Polyoxygenated Terpenoids and Polyketides from the Roots of *Flueggea virosa* and Their Inhibitory Effect against SARS-CoV-2-Induced Inflammation

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analysis.

Figure S49. H-6/H-7 distance of 6α-OH and 6β-OH possible candidates of compound **2.** Conformers were generated by MM2 energy minimizations.

Table S1. DP4+ analysis table for compound **1** (isomer 1: 3β-OH; isomer 2: 3α-OH).

Table S2. Conformers and Boltzmann populations of 3α-OH isomer of **1**.

Table S3. Conformers and Boltzmann populations of 3β-OH isomer of **1**.

Table S4. DP4+ analysis table for compound **2** (isomer 1: 6α-OH; isomer 2: 6β-OH).

Table S5. Conformers and Boltzmann populations of 6α-OH isomer of **2**.

Table S6. Conformers and Boltzmann populations of 6β-OH isomer of **2**.

Table S7. DP4+ analysis table for compound **6** (isomer 1: 2α,10α-OH; isomer 2: 2β,10α-OH; isomer 3: 2α,10β-OH; isomer 4: 2β,10β-OH).

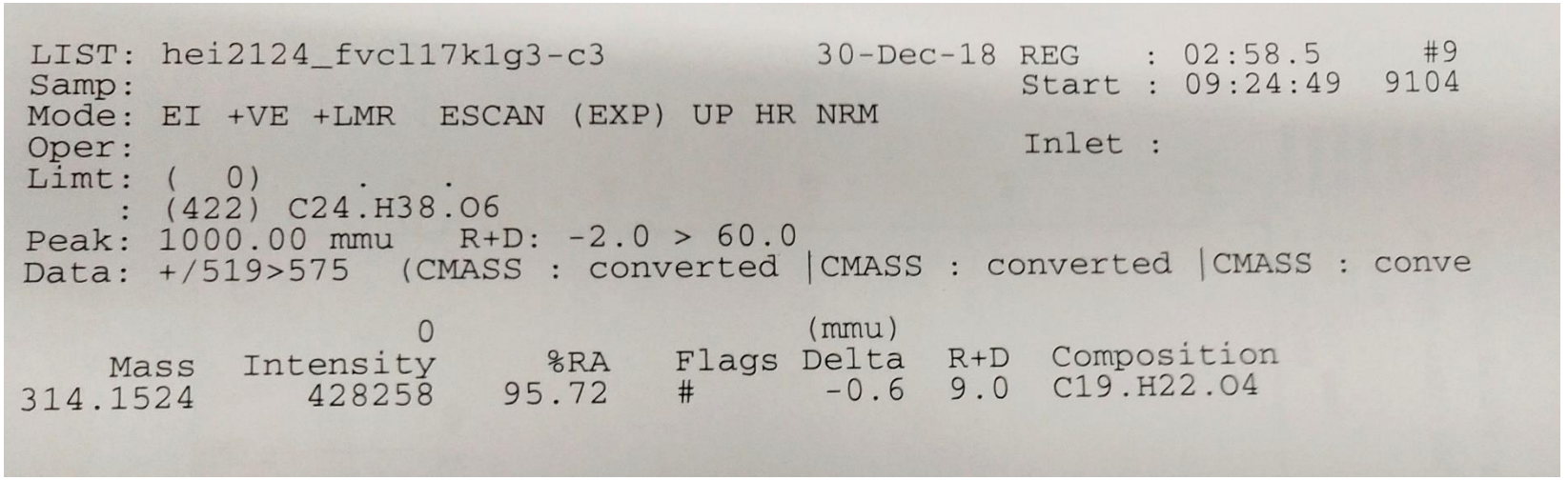
Table S8. Conformers and Boltzmann populations of 2α,10α-OH isomer of **6**.

Table S9. Conformers and Boltzmann populations of 2β,10α-OH isomer of **6**.

Table S10. Conformers and Boltzmann populations of 2α,10β-OH isomer of **6**.

Table S11. Conformers and Boltzmann populations of 2β,10β-OH isomer of **6**.

Table S12. ^{1}H NMR spectroscopic data of compounds **1**–**6**.



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Samp:                                          Start  : 09:24:49  9104
Mode: EI +VE +LMR  ESCAN (EXP) UP HR NRM
Oper:                                          Inlet  :
Limt: (  0)     .    .
    : (422) C24.H38.O6
Peak: 1000.00 mmu   R+D: -2.0 > 60.0
Data: +/519>575  (CMASS : converted |CMASS : converted |CMASS : conve

                    0                        (mmu)
    Mass  Intensity      %RA   Flags Delta  R+D  Composition
314.1524     428258    95.72   #      -0.6  9.0  C19.H22.O4
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Figure S1. (+)-HR-EIMS spectrum of **1**.

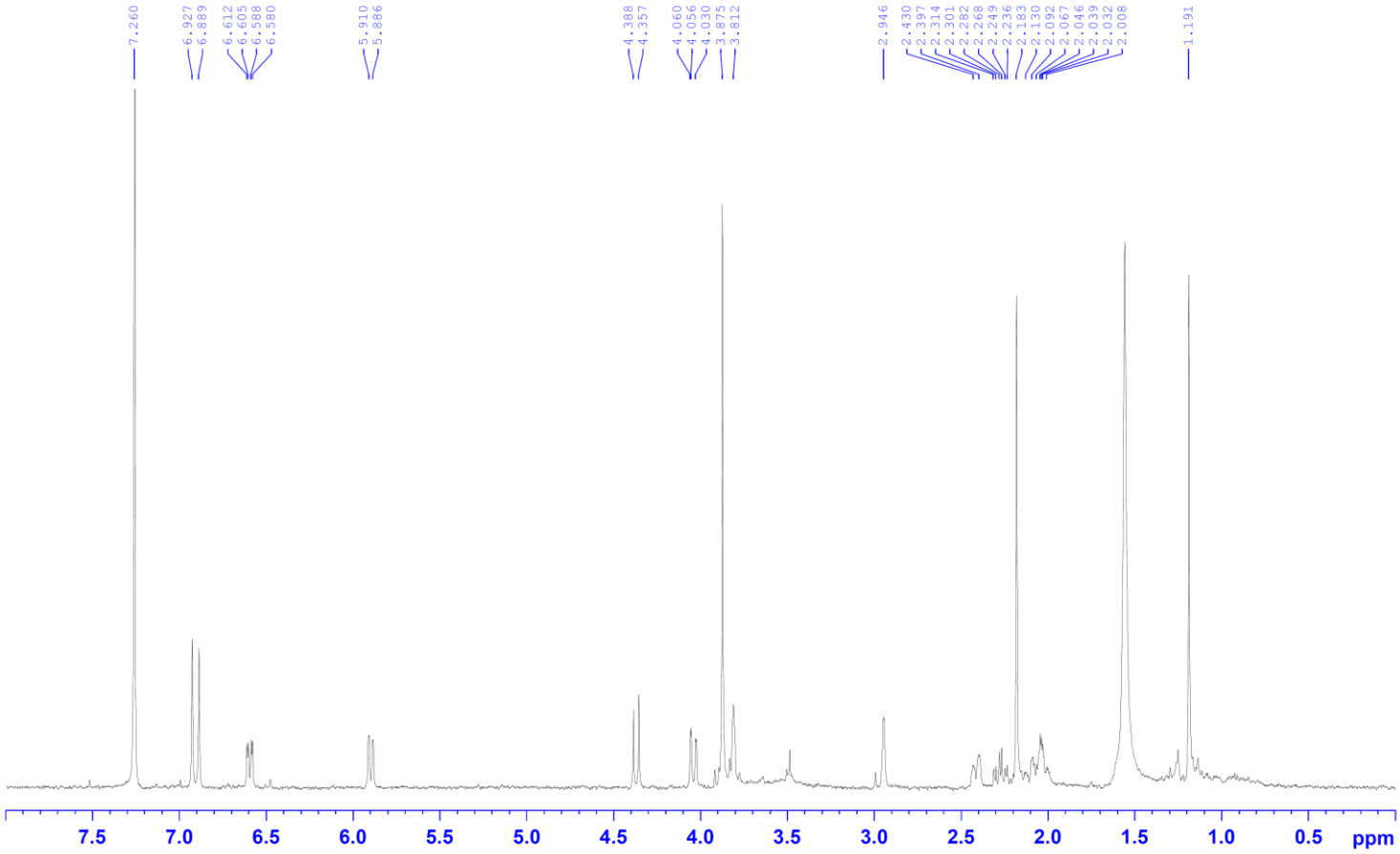

Figure S2. ^{1}H NMR spectrum of **1**.

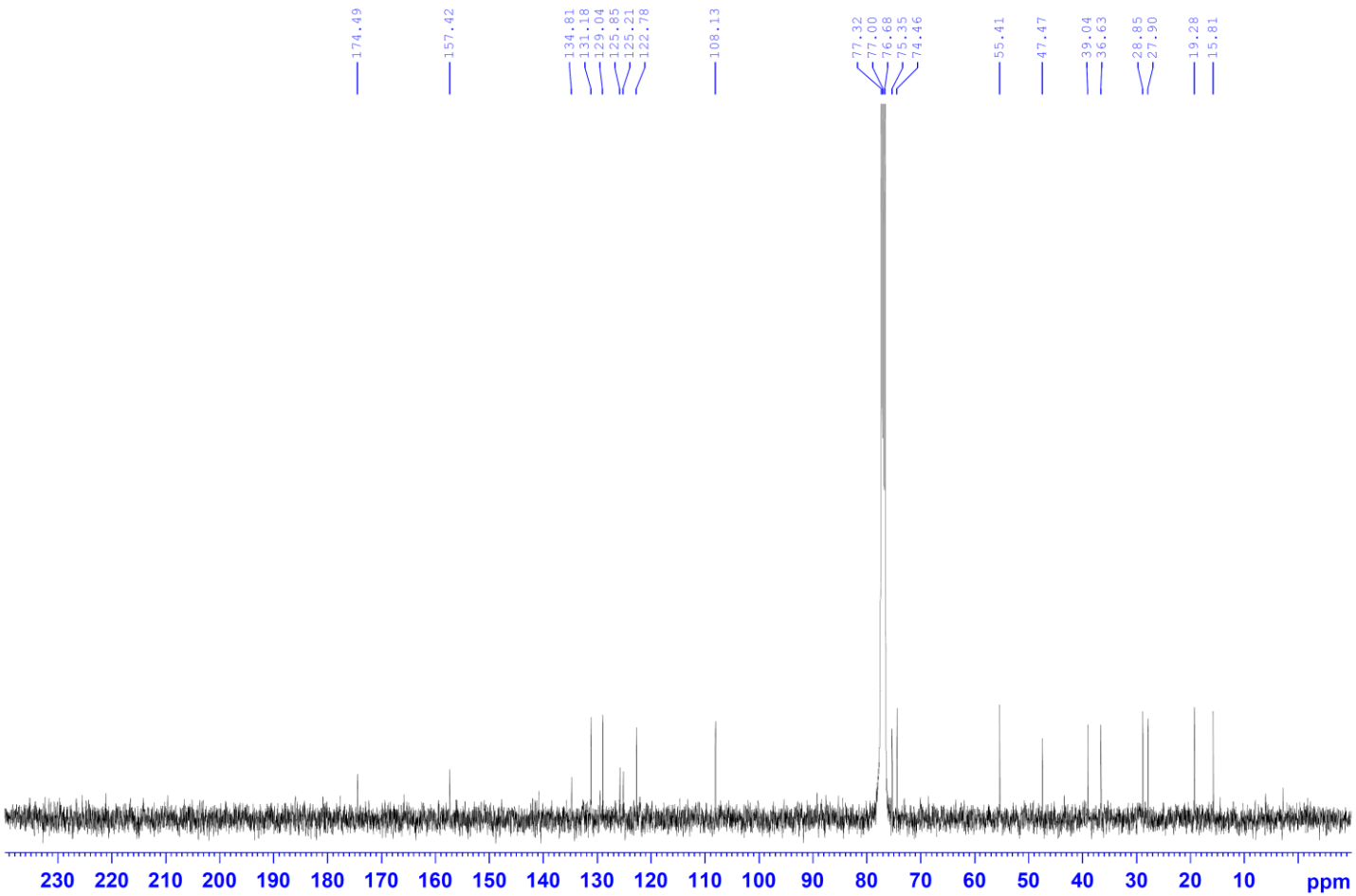

Figure S3. ^{13}C NMR spectrum of **1**.

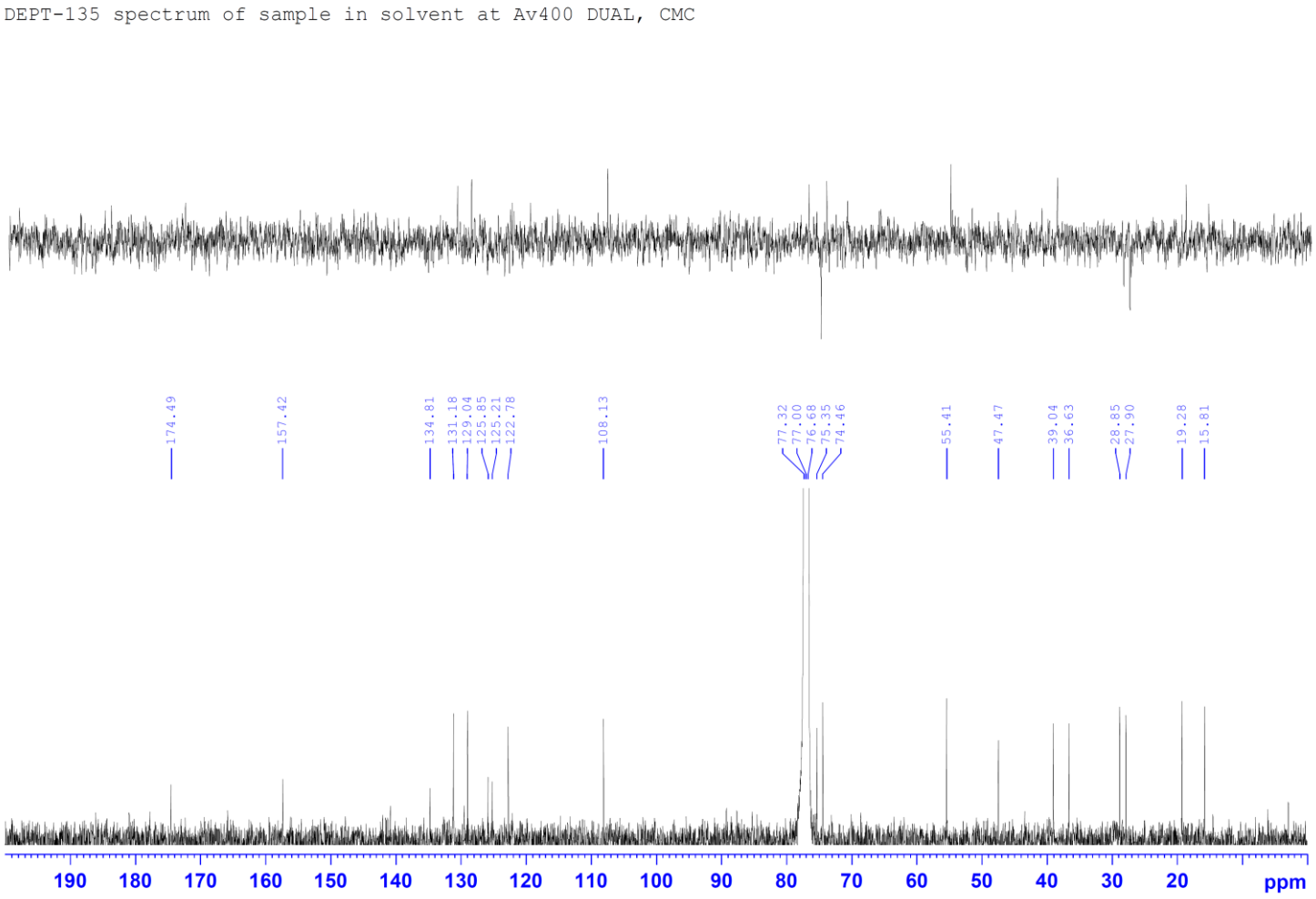

Figure S4. DEPT spectrum of **1**.

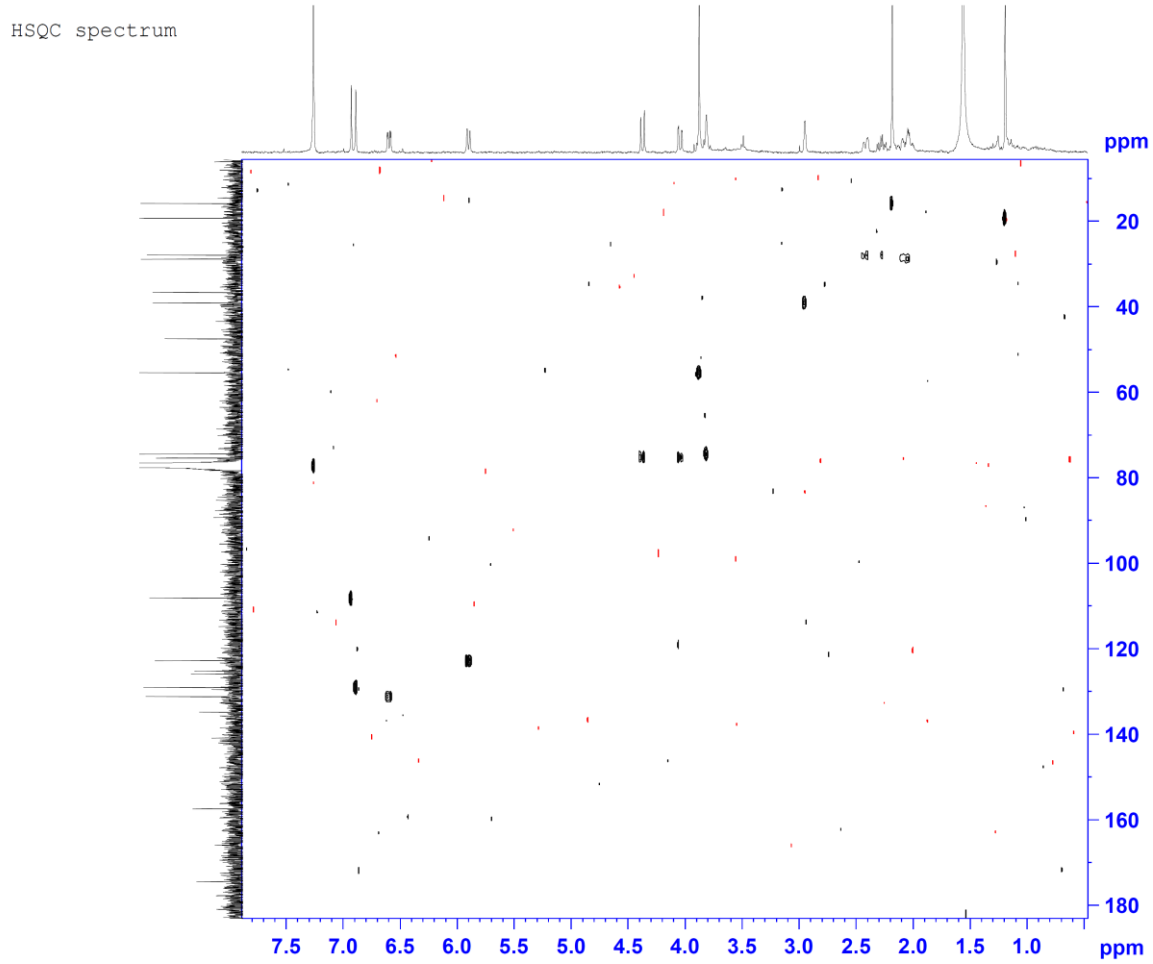

Figure S5. HSQC spectrum of **1**.

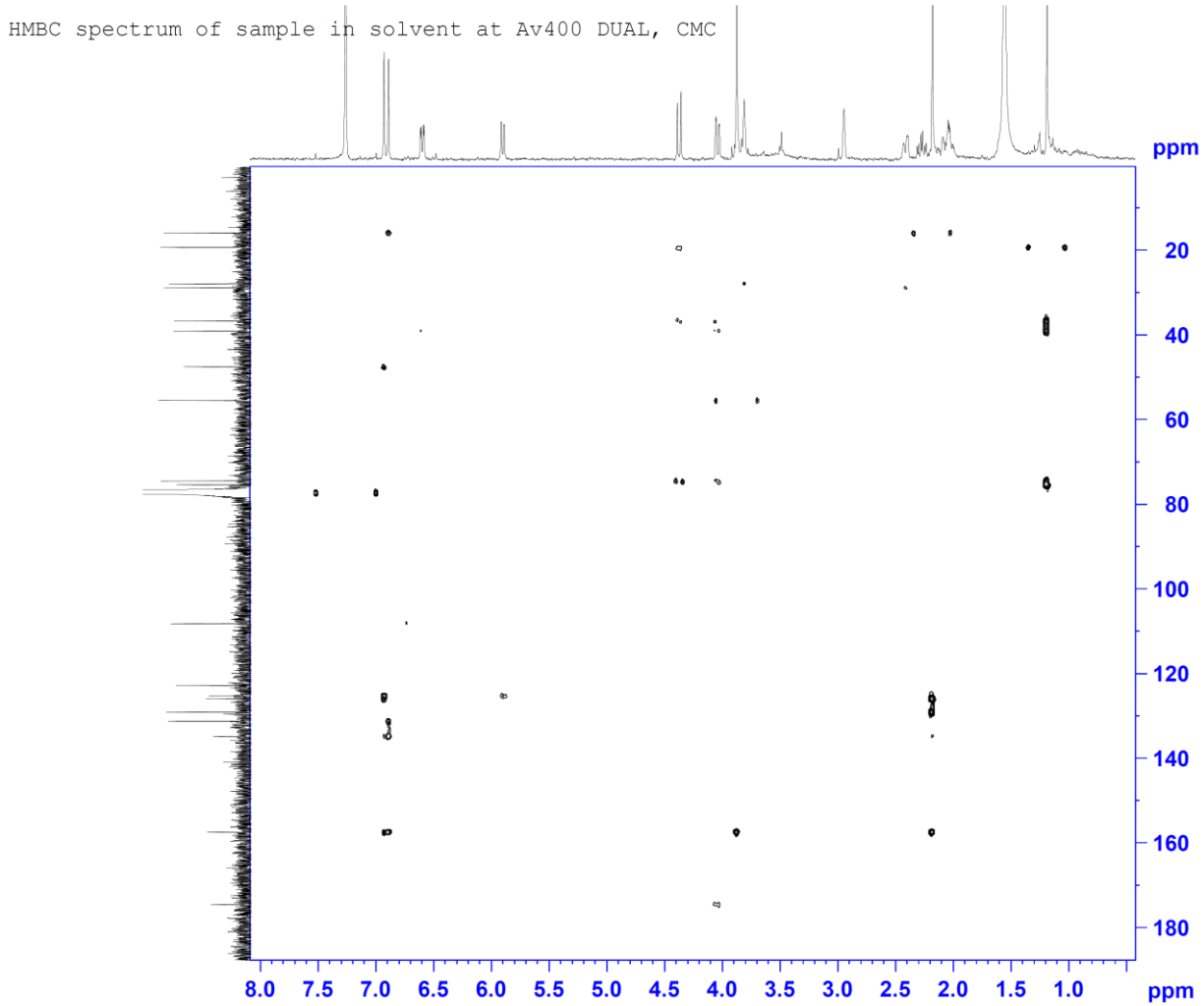

Figure S6. HMBC spectrum of **1**.

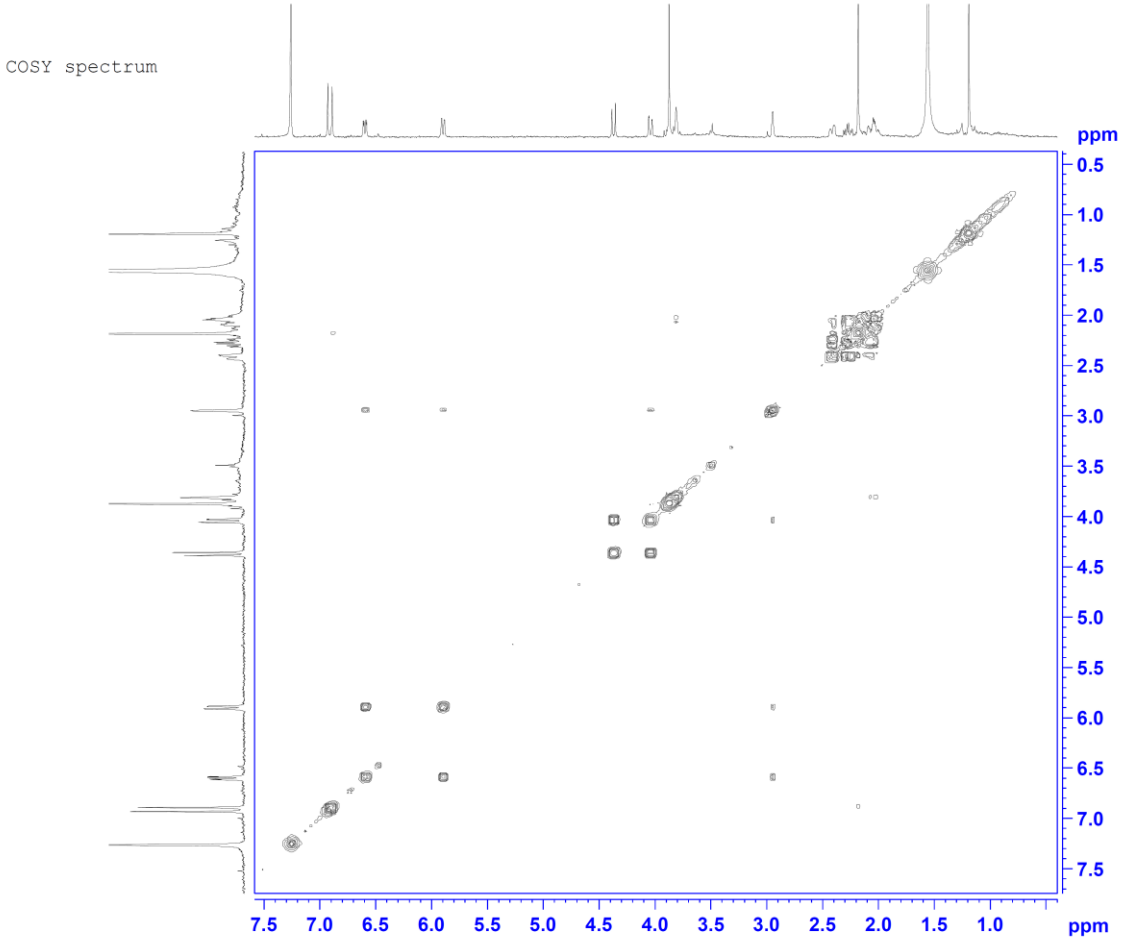

Figure S7. COSY spectrum of **1**.

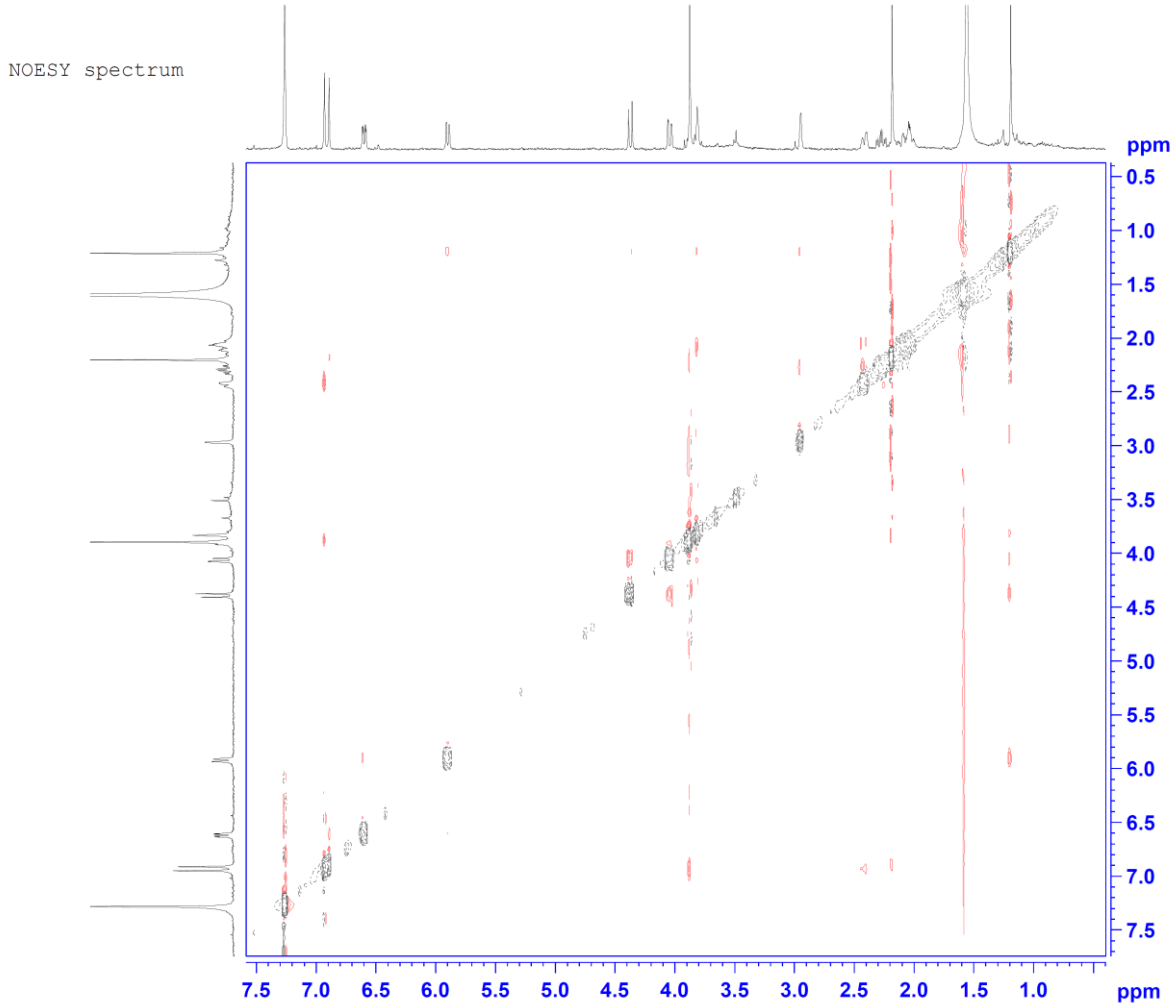

Figure S8. NOESY spectrum of **1**.

F:\Exp_data\...\85-FV-Cl-17K1D2-APCI-H 2017/9/26 下午 05:18:08

85-FV-Cl-17K1D2-APCI-H#1-20 RT: 0.01-0.53 AV: 20
T: FTMS - p APCI corona Full ms [250.00-400.00]
m/z= 317.1718-317.1777
Isotope Min Max
O-16 0 4
C-12 0 19
H-1 0 27
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
317.1748	113607.6	100.00	317.1747	0.15	$C_{19}H_{25}O_4$

Figure S9. (–)-HR-APCIMS spectrum of **2**.

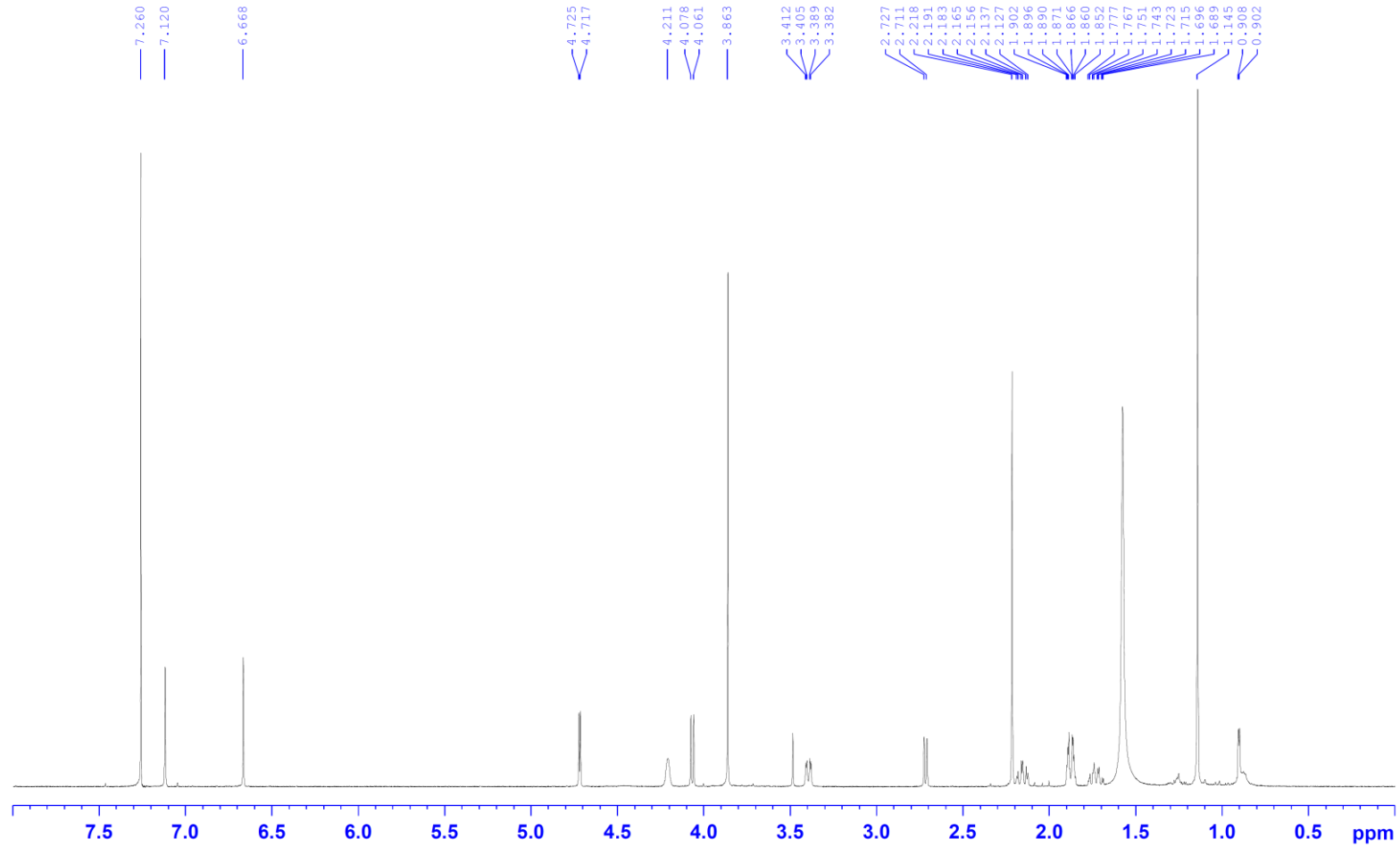

Figure S10. ^{1}H NMR spectrum of **2**.

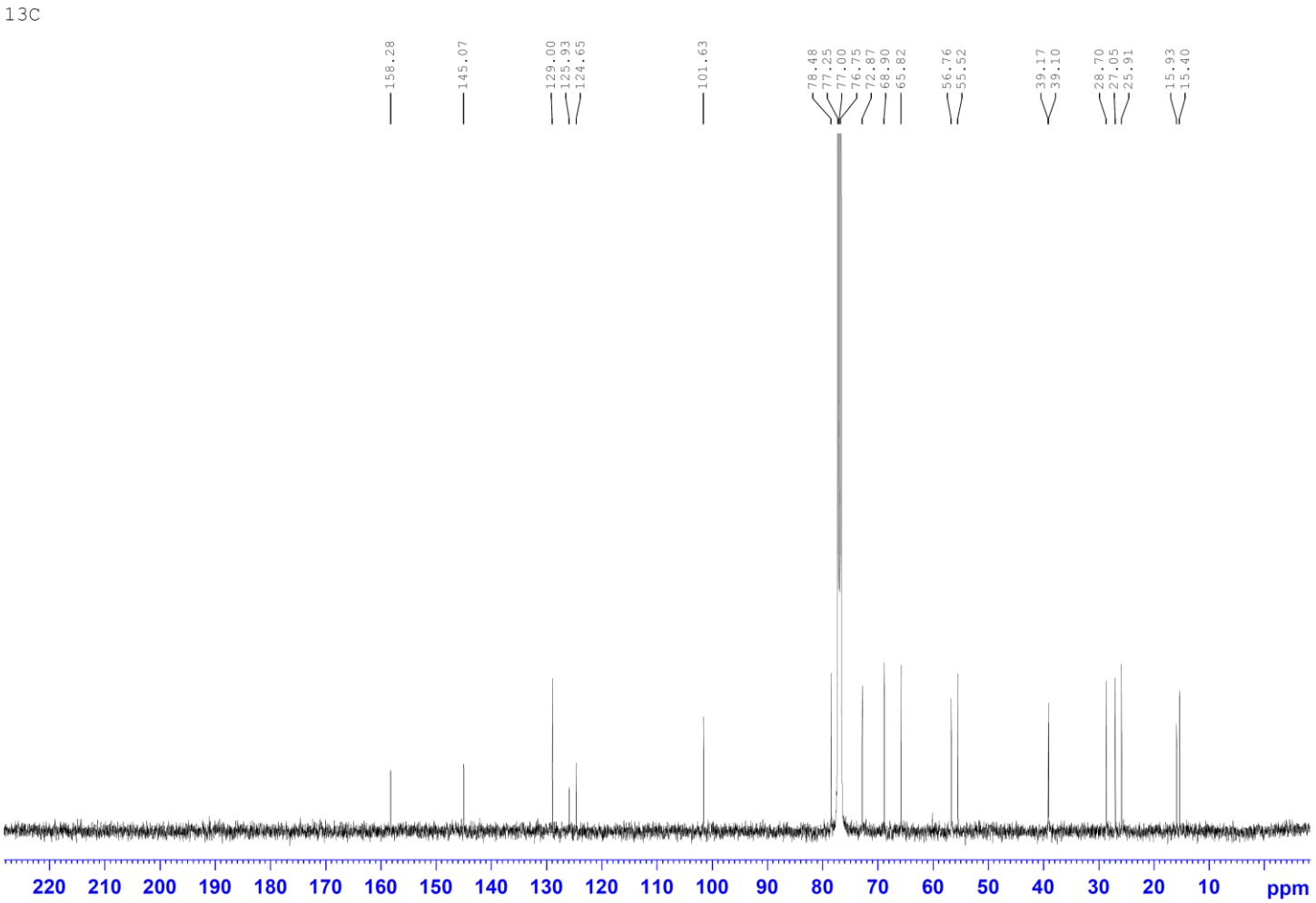

Figure S11. ^{13}C NMR spectrum of **2**.

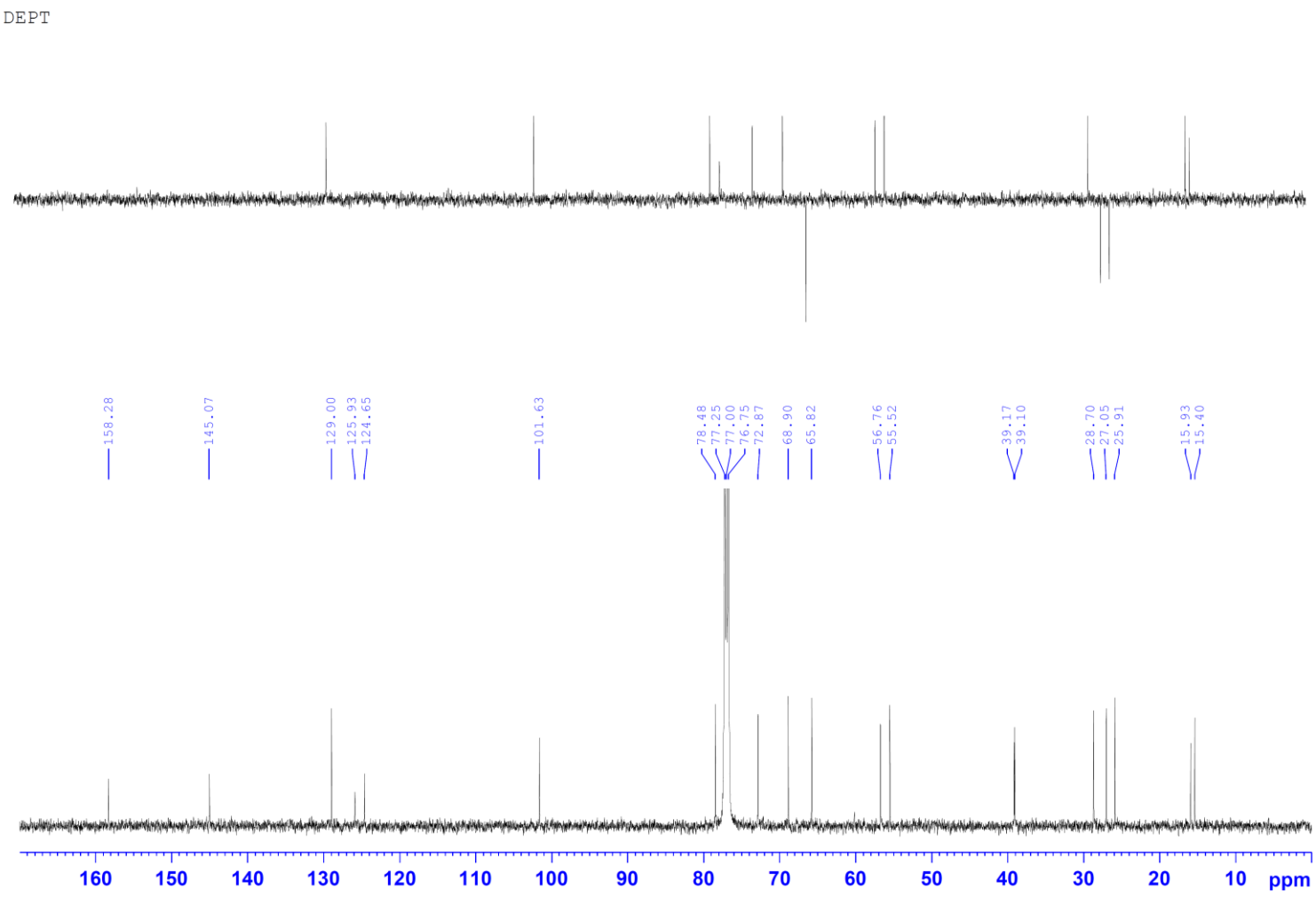

Figure S12. DEPT spectrum of **2**.

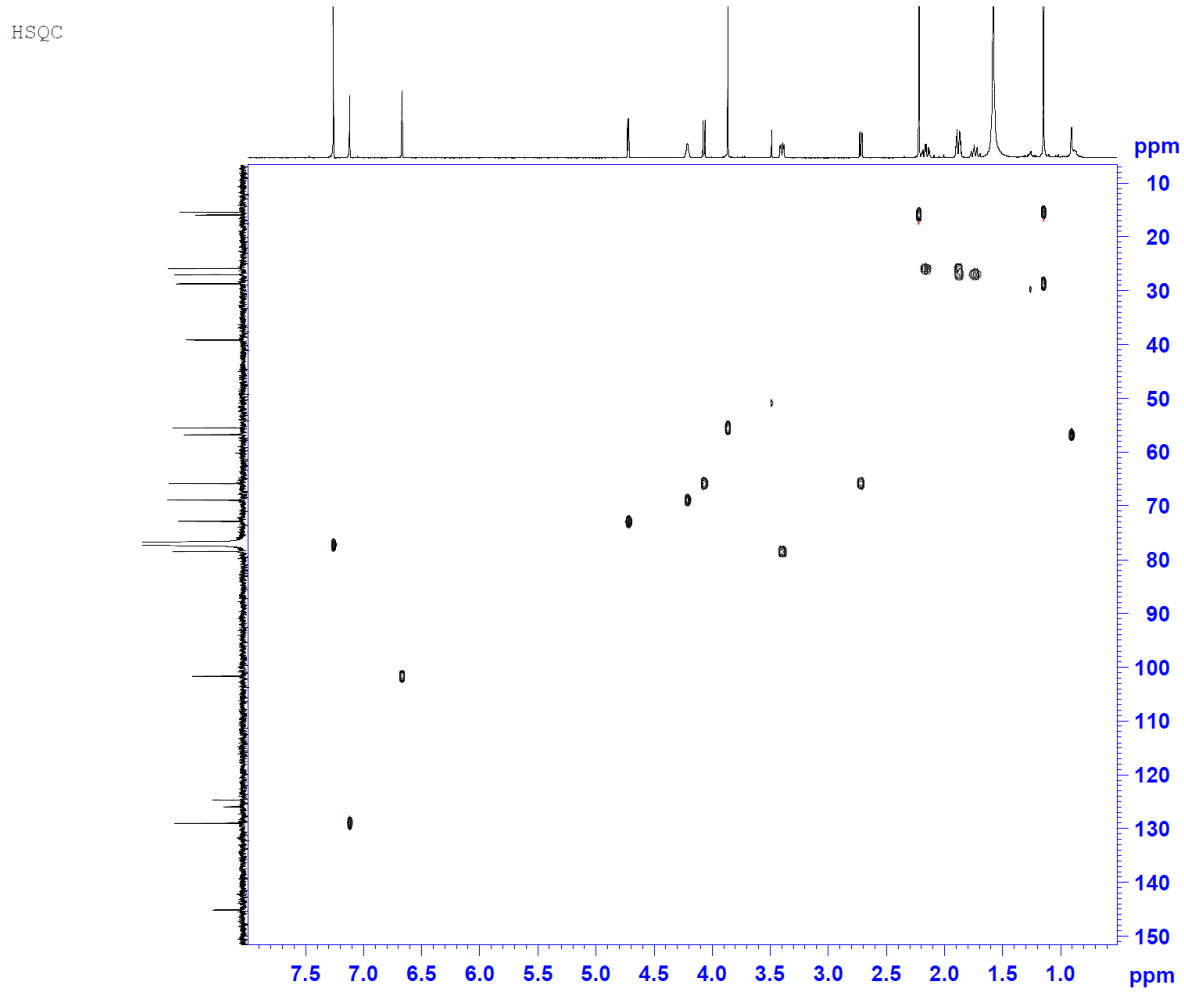

Figure S13. HSQC spectrum of **2**.

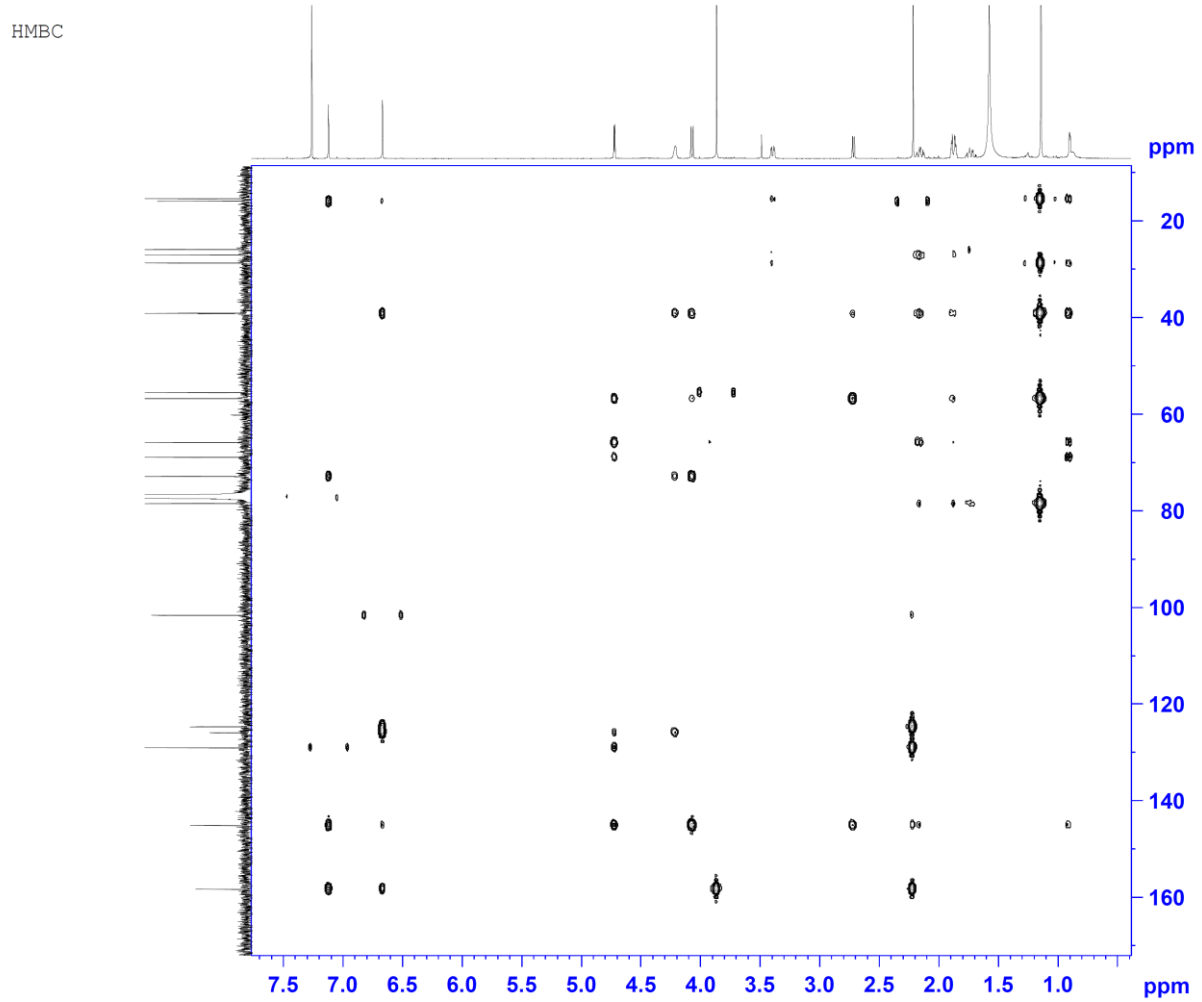

Figure S14. HMBC spectrum of **2**.

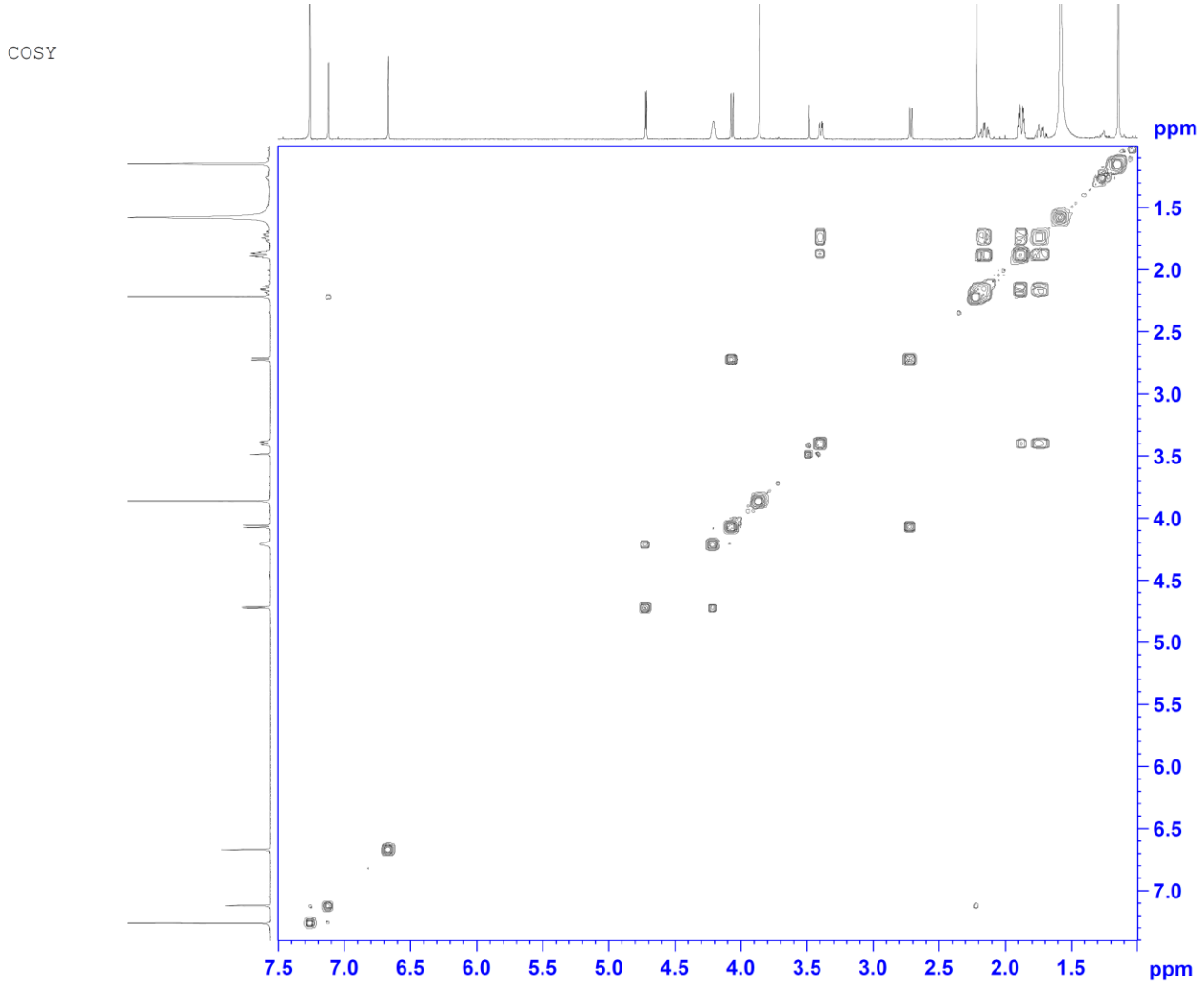

Figure S15. COSY spectrum of **2**.

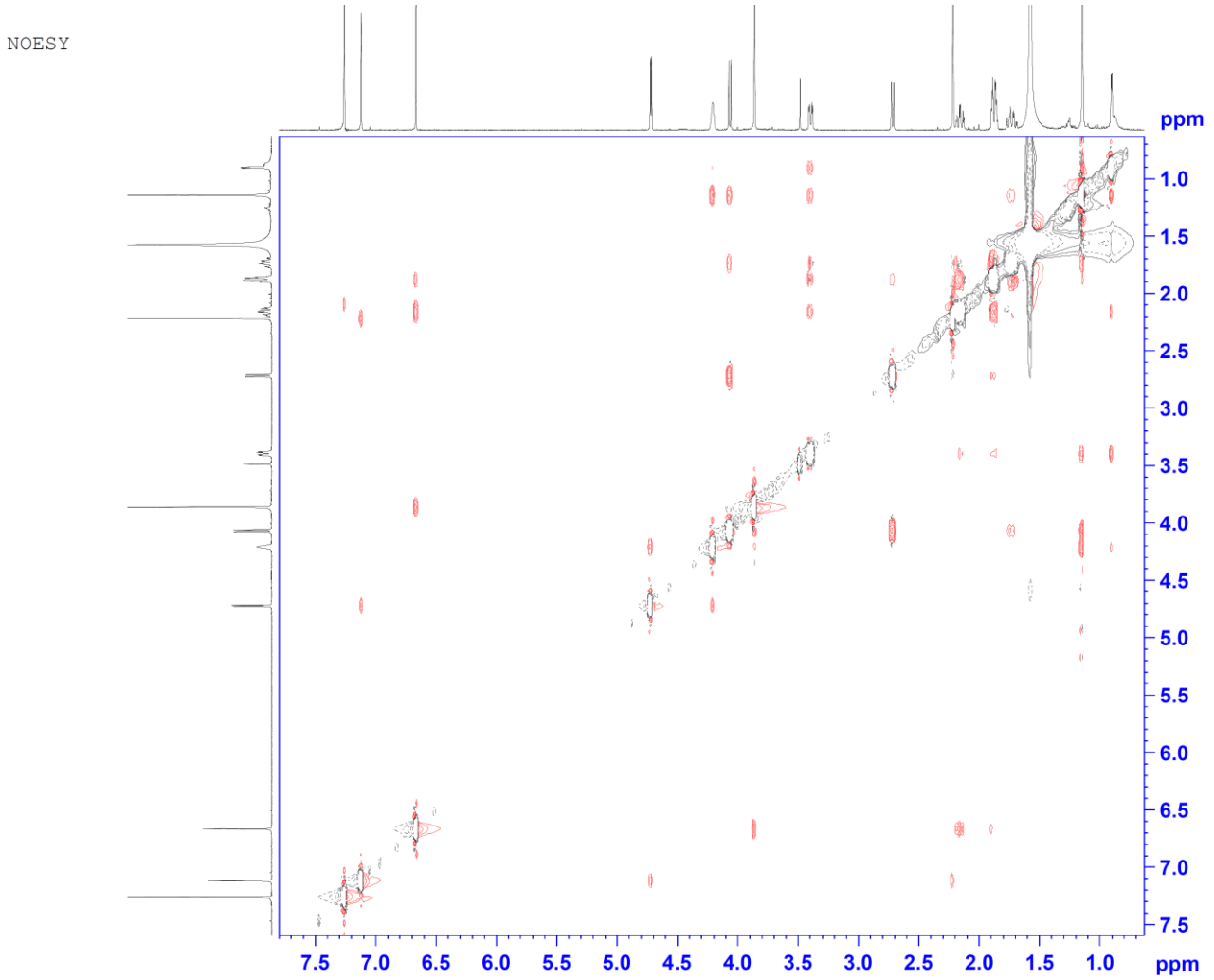

Figure S16. NOESY spectrum of **2**.

F:\Exp_data\...\51-FV-Cl-17J3D-H 2017/9/20 上午 11:31:15

51-FV-Cl-17J3D-H#1-20 RT: 0.01-0.53 AV: 20
T: FTMS - p ESI Full ms [310.00-325.00]
m/z= 317.1416-317.2115
Isotope Min Max
O-16 0 4
C-12 0 19
H-1 0 27
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
317.1753	3564591.0	100.00	317.1747	1.90	$C_{19}H_{25}O_4$

Figure S17. (–)-HR-ESIMS spectrum of **3**.

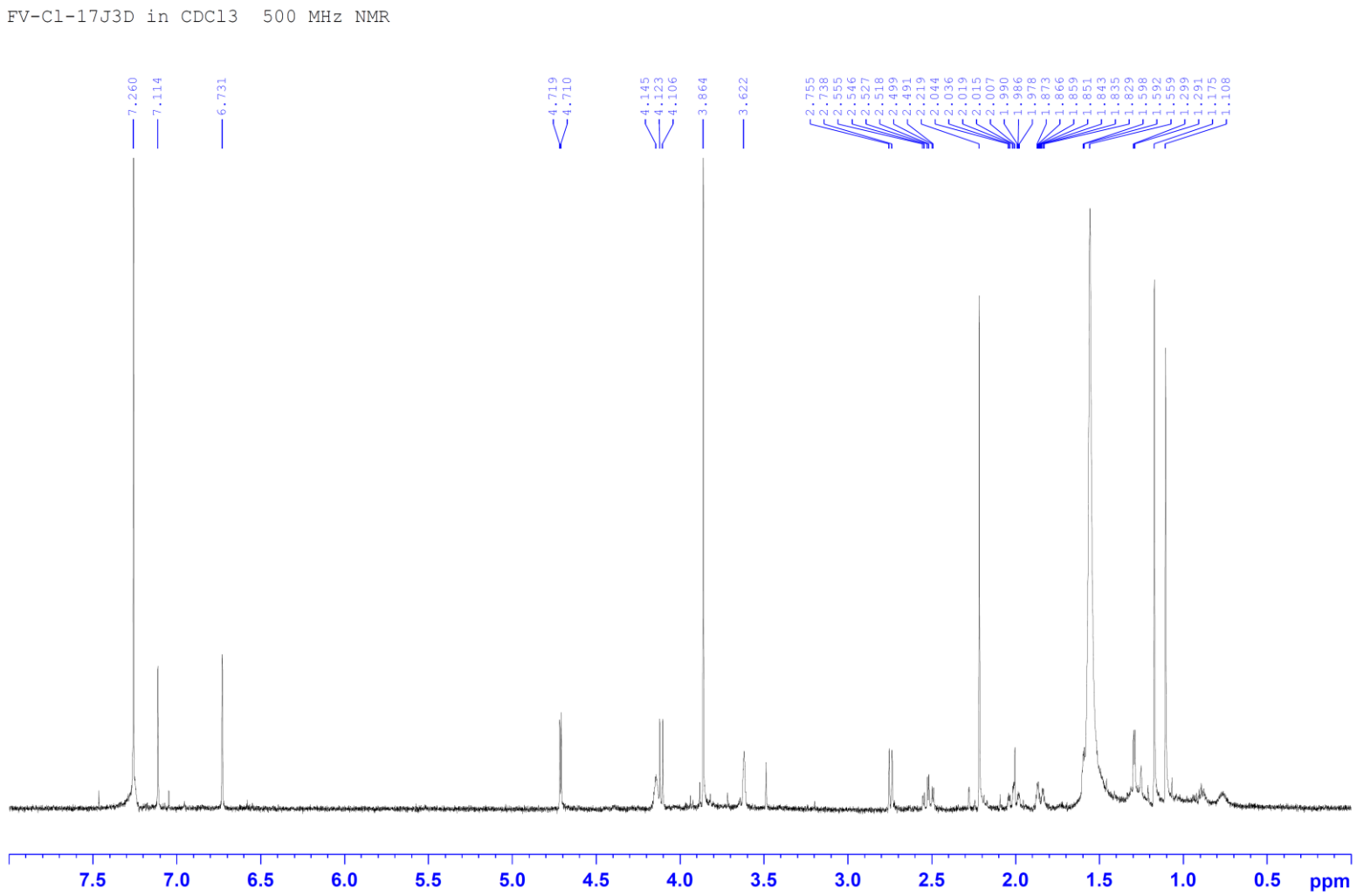

Figure S18. ^{1}H NMR spectrum of **3**.

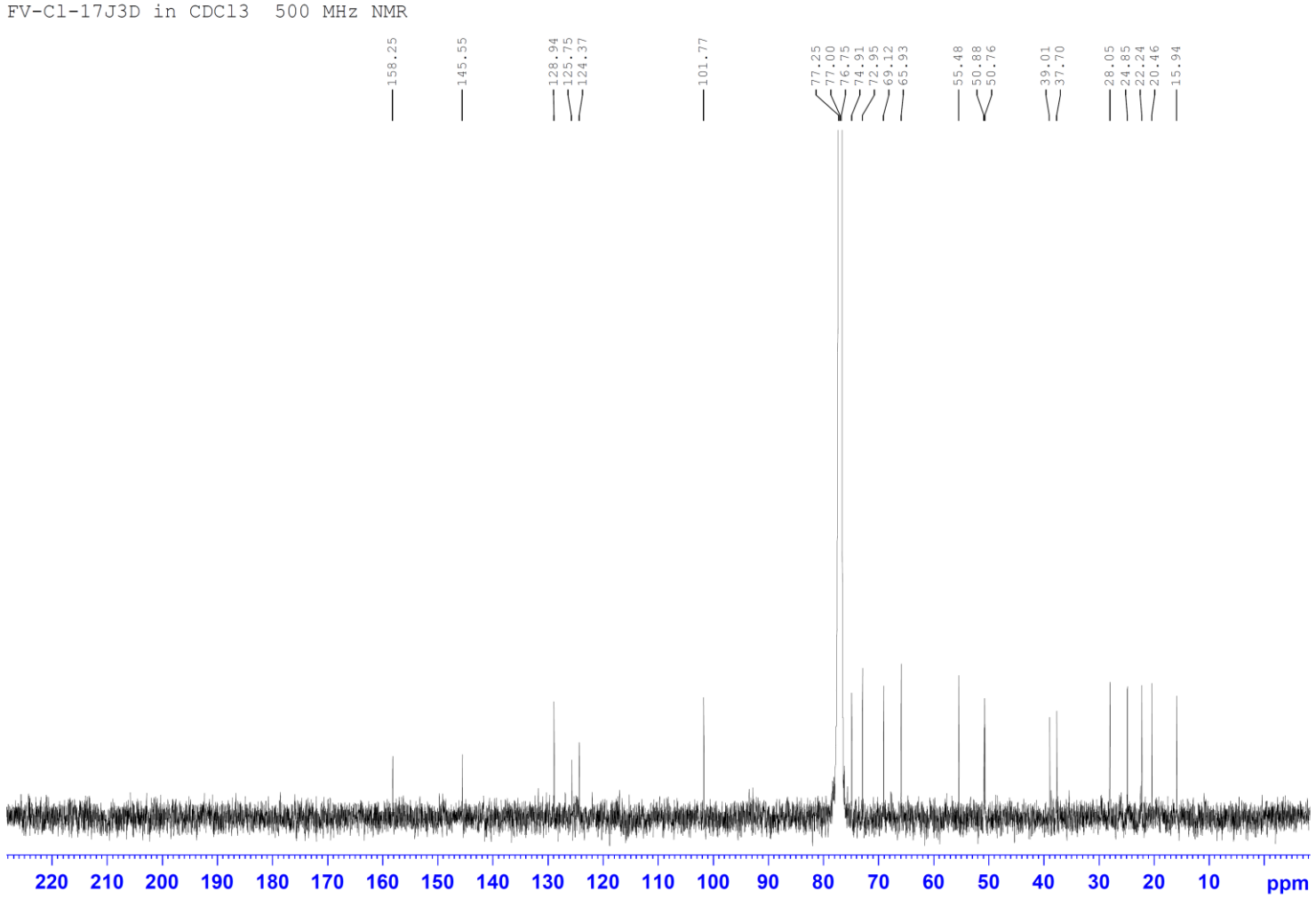

Figure S19. ^{13}C NMR spectrum of **3**.

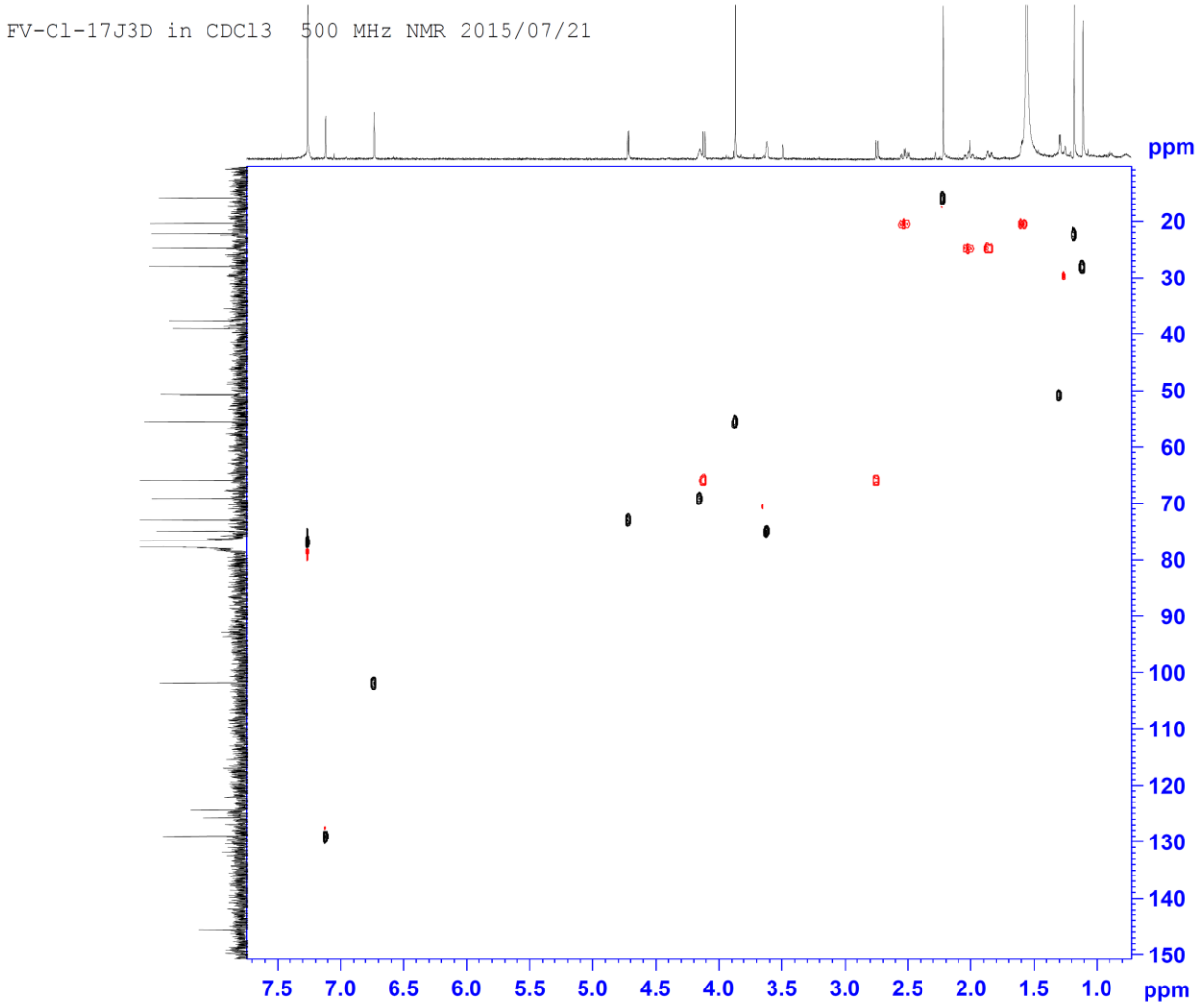

Figure S20. HSQC spectrum of **3**.

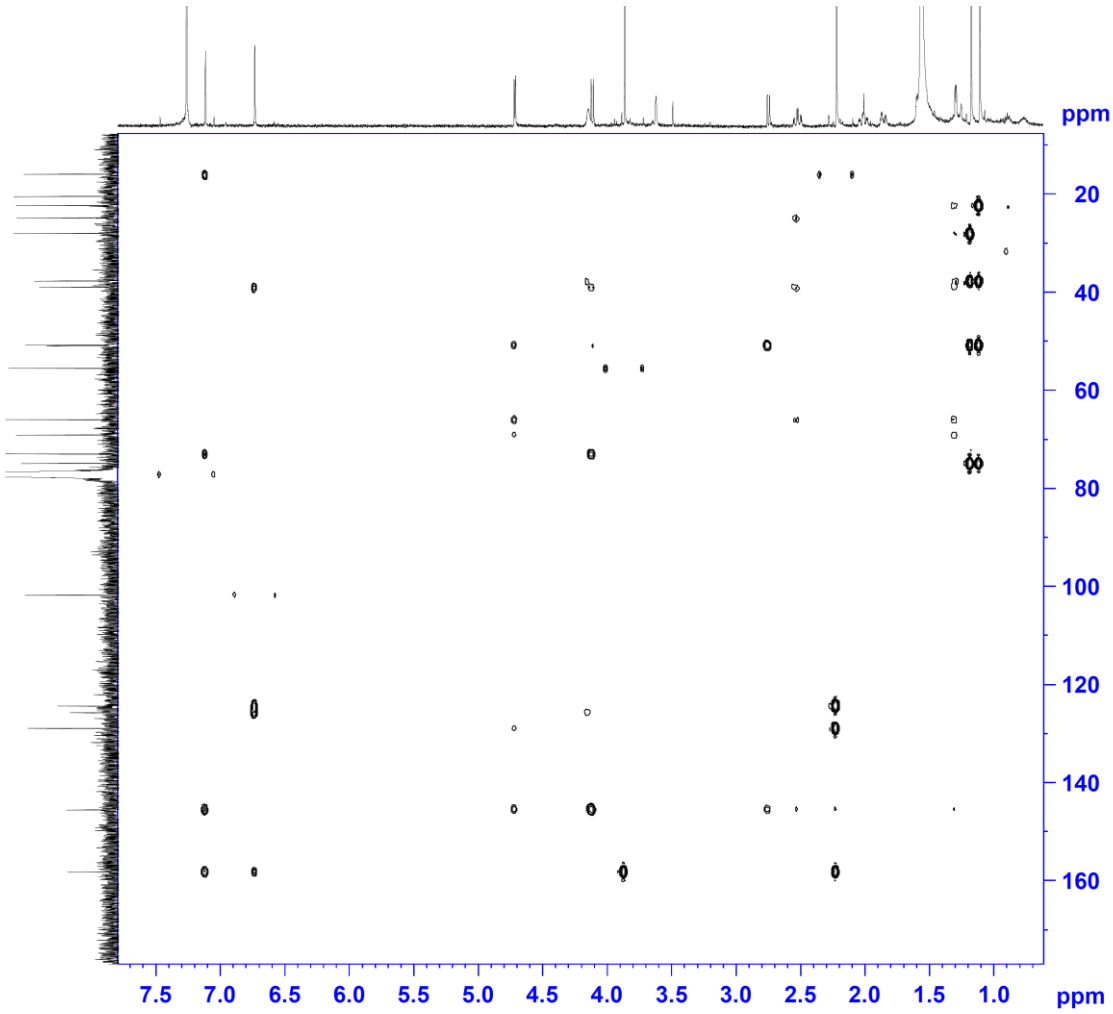

Figure S21. HMBC spectrum of **3**.

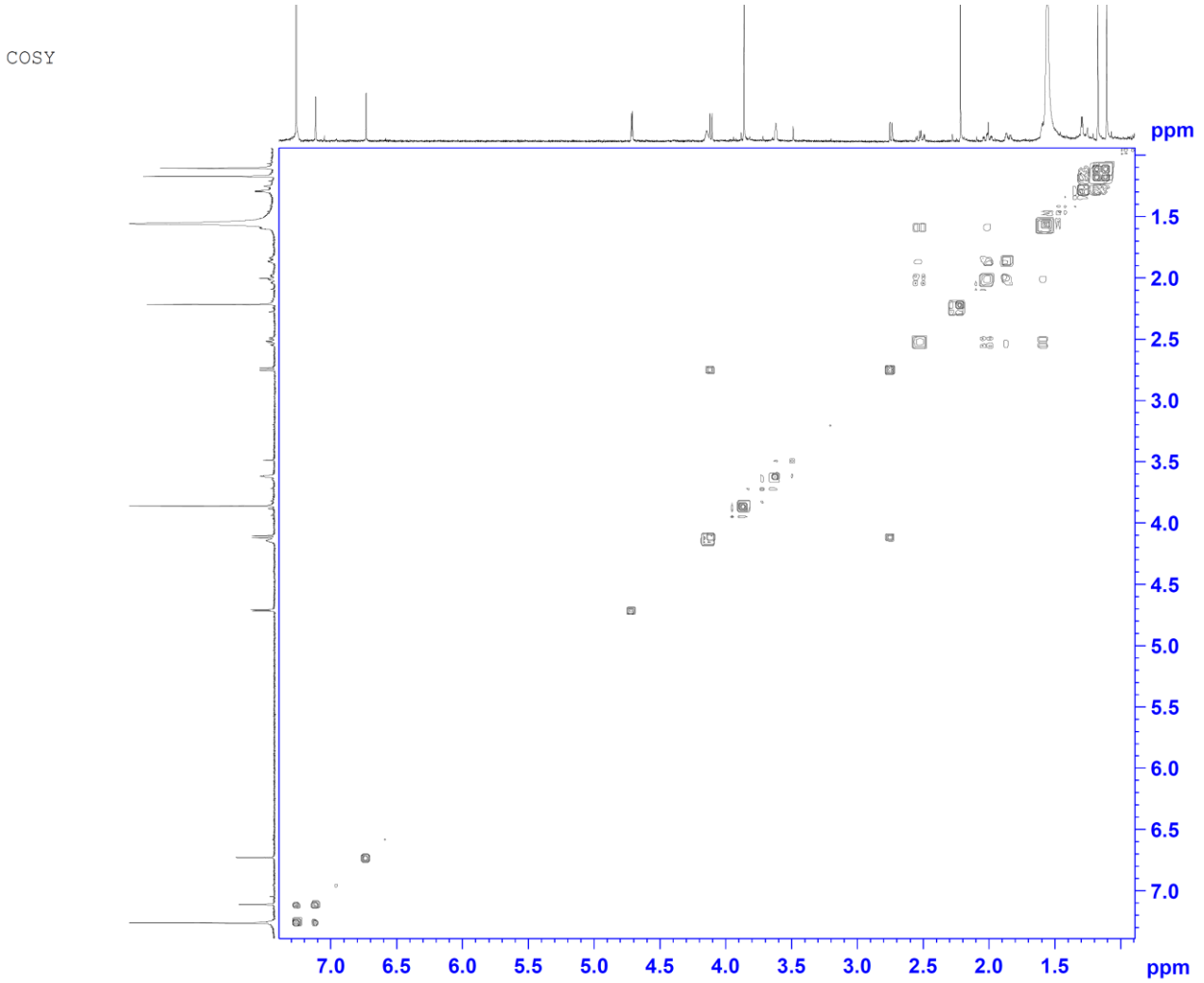

Figure S22. COSY spectrum of **3**.

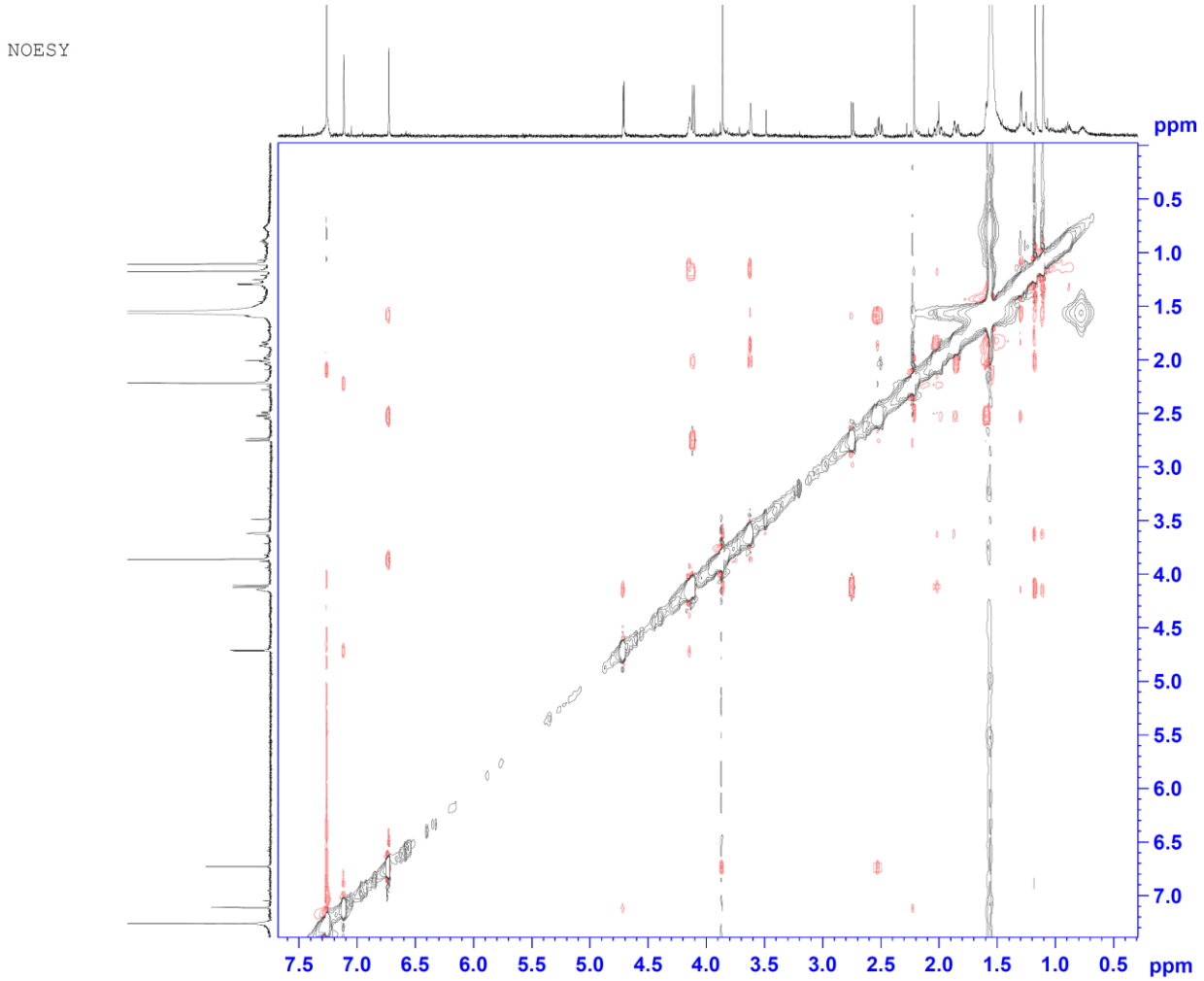

Figure S23. NOESY spectrum of **3**.

F:\Exp_data\...\80-FV-Cl-17K1L-H 2017/9/19 下午 03:51:33

80-FV-Cl-17K1L-H#1-20 RT: 0.02-0.54 AV: 20
T: FTMS - p ESI Full ms [300.00-350.00]
m/z= 335.1955-335.2456
Isotope Min Max
O-16 0 4
C-12 0 20
H-1 0 33
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
335.2221	5521533.5	100.00	335.2217	1.27	$C_{20}H_{31}O_4$

Figure S24. (–)-HR-ESIMS spectrum of **4**.

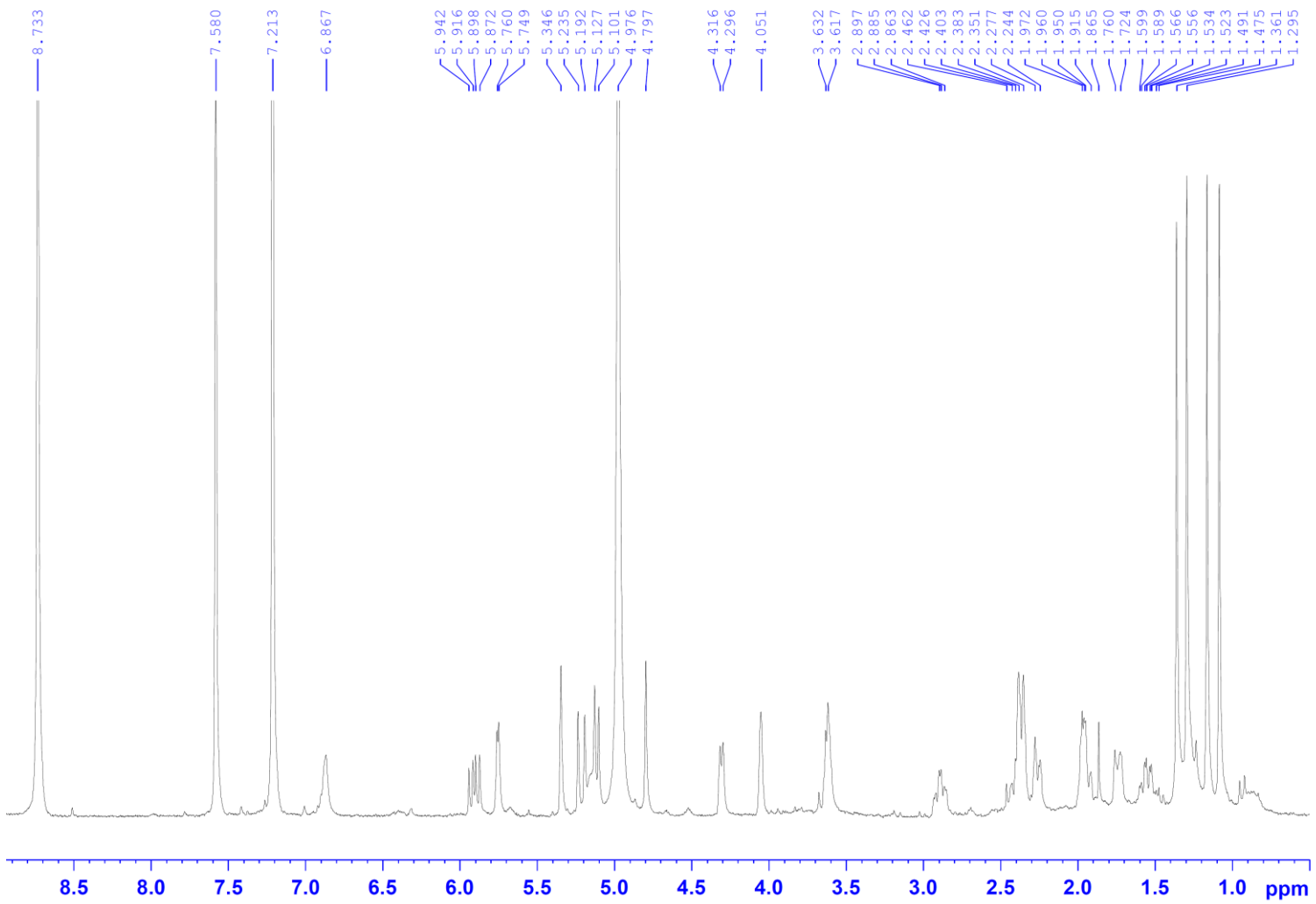

Figure S25. ^{1}H NMR spectrum of **4**.

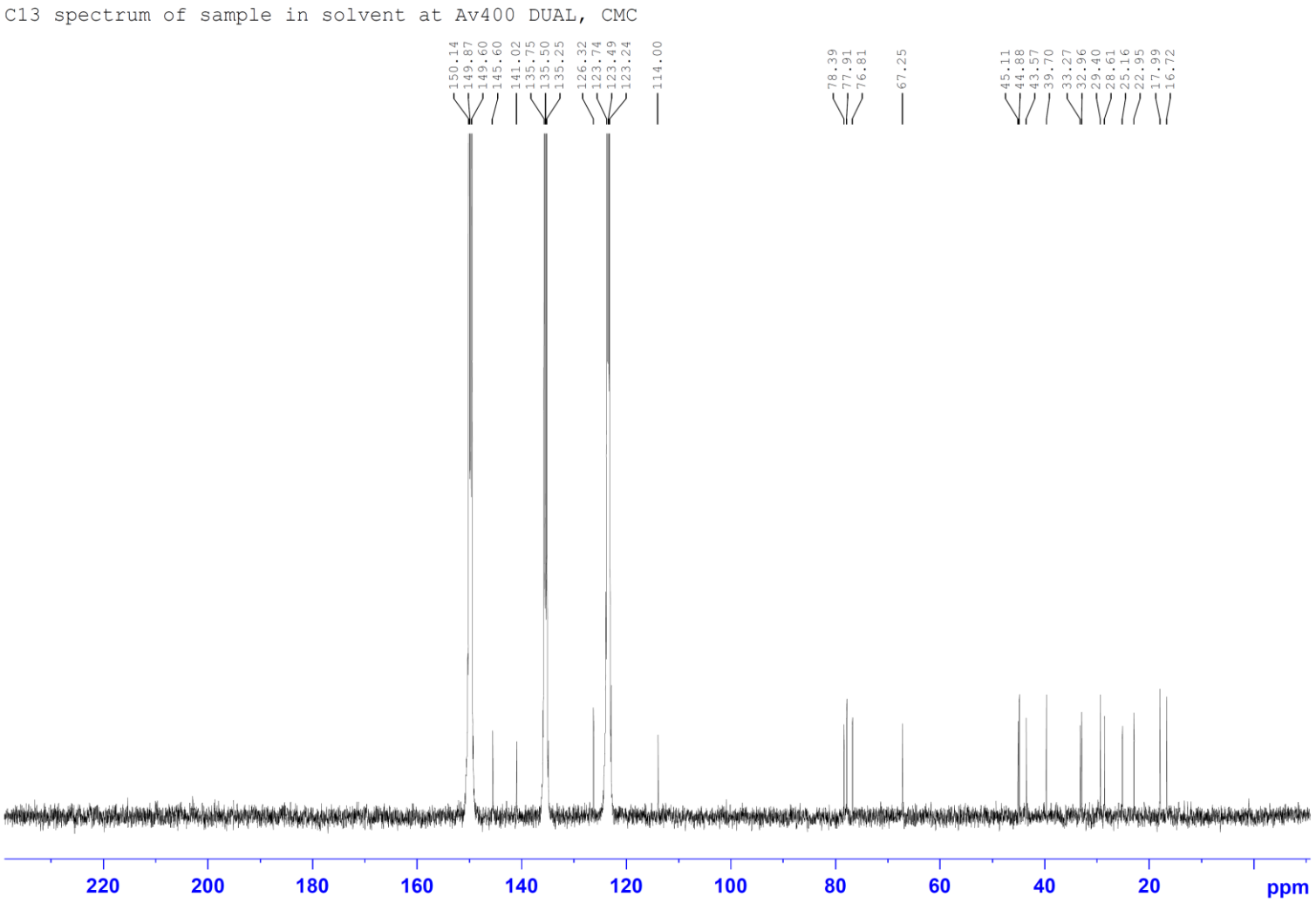

Figure S26. ^{13}C NMR spectrum of **4**.

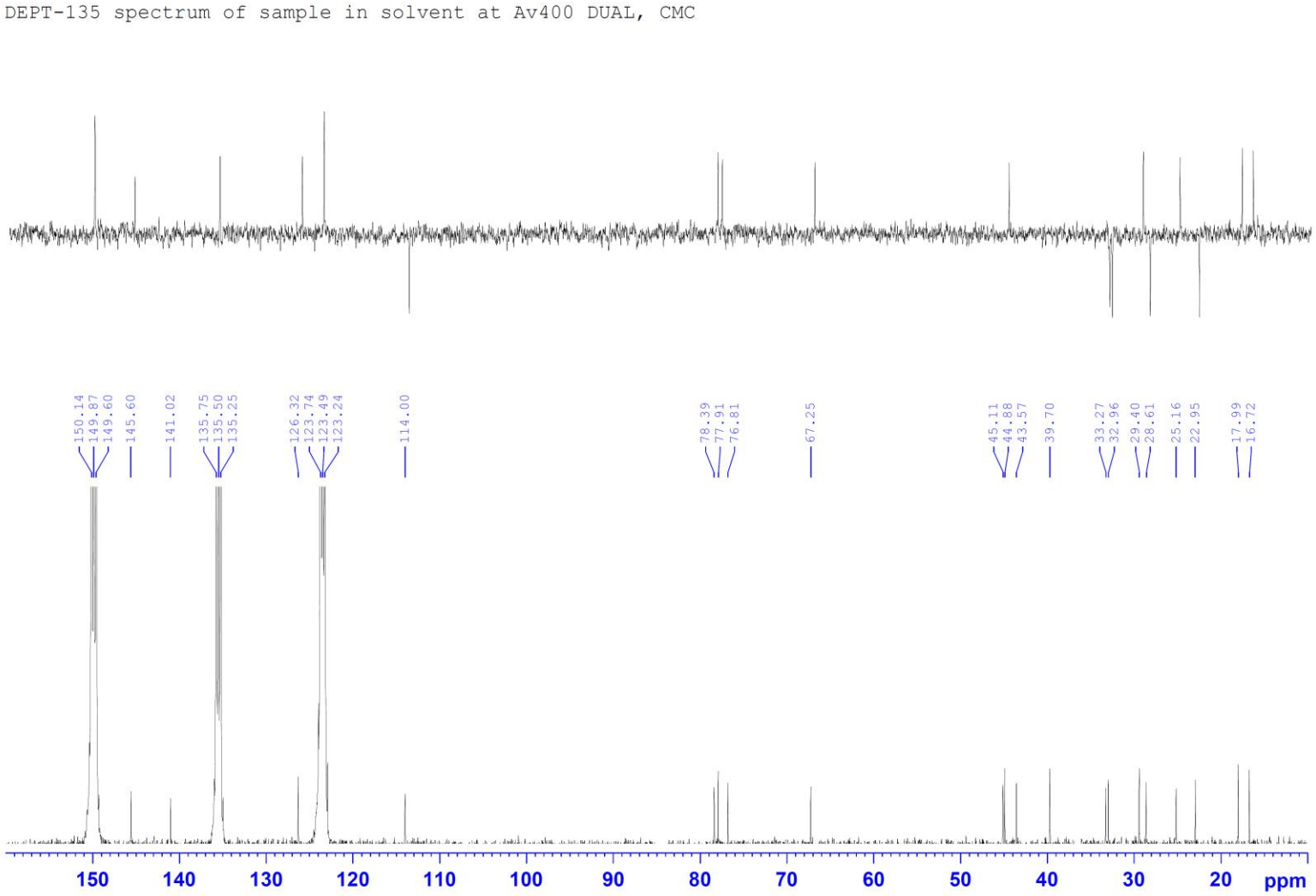

Figure S27. DEPT spectrum of **4**.

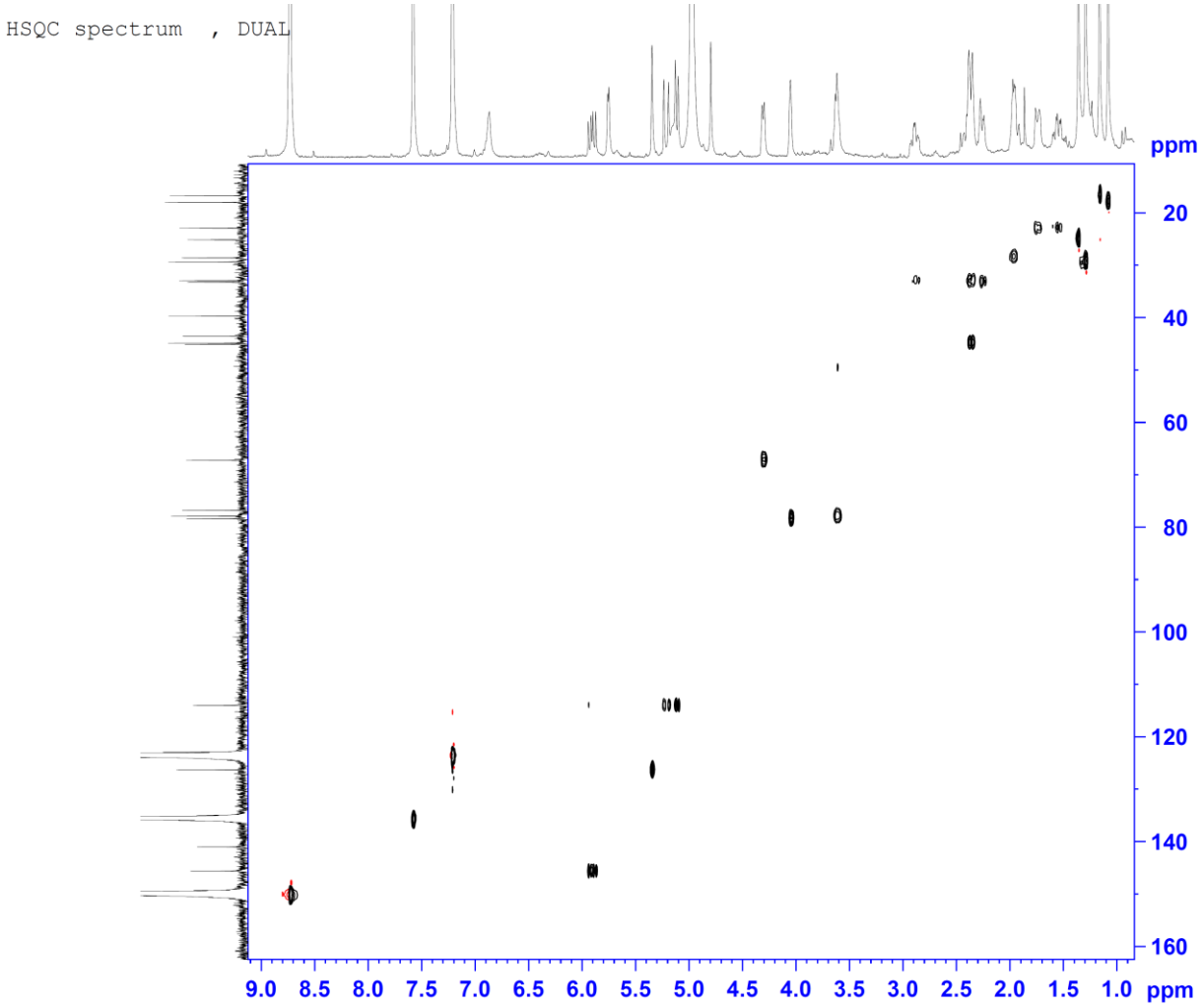

Figure S28. HSQC spectrum of **4**.

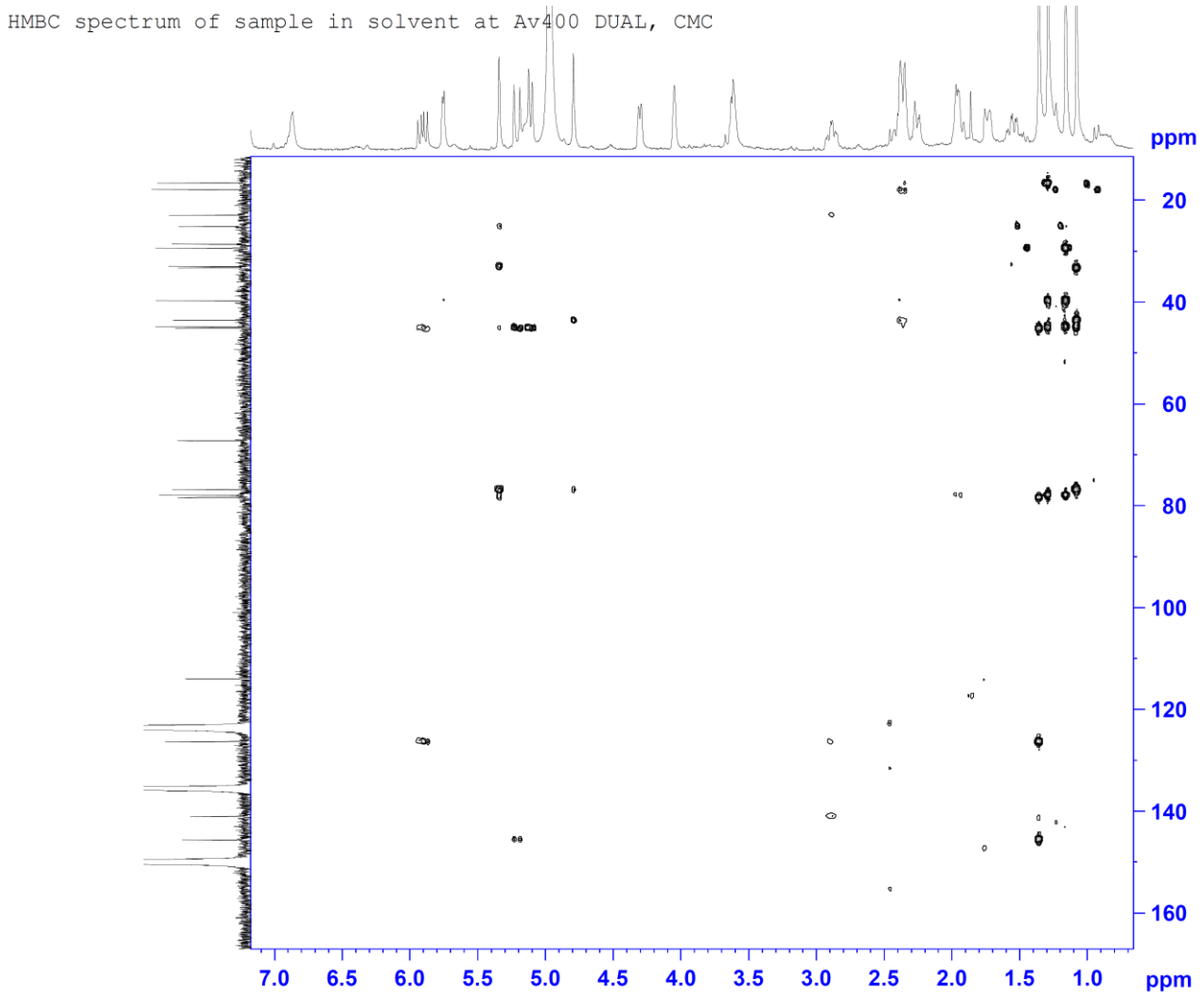

Figure S29. HMBC spectrum of **4**.

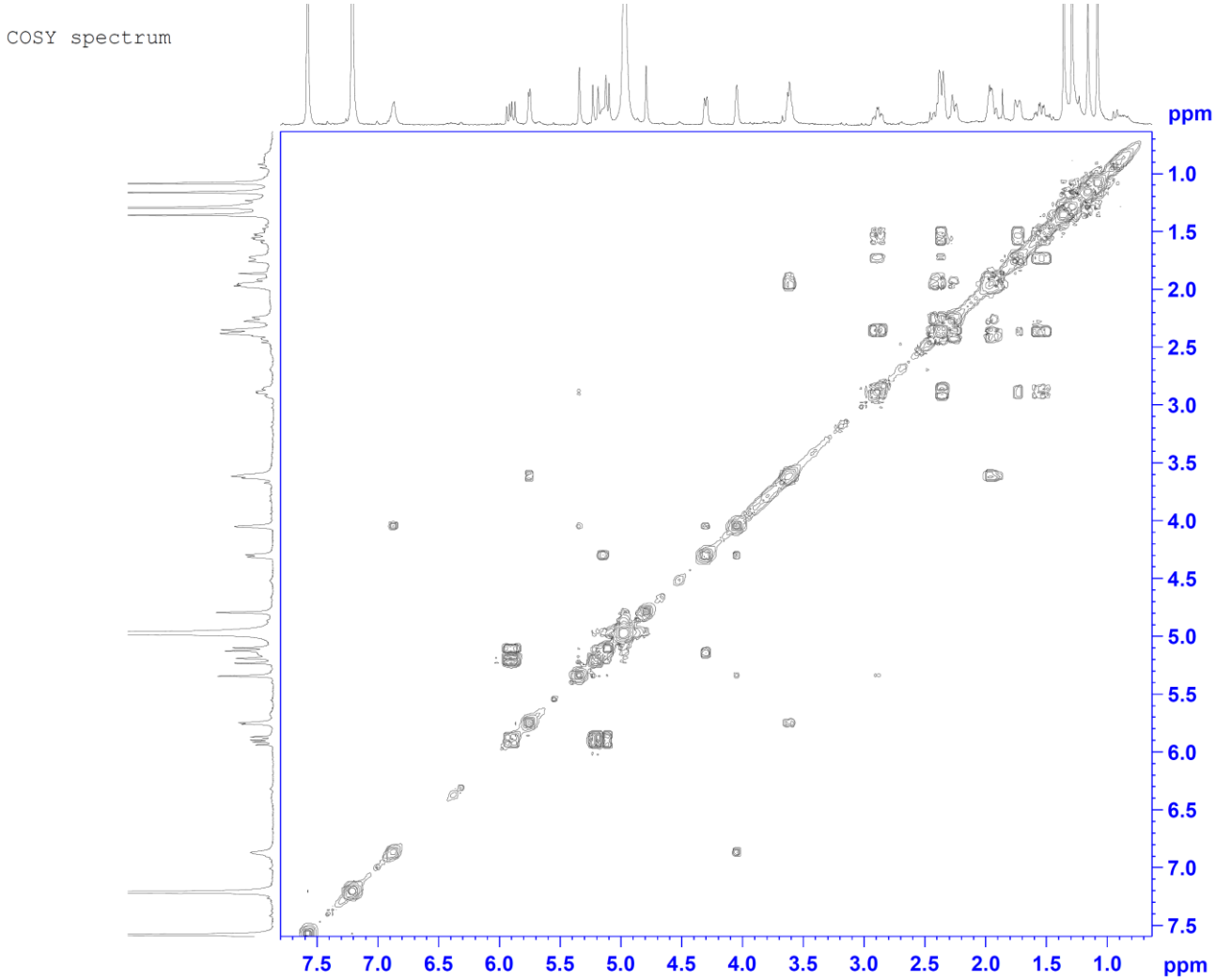

Figure S30. COSY spectrum of **4**.

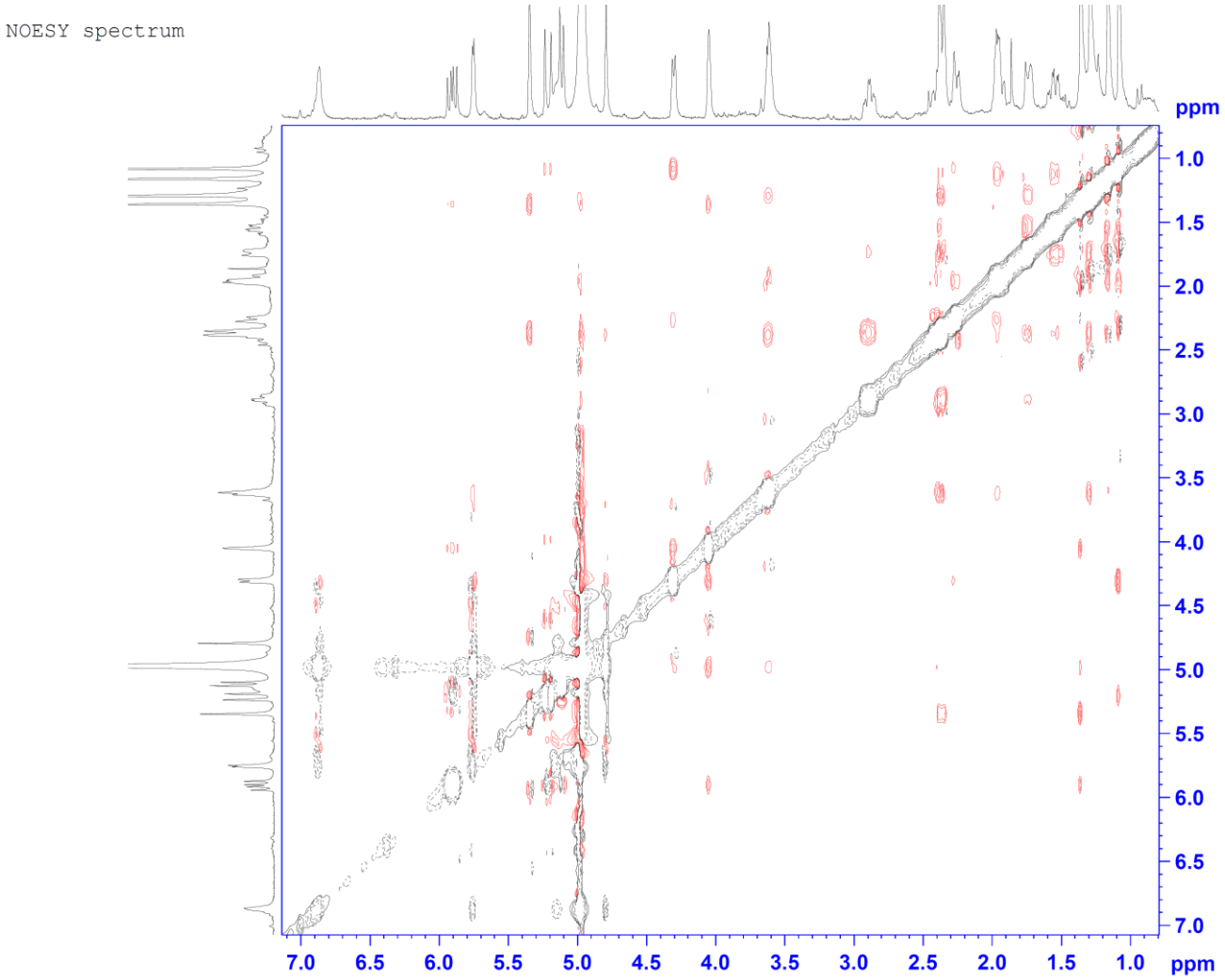

Figure S31. NOESY spectrum of **4**.

F:\Exp_data\...\30-FV-Cl-17J3C-APCI-H 2017/9/12 上午 11:28:26

30-FV-Cl-17J3C-APCI-H#1-20 RT: 0.00-0.52 AV: 20
T: FTMS - p APCI corona Full ms [300.00-340.00]
m/z= 317.1727-317.1781
Isotope Min Max
O-16 0 4
C-12 0 19
H-1 0 27
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
317.1752	329827.7	100.00	317.1747	1.46	$C_{19}H_{25}O_4$

Figure S32. (–)-HR-APCIMS spectrum of **5**.

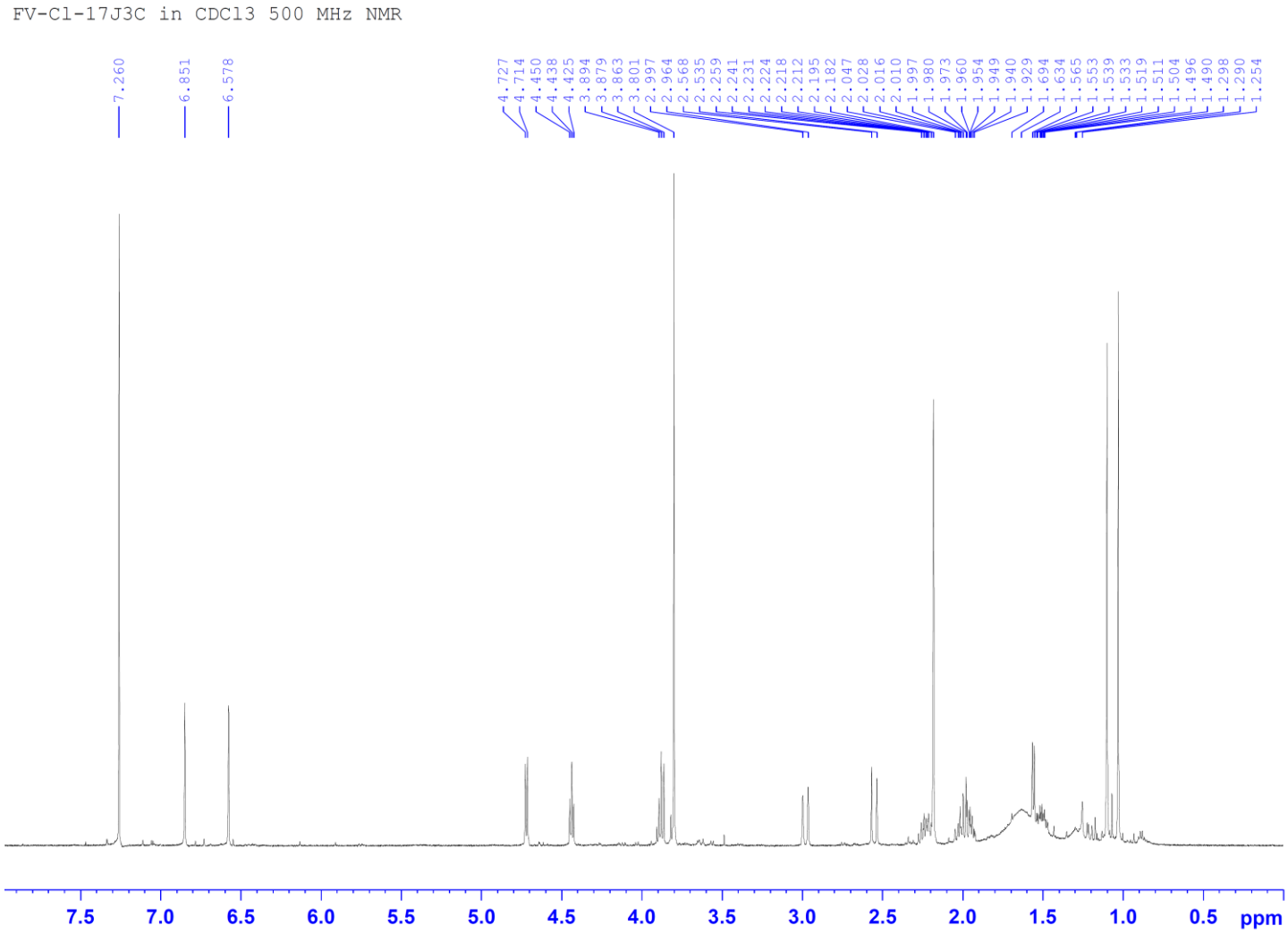

Figure S33. ^{1}H NMR spectrum of **5**.

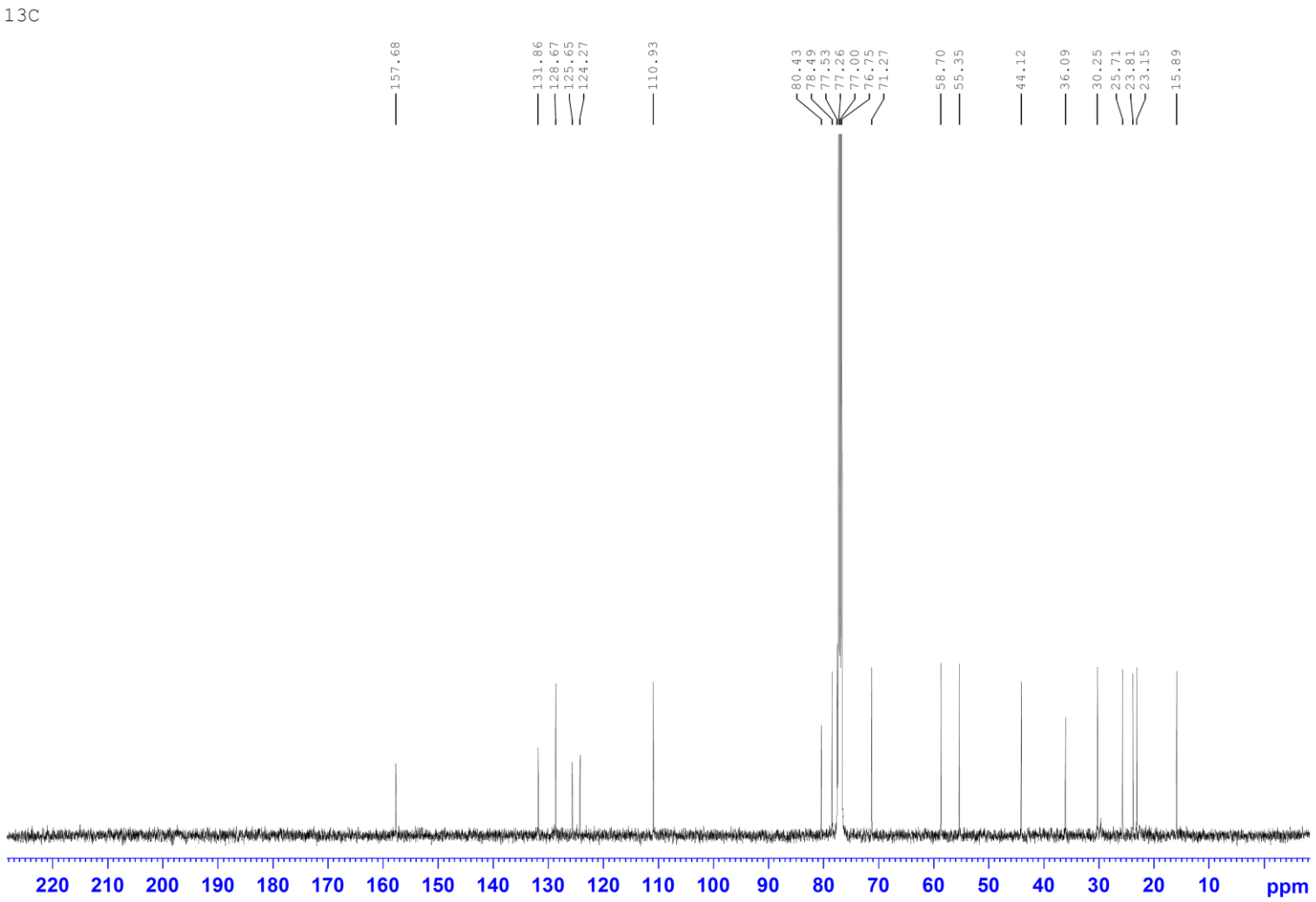

Figure S34. ^{13}C NMR spectrum of **5**.

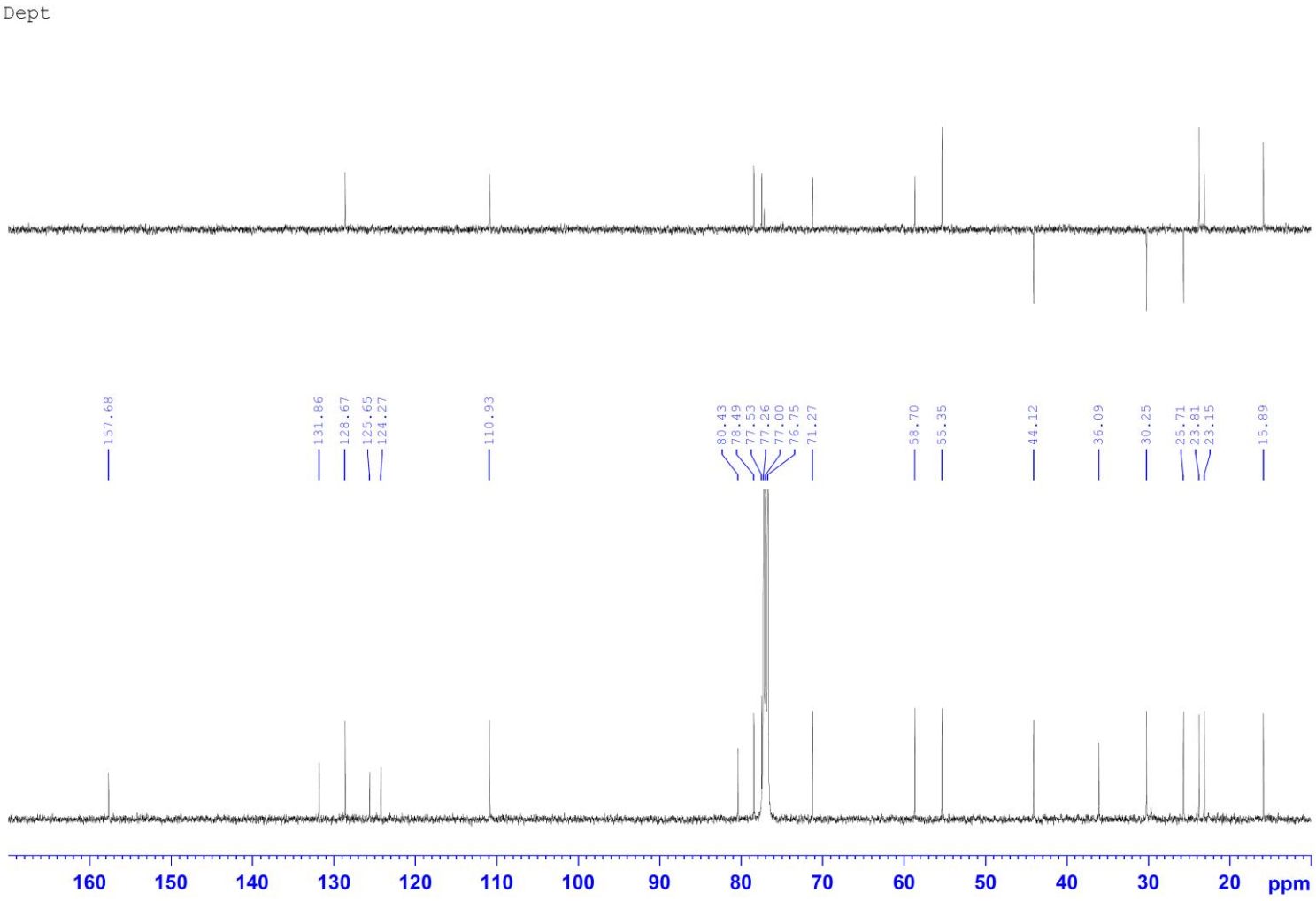

Figure S35. DEPT spectrum of **5**.

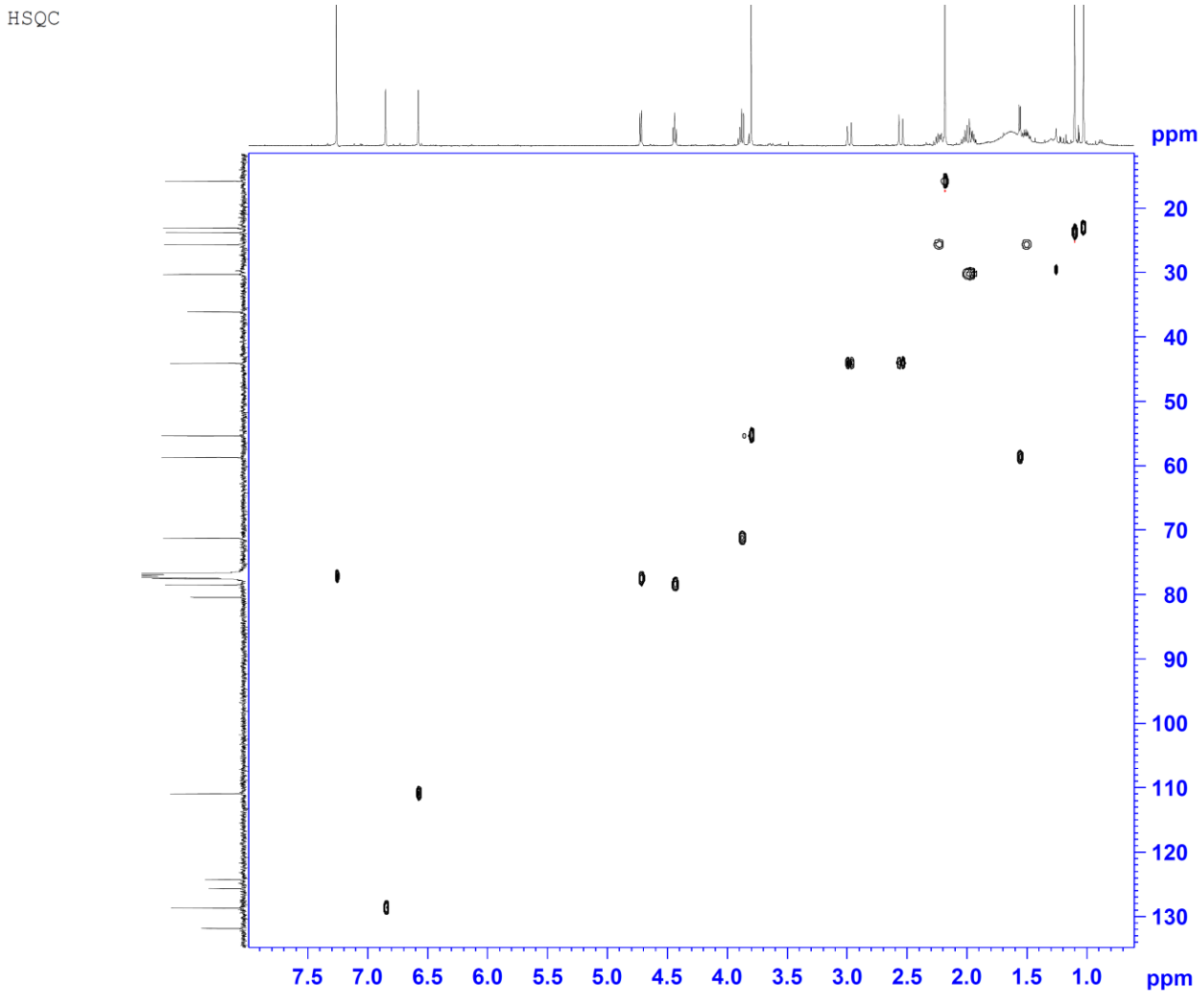

Figure S36. HSQC spectrum of **5**.

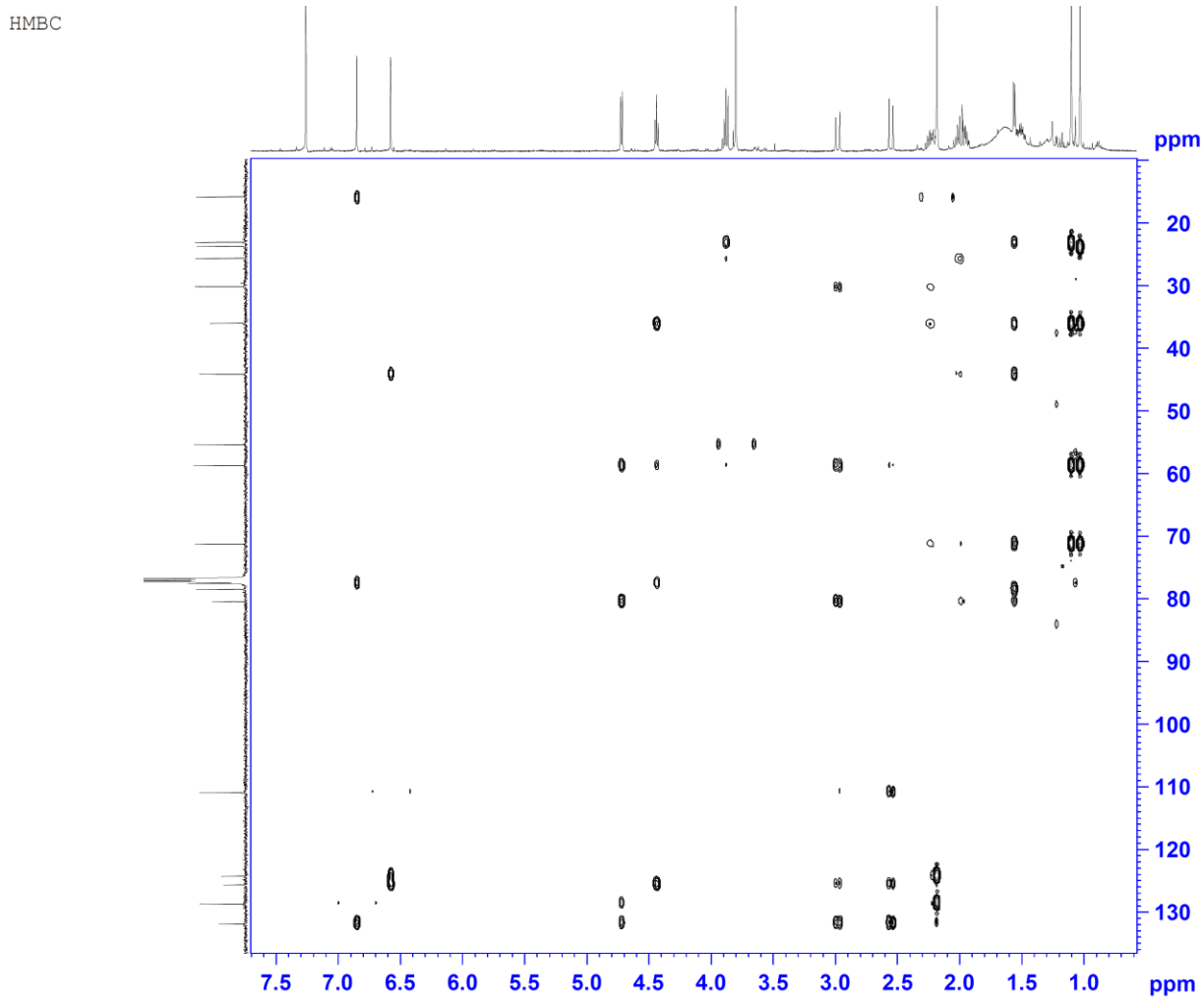

Figure S37. HMBC spectrum of **5**.

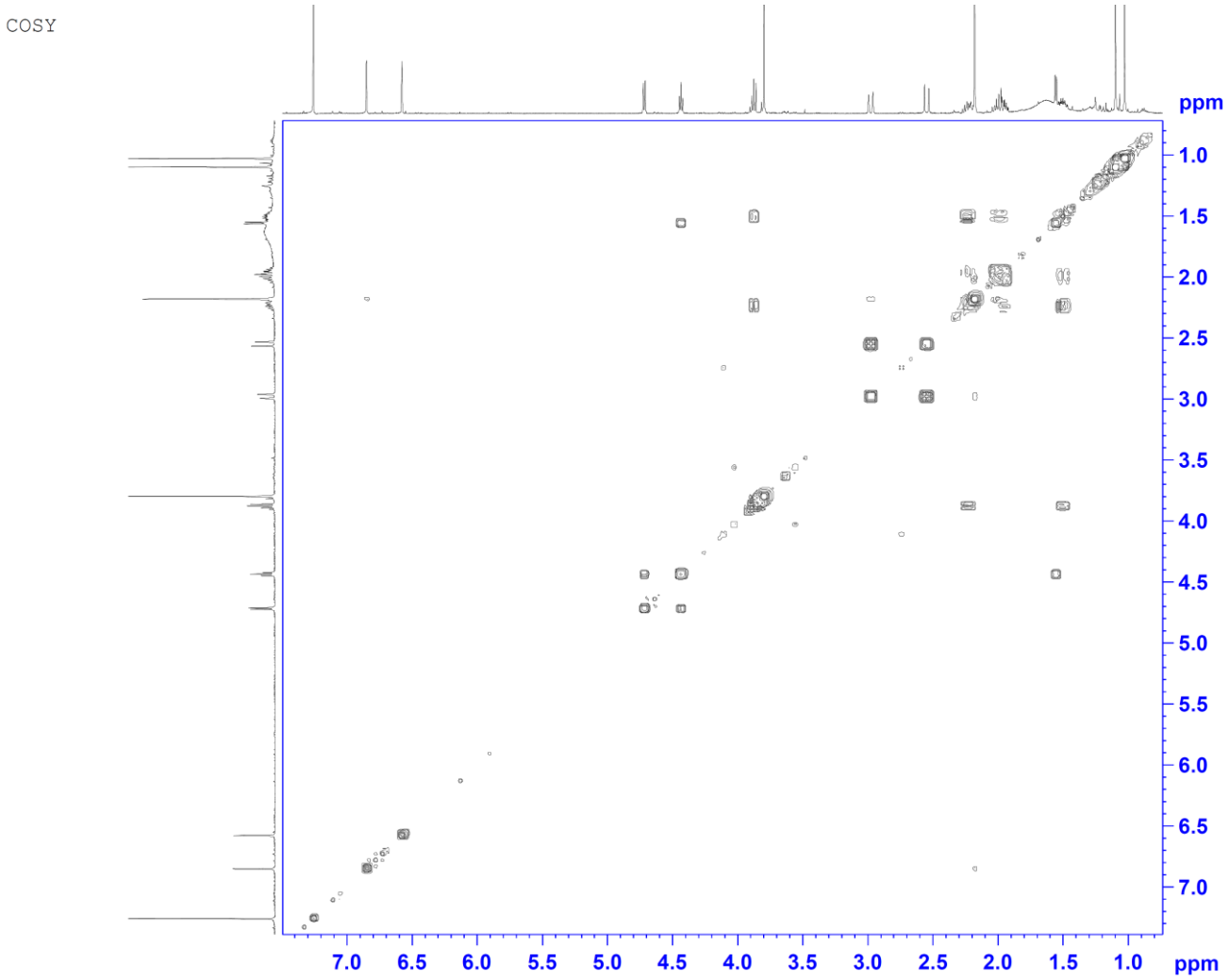

Figure S38. COSY spectrum of **5**.

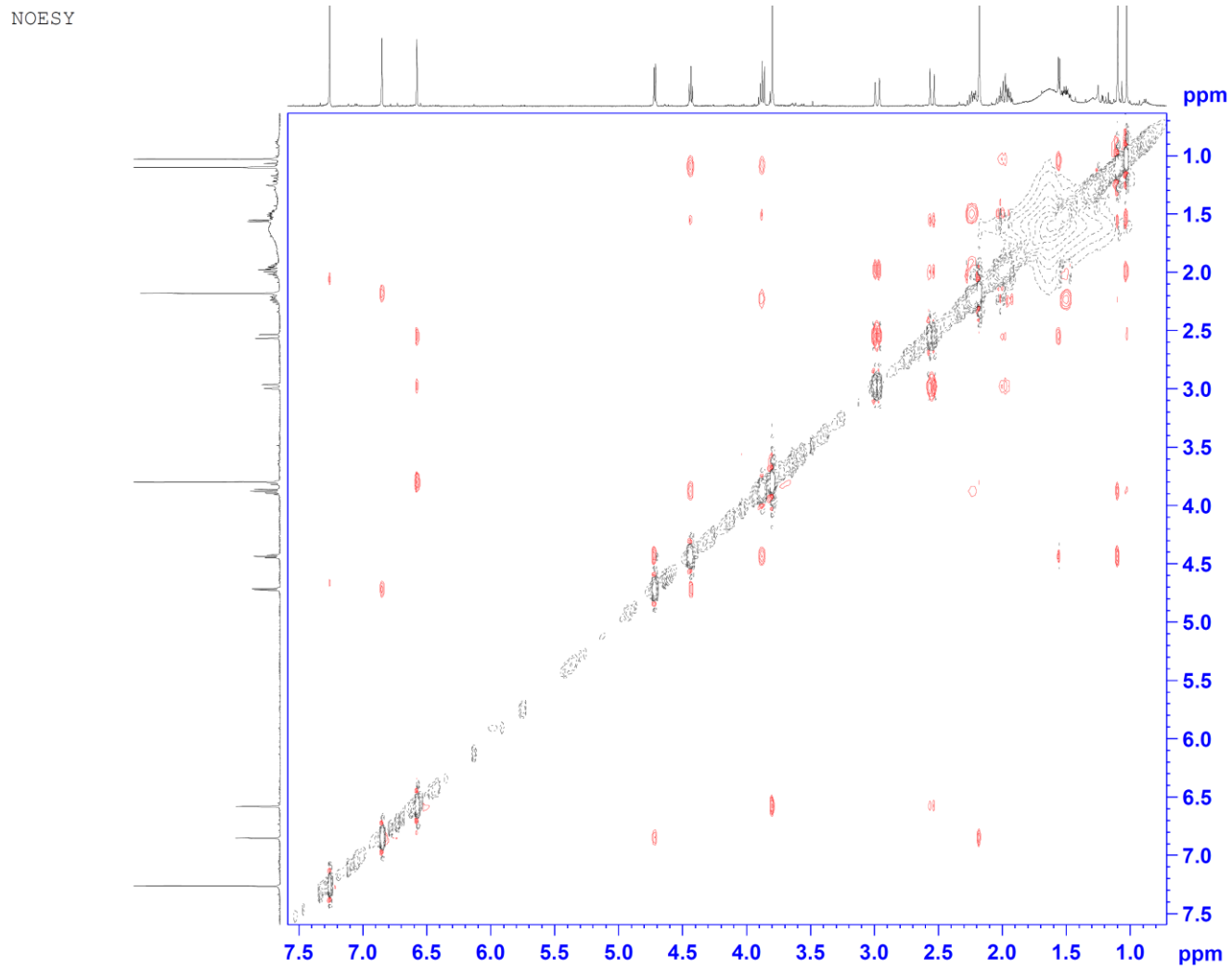

Figure S39. NOESY spectrum of **5**.

F:\Exp_data\...\07-FV-Cl-17J6C-H 2017/9/14 下午 02:11:36

07-FV-Cl-17J6C-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-500.00]
m/z= 341.1300-341.1982

Isotope	Min	Max
O-16	0	4
C-12	0	19
H-1	0	27
Na-23	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
341.1720	2807975.5	100.00	341.1723	-0.83	$C_{19}H_{26}O_4Na$

Figure S40. (+)-HR-ESIMS spectra of **6**.

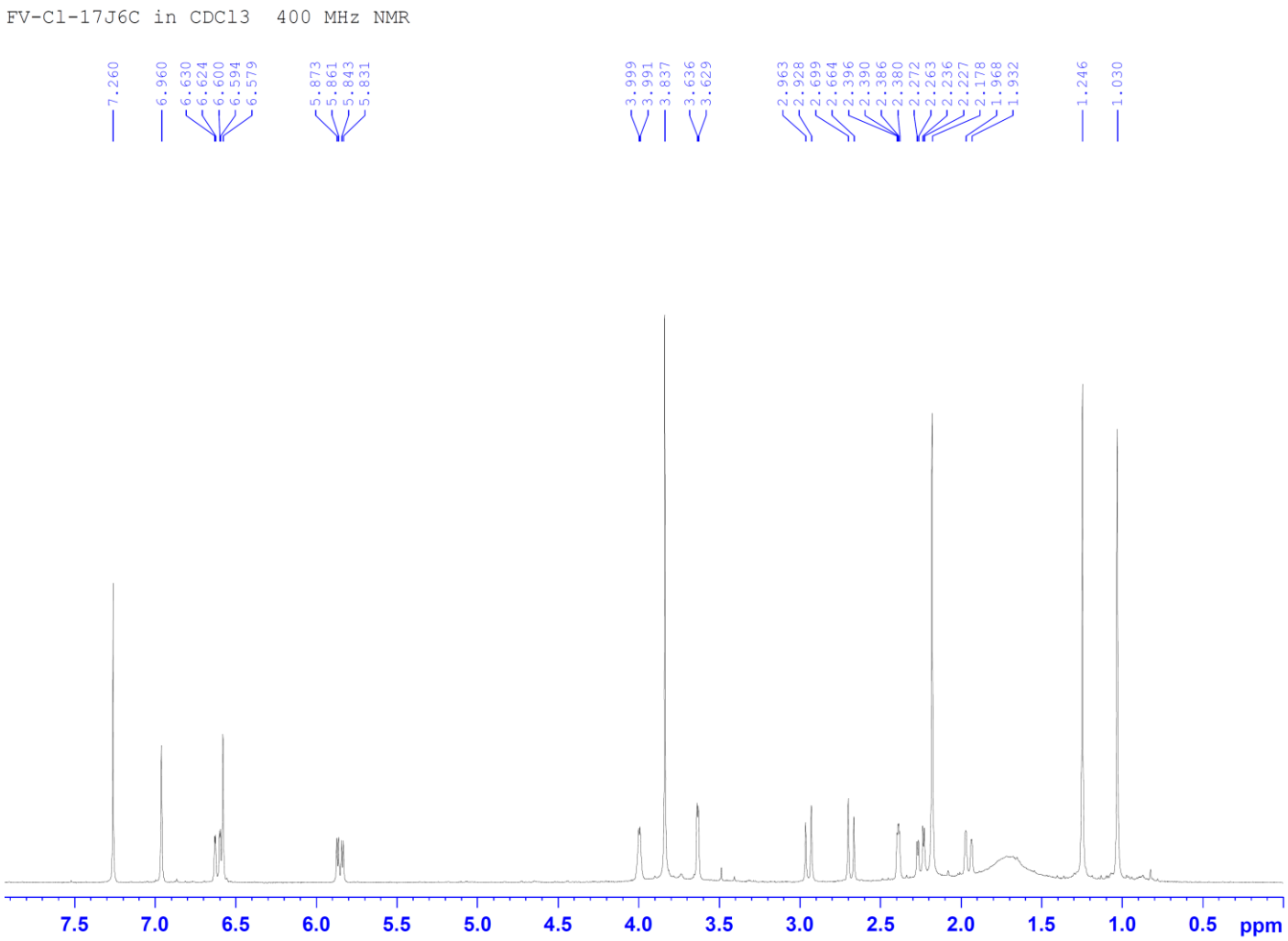

Figure S41. ^{1}H NMR spectrum of **6**.

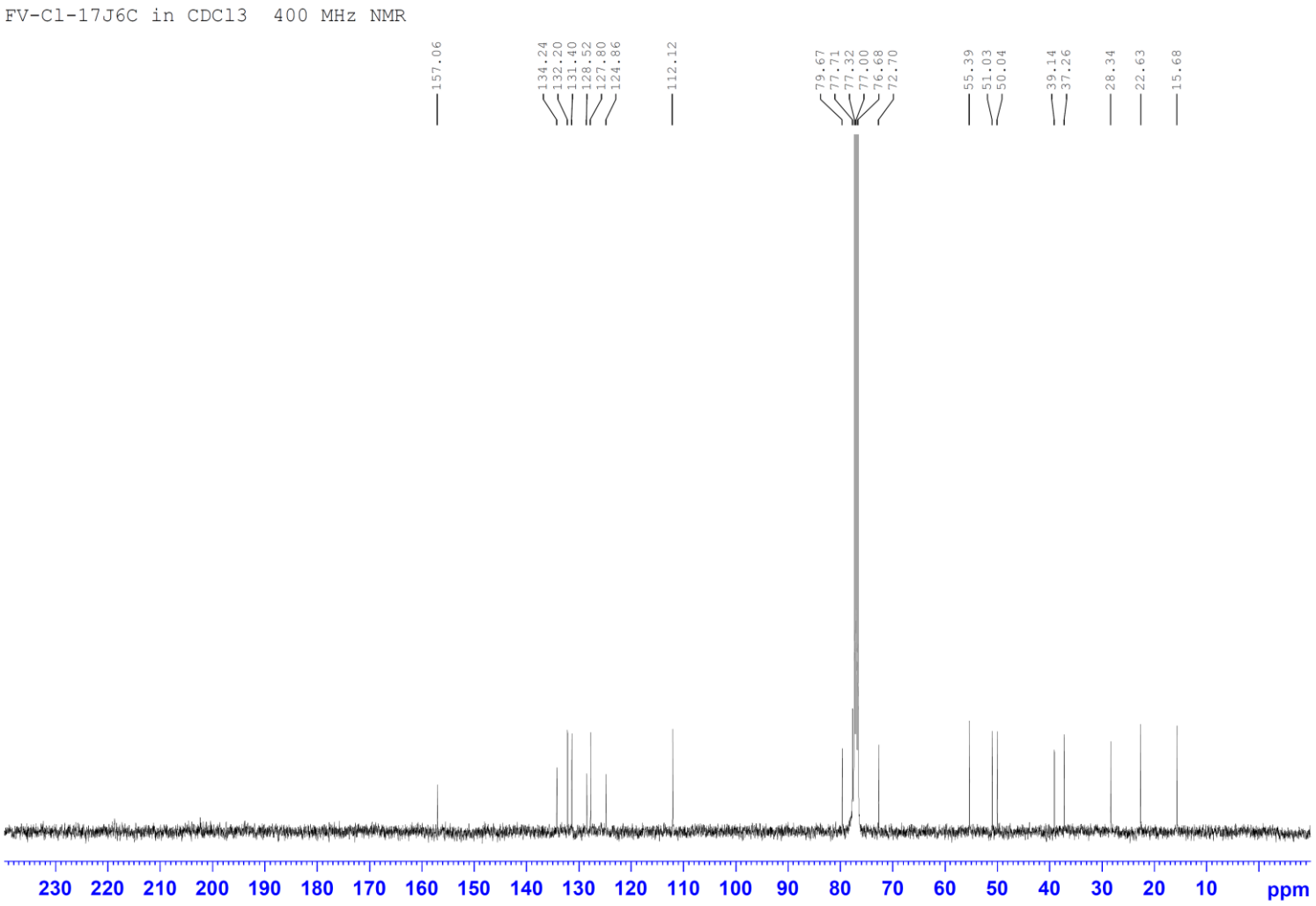

Figure S42. ^{13}C NMR spectrum of **6**.

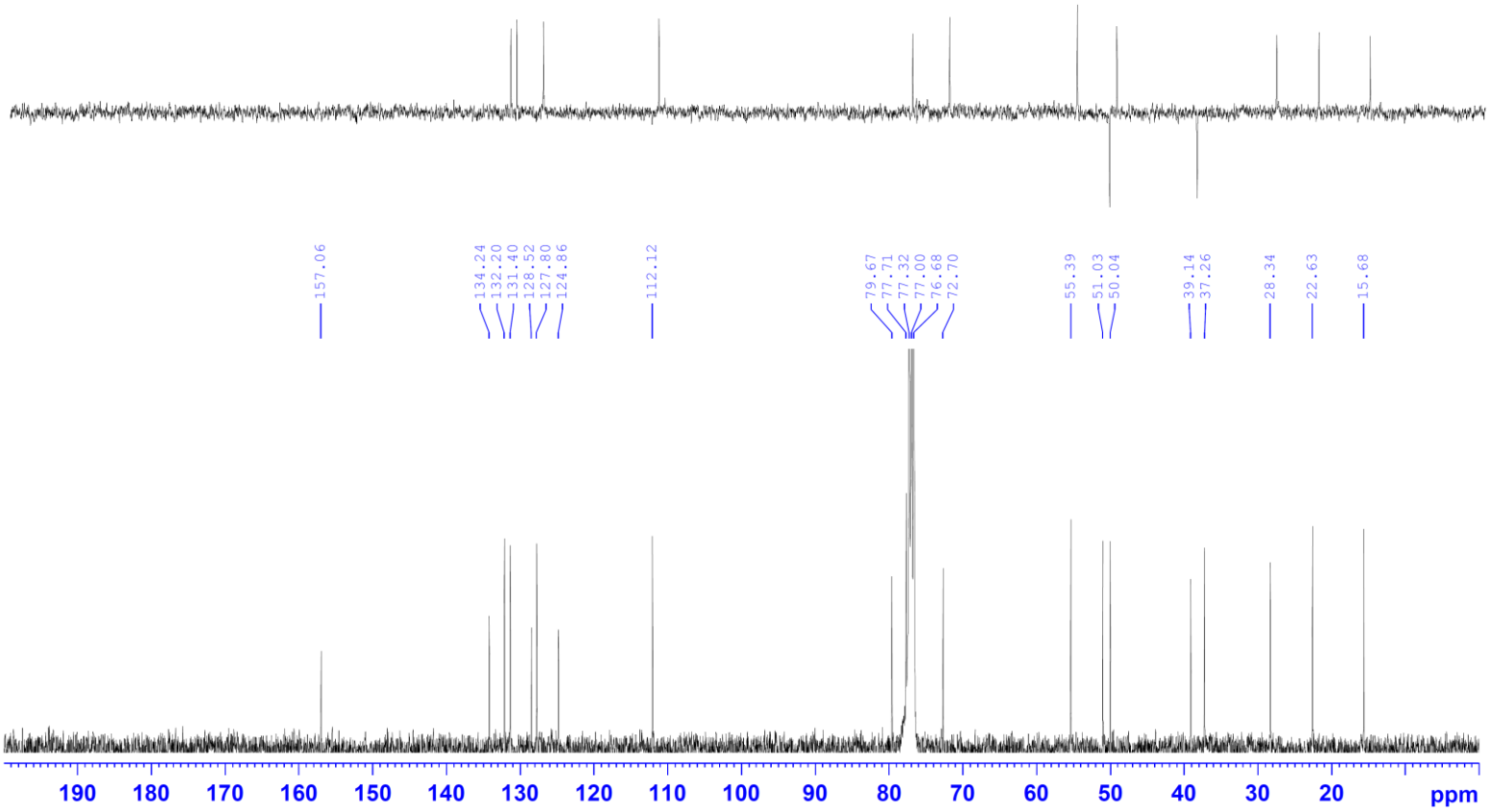

Figure S43. DEPT spectrum of **6**.

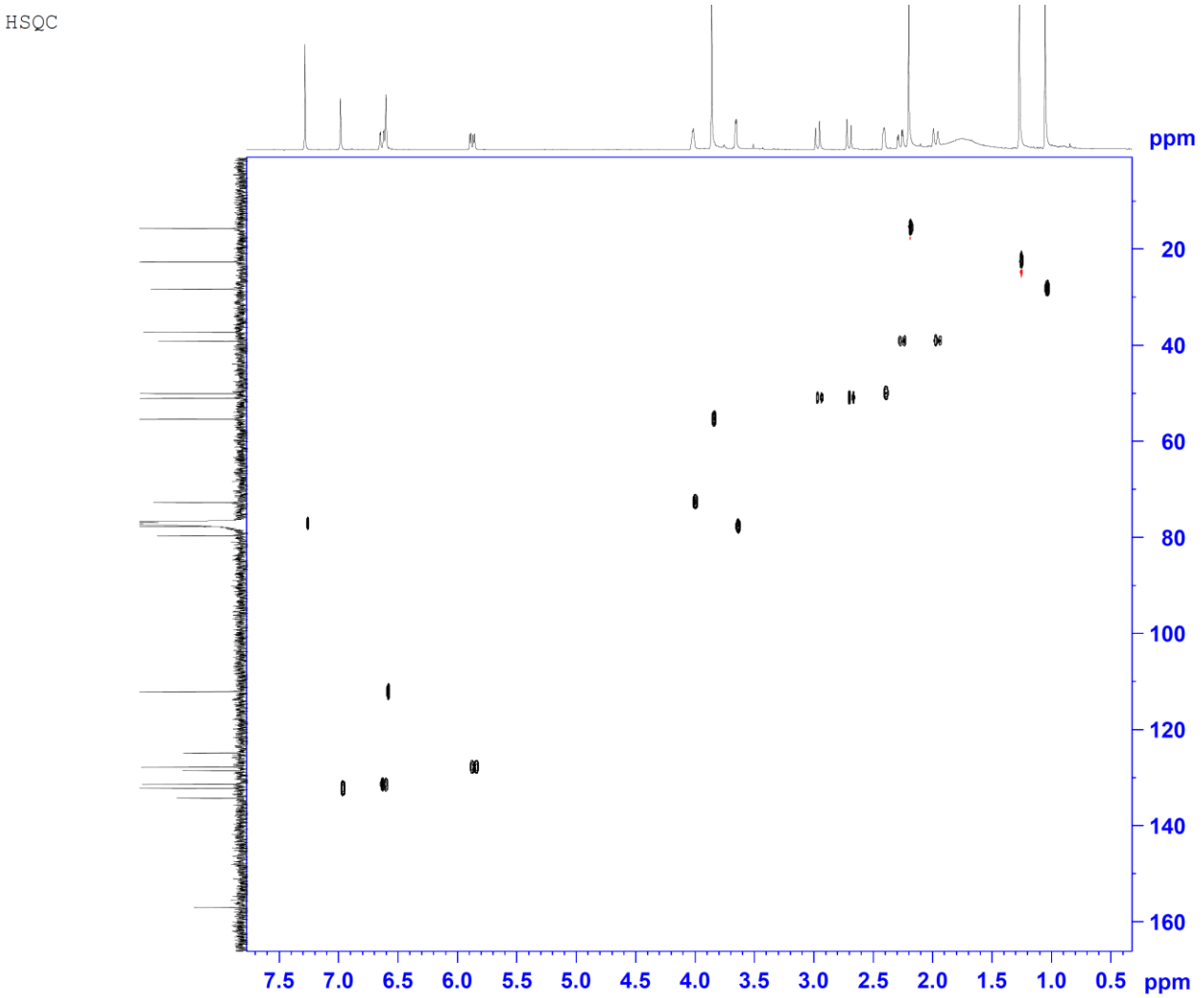

Figure S44. HSQC spectrum of **6**.

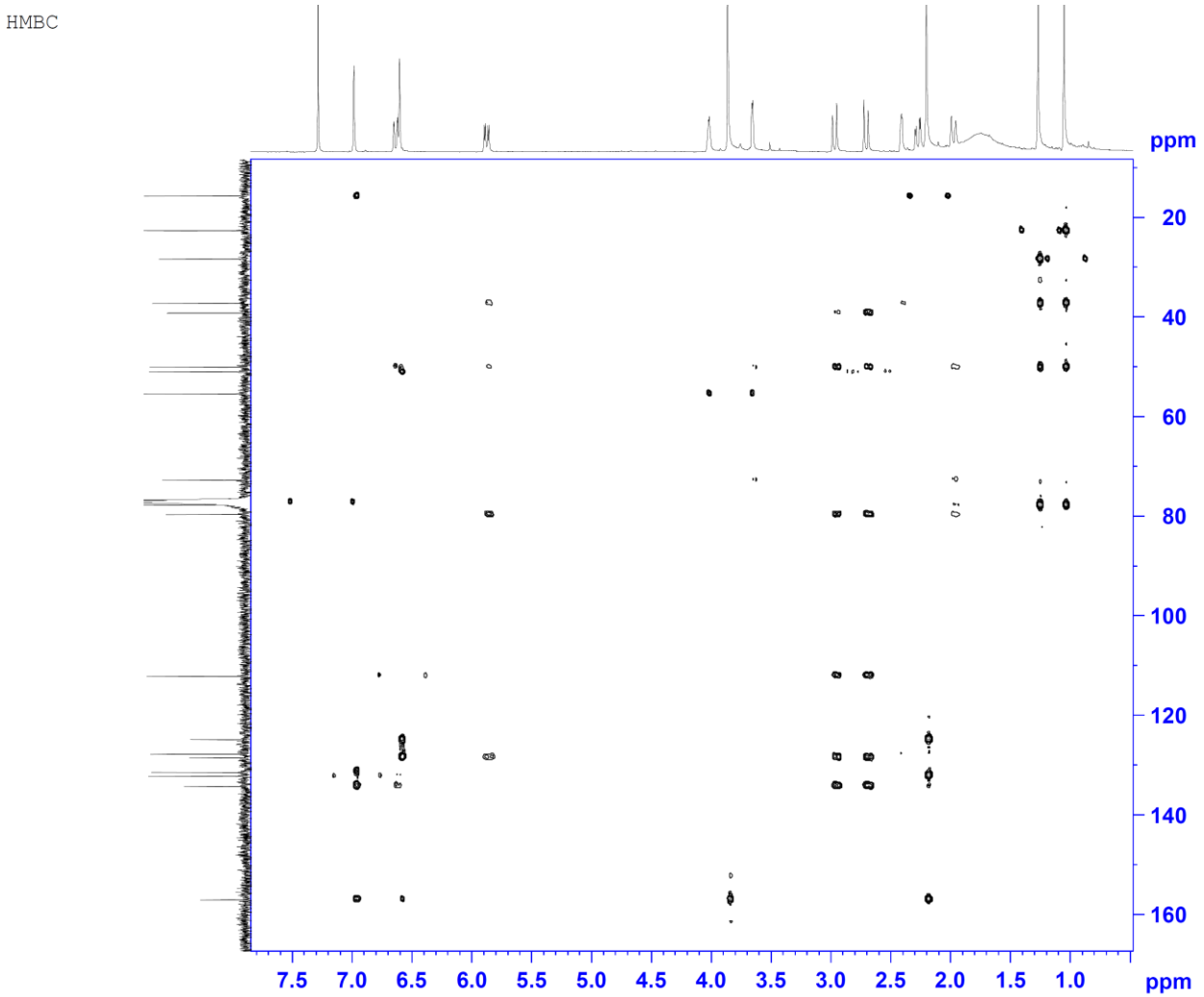

Figure S45. HMBC spectrum of **6**.

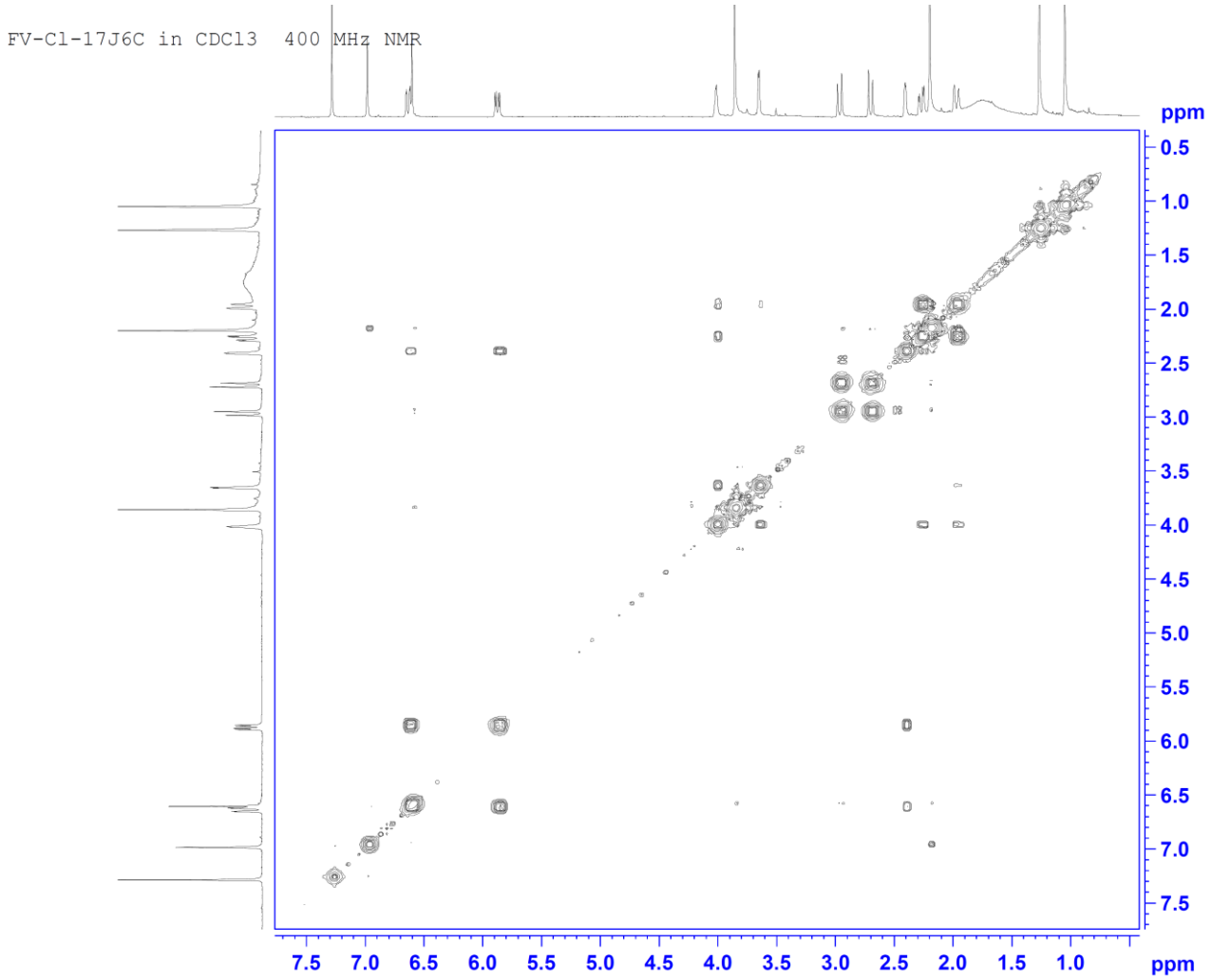

Figure S46. COSY spectrum of **6**.

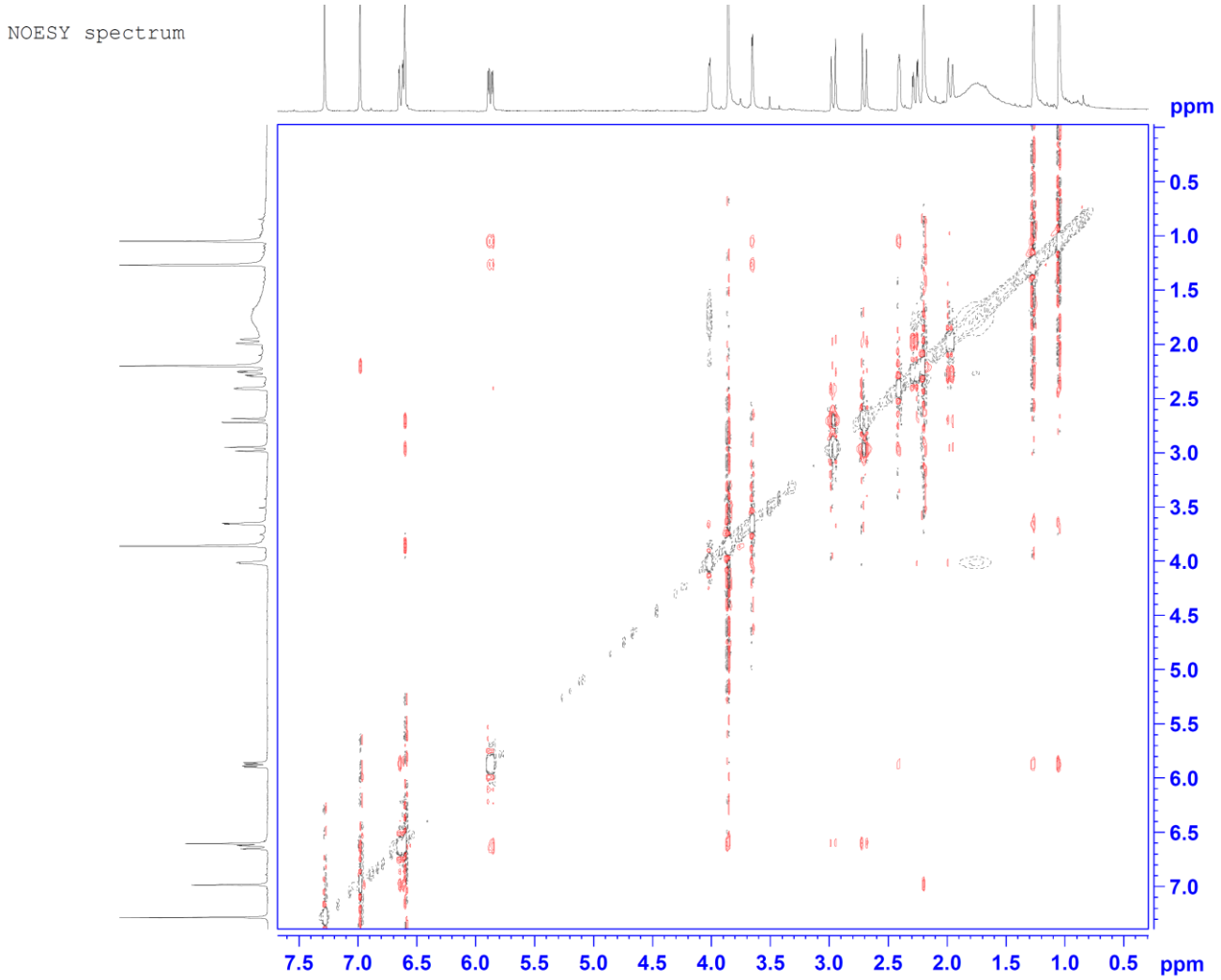

Figure S47. NOESY spectrum of **6**.

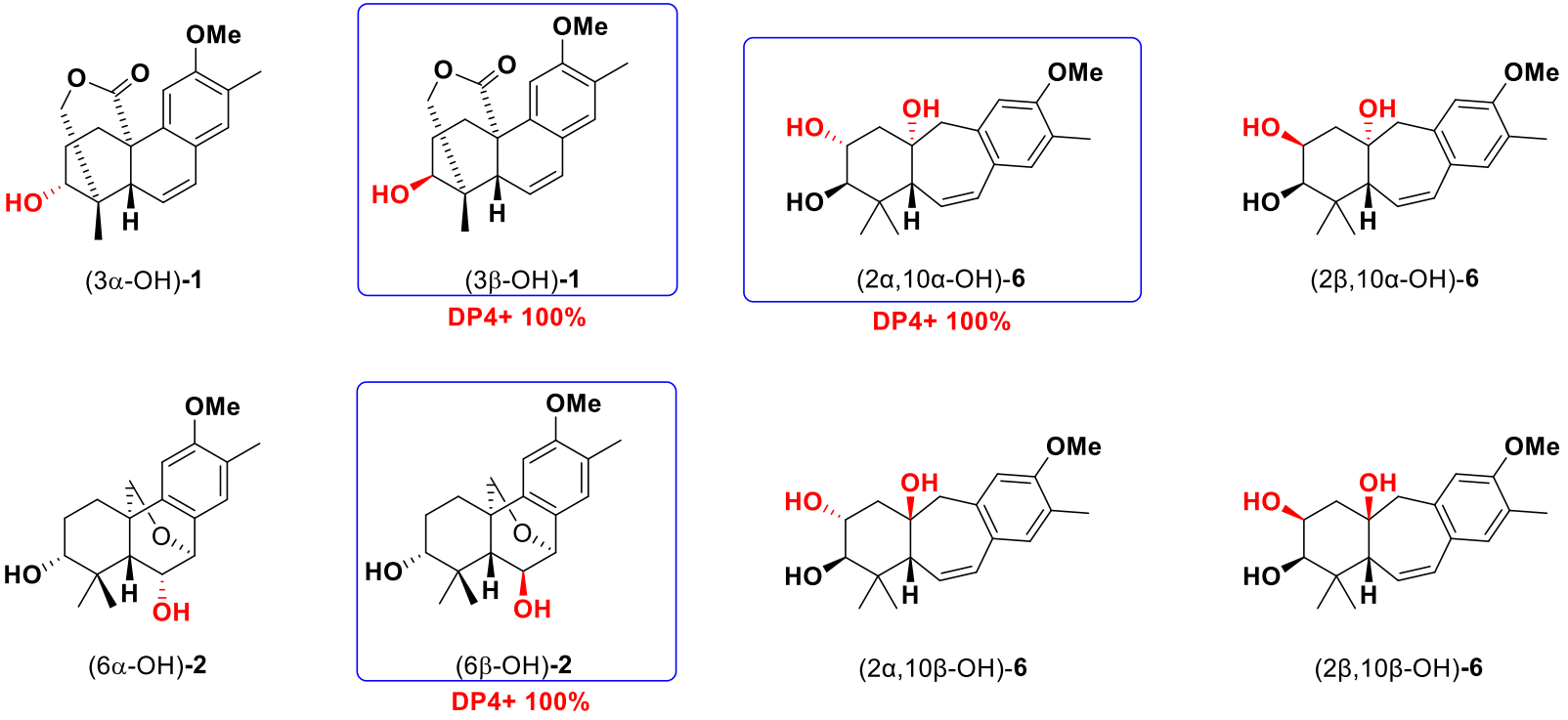

Figure S48. Possible candidates of compounds **1**, **2**, and **6** for DP4+ probability analysis.

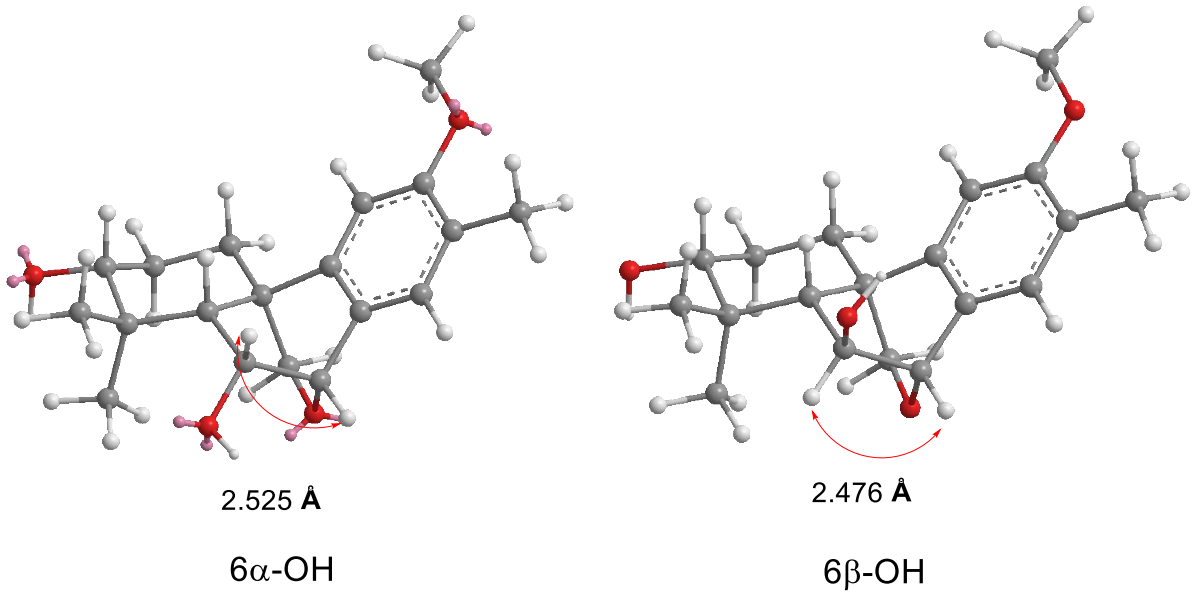

Figure S49. H-6/H-7 distance of 6α-OH and 6β-OH possible candidates of compound **2.** Conformers were generated by MM2 energy minimizations.

Table S1. DP4+ analysis table for compound **1** (isomer **1**: 3β-OH; isomer **2**: 3α-OH).

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-31+G(d,p)

Isomer №			1	2	3
DP4+ (%)		H data	100.00%	0.00%	-
		C data	100.00%	0.00%	-
		All data	100.00%	0.00%	-
Type	sp2?	Exp	1	2	3
C	x	108.1	89.59574001	89.2967897	
C	x	134.8	61.9701478	62.489968	
C	x	125.2	72.23589959	72.5038408	
C	x	129	69.60684022	69.4925838	
C	x	125.9	71.8181605	71.6585755	
C	x	157.4	41.8256481	41.7256232	
C		47.5	143.8645873	144.333204	
C		39	153.4398502	147.823136	
C	x	122.8	73.78434471	74.8083597	
C	x	131.2	66.20999243	66.4814807	
C		15.8	177.347593	177.423368	
C		27.9	163.9664729	160.691371	
C		28.9	164.7070977	163.300495	
C		74.5	119.3974051	120.03775	
C		36.6	155.7825877	155.226002	
C		19.3	176.4108609	176.814747	
C	x	174.5	24.27630265	24.4480983	
C		75.4	121.5269572	124.880552	
C		55.4	142.015428	142.109266	
H	x	6.93	24.51803458	24.5233053	
H	x	6.89	24.39986759	24.42251	
H		2.94	28.42534812	29.0671563	
H	x	5.9	25.34491231	25.2815031	
H	x	6.6	24.54488507	24.6163656	
H		2.18	29.33899984	29.3323841	
H		2.42	29.32183365	29.0578319	
H		2.28	29.33693171	29.660755	
H		2.1	29.66138839	29.5900136	
H		2.05	29.47941688	29.7443486	
H		3.81	27.72538307	27.8833957	
H		1.19	30.47799693	30.3829288	
H		4.04	27.52986444	26.8409481	
H		4.37	27.11379826	27.3127916	
H		3.88	27.62024425	27.6388816	

Table S2. Conformers and Boltzmann populations of 3α-OH isomer of **1**.

3α1 (69.69%)			**3α2** (30.31%)		
C	1.99573	−0.7934 −0.17558	C	1.996059	−0.78716 −0.18317
C	0.972396	0.154266 −0.09847	C	0.972865	0.160853 −0.10569
C	1.314187	1.519463 −0.05034	C	1.315497	1.525083 −0.04084
C	2.667677	1.889923 −0.08531	C	2.669846	1.894231 −0.0618
C	3.697269	0.960313 −0.17587	C	3.69915	0.964633 −0.15348
C	3.337629	−0.40112 −0.21977	C	3.338642	−0.39609 −0.21317
C	−0.50657	−0.23837 0.025388	C	−0.50676	−0.23444 0.003024
C	−1.42088	0.831768 −0.63714	C	−1.42406	0.848296 −0.63578
C	−1.0211	2.229962 −0.21788	C	−1.01765	2.243124 −0.21326
C	0.261177	2.527135 0.035394	C	0.264722	2.535009 0.045192
C	5.147789	1.366235 −0.21767	C	5.150315	1.369428 −0.18045
C	−0.81086	−1.61655 −0.62888	C	−0.81206	−1.59208 −0.69457
C	−2.28814	−2.0092 −0.50429	C	−2.28579	−1.99869 −0.57227
C	−3.2263	−0.89451 −0.97142	C	−3.24888	−0.87673 −0.96675
C	−2.90694	0.491353 −0.35109	C	−2.90762	0.509558 −0.33479
O	−4.58612	−1.20387 −0.66161	O	−4.60244	−1.26046 −0.7234
C	−3.87369	1.515003 −0.9813	C	−3.88071	1.539038 −0.94214
C	−0.83933	−0.41502 1.529567	C	−0.83989	−0.46484 1.500359
O	−0.04477	−0.86407 2.320824	O	−0.05291	−0.95579 2.272872
O	−2.11163	−0.19585 1.943429	O	−2.1139	−0.25306 1.926113
C	−3.10804	0.507705 1.16877	C	−3.07906	0.522849 1.185637
O	4.38523	−1.27694 −0.30092	O	4.385806	−1.27191 −0.29407
C	4.11272	−2.66862 −0.28801	C	4.112096	−2.66366 −0.30147
H	1.753506	−1.8468 −0.18163	H	1.752946	−1.84018 −0.19978
H	2.920438	2.947843 −0.04472	H	2.923283	2.951438 −0.00925
H	−1.26557	0.755542 −1.72889	H	−1.28388	0.779997 −1.73017
H	−1.77464	3.010331 −0.19007	H	−1.76876	3.026315 −0.18988
H	0.554095	3.546309 0.280149	H	0.560452	3.552757 0.292573
H	5.249113	2.454567 −0.16581	H	5.252283	2.457208 −0.1193
H	5.708023	0.927018 0.616215	H	5.703421	0.923052 0.654381
H	5.634288	1.017913 −1.13669	H	5.643603	1.027651 −1.09826
H	−0.19982	−2.3958 −0.16531	H	−0.19372	−2.38481 −0.26511
H	−0.51791	−1.55806 −1.68543	H	−0.52986	−1.49527 −1.75092
H	−2.47525	−2.91475 −1.09911	H	−2.48791	−2.87497 −1.19907
H	−2.53162	−2.25966 0.534101	H	−2.4958	−2.30144 0.463059
H	−3.1148	−0.77738 −2.06427	H	−3.19515	−0.73582 −2.05473

H -4.76492 -2.10186 -0.98033	H -4.63327 -1.70469 0.138719
H -3.67739 1.611664 -2.05582	H -3.66687 1.683793 -2.00782
H -4.90696 1.181262 -0.85761	H -4.90772 1.174645 -0.85288
H -3.78222 2.508334 -0.53301	H -3.82198 2.516018 -0.45313
H -4.05924 0.04338 1.437047	H -4.05418 0.121034 1.478199
H -3.11053 1.542355 1.529789	H -3.01852 1.551593 1.558526
H 3.595822 -2.9698 0.632308	H 3.588017 -2.9763 0.610889
H 3.510865 -2.97114 -1.15559	H 3.516766 -2.95403 -1.17756
H 5.08464 -3.1636 -0.33568	H 5.084028 -3.15862 -0.34813

Table S3. Conformers and Boltzmann populations of 3β-OH isomer of **1**.

3β1 (46.15%)	**3β2** (45.62%)	**3β3** (8.23%)
C 1.941671 -0.77581 -0.09939	C 1.943799 -0.77349 -0.10511	C 1.94132 -0.77485 -0.09879
C 0.898418 0.151465 -0.04939	C 0.900018 0.152633 -0.04962	C 0.89835 0.152885 -0.04836
C 1.206661 1.524348 -0.10651	C 1.207574 1.526065 -0.09838	C 1.206942 1.525684 -0.10544
C 2.548512 1.922298 -0.21176	C 2.549227 1.925754 -0.201	C 2.54882 1.923428 -0.21295
C 3.597651 1.01218 -0.27457	C 3.598835 1.016753 -0.26925	C 3.597501 1.013185 -0.27731
C 3.27111 -0.35682 -0.21643	C 3.272982 -0.35295 -0.21967	C 3.270869 -0.3561 -0.21737
C -0.56615 -0.26144 0.153777	C -0.56344 -0.26564 0.150659	C -0.56585 -0.26068 0.154867
C -1.52124 0.730938 -0.57301	C -1.52135 0.73383 -0.56113	C -1.52279 0.735734 -0.56441
C -1.14912 2.164769 -0.26346	C -1.14869 2.166619 -0.24786	C -1.1491 2.168692 -0.25207
C 0.130542 2.510609 -0.06223	C 0.131478 2.511696 -0.04819	C 0.131741 2.512103 -0.0546
C 5.035418 1.447565 -0.39323	C 5.036374 1.45346 -0.38529	C 5.035155 1.447937 -0.39805
C -0.85677 -1.70205 -0.35921	C -0.85498 -1.69824 -0.3852	C -0.85537 -1.70101 -0.35971
C -2.31906 -2.11517 -0.1477	C -2.3166 -2.11923 -0.18235	C -2.32071 -2.11916 -0.16265
C -3.29522 -1.07577 -0.70594	C -3.29736 -1.07618 -0.71279	C -3.29883 -1.0799 -0.71844
C -2.99023 0.369242 -0.22687	C -2.98649 0.368661 -0.21093	C -2.9918 0.369626 -0.2251
O -3.24113 -1.04877 -2.13684	O -3.22825 -1.15894 -2.13945	O -3.35788 -1.14251 -2.1468
C -4.01287 1.312666 -0.89185	C -4.00354 1.329829 -0.86012	C -4.01595 1.313017 -0.88415
C -0.84932 -0.30648 1.675857	C -0.84317 -0.3329 1.671945	C -0.85027 -0.31128 1.677631
O -0.02256 -0.64194 2.488654	O -0.01494 -0.67804 2.478795	O -0.02101 -0.65221 2.485601
O -2.1263 -0.10631 2.101864	O -2.12034 -0.14118 2.104835	O -2.1233 -0.10603 2.104801
C -3.15377 0.4991 1.292522	C -3.14767 0.479799 1.310766	C -3.15578 0.492817 1.295331
O 4.337394 -1.21223 -0.2766	O 4.339362 -1.20707 -0.28541	O 4.336336 -1.21098 -0.27778
C 4.099361 -2.60592 -0.17094	C 4.101731 -2.60218 -0.19172	C 4.100397 -2.60496 -0.16352
H 1.725293 -1.83264 -0.0298	H 1.727327 -1.83065 -0.04251	H 1.725633 -1.83167 -0.02674
H 2.776005 2.985946 -0.25233	H 2.776041 2.989812 -0.23509	H 2.776402 2.987016 -0.2532

H -1.39384 0.572838 -1.65526	H -1.40206 0.577778 -1.64553	H -1.38347 0.593969 -1.65159
H -1.92028 2.928655 -0.27703	H -1.91988 2.931028 -0.25474	H -1.92137 2.931052 -0.25664
H 0.403323 3.551522 0.100598	H 0.404354 3.551912 0.119175	H 0.405232 3.55189 0.11379
H 5.110735 2.538997 -0.41783	H 5.11131 2.545042 -0.40389	H 5.111052 2.539233 -0.4233
H 5.633844 1.079037 0.448357	H 5.634774 1.080499 0.454363	H 5.634121 1.079303 0.443031
H 5.50023 1.049293 -1.30315	H 5.501429 1.060208 -1.29726	H 5.498478 1.048698 -1.30826
H -0.2094 -2.41889 0.153877	H -0.20882 -2.42245 0.119207	H -0.21292 -2.41867 0.157816
H -0.60911 -1.73428 -1.42638	H -0.6052 -1.71659 -1.4519	H -0.57429 -1.74121 -1.42204
H -2.50564 -3.08265 -0.63607	H -2.50731 -3.06276 -0.70514	H -2.50946 -3.07614 -0.66267
H -2.52271 -2.27173 0.917524	H -2.51749 -2.29457 0.879799	H -2.51848 -2.27497 0.903345
H -4.3198 -1.32696 -0.38199	H -4.31606 -1.33571 -0.37775	H -4.31774 -1.33225 -0.40038
H -3.4011 -1.95113 -2.45354	H -3.95498 -0.63657 -2.51024	H -2.45047 -1.12911 -2.48862
H -3.88984 1.306827 -1.97684	H -3.82111 1.429784 -1.93576	H -3.92503 1.273501 -1.97181
H -5.03456 0.978916 -0.67144	H -5.02896 0.964074 -0.71652	H -5.03586 0.998459 -0.63009
H -3.92175 2.341982 -0.53326	H -3.96054 2.335429 -0.43274	H -3.90306 2.350381 -0.55678
H -4.08943 0.041442 1.632556	H -4.08414 0.019279 1.645994	H -4.08714 0.023131 1.630603
H -3.18299 1.56054 1.563956	H -3.17344 1.53699 1.600037	H -3.19611 1.551683 1.575355
H 5.080792 -3.08142 -0.22325	H 5.083424 -3.07659 -0.24786	H 5.082531 -3.07893 -0.21359
H 3.621604 -2.86261 0.783502	H 3.62394 -2.86684 0.760435	H 3.623671 -2.85603 0.792783
H 3.475737 -2.97385 -0.99689	H 3.478359 -2.96287 -1.02086	H 3.47712 -2.97855 -0.98709

Table S4. DP4+ analysis table for compound **2** (isomer **1**: 6α-OH; isomer **2**: 6β-OH).

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-31+G(d,p)

Isomer Nº		1	2	3
DP4+ (%)	H data	0.00%	100.00%	-
	C data	0.00%	100.00%	-
	All data	0.00%	100.00%	-

Type	sp2?	Exp	1	2	3
C		27	166.9032247	166.529575	
C		78.5	116.7934818	116.806488	
C		39.1	151.6956414	152.89649	
c		56.8	148.2454013	137.615652	
c		39.2	153.5290984	152.479861	
c		25.9	167.5768392	167.609611	
c		68.9	122.6160673	125.022165	
c		72.9	118.1037707	120.823519	
c	x	125.9	70.7826572	72.0894995	
c	x	145.1	51.37148232	51.1426929	
c	x	129	71.24476556	69.4267738	
c	x	124.6	73.08509916	73.0708289	
c	x	158.3	40.89726929	40.6921424	
c	x	101.6	97.17987369	97.5057014	
c		15.9	177.3707034	177.330815	
c		65.8	127.5627827	129.543047	
c		28.7	169.6653998	167.531664	
c		15.4	179.5177543	179.92844	
c		55.5	142.1017936	142.192915	
H		0.91	30.43274742	30.818264	
H		1.88	29.95801379	29.8915114	
H		1.73	29.79565981	29.8576739	
H		3.4	28.22982641	28.148608	
H		2.16	29.36782698	29.4270667	
H		1.88	29.85722374	29.7747043	
H		4.21	27.6502101	27.4409883	
H		4.72	27.04143838	26.960035	
H	x	7.12	24.21051712	24.2096163	
H	x	6.67	24.76929582	24.7275913	
H		2.22	29.3598753	29.338014	
H		4.07	27.09451381	27.3561901	
H		2.72	28.73106972	28.8548811	
H		1.14	30.42756119	30.4905711	
H		1.14	30.1676364	30.4267473	
H		3.86	27.64320049	27.6226388	

Table S5. Conformers and Boltzmann populations of 6α-OH isomer of **2**.

6α1 (52.98%)			**6α2** (26.20%)			**6α3** (20.82%)		
C	2.237828	2.146824	0.890175	C	2.237042	2.140624	0.88706	C	2.22783	2.158625	0.871023
C	2.856339	1.689916	-0.42712	C	2.859168	1.681081	-0.43441	C	2.863252	1.691807	-0.44127
C	2.816024	0.136741	-0.58713	C	2.81804	0.136438	-0.598	C	2.818721	0.13874	-0.60201
C	1.301176	-0.27778	-0.52899	C	1.302602	-0.2805	-0.52861	C	1.304456	-0.28401	-0.52761
C	0.438756	0.315256	0.658973	C	0.439726	0.311833	0.659733	C	0.440835	0.308818	0.658602
C	0.746981	1.799189	0.919802	C	0.745373	1.796186	0.918351	C	0.74111	1.795464	0.911254
C	0.991022	-1.823	-0.66865	C	0.993017	-1.82643	-0.66589	C	0.993033	-1.83052	-0.66538
C	-0.12728	-2.16752	0.333819	C	-0.12959	-2.16869	0.333004	C	-0.1341	-2.17064	0.32893
C	-1.32062	-1.28824	0.132754	C	-1.32166	-1.28842	0.131514	C	-1.324	-1.28911	0.128275
C	-1.02416	0.069076	0.285914	C	-1.02395	0.068066	0.287915	C	-1.02408	0.065981	0.288503
C	-2.61596	-1.6998	-0.17982	C	-2.61715	-1.6982	-0.18252	C	-2.62005	-1.69739	-0.18575
C	-3.64512	-0.7735	-0.34821	C	-3.64558	-0.77081	-0.34933	C	-3.64753	-0.76871	-0.34927
C	-3.33689	0.59349	-0.17972	C	-3.33631	0.595374	-0.1774	C	-3.33656	0.596812	-0.1737
C	-2.04041	1.016874	0.141235	C	-2.03968	1.016942	0.145191	C	-2.03937	1.016162	0.149296
C	-5.05177	-1.19391	-0.69062	C	-5.05228	-1.1894	-0.69385	C	-5.05485	-1.18469	-0.6941
C	0.631295	-0.54932	1.934856	C	0.635324	-0.55288	1.934897	C	0.642785	-0.55751	1.931228
O	4.176536	2.228559	-0.47532	O	4.216301	2.110112	-0.55325	O	4.173953	2.233548	-0.60622
H	0.867368	0.189651	-1.42325	H	0.865306	0.183309	-1.42258	H	0.867849	0.178764	-1.42239
C	3.347521	-0.22921	-1.99185	C	3.344423	-0.21778	-2.00674	C	3.343083	-0.21857	-2.00958
C	3.771431	-0.50007	0.45208	C	3.778731	-0.5042	0.436002	C	3.780947	-0.50273	0.42714
O	0.470742	-1.9467	1.642556	O	0.463888	-1.94909	1.64446	O	0.457786	-1.95348	1.64258
O	2.079651	-2.70322	-0.42899	O	2.076061	-2.71118	-0.42033	O	2.071588	-2.71986	-0.40854
O	-4.39395	1.446435	-0.34984	O	-4.39286	1.449753	-0.34602	O	-4.39193	1.452521	-0.33933
C	-4.1778	2.838642	-0.19324	C	-4.17541	2.841249	-0.18768	C	-4.17223	2.844122	-0.1821
H	2.369755	3.230734	0.983621	H	2.356336	3.229129	0.989745	H	2.344893	3.245838	0.950821
H	2.778091	1.694046	1.729535	H	2.779099	1.690352	1.726297	H	2.764613	1.722585	1.725111
H	2.260047	2.122926	-1.25122	H	2.268263	2.117764	-1.26042	H	2.293654	2.128716	-1.27304
H	0.255501	2.394976	0.139535	H	0.255571	2.388929	0.134549	H	0.245143	2.38178	0.12704
H	0.295581	2.109902	1.871935	H	0.292331	2.110624	1.868457	H	0.288976	2.110888	1.861585
H	0.664227	-2.04001	-1.68997	H	0.670378	-2.04349	-1.68837	H	0.677026	-2.04791	-1.68979
H	-0.3574	-3.23495	0.294884	H	-0.36076	-3.23581	0.293573	H	-0.36694	-3.23743	0.28894
H	-2.83508	-2.75967	-0.29488	H	-2.83687	-2.75765	-0.30014	H	-2.84053	-2.75635	-0.3061
H	-1.83351	2.070487	0.279556	H	-1.83273	2.070252	0.285898	H	-1.83204	2.068939	0.292486
H	-5.12089	-2.28225	-0.78059	H	-5.12241	-2.27761	-0.78458	H	-5.12586	-2.2724	-0.7901
H	-5.76491	-0.86535	0.074742	H	-5.76613	-0.86049	0.070692	H	-5.7675	-0.85905	0.072957
H	-5.38381	-0.74821	-1.63592	H	-5.38247	-0.74289	-1.63943	H	-5.38578	-0.73316	-1.63697

H 1.623932 -0.42253 2.375108	H 1.632633 -0.43191 2.366634	H 1.646614 -0.4445 2.351181
H -0.11085 -0.24874 2.688096	H -0.09944 -0.24792 2.693786	H -0.08058 -0.24904 2.699262
H 4.548758 2.024453 -1.34685	H 4.223864 3.076049 -0.47319	H 4.679446 2.030252 0.196037
H 3.273672 -1.30638 -2.16155	H 3.314176 -1.29903 -2.16639	H 3.356845 -1.3024 -2.15522
H 4.407785 0.036494 -2.09545	H 4.377469 0.122655 -2.12098	H 4.358506 0.166742 -2.1418
H 2.788065 0.287205 -2.78339	H 2.744341 0.266689 -2.78831	H 2.715587 0.228823 -2.79126
H 3.365632 -0.52267 1.466224	H 3.396035 -0.4894 1.460148	H 3.463887 -0.38389 1.467251
H 4.027222 -1.52136 0.170264	H 3.991065 -1.53921 0.170864	H 3.904999 -1.56546 0.228004
H 4.691567 0.091542 0.486195	H 4.719979 0.052108 0.431787	H 4.771944 -0.04283 0.330378
H 2.163661 -2.73925 0.541295	H 2.155977 -2.74664 0.550254	H 2.117565 -2.77902 0.563563
H -5.14371 3.313704 -0.37526	H -5.14073 3.317665 -0.36944	H -5.13696 3.321647 -0.36388
H -3.83954 3.084094 0.822279	H -3.83727 3.085317 0.828308	H -3.83353 3.088306 0.833615
H -3.44521 3.218609 -0.91777	H -3.44216 3.221474 -0.9115	H -3.43873 3.222435 -0.90651

Table S6. Conformers and Boltzmann populations of 6β-OH isomer of **2**.

6β1 (26.78%)	**6β2** (23.81%)	**6β3** (30.93%)
C 2.41495 2.122268 0.732579	C 2.409895 2.128151 0.703814	C 2.403378 2.151761 0.665434
C 3.062606 1.470365 -0.4864	C 3.078819 1.451477 -0.49812	C 3.099936 1.450906 -0.50734
C 2.879224 -0.07758 -0.5172	C 2.886717 -0.08757 -0.51506	C 2.889132 -0.0932 -0.51047
C 1.341606 -0.37033 -0.43396	C 1.344788 -0.36853 -0.4431	C 1.345518 -0.3649 -0.45634
C 0.519659 0.395444 0.676883	C 0.520027 0.39994 0.661932	C 0.52012 0.408768 0.641595
C 0.900373 1.882055 0.73384	C 0.895054 1.888075 0.701283	C 0.890448 1.898443 0.660869
C 0.971197 -1.887 -0.39181	C 0.963323 -1.88253 -0.40824	C 0.952438 -1.87661 -0.43024
C -0.09996 -2.0937 0.699515	C -0.09646 -2.08879 0.694772	C -0.09046 -2.08237 0.689294
C -1.2832 -1.21951 0.383165	C -1.2833 -1.21731 0.385016	C -1.28227 -1.21455 0.389771
C -0.95029 0.141486 0.34906	C -0.95121 0.143424 0.342459	C -0.9524 0.146073 0.333095
C -2.59225 -1.62953 0.126384	C -2.59375 -1.62916 0.13878	C -2.5945 -1.63022 0.159255
C -3.596 -0.70381 -0.16328	C -3.60005 -0.70541 -0.14827	C -3.6045 -0.71002 -0.12572
C -3.24891 0.664282 -0.18141	C -3.25378 0.662663 -0.17523	C -3.26013 0.658356 -0.168
C -1.93843 1.089643 0.075805	C -1.94193 1.089828 0.071259	C -1.94659 1.089105 0.062749
C -5.01593 -1.12586 -0.44355	C -5.02146 -1.12963 -0.41749	C -5.02785 -1.13802 -0.37799
C 0.701502 -0.29787 2.05435	C 0.711827 -0.2876 2.040777	C 0.722637 -0.2716 2.022158
O 4.431452 1.874144 -0.49419	O 4.480329 1.724563 -0.53555	O 4.47812 1.818792 -0.58064
H 0.933855 0.00552 -1.38304	H 0.949157 0.011356 -1.39533	H 0.965076 0.020122 -1.41249
C 3.381466 -0.60574 -1.88174	C 3.404148 -0.62828 -1.86768	C 3.424878 -0.65386 -1.84637
C 3.738216 -0.73889 0.582011	C 3.731628 -0.73934 0.602921	C 3.711117 -0.73732 0.630977

O 0.502639 -1.70909 1.952231	O 0.513672 -1.69933 1.942546	O 0.538306 -1.68598 1.92648
O 0.550747 -2.39549 -1.654	O 0.520041 -2.37804 -1.66721	O 0.485127 -2.35651 -1.68586
O -4.28174 1.51598 -0.46451	O -4.28913 1.51266 -0.45558	O -4.29877 1.504335 -0.44617
C -4.02609 2.910272 -0.49547	C -4.03407 2.906488 -0.49639	C -4.04563 2.898247 -0.50466
H 2.623677 3.197651 0.702464	H 2.604082 3.20976 0.661782	H 2.602537 3.227161 0.592031
H 2.882978 1.742124 1.648069	H 2.872215 1.769915 1.63057	H 2.846749 1.820894 1.615105
H 2.559905 1.872945 -1.3852	H 2.603871 1.847582 -1.41466	H 2.671859 1.843328 -1.43983
H 0.476461 2.386612 -0.14526	H 0.474815 2.376808 -0.18864	H 0.471952 2.370987 -0.23835
H 0.438377 2.35318 1.611869	H 0.427491 2.372609 1.56902	H 0.416758 2.394702 1.518743
H 1.836097 -2.49454 -0.11934	H 1.827077 -2.49936 -0.1548	H 1.815805 -2.50339 -0.19948
H -0.35842 -3.15089 0.794456	H -0.35294 -3.14591 0.795175	H -0.34374 -3.13937 0.798545
H -2.84278 -2.68831 0.155747	H -2.84306 -2.68803 0.173717	H -2.84198 -2.6891 0.204538
H -1.69662 2.145266 0.066664	H -1.70127 2.145663 0.055369	H -1.7072 2.144928 0.035457
H -5.11586 -2.21405 -0.38781	H -5.12024 -2.21762 -0.35606	H -5.12487 -2.22554 -0.30649
H -5.71447 -0.67861 0.273587	H -5.71579 -0.67951 0.301962	H -5.71578 -0.68248 0.344152
H -5.34207 -0.80005 -1.43854	H -5.35409 -0.80878 -1.41195	H -5.37001 -0.82579 -1.37192
H 1.700117 -0.13855 2.46941	H 1.714318 -0.12861 2.446003	H 1.725655 -0.10437 2.423186
H -0.02487 0.128635 2.762495	H -0.00933 0.139405 2.754162	H 0.001359 0.150063 2.738343
H 4.827638 1.563828 -1.32278	H 4.58976 2.686782 -0.58003	H 4.887142 1.584623 0.267464
H 3.176119 -1.67389 -1.99835	H 3.278016 -1.71327 -1.9381	H 3.354568 -1.74588 -1.88312
H 4.466338 -0.47226 -1.98387	H 4.46527 -0.39202 -1.9871	H 4.472413 -0.36681 -1.97785
H 2.891192 -0.08861 -2.71626	H 2.858272 -0.18139 -2.70763	H 2.856066 -0.26102 -2.69736
H 3.42641 -0.48133 1.595676	H 3.50124 -0.36218 1.601722	H 3.573185 -0.24884 1.60008
H 3.722252 -1.82995 0.500866	H 3.598744 -1.82488 0.623668	H 3.462695 -1.79278 0.769323
H 4.775614 -0.41044 0.471247	H 4.789302 -0.53556 0.417577	H 4.778601 -0.69173 0.387187
H -0.28284 -1.94655 -1.87548	H -0.31082 -1.91787 -1.875	H -0.34948 -1.89392 -1.87238
H -4.97969 3.383773 -0.73657	H -4.98934 3.378561 -0.73378	H -5.00363 3.366497 -0.73836
H -3.67456 3.278777 0.477347	H -3.67602 3.28092 0.471865	H -3.67922 3.283486 0.456131
H -3.28813 3.169382 -1.26632	H -3.30137 3.161366 -1.27375	H -3.32047 3.14509 -1.29148

6β4 (4.42%)	**6β5** (3.81%)	**6β6** (2.07%)
C 2.397297 2.12492 0.749566	C 2.392497 2.13196 0.717998	C 2.389043 2.145933 0.692129
C 3.038484 1.489432 -0.48048	C 3.056073 1.469135 -0.49364	C 3.059722 1.465235 -0.50605
C 2.876214 -0.06061 -0.51353	C 2.884558 -0.07214 -0.51008	C 2.885895 -0.07536 -0.49505
C 1.341977 -0.37545 -0.42504	C 1.345306 -0.37344 -0.43308	C 1.346594 -0.37255 -0.43193
C 0.51017 0.384762 0.683905	C 0.510763 0.389942 0.669295	C 0.509586 0.396857 0.663077
C 0.885383 1.872422 0.754031	C 0.880398 1.879274 0.719571	C 0.877381 1.887366 0.699915
C 0.9999 -1.88722 -0.36382	C 0.9901 -1.88233 -0.38186	C 0.982554 -1.88968 -0.38414

C -0.1138 -2.09666 0.686462	C -0.11034 -2.09126 0.682831	C -0.10771 -2.09144 0.682126
C -1.29108 -1.22292 0.366394	C -1.29132 -1.2203 0.369902	C -1.28873 -1.21913 0.36806
C -0.95799 0.135377 0.345669	C -0.95887 0.137709 0.339541	C -0.95953 0.139351 0.334337
C -2.59808 -1.63137 0.108249	C -2.59974 -1.6308 0.12296	C -2.59642 -1.63293 0.12321
C -3.60088 -0.70422 -0.17741	C -3.6051 -0.70585 -0.16074	C -3.60408 -0.71015 -0.15902
C -3.25327 0.663272 -0.18842	C -3.25819 0.661577 -0.1819	C -3.26083 0.658154 -0.18161
C -1.94428 1.0866 0.075886	C -1.94771 1.086949 0.071183	C -1.95071 1.086887 0.066938
C -5.02033 -1.1242 -0.46332	C -5.02617 -1.12826 -0.43484	C -5.02439 -1.13654 -0.43125
C 0.683696 -0.31538 2.059673	C 0.693968 -0.30388 2.046772	C 0.692851 -0.29294 2.041907
O 4.402085 1.911484 -0.50582	O 4.453579 1.761756 -0.54867	O 4.457953 1.753555 -0.55812
H 0.91784 -0.02853 -1.37603	H 0.934365 -0.02041 -1.38731	H 0.941549 -0.01048 -1.38635
C 3.384065 -0.57755 -1.87997	C 3.406788 -0.60491 -1.86378	C 3.426412 -0.6343 -1.83182
C 3.75071 -0.70866 0.582052	C 3.744971 -0.70926 0.604811	C 3.73475 -0.69403 0.639277
O 0.472221 -1.72645 1.953514	O 0.485733 -1.71575 1.943943	O 0.493232 -1.70486 1.938307
O 0.61366 -2.3032 -1.67424	O 0.576087 -2.28012 -1.6889	O 0.478245 -2.38417 -1.62255
O -4.28649 1.517897 -0.46908	O -4.29398 1.514342 -0.46036	O -4.29971 1.508726 -0.45786
C -4.02575 2.910229 -0.50371	C -4.03368 2.906071 -0.50683	C -4.04363 2.900853 -0.50132
H 2.597412 3.202185 0.728615	H 2.577499 3.215478 0.682527	H 2.569415 3.229379 0.636992
H 2.873809 1.738799 1.658261	H 2.863575 1.770554 1.639163	H 2.86122 1.803834 1.619878
H 2.518773 1.888358 -1.3708	H 2.564528 1.860288 -1.40324	H 2.57356 1.842394 -1.42472
H 0.456071 2.382403 -0.11894	H 0.454507 2.371965 -0.16513	H 0.446927 2.371139 -0.18747
H 0.421662 2.331611 1.637366	H 0.411253 2.353433 1.592068	H 0.41077 2.369012 1.569573
H 1.865639 -2.46827 -0.02188	H 1.855656 -2.47579 -0.06286	H 1.847045 -2.4857 -0.06732
H -0.38016 -3.15495 0.779611	H -0.37448 -3.14942 0.782252	H -0.36678 -3.14801 0.778994
H -2.84976 -2.69028 0.128014	H -2.85032 -2.68981 0.149554	H -2.84141 -2.69282 0.145914
H -1.70262 2.142236 0.074563	H -1.70723 2.142847 0.062206	H -1.71293 2.143445 0.056799
H -5.12156 -2.21256 -0.40999	H -5.12623 -2.21638 -0.37478	H -5.12042 -2.225 -0.37258
H -5.72206 -0.67769 0.251313	H -5.72353 -0.67828 0.281918	H -5.72198 -0.68964 0.287273
H -5.34174 -0.79705 -1.45945	H -5.35436 -0.80698 -1.43067	H -5.35513 -0.81519 -1.42622
H 1.682723 -0.16651 2.478392	H 1.696195 -0.15398 2.456846	H 1.693037 -0.13767 2.45544
H -0.04163 0.113305 2.767036	H -0.0275 0.124209 2.7587	H -0.03243 0.133653 2.751036
H 4.787846 1.616586 -1.34486	H 4.548006 2.725621 -0.59079	H 4.556825 2.717292 -0.59415
H 3.187413 -1.64686 -1.99961	H 3.29002 -1.69101 -1.93447	H 3.385845 -1.73104 -1.8508
H 4.467746 -0.43323 -1.98081	H 4.465678 -0.35889 -1.98362	H 4.470669 -0.34181 -1.97179
H 2.887224 -0.06373 -2.7123	H 2.854715 -0.1637 -2.70218	H 2.853169 -0.25304 -2.68694
H 3.410856 -0.49611 1.59727	H 3.48405 -0.36835 1.609142	H 3.503126 -0.28765 1.625738
H 3.789532 -1.79671 0.470822	H 3.663062 -1.80016 0.597705	H 3.602539 -1.7784 0.693548
H 4.772209 -0.32723 0.495359	H 4.794185 -0.45271 0.437643	H 4.792099 -0.4929 0.448257

H 0.472913 -3.26345 -1.65103	H 0.449798 -3.24249 -1.68006	H 1.186318 -2.30331 -2.27963
H -4.97677 3.387213 -0.74886	H -4.98639 3.381405 -0.74881	H -4.99826 3.374438 -0.73934
H -3.67537 3.281432 0.468792	H -3.67659 3.28453 0.460524	H -3.68467 3.278054 0.465929
H -3.28438 3.164507 -1.27305	H -3.29765 3.154957 -1.28313	H -3.31046 3.154425 -1.27902

6β7 (1.47%)	**6β8** (4.47%)	**6β9** (2.47%)
C 2.39374 2.142518 0.710214	C 2.386029 2.155687 0.677909	C 2.384377 2.164814 0.661537
C 3.055623 1.477677 -0.49443	C 3.077885 1.467584 -0.50411	C 3.080005 1.465629 -0.51174
C 2.884014 -0.07226 -0.49257	C 2.887635 -0.07929 -0.50457	C 2.886535 -0.08027 -0.49504
C 1.345875 -0.37423 -0.43049	C 1.346329 -0.37046 -0.44499	C 1.346082 -0.36982 -0.44332
C 0.510197 0.39433 0.667645	C 0.51105 0.398239 0.649895	C 0.50949 0.404635 0.646062
C 0.882738 1.883379 0.715477	C 0.876075 1.889241 0.678838	C 0.874245 1.896089 0.665668
C 0.981524 -1.89202 -0.38261	C 0.978087 -1.87704 -0.40444	C 0.972857 -1.88547 -0.40055
C -0.10938 -2.09395 0.683195	C -0.10541 -2.0851 0.678138	C -0.10364 -2.08536 0.680063
C -1.28911 -1.21973 0.36833	C -1.29109 -1.2175 0.375723	C -1.28869 -1.21615 0.374145
C -0.95836 0.138497 0.334983	C -0.96006 0.140247 0.330936	C -0.96089 0.142115 0.327221
C -2.59686 -1.63201 0.121071	C -2.6014 -1.63138 0.14465	C -2.59792 -1.63309 0.143029
C -3.60279 -0.70788 -0.16293	C -3.61002 -0.70966 -0.13755	C -3.60834 -0.7133 -0.13861
C -3.25786 0.660126 -0.18503	C -3.2643 0.657884 -0.17453	C -3.26622 0.65515 -0.17566
C -1.9476 1.087311 0.065698	C -1.95193 1.086425 0.063045	C -1.95457 1.086857 0.059444
C -5.02324 -1.13239 -0.43734	C -5.03326 -1.13534 -0.39464	C -5.03042 -1.14272 -0.39625
C 0.685622 -0.29823 2.046352	C 0.704791 -0.28842 2.029088	C 0.702113 -0.2779 2.026848
O 4.422377 1.891531 -0.49563	O 4.450476 1.853901 -0.59407	O 4.454178 1.846103 -0.60187
H 0.938029 -0.01056 -1.38356	H 0.950854 -0.01021 -1.40295	H 0.9519 -0.00319 -1.40054
C 3.419445 -0.62848 -1.83295	C 3.426808 -0.6339 -1.84139	C 3.437324 -0.64981 -1.82169
C 3.735981 -0.69679 0.633641	C 3.726264 -0.70748 0.633193	C 3.718755 -0.69893 0.65292
O 0.492901 -1.71062 1.939225	O 0.510501 -1.70298 1.92851	O 0.514124 -1.69209 1.926974
O 0.474688 -2.38821 -1.61973	O 0.53945 -2.25546 -1.70834	O 0.449874 -2.36968 -1.63469
O -4.29503 1.511776 -0.46306	O -4.3029 1.507084 -0.45135	O -4.30746 1.502335 -0.45129
C -4.03765 2.904022 -0.5037	C -4.04378 2.89862 -0.51613	C -4.05226 2.894322 -0.51205
H 2.58883 3.219646 0.659918	H 2.575072 3.233327 0.609458	H 2.571898 3.241906 0.581627
H 2.866015 1.786656 1.633072	H 2.838748 1.822445 1.622449	H 2.837031 1.842604 1.609855
H 2.557741 1.860597 -1.40403	H 2.632985 1.854446 -1.43088	H 2.63854 1.84419 -1.44379
H 0.452101 2.377365 -0.16612	H 0.451255 2.365075 -0.2153	H 0.447276 2.366501 -0.23033
H 0.417642 2.356848 1.590454	H 0.401431 2.375831 1.541598	H 0.401452 2.388201 1.526209
H 1.846495 -2.48755 -0.06484	H 1.843773 -2.48324 -0.10921	H 1.838193 -2.48967 -0.10079
H -0.36966 -3.15048 0.77746	H -0.36637 -3.14314 0.786588	H -0.36017 -3.1417 0.785589
H -2.84338 -2.69156 0.143495	H -2.8508 -2.69035 0.182411	H -2.84181 -2.69298 0.17566

H -1.70794 2.143419 0.056248	H -1.71237 2.142304 0.042359	H -1.71742 2.143347 0.03836
H -5.1209 -2.22071 -0.37878	H -5.13215 -2.22293 -0.32382	H -5.12541 -2.2307 -0.32787
H -5.72127 -0.68449 0.280118	H -5.72415 -0.67919 0.324452	H -5.72261 -0.69018 0.32394
H -5.35208 -0.81054 -1.43277	H -5.37072 -0.82315 -1.39023	H -5.36893 -0.82964 -1.39121
H 1.680495 -0.13852 2.470663	H 1.707629 -0.13046 2.43506	H 1.702959 -0.11512 2.436584
H -0.04764 0.125136 2.749028	H -0.01692 0.134259 2.743783	H -0.02295 0.144993 2.738192
H 4.814932 1.630536 -1.34227	H 4.867214 1.646263 0.257084	H 4.863954 1.663076 0.258343
H 3.32672 -1.72055 -1.8795	H 3.366483 -1.72677 -1.87641	H 3.424136 -1.74739 -1.82608
H 4.488358 -0.41366 -1.95561	H 4.471449 -0.33741 -1.97513	H 4.472994 -0.32941 -1.968
H 2.886417 -0.20146 -2.6925	H 2.851204 -0.24838 -2.69069	H 2.855115 -0.29436 -2.68161
H 3.44438 -0.36699 1.631808	H 3.553986 -0.2494 1.611311	H 3.556062 -0.21452 1.619493
H 3.6822 -1.78943 0.62114	H 3.529518 -1.77723 0.742815	H 3.501063 -1.7613 0.789543
H 4.781921 -0.40848 0.494376	H 4.792795 -0.605 0.402388	H 4.7864 -0.61928 0.418313
H 1.174105 -2.2963 -2.28424	H 0.392769 -3.21502 -1.70657	H 1.151958 -2.29547 -2.29908
H -4.99148 3.378676 -0.74264	H -4.99894 3.370525 -0.75493	H -5.00893 3.364717 -0.74798
H -3.68012 3.279077 0.464828	H -3.67836 3.288161 0.443634	H -3.68625 3.282095 0.448302
H -3.30287 3.158208 -1.2796	H -3.31493 3.138736 -1.30178	H -3.32517 3.139317 -1.29802

Table S7. DP4+ analysis table for compound **6** (isomer **1**: 2α,10α-OH; isomer **2**: 2β,10α-OH; isomer **3**: 2α,10β-OH; isomer **4**: 2β,10β-OH).

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-31+G(d,p)

Isomer №			1	2	3	4
DP4+ (%)		H data	100.00%	0.00%	0.00%	0.00%
		C data	100.00%	0.00%	0.00%	0.00%
		All data	100.00%	0.00%	0.00%	0.00%
Type	sp2?	Exp	1	2	3	4
C		72.7	120.7953331	127.020847	126.211219	124.442926
C		77.7	116.5362693	116.694796	114.929367	119.014128
C		37.3	153.9252959	152.490488	155.170259	154.171779
C		50	143.3648261	142.043119	140.297437	140.103775
C		79.7	112.4088318	123.48581	103.278112	108.419972
C		39.1	156.0973405	152.299242	152.504518	155.529593
C	x	127.8	68.74998702	69.7097748	64.2909436	66.5446592
C	x	131.4	65.66996402	67.949571	66.301696	66.5728773
C	x	128.5	69.9068492	71.40063	67.3098119	68.9206392
C	x	134.2	61.83062617	63.0448967	60.1248338	61.1021805
C		51	143.6634072	143.901219	144.300485	145.487762
C	x	132.2	66.47120351	64.8270532	68.3394601	66.909215
C	x	124.9	72.13857427	72.4637203	72.0923715	72.0763857
C	x	157.1	41.93049285	41.8105599	42.7036606	42.2558289
C	x	112.1	88.01266816	87.1747742	88.9495896	87.9801737
C		15.7	177.3512926	177.510522	177.233878	177.381132
C		22.6	173.8083769	174.504133	169.285563	169.615151
C		28.3	168.20238	168.965692	173.345005	169.563666
C		55.4	142.0480025	141.99879	142.029988	142.002335
H		2.39	28.98027259	28.7309236	29.9403773	29.4400876
H		4	27.65355522	27.2137399	27.5696957	27.5766669
H		3.63	27.98681306	27.9937538	28.0491576	28.0410469
H		2.25	29.26460226	29.6443504	29.9015043	29.3582693
H		1.95	29.74291214	29.8047291	29.5093268	29.7069854
H	x	5.85	25.35061201	25.6049567	24.9943284	25.2235858
H	x	6.61	24.488405	24.7195182	24.4952257	24.5718205
H		2.95	28.65257945	28.3044752	28.8461367	28.9933741
H		2.68	28.88944676	28.8944254	29.2406099	28.6411592
H	x	6.96	24.29783461	24.3481814	24.2194392	24.2537939
H	x	6.58	24.78408735	24.84541	24.6651408	24.735873
H		2.18	29.36601359	29.3816894	29.343001	29.338541
H		1.25	30.41075391	30.5438934	30.6497439	30.6399623
H		1.03	30.63006629	30.423395	30.4301909	30.4725995
H		3.84	27.63462954	27.6419699	27.6233845	27.6472857

Table S8. Conformers and Boltzmann populations of 2α,10α-OH isomer of **6**.

2α10α1 (21.64%)			**2α10α2** (36.78%)			**2α10α3** (11.89%)		
C	-3.16462	-1.77871	0.386831	C	-3.1668	-1.79014	0.377929	C	2.885733	-1.74389	0.546028
C	-3.93889	-0.48279	0.057025	C	-3.9383	-0.49699	0.049076	C	3.042049	-0.44262	1.371303
C	-3.1218	0.833814	0.161924	C	-3.11862	0.825041	0.171262	C	2.72213	0.874681	0.608689
C	-1.75105	0.662447	-0.60737	C	-1.75089	0.658389	-0.60123	C	1.346458	0.709815	-0.12276
C	-0.97302	-0.63909	-0.26787	C	-0.97167	-0.64403	-0.26553	C	1.207388	-0.58222	-0.98163
C	-1.88425	-1.86133	-0.45051	C	-1.8818	-1.86707	-0.45189	C	1.502069	-1.81193	-0.11545
C	-0.922	1.926428	-0.55061	C	-0.92381	1.923745	-0.54861	C	0.874181	1.950583	-0.85179
C	0.402445	2.147337	-0.4273	C	0.400376	2.146818	-0.4263	C	-0.42957	2.218508	-1.05778
C	1.553877	1.241658	-0.31841	C	1.552786	1.242668	-0.31789	C	-1.51851	1.300499	-0.69204
C	1.526589	-0.12578	-0.65635	C	1.526626	-0.12469	-0.65671	C	-1.38321	-0.09338	-0.86827
C	0.275419	-0.78658	-1.18568	C	0.275838	-0.7867	-1.18538	C	-0.20315	-0.6524	-1.63402
C	2.775568	1.789206	0.128073	C	2.774011	1.791681	0.12822	C	-2.71762	1.7978	-0.15059
C	3.941039	1.048175	0.270742	C	3.940256	1.051869	0.270229	C	-3.75512	0.973069	0.268851
C	3.882823	-0.32243	-0.05587	C	3.883298	-0.31881	-0.0568	C	-3.58347	-0.42014	0.122927
C	2.690275	-0.89053	-0.50915	C	2.691246	-0.88808	-0.51004	C	-2.42	-0.93826	-0.45063
C	5.230606	1.660584	0.754187	C	5.229382	1.665317	0.753477	C	-5.02661	1.521445	0.864485
C	-2.94288	1.231586	1.644681	C	-2.94678	1.219832	1.654966	C	3.90318	1.235619	-0.32223
C	-3.96015	1.953611	-0.50361	C	-3.95445	1.948812	-0.49197	C	2.595409	2.021053	1.638647
H	-2.05244	0.536415	-1.65872	H	-2.05776	0.527741	-1.65087	H	0.618234	0.54363	0.682832
O	-0.56329	-0.69389	1.115971	O	-0.55975	-0.69979	1.117301	O	2.171687	-0.6457	-2.06154
O	-4.41597	-0.58005	-1.2953	O	-4.40574	-0.70428	-1.29402	O	2.147647	-0.51551	2.49253
O	-2.92403	-1.94502	1.776737	O	-2.92859	-1.94312	1.771176	O	3.943422	-1.93934	-0.38306
O	5.051633	-1.01179	0.101615	O	5.05264	-1.00684	0.100243	O	-4.63048	-1.18432	0.558575
C	5.069524	-2.39759	-0.20263	C	5.071801	-2.39301	-0.2033	C	-4.53553	-2.59448	0.442506
H	-3.82146	-2.61559	0.1006	H	-3.8261	-2.61536	0.084454	H	2.96848	-2.57636	1.262576
H	-4.78973	-0.40651	0.752055	H	-4.79328	-0.43323	0.739492	H	4.08396	-0.38826	1.723691
H	-2.15192	-1.94327	-1.50937	H	-2.14539	-1.95343	-1.51151	H	0.731799	-1.88154	0.659978
H	-1.3278	-2.764	-0.17173	H	-1.32398	-2.76797	-0.16947	H	1.442823	-2.71601	-0.7335
H	-1.51778	2.831964	-0.63226	H	-1.51952	2.82974	-0.62993	H	1.609242	2.693654	-1.1533
H	0.69026	3.198277	-0.38792	H	0.686755	3.198195	-0.38761	H	-0.7136	3.181965	-1.48135
H	0.031582	-0.3843	-2.1782	H	0.03005	-0.38323	-2.17696	H	-0.12801	-0.08764	-2.57255
H	0.48007	-1.85429	-1.32225	H	0.481671	-1.85376	-1.32413	H	-0.39561	-1.6935	-1.9175
H	2.80529	2.848277	0.377345	H	2.802675	2.85071	0.377864	H	-2.83187	2.874319	-0.03771
H	2.650065	-1.94384	-0.76371	H	2.652028	-1.94132	-0.76494	H	-2.31272	-2.00685	-0.6029
H	6.029827	1.545249	0.012421	H	6.028504	1.550814	0.011482	H	-5.18154	1.151248	1.885008
H	5.102238	2.727767	0.958881	H	5.100147	2.732345	0.95847	H	-5.00135	2.614913	0.895933

H 5.58475 1.173849 1.670732	H 5.584155 1.17864 1.669801	H -5.905 1.212655 0.285342
H -2.49175 0.448939 2.250543	H -2.48669 0.43782 2.254153	H 4.151844 0.45108 -1.03366
H -2.31934 2.129501 1.72221	H -2.33511 2.125437 1.740444	H 3.695094 2.156229 -0.87992
H -3.91905 1.468667 2.084392	H -3.92638 1.439835 2.096903	H 4.798709 1.426447 0.280752
H -3.56175 2.946225 -0.26898	H -3.56927 2.943062 -0.24642	H 2.466718 2.983846 1.131518
H -4.01166 1.841219 -1.58922	H -3.97976 1.863024 -1.58395	H 1.749798 1.868565 2.312422
H -4.98681 1.922047 -0.12069	H -4.98722 1.919365 -0.1179	H 3.504113 2.085382 2.249401
H -0.01437 0.085224 1.304508	H 0.00332 0.070126 1.301837	H 2.126478 0.195645 -2.54561
H -4.97273 -1.37243 -1.34983	H -5.09082 -0.04529 -1.47677	H 2.382667 -1.30837 2.999275
H -2.04533 -1.55882 1.946906	H -2.04552 -1.56837 1.940693	H 3.638103 -1.55408 -1.22458
H 6.087925 -2.73466 -0.0007	H 6.090552 -2.72888 -0.00123	H -4.4472 -2.90877 -0.60592
H 4.369123 -2.95819 0.430057	H 4.371972 -2.95375 0.429806	H -3.68215 -2.98936 1.009399
H 4.828937 -2.58186 -1.25789	H 4.831316 -2.57794 -1.25842	H -5.46209 -2.99234 0.860751

2α10α4 (24.00%)

C 2.877282 -1.75026 0.560856	C 2.873925 -1.74938 0.569382	C 2.853166 -1.74052 0.594148
C 3.026565 -0.45009 1.381388	C 3.032847 -0.44276 1.386639	C 3.022577 -0.42171 1.388017
C 2.719136 0.8701 0.603745	C 2.720967 0.875234 0.605483	C 2.722418 0.881474 0.59103
C 1.347829 0.705597 -0.13225	C 1.350056 0.708895 -0.13629	C 1.353237 0.710072 -0.15062
C 1.209908 -0.59048 -0.98547	C 1.20852 -0.5899 -0.98772	C 1.204251 -0.59686 -0.97373
C 1.500554 -1.81762 -0.11383	C 1.498864 -1.81795 -0.11484	C 1.466649 -1.80817 -0.06445
C 0.877655 1.944782 -0.86487	C 0.878525 1.946457 -0.871	C 0.886572 1.937971 -0.90201
C -0.4258 2.214339 -1.07146	C -0.4256 2.214222 -1.07511	C -0.4153 2.213897 -1.09656
C -1.51524 1.298335 -0.70264	C -1.51398 1.298425 -0.70184	C -1.50517 1.303533 -0.70709
C -1.37982 -0.09642 -0.87343	C -1.38044 -0.0965 -0.87404	C -1.37685 -0.09073 -0.88166
C -0.20078 -0.6593 -1.63815	C -0.20232 -0.65898 -1.64048	C -0.19452 -0.65113 -1.64441
C -2.71406 1.79811 -0.16268	C -2.71066 1.798548 -0.15697	C -2.69775 1.802942 -0.15487
C -3.7508 0.975079 0.261838	C -3.74715 0.976032 0.269061	C -3.73515 0.98083 0.271902
C -3.57837 -0.41893 0.123227	C -3.57773 -0.41826 0.126457	C -3.56989 -0.41248 0.12452
C -2.4157 -0.93936 -0.45002	C -2.41642 -0.93939 -0.44948	C -2.41161 -0.93417 -0.4563
C -5.02215 1.525627 0.855758	C -5.01624 1.527259 0.867024	C -5.0003 1.5336 0.87706
C 3.909084 1.228961 -0.31515	C 3.90507 1.224905 -0.32576	C 3.911745 1.223222 -0.33582
C 2.583913 2.023026 1.626314	C 2.593282 2.03119 1.623041	C 2.591045 2.049054 1.596822
H 0.618271 0.538304 0.672425	H 0.602081 0.555534 0.658467	H 0.623051 0.559985 0.656184
O 2.17486 -0.65658 -2.06402	O 2.173716 -0.65952 -2.06206	O 2.190758 -0.59475 -2.04726
O 2.131094 -0.63608 2.487842	O 2.259569 -0.56005 2.589855	O 2.122488 -0.45911 2.507153
O 3.943214 -1.93169 -0.36356	O 3.933815 -1.95189 -0.35873	O 3.903078 -1.96534 -0.33699
O -4.62357 -1.18123 0.564985	O -4.62316 -1.17927 0.567907	O -4.61684 -1.17395 0.56778

2α10α14 (1.78%)

2α10α15 (1.32%)

C -4.52497 -2.59266 0.462667	C -4.53495 -2.59032 0.449222	C -4.52637 -2.58374 0.451238
H 2.954618 -2.56919 1.285333	H 2.947853 -2.56462 1.298592	H 2.93453 -2.55953 1.324991
H 4.065575 -0.40382 1.742331	H 4.069357 -0.39702 1.736441	H 4.063378 -0.37212 1.743663
H 0.72493 -1.8911 0.655982	H 0.703512 -1.90678 0.637181	H 0.694527 -1.84444 0.712249
H 1.448054 -2.72186 -0.73258	H 1.451934 -2.72233 -0.73311	H 1.393095 -2.73587 -0.64853
H 1.614836 2.683725 -1.17231	H 1.615921 2.685365 -1.17595	H 1.630734 2.650583 -1.24766
H -0.70851 3.176275 -1.49951	H -0.70978 3.175956 -1.50216	H -0.69849 3.164859 -1.54761
H -0.12558 -0.09746 -2.57852	H -0.12659 -0.09631 -2.58007	H -0.09385 -0.07043 -2.56988
H -0.39486 -1.70095 -1.91796	H -0.396 -1.70046 -1.92129	H -0.40221 -1.69118 -1.93196
H -2.82878 2.875206 -0.05528	H -2.82384 2.875491 -0.0476	H -2.80813 2.879728 -0.04114
H -2.30785 -2.00864 -0.59635	H -2.31184 -2.00843 -0.60061	H -2.30761 -2.00352 -0.60635
H -5.17657 1.159706 1.877904	H -5.16902 1.159202 1.888594	H -5.14946 1.163052 1.898327
H -4.99749 2.619276 0.882266	H -4.98985 2.620696 0.895947	H -4.97047 2.62691 0.909272
H -5.90069 1.213913 0.278442	H -5.89617 1.217897 0.290668	H -5.88401 1.228815 0.303878
H 4.155949 0.442683 -1.02475	H 4.154609 0.431417 -1.02671	H 4.122158 0.462154 -1.0835
H 3.713581 2.152537 -0.87309	H 3.704763 2.140681 -0.89487	H 3.729618 2.165205 -0.86432
H 4.802662 1.409819 0.294549	H 4.797826 1.41771 0.280475	H 4.817123 1.3619 0.267051
H 2.489294 2.989043 1.119603	H 2.463473 2.990608 1.110063	H 2.461752 2.999556 1.067623
H 1.701127 1.907133 2.264229	H 1.748979 1.890068 2.30262	H 1.744413 1.910007 2.272141
H 3.475335 2.080561 2.266145	H 3.499526 2.097873 2.235973	H 3.498559 2.128275 2.207625
H 2.120834 0.177918 -2.55894	H 2.128678 0.176951 -2.55463	H 1.912345 -1.26749 -2.69117
H 2.325912 0.044589 3.14802	H 1.32003 -0.57553 2.349889	H 2.354606 -1.2359 3.039404
H 3.63623 -1.56168 -1.21057	H 3.638842 -1.56776 -1.2034	H 3.633085 -1.49826 -1.14946
H -4.43857 -2.91679 -0.58286	H -4.45171 -2.90267 -0.60003	H -4.44552 -2.89881 -0.59774
H -3.66912 -2.97916 1.031345	H -3.68165 -2.98981 1.012869	H -3.67049 -2.98138 1.012724
H -5.44951 -2.98857 0.887089	H -5.46183 -2.98422 0.870128	H -5.45125 -2.97955 0.87526

2α10α17 (2.57%)

C 2.821348 -1.72873 0.626719
C 3.029133 -0.40243 1.377941
C 2.721045 0.891384 0.555836
C 1.344526 0.715282 -0.16531
C 1.203173 -0.60287 -0.99531
C 1.449246 -1.79626 -0.05278
C 0.873422 1.93978 -0.91445
C -0.42961 2.21243 -1.1063
C -1.51481 1.300045 -0.71113
C -1.37927 -0.09502 -0.88098

C -0.20254 -0.6628 -1.64593

C -2.70817 1.799486 -0.16036

C -3.74347 0.977247 0.271326

C -3.57324 -0.41577 0.130175

C -2.41374 -0.93642 -0.44875

C -5.01067 1.529554 0.872986

C 3.908322 1.213546 -0.38061

C 2.607748 2.07643 1.544859

H 0.623204 0.568942 0.651439

O 2.100084 -0.67043 -2.10935

O 2.170826 -0.54675 2.515609

O 3.895158 -1.87694 -0.3302

O -4.61852 -1.17917 0.577643

C -4.52517 -2.5883 0.460611

H 2.904464 -2.5231 1.379534

H 4.080946 -0.36372 1.702946

H 0.678916 -1.8212 0.72617

H 1.366587 -2.73158 -0.62464

H 1.613603 2.650138 -1.27454

H -0.71587 3.159596 -1.56361

H -0.09894 -0.10105 -2.58143

H -0.40461 -1.70357 -1.92592

H -2.82205 2.876878 -0.0536

H -2.30787 -2.00604 -0.59574

H -5.16088 1.163815 1.895979

H -4.98365 2.623249 0.899915

H -5.89341 1.220491 0.300441

H 4.153971 0.408457 -1.0693

H 3.702376 2.109478 -0.97498

H 4.804384 1.420232 0.218331

H 2.532151 3.024943 1.004367

H 1.718523 2.003153 2.181006

H 3.498575 2.140589 2.185665

H 2.939404 -1.03087 -1.7702

H 2.318977 0.212957 3.097042

H 3.888026 -2.80063 -0.6276

H -4.44331 -2.90314 -0.58837

H -3.66833 -2.98483 1.02161

H -5.44922 -2.9865 0.884605

Table S9. Conformers and Boltzmann populations of 2β,10α-OH isomer of **6**.

2β10α1 (20.69%)	**2β10α2** (26.62%)	**2β10α3** (29.01%)
C 3.188918 1.524535 0.644379	C 3.176744 1.535417 0.63175	C 3.185267 1.555423 0.637164
C 3.912973 0.264903 0.161706	C 3.903277 0.26186 0.173736	C 3.901848 0.278277 0.188516
C 3.039611 -1.01239 0.221838	C 3.030907 -1.01658 0.227927	C 3.024975 -1.00248 0.241223
C 1.677732 -0.73931 -0.52915	C 1.676556 -0.74054 -0.53487	C 1.67426 -0.73209 -0.52848
C 0.944596 0.55841 -0.07908	C 0.944976 0.559631 -0.08957	C 0.941114 0.570092 -0.089
C 1.906054 1.753262 -0.15194	C 1.900463 1.757848 -0.16744	C 1.901337 1.76515 -0.17117
C 0.801932 -1.97127 -0.56507	C 0.800005 -1.97175 -0.57857	C 0.801465 -1.9663 -0.57522
C -0.53274 -2.14589 -0.48828	C -0.53465 -2.14629 -0.50158	C -0.53298 -2.14331 -0.50176
C -1.65265 -1.20561 -0.34692	C -1.65336 -1.20574 -0.3539	C -1.65374 -1.20526 -0.3564
C -1.56516 0.182992 -0.57085	C -1.56489 0.182964 -0.57697	C -1.5676 0.183642 -0.58012
C -0.2761 0.839646 -1.00684	C -0.27647 0.837721 -1.01703	C -0.28003 0.841225 -1.01868
C -2.9084 -1.73963 0.013394	C -2.90836 -1.73886 0.010366	C -2.90795 -1.74138 0.00631
C -4.05213 -0.96948 0.176591	C -4.05027 -0.96721 0.179123	C -4.05147 -0.97212 0.174222
C -3.93428 0.419412 -0.03499	C -3.93129 0.421925 -0.03092	C -3.93491 0.417457 -0.03526
C -2.70673 0.976175 -0.39978	C -2.70458 0.977562 -0.40021	C -2.7091 0.97568 -0.40395
C -5.37897 -1.57021 0.56447	C -5.3765 -1.56646 0.571357	C -5.37682 -1.57383 0.565579
C 2.838655 -1.43581 1.692962	C 2.817822 -1.43575 1.698572	C 2.81165 -1.41609 1.713301
C 3.833462 -2.13369 -0.48931	C 3.829461 -2.1401 -0.47396	C 3.821471 -2.13359 -0.45269
H 1.986565 -0.54464 -1.56764	H 1.995082 -0.54672 -1.57068	H 1.995823 -0.53743 -1.564
O 0.521953 0.516075 1.289992	O 0.523237 0.518823 1.28044	O 0.518078 0.530958 1.279818
O 4.341986 0.472271 -1.18417	O 4.361383 0.464388 -1.16061	O 4.35453 0.572934 -1.1504
O 4.129435 2.594173 0.439491	O 4.028104 2.671642 0.377028	O 4.063512 2.668883 0.52443
O -5.08372 1.138075 0.138702	O -5.07886 1.141912 0.148729	O -5.08354 1.134953 0.14412
C -5.04207 2.542657 -0.05501	C -5.03548 2.547051 -0.04203	C -5.04196 2.541218 -0.04123
H 2.956721 1.435536 1.712004	H 2.939322 1.477824 1.699804	H 2.935057 1.474948 1.697659
H 4.793863 0.107683 0.806608	H 4.773621 0.098873 0.838504	H 4.779496 0.129623 0.835911
H 2.173239 1.940965 -1.19765	H 2.167912 1.941768 -1.21386	H 2.164141 1.945095 -1.2208
H 1.379728 2.638904 0.229336	H 1.385787 2.648175 0.208584	H 1.388099 2.657816 0.201729
H 1.362574 -2.89397 -0.69078	H 1.360102 -2.89395 -0.7112	H 1.362373 -2.8887 -0.70594
H -0.86159 -3.18483 -0.52452	H -0.86419 -3.18483 -0.54393	H -0.86019 -3.18259 -0.54456
H -0.02374 0.524638 -2.02836	H -0.02528 0.518004 -2.03742	H -0.02682 0.520713 -2.03847
H -0.43913 1.922666 -1.04582	H -0.43821 1.92053 -1.05998	H -0.44405 1.92345 -1.06331
H -2.98416 -2.81335 0.174834	H -2.98499 -2.81274 0.170493	H -2.98247 -2.81539 0.166594
H -2.62073 2.044299 -0.56626	H -2.61746 2.045726 -0.56556	H -2.62393 2.044032 -0.5688

H -6.14569 -1.36683 -0.19259	H -6.14595 -1.36062 -0.18228	H -6.14607 -1.36975 -0.18874
H -5.29478 -2.65433 0.686453	H -5.2936 -2.65093 0.691251	H -5.29189 -2.65809 0.686021
H -5.75029 -1.14528 1.504674	H -5.7434 -1.14246 1.513726	H -5.74522 -1.15006 1.507429
H 2.331209 -0.67301 2.28503	H 2.314616 -0.66665 2.286251	H 2.305251 -0.64316 2.291989
H 2.232914 -2.34782 1.743254	H 2.201957 -2.34092 1.747135	H 2.198652 -2.323 1.766976
H 3.807276 -1.65852 2.157438	H 3.781623 -1.66918 2.168444	H 3.775312 -1.64098 2.188072
H 3.37862 -3.11681 -0.33128	H 3.372274 -3.12238 -0.31735	H 3.37948 -3.11766 -0.27145
H 3.92034 -1.95205 -1.56359	H 3.924499 -1.9609 -1.54804	H 3.883616 -1.99057 -1.53738
H 4.849775 -2.18123 -0.08049	H 4.842756 -2.18826 -0.05733	H 4.843477 -2.17524 -0.05122
H -0.11396 -0.21281 1.380281	H -0.1232 -0.20098 1.368971	H -0.1453 -0.17362 1.365192
H 4.709225 1.373943 -1.19019	H 4.638253 1.399144 -1.1843	H 5.076496 -0.03493 -1.36468
H 3.663886 3.43289 0.580024	H 4.737626 2.660853 1.039593	H 4.474186 2.57084 -0.35257
H -6.05496 2.901266 0.137695	H -6.04685 2.906977 0.156078	H -6.0538 2.898834 0.158447
H -4.34673 3.025789 0.643912	H -4.33604 3.027233 0.654734	H -4.343 3.019269 0.657313
H -4.75574 2.799924 -1.08331	H -4.75337 2.806027 -1.07103	H -4.76043 2.804327 -1.06929

2β10α4 (20.69%)

C 3.188844 1.524588 0.644413	C 3.186204 1.554034 0.644	C 3.186025 1.55408 0.644103
C 3.912954 0.264903 0.161878	C 3.910438 0.275615 0.1961	C 3.910376 0.275641 0.196414
C 3.039553 -1.01238 0.221933	C 3.032907 -1.00567 0.228523	C 3.032762 -1.00564 0.228594
C 1.677754 -0.73928 -0.52925	C 1.672917 -0.73414 -0.53076	C 1.672965 -0.73406 -0.53103
C 0.944601 0.558407 -0.07928	C 0.939669 0.569919 -0.09075	C 0.939675 0.569985 -0.09102
C 1.906038 1.75327 -0.15203	C 1.902264 1.764505 -0.16747	C 1.902232 1.764544 -0.16759
C 0.80196 -1.97123 -0.56527	C 0.800017 -1.96933 -0.57048	C 0.800069 -1.96923 -0.57119
C -0.53271 -2.14588 -0.48836	C -0.53469 -2.14235 -0.49494	C -0.53462 -2.14228 -0.49536
C -1.65262 -1.2056 -0.347	C -1.65523 -1.20365 -0.35309	C -1.65511 -1.20361 -0.35323
C -1.56514 0.182972 -0.57097	C -1.56995 0.184927 -0.57866	C -1.56992 0.184949 -0.57881
C -0.27609 0.839557 -1.00708	C -0.28281 0.843002 -1.01834	C -0.28283 0.843021 -1.01859
C -2.90837 -1.73964 0.013367	C -2.90935 -1.73979 0.010256	C -2.9092 -1.73981 0.010268
C -4.05207 -0.96947 0.176603	C -4.05309 -0.97079 0.176852	C -4.05294 -0.97087 0.177029
C -3.93423 0.419439 -0.03495	C -3.93719 0.418686 -0.03464	C -3.93709 0.418669 -0.03446
C -2.7067 0.976168 -0.39985	C -2.71141 0.977 -0.40411	C -2.7114 0.976999 -0.4041
C -5.37889 -1.57017 0.564613	C -5.37817 -1.5724 0.569046	C -5.37791 -1.57239 0.569599
C 2.838423 -1.43581 1.693009	C 2.81181 -1.4262 1.698502	C 2.811333 -1.42625 1.698524
C 3.833414 -2.13371 -0.48912	C 3.829696 -2.13334 -0.4688	C 3.829706 -2.13336 -0.46851
H 1.986776 -0.54464 -1.56768	H 1.967205 -0.55173 -1.58107	H 1.967564 -0.55152 -1.58123
O 0.521846 0.51611 1.289791	O 0.521192 0.527966 1.276867	O 0.521182 0.527965 1.276651
O 4.342216 0.472227 -1.18391	O 4.506308 0.524436 -1.09566	O 4.506745 0.524362 -1.0951

2β10α6 (1.50%)

2β10α9 (1.51%)

O 4.129374 2.59422 0.439505	O 4.061935 2.667411 0.525153	O 4.061671 2.667491 0.525336
O -5.08366 1.138077 0.138907	O -5.08545 1.135503 0.14347	O -5.08532 1.135435 0.144
C -5.04213 2.542627 -0.05498	C -5.04521 2.542174 -0.04195	C -5.04547 2.541966 -0.04252
H 2.956582 1.435665 1.712023	H 2.925352 1.477229 1.702743	H 2.925035 1.477285 1.702827
H 4.793727 0.107686 0.806947	H 4.777179 0.120558 0.847879	H 4.776839 0.120574 0.848562
H 2.173323 1.941039 -1.19771	H 2.158788 1.959235 -1.21924	H 2.159006 1.959303 -1.21928
H 1.379648 2.638902 0.229179	H 1.389948 2.659322 0.200347	H 1.389899 2.659401 0.200132
H 1.362606 -2.89391 -0.69113	H 1.362052 -2.89123 -0.69492	H 1.362064 -2.89108 -0.69614
H -0.86153 -3.18482 -0.52466	H -0.86215 -3.18172 -0.53024	H -0.86208 -3.18164 -0.53095
H -0.02378 0.524381 -2.02856	H -0.03347 0.524556 -2.04002	H -0.03354 0.524405 -2.04024
H -0.4391 1.922574 -1.04626	H -0.44647 1.925362 -1.06038	H -0.44648 1.925372 -1.0608
H -2.98416 -2.81335 0.174766	H -2.98341 -2.81345 0.172452	H -2.98316 -2.8135 0.17234
H -2.62067 2.044282 -0.56638	H -2.62699 2.04515 -0.57052	H -2.62702 2.045163 -0.57046
H -6.14611 -1.3653 -0.19152	H -6.14699 -1.37049 -0.18622	H -6.14786 -1.36708 -0.18355
H -5.2951 -2.65452 0.684917	H -5.29265 -2.65625 0.692174	H -5.29337 -2.65673 0.689062
H -5.74927 -1.14657 1.505803	H -5.74704 -1.14636 1.509611	H -5.74459 -1.14912 1.512312
H 2.331059 -0.67295 2.285076	H 2.31765 -0.65121 2.28506	H 2.317074 -0.65125 2.284995
H 2.232597 -2.34776 1.743233	H 2.187085 -2.32526 1.746035	H 2.18658 -2.32529 1.745884
H 3.806986 -1.65862 2.15757	H 3.773658 -1.66752 2.167428	H 3.773087 -1.66758 2.167608
H 3.37854 -3.11682 -0.3311	H 3.377224 -3.11524 -0.29916	H 3.377274 -3.11525 -0.29872
H 3.920345 -1.95211 -1.56341	H 3.91801 -1.9769 -1.54845	H 3.918015 -1.97713 -1.5482
H 4.849706 -2.18127 -0.08025	H 4.847055 -2.17175 -0.06331	H 4.847055 -2.17162 -0.06301
H -0.11352 -0.21323 1.380178	H -0.14229 -0.17639 1.364026	H -0.14277 -0.17597 1.363592
H 4.709552 1.373865 -1.18992	H 3.79921 0.524536 -1.76041	H 3.800026 0.523931 -1.76024
H 3.663845 3.432942 0.580112	H 4.564603 2.49955 -0.2927	H 4.564652 2.499479 -0.29228
H -6.05502 2.901195 0.13779	H -6.0573 2.898553 0.158208	H -6.05767 2.898259 0.157197
H -4.34679 3.025908 0.643834	H -4.3465 3.020531 0.656503	H -4.34702 3.021081 0.655673
H -4.75598 2.799802 -1.08335	H -4.76461 2.805187 -1.07022	H -4.76477 2.804244 -1.07095

Table S10. Conformers and Boltzmann populations of 2α,10β-OH isomer of **6**.

2α10β1 (28.98%)	**2α10β2** (23.10%)	**2α10β3** (15.17%)
C 3.479124 -1.19501 -0.28603	C 3.482507 -1.22152 -0.29927	C 3.486109 -1.20517 -0.3245
C 3.655695 0.300564 -0.0243	C 3.650964 0.274401 -0.03216	C 3.653679 0.287416 -0.01751
C 2.512832 0.898151 0.827743	C 2.514883 0.879696 0.830686	C 2.505862 0.887017 0.834274
C 1.137269 0.585178 0.128397	C 1.137456 0.577145 0.132019	C 1.135005 0.573259 0.124874
C 0.946928 -0.92152 -0.27918	C 0.944501 -0.93113 -0.27241	C 0.952424 -0.93333 -0.28314
C 2.172088 -1.46425 -1.02855	C 2.16479 -1.48423 -1.01936	C 2.170315 -1.46506 -1.04836
C 0.80218 1.528888 -1.01496	C 0.808419 1.523484 -1.01055	C 0.810634 1.513913 -1.02308

C -0.45754 1.780027 -1.41437	C -0.45027 1.779631 -1.41025	C -0.44799 1.765833 -1.4253
C -1.62725 1.049693 -0.90085	C -1.62223 1.052117 -0.89814	C -1.61979 1.042523 -0.90592
C -1.55262 -0.34528 -0.70425	C -1.55166 -0.34357 -0.70317	C -1.5501 -0.35184 -0.70087
C -0.32286 -1.10355 -1.15415	C -0.32377 -1.10599 -1.15141	C -0.3243 -1.11866 -1.1479
C -2.83585 1.707159 -0.61302	C -2.82912 1.713241 -0.61135	C -2.82564 1.706479 -0.62157
C -3.94482 1.049266 -0.09108	C -3.94065 1.05843 -0.09113	C -3.93703 1.056161 -0.09527
C -3.83676 -0.33923 0.138022	C -3.83703 -0.33067 0.136816	C -3.83451 -0.33149 0.141585
C -2.65981 -1.02415 -0.17627	C -2.66181 -1.01902 -0.17708	C -2.66017 -1.0229 -0.16898
C -5.22911 1.771144 0.228448	C -5.22329 1.783763 0.227153	C -5.21855 1.784809 0.219833
C 2.732752 2.422377 0.958592	C 2.73604 2.404233 0.967992	C 2.719269 2.410311 0.976531
C 2.540165 0.3293 2.266511	C 2.544031 0.304476 2.266025	C 2.510053 0.309817 2.271529
H 0.36143 0.762931 0.889264	H 0.362539 0.758853 0.892826	H 0.352456 0.752065 0.878323
O 0.814009 -1.74828 0.888993	O 0.796688 -1.74712 0.90069	O 0.830712 -1.75462 0.890416
O 4.904454 0.543379 0.608949	O 4.950663 0.416332 0.564033	O 4.960774 0.511667 0.536702
O 4.623145 -1.57642 -1.07201	O 4.537177 -1.68519 -1.13617	O 4.549942 -1.64164 -1.16282
O -4.9538 -0.93192 0.659276	O -4.95606 -0.92023 0.656181	O -4.95357 -0.91669 0.66587
C -4.9291 -2.32855 0.903704	C -4.93669 -2.31782 0.897887	C -4.93691 -2.31331 0.912673
H 3.497121 -1.73282 0.669374	H 3.501039 -1.75912 0.659124	H 3.501327 -1.77066 0.6217
H 3.645524 0.79626 -1.01311	H 3.65577 0.77384 -1.01554	H 3.6907 0.811863 -0.98093
H 2.235484 -0.98566 -2.01324	H 2.223613 -1.01613 -2.00979	H 2.222923 -0.9733 -2.02745
H 2.038157 -2.54119 -1.1942	H 2.037924 -2.56119 -1.17462	H 2.049702 -2.53906 -1.22823
H 1.612638 2.075801 -1.48816	H 1.620621 2.065438 -1.48746	H 1.624312 2.050825 -1.5028
H -0.63668 2.559045 -2.15542	H -0.62621 2.55848 -2.15227	H -0.62425 2.53802 -2.17404
H -0.08294 -0.78699 -2.17546	H -0.07979 -0.78948 -2.17156	H -0.08859 -0.81385 -2.17354
H -0.53194 -2.17859 -1.18515	H -0.53648 -2.18006 -1.18492	H -0.536 -2.19331 -1.16846
H -2.90312 2.778958 -0.79019	H -2.89324 2.785313 -0.78831	H -2.88904 2.777348 -0.80571
H -2.59715 -2.09916 -0.04372	H -2.60314 -2.09451 -0.04678	H -2.60287 -2.09772 -0.03235
H -5.14861 2.834592 -0.01616	H -5.1395 2.847179 -0.01662	H -5.134 2.846534 -0.0308
H -6.07337 1.350987 -0.33101	H -6.06789 1.3664 -0.33385	H -6.06415 1.364674 -0.33757
H -5.48505 1.680543 1.290923	H -5.4811 1.693058 1.289166	H -5.47526 1.701114 1.28269
H 1.876686 2.895896 1.454038	H 1.87089 2.882451 1.441193	H 1.876435 2.872664 1.503875
H 3.626927 2.613317 1.558646	H 3.604645 2.603574 1.607267	H 3.631225 2.606009 1.548863
H 2.878981 2.917187 -0.00644	H 2.90523 2.905062 0.008405	H 2.83053 2.916305 0.013312
H 3.524613 0.50011 2.710691	H 3.538043 0.445047 2.701493	H 3.44729 0.555303 2.788364
H 1.795093 0.848706 2.882729	H 1.820235 0.838953 2.894574	H 1.708305 0.775469 2.857446
H 2.315792 -0.73698 2.302838	H 2.293552 -0.75547 2.295655	H 2.355156 -0.7688 2.298472
H 0.047758 -1.41593 1.386361	H 0.006776 -1.42881 1.369811	H 0.032644 -1.4588 1.360523
H 5.538544 -0.01574 0.127419	H 5.223649 1.341653 0.479325	H 4.97484 0.10203 1.417479

H 4.690481 -2.54289 -1.05329	H 5.348445 -1.32995 -0.73412	H 5.341823 -1.19237 -0.81774
H -5.90673 -2.57688 1.321133	H -5.91569 -2.56314 1.313809	H -5.91628 -2.55524 1.329679
H -4.77484 -2.89838 -0.02212	H -4.78362 -2.88607 -0.02897	H -4.78509 -2.88529 -0.01211
H -4.14718 -2.59847 1.625934	H -4.15653 -2.59181 1.620365	H -4.15721 -2.5863 1.636108

2α10β4 (17.23%)	**2α10β5** (3.84%)	**2α10β7** (2.90%)
C 3.478164 -1.20117 -0.28657	C 3.489638 -1.19881 -0.33347	C 3.492783 -1.18047 -0.36069
C 3.654699 0.297045 -0.01901	C 3.650434 0.291948 -0.03478	C 3.652493 0.306179 -0.0198
C 2.513273 0.897201 0.833645	C 2.515537 0.872332 0.847454	C 2.505462 0.878476 0.852092
C 1.138685 0.585179 0.131322	C 1.132734 0.561319 0.15918	C 1.129963 0.556275 0.152468
C 0.947661 -0.92206 -0.27663	C 0.952092 -0.93198 -0.269	C 0.960517 -0.93495 -0.28106
C 2.171625 -1.47208 -1.02585	C 2.170892 -1.4463 -1.05659	C 2.176274 -1.42493 -1.08824
C 0.803812 1.530903 -1.01054	C 0.801967 1.512215 -0.98133	C 0.804672 1.50195 -0.99328
C -0.45585 1.781699 -1.4109	C -0.45304 1.76999 -1.38948	C -0.4501 1.756158 -1.404
C -1.62584 1.050395 -0.89995	C -1.63025 1.044771 -0.88903	C -1.62736 1.035239 -0.89654
C -1.55138 -0.34453 -0.70311	C -1.5601 -0.34745 -0.67995	C -1.55833 -0.35563 -0.67762
C -0.32179 -1.10314 -1.15255	C -0.33223 -1.11309 -1.12285	C -0.33268 -1.12588 -1.11958
C -2.8349 1.7079 -0.61371	C -2.84015 1.70901 -0.62264	C -2.83622 1.702291 -0.63269
C -3.94422 1.050009 -0.09276	C -3.95696 1.058231 -0.11009	C -3.95305 1.056025 -0.11434
C -3.83626 -0.33857 0.136869	C -3.85263 -0.32808 0.133415	C -3.85 -0.32875 0.138053
C -2.65897 -1.02349 -0.17627	C -2.6743 -1.01786 -0.16119	C -2.67255 -1.0216 -0.15311
C -5.22892 1.771691 0.225367	C -5.2438 1.784807 0.187772	C -5.23878 1.78593 0.180127
C 2.734137 2.420674 0.968891	C 2.718479 2.399287 0.994695	C 2.698718 2.403814 1.008126
C 2.541722 0.322813 2.269952	C 2.569474 0.290778 2.27926	C 2.535412 0.291013 2.284698
H 0.361731 0.761543 0.891266	H 0.360172 0.714047 0.924965	H 0.3494 0.70629 0.910419
O 0.814967 -1.74725 0.890683	O 0.797676 -1.67709 0.952649	O 0.835475 -1.68905 0.939266
O 4.907945 0.535684 0.60294	O 4.954632 0.425674 0.552712	O 4.962264 0.523017 0.530323
O 4.624294 -1.69368 -1.00188	O 4.546298 -1.64604 -1.17547	O 4.559896 -1.598 -1.20292
O -4.95338 -0.93097 0.657133	O -4.97676 -0.91401 0.648265	O -4.97427 -0.91025 0.657542
C -4.92904 -2.32774 0.902457	C -4.94835 -2.30344 0.92891	C -4.94812 -2.29836 0.944538
H 3.499987 -1.74707 0.659383	H 3.507462 -1.75286 0.616292	H 3.506733 -1.76377 0.575215
H 3.637096 0.801121 -1.00821	H 3.646292 0.811484 -1.00775	H 3.68118 0.851411 -0.97188
H 2.217847 -0.99046 -2.01379	H 2.218752 -0.94596 -2.03186	H 2.216781 -0.90017 -2.0508
H 2.046579 -2.54826 -1.18858	H 2.060615 -2.52 -1.26501	H 2.072121 -2.49416 -1.32173
H 1.613417 2.082764 -1.47974	H 1.615422 2.058574 -1.45079	H 1.620003 2.042903 -1.46538
H -0.63477 2.563419 -2.14919	H -0.62104 2.552412 -2.12984	H -0.61802 2.532254 -2.15084
H -0.08214 -0.78601 -2.17389	H -0.09945 -0.81742 -2.15245	H -0.1087 -0.84202 -2.15443
H -0.53077 -2.17806 -1.18414	H -0.55646 -2.18794 -1.15082	H -0.55665 -2.20112 -1.13462

H -2.90208 2.779668 -0.79104	H -2.90153 2.779635 -0.8093	H -2.89676 2.771665 -0.82643
H -2.5963 -2.09844 -0.0435	H -2.61174 -2.0892 -0.00463	H -2.61132 -2.09213 0.009727
H -5.14837 2.835177 -0.01902	H -5.15854 2.846069 -0.06511	H -5.15277 2.845318 -0.08013
H -6.07243 1.351373 -0.33507	H -6.08251 1.36159 -0.37783	H -6.07853 1.359621 -0.38156
H -5.48596 1.680836 1.287529	H -5.51226 1.704009 1.247963	H -5.50602 1.712677 1.241174
H 1.879945 2.893167 1.468557	H 1.850581 2.861182 1.478533	H 1.856054 2.846582 1.551888
H 3.629966 2.608921 1.567542	H 3.588491 2.604759 1.630399	H 3.614702 2.606172 1.571786
H 2.87776 2.919281 0.00529	H 2.874668 2.911498 0.039055	H 2.79018 2.923625 0.050311
H 3.525503 0.495464 2.714753	H 3.566244 0.445343 2.703973	H 3.470073 0.558627 2.795996
H 1.794635 0.837137 2.887872	H 1.842521 0.809379 2.915992	H 1.723949 0.727906 2.877554
H 2.321514 -0.7444 2.3022	H 2.33005 -0.77084 2.309591	H 2.404457 -0.79017 2.308066
H 0.049564 -1.41455 1.389058	H 0.768826 -2.61737 0.712083	H 0.787332 -2.6267 0.691542
H 5.513492 -0.11095 0.197925	H 5.212394 1.358248 0.508944	H 4.972502 0.124838 1.416339
H 4.582579 -1.32781 -1.9019	H 5.354051 -1.27848 -0.77685	H 5.347165 -1.14579 -0.85037
H -5.90715 -2.57553 1.318983	H -5.92885 -2.54537 1.343663	H -5.9287 -2.53663 1.361193
H -4.77396 -2.89792 -0.02294	H -4.784 -2.8966 0.019375	H -4.78558 -2.896 0.037614
H -4.14794 -2.5971 1.625684	H -4.17153 -2.5506 1.664451	H -4.1712 -2.54364 1.680662

2α10β8 (2.59%)	**2α10β11** (3.85%)	**2α10β14** (2.34%)
C 3.490859 -1.17363 -0.32114	C 3.489769 -1.19851 -0.33389	C 3.487442 -1.17882 -0.32186
C 3.655656 0.318178 -0.02857	C 3.65047 0.292224 -0.03453	C 3.656332 0.314128 -0.02128
C 2.515542 0.887521 0.846832	C 2.515291 0.872281 0.847647	C 2.515451 0.888182 0.851355
C 1.134545 0.56799 0.159072	C 1.132656 0.561241 0.159166	C 1.13521 0.569063 0.160118
C 0.953472 -0.92573 -0.26655	C 0.952148 -0.93206 -0.26911	C 0.954573 -0.92439 -0.26866
C 2.177004 -1.43617 -1.05448	C 2.170971 -1.44606 -1.05685	C 2.177262 -1.43597 -1.05934
C 0.800033 1.513765 -0.9849	C 0.801988 1.512158 -0.98137	C 0.799687 1.517677 -0.98128
C -0.45559 1.767201 -1.39374	C -0.45304 1.770017 -1.38945	C -0.45616 1.770219 -1.39057
C -1.63185 1.041514 -0.89093	C -1.63024 1.04481 -0.88905	C -1.63202 1.042482 -0.89045
C -1.56027 -0.34984 -0.67852	C -1.56003 -0.34746 -0.68007	C -1.55957 -0.34892 -0.67868
C -0.32986 -1.11255 -1.1194	C -0.33222 -1.11308 -1.12302	C -0.32953 -1.1113 -1.12077
C -2.84299 1.703867 -0.62588	C -2.84018 1.708975 -0.62271	C -2.84376 1.704025 -0.62569
C -3.95918 1.052087 -0.11295	C -3.95702 1.058184 -0.11022	C -3.95941 1.051352 -0.11299
C -3.85344 -0.33365 0.132353	C -3.85262 -0.32814 0.133239	C -3.8526 -0.33446 0.132354
C -2.67375 -1.02193 -0.16014	C -2.67427 -1.01787 -0.1614	C -2.67247 -1.02193 -0.16047
C -5.24697 1.777569 0.183549	C -5.24388 1.784675 0.187592	C -5.24778 1.775689 0.183593
C 2.715325 2.41373 0.993044	C 2.718004 2.3992 0.995281	C 2.717439 2.413764 0.999277
C 2.570989 0.30582 2.279281	C 2.569193 0.290437 2.279299	C 2.569418 0.304326 2.282818
H 0.361718 0.72033 0.92429	H 0.359934 0.713868 0.924809	H 0.361498 0.718509 0.925008

O 0.808414 -1.67393 0.954444	O 0.797788 -1.6773 0.952389	O 0.813862 -1.67426 0.949625
O 4.90925 0.557903 0.595847	O 4.954422 0.425428 0.553638	O 4.912369 0.545778 0.597524
O 4.629887 -1.52917 -1.12594	O 4.546215 -1.64513 -1.17634	O 4.631141 -1.65479 -1.05154
O -4.97759 -0.9207 0.646768	O -4.97671 -0.91421 0.647955	O -4.97593 -0.92215 0.646752
C -4.94713 -2.30909 0.930317	C -4.94764 -2.30336 0.929781	C -4.94406 -2.31035 0.932525
H 3.522703 -1.72891 0.624363	H 3.507925 -1.75278 0.615748	H 3.514821 -1.74229 0.613976
H 3.631718 0.832851 -1.00727	H 3.646844 0.812154 -1.00725	H 3.630468 0.838507 -0.99963
H 2.225017 -0.93485 -2.02906	H 2.218646 -0.94552 -2.03203	H 2.210534 -0.92301 -2.03217
H 2.059891 -2.51176 -1.261	H 2.060939 -2.51974 -1.26544	H 2.069625 -2.50868 -1.27321
H 1.612407 2.063309 -1.45159	H 1.615466 2.058405 -1.45092	H 1.610648 2.073161 -1.44366
H -0.62586 2.548243 -2.13497	H -0.62106 2.552492 -2.12975	H -0.62694 2.554477 -2.12833
H -0.09726 -0.81679 -2.14901	H -0.09939 -0.81733 -2.15259	H -0.09886 -0.81508 -2.15087
H -0.5522 -2.18865 -1.14899	H -0.55651 -2.18791 -1.15108	H -0.55097 -2.18723 -1.14952
H -2.90571 2.774126 -0.81379	H -2.90153 2.779617 -0.8093	H -2.90719 2.774306 -0.81321
H -2.61053 -2.09323 -0.00263	H -2.6118 -2.08924 -0.00496	H -2.60824 -2.09313 -0.00308
H -5.16257 2.838643 -0.07021	H -5.15873 2.84594 -0.06529	H -5.16451 2.836801 -0.07036
H -6.08499 1.352947 -0.38204	H -6.08256 1.361387 -0.37801	H -6.08545 1.350067 -0.38173
H -5.51569 1.697514 1.243715	H -5.51237 1.703875 1.247786	H -5.51615 1.69548 1.243821
H 1.858846 2.867083 1.50593	H 1.850154 2.860763 1.479553	H 1.862208 2.868147 1.513331
H 3.614038 2.609987 1.584557	H 3.58813 2.604613 1.630869	H 3.616605 2.607591 1.591162
H 2.84159 2.924142 0.033346	H 2.873868 2.911715 0.039786	H 2.844074 2.925793 0.040362
H 3.556668 0.494998 2.713436	H 3.565882 0.445058 2.704181	H 3.554022 0.494695 2.718666
H 1.819382 0.800775 2.906065	H 1.842039 0.808676 2.916099	H 1.81572 0.796906 2.90885
H 2.364771 -0.76347 2.311362	H 2.329999 -0.77125 2.309417	H 2.365256 -0.76532 2.312724
H 0.66819 -2.60201 0.706	H 0.768949 -2.61755 0.711699	H 0.714332 -2.60826 0.703318
H 5.545624 0.025771 0.087797	H 5.212872 1.357783 0.509243	H 5.521153 -0.08445 0.172515
H 4.717265 -2.49404 -1.11701	H 5.354196 -1.27905 -0.77686	H 4.592076 -1.25966 -1.93923
H -5.92764 -2.55209 1.344458	H -5.92782 -2.5453 1.345287	H -5.92407 -2.55334 1.347783
H -4.78071 -2.90418 0.022286	H -4.7836 -2.89728 0.020678	H -4.77796 -2.90655 0.025231
H -4.1708 -2.55354 1.667424	H -4.17031 -2.54962 1.665097	H -4.16695 -2.55277 1.669361

Table S11. Conformers and Boltzmann populations of 2β,10β-OH isomer of **6**.

2β10β1 (55.19%)	**2β10β2** (4.00%)	**2β10β3** (5.94%)
C 3.538389 -1.05381 -0.78035	C 3.532959 -1.028 -0.81102	C 3.035186 1.621854 0.364075
C 3.737156 0.342326 -0.15577	C 3.704526 0.360306 -0.18065	C 3.806451 0.295728 0.409955
C 2.566948 0.853018 0.745243	C 2.555945 0.829494 0.762901	C 2.885599 -0.93833 0.564121
C 1.178772 0.611296 0.039975	C 1.166614 0.582172 0.06374	C 1.727746 -0.88085 -0.51931

C 1.004042 -0.81758 -0.5714	C 1.001032 -0.85646 -0.5468	C 0.98992 0.479233 -0.68674
C 2.184597 -1.18366 -1.47901	C 2.175457 -1.17411 -1.49124	C 2.022903 1.615891 -0.77585
C 0.790714 1.682342 -0.96645	C 0.788056 1.66181 -0.93618	C 0.817656 -2.07887 -0.41665
C -0.48797 1.961467 -1.27709	C -0.4865 1.948579 -1.25837	C -0.51225 -2.20533 -0.23216
C -1.62679 1.163418 -0.79551	C -1.63245 1.154948 -0.79192	C -1.59716 -1.2295 -0.06191
C -1.53425 -0.24389 -0.75973	C -1.53872 -0.25144 -0.73882	C -1.42598 0.145731 0.199189
C -0.32783 -0.93478 -1.35933	C -0.33527 -0.9551 -1.32924	C -0.0653 0.768353 0.419502
C -2.824 1.771002 -0.37893	C -2.83527 1.768987 -0.4004	C -2.91734 -1.71894 -0.17766
C -3.9029 1.04635 0.116541	C -3.92004 1.050513 0.089635	C -4.04787 -0.9221 -0.06641
C -3.77606 -0.35801 0.181903	C -3.7897 -0.35233 0.178463	C -3.84931 0.453009 0.173384
C -2.61107 -0.99008 -0.26151	C -2.62075 -0.98928 -0.24345	C -2.55785 0.966441 0.300562
C -5.17487 1.713188 0.574583	C -5.1986 1.721467 0.523013	C -5.44235 -1.47853 -0.19829
C 2.797284 2.359005 1.01042	C 2.755479 2.33883 1.055829	C 2.38195 -1.00971 2.023407
C 2.585478 0.187639 2.143545	C 2.592973 0.134201 2.146361	C 3.747066 -2.2004 0.322051
H 0.416587 0.672057 0.8332	H 0.411968 0.618119 0.860401	H 2.259596 -0.99093 -1.47548
O 1.002349 -1.8216 0.473271	O 0.922638 -1.843 0.486743	O 0.357741 0.517554 -1.97244
O 4.981493 0.357163 0.53155	O 4.982619 0.298375 0.466873	O 4.570315 0.168256 -0.78473
O 3.762043 -2.07741 0.19535	O 3.669412 -2.06294 0.17401	O 4.040312 2.62953 0.16274
O -4.86354 -1.01759 0.683169	O -4.88155 -1.0069 0.680416	O -4.9884 1.201853 0.268791
C -4.82245 -2.43316 0.762209	C -4.82285 -2.41798 0.80986	C -4.8672 2.596122 0.500047
H 4.339163 -1.18693 -1.51774	H 4.334882 -1.14745 -1.55542	H 2.539424 1.796923 1.329776
H 3.842683 1.052624 -0.98869	H 3.757935 1.074884 -1.01912	H 4.485865 0.326126 1.279027
H 2.058828 -2.20662 -1.85405	H 2.071769 -2.19417 -1.88062	H 2.568389 1.491911 -1.71637
H 2.170418 -0.51249 -2.34647	H 2.147975 -0.49187 -2.34984	H 1.490047 2.575418 -0.82925
H 1.576118 2.288466 -1.40866	H 1.576914 2.26768 -1.37541	H 1.341809 -3.02296 -0.55248
H -0.70741 2.818076 -1.91427	H -0.69417 2.809407 -1.89443	H -0.8797 -3.2316 -0.25443
H -0.52653 -2.0046 -1.48501	H -0.54579 -2.02317 -1.44155	H -0.19926 1.85394 0.489346
H -0.16351 -0.51682 -2.35912	H -0.17099 -0.54582 -2.33305	H 0.31872 0.440337 1.390508
H -2.90578 2.855054 -0.43093	H -2.91581 2.852622 -0.4669	H -3.05569 -2.78119 -0.36995
H -2.53645 -2.07242 -0.25408	H -2.53555 -2.06939 -0.20305	H -2.40968 2.023638 0.491199
H -5.11228 2.798259 0.44871	H -5.13637 2.804983 0.382135	H -5.41567 -2.55715 -0.38029
H -6.04182 1.349396 0.010427	H -6.05909 1.348641 -0.04544	H -6.03218 -1.2961 0.707897
H -5.38003 1.500114 1.630512	H -5.41594 1.5237 1.579618	H -5.98555 -1.00299 -1.02365
H 1.976384 2.785869 1.599296	H 1.883881 2.746349 1.579282	H 1.612688 -1.78112 2.129922
H 3.727609 2.487191 1.572032	H 3.620582 2.499077 1.714539	H 3.213106 -1.27011 2.689276
H 2.890732 2.946341 0.091967	H 2.91251 2.938659 0.1541	H 1.963544 -0.06887 2.392813
H 3.552574 0.365264 2.622434	H 3.587776 0.221327 2.596487	H 4.654058 -2.15569 0.936177
H 1.814246 0.642122 2.778374	H 1.881766 0.630202 2.81706	H 3.206887 -3.11015 0.603267

H 2.409713 -0.88662 2.12186	H 2.320064 -0.91654 2.108995	H 4.060524 -2.28143 -0.72169
H 0.32528 -1.57141 1.123816	H 1.828103 -2.17748 0.629992	H -0.35724 -0.1398 -1.96813
H 5.041682 -0.52695 0.939208	H 5.118021 1.120732 0.96138	H 4.962681 1.048655 -0.92337
H 2.897111 -2.25238 0.610074	H 4.399983 -1.77867 0.751757	H 3.598975 3.435554 -0.14667
H -5.77938 -2.7368 1.190699	H -4.0071 -2.7285 1.475633	H -5.88717 2.983842 0.53124
H -4.00802 -2.77774 1.413183	H -4.69691 -2.90845 -0.16454	H -4.37059 2.804901 1.456837
H -4.70783 -2.89003 -0.22955	H -5.77873 -2.71875 1.24337	H -4.31454 3.092439 -0.3084

2β10β6 (9.56%)

C 3.030227 1.645602 0.357773
C 3.794362 0.316652 0.417439
C 2.878313 -0.92768 0.564714
C 1.724943 -0.87576 -0.52165
C 0.988748 0.485215 -0.69919
C 2.017847 1.624734 -0.78914
C 0.817499 -2.07617 -0.41579
C -0.51172 -2.20264 -0.22691
C -1.59732 -1.22774 -0.05806
C -1.42785 0.150106 0.19183
C -0.06907 0.780197 0.402674
C -2.91665 -1.72159 -0.16501
C -4.04868 -0.9267 -0.05606
C -3.85234 0.450864 0.171732
C -2.56159 0.968408 0.290339
C -5.44235 -1.48725 -0.17874
C 2.375166 -1.00033 2.024062
C 3.742256 -2.18897 0.3257
H 2.258357 -0.98727 -1.47747
O 0.358514 0.504905 -1.98651
O 4.569332 0.293897 -0.7956
O 3.945775 2.725434 0.22707
O -4.9923 1.197801 0.264493
C -4.87332 2.594724 0.484156
H 2.522793 1.810502 1.314328
H 4.47944 0.351757 1.278689
H 2.561431 1.50375 -1.73258
H 1.497274 2.586811 -0.83901
H 1.340265 -3.0215 -0.55233

2β10β8 (4.84%)

C 3.529193 -1.01608 -0.81632
C 3.70141 0.368457 -0.1672
C 2.553092 0.831264 0.769541
C 1.165811 0.579803 0.066907
C 0.999657 -0.85678 -0.54788
C 2.172306 -1.16698 -1.49726
C 0.787258 1.659209 -0.93327
C -0.48659 1.9465 -1.25755
C -1.63371 1.153795 -0.79214
C -1.54097 -0.2525 -0.73858
C -0.33766 -0.9564 -1.3289
C -2.83645 1.76844 -0.40157
C -3.92201 1.050536 0.087734
C -3.79249 -0.35226 0.177097
C -2.62357 -0.98991 -0.24377
C -5.20042 1.722392 0.520243
C 2.760385 2.335987 1.069172
C 2.592053 0.131662 2.151947
H 0.410352 0.614651 0.862622
O 0.925589 -1.84934 0.47957
O 4.929425 0.363071 0.585104
O 3.683461 -2.05218 0.162043
O -4.88518 -1.0063 0.678546
C -4.82604 -2.41698 0.810649
H 4.326648 -1.12994 -1.57252
H 3.777812 1.099682 -0.98724
H 2.071864 -2.18513 -1.8928
H 2.140536 -0.47963 -2.35197
H 1.576376 2.267371 -1.36887

2β10β10 (5.39 %)

C 3.032259 1.625254 0.350364
C 3.801572 0.294135 0.402903
C 2.884207 -0.94209 0.560722
C 1.725556 -0.88272 -0.52064
C 0.989988 0.479051 -0.68845
C 2.016511 1.620846 -0.78159
C 0.814986 -2.08031 -0.41482
C -0.51459 -2.20574 -0.22704
C -1.59878 -1.22921 -0.05686
C -1.42632 0.146656 0.200327
C -0.06536 0.769409 0.417941
C -2.91931 -1.71831 -0.16982
C -4.0492 -0.9203 -0.06033
C -3.84946 0.455534 0.174414
C -2.55758 0.968428 0.299577
C -5.44419 -1.47606 -0.1898
C 2.382793 -1.00973 2.020957
C 3.745685 -2.20397 0.319172
H 2.256138 -0.99406 -1.47736
O 0.356292 0.512498 -1.97346
O 4.57234 0.169283 -0.78536
O 3.960327 2.688552 0.064861
O -4.98783 1.205688 0.267243
C -4.86499 2.601493 0.489208
H 2.541664 1.817515 1.314827
H 4.479557 0.319248 1.278824
H 2.555588 1.503053 -1.72652
H 1.495569 2.582854 -0.82508
H 1.337864 -3.02513 -0.55112

H -0.87827 -3.22938 -0.24531	H -0.69326 2.808107 -1.89291	H -0.88256 -3.2319 -0.24741
H -0.20541 1.865736 0.459253	H -0.54793 -2.02467 -1.4402	H -0.19823 1.855044 0.485052
H 0.31534 0.466015 1.37838	H -0.17481 -0.5478 -2.33327	H 0.31838 0.443036 1.389827
H -3.05325 -2.78563 -0.3487	H -2.91621 2.85213 -0.46788	H -3.05856 -2.78102 -0.35901
H -2.41501 2.027442 0.471215	H -2.53882 -2.07005 -0.20287	H -2.4083 2.026193 0.485942
H -5.41392 -2.56721 -0.3526	H -5.13737 2.805825 0.379111	H -5.41844 -2.5553 -0.36833
H -6.02941 -1.29915 0.72809	H -6.06091 1.349958 -0.0485	H -6.03359 -1.29022 0.715986
H -5.98949 -1.01918 -1.00573	H -5.41835 1.525112 1.576814	H -5.98731 -1.00277 -1.0165
H 1.607739 -1.77329 2.131898	H 1.910979 2.734067 1.63548	H 1.611867 -1.77897 2.129879
H 3.205846 -1.25561 2.693312	H 3.665547 2.472025 1.669326	H 3.213784 -1.27106 2.687033
H 1.953977 -0.05918 2.387723	H 2.87036 2.943497 0.165432	H 1.965239 -0.06745 2.388336
H 4.653228 -2.14838 0.938769	H 3.5742 0.262702 2.615673	H 4.652413 -2.16056 0.934178
H 3.211373 -3.10097 0.614189	H 1.848535 0.600939 2.806531	H 3.205297 -3.11401 0.598944
H 4.037298 -2.29021 -0.72431	H 2.356273 -0.92866 2.112131	H 4.059444 -2.28399 -0.7246
H -0.37054 -0.13659 -1.9686	H 1.833343 -2.17472 0.626833	H -0.36263 -0.14035 -1.96443
H 5.294775 -0.33602 -0.67876	H 5.664936 0.392004 -0.04727	H 4.874717 1.074494 -0.98431
H 4.547274 2.453727 -0.48837	H 4.357836 -1.71767 0.782277	H 4.514796 2.814687 0.852138
H -5.89413 2.980071 0.516078	H -5.78202 -2.71741 1.244246	H -5.88455 2.990514 0.517796
H -4.37354 2.811951 1.43726	H -4.01047 -2.72598 1.477363	H -4.36819 2.816042 1.444605
H -4.32483 3.085426 -0.33033	H -4.6994 -2.90937 -0.16275	H -4.31165 3.091637 -0.32243

2β10β13 (1.93%)

C 3.536821 -0.9995 -0.80997
C 3.716756 0.38007 -0.15941
C 2.552399 0.844944 0.771438
C 1.163765 0.58957 0.07158
C 1.001632 -0.84509 -0.54553
C 2.177798 -1.14858 -1.49401
C 0.78228 1.664785 -0.93271
C -0.49202 1.946847 -1.25939
C -1.63747 1.152382 -0.79236
C -1.5412 -0.25335 -0.73566
C -0.33509 -0.95461 -1.32408
C -2.84214 1.76429 -0.40379
C -3.92632 1.044285 0.085684
C -3.79342 -0.35795 0.177291
C -2.6223 -0.99317 -0.24119
C -5.20673 1.713653 0.516071

2β10β19 (9.57%)

C 3.03024 1.645495 0.358409
C 3.794289 0.316461 0.417659
C 2.878235 -0.9279 0.564291
C 1.724903 -0.87551 -0.52207
C 0.988718 0.48558 -0.69907
C 2.0179 1.625079 -0.78853
C 0.817501 -2.07598 -0.41665
C -0.51166 -2.20256 -0.22749
C -1.59724 -1.22775 -0.05809
C -1.42782 0.150054 0.19196
C -0.06904 0.780141 0.402898
C -2.91661 -1.72166 -0.16478
C -4.04864 -0.92684 -0.05557
C -3.85234 0.450759 0.172206
C -2.56161 0.9683 0.290771
C -5.44231 -1.48743 -0.178

2β10β20 (3.59%)

C -3.52761 1.311417 -0.47511
C -3.55687 0.325782 0.723978
C -2.90619 -1.03813 0.376455
C -1.37383 -0.84257 0.046214
C -1.02281 0.580646 -0.55792
C -2.20549 1.223816 -1.28766
C -0.78309 -2.04485 -0.67308
C 0.52768 -2.29113 -0.85043
C 1.615313 -1.3542 -0.54401
C 1.466462 0.022606 -0.80122
C 0.21529 0.540354 -1.4749
C 2.838347 -1.81225 -0.02128
C 3.885645 -0.95813 0.306135
C 3.701854 0.423418 0.080743
C 2.511041 0.900789 -0.47421
C 5.183496 -1.46384 0.882092

C 2.761383 2.350814 1.059883
C 2.598532 0.159055 2.159167
H 0.405283 0.622283 0.864612
O 0.930479 -1.84541 0.477007
O 4.99019 0.442176 0.472027
O 3.726515 -1.99051 0.236595
O -4.88518 -1.01408 0.678479
C -4.82264 -2.42407 0.813591
H 4.347541 -1.1206 -1.54103
H 3.772622 1.094754 -0.99122
H 2.068836 -2.16167 -1.90567
H 2.148557 -0.45394 -2.34341
H 1.569907 2.273611 -1.36926
H -0.70069 2.805549 -1.89794
H -0.54161 -2.02427 -1.43158
H -0.17393 -0.54933 -2.32998
H -2.9246 2.847617 -0.4719
H -2.53515 -2.07311 -0.19855
H -5.14634 2.796932 0.372899
H -6.06586 1.337839 -0.05247
H -5.42471 1.51785 1.572899
H 1.92902 2.75075 1.650264
H 3.686057 2.489381 1.62861
H 2.846033 2.954617 0.151412
H 3.57323 0.328999 2.628626
H 1.839264 0.60901 2.808985
H 2.407498 -0.91121 2.13657
H 1.846407 -2.09778 0.690773
H 5.060856 -0.37651 0.991769
H 3.962467 -2.83036 -0.18706
H -5.77829 -2.72611 1.246794
H -4.00703 -2.72972 1.481918
H -4.69373 -2.91835 -0.15862
C 2.37504 -1.00138 2.023591
C 3.742199 -2.18902 0.324547
H 2.258314 -0.9867 -1.47793
O 0.358598 0.505829 -1.9864
O 4.569326 0.293962 -0.79538
O 3.945829 2.725298 0.228097
O -4.99234 1.197587 0.265195
C -4.87335 2.594914 0.482256
H 2.522764 1.810151 1.314977
H 4.479352 0.35116 1.278919
H 2.561484 1.50449 -1.73203
H 1.49736 2.587203 -0.83811
H 1.340253 -3.02124 -0.55372
H -0.87819 -3.2293 -0.24623
H -0.20547 1.865659 0.459895
H 0.315405 0.465702 1.378509
H -3.05319 -2.7857 -0.34847
H -2.41502 2.027276 0.471979
H -5.41391 -2.56756 -0.35078
H -6.02957 -1.29839 0.728486
H -5.98922 -1.02022 -1.00565
H 1.607669 -1.77444 2.131014
H 3.205713 -1.25701 2.692733
H 1.953853 -0.06044 2.387811
H 4.65301 -2.1489 0.937884
H 3.211192 -3.10121 0.612208
H 4.037568 -2.28938 -0.72545
H -0.37157 -0.13441 -1.96829
H 5.295766 -0.33469 -0.67794
H -3.53028 2.616669 0.926277
H -5.89416 2.980427 0.512633
H -4.37438 2.813951 1.435372
H -4.32418 3.083966 -0.33274
C -3.71301 -1.65817 -0.79282
C -3.03273 -1.97457 1.594299
H -0.8639 -0.82386 1.019875
O -0.71192 1.481241 0.542859
O -2.99536 0.94796 1.882053
O -3.78923 2.626155 -0.01492
O 4.758837 1.21612 0.427021
C 4.657048 2.615861 0.215484
H -4.34928 1.052782 -1.15336
H -4.60326 0.146859 0.996468
H -1.93114 2.240793 -1.58476
H -2.37439 0.651702 -2.20811
H -1.47193 -2.82823 -0.97292
H 0.820191 -3.26439 -1.24503
H 0.385648 1.558918 -1.84087
H -0.01929 -0.08973 -2.34078
H 2.966046 -2.87956 0.148915
H 2.389417 1.957063 -0.68973
H 5.165616 -2.55291 0.984949
H 6.034559 -1.1903 0.247289
H 5.379101 -1.0273 1.868746
H -3.52663 -2.73264 -0.88474
H -4.78731 -1.54338 -0.60568
H -3.49375 -1.2022 -1.76302
H -4.08514 -2.21024 1.794938
H -2.50531 -2.91998 1.419913
H -2.61912 -1.50371 2.490608
H 0.153139 1.205163 0.895858
H -2.0669 1.179999 1.655915
H -3.53028 2.616669 0.926277
H 5.599333 3.040241 0.566543
H 3.827336 3.050815 0.787967
H 4.525316 2.854499 -0.84793

Table S12. ^{1}H NMR spectroscopic data of compounds **1**–**6**.

	1 [a]	**2** [b]	**3** [b]	**4** [c]	**5** [b]	**6** [a]
No.	δ_H (*J* in Hz)	δ_H (*J* in Hz)	δ_H (*J* in Hz)	δ_H (*J* in Hz)	δ_H (*J* in Hz)	δ_H (*J* in Hz)
1	2.42 br d (13.2)	2.16 td (14.2, 4.4)	2.52 td (14.0, 4.3)	2.39 m	1.98 m	2.25 dd (14.5, 3.7)
	2.28 td (13.2, 5.4)	1.88 m	1.59 m	2.25 m	1.98 m	1.95 d (14.5, 2.0)
2	2.10 m	1.88 m	2.01 m	1.97 m	2.24 m	4.00 ddd (3.7, 3.0, 2.0)
	2.05 m	1.73 m	1.85 m	1.97 m	1.50 m	
3	3.81 br s	3.40 dd (11.7, 3.4)	3.62 br s	3.62 m	3.88 t (8.0)	3.63 br d (3.0)
5	2.94 br s	0.91 d (2.4)	1.29 d (3.6)	2.37 m	1.56 d (6.2)	2.39 dd (4.6, 2.2)
6	5.90 br d (9.8)	4.21 m	4.15 m	1.75 m	4.44 t (6.2)	5.85 dd (12.0, 4.6)
				1.56 m		
7	6.60 dd (9.8, 2.9)	4.72 d (4.4)	4.71 d (4.3)	2.89 m	4.72 d (6.2)	6.61 dd (12.0, 2.2)
				2.37 m		
11	6.93 s	6.67 s	6.73 s	4.31 br d (8.0)	6.58 s	6.58 s
12				4.05 br s		
14	6.89 s	7.12 s	7.11 s	5.35 s	6.85 s	6.96 s
15	2.18 s	2.22 s	2.21 s	5.91 dd (17.4, 10.4)	2.18 s	2.18 s
16				5.21 d (17.4)		
				5.11 d (10.4)		
17				1.36 s		
18	1.19 s	1.14 s	1.11 s	1.29 s	1.03 s	1.03 s
19	4.37 d (12.2)	1.14 s	1.17 s	1.16 s	1.10 s	1.25 s
	4.04 dd (12.2, 1.7)					
20		4.07 d (8.5)	4.11 d (8.5)	1.08 s	2.98 d (16.3)	2.95 d (14.0)
		2.72 d (8.5)	2.75 d (8.5)		2.55 d (16.3)	2.68 d (14.0)
OMe	3.88 s	3.86 s	3.86 s		3.80 s	3.84 s
3-O*H*				5.75 br d (4.6)		
9-O*H*				4.79 br s		
11-O*H*				5.15 overlapped		
12-O*H*				6.87 br s		

[a] Spectra recorded at 400 MHz in $CDCl_3$; [b] Spectra recorded at 500 MHz in $CDCl_3$; [c] Spectra recorded at 400 MHz in pyridine-d_5.