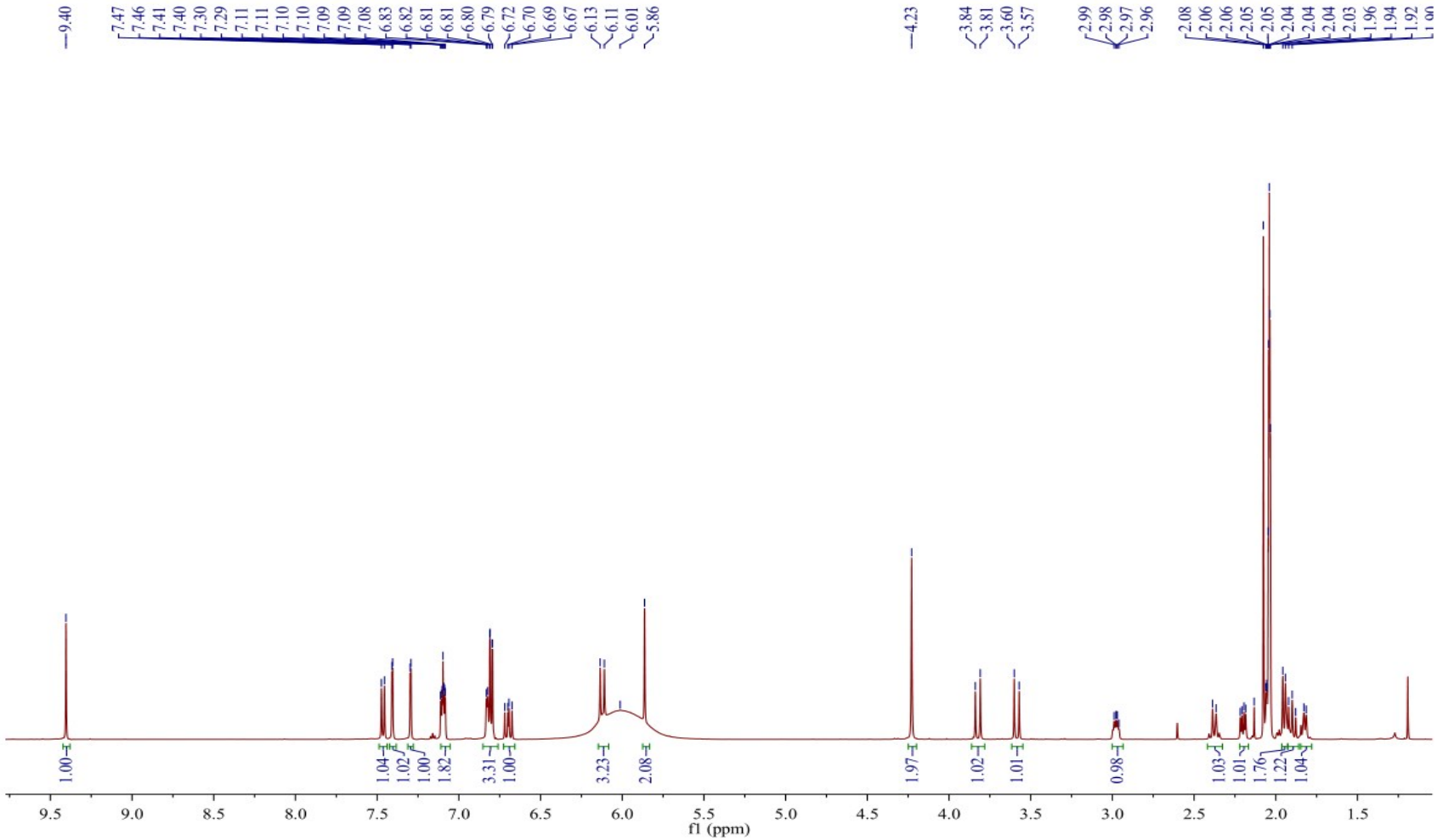


Figure S2. ^{13}C NMR (150 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).

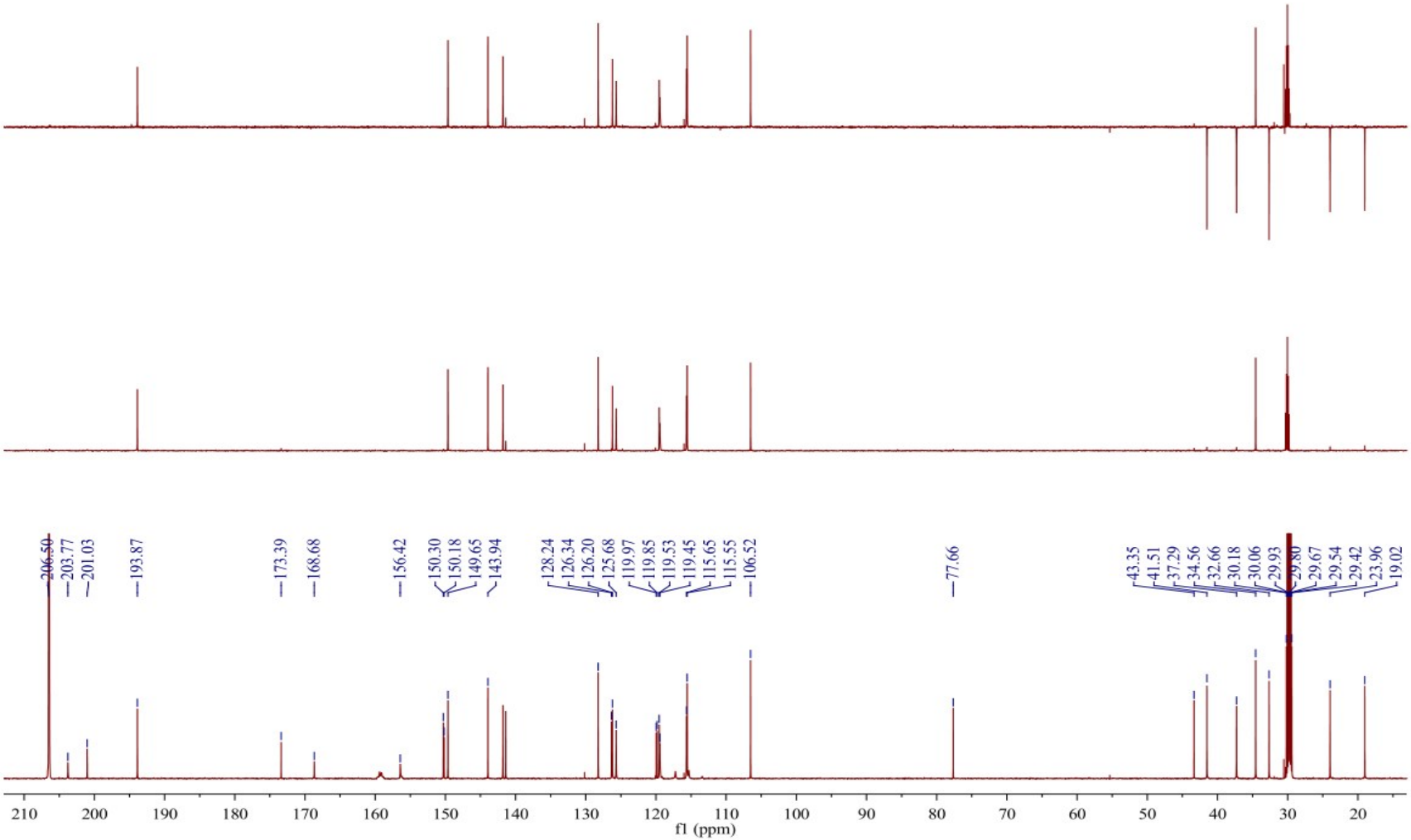


Figure S3. ^{1}H-^{1}H COSY (600 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).

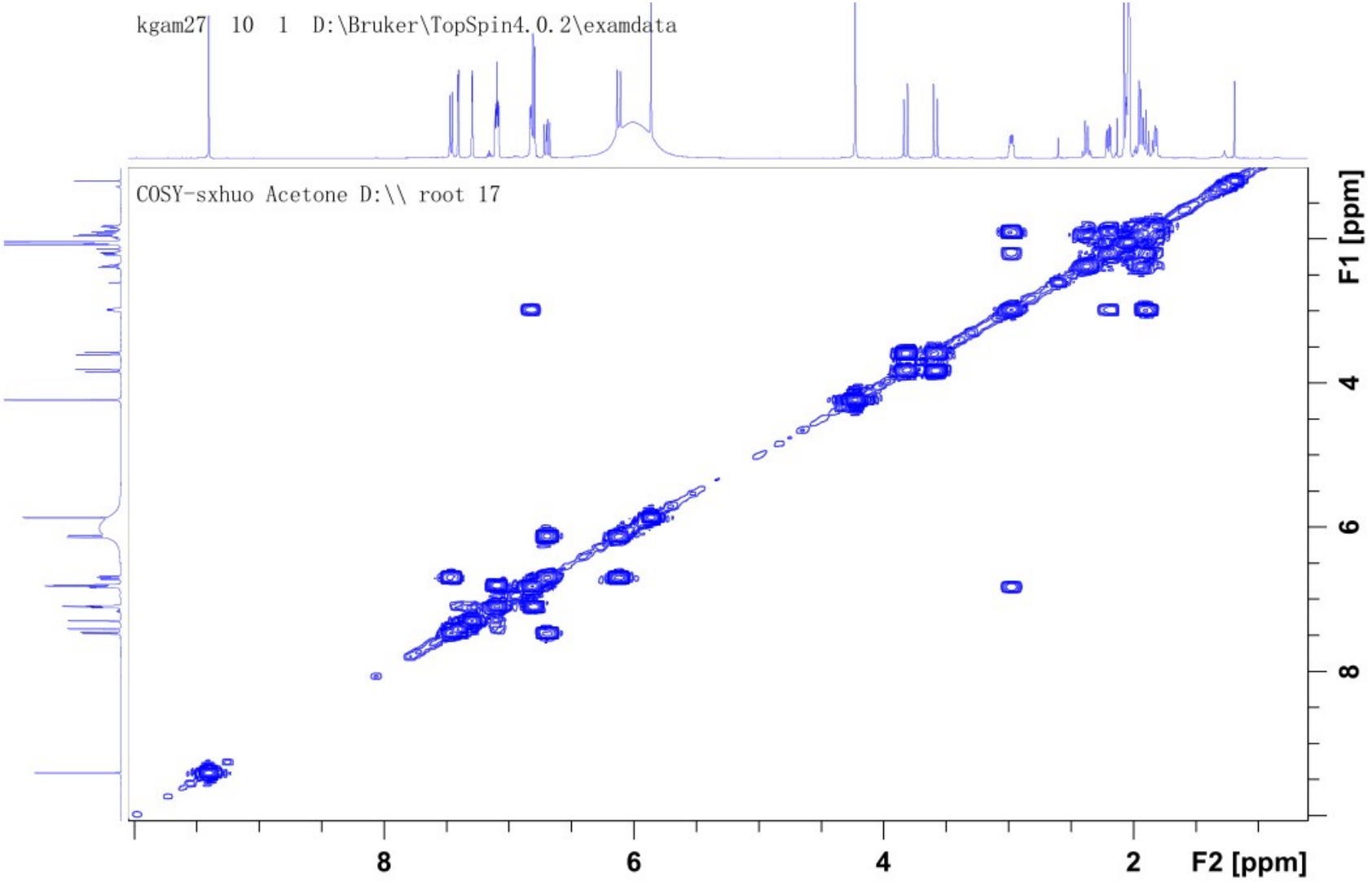


Figure S4. HSQC (600/150 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).

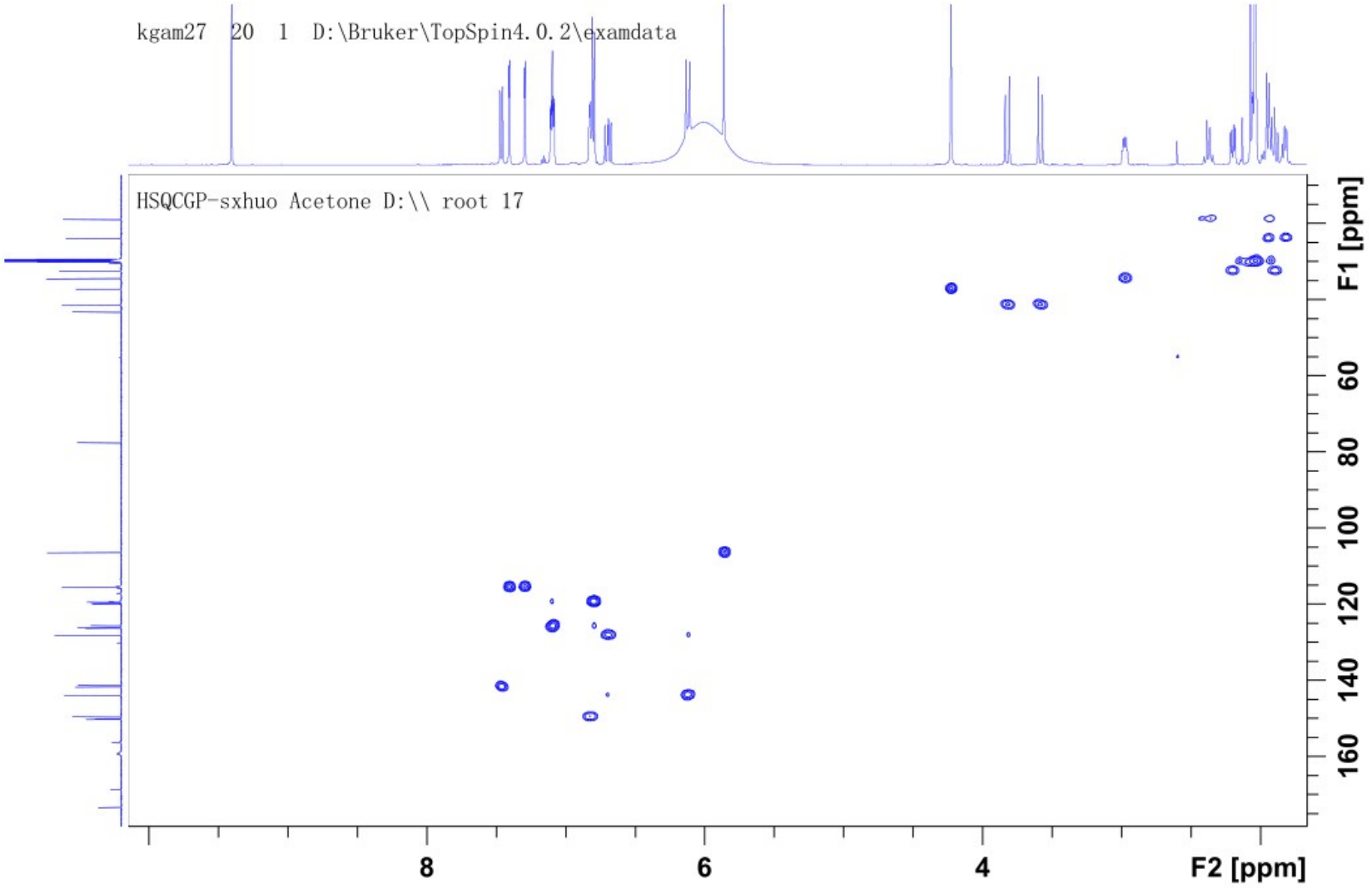


Figure S5. HMBC (600/150 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).

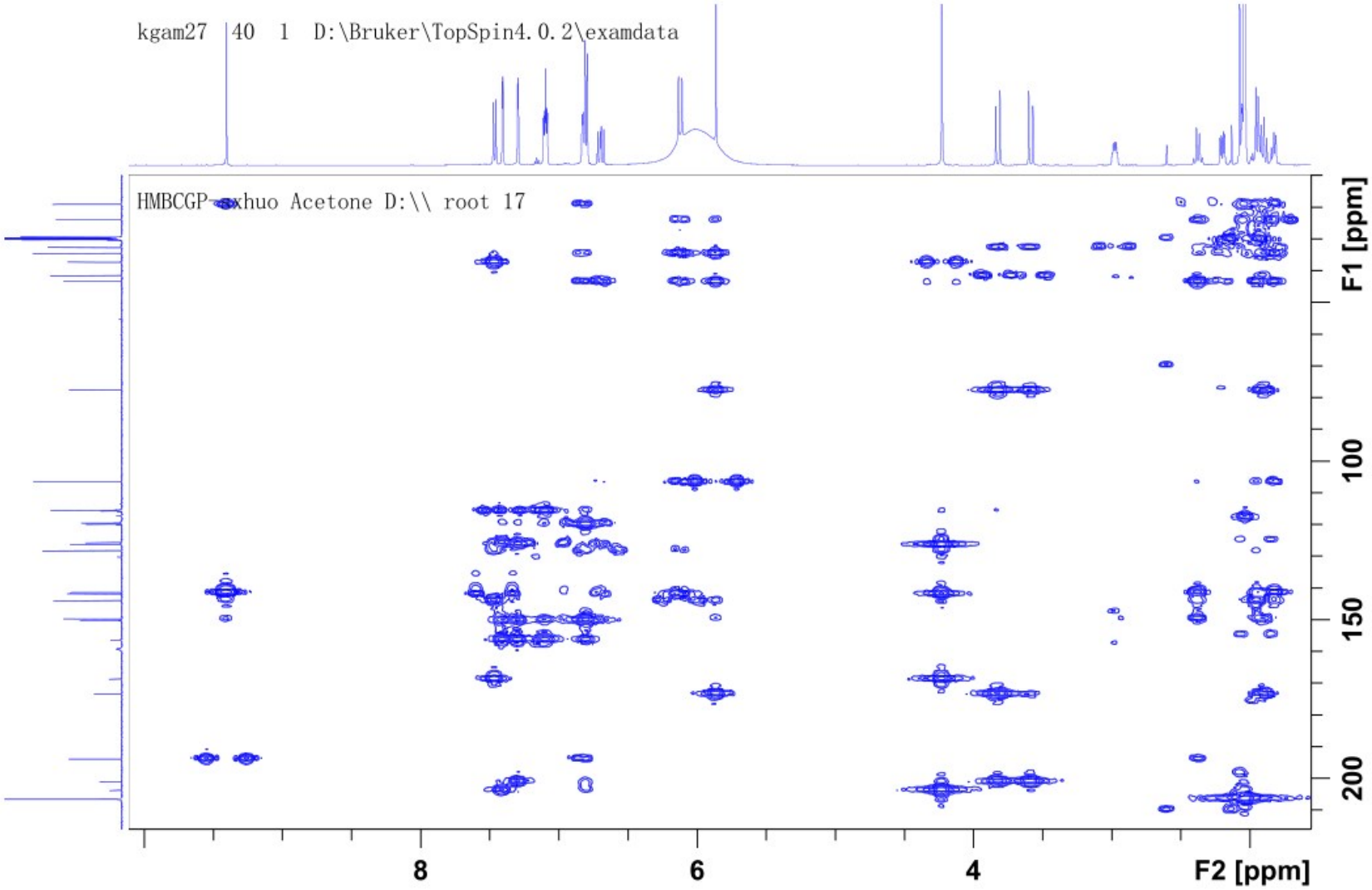
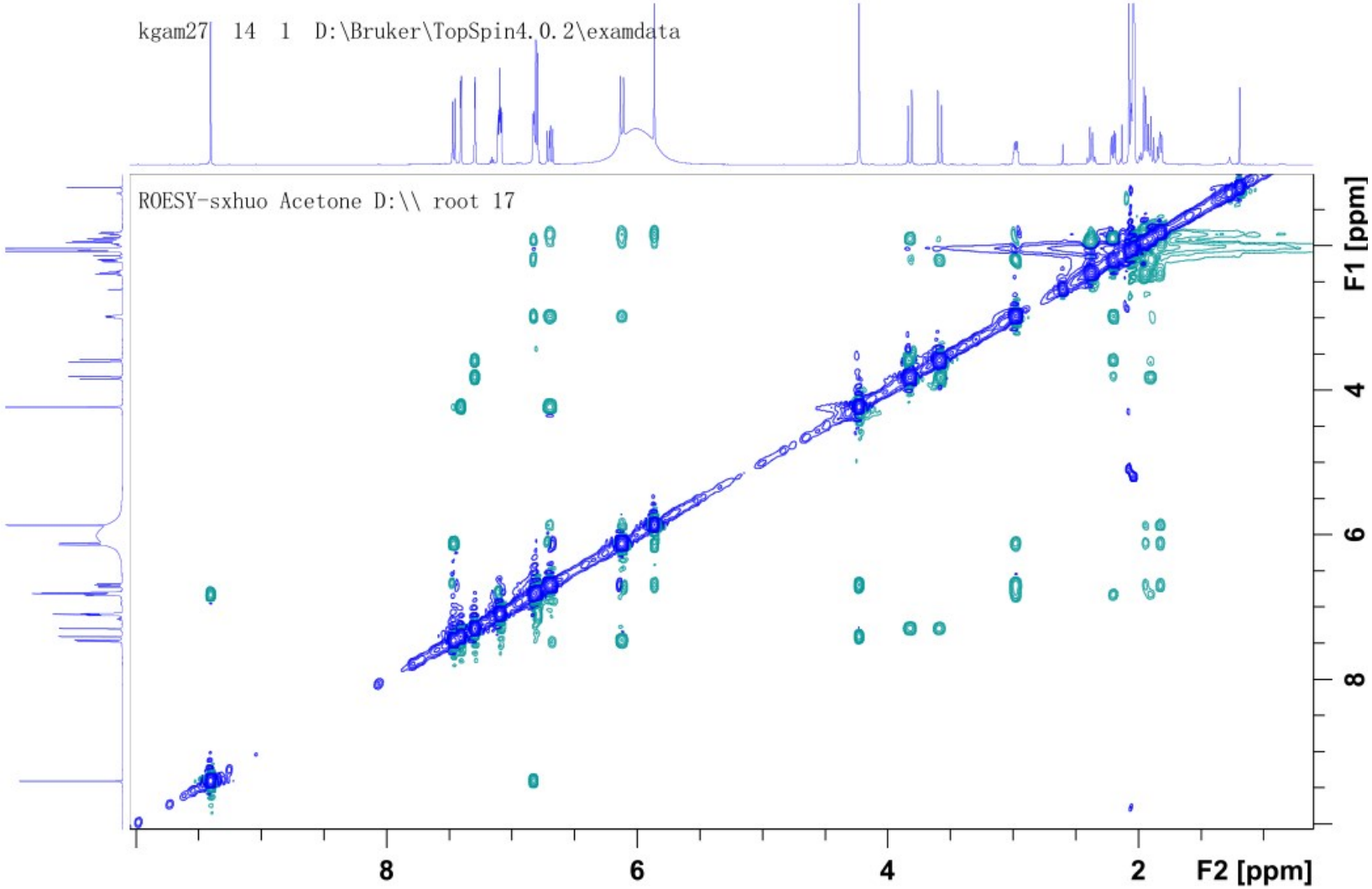
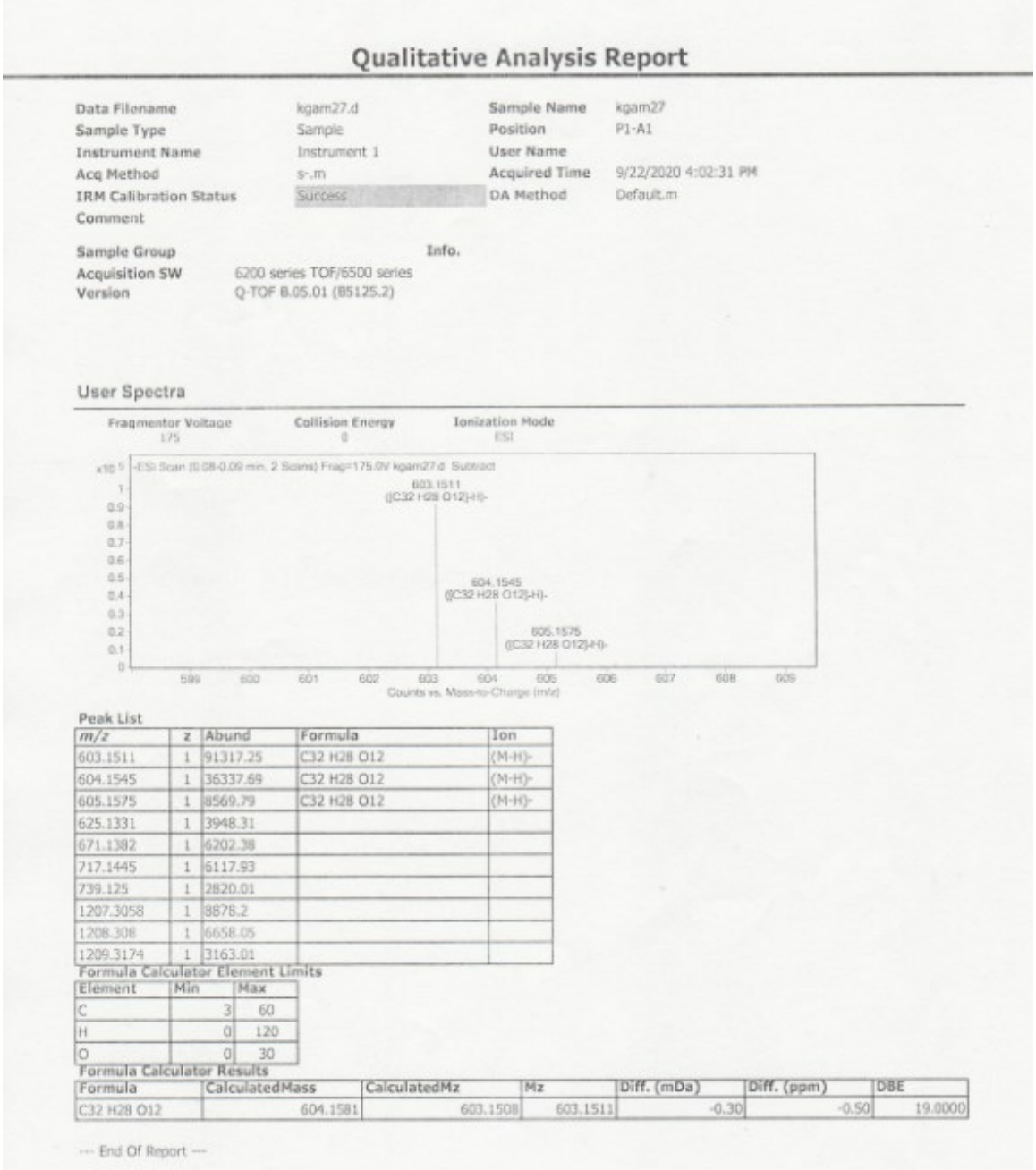


Figure S6. ROESY (600 MHz, $CO(CD_3)_2$) spectrum of applanmerotic acid A (1).



HRESIMS, CD spectra, as well as computational NMR and ECD data of 1

Figure S7. HRESIMS spectrum of applanmerotic acid A (1).



Qualitative Analysis Report

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Instrument Name	Instrument 1	User Name	
Acq Method	s-.m	Acquired Time	9/22/2020 4:02:31 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group — Info.

Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
603.1511	1	91317.25	C32 H28 O12	(M-H)-
604.1545	1	36337.69	C32 H28 O12	(M-H)-
605.1575	1	8569.79	C32 H28 O12	(M-H)-
625.1331	1	3948.31		
671.1382	1	6202.38		
717.1445	1	6117.93		
739.125	1	2820.01		
1207.3058	1	8878.2		
1208.308	1	6658.05		
1209.3174	1	3163.01		

Formula Calculator Element Limits

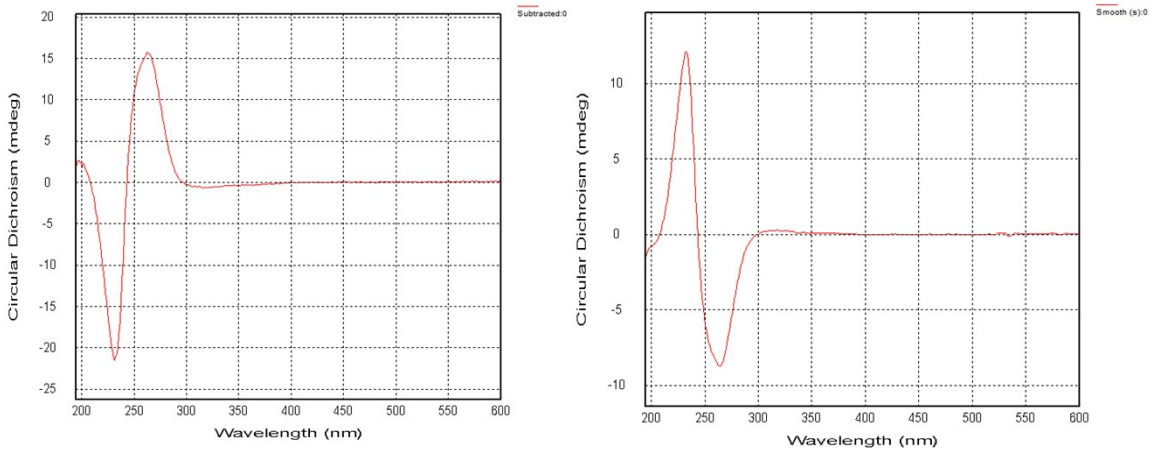
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C32 H28 O12	604.1581	603.1508	603.1511	-0.30	-0.50	19.0000

--- End Of Report ---

Figure S8. CD spectrum of applanmerotic acid A (1).



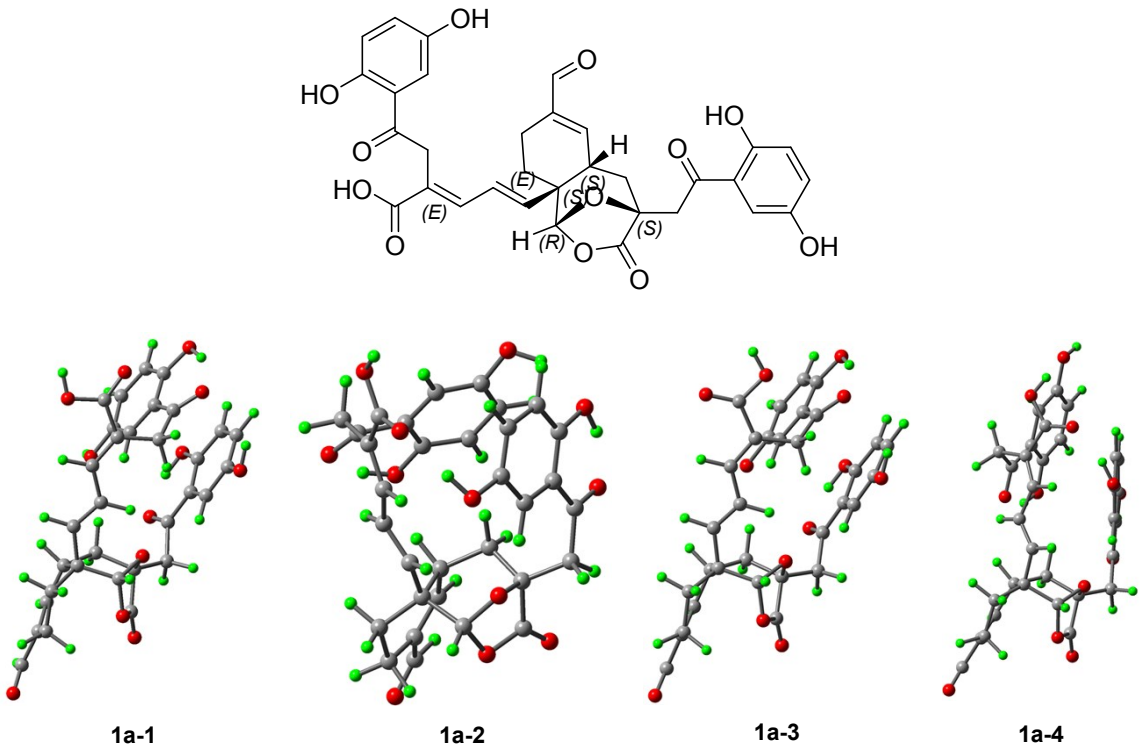


Figure S9. Four optimized conformers of 1a.

Table S2. Conformational analysis of the four optimized conformers of **1a** in the gas phase (T = 298.15 K)

Conformer	E (Hartree)	C (Hartree)	G (kcal/mol)	ΔG (kcal/mol)	Population
1a-1	-2138.819426	0.478133	-1341809.161188	0.0	50.43%
1a-2	-2138.823225	0.48257	-1341808.760818	0.40037	25.64%
1a-3	-2138.81886	0.478321	-1341808.688185	0.473003	22.68%
1a-4	-2138.818979	0.48118	-1341806.968697	2.192491	1.24%

Electronic energy obtained at M062X/6-311+G(2d,p) (Solvent=Methanol) level of theory; Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d), EmpiricalDispersion=GD3 level of theory; Gibbs free energy (E + C); The relative Gibbs free energy; The Boltzmann distribution of each conformer.

Table S3. Experimental and calculated ^{13}C-NMR chemical shifts of **1a**

No.	$\delta_{exptl.}$	**1a**-$\delta_{calcd.}$
1a	156.4	154.1
2a	119.9	116
3a	115.5	116.7
4a	150.2	143.4
5a	125.7	123.8
6a	119.4	115.9
7a	203.8	205.5
8a	37.3	43.7
9a	126.3	123.6
10a	141.8	144.7
11a	128.2	124.2
12a	143.9	153.3
13a	43.4	44.5
14a	24.0	31.9
15a	106.5	106.6
16a	168.7	166
1b	156.4	153.5
2b	120.0	119
3b	115.7	116.8
4b	150.3	144.8
5b	125.7	125.6
6b	119.5	118.3
7b	201.0	201.4
8b	41.5	46.6
9b	77.7	80.1
10b	32.7	32.6
11b	34.6	40.8
12b	149.6	156.6
13b	141.4	140.9
14b	19.0	22.2
15b	193.9	191.6
16b	173.4	172

Table S4. Atomic coordinates (Å) of **1a-1** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	4.513413	-0.105604	-1.031035	H	1.585254	1.381562	1.744490
C	3.370260	0.478922	-0.426842	H	0.276302	3.886232	-0.740818
C	2.110155	0.275310	-1.020250	H	-0.342138	1.564696	1.231766
C	1.980484	-0.455921	-2.188531	H	-1.871267	2.921858	-1.046351
C	3.124741	-0.965357	-2.819694	H	-4.106351	3.018206	-0.684785
C	4.376019	-0.789861	-2.244805	H	-3.978751	3.027538	1.066630
C	3.507529	1.188247	0.849815	H	-2.582426	1.257539	2.261783
C	2.370671	2.051851	1.386296	H	0.345025	-1.359372	2.150200
C	1.823157	3.055866	0.399981	H	4.593180	-1.864416	1.988411
C	0.532932	3.132548	-0.001477	H	4.371070	-3.238320	-0.063854
C	-0.535785	2.252185	0.417829	H	-1.330491	-2.792489	1.839355
C	-1.724731	2.236187	-0.211511	H	-2.202230	-3.490486	0.468269
C	-2.940686	1.390427	0.089171	H	-1.268966	-0.695494	-1.254832
C	-4.138398	2.374158	0.201582	H	-2.680341	-1.696369	-1.582961
C	-2.739551	0.607761	1.401672	H	-2.815964	0.871511	-2.015685
C	2.838553	3.964386	-0.170575	H	-4.785494	-0.752663	-2.059115
C	2.235431	-3.077291	-0.138476	H	-6.292071	2.481944	0.088386
C	1.070204	-2.587855	0.513316	H	-5.723985	1.324678	1.272442
C	1.213857	-1.798688	1.675084	H	-7.033666	-0.680339	-1.831216
C	2.471240	-1.513924	2.182298	H	3.102214	5.451484	-1.291006
C	3.609814	-2.074388	1.578363	O	2.184489	-3.776319	-1.288348
C	3.492860	-2.840417	0.431577	O	-1.673359	-0.311338	1.305794
C	-0.243254	-2.916943	-0.039996	O	-4.444060	-2.346802	1.126578
C	-1.513509	-2.695577	0.766766	O	4.530985	1.061291	1.545549
C	-2.241661	-1.377298	0.518809	O	-3.894549	-0.225045	1.681965

C	-2.294943	-0.900187	-0.939146	O	4.037435	3.846032	0.035319
C	-3.162193	0.381138	-1.095014	O	-8.040861	0.584089	-0.606118
C	-4.608405	0.036897	-1.328874	O	2.338977	4.943545	-0.957668
C	-5.663354	0.621635	-0.736631	O	2.564383	-0.679409	3.270323
C	-5.522892	1.723955	0.272815	O	-0.361341	-3.443406	-1.161422
C	-7.006909	0.140740	-1.084663	H	0.719766	-1.354028	-3.340629
C	-3.657081	-1.435720	1.120384	H	5.612021	0.361001	0.425143
H	1.209713	0.637992	-0.547068	H	3.456410	-0.292082	3.288910
H	3.029983	-1.524964	-3.746416	H	1.228594	-3.795109	-1.557252
H	5.262095	-1.214644	-2.704387	O	0.711353	-0.643295	-2.680245
H	2.779573	2.561368	2.263593	O	5.740936	-0.041834	-0.470782

Table S5. Atomic coordinates (Å) of **1a-2** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	0.352482	-1.443074	2.635071	H	3.430767	-3.444403	0.505144
C	1.477298	-1.853232	1.870497	H	1.563115	-1.285079	-2.590825
C	2.622198	-1.028943	1.839737	H	-0.317139	-2.548131	-0.471921
C	2.660880	0.160862	2.551213	H	-0.514965	-0.457582	-2.694405
C	1.513169	0.588163	3.244366	H	-2.839415	-2.770556	-1.167372
C	0.373905	-0.200395	3.280366	H	-3.301096	-2.034431	-2.696166
C	1.408536	-3.109521	1.117907	H	-2.823526	0.471786	-3.107878
C	2.439433	-3.426540	0.046347	H	0.416690	2.081915	-2.082696
C	2.452940	-2.479261	-1.143114	H	4.548073	1.022037	-1.825918
C	1.367394	-1.915084	-1.729938	H	4.718735	2.151845	0.375785
C	-0.009718	-1.919473	-1.298282	H	-1.071099	3.859946	-1.253408
C	-0.870915	-1.043747	-1.850924	H	-1.766893	3.953605	0.374076
C	-2.255818	-0.713929	-1.326578	H	-0.369856	0.741831	0.394980
C	-3.251571	-1.859675	-1.615866	H	-1.640134	1.239552	1.511894
C	-2.641732	0.602742	-2.041087	H	-1.556765	-1.217241	0.661725
C	3.753958	-2.135142	-1.757372	H	-3.530743	-0.206307	1.935904
C	2.658654	2.737252	0.417352	H	-5.235288	-2.538194	-1.080532
C	1.417674	2.736865	-0.271418	H	-5.204693	-0.891628	-1.670969
C	1.348954	2.114481	-1.537548	H	-5.714984	-0.760299	2.212399
C	2.455048	1.478600	-2.081774	H	5.609680	-2.403778	-1.597656
C	3.680174	1.508984	-1.393537	O	2.804778	3.273522	1.659395
C	3.780727	2.141898	-0.165783	O	-1.612845	1.547409	-1.851847
C	0.232950	3.304539	0.385968	O	-4.100537	2.801465	0.143805
C	-1.137651	3.351817	-0.285703	O	0.485904	-3.922007	1.309928
C	-1.837494	2.009364	-0.505590	O	-3.807888	1.237887	-1.466142

C	-1.446187	0.900879	0.489872	O	3.926817	-1.396629	-2.726435
C	-2.176395	-0.436912	0.208594	O	-6.887511	-1.625688	0.801335
C	-3.502979	-0.554569	0.903668	O	4.803743	-2.708166	-1.138168
C	-4.607103	-1.097826	0.362512	O	2.328492	0.842395	-3.288205
C	-4.654727	-1.610056	-1.050835	O	0.308907	3.775886	1.534889
C	-5.820930	-1.166270	1.184646	H	3.599790	1.827644	2.602133
C	-3.370998	2.120391	-0.527760	H	-0.564389	-3.056746	2.297133
H	3.498445	-1.320898	1.272824	H	2.980995	0.108177	-3.308251
H	1.531352	1.536036	3.773620	H	1.902556	3.612407	1.918688
H	-0.506286	0.114693	3.830681	O	3.827223	0.874567	2.588799
H	2.227514	-4.447065	-0.289047	O	-0.770005	-2.190426	2.737650

Table S6. Atomic coordinates (Å) of **1a-3** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	4.484219	-0.161242	-1.062397	H	1.604092	1.416334	1.712014
C	3.353243	0.451235	-0.460784	H	0.289542	3.890479	-0.783284
C	2.086529	0.255974	-1.043943	H	-0.323447	1.558608	1.187000
C	1.939238	-0.491824	-2.199119	H	-1.869870	2.925448	-1.073143
C	3.071788	-1.031876	-2.826754	H	-4.099605	3.022117	-0.712761
C	4.328552	-0.866183	-2.262266	H	-3.963809	3.049509	1.037853
C	3.512522	1.186085	0.797590	H	-2.568562	1.287062	2.244878
C	2.392998	2.073644	1.336470	H	0.332450	-1.326279	2.156571
C	1.834354	3.072446	0.349588	H	4.580714	-1.844023	2.029616
C	0.541949	3.130606	-0.047182	H	4.367571	-3.248882	-0.002196
C	-0.522148	2.248809	0.376246	H	-1.339629	-2.774933	1.859862
C	-1.718013	2.238262	-0.240579	H	-2.208531	-3.480352	0.490688
C	-2.935485	1.398872	0.072759	H	-1.277610	-0.707004	-1.256983
C	-4.129519	2.387571	0.180468	H	-2.694171	-1.705916	-1.568327
C	-2.731950	0.628970	1.392338	H	-2.821359	0.858015	-2.027180
C	2.757122	4.062940	-0.255264	H	-4.797230	-0.758923	-2.045957
C	2.232957	-3.082685	-0.094001	H	-6.283296	2.501465	0.076478
C	1.065131	-2.579303	0.542247	H	-5.713457	1.354242	1.269410
C	1.203219	-1.774008	1.693143	H	-7.043848	-0.677775	-1.807797
C	2.458213	-1.484581	2.203975	H	4.572578	4.577233	-0.273080
C	3.599153	-2.056963	1.616449	O	2.187355	-3.799941	-1.232871
C	3.487203	-2.840618	0.480825	O	-1.669637	-0.294973	1.301520
C	-0.246259	-2.913454	-0.013991	O	-4.447749	-2.322544	1.155166
C	-1.519532	-2.684562	0.786129	O	4.552357	1.082577	1.472471
C	-2.244850	-1.366828	0.527841	O	-3.888577	-0.197011	1.686194

C	-2.302741	-0.904571	-0.934554	O	2.451220	4.929124	-1.057883
C	-3.165732	0.378426	-1.100159	O	-8.041521	0.601447	-0.590291
C	-4.614204	0.037087	-1.324227	O	4.029803	3.904671	0.180150
C	-5.664549	0.630903	-0.732816	O	2.543790	-0.633136	3.278995
C	-5.515772	1.742781	0.264899	O	-0.359041	-3.451267	-1.130337
C	-7.011159	0.150567	-1.069535	H	0.658261	-1.387237	-3.330825
C	-3.657726	-1.414285	1.136156	H	5.602191	0.326217	0.371593
H	1.194880	0.642311	-0.573346	H	3.448483	-0.280647	3.326901
H	2.962806	-1.605942	-3.742992	H	1.233975	-3.817398	-1.509876
H	5.205278	-1.312921	-2.718861	O	0.665584	-0.664002	-2.684168
H	2.818755	2.585018	2.204255	O	5.716460	-0.104817	-0.513675

Table S7. Atomic coordinates (Å) of **1a-4** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-2.867989	1.147882	-2.106212	H	-2.949813	-2.993662	-1.653822
C	-3.035665	-0.214854	-1.733438	H	-0.601309	-2.834834	1.871396
C	-4.323875	-0.674650	-1.384576	H	0.589758	-2.091716	-0.892947
C	-5.415073	0.178236	-1.407862	H	1.662279	-2.149089	1.975482
C	-5.240951	1.517456	-1.799226	H	3.526750	-3.060538	-0.744066
C	-3.985427	1.992247	-2.142091	H	4.182449	-3.052962	0.887747
C	-1.875573	-1.105217	-1.733345	H	3.755639	-1.029020	2.425148
C	-1.999028	-2.575720	-1.326992	H	0.392921	0.736069	2.538231
C	-1.830319	-2.760937	0.172666	H	-3.763380	-0.199652	2.234432
C	-0.629648	-2.668481	0.799675	H	-4.132441	1.815070	0.834050
C	0.605833	-2.271072	0.173910	H	1.824557	2.734561	2.504289
C	1.695536	-1.968365	0.901778	H	2.356042	3.584490	1.043981
C	2.965702	-1.325654	0.379947	H	0.880957	0.660281	-0.277005
C	3.994970	-2.421001	0.012434	H	2.015723	1.654714	-1.192189
C	3.443908	-0.444243	1.559424	H	2.000711	-0.922254	-1.525510
C	-3.001463	-3.048409	1.020707	H	3.814104	0.649482	-2.423660
C	-2.085421	2.439759	0.890848	H	5.892754	-2.677172	-0.995860
C	-0.775831	2.137535	1.359971	H	5.940781	-1.469982	0.269941
C	-0.590417	0.998113	2.174337	H	5.943191	0.417156	-3.159970
C	-1.649247	0.161187	2.490019	H	-4.794237	-3.628149	0.977740
C	-2.933853	0.460659	1.999843	O	-2.356436	3.520340	0.133616
C	-3.146524	1.585776	1.220113	O	2.406184	0.432452	1.931648
C	0.346936	2.979639	0.938752	O	4.640833	2.557049	0.427700
C	1.779114	2.732089	1.410019	O	-0.747891	-0.686856	-2.060031
C	2.467909	1.457339	0.918560	O	4.536850	0.434508	1.203352

C	1.939562	0.889874	-0.412402	O	-3.053179	-2.912821	2.243074
C	2.684483	-0.401930	-0.844450	O	7.291214	-0.912969	-2.433069
C	3.914841	-0.126160	-1.664635	O	-4.070678	-3.496766	0.335083
C	5.082050	-0.783791	-1.553400	O	-1.412128	-0.925097	3.288432
C	5.314362	-1.867744	-0.537703	O	0.172579	3.949821	0.178903
C	6.181521	-0.399224	-2.446501	H	-7.304764	0.366630	-1.109082
C	3.994067	1.616213	0.807866	H	-1.017644	0.930776	-2.373226
H	-4.484752	-1.701040	-1.082964	H	-2.064771	-1.627745	3.068523
H	-6.096642	2.187650	-1.828396	H	-1.480012	3.944985	-0.059826
H	-3.839660	3.028682	-2.422352	O	-6.635254	-0.333606	-1.052033
H	-1.206509	-3.106039	-1.860353	O	-1.670796	1.675694	-2.428918

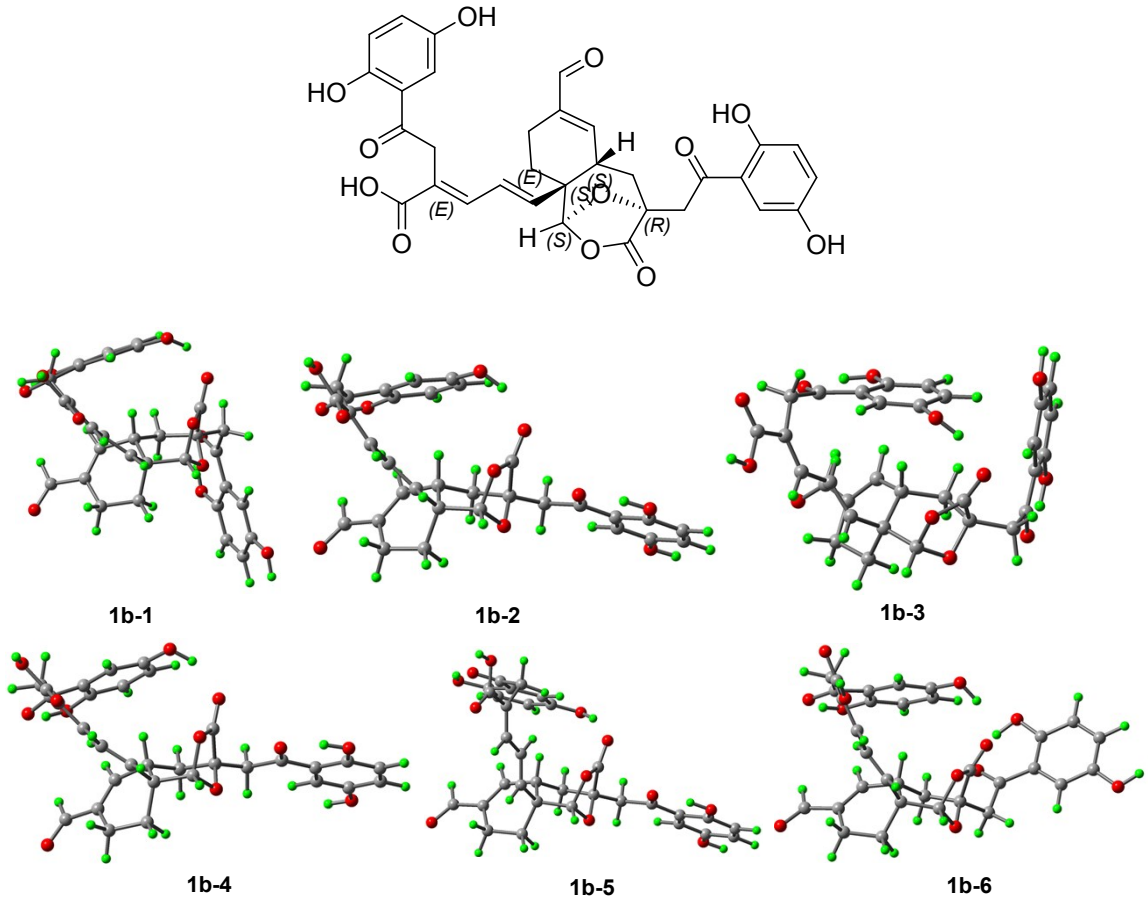


Figure S10. Six optimized conformers of 1b.

Table S8. Conformational analysis of the six optimized conformers of **1b** in the gas phase (T = 298.15 K)

Conformer	E (Hartree)	C (Hartree)	G (kcal/mol)	ΔG (kcal/mol)	Population
1b-1	-2138.816862	0.475607	-1341829.238	0	52.07%
1b-2	-2138.817508	0.477072	-1341828.724	0.51371057	21.87%
1b-3	-2138.818121	0.478368	-1341828.295	0.942638346	10.60%
1b-4	-2138.816881	0.477272	-1341828.205	1.032648294	9.10%
1b-5	-2138.815366	0.476522	-1341827.725	1.512956539	4.04%
1b-6	-2138.815463	0.477144	-1341827.396	1.842254647	2.32%

Electronic energy obtained at M062X/6-311+G(2d,p) (Solvent=Methanol) level of theory; Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d), EmpiricalDispersion=GD3 level of theory; Gibbs free energy (E + C); The relative Gibbs free energy; The Boltzmann distribution of each conformer.

Table S9. Experimental and calculated ^{13}C-NMR chemical shifts of **1b**

No.	$\delta_{exptl.}$	**1b**-$\delta_{calcd.}$
1a	156.4	154.9
2a	119.9	118.9
3a	115.5	119.7
4a	150.2	146.2
5a	125.7	129.1
6a	119.4	117.0
7a	203.8	206.7
8a	37.3	45.3
9a	126.3	122.5
10a	141.8	140.5
11a	128.2	127.6
12a	143.9	145.1
13a	43.4	45.9
14a	24.0	25.2
15a	106.5	109.9
16a	168.7	165.3
1b	156.4	155.8
2b	120.0	116.4
3b	115.7	114.9
4b	150.3	144.6
5b	125.7	124.0
6b	119.5	117.6
7b	201.0	200.1
8b	41.5	43.3
9b	77.7	81.3
10b	32.7	32.0
11b	34.6	36.0
12b	149.6	152.7
13b	141.4	139.9
14b	19.0	21.5
15b	193.9	194.3
16b	173.4	174.8

Table S10. Parameters of calculated ^{13}C NMR method for **1a** and **1b**

	1a (green)	**1b (red)**
Liner equation	y = 0.9649x + 4.5486	y = 0.9787x + 2.6778
R^2	0.9952	0.9973
MAE	3.1	2.4
CMAE	2.7	2.2

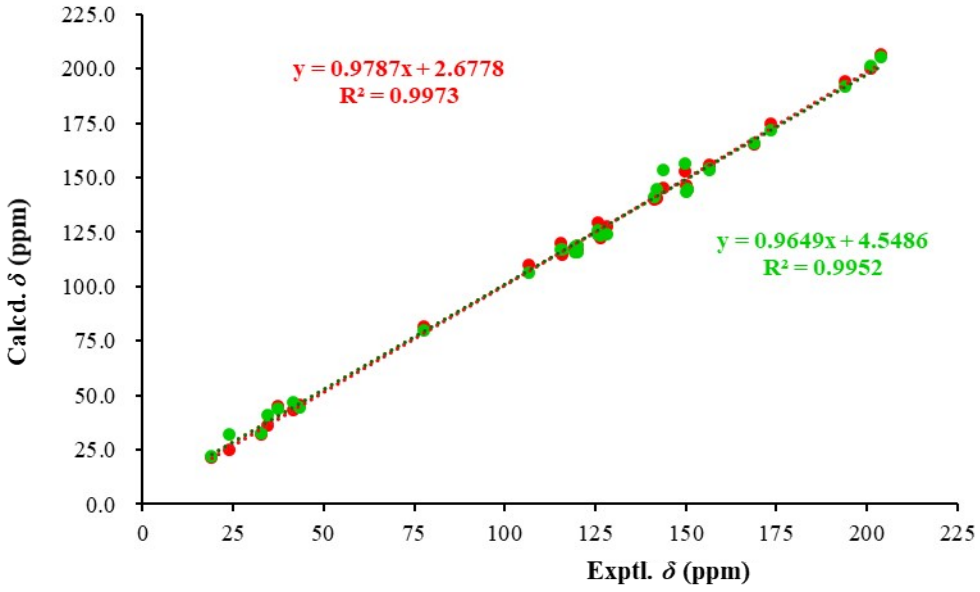


Table S11. Atomic coordinates (Å) of **1b-1** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-2.647976	0.638272	2.776362	H	-3.276376	-2.252624	1.046006
C	-3.36645	-0.300271	1.989895	H	0.189671	-1.165065	3.298456
C	-2.768683	-1.542589	1.687846	H	-0.846209	1.019892	3.874379
C	-1.488765	-1.845504	2.124477	H	-6.504992	-0.484558	0.604327
C	-0.806302	-0.92316	2.942973	H	-5.583565	-1.822985	1.255105
C	-1.378158	0.297809	3.263856	H	-3.994596	-1.482995	-2.497225
C	-4.652909	0.086727	1.397657	H	-3.021387	0.512977	-0.32933
C	-5.501558	-0.919581	0.637489	H	-1.775169	-0.718825	-2.831881
C	-5.116035	-1.347206	-0.768916	H	0.473777	2.418809	-2.382345
C	-4.051118	-0.994087	-1.526884	H	-0.500847	1.605639	-3.604995
C	-2.950008	-0.115987	-1.203989	H	0.638036	-0.620037	-2.952086
C	-1.821277	-0.101594	-1.933844	H	5.665974	1.448097	0.942195
C	-0.567425	0.681324	-1.629162	H	9.601521	-0.106514	0.323587
C	-0.486205	1.922446	-2.556294	H	8.660583	-2.073924	-0.854156
C	0.632291	-0.238699	-1.931173	H	3.715632	1.479766	-0.078026
C	-6.043239	-2.324219	-1.408395	H	3.409056	0.468439	1.326067
C	6.623078	-1.446068	-0.635498	H	1.339588	2.336034	0.048717
C	5.752629	-0.441975	-0.131462	H	0.983165	1.324658	1.455719
C	6.304004	0.6706	0.539857	H	-0.893308	0.309191	0.468334
C	7.674038	0.795628	0.707977	H	-1.478082	2.585652	1.188009
C	8.525826	-0.200132	0.198553	H	-1.4552	3.849023	-2.791268
C	8.006519	-1.302601	-0.461918	H	-2.573919	2.505589	-2.701225
C	4.306232	-0.586927	-0.30847	H	-2.756065	4.388533	0.719707
C	3.373576	0.487603	0.230451	H	-3.981807	1.951672	2.563637
C	1.938436	0.306391	-0.218357	H	0.025712	-2.855359	1.558863

C	0.972974	1.354153	0.361965	H	5.19117	-2.479058	-1.298259
C	-0.483314	1.123955	-0.137939	H	9.109041	1.857776	1.420975
C	-1.303936	2.346228	0.140649	H	-7.617222	-3.308492	-1.095418
C	-1.823764	3.142415	-0.811167	O	-5.104158	1.235778	1.54424
C	-1.636225	2.895583	-2.283944	O	-3.184951	5.069182	-1.142942
C	-2.643914	4.282522	-0.379564	O	8.140574	1.898849	1.370556
C	1.358851	-1.088088	0.03153	O	-7.069991	-2.671948	-0.597793

Table S12. Atomic coordinates (Å) of **1b-2** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-2.647976	0.638272	2.776362	H	-3.276376	-2.252624	1.046006
C	-3.36645	-0.300271	1.989895	H	0.189671	-1.165065	3.298456
C	-2.768683	-1.542589	1.687846	H	-0.846209	1.019892	3.874379
C	-1.488765	-1.845504	2.124477	H	-6.504992	-0.484558	0.604327
C	-0.806302	-0.92316	2.942973	H	-5.583565	-1.822985	1.255105
C	-1.378158	0.297809	3.263856	H	-3.994596	-1.482995	-2.497225
C	-4.652909	0.086727	1.397657	H	-3.021387	0.512977	-0.32933
C	-5.501558	-0.919581	0.637489	H	-1.775169	-0.718825	-2.831881
C	-5.116035	-1.347206	-0.768916	H	0.473777	2.418809	-2.382345
C	-4.051118	-0.994087	-1.526884	H	-0.500847	1.605639	-3.604995
C	-2.950008	-0.115987	-1.203989	H	0.638036	-0.620037	-2.952086
C	-1.821277	-0.101594	-1.933844	H	5.665974	1.448097	0.942195
C	-0.567425	0.681324	-1.629162	H	9.601521	-0.106514	0.323587
C	-0.486205	1.922446	-2.556294	H	8.660583	-2.073924	-0.854156
C	0.632291	-0.238699	-1.931173	H	3.715632	1.479766	-0.078026
C	-6.043239	-2.324219	-1.408395	H	3.409056	0.468439	1.326067
C	6.623078	-1.446068	-0.635498	H	1.339588	2.336034	0.048717
C	5.752629	-0.441975	-0.131462	H	0.983165	1.324658	1.455719
C	6.304004	0.6706	0.539857	H	-0.893308	0.309191	0.468334
C	7.674038	0.795628	0.707977	H	-1.478082	2.585652	1.188009
C	8.525826	-0.200132	0.198553	H	-1.4552	3.849023	-2.791268
C	8.006519	-1.302601	-0.461918	H	-2.573919	2.505589	-2.701225
C	4.306232	-0.586927	-0.30847	H	-2.756065	4.388533	0.719707
C	3.373576	0.487603	0.230451	H	-3.981807	1.951672	2.563637
C	1.938436	0.306391	-0.218357	H	0.025712	-2.855359	1.558863

C	0.972974	1.354153	0.361965	H	5.19117	-2.479058	-1.298259
C	-0.483314	1.123955	-0.137939	H	9.109041	1.857776	1.420975
C	-1.303936	2.346228	0.140649	H	-7.617222	-3.308492	-1.095418
C	-1.823764	3.142415	-0.811167	O	-5.104158	1.235778	1.54424
C	-1.636225	2.895583	-2.283944	O	-3.184951	5.069182	-1.142942
C	-2.643914	4.282522	-0.379564	O	8.140574	1.898849	1.370556
C	1.358851	-1.088088	0.03153	O	-7.069991	-2.671948	-0.597793

Table S13. Atomic coordinates (Å) of **1b-3** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-0.759887	-1.801126	1.856241	H	-2.824661	-2.194512	-0.851325
C	-1.96664	-1.821536	1.107345	H	1.376653	-2.945523	-0.528505
C	-1.926826	-2.222311	-0.245464	H	1.344306	-2.227293	1.840666
C	-0.731627	-2.580245	-0.848044	H	-5.301148	-1.315369	1.783383
C	0.447129	-2.615244	-0.077754	H	-4.645729	-2.503849	0.682185
C	0.432414	-2.226028	1.252407	H	-4.657648	0.883672	-1.635016
C	-3.206339	-1.321392	1.715484	H	-2.430697	0.564846	0.492951
C	-4.543525	-1.460555	1.006915	H	-2.621291	1.993369	-2.201823
C	-4.904327	-0.578783	-0.176457	H	0.385821	3.866415	-0.584855
C	-4.199443	0.414013	-0.769198	H	-1.154638	4.192398	-1.376743
C	-2.872677	0.882606	-0.439475	H	-0.480233	2.521728	-3.23073
C	-2.155365	1.650091	-1.277484	H	3.430879	-1.451524	-1.387533
C	-0.720405	2.07532	-1.077433	H	5.073337	-3.351732	2.07363
C	-0.663956	3.559235	-0.629527	H	6.086831	-1.206463	2.795212
C	-0.007959	1.944466	-2.436248	H	3.671242	0.215103	-2.704478
C	-6.241139	-0.932517	-0.720964	H	3.675159	1.98117	-2.631577
C	5.352068	-0.096611	1.114576	H	2.034094	2.028752	0.169053
C	4.592452	-0.150023	-0.085962	H	1.959804	0.266653	0.267999
C	4.026733	-1.37987	-0.486151	H	-0.33203	0.150477	-0.191641
C	4.197552	-2.522176	0.278083	H	0.029775	0.85497	2.137688
C	4.941381	-2.458143	1.468893	H	-1.101082	4.748383	1.130715
C	5.511289	-1.262167	1.877535	H	-2.417009	3.700701	0.644997
C	4.358126	1.080973	-0.844915	H	-0.783753	2.119772	3.828668
C	3.450146	1.074644	-2.067596	H	-1.618051	-1.050702	3.3566
C	1.941748	1.104754	-1.746483	H	0.093416	-2.534393	-2.566604

C	1.56141	1.138139	-0.255173	H	5.691392	1.74417	0.906977
C	0.02371	1.176827	-0.049138	H	3.752071	-4.38696	0.480495
C	-0.271472	1.563822	1.368587	H	-7.526686	-0.49415	-2.019357
C	-0.871803	2.712413	1.728796	O	-3.201917	-0.825739	2.85601
C	-1.324158	3.750933	0.738094	O	-1.678244	3.927786	3.612157
C	-1.126589	2.935733	3.158948	O	3.617577	-3.680551	-0.171628
C	1.14265	0.001757	-2.454822	O	-6.650209	-0.15881	-1.753415

Table S14. Atomic coordinates (Å) of **1b-4** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-2.641604	0.634362	2.777577	H	-3.272522	-2.254388	1.044534
C	-3.361211	-0.303241	1.991014	H	0.196574	-1.169827	3.29372
C	-2.763914	-1.545201	1.686596	H	-0.838429	1.014517	3.87378
C	-1.48336	-1.848598	2.120976	H	-6.501919	-0.48555	0.610266
C	-0.799807	-0.92734	2.939814	H	-5.579806	-1.824917	1.258128
C	-1.371153	0.293274	3.262934	H	-3.997265	-1.481538	-2.496662
C	-4.648506	0.084501	1.4011	H	-3.019939	0.511648	-0.328099
C	-5.498564	-0.9209	0.641333	H	-1.777561	-0.716859	-2.834167
C	-5.115613	-1.347193	-0.766223	H	0.471475	2.420415	-2.384341
C	-4.051884	-0.993703	-1.525677	H	-0.504599	1.608144	-3.606407
C	-2.949984	-0.116271	-1.203625	H	0.636031	-0.617953	-2.956761
C	-1.822418	-0.100843	-1.935233	H	5.65619	1.448787	0.928469
C	-0.568336	0.68198	-1.631338	H	9.598923	-0.101325	0.343201
C	-0.488615	1.923974	-2.557436	H	8.659157	-2.08543	-0.838412
C	0.631462	-0.237328	-1.935587	H	3.71538	1.482117	-0.089178
C	-6.044445	-2.323061	-1.405144	H	3.41114	0.474256	1.31843
C	6.622457	-1.448202	-0.629319	H	1.339486	2.336584	0.045032
C	5.753532	-0.441399	-0.132953	H	0.985856	1.323931	1.451823
C	6.307764	0.675011	0.536933	H	-0.891131	0.30766	0.466304
C	7.676764	0.794403	0.707438	H	-1.477032	2.582936	1.188769
C	8.52767	-0.207819	0.205345	H	-1.458295	3.850592	-2.789328
C	8.008168	-1.309027	-0.451003	H	-2.576636	2.506842	-2.699249
C	4.308688	-0.584846	-0.313859	H	-2.755762	4.386115	0.7236
C	3.375106	0.490294	0.22277	H	-3.975715	1.948017	2.568319
C	1.939623	0.307535	-0.224333	H	0.030437	-2.857592	1.552164

C	0.974139	1.354164	0.358092	H	5.191009	-2.479317	-1.294688
C	-0.482671	1.123285	-0.139848	H	7.589243	2.472181	1.643471
C	-1.303654	2.344832	0.140976	H	-7.618608	-3.306574	-1.090624
C	-1.824538	3.141914	-0.809502	O	-5.099428	1.233455	1.549562
C	-1.638513	2.896614	-2.282731	O	-3.186023	5.069089	-1.13788
C	-2.644406	4.281492	-0.375893	O	8.271231	1.848047	1.346822
C	1.36136	-1.087491	0.025586	O	-7.070066	-2.670982	-0.593213

Table S15. Atomic coordinates (Å) of **1b-5** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-3.711628	1.074807	2.678334	H	-1.54456	-1.489705	1.963957
C	-3.272839	-0.181145	2.173314	H	-0.73928	2.251423	3.862496
C	-1.905368	-0.530898	2.318414	H	-3.140751	2.89575	3.654556
C	-1.002742	0.336962	2.919707	H	-4.352857	-3.153659	1.317808
C	-1.456347	1.580206	3.400735	H	-2.783844	-2.532404	0.837416
C	-2.785593	1.939867	3.284533	H	-4.085391	-1.597161	-2.618985
C	-4.252313	-1.044918	1.49876	H	-2.099679	-0.865262	-0.348422
C	-3.854607	-2.337664	0.789766	H	-2.188552	-0.053215	-3.294526
C	-4.323766	-2.297475	-0.654387	H	0.570401	2.332951	-2.820253
C	-3.675079	-1.592891	-1.612533	H	-0.34241	1.426342	-4.022526
C	-2.479175	-0.828165	-1.360201	H	0.69909	-0.753223	-3.151874
C	-1.822841	-0.086934	-2.269083	H	5.579748	1.369767	0.860179
C	-0.541745	0.675912	-1.991079	H	9.416929	-0.508484	0.677613
C	-0.383414	1.829595	-3.004012	H	8.396898	-2.541287	-0.309887
C	0.647888	-0.305291	-2.161004	H	3.695964	1.40703	-0.252213
C	-5.567774	-2.99671	-1.050468	H	3.217592	0.581242	1.223222
C	6.402503	-1.756439	-0.294255	H	1.349841	2.421776	-0.417427
C	5.58319	-0.641349	0.030578	H	0.892529	1.604283	1.086763
C	6.178985	0.507343	0.594702	H	-0.944729	0.516194	0.140046
C	7.543662	0.560758	0.829598	H	-1.573461	2.804953	0.607456
C	8.345357	-0.545702	0.498016	H	-1.307033	3.742391	-3.452688
C	7.781788	-1.685025	-0.054858	H	-2.450975	2.427684	-3.331942
C	4.142117	-0.709947	-0.214747	H	-2.810511	4.582903	-0.08796
C	3.260906	0.480009	0.132111	H	-5.490456	0.752677	2.160679
C	1.851368	0.347069	-0.407633	H	0.604391	-0.659759	2.483429

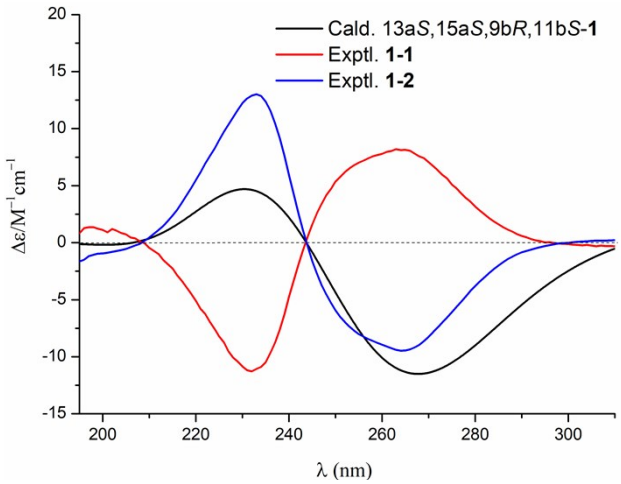
C	0.925312	1.503639	-0.001491	H	4.93519	-2.767575	-0.91315
C	-0.508943	1.251731	-0.539744	H	9.014529	1.607188	1.489742
C	-1.346331	2.486218	-0.409038	H	-6.938148	-4.106168	-0.394219
C	-1.810725	3.199601	-1.44993	O	-5.454535	-0.728707	1.448473
C	-1.53407	2.834332	-2.88418	O	-3.130806	5.097596	-2.023838
C	-2.641876	4.37695	-1.1657	O	8.055069	1.704701	1.380156
C	1.160295	-0.985446	-0.078663	O	-6.136029	-3.684286	-0.032682

Table S16. Atomic coordinates (Å) of **1b-6** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-1.549816	-0.732143	2.657221	H	-2.033374	-2.780674	-0.046175
C	-2.253671	-1.464138	1.664796	H	1.6302	-1.630746	1.843166
C	-1.523223	-2.250756	0.749462	H	0.371259	-0.25966	3.484542
C	-0.13891	-2.30208	0.794023	H	-5.547532	-2.066189	0.891872
C	0.546119	-1.593707	1.802092	H	-4.22247	-3.188293	0.695448
C	-0.151751	-0.82305	2.718954	H	-3.921237	-0.925933	-2.713715
C	-3.706602	-1.295671	1.531432	H	-2.838254	0.248787	-0.062057
C	-4.508893	-2.138493	0.554571	H	-2.137208	0.637734	-3.011633
C	-4.478267	-1.853431	-0.938019	H	-0.581976	3.856295	-1.479338
C	-3.80447	-0.906449	-1.633807	H	-1.633397	3.34144	-2.797545
C	-2.887406	0.089692	-1.128671	H	0.105523	1.558383	-3.398834
C	-2.059743	0.779136	-1.933045	H	5.486148	0.884847	-1.619312
C	-0.979126	1.732125	-1.478367	H	7.75091	-2.535691	-0.425759
C	-1.418661	3.197071	-1.732804	H	6.487674	-2.651992	1.705903
C	0.274407	1.443508	-2.328699	H	3.821777	1.870735	-1.388082
C	-5.330945	-2.816646	-1.682641	H	3.325765	2.943993	-0.072932
C	5.270888	-0.942653	1.276742	H	0.899673	3.049339	0.474825
C	4.959211	0.072505	0.329569	H	1.119773	1.519819	1.329657
C	5.684575	0.120286	-0.879015	H	-0.676009	0.457399	0.232013
C	6.686154	-0.799289	-1.150954	H	-1.524284	1.953655	1.991873
C	6.97249	-1.806819	-0.215114	H	-2.823942	4.641607	-0.930021
C	6.27059	-1.876848	0.9788	H	-3.546373	3.093101	-1.31241
C	3.862145	0.997611	0.625108	H	-3.231907	3.310747	2.584192
C	3.278971	1.915841	-0.445517	H	-3.131419	0.07615	3.286817
C	1.816694	1.563698	-0.727178	H	1.31477	-2.533078	-0.416526

C	0.827959	1.961555	0.376444	H	4.016504	-0.28669	2.520484
C	-0.618252	1.531163	0.0218	H	8.021034	-1.384703	-2.404919
C	-1.582304	2.220642	0.938396	H	-5.968591	-3.294828	-3.384232
C	-2.491033	3.128657	0.538794	O	-4.324449	-0.49454	2.254181
C	-2.645841	3.561827	-0.894022	O	-4.27219	4.506103	1.317268
C	-3.393531	3.689644	1.553444	O	7.355532	-0.681169	-2.339617
C	1.624597	0.095166	-1.130385	O	-5.390203	-2.600367	-3.017494

Figure S11. Calculated and experimental ECD curves of 1b, 1-1 and 1-2.



1D and 2D NMR spectra of compound 2

Figure S12. ^{1}H NMR spectrum (600 MHz, $CO(CD)_3$) of compound 2.

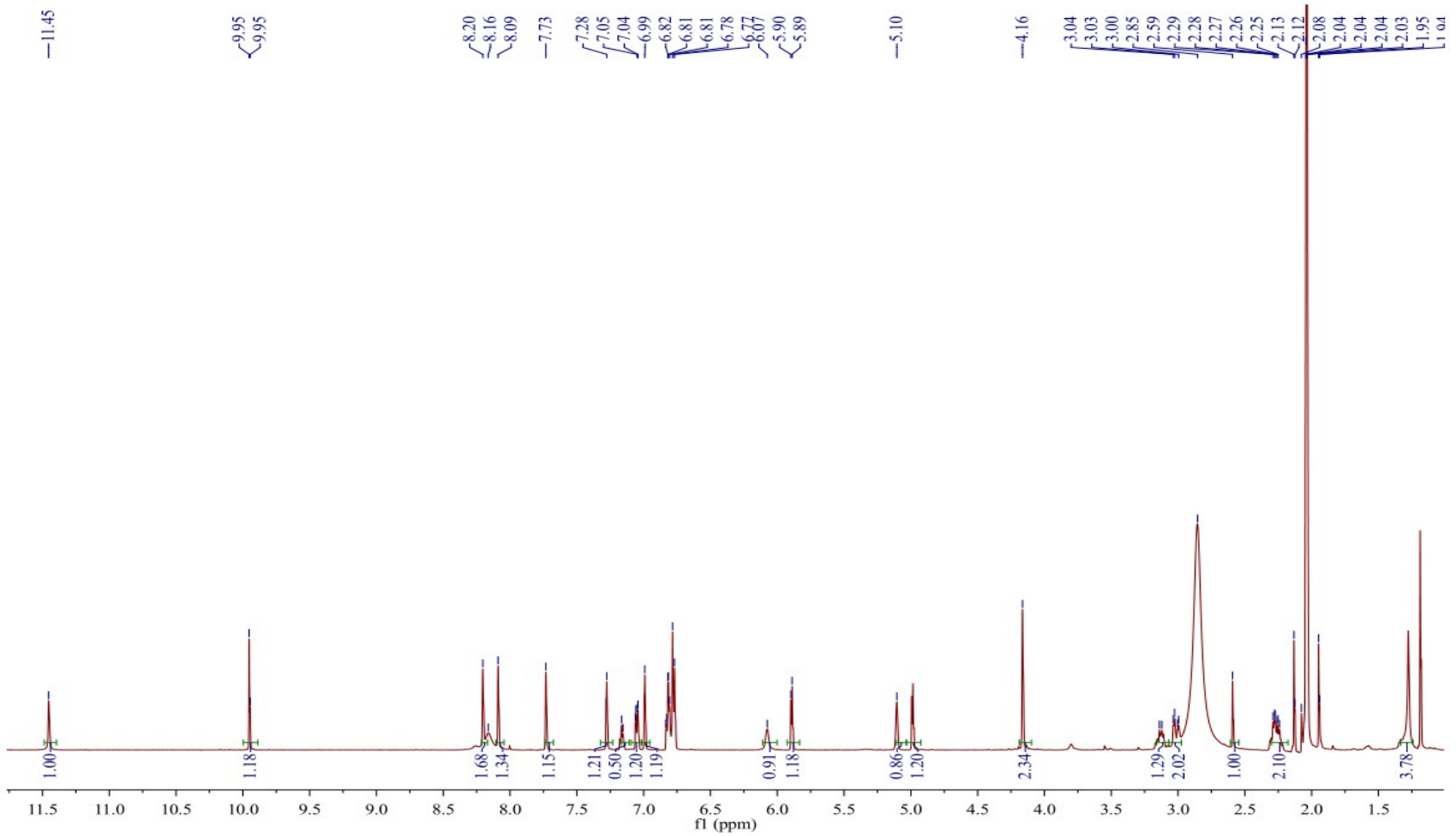


Figure S13. ^{13}C NMR spectrum (150 MHz, $CO(CD)_3$) of compound 2.

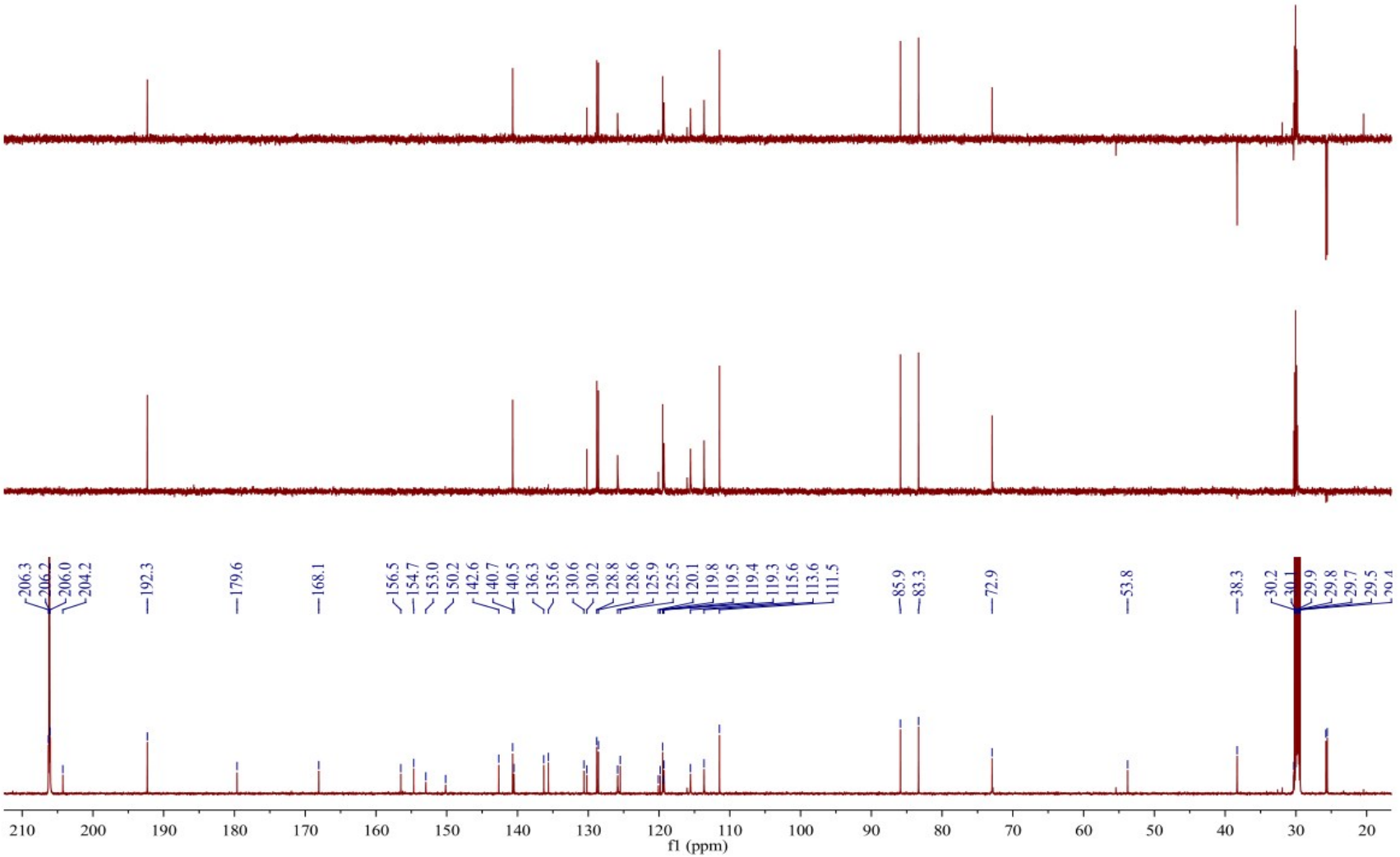


Figure S14. HSQC spectrum (100/150 MHz, $CO(CD)_3$) of compound 2.

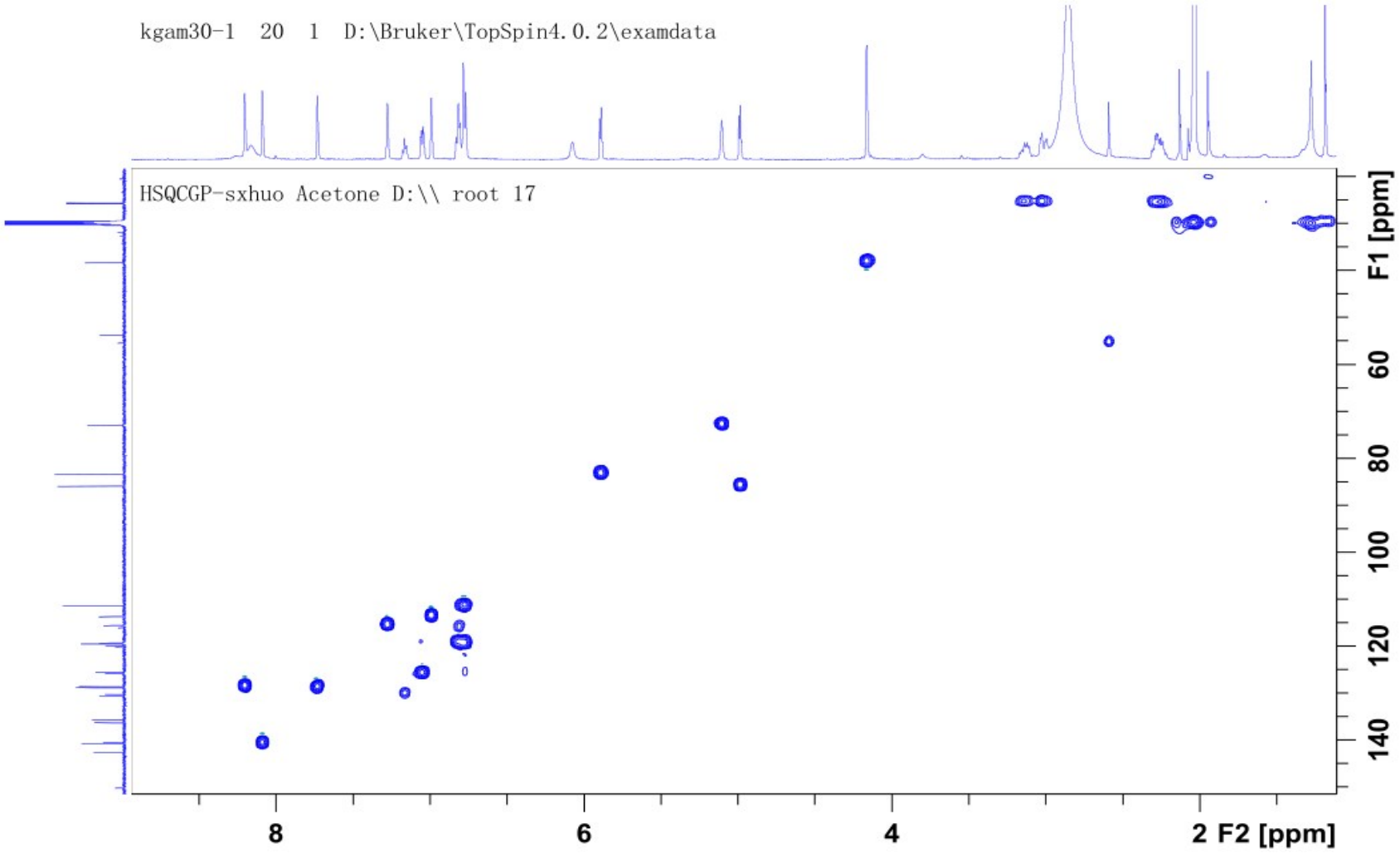


Figure S15. HMBC spectrum (600/150 MHz, $CO(CD)_3$) of compound 2.

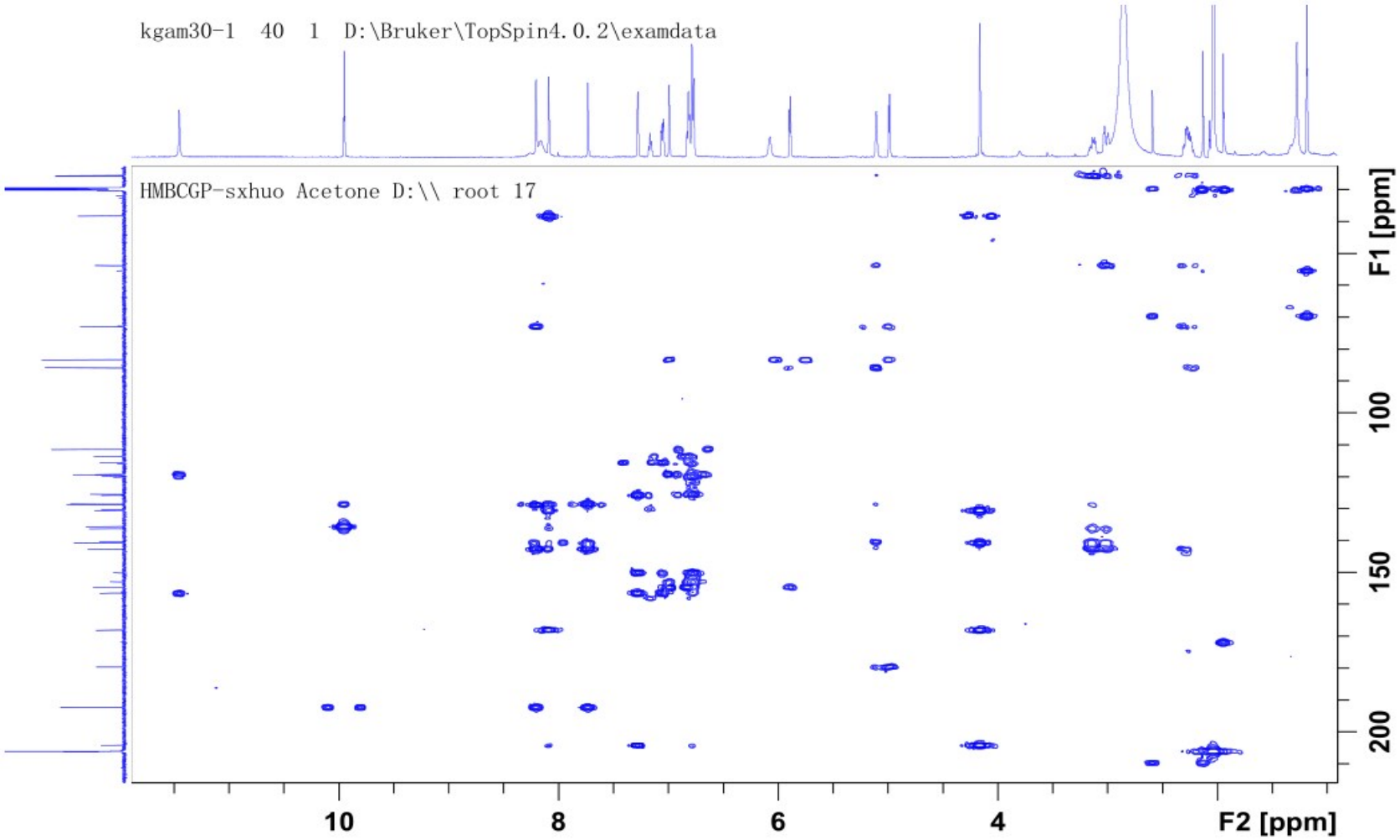


Figure S16. ^{1}H-^{1}H COSY spectrum (600 MHz, $CO(CD)_3$) of compound 2.

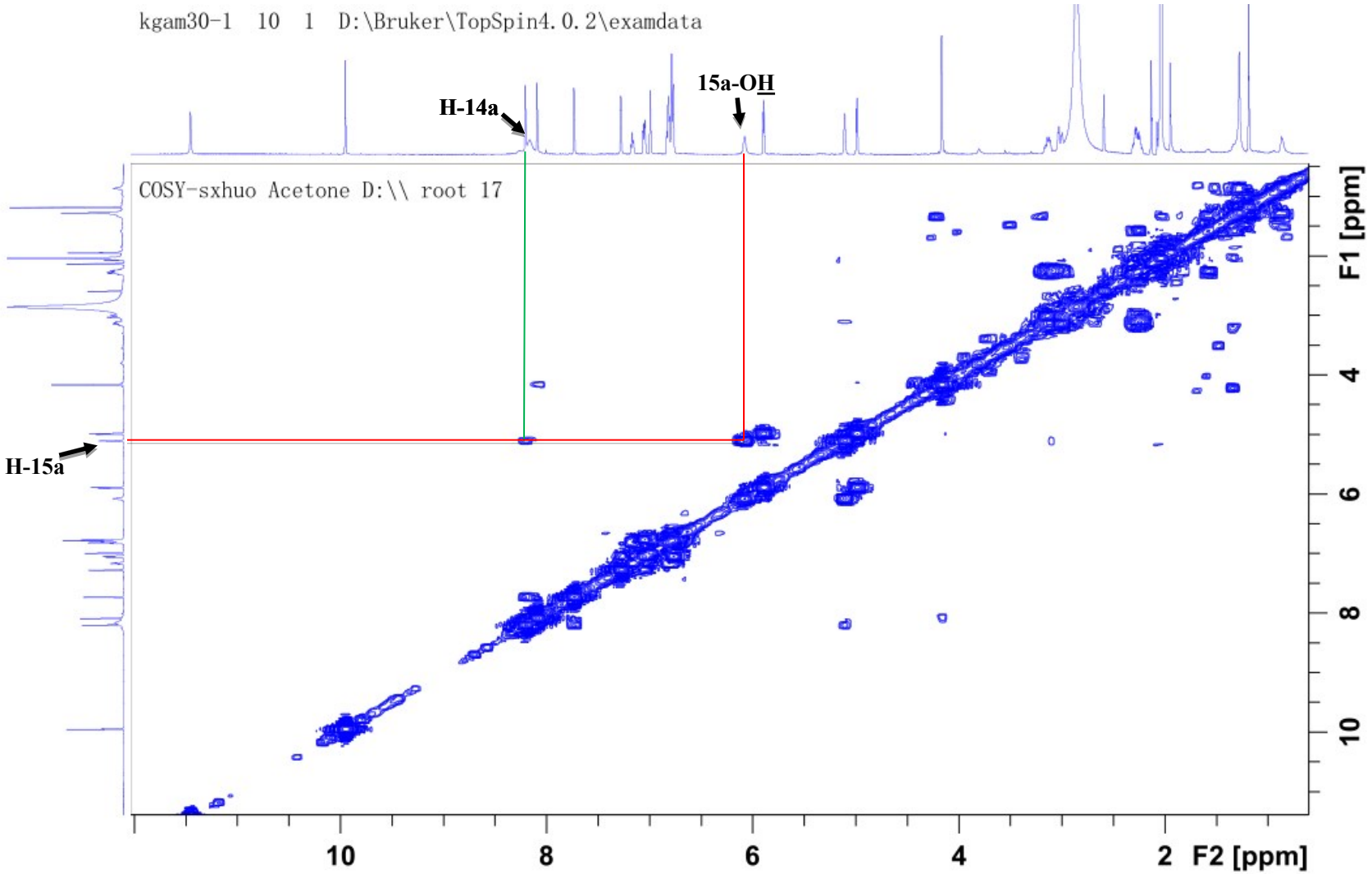


Figure S17. ROESY spectrum (600 MHz, $CO(CD)_3$) of compound 2.

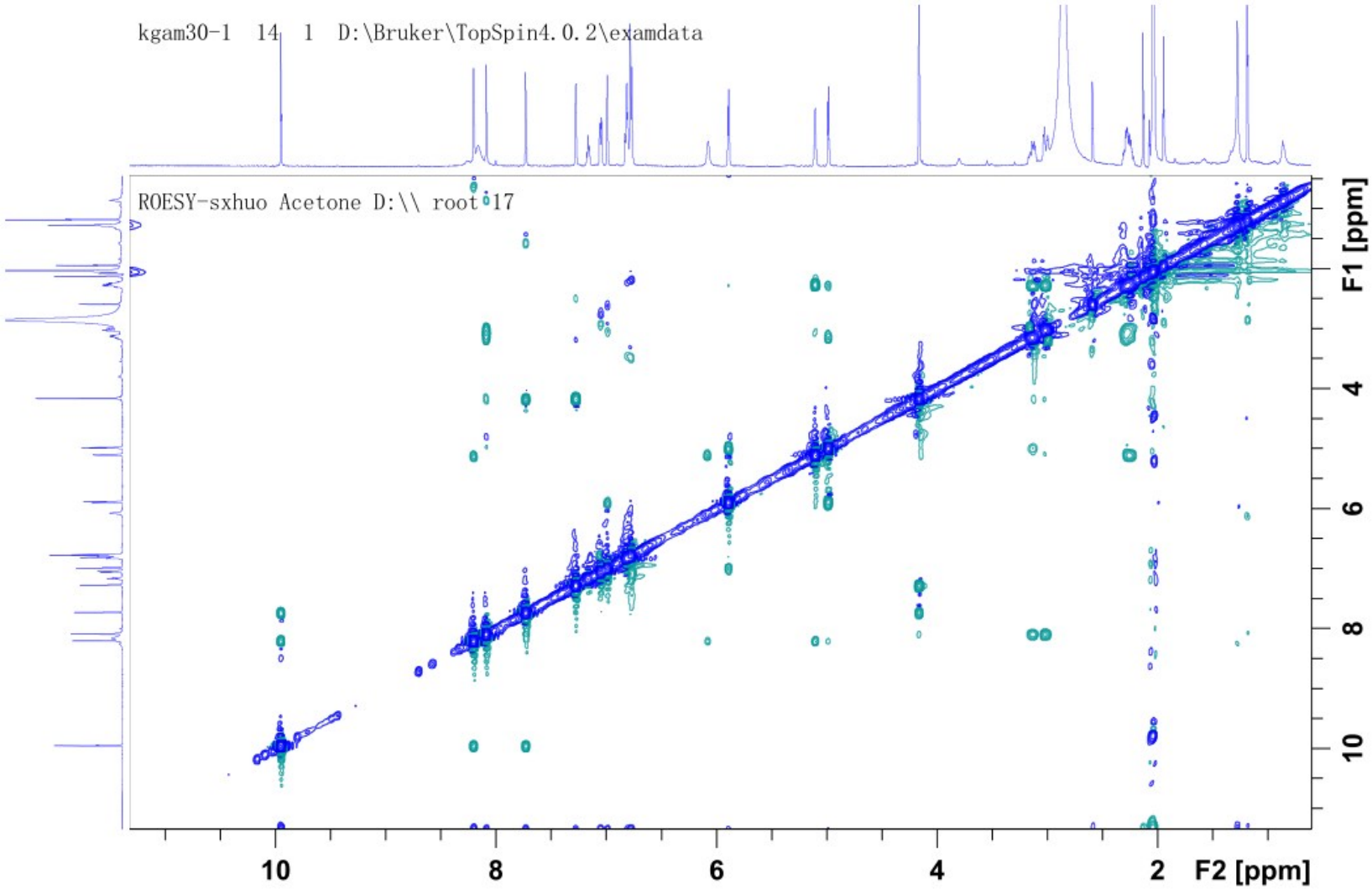
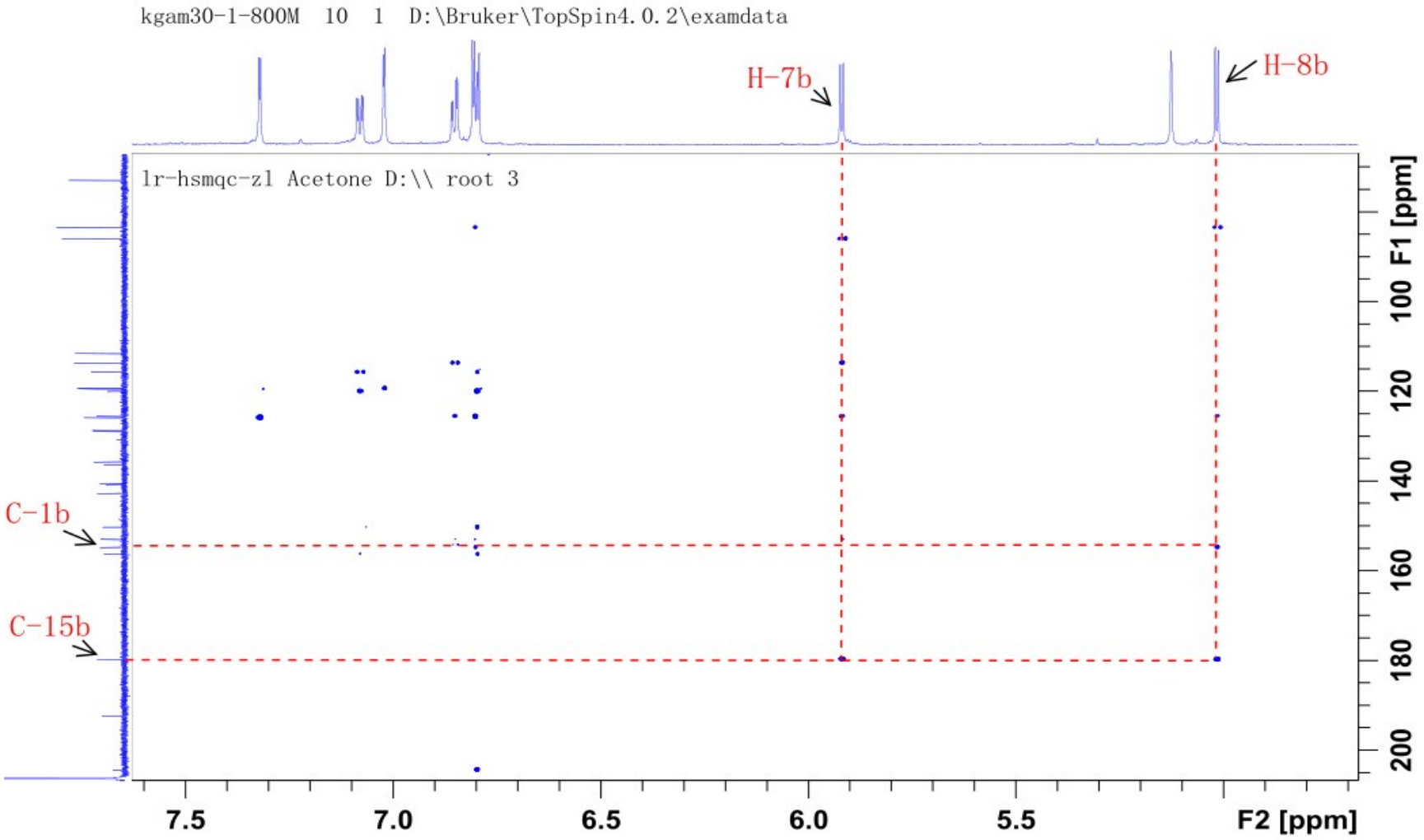


Figure S18. HSMQC spectrum (800 MHz, $CO(CD)_3$) of compound 2.



HRESIMS, CD spectra, as well as computational ECD data of 2

Figure S19. HRESIMS spectrum of applanmerotic acid B (2).

Qualitative Analysis Report

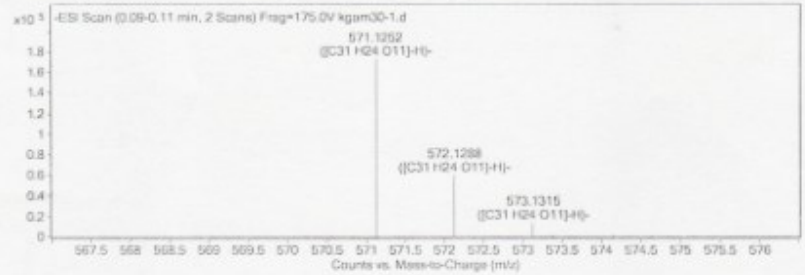
Data Filename	kgam30-1.d	Sample Name	kgam30-1
Sample Type	Sample	Position	P1-A1
Instrument Name	Instrument 1	User Name	
Acq Method	s-.m	Acquired Time	9/27/2020 2:30:01 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group — Info.

Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage: 175 | Collision Energy: 0 | Ionization Mode: ESI



Peak List

m/z	z	Abund	Formula	Ion
571.1252	1	173006.06	C31 H24 O11	(M-H)-
572.1288	1	60295.36	C31 H24 O11	(M-H)-
573.1315	1	14236.5	C31 H24 O11	(M-H)-
607.1017	1	12855.13		
639.1127	1	18656.18		
955.9725	1	10250.2		
966.0007	1	53633.28		
967.0034	1	11619.97		
982.9908	1	10941.17		
1033.9882	1	35262.84		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C31 H24 O11	572.1319	571.1246	571.1252	-0.60	-1.05	20.0000

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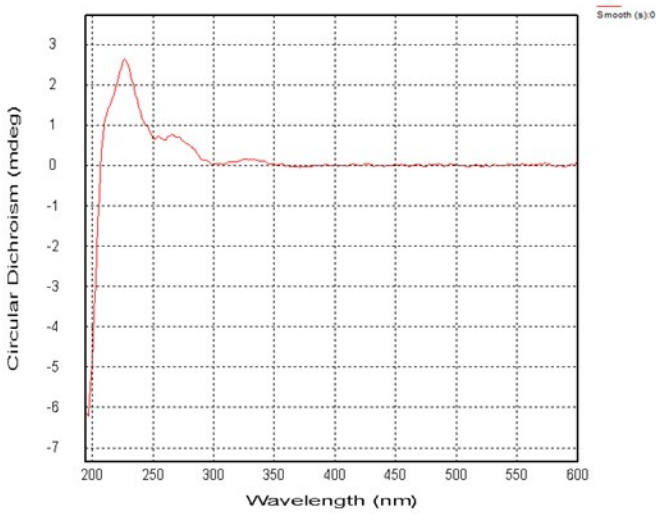
Figure S20. CD spectrum of applanmerotic acid B (2).



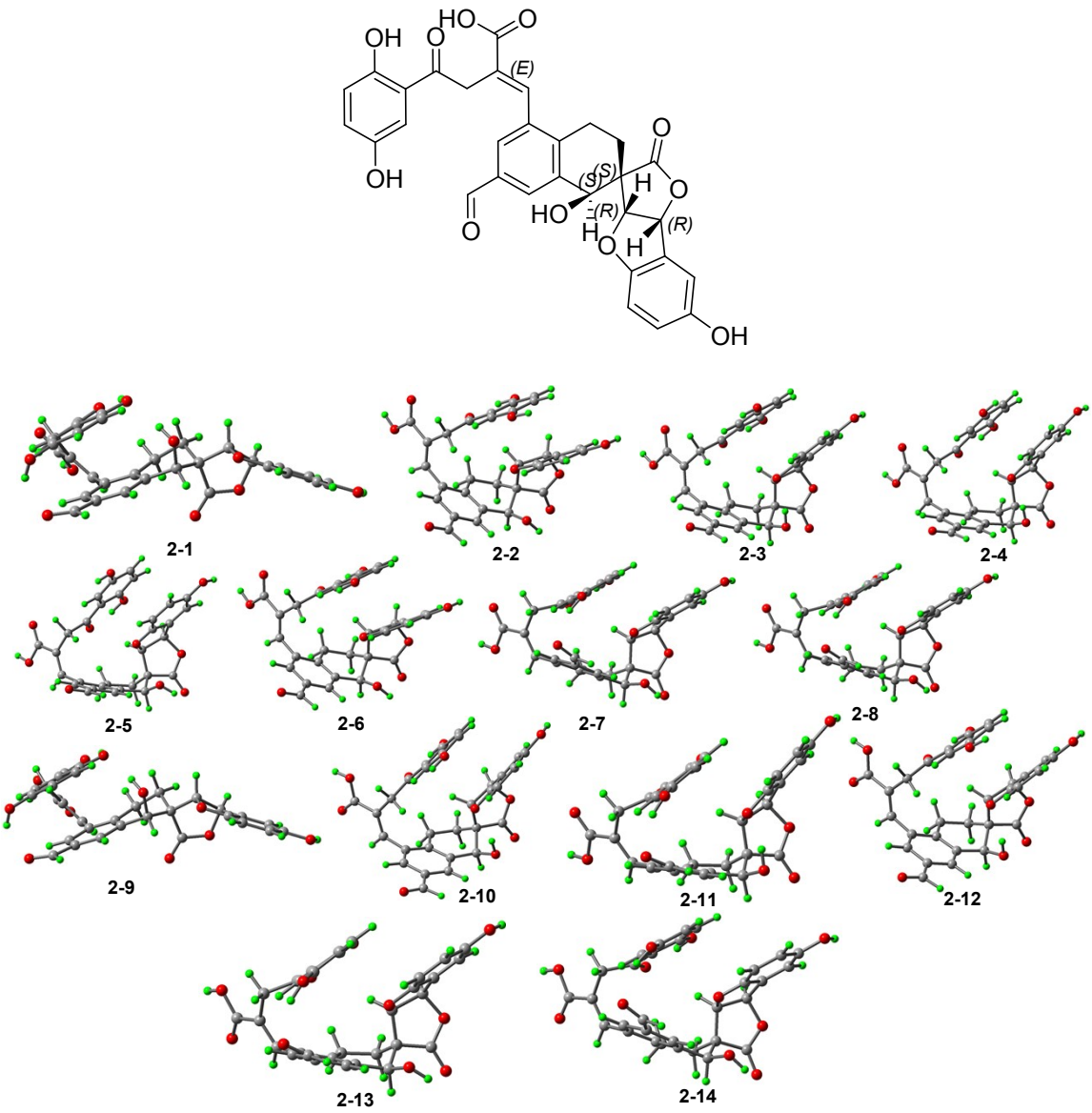


Figure S21. Fourteen optimized conformers of 2.

Table S17. Conformational analysis of the 14 optimized conformers of **2** in the gas phase (T = 298.15 K)

Conformer	E (Hartree)	C (Hartree)	G (kcal/mol)	ΔG (kcal/mol)	Population
2b-1	-2023.111577	0.428064	-1269252.918	0	28.25%
2b-2	-2023.108869	0.426017	-1269252.503	0.414626836	14.02%
2b-3	-2023.10953	0.427011	-1269252.294	0.624051823	9.85%
2b-4	-2023.109522	0.427025	-1269252.28	0.637417773	9.63%
2b-5	-2023.108054	0.426126	-1269251.923	0.994727901	5.26%
2b-6	-2023.108052	0.426137	-1269251.915	1.002496467	5.20%
2b-7	-2023.109773	0.427892	-1269251.894	1.023825512	5.01%
2b-8	-2023.109774	0.427893	-1269251.894	1.023938464	5.01%
2b-9	-2023.109696	0.428045	-1269251.749	1.168253075	3.93%

2b-10	-2023.108473	0.42691	-1269251.694	1.223367226	3.58%
2b-11	-2023.111362	0.429818	-1269251.682	1.235892314	3.50%
2b-12	-2023.108621	0.427412	-1269251.472	1.445718907	2.46%
2b-13	-2023.108401	0.427924	-1269251.013	1.905024412	1.13%
2b-14	-2023.1084	0.42793	-1269251.008	1.909831134	1.12%

Electronic energy obtained at M062X/6-311+G(2d,p) (Solvent=Methanol) level of theory; Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d), EmpiricalDispersion=GD3 level of theory; Gibbs free energy (E + C); The relative Gibbs free energy; The Boltzmann distribution of each conformer.

Table S18. Atomic coordinates (Å) of **2-1** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	2.235245	-1.6632	-1.822606	H	1.174673	-3.509724	-2.050217
C	3.360399	-1.004427	-1.262675	H	5.096442	0.647026	0.045194
C	4.276722	-1.768799	-0.512913	H	5.210031	1.667696	-1.376335
C	4.075587	-3.125019	-0.29891	H	2.367625	3.21432	1.323676
C	2.96235	-3.75961	-0.870792	H	3.759905	0.155521	2.163447
C	2.053491	-3.036097	-1.626975	H	0.398109	-2.43016	1.525391
C	3.46997	0.454808	-1.40035	H	2.316683	-3.304857	2.642291
C	4.510626	1.261954	-0.638295	H	-7.075657	2.03586	-0.049604
C	3.884997	2.426835	0.10641	H	-8.259848	-2.084359	0.322863
C	2.788863	2.317383	0.878016	H	-5.910047	-2.835383	-0.108513
C	2.096197	1.030573	1.112442	H	-4.308557	2.183297	-1.154142
C	2.756195	0.006896	1.780255	H	-3.127048	0.194423	-2.04811
C	2.148831	-1.246828	1.934012	H	-0.749381	0.934872	-1.880824
C	0.864972	-1.453265	1.428968	H	-1.655698	2.337461	-1.335888
C	2.896849	-2.370843	2.510519	H	0.844562	2.408117	-0.830916
C	4.541742	3.744258	-0.099773	H	-0.193501	2.703306	0.552565
C	-5.202521	-0.803412	-0.317426	H	-1.747915	-1.349949	0.885413
C	-5.524489	0.551282	-0.303999	O	5.4936	3.921871	-0.840787
C	-6.825922	0.97834	-0.064753	H	4.482584	5.557844	0.39573
C	-7.808005	0.005263	0.15846	O	2.688679	1.081518	-2.139701
C	-7.473371	-1.357568	0.147049	O	1.282062	-0.992966	-2.5217
C	-6.164699	-1.78139	-0.094014	O	-1.968741	1.37575	2.116506
C	-4.252486	1.311966	-0.501787	O	-3.735772	1.763487	0.793952
C	-3.269604	0.212451	-0.966007	O	-9.120225	0.321442	0.394913
C	-1.988809	0.500187	-0.187713	O	-3.874214	-1.045755	-0.570116
C	-1.08725	1.470068	-0.986388	O	-1.034388	-1.602397	-0.977192
C	0.116512	1.932942	-0.165574	H	-0.304531	-1.264557	-1.533978

C	0.794807	0.81738	0.591983	H	5.123359	-3.371626	1.286134
C	0.181436	-0.431006	0.763972	H	1.615081	-0.053327	-2.601172
C	-1.175614	-0.760676	0.165142	O	3.986875	4.746566	0.614575
C	-2.517423	1.22753	1.048489	O	4.088433	-2.334138	2.800379
H	5.143498	-1.299921	-0.063614	O	4.925769	-3.876822	0.475076
H	2.812511	-4.818812	-0.689498	H	-9.223111	1.28664	0.384266

Table S19. Atomic coordinates (Å) of **2-2** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.047714	2.622331	-1.257237	H	3.116943	3.062154	-1.594136
C	0.010235	2.51407	-0.293862	H	-2.016	1.213424	1.124674
C	0.305235	2.786509	1.05853	H	-2.629226	2.829874	0.78989
C	1.583999	3.147247	1.449719	H	-4.86971	-0.400389	-0.680805
C	2.599158	3.262486	0.485046	H	-3.921396	-0.615896	2.449216
C	2.332624	2.999426	-0.847894	H	-0.538094	-3.259979	2.370656
C	-1.318778	2.059176	-0.709669	H	-1.580915	-2.818574	4.460322
C	-2.409717	1.857767	0.334961	H	5.035447	-0.035614	-1.225595
C	-3.661154	1.263171	-0.256634	H	4.334192	0.652634	2.963766
C	-3.967257	-0.043514	-0.19073	H	1.905428	0.106107	2.678
C	-3.097798	-1.029636	0.500804	H	2.290908	0.006727	-2.563079
C	-3.178951	-1.168006	1.882381	H	0.107491	-0.097797	-1.604865
C	-2.281428	-2.003395	2.561436	H	-0.657423	-1.755122	-3.363976
C	-1.278066	-2.662298	1.849208	H	-1.10184	-3.319561	-2.694902
C	-2.355511	-2.154279	4.024362	H	-2.114742	-0.547358	-1.992079
C	-4.526987	2.2225	-0.987628	H	-3.012243	-2.029879	-2.160298
C	2.145574	-0.2746	0.566812	H	-0.341552	-4.120776	-0.702521
C	3.010434	-0.32013	-0.522383	O	-4.301118	3.418576	-1.053122
C	4.358613	-0.010452	-0.375696	H	-6.092533	2.373681	-2.019078
C	4.820448	0.344054	0.897016	O	-1.562228	1.79562	-1.902229
C	3.941804	0.37291	1.991369	O	0.861878	2.342036	-2.568369
C	2.590513	0.062363	1.839185	O	1.67862	-4.040399	-2.522009
C	2.214472	-0.69746	-1.733822	O	2.578838	-2.005235	-2.266881
C	0.778098	-0.831404	-1.164759	O	6.128539	0.675648	1.141736
C	0.342256	-2.270956	-1.49617	O	0.843001	-0.54822	0.248287
C	-0.880803	-2.281109	-2.430096	O	1.065744	-3.364208	0.598409
C	-2.08725	-1.612563	-1.741999	H	1.545738	-4.142873	0.276386

C	-2.127471	-1.751453	-0.232834	H	2.756194	3.527346	2.922674
C	-1.188471	-2.528731	0.464902	H	-0.09822	2.111011	-2.667119
C	-0.031838	-3.155037	-0.28155	O	-5.599762	1.655082	-1.580138
C	1.567652	-2.891078	-2.155122	O	-3.183563	-1.611543	4.740134
H	-0.45993	2.696136	1.81991	O	1.810031	3.363259	2.782241
H	3.606473	3.532495	0.789446	H	6.631064	0.619844	0.313156

Table S20. Atomic coordinates (Å) of **2-3** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-1.312731	-2.487626	-1.028187	H	-3.417648	-2.869455	-1.154649
C	-0.173009	-2.450802	-0.183738	H	2.121596	-1.382569	1.02355
C	-0.32744	-2.769617	1.186531	H	2.537649	-3.026079	0.548578
C	-1.565746	-3.114514	1.698621	H	4.844768	0.076274	-1.092722
C	-2.683173	-3.165479	0.844292	H	4.303068	0.296354	2.126248
C	-2.55706	-2.855818	-0.495876	H	1.179536	3.220289	2.487157
C	1.126369	-2.073964	-0.740401	H	2.429884	2.655513	4.428354
C	2.35186	-2.017399	0.164098	H	-5.01032	0.105209	-1.539886
C	3.568278	-1.503016	-0.560327	H	-4.84655	-0.659003	2.692558
C	3.980604	-0.225782	-0.506224	H	-2.440953	0.036354	2.758212
C	3.278465	0.805692	0.29972	H	-2.193479	0.37626	-2.537606
C	3.542714	0.91479	1.660629	H	-0.190112	0.219941	-1.211815
C	2.810585	1.810622	2.45167	H	0.46592	1.840424	-3.230073
C	1.788025	2.563817	1.873169	H	1.142803	3.330523	-2.589891
C	3.080775	1.932527	3.894867	H	1.940425	0.452968	-2.055479
C	4.261145	-2.502258	-1.412578	H	2.954838	1.842761	-2.318716
C	-2.418444	0.463447	0.640691	H	0.637924	4.181885	-0.471489
C	-3.123055	0.486393	-0.557035	O	3.924849	-3.671488	-1.487693
C	-4.45697	0.095455	-0.604761	H	5.682349	-2.741812	-2.621047
C	-5.065496	-0.318165	0.586373	O	1.244674	-1.769337	-1.94302
C	-4.34383	-0.327193	1.790176	O	-1.262727	-2.15988	-2.338659
C	-3.005038	0.06299	1.832824	O	-1.495176	4.344909	-2.140915
C	-2.204615	0.980592	-1.630414	O	-2.515734	2.35117	-2.025193
C	-0.837549	1.039679	-0.911968	O	-6.369405	-0.731299	0.644167
C	-0.265725	2.42051	-1.255967	O	-1.104845	0.867653	0.510777
C	0.847826	2.31218	-2.318878	O	-0.650948	3.528378	0.914069
C	2.050645	1.509484	-1.793337	H	-0.955741	2.668424	1.258277

C	2.286539	1.616153	-0.301823	H	-0.94545	-3.350688	3.502747
C	1.513404	2.463569	0.508911	H	-0.30965	-1.964907	-2.538381
C	0.321892	3.213871	-0.067809	O	5.306979	-2.003328	-2.105623
C	-1.457657	3.175159	-1.839047	O	3.940351	1.307326	4.496562
H	0.532752	-2.739707	1.846811	O	-1.783237	-3.413275	3.016049
H	-3.648224	-3.432084	1.261154	H	-6.763161	-0.675309	-0.241283

Table S21. Atomic coordinates (Å) of **2-4** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	-1.28874	-2.540472	-1.007121	H	-3.389989	-2.925697	-1.165121
C	-0.171701	-2.452401	-0.133865	H	2.093396	-1.331261	1.074873
C	-0.366225	-2.669644	1.247749	H	2.523651	-2.995004	0.694488
C	-1.621679	-2.967014	1.750324	H	4.872251	0.027214	-1.031738
C	-2.71266	-3.081662	0.870655	H	4.29589	0.398212	2.151558
C	-2.546785	-2.868076	-0.486421	H	1.160265	3.324016	2.356259
C	1.145433	-2.11493	-0.67717	H	2.400378	2.855699	4.329012
C	2.346263	-2.007531	0.254653	H	-5.012532	0.032561	-1.506778
C	3.578769	-1.52601	-0.464951	H	-4.830752	-0.530909	2.756339
C	3.993718	-0.248555	-0.453731	H	-2.420367	0.15198	2.776397
C	3.280119	0.816363	0.297274	H	-2.195132	0.234601	-2.527863
C	3.536033	0.990983	1.652919	H	-0.184575	0.146795	-1.208891
C	2.796008	1.920131	2.396649	H	0.483155	1.671229	-3.292707
C	1.774379	2.641416	1.777335	H	1.149878	3.193337	-2.721262
C	3.05747	2.111268	3.833962	H	1.959975	0.349275	-2.049401
C	4.288462	-2.561339	-1.25837	H	2.967401	1.731561	-2.368611
C	-2.407638	0.480572	0.641318	H	0.634176	4.142262	-0.649414
C	-3.11816	0.450323	-0.552647	O	3.959045	-3.734643	-1.282273
C	-4.454426	0.065237	-0.575015	H	5.729484	-2.850916	-2.431974
C	-5.058675	-0.288938	0.637214	O	1.297005	-1.884015	-1.891751
C	-4.330951	-0.244972	1.836713	O	-1.201378	-2.295308	-2.334275
C	-2.989942	0.139865	1.854096	O	-1.49017	4.218372	-2.336542
C	-2.20196	0.885748	-1.653373	O	-2.511445	2.233887	-2.118452
C	-0.831713	0.9786	-0.943422	O	-6.363836	-0.693618	0.720575
C	-0.261512	2.342647	-1.352224	O	-1.092803	0.871199	0.486312
C	0.857906	2.187859	-2.403145	O	-0.660691	3.554274	0.759171
C	2.061904	1.417036	-1.833936	H	-0.960299	2.712388	1.149069

C	2.288547	1.59336	-0.347544	H	-2.68321	-3.291915	3.317673
C	1.508214	2.475743	0.417818	H	-0.243503	-2.11162	-2.518901
C	0.318262	3.194223	-0.200765	O	5.342339	-2.090487	-1.958985
C	-1.452913	3.065817	-1.9747	O	3.916479	1.519445	4.469205
H	0.462964	-2.595356	1.940803	O	-1.750366	-3.131766	3.10298
H	-3.699337	-3.31297	1.261595	H	-6.761428	-0.678082	-0.164785

Table S22. Atomic coordinates (Å) of **2-5** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.071301	2.548247	-1.309539	H	3.144196	2.999252	-1.61378
C	0.003897	2.49631	-0.377559	H	-2.067609	1.296038	1.067105
C	0.247363	2.886816	0.959728	H	-2.669915	2.878226	0.582184
C	1.504081	3.306624	1.359366	H	-4.841429	-0.470833	-0.725736
C	2.552091	3.358685	0.422465	H	-3.920221	-0.447152	2.446233
C	2.337234	2.982524	-0.889672	H	-0.53722	-3.090713	2.570114
C	-1.304125	1.99556	-0.802371	H	-1.581482	-2.492325	4.620026
C	-2.43283	1.873846	0.214665	H	5.03146	-0.113635	-1.289648
C	-3.662513	1.229936	-0.371058	H	4.368019	0.863412	2.84773
C	-3.957887	-0.073623	-0.232277	H	1.940814	0.282553	2.627869
C	-3.094018	-1.006067	0.535586	H	2.276862	-0.189232	-2.598931
C	-3.176949	-1.040222	1.923558	H	0.103927	-0.228456	-1.610162
C	-2.280264	-1.822428	2.664395	H	-0.646703	-2.013879	-3.259882
C	-1.276523	-2.533592	2.004661	H	-1.092809	-3.52389	-2.477293
C	-2.354593	-1.861483	4.134592	H	-2.102275	-0.705149	-1.979201
C	-4.512965	2.130543	-1.18968	H	-3.003808	-2.194142	-2.046498
C	2.161212	-0.24233	0.545588	H	-0.338773	-4.177573	-0.433997
C	3.015423	-0.358433	-0.546846	O	-4.283886	3.318043	-1.342599
C	4.363209	-0.032178	-0.436537	H	-6.055676	2.201174	-2.263378
C	4.836022	0.411323	0.803699	O	-1.503031	1.634486	-1.978148
C	3.967994	0.512633	1.901968	O	0.934627	2.167985	-2.600718
C	2.617022	0.186028	1.786143	O	1.690823	-4.226106	-2.247453
C	2.211469	-0.829848	-1.718976	O	2.580533	-2.172362	-2.154684
C	0.781158	-0.928993	-1.128625	O	6.145183	0.76339	1.011486
C	0.348925	-2.389516	-1.356034	O	0.857929	-0.549051	0.261714
C	-0.872031	-2.468661	-2.28993	O	1.066553	-3.332705	0.813171
C	-2.079044	-1.750599	-1.655572	H	1.54813	-4.131055	0.546423

C	-2.123056	-1.781178	-0.140609	H	1.015039	3.573534	3.198957
C	-1.18538	-2.504603	0.614288	H	-0.018892	1.915514	-2.713686
C	-0.028009	-3.184766	-0.08245	O	-5.574441	1.51915	-1.758278
C	1.57546	-3.052435	-1.969363	O	-3.181013	-1.26352	4.807001
H	-0.556053	2.84637	1.687495	O	1.805175	3.671535	2.643364
H	3.534793	3.676724	0.753443	H	6.639962	0.649744	0.184149

Table S23. Atomic coordinates (Å) of **2-6** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.072199	2.549107	-1.309385	H	3.14515	2.999504	-1.613988
C	0.00506	2.497052	-0.377111	H	-2.065528	1.294765	1.067275
C	0.249015	2.886863	0.960289	H	-2.668118	2.877635	0.584754
C	1.505993	3.306048	1.359792	H	-4.841925	-0.468893	-0.724604
C	2.553766	3.358133	0.422629	H	-3.920359	-0.44884	2.446946
C	2.338396	2.982695	-0.88964	H	-0.537497	-3.092731	2.568088
C	-1.303145	1.996697	-0.801737	H	-1.581571	-2.496274	4.618643
C	-2.43126	1.873719	0.21585	H	5.031772	-0.115644	-1.287162
C	-3.661424	1.230737	-0.369941	H	4.365239	0.860469	2.849948
C	-3.957829	-0.072613	-0.231395	H	1.937757	0.281554	2.627585
C	-3.094313	-1.006003	0.53577	H	2.278012	-0.188101	-2.598842
C	-3.177212	-1.041551	1.923684	H	0.104074	-0.227373	-1.612459
C	-2.280537	-1.824567	2.663697	H	-0.648583	-2.013032	-3.261422
C	-1.276822	-2.535053	2.003197	H	-1.094715	-3.522614	-2.478042
C	-2.354858	-1.865133	4.133855	H	-2.10191	-0.702974	-1.978973
C	-4.511799	2.132437	-1.187465	H	-3.004878	-2.191013	-2.047405
C	2.159701	-0.242591	0.545301	H	-0.338437	-4.176972	-0.436127
C	3.014854	-0.359169	-0.546343	O	-4.283668	3.320484	-1.337439
C	4.362774	-0.033923	-0.434657	H	-6.053775	2.204138	-2.262182
C	4.83476	0.408862	0.806157	O	-1.50267	1.636784	-1.977784
C	3.965801	0.510418	1.903666	O	0.935004	2.169444	-2.600685
C	2.614683	0.184893	1.786448	O	1.689171	-4.224794	-2.25133
C	2.211564	-0.829374	-1.71944	O	2.580093	-2.171701	-2.155905
C	0.780713	-0.92804	-1.13029	O	6.143972	0.760006	1.015228
C	0.348139	-2.388453	-1.358035	O	0.856407	-0.548021	0.260043
C	-0.873418	-2.467389	-2.291172	O	1.066839	-3.331639	0.810782
C	-2.079622	-1.74872	-1.656208	H	1.547579	-4.130833	0.545077

C	-2.123468	-1.780575	-0.141276	H	1.017625	3.571896	3.199696
C	-1.185695	-2.504675	0.612858	H	-0.018718	1.917724	-2.713582
C	-0.028146	-3.184081	-0.08445	O	-5.572071	1.521317	-1.758603
C	1.574383	-3.051415	-1.971889	O	-3.181419	-1.268055	4.806868
H	-0.554271	2.846422	1.688208	O	1.807517	3.67036	2.643846
H	3.536677	3.675668	0.753486	H	6.639476	0.646034	0.188371

Table S24. Atomic coordinates (Å) of **2-7** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	0.054128	1.931362	-1.68359	H	1.856227	3.083838	-1.787014
C	-1.230248	1.808526	-1.088924	H	-3.865088	1.530288	-0.482951
C	-1.603196	2.729332	-0.084028	H	-4.095439	1.115376	-2.162735
C	-0.735959	3.725919	0.336247	H	-4.152806	-2.313806	0.287285
C	0.506308	3.870233	-0.306328	H	-3.640156	0.835729	1.778655
C	0.88819	2.993341	-1.308164	H	0.309393	0.163275	3.33759
C	-2.125041	0.739004	-1.537562	H	-0.864168	2.153876	3.979196
C	-3.617045	0.782553	-1.234572	H	5.372327	-0.729872	-2.111372
C	-4.189947	-0.568159	-0.87023	H	5.087639	2.886709	0.202611
C	-3.728196	-1.32443	0.141046	H	2.795125	2.242538	0.983929
C	-2.628863	-0.916858	1.039915	H	2.60697	-1.971253	-2.26379
C	-2.738474	0.234298	1.811607	H	0.563811	-1.232594	-1.166396
C	-1.675632	0.641743	2.629709	H	0.309109	-3.842011	-0.964757
C	-0.523403	-0.144467	2.715196	H	0.145729	-4.354316	0.707762
C	-1.699019	1.953021	3.281367	H	-1.533882	-2.419612	-0.896395
C	-5.283303	-1.063819	-1.746188	H	-2.03429	-3.592135	0.294236
C	2.826488	0.402189	-0.143751	H	0.689952	-3.049643	2.493423
C	3.540713	-0.42805	-1.001479	O	-5.697735	-0.464133	-2.72385
C	4.812744	-0.079004	-1.444799	H	-6.484395	-2.486861	-2.010727
C	5.356864	1.131816	-1.001167	O	-1.704573	-0.191141	-2.252965
C	4.633791	1.957142	-0.125614	O	0.513097	1.069522	-2.616312
C	3.358066	1.602513	0.315144	O	2.923093	-4.090258	1.261979
C	2.731318	-1.666632	-1.224538	O	3.334491	-2.804161	-0.527757
C	1.404163	-1.346036	-0.483513	O	6.60004	1.567014	-1.382597
C	1.219971	-2.510267	0.505905	O	1.583218	-0.070918	0.171478
C	0.110486	-3.481201	0.049414	O	1.915101	-1.403374	2.61299
C	-1.281143	-2.819887	0.092986	H	2.544373	-2.068982	2.932745

C	-1.436879	-1.681091	1.077834	H	-1.742397	4.212988	1.902182
C	-0.399815	-1.296579	1.941592	H	-0.192647	0.380291	-2.722098
C	0.874135	-2.10811	1.957966	O	-5.790562	-2.256019	-1.364974
C	2.559643	-3.230927	0.488197	O	-2.537271	2.822599	3.051754
H	-2.561408	2.641087	0.410312	O	-1.035053	4.597494	1.348344
H	1.17154	4.667071	0.011327	H	6.998647	0.910187	-1.975798

Table S25. Atomic coordinates (Å) of **2-8** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	0.054072	1.93142	-1.683031	H	1.856205	3.08391	-1.785732
C	-1.230523	1.808578	-1.088813	H	-3.86559	1.53022	-0.483688
C	-1.60385	2.729372	-0.084049	H	-4.095411	1.114853	-2.163433
C	-0.736776	3.72593	0.336586	H	-4.152353	-2.314197	0.286609
C	0.505749	3.870234	-0.305512	H	-3.640203	0.835398	1.778074
C	0.887997	2.993393	-1.307239	H	0.309049	0.163053	3.337754
C	-2.125091	0.739053	-1.537732	H	-0.864517	2.15367	3.978946
C	-3.617167	0.782361	-1.235073	H	5.372084	-0.729436	-2.112151
C	-4.189895	-0.568403	-0.870632	H	5.088141	2.886856	0.202355
C	-3.727916	-1.324728	0.140497	H	2.795902	2.242557	0.984385
C	-2.628703	-0.917111	1.03945	H	2.606881	-1.9711	-2.263633
C	-2.738494	0.234022	1.811152	H	0.564013	-1.232095	-1.165923
C	-1.675848	0.641473	2.629505	H	0.30978	-3.841797	-0.964962
C	-0.523604	-0.144697	2.715174	H	0.146272	-4.354366	0.707462
C	-1.699433	1.952698	3.281228	H	-1.53347	-2.419766	-0.896644
C	-5.283403	-1.064063	-1.746409	H	-2.03379	-3.592412	0.293909
C	2.826906	0.402358	-0.14353	H	0.689878	-3.049882	2.493416
C	3.540846	-0.427765	-1.001617	O	-5.698004	-0.464389	-2.723997
C	4.812722	-0.078654	-1.445313	H	-6.484448	-2.48718	-2.010825
C	5.356969	1.132126	-1.001732	O	-1.704324	-0.191026	-2.253075
C	4.634191	1.957327	-0.125824	O	0.513361	1.069619	-2.615607
C	3.358629	1.602625	0.315331	O	2.923709	-4.089719	1.262291
C	2.731438	-1.666382	-1.224433	O	3.3348	-2.803783	-0.527639
C	1.404436	-1.345757	-0.483163	O	6.599995	1.567389	-1.383557
C	1.220274	-2.510145	0.506049	O	1.583739	-0.070795	0.172034
C	0.11099	-3.481162	0.049236	O	1.914905	-1.403583	2.613533
C	-1.28074	-2.82005	0.092737	H	2.54424	-2.069224	2.933099

C	-1.436714	-1.681313	1.07761	H	-1.743506	4.212735	1.90239
C	-0.399842	-1.296796	1.94159	H	-0.192354	0.380395	-2.721888
C	0.874135	-2.108261	1.95814	O	-5.790558	-2.256298	-1.365153
C	2.560075	-3.230574	0.488408	O	-2.537886	2.822134	3.051811
H	-2.562268	2.641116	0.409896	O	-1.036274	4.597485	1.348571
H	1.170855	4.667064	0.012421	H	6.998352	0.910715	-1.977091

Table S26. Atomic coordinates (Å) of **2-9** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	2.232047	-1.64908	-1.823236	H	1.173686	-3.495626	-2.060547
C	3.356914	-0.991947	-1.260318	H	5.103103	0.65649	0.04507
C	4.275379	-1.759559	-0.516498	H	5.201836	1.668486	-1.379671
C	4.07655	-3.117307	-0.310728	H	2.376656	3.202239	1.353282
C	2.963456	-3.750054	-0.885099	H	3.749789	0.130895	2.165705
C	2.052496	-3.023421	-1.635679	H	0.381389	-2.441734	1.510815
C	3.46393	0.467935	-1.389581	H	2.296112	-3.327425	2.625822
C	4.510431	1.274262	-0.630288	H	-7.081469	2.049637	-0.038087
C	3.882702	2.429992	0.132019	H	-8.27413	-2.070988	0.301656
C	2.784478	2.302808	0.897327	H	-5.925423	-2.823322	-0.133492
C	2.089003	1.016933	1.118859	H	-4.313328	2.200035	-1.1394
C	2.74601	-0.012728	1.780807	H	-3.135231	0.215763	-2.047821
C	2.135041	-1.265526	1.927419	H	-0.756909	0.950177	-1.874084
C	0.851034	-1.465609	1.420225	H	-1.660246	2.350523	-1.31855
C	2.879026	-2.394352	2.499607	H	0.840196	2.41227	-0.812641
C	4.475615	3.79303	0.029293	H	-0.197042	2.69854	0.573139
C	-5.213722	-0.791199	-0.326213	H	-1.7609	-1.353461	0.87488
C	-5.533016	0.563999	-0.30259	O	4.048164	4.785731	0.591633
C	-6.833803	0.991771	-0.061155	H	5.881358	4.753771	-0.775035
C	-7.818024	0.018942	0.153688	O	2.680264	1.09831	-2.122913
C	-7.486068	-1.344416	0.132107	O	1.277753	-0.976406	-2.518072
C	-6.178006	-1.768965	-0.111109	O	-1.977043	1.36297	2.126345
C	-4.259345	1.323684	-0.493625	O	-3.742571	1.764247	0.805759
C	-3.278335	0.225817	-0.965678	O	-9.129844	0.335879	0.391356
C	-1.997385	0.505176	-0.184569	O	-3.885681	-1.034195	-0.579731
C	-1.093636	1.479314	-0.97561	O	-1.046148	-1.59329	-0.989155
C	0.111083	1.933286	-0.151241	H	-0.313006	-1.254204	-1.540893

C	0.786829	0.810468	0.597583	H	5.116104	-3.376274	1.277278
C	0.170407	-0.437423	0.761349	H	1.608254	-0.035451	-2.591442
C	-1.186941	-0.75991	0.159466	O	5.566914	3.829711	-0.766544
C	-2.525234	1.224232	1.056815	O	4.070075	-2.362159	2.792445
H	5.141862	-1.292243	-0.065002	O	4.929274	-3.872027	0.45775
H	2.815451	-4.810537	-0.709897	H	-9.230863	1.301334	0.387859

Table S27. Atomic coordinates (Å) of **2-10** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.32115	2.503491	-1.001607	H	3.427459	2.880385	-1.120567
C	0.181841	2.451923	-0.157456	H	-2.107604	1.33193	1.014077
C	0.338523	2.736775	1.220111	H	-2.519263	2.992963	0.621912
C	1.578605	3.063633	1.739346	H	-4.848582	-0.032043	-1.116429
C	2.695456	3.131737	0.885339	H	-4.330087	-0.33844	2.10467
C	2.567254	2.854424	-0.461622	H	-1.214157	-3.275137	2.425489
C	-1.118504	2.090845	-0.721419	H	-2.477169	-2.7495	4.369268
C	-2.341528	2.004992	0.184407	H	5.007723	-0.098386	-1.507901
C	-3.561132	1.51314	-0.552422	H	4.817075	0.595938	2.735477
C	-3.983019	0.239047	-0.514759	H	2.408463	-0.090476	2.772719
C	-3.295284	-0.812705	0.274463	H	2.195967	-0.340471	-2.528841
C	-3.568459	-0.949199	1.631122	H	0.183559	-0.203401	-1.215311
C	-2.843292	-1.863016	2.408071	H	-0.468409	-1.790636	-3.262213
C	-1.817892	-2.605576	1.821012	H	-1.151795	-3.288208	-2.646913
C	-3.12296	-2.014055	3.84671	H	-1.938605	-0.41595	-2.065517
C	-4.304948	2.457828	-1.430102	H	-2.958668	-1.794379	-2.362118
C	2.399293	-0.48298	0.648397	H	-0.652084	-4.17778	-0.544945
C	3.112162	-0.488562	-0.544614	O	-5.262568	2.171036	-2.125645
C	4.447953	-0.102415	-0.576537	H	-4.330986	4.260504	-1.979711
C	5.049663	0.288845	0.625532	O	-1.240583	1.817687	-1.931213
C	4.319597	0.280793	1.824267	O	1.269278	2.205212	-2.318901
C	2.979035	-0.104641	1.851058	O	1.485534	-4.313975	-2.206649
C	2.199432	-0.96105	-1.632545	O	2.509552	-2.32493	-2.049925
C	0.827378	-1.029164	-0.924118	O	6.354598	0.696105	0.69928
C	0.255045	-2.403174	-1.29427	O	1.085229	-0.880463	0.502817
C	-0.854293	-2.275123	-2.359434	O	0.628924	-3.548086	0.85859
C	-2.05578	-1.476865	-1.824887	H	0.930385	-2.694448	1.220846

C	-2.300939	-1.61306	-0.337229	H	0.962459	3.249132	3.550741
C	-1.533915	-2.477558	0.460884	H	0.315484	2.018445	-2.522714
C	-0.338809	-3.216775	-0.122813	O	-3.79731	3.709206	-1.376412
C	1.448625	-3.149663	-1.884419	O	-3.984886	-1.399304	4.455762
H	-0.52095	2.693037	1.880495	O	1.798761	3.327206	3.063706
H	3.66182	3.384381	1.307726	H	6.754175	0.653649	-0.184293

Table S28. Atomic coordinates (Å) of **2-11** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	0.096167	1.978081	-1.490653	H	1.84668	3.204973	-1.377979
C	-1.241729	1.794006	-1.049331	H	-3.913513	1.381406	-0.741404
C	-1.76703	2.686321	-0.08705	H	-3.942066	0.970961	-2.438468
C	-0.995737	3.70975	0.441608	H	-4.066002	-2.478253	-0.016562
C	0.307685	3.910245	-0.047245	H	-3.917111	0.670196	1.53518
C	0.837705	3.065672	-1.008274	H	-0.106203	0.263675	3.476166
C	-2.031365	0.693385	-1.607794	H	-1.481014	2.145845	4.021776
C	-3.546948	0.656027	-1.465988	H	5.356184	-0.860547	-2.235567
C	-4.078771	-0.728188	-1.169551	H	5.32062	2.945906	-0.227409
C	-3.685713	-1.465336	-0.116177	H	3.137354	2.383522	0.867906
C	-2.713946	-0.997796	0.894288	H	2.666764	-2.147769	-1.948516
C	-2.982738	0.133372	1.656512	H	0.718243	-1.078708	-0.918882
C	-2.0388	0.604527	2.578359	H	0.572653	-3.827576	-0.710211
C	-0.844749	-0.095677	2.767219	H	0.223264	-4.239229	0.960738
C	-2.220789	1.900916	3.236271	H	-1.27353	-2.394045	-0.928636
C	-5.04201	-1.276213	-2.159801	H	-1.900709	-3.593291	0.171445
C	3.050348	0.455009	-0.100241	H	0.669424	-2.823232	2.770014
C	3.661973	-0.453737	-0.954876	O	-5.38592	-0.689097	-3.171692
C	4.87294	-0.151544	-1.568899	H	-6.121537	-2.764234	-2.55818
C	5.456926	1.092164	-1.297984	O	-1.490236	-0.203339	-2.284031
C	4.836537	1.993992	-0.419185	O	0.694383	1.152179	-2.37596
C	3.621143	1.685723	0.194601	O	2.945609	-3.934896	1.697295
C	2.836079	-1.701012	-0.968561	O	3.448834	-2.728455	-0.12605
C	1.544938	-1.270425	-0.237177	O	6.642003	1.487817	-1.857324
C	1.281001	-2.389175	0.775728	O	1.853438	0.000681	0.412479
C	0.246137	-3.409635	0.247517	O	1.741818	-1.137083	2.855873
C	-1.152533	-2.795495	0.085466	H	1.926485	-0.376081	2.273644

C	-1.479835	-1.67645	1.046533	H	-2.207938	4.147721	1.871324
C	-0.555859	-1.225563	2.002786	H	0.032016	0.441324	-2.578147
C	0.789889	-1.920166	2.161649	O	-5.513949	-2.500749	-1.841831
C	2.625854	-3.102353	0.882073	O	-3.08553	2.716032	2.922949
H	-2.773738	2.556157	0.287399	O	-1.445095	4.556385	1.4181
H	0.897219	4.729358	0.352598	H	6.972971	0.783566	-2.437636

Table S29. Atomic coordinates (Å) of **2-12** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.297717	2.559208	-0.978271	H	3.401509	2.933538	-1.129095
C	0.181139	2.457319	-0.105993	H	-2.07553	1.275459	1.060928
C	0.378333	2.639736	1.28031	H	-2.503155	2.95362	0.774844
C	1.635962	2.917835	1.788296	H	-4.877286	0.021416	-1.053737
C	2.726855	3.04626	0.910411	H	-4.328645	-0.447496	2.124792
C	2.55847	2.865544	-0.451108	H	-1.200743	-3.384213	2.285274
C	-1.137527	2.136937	-0.655356	H	-2.457813	-2.962831	4.25727
C	-2.334138	1.992746	0.277266	H	5.012469	-0.029511	-1.470548
C	-3.570678	1.536534	-0.45404	H	4.804019	0.455098	2.800868
C	-3.996545	0.26328	-0.461747	H	2.390288	-0.21565	2.791747
C	-3.298709	-0.823679	0.269293	H	2.199642	-0.195007	-2.513572
C	-3.566433	-1.030295	1.618133	H	0.180347	-0.127481	-1.208078
C	-2.83482	-1.979214	2.34519	H	-0.482618	-1.613242	-3.323609
C	-1.808972	-2.687089	1.717561	H	-1.158085	-3.141753	-2.780428
C	-3.108561	-2.204403	3.775263	H	-1.953277	-0.305281	-2.055694
C	-4.331197	2.520829	-1.271883	H	-2.968696	-1.671275	-2.414363
C	2.390523	-0.504372	0.650848	H	-0.647777	-4.133586	-0.729225
C	3.109274	-0.455187	-0.537501	O	-5.29927	2.265316	-1.965179
C	4.447643	-0.076982	-0.543519	H	-4.37233	4.348645	-1.729651
C	5.045303	0.251531	0.679101	O	-1.294236	1.943157	-1.87567
C	4.30927	0.188724	1.872674	O	1.207577	2.345712	-2.310616
C	2.966259	-0.18956	1.873737	O	1.480189	-4.18032	-2.40539
C	2.198404	-0.864199	-1.652723	O	2.505661	-2.203289	-2.143958
C	0.823114	-0.966084	-0.953402	O	6.351651	0.648571	0.778474
C	0.251513	-2.320764	-1.391288	O	1.074666	-0.88514	0.479694
C	-0.862683	-2.143187	-2.444204	O	0.636982	-3.572008	0.699228
C	-2.064731	-1.376967	-1.865826	H	0.932874	-2.737539	1.107407

C	-2.303414	-1.587753	-0.385747	H	2.701302	3.197031	3.361714
C	-1.530652	-2.489145	0.364707	H	0.248351	2.173807	-2.499088
C	-0.335756	-3.194187	-0.260144	O	-3.826778	3.76989	-1.163873
C	1.444212	-3.034847	-2.021582	O	-3.970833	-1.625352	4.417817
H	-0.450204	2.552627	1.972663	O	1.766997	3.049732	3.144219
H	3.715279	3.262071	1.305693	H	6.754183	0.649984	-0.104811

Table S30. Atomic coordinates (Å) of **2-13** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	1.047714	2.622331	-1.257237	H	3.116943	3.062154	-1.594136
C	0.010235	2.51407	-0.293862	H	-2.016	1.213424	1.124674
C	0.305235	2.786509	1.05853	H	-2.629226	2.829874	0.78989
C	1.583999	3.147247	1.449719	H	-4.86971	-0.400389	-0.680805
C	2.599158	3.262486	0.485046	H	-3.921396	-0.615896	2.449216
C	2.332624	2.999426	-0.847894	H	-0.538094	-3.259979	2.370656
C	-1.318778	2.059176	-0.709669	H	-1.580915	-2.818574	4.460322
C	-2.409717	1.857767	0.334961	H	5.035447	-0.035614	-1.225595
C	-3.661154	1.263171	-0.256634	H	4.334192	0.652634	2.963766
C	-3.967257	-0.043514	-0.19073	H	1.905428	0.106107	2.678
C	-3.097798	-1.029636	0.500804	H	2.290908	0.006727	-2.563079
C	-3.178951	-1.168006	1.882381	H	0.107491	-0.097797	-1.604865
C	-2.281428	-2.003395	2.561436	H	-0.657423	-1.755122	-3.363976
C	-1.278066	-2.662298	1.849208	H	-1.10184	-3.319561	-2.694902
C	-2.355511	-2.154279	4.024362	H	-2.114742	-0.547358	-1.992079
C	-4.526987	2.2225	-0.987628	H	-3.012243	-2.029879	-2.160298
C	2.145574	-0.2746	0.566812	H	-0.341552	-4.120776	-0.702521
C	3.010434	-0.32013	-0.522383	O	-4.301118	3.418576	-1.053122
C	4.358613	-0.010452	-0.375696	H	-6.092533	2.373681	-2.019078
C	4.820448	0.344054	0.897016	O	-1.562228	1.79562	-1.902229
C	3.941804	0.37291	1.991369	O	0.861878	2.342036	-2.568369
C	2.590513	0.062363	1.839185	O	1.67862	-4.040399	-2.522009
C	2.214472	-0.69746	-1.733822	O	2.578838	-2.005235	-2.266881
C	0.778098	-0.831404	-1.164759	O	6.128539	0.675648	1.141736
C	0.342256	-2.270956	-1.49617	O	0.843001	-0.54822	0.248287
C	-0.880803	-2.281109	-2.430096	O	1.065744	-3.364208	0.598409
C	-2.08725	-1.612563	-1.741999	H	1.545738	-4.142873	0.276386

C	-2.127471	-1.751453	-0.232834	H	2.756194	3.527346	2.922674
C	-1.188471	-2.528731	0.464902	H	-0.09822	2.111011	-2.667119
C	-0.031838	-3.155037	-0.28155	O	-5.599762	1.655082	-1.580138
C	1.567652	-2.891078	-2.155122	O	-3.183563	-1.611543	4.740134
H	-0.45993	2.696136	1.81991	O	1.810031	3.363259	2.782241
H	3.606473	3.532495	0.789446	H	6.631064	0.619844	0.313156

Table S31. Atomic coordinates (Å) of **2-14** obtained at the B3LYP/6-31G(d,p) level of theory in the gas phase.

C	0.019594	1.930515	-1.668455	H	1.809144	3.102189	-1.772888
C	-1.262086	1.792337	-1.071001	H	-3.89013	1.474607	-0.449578
C	-1.642457	2.706837	-0.062989	H	-4.113112	1.095511	-2.133874
C	-0.784861	3.711436	0.357837	H	-4.127691	-2.36291	0.290678
C	0.454513	3.870344	-0.286975	H	-3.641053	0.785648	1.800609
C	0.843287	3.000238	-1.291963	H	0.3217	0.154231	3.342656
C	-2.145608	0.713938	-1.520205	H	-0.874353	2.127772	3.997248
C	-3.639607	0.740242	-1.213721	H	5.379089	-0.681394	-2.131452
C	-4.192011	-0.622768	-0.853296	H	5.063314	2.93522	0.178547
C	-3.707879	-1.368686	0.15477	H	2.781883	2.266103	0.970982
C	-2.611478	-0.951441	1.050155	H	2.627561	-1.953131	-2.271571
C	-2.732016	0.19512	1.827256	H	0.580959	-1.2324	-1.169402
C	-1.671447	0.611726	2.643583	H	0.351023	-3.845027	-0.967589
C	-0.509411	-0.160749	2.721626	H	0.194935	-4.357731	0.705543
C	-1.709071	1.919558	3.301428	H	-1.501338	-2.433541	-0.89557
C	-5.292011	-1.222974	-1.658327	H	-1.992802	-3.614034	0.290579
C	2.829007	0.424745	-0.154574	H	0.734949	-3.049966	2.489627
C	3.548947	-0.398632	-1.014238	O	-5.804862	-2.307685	-1.4444
C	4.815045	-0.035825	-1.463484	H	-6.397178	-0.90671	-3.149661
C	5.347264	1.181812	-1.024024	O	-1.717549	-0.208707	-2.240172
C	4.618687	2.000061	-0.146404	O	0.485522	1.07678	-2.604989
C	3.349001	1.631609	0.300461	O	2.97278	-4.068843	1.251946
C	2.752042	-1.646055	-1.233037	O	3.368776	-2.776575	-0.536831
C	1.423918	-1.338327	-0.488487	O	6.58359	1.630806	-1.411652
C	1.253095	-2.504517	0.500815	O	1.592551	-0.061924	0.166665
C	0.151256	-3.485323	0.04675	O	1.943296	-1.391091	2.60616
C	-1.245435	-2.835451	0.092399	H	2.579725	-2.050271	2.925063

C	-1.410332	-1.701729	1.081402	H	-1.79024	4.182474	1.929267
C	-0.374913	-1.308324	1.943047	H	-0.212568	0.380011	-2.711369
C	0.907631	-2.106327	1.954068	O	-5.683666	-0.432449	-2.682035
C	2.599659	-3.212256	0.479769	O	-2.559239	2.779389	3.078909
H	-2.598578	2.607453	0.433315	O	-1.090908	4.577437	1.372588
H	1.112005	4.673305	0.031365	H	6.986473	0.978695	-2.007154

Figure S22. Parameters of calculated ^{13}C NMR method for 2

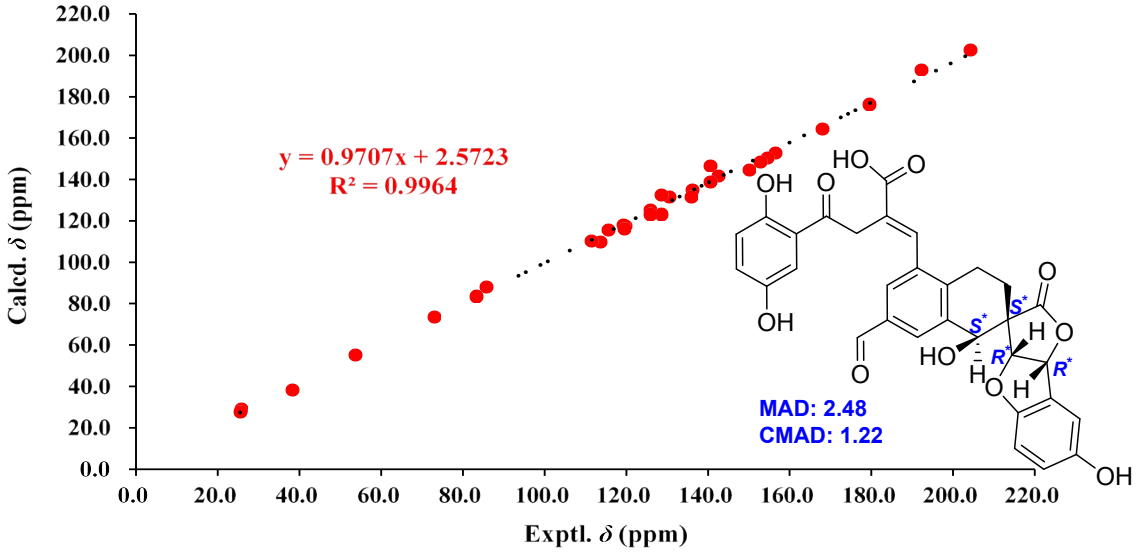


Figure S23. Calculated and experimental ECD curves of 2.