Supporting Information

The Isolation of novel pregnane steroids from *Aglaia pachyphylla* Miq and the cytotoxicity against breast cancer cell (MCF-7)

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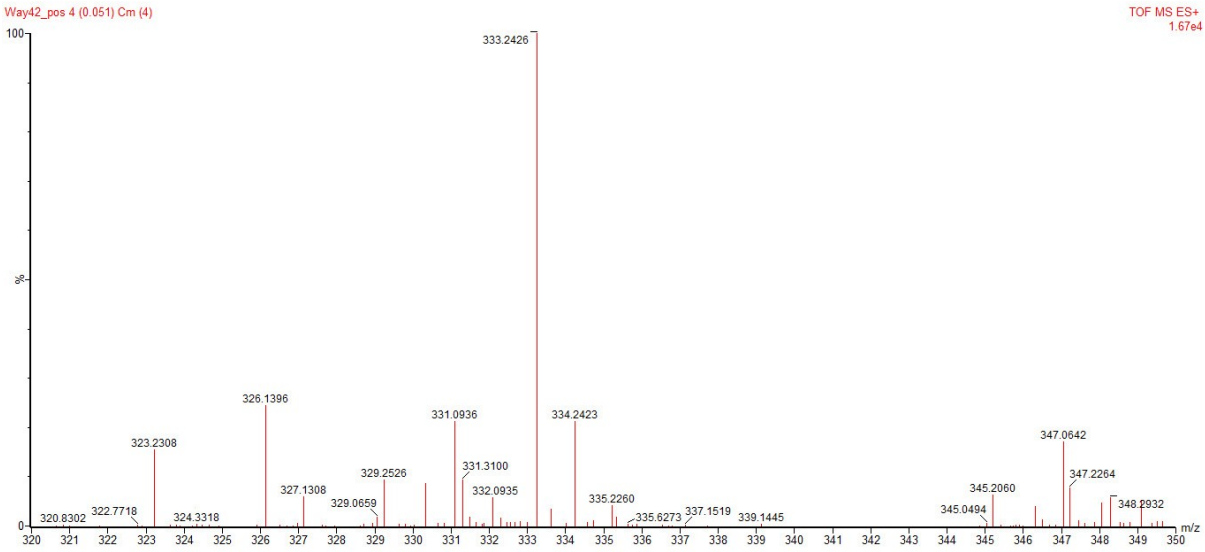
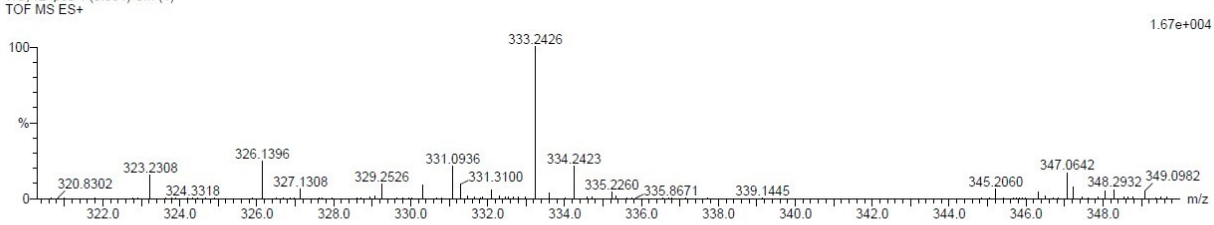
***Corresponding author:** desi.harneti@unpad.ac.id



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 3 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-50 O: 0-6
Way42_pos 4 (0.051) Cm (4)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
333.2426	333.2430	-0.4	-1.2	5.5	83.4	0.0	C21 H33 O3

Figure S1 HRTOF-MS spectrum of compound **1** (range of magnification *m/z* 320-350)

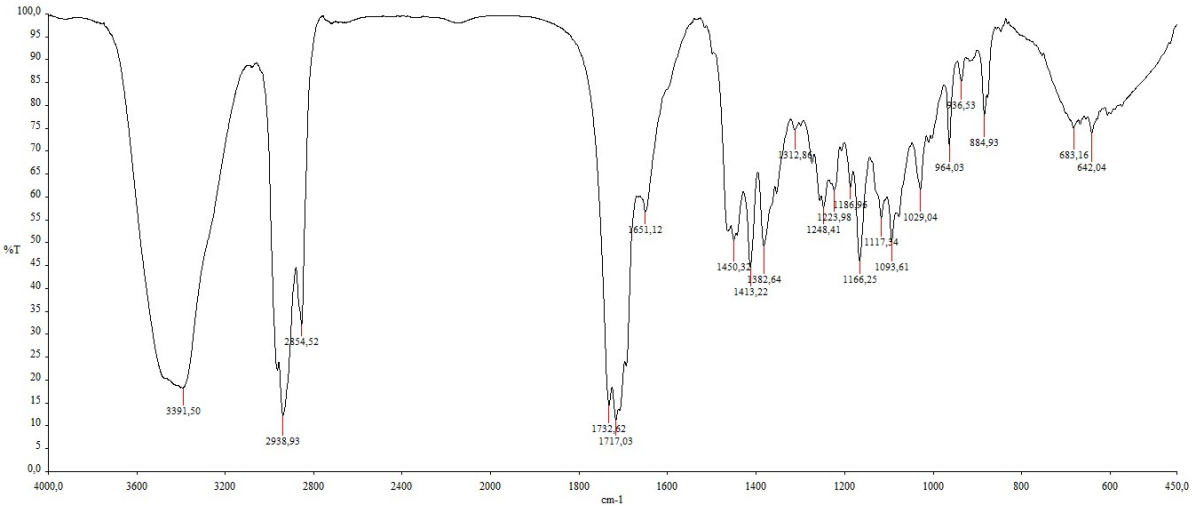


Figure S2 FTIR spectrum of compound **1**

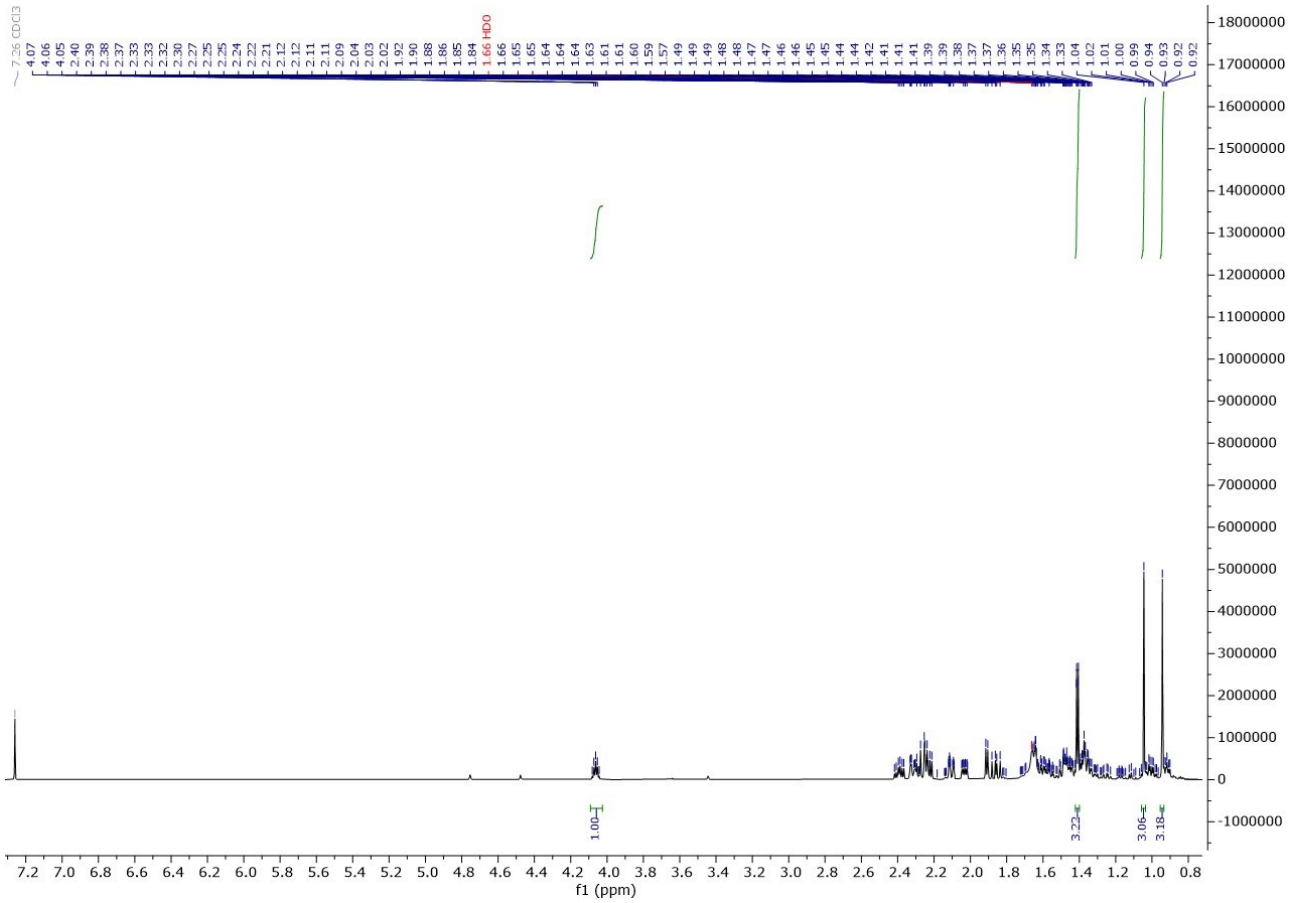


Figure S3 ^{1}H NMR spectrum (700 MHz, $CDCl_3$) of compound **1**

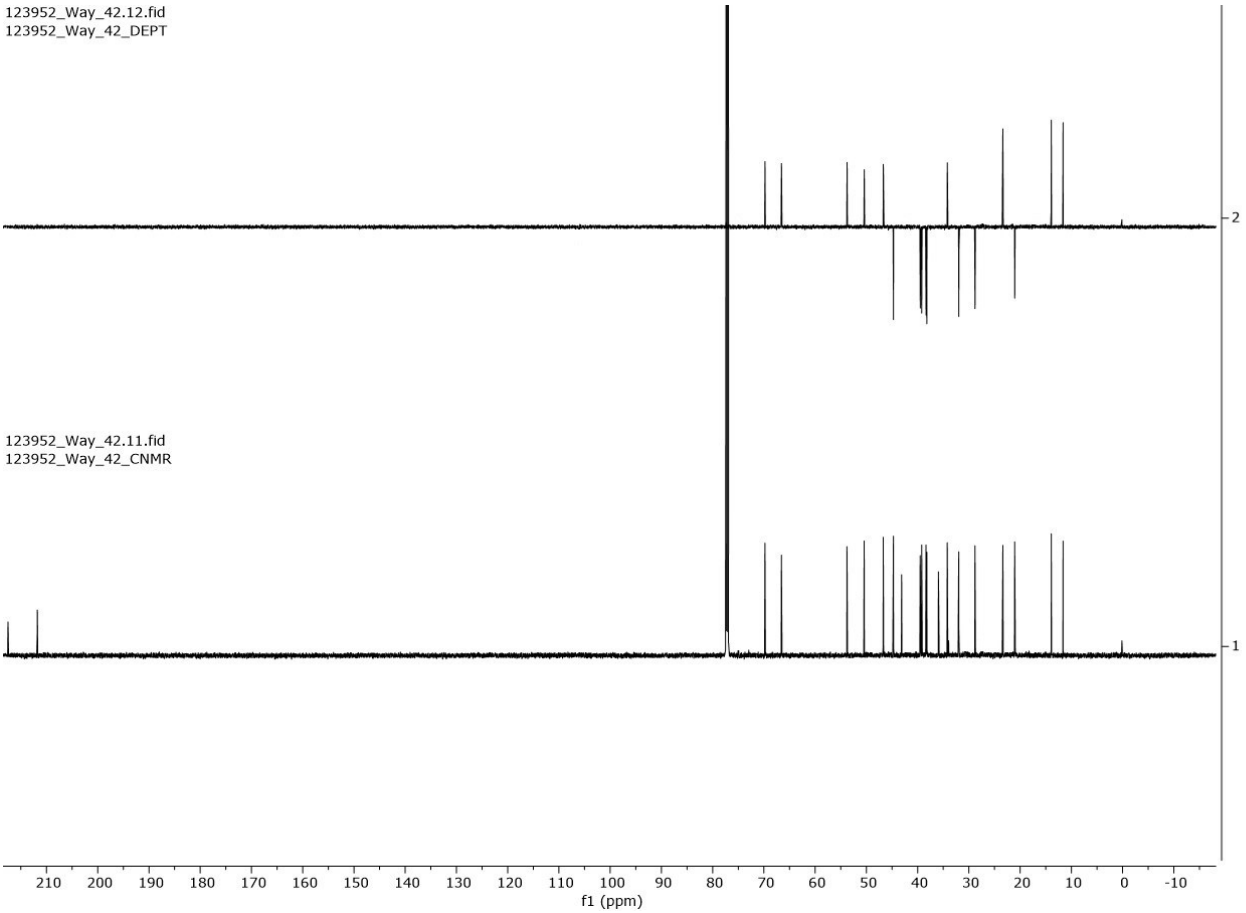


Figure S4 ^{13}C NMR (175 MHz, $CDCl_3$) and DEPT 135˚ of compound **1**

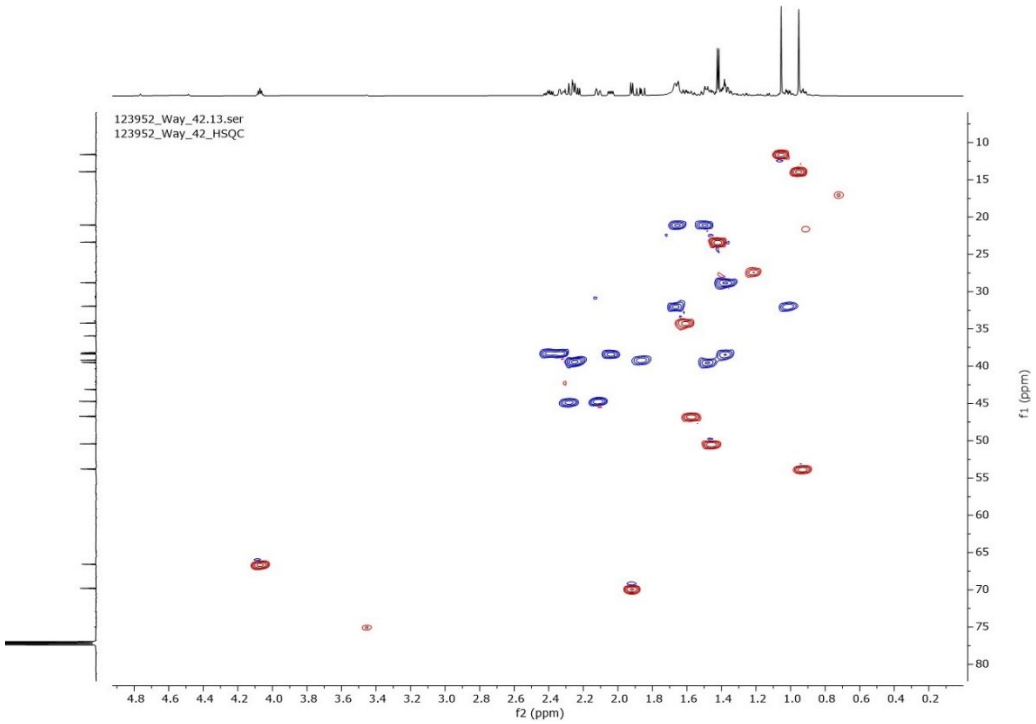


Figure S5 HSQC spectrum of compound **1**

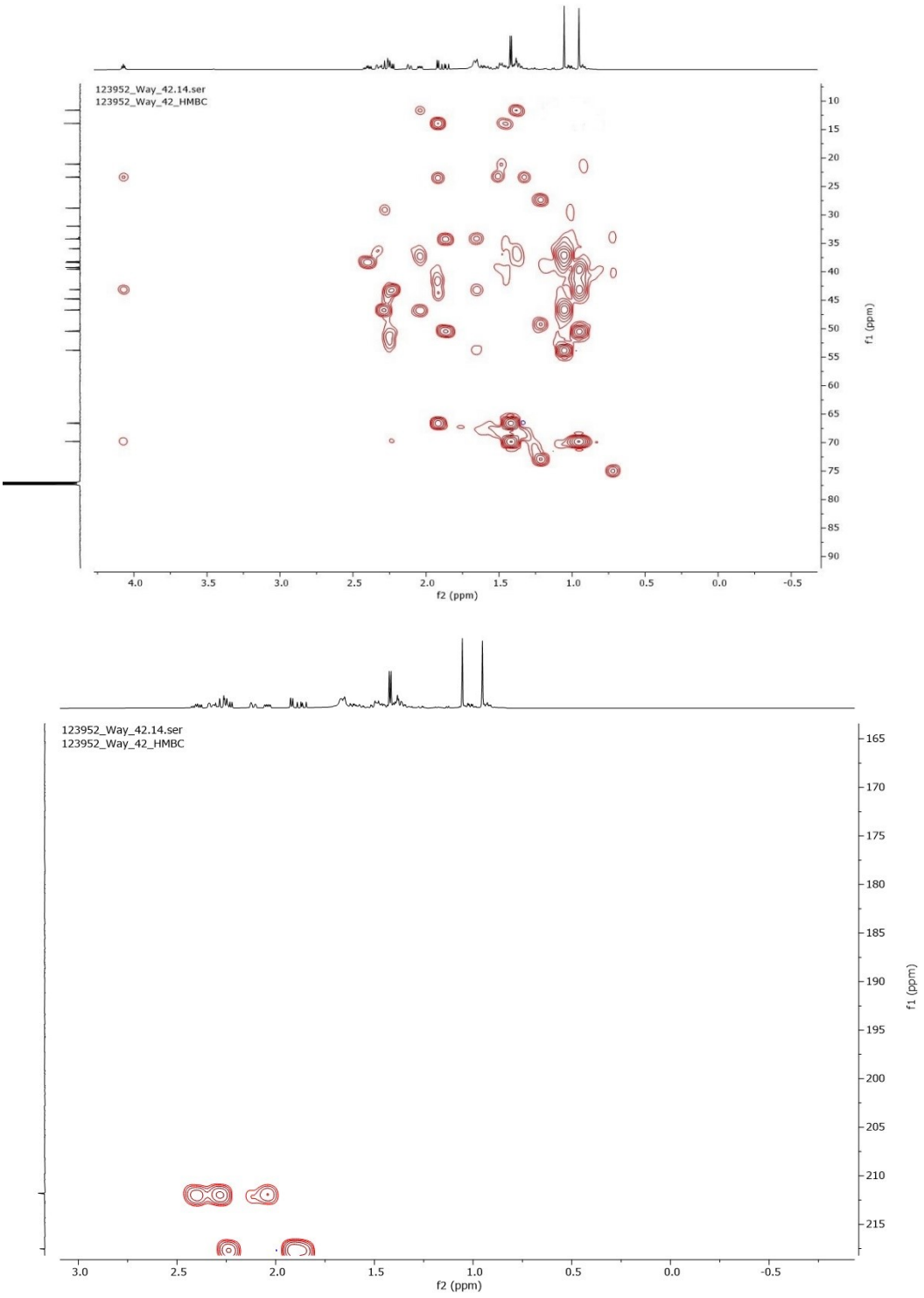


Figure S6. HMBC spectrum of compound **1**

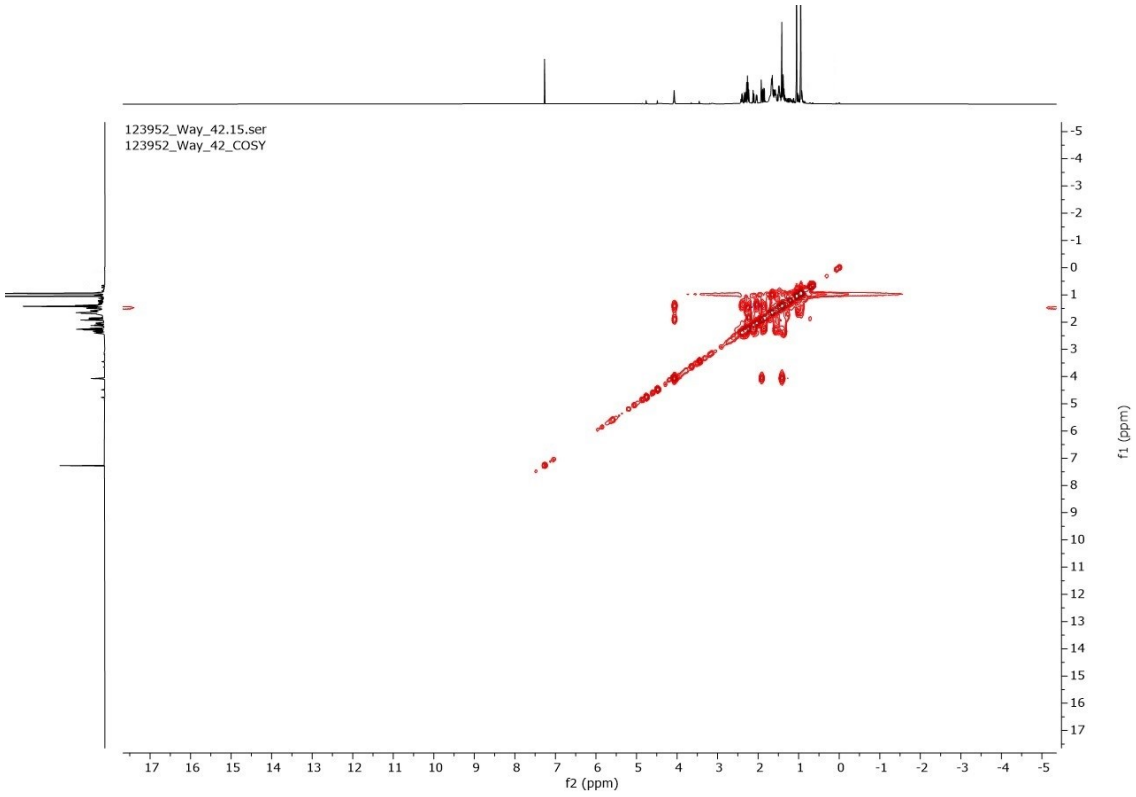


Figure S7 ^{1}H-^{1}H COSY spectrum of compound **1**

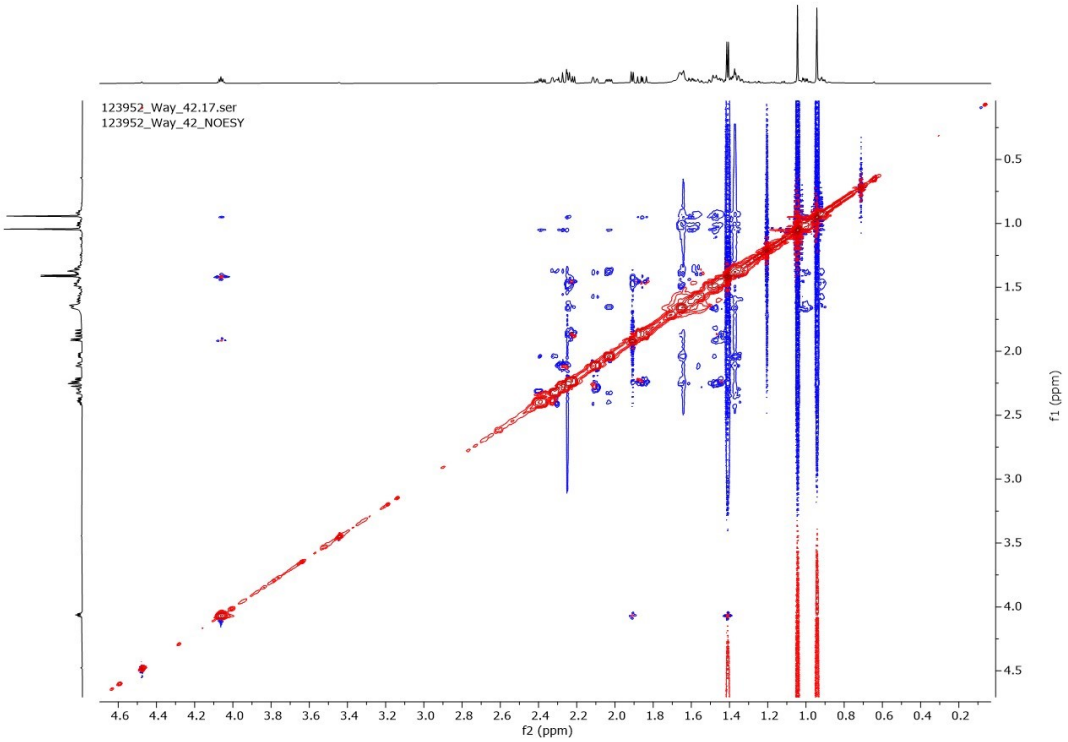
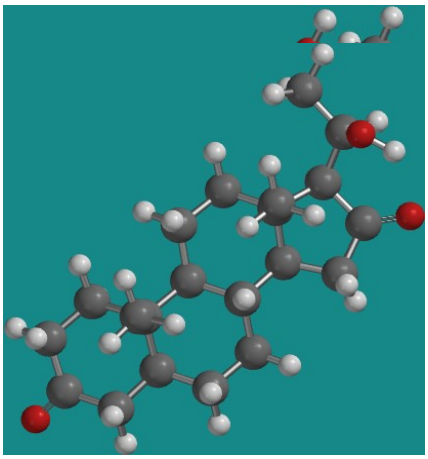


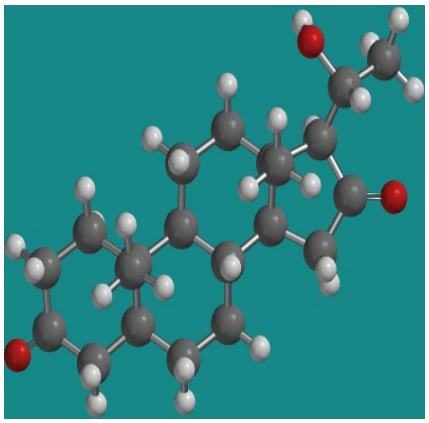
Figure S8 NOESY spectrum of compound **1**

ECD calculation of compound **1**

Conformation search of **1** at MMFF94s force field gave three conformers **1-1**-**1-3**. These conformers were optimized at B3LYP/6-31G(d) level, and then calculated the ECD at B3LYP/6-311G(d,p) level, nstates=20, IEFPCM, solvent=methanol.



1-1



1-2 **1-3**

Conformers	Gibbs Free Energies (Hartree)	Population (%)
1-1	-1045.18765	35.5
1-2	-1045.18775	32.0
1-3	-1045.18773	32.5

Table S1 Cartesian coordinates for the re-optimized conformers of compound **1** in the gas phase (Å) at B3LYP/6-31G (d) level.

Conf-**1-1**	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.163513	-1.5925	-0.42059
2	6	0	3.112608	0.904865	-0.21916
3	6	0	5.346937	-0.2715	-0.51815
4	6	0	4.63228	0.944405	0.052077
5	6	0	4.692445	-1.60867	-0.20535
6	6	0	2.434137	-0.41315	0.27714
7	6	0	0.93325	-0.36967	-0.18523
8	6	0	0.18856	0.906245	0.31039
9	6	0	0.932446	2.183791	-0.11561
10	6	0	2.408548	2.166806	0.296972
11	6	0	-1.24683	0.880362	-0.2334
12	6	0	-2.07067	-0.37322	0.196127

13	6	0	-1.33549	-1.60887	-0.35068
14	6	0	0.130906	-1.6558	0.126651
15	6	0	-3.44648	-0.04466	-0.46243
16	6	0	-3.57856	1.475179	-0.21648
17	6	0	-2.18437	2.063079	0.037577
18	6	0	2.541901	-0.58043	1.810432
19	6	0	-2.25198	-0.48445	1.727117
20	6	0	-4.6915	-0.83722	-0.03923
21	8	0	-4.3238	-2.22368	-0.04043
22	6	0	-5.88507	-0.59672	-0.96396
23	8	0	-4.61143	2.111883	-0.19872
24	8	0	6.365313	-0.18081	-1.17791
25	1	0	2.994012	0.906104	-1.31549
26	1	0	0.96716	-0.28426	-1.28537
27	1	0	0.146851	0.895234	1.409014
28	1	0	-1.15257	0.80847	-1.33036
29	1	0	-3.32264	-0.17061	-1.55198
30	1	0	2.75723	-2.55007	-0.07712
31	1	0	2.962201	-1.53979	-1.5
32	1	0	4.821426	0.980408	1.135359
33	1	0	5.084224	1.842091	-0.38232
34	1	0	4.914858	-1.84668	0.845257
35	1	0	5.17163	-2.3799	-0.816
36	1	0	0.434417	3.066024	0.306008
37	1	0	0.868891	2.285332	-1.21015
38	1	0	2.496149	2.225867	1.390832
39	1	0	2.916977	3.056106	-0.09817
40	1	0	-1.85441	-2.52645	-0.05943
41	1	0	-1.35642	-1.57401	-1.45008
42	1	0	0.151221	-1.85763	1.204424
43	1	0	0.616299	-2.51603	-0.34791
44	1	0	-2.14006	2.412609	1.078181
45	1	0	-2.02344	2.940081	-0.59743
46	1	0	1.988743	0.189417	2.356079
47	1	0	2.146905	-1.55237	2.124012
48	1	0	3.578627	-0.53247	2.156965
49	1	0	-2.78219	0.3774	2.149727
50	1	0	-1.29826	-0.56549	2.254901
51	1	0	-2.83729	-1.37934	1.958821
52	1	0	-4.9699	-0.53251	0.981955
53	1	0	-5.12453	-2.73285	0.162214
54	1	0	-6.75151	-1.18265	-0.62859
55	1	0	-5.64024	-0.90769	-1.9864

56	1	0	-6.16456	0.459239	-0.96588

Conf-**1**-**2**	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.161578	-1.59303	-0.41805
2	6	0	3.112112	0.904837	-0.22016
3	6	0	5.344908	-0.27307	-0.522
4	6	0	4.632262	0.943865	0.048564
5	6	0	4.690816	-1.60951	-0.2051
6	6	0	2.433779	-0.41219	0.278965
7	6	0	0.932353	-0.36823	-0.18166
8	6	0	0.188539	0.908922	0.312175
9	6	0	0.933025	2.18538	-0.11591
10	6	0	2.40944	2.167745	0.295454
11	6	0	-1.24701	0.883084	-0.23138
12	6	0	-2.07224	-0.36886	0.198896
13	6	0	-1.33598	-1.60703	-0.34093
14	6	0	0.13066	-1.65324	0.135694
15	6	0	-3.44744	-0.04423	-0.46146
16	6	0	-3.57869	1.478586	-0.22491
17	6	0	-2.18544	2.065369	0.039422
18	6	0	2.543068	-0.57736	1.812375
19	6	0	-2.25553	-0.4773	1.730002
20	6	0	-4.69309	-0.84866	-0.03275
21	8	0	-4.406	-2.24982	0.067417
22	6	0	-5.89204	-0.60846	-0.94928
23	8	0	-4.61061	2.116521	-0.22181
24	8	0	6.360827	-0.18378	-1.18557
25	1	0	2.991855	0.90474	-1.31633
26	1	0	0.964831	-0.28583	-1.28212
27	1	0	0.147284	0.899274	1.410696
28	1	0	-1.15248	0.811531	-1.32859
29	1	0	-3.3231	-0.16548	-1.55335
30	1	0	2.755711	-2.55003	-0.07236
31	1	0	2.958828	-1.54189	-1.49733
32	1	0	4.82337	0.980964	1.131427
33	1	0	5.083716	1.840853	-0.3877
34	1	0	4.914675	-1.84554	0.845594
35	1	0	5.168538	-2.38215	-0.81508
36	1	0	0.435843	3.068209	0.305299
37	1	0	0.868615	2.285927	-1.21051
38	1	0	2.498086	2.227931	1.38913
39	1	0	2.918013	3.056253	-0.10114
40	1	0	-1.85168	-2.52322	-0.03599

41	1	0	-1.35452	-1.57936	-1.44152
42	1	0	0.149084	-1.85003	1.21414
43	1	0	0.615686	-2.51584	-0.33476
44	1	0	-2.14509	2.410618	1.081577
45	1	0	-2.02133	2.944459	-0.59174
46	1	0	1.989907	0.192727	2.35763
47	1	0	2.149533	-1.54926	2.127977
48	1	0	3.580093	-0.52802	2.157633
49	1	0	-2.79584	0.380689	2.147326
50	1	0	-1.30157	-0.54406	2.25946
51	1	0	-2.83101	-1.37691	1.966972
52	1	0	-4.9647	-0.55959	0.987759
53	1	0	-4.29011	-2.58657	-0.83599
54	1	0	-6.7467	-1.20003	-0.60553
55	1	0	-5.65664	-0.91335	-1.97941
56	1	0	-6.1633	0.449776	-0.96116

Conf-**1**-**3**	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.168228	-1.59604	-0.36145
2	6	0	3.106667	0.903168	-0.18224
3	6	0	5.351581	-0.2725	-0.38139
4	6	0	4.613857	0.946494	0.151697
5	6	0	4.6871	-1.60823	-0.08365
6	6	0	2.410264	-0.41205	0.29673
7	6	0	0.929723	-0.3725	-0.22727
8	6	0	0.163154	0.904467	0.230029
9	6	0	0.921747	2.179883	-0.17624
10	6	0	2.380574	2.168188	0.294308
11	6	0	-1.24779	0.870504	-0.3736
12	6	0	-2.09276	-0.38093	0.036198
13	6	0	-1.33013	-1.61792	-0.47195
14	6	0	0.118906	-1.65873	0.05883
15	6	0	-3.43141	-0.04581	-0.6952
16	6	0	-3.5774	1.457212	-0.40984
17	6	0	-2.19385	2.061651	-0.15766
18	6	0	2.455186	-0.56622	1.834414
19	6	0	-2.32396	-0.47054	1.562094
20	6	0	-4.76635	-0.7916	-0.46028
21	8	0	-5.33297	-0.50753	0.816266
22	6	0	-4.68647	-2.30785	-0.59467
23	8	0	-4.63445	2.055432	-0.33215

24	8	0	6.393802	-0.18525	-1.00302
25	1	0	3.033781	0.895231	-1.28254
26	1	0	1.009309	-0.29317	-1.32538
27	1	0	0.076634	0.901476	1.325929
28	1	0	-1.10628	0.785595	-1.46434
29	1	0	-3.2187	-0.1198	-1.77708
30	1	0	2.749499	-2.5516	-0.02724
31	1	0	3.011525	-1.55192	-1.44866
32	1	0	4.757283	0.989545	1.241555
33	1	0	5.082419	1.841839	-0.26958
34	1	0	4.866584	-1.83696	0.977173
35	1	0	5.191465	-2.38389	-0.66777
36	1	0	0.406778	3.064605	0.218839
37	1	0	0.900982	2.273014	-1.27319
38	1	0	2.424565	2.237182	1.390116
39	1	0	2.903003	3.054757	-0.08825
40	1	0	-1.8385	-2.54512	-0.18462
41	1	0	-1.31162	-1.59915	-1.57189
42	1	0	0.098053	-1.85697	1.136706
43	1	0	0.622268	-2.51977	-0.3948
44	1	0	-2.16789	2.452265	0.868237
45	1	0	-2.01999	2.913378	-0.82364
46	1	0	1.877385	0.206277	2.34976
47	1	0	2.051561	-1.53698	2.140848
48	1	0	3.476776	-0.51121	2.222268
49	1	0	-2.83483	0.412656	1.958265
50	1	0	-1.38541	-0.58228	2.111586
51	1	0	-2.96095	-1.32512	1.803697
52	1	0	-5.44612	-0.41745	-1.24282
53	1	0	-5.5751	0.434154	0.79038
54	1	0	-5.6931	-2.73257	-0.53119
55	1	0	-4.08889	-2.74566	0.210214
56	1	0	-4.24479	-2.59745	-1.5545

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311+G(d,p)

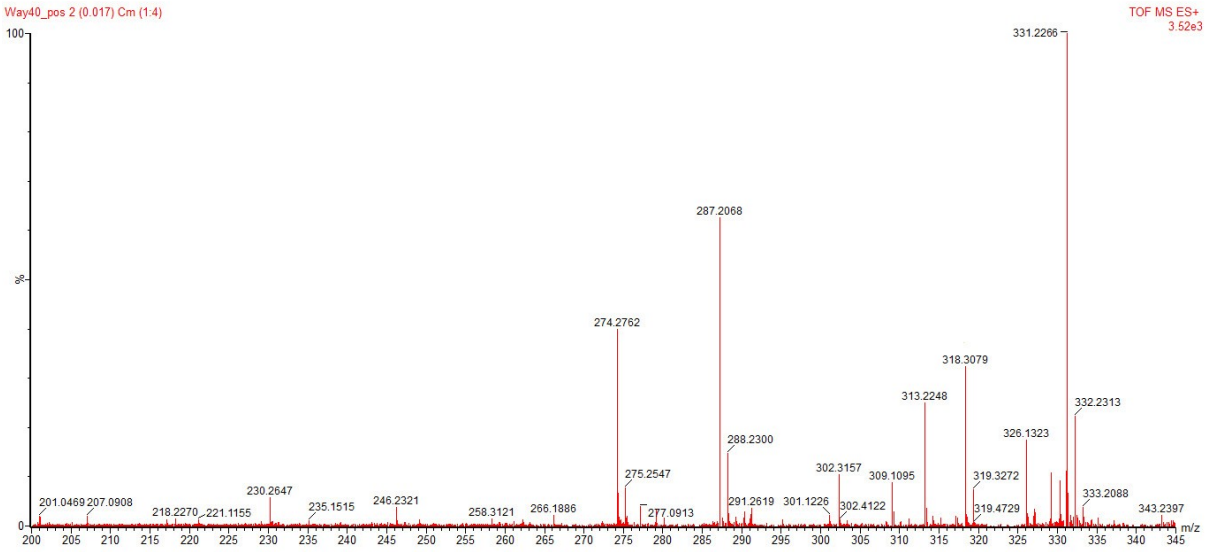
		DP4+	100.00%	0.00%	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3
C		38.2	37.0	36.8	
C		38.5	37.1	37.0	
C	x	211.7	216.2	216.0	
C		44.7	43.7	43.6	
C		46.7	46.1	45.9	
C		28.8	26.8	26.7	
C		31.9	30.1	29.8	
C		34.4	33.2	33.2	
C		53.8	51.7	51.4	
C		35.9	36.4	36.4	
C		21	19.3	19.2	
C		39.2	37.10	36.60	
C		43.1	43.50	41.60	
C		50.3	47.70	48.50	
C		39.5	38.30	38.20	
C	x	217.5	225.30	233.50	
C		69.7	67.30	69.10	
C		13.9	7.60	8.50	
C		11.6	6.80	6.70	
C		66.5	66.00	64.90	
C		23.3	20.48	17.00	

H	2.04	2.10	2.09	
H	1.37	1.42	1.41	
H	2.37	2.65	2.64	
H	2.33	2.24	2.25	
H	2.28	2.48	2.48	
H	2.11	2	2.01	
H	1.58	1.6	1.58	
H	1.38	1.59	1.59	
H	1.38	1.33	1.32	
H	1.66	1.75	1.73	
H	1.01	1.1	1.1	
H	1.6	1.78	1.75	
H	0.93	1.02	1.03	
H	1.65	1.6	1.59	
H	1.49	1.58	1.6	
H	1.86	2.45	1.98	
H	1.86	1.54	1.58	
H	1.46	1.58	1.66	
H	1.48	2.02	2.14	
H	2.25	2.19	2.3	
H	1.91	1.96	1.65	
H	0.95	0.62	1.31	
H	1.05	1.24	0.84	
H	4.06	4.1	4.13	
H	1.42	1.21	1.04	

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311+G(d,p)

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	80.79%	19.21%	-	-
sDP4+ (C data)	99.81%	0.19%	-	-
sDP4+ (all data)	99.95%	0.05%	-	-
uDP4+ (H data)	69.79%	30.21%	-	-
uDP4+ (C data)	100.00%	0.00%	-	-
uDP4+ (all data)	100.00%	0.00%	-	-
DP4+ (H data)	90.67%	9.33%	-	-
DP4+ (C data)	100.00%	0.00%	-	-
DP4+ (all data)	100.00%	0.00%	-	-

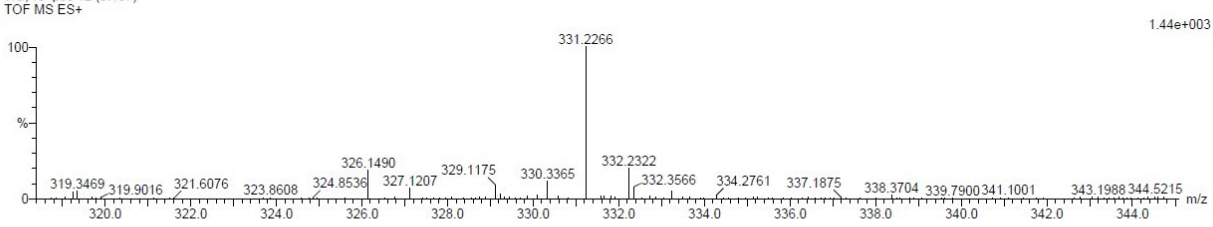
Figure S9 NMR calculation (DP4+ analysis) of compound **1**



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-35 O: 0-6
Way40_pos 12 (0.187)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
331.2266	331.2273	-0.7	-2.1	6.5	75.4	0.0	C21 H31 O3

Figure S10 HRTOF-MS spectrum of compound **2** (range of magnification *m/z* 319-345)

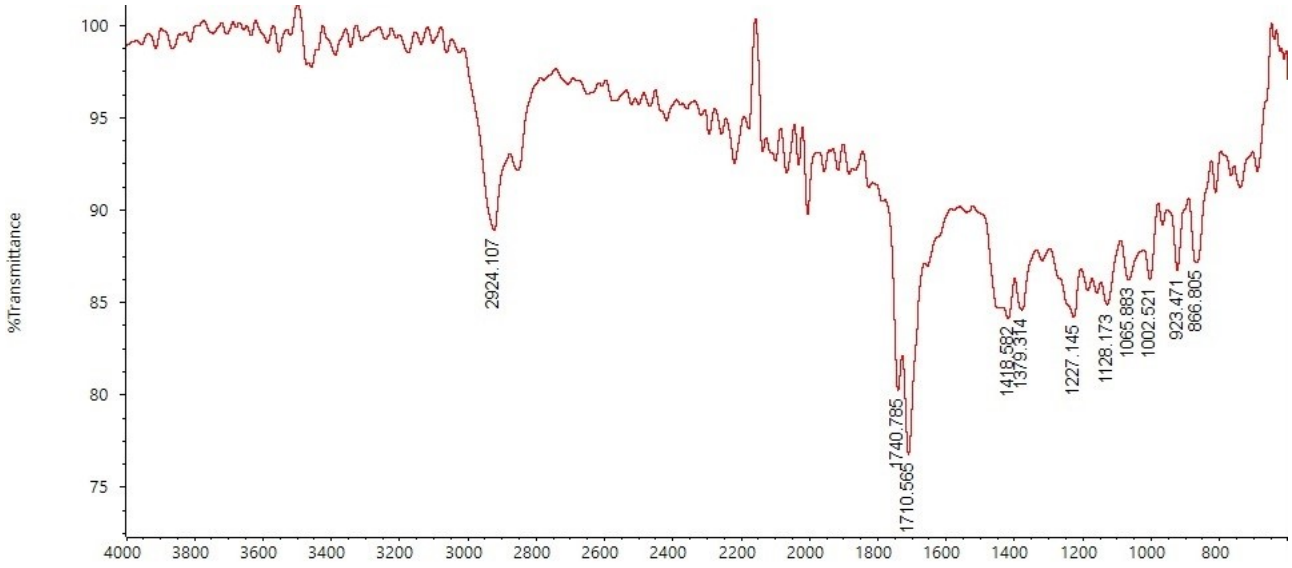


Figure S11 FTIR spectrum of compound **2**

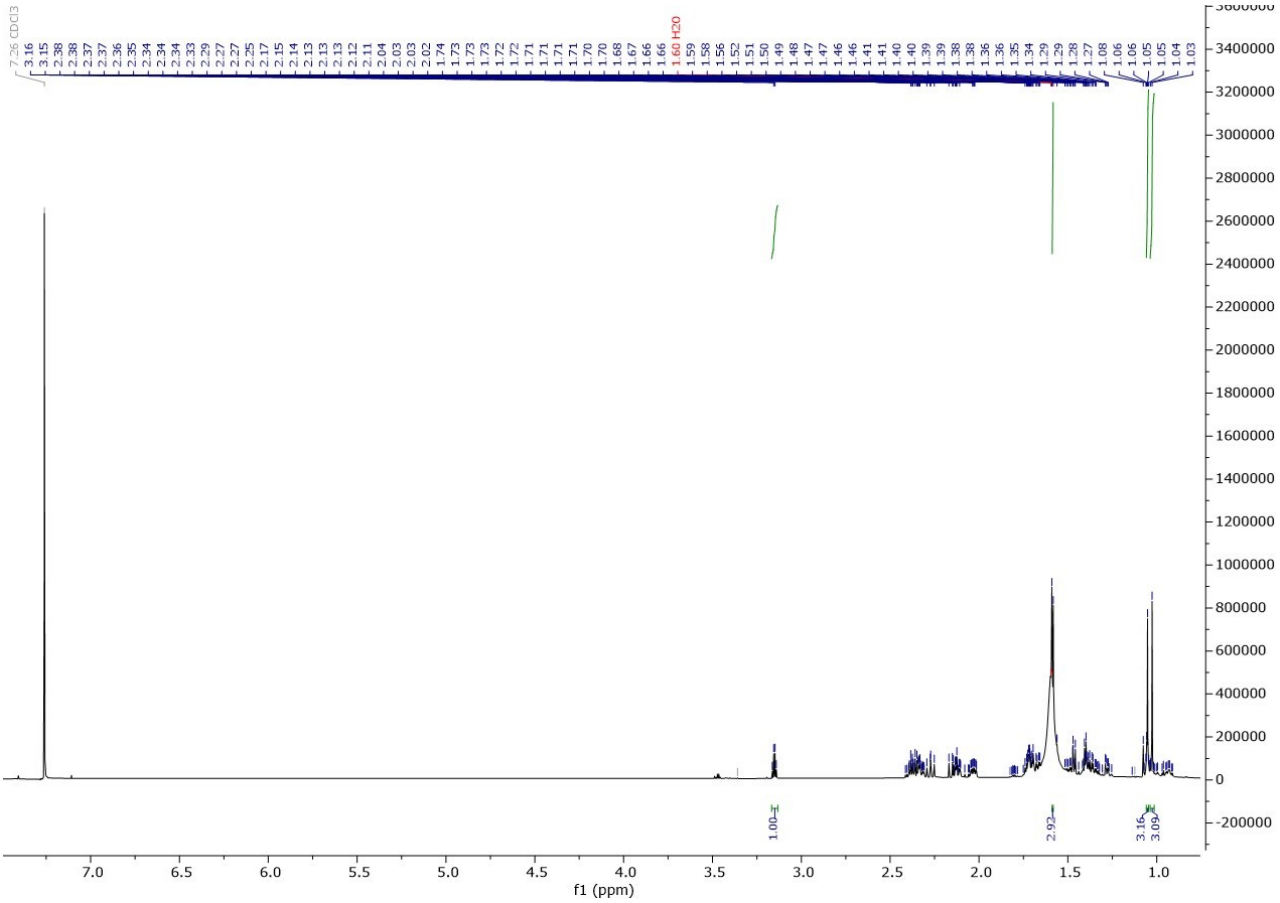


Figure S12 ^{1}H NMR (700 MHz, $CDCl_3$) spectrum of compound **2**

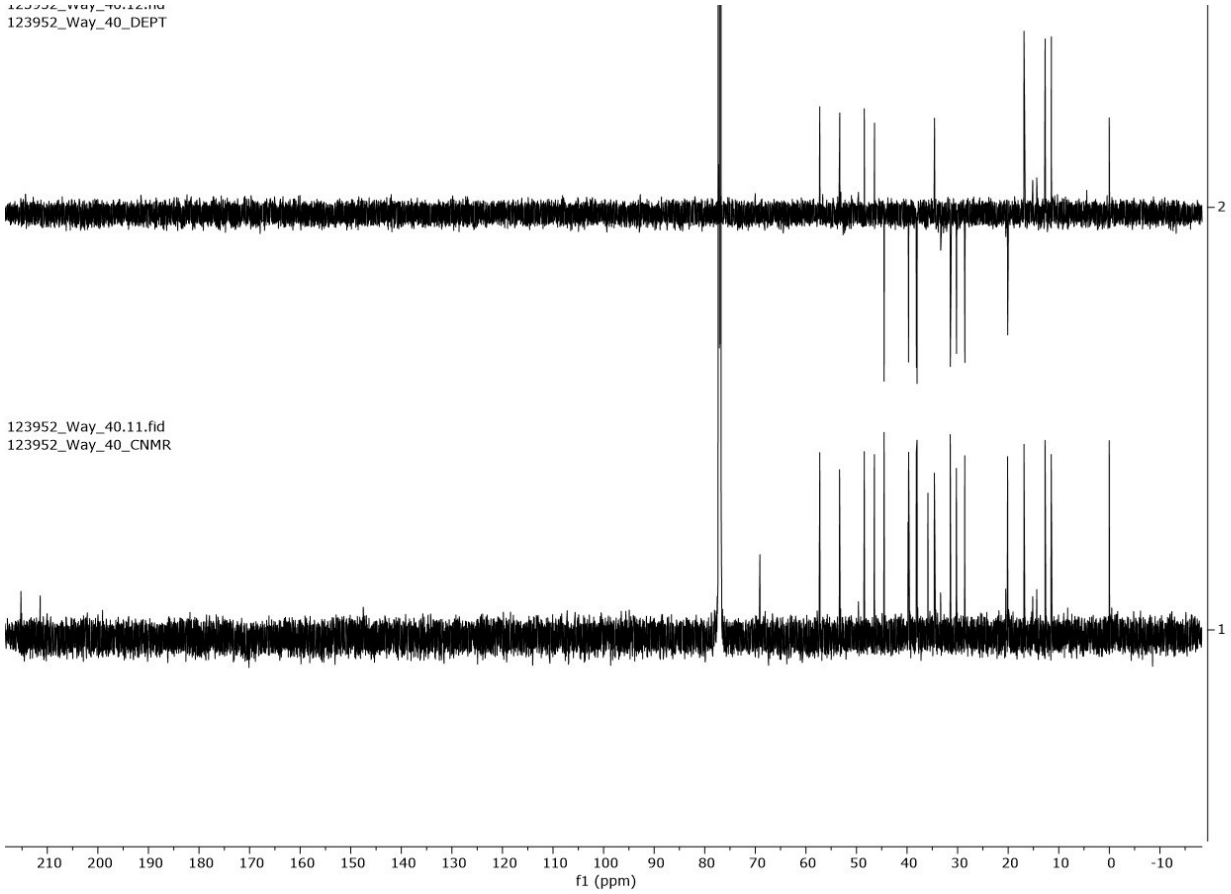


Figure S13 ^{13}C NMR (175 MHz, $CDCl_3$) and DEPT 135˚ spectrum of compound **2**

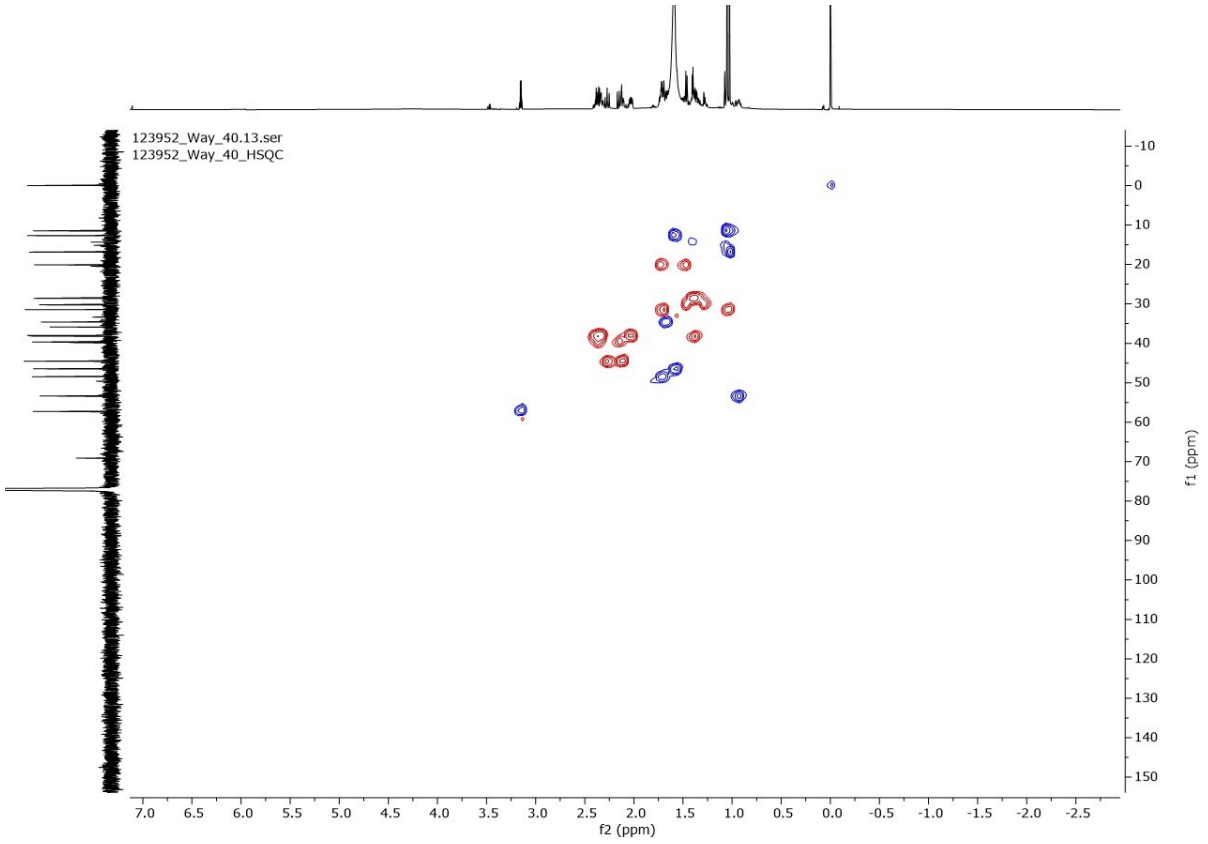


Figure S14 HSQC spectrum of compound **2**

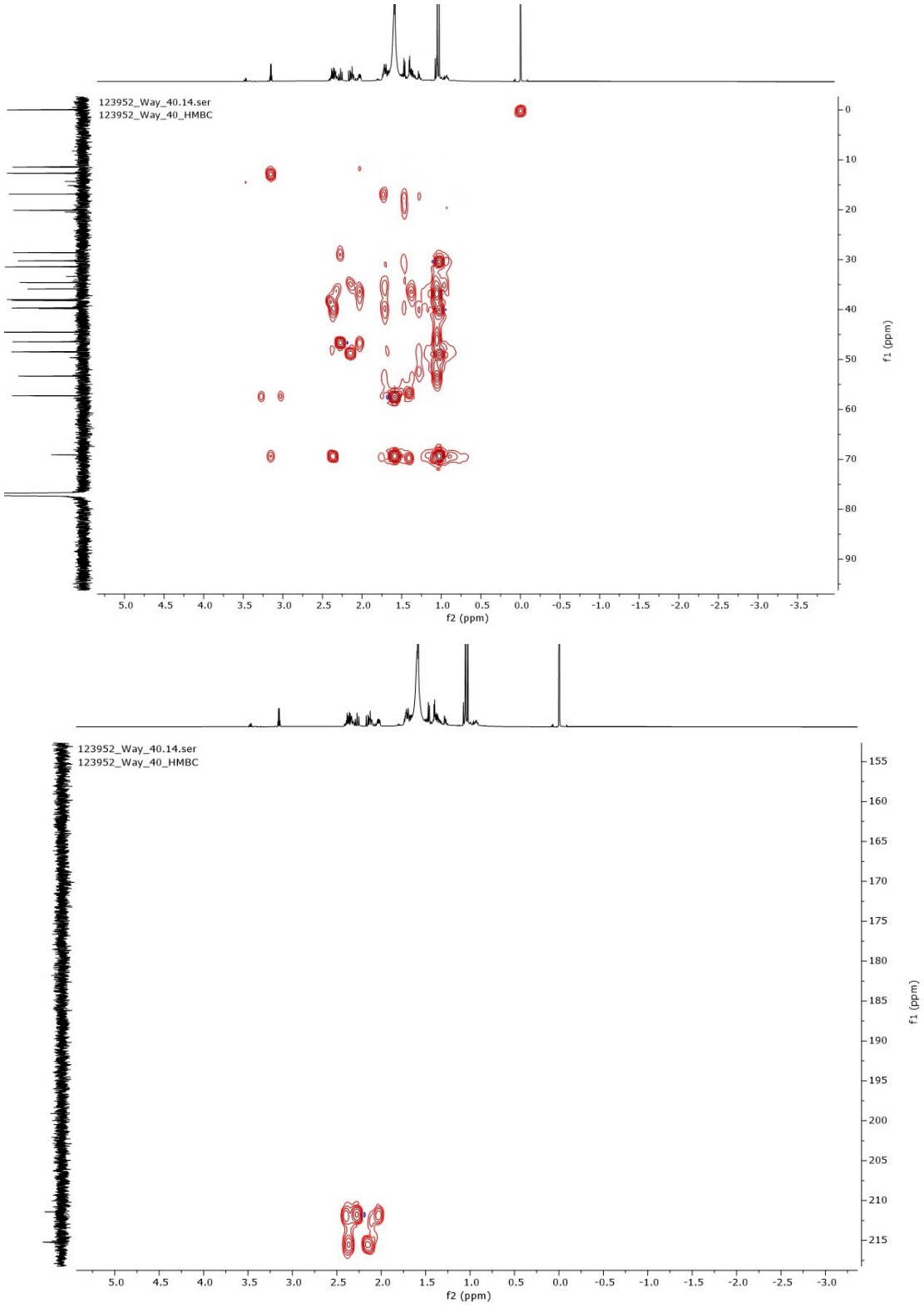


Figure S15 HMBC spectrum of compound **2**

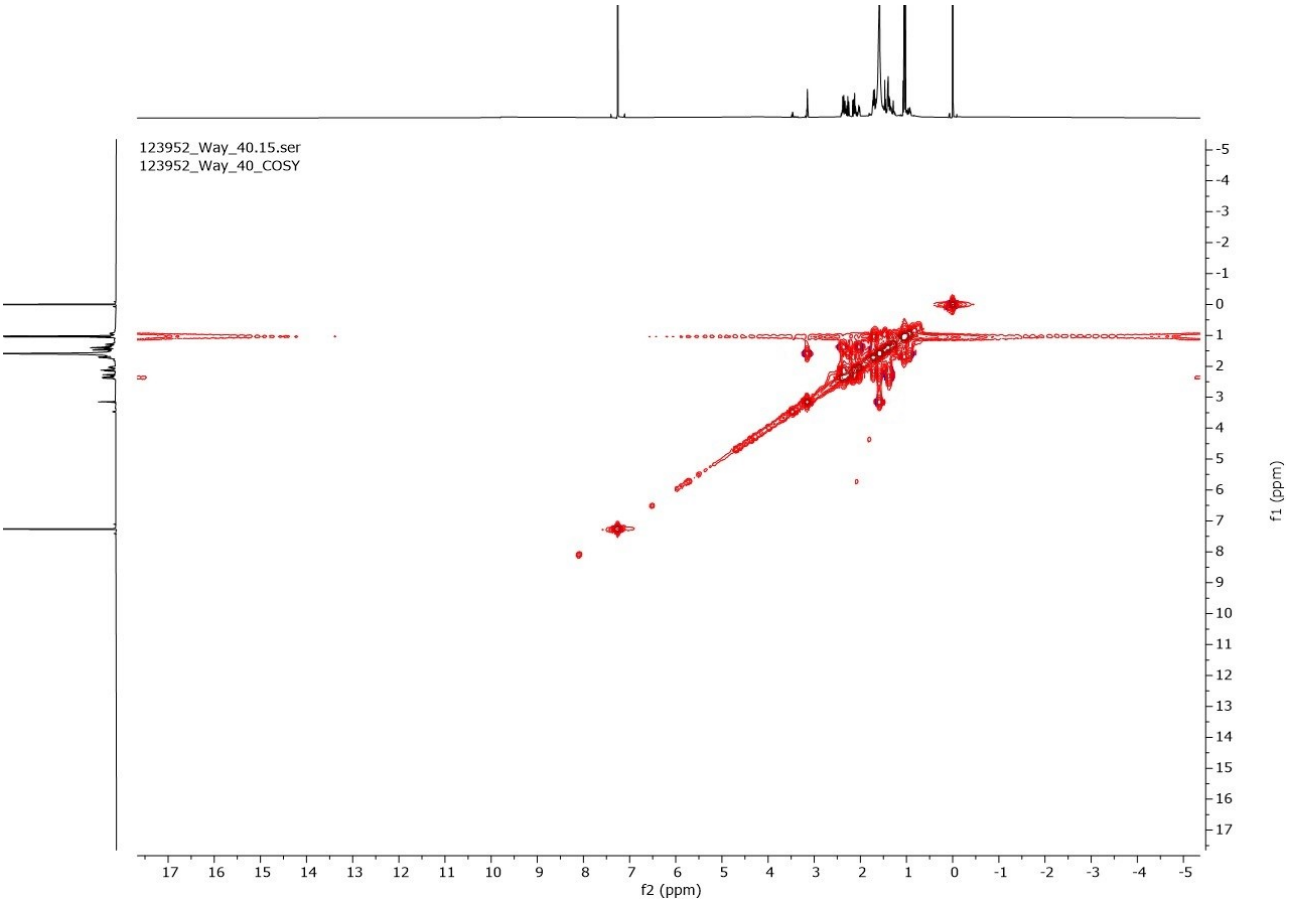


Figure S16 COSY spectrum of compound **2**

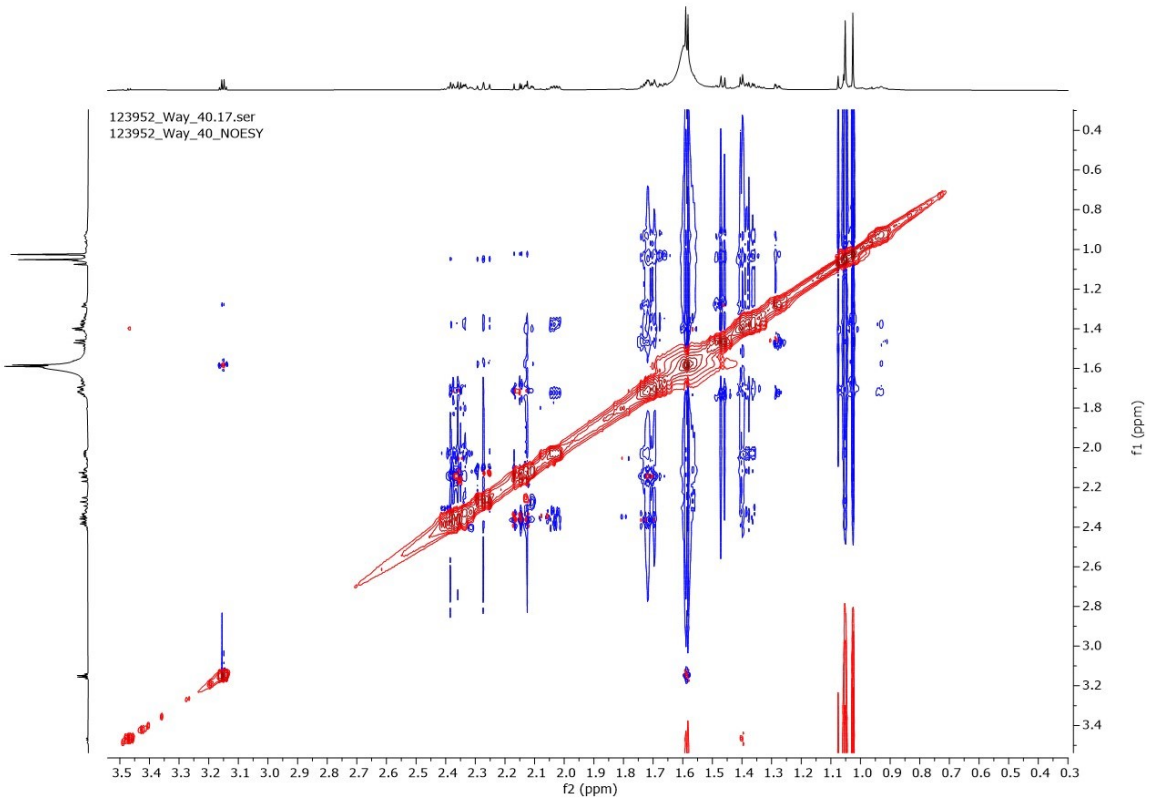
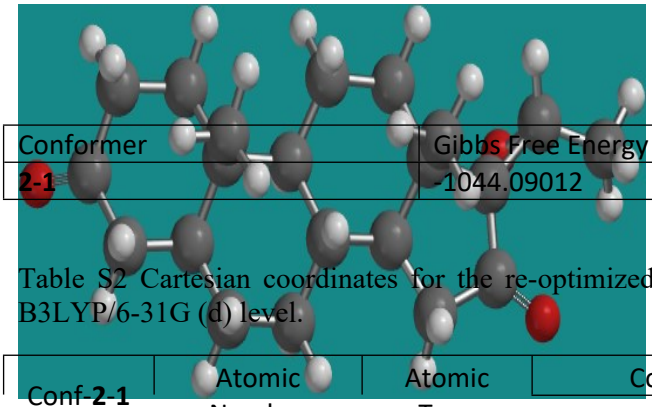


Figure S17 NOESY spectrum of compound **2**

ECD calculation

Conformation search of **2** at MMFF94s force field gave one conformer of **2**. These conformers were optimized at B3LYP/6-31G(d) level, and then calculated the ECD at B3LYP/6-311G(d,p) level, nstates=20, IEFPCM, solvent=methanol.



Conformer	Gibbs Free Energy (Hartree)	Population (%)
2-1	-1044.09012	100

Table S2 Cartesian coordinates for the re-optimized conformers of compound **2** in the gas phase (Å) at B3LYP/6-31G (d) level.

Conf-**2-1**	Atomic Number	Atomic Type	Coordinates (Angstroms)		
2-1					
			X	Y	Z
1	6	0	3.128114	-1.56955	-0.39993
2	6	0	3.004397	0.927426	-0.2299
3	6	0	5.266308	-0.18474	-0.57735
4	6	0	4.529573	1.018426	-0.0077
5	6	0	4.661784	-1.53635	-0.22749
6	6	0	2.382753	-0.40397	0.304169
7	6	0	0.86774	-0.41387	-0.11225
8	6	0	0.098318	0.849608	0.382013
9	6	0	0.791169	2.141925	-0.08212
10	6	0	2.277241	2.174222	0.290911
11	6	0	-1.34574	0.765555	-0.12737
12	6	0	-2.10848	-0.50791	0.347395
13	6	0	-1.35989	-1.73565	-0.18676
14	6	0	0.119257	-1.71959	0.253933
15	6	0	-3.50043	-0.24264	-0.24046
16	6	0	-3.6883	1.281811	-0.20731
17	6	0	-2.33269	1.915608	0.13418
18	6	0	2.54094	-0.54633	1.835678
19	1	0	0.083606	0.854506	1.481432
20	6	0	-2.2753	-0.58484	1.883916
21	1	0	-1.27961	0.671192	-1.22415
22	1	0	0.86389	-0.35133	-1.2141
23	1	0	2.851912	0.909363	-1.32176

24	8	0	6.264891	-0.07381	-1.2634
25	8	0	-4.70704	1.886076	-0.46141
26	6	0	-4.59958	-1.22638	-0.3039
27	8	0	-3.87125	-0.86576	-1.48894
28	6	0	-6.06971	-0.89545	-0.25069
29	1	0	2.762213	-2.53488	-0.03362
30	1	0	2.895372	-1.53672	-1.47376
31	1	0	4.751933	1.082552	1.067927
32	1	0	4.938535	1.921278	-0.47281
33	1	0	4.92078	-1.75207	0.819504
34	1	0	5.147045	-2.30167	-0.84069
35	1	0	0.277767	3.014787	0.340525
36	1	0	0.695369	2.225039	-1.17568
37	1	0	2.392845	2.250064	1.38114
38	1	0	2.747345	3.07313	-0.12888
39	1	0	-1.83019	-2.66563	0.160037
40	1	0	-1.426	-1.74148	-1.28103
41	1	0	0.174366	-1.88935	1.336173
42	1	0	0.622211	-2.57476	-0.21051
43	1	0	-2.33486	2.237667	1.184927
44	1	0	-2.17781	2.809143	-0.47697
45	1	0	3.584586	-0.45746	2.152265
46	1	0	2.191034	-1.52754	2.173293
47	1	0	1.976182	0.210574	2.387635
48	1	0	-2.82113	-1.497	2.150883
49	1	0	-1.31719	-0.6086	2.410128
50	1	0	-2.84539	0.260592	2.285244
51	1	0	-4.34096	-2.22724	0.054497
52	1	0	-6.63025	-1.59616	-0.88043
53	1	0	-6.25173	0.123942	-0.59164
54	1	0	-6.43959	-0.99802	0.776663

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311+G(d,p)

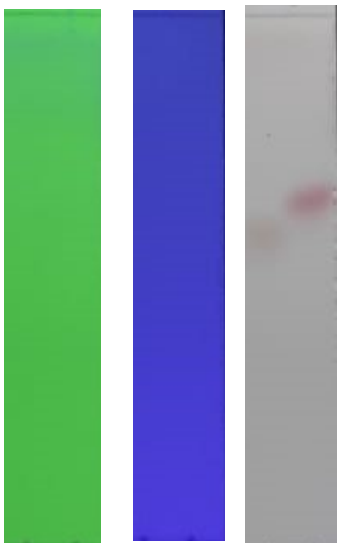
		DP4+	100.00%	0.00%	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3
C		38.1	36.7	36.8	
C		38	37.0	37.0	
C	x	211.4	216.0	216.1	
C		44.5	43.7	43.6	
C		46.5	45.5	45.5	
C		28.6	26.6	26.4	
C		31.4	29.5	29.4	
C		34.6	33.8	33.3	
C		53.4	51.4	51.0	
C		35.9	36.3	36.3	
C		20.1	18.6	18.8	
C		30.2	28.20	31.40	
C		39.8	40.00	39.80	
C		48.5	46.00	47.40	
C		39.7	39.40	37.20	
C	x	215.2	226.00	224.40	
C		69	66.60	67.90	
C		16.8	11.50	9.80	
C		11.5	6.80	6.70	
C		57.2	57.50	56.30	
C		12.7	9.00	10.90	

H		2.03	2.10	2.10
H		1.46	1.45	1.45
H		2.35	2.65	2.65
H		2.03	2.29	2.27
H		2.27	2.49	2.47
H		2.11	2.08	2.05
H		1.58	1.61	1.61
H		1.37	1.61	1.6
H		1.37	1.33	1.35
H		1.7	1.77	1.76
H		1.03	1.12	1.12
H		1.67	1.8	1.85
H		0.93	0.99	1.05
H		1.46	1.64	1.63
H		1.71	1.71	1.7
H		1.28	1.28	1.58
H		1.46	1.57	1.81
H		1.71	1.8	1.89
H		2.37	2.4	2.25
H		2.15	2.4	2.37
H		1.02	1.21	1.54
H		1.05	1.26	1.37
H		3.15	3.33	3.53
H		1.58	1.51	1.74

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311+G(d,p)

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	99.97%	0.03%	-	-
sDP4+ (C data)	51.93%	48.07%	-	-
sDP4+ (all data)	99.97%	0.03%	-	-
uDP4+ (H data)	99.99%	0.01%	-	-
uDP4+ (C data)	9.29%	90.71%	-	-
uDP4+ (all data)	99.93%	0.07%	-	-
DP4+ (H data)	100.00%	0.00%	-	-
DP4+ (C data)	9.96%	90.04%	-	-
DP4+ (all data)	100.00%	0.00%	-	-

Figure S18 NMR calculation (DP4+ analysis) of compound **2**



a. b. c.

Figure S19 TLC profile of compounds **1** (left) and **2** (right) in Merck pre-coated silica gel 60 F_{254} plates in *n*-hexane: DCM: EtOAc (7:2:1) at a. UV 254 nm, b. UV 365 nm, c. H_2SO_4 spray