Supplementary Material

Polycyclic polyprenylated acylphloroglucinols from the fruit of *Hypericum addingtonii* N. Robson and their *α*-glucosidase inhibitory activity

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Figure S1. Key ROSEY correlations of 1, 5

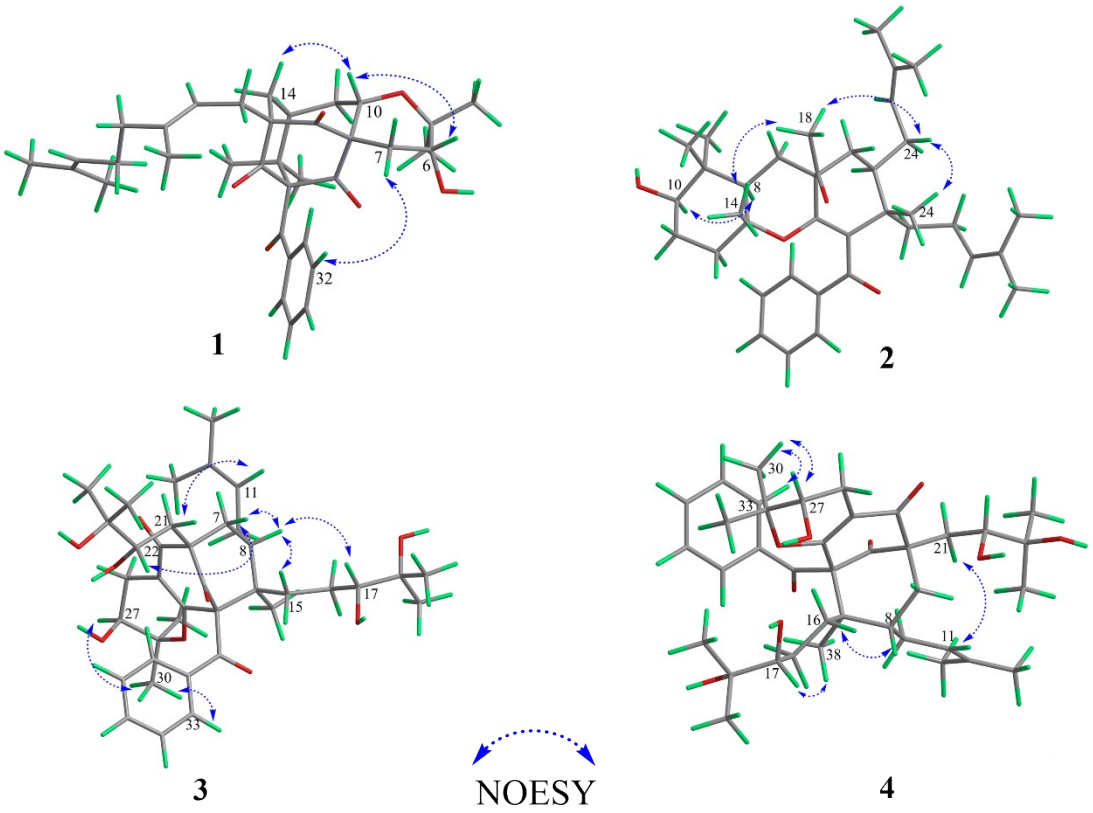

Figure S2. Experimental ECD spectra of 19

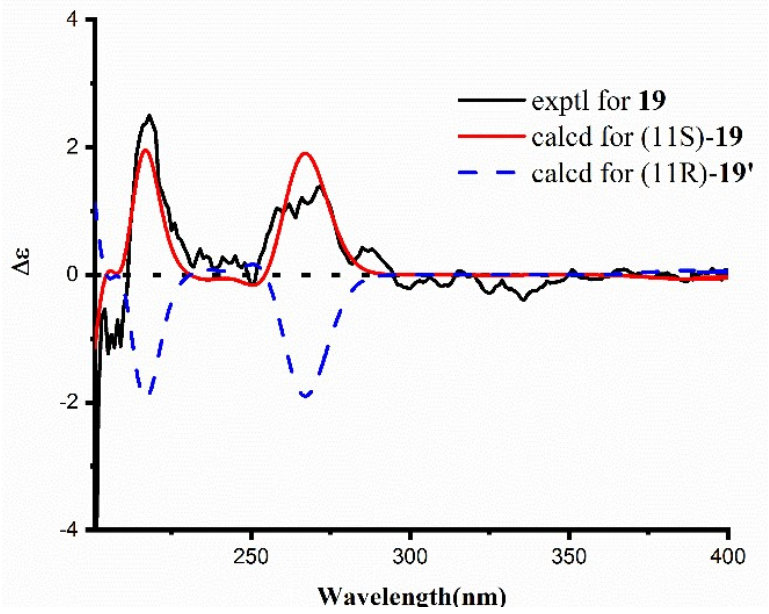

Figure S3. Regression analysis of calculated ^{13}C NMR chemical shifts of (1*S, 3*S**, 8*S**, 9*R**, 17*R**, 22*S**, 27*S**) vs experimental data of 3 and 4 at the PCM/mPW1PW91/6-311+G (d, p) level using DP4+ method.**

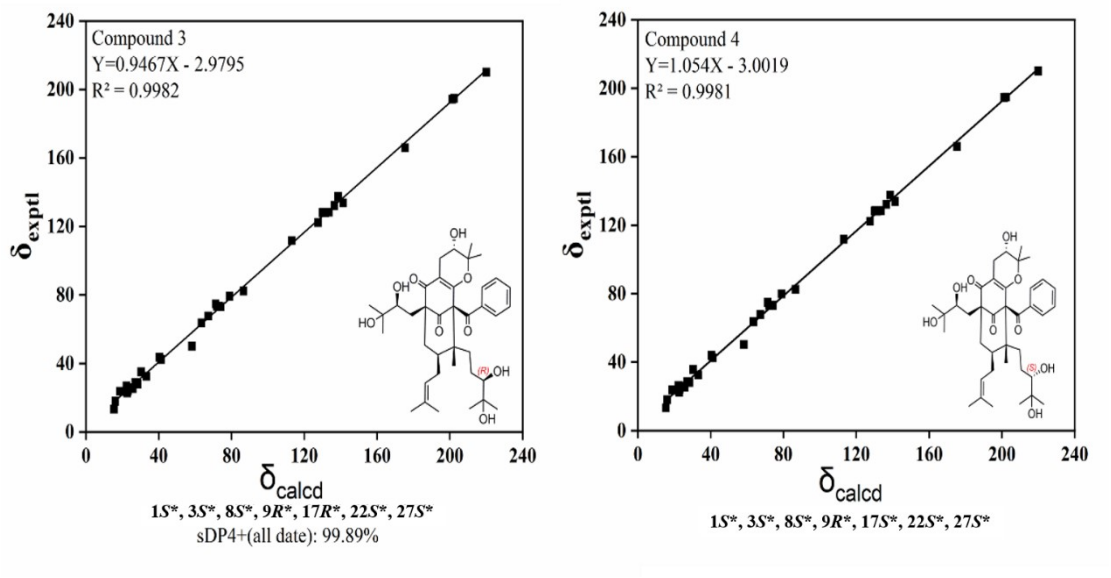

Figure S4. Inhibitory activities of active compounds. Each point indicates the average ± standard deviation of triplicate measurements

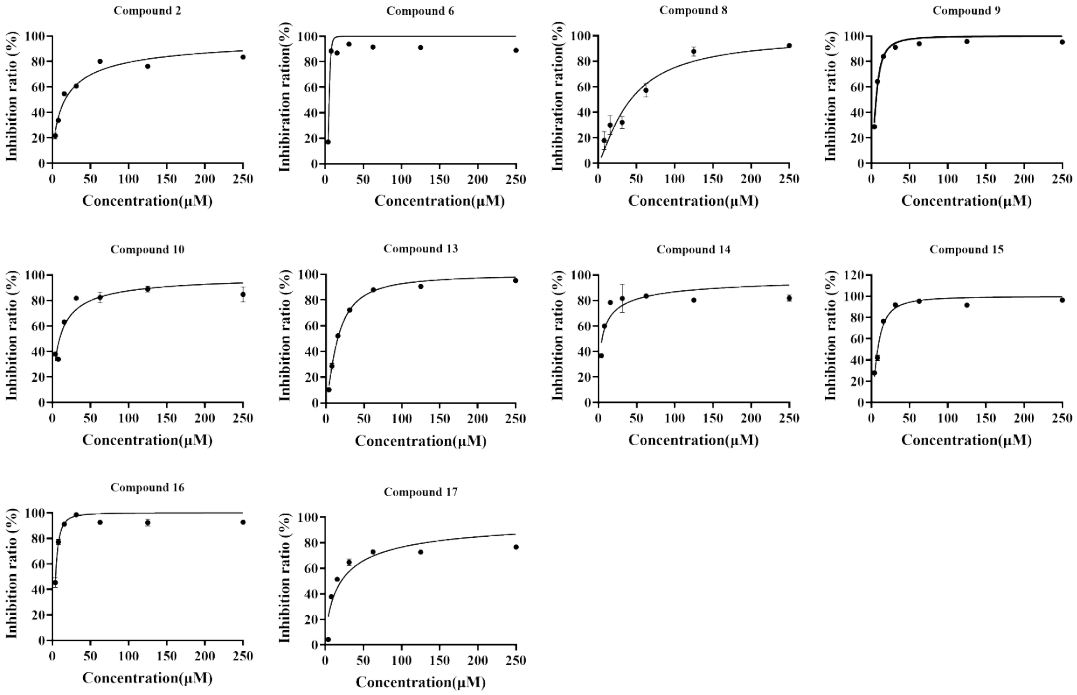

Table S1. Gibbs free energies and equilibrium populations of low-energy conformers of Compound 1 (1S，2R，4S，6R，7R，9R).

no	Conformational search		Calculation result	
	ΔE (kcal/mol)	Boltzman distribution	Extracted heat	Boltzman-calculated contribution
1-1	0.00	0.274	-1742.2498769	0.810709475
1-2	0.85	0.195	-1742.2478843	0.098238556
1-3	1.82	0.132	-1742.2477671	0.086770224
1-4	2.45	0.102	-1742.2449263	0.004281746

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 1(1S，2R，4S，6R，7R，9R) at B3LYP/6-31G(d) level of theory in Methanol.

Table S2. 1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.400344	-2.596656	2.899696
2	6	0	-3.696633	-1.925634	2.428496
3	6	0	-3.424115	-0.827739	1.391696
4	6	0	-2.642824	-1.369752	0.183496
5	6	0	-1.348436	-2.067073	0.686196
6	6	0	-1.553654	-3.202670	1.744796
7	8	0	-2.237504	-0.168058	-0.590004
8	6	0	-0.896402	-0.035481	-0.880304
9	6	0	-0.277722	-1.258191	-1.508704
10	6	0	-0.396842	-2.424789	-0.474904
11	6	0	-0.264983	1.107609	-0.563304
12	6	0	1.240121	1.340884	-0.818204
13	6	0	1.928598	-0.060427	-0.934004
14	6	0	1.193882	-0.979415	-1.920404
15	6	0	-1.079466	2.149422	0.183496
16	6	0	-1.840748	3.192935	-0.574304
17	6	0	-2.407331	4.257545	0.146296
18	6	0	-3.128714	5.248256	-0.511404
19	6	0	-3.302015	5.183559	-1.898104
20	6	0	-2.750433	4.125050	-2.621904
21	6	0	-2.019949	3.135738	-1.963604
22	8	0	-1.100366	2.147823	1.409496
23	6	0	3.438499	-0.004752	-1.286604

24	6	0	4.144277	-1.305064	-0.998604
25	6	0	4.839064	-2.093876	-1.833904
26	6	0	5.488843	-3.362686	-1.332504
27	6	0	1.863235	2.166774	0.351596
28	6	0	5.059068	-1.821379	-3.302304
29	6	0	-2.207176	-4.488959	1.196396
30	6	0	-0.178461	-3.594992	2.333996
31	6	0	-3.558737	-2.169036	-0.751804
32	1	0	-0.840922	-1.268281	1.248096
33	6	0	-0.984029	-1.642279	-2.842104
34	6	0	-1.528610	-0.530970	-3.720204
35	6	0	1.432135	2.185081	-2.103704
36	8	0	-1.048548	-2.804278	-3.197104
37	6	0	1.967023	1.479972	1.730896
38	6	0	2.288940	2.474467	2.814696
39	6	0	3.402742	2.584348	3.555396
40	6	0	3.531260	3.668146	4.600496
41	6	0	4.607727	1.680928	3.447496
42	8	0	-2.671362	-3.638651	3.839896
43	1	0	-1.776332	-1.822166	3.379996
44	1	0	-4.373746	-2.691123	2.031096
45	1	0	-4.207226	-1.486226	3.297296
46	1	0	-4.361707	-0.372823	1.049996
47	1	0	-2.828802	-0.025648	1.844096
48	1	0	0.595855	-2.627305	-0.061904
49	1	0	-0.707256	-3.326284	-1.009604
50	1	0	1.845890	-0.524526	0.057696
51	1	0	1.718767	-1.936524	-2.005604
52	1	0	1.228290	-0.525416	-2.919604
53	1	0	-2.266030	4.283242	1.221796
54	1	0	-3.558601	6.071964	0.052296
55	1	0	-3.867302	5.956769	-2.411904
56	1	0	-2.889834	4.069353	-3.698104
57	1	0	-1.596863	2.308831	-2.522804
58	1	0	3.916512	0.783640	-0.689404
59	1	0	3.564303	0.287845	-2.334404
60	1	0	4.072072	-1.628263	0.042396
61	1	0	5.304640	-3.523183	-0.265604
62	1	0	5.116228	-4.240780	-1.878404
63	1	0	6.576543	-3.339205	-1.489604
64	1	0	2.865540	2.494557	0.050096
65	1	0	1.284550	3.091883	0.462496
66	1	0	4.567784	-0.911371	-3.654204
67	1	0	6.132070	-1.728697	-3.521404

68	1	0	4.690855	-2.659373	-3.910104
69	1	0	-2.203389	-5.259559	1.971696
70	1	0	-1.649782	-4.872968	0.335596
71	1	0	-3.244473	-4.349342	0.885796
72	1	0	0.396754	-2.709502	2.633396
73	1	0	-0.324571	-4.219890	3.219396
74	1	0	0.422530	-4.162802	1.615996
75	1	0	-4.227126	-1.464225	-1.257804
76	1	0	-3.007647	-2.726746	-1.511904
77	1	0	-4.183049	-2.877626	-0.202804
78	1	0	-1.831717	-0.948665	-4.682304
79	1	0	-2.393703	-0.076256	-3.224604
80	1	0	-0.790497	0.263118	-3.876404
81	1	0	1.031827	1.684087	-2.991504
82	1	0	0.919551	3.148389	-2.012104
83	1	0	2.492838	2.392963	-2.283104
84	1	0	1.003415	1.011888	1.964796
85	1	0	2.716310	0.682760	1.696596
86	1	0	1.492752	3.198580	2.996496
87	1	0	4.393770	4.318332	4.394696
88	1	0	3.698952	3.239343	5.598996
89	1	0	2.636670	4.297061	4.648696
90	1	0	4.503314	0.906730	2.683596
91	1	0	4.805918	1.180725	4.405996
92	1	0	5.509536	2.263913	3.212396
93	1	0	-3.137955	-3.239243	4.589996

Table S3. 1-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.044291	-1.932816	3.012802
2	6	0	-4.094697	-0.921122	2.540302
3	6	0	-3.505703	0.073681	1.533002
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6	6	0	-2.378286	-2.732812	1.857002
7	8	0	-2.146805	0.411390	-0.399198
8	6	0	-0.832004	0.178198	-0.726998
9	6	0	-0.567896	-1.167101	-1.358398
10	6	0	-1.035089	-2.276204	-0.350898
11	6	0	0.068590	1.145303	-0.496198
12	6	0	1.563991	0.994912	-0.831798

13	6	0	1.893801	-0.535186	-0.847498
14	6	0	0.932905	-1.317692	-1.754098
15	6	0	-0.447517	2.422200	0.140602
16	6	0	-1.136123	3.441596	-0.714198
17	6	0	-1.385731	4.707494	-0.157298
18	6	0	-2.018937	5.694090	-0.905398
19	6	0	-2.420735	5.423588	-2.217798
20	6	0	-2.186728	4.165089	-2.774498
21	6	0	-1.542922	3.175293	-2.031098
22	8	0	-0.276118	2.634101	1.336602
23	6	0	3.358703	-0.865077	-1.240198
24	6	0	3.740911	-2.288675	-0.927198
25	6	0	4.205817	-3.240872	-1.752098
26	6	0	4.555225	-4.613670	-1.225798
27	6	0	2.443387	1.734117	0.222402
28	6	0	4.442116	-3.064971	-3.232698
29	6	0	-3.356080	-3.777618	1.278002
30	6	0	-1.178581	-3.502404	2.458102
31	6	0	-3.962896	-1.129521	-0.645998
32	1	0	-1.129096	-1.077604	1.394802
33	6	0	-1.305095	-1.231205	-2.724098
34	6	0	-1.470387	-2.595806	-3.384198
35	6	0	1.841887	1.666114	-2.201598
36	8	0	-1.661701	-0.225007	-3.306398
37	6	0	2.464990	1.154417	1.653602
38	6	0	3.057185	2.134521	2.631202
39	6	0	4.219985	2.063628	3.297502
40	6	0	4.640878	3.170831	4.235902
41	6	0	5.204892	0.923234	3.200702
42	8	0	-3.606885	-2.875019	3.928502
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45	1	0	-4.479100	-0.373024	3.412202
46	1	0	-4.269407	0.780377	1.187502
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49	1	0	-1.609084	-3.047907	-0.872498
50	1	0	1.741103	-0.893987	0.179202
51	1	0	1.204012	-2.379090	-1.741498
52	1	0	1.080303	-0.977291	-2.787198
53	1	0	-1.071632	4.891296	0.865102
54	1	0	-2.202343	6.673089	-0.470198
55	1	0	-2.917840	6.193285	-2.802998
56	1	0	-2.508326	3.949787	-3.789898

57	1	0	-1.384816	2.192494	-2.462898
58	1	0	4.033199	-0.200973	-0.683398
59	1	0	3.513701	-0.638176	-2.299998
60	1	0	3.626313	-2.558476	0.125402
61	1	0	4.370126	-4.699771	-0.150398
62	1	0	3.973230	-5.394573	-1.735598
63	1	0	5.613427	-4.849164	-1.407898
64	1	0	3.473087	1.780924	-0.153098
65	1	0	2.111181	2.776815	0.273602
66	1	0	4.165710	-2.075072	-3.602698
67	1	0	5.500817	-3.229464	-3.477698
68	1	0	3.874020	-3.810174	-3.806898
69	1	0	-3.593875	-4.517419	2.046602
70	1	0	-2.907077	-4.307715	0.431002
71	1	0	-4.301482	-3.348523	0.939702
72	1	0	-0.386986	-2.816600	2.785902
73	1	0	-1.509778	-4.078006	3.326802
74	1	0	-0.742477	-4.202602	1.737702
75	1	0	-4.383201	-0.257424	-1.155298
76	1	0	-3.571992	-1.804719	-1.411398
77	1	0	-4.774893	-1.646526	-0.129398
78	1	0	-1.547988	-2.453007	-4.464198
79	1	0	-0.645483	-3.276401	-3.151698
80	1	0	-2.396484	-3.072812	-3.040598
81	1	0	1.246390	1.222310	-3.005298
82	1	0	1.583681	2.729712	-2.159698
83	1	0	2.901488	1.595220	-2.473098
84	1	0	1.433492	0.942411	1.958602
85	1	0	3.011996	0.205821	1.668302
86	1	0	2.439879	3.020417	2.789002
87	1	0	5.601876	3.608636	3.929202
88	1	0	4.786081	2.792531	5.258202
89	1	0	3.899473	3.975126	4.275302
90	1	0	4.887297	0.134432	2.514402
91	1	0	5.368895	0.464335	4.186202
92	1	0	6.186290	1.285740	2.863102
93	1	0	-3.955388	-2.375321	4.682702

Table S4. 1-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911833	-2.918376	2.829505

2	6	0	-3.235825	-2.148362	2.752905
3	6	0	-3.132312	-0.928763	1.827005
4	6	0	-2.669617	-1.325468	0.416005
5	6	0	-1.341625	-2.124982	0.521205
6	6	0	-1.379038	-3.388082	1.446705
7	8	0	-2.371103	-0.041471	-0.269995
8	6	0	-1.120102	0.086116	-0.834395
9	6	0	-0.732014	-1.054388	-1.736895
10	6	0	-0.691427	-2.348289	-0.861295
11	6	0	-0.360990	1.149708	-0.522495
12	6	0	1.066612	1.366093	-1.070195
13	6	0	1.629297	-0.019913	-1.543995
14	6	0	0.624189	-0.765403	-2.436995
15	6	0	-0.931080	2.105614	0.512405
16	6	0	-1.768468	3.269323	0.078805
17	6	0	-2.103458	4.240826	1.036805
18	6	0	-2.882946	5.337634	0.684905
19	6	0	-3.347245	5.473639	-0.627795
20	6	0	-3.027755	4.508936	-1.584695
21	6	0	-2.238967	3.413328	-1.233995
22	8	0	-0.695082	1.933411	1.703205
23	6	0	3.009798	0.079772	-2.253795
24	6	0	3.674484	-1.253635	-2.489795
25	6	0	4.797579	-1.738447	-1.935495
26	6	0	5.310165	-3.109452	-2.311195
27	6	0	1.971718	1.976583	0.046805
28	6	0	5.654087	-1.013556	-0.926695
29	6	0	-2.214951	-4.565773	0.902005
30	6	0	0.065056	-3.901097	1.655505
31	6	0	-3.815023	-1.960156	-0.382895
32	1	0	-0.675218	-1.426889	1.050505
33	6	0	-1.736116	-1.226378	-2.915195
34	6	0	-2.386602	0.014429	-3.498095
35	6	0	1.030623	2.399893	-2.224695
36	8	0	-1.948927	-2.324976	-3.392695
37	6	0	2.287909	1.088780	1.272105
38	6	0	2.772318	1.916275	2.433805
39	6	0	3.969818	1.913262	3.039505
40	6	0	4.248927	2.841459	4.199105
41	6	0	5.129308	1.023050	2.664205
42	8	0	-2.033246	-4.069875	3.668005
43	1	0	-1.150426	-2.237884	3.250105
44	1	0	-4.030233	-2.830854	2.428105
45	1	0	-3.513222	-1.814659	3.763105

46	1	0	-4.092807	-0.402853	1.765905
47	1	0	-2.404505	-0.214471	2.229905
48	1	0	0.353770	-2.634900	-0.711995
49	1	0	-1.165836	-3.157284	-1.423195
50	1	0	1.774891	-0.625015	-0.640595
51	1	0	1.037279	-1.723207	-2.767695
52	1	0	0.461196	-0.176401	-3.349595
53	1	0	-1.738659	4.110922	2.050405
54	1	0	-3.132338	6.088237	1.430105
55	1	0	-3.957936	6.329846	-0.902395
56	1	0	-3.393054	4.609240	-2.603095
57	1	0	-1.994875	2.659625	-1.974095
58	1	0	3.667505	0.732965	-1.674095
59	1	0	2.869803	0.573174	-3.226595
60	1	0	3.176977	-1.895530	-3.217195
61	1	0	4.664259	-3.601345	-3.045195
62	1	0	6.323265	-3.051363	-2.733895
63	1	0	5.380358	-3.761153	-1.428795
64	1	0	2.916922	2.300573	-0.405695
65	1	0	1.496828	2.900988	0.397205
66	1	0	6.680088	-0.897867	-1.302995
67	1	0	5.279597	-0.020152	-0.670195
68	1	0	5.731481	-1.593857	0.003405
69	1	0	-2.087760	-5.434974	1.552605
70	1	0	-1.885954	-4.845576	-0.104195
71	1	0	-3.284849	-4.352861	0.854705
72	1	0	0.745665	-3.084104	1.927005
73	1	0	0.078048	-4.636797	2.464405
74	1	0	0.457451	-4.383801	0.754405
75	1	0	-3.477528	-2.429959	-1.309095
76	1	0	-4.349131	-2.714050	0.199805
77	1	0	-4.531115	-1.171248	-0.636495
78	1	0	-1.652994	0.803721	-3.694095
79	1	0	-2.903105	-0.250065	-4.422895
80	1	0	-3.105798	0.413237	-2.773795
81	1	0	0.438019	2.047599	-3.075695
82	1	0	0.587233	3.341098	-1.884495
83	1	0	2.039125	2.625382	-2.587495
84	1	0	1.370803	0.572489	1.580105
85	1	0	3.017401	0.319072	1.000505
86	1	0	2.020925	2.611083	2.813005
87	1	0	5.100134	3.502950	3.982305
88	1	0	4.518421	2.277656	5.103805
89	1	0	3.384034	3.468868	4.436905

90	1	0	4.906701	0.351152	1.832305
91	1	0	5.437702	0.405447	3.519705
92	1	0	6.007315	1.623440	2.386105
93	1	0	-2.295942	-3.761572	4.548805

Table S5. 1-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.228834	4.209697	1.195099
2	6	0	2.689831	3.891483	0.853699
3	6	0	2.882117	2.412881	0.490199
4	6	0	1.962114	1.988390	-0.666401
5	6	0	0.493317	2.335204	-0.298601
6	6	0	0.226731	3.836206	0.066699
7	8	0	2.079500	0.512789	-0.729001
8	6	0	0.912393	-0.220600	-0.712701
9	6	0	-0.136403	0.254109	-1.683901
10	6	0	-0.518289	1.717013	-1.287901
11	6	0	0.800984	-1.245299	0.149999
12	6	0	-0.452825	-2.141088	0.247999
13	6	0	-1.668717	-1.331976	-0.314801
14	6	0	-1.358111	-0.706179	-1.684401
15	6	0	1.950082	-1.426010	1.126999
16	6	0	3.120074	-2.288321	0.764399
17	6	0	4.070471	-2.573630	1.758799
18	6	0	5.176664	-3.365540	1.469099
19	6	0	5.352759	-3.876641	0.178899
20	6	0	4.418262	-3.592233	-0.818201
21	6	0	3.305269	-2.803822	-0.526101
22	8	0	1.912787	-0.873210	2.220499
23	6	0	-2.983625	-2.150064	-0.418801
24	6	0	-4.196917	-1.272853	-0.588601
25	6	0	-5.095017	-1.254845	-1.586401
26	6	0	-6.261908	-0.295134	-1.554701
27	6	0	-0.688429	-2.575685	1.730499
28	6	0	-5.063125	-2.151445	-2.800801
29	6	0	0.334540	4.821905	-1.116301
30	6	0	-1.200268	3.967819	0.647399
31	6	0	2.496218	2.505785	-2.009001
32	1	0	0.343612	1.796705	0.649899
33	6	0	0.372897	0.211105	-3.155901
34	6	0	1.347287	-0.881604	-3.555701

35	6	0	-0.216237	-3.450490	-0.549201
36	8	0	-0.046896	1.002309	-3.979501
37	6	0	-1.080119	-1.498082	2.772599
38	6	0	-2.566617	-1.351468	2.992399
39	6	0	-3.272707	-0.240961	3.259899
40	6	0	-4.760008	-0.311048	3.517999
41	6	0	-2.683094	1.144233	3.363699
42	8	0	1.059847	5.597698	1.491799
43	1	0	0.951229	3.609199	2.079699
44	1	0	3.019137	4.547480	0.039199
45	1	0	3.320633	4.137977	1.719799
46	1	0	3.926316	2.210272	0.223199
47	1	0	2.648212	1.780484	1.355099
48	1	0	-1.502789	1.703222	-0.810901
49	1	0	-0.618284	2.302014	-2.206101
50	1	0	-1.849310	-0.514775	0.395399
51	1	0	-2.231506	-0.155971	-2.049001
52	1	0	-1.195219	-1.517981	-2.406201
53	1	0	3.917275	-2.160928	2.750599
54	1	0	5.904662	-3.586347	2.245199
55	1	0	6.218153	-4.494150	-0.047601
56	1	0	4.556658	-3.982734	-1.822701
57	1	0	2.581971	-2.575616	-1.300901
58	1	0	-3.113730	-2.733663	0.501199
59	1	0	-2.902932	-2.875065	-1.235801
60	1	0	-4.346910	-0.568152	0.231399
61	1	0	-6.249202	0.335566	-0.660101
62	1	0	-6.258402	0.362966	-2.435201
63	1	0	-7.219413	-0.834925	-1.576001
64	1	0	-1.451336	-3.364578	1.733999
65	1	0	0.229067	-3.069994	2.069299
66	1	0	-5.028619	-1.553545	-3.722201
67	1	0	-4.211331	-2.835053	-2.813901
68	1	0	-5.978830	-2.756436	-2.859401
69	1	0	-0.005451	5.810908	-0.798101
70	1	0	-0.295763	4.500811	-1.952001
71	1	0	1.352341	4.938896	-1.492801
72	1	0	-1.391175	3.212021	1.419299
73	1	0	-1.320759	4.954920	1.102399
74	1	0	-1.964269	3.858826	-0.129401
75	1	0	3.390813	1.928077	-2.264801
76	1	0	1.775117	2.404492	-2.822701
77	1	0	2.789128	3.556282	-1.951701
78	1	0	1.011578	-1.867801	-3.218501

79	1	0	1.462787	-0.880705	-4.641401
80	1	0	2.315589	-0.689313	-3.080001
81	1	0	-0.052335	-3.261591	-1.615101
82	1	0	0.665658	-3.977098	-0.170101
83	1	0	-1.069943	-4.130782	-0.455701
84	1	0	-0.627022	-1.801086	3.728599
85	1	0	-0.602010	-0.546686	2.526799
86	1	0	-3.118326	-2.294463	2.983999
87	1	0	-5.317802	0.316157	2.807799
88	1	0	-5.005804	0.065655	4.521199
89	1	0	-5.140917	-1.334044	3.437599
90	1	0	-1.618394	1.175423	3.120599
91	1	0	-2.801691	1.539034	4.382899
92	1	0	-3.207288	1.845138	2.699299
93	1	0	1.644349	5.809393	2.235799

Table S6. Gibbs free energies and equilibrium populations of low-energy conformers of Compound 2 (1R, 3R, 5R, 7S, 9S, and 11R).

no	Conformational search		Calculation result	
	ΔE (kcal/mol)	Boltzman distribution	Extracted heat	Boltzman-calculated contribution
1-1	0.00	0.429	-1811.6486045	0.300698471
1-2	2.91	0.133	-1811.6483976	0.241523026
1-3	3.05	0.125	-1811.6479941	0.157525591
1-4	3.44	0.107	-1811.6486031	0.300252913

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 2 (1R, 3R, 5R, 7S, 9S, and 11R) at B3LYP/6-31+G(d, p) level of theory in Methanol.

Table S7. 2-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.840761	-0.659369	-2.302224
2	6	0	-6.165149	-1.003607	-2.027231
3	6	0	-6.503005	-1.512439	-0.770872
4	6	0	-5.521431	-1.675297	0.201545
5	6	0	-4.186231	-1.326593	-0.059584

6	6	0	-3.860338	-0.817042	-1.324740
7	6	0	-3.202179	-1.542557	1.056513
8	6	0	-1.743094	-0.998958	0.916673
9	6	0	-1.014543	-1.780492	-0.179295
10	6	0	0.326757	-1.174425	-0.619588
11	6	0	-0.040501	0.215346	-1.164356
12	6	0	-0.739076	1.198649	-0.222520
13	6	0	-1.820191	0.515225	0.631962
14	8	0	-1.439721	-2.830182	-0.617651
15	8	0	0.207544	0.529115	-2.315727
16	6	0	-0.833235	-1.189444	2.231072
17	6	0	0.407567	1.781426	0.726487
18	6	0	0.573749	-0.548768	1.945641
19	6	0	0.651057	0.996733	2.019083
20	6	0	-0.628904	-2.694800	2.535518
21	6	0	-1.484606	-0.557433	3.480104
22	8	0	-3.552853	-2.137075	2.059492
23	8	0	-2.725683	1.161102	1.123628
24	6	0	0.989842	-2.052508	-1.710677
25	6	0	2.373316	-1.610805	-2.112598
26	6	0	3.542219	-2.239020	-1.901797
27	6	0	4.829352	-1.636685	-2.431704
28	6	0	5.869918	-1.247573	-1.350951
29	6	0	5.393862	-0.157003	-0.428290
30	6	0	5.474561	-0.090801	0.910501
31	6	0	4.980634	1.127466	1.656210
32	6	0	6.069005	-1.160108	1.795374
33	6	0	3.698301	-3.554445	-1.176135
34	6	0	1.229797	-1.106916	0.662359
35	6	0	-1.348702	2.389805	-1.000279
36	6	0	-0.323061	3.499759	-1.249462
37	6	0	0.144424	4.120281	0.093540
38	8	0	0.095383	3.093395	1.122608
39	6	0	1.573771	4.660781	-0.020480
40	6	0	-0.810765	5.203812	0.596407
41	8	0	-0.862532	4.549632	-2.048372
42	1	0	-4.568454	-0.270210	-3.279188
43	1	0	-6.929502	-0.877173	-2.789289
44	1	0	-7.532091	-1.782460	-0.550437
45	1	0	-5.765698	-2.072859	1.180454
46	1	0	-2.838716	-0.553180	-1.577615
47	1	0	1.326975	1.780330	0.121028
48	1	0	1.197481	-0.901709	2.777153
49	1	0	-0.046935	1.384593	2.764538

50	1	0	1.650473	1.278094	2.370704
51	1	0	-0.125695	-3.241092	1.733607
52	1	0	-1.587746	-3.179330	2.719254
53	1	0	-0.015350	-2.790019	3.439272
54	1	0	-1.872220	0.447936	3.305953
55	1	0	-0.739235	-0.503205	4.283350
56	1	0	-2.315345	-1.173619	3.823826
57	1	0	0.338701	-2.035347	-2.591998
58	1	0	0.980503	-3.082202	-1.345311
59	1	0	2.399532	-0.670031	-2.659071
60	1	0	4.595093	-0.748444	-3.031874
61	1	0	5.310066	-2.355265	-3.113006
62	1	0	6.178828	-2.137631	-0.793202
63	1	0	6.770810	-0.898520	-1.879236
64	1	0	4.951645	0.699363	-0.942438
65	1	0	4.550130	1.875077	0.981940
66	1	0	4.218005	0.857564	2.401189
67	1	0	5.796675	1.607689	2.214751
68	1	0	6.388121	-2.049055	1.246571
69	1	0	5.348173	-1.476494	2.562127
70	1	0	6.943436	-0.772088	2.336553
71	1	0	2.743640	-4.030026	-0.939521
72	1	0	4.282838	-4.262123	-1.779784
73	1	0	4.245061	-3.424503	-0.232533
74	1	0	1.554561	-2.136173	0.843614
75	1	0	2.143546	-0.552498	0.424268
76	1	0	-2.186026	2.788633	-0.424779
77	1	0	-1.732517	2.034469	-1.962505
78	1	0	0.546265	3.066519	-1.764272
79	1	0	1.626640	5.406757	-0.820745
80	1	0	1.885442	5.128644	0.918824
81	1	0	2.285703	3.861449	-0.259341
82	1	0	-1.835842	4.828160	0.658036
83	1	0	-0.499915	5.513129	1.599563
84	1	0	-0.797085	6.071129	-0.066711
85	1	0	-1.021209	4.184641	-2.932802

Table S8. 2-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.826783	-0.715509	-2.299733
2	6	0	-6.147393	-1.073721	-2.024214

3	6	0	-6.481519	-1.576403	-0.764327
4	6	0	-5.500004	-1.719234	0.211295
5	6	0	-4.168536	-1.356821	-0.050390
6	6	0	-3.846460	-0.853717	-1.319178
7	6	0	-3.184179	-1.551336	1.069326
8	6	0	-1.728525	-0.999723	0.922693
9	6	0	-0.996080	-1.788032	-0.166614
10	6	0	0.340936	-1.180230	-0.614042
11	6	0	-0.025497	0.206363	-1.168516
12	6	0	-0.741082	1.192224	-0.239557
13	6	0	-1.816638	0.509493	0.622210
14	8	0	-1.416765	-2.844866	-0.591974
15	8	0	0.242298	0.520134	-2.314108
16	6	0	-0.815634	-1.171184	2.237475
17	6	0	0.395431	1.795343	0.704928
18	6	0	0.588420	-0.527811	1.942581
19	6	0	0.660156	1.018315	1.999022
20	6	0	-0.604167	-2.672043	2.558492
21	6	0	-1.467828	-0.527936	3.480235
22	8	0	-3.531400	-2.134486	2.080165
23	8	0	-2.727068	1.154831	1.106742
24	6	0	1.006030	-2.064966	-1.698917
25	6	0	2.390567	-1.627993	-2.102552
26	6	0	3.558503	-2.254348	-1.880966
27	6	0	4.847250	-1.659832	-2.415748
28	6	0	5.882184	-1.250200	-1.337203
29	6	0	5.403194	-0.138546	-0.441699
30	6	0	5.479632	-0.041162	0.895420
31	6	0	4.984534	1.194913	1.610538
32	6	0	6.070390	-1.089785	1.807166
33	6	0	3.712320	-3.560488	-1.138060
34	6	0	1.245745	-1.097460	0.665548
35	6	0	-1.366396	2.364201	-1.035740
36	6	0	-0.381783	3.511297	-1.278942
37	6	0	0.094200	4.126512	0.072872
38	8	0	0.060918	3.102233	1.103734
39	6	0	1.514094	4.687194	-0.053093
40	6	0	-0.867834	5.198825	0.589896
41	8	0	-0.921719	4.495717	-2.154316
42	1	0	-4.556977	-0.330910	-3.279148
43	1	0	-6.911674	-0.963197	-2.788818
44	1	0	-7.507606	-1.857545	-0.543745
45	1	0	-5.741302	-2.111775	1.192975
46	1	0	-2.827722	-0.579570	-1.572900

47	1	0	1.311179	1.813549	0.094458
48	1	0	1.214484	-0.867841	2.777779
49	1	0	-0.029132	1.409049	2.751109
50	1	0	1.662988	1.306048	2.335475
51	1	0	-0.100365	-3.225216	1.761745
52	1	0	-1.560502	-3.158592	2.749739
53	1	0	0.011705	-2.754261	3.461946
54	1	0	-1.857129	0.475060	3.296201
55	1	0	-0.722490	-0.464453	4.282849
56	1	0	-2.297469	-1.142188	3.830019
57	1	0	0.356219	-2.052973	-2.581349
58	1	0	0.995273	-3.092247	-1.326832
59	1	0	2.418291	-0.694525	-2.661096
60	1	0	4.614751	-0.782654	-3.032545
61	1	0	5.331886	-2.389852	-3.081865
62	1	0	6.185251	-2.128563	-0.758077
63	1	0	6.787244	-0.914668	-1.867129
64	1	0	4.963439	0.705893	-0.977184
65	1	0	4.555335	1.925665	0.917244
66	1	0	4.220713	0.943164	2.360680
67	1	0	5.799628	1.688766	2.158521
68	1	0	6.388502	-1.992568	1.280777
69	1	0	5.347587	-1.385778	2.580181
70	1	0	6.944791	-0.690570	2.340232
71	1	0	4.255682	-3.418881	-0.194110
72	1	0	2.756957	-4.033491	-0.898945
73	1	0	4.299241	-4.275465	-1.730682
74	1	0	1.574661	-2.123475	0.857320
75	1	0	2.157003	-0.541807	0.420507
76	1	0	-2.225811	2.729997	-0.465690
77	1	0	-1.719805	2.005880	-2.006149
78	1	0	0.483453	3.123066	-1.824636
79	1	0	1.550587	5.430420	-0.856973
80	1	0	1.830831	5.160793	0.881855
81	1	0	2.232888	3.896354	-0.298768
82	1	0	-1.892398	4.815769	0.659101
83	1	0	-0.563631	5.499013	1.597132
84	1	0	-0.853423	6.082460	-0.054039
85	1	0	-1.776739	4.776418	-1.790353

Table S9. 2-3

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

1	6	0	-4.833647	-0.685505	-2.295295
2	6	0	-6.152318	-1.053534	-2.023734
3	6	0	-6.483317	-1.574923	-0.770616
4	6	0	-5.500647	-1.726056	0.202490
5	6	0	-4.171037	-1.353942	-0.055234
6	6	0	-3.852091	-0.832698	-1.317388
7	6	0	-3.185230	-1.557614	1.061044
8	6	0	-1.729888	-1.004125	0.917643
9	6	0	-0.997460	-1.784869	-0.176343
10	6	0	0.340538	-1.174284	-0.618010
11	6	0	-0.025349	0.215272	-1.165527
12	6	0	-0.743030	1.196086	-0.232949
13	6	0	-1.817429	0.507909	0.627175
14	8	0	-1.418214	-2.837672	-0.611682
15	8	0	0.247528	0.535202	-2.308622
16	6	0	-0.817848	-1.183388	2.231777
17	6	0	0.393709	1.792618	0.715308
18	6	0	0.584915	-0.535251	1.942482
19	6	0	0.652616	1.011031	2.007671
20	6	0	-0.603529	-2.686107	2.542343
21	6	0	-1.471632	-0.550315	3.478977
22	8	0	-3.529915	-2.151034	2.066907
23	8	0	-2.724246	1.150199	1.121004
24	6	0	1.007086	-2.053606	-1.706342
25	6	0	2.392250	-1.615508	-2.106439
26	6	0	3.559630	-2.244298	-1.888864
27	6	0	4.848909	-1.647808	-2.420246
28	6	0	5.884449	-1.244926	-1.339709
29	6	0	5.406130	-0.138503	-0.437418
30	6	0	5.481020	-0.049782	0.900359
31	6	0	4.985285	1.181651	1.622964
32	6	0	6.069650	-1.104812	1.806008
33	6	0	3.712257	-3.555165	-1.154148
34	6	0	1.244182	-1.096820	0.662762
35	6	0	-1.370575	2.370304	-1.021919
36	6	0	-0.377727	3.503288	-1.265651
37	6	0	0.083670	4.125864	0.088355
38	8	0	0.063828	3.099890	1.117269
39	6	0	1.505163	4.693671	-0.017320
40	6	0	-0.894093	5.186298	0.595794
41	8	0	-1.029026	4.453828	-2.106110
42	1	0	-4.566658	-0.284521	-3.268826
43	1	0	-6.917799	-0.935244	-2.785966

44	1	0	-7.508049	-1.863377	-0.553157
45	1	0	-5.739532	-2.132237	1.179192
46	1	0	-2.835053	-0.549043	-1.567436
47	1	0	1.311785	1.808176	0.107732
48	1	0	1.210986	-0.878658	2.776310
49	1	0	-0.042467	1.396508	2.757104
50	1	0	1.652696	1.299718	2.351627
51	1	0	-0.099296	-3.232948	1.741463
52	1	0	-1.559071	-3.175384	2.730487
53	1	0	0.012939	-2.773772	3.444914
54	1	0	-1.864197	0.452544	3.301502
55	1	0	-0.726212	-0.489908	4.281804
56	1	0	-2.299323	-1.169333	3.824939
57	1	0	0.358397	-2.037043	-2.589517
58	1	0	0.995541	-3.082812	-1.339641
59	1	0	2.420959	-0.678445	-2.658905
60	1	0	4.617004	-0.766948	-3.032116
61	1	0	5.333026	-2.374296	-3.090612
62	1	0	6.187289	-2.126842	-0.765930
63	1	0	6.789579	-0.906752	-1.867900
64	1	0	4.967186	0.709603	-0.967852
65	1	0	4.558713	1.917758	0.933662
66	1	0	4.218866	0.925435	2.368860
67	1	0	5.799302	1.670645	2.176879
68	1	0	6.389133	-2.003697	1.273858
69	1	0	5.344904	-1.406480	2.574965
70	1	0	6.942654	-0.709346	2.344118
71	1	0	4.257728	-3.420367	-0.210411
72	1	0	2.756335	-4.027407	-0.915932
73	1	0	4.296443	-4.267920	-1.752171
74	1	0	1.574715	-2.123263	0.849470
75	1	0	2.154793	-0.538448	0.421428
76	1	0	-2.223174	2.749191	-0.454869
77	1	0	-1.731061	2.017811	-1.991411
78	1	0	0.496014	3.095100	-1.793030
79	1	0	1.557908	5.469027	-0.792308
80	1	0	1.812907	5.142432	0.932346
81	1	0	2.229281	3.913507	-0.280861
82	1	0	-1.911526	4.789344	0.644518
83	1	0	-0.596881	5.494414	1.603395
84	1	0	-0.899684	6.063827	-0.055195
85	1	0	-0.354423	5.055245	-2.456659

Table S10. 2-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.774742	-0.457048	-2.509019
2	6	0	-6.136516	-0.698633	-2.320619
3	6	0	-6.599626	-1.123451	-1.073021
4	6	0	-5.705206	-1.304846	-0.022931
5	6	0	-4.333368	-1.059047	-0.196904
6	6	0	-3.881448	-0.633583	-1.454375
7	6	0	-3.450549	-1.287500	0.998338
8	6	0	-1.946323	-0.864925	0.940389
9	6	0	-1.210297	-1.758406	-0.060558
10	6	0	0.204532	-1.285054	-0.427673
11	6	0	-0.003146	0.099864	-1.063248
12	6	0	-0.688922	1.183037	-0.227257
13	6	0	-1.879987	0.632942	0.575641
14	8	0	-1.689880	-2.792104	-0.480283
15	8	0	0.364048	0.333449	-2.201563
16	6	0	-1.147523	-1.055932	2.325108
17	6	0	0.426541	1.728754	0.779933
18	6	0	0.322034	-0.539027	2.115488
19	6	0	0.515372	0.997567	2.122423
20	6	0	-1.083618	-2.554553	2.713692
21	6	0	-1.832541	-0.311875	3.491792
22	8	0	-3.915770	-1.800354	1.999824
23	8	0	-2.762827	1.373186	0.964635
24	6	0	0.867890	-2.271002	-1.421328
25	6	0	2.319171	-1.984701	-1.708299
26	6	0	3.385363	-2.766172	-1.465646
27	6	0	4.768499	-2.305811	-1.887935
28	6	0	5.793600	-2.122736	-0.735641
29	6	0	5.375647	-1.103521	0.290141
30	6	0	5.919538	0.096630	0.547641
31	6	0	5.351203	0.988076	1.627380
32	6	0	7.112641	0.679012	-0.170882
33	6	0	3.328315	-4.131432	-0.820467
34	6	0	1.019395	-1.212582	0.911426
35	6	0	-1.138639	2.373869	-1.108348
36	6	0	-0.010149	3.387233	-1.324043
37	6	0	0.399040	4.042083	0.021473
38	8	0	0.186039	3.078677	1.089723
39	6	0	1.872691	4.462420	0.001078
40	6	0	-0.501452	5.221761	0.390726

41	8	0	-0.398260	4.430370	-2.214465
42	1	0	-4.405687	-0.133517	-3.478120
43	1	0	-6.832739	-0.557714	-3.143025
44	1	0	-7.658390	-1.313472	-0.920004
45	1	0	-6.047106	-1.637863	0.950818
46	1	0	-2.828213	-0.449843	-1.639629
47	1	0	1.384925	1.630756	0.247597
48	1	0	0.855268	-0.894993	3.006308
49	1	0	-0.202115	1.473945	2.794289
50	1	0	1.505800	1.221706	2.535675
51	1	0	-0.571958	-3.178469	1.976207
52	1	0	-2.087627	-2.955780	2.851528
53	1	0	-0.541573	-2.648150	3.662276
54	1	0	-2.129490	0.708256	3.241230
55	1	0	-1.142325	-0.268863	4.343513
56	1	0	-2.729538	-0.846925	3.803066
57	1	0	0.301372	-2.228219	-2.358889
58	1	0	0.722941	-3.277713	-1.023119
59	1	0	2.498976	-1.030803	-2.200853
60	1	0	4.685347	-1.358760	-2.433416
61	1	0	5.189110	-3.042231	-2.590490
62	1	0	5.946655	-3.090437	-0.236341
63	1	0	6.758482	-1.861555	-1.182449
64	1	0	4.509930	-1.392981	0.887996
65	1	0	4.497217	0.525610	2.133729
66	1	0	6.108469	1.221814	2.389095
67	1	0	5.022382	1.952693	1.214471
68	1	0	7.503516	0.031288	-0.958724
69	1	0	7.930251	0.881139	0.535210
70	1	0	6.854649	1.644289	-0.628478
71	1	0	2.309424	-4.472653	-0.624409
72	1	0	3.812075	-4.880067	-1.462860
73	1	0	3.871481	-4.147879	0.134025
74	1	0	1.257627	-2.250094	1.165599
75	1	0	1.982531	-0.732032	0.709068
76	1	0	-1.984315	2.865675	-0.623970
77	1	0	-1.472133	1.997513	-2.081292
78	1	0	0.859406	2.861464	-1.743237
79	1	0	2.052167	5.153657	-0.829412
80	1	0	2.145168	4.958972	0.937879
81	1	0	2.532835	3.596950	-0.133694
82	1	0	-1.555231	4.929590	0.388145
83	1	0	-0.244760	5.562646	1.398940
84	1	0	-0.366969	6.046371	-0.312145

85	1	0	-0.509161	4.032409	-3.091934

Table S11. Gibbs free energies and equilibrium populations of low-energy conformers of Compound 3 (2S, 3R, 4S, 6S, 20R, 30S, 35S).

no	Conformational search		Calculation result	
	ΔE (kcal/mol)	Boltzman distribution	Extracted heat	Boltzman-calculated contribution
3-1	0.00	0.839	-2082.4918226	0.579112031
3-2	5.88	0.078	-2082.4915213	0.420887969

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 3 (2S, 3R, 4S, 6S, 20R, 30S, 35S) at B3LYP/6-31+G(d, p) level of theory in Methanol.

Table S12. 3-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954587	1.625464	0.786103
2	6	0	-0.111169	1.460946	-0.323247
3	6	0	-0.021348	0.110776	-1.003647
4	6	0	0.050057	-1.074742	-0.033084
5	6	0	1.115950	-0.800108	1.019731
6	6	0	1.586934	0.431353	1.339467
7	6	0	0.503031	-2.366475	-0.807030
8	6	0	1.882120	-2.438053	-1.416663
9	6	0	2.350476	-3.726499	-1.724835
10	6	0	3.617304	-3.916479	-2.269351
11	6	0	4.439990	-2.817379	-2.525364
12	6	0	3.980336	-1.531232	-2.238421
13	6	0	2.711797	-1.335805	-1.687083
14	6	0	-0.022620	2.648135	-1.304975
15	6	0	1.191413	2.623613	-2.248209
16	6	0	1.589122	4.007351	-2.823473
17	6	0	0.498943	4.570602	-3.739892
18	6	0	1.999969	5.009844	-1.739041
19	8	0	1.580809	-1.945304	1.563969
20	8	0	-0.219981	-3.343340	-0.881349
21	8	0	-0.147739	-0.055291	-2.202796
22	6	0	-1.524919	1.450791	0.361916
23	6	0	-1.446536	-1.159298	0.595446
24	6	0	-1.847406	0.225017	1.257786
25	6	0	-1.459461	0.485319	2.747500

26	6	0	-2.433846	1.429920	3.406806
27	6	0	-2.201704	2.613615	3.997183
28	6	0	-3.334276	3.382474	4.638085
29	6	0	-0.852127	3.280828	4.114444
30	6	0	-1.535219	-2.310174	1.617036
31	6	0	-2.465197	-1.413622	-0.575230
32	6	0	-3.876408	-1.852980	-0.151848
33	6	0	-4.807349	-2.142465	-1.336781
34	6	0	-5.092899	-0.948665	-2.281116
35	6	0	-5.995467	-1.386346	-3.447384
36	6	0	-5.699366	0.257217	-1.548848
37	8	0	2.316074	2.067051	-1.560850
38	8	0	2.753470	3.667356	-3.620243
39	6	0	2.577210	-1.906103	2.652567
40	6	0	3.519139	-0.697273	2.441201
41	6	0	2.712440	0.602348	2.328055
42	6	0	1.814610	-1.813539	3.978736
43	6	0	3.314712	-3.236622	2.535192
44	8	0	4.382546	-0.880594	1.327635
45	8	0	1.200747	2.740910	1.234007
46	8	0	-6.014085	-2.645865	-0.746890
47	1	0	1.700521	-4.570857	-1.523260
48	1	0	3.963715	-4.921889	-2.492991
49	1	0	5.430022	-2.961268	-2.949639
50	1	0	4.606361	-0.668915	-2.451342
51	1	0	2.385839	-0.317055	-1.512529
52	1	0	-0.927608	2.665558	-1.920538
53	1	0	-0.016924	3.549898	-0.687828
54	1	0	0.955099	1.982417	-3.106470
55	1	0	0.847455	5.490763	-4.225066
56	1	0	0.245760	3.849144	-4.523650
57	1	0	-0.410531	4.816171	-3.180783
58	1	0	2.713489	4.555230	-1.047193
59	1	0	1.140855	5.360083	-1.159228
60	1	0	2.461439	5.893981	-2.199398
61	1	0	-2.261827	1.521288	-0.445981
62	1	0	-1.621386	2.368353	0.952991
63	1	0	-2.942887	0.177299	1.284848
64	1	0	-0.438937	0.856227	2.841393
65	1	0	-1.494141	-0.463563	3.295646
66	1	0	-3.466351	1.071809	3.404600
67	1	0	-4.290630	2.857470	4.548368
68	1	0	-3.139771	3.553190	5.706571
69	1	0	-3.445529	4.376376	4.182248

70	1	0	-0.919664	4.333832	3.810093
71	1	0	-0.512919	3.284339	5.160618
72	1	0	-0.074973	2.818703	3.503213
73	1	0	-0.727507	-2.277057	2.349234
74	1	0	-2.482979	-2.257858	2.162941
75	1	0	-1.483708	-3.274364	1.109348
76	1	0	-2.543270	-0.509069	-1.185086
77	1	0	-2.058711	-2.185778	-1.228916
78	1	0	-3.828708	-2.781865	0.424422
79	1	0	-4.363282	-1.114727	0.496808
80	1	0	-4.339920	-2.936256	-1.945559
81	1	0	-4.129003	-0.649988	-2.716405
82	1	0	-5.586835	-2.263081	-3.965947
83	1	0	-7.007852	-1.633494	-3.101112
84	1	0	-6.099338	-0.583324	-4.185411
85	1	0	-5.967309	1.048848	-2.258213
86	1	0	-5.003421	0.689644	-0.821299
87	1	0	-6.605263	-0.039789	-1.009293
88	1	0	3.068755	2.239050	-2.155757
89	1	0	3.207240	4.492710	-3.851111
90	1	0	4.187674	-0.646453	3.307167
91	1	0	2.331743	0.914512	3.310057
92	1	0	3.373510	1.406869	1.991738
93	1	0	1.182928	-2.697383	4.111479
94	1	0	2.520881	-1.771706	4.815626
95	1	0	1.176396	-0.927367	4.025719
96	1	0	4.039149	-3.332809	3.351154
97	1	0	2.604354	-4.066626	2.600502
98	1	0	3.853454	-3.296947	1.588498
99	1	0	3.846402	-0.909156	0.516285
100	1	0	-6.563522	-3.005024	-1.459818

Table S13. 3-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303080	1.596539	0.871719
2	6	0	0.433489	1.598239	-0.407663
3	6	0	0.332615	0.226702	-1.041643
4	6	0	-0.010987	-0.893491	-0.053068
5	6	0	0.928087	-0.800107	1.144653
6	6	0	1.593692	0.320942	1.520493
7	6	0	0.259788	-2.292819	-0.718112

8	6	0	1.663937	-2.682707	-1.116744
9	6	0	2.746563	-1.798923	-1.269902
10	6	0	4.006992	-2.286620	-1.622980
11	6	0	4.209082	-3.652485	-1.826224
12	6	0	3.136561	-4.535698	-1.685908
13	6	0	1.877764	-4.053570	-1.338745
14	6	0	0.937243	2.686805	-1.377493
15	6	0	2.259225	2.359839	-2.090254
16	6	0	3.026043	3.597463	-2.624250
17	6	0	2.255575	4.295279	-3.748981
18	6	0	3.428901	4.573987	-1.513235
19	8	0	1.055324	-1.992092	1.766130
20	8	0	-0.634596	-3.104611	-0.865419
21	8	0	0.363634	0.031588	-2.242680
22	6	0	-1.040028	1.915570	0.018412
23	6	0	-1.573444	-0.623412	0.332964
24	6	0	-1.752264	0.849967	0.893409
25	6	0	-1.550780	1.045157	2.431726
26	6	0	-1.773222	2.464269	2.899433
27	6	0	-2.904235	3.001043	3.385696
28	6	0	-2.950032	4.446583	3.821321
29	6	0	-4.206616	2.255827	3.551846
30	6	0	-2.054190	-1.666228	1.361948
31	6	0	-2.436822	-0.741275	-0.971342
32	6	0	-3.962890	-0.774785	-0.773201
33	6	0	-4.709298	-0.804815	-2.111303
34	6	0	-6.235982	-0.576862	-1.982959
35	6	0	-6.892383	-0.517356	-3.371557
36	6	0	-6.923044	-1.632225	-1.104052
37	8	0	3.110755	1.637114	-1.196462
38	8	0	4.220648	2.984563	-3.174836
39	6	0	1.882380	-2.123964	2.981874
40	6	0	3.064113	-1.126523	2.917742
41	6	0	2.556657	0.301032	2.679873
42	6	0	0.975500	-1.858735	4.188680
43	6	0	2.354639	-3.574944	2.961475
44	8	0	4.034991	-1.506477	1.951800
45	8	0	1.672890	2.659689	1.358719
46	8	0	-4.411694	-2.067884	-2.717090
47	1	0	2.632651	-0.727593	-1.153843
48	1	0	4.831245	-1.589511	-1.747877
49	1	0	5.193698	-4.024500	-2.096558
50	1	0	3.281338	-5.600717	-1.846288
51	1	0	1.035726	-4.728048	-1.229210

52	1	0	0.173253	2.860119	-2.142263
53	1	0	1.032419	3.598743	-0.782912
54	1	0	2.043028	1.724096	-2.958010
55	1	0	2.865395	5.094006	-4.189160
56	1	0	2.006085	3.582861	-4.542040
57	1	0	1.329578	4.751413	-3.381936
58	1	0	4.146593	5.310215	-1.899747
59	1	0	3.884522	4.036289	-0.677830
60	1	0	2.569918	5.132784	-1.130106
61	1	0	-1.609963	2.053731	-0.907407
62	1	0	-1.043527	2.882651	0.530265
63	1	0	-2.818878	1.065041	0.759122
64	1	0	-0.549079	0.740428	2.740597
65	1	0	-2.243592	0.372152	2.943888
66	1	0	-0.900891	3.114329	2.829922
67	1	0	-1.986261	4.945836	3.680898
68	1	0	-3.709861	5.007303	3.258367
69	1	0	-3.226281	4.532025	4.882037
70	1	0	-4.146801	1.207604	3.248791
71	1	0	-4.542056	2.286221	4.598079
72	1	0	-5.002264	2.729853	2.960073
73	1	0	-1.402424	-1.716428	2.235713
74	1	0	-3.060038	-1.413064	1.713384
75	1	0	-2.090589	-2.657872	0.909087
76	1	0	-2.199192	0.089296	-1.645456
77	1	0	-2.163883	-1.651873	-1.501243
78	1	0	-4.249495	-1.666161	-0.206023
79	1	0	-4.320773	0.096019	-0.207329
80	1	0	-4.309695	0.006860	-2.745109
81	1	0	-6.363617	0.410317	-1.512722
82	1	0	-7.954406	-0.259190	-3.294820
83	1	0	-6.412709	0.232222	-4.014237
84	1	0	-6.833584	-1.489490	-3.878040
85	1	0	-8.008977	-1.482313	-1.094039
86	1	0	-6.574644	-1.592012	-0.066645
87	1	0	-6.719818	-2.637652	-1.488075
88	1	0	3.974427	1.621610	-1.648047
89	1	0	4.865827	3.688553	-3.343926
90	1	0	3.589817	-1.180386	3.877039
91	1	0	3.407786	0.952345	2.459317
92	1	0	2.089828	0.709841	3.586528
93	1	0	0.538133	-0.857146	4.163538
94	1	0	0.159155	-2.587307	4.212161
95	1	0	1.548110	-1.958246	5.117771

96	1	0	2.923775	-3.792679	3.871727
97	1	0	1.493927	-4.249531	2.918920
98	1	0	2.999508	-3.758949	2.101138
99	1	0	3.636710	-1.443906	1.066411
100	1	0	-4.639021	-2.011488	-3.657072

Table S14. Gibbs free energies and equilibrium populations of low-energy conformers of Compound 4 (2S, 3R, 4S, 6S, 20S, 30S, 35S).

no	Conformational search		Calculation result	
	ΔE (kcal/mol)	Boltzman distribution	Extracted heat	Boltzman-calculated contribution
1-1	0.00	0.429	-2082.4943106	0.495069641
1-2	2.91	0.133	-2082.493924	0.328725022
1-3	3.05	0.125	-2082.4929982	0.123302157
1-4	3.44	0.107	-2082.4921993	0.052903179

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 4 (2S, 3R, 4S, 6S, 20S, 30S, 35S) at B3LYP/6-31+G(d, p) level of theory in Methanol.

Table S11. 4-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.306048	1.460745	0.713302
2	6	0	0.268636	1.504364	-0.399788
3	6	0	0.080142	0.156187	-1.054047
4	6	0	-0.151328	-0.997651	-0.087698
5	6	0	0.938332	-0.949668	1.000176
6	6	0	1.662646	0.141169	1.306866
7	6	0	0.031693	-2.372693	-0.819904
8	6	0	1.362139	-2.798172	-1.400335
9	6	0	1.559232	-4.175327	-1.603474
10	6	0	2.772434	-4.666267	-2.092025
11	6	0	3.808050	-3.786392	-2.388366
12	6	0	3.627004	-2.418923	-2.202399
13	6	0	2.411925	-1.926199	-1.713124
14	6	0	0.670189	2.590056	-1.439659
15	6	0	1.936908	2.287383	-2.276393

16	6	0	2.503491	3.522370	-3.035911
17	6	0	3.717406	3.122473	-3.885055
18	6	0	1.452591	4.201784	-3.915901
19	8	0	1.159952	-2.170194	1.620126
20	8	0	-0.876600	-3.206696	-0.882657
21	8	0	-0.010617	0.020044	-2.274508
22	6	0	-1.105979	1.856620	0.215674
23	6	0	-1.639722	-0.727263	0.473461
24	6	0	-1.776491	0.751074	1.096964
25	6	0	-1.440694	0.901900	2.609408
26	6	0	-1.916180	2.215675	3.180358
27	6	0	-1.202211	3.165614	3.815397
28	6	0	-1.871273	4.427856	4.297389
29	6	0	0.270588	3.107607	4.109724
30	6	0	-2.033657	-1.788863	1.530820
31	6	0	-2.681041	-0.795094	-0.728508
32	6	0	-4.166011	-0.966780	-0.345156
33	6	0	-5.082982	-0.815983	-1.570383
34	6	0	-6.542313	-1.235135	-1.277864
35	6	0	-7.223608	-0.353318	-0.227073
36	6	0	-7.382416	-1.230869	-2.559948
37	8	0	2.955335	1.770000	-1.411783
38	8	0	2.961030	4.464868	-2.053413
39	6	0	2.037318	-2.236632	2.765599
40	6	0	3.253150	-1.296682	2.601613
41	6	0	2.809808	0.129386	2.275442
42	6	0	1.227838	-1.908280	4.029643
43	6	0	2.493100	-3.701760	2.850154
44	8	0	4.133348	-1.752415	1.563768
45	8	0	1.812956	2.480883	1.180954
46	8	0	-5.028056	0.545119	-1.998062
47	1	0	0.764562	-4.883181	-1.371953
48	1	0	2.904761	-5.735164	-2.239335
49	1	0	4.753435	-4.164354	-2.769511
50	1	0	4.431977	-1.726618	-2.441818
51	1	0	2.334577	-0.851427	-1.606111
52	1	0	-0.163667	2.752938	-2.134963
53	1	0	0.811202	3.540144	-0.907666
54	1	0	1.716298	1.505904	-3.009824
55	1	0	4.135549	3.993816	-4.402313
56	1	0	4.525786	2.723179	-3.262711
57	1	0	3.451015	2.371655	-4.636024
58	1	0	0.649916	4.641413	-3.314435
59	1	0	1.014374	3.499189	-4.631943

60	1	0	1.893928	5.033773	-4.476931
61	1	0	-1.803605	2.074668	-0.605566
62	1	0	-1.028193	2.797842	0.772275
63	1	0	-2.847120	0.994424	1.059995
64	1	0	-0.382563	0.749244	2.793253
65	1	0	-1.963017	0.133558	3.188634
66	1	0	-2.985841	2.387767	3.049894
67	1	0	-2.939929	4.450581	4.059346
68	1	0	-1.771098	4.519153	5.383905
69	1	0	-1.408862	5.303240	3.829654
70	1	0	0.725447	2.148332	3.861669
71	1	0	0.797575	3.886306	3.549184
72	1	0	0.446867	3.274126	5.177867
73	1	0	-1.297131	-1.868798	2.333401
74	1	0	-2.989696	-1.542738	2.006285
75	1	0	-2.147523	-2.785356	1.096233
76	1	0	-2.582757	0.106513	-1.342769
77	1	0	-2.441164	-1.618946	-1.404850
78	1	0	-4.314546	-1.961412	0.089804
79	1	0	-4.440173	-0.222160	0.407272
80	1	0	-4.687406	-1.437046	-2.383906
81	1	0	-6.530965	-2.265660	-0.899378
82	1	0	-7.249077	0.696757	-0.536146
83	1	0	-6.710039	-0.413687	0.737057
84	1	0	-8.257087	-0.678154	-0.063141
85	1	0	-6.917573	-1.852538	-3.332265
86	1	0	-7.505126	-0.220039	-2.962373
87	1	0	-8.381926	-1.635275	-2.366479
88	1	0	3.294587	2.559389	-0.933174
89	1	0	3.312643	5.240769	-2.524580
90	1	0	3.853680	-1.287259	3.518522
91	1	0	3.656117	0.682678	1.850062
92	1	0	2.503112	0.640986	3.194631
93	1	0	0.815189	-0.896064	4.002564
94	1	0	0.369322	-2.582704	4.126897
95	1	0	1.842287	-2.001171	4.931272
96	1	0	3.193117	-3.858248	3.677347
97	1	0	1.634360	-4.368317	2.993067
98	1	0	2.971470	-4.026588	1.919444
99	1	0	3.589053	-1.990110	0.790964
100	1	0	-5.413475	0.585935	-2.889615

Table S15. 4-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.203747	1.436702	0.902327
2	6	0	0.269569	1.522148	-0.326384
3	6	0	0.211981	0.204026	-1.068505
4	6	0	-0.066407	-1.010844	-0.174222
5	6	0	0.859129	-0.979205	1.031677
6	6	0	1.492151	0.130978	1.488122
7	6	0	0.275213	-2.320824	-0.970938
8	6	0	1.700769	-2.588501	-1.392771
9	6	0	1.992253	-3.909334	-1.772638
10	6	0	3.277569	-4.275388	-2.162363
11	6	0	4.298705	-3.322888	-2.187729
12	6	0	4.020413	-2.003629	-1.826402
13	6	0	2.733484	-1.634392	-1.429367
14	6	0	0.677637	2.705873	-1.227399
15	6	0	2.009362	2.510484	-1.986067
16	6	0	2.587311	3.830755	-2.558678
17	6	0	3.854149	3.537784	-3.374482
18	6	0	1.564267	4.595819	-3.409474
19	8	0	1.022664	-2.208510	1.562465
20	8	0	-0.577971	-3.153354	-1.218675
21	8	0	0.238428	0.100990	-2.281195
22	6	0	-1.201423	1.739770	0.189304
23	6	0	-1.627509	-0.845947	0.237293
24	6	0	-1.862785	0.555207	0.943430
25	6	0	-1.656955	0.658577	2.487182
26	6	0	-2.489106	1.770269	3.076615
27	6	0	-2.093435	2.849513	3.770929
28	6	0	-3.111726	3.829560	4.306969
29	6	0	-0.662579	3.194936	4.107998
30	6	0	-2.076499	-2.011379	1.140144
31	6	0	-2.486967	-0.841615	-1.073412
32	6	0	-4.006529	-1.009575	-0.885689
33	6	0	-4.763350	-0.635080	-2.163711
34	6	0	-6.268910	-0.994726	-2.172468
35	6	0	-6.503923	-2.511397	-2.229687
36	6	0	-7.045813	-0.339731	-1.021951
37	8	0	2.993891	1.877871	-1.163102
38	8	0	2.930272	4.601295	-1.389795
39	6	0	1.840373	-2.399608	2.777673
40	6	0	3.001377	-1.376979	2.784793
41	6	0	2.465000	0.052647	2.637810

42	6	0	0.917529	-2.224835	3.988604
43	6	0	2.341661	-3.836624	2.671739
44	8	0	3.986087	-1.675006	1.805168
45	8	0	1.647256	2.465745	1.409588
46	8	0	-4.580899	0.779741	-2.327256
47	1	0	1.189288	-4.637999	-1.752484
48	1	0	3.483225	-5.304163	-2.445679
49	1	0	5.303174	-3.605129	-2.491580
50	1	0	4.800149	-1.248006	-1.859712
51	1	0	2.563004	-0.593093	-1.184979
52	1	0	-0.118993	2.873193	-1.959329
53	1	0	0.745076	3.592184	-0.590370
54	1	0	1.847343	1.819665	-2.815640
55	1	0	4.326142	4.475554	-3.697136
56	1	0	4.568097	2.968472	-2.775144
57	1	0	3.618731	2.960235	-4.275787
58	1	0	0.714538	4.924159	-2.805237
59	1	0	1.190382	3.978587	-4.235090
60	1	0	2.029525	5.487825	-3.848106
61	1	0	-1.804723	1.990444	-0.689519
62	1	0	-1.203747	2.626793	0.832275
63	1	0	-2.939759	0.719190	0.818238
64	1	0	-0.606391	0.782574	2.750220
65	1	0	-1.981277	-0.280627	2.951713
66	1	0	-3.563217	1.654623	2.911829
67	1	0	-4.136333	3.536409	4.056802
68	1	0	-3.040118	3.913960	5.400826
69	1	0	-2.937525	4.838555	3.907625
70	1	0	0.075434	2.586649	3.582160
71	1	0	-0.453775	4.243206	3.856605
72	1	0	-0.485186	3.095703	5.188843
73	1	0	-1.418358	-2.151105	1.998968
74	1	0	-3.085923	-1.821953	1.521408
75	1	0	-2.090978	-2.944995	0.575753
76	1	0	-2.325233	0.091405	-1.617384
77	1	0	-2.142374	-1.645809	-1.724255
78	1	0	-4.241824	-2.045078	-0.617324
79	1	0	-4.388622	-0.374496	-0.077713
80	1	0	-4.292701	-1.162907	-3.011378
81	1	0	-6.659519	-0.574007	-3.114649
82	1	0	-6.196334	-3.003129	-1.299296
83	1	0	-5.946996	-2.975770	-3.052847
84	1	0	-7.566983	-2.732222	-2.379481
85	1	0	-6.826630	0.731218	-0.966742

86	1	0	-6.787739	-0.790314	-0.055983
87	1	0	-8.125850	-0.463900	-1.162719
88	1	0	3.202985	2.524570	-0.464463
89	1	0	3.462700	5.358996	-1.677093
90	1	0	3.522116	-1.481130	3.742664
91	1	0	3.302933	0.732367	2.456814
92	1	0	1.998076	0.392947	3.572372
93	1	0	0.448973	-1.237484	4.009567
94	1	0	0.125048	-2.979349	3.968594
95	1	0	1.486923	-2.353760	4.916004
96	1	0	2.912475	-4.097283	3.569487
97	1	0	1.494920	-4.524539	2.585115
98	1	0	2.992699	-3.955028	1.804532
99	1	0	3.596726	-1.563836	0.920554
100	1	0	-4.929799	1.022195	-3.199049

Table S16. 4-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.168165	1.317138	1.292798
2	6	0	0.364728	1.610098	0.005277
3	6	0	0.400344	0.444176	-0.958729
4	6	0	0.072679	-0.910212	-0.319876
5	6	0	0.902613	-1.086436	0.943474
6	6	0	1.459306	-0.069374	1.648220
7	6	0	0.503794	-2.058080	-1.302749
8	6	0	1.961402	-2.227247	-1.661589
9	6	0	2.307916	-3.445155	-2.270285
10	6	0	3.625813	-3.719412	-2.625277
11	6	0	4.626267	-2.775095	-2.384653
12	6	0	4.294693	-1.555188	-1.792789
13	6	0	2.974559	-1.279107	-1.431117
14	6	0	0.833094	2.935069	-0.630058
15	6	0	2.235866	2.878024	-1.274252
16	6	0	2.843955	4.279161	-1.542477
17	6	0	4.187460	4.136588	-2.270871
18	6	0	1.893925	5.186739	-2.335681
19	8	0	1.058102	-2.389847	1.253855
20	8	0	-0.307143	-2.848751	-1.749818
21	8	0	0.526706	0.560018	-2.164154
22	6	0	-1.153364	1.722566	0.390119
23	6	0	-1.525094	-0.832914	-0.017152

24	6	0	-1.850710	0.427916	0.888819
25	6	0	-1.783946	0.218066	2.436120
26	6	0	-2.165431	1.444177	3.231963
27	6	0	-3.374384	1.761143	3.723159
28	6	0	-3.580589	3.031762	4.513291
29	6	0	-4.617146	0.921070	3.552650
30	6	0	-2.007116	-2.136978	0.648196
31	6	0	-2.277246	-0.628132	-1.376166
32	6	0	-3.802748	-0.836833	-1.340735
33	6	0	-4.465084	-0.272985	-2.601812
34	6	0	-5.951600	-0.656587	-2.799026
35	6	0	-6.129663	-2.146260	-3.127236
36	6	0	-6.840106	-0.219347	-1.626429
37	8	0	3.145208	2.111003	-0.479215
38	8	0	3.060453	4.824071	-0.225319
39	6	0	1.794735	-2.796495	2.467131
40	6	0	2.904262	-1.762410	2.775413
41	6	0	2.320915	-0.345379	2.854423
42	6	0	0.778941	-2.902254	3.609865
43	6	0	2.368912	-4.166425	2.117161
44	8	0	3.980891	-1.837083	1.851089
45	8	0	1.505528	2.241822	2.028903
46	8	0	-4.317613	1.152894	-2.517420
47	1	0	1.521292	-4.168610	-2.454478
48	1	0	3.872840	-4.670514	-3.089337
49	1	0	5.655987	-2.985871	-2.660748
50	1	0	5.058926	-0.803536	-1.616483
51	1	0	2.766178	-0.307609	-0.999596
52	1	0	0.107488	3.226937	-1.395974
53	1	0	0.821283	3.694758	0.156625
54	1	0	2.170087	2.344807	-2.224743
55	1	0	4.673952	5.116153	-2.371058
56	1	0	4.849518	3.465759	-1.718694
57	1	0	4.047760	3.733461	-3.280404
58	1	0	0.986786	5.402704	-1.765330
59	1	0	1.607791	4.728077	-3.289680
60	1	0	2.384862	6.141818	-2.561952
61	1	0	-1.675994	2.079351	-0.503862
62	1	0	-1.251395	2.513483	1.139739
63	1	0	-2.915451	0.619931	0.712085
64	1	0	-0.785124	-0.090556	2.750702
65	1	0	-2.451187	-0.610398	2.688864
66	1	0	-1.350473	2.142413	3.424265
67	1	0	-2.654388	3.606581	4.611298

68	1	0	-4.333158	3.676843	4.037971
69	1	0	-3.954440	2.813128	5.523806
70	1	0	-4.442408	-0.000970	2.992564
71	1	0	-5.040317	0.648400	4.529718
72	1	0	-5.397389	1.488147	3.026063
73	1	0	-1.444593	-2.377401	1.551870
74	1	0	-3.061677	-2.046178	0.929638
75	1	0	-1.908462	-2.975339	-0.042941
76	1	0	-2.092070	0.380892	-1.750524
77	1	0	-1.865991	-1.315335	-2.115907
78	1	0	-4.035804	-1.903949	-1.257163
79	1	0	-4.259986	-0.340456	-0.476444
80	1	0	-3.908033	-0.644625	-3.479395
81	1	0	-6.278577	-0.090877	-3.687979
82	1	0	-5.883864	-2.781995	-2.268440
83	1	0	-5.491119	-2.454323	-3.964329
84	1	0	-7.168582	-2.359119	-3.404096
85	1	0	-6.660739	0.831052	-1.376633
86	1	0	-6.646055	-0.820909	-0.730238
87	1	0	-7.900617	-0.338514	-1.877151
88	1	0	3.286073	2.635369	0.330440
89	1	0	3.612078	5.616252	-0.315902
90	1	0	3.346288	-2.036291	3.739275
91	1	0	3.141266	0.377395	2.894754
92	1	0	1.751274	-0.206456	3.783790
93	1	0	0.278476	-1.950487	3.806321
94	1	0	0.014452	-3.645851	3.364360
95	1	0	1.281284	-3.221126	4.530081
96	1	0	2.889312	-4.583619	2.985995
97	1	0	1.563548	-4.850170	1.831483
98	1	0	3.082492	-4.087564	1.295773
99	1	0	3.661431	-1.568288	0.972437
100	1	0	-4.592575	1.527882	-3.368533

Table S17. 4-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.170521	1.209861	1.394820
2	6	0	0.264493	1.576139	0.197600
3	6	0	0.297678	0.518744	-0.883897
4	6	0	0.103464	-0.912172	-0.371402
5	6	0	1.029503	-1.157970	0.812141

6	6	0	1.573264	-0.181458	1.581455
7	6	0	0.538935	-1.922822	-1.493066
8	6	0	1.975149	-1.947760	-1.958940
9	6	0	2.357506	-3.070146	-2.712663
10	6	0	3.661116	-3.208430	-3.180888
11	6	0	4.610327	-2.220557	-2.909646
12	6	0	4.241876	-1.094296	-2.171882
13	6	0	2.936166	-0.954692	-1.697150
14	6	0	0.608331	2.987303	-0.322053
15	6	0	1.961887	3.085829	-1.059146
16	6	0	2.466019	4.543122	-1.224588
17	6	0	3.756275	4.561129	-2.055797
18	6	0	1.407777	5.460444	-1.851744
19	8	0	1.283784	-2.472387	0.974339
20	8	0	-0.247369	-2.723092	-1.966357
21	8	0	0.313155	0.765938	-2.076696
22	6	0	-1.228393	1.546274	0.683033
23	6	0	-1.473824	-0.975826	0.038138
24	6	0	-1.810612	0.165247	1.087719
25	6	0	-1.618247	-0.195174	2.596582
26	6	0	-1.973351	0.927465	3.542535
27	6	0	-3.141851	1.135157	4.171043
28	6	0	-3.321068	2.311702	5.101062
29	6	0	-4.360709	0.255303	4.033233
30	6	0	-1.824025	-2.367410	0.600638
31	6	0	-2.328609	-0.704334	-1.247802
32	6	0	-3.841779	-0.957975	-1.142631
33	6	0	-4.570318	-0.570692	-2.442499
34	6	0	-6.079443	-0.891684	-2.429699
35	6	0	-6.859398	-0.058378	-1.399779
36	6	0	-6.677906	-0.715415	-3.833784
37	8	0	2.969039	2.306621	-0.406496
38	8	0	2.749618	4.968265	0.123408
39	6	0	2.119243	-2.947524	2.096103
40	6	0	3.188861	-1.881188	2.435230
41	6	0	2.535376	-0.517151	2.693091
42	6	0	1.188555	-3.221350	3.282348
43	6	0	2.742183	-4.241223	1.579709
44	8	0	4.200826	-1.800421	1.441336
45	8	0	1.496005	2.076124	2.203434
46	8	0	-4.431332	0.830474	-2.721626
47	1	0	1.610070	-3.828241	-2.919275
48	1	0	3.937023	-4.087447	-3.757150
49	1	0	5.628820	-2.325215	-3.273804

50	1	0	4.964617	-0.309388	-1.967883
51	1	0	2.696011	-0.049856	-1.152189
52	1	0	-0.185816	3.309503	-1.003257
53	1	0	0.609293	3.659855	0.540415
54	1	0	1.859293	2.643246	-2.051856
55	1	0	4.172392	5.576807	-2.093445
56	1	0	4.499009	3.889020	-1.620163
57	1	0	3.564577	4.245051	-3.087601
58	1	0	0.534031	5.555590	-1.201886
59	1	0	1.080234	5.083947	-2.828136
60	1	0	1.822823	6.464370	-2.007008
61	1	0	-1.827946	1.955872	-0.137501
62	1	0	-1.325754	2.251853	1.513487
63	1	0	-2.895248	0.300847	1.004220
64	1	0	-0.588744	-0.495552	2.800793
65	1	0	-2.237174	-1.070941	2.809448
66	1	0	-1.172352	1.642560	3.731312
67	1	0	-2.415336	2.922584	5.166229
68	1	0	-4.145162	2.958560	4.768278
69	1	0	-3.580744	1.977697	6.115785
70	1	0	-4.204995	-0.601207	3.372513
71	1	0	-4.676473	-0.127981	5.013694
72	1	0	-5.210290	0.830405	3.639429
73	1	0	-1.176068	-2.652965	1.430436
74	1	0	-2.855653	-2.375462	0.968084
75	1	0	-1.731531	-3.126985	-0.177197
76	1	0	-2.186851	0.336249	-1.554739
77	1	0	-1.942152	-1.325327	-2.057379
78	1	0	-4.037728	-2.019836	-0.949572
79	1	0	-4.283429	-0.390551	-0.315458
80	1	0	-4.119985	-1.150147	-3.266119
81	1	0	-6.165782	-1.953205	-2.152677
82	1	0	-6.745985	1.011050	-1.604396
83	1	0	-6.521975	-0.244708	-0.374452
84	1	0	-7.927359	-0.302063	-1.442954
85	1	0	-6.166979	-1.351002	-4.567724
86	1	0	-6.581597	0.324157	-4.163327
87	1	0	-7.741221	-0.981829	-3.843356
88	1	0	3.144935	2.764011	0.436298
89	1	0	3.237678	5.804850	0.077833
90	1	0	3.711007	-2.218436	3.336887
91	1	0	3.315900	0.247581	2.748679
92	1	0	2.029327	-0.501144	3.668105
93	1	0	0.647667	-2.325790	3.599278

94	1	0	0.454349	-3.986995	3.013570
95	1	0	1.767980	-3.590193	4.136096
96	1	0	3.341898	-4.705405	2.369986
97	1	0	1.957368	-4.942769	1.280205
98	1	0	3.393211	-4.043530	0.727128
99	1	0	3.807536	-1.463677	0.617932
100	1	0	-3.556360	0.971457	-3.110908

Table S18 Gibbs free energies and equilibrium populations of low-energy conformers of Compound 19 (11S).

no	Conformational search		Calculation result	
	ΔE (kcal/mol)	Boltzman distribution	Extracted heat	Boltzman-calculated contribution
3-1	0.00	0.722	-1069.5592299	0.287024241
3-2	3.89	0.150	-1069.5591272	0.257440715
3-3	5.60	0.075	-1069.559666	0.455535044

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 19 (11S) at B3LYP/6-31+G(d, p) level of theory in Methanol.

Table S19. 19-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.969927	0.183407	0.745425
2	6	0	3.784102	-0.986969	-0.003893
3	6	0	2.563200	-1.220782	-0.628856
4	6	0	1.496425	-0.280021	-0.512212
5	6	0	1.740580	0.884327	0.260652
6	6	0	2.948108	1.132623	0.887691
7	6	0	0.218868	-0.516385	-1.166214
8	6	0	-0.741905	0.546550	-0.931986
9	6	0	-0.408561	1.612095	-0.180528
10	8	0	0.759982	1.844011	0.424430
11	8	0	-0.030029	-1.530692	-1.857517
12	8	0	2.402237	-2.345977	-1.344691
13	8	0	5.139228	0.457618	1.368265
14	6	0	-2.153848	0.721888	-1.408254
15	8	0	-2.551656	2.007025	-0.827542

16	6	0	-1.548284	2.557889	-0.095727
17	6	0	-3.149124	-0.374251	-0.991290
18	6	0	-3.282717	-0.561251	0.496881
19	6	0	-2.957149	-1.641155	1.226289
20	6	0	-3.202757	-1.659357	2.716911
21	6	0	-2.348896	-2.910100	0.679549
22	8	0	-1.631759	3.615555	0.482272
23	1	0	4.580740	-1.716898	-0.107667
24	1	0	3.100710	2.033087	1.469647
25	1	0	1.474123	-2.327475	-1.706642
26	1	0	5.779674	-0.254862	1.202610
27	1	0	-2.192302	0.853537	-2.494929
28	1	0	-2.829800	-1.288578	-1.498841
29	1	0	-4.121212	-0.096208	-1.419851
30	1	0	-3.718547	0.288418	1.022254
31	1	0	-3.658973	-0.729036	3.069343
32	1	0	-3.863795	-2.492033	2.994755
33	1	0	-2.264283	-1.812424	3.267383
34	1	0	-2.077986	-2.847709	-0.376293
35	1	0	-1.440506	-3.166395	1.241103
36	1	0	-3.039699	-3.754780	0.808756

Table S20. 19-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.968481	0.169607	0.740857
2	6	0	3.780609	-1.001548	-0.007143
3	6	0	2.561759	-1.233409	-0.632085
4	6	0	1.495339	-0.288784	-0.518888
5	6	0	1.740722	0.875795	0.249822
6	6	0	2.950070	1.122629	0.878948
7	6	0	0.216256	-0.523871	-1.171155
8	6	0	-0.742154	0.541475	-0.938149
9	6	0	-0.405751	1.608845	-0.190834
10	8	0	0.764780	1.839209	0.411396
11	8	0	-0.035832	-1.539131	-1.859564
12	8	0	2.396398	-2.359907	-1.346215
13	8	0	5.180803	0.329164	1.319955
14	6	0	-2.155329	0.717089	-1.410665
15	8	0	-2.549112	2.005554	-0.834501
16	6	0	-1.543206	2.557173	-0.106735
17	6	0	-3.150626	-0.375542	-0.984221

18	6	0	-3.278864	-0.553843	0.505522
19	6	0	-2.949723	-1.629017	1.240305
20	6	0	-3.189231	-1.638039	2.732014
21	6	0	-2.342922	-2.901010	0.699152
22	8	0	-1.623390	3.617007	0.467720
23	1	0	4.584626	-1.722783	-0.097425
24	1	0	3.088382	2.029918	1.456843
25	1	0	1.468724	-2.339558	-1.707812
26	1	0	5.207930	1.167263	1.811650
27	1	0	-2.197490	0.843546	-2.497781
28	1	0	-2.834341	-1.293121	-1.487783
29	1	0	-4.123871	-0.098539	-1.410768
30	1	0	-3.713100	0.298790	1.027392
31	1	0	-3.643968	-0.705552	3.080604
32	1	0	-3.849088	-2.468988	3.017700
33	1	0	-2.248489	-1.787742	3.279532
34	1	0	-2.078656	-2.846134	-0.358788
35	1	0	-1.430716	-3.151908	1.256968
36	1	0	-3.031690	-3.745669	0.838875

Table S21. 19-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.135002	0.797794	0.719961
2	6	0	4.161444	-0.593329	0.547311
3	6	0	3.029602	-1.252677	0.078011
4	6	0	1.841816	-0.524815	-0.231061
5	6	0	1.873264	0.880253	-0.037924
6	6	0	2.989132	1.551165	0.428795
7	6	0	0.654702	-1.208624	-0.720498
8	6	0	-0.451087	-0.304641	-0.980770
9	6	0	-0.316627	1.017262	-0.765819
10	8	0	0.765123	1.658604	-0.314258
11	8	0	0.588617	-2.446289	-0.897122
12	8	0	3.070417	-2.585997	-0.080608
13	8	0	5.208886	1.483747	1.174592
14	6	0	-1.841327	-0.565536	-1.481232
15	8	0	-2.434999	0.769247	-1.550498
16	6	0	-1.574058	1.724018	-1.113621
17	6	0	-2.713438	-1.477404	-0.597615
18	6	0	-2.801684	-1.044863	0.842810

19	6	0	-3.809895	-0.385658	1.437217
20	6	0	-3.741672	-0.040021	2.906035
21	6	0	-5.074590	0.062175	0.746667
22	8	0	-1.838546	2.901607	-1.054985
23	1	0	5.053611	-1.168413	0.774781
24	1	0	2.978754	2.625418	0.565449
25	1	0	2.174874	-2.864254	-0.417476
26	1	0	5.944951	0.872314	1.345980
27	1	0	-1.833023	-0.951616	-2.505910
28	1	0	-2.262931	-2.475799	-0.662054
29	1	0	-3.697334	-1.541736	-1.070575
30	1	0	-1.938211	-1.303497	1.455973
31	1	0	-2.807622	-0.379276	3.364636
32	1	0	-3.825543	1.044787	3.058132
33	1	0	-4.578150	-0.494821	3.454613
34	1	0	-5.102818	-0.187364	-0.315824
35	1	0	-5.954967	-0.384275	1.228674
36	1	0	-5.191081	1.150589	0.837035

HRESIMS, UV, IR and NMR spectra of 1–4 and 19-21

Figure S5. HRESIMS spectrum of 1

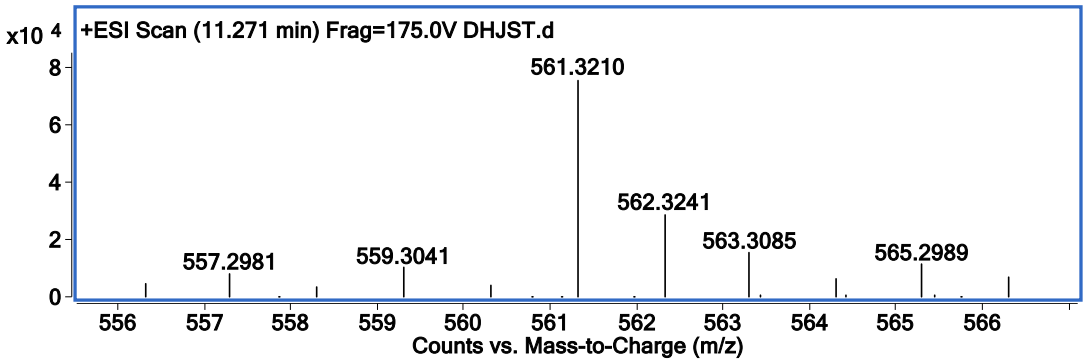

Figure S6. UV spectrum of 1

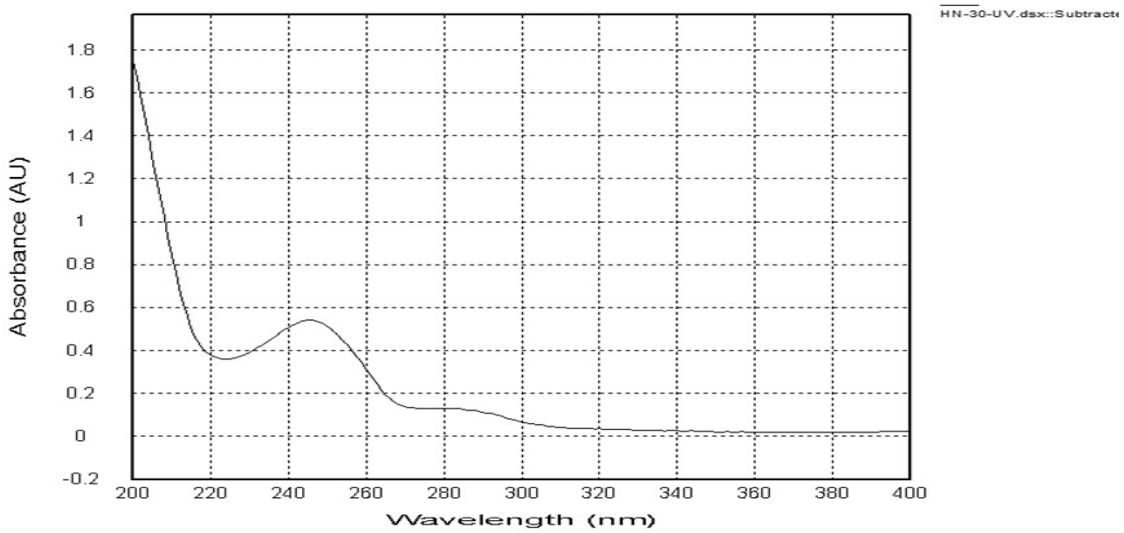

Figure S7 IR spectrum of 1.

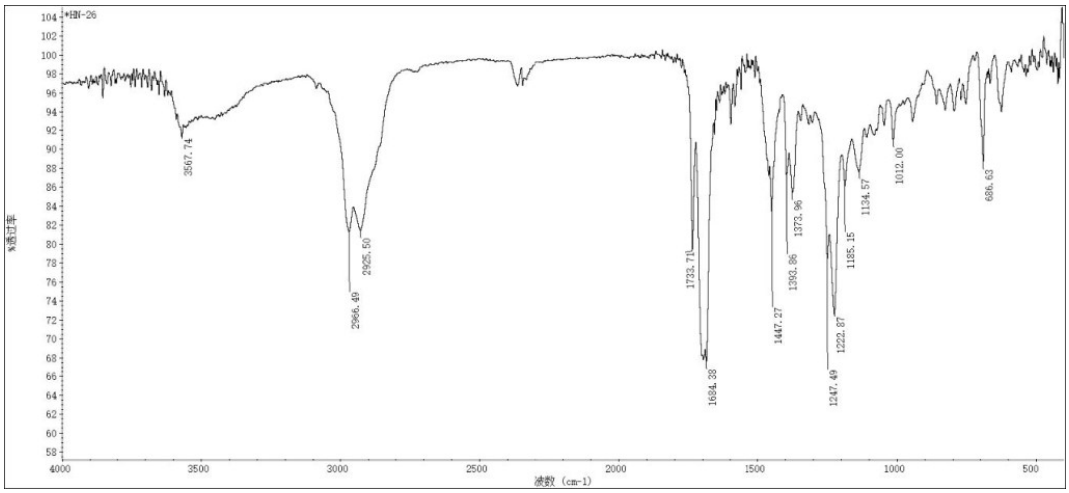

Figure S8. ^{1}H NMR (400 MHz) spectrum of 1 in $CDCl_3$

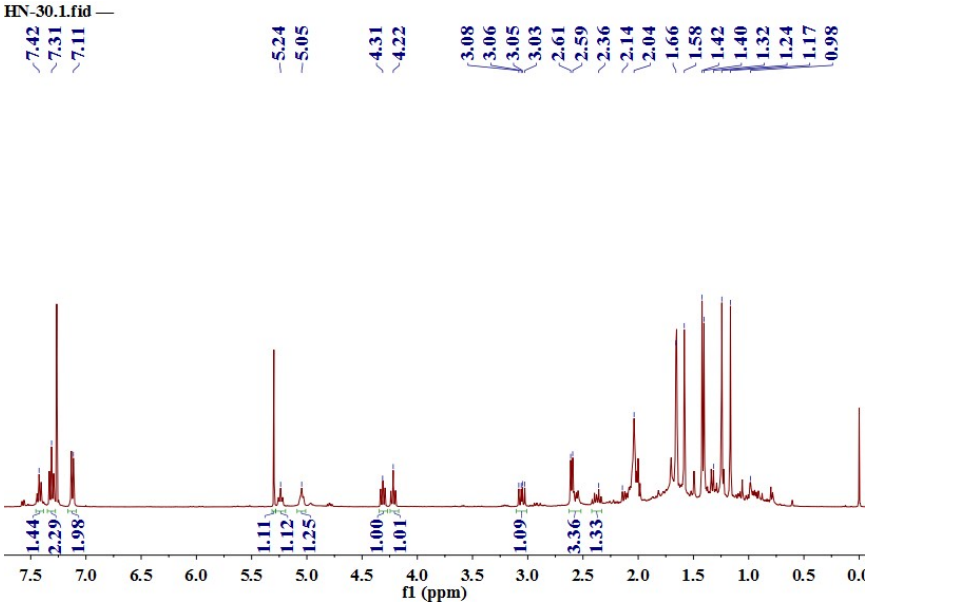

Figure S9. ^{13}C NMR (100 MHz) spectrum of 1 in $CDCl_3$

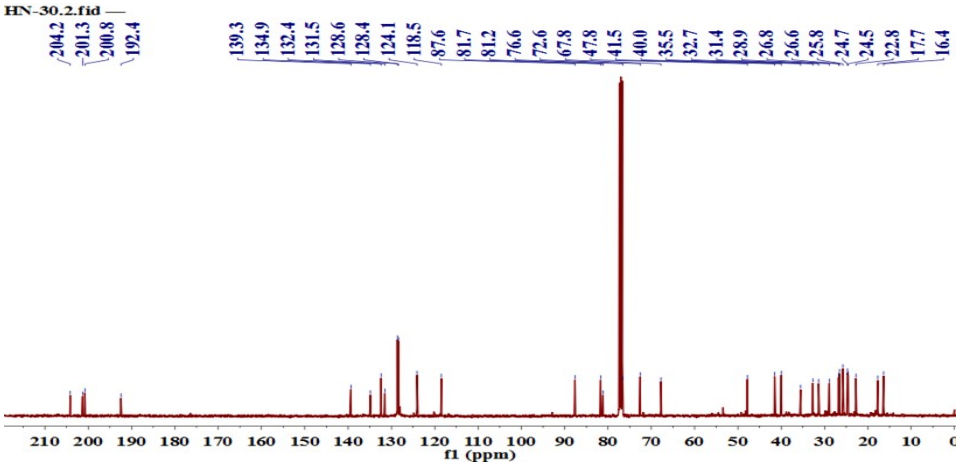

Figure S10. DEPT spectrum of 1 in $CDCl_3$

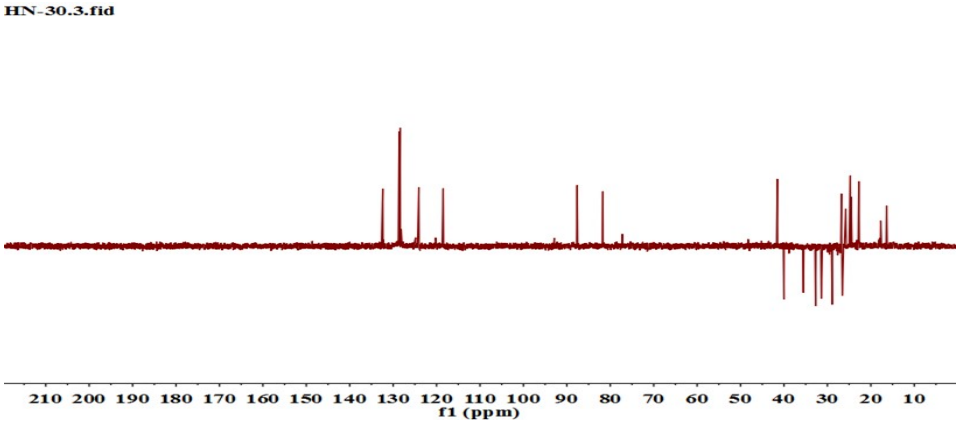

Figure S11. ^{1}H-^{1}H COSY spectrum of 1 in $CDCl_3$

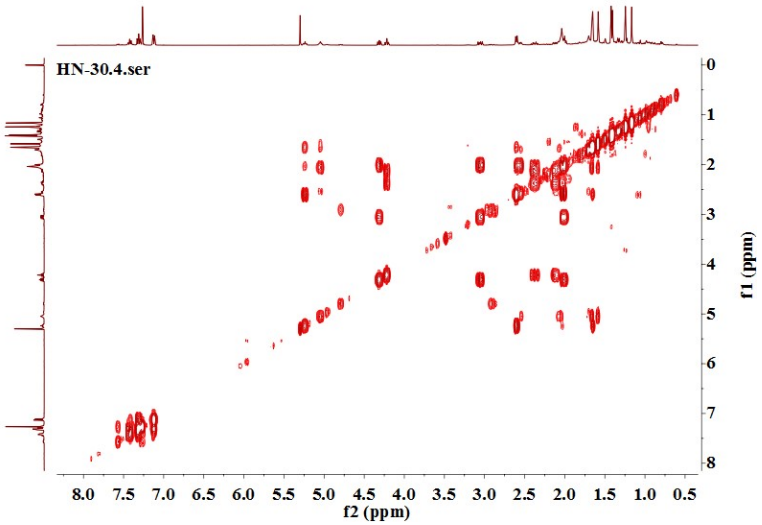

Figure S12. HSQC spectrum of 1 in $CDCl_3$

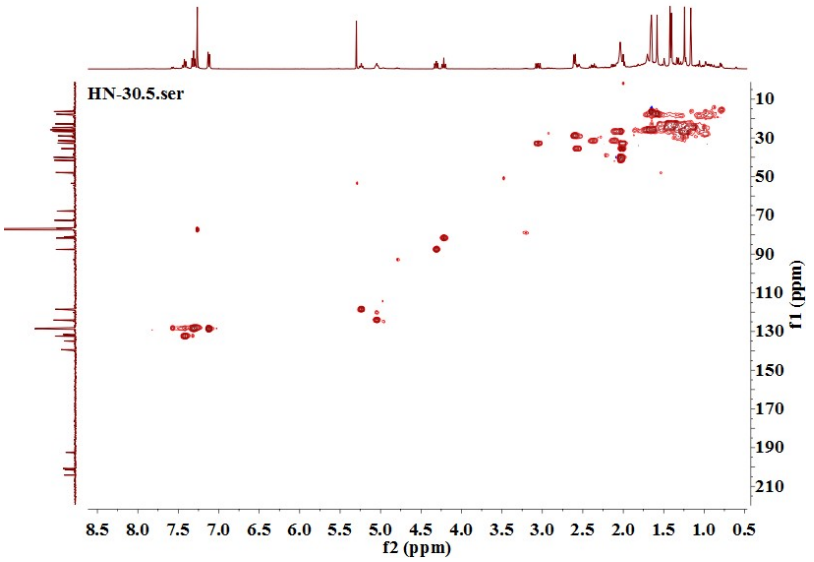

Figure S13. HMBC spectrum of 1 in $CDCl_3$

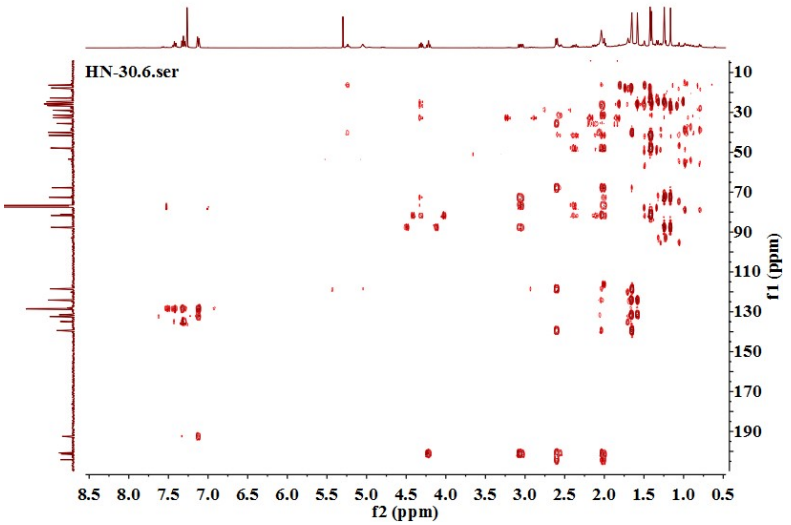

Figure S14. ^{1}H-^{1}H ROESY spectrum of 1 in $CDCl_3$

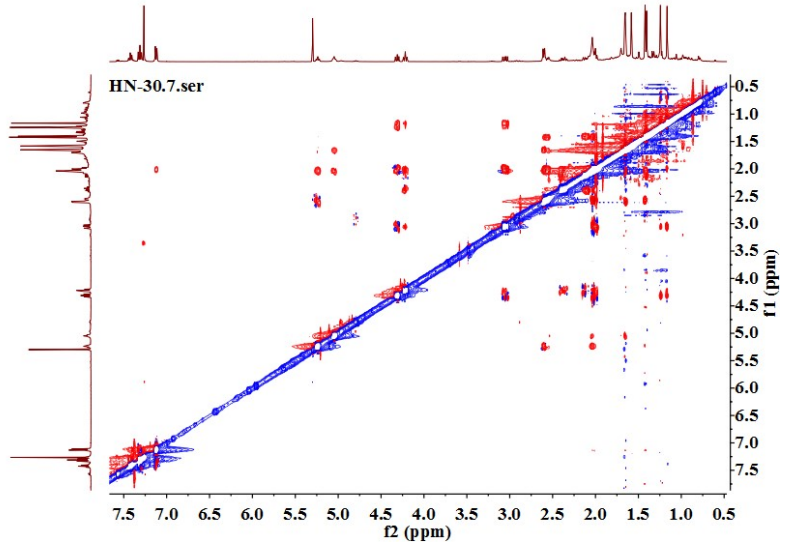

Figure S15. HRESIMS spectrum of 2

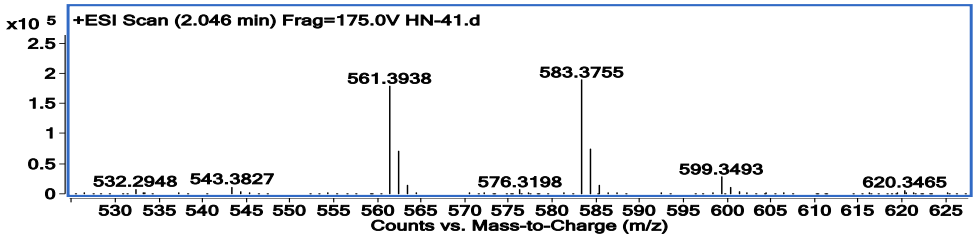

Figure S16. IR spectrum of 2

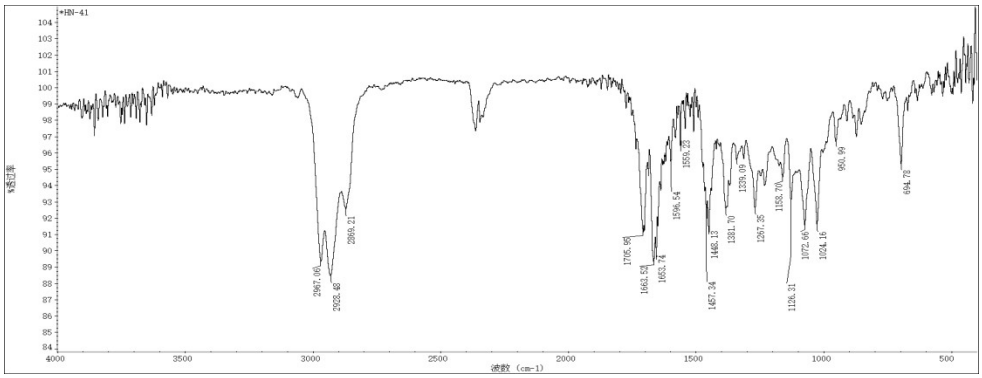

Figure S17. UV spectrum of 2

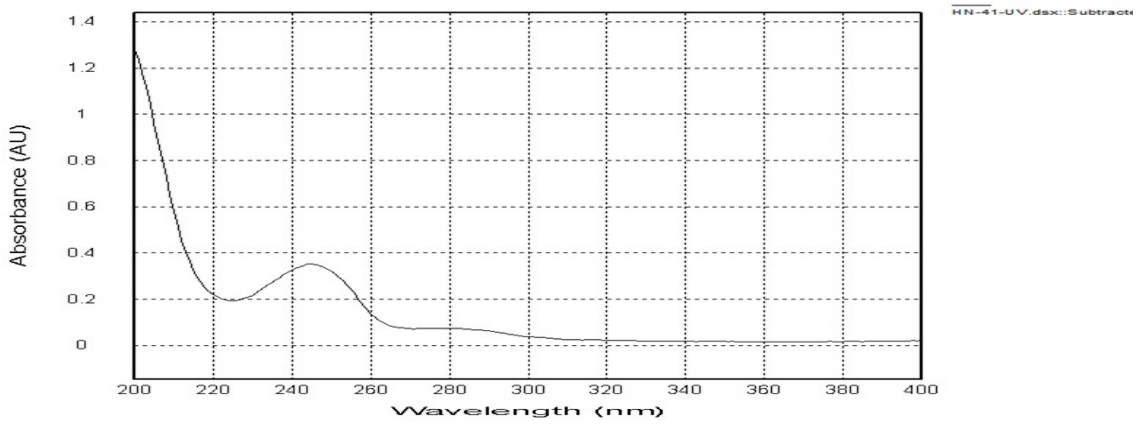

Figure S18. ^{1}H NMR (400 MHz) spectrum of 2 in $CDCl_3$

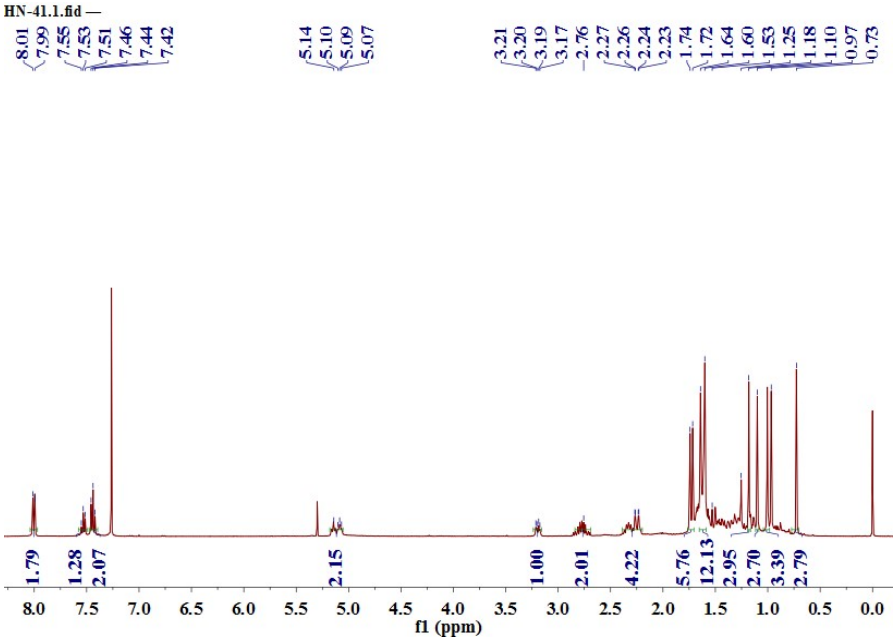

Figure S19. ^{13}C NMR (100 MHz) spectrum of 2 in $CDCl_3$

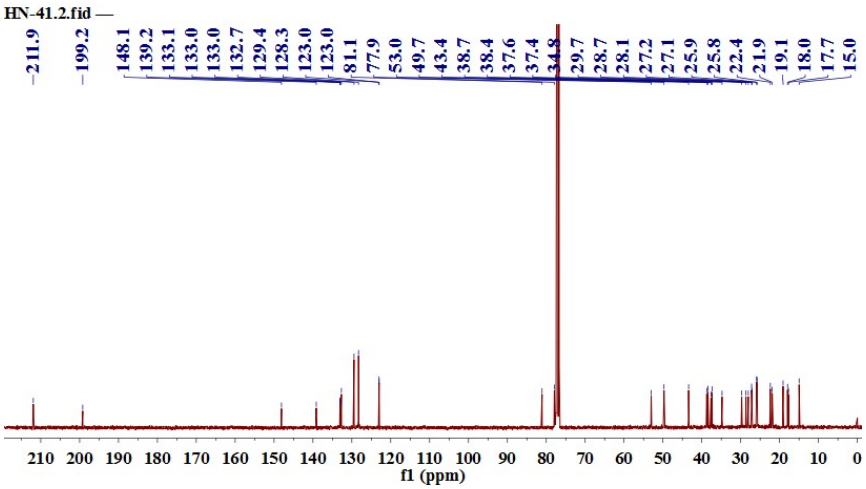

Figure S20. DEPT spectrum of 2 in $CDCl_3$

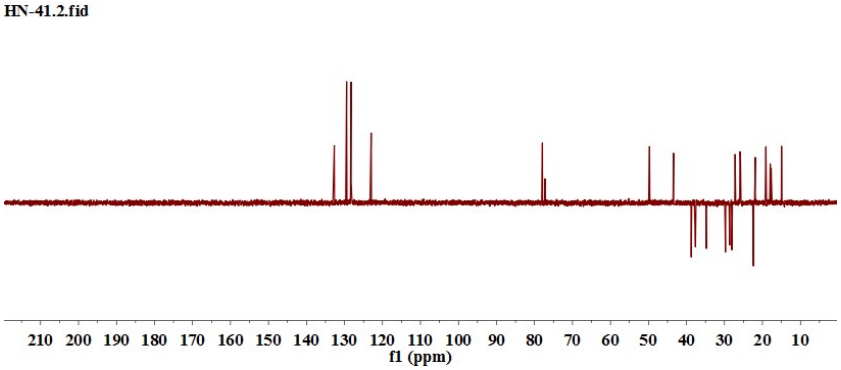

Figure S21. ^{1}H-^{1}H COSY spectrum of 2 in $CDCl_3$

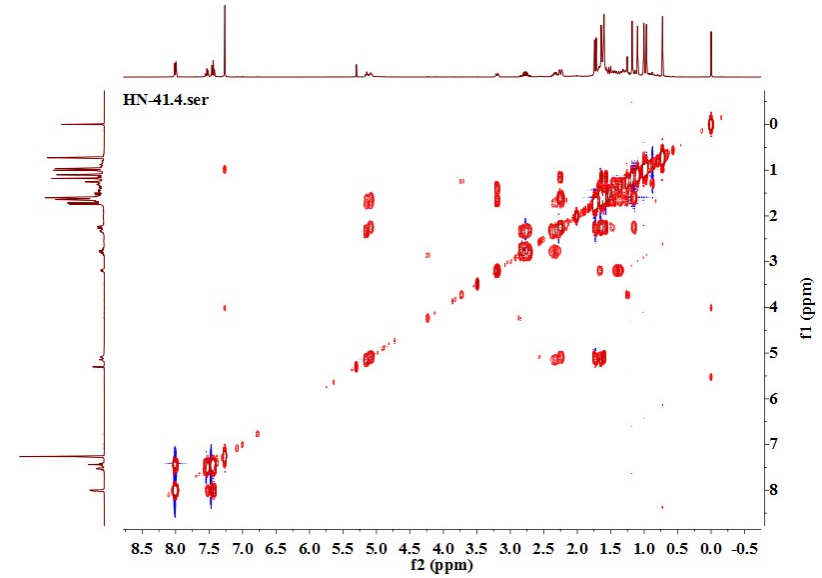

Figure S22. HSQC spectrum of 2 in $CDCl_3$

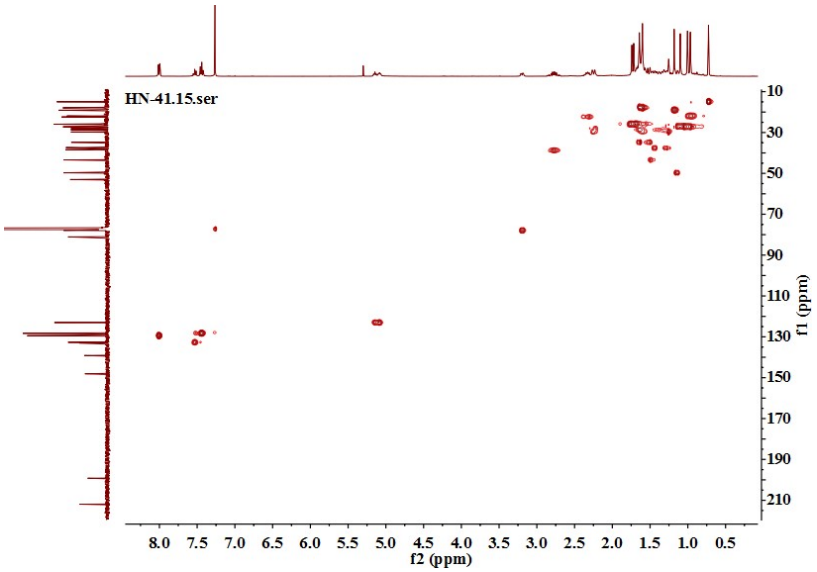

Figure S23. HMBC spectrum of 2 in $CDCl_3$

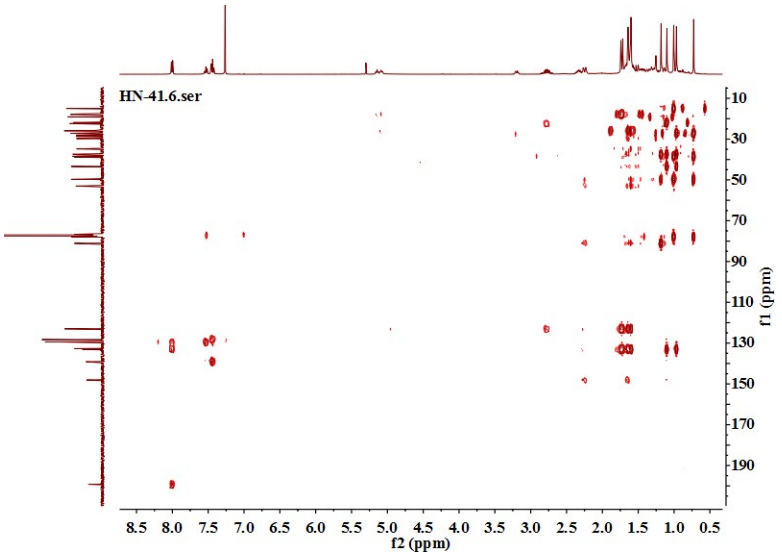

Figure S24. ^{1}H-^{1}H ROESY spectrum of 2 in $CDCl_3$

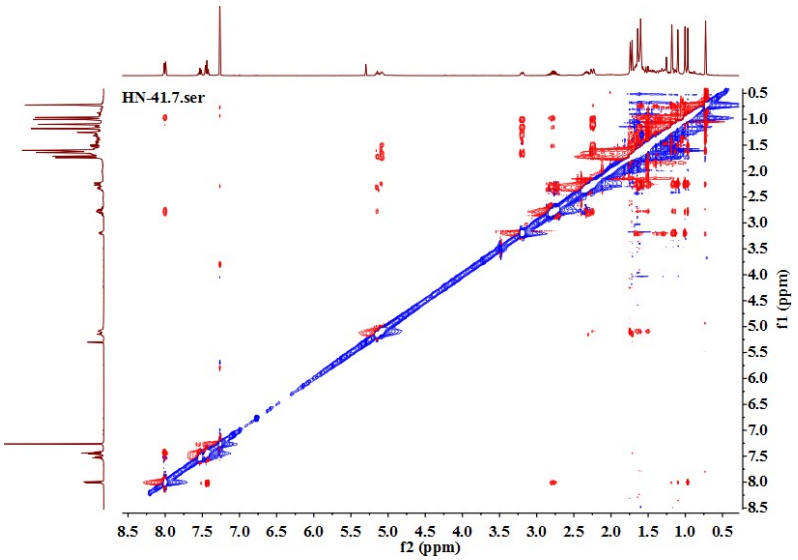

Figure S25. HRESIMS spectrum of 3

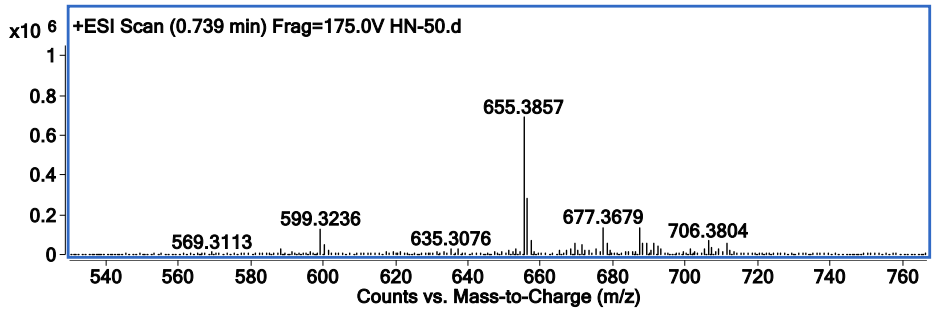

Figure S26. UV spectrum of 3

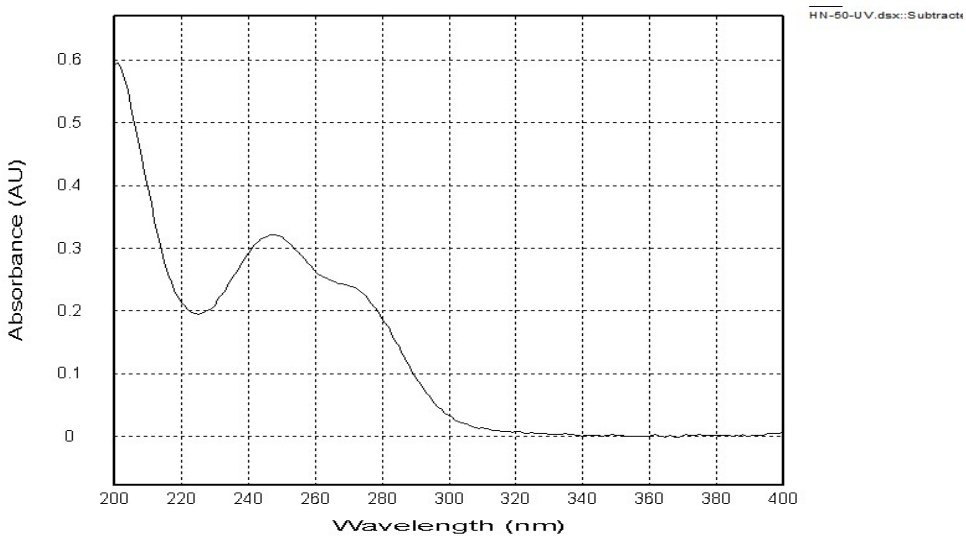

Figure S27. IR spectrum of 3

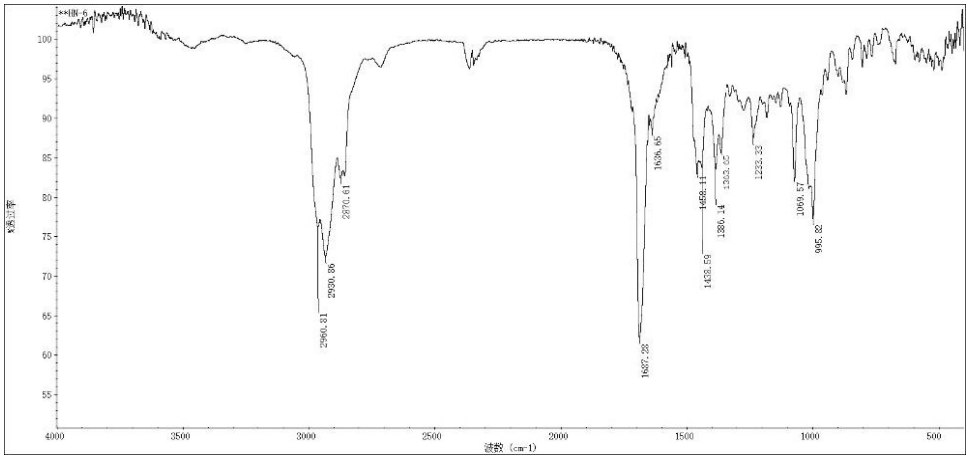

Figure S28. ^{1}H NMR (400 MHz) spectrum of 3 in $CDCl_3$

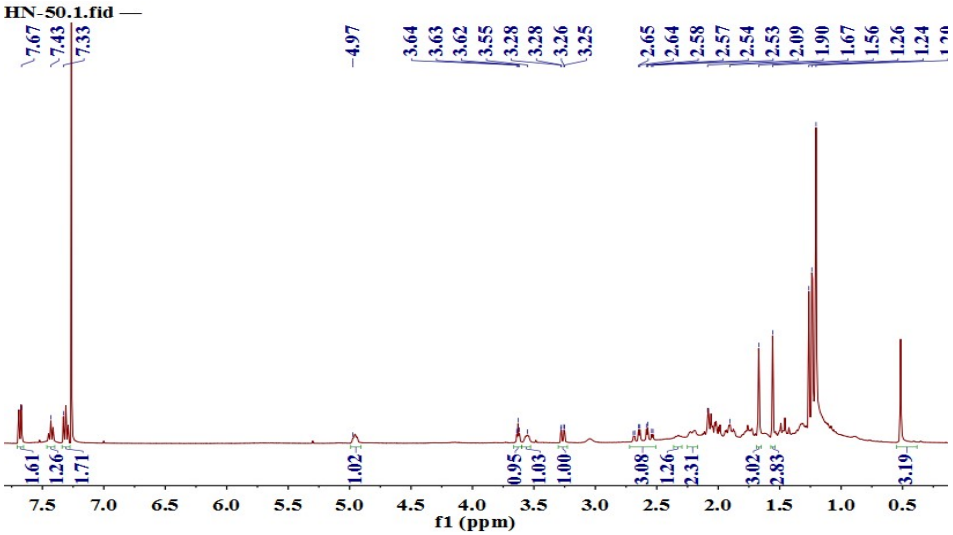

Figure S29. ^{13}C NMR (100 MHz) spectrum of 3 in $CDCl_3$

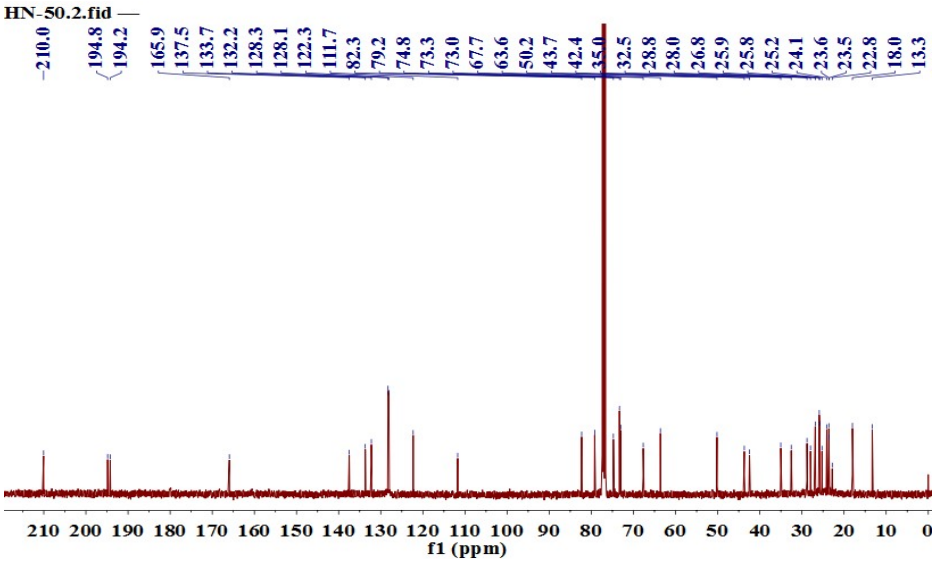

Figure S30. DEPT spectrum of 3 in $CDCl_3$

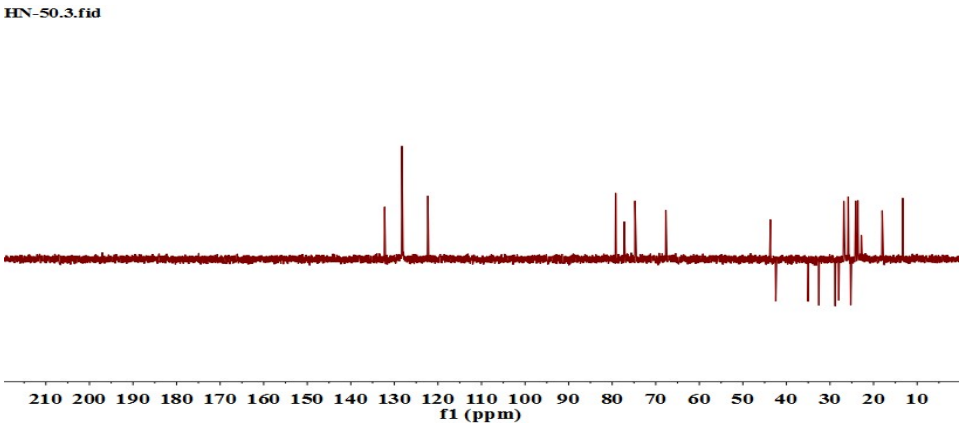

Figure S31. ^1H-^1H COSY spectrum of 3 in $CDCl_3$

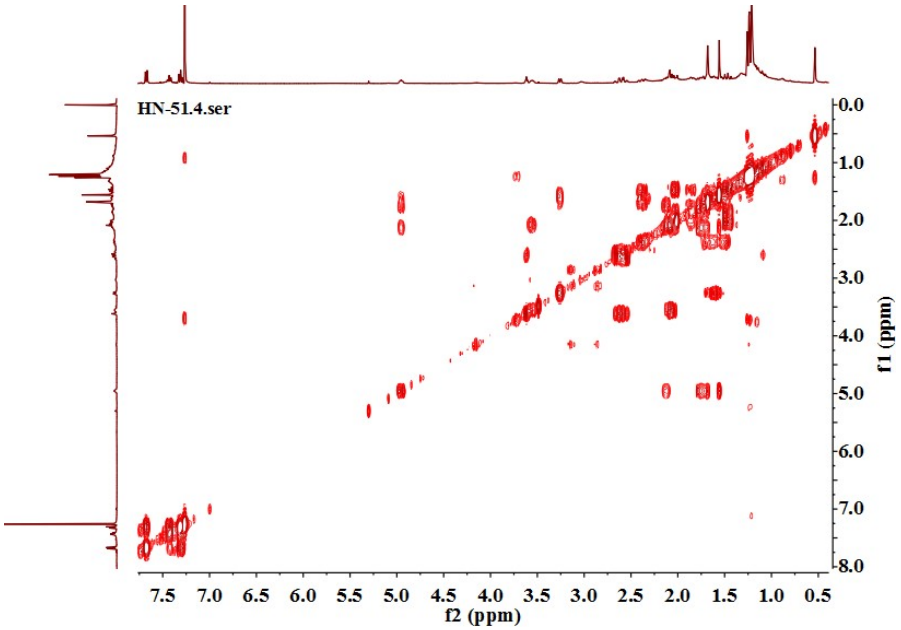

Figure S32. HSQC spectrum of 3 in $CDCl_3$

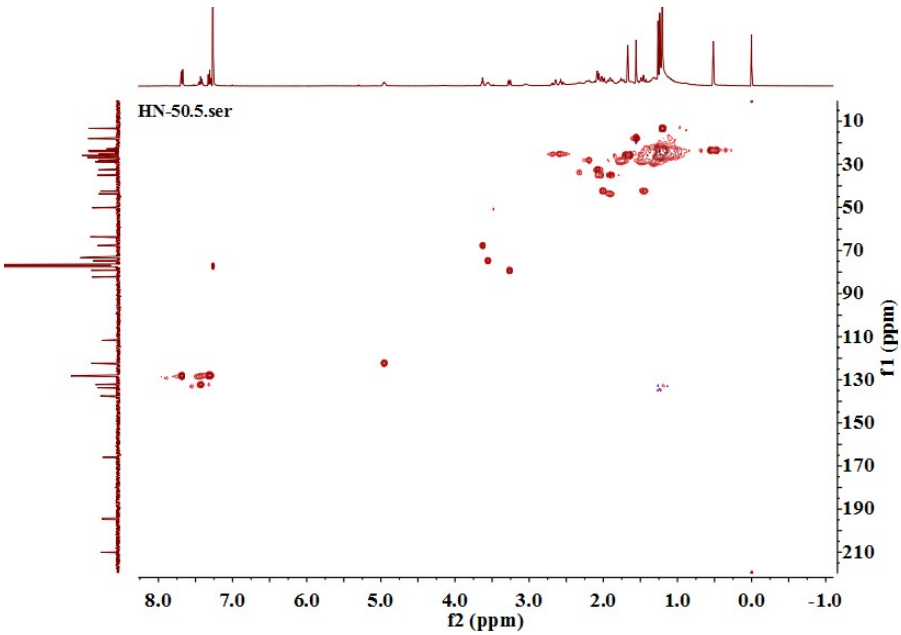

Figure S33. HMBC spectrum of 3 in $CDCl_3$

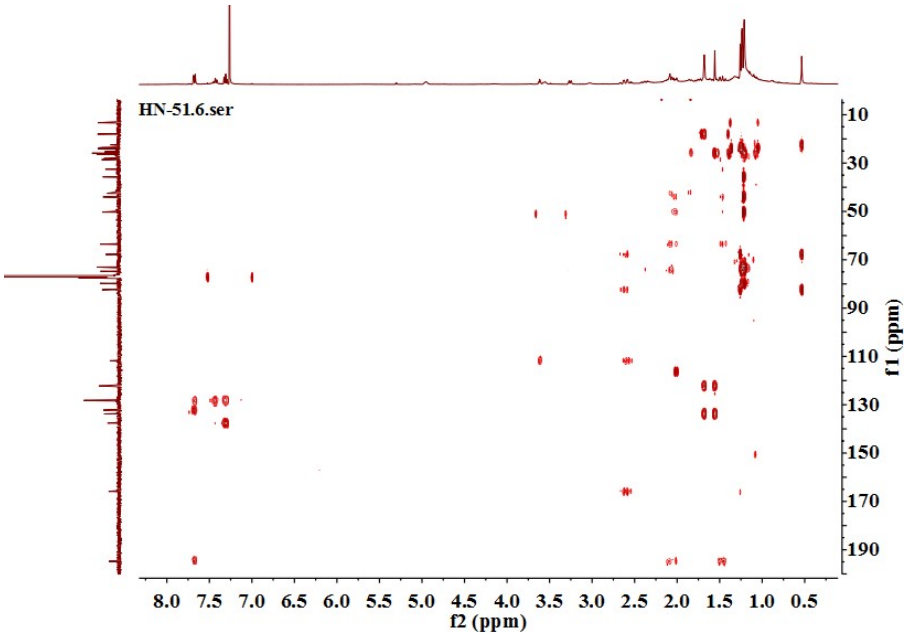

Figure S34. ^1H-^1H ROESY spectrum of 3 in $CDCl_3$

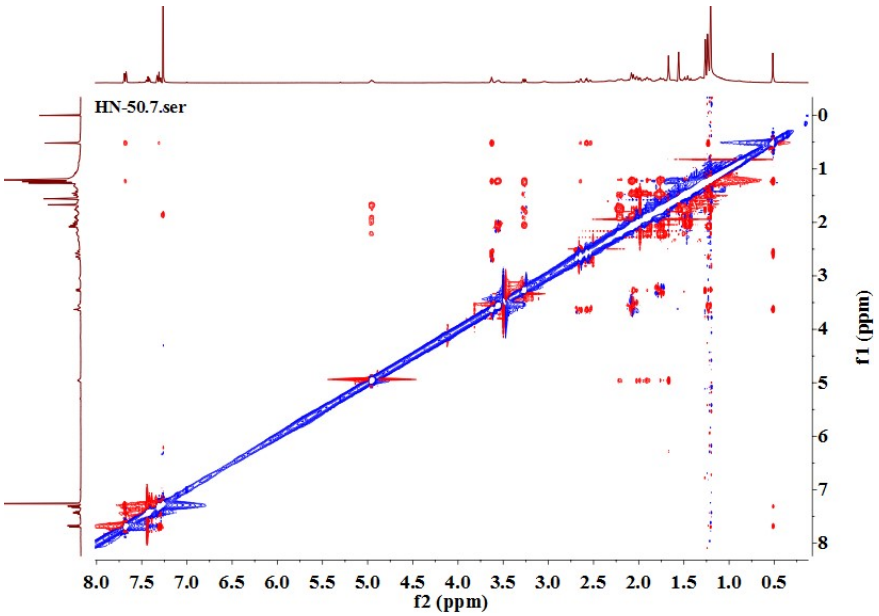

Figure S35. HRESIMS spectrum of 4

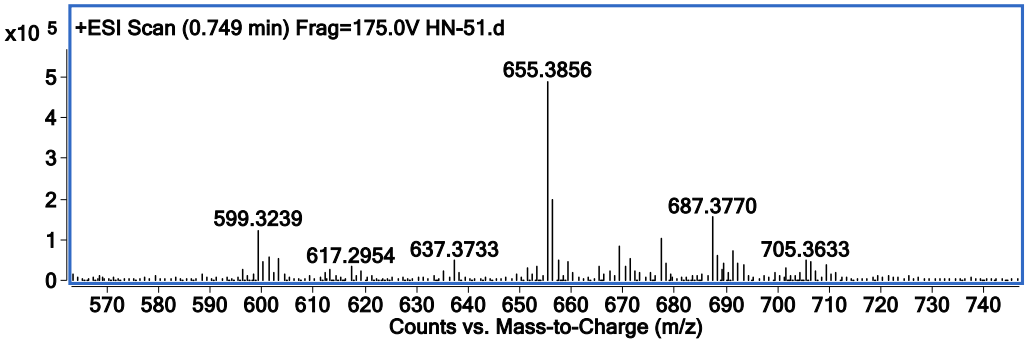

Figure S36. UV spectrum of 4

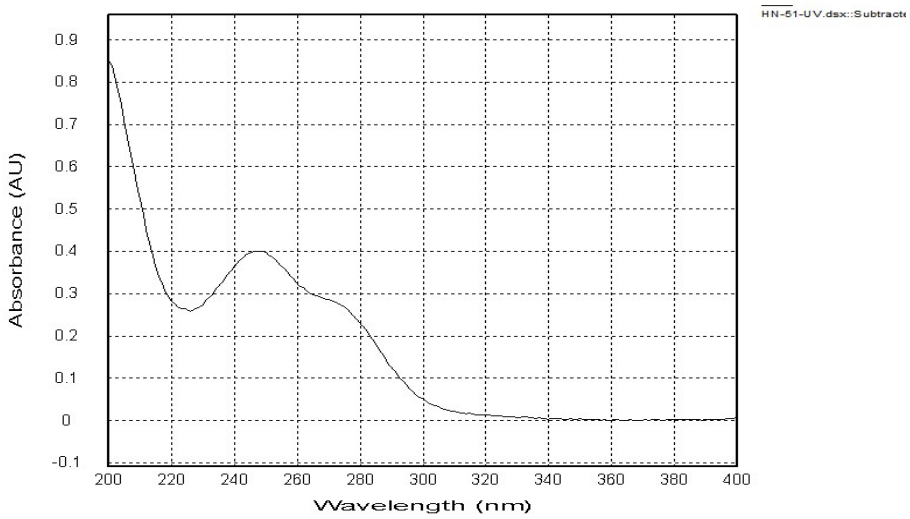

Figure S37. IR spectrum of 4

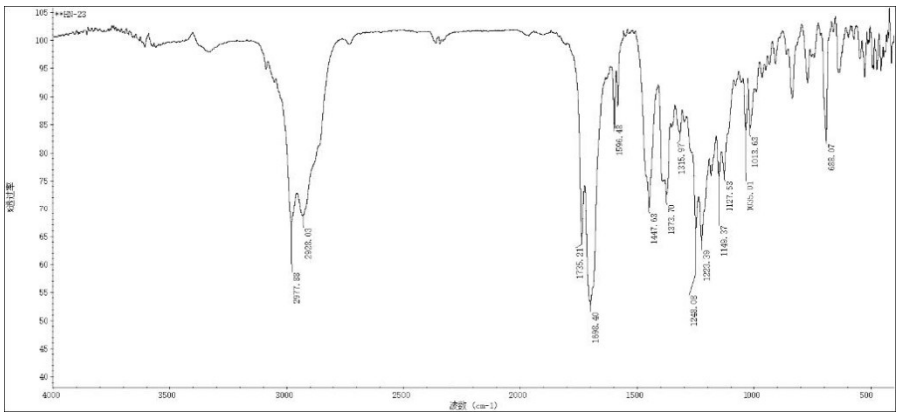

Figure S38. ^{1}H NMR (400 MHz) spectrum of 4 in $CDCl_3$

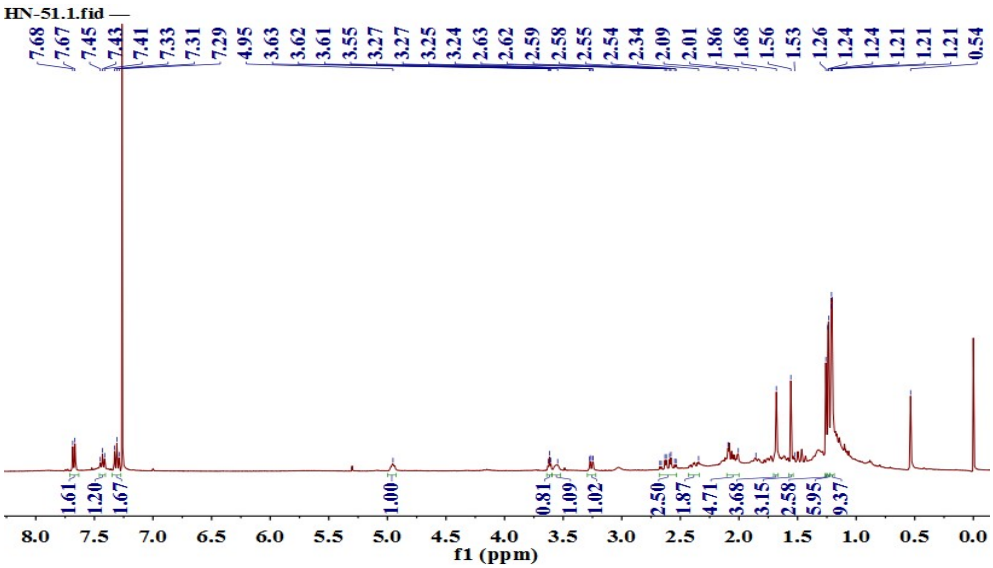

Figure S39. ^{13}C NMR (400 MHz) spectrum of 4 in $CDCl_3$

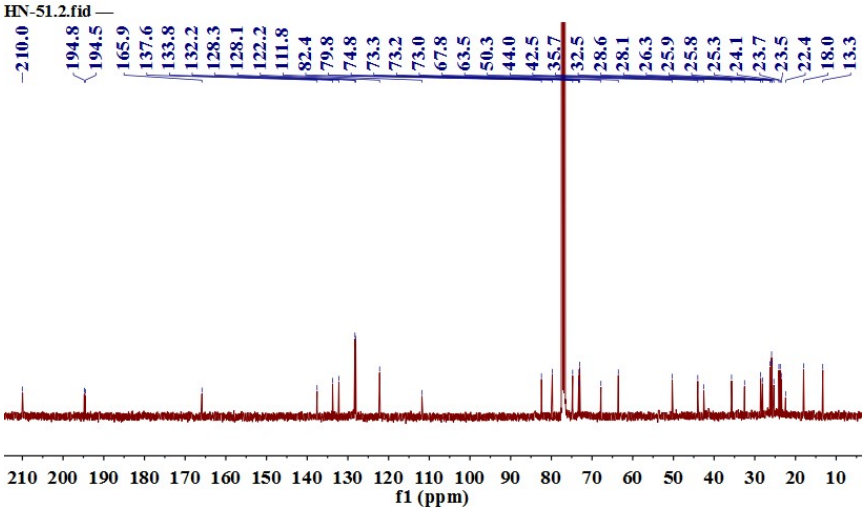

Figure S40. DEPT spectrum of 4 in $CDCl_3$

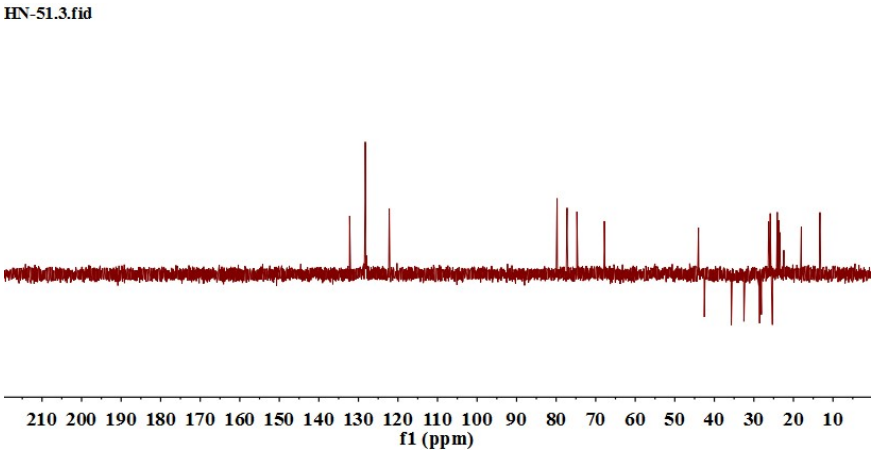

Figure S41. ^{1}H-^{1}H ROESY spectrum of 4 in $CDCl_3$

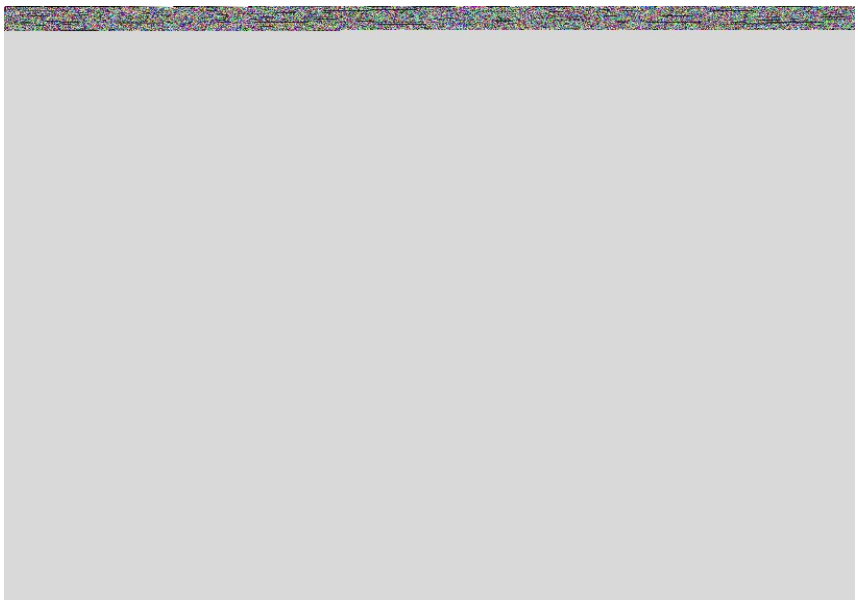

Figure S42. HSQC spectrum of 4 in $CDCl_3$

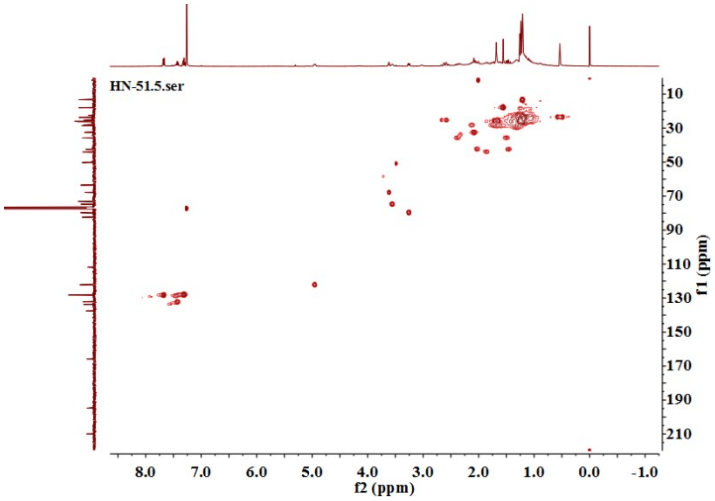

Figure S43. HMBC spectrum of 4 in $CDCl_3$

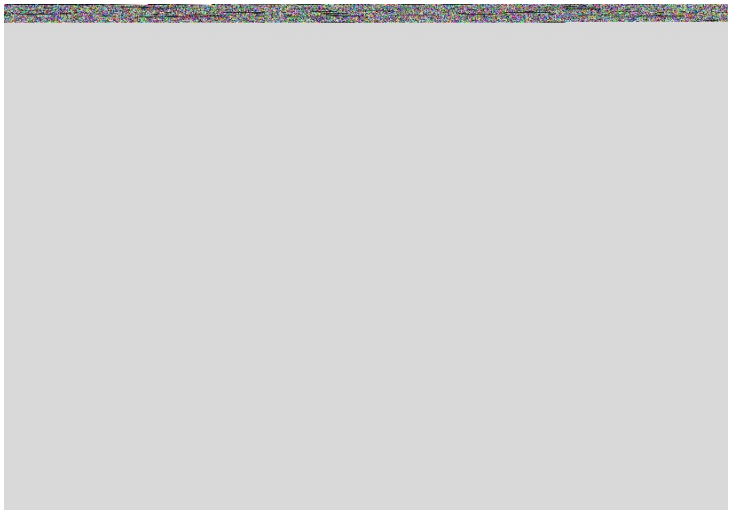

Figure S44. ^{1}H-^{1}H ROESY spectrum of 4 in $CDCl_3$

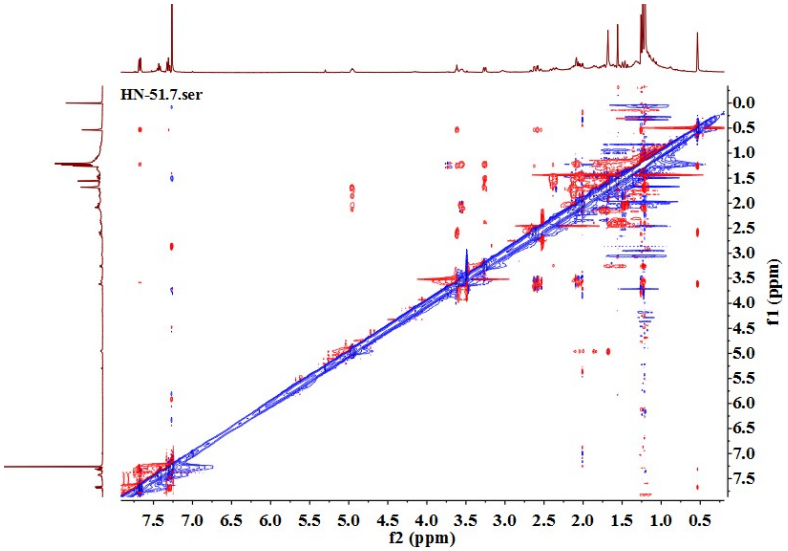

Figure S45. HRESIMS spectrum of 19

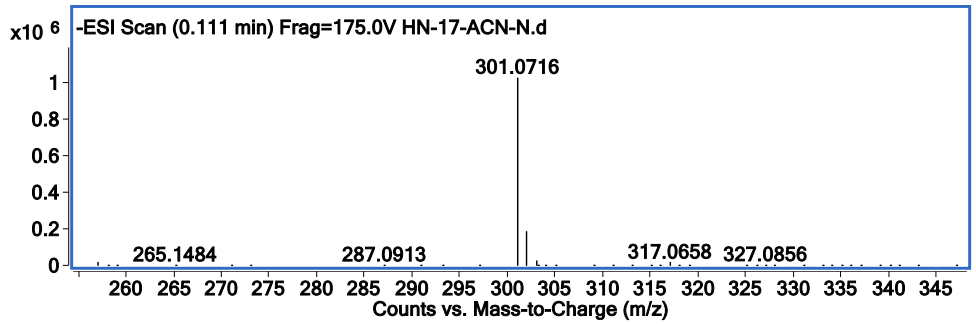

Figure S46. UV spectrum of 19

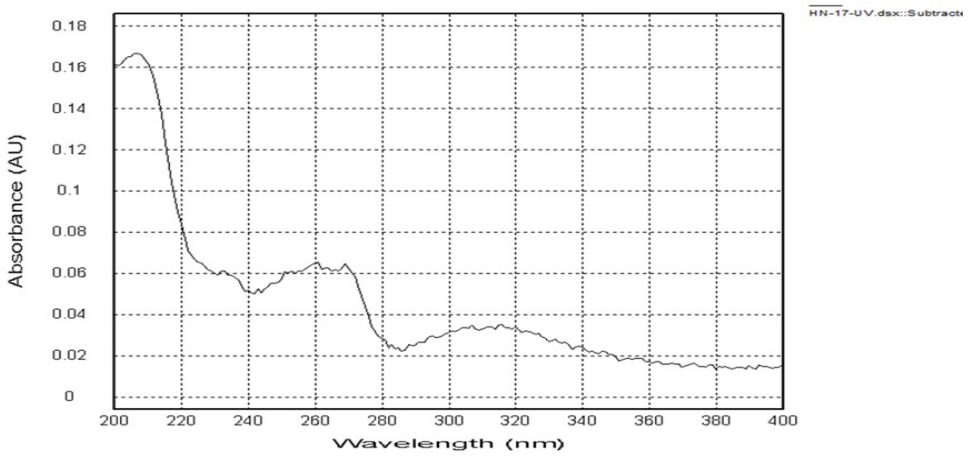

Figure S47. IR spectrum of 19

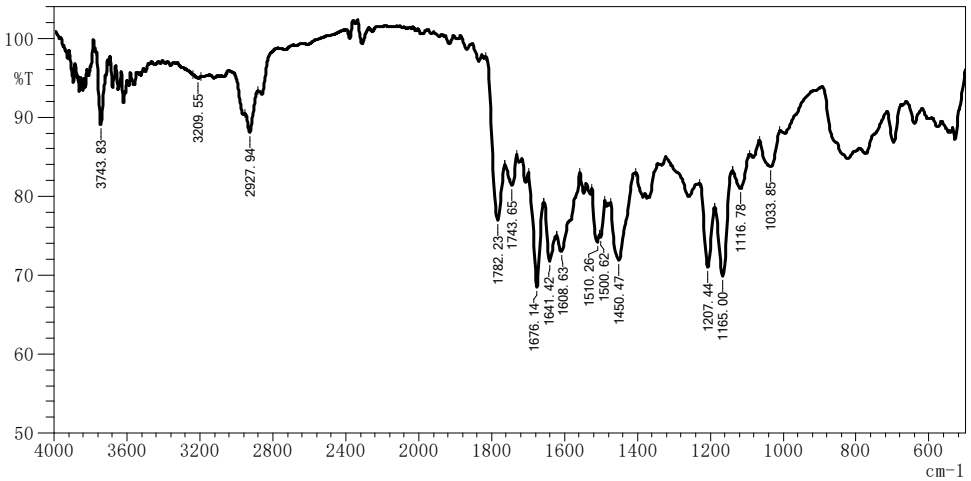

Figure S48. ^{1}H NMR (400 MHz) spectrum of 19 in $(CD_3)_2CO$

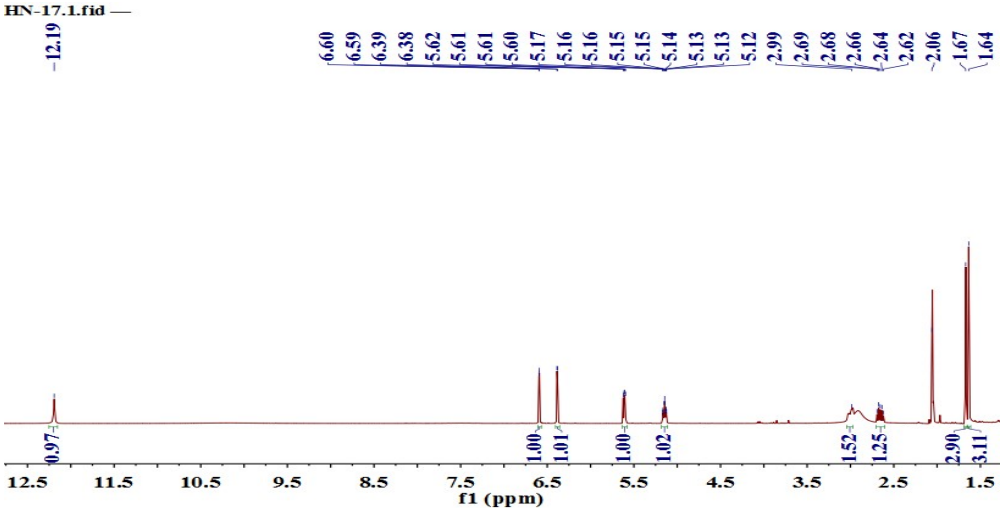

Figure S49. ^{13}C NMR (100 MHz) spectrum of 19 in $(CD_3)_2CO$

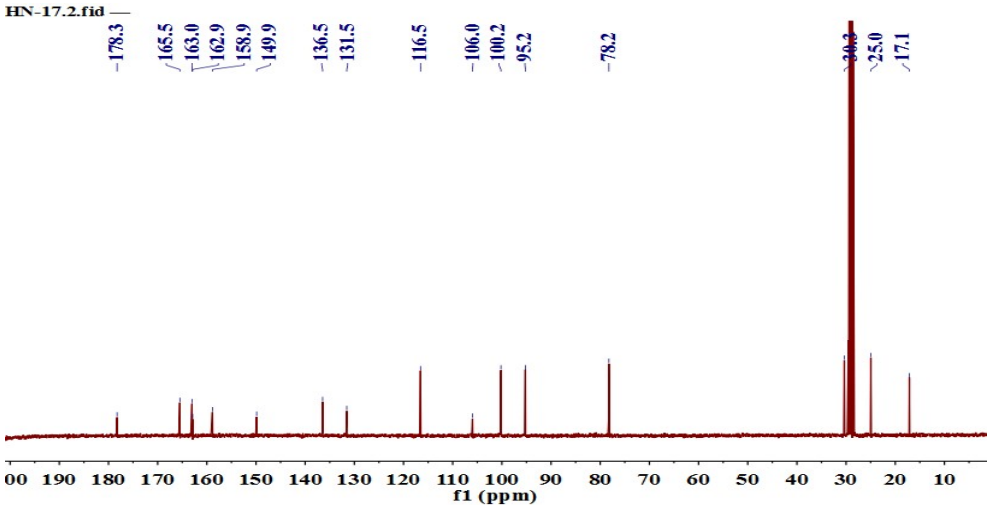

Figure S50. DEPT spectrum of 19 in $(CD_3)_2CO$

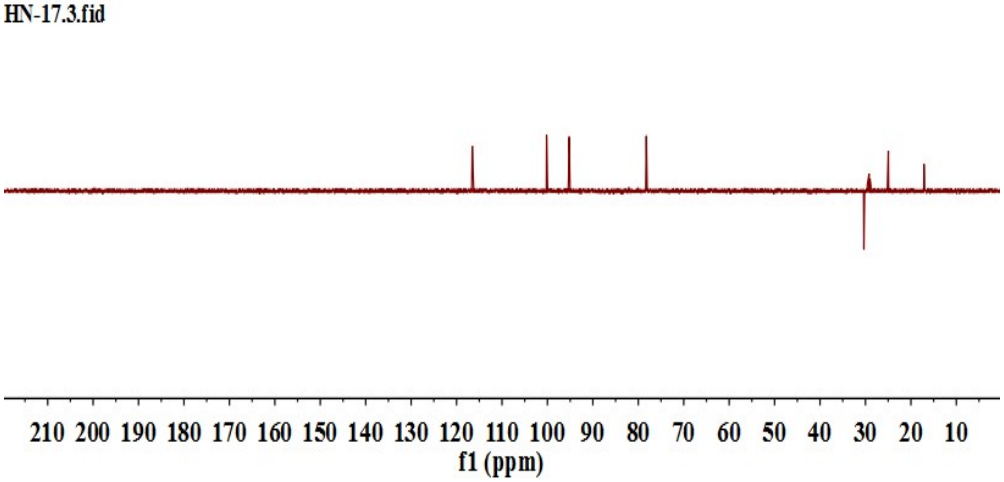

Figure S51. ^{1}H-^{1}H COSY spectrum of 19 in $(CD_3)_2CO$

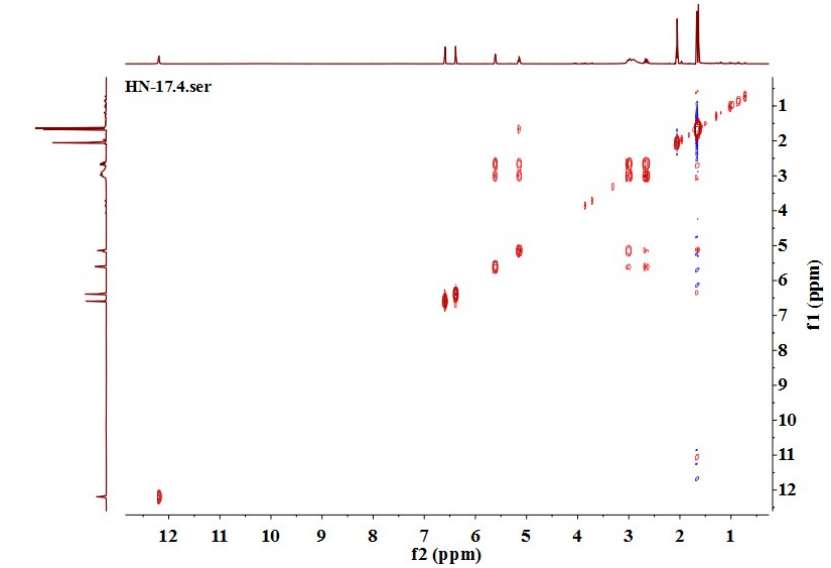

Figure S52. HSQC spectrum of 19 in $(CD_3)_2CO$

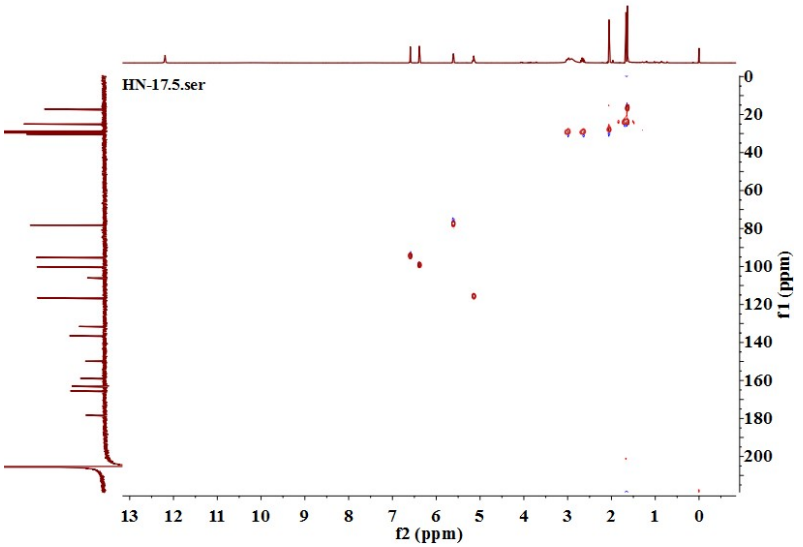

Figure S53. HMBC spectrum of 19 in $(CD_3)_2CO$

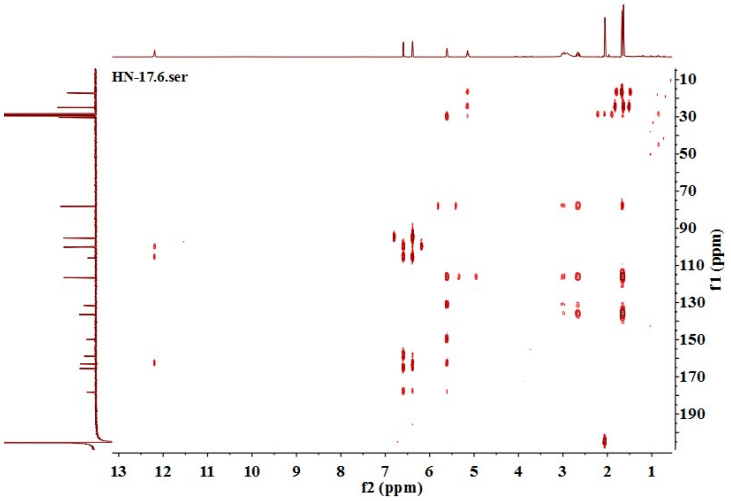

Figure S54. ^{1}H-^{1}H ROESY spectrum of 19 in $(CD_3)_2CO$

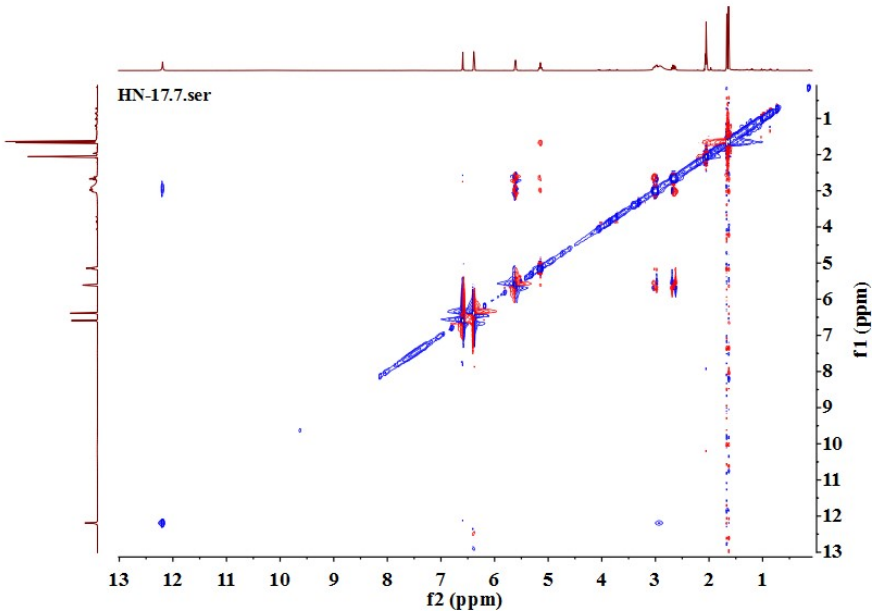

Figure S55. HRESIMS spectrum of 20

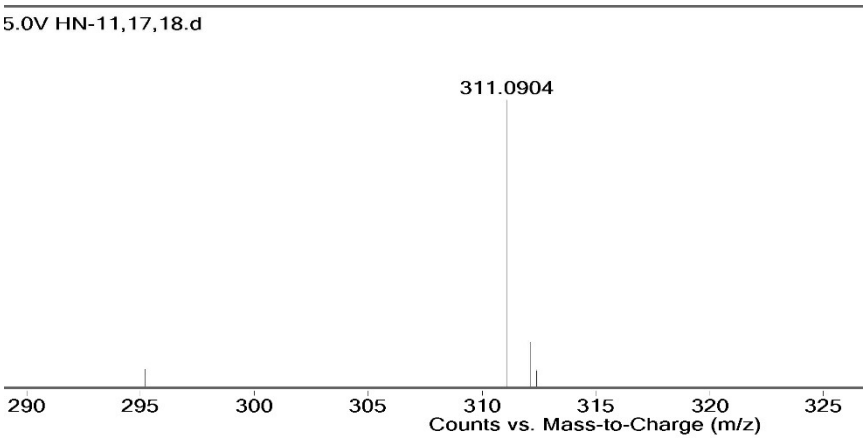

Figure S56. UV spectrum of 20

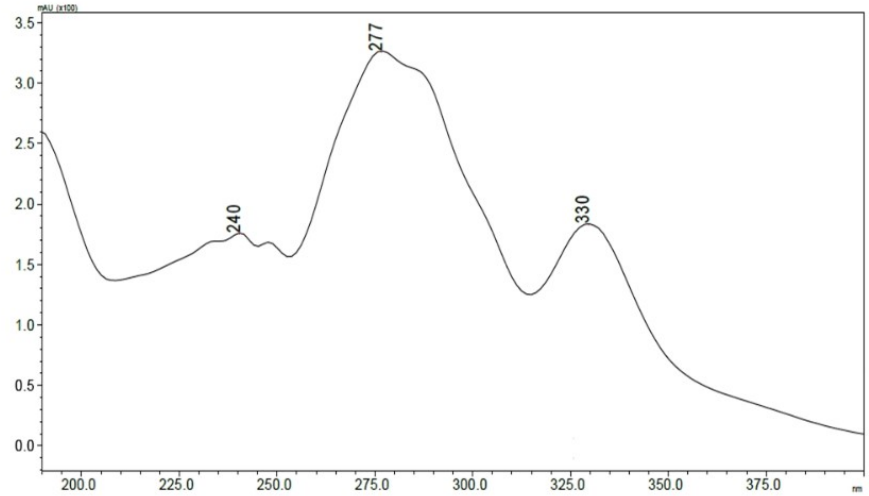

Figure S57. IR spectrum of 20

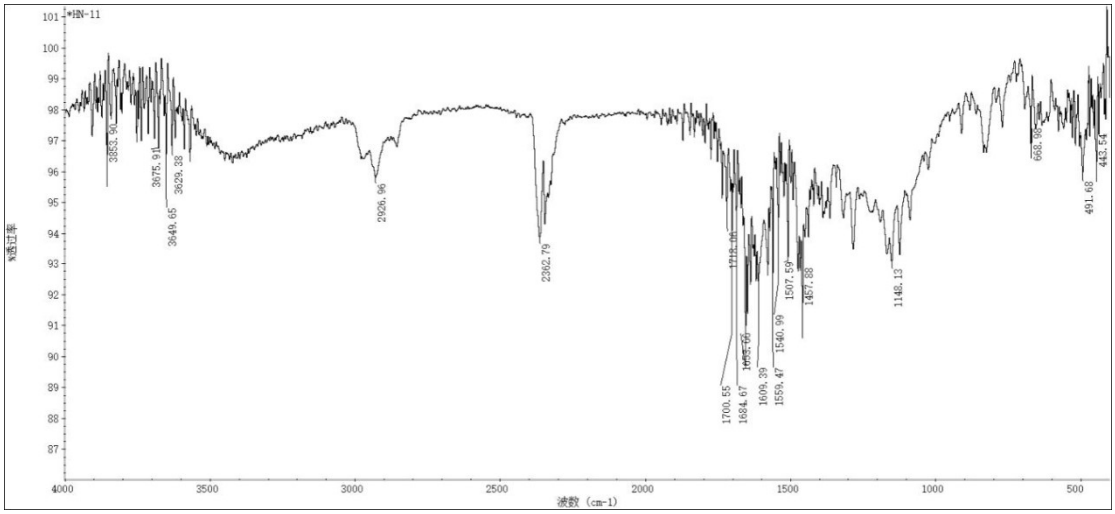

Figure S58. ^{1}H NMR (400 MHz) spectrum of 20 in $(CD_3)_2CO$

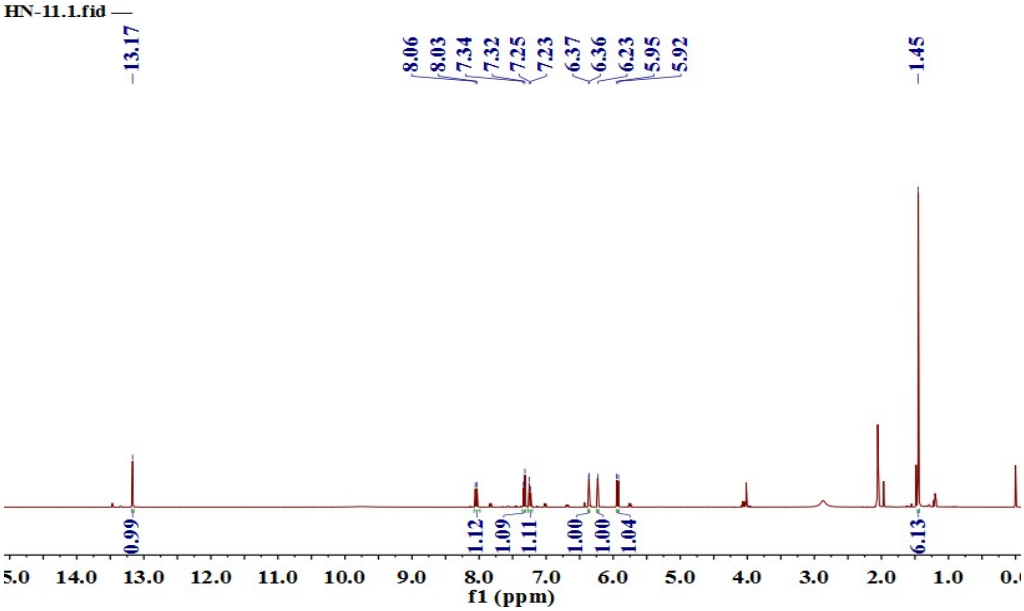

Figure S59. ^{13}C NMR (100 MHz) spectrum of 20 in $(CD_3)_2CO$

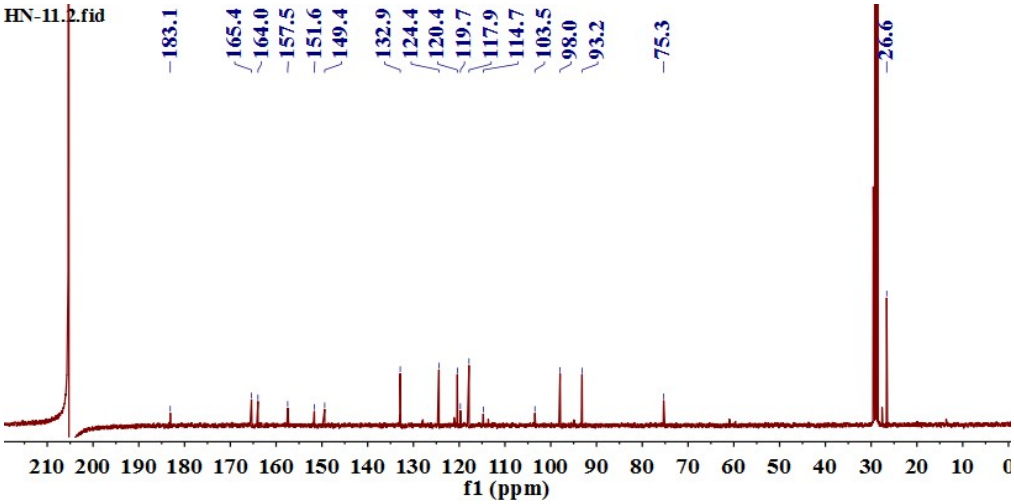

Figure S60. DEPT spectrum of 20 in $(CD_3)_2CO$

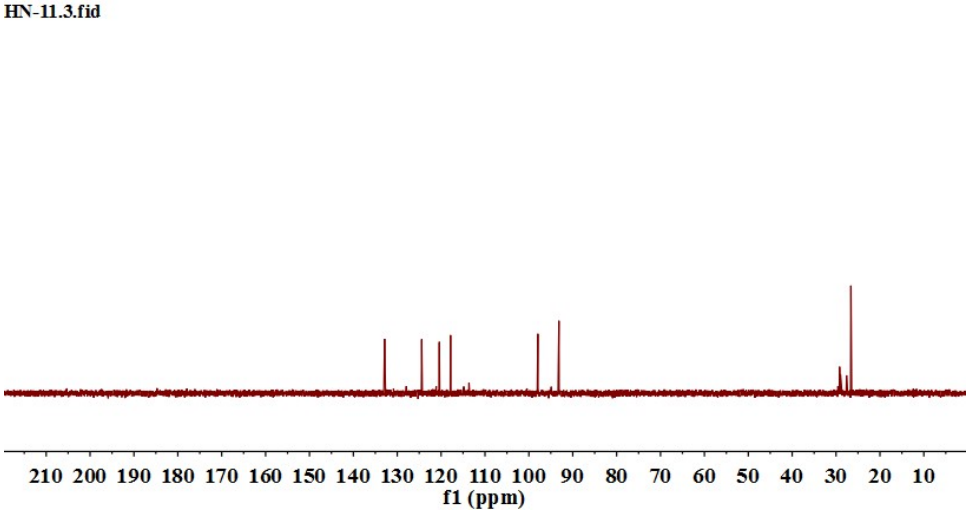

Figure S61. ^1H-^1H COSY spectrum of 20 in $(CD_3)_2CO$

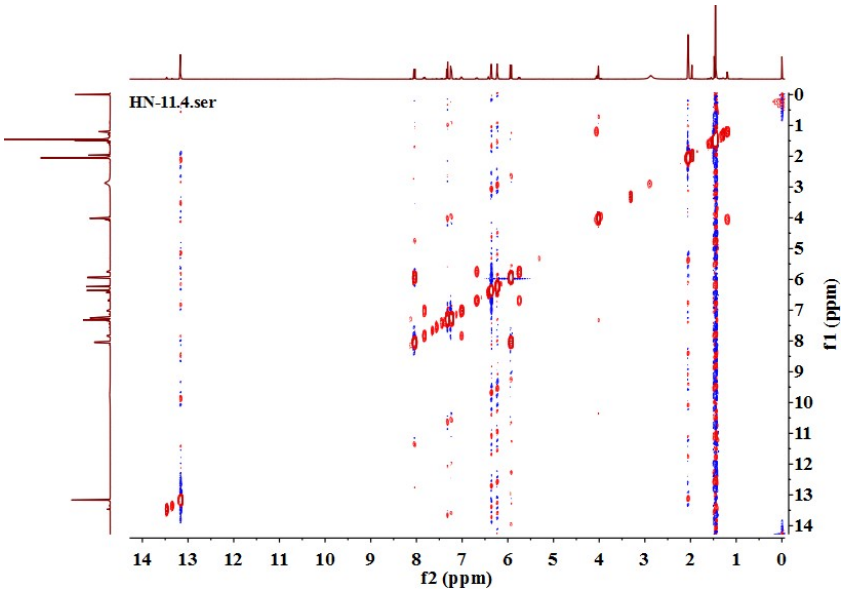

Figure S62. HSQC spectrum of 20 in $(CD_3)_2CO$

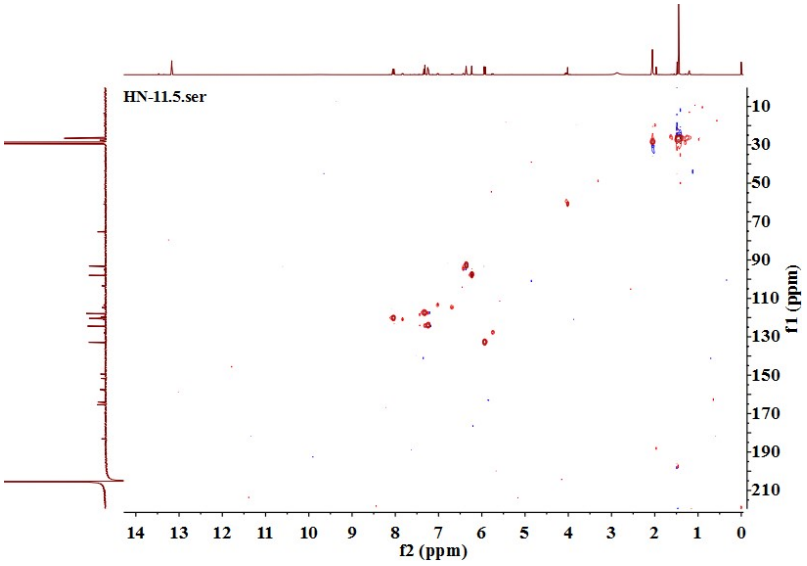

Figure S63. HMBC spectrum of 20 in $(CD_3)_2CO$

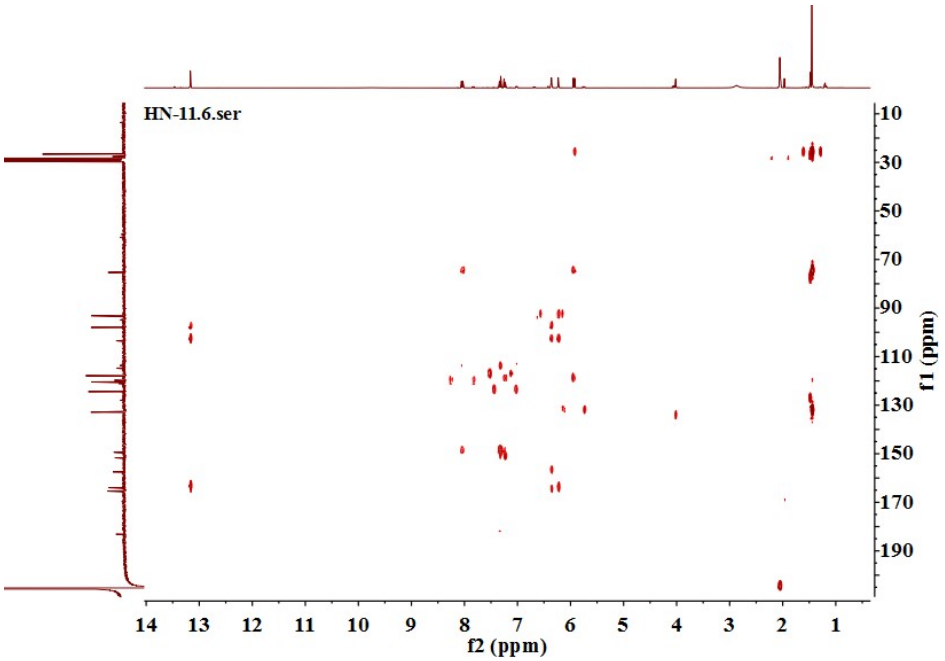

Figure S64. HRESIMS spectrum of 21

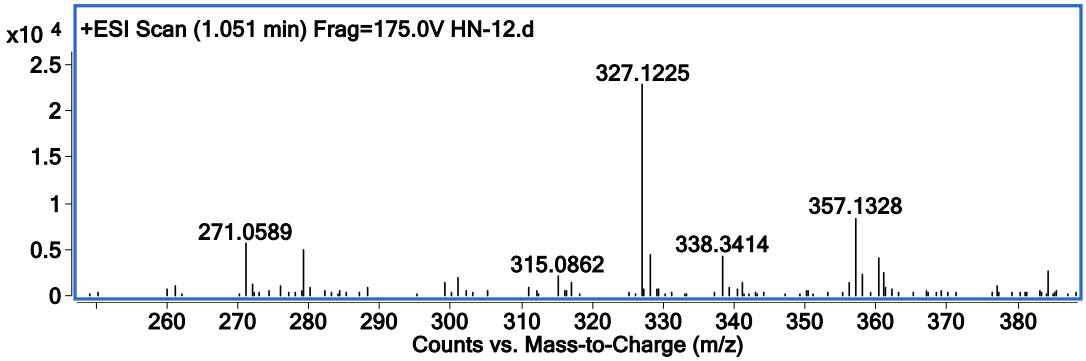

Figure S65. UV spectrum of 21

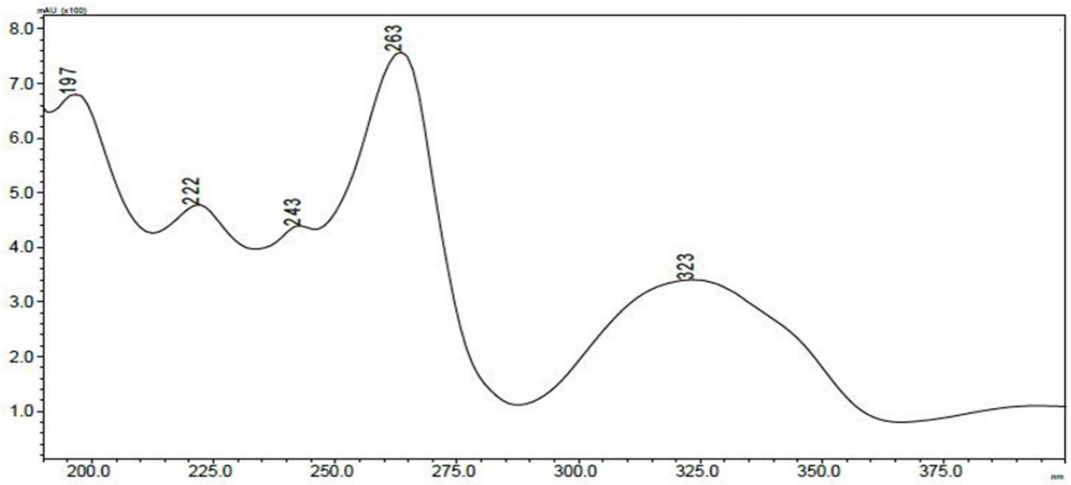

Figure S66. IR spectrum of 21

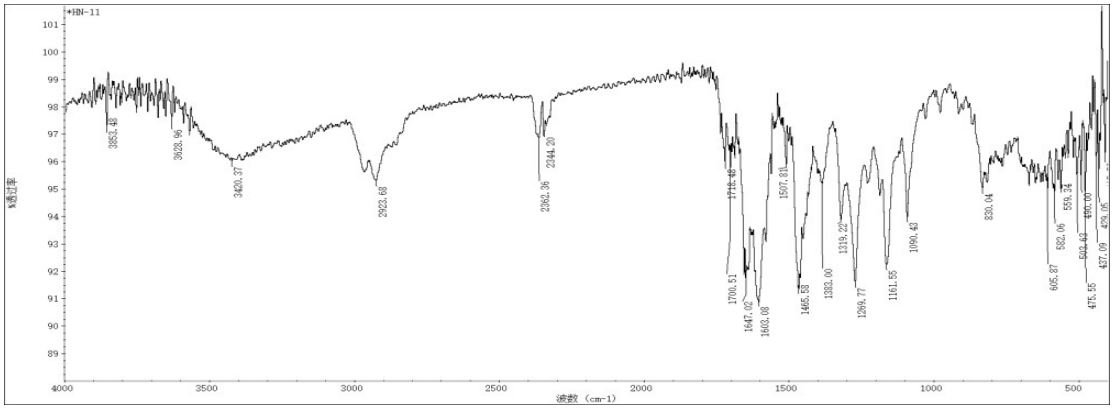

Figure S67. ^{1}H NMR (400 MHz) spectrum of 21 in $(CD_3)_2CO$

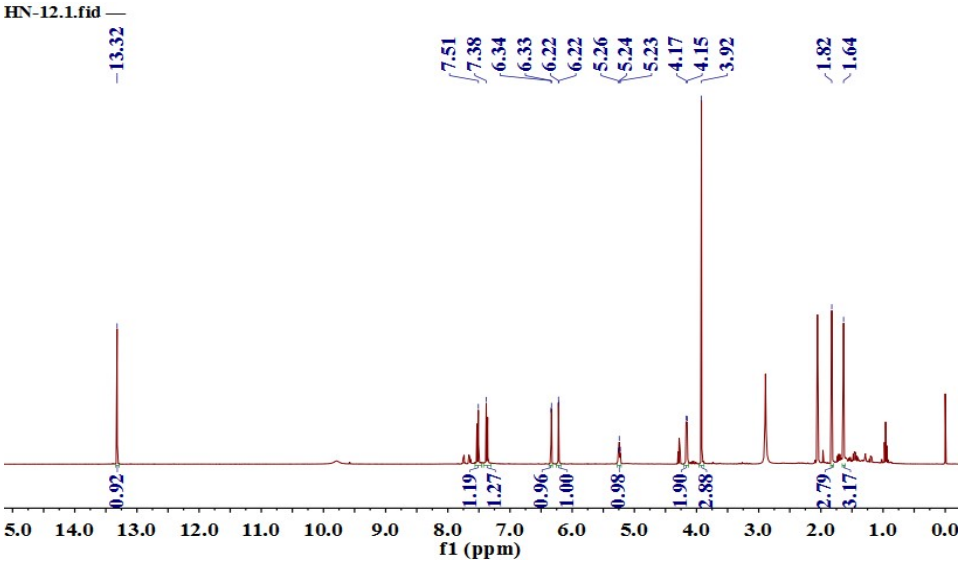

Figure S68. ^{13}C NMR (100 MHz) spectrum of 21 in $(CD_3)_2CO$

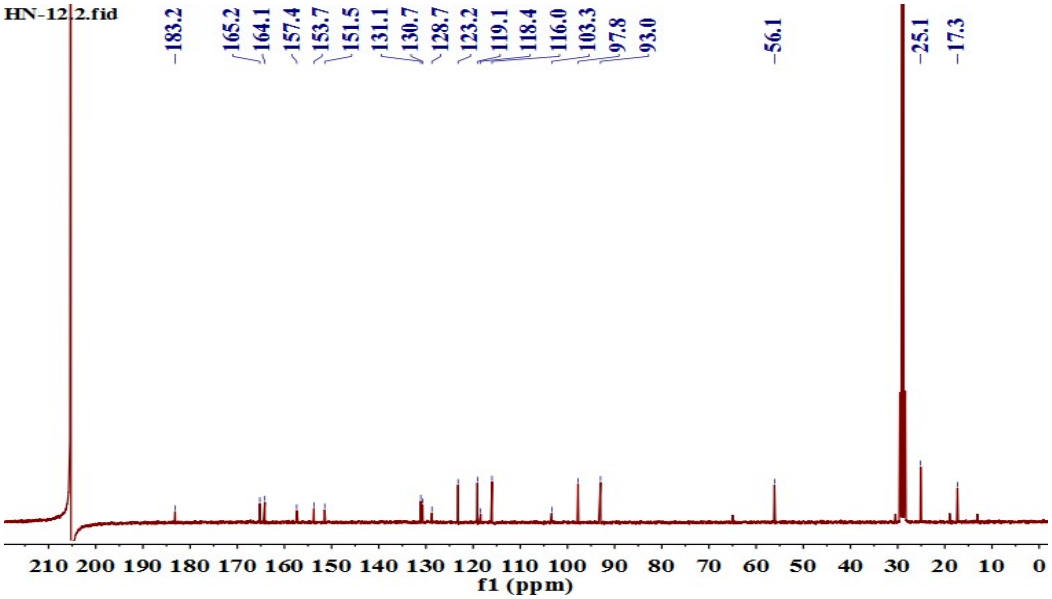

Figure S69. DEPT spectrum of 20 in $(CD_3)_2CO$

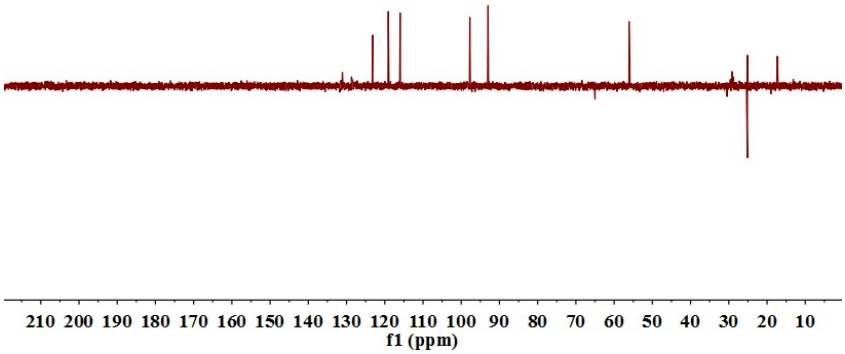

Figure S70. ^1H-^1H COSY spectrum of 21 in $(CD_3)_2CO$

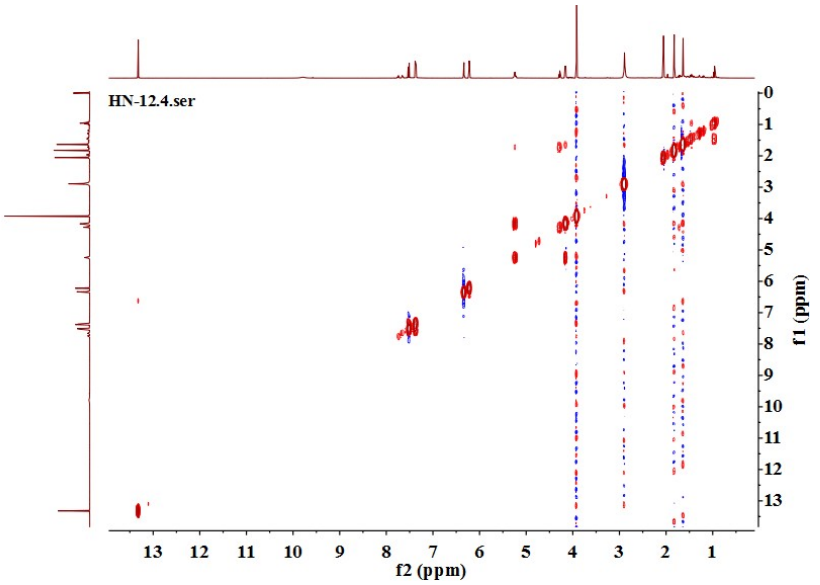

Figure S71. HSQC spectrum of 21 in $(CD_3)_2CO$

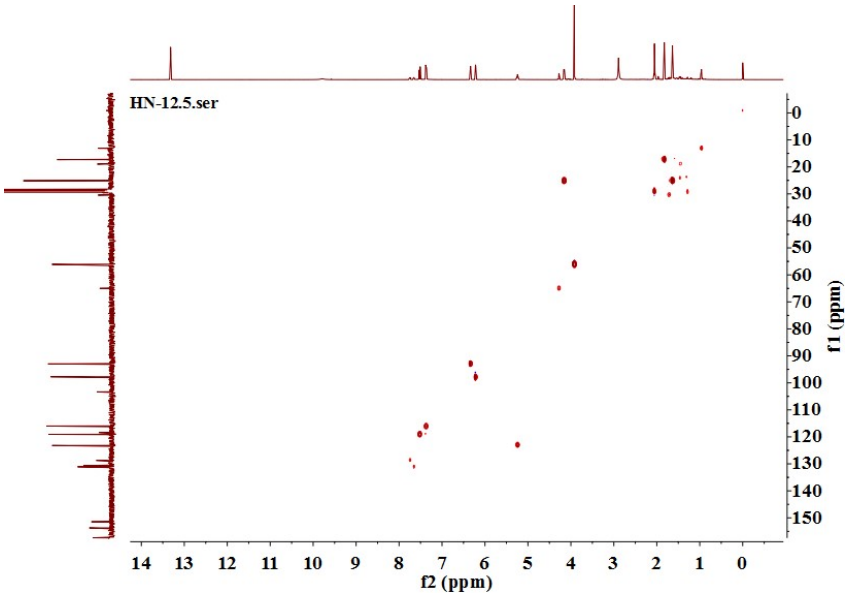

Figure S72. HMBC spectrum of 21 in $(CD_3)_2CO$