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Supporting Information

Dysoticans F-H: three unprecedented dimeric cadinanes from *Dysoxylum parasiticum* (Osbeck) Kosterm. stem bark

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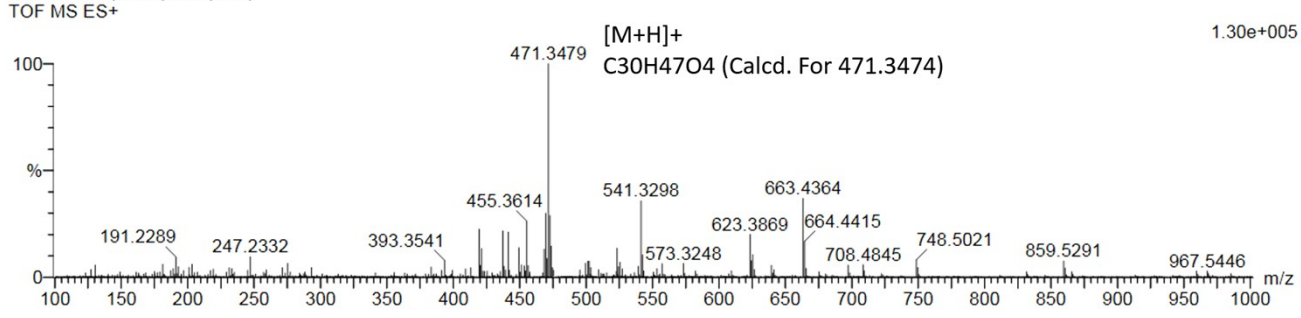
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
226 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

NAINI 28 3 (0.068) Cm (2:11)
TOF MS ES+



Minimum:				-1.5			
Maximum:		10.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
471.3479	471.3474	0.5	1.1	7.5	13.9	1.9	C30 H47 O4

Figure S1. Mass Spectrum of **1**

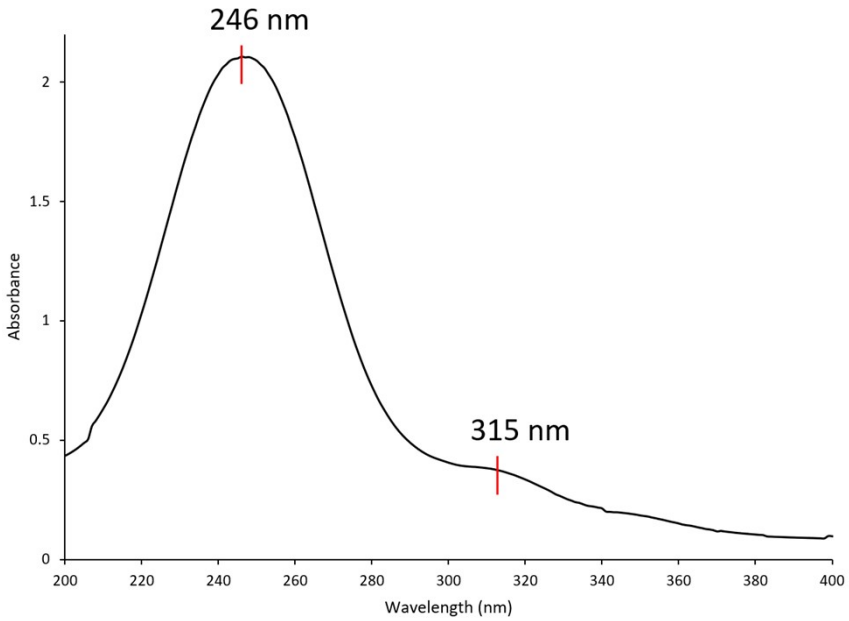


Figure S2. UV spectrum of **1**

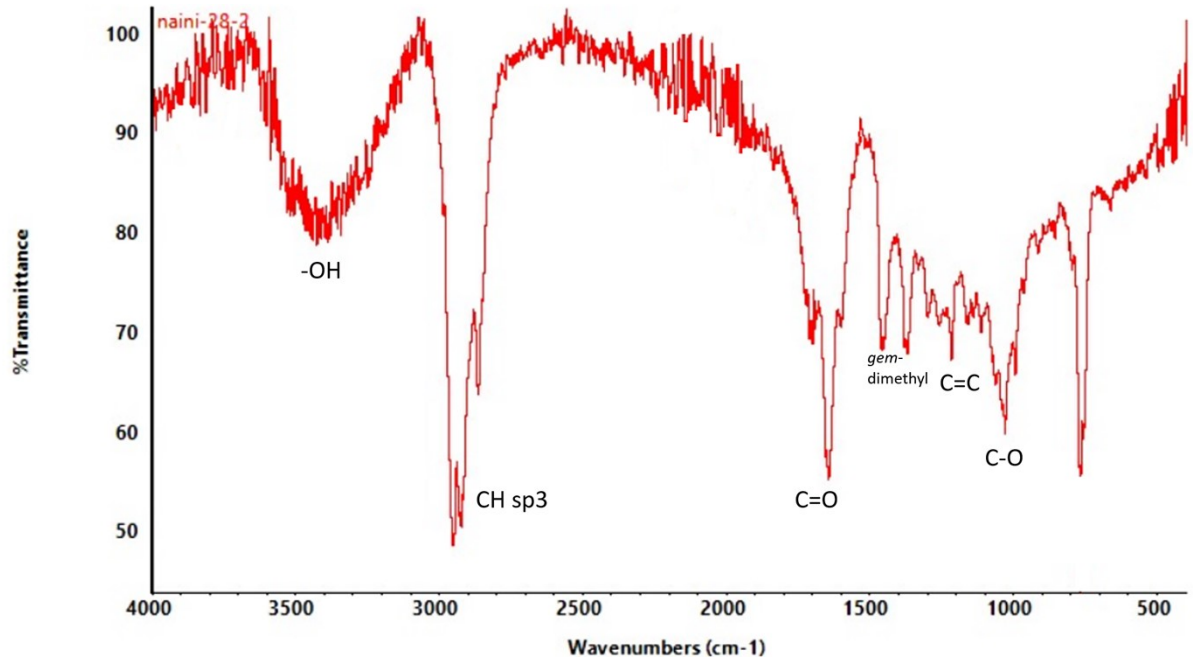
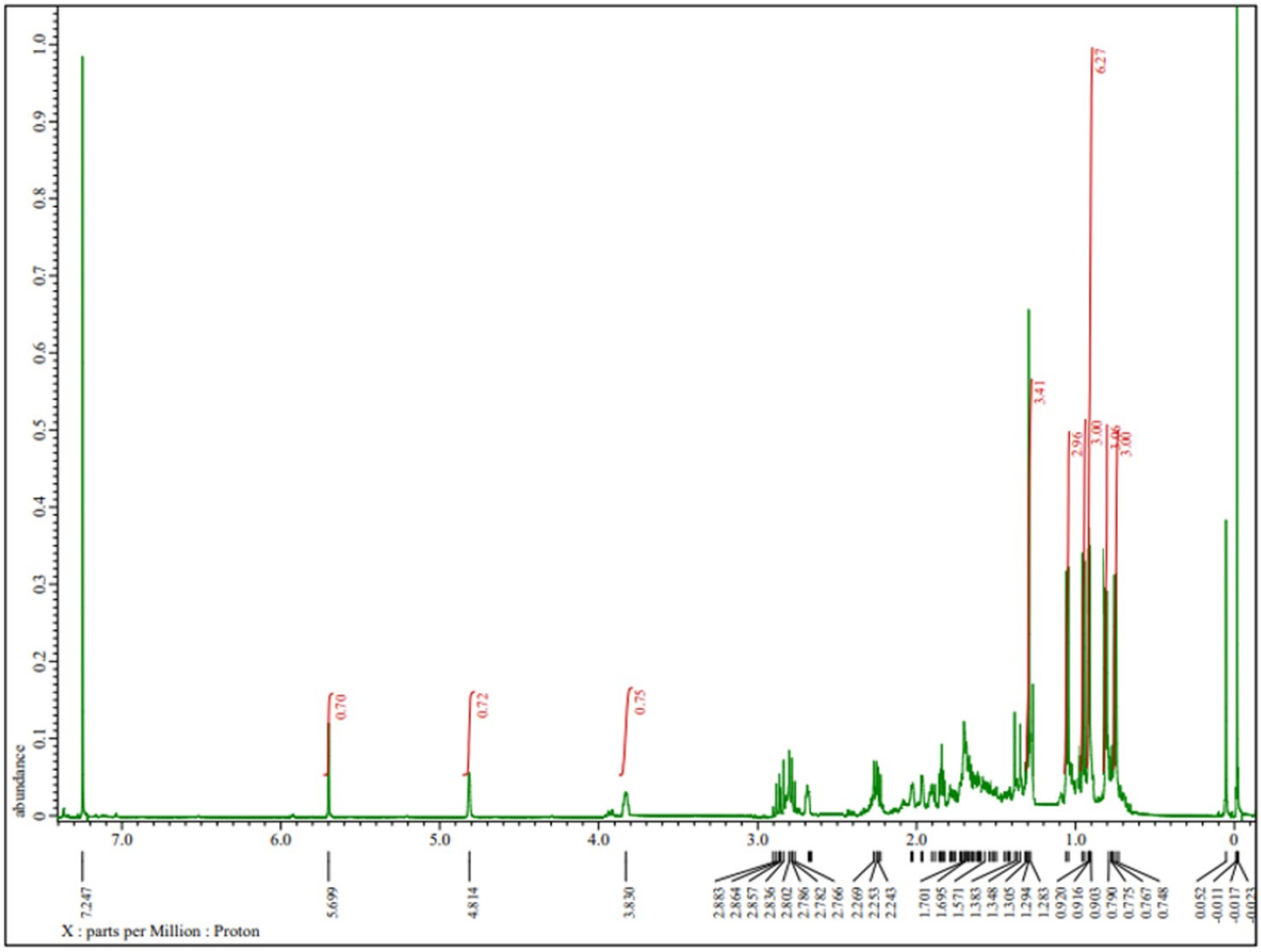


Figure S3. IR spectrum of **1**



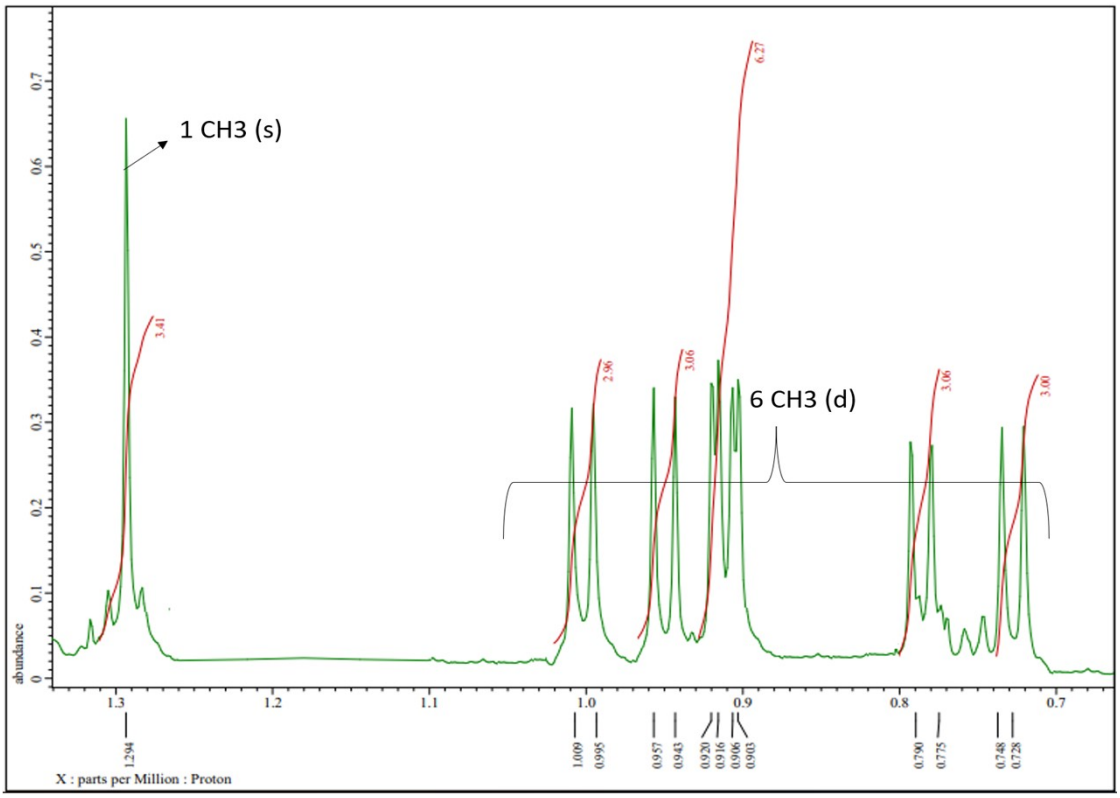


Figure S4. ^{1}H NMR of **1**

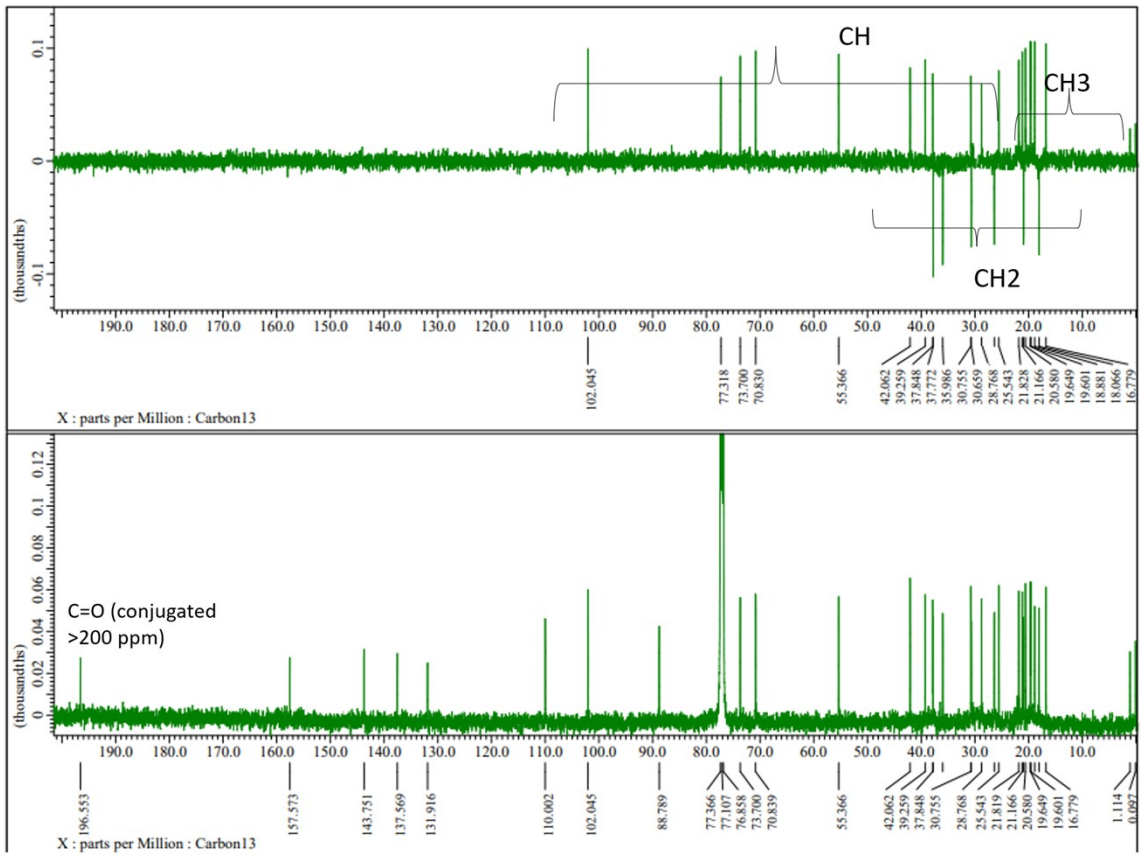


Figure S5. ^{13}C-DEPT NMR of **1**

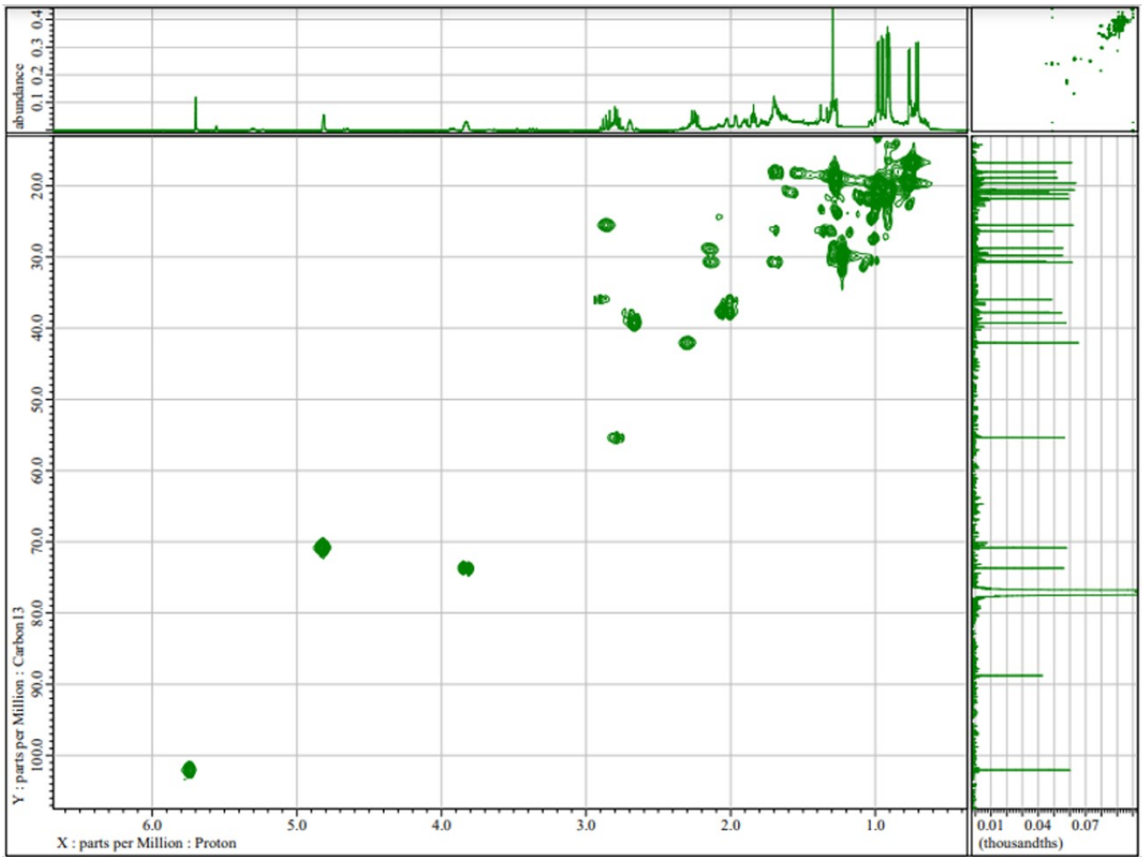
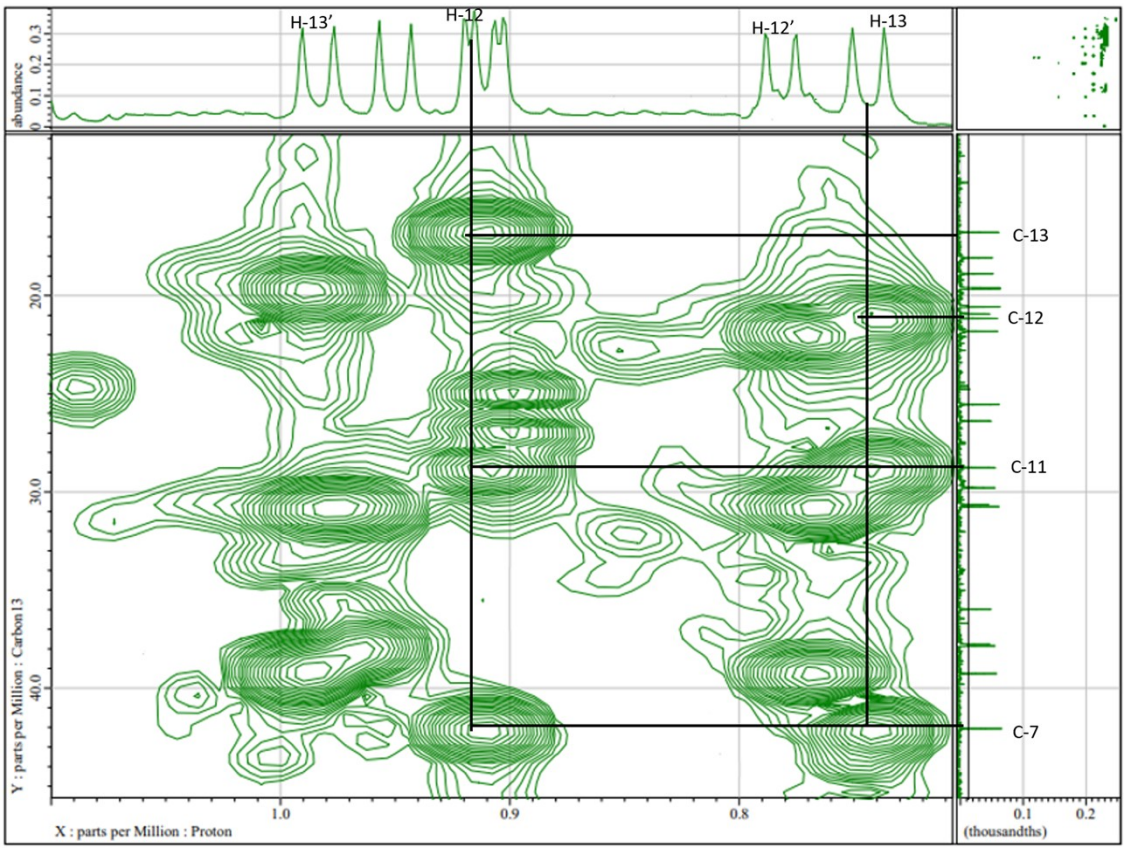


Figure S6. HMQC spectrum of **1**



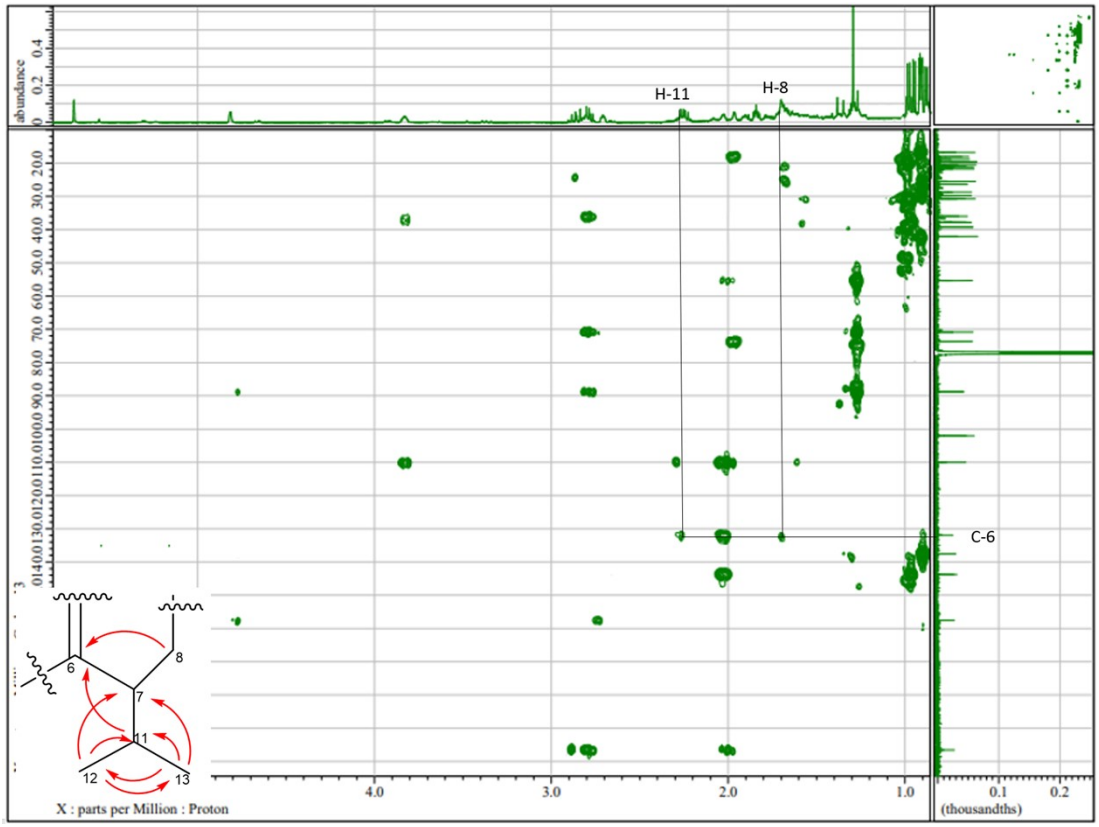
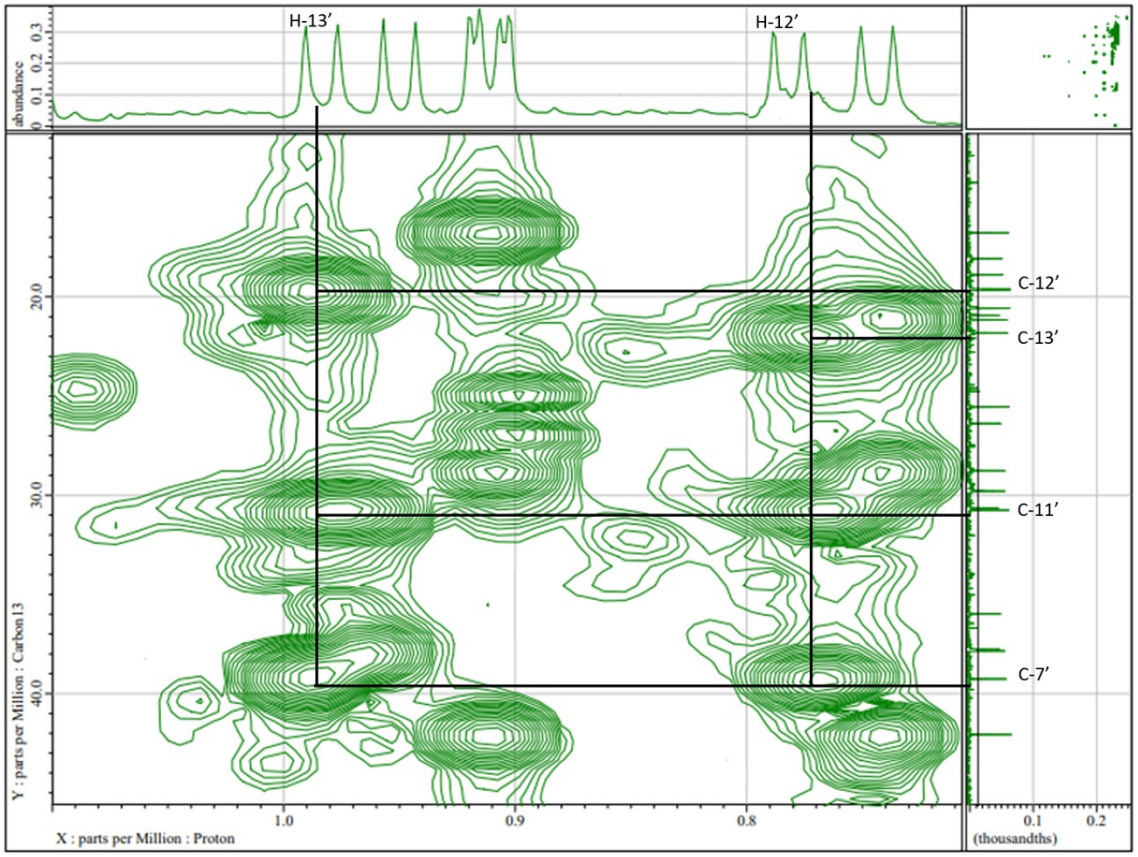
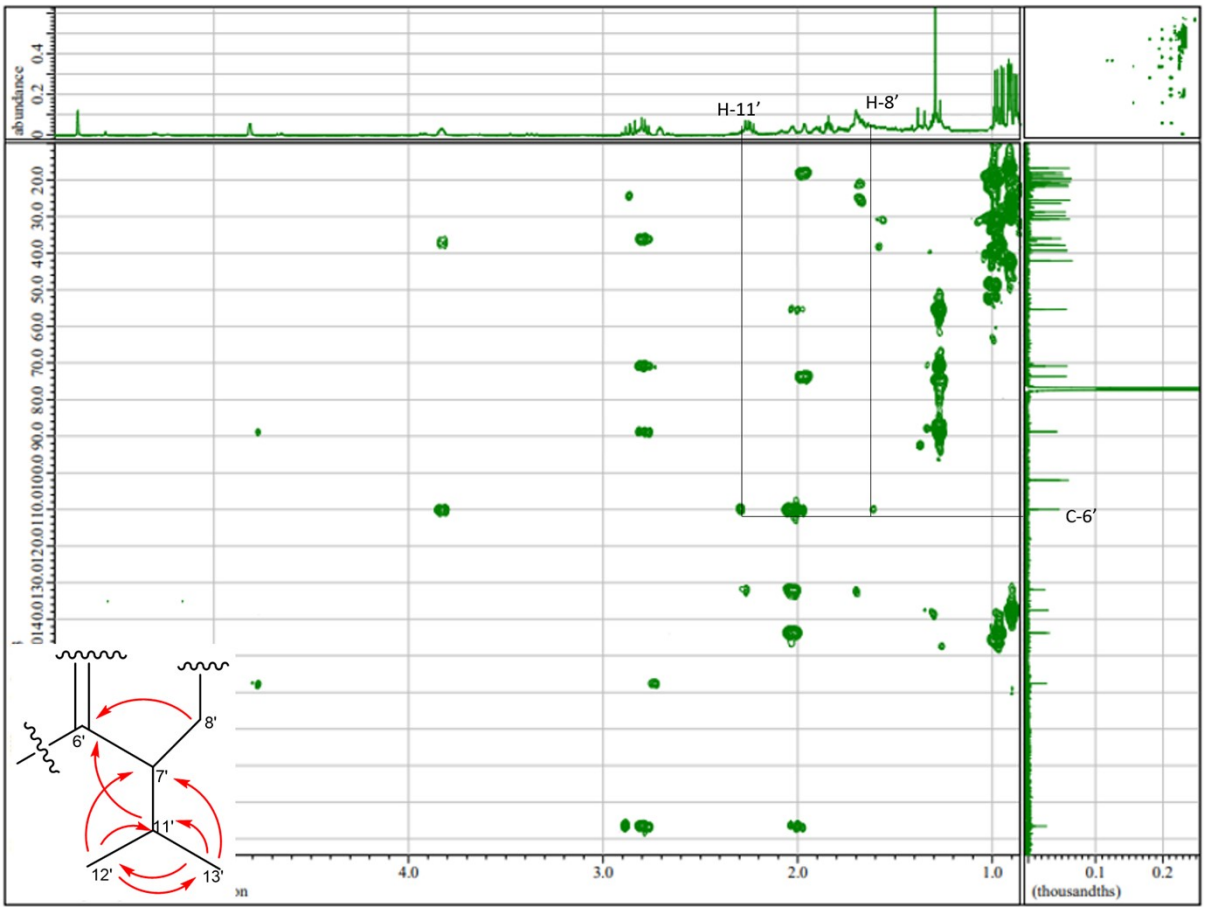
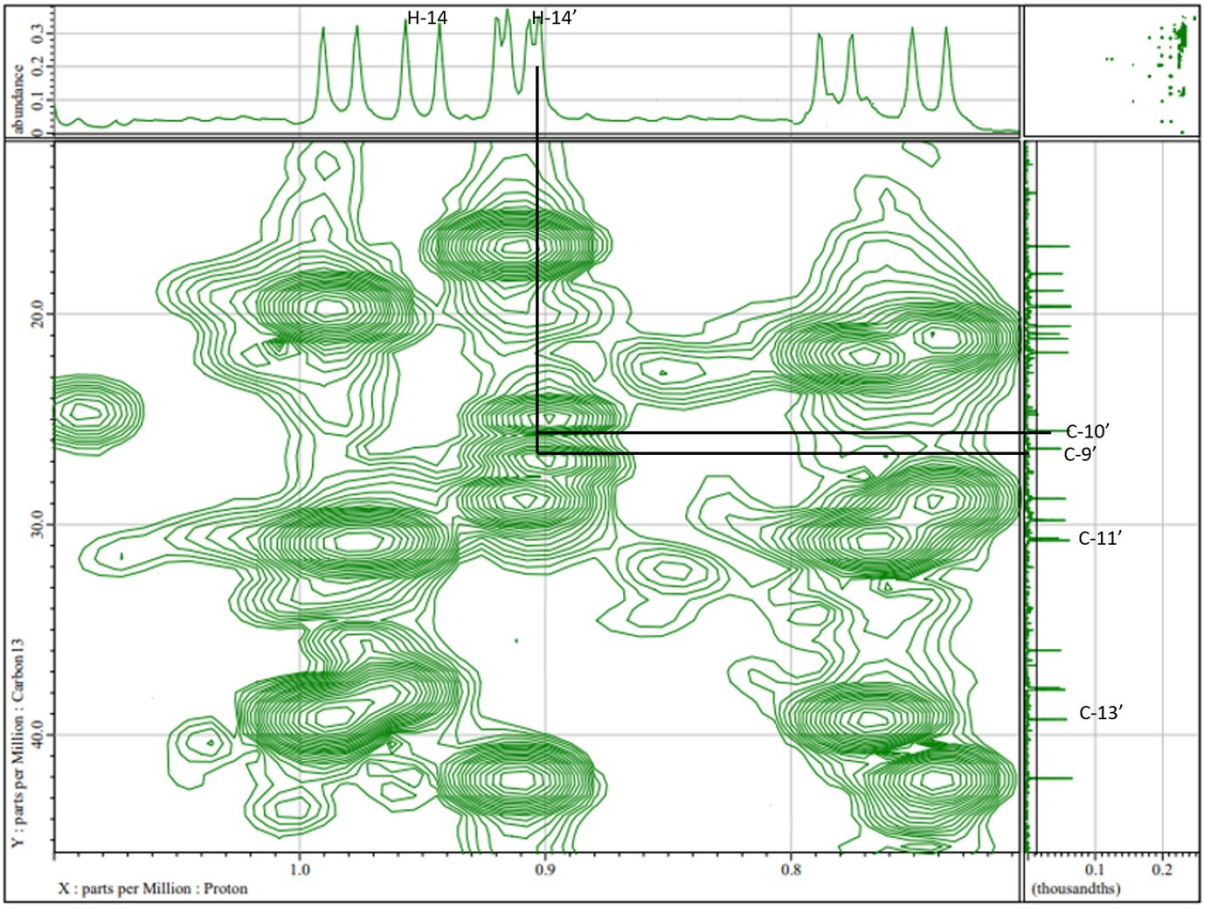


Figure S7. HMBC of **1** (A Unit)




abundance
H-11′
H-8′
C-6′
6'
8'
7'
11'
12'
13'
4.0
3.0
2.0
1.0
0.1
0.2
(thousandths)


abundance
H-14
H-14′
C-10′
C-9′
C-11′
C-13′
Y : parts per Million : Carbon 13
X : parts per Million : Proton
1.0
0.9
0.8
0.1
0.2
(thousandths)

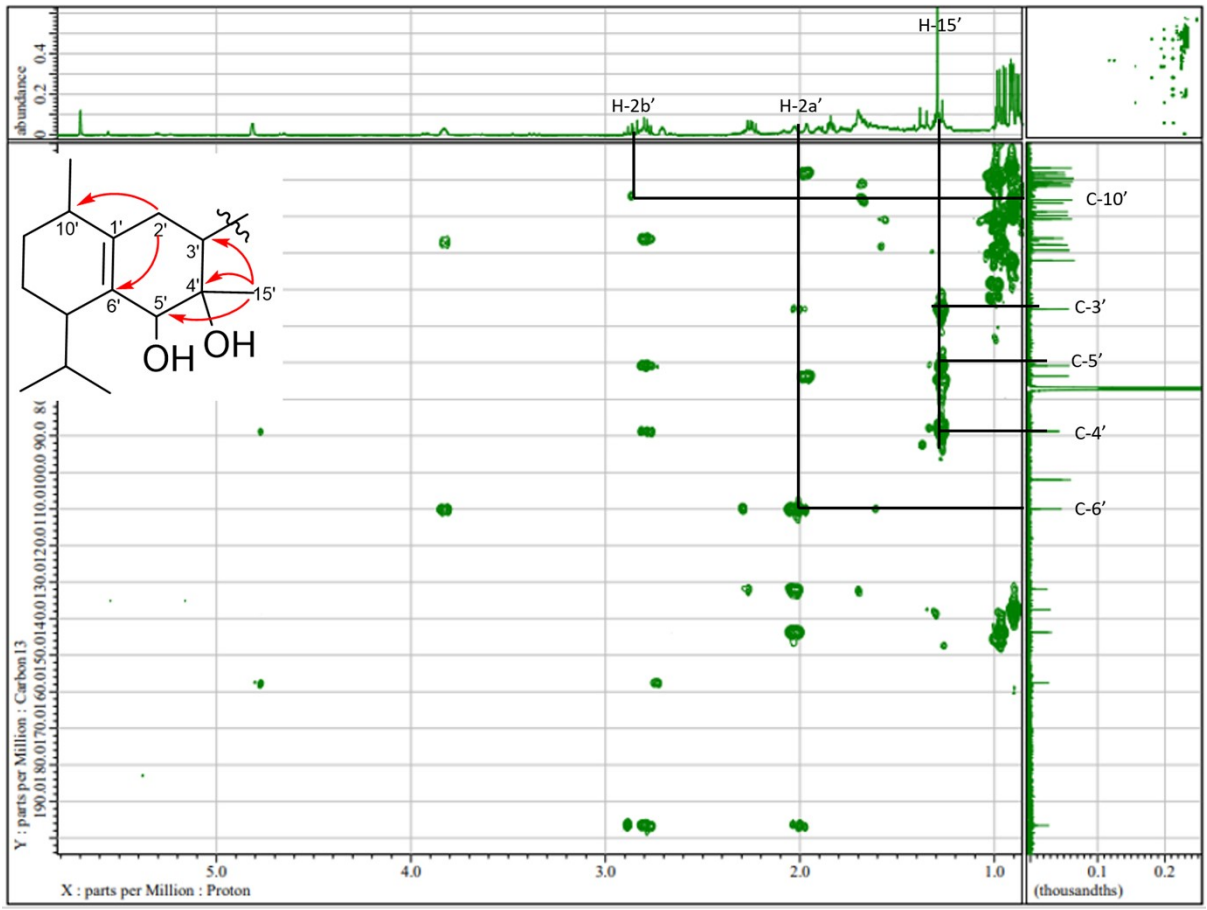


Figure S8. HMBC of **1** (B Unit)

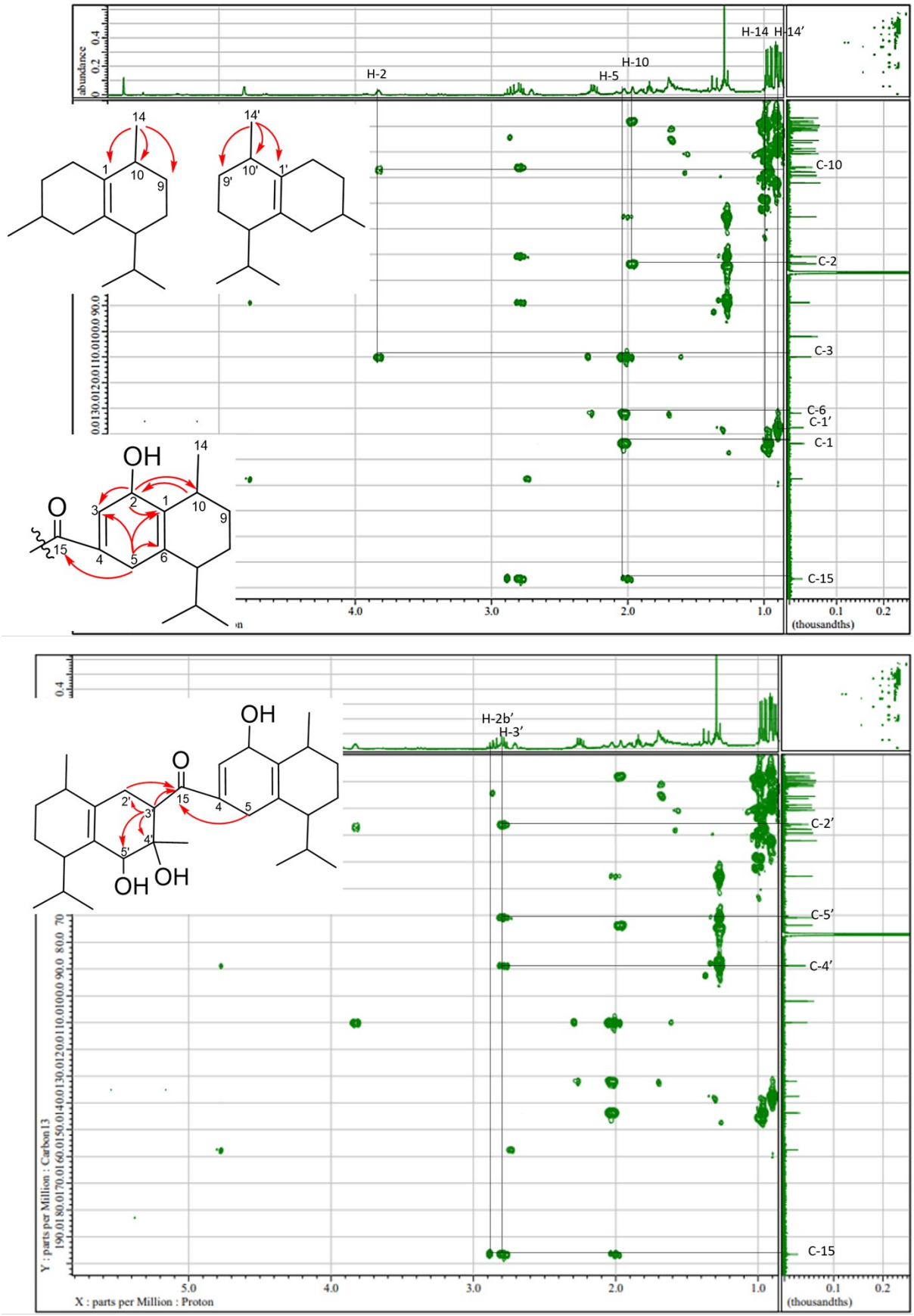


Figure S9. HMBC of **1** (A and B units)

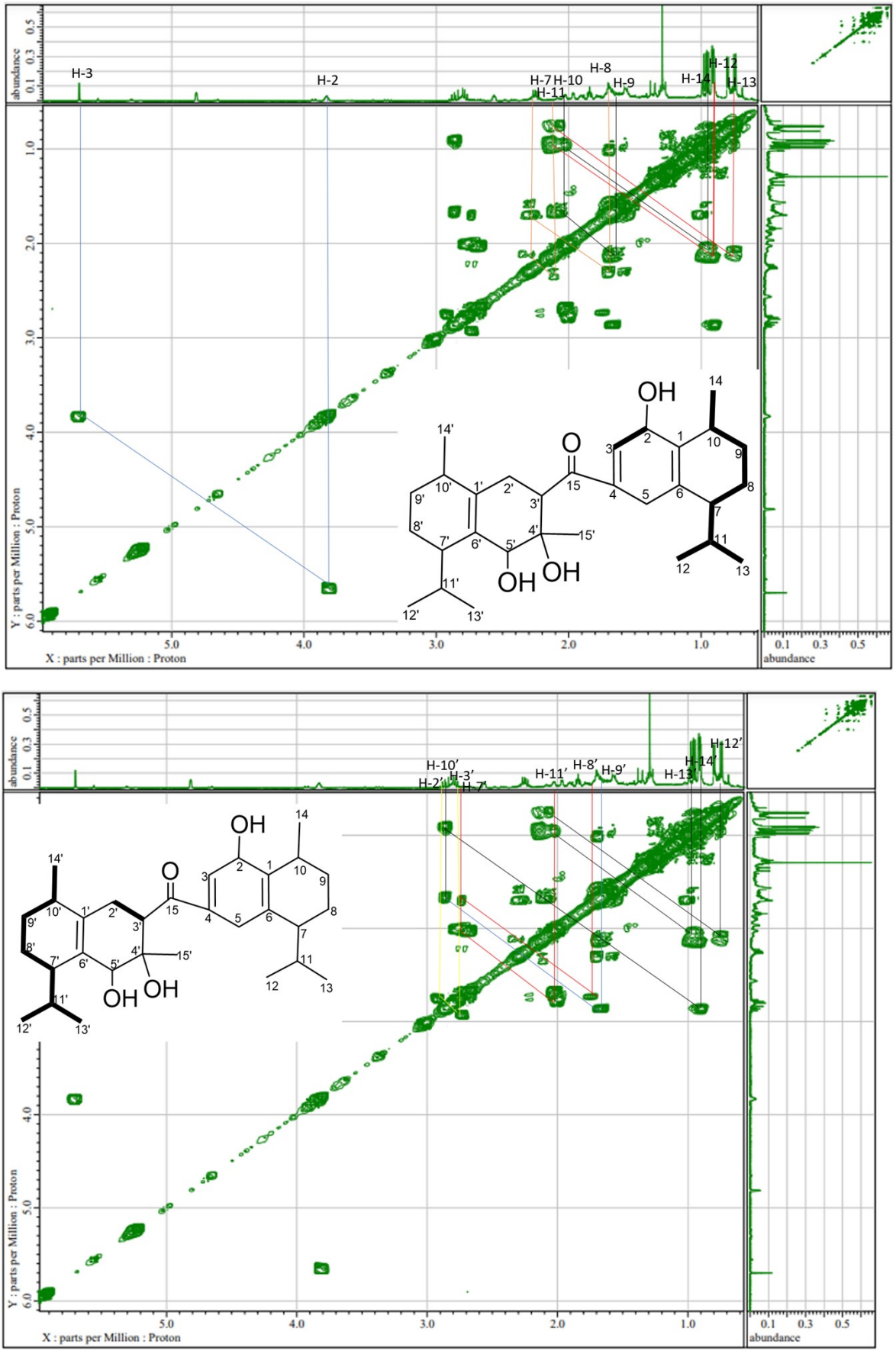


Figure S10. ^{1}H-^{1}H COSY of **1**

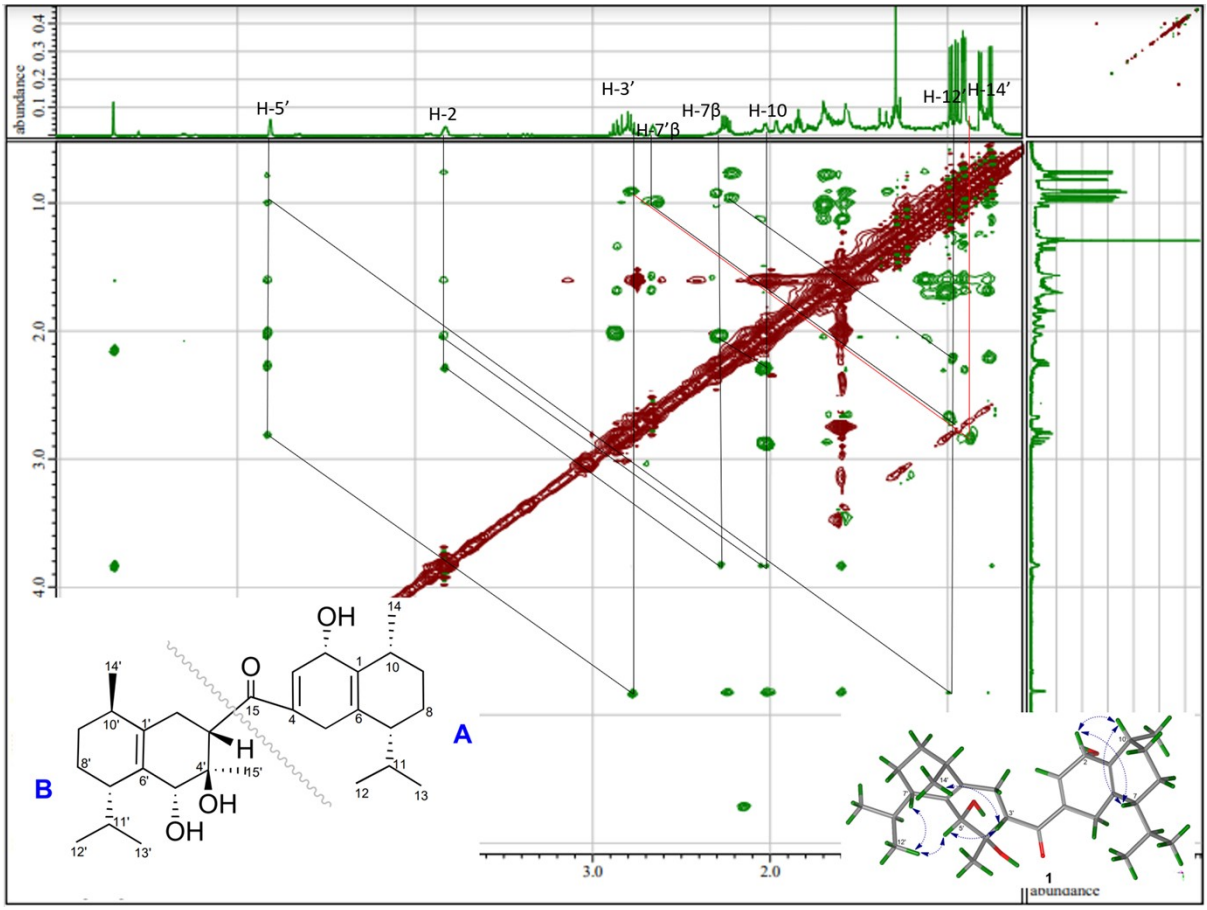
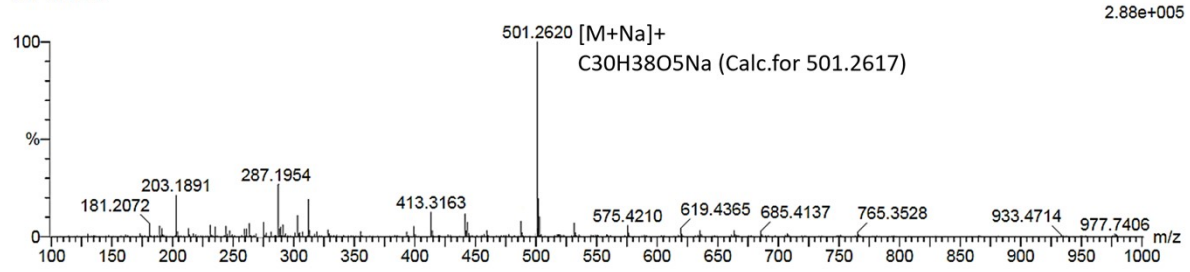


Figure S11. ^{1}H-^{1}H NOESY of **1**

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1
NAINI 30 14 (0.255) Cm (12:16)
TOF MS ES+



Minimum:			-1.5				
Maximum:		10.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
501.2620	501.2617	0.3	0.6	11.5	14.0	2.0	C30 H38 O5 Na

Figure S12. Mass spectrum of **2**

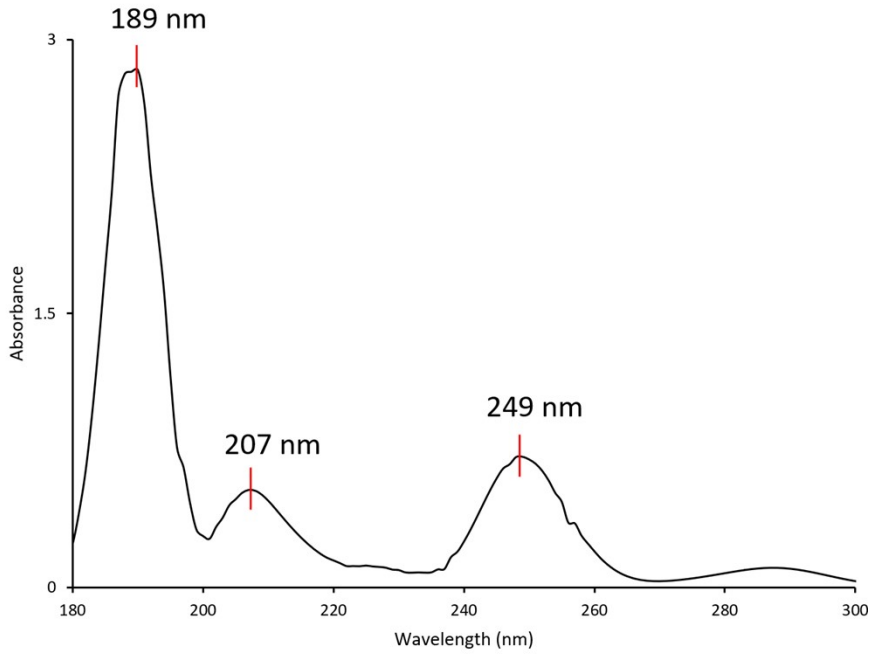


Figure S13. UV spectrum of **2**

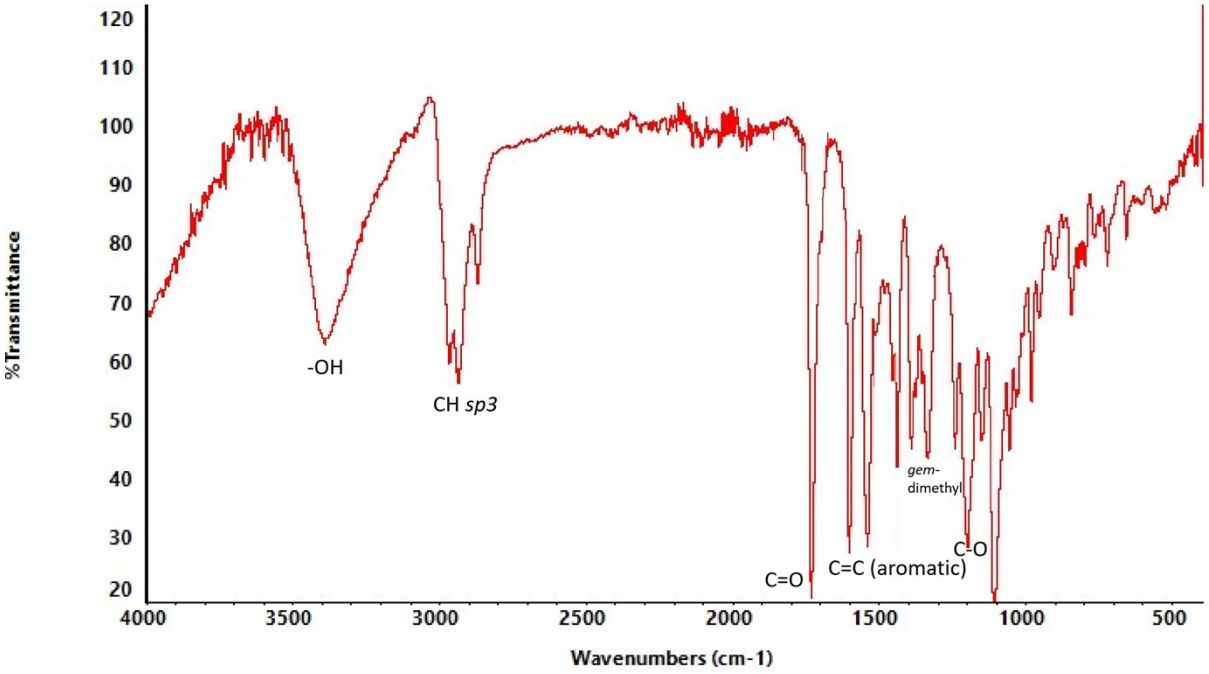


Figure S14. IR spectrum of **2**

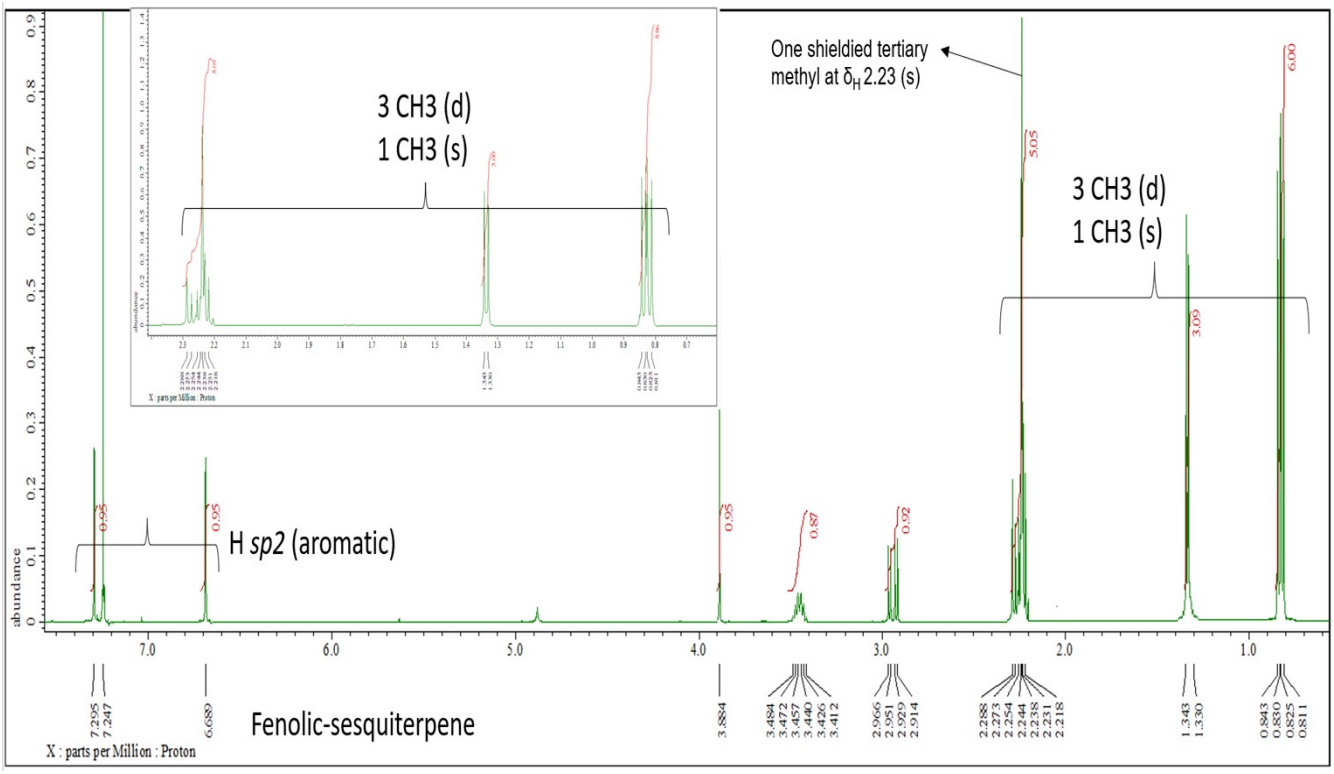


Figure S15. ^{1}H NMR of **2**

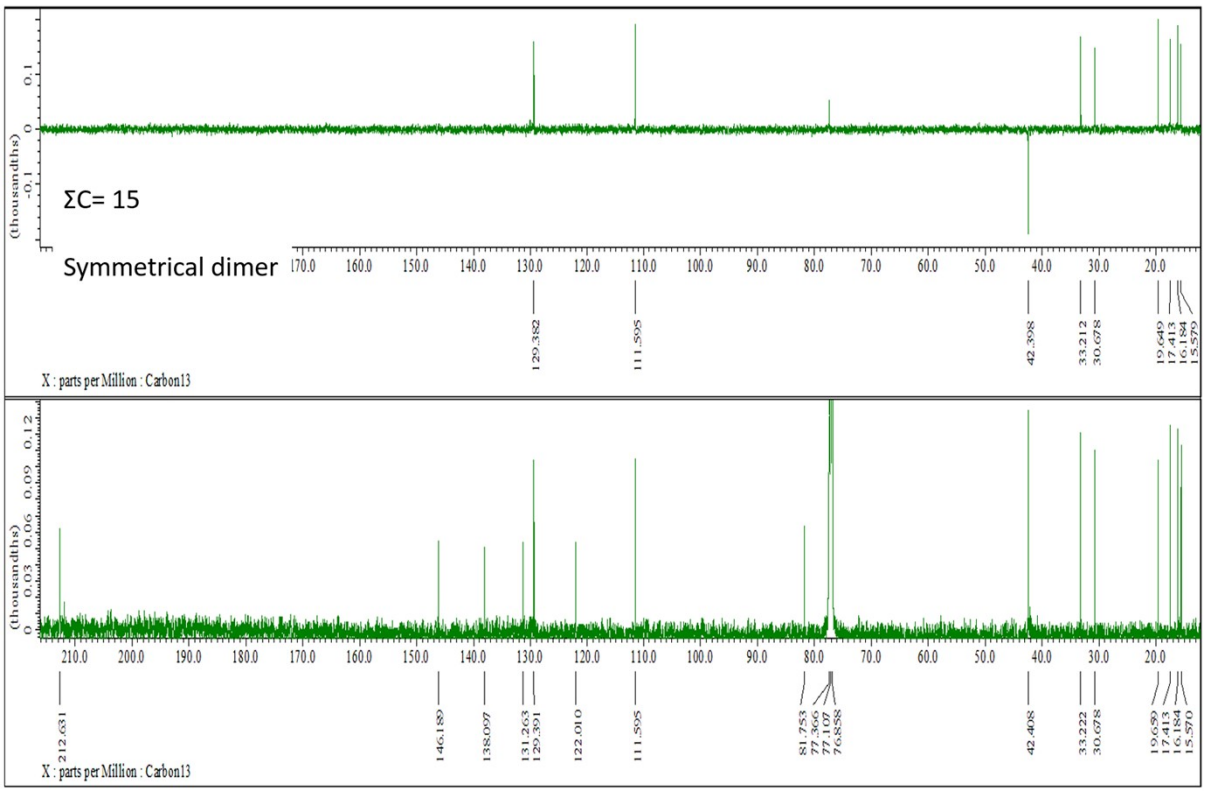


Figure S16. ^{13}C-DEPT NMR of **2**

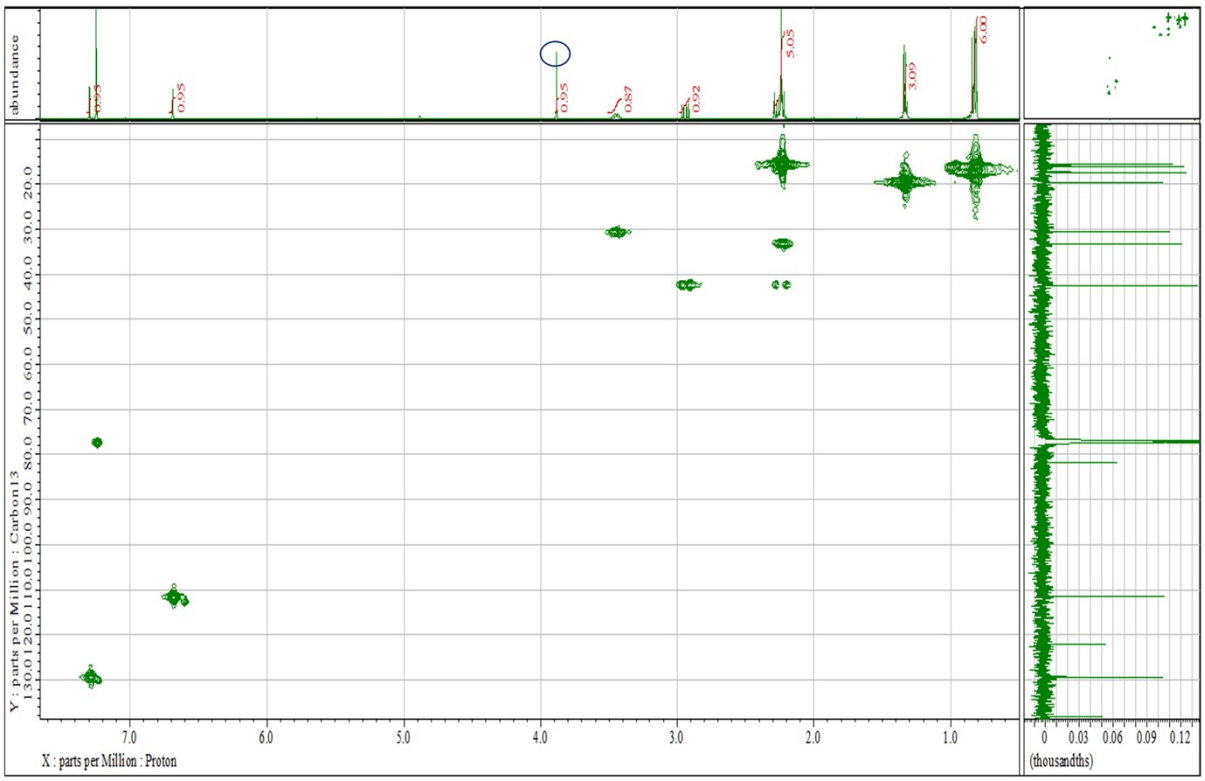


Figure S17. HMQC spectrum of **2**

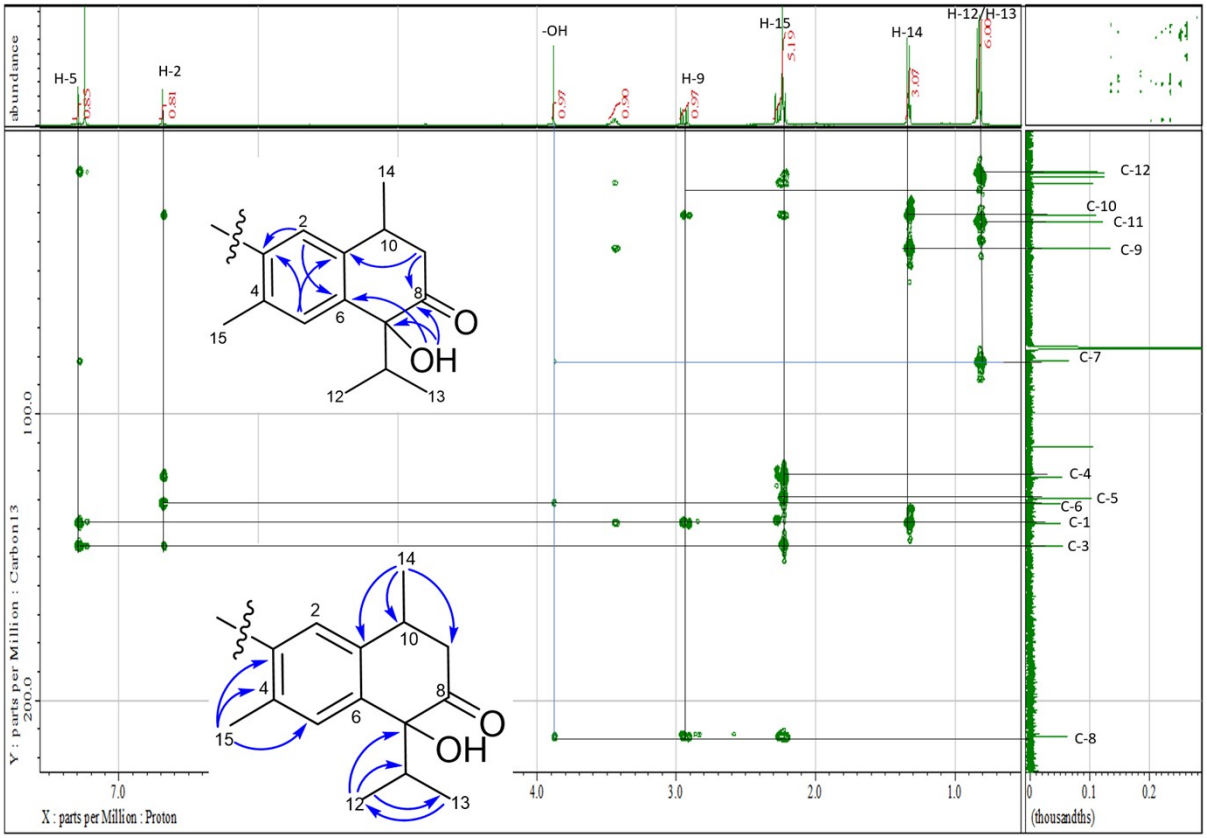


Figure S18. HMBC spectrum of **2**

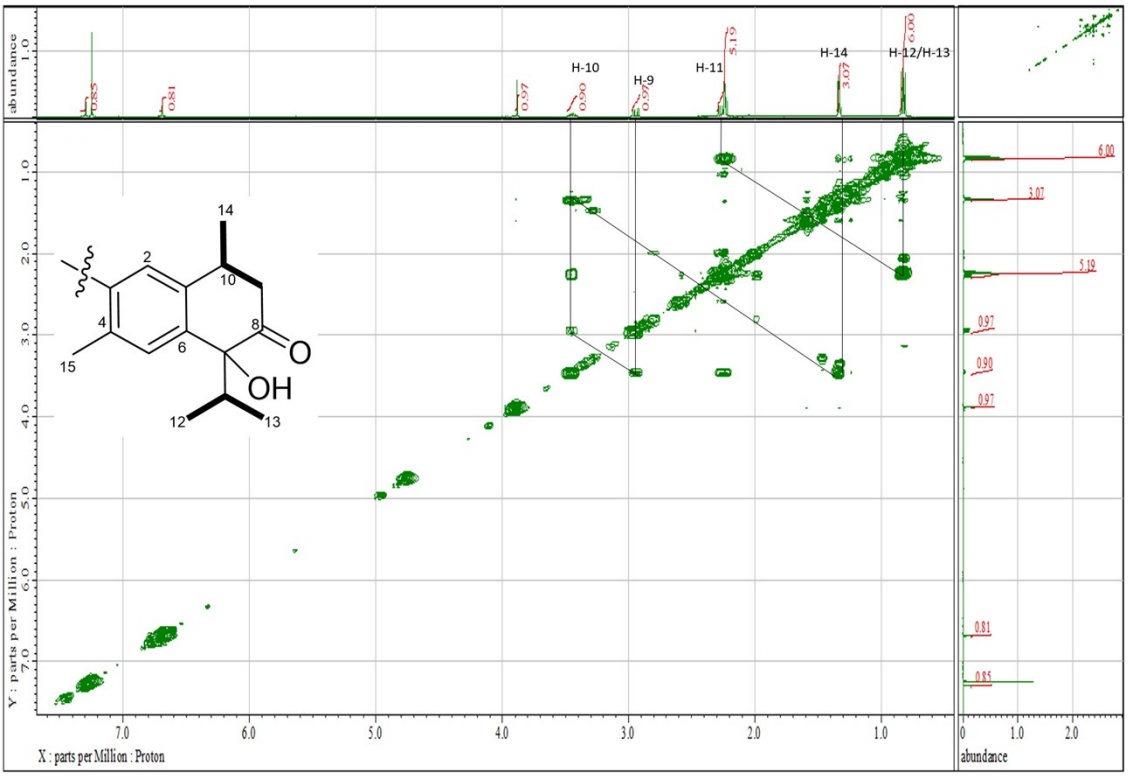


Figure S19. ^{1}H-^{1}H COSY of **2**

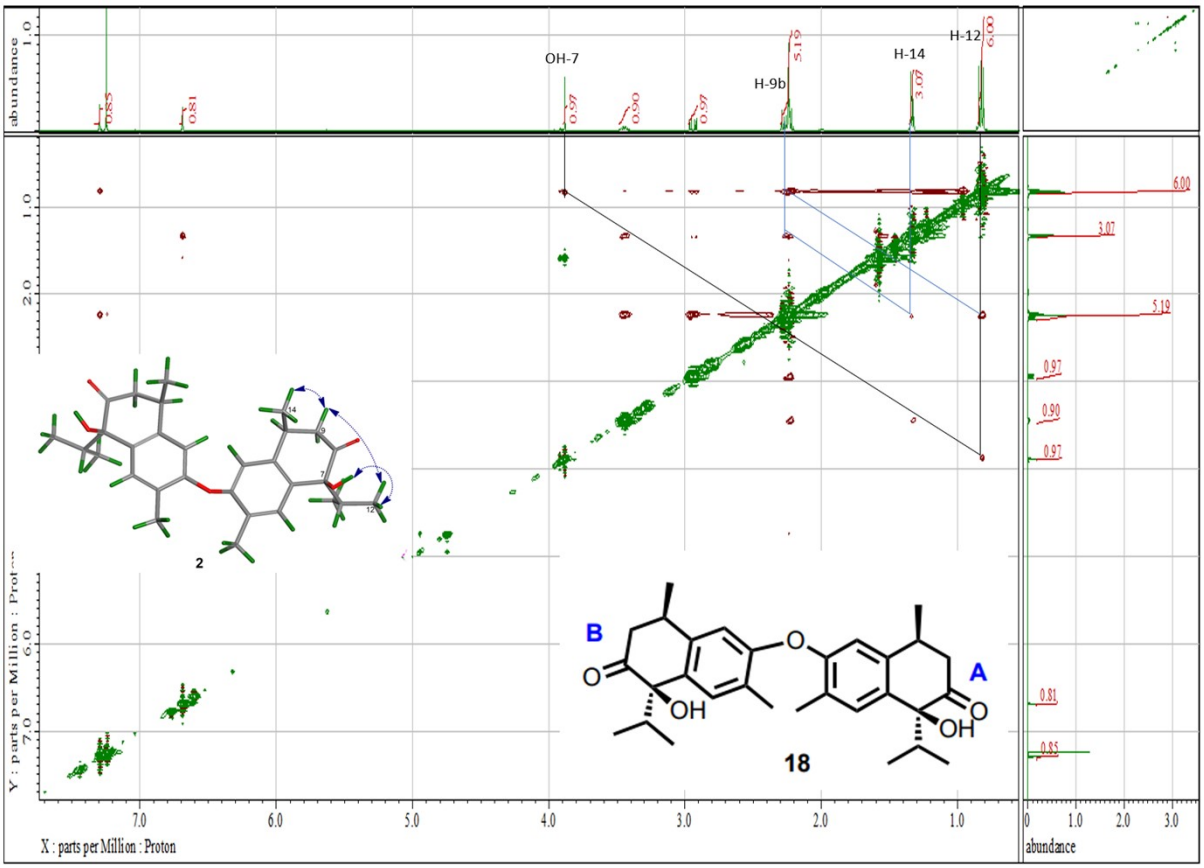
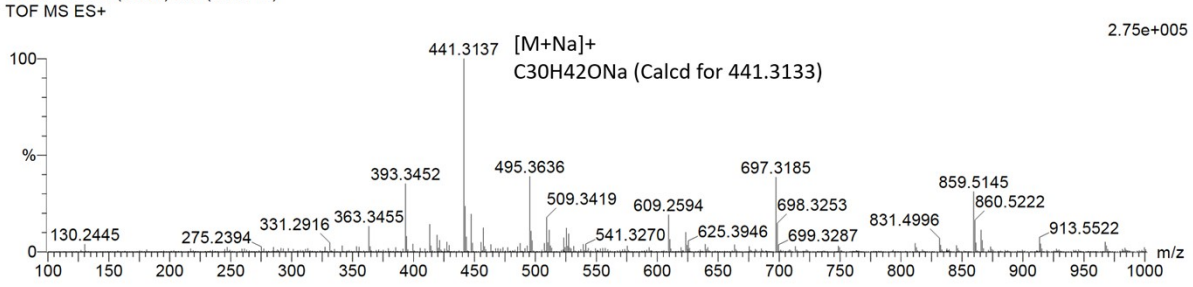


Figure S20. ^{1}H-^{1}H NOESY of **2**

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
155 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1
NAINI 39 108 (1.853) Cm (108:113)
TOF MS ES+



Minimum:				-1.5					
Maximum:		10.0	10.0	100.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula		
441.3137	441.3133	0.4	0.9	9.5	13.6	1.5	C30	H42	O Na

Figure S21. Mass spectrum of **3**

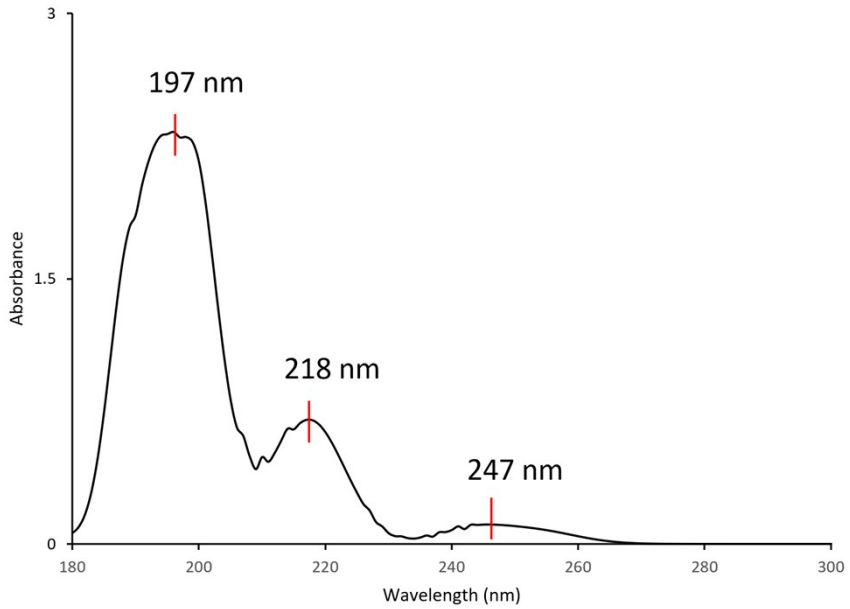


Figure S22. UV spectrum of **3**

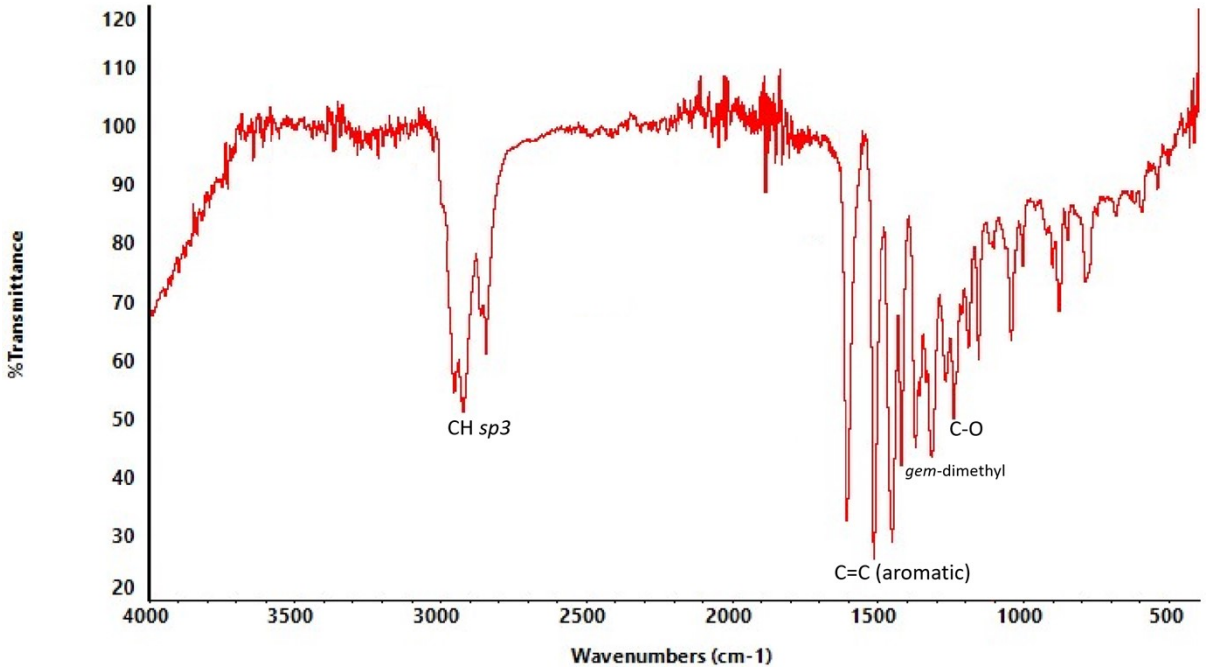


Figure S.23. IR spectrum of **3**

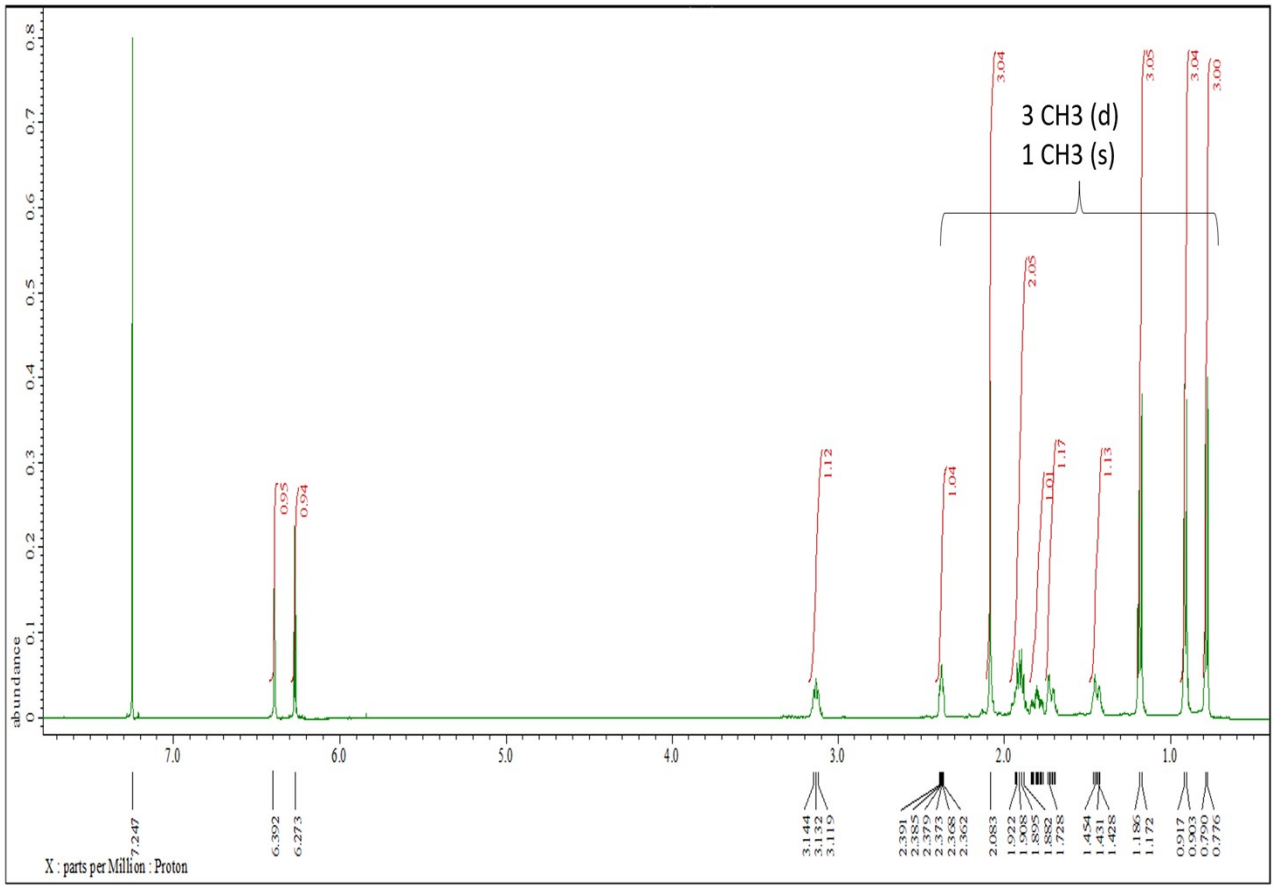


Figure S24. ^{1}H NMR of **3**

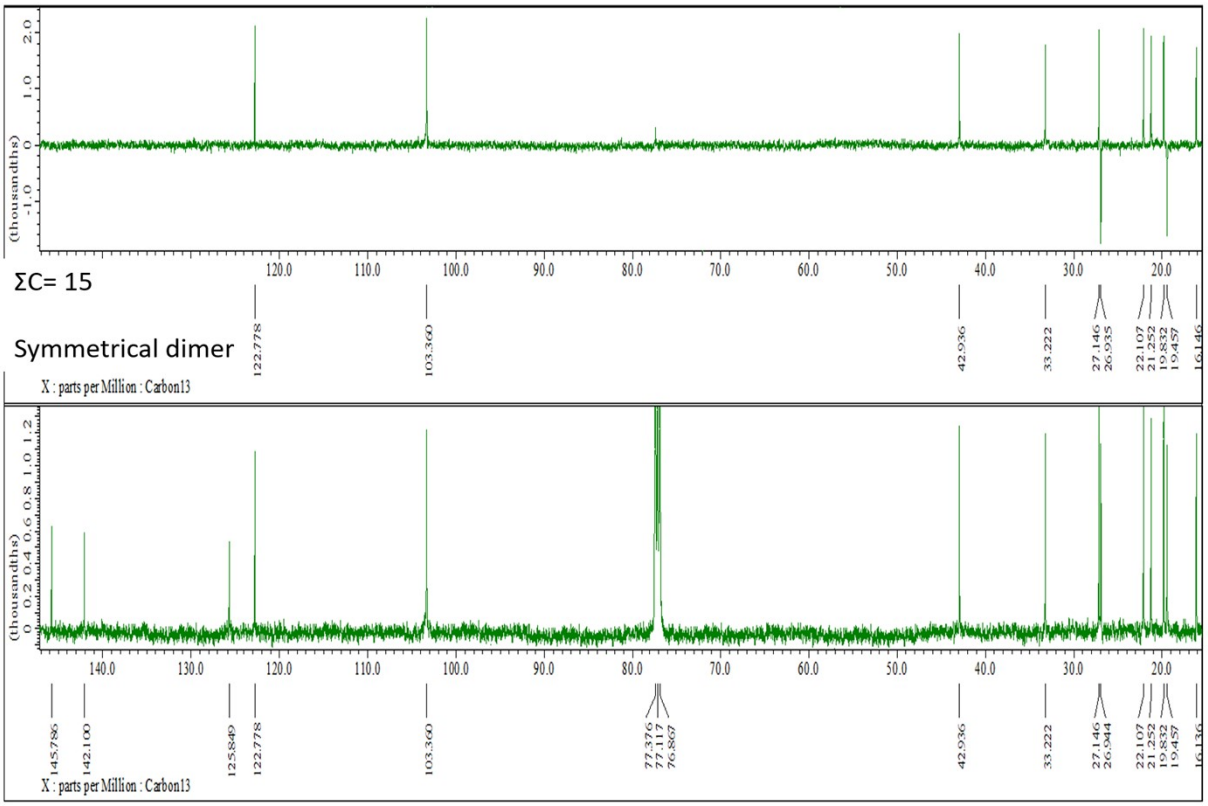


Figure S25. ^{13}C-DEPT NMR of **3**

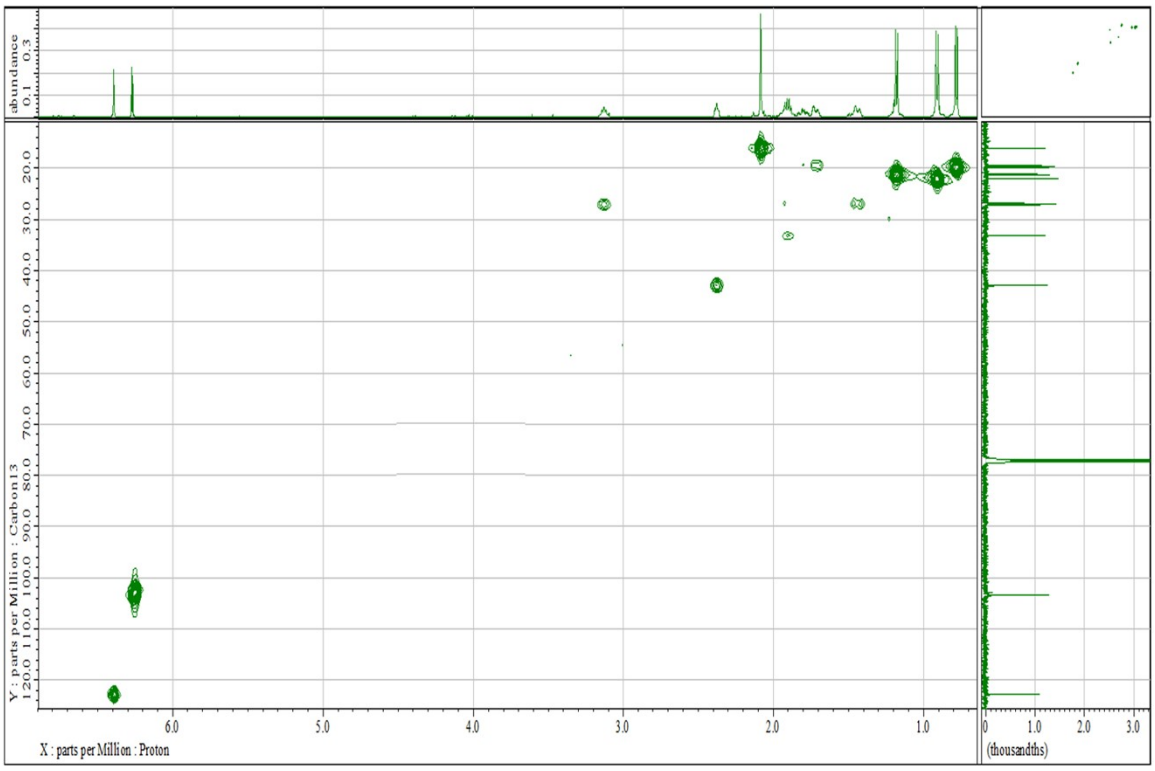


Figure S26. HMQC spectrum of **3**

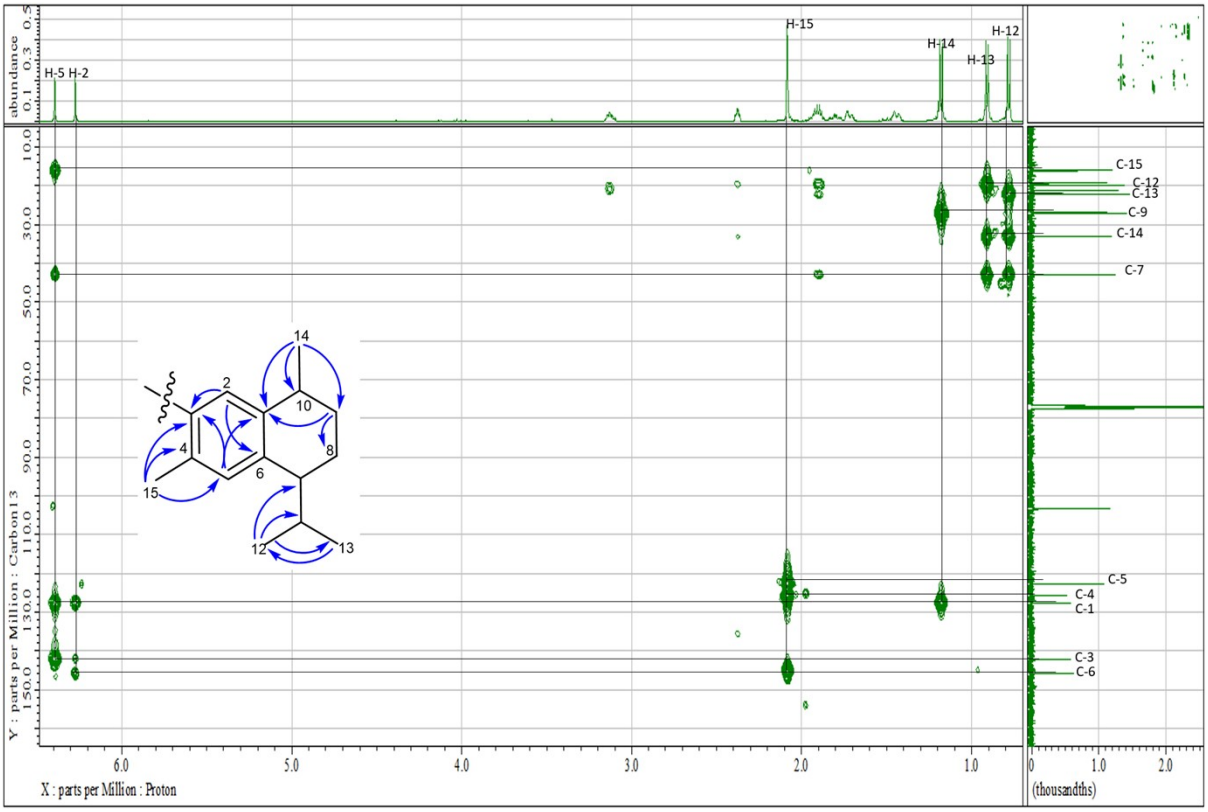


Figure S27. HMBC spectrum of **3**

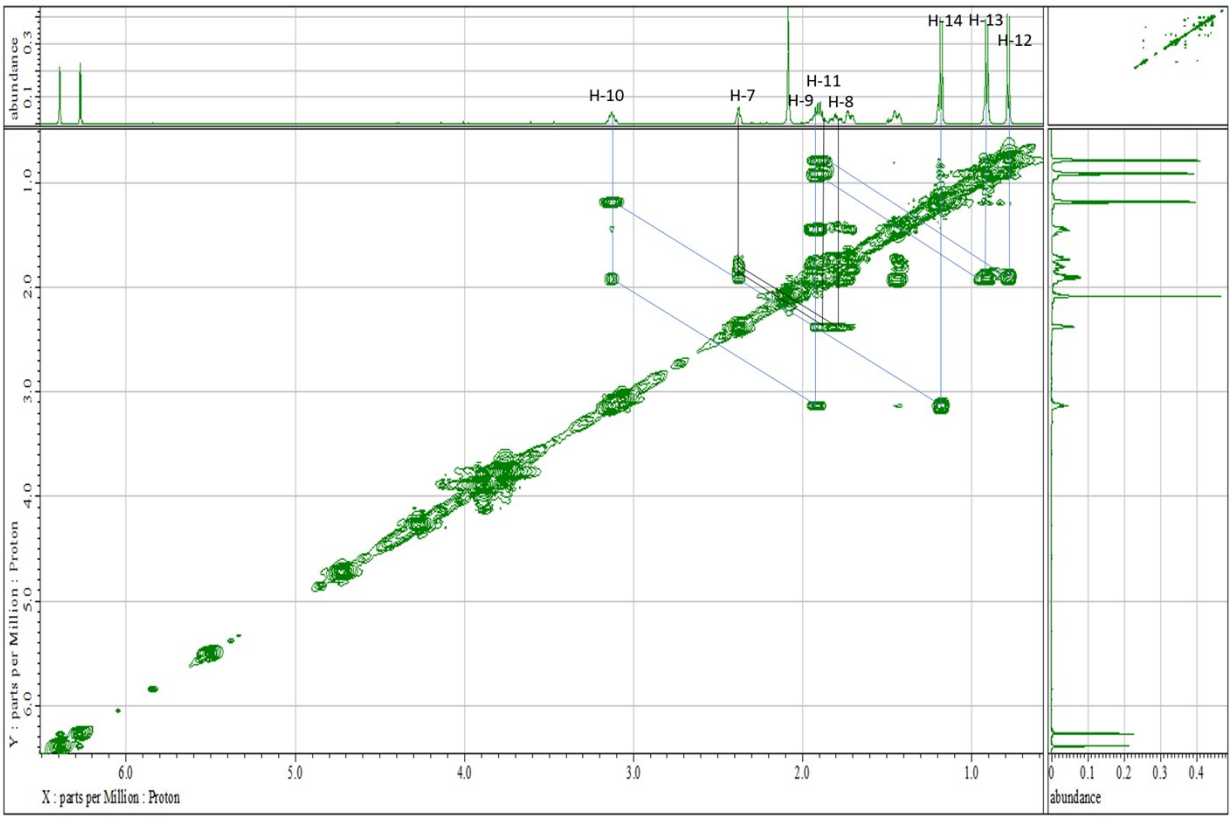


Figure S28. ^{1}H-^{1}H COSY of **3**

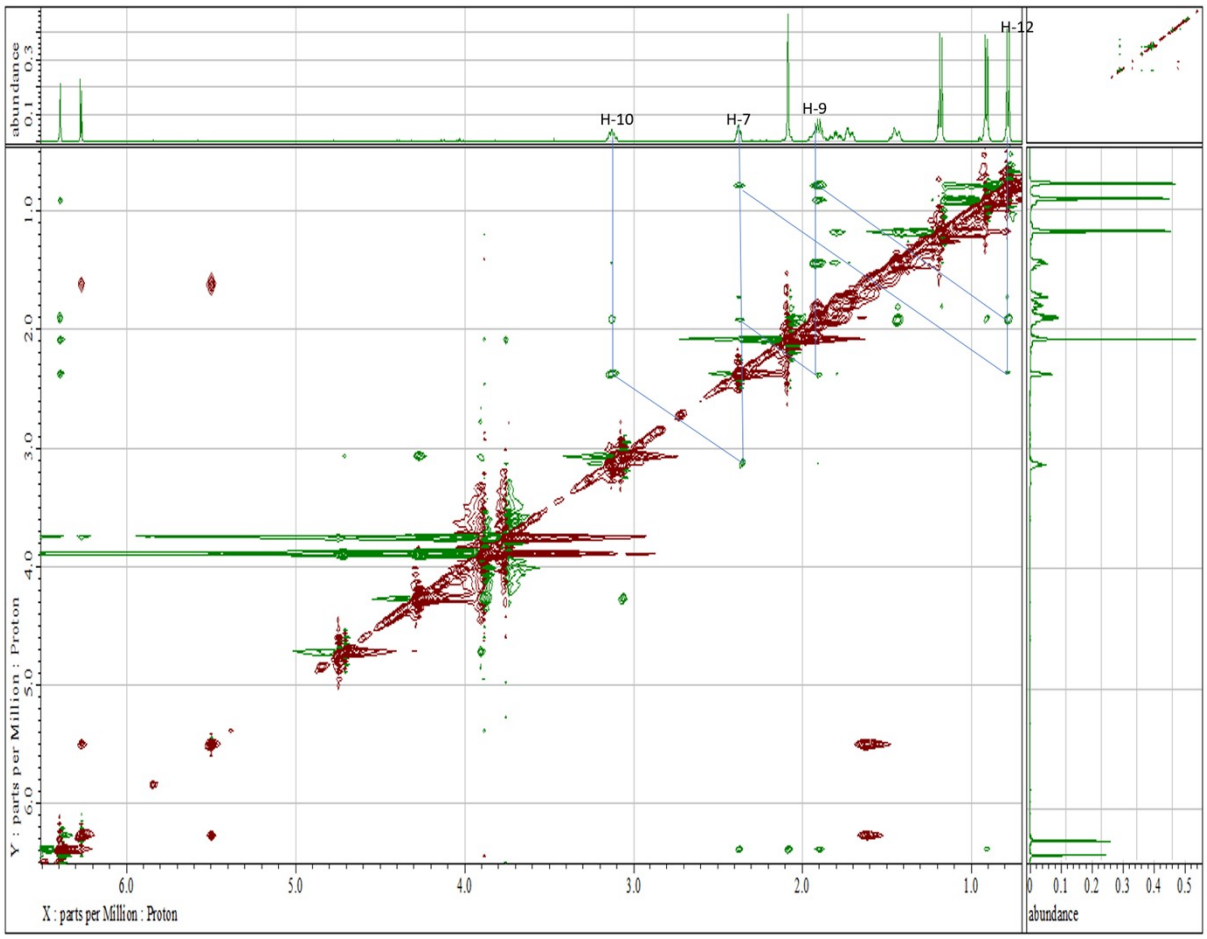
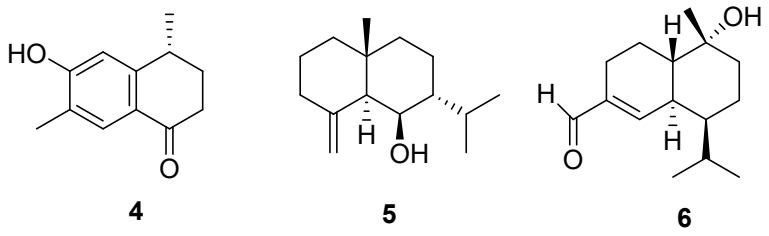


Figure S29. ^{1}H-^{1}H NOESY of **3**

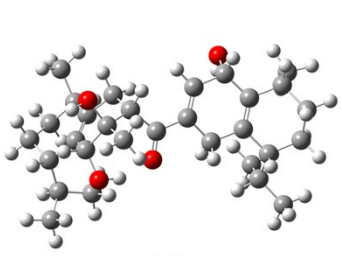


4 **5** **6**

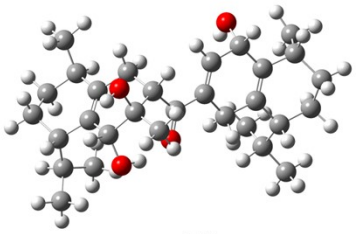
Figure S30. Chemical structure of known compounds (**4-6**).

Computational section

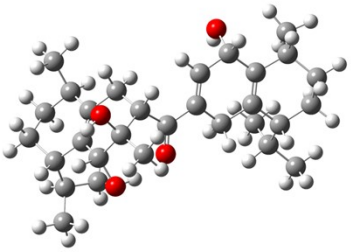
- **For compound 1**



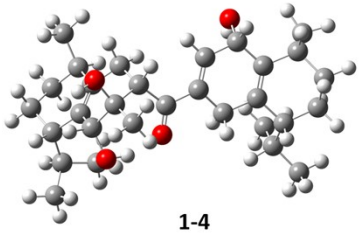
1-1



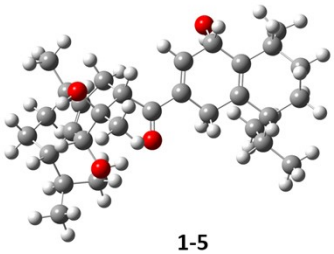
1-2



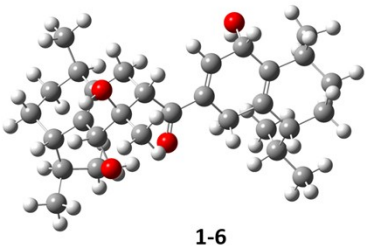
1-3



1-4



1-5



1-6

Table S1. Gibbs free energies and equilibrium populations of low-energy conformer of **1**

Conformer	**G HF hartree**	**ΔG hartree**	**ΔG kJ/mol**	**ΔG kcal/mol**	**(-)ΔG/RT**	**e(-ΔG/RT)**	**Mole fraction**	**Population%**
1-1	-1471.843661	0	0	0	0	1	0.26425467	26.42546697
1-2	-1471.843504	-0.000157	0.4122035	0.09851901	-0.16628102	0.846808233	0.22377303	22.37730299
1-3	-1471.843422	-0.000239	1.2051046	0.28802691	-0.48613367	0.614999592	0.162516514	16.25165141
1-4	-1471.843202	-0.000459	1.2051046	0.28802691	-0.48613367	0.614999592	0.162516514	16.25165141
1-5	-1471.843021	-0.00064	1.6803201	0.40160615	-0.67783345	0.507715795	0.13416627	13.41662696
1-6	-1471.84214	-0.001521	3.9933858	0.95444211	-1.61091355	0.19970509	0.052773003	5.277300268
SUM						3.784228302	1	100

Table S2. Cartesian coordinates for the low-energy reoptimized of compound **1** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

Center Number	Atomic Number	Atomic Type	Conformer 1-1	Coordinates (Angstroms)			Conformer 1-2	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		2.243	-0.450353	-2.868292		-1.8989082	-1.24999286	-2.88896473
2	6	0		3.1821	-0.756876	-2.383076		-4.5583963	-0.67011604	-2.19396718
3	6	0		4.2896	0.232113	-2.803588		4.7071827	-0.71132536	-1.94845774
4	1	0		4.7017	-0.074149	-3.772165		6.8880669	-0.38815945	-1.81523832
5	1	0		3.8648	1.230111	-2.956174		6.8542321	0.4048649	-0.21213239
6	6	0		5.3921	0.311942	-1.7469		6.7686251	0.12934888	-2.61643375
7	1	0		5.8337	-0.681858	-1.596818		-5.4256461	-0.32955989	-0.71445481
8	1	0		6.2026	0.968862	-2.084558		-0.1806082	0.53175741	-2.31189543
9	6	0		4.8209	0.824018	-0.410644		-1.7842561	0.27393248	-2.22997613
10	1	0		5.606	0.694008	0.346857		-3.9111416	0.44810246	1.10635083
11	6	0		3.6576	-0.072414	0.017083		-2.8569615	-1.76318264	1.25166907
12	6	0		2.9248	-0.769679	-0.87515		-4.4526745	-1.22517828	-0.13335763
13	6	0		1.8088	-1.707536	-0.460915		-6.4845174	-0.96304644	-0.35884087
14	1	0		2.1576	-2.741461	-0.546836		-2.5118408	-1.55626237	-0.08960165
15	1	0		0.9735	-1.613625	-1.165663		-4.5374639	-0.42368105	-0.67980168
16	6	0		1.2994	-1.52533	0.991353		-1.9975054	-1.8691082	0.66868029
17	1	0		0.8086	-2.457179	1.284342		-5.6428102	-0.64324786	0.94650899
18	6	0		2.5127	-1.380758	1.940236		-4.0888133	-1.12275928	1.06136642
19	6	0		3.4628	-0.222308	1.524094		-0.8441488	-0.72337246	0.13859747

20	1	0		4.4448	-0.482245	1.947325		-6.9259156	-1.98682857	1.41463978
21	6	0		3.5043	-2.176089	-2.908851		-6.3812287	-0.81080051	-1.93218767
22	1	0		2.7099	-2.894001	-2.689685		-0.4106838	-0.01877652	-1.54914621
23	1	0		4.4319	-2.557914	-2.468052		0.114066	-1.50068164	-2.22663809
24	1	0		3.6333	-2.1503	-3.995702		5.0186115	-0.24535411	-1.49854111
25	6	0		4.5406	2.379488	-0.482298		3.3884682	0.00666487	-3.99481825
26	1	0		5.0769	2.732734	-1.374619		0.484988	2.8406353	-1.19500433
27	6	0		3.0706	2.786627	-0.66678		1.3977071	1.61107599	-3.4803525
28	1	0		2.4792	2.542978	0.218016		3.3136543	2.83264483	2.24004448
29	1	0		2.6037	2.291475	-1.522716		6.6173583	2.15462406	-1.39084998
30	1	0		3.0022	3.868446	-0.830706		2.0281648	1.86927185	-1.49535734
31	6	0		5.1522	3.119352	0.718402		0.6936796	2.68677322	1.56559489
32	1	0		6.2276	2.921802	0.798326		1.6944159	0.08701655	1.37727624
33	1	0		4.6733	2.797236	1.646789		0.5379775	2.05816562	0.9045103
34	1	0		5.0208	4.203329	0.61841		6.7883864	4.33842433	1.6608979
35	8	0		3.121	1.009312	2.162876		3.0775943	1.17793085	1.34174063
36	1	0		2.1906	1.169422	1.908882		0.9471888	3.33612695	0.08796642
37	6	0		-3.0092	-2.224844	-0.072261		-6.2681807	-0.40883899	0.85474393
38	1	0		-3.3954	-3.065184	0.520608		-6.7661075	-1.25434599	1.07476254
39	6	0		-1.6033	-1.93598	0.365453		-5.8545151	-0.82412947	0.93817087
40	1	0		-0.9447	-2.798546	0.366228		-0.9995261	-0.52473352	1.70143779
41	6	0		-1.1585	-0.706259	0.67213		-6.9189294	-2.48734639	0.18883822
42	6	0		-2.0834	0.481035	0.643604		-5.149826	2.15231262	-0.47854012
43	1	0		-2.0121	1.012715	1.602798		-0.4400818	1.41196283	-0.10131289
44	1	0		-1.6867	1.201973	-0.083481		-2.5984876	1.23401897	-0.33534644
45	6	0		-3.5375	0.1821	0.352829		-2.3731954	1.25421208	-0.70478128
46	6	0		-3.9676	-1.059626	0.048325		-0.5201117	-0.80015537	-0.1656459
47	6	0		-5.4424	-1.407835	-0.116705		-3.8702623	-0.12659367	-0.16521137
48	1	0		-5.5871	-2.395395	0.345735		-3.5784425	-1.8558185	-0.78778872
49	6	0		-6.3079	-0.395924	0.651821		-3.9915177	-1.8475366	-0.56783917
50	1	0		-6.1464	-0.529895	1.72957		-2.4272922	-1.1918549	-1.38116424
51	1	0		-7.3703	-0.591649	0.462883		-4.9510808	-1.51566709	-1.50006902
52	6	0		-5.954	1.03821	0.258244		-2.4785641	0.95477587	-1.01497017
53	1	0		-6.5967	1.743856	0.79441		-3.6776111	2.05762494	-0.72219312
54	1	0		-6.1685	1.180308	-0.806847		-0.1234053	2.01972651	-0.92480357
55	6	0		-4.4775	1.372814	0.549497		-3.601072	0.41865717	0.35817226
56	1	0		-4.4044	1.620291	1.622336		-4.4888972	1.24249732	1.52690378
57	6	0		-3.9999	2.658248	-0.200072		-1.5764943	1.99818837	0.48744261
58	1	0		-2.9946	2.888462	0.17344		-1.896218	1.38570062	0.72862143
59	6	0		-3.8897	2.474459	-1.721935		-3.3977436	1.51532138	-1.78002176
60	1	0		-3.255	1.62176	-1.984308		-4.4298246	1.93186949	-1.60704764
61	1	0		-3.4571	3.368528	-2.183434		-1.3994545	0.19162183	-0.02548184
62	1	0		-4.8697	2.31262	-2.18364		-1.1380514	1.10278795	-0.32865728
63	6	0		-4.8761	3.873237	0.142987		-2.2066933	3.34353661	0.56903302
64	1	0		-5.8874	3.775374	-0.265458		-3.4640818	4.65263946	-0.55198775
65	1	0		-4.4414	4.787408	-0.275198		-3.9022719	4.20516323	-0.38763857
66	1	0		-4.9633	4.009942	1.226784		-0.9232317	1.5415053	0.84429724
67	6	0		-5.8796	-1.547054	-1.591292		-0.0472064	-0.65384926	-1.04804231
68	1	0		-6.9327	-1.845042	-1.648782		-3.589284	-1.99807742	-2.1020368
69	1	0		-5.2761	-2.300278	-2.101123		-1.6922053	-0.67981928	-2.36453941
70	1	0		-5.7657	-0.60371	-2.134912		-2.6709299	-2.30304371	-1.93174705
71	8	0		-2.957	-2.771356	-1.414583		-0.2464959	-1.54386641	-1.24718607
72	1	0		-2.6892	-2.043615	-1.995684		-4.159719	-0.38125744	-1.56149507
73	6	0		0.2559	-0.415639	1.049808		4.8044929	-1.2162803	3.15409111
74	8	0		0.5379	0.746003	1.363377		5.6774669	0.51589809	3.19195074
75	8	0		3.2116	-2.627604	1.742982		1.3625117	-1.6091743	2.88220407
76	1	0		3.9582	-2.638454	2.358401		0.3674191	-0.0687472	1.37285288
77	6	0		2.0949	-1.278136	3.410521		5.3743726	-1.02273695	3.75710982
78	1	0		1.5208	-2.168198	3.685481		6.827391	-0.53551915	0.08459413
79	1	0		1.4934	-0.391179	3.612046		5.0641513	-0.34905722	1.23173899
80	1	0		2.9815	-1.228399	4.052463		9.4737836	-2.24003941	3.3042033

Center Number	Atomic Number	Atomic Type	Conformer 1-3	Coordinates (Angstroms)			Conformer 1-4	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		2.6877936	-1.0592333	-3.3740814		-2.5488815	-0.63659803	-2.11919384
2	6	0		1.0070542	-0.6470359	-3.3811396		-2.7199686	-0.16627601	-0.58990714
3	6	0		4.1424328	-0.2911403	-1.8588457		-1.6395269	1.24022795	-3.3272539
4	1	0		1.4300412	-0.1204547	-0.0565557		-4.605148	-0.05702905	-1.92965599
5	1	0		3.0330278	-0.0428246	-4.1439086		5.1300668	1.98074786	-3.54146881
6	6	0		2.7252502	-1.2156772	-4.851016		1.5110103	0.79421018	-2.80173423
7	1	0		3.2145557	-1.9228802	-2.0093215		0.9134834	-0.35276942	-1.29679299

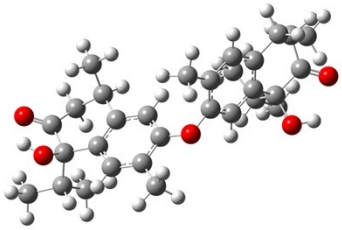
8	1	0		1.4115949	-1.6942549	-0.2518817		0.6413906	0.60546226	-2.91039389
9	6	0		1.5102234	-0.1850531	-1.4442399		1.9497415	1.03235326	-3.40280815
10	1	0		-3.561122	-0.6187356	0.9813144		1.3930704	1.15955643	1.93724351
11	6	0		-1.1311535	-1.9861346	1.0607955		4.4787359	-0.99875694	1.13962093
12	6	0		-1.6166998	-1.4887875	-4.6470168		1.5913759	-1.00139258	-1.77488058
13	6	0		-0.2550316	-0.9875308	-2.3754856		2.129382	-0.13287451	-2.01228091
14	1	0		-0.1783172	-1.8753155	-3.2790608		1.21306	-1.45590241	-1.3714064
15	1	0		-4.8754468	-1.2801002	-2.1765434		3.6655939	-1.94857825	-1.93850989
16	6	0		-1.872	-0.2566732	0.9566637		2.2640329	-1.19931739	-3.06983875
17	1	0		0.0721831	-2.754349	2.134577		4.5291534	-1.17106422	3.30208202
18	6	0		0.5989836	-1.4775503	3.8100867		3.7091475	-1.09270659	3.11988036
19	6	0		0.4064947	-2.3414749	2.6263367		0.4811026	-1.76692861	2.80008592
20	1	0		1.543079	-1.0591476	3.5678019		3.6579913	-1.05699292	1.84286861
21	6	0		1.6723684	-0.7035432	-1.3824061		-1.5404863	-0.77985655	0.06933701
22	1	0		1.1758195	-1.6249067	-4.6753298		-3.5972762	-2.01227581	-2.29943133
23	1	0		2.8157481	-2.0000038	-4.666707		-1.9516785	-0.39652384	-1.75885652
24	1	0		3.6623387	-1.5244444	-3.7935897		-3.0641725	-1.98003091	-0.3054036
25	6	0		0.3924331	2.7739738	-4.5187211		-0.647246	1.87167205	-0.1606125
26	1	0		0.2276335	0.0154903	-4.348822		-1.5236878	1.25829612	-2.32409604
27	6	0		0.3526735	1.4351691	-2.6533242		1.1002967	2.56098888	-0.39373758
28	1	0		2.0554971	0.4067906	3.3650616		4.0511239	0.42493266	0.16291972
29	1	0		4.7832289	1.0159039	-0.8683408		0.3010681	1.32955978	-0.16617191
30	1	0		4.6688169	1.9928884	-2.975454		0.2594605	2.18183509	-2.32577985
31	6	0		3.1000663	0.5333744	1.5223197		0.2043493	0.0828071	2.19103247
32	1	0		3.5965541	1.0870856	4.6220551		5.4692075	0.75296281	3.169449
33	1	0		1.3584089	0.7808592	0.316641		2.331018	0.15254989	0.49845607
34	1	0		2.3448821	2.4642722	3.4646947		4.6870481	1.00685787	3.96131718
35	8	0		1.3770196	0.6242238	2.5224567		4.6729213	-0.4151176	0.65081439
36	1	0		3.3699912	2.7409996	3.8846074		3.0830569	-2.05176029	0.21894821
37	6	0		2.3653333	-3.9338144	-2.2112628		2.7518395	-0.13370135	-0.77649329
38	1	0		-0.1625532	-1.0194841	3.9167644		-3.6094297	-1.52082056	3.5290171
39	6	0		-2.163936	-3.3604555	1.1494319		-3.3803363	-2.12651122	-1.891592
40	1	0		-1.5068103	-2.0205907	1.4531949		-0.7833649	-1.57172163	-0.94892238
41	6	0		-2.690061	-1.2344275	2.0442556		-3.5132636	-0.35602928	-0.5038114
42	6	0		-2.2690333	1.4158586	3.403929		-2.832914	2.23063953	-1.6269453
43	1	0		-2.5301097	0.0321544	1.2316792		-0.4296732	0.15314137	-3.92546317
44	1	0		-2.5731685	1.0253621	-1.4344138		-3.9952586	0.27745337	-0.56298394
45	6	0		-0.6155911	1.0183046	4.5160076		-0.4036298	-2.13568925	-2.88317272
46	6	0		-0.8194809	-0.9541673	2.576569		-4.0637153	-1.12804313	-0.37769767
47	6	0		-0.0012974	-0.4682194	-4.8236308		-0.530713	-2.78313781	-0.76627126
48	1	0		-2.4193088	-0.7956763	0.9557495		-3.3239334	-0.08565893	-1.16983534
49	6	0		-6.9106966	-0.1578849	4.6998433		-1.0795583	-2.06189846	-3.51051053
50	1	0		-2.9672855	-0.4293482	0.2741651		-1.0211765	-1.02081429	-0.80654721
51	1	0		-4.0087897	-1.4098627	1.0918841		-4.5796419	-0.53014159	-1.04575528
52	6	0		-4.7851004	0.0313479	4.6753671		-3.6987026	2.94824921	-3.67855568
53	1	0		-1.0553979	1.1912244	4.7903881		-4.5433002	2.52336682	-2.98247917
54	1	0		-0.0678328	0.8539029	-4.8773945		-0.9516216	1.22362291	-0.99884517
55	6	0		-1.422062	1.8615152	-0.9477818		-0.4518133	0.98353035	-3.62879611
56	1	0		-6.8424427	1.6007491	-3.2475723		-4.3739229	1.59688993	-3.89283415
57	6	0		-3.8827961	1.5690434	-2.5657593		-3.4674908	0.71781566	-0.55493865
58	1	0		-3.4353789	1.0374124	-3.6091718		-1.5255822	1.48936933	0.89814846
59	6	0		-3.6785176	0.7256227	-3.1475884		-3.4946726	0.53094214	-3.78524128
60	1	0		-5.8884763	0.7886187	-1.6575442		-0.660039	2.48012663	-3.86376384
61	1	0		-3.258942	3.7044474	-4.383903		-4.0307811	3.98037199	-2.9397691
62	1	0		-5.6330164	1.549222	-3.1636695		-2.0383148	1.7586414	-0.78810503
63	6	0		-1.8429395	3.8871653	2.0209839		-4.3873028	3.16243123	0.46450401
64	1	0		-0.49372	3.3337095	-2.4872021		-2.9422125	0.21538234	2.57115067
65	1	0		-4.9723421	1.3113228	-2.8396389		-4.9102097	3.57175427	2.22133534
66	1	0		-5.8921984	4.2222495	-1.4349743		-3.0664128	3.57493291	-0.46565983
67	6	0		-3.2654852	-1.7401056	-3.9527081		-3.2999233	-1.86764269	-0.1281905
68	1	0		-2.1296038	-3.3836845	-2.4710818		-3.1662212	-0.39258956	-0.23984336
69	1	0		-6.6017474	-1.5590584	-4.5069534		-3.9693863	-0.04781516	-3.84053741
70	1	0		-0.4028579	-1.7327619	-1.9647891		-4.6432083	-2.31981783	-2.35603225
71	8	0		-5.8014023	-2.1133917	-2.6460585		-3.7145703	-1.23060729	-1.66654225
72	1	0		-4.2789509	-3.7605479	-2.1420953		-3.4682875	-1.96624052	-2.10290358
73	6	0		0.5348347	-3.6969453	-0.1499462		0.7317112	-2.1911063	1.34743976
74	8	0		0.2406334	-3.749506	2.2052428		4.2906934	1.16373187	-3.42985065
75	8	0		1.7338436	-2.772887	3.9223571		2.8127209	-1.99352909	-3.9769751
76	1	0		2.4843488	-0.5802137	-2.4663991		1.194981	-1.84399095	-2.40502818
77	6	0		2.982994	-2.2150046	-2.8663215		1.0216172	-0.59452951	-3.35684451
78	1	0		2.1933771	-2.3342689	-4.2003915		0.203229	-2.3912	-0.27784921

79	1	0		2.2068831	-0.3346067	-4.2331215		4.9420787	-2.44716977	-2.41670227
80	1	0		2.2322536	-2.3641917	-0.7913545		2.7931219	-1.81773276	-3.79467177

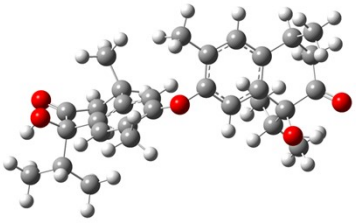
Center Number	Atomic Number	Atomic Type	Conformer 1-5	Coordinates (Angstroms)			Conformer 1-6	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		-1.475140	1.91962	0.295949		-1.476225	2.79104	0.265069
2	6	0		-3.962206	-0.188571	0.089733		-3.968106	0.191544	-0.103367
3	6	0		-3.750759	-1.488479	-0.208916		-3.759197	1.495901	0.176939
4	1	0		-1.292266	-0.996245	-0.621762		-1.292119	1.015536	0.562893
5	1	0		-0.309755	-1.378788	-0.883949		-0.30971	1.401466	0.820225
6	6	0		-4.775463	-2.588599	0.047026		-4.803564	2.582758	-0.057735
7	1	0		-4.224111	-3.417916	0.515776		-4.272812	3.424479	-0.527827
8	1	0		-5.833076	-2.099172	1.04739		-5.86673	2.081796	-1.046649
9	6	0		-5.381805	-2.00792	2.044369		-5.424053	1.990456	-2.047462
10	1	0		-6.640934	-2.836051	1.129732		-6.681223	2.811965	-1.123808
11	6	0		-6.385751	-0.745464	0.609485		-6.405124	0.725955	-0.597428
12	6	0		-7.217869	-0.444461	1.253253		-7.238075	0.413435	-1.234753
13	6	0		-6.796771	-0.844387	-0.401201		-6.812293	0.828508	0.414147
14	1	0		-5.298981	0.345642	0.628689		-5.309909	-0.356831	-0.615439
15	1	0		-5.119851	0.597469	1.687876		-5.141363	-0.619141	-1.673834
16	6	0		-5.415732	-3.163845	-1.234942		-5.437405	3.13774	1.236528
17	1	0		-4.651263	-3.530539	-1.921394		-4.670324	3.51885	1.911811
18	6	0		-6.089137	-3.990353	-0.980829		-6.133344	3.949709	0.996286
19	6	0		-5.998097	-2.40503	-1.767767		-5.994444	2.364034	1.774825
20	1	0		-5.759631	1.686889	-0.069656		-5.750638	-1.694639	0.10243
21	6	0		-5.346609	1.688312	-1.087879		-5.313374	-1.688821	1.110397
22	1	0		-7.286819	1.83512	-0.213603		-7.273189	-1.847727	0.284704
23	1	0		-7.514199	2.789775	-0.699743		-7.484663	-2.800714	0.781204
24	1	0		-7.738076	1.045884	-0.818906		-7.71227	-1.057213	0.897308
25	6	0		-7.784676	1.840101	0.762829		-7.795384	-1.859555	-0.678823
26	1	0		-5.243335	2.937764	0.66796		-5.246698	-2.947429	-0.640322
27	6	0		-5.668328	2.981149	1.67832		-5.699173	-3.000649	-1.638209
28	1	0		-4.157517	2.969876	0.766278		-4.163716	-2.971932	-0.76883
29	1	0		-5.552171	3.847676	0.141925		-5.534108	-3.855904	-0.099852
30	1	0		-0.36783	1.290453	-0.296228		-0.370506	-1.279247	0.291799
31	6	0		-0.65614	2.490197	-0.350163		-0.66128	-2.477356	0.365079
32	1	0		-2.422673	-1.974384	-0.750986		-2.416493	2.003823	0.660451
33	1	0		-2.150383	-2.90121	-0.223588		-2.153587	2.895612	0.070434
34	1	0		-2.847187	0.829779	0.006065		-2.847369	-0.821336	-0.031474
35	8	0		-3.079411	1.605721	-0.734274		-3.071459	-1.600779	0.707289
36	1	0		-2.800575	1.374937	0.95855		-2.804649	-1.363317	-0.986372
37	6	0		-2.5805	-2.286891	-2.162131		-2.53684	2.403811	2.052118
38	1	0		-1.920138	-2.957964	-2.386678		-1.874245	3.089895	2.216197
39	6	0		3.86606	0.240033	0.117819		3.868992	-0.245156	-0.104227
40	1	0		3.007961	-0.210725	1.063506		3.020847	0.187329	-1.067289
41	6	0		1.49132	0.028927	1.000826		1.503166	-0.048237	-1.014092
42	6	0		1.064141	-0.975712	0.875306		1.077237	0.959709	-0.913342
43	1	0		1.088076	0.833369	-0.272819		1.086486	-0.825386	0.27206
44	1	0		1.197502	0.144805	-1.119942		1.189863	-0.119853	1.105803
45	6	0		2.1023	1.959275	-0.578112		2.09541	-1.946944	0.609492
46	6	0		3.410869	1.229898	-0.945771		3.401994	-1.212783	0.974685
47	6	0		4.195825	1.995299	-1.059003		4.184364	-1.97719	1.110291
48	1	0		5.350057	-0.155534	0.040026		5.35278	0.149823	-0.020208
49	6	0		5.920701	0.783095	-0.011948		5.921423	-0.788277	0.056803
50	1	0		5.811057	-0.878113	1.32006		5.827374	0.844682	-1.310553
51	1	0		6.00285	-0.129838	2.096644		6.02536	0.079844	-2.069249
52	6	0		6.766897	-1.380061	1.156218		6.782565	1.348309	-1.148001
53	1	0		4.755068	-1.86306	1.825107		4.778296	1.820615	-1.846576
54	1	0		5.13028	-2.42512	2.688746		5.162975	2.363366	-2.718358
55	6	0		4.521331	-2.596903	1.044044		4.538645	2.57148	-1.083699
56	1	0		3.476157	-1.104709	2.215345		3.501526	1.056596	-2.2328
57	6	0		2.683213	-1.840638	2.410349		2.711874	1.789768	-2.450245
58	1	0		5.676631	-0.929852	-1.31047		5.667472	0.951686	1.31689
59	6	0		4.727408	-1.284249	-1.722939		4.714847	1.316236	1.71235
60	1	0		6.303265	0.022723	-2.343758		6.282202	0.020056	2.376053
61	1	0		6.491705	-0.498122	-3.289841		6.461764	0.560282	3.31294
62	1	0		5.650475	0.870533	-2.559125		5.626036	-0.822239	2.602336
63	6	0		7.265243	0.406473	-1.98068		7.247301	-0.372246	2.030864
64	1	0		6.589539	-2.159854	-1.163914		6.584014	2.176865	1.153518
65	1	0		7.593299	-1.888662	-0.81652		7.590671	1.896749	0.821961

66	1	0		6.187674	-2.912112	-0.479467		6.190358	2.915085	0.449316
67	6	0		6.706067	-2.639159	-2.142408		6.691705	2.676575	2.122762
68	1	0		0.845609	0.569988	2.29745		0.867996	-0.614512	-2.305162
69	1	0		-0.231382	0.700278	2.157841		-0.210552	-0.739489	-2.172727
70	1	0		0.965104	-0.141482	3.115949		0.996814	0.079514	-3.137142
71	8	0		1.259878	1.52913	2.614573		1.282635	-1.58103	-2.598497
72	1	0		3.22724	0.564403	-2.205414		3.208157	-0.522097	2.219168
73	6	0		2.735299	1.20859	-2.743416		2.710179	-1.154577	2.765397
74	8	0		3.713857	-0.330448	3.536749		3.749862	0.25493	-3.535758
75	8	0		4.474088	0.445778	3.414563		4.510127	-0.517459	-3.391506
76	1	0		2.814741	0.156211	3.913106		2.854214	-0.240875	-3.908385
77	6	0		4.063182	-1.023794	4.310046		4.104174	0.93226	-4.320884
78	1	0		2.330857	2.999943	0.524567		2.3323	-3.010103	-0.46977
79	1	0		2.992284	3.778704	0.132672		2.988354	-3.782065	-0.056001
80	1	0		1.388684	3.466389	0.819208		1.391973	-3.48049	-0.763971

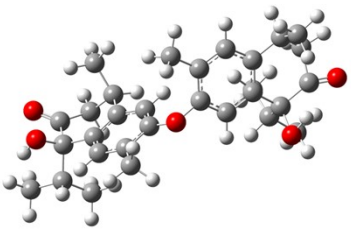
- **For compound 2**



2-1



2-2



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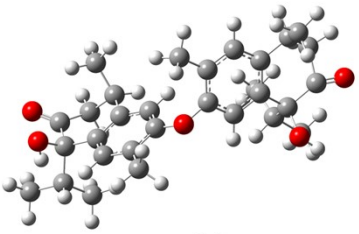

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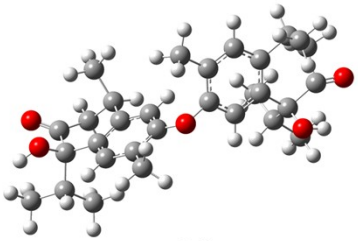

2-5

Table S3. Gibbs free energies and equilibrium populations of low-energy conformer of **2**

Conformer	**G HF hartree**	**ΔG hartree**	**ΔG kJ/mol**	**ΔG kcal/mol**	**(-)ΔG/RT**	**e(-ΔG/RT)**	**Mole fraction**	**Population%**
2-1	-1542.290499	0	0	0	0	1	0.404084077	40.40840774
2-2	-1542.290215	-0.000284	0.7456421	0.17821273	-0.30078859	0.740234248	0.299116873	29.9116873
2-3	-1542.290112	-0.000387	1.0160686	0.24284622	-0.40987741	0.663731611	0.268203376	26.82033758
2-4	-1542.287532	-0.002967	7.7898591	1.86182101	-3.1423935	0.043179325	0.017448078	1.744807755
2-5	-1542.287109	-0.00339	8.9004457	2.1272576	-3.59039908	0.027587319	0.011147596	1.11475962
SUM						2.474732502	1	100

Table S4. Cartesian coordinates for the low-energy reoptimized of compound **2** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

Center Number	Atomic Number	Atomic Type	Conformer 2-1	Coordinates (Angstroms)			Conformer 2-2	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		1.113267	0.942125	0.200815		3.649870	0.794659	1.650038
2	6	0		0.322128	1.570298	0.591433		3.276088	-2.480829	0.884394
3	6	0		-1.663298	3.141785	1.682127		3.891001	-2.369465	2.54748
4	6	0		3.25612	2.778093	-0.046006		2.566471	-0.725095	1.937732
5	6	0		-0.349754	1.155879	1.737229		1.620196	-1.25418	2.098059

6	6	0		-1.357778	1.940522	2.319106		4.771895	-0.26543	-0.126679
7	6	0		-1.020941	3.571787	0.511466		3.424934	0.461004	-0.171299
8	1	0		-2.428983	3.775837	2.118666		2.394965	0.213962	0.751181
9	6	0		0.81943	3.228431	-1.256702		3.221533	1.421367	-1.174479
10	1	0		1.740731	3.685706	-0.867282		4.029118	1.633936	-1.868717
11	6	0		0.086745	4.324504	-2.070271		2.027393	2.125183	-1.317693
12	1	0		-0.731938	3.857761	-2.627945		0.999984	1.836171	-0.402121
13	1	0		0.766227	4.796084	-2.784133		1.183749	0.907762	0.617549
14	6	0		-0.464492	5.369971	-1.148036		0.379828	0.722626	1.322888
15	6	0		-1.464015	4.912905	-0.081649		1.828941	3.153573	-2.401555
16	6	0		1.234006	2.088296	-2.200636		2.707388	3.208616	-3.048797
17	1	0		0.356985	1.54259	-2.564569		1.651934	4.149537	-1.980594
18	1	0		1.904399	1.37461	-1.715875		0.957783	2.915101	-3.020815
19	1	0		1.765762	2.495865	-3.065905		2.889043	0.061015	3.225043
20	6	0		-2.937016	4.841773	-0.651712		3.838814	0.598951	3.135205
21	1	0		-3.525896	4.648752	0.253923		2.961101	-0.616775	4.081869
22	6	0		-3.232465	3.702788	-1.637301		2.107548	0.79631	3.435825
23	1	0		-4.316032	3.597272	-1.752744		4.993988	-1.15232	-1.416867
24	1	0		-2.840099	2.742701	-1.291476		4.987731	-0.406392	-2.221471
25	1	0		-2.827382	3.902301	-2.634841		6.374309	-1.824396	-1.423865
26	6	0		-3.394394	6.192164	-1.22118		6.553294	-2.293807	-2.396417
27	1	0		-3.220357	7.001381	-0.508464		6.449961	-2.607403	-0.661425
28	1	0		-4.466024	6.160124	-1.441985		7.170427	-1.097073	-1.249656
29	1	0		-2.874214	6.436845	-2.154119		3.888519	-2.170968	-1.728286
30	8	0		-1.468778	5.895603	0.954309		4.014316	-2.54219	-2.750427
31	1	0		-1.024334	6.669076	0.56028		2.889016	-1.733777	-1.654485
32	8	0		-0.111321	6.542412	-1.170704		3.933897	-3.043038	-1.067445
33	6	0		-2.060364	1.496705	3.576348		5.815217	0.710209	-0.096627
34	1	0		-2.852599	2.19908	3.845937		6.458108	0.362465	0.548351
35	1	0		-1.364514	1.427238	4.419814		4.889906	-1.109006	1.150609
36	1	0		-2.505734	0.503894	3.453681		5.961183	-1.138768	1.743135
37	8	0		0	0	2.415522		-0.157242	2.582805	-0.53144
38	1	0		-1.113267	-0.942125	0.200815		-1.393298	2.060323	-0.180377
39	6	0		-0.322128	-1.570298	0.591433		-1.795602	0.79563	-0.595265
40	6	0		1.663298	-3.141785	1.682127		-1.109208	0.179488	-1.164983
41	6	0		0.349754	-1.155879	1.737229		-3.080703	0.322477	-0.298202
42	6	0		0	-2.778093	-0.046006		-2.25738	2.905719	0.535183
43	6	0		1.020941	-3.571787	0.511466		-3.974488	1.152574	0.397119
44	6	0		1.357778	-1.940522	2.319106		-3.538404	2.422525	0.802783
45	1	0		2.428983	-3.775837	2.118666		-4.229277	3.061908	1.347538
46	6	0		-0.81943	-3.228431	-1.256702		-5.629312	-0.791421	0.664067
47	1	0		-1.740731	-3.685706	-0.867282		-5.080458	-1.193913	1.523546
48	6	0		-0.086745	-4.324504	-2.070271		-3.462249	-1.081196	-0.773524
49	1	0		0.731938	-3.857761	-2.627945		-2.599881	-2.192006	-0.051025
50	1	0		-0.766227	-4.796084	-2.784133		-1.583149	-1.955045	-0.389162
51	6	0		0.464492	-5.369971	-1.148036		-2.590482	-2.151112	1.483536
52	6	0		1.464015	-4.912905	-0.081649		-1.777807	-2.782527	1.857035
53	6	0		-1.234006	-2.088296	-2.200636		-3.517877	-2.543197	1.913995
54	1	0		-1.904399	-1.37461	-1.715875		-2.431352	-1.14107	1.871032
55	1	0		-1.765762	-2.495865	-3.065905		-2.936756	-3.600795	-0.559602
56	1	0		-0.356985	-1.54259	-2.564569		-2.903646	-3.646611	-1.650457
57	6	0		2.937016	-4.841773	-0.651712		-3.930272	-3.925448	-0.231205
58	1	0		3.525896	-4.648752	0.253923		-2.210221	-4.320404	-0.169168
59	6	0		3.394394	-6.192164	-1.22118		-3.183656	-1.177316	-2.170802
60	1	0		3.220357	-7.001381	-0.508464		-3.958038	-1.636934	-2.544787
61	1	0		4.466024	-6.160124	-1.441985		-4.969009	-1.328497	-0.584002
62	1	0		2.874214	-6.436845	-2.154119		-5.58186	-1.904913	-1.473408
63	6	0		3.232465	-3.702788	-1.637301		-1.810592	4.275795	0.976409
64	1	0		2.827382	-3.902301	-2.634841		-0.897431	4.22161	1.578163
65	1	0		4.316032	-3.597272	-1.752744		-2.586586	4.763933	1.570624
66	1	0		2.840099	-2.742701	-1.291476		-1.584084	4.917125	0.117611
67	8	0		1.468778	-5.895603	0.954309		-5.407349	0.740687	0.666819
68	1	0		1.024334	-6.669076	0.56028		-5.741842	1.144448	1.628135
69	8	0		0.111321	-6.542412	-1.170704		-6.0627	1.186274	-0.094978
70	6	0		2.060364	-1.496705	3.576348		-7.104423	-1.174877	0.770198
71	1	0		1.364514	-1.427238	4.419814		-7.228478	-2.260803	0.789879
72	1	0		2.505734	-0.503894	3.453681		-7.535859	-0.763353	1.687149
73	1	0		2.852599	-2.19908	3.845937		-7.671832	-0.788155	-0.081213

Center Number	Atomic Number	Atomic Type	Conformer 2-3	Coordinates (Angstroms)			Conformer 2-4	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		-3.685766	-1.827725	-1.436793		-3.794942	-1.740004	-1.463418
2	6	0		-3.360645	-2.372582	-0.542706		-3.496072	-2.287658	-0.561894
3	6	0		-4.757892	-0.02362	0.12678		-4.856808	0.093101	0.07362
4	6	0		-3.386462	0.653652	0.114825		-3.472481	0.743641	0.080756
5	6	0		-2.356364	0.255006	-0.750792		-2.43586	0.319481	-0.764624
6	6	0		-3.160201	1.726675	0.990576		-3.240193	1.817732	0.953723
7	6	0		-3.966749	2.053658	1.640149		-4.051248	2.164672	1.587135
8	1	0		-1.943563	2.402623	1.058386		-2.011687	2.469751	1.038674
9	6	0		-0.918167	1.96535	0.200424		-0.980391	2.006657	0.20156
10	1	0		-1.122328	0.917646	-0.692189		-1.190114	0.958092	-0.688667
11	6	0		-0.319792	0.615319	-1.356924		-0.383042	0.636761	-1.338748
12	1	0		-1.719024	3.554918	2.003792		-1.780267	3.623159	1.981018
13	1	0		-2.60123	3.722935	2.626034		-2.670893	3.815547	2.583901
14	6	0		-1.5025	4.481659	1.460797		-1.531329	4.540872	1.436591
15	6	0		-0.862934	3.369169	2.661084		-0.942269	3.422454	2.657009
16	6	0		-5.041237	-0.742154	1.50646		-5.176425	-0.61235	1.452091
17	1	0		-5.03718	0.097232	2.213159		-5.166314	0.230252	2.1549
18	1	0		-6.440221	-1.373084	1.550985		-6.588513	-1.214475	1.477403
19	1	0		-6.664173	-1.709232	2.568377		-6.834836	-1.541958	2.49245
20	6	0		-6.514701	-2.245622	0.892585		-6.670731	-2.08785	0.821051
21	1	0		-7.208654	-0.654647	1.256841		-7.337513	-0.481713	1.168848
22	6	0		-3.975644	-1.741074	1.978925		-4.138958	-1.630494	1.945596
23	1	0		-4.142748	-1.976682	3.034943		-4.32725	-1.857936	2.999823
24	1	0		-2.962258	-1.341664	1.884022		-3.116278	-1.252215	1.864803
25	1	0		-4.0258	-2.688623	1.432156		-4.199961	-2.579166	1.401906
26	6	0		-5.761378	0.981072	-0.036654		-5.837827	1.116035	-0.111366
27	1	0		-6.398686	0.59168	-0.663324		-6.472842	0.735176	-0.745548
28	1	0		-4.892499	-1.004402	-1.050805		-4.991447	-0.891476	-1.100818
29	1	0		-5.952919	-1.042452	-1.661809		-6.042807	-0.912921	-1.728075
30	8	0		0.261724	2.684735	0.25332		0.212316	2.703296	0.270616
31	1	0		1.475007	2.096738	-0.076006		1.415212	2.085786	-0.036498
32	8	0		1.881755	0.902776	0.509017		1.799002	0.886612	0.550812
33	6	0		1.215054	0.395007	1.197024		1.130385	0.381204	1.237826
34	1	0		3.145963	0.366343	0.231184		3.062385	0.348559	0.272208
35	1	0		2.313001	2.8078	-0.950116		3.953572	1.027825	-0.578169
36	1	0		4.014445	1.064421	-0.623489		3.554902	2.256466	-1.157349
37	8	0		3.574414	2.26554	-1.198647		5.560714	-0.993354	-0.52626
38	1	0		4.246175	2.801542	-1.865161		4.990759	-1.553439	-1.276667
39	6	0		5.632954	-0.927712	-0.662748		3.424637	-0.970969	0.963776
40	6	0		5.038052	-1.447806	-1.422705		2.534031	-2.166916	0.438249
41	6	0		3.536319	-0.952448	0.902168		1.531226	-1.870167	0.7704
42	6	0		2.629157	-2.147863	0.405169		2.469776	-2.356223	-1.083788
43	6	0		1.632273	-1.843877	0.748675		1.63455	-3.020187	-1.329182
44	6	0		2.546126	-2.3487	-1.114553		3.373973	-2.827662	-1.482556
45	1	0		1.710069	-3.016578	-1.345964		2.311172	-1.413097	-1.613788
46	6	0		3.447849	-2.819831	-1.519507		2.880441	-3.486798	1.14173
47	1	0		2.379058	-1.409629	-1.649296		2.891724	-3.365553	2.227249
48	6	0		2.977719	-3.464622	1.113378		3.857789	-3.870423	0.82804
49	1	0		2.995336	-3.338498	2.198233		2.134188	-4.248197	0.893895
50	1	0		3.952247	-3.851792	0.796033		3.154408	-0.838236	2.359026
51	6	0		2.227894	-4.225207	0.873844		3.943401	-1.207199	2.798065
52	6	0		3.325974	-0.822784	2.308676		4.923475	-1.269354	0.811123
53	6	0		4.111993	-1.23371	2.713746		5.544761	-1.670322	1.78705
54	1	0		5.02933	-1.253308	0.683232		5.354776	0.508933	-0.838505
55	1	0		5.679032	-1.695656	1.621822		5.63612	0.675835	-1.882816
56	1	0		1.8622	4.103872	-1.573509		6.072448	1.089691	-0.240586
57	6	0		0.920363	3.97759	-2.117401		7.030419	-1.407279	-0.586947
58	1	0		2.614334	4.481316	-2.270199		7.145462	-2.478592	-0.402316
59	6	0		1.685966	4.871841	-0.812408		7.44499	-1.182799	-1.573912
60	1	0		5.427943	0.589535	-0.892189		7.619093	-0.872143	0.163702
61	1	0		5.719592	0.834081	-1.918936		-2.63983	-0.766669	-1.801183
62	1	0		6.124409	1.135105	-0.239794		-2.850143	-0.302889	-2.775368
63	6	0		7.096916	-1.349474	-0.7776		-1.718017	-1.342968	-1.93165
64	1	0		7.208573	-2.427663	-0.635951		-4.084339	-2.727043	-2.59315
65	1	0		7.487045	-1.090933	-1.76616		-4.885566	-3.41768	-2.317273
66	1	0		7.70937	-0.846951	-0.023421		-4.392323	-2.202303	-3.502113
67	8	0		-2.556648	-0.829538	-1.789765		-3.189178	-3.313116	-2.820273
68	1	0		-2.793674	-0.365113	-2.757483		4.486027	3.033766	-2.058689
69	8	0		-1.625847	-1.386326	-1.939655		4.744115	2.467376	-2.961303

70	6	0		-3.974182	-2.816065	-2.565619		4.026362	3.972693	-2.375369
71	1	0		-4.75681	-3.523588	-2.279323		5.429181	3.274165	-1.555164
72	1	0		-4.30761	-2.294219	-3.467229		2.284445	2.767212	-0.886806
73	1	0		-3.071441	-3.383329	-2.809865		1.962692	3.707179	-1.323886

Center Number	Atomic Number	Atomic Type	Conformer 2-5	Coordinates (Angstroms)		
				X	Y	Z
1	1	0		-3.664021	-1.655893	-1.529278
2	6	0		-3.35661	-2.215125	-0.638756
3	6	0		-4.783354	0.105425	0.052163
4	6	0		-3.414187	0.812292	0.118417
5	6	0		-2.369239	0.42253	-0.747651
6	6	0		-3.178401	1.872479	1.034112
7	6	0		-0.891432	2.06596	0.226881
8	1	0		-1.115106	1.042659	-0.685717
9	6	0		-0.327061	0.730353	-1.362339
10	1	0		-5.114285	-0.71027	1.370736
11	6	0		-5.244247	0.078166	2.11643
12	1	0		-6.456293	-1.451207	1.267361
13	1	0		-6.743964	-1.834578	2.251449
14	6	0		-6.40272	-2.306862	0.585147
15	6	0		-7.25064	-0.786051	0.920276
16	6	0		-4.010889	-1.64381	1.889201
17	1	0		-4.243081	-1.938541	2.917842
18	1	0		-3.0295	-1.162075	1.89508
19	1	0		-3.937045	-2.568049	1.306899
20	6	0		-5.815245	1.078909	-0.118518
21	1	0		-6.385238	0.708197	-0.818931
22	6	0		-4.870722	-0.831917	-1.169663
23	1	0		-5.899393	-0.827522	-1.834357
24	1	0		0.291563	2.775411	0.30304
25	1	0		1.505101	2.163342	0.031781
26	6	0		1.846828	0.92069	0.550804
27	1	0		1.137785	0.371076	1.158417
28	1	0		3.12156	0.391758	0.307148
29	1	0		4.066665	1.122025	-0.435055
30	8	0		3.710149	2.39433	-0.943844
31	1	0		5.65856	-0.91248	-0.433442
32	8	0		5.136823	-1.411693	-1.258114
33	6	0		3.430702	-0.982023	0.913503
34	1	0		2.569976	-2.122255	0.235738
35	1	0		1.549324	-1.840809	0.523963
36	1	0		2.605564	-2.18892	-1.297536
37	8	0		1.783692	-2.820789	-1.649613
38	1	0		3.530757	-2.638337	-1.673014
39	6	0		2.489209	-1.204599	-1.75914
40	6	0		2.860442	-3.497733	0.852551
41	6	0		2.803288	-3.46204	1.942769
42	6	0		3.852706	-3.868103	0.57142
43	6	0		2.125662	-4.227782	0.498692
44	6	0		3.069168	-0.959692	2.293977
45	1	0		3.828013	-1.365771	2.753012
46	6	0		4.934723	-1.282094	0.83556
47	1	0		5.489507	-1.76214	1.815924
48	6	0		5.478333	0.610104	-0.648162
49	1	0		5.823232	0.849067	-1.658919
50	1	0		6.161418	1.139902	0.03191
51	6	0		7.127733	-1.33271	-0.429528
52	6	0		7.227141	-2.415699	-0.318783
53	6	0		7.606605	-1.038502	-1.367866
54	1	0		7.667756	-0.859851	0.395776
55	1	0		-2.550435	-0.628665	-1.827456
56	1	0		-2.784322	-0.130225	-2.778958
57	6	0		-1.608439	-1.162585	-1.987362
58	1	0		-3.912069	-2.619237	-2.688315
59	6	0		-4.697888	-3.337997	-2.44104
60	1	0		-4.222103	-2.079133	-3.587362
61	1	0		-2.998597	-3.17538	-2.917767
62	1	0		4.698144	3.226498	-1.728027
63	6	0		5.007768	2.725009	-2.652564
64	1	0		4.263415	4.190381	-2.002082

65	1	0		5.610149	3.420493	-1.15223
66	1	0		2.428929	2.896141	-0.712684
67	8	0		2.139045	3.868568	-1.098063
68	1	0		-1.920417	2.479995	1.069057
69	8	0		-1.72816	3.291782	1.763707
70	6	0		-4.207052	2.401166	2.016051
71	1	0		-5.219552	2.34779	1.62021
72	1	0		-4.179507	1.838629	2.957084
73	1	0		-3.982947	3.442366	2.264052

- **For compound 3**

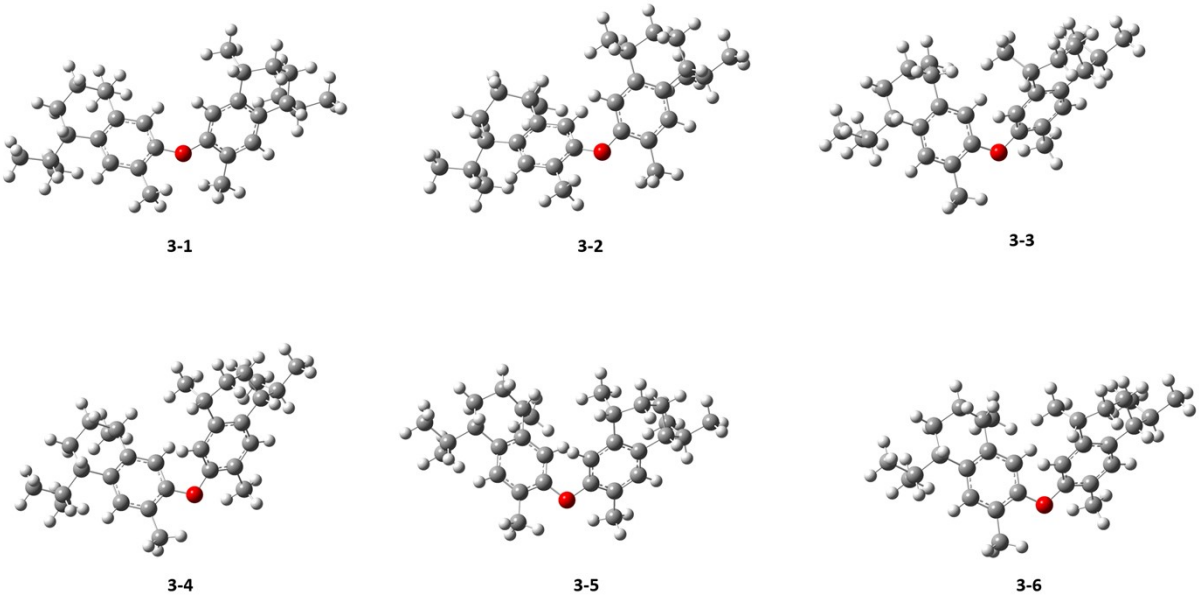

Table S5. Gibbs free energies and equilibrium populations of low-energy conformer of **3**

Conformer	**G HF hartree**	**ΔG hartree**	**ΔG kJ/mol**	**ΔG kcal/mol**	**(-)ΔG/RT**	**e(-ΔG/RT)**	**Mole fraction**	**Population%**
3-1	-1243.824904	0	0	0	0	1	0.230891909	23.0891909
3-2	-1243.824831	-7.3E-05	0.1916615	0.0458082	-0.07731538	0.925597896	0.213713065	21.37130651
3-3	-1243.824754	-0.00015	0.393825	0.09412644	-0.15886721	0.853109633	0.196976112	19.69761118
3-4	-1243.824612	-0.000292	0.7666461	0.18323281	-0.30926151	0.733988799	0.169472075	16.94720751
3-5	-1243.8245	-0.000404	1.0607021	0.25351388	-0.42788236	0.651888096	0.150515687	15.0515687
3-6	-1243.823211	-0.001693	4.4449718	1.06237377	-1.79308129	0.166446508	0.038431152	3.843115203
SUM						4.331030932	1	100

Table S6. Cartesian coordinates for the low-energy reoptimized of compound **3** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

Center Number	Atomic Number	Atomic Type	Conformer 3-1	Coordinates (Angstroms)			Conformer 3-2	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		-0.365152	0.357286	0.228129		0.576751	-0.662114	0.102653
2	6	0		-1.29746	0.196412	0.222763		1.442765	-0.061245	-0.151854
3	6	0		-3.632831	1.652599	0.296321		3.604408	1.47448	-0.89315
4	6	0		-2.51245	-0.483676	0.418304		2.722786	-0.643062	-0.136735
5	6	0		-1.260854	1.575749	0.049037		1.257484	1.268537	-0.514281
6	6	0		-2.439747	2.34159	0.089985		2.345524	2.070879	-0.902458
7	6	0		-3.708133	0.25672	0.444923		3.830003	0.142248	-0.505075
8	1	0		-4.552005	2.230965	0.353124		4.454258	2.07293	-1.212841
9	6	0		-2.458913	-1.989618	0.688673		2.831319	-2.134503	0.19114
10	1	0		-1.868229	-2.104743	1.610086		2.243463	-2.651952	-0.582023

11	6	0		-3.84374	-2.619235	0.951678		4.273118	-2.680888	0.111902
12	1	0		-3.714876	-3.5068	1.581901		4.233728	-3.750119	-0.1263
13	1	0		-4.264025	-2.981764	0.005148		4.743268	-2.610917	1.100874
14	6	0		-4.82657	-1.639283	1.595863		5.134053	-1.933089	-0.908255
15	1	0		-4.420675	-1.28763	2.553548		4.679312	-2.016064	-1.904199
16	1	0		-5.770822	-2.14062	1.827087		6.124272	-2.391735	-0.982789
17	6	0		-5.055522	-0.415756	0.684425		5.239702	-0.437752	-0.543606
18	1	0		-5.694089	0.298175	1.224877		5.788787	0.072119	-1.348642
19	6	0		-1.725421	-2.76911	-0.418891		2.204151	-2.492944	1.551507
20	1	0		-0.695778	-2.427812	-0.557684		1.145714	-2.223755	1.606786
21	1	0		-2.247516	-2.662985	-1.37643		2.725978	-1.976841	2.36518
22	1	0		-1.690358	-3.835673	-0.170805		2.282043	-3.57083	1.731642
23	6	0		-5.812466	-0.7596	-0.641868		6.047736	-0.17193	0.770365
24	1	0		-5.155785	-1.397599	-1.248789		5.47402	-0.589104	1.609066
25	6	0		-7.115731	-1.533603	-0.380335		7.425005	-0.856551	0.750918
26	1	0		-7.771131	-0.97809	0.302198		8.005887	-0.543207	-0.125665
27	1	0		-6.939368	-2.521044	0.054394		7.353408	-1.94731	0.732586
28	1	0		-7.664971	-1.682416	-1.316159		7.999598	-0.582172	1.642053
29	6	0		-6.124488	0.4934	-1.475292		6.230531	1.32865	1.04751
30	1	0		-6.775652	1.182011	-0.922061		6.793285	1.812484	0.239134
31	1	0		-6.646119	0.216403	-2.397763		6.79275	1.478322	1.975563
32	1	0		-5.220231	1.039399	-1.754199		5.275356	1.84928	1.148362
33	8	0		-0.091894	2.291791	-0.145358		0.02037	1.889491	-0.543848
34	1	0		1.542286	1.879006	1.829204		-1.44854	0.513175	-2.171305
35	6	0		1.917201	1.492301	0.885251		-1.84736	0.520564	-1.16135
36	6	0		2.840661	0.594962	-1.545311		-2.75186	0.548148	1.437476
37	6	0		1.124004	1.619172	-0.246412		-1.1231	1.181871	-0.177828
38	6	0		3.187244	0.899899	0.823911		-3.05263	-0.13574	-0.86713
39	6	0		3.657459	0.418763	-0.413933		-3.51832	-0.111411	0.462866
40	6	0		1.574815	1.182494	-1.500831		-1.55595	1.211797	1.155362
41	1	0		3.205817	0.271162	-2.515838		-3.10219	0.538654	2.46664
42	6	0		4.019001	0.830795	2.097662		-3.74846	-0.91863	-1.983061
43	1	0		3.865971	1.775441	2.636357		-5.02411	-1.654122	-1.518748
44	6	0		5.512812	0.716045	1.754085		-5.17849	-2.531623	-2.157009
45	1	0		6.094391	0.56473	2.671183		-5.89605	-1.008146	-1.680576
46	1	0		5.854845	1.66298	1.31543		-4.96742	-2.063633	-0.045535
47	6	0		5.771205	-0.423706	0.766976		-5.8585	-2.635927	0.227536
48	1	0		6.846186	-0.519752	0.585057		-4.11019	-2.729656	0.118909
49	1	0		5.453964	-1.369388	1.220938		2.136901	3.503729	-1.321144
50	6	0		5.047041	-0.212086	-0.57881		1.442611	3.577627	-2.165625
51	1	0		5.644273	0.519146	-1.146598		3.083735	3.964191	-1.614305
52	6	0		5.032324	-1.506783	-1.452019		1.704098	4.099355	-0.509266
53	1	0		4.59969	-1.230923	-2.421342		-0.76376	1.924834	2.221753
54	6	0		4.159106	-2.632063	-0.875097		-1.27502	1.871373	3.185958
55	1	0		4.560354	-3.017249	0.068635		-0.61791	2.980503	1.969032
56	1	0		4.113507	-3.473429	-1.57494		0.233478	1.487087	2.341071
57	1	0		3.135024	-2.292976	-0.692156		-4.05527	-0.049567	-3.217019
58	6	0		6.454962	-2.011296	-1.7424		-4.7451	0.761028	-2.957102
59	1	0		7.087789	-1.213658	-2.147858		-3.15459	0.399178	-3.645235
60	1	0		6.429513	-2.823575	-2.476641		-4.52672	-0.6561	-3.998002
61	1	0		6.94166	-2.400424	-0.841903		-3.02664	-1.686369	-2.299648
62	6	0		3.538025	-0.297124	3.034082		-6.05323	0.118845	0.857143
63	1	0		2.483376	-0.163968	3.294726		-6.13972	0.559351	-0.145272
64	1	0		4.11823	-0.298658	3.963507		-5.90847	1.280655	1.852821
65	1	0		3.639099	-1.282483	2.568694		-5.0383	1.90498	1.636751
66	6	0		-2.392895	3.839783	-0.068493		-6.79583	1.921773	1.819224
67	1	0		-1.758973	4.304422	0.695068		-5.80885	0.908702	2.880352
68	1	0		-3.394613	4.269725	0.010022		-7.35477	-0.645358	1.153263
69	1	0		-1.972508	4.126924	-1.039031		-8.19608	0.051661	1.229049
70	6	0		0.733667	1.360792	-2.739477		-7.6033	-1.372414	0.375616
71	1	0		1.283054	1.048151	-3.630755		-7.28482	-1.183499	2.10685
72	1	0		0.433381	2.40591	-2.868538		-4.80503	-0.825911	0.86122
73	1	0		-0.188205	0.770827	-2.68559		-4.68636	-1.173251	1.897594

Center Number	Atomic Number	Atomic Type	Conformer 3-3	Coordinates (Angstroms)			Conformer 3-4	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		3.748671	-2.651454	-0.329076		3.932854	2.687009	0.146
2	6	0		3.467284	-2.813917	0.722505		3.563725	-2.80002	0.885
3	6	0		4.969642	-0.519003	0.425568		5.031318	-0.48166	0.588
4	6	0		3.609449	0.174656	0.277644		3.673422	0.163948	0.284
5	6	0		2.52459	-0.435747	-0.379449		2.664981	-0.51396	-0.428

6	6	0		3.396522	1.433913	0.863638		3.380993	1.446951	0.776
7	6	0		4.208852	1.910346	1.405608		4.131908	1.975718	1.356
8	1	0		2.180947	2.117458	0.803124		2.158371	2.090647	0.573
9	6	0		1.126875	1.490248	0.120723		1.184177	1.395594	-0.159
10	1	0		1.296647	0.235645	-0.456453		1.433176	0.11678	-0.647
11	6	0		0.461505	-0.234866	-0.966197		0.655055	-0.40314	-1.198
12	1	0		1.994369	3.472524	1.43821		1.885195	3.473072	1.11
13	1	0		1.792042	4.244387	0.686819		1.736024	4.196733	0.301
14	6	0		2.888777	3.767147	1.992896		2.718734	3.8215	1.725
15	1	0		1.143877	3.477137	2.128163		0.975674	3.49282	1.72
16	1	0		6.17412	0.426499	0.117894		6.235897	0.47924	0.333
17	6	0		6.078907	1.286957	0.791594		6.061774	1.371888	0.947
18	1	0		7.519622	-0.237185	0.452205		7.561604	-0.12755	0.82
19	6	0		8.334487	0.490683	0.375636		8.362854	0.617772	0.774
20	1	0		7.750746	-1.059014	-0.233726		7.871515	-0.97824	0.204
21	1	0		7.52538	-0.63955	1.471644		7.486633	-0.47414	1.857
22	1	0		6.176688	0.977885	-1.316505		6.35228	0.951731	-1.124
23	6	0		6.980089	1.712188	-1.43964		7.1474	1.699156	-1.219
24	1	0		5.230912	1.471883	-1.558596		5.421042	1.406859	-1.475
25	6	0		6.343422	0.187936	-2.056858		6.600113	0.127373	-1.802
26	1	0		-2.266545	2.087846	-0.842233		-2.237287	1.877047	-1.183
27	1	0		-3.536763	1.514804	-0.764657		-3.500058	1.302313	-1.031
28	1	0		-4.301665	1.911832	-1.426057		-4.289519	1.650302	-1.692
29	6	0		-3.867642	0.468406	0.114209		-3.793022	0.312932	-0.077
30	1	0		-1.285139	1.585522	0.025789		-1.225272	1.438034	-0.315
31	1	0		-2.866719	0.007665	0.992215		-2.76319	-0.08286	0.797
32	1	0		-1.58669	0.577569	0.934866		-1.490151	0.489218	0.668
33	8	0		-0.817032	0.232883	1.619334		-0.699162	0.192009	1.35
34	1	0		-3.128066	-1.071913	2.03472		-5.217854	-0.24312	0.033
35	6	0		-2.605452	-0.770921	2.952527		-5.806665	-0.67873	-1.348
36	6	0		-2.53255	-2.430658	1.610627		-5.757885	0.20163	-2.001
37	6	0		-2.988256	-2.803574	0.688093		-5.005722	-1.79278	-2.04
38	6	0		-2.688401	-3.18048	2.394261		-5.402829	-1.97777	-3.044
39	6	0		-5.303495	-0.073956	0.141628		-5.061561	-2.73886	-1.49
40	6	0		-5.890039	-0.336502	-1.281395		-3.949897	-1.52419	-2.141
41	1	0		-5.831112	0.612062	-1.829006		-7.292289	-1.05741	-1.24
42	6	0		-5.099901	-1.373932	-2.094322		-7.871473	-0.26899	-0.745
43	1	0		-5.500113	-1.444401	-3.111532		-7.436446	-1.98373	-0.673
44	6	0		-5.163627	-2.373753	-1.651178		-7.721183	-1.21316	-2.235
45	1	0		-4.041922	-1.105187	-2.168284		-1.960692	2.935839	-2.221
46	1	0		-7.380705	-0.707102	-1.221833		-1.140375	2.64063	-2.884
47	6	0		-7.951726	0.022826	-0.636773		-1.66363	3.884245	-1.759
48	1	0		-7.538557	-1.693499	-0.773099		-2.847153	3.119705	-2.833
49	1	0		-7.808006	-0.735025	-2.22993		0.002689	2.070407	-0.431
50	6	0		-1.952535	3.208478	-1.801291		5.039071	-0.67978	1.672
51	1	0		-1.11188	2.951134	-2.454577		5.214117	-1.84553	-0.111
52	6	0		-1.667866	4.124049	-1.270701		6.010119	-2.40294	0.395
53	1	0		-2.817603	3.435419	-2.429355		5.548959	-1.69856	-1.147
54	6	0		-0.049159	2.214693	0.00112		-5.849037	0.595783	0.364
55	1	0		5.066666	-0.779235	1.491726		-4.476058	-1.13979	2.343
56	1	0		5.051816	-1.844189	-0.361121		-4.604423	-2.01466	2.994
57	1	0		5.872645	-2.448495	0.039946		-5.34846	-1.35729	1.096
58	6	0		5.299071	-1.645626	-1.412949		-6.399356	-1.44994	1.39
59	1	0		-5.923161	0.72992	0.570702		-5.064797	-2.32116	0.655
60	1	0		-4.629774	-1.159674	2.35027		4.182074	-4.08353	-0.724
61	1	0		-4.93754	-0.254913	2.891456		4.917337	-4.63355	-0.127
62	6	0		-4.819725	-2.007373	3.019354		3.259705	-4.67425	-0.749
63	1	0		-5.460668	-1.293596	1.072862		4.565382	-4.0201	-1.75
64	1	0		-6.517534	-1.416665	1.329542		-4.879062	0.101403	3.153
65	1	0		-5.166199	-2.209426	0.547723		-5.933788	0.051824	3.445
66	6	0		-1.455745	-2.346049	1.433673		-4.281466	0.178665	4.068
67	1	0		3.906511	-4.018514	-1.001715		-4.732776	1.025884	2.585
68	1	0		4.674472	-4.619099	-0.502339		-3.005614	-1.09904	1.897
69	1	0		2.968727	-4.584536	-0.977882		-2.71829	-2.09865	1.54
70	6	0		4.201289	-3.906251	-2.052249		-2.348563	-0.88123	2.747
71	1	0		2.645544	-1.817352	-0.991292		2.872986	-1.9224	-0.948
72	1	0		1.679703	-2.332419	-0.924179		1.917704	-2.46077	-0.937
73	1	0		2.868846	-1.732111	-2.066161		3.189069	-1.88857	-2.002

Center Number	Atomic Number	Atomic Type	Conformer 3-5	Coordinates (Angstroms)			Conformer 3-6	Coordinates (Angstroms)		
				X	Y	Z		X	Y	Z
1	1	0		3.688034	2.587342	-0.31455		-4.150324	1.549481	1.960956
2	6	0		3.203018	-2.596759	0.955694		-4.091319	0.724645	2.686227
3	6	0		5.016334	-0.399005	0.480191		-5.162467	0.021237	0.104442
4	6	0		3.637134	0.255958	0.360916		-3.747884	-0.563856	0.063452
5	6	0		2.609369	-0.356131	-0.388428		-2.638509	0.19404	0.492775
6	6	0		3.356431	1.482322	1.014342		-3.52141	-1.889162	-0.388741
7	6	0		1.118761	1.488589	0.068119		-1.126609	-1.597299	-0.093743
8	1	0		1.364436	0.262582	-0.543186		-1.3382	-0.317584	0.41073
9	6	0		0.587113	-0.22361	-1.123848		-0.501113	0.278331	0.758961
10	1	0		6.113883	0.416	-0.285312		-5.7311	0.270955	-1.333902
11	6	0		6.070876	1.439732	0.101338		-5.660874	-0.682117	-1.868865
12	1	0		7.524056	-0.112919	0.020444		-7.220887	0.646352	-1.293906
13	1	0		8.283773	0.535478	-0.429358		-7.630125	0.705409	-2.308304
14	6	0		7.677174	-1.121315	-0.378763		-7.383773	1.619655	-0.818607
15	1	0		7.710989	-0.148395	1.099773		-7.804696	-0.098075	-0.740548
16	1	0		5.873026	0.508777	-1.799953		-4.924238	1.292447	-2.150194
17	6	0		6.61211	1.173975	-2.259465		-5.306287	1.342684	-3.175598
18	1	0		4.878945	0.907958	-2.023822		-3.865877	1.018594	-2.200335
19	6	0		5.964111	-0.464764	-2.293917		-4.991047	2.302498	-1.731316
20	1	0		-2.277024	2.076977	-0.942729		2.579217	0.192987	-1.478073
21	1	0		-3.539647	1.484483	-0.886371		2.67749	0.872472	-2.318864
22	1	0		-4.313763	1.897269	-1.527792		3.638897	0.053133	-0.565644
23	6	0		-3.85052	0.398104	-0.051198		1.262241	-1.412568	-0.274293
24	1	0		-1.285878	1.551896	-0.098924		3.503548	-0.885504	0.477156
25	6	0		-2.84197	-0.083982	0.804481		2.297324	-1.609473	0.646317
26	1	0		-1.5702	0.504091	0.771358		4.912019	0.885021	-0.771422
27	1	0		-0.795446	0.14133	1.439995		4.608429	2.399068	-1.015342
28	1	0		-5.273286	-0.173678	-0.041727		3.940275	2.450745	-1.883578
29	6	0		-5.818755	-0.464013	-1.476922		3.878221	3.081293	0.152196
30	1	0		-5.759658	0.480847	-2.031348		3.601937	4.105557	-0.120481
31	1	0		-4.988161	-1.493587	-2.258912		4.506369	3.143066	1.047423
32	1	0		-5.354448	-1.573544	-3.288125		2.961597	2.547315	0.420291
33	8	0		-5.051137	-2.492794	-1.814484		5.876525	3.178638	-1.398376
34	1	0		-3.932341	-1.209312	-2.299959		6.407679	2.697143	-2.227337
35	6	0		-7.303371	-0.860956	-1.452971		6.573186	3.262893	-0.557687
36	6	0		-7.903294	-0.133509	-0.894327		5.619199	4.195929	-1.712296
37	6	0		-7.455388	-1.843581	-0.993969		0.118001	-2.197162	-0.164803
38	6	0		-7.702503	-0.911267	-2.471732		-5.808052	-0.753347	0.539321
39	6	0		-1.97963	3.240375	-1.855009		-5.314154	1.286936	0.999043
40	6	0		-1.1392	3.019993	-2.522038		-6.252818	1.218826	1.560192
41	1	0		-1.702135	4.136033	-1.28774		-5.408826	2.178105	0.366016
42	6	0		-2.850085	3.484014	-2.469255		5.365421	0.526747	-1.708298
43	1	0		-0.058455	2.197367	-0.111248		6.02483	-0.76659	0.854678
44	6	0		5.298835	-0.338646	1.539471		6.751075	-0.79694	1.677627
45	1	0		5.055779	-1.906351	0.089513		5.953381	0.679283	0.34725
46	1	0		5.677845	-2.447404	0.811186		6.937601	0.99764	-0.012663
47	6	0		5.554166	-2.023301	-0.880837		5.711643	1.323657	1.201504
48	1	0		-5.920499	0.622292	0.357566		-4.343205	2.858096	2.73341
49	1	0		-4.589397	-1.304658	2.181173		-5.275394	2.844719	3.308778
50	6	0		-4.729408	-2.243416	2.733281		-3.518783	3.031301	3.433706
51	1	0		-5.4246	-1.3945	0.89362		-4.386375	3.714557	2.049561
52	6	0		-6.482567	-1.523123	1.146523		6.503403	-1.758893	-0.216602
53	1	0		-5.12071	-2.305174	0.362854		7.473567	-1.45522	-0.625229
54	6	0		3.82129	-4.034028	-0.516954		6.618478	-2.762211	0.207906
55	1	0		4.447351	-4.623458	0.161861		5.798074	-1.833648	-1.05053
56	1	0		2.843146	-4.523	-0.581444		4.653785	-1.149316	1.433876
57	1	0		4.280881	-4.073061	-1.512065		4.490257	-0.589849	2.367079
58	6	0		-5.024356	-0.156962	3.104867		4.659938	-2.206171	1.721024
59	1	0		-6.086523	-0.241582	3.359865		-2.851577	1.544848	1.142816
60	1	0		-4.453505	-0.173399	4.039794		-1.989685	1.785655	1.775494
61	1	0		-4.868939	0.822598	2.641446		-2.910246	2.340634	0.384684
62	6	0		-3.10744	-1.211091	1.783946		-4.639626	-2.832578	-0.78414
63	1	0		-2.803427	-2.166616	1.332623		-5.532388	-2.702968	-0.166005
64	1	0		-2.475766	-1.081027	2.670866		-4.948497	-2.693055	-1.826363
65	1	0		2.818964	-1.738205	-0.969734		-4.311655	-3.87074	-0.683778
66	6	0		1.846688	-2.214033	-1.140497		-2.2149	-2.382226	-0.469098
67	1	0		3.312749	-1.68136	-1.95166		-2.03218	-3.395044	-0.815865
68	1	0		4.347078	2.187456	1.918592		2.121147	-2.583661	1.788423

69	1	0		4.958123	1.487393	2.495049		2.405692	-2.133786	2.744955
70	6	0		5.036579	2.826373	1.355125		1.084628	-2.913508	1.858271
71	1	0		3.819941	2.83218	2.626956		2.745222	-3.476433	1.658007
72	1	0		2.101159	2.081698	0.855175		1.40236	-0.529928	-1.346237
73	1	0		1.874974	3.019625	1.353459		0.595254	-0.419435	-2.062912

- **NMR calculation of compound 1**

Table S7. Cartesian coordinates for the low-energy reoptimized of **1a** and **1b** in the gas phase (Å) at B3LYP/6-31G (d,p) level

Center Number	Atomic Number	Atomic Type	Conformer 1	Coordinates (Angstroms)		
				X	Y	Z
1	1	0		2.242966	-0.450353	-2.868292
2	6	0		3.182111	-0.756876	-2.383076
3	6	0		4.289569	0.232113	-2.803588
4	1	0		4.701695	-0.074149	-3.772165
5	1	0		3.864845	1.230111	-2.956174
6	6	0		5.392072	0.311942	-1.7469
7	1	0		5.833694	-0.681858	-1.596818
8	1	0		6.202567	0.968862	-2.084558
9	6	0		4.820877	0.824018	-0.410644
10	1	0		5.606006	0.694008	0.346857
11	6	0		3.65758	-0.072414	0.017083
12	6	0		2.924773	-0.769679	-0.87515
13	6	0		1.80876	-1.707536	-0.460915
14	1	0		2.1576	-2.741461	-0.546836
15	1	0		0.973549	-1.613625	-1.165663
16	6	0		1.299415	-1.52533	0.991353
17	1	0		0.80864	-2.457179	1.284342
18	6	0		2.512713	-1.380758	1.940236
19	6	0		3.462838	-0.222308	1.524094
20	1	0		4.444783	-0.482245	1.947325
21	6	0		3.504298	-2.176089	-2.908851
22	1	0		2.709947	-2.894001	-2.689685
23	1	0		4.43191	-2.557914	-2.468052
24	1	0		3.633289	-2.1503	-3.995702
25	6	0		4.540632	2.379488	-0.482298
26	1	0		5.076947	2.732734	-1.374619
27	6	0		3.070575	2.786627	-0.66678
28	1	0		2.479157	2.542978	0.218016
29	1	0		2.603699	2.291475	-1.522716
30	1	0		3.002219	3.868446	-0.830706
31	6	0		5.152206	3.119352	0.718402
32	1	0		6.227598	2.921802	0.798326
33	1	0		4.673304	2.797236	1.646789
34	1	0		5.020826	4.203329	0.61841
35	8	0		3.121022	1.009312	2.162876
36	1	0		2.190585	1.169422	1.908882
37	6	0		-3.009226	-2.224844	-0.072261
38	1	0		-3.395391	-3.065184	0.520608
39	6	0		-1.603298	-1.93598	0.365453
40	1	0		-0.944696	-2.798546	0.366228
41	6	0		-1.158513	-0.706259	0.67213
42	6	0		-2.083439	0.481035	0.643604
43	1	0		-2.012065	1.012715	1.602798
44	1	0		-1.686722	1.201973	-0.083481
45	6	0		-3.537471	0.1821	0.352829
46	6	0		-3.967557	-1.059626	0.048325
47	6	0		-5.44237	-1.407835	-0.116705
48	1	0		-5.587061	-2.395395	0.345735
49	6	0		-6.307885	-0.395924	0.651821
50	1	0		-6.146449	-0.529895	1.72957
51	1	0		-7.370305	-0.591649	0.462883
52	6	0		-5.954028	1.03821	0.258244
53	1	0		-6.596713	1.743856	0.79441
54	1	0		-6.168498	1.180308	-0.806847
55	6	0		-4.477469	1.372814	0.549497

56	1	0		-4.404384	1.620291	1.622336
57	6	0		-3.99985	2.658248	-0.200072
58	1	0		-2.994625	2.888462	0.17344
59	6	0		-3.889673	2.474459	-1.721935
60	1	0		-3.255038	1.62176	-1.984308
61	1	0		-3.4571	3.368528	-2.183434
62	1	0		-4.869713	2.31262	-2.18364
63	6	0		-4.876108	3.873237	0.142987
64	1	0		-5.887374	3.775374	-0.265458
65	1	0		-4.441385	4.787408	-0.275198
66	1	0		-4.963275	4.009942	1.226784
67	6	0		-5.879567	-1.547054	-1.591292
68	1	0		-6.932721	-1.845042	-1.648782
69	1	0		-5.276058	-2.300278	-2.101123
70	1	0		-5.765691	-0.60371	-2.134912
71	8	0		-2.956995	-2.771356	-1.414583
72	1	0		-2.689163	-2.043615	-1.995684
73	6	0		0.255918	-0.415639	1.049808
74	8	0		0.537923	0.746003	1.363377
75	8	0		3.211557	-2.627604	1.742982
76	1	0		3.958221	-2.638454	2.358401
77	6	0		2.094898	-1.278136	3.410521
78	1	0		1.520809	-2.168198	3.685481
79	1	0		1.493362	-0.391179	3.612046
80	1	0		2.98148	-1.228399	4.052463

- **NMR Calculation of compound 2**

Table S8. Cartesian coordinates for the low-energy reoptimized of **2** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

Center Number	Atomic Number	Atomic Type	Conformer 2a	Coordinates (Angstroms)		
				X	Y	Z
1	1	0		1.113267	0.942125	0.200815
2	6	0		0.322128	1.570298	0.591433
3	6	0		-1.663298	3.141785	1.682127
4	6	0		3.25612	2.778093	-0.046006
5	6	0		-0.349754	1.155879	1.737229
6	6	0		-1.357778	1.940522	2.319106
7	6	0		-1.020941	3.571787	0.511466
8	1	0		-2.428983	3.775837	2.118666
9	6	0		0.81943	3.228431	-1.256702
10	1	0		1.740731	3.685706	-0.867282
11	6	0		0.086745	4.324504	-2.070271
12	1	0		-0.731938	3.857761	-2.627945
13	1	0		0.766227	4.796084	-2.784133
14	6	0		-0.464492	5.369971	-1.148036
15	6	0		-1.464015	4.912905	-0.081649
16	6	0		1.234006	2.088296	-2.200636
17	1	0		0.356985	1.54259	-2.564569
18	1	0		1.904399	1.37461	-1.715875
19	1	0		1.765762	2.495865	-3.065905
20	6	0		-2.937016	4.841773	-0.651712
21	1	0		-3.525896	4.648752	0.253923
22	6	0		-3.232465	3.702788	-1.637301
23	1	0		-4.316032	3.597272	-1.752744
24	1	0		-2.840099	2.742701	-1.291476
25	1	0		-2.827382	3.902301	-2.634841
26	6	0		-3.394394	6.192164	-1.22118
27	1	0		-3.220357	7.001381	-0.508464
28	1	0		-4.466024	6.160124	-1.441985
29	1	0		-2.874214	6.436845	-2.154119
30	8	0		-1.468778	5.895603	0.954309
31	1	0		-1.024334	6.669076	0.56028
32	8	0		-0.111321	6.542412	-1.170704
33	6	0		-2.060364	1.496705	3.576348
34	1	0		-2.852599	2.19908	3.845937
35	1	0		-1.364514	1.427238	4.419814

36	1	0		-2.505734	0.503894	3.453681
37	8	0		0	0	2.415522
38	1	0		-1.113267	-0.942125	0.200815
39	6	0		-0.322128	-1.570298	0.591433
40	6	0		1.663298	-3.141785	1.682127
41	6	0		0.349754	-1.155879	1.737229
42	6	0		0	-2.778093	-0.046006
43	6	0		1.020941	-3.571787	0.511466
44	6	0		1.357778	-1.940522	2.319106
45	1	0		2.428983	-3.775837	2.118666
46	6	0		-0.81943	-3.228431	-1.256702
47	1	0		-1.740731	-3.685706	-0.867282
48	6	0		-0.086745	-4.324504	-2.070271
49	1	0		0.731938	-3.857761	-2.627945
50	1	0		-0.766227	-4.796084	-2.784133
51	6	0		0.464492	-5.369971	-1.148036
52	6	0		1.464015	-4.912905	-0.081649
53	6	0		-1.234006	-2.088296	-2.200636
54	1	0		-1.904399	-1.37461	-1.715875
55	1	0		-1.765762	-2.495865	-3.065905
56	1	0		-0.356985	-1.54259	-2.564569
57	6	0		2.937016	-4.841773	-0.651712
58	1	0		3.525896	-4.648752	0.253923
59	6	0		3.394394	-6.192164	-1.22118
60	1	0		3.220357	-7.001381	-0.508464
61	1	0		4.466024	-6.160124	-1.441985
62	1	0		2.874214	-6.436845	-2.154119
63	6	0		3.232465	-3.702788	-1.637301
64	1	0		2.827382	-3.902301	-2.634841
65	1	0		4.316032	-3.597272	-1.752744
66	1	0		2.840099	-2.742701	-1.291476
67	8	0		1.468778	-5.895603	0.954309
68	1	0		1.024334	-6.669076	0.56028
69	8	0		0.111321	-6.542412	-1.170704
70	6	0		2.060364	-1.496705	3.576348
71	1	0		1.364514	-1.427238	4.419814
72	1	0		2.505734	-0.503894	3.453681
73	1	0		2.852599	-2.19908	3.845937

- **NMR Calculation of compound 3**

Table S9. Cartesian coordinates for the low-energy reoptimized of **3** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

Center Number	Atomic Number	Atomic Type	Conformer 3	Coordinates (Angstroms)		
				X	Y	Z
1	1	0		-0.365152	0.357286	0.228129
2	6	0		-1.29746	0.196412	0.222763
3	6	0		-3.632831	1.652599	0.296321
4	6	0		-2.51245	-0.483676	0.418304
5	6	0		-1.260854	1.575749	0.049037
6	6	0		-2.439747	2.34159	0.089985
7	6	0		-3.708133	0.25672	0.444923
8	1	0		-4.552005	2.230965	0.353124
9	6	0		-2.458913	-1.989618	0.688673
10	1	0		-1.868229	-2.104743	1.610086
11	6	0		-3.84374	-2.619235	0.951678
12	1	0		-3.714876	-3.5068	1.581901
13	1	0		-4.264025	-2.981764	0.005148
14	6	0		-4.82657	-1.639283	1.595863
15	1	0		-4.420675	-1.28763	2.553548
16	1	0		-5.770822	-2.14062	1.827087
17	6	0		-5.055522	-0.415756	0.684425
18	1	0		-5.694089	0.298175	1.224877
19	6	0		-1.725421	-2.76911	-0.418891
20	1	0		-0.695778	-2.427812	-0.557684
21	1	0		-2.247516	-2.662985	-1.37643
22	1	0		-1.690358	-3.835673	-0.170805
23	6	0		-5.812466	-0.7596	-0.641868

24	1	0		-5.155785	-1.397599	-1.248789
25	6	0		-7.115731	-1.533603	-0.380335
26	1	0		-7.771131	-0.97809	0.302198
27	1	0		-6.939368	-2.521044	0.054394
28	1	0		-7.664971	-1.682416	-1.316159
29	6	0		-6.124488	0.4934	-1.475292
30	1	0		-6.775652	1.182011	-0.922061
31	1	0		-6.646119	0.216403	-2.397763
32	1	0		-5.220231	1.039399	-1.754199
33	8	0		-0.091894	2.291791	-0.145358
34	1	0		1.542286	1.879006	1.829204
35	6	0		1.917201	1.492301	0.885251
36	6	0		2.840661	0.594962	-1.545311
37	6	0		1.124004	1.619172	-0.246412
38	6	0		3.187244	0.899899	0.823911
39	6	0		3.657459	0.418763	-0.413933
40	6	0		1.574815	1.182494	-1.500831
41	1	0		3.205817	0.271162	-2.515838
42	6	0		4.019001	0.830795	2.097662
43	1	0		3.865971	1.775441	2.636357
44	6	0		5.512812	0.716045	1.754085
45	1	0		6.094391	0.56473	2.671183
46	1	0		5.854845	1.66298	1.31543
47	6	0		5.771205	-0.423706	0.766976
48	1	0		6.846186	-0.519752	0.585057
49	1	0		5.453964	-1.369388	1.220938
50	6	0		5.047041	-0.212086	-0.57881
51	1	0		5.644273	0.519146	-1.146598
52	6	0		5.032324	-1.506783	-1.452019
53	1	0		4.59969	-1.230923	-2.421342
54	6	0		4.159106	-2.632063	-0.875097
55	1	0		4.560354	-3.017249	0.068635
56	1	0		4.113507	-3.473429	-1.57494
57	1	0		3.135024	-2.292976	-0.692156
58	6	0		6.454962	-2.011296	-1.7424
59	1	0		7.087789	-1.213658	-2.147858
60	1	0		6.429513	-2.823575	-2.476641
61	1	0		6.94166	-2.400424	-0.841903
62	6	0		3.538025	-0.297124	3.034082
63	1	0		2.483376	-0.163968	3.294726
64	1	0		4.11823	-0.298658	3.963507
65	1	0		3.639099	-1.282483	2.568694
66	6	0		-2.392895	3.839783	-0.068493
67	1	0		-1.758973	4.304422	0.695068
68	1	0		-3.394613	4.269725	0.010022
69	1	0		-1.972508	4.126924	-1.039031
70	6	0		0.733667	1.360792	-2.739477
71	1	0		1.283054	1.048151	-3.630755
72	1	0		0.433381	2.40591	-2.868538
73	1	0		-0.188205	0.770827	-2.68559