Lipid Peroxidation and Cyclooxygenase Enzyme Inhibitory Compounds from *Prangos haussknechtii*

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Supplemental data

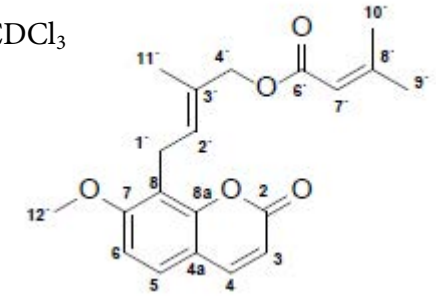
For compound **4**

Bio assay results

For known compounds

Bio assay results

Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	3800.7	7.606	18.3
2	3791.4	7.587	17.9
3	3644.7	7.294	13.3
4	3635.9	7.276	15.5
5	3617.8	7.240	67.3
6	3404.1	6.812	15.1
7	3395.3	6.795	14.4
8	3113.6	6.231	15.9
9	3104.3	6.212	17.3
10	2851.4	5.706	9.1
11	2850.5	5.704	10.6
12	2849.0	5.701	8.6
13	2847.5	5.699	3.5
14	2753.1	5.510	2.6
15	2745.8	5.495	5.5
16	2744.8	5.493	5.4
17	2738.0	5.479	2.8
18	2426.4	4.856	42.3
19	1944.7	3.892	4.2
20	1939.8	3.882	107.1
21	1808.3	3.619	14.3
22	1800.9	3.604	14.3
23	1734.4	3.471	4.0
24	1086.4	2.174	52.0
25	1084.9	2.171	45.4
26	942.1	1.885	53.7
27	941.2	1.883	49.0
28	853.6	1.708	43.1
29	852.6	1.706	39.8
30	788.1	1.577	2.7
31	615.4	1.232	2.1
32	480.5	0.961	2.5
33	474.1	0.949	3.1

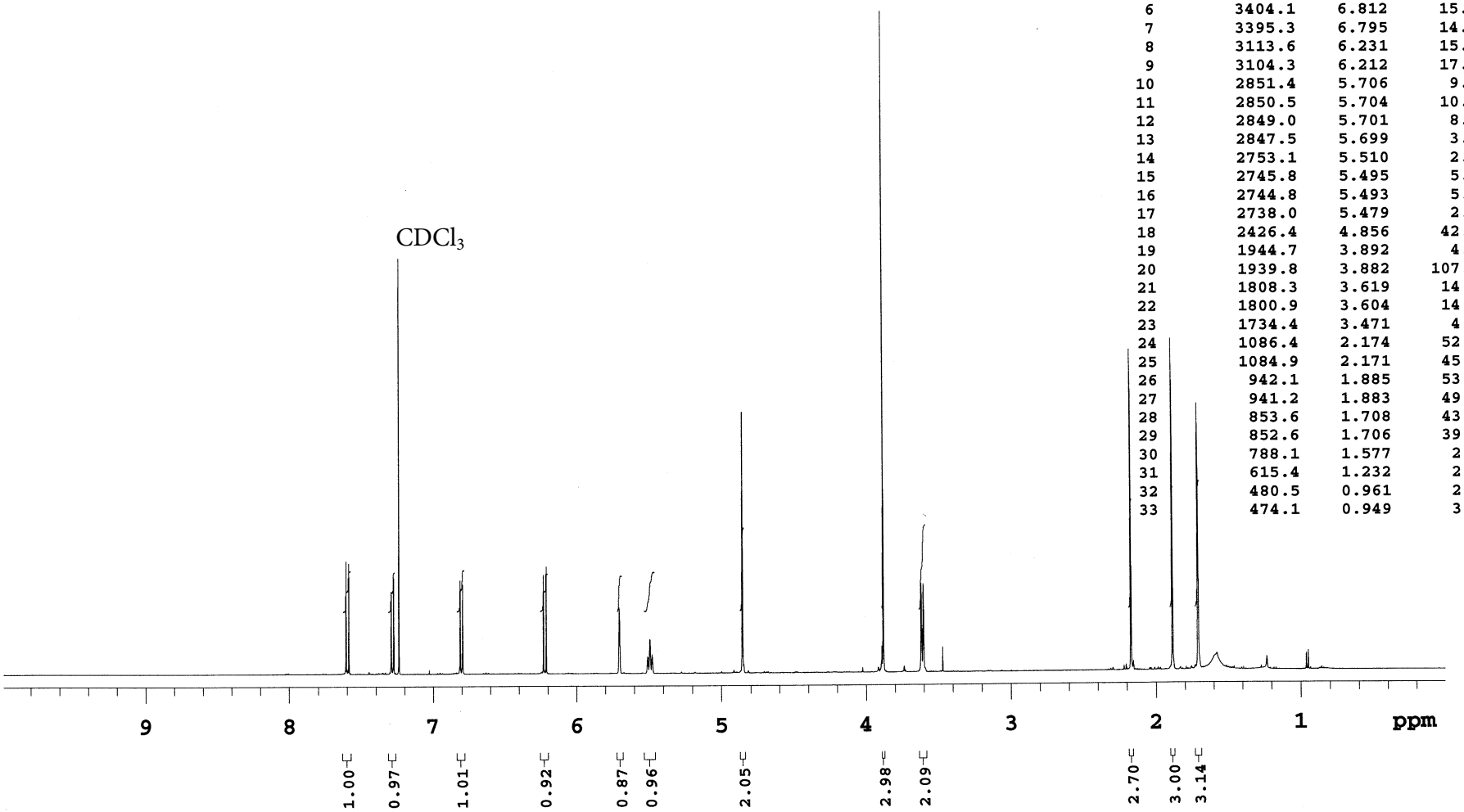
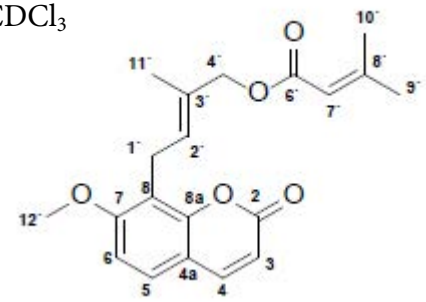


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$



$CDCl_3$

INDEX	FREQUENCY	PPM	HEIGHT
1	20963.6	166.843	29.9
2	20254.1	161.196	18.8
3	20115.8	160.095	31.1
4	19662.8	156.490	26.6
5	19207.9	152.870	24.5
6	18053.9	143.686	73.2
7	16491.8	131.253	46.2
8	15897.7	126.525	90.5
9	15891.9	126.479	88.2
10	14658.8	116.665	26.4
11	14584.5	116.073	74.8
12	14206.8	113.068	78.4
13	14188.7	112.924	30.9
14	13482.0	107.299	95.8
15	9707.4	77.258	1110.1
16	9674.9	77.000	996.2
17	9643.5	76.750	1121.7
18	7842.0	62.412	97.8
19	7039.0	56.021	105.8
20	3445.5	27.422	81.0
21	2716.0	21.616	87.2
22	2697.9	21.471	86.5
23	2540.5	20.219	55.8

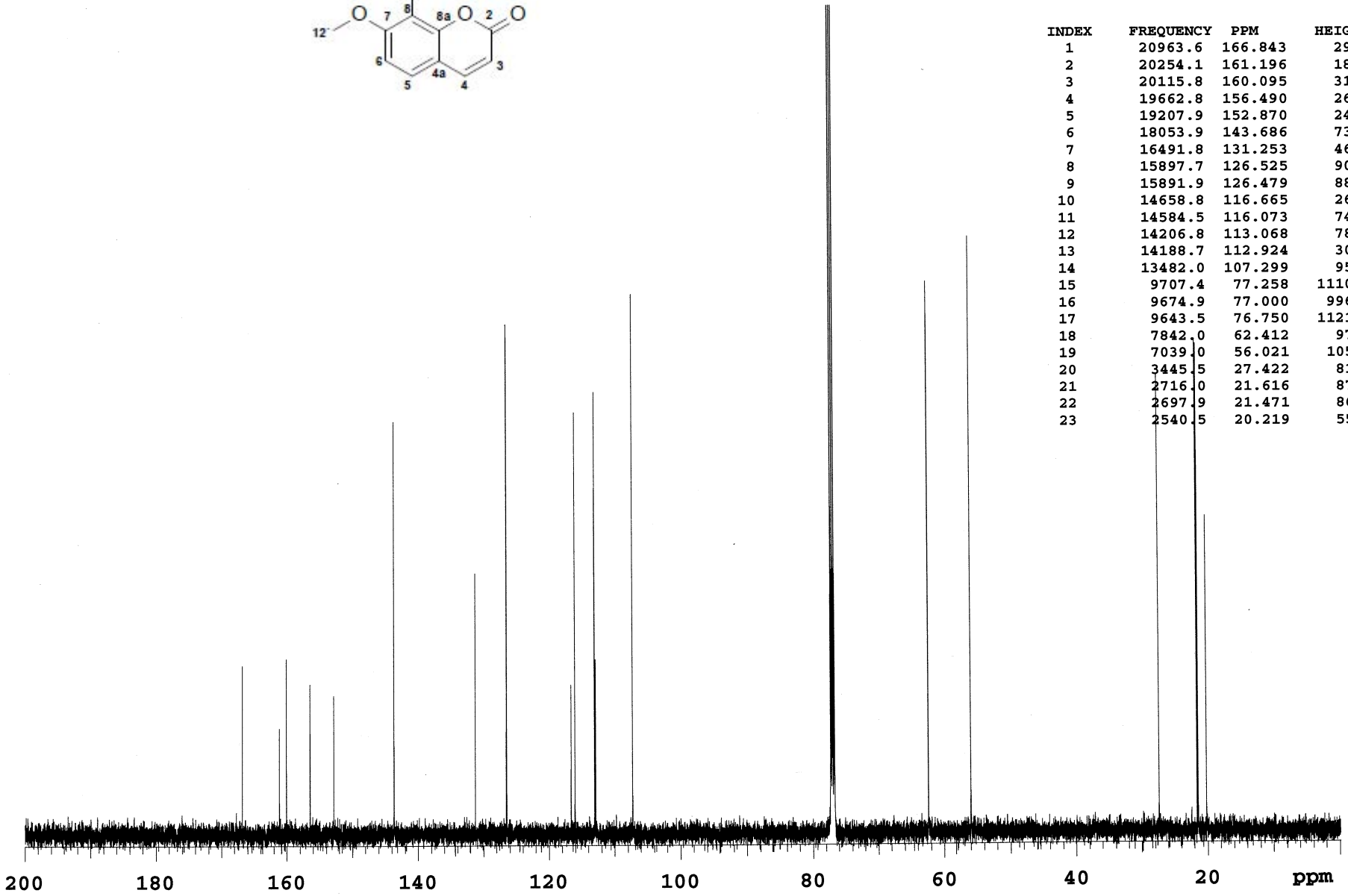


Figure S3. HSQC spectrum of **1** in $CDCl_3$

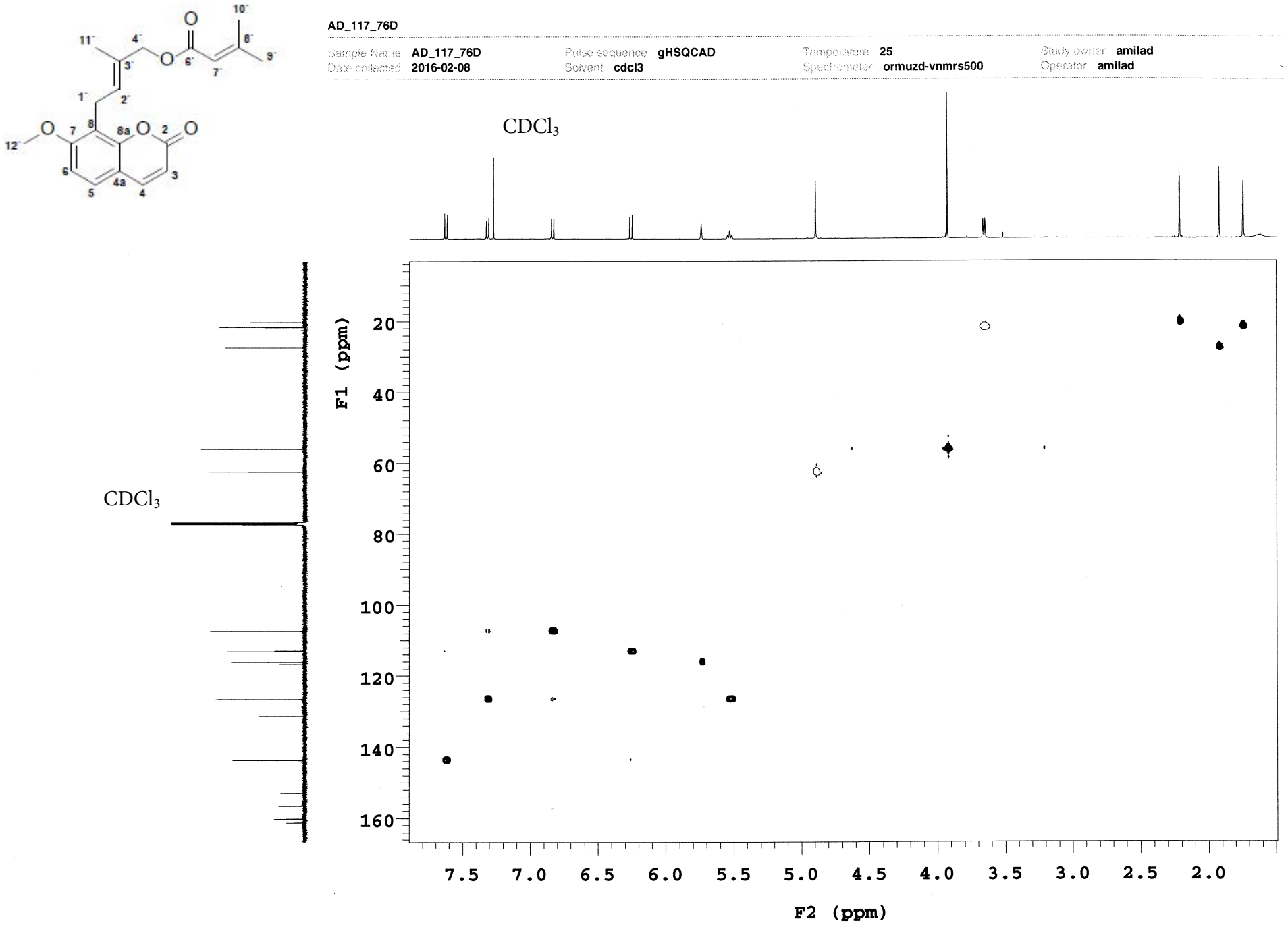


Figure S4. HMBC spectrum of **1** in $CDCl_3$

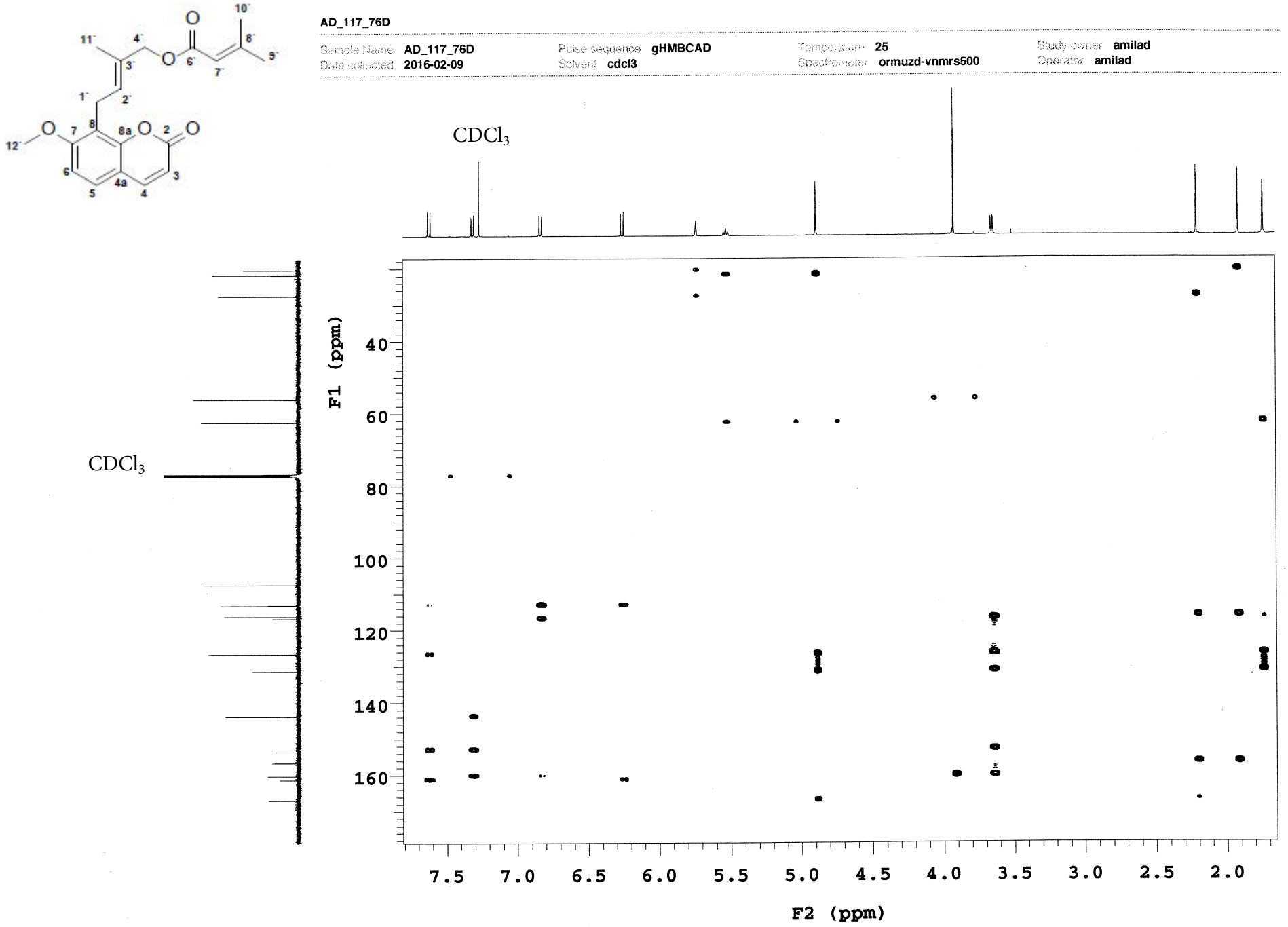


Figure S5. $^{1}H–^{1}H$ COSY spectrum of **1** in $CDCl_3$

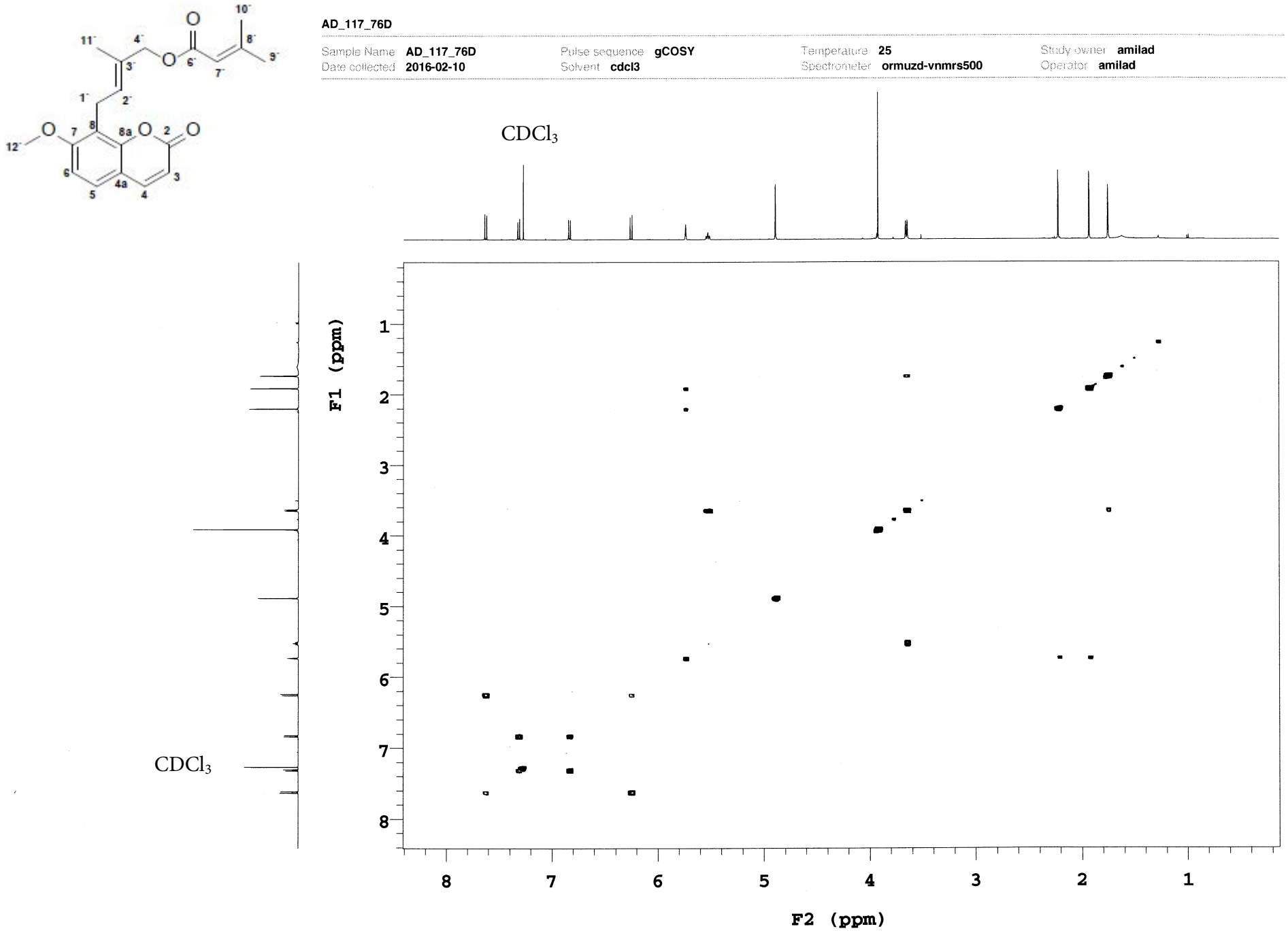
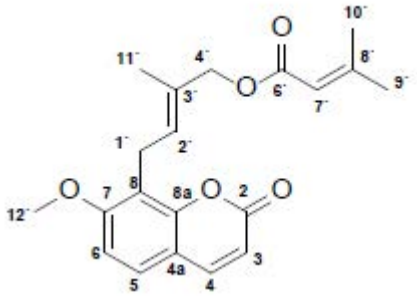


Figure S6. NOESY spectrum of **1** in $CDCl_3$ ($\delta H = 4.85$)



INDEX	FREQUENCY	PPM	HEIGHT
1	2763.5	5.530	52.8
2	2755.6	5.515	109.8
3	2747.8	5.499	53.2
4	859.5	1.720	10.7

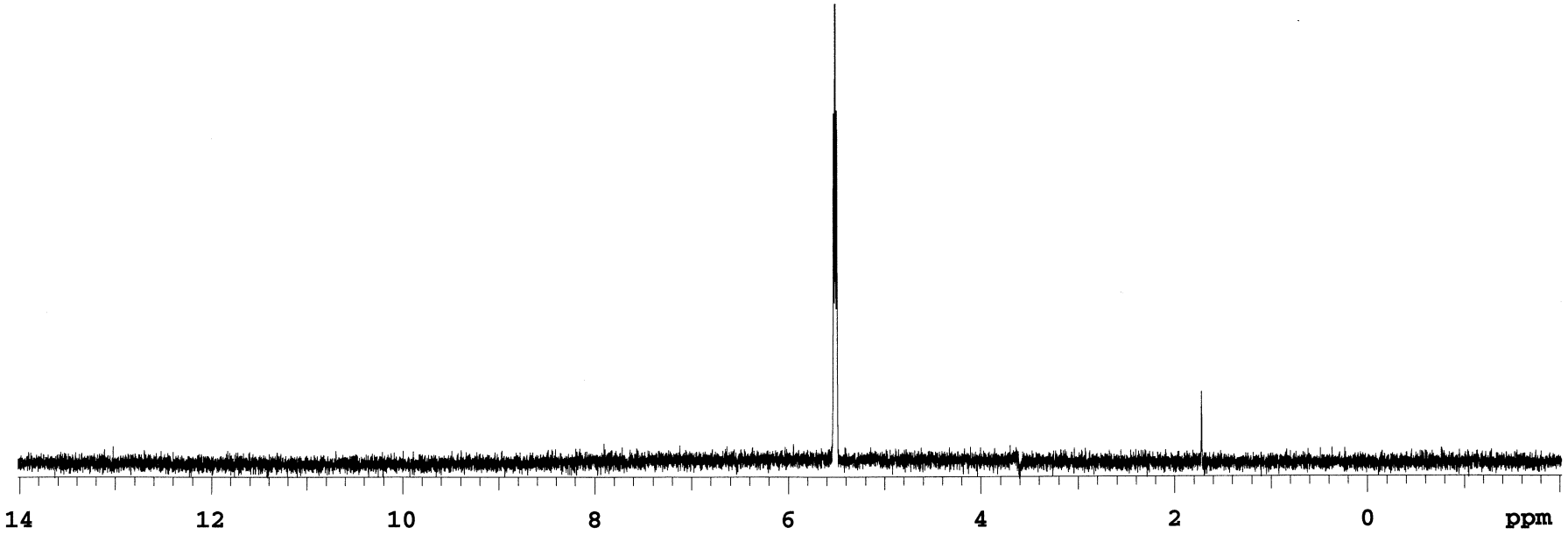


Figure S7. HR-ESITOFMS (positive) of **1**

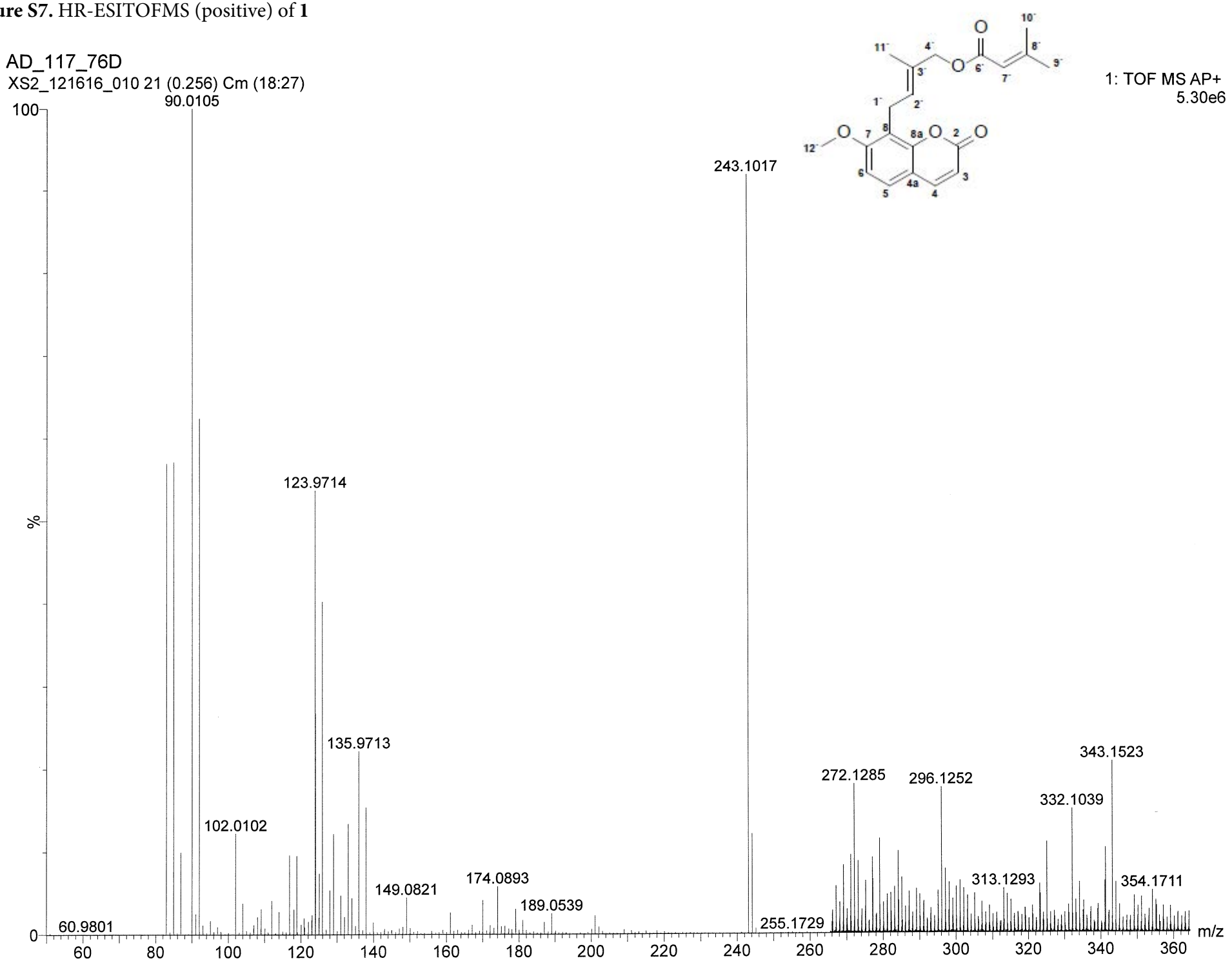
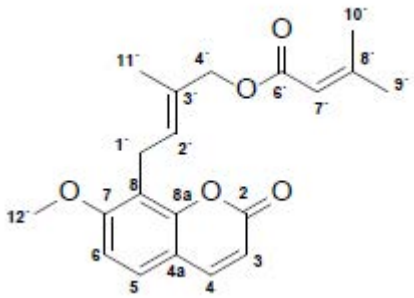


Figure S8. Elemental composition of **1** calculated by single mass analysis



Elemental Composition Report

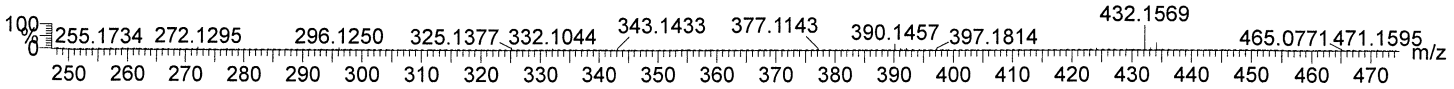
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-20 H: 0-60 O: 0-5

AD_117_76D
XS2_121616_010 21 (0.256)

1: TOF MS AP+
2.38e+004



Minimum:				-1.5				
Maximum:		10.0	10.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
343.1523	343.1545	-2.2	-6.4	9.5	226.9	n/a	n/a	C20 H23 O5

Figure S9. IR spectrum of **1** in KBr

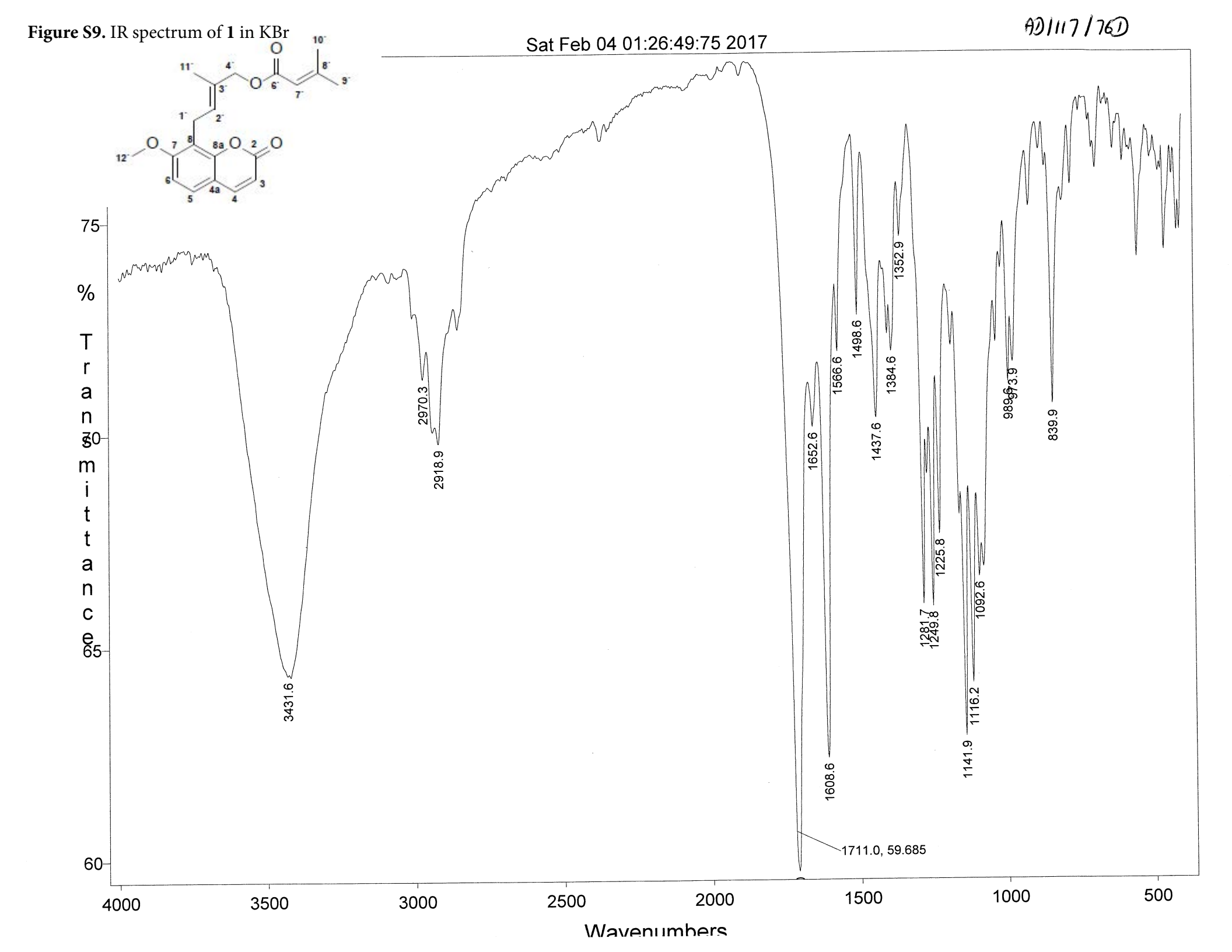


Figure S10. UV/Vis spectrum of **1** in methanol

Overlay Spectrum Graph Report

02/03/2017 12:27:14 PM

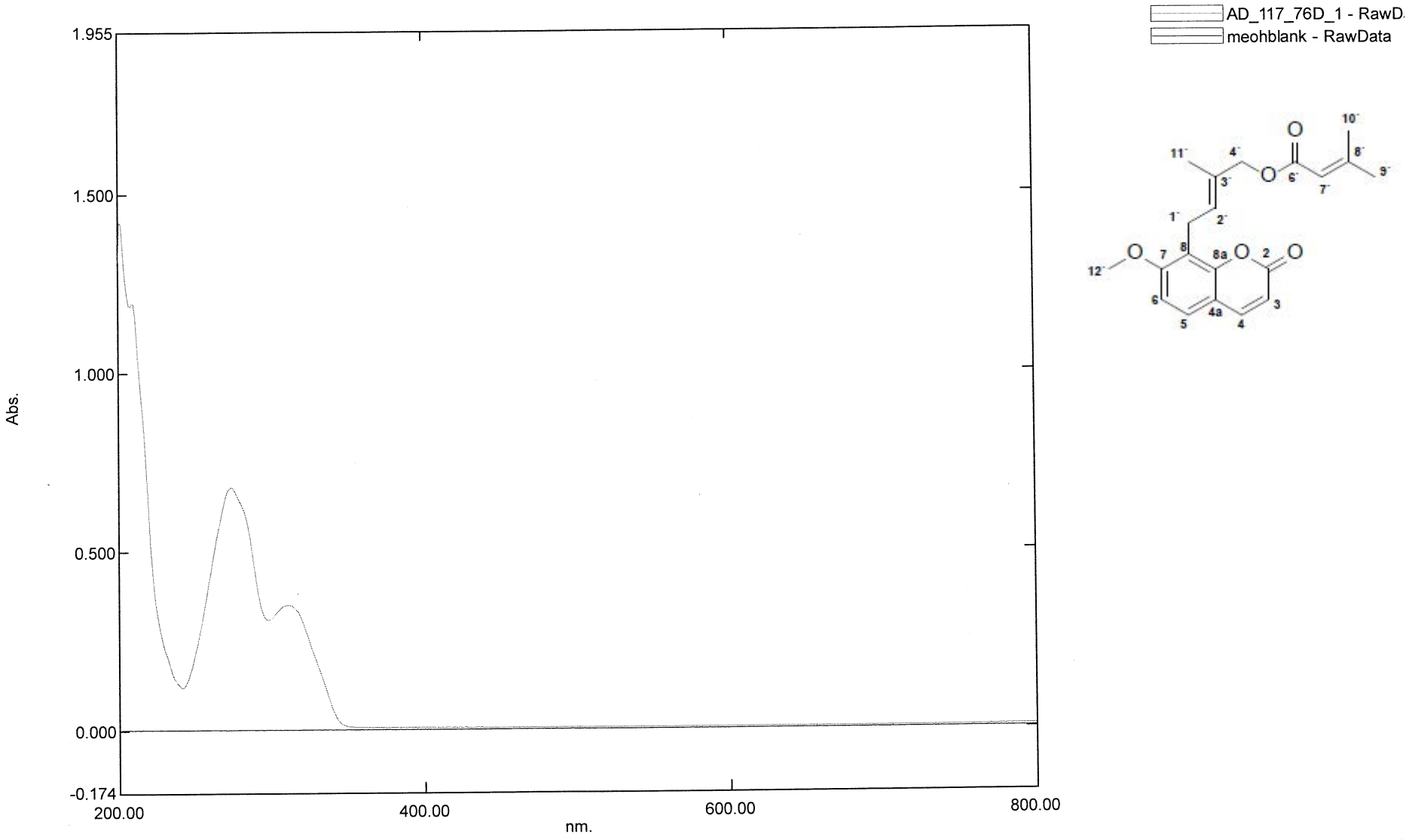
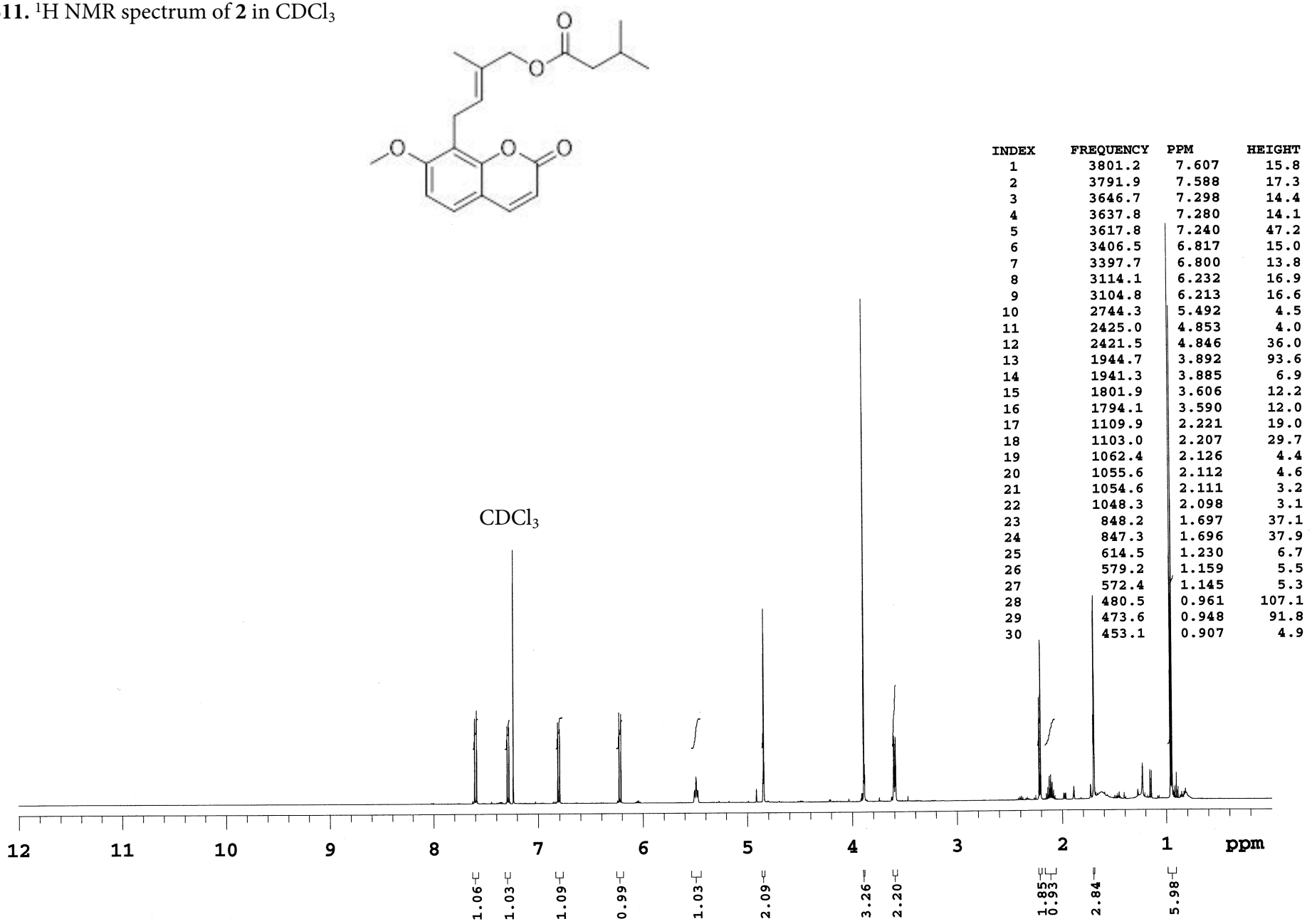
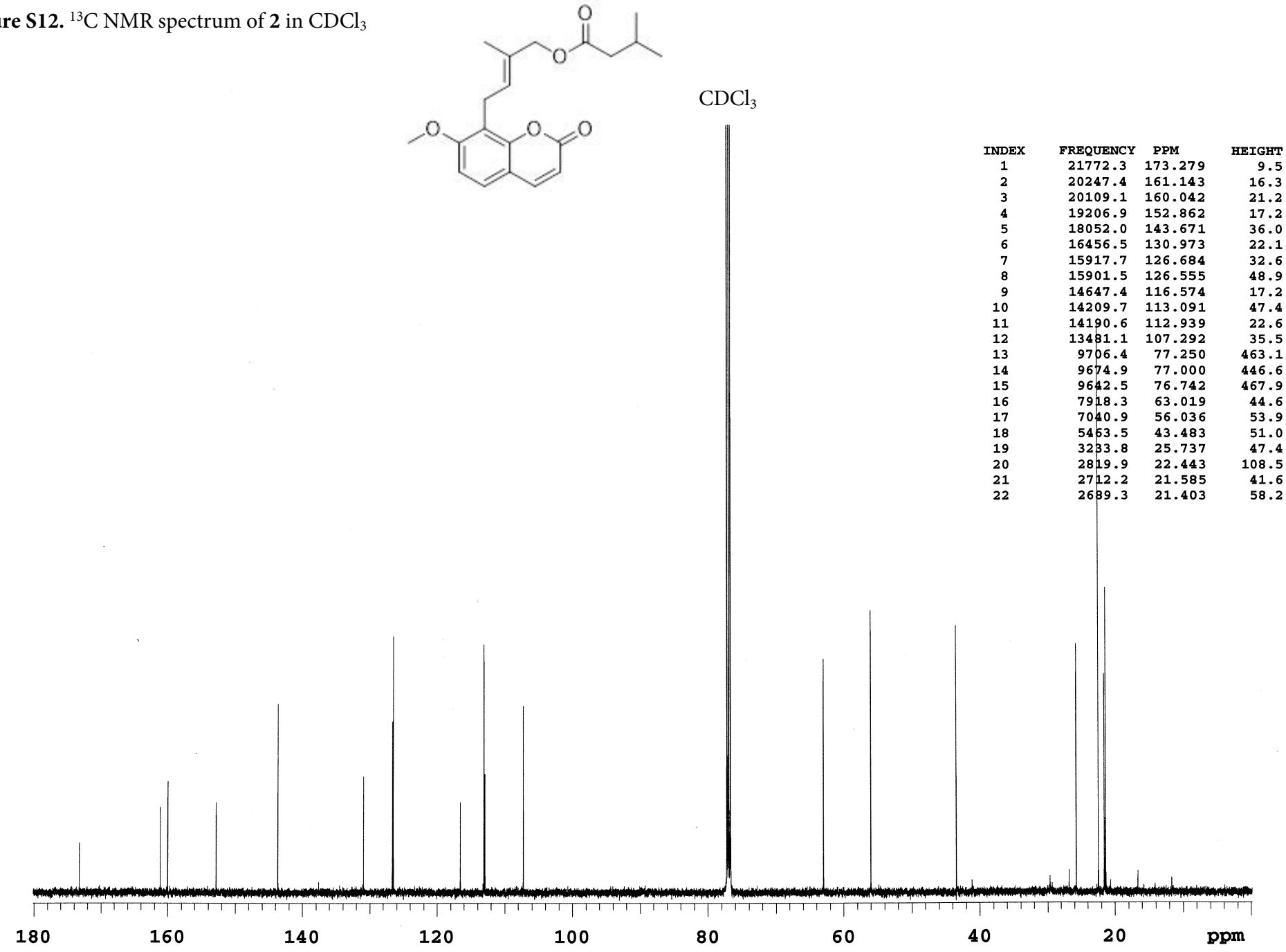


Figure S11. ^{1}H NMR spectrum of **2** in $CDCl_3$



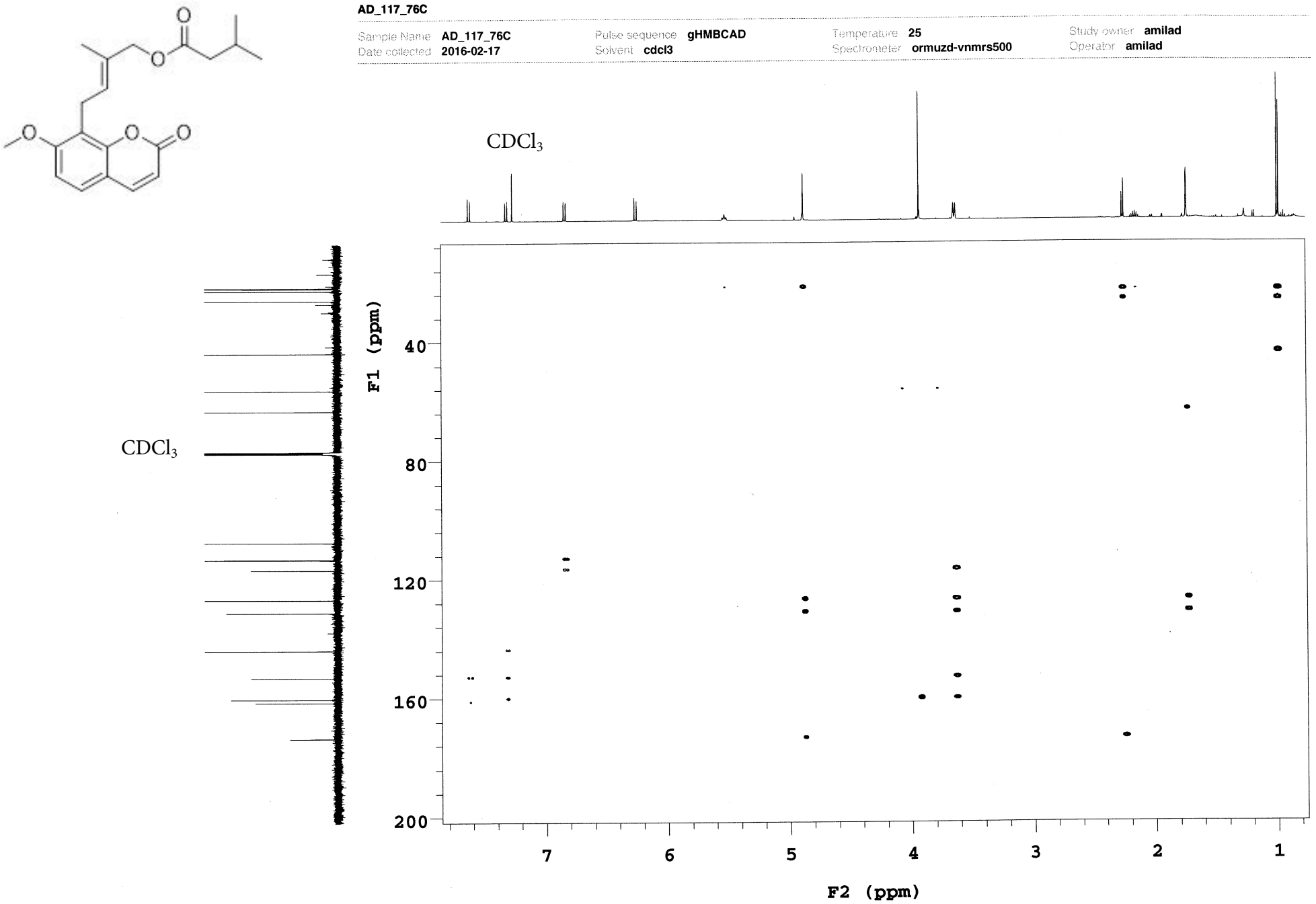
INDEX	FREQUENCY	PPM	HEIGHT
1	3801.2	7.607	15.8
2	3791.9	7.588	17.3
3	3646.7	7.298	14.4
4	3637.8	7.280	14.1
5	3617.8	7.240	47.2
6	3406.5	6.817	15.0
7	3397.7	6.800	13.8
8	3114.1	6.232	16.9
9	3104.8	6.213	16.6
10	2744.3	5.492	4.5
11	2425.0	4.853	4.0
12	2421.5	4.846	36.0
13	1944.7	3.892	93.6
14	1941.3	3.885	6.9
15	1801.9	3.606	12.2
16	1794.1	3.590	12.0
17	1109.9	2.221	19.0
18	1103.0	2.207	29.7
19	1062.4	2.126	4.4
20	1055.6	2.112	4.6
21	1054.6	2.111	3.2
22	1048.3	2.098	3.1
23	848.2	1.697	37.1
24	847.3	1.696	37.9
25	614.5	1.230	6.7
26	579.2	1.159	5.5
27	572.4	1.145	5.3
28	480.5	0.961	107.1
29	473.6	0.948	91.8
30	453.1	0.907	4.9

Figure S12. ^{13}C NMR spectrum of **2** in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	21772.3	173.279	9.5
2	20247.4	161.143	16.3
3	20109.1	160.042	21.2
4	19206.9	152.862	17.2
5	18052.0	143.671	36.0
6	16456.5	130.973	22.1
7	15917.7	126.684	32.6
8	15901.5	126.555	48.9
9	14647.4	116.574	17.2
10	14209.7	113.091	47.4
11	14190.6	112.939	22.6
12	13481.1	107.292	35.5
13	9706.4	77.250	463.1
14	9674.9	77.000	446.6
15	9642.5	76.742	467.9
16	7918.3	63.019	44.6
17	7040.9	56.036	53.9
18	5463.5	43.483	51.0
19	3233.8	25.737	47.4
20	2819.9	22.443	108.5
21	2712.2	21.585	41.6
22	2689.3	21.403	58.2

Figure S13. HMBC spectrum of **2** in $CDCl_3$



Data file /net/ormuzd/home/walkup/vnmrsys/data/amilad/AD_117_76C_20160217_01/AD_117_76C_gHMBCAD_01.fid

Plot date 2016-02-18

Figure S14. NOESY spectrum of **2** in $CDCl_3$ (δH = 4.84)

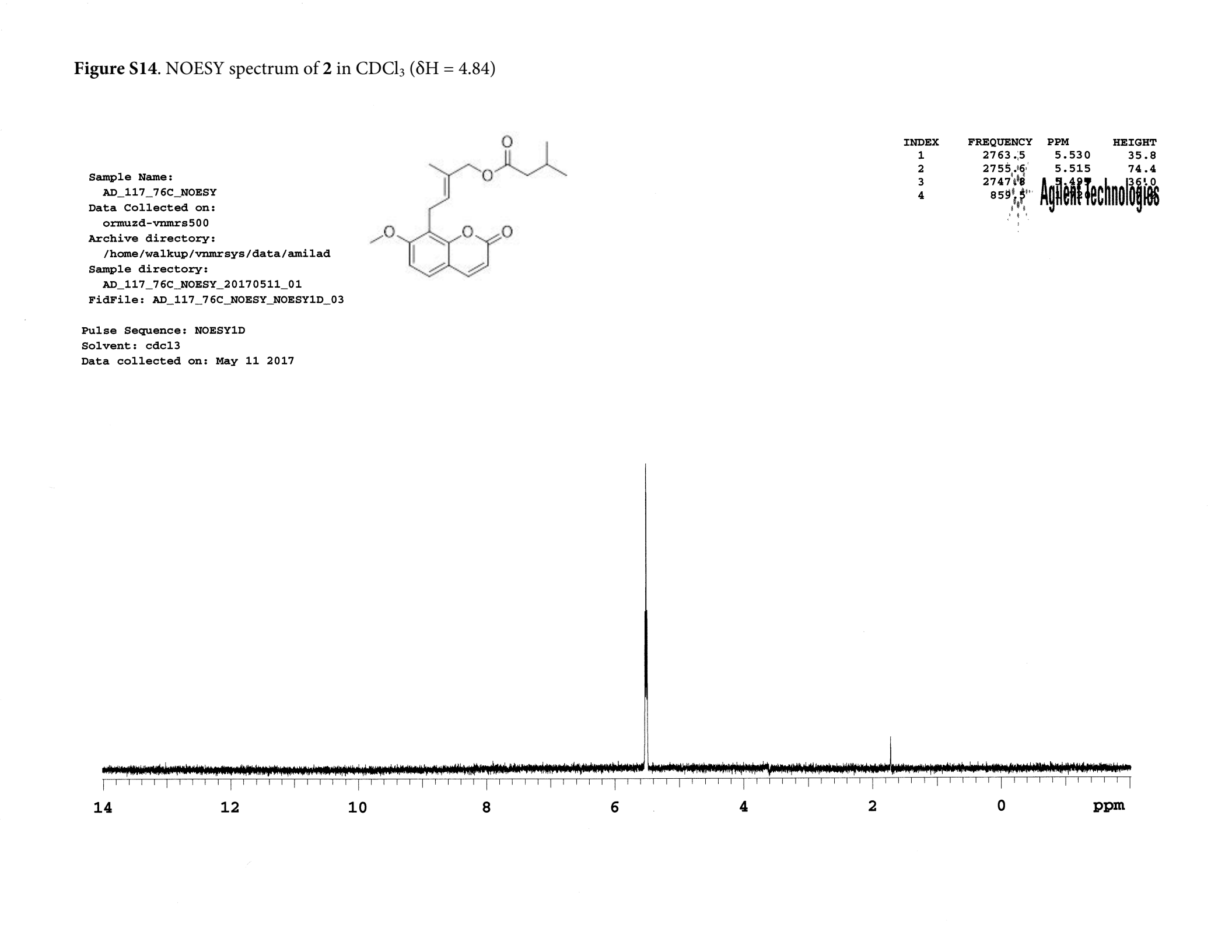


Figure S15. HR-ESITOFMS (positive) of **2**

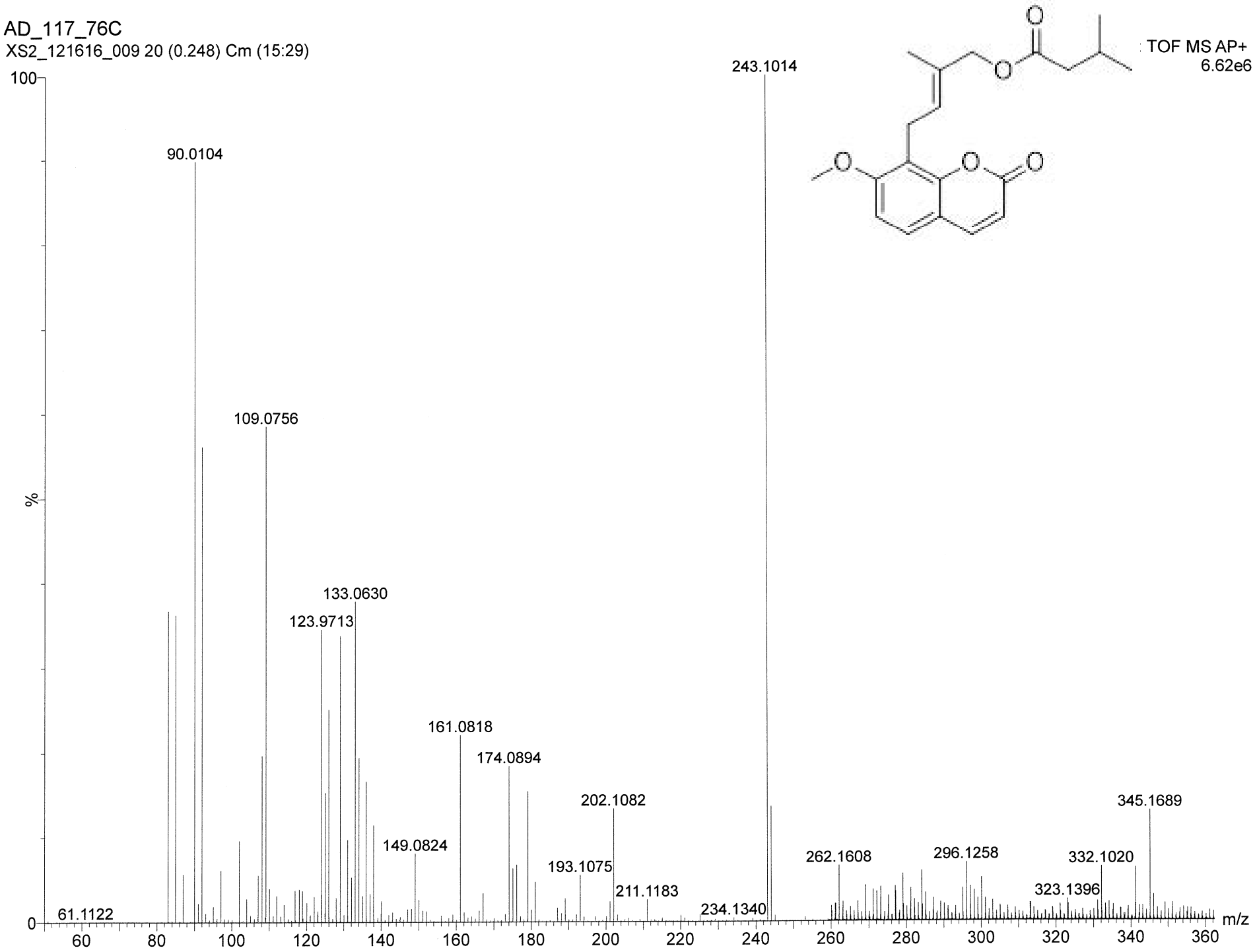
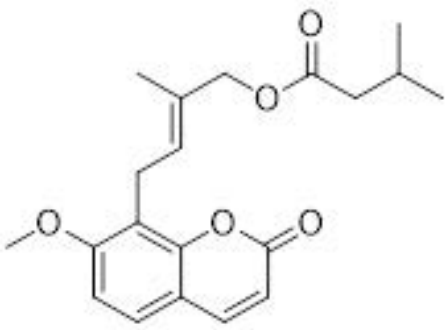


Figure S16. Elemental composition of **2** calculated by single mass analysis

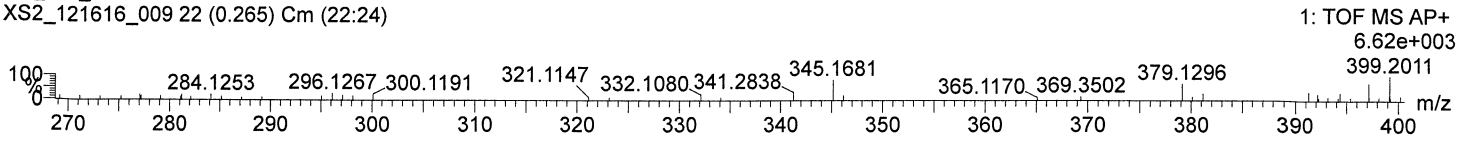


Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: On (Carbon range ± 5) (Set 0 < Cl < 9, 0< Br < 9 and 0 < S < 7 for
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-50 O: 0-5
AD_117_76C
XS2_121616_009 22 (0.265) Cm (22:24)



Minimum:				-1.5				
Maximum:		10.0	10.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
345.1689	345.1702	-1.3	-3.8	8.5	25.0	n/a	n/a	C20 H25 O5

Figure S17. IR spectrum of **2** in KBr

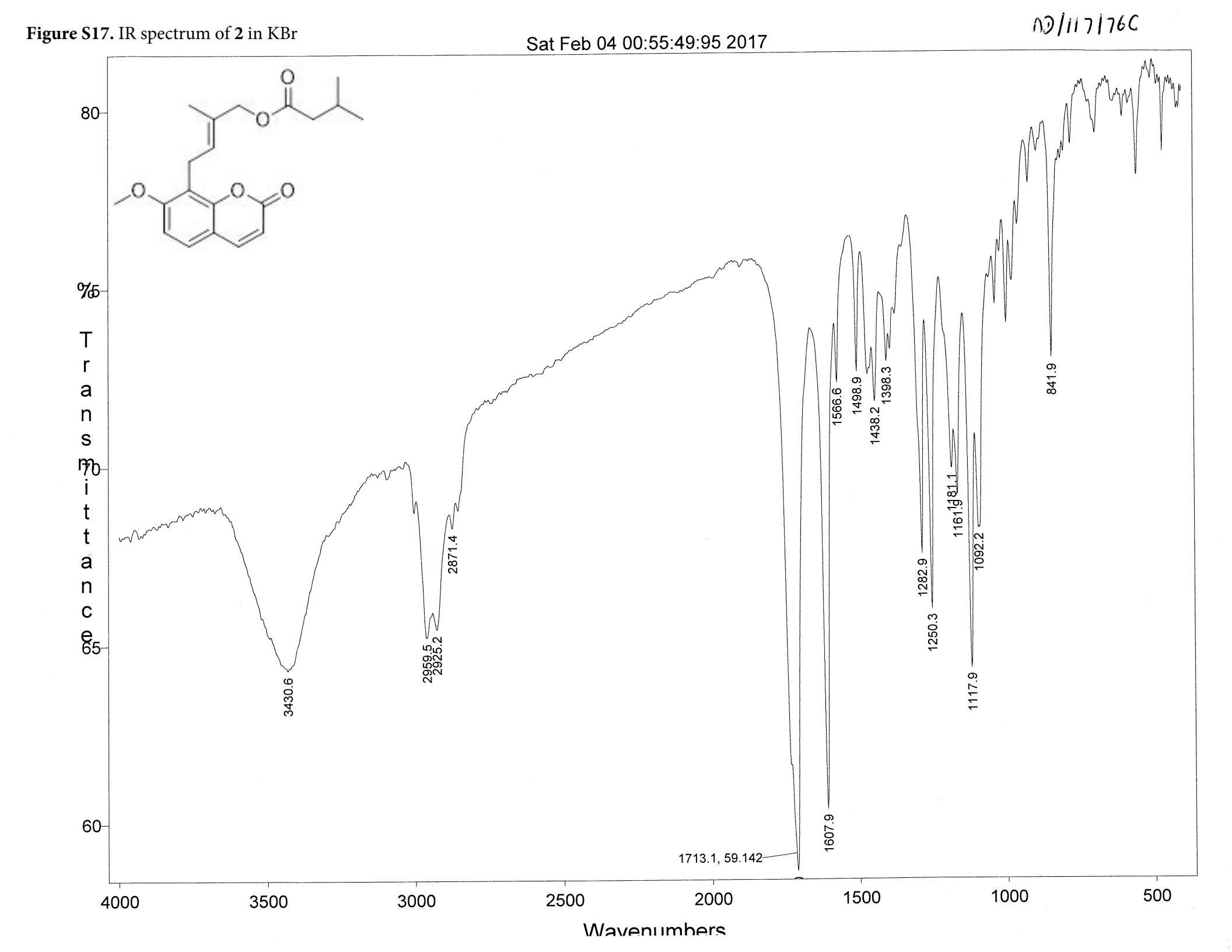


Figure S18. UV/Vis spectrum of **2** in methanol

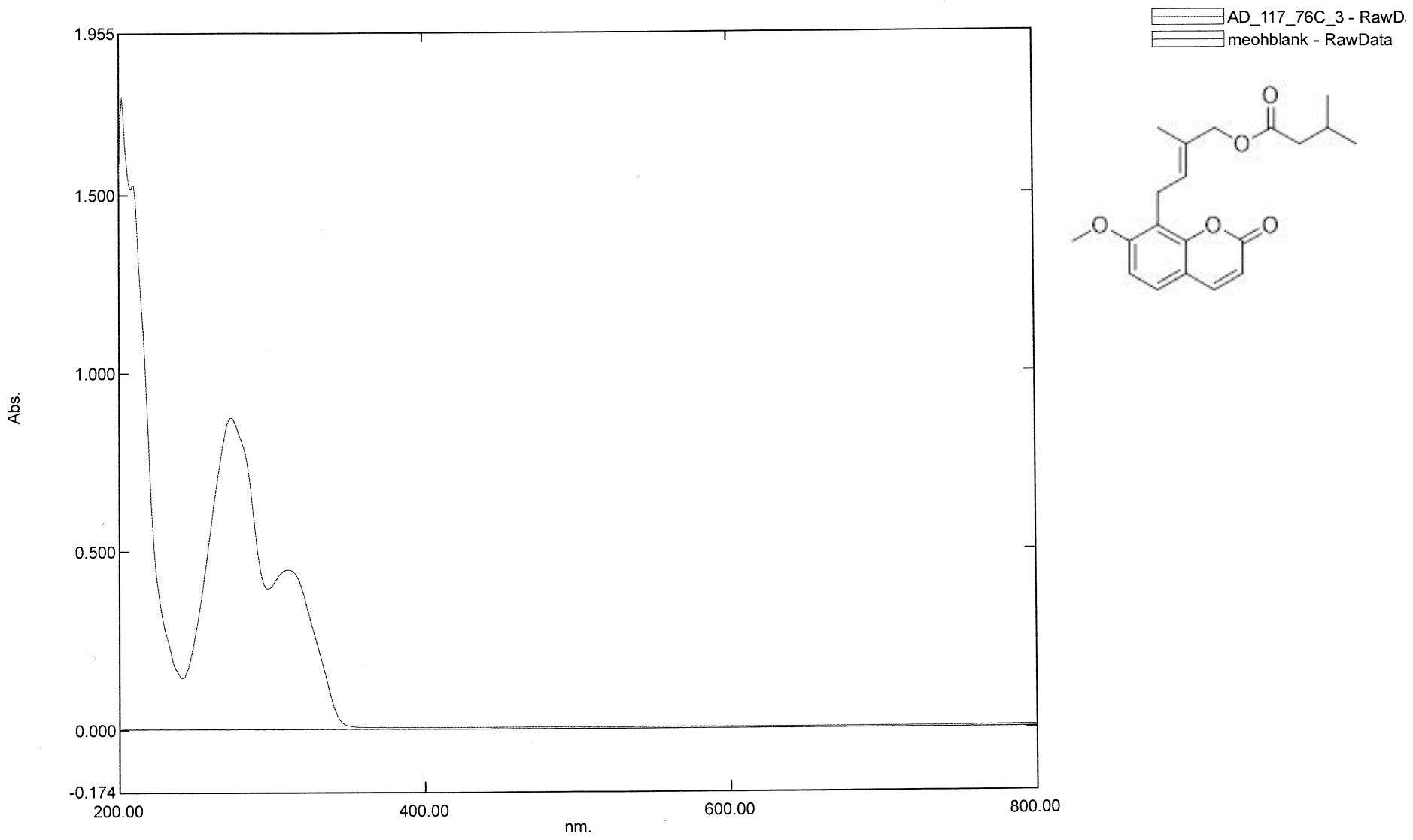
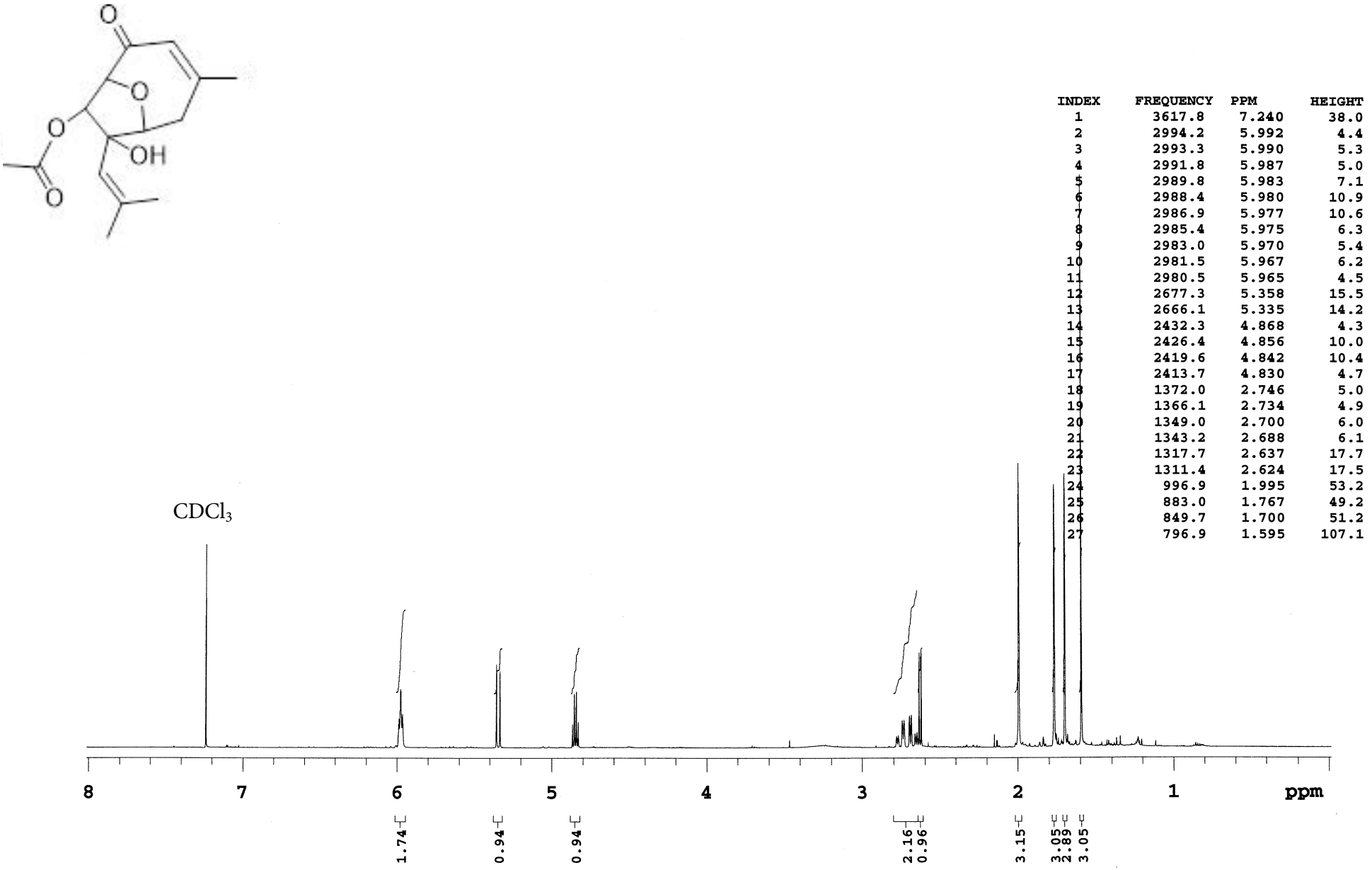
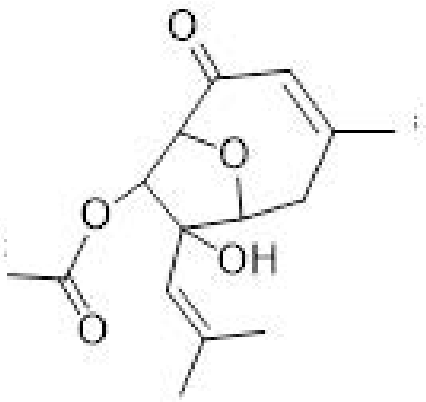


Figure S19. ^{1}H NMR spectrum of **3** in $CDCl_3$



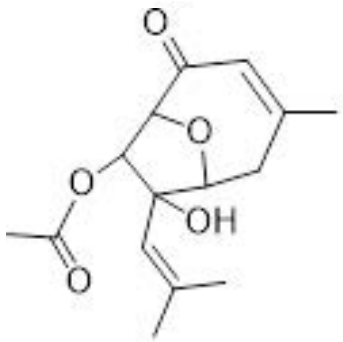
INDEX	FREQUENCY	PPM	HEIGHT
1	3617.8	7.240	38.0
2	2994.2	5.992	4.4
3	2993.3	5.990	5.3
4	2991.8	5.987	5.0
5	2989.8	5.983	7.1
6	2988.4	5.980	10.9
7	2986.9	5.977	10.6
8	2985.4	5.975	6.3
9	2983.0	5.970	5.4
10	2981.5	5.967	6.2
11	2980.5	5.965	4.5
12	2677.3	5.358	15.5
13	2666.1	5.335	14.2
14	2432.3	4.868	4.3
15	2426.4	4.856	10.0
16	2419.6	4.842	10.4
17	2413.7	4.830	4.7
18	1372.0	2.746	5.0
19	1366.1	2.734	4.9
20	1349.0	2.700	6.0
21	1343.2	2.688	6.1
22	1317.7	2.637	17.7
23	1311.4	2.624	17.5
24	996.9	1.995	53.2
25	883.0	1.767	49.2
26	849.7	1.700	51.2
27	796.9	1.595	107.1

Figure S20. ^{13}C NMR spectrum of **3** in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	24746.0	196.865	21.8
2	20126.4	160.114	21.8
3	19880.4	158.157	33.6
4	16669.4	132.612	27.2
5	15989.4	127.202	48.7
6	14794.4	117.696	78.0
7	11856.2	94.321	73.1
8	9875.4	78.563	53.4
9	9710.4	77.250	376.0
10	9704.7	77.205	22.0
11	9678.9	77.000	396.6
12	9646.5	76.742	380.8
13	9567.3	76.112	81.8
14	6729.2	53.534	73.7
15	4384.1	34.878	77.6
16	3440.0	27.367	55.9
17	3274.1	26.046	77.0
18	3095.7	24.628	68.8
19	2286.0	18.186	68.4

Figure S21. DEPT spectrum of **3** in $CDCl_3$



AD_117_73C

Sample Name **AD_117_73C**	Pulse sequence **DEPT**	Temperature **25**	Study owner **amilad**
Date collected **2016-01-24**	Solvent **cdcl3**	Spectrometer **agilentNMR-inova500**	Operator **process**

CH3 carbons

CH2 carbons

CH carbons

quaternary carbons

$CDCl_3$

220 200 180 160 140 120 100 80 60 40 20 0 ppm

Data file /net/ahriman/home/walkup/vnmrsys/data/amilad/AD_117_73C_20160123_01/AD_117_73C_DEPT_01.fid

Plot date 2016-01-25

Figure S22. HSQC spectrum of **3** in $CDCl_3$

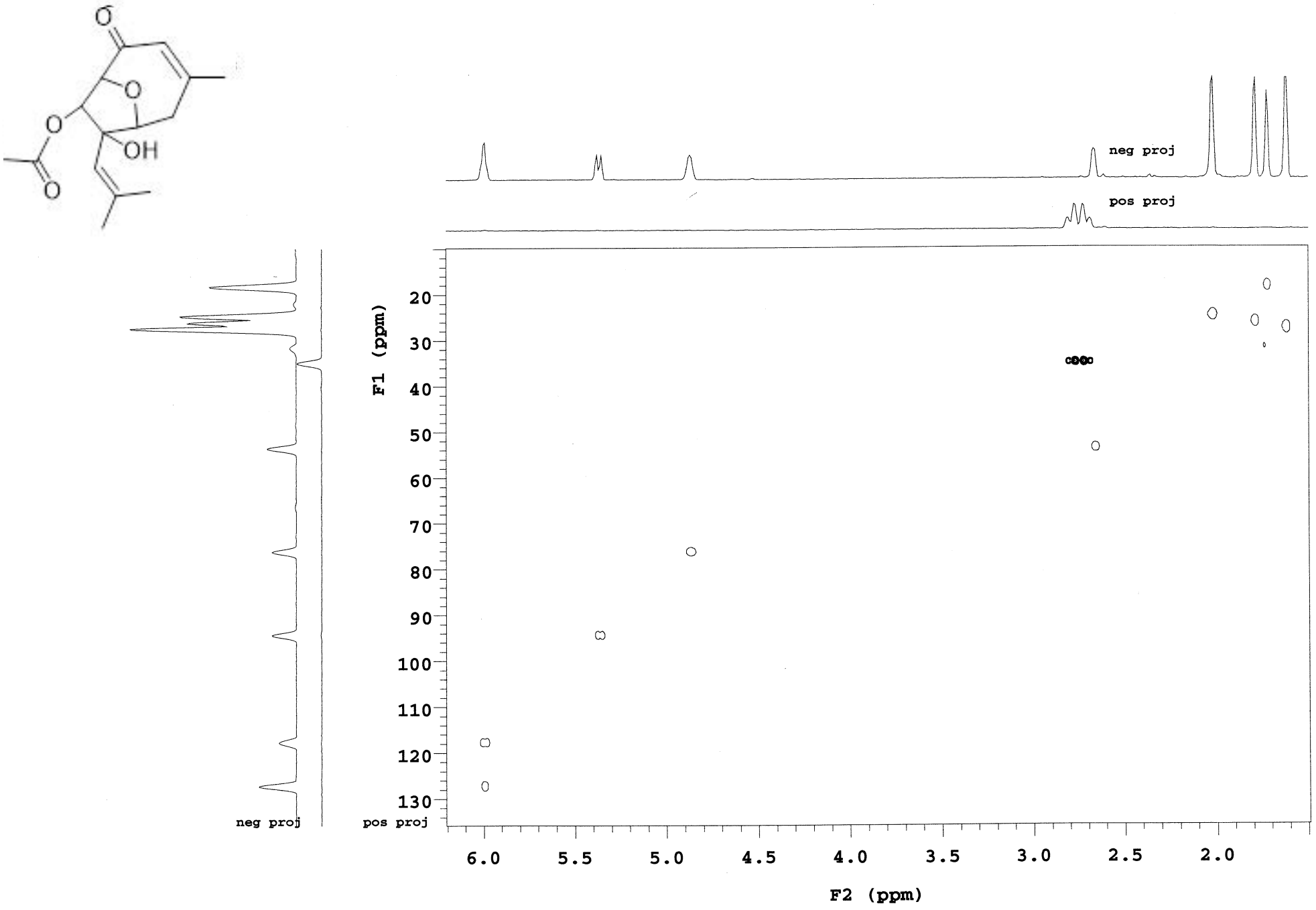
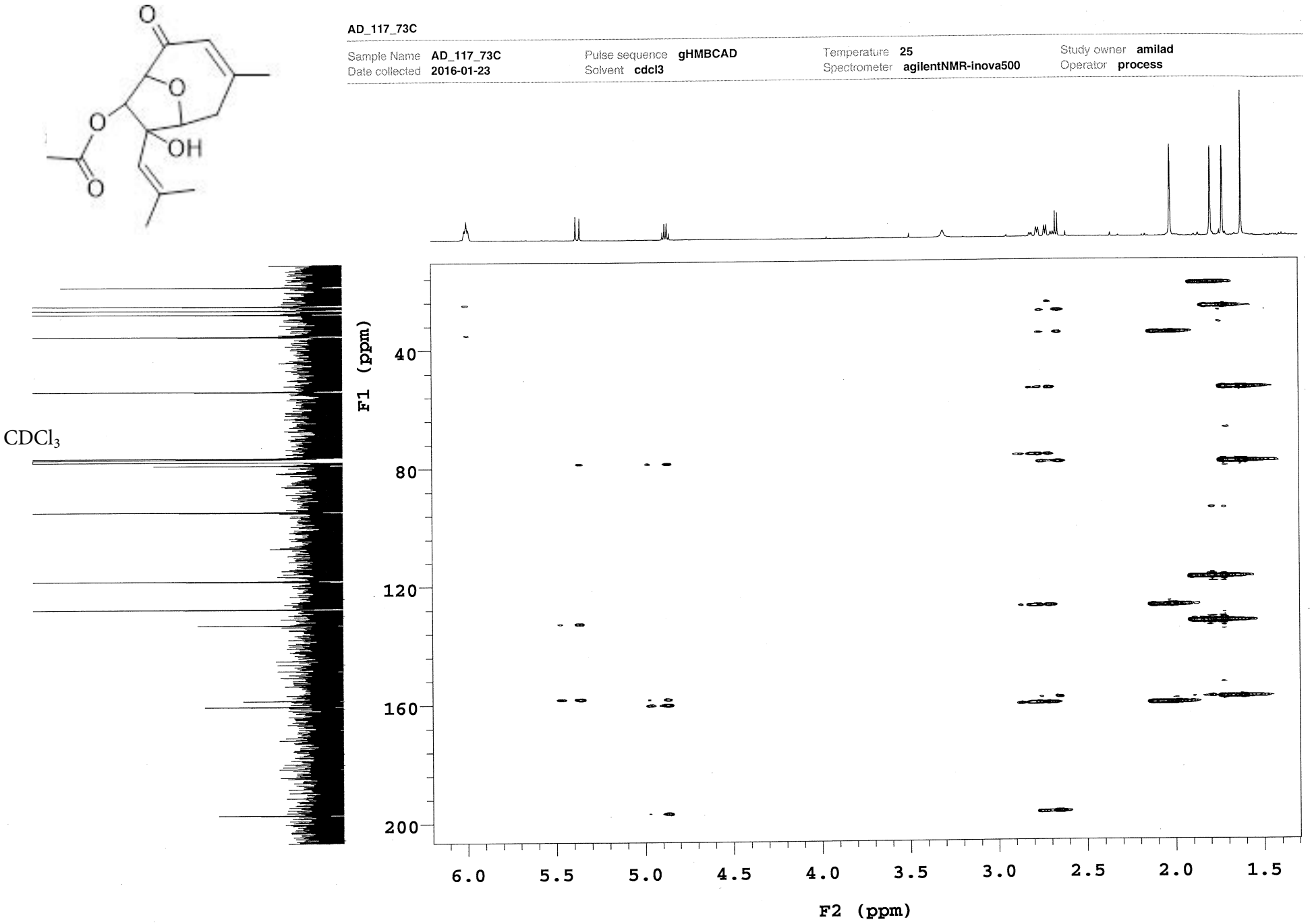


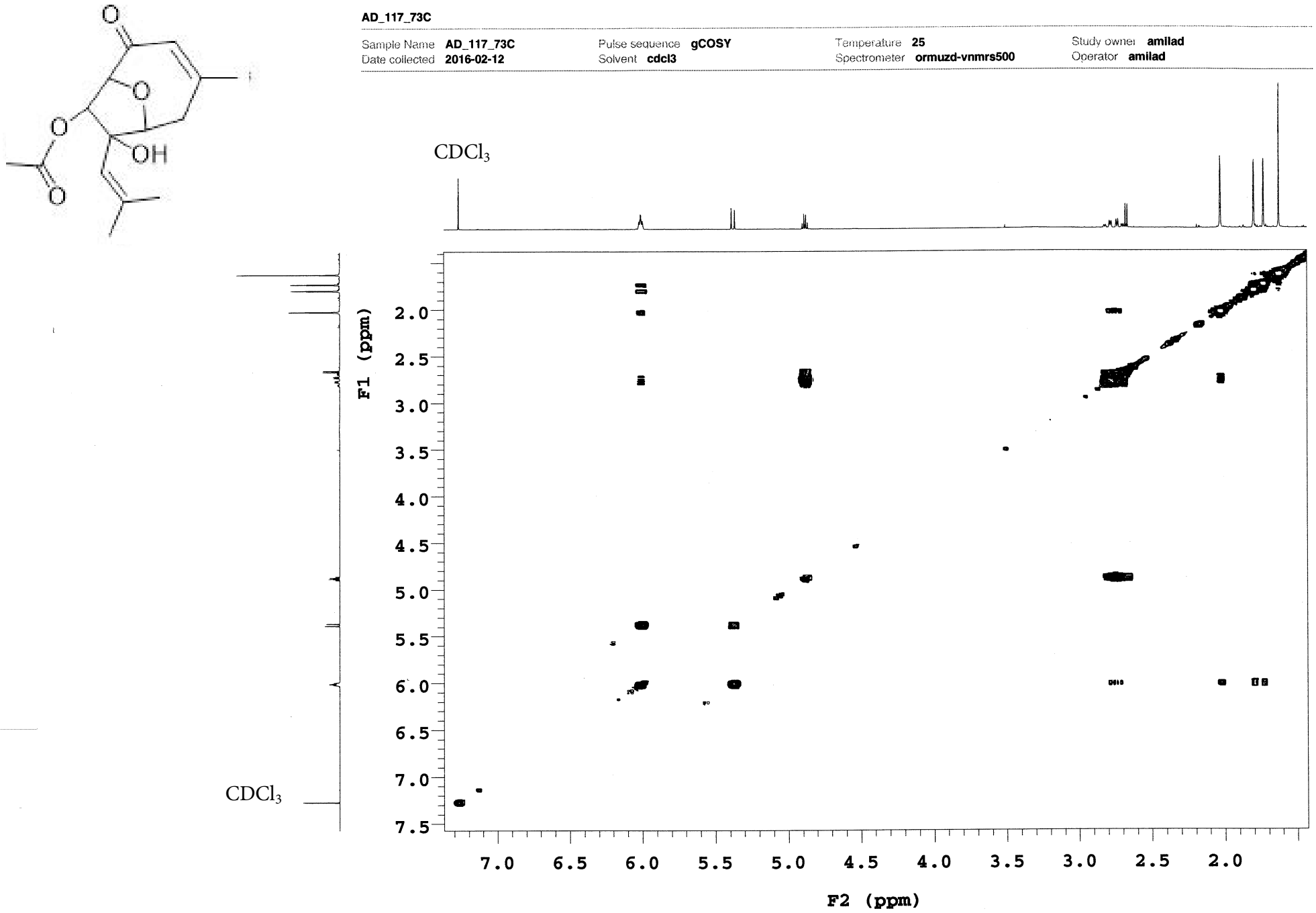
Figure S23. HMBC spectrum of **3** in $CDCl_3$



Data file /net/ahriman/home/walkup/vnmrsys/data/amilad/AD_117_73C_20160123_01/AD_117_73C_gHMBCAD_01.fid

Plot date 2016-01-25

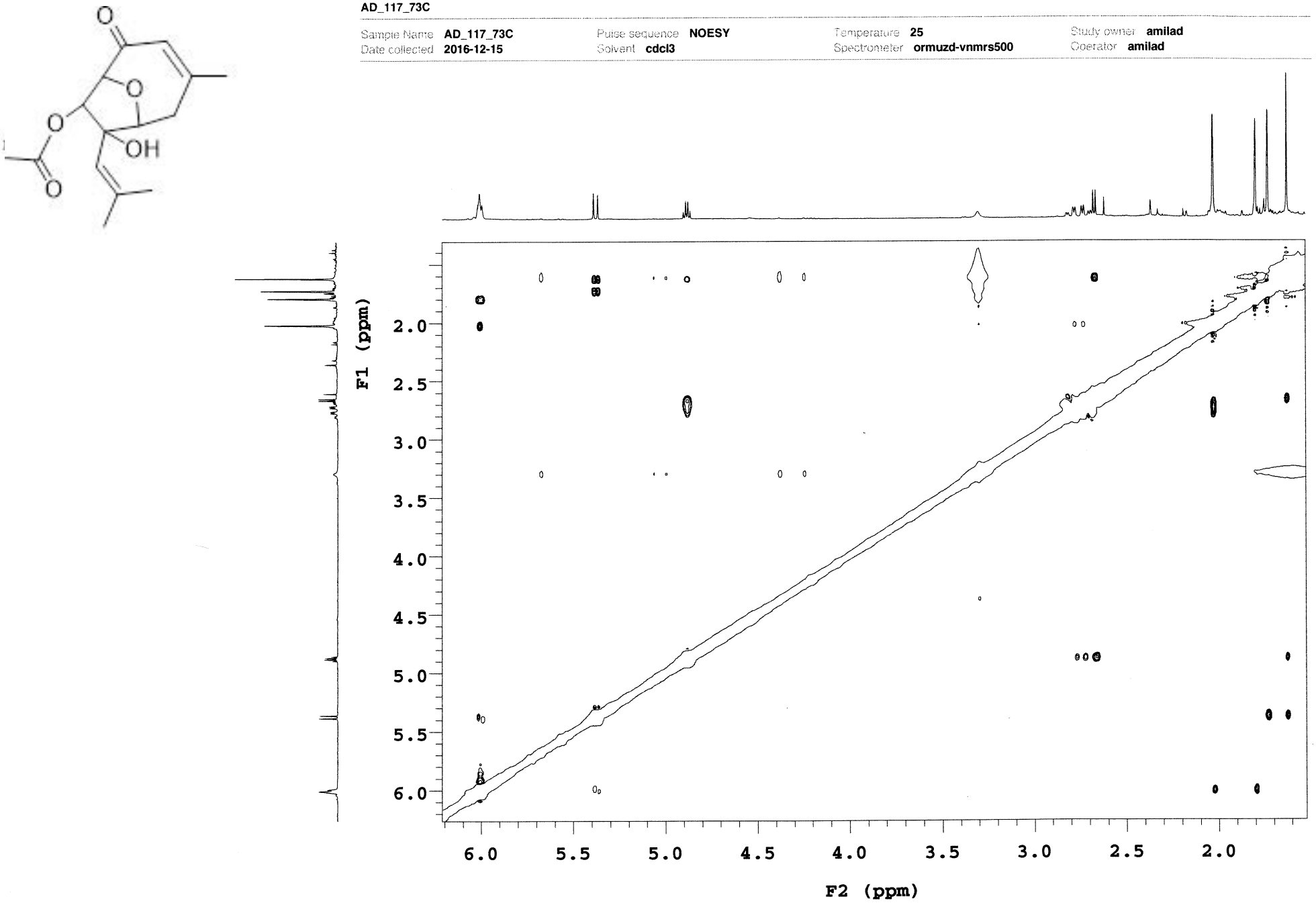
Figure S24. $^{1}H-^{1}H$ COSY spectrum of **3** in $CDCl_3$



Data file /net/ormuzd/home/walkup/vnmrsys/data/amilad/AD_117_73C_20160212_01/AD_117_73C_gCOSY_01.fid

Plot date 2016-02-12

Figure S25. NOESY spectrum of 3 **in $CDCl_3$**



Data file /net/ormuzd/home/walkup/vnmrsys/data/amilad/AD_117_73C_20161215_01/AD_117_73C_NOESY_01.fid

Plot date 2016-12-19

Figure S26. HR-ESITOFMS (positive) of **3**

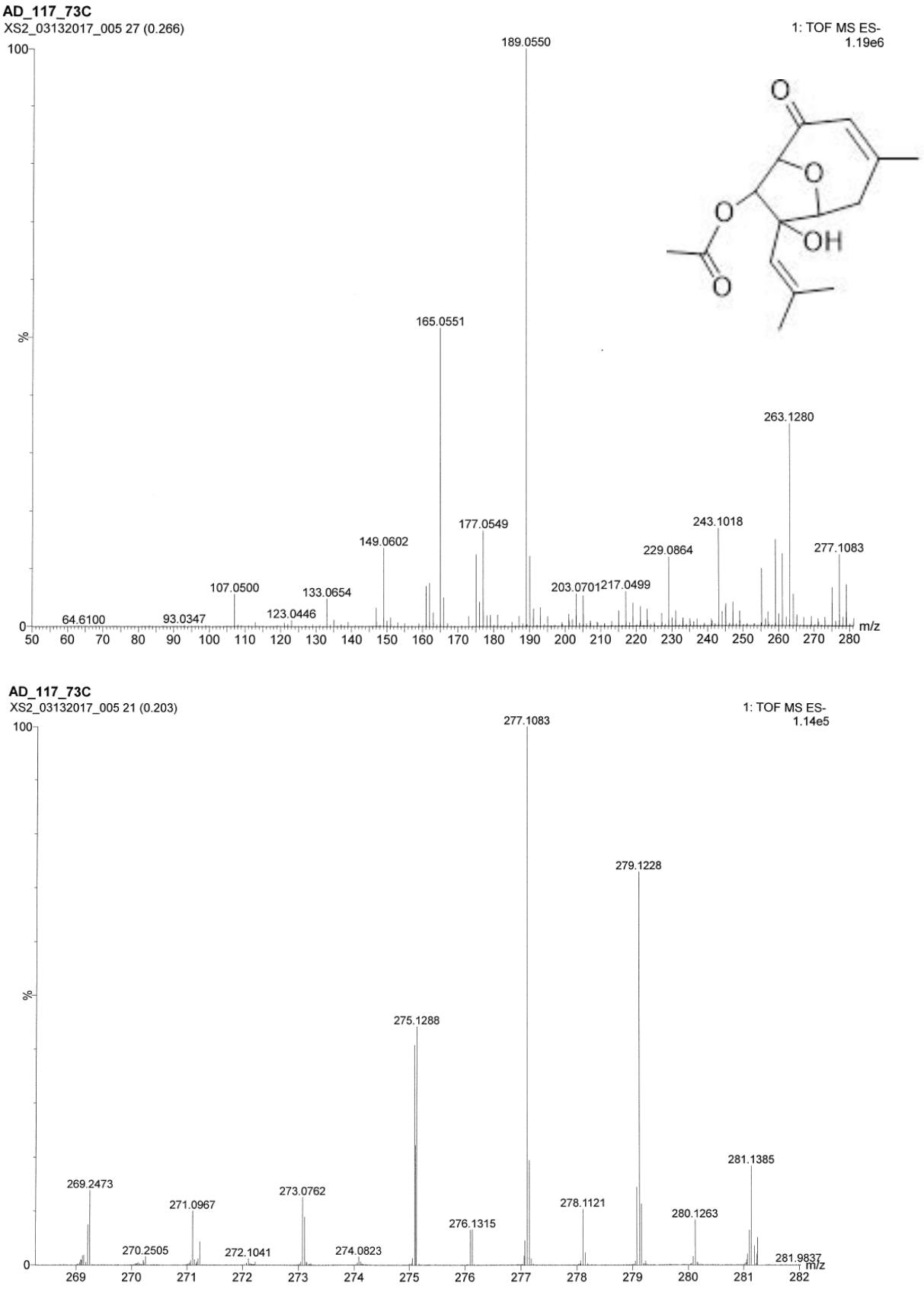
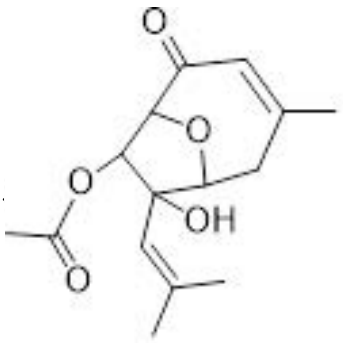


Figure S27. Elemental composition of **3** calculated by single mass analysis



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: On (Carbon range ± 5) (Set 0 < Cl < 9, 0< Br < 9 and 0 < S < 7 for enhanced

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

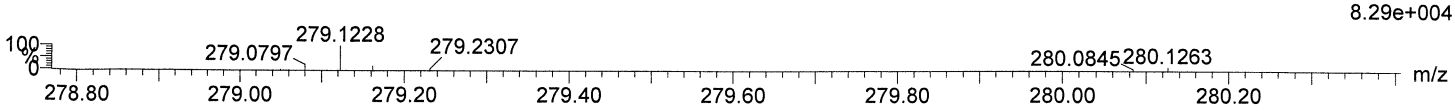
Elements Used:

C: 0-30 H: 0-60 O: 0-8

AD_117_73C

XS2_03132017_005 21 (0.203)

1: TOF MS ES-
8.29e+004



Minimum:				-1.5				
Maximum:		10.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
279.1228	279.1232	-0.4	-1.4	6.5	77.8	n/a	n/a	C15 H19 O5

Figure S28. IR spectrum of **3** in KBr

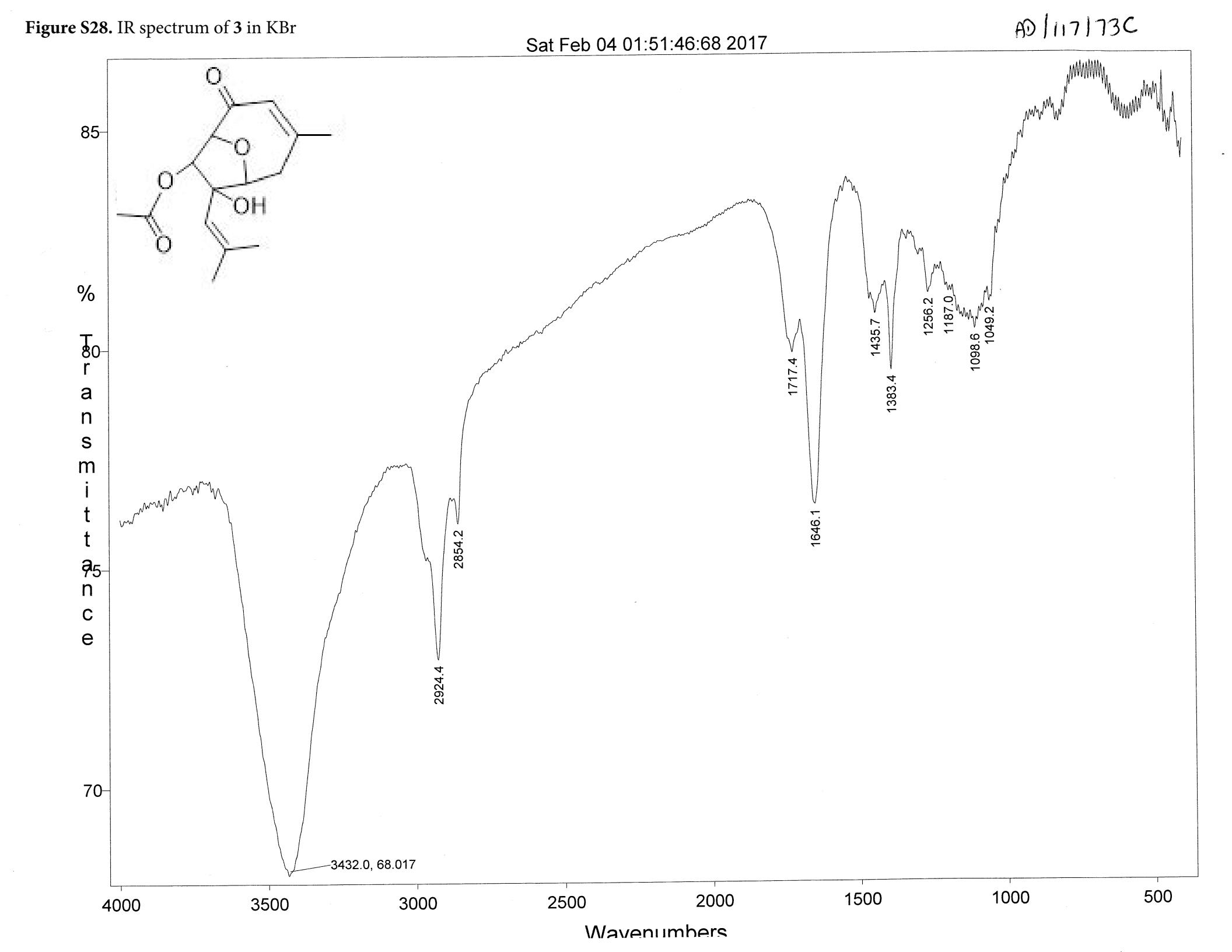


Figure S29. UV/Vis spectrum of **3** in methanol

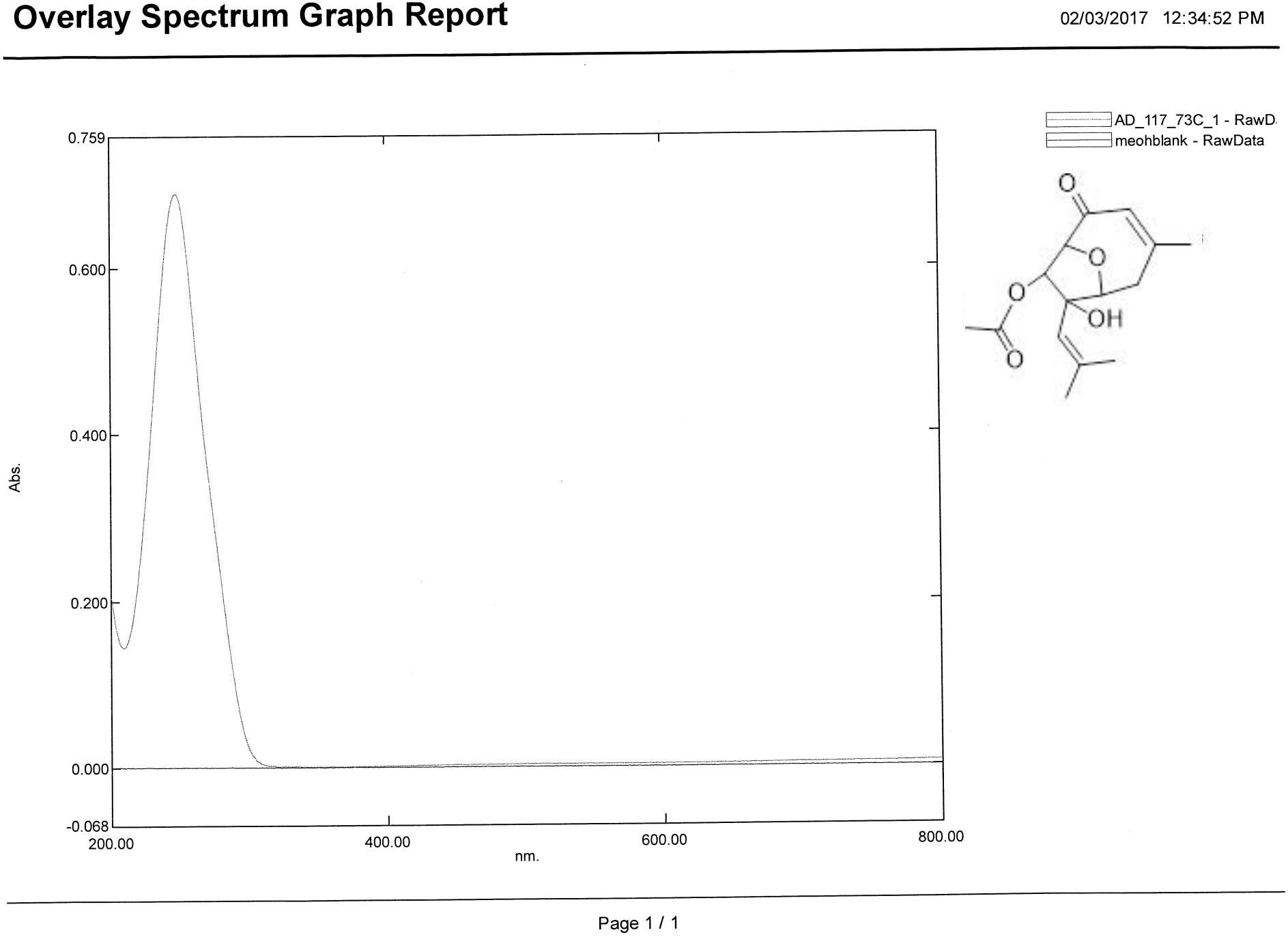


Figure S30. 1H NMR spectrum of **4** in D_2O

INDEX	FREQUENCY	PPM	HEIGHT
1	1858.6	3.719	5.9
2	1849.8	3.702	9.9
3	1844.4	3.691	4.7
4	1820.5	3.643	31.9
5	1816.6	3.635	31.2
6	980.3	1.962	5.1
7	977.8	1.957	5.3
8	975.4	1.952	5.4
9	972.9	1.947	5.3
10	859.5	1.720	4.8
11	849.2	1.699	8.0
12	847.7	1.696	5.5
13	845.3	1.692	5.4
14	841.4	1.684	7.2
15	839.9	1.681	6.0
16	837.9	1.677	5.1
17	836.5	1.674	5.7
18	834.5	1.670	7.4
19	827.2	1.655	5.8
20	734.3	1.469	4.6
21	729.4	1.460	5.2
22	726.9	1.455	5.2
23	721.1	1.443	7.1
24	716.2	1.433	6.0
25	713.2	1.427	6.5
26	708.3	1.418	5.7
27	630.6	1.262	5.8
28	623.2	1.247	7.1
29	621.3	1.243	5.9
30	617.4	1.235	5.4
31	614.0	1.229	6.5
32	610.0	1.221	5.4
33	608.1	1.217	5.0
34	494.1	0.989	83.7
35	487.3	0.975	90.8
36	472.1	0.945	33.7
37	466.3	0.933	64.3
38	462.3	0.925	57.6
39	459.9	0.920	32.5
40	455.0	0.911	95.4
41	447.7	0.896	40.0

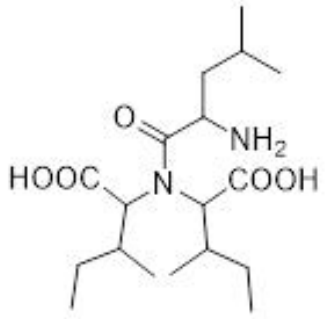
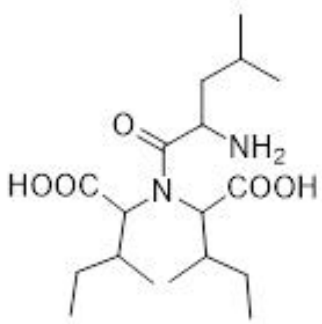


Figure S31. ^{13}C NMR spectrum of **4** in D_2O



INDEX	FREQUENCY	PPM	HEIGHT
1	22050.6	175.494	16.2
2	21873.7	174.086	29.6
3	7466.8	59.426	72.0
4	6695.7	53.289	35.9
5	4985.6	39.679	48.1
6	4494.2	35.768	94.9
7	3056.0	24.322	92.8
8	3019.6	24.032	54.8
9	2751.1	21.895	54.1
10	2604.5	20.728	53.9
11	1829.1	14.558	94.5
12	1378.3	10.969	104.5

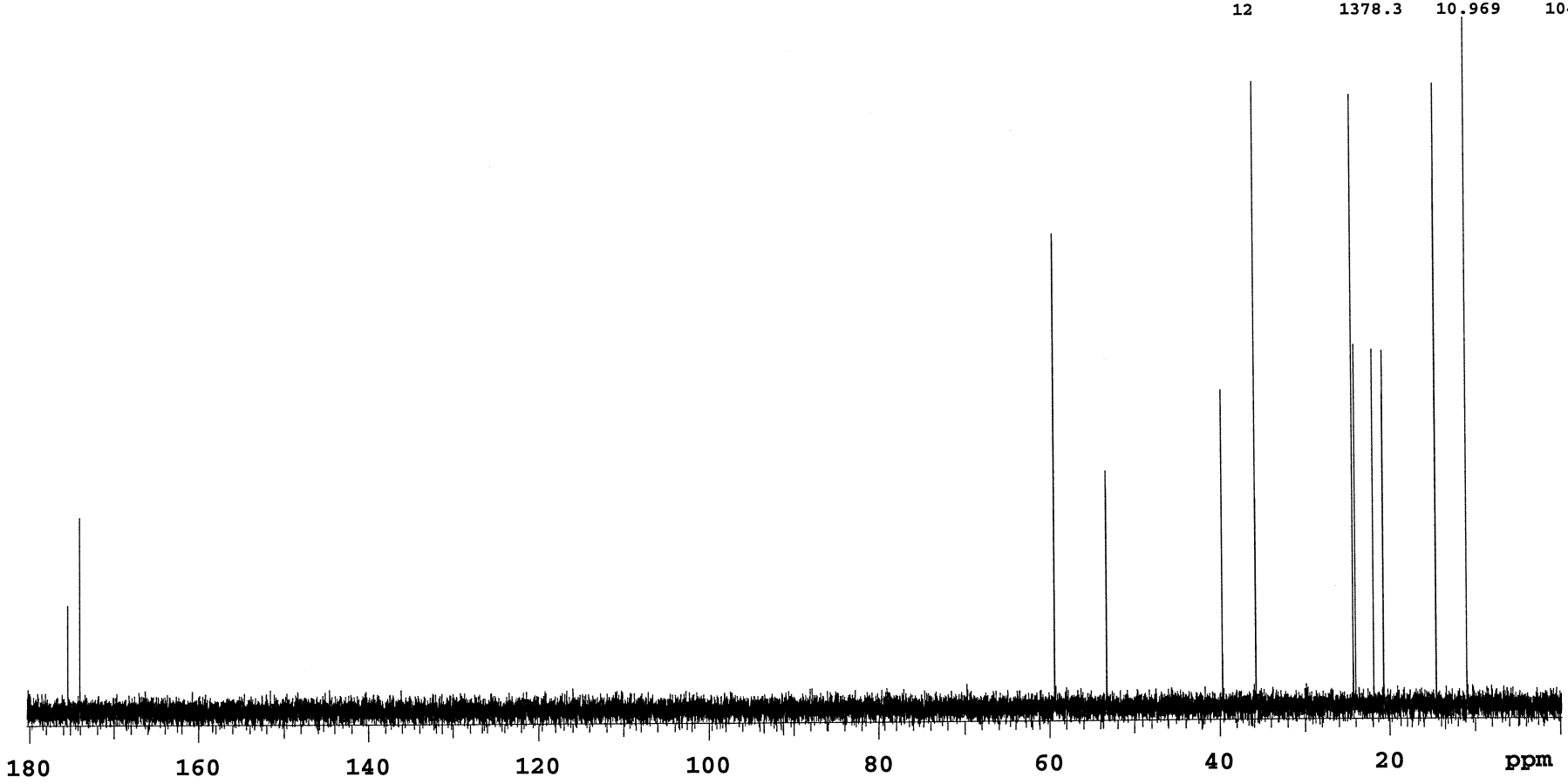
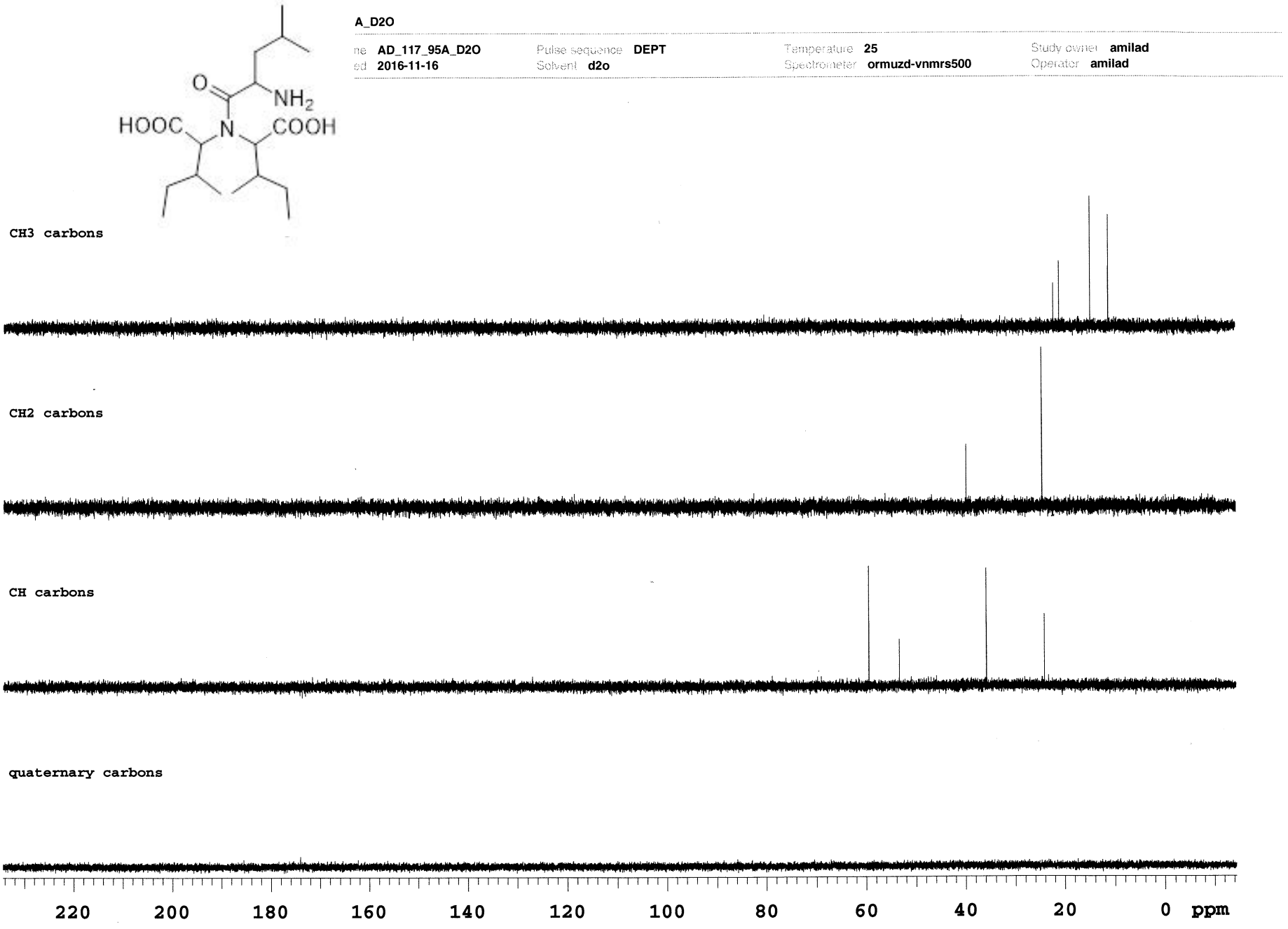


Figure S32. DEPT spectrum of **4** in D_2O



Data file /net/ormuzd/home/walkup/vnmrsys/data/amilad/AD_117_95A_D2O_20161116_02/AD_117_95A_D2O_DEPT_01.fid

Plot date 2016-11-17

Figure S33. HSQC spectrum of **4** in D_2O

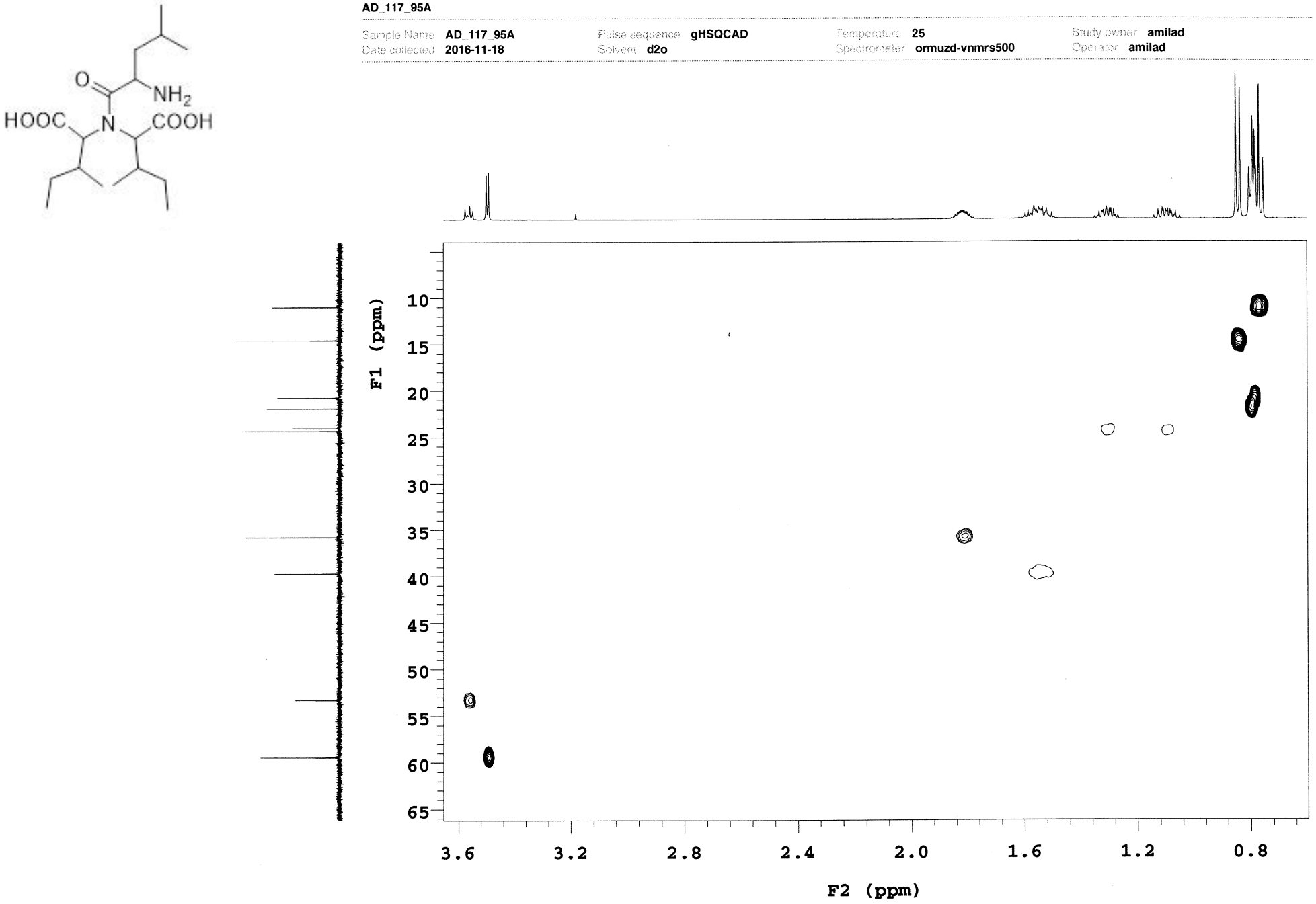


Figure S34. HR-ESITOFMS (positive) of **4**

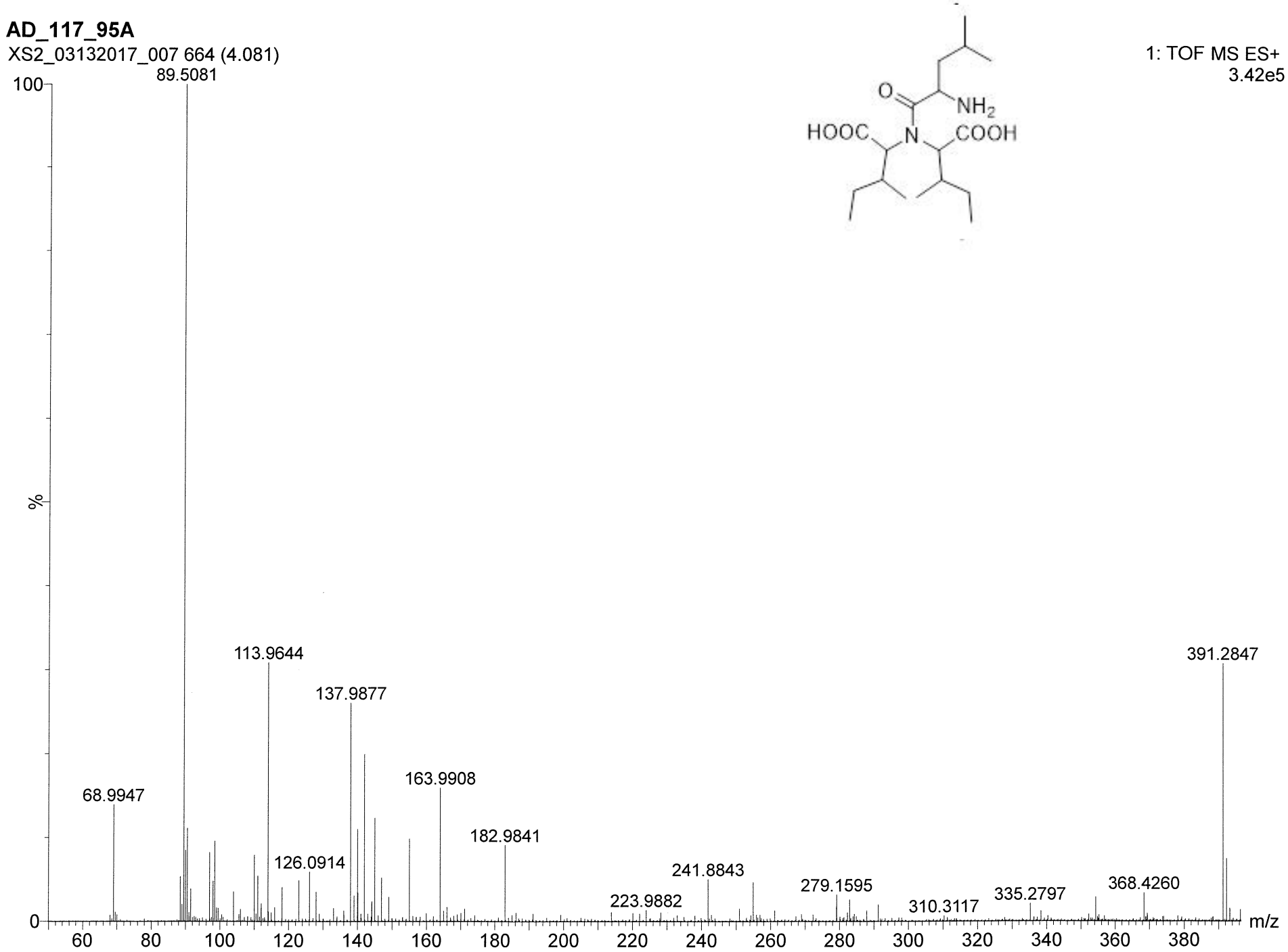
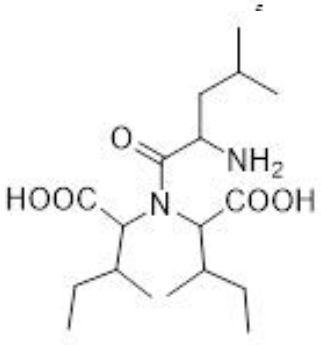


Figure S35. Elemental composition of **4** calculated by single mass analysis



Elemental Composition Report

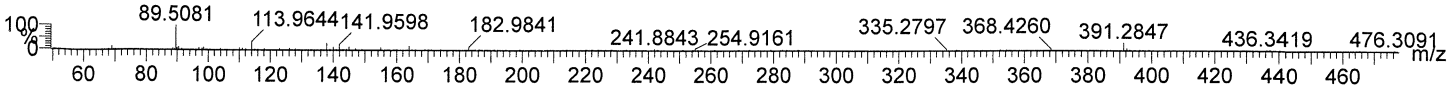
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: On (Carbon range ± 5) (Set 0 < Cl < 9, 0< Br < 9 and 0 < S < 7 for enhanced filter
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-22 H: 0-60 N: 0-2 O: 0-6

AD_117_95A
XS2_03132017_007 664 (4.081)

1: TOF MS ES+
3.42e+005



Minimum:				-1.5				
Maximum:		10.0	10.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
391.2847	391.2808	3.9	10.0	1.5	581.8	n/a	n/a	C19 H39 N2 O6

Figure S36. IR spectrum of **4** in KBr

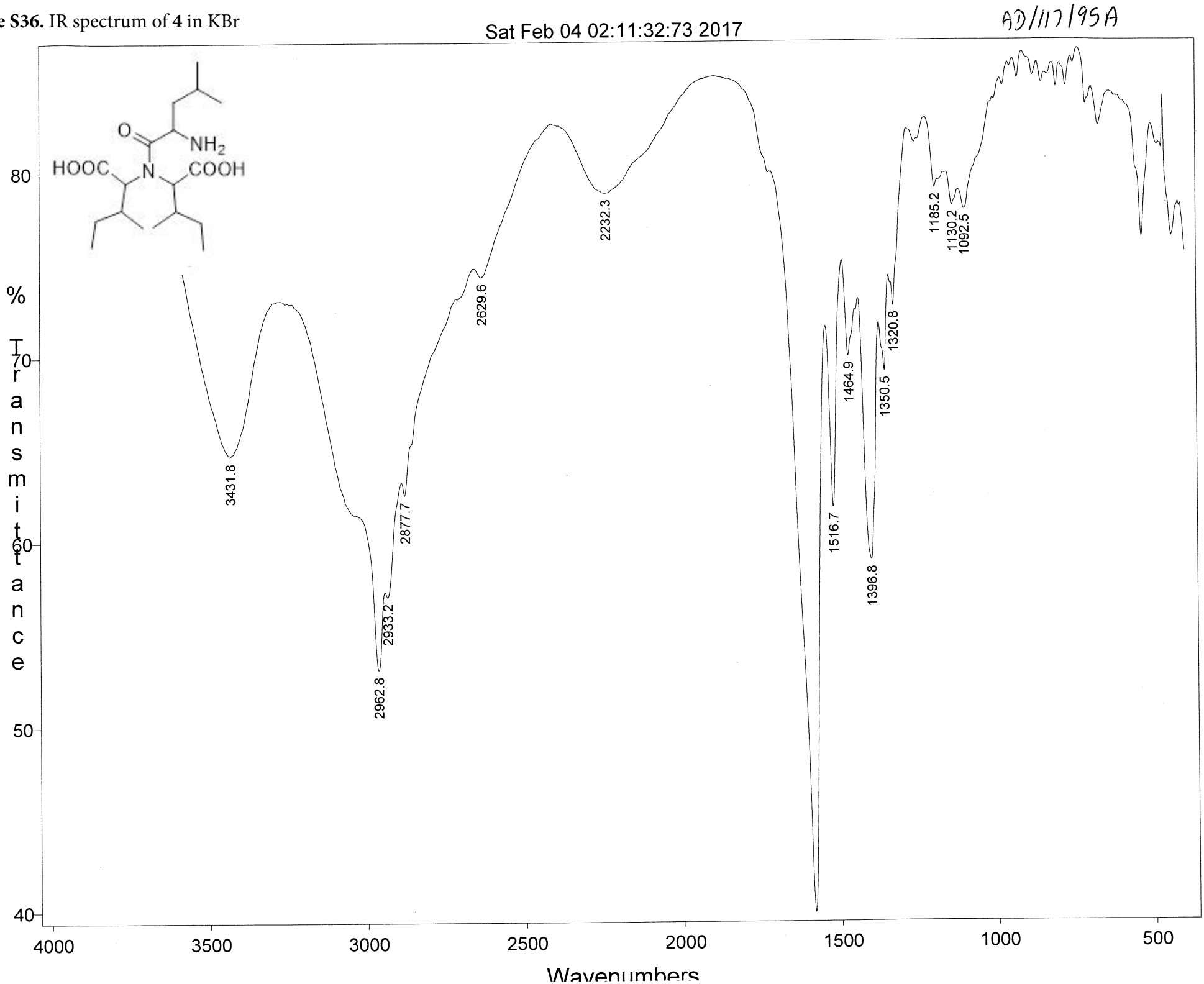


Figure S37. UV/Vis spectrum of **4** water

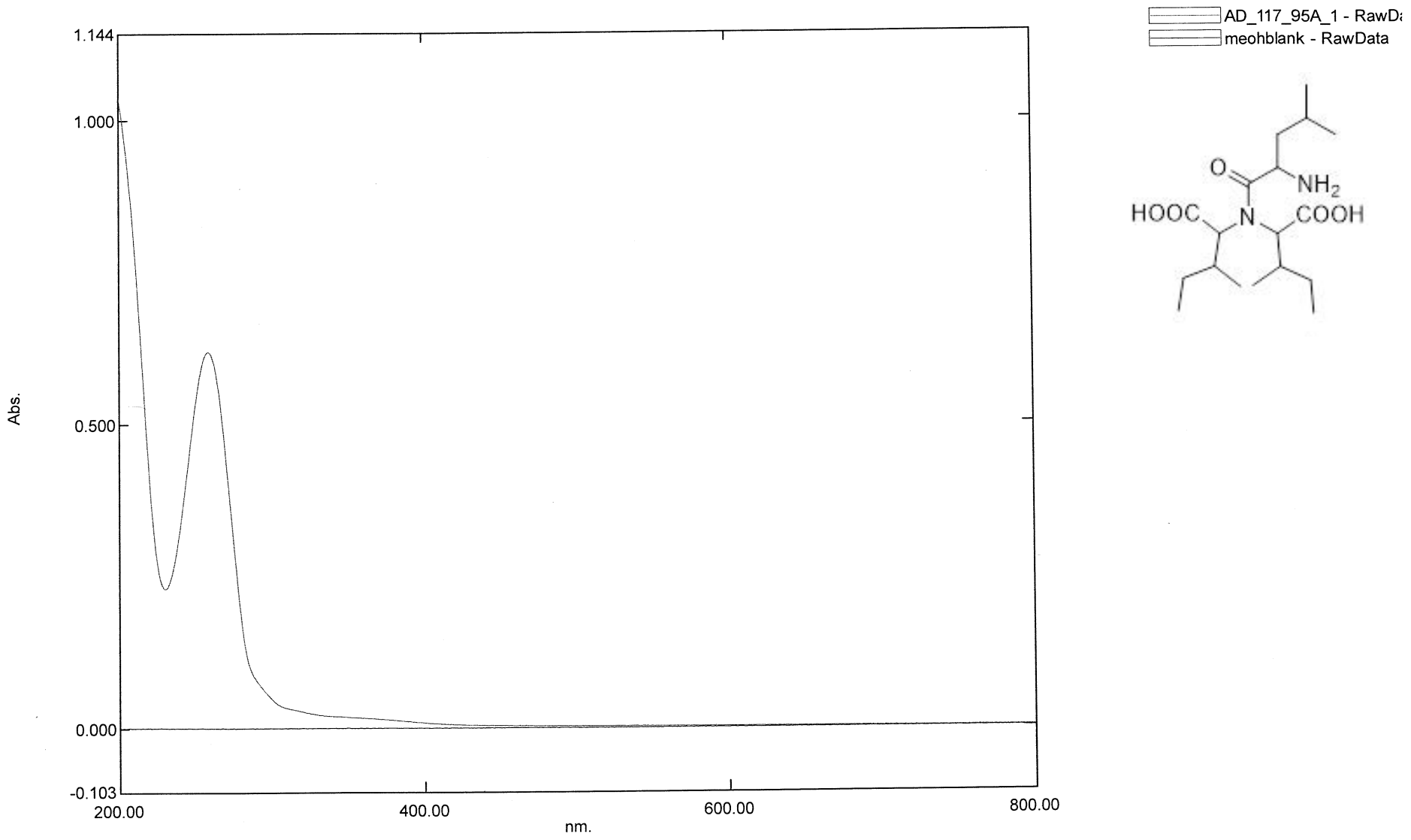
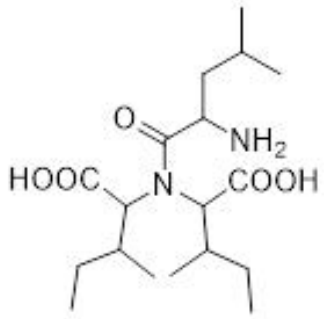


Figure S38. HOMODEC NMR spectrum of **4** D_2O (δH = 3.71)



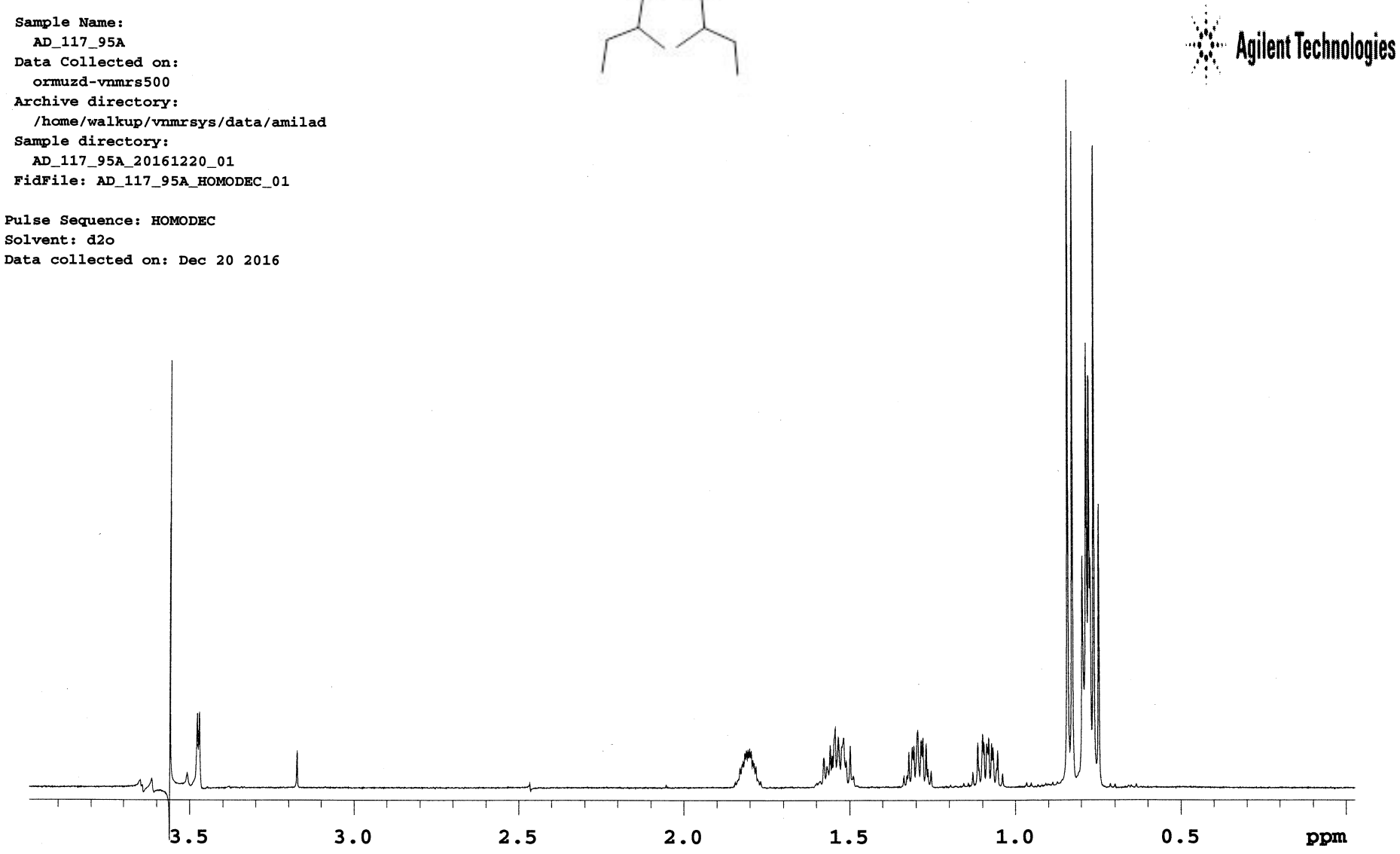


Figure S39. HOMODEC NMR spectrum of **4** D_2O (δH = 1.67)

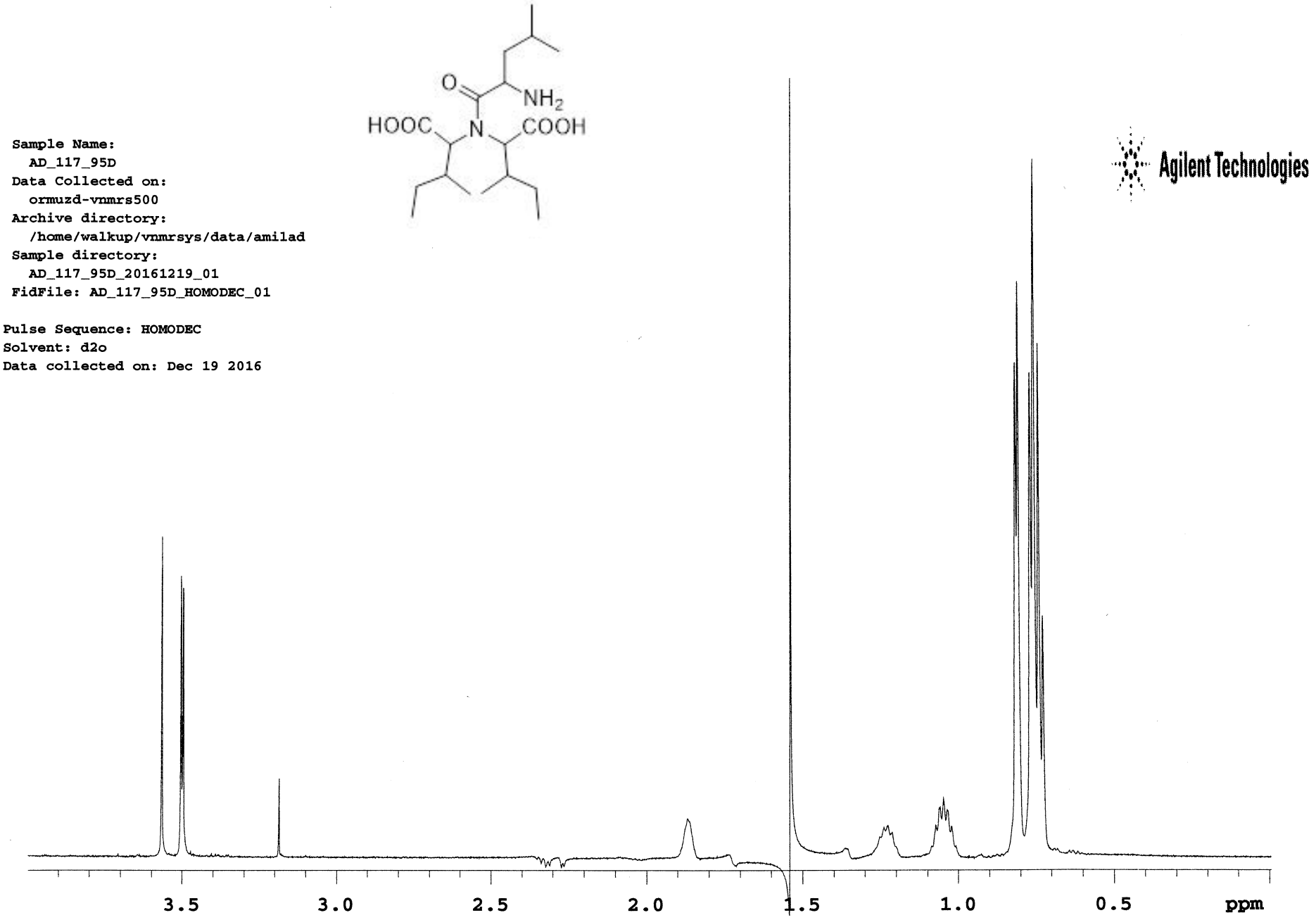


Figure S40. HOMODEC NMR spectrum of **4** D_2O (δH = 3.64)

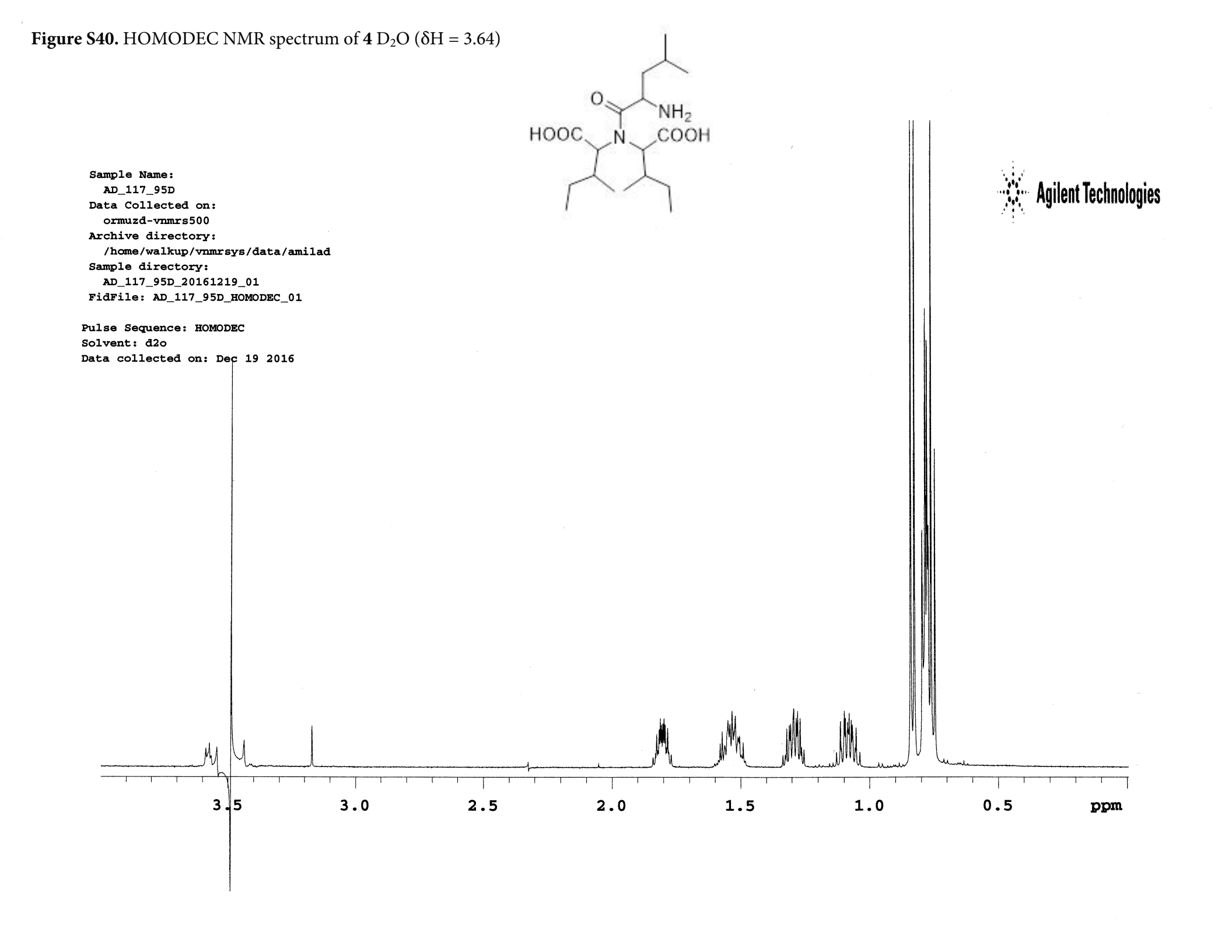


Figure S41. HOMODEC NMR spectrum of **4** D_2O (δH = 1.94)

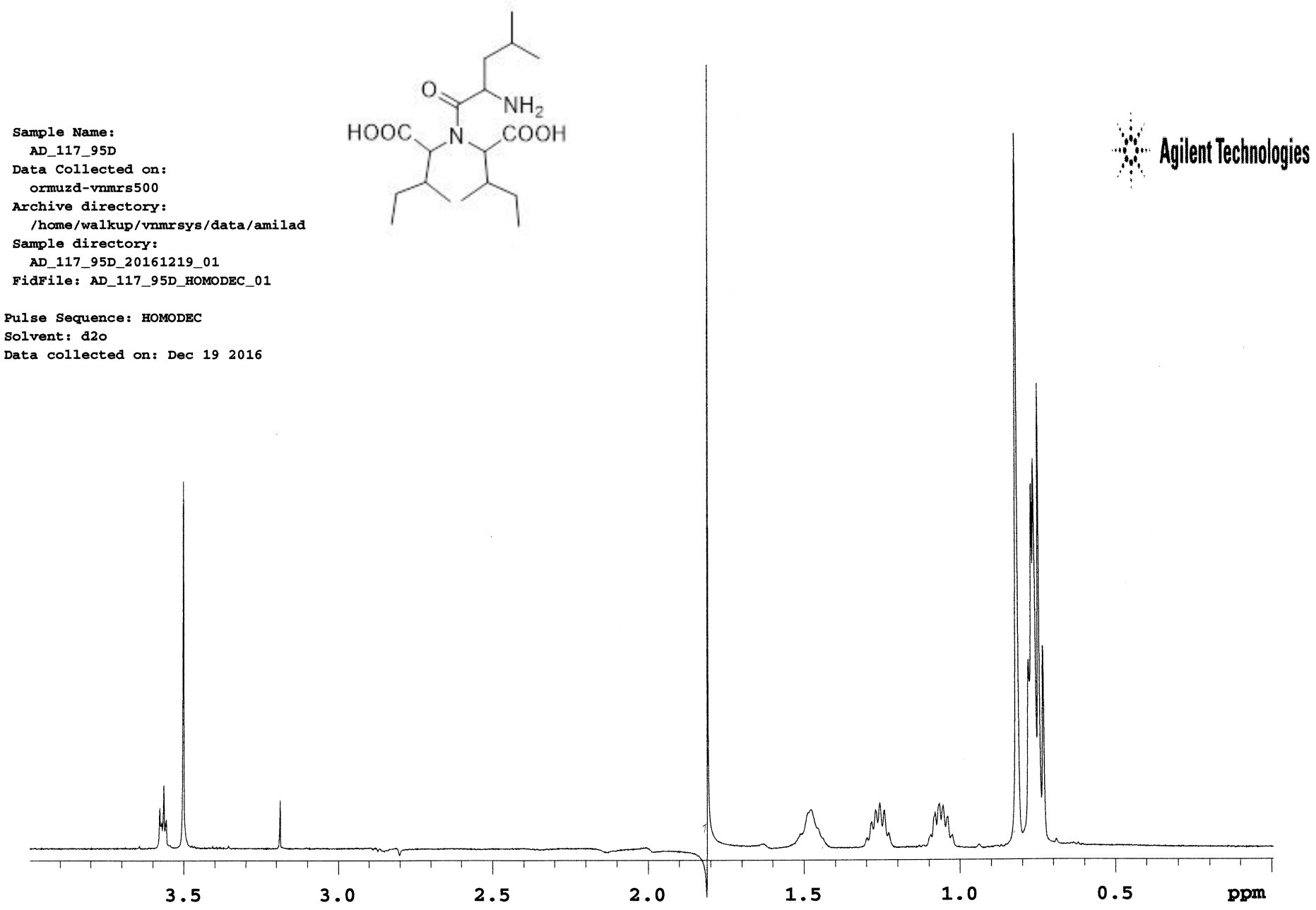


Figure S42. HOMODEC NMR spectrum of **4** D_2O (δH = 1.45)

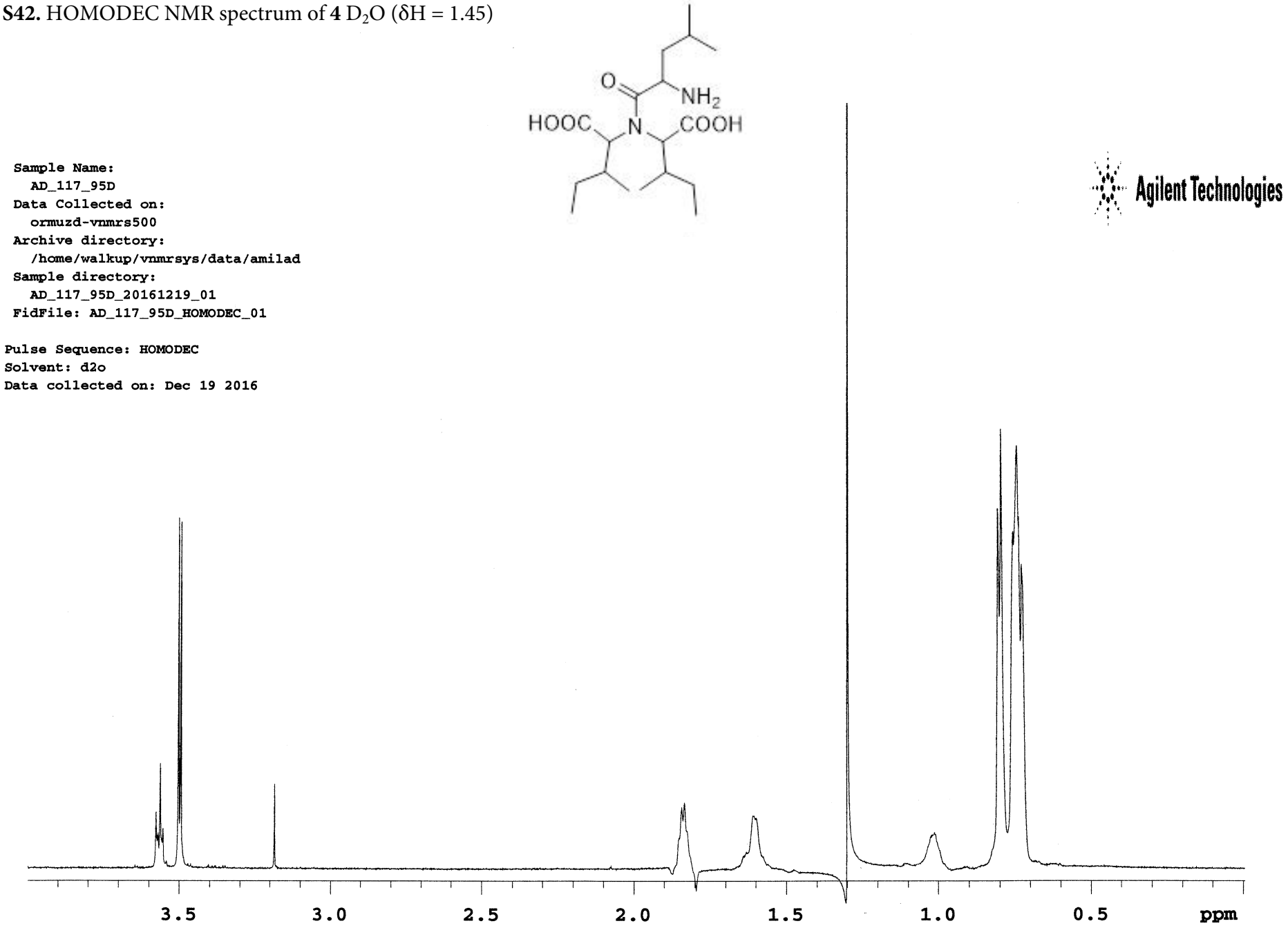


Figure S43. HOMODEC NMR spectrum of **4** D_2O (δH = 0.97)

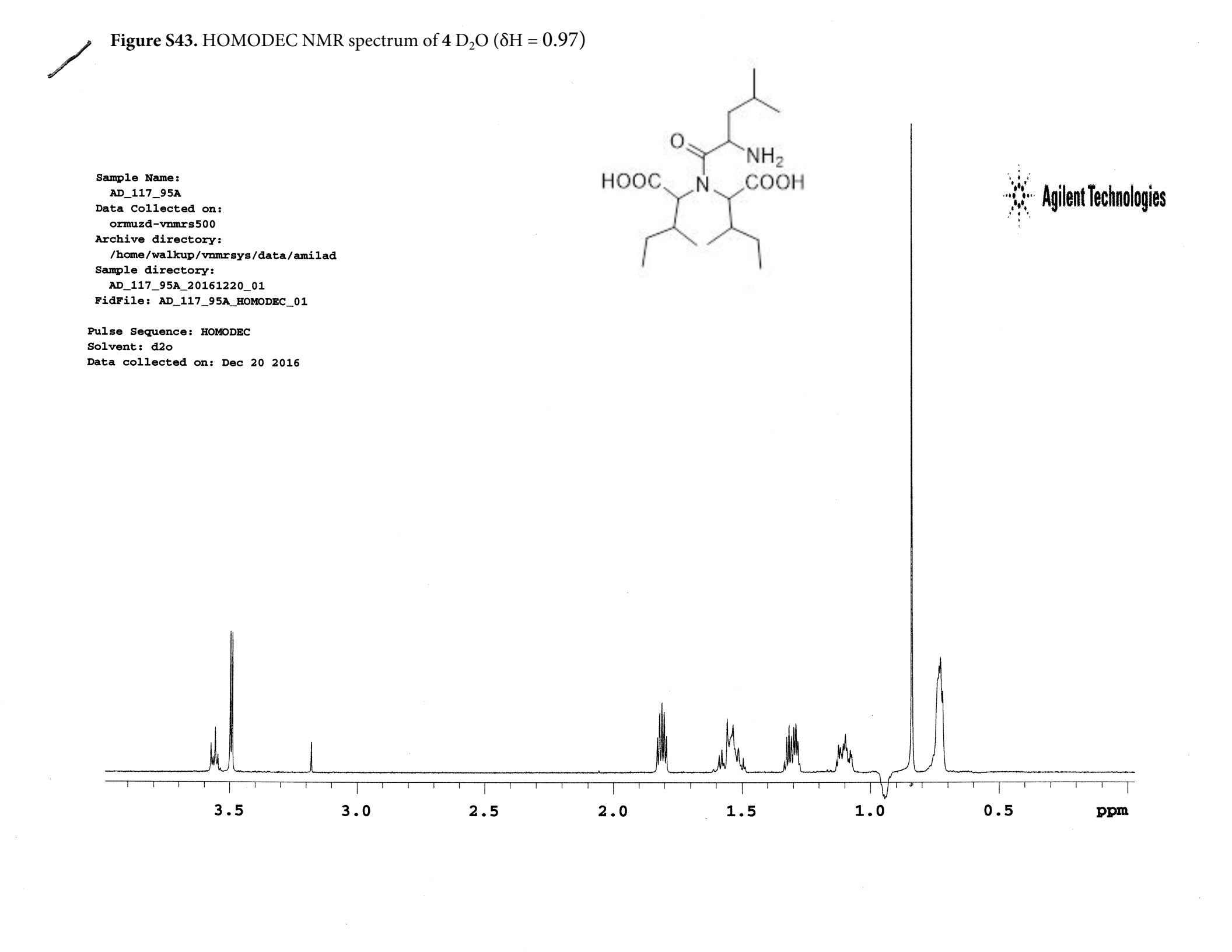


Figure S44. HMBC spectrum of **4** in D_2O

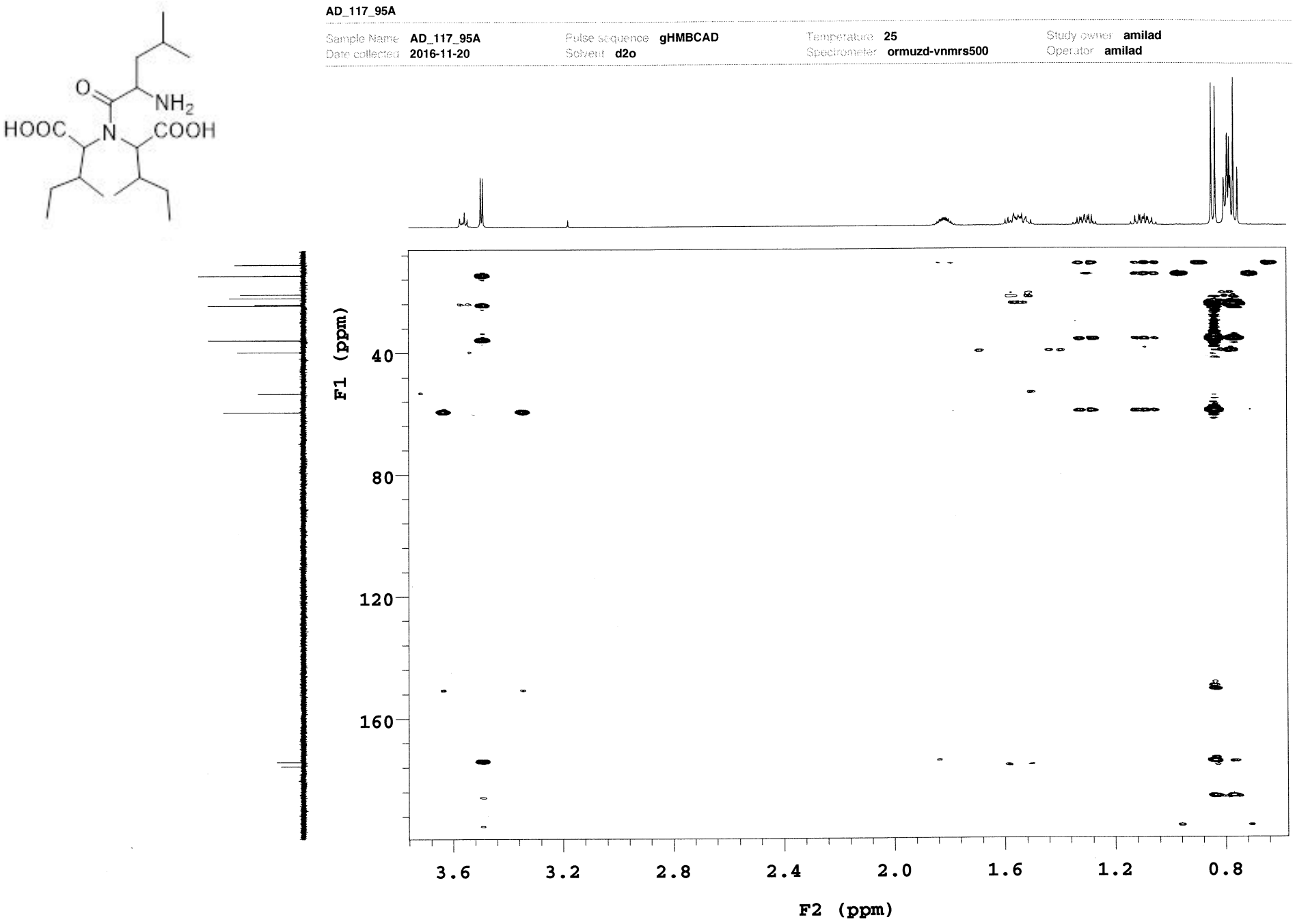
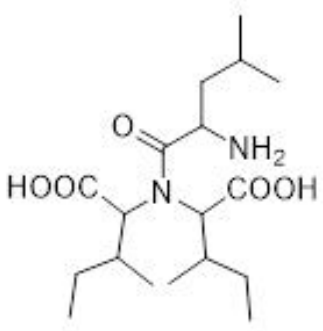
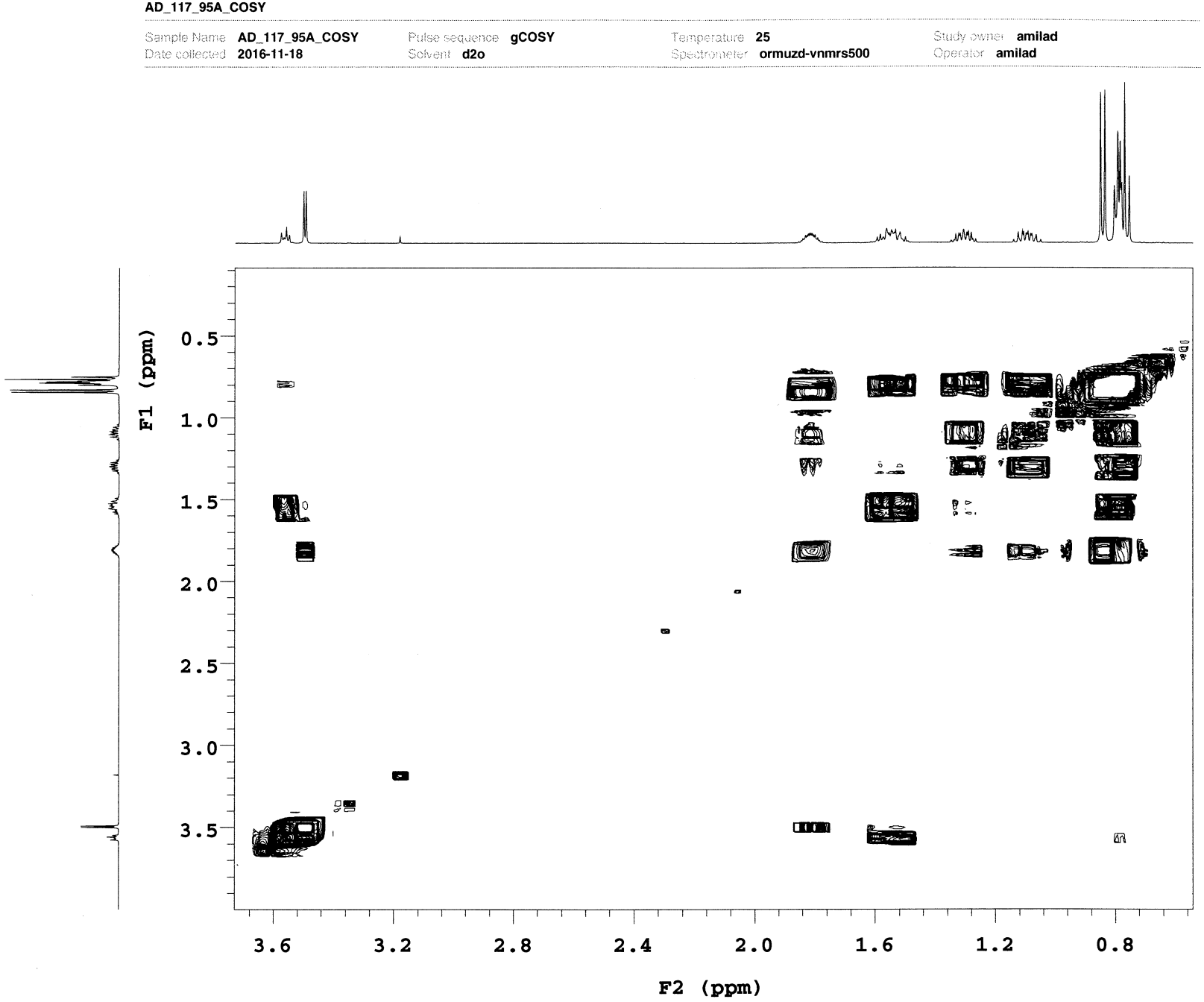


Figure S45. $^{1}H-^{1}H$ COSY spectrum of **4** in D_2O





Data file /net/ormuzd/home/walkup/vnmrsys/data/amilad/AD_117_95A_COSY_20161118_01/AD_117_95A_COSY_gCOSY_01.fid

Plot date 2016-11-18

Figure S46. NOESY spectrum of **4** in D_2O

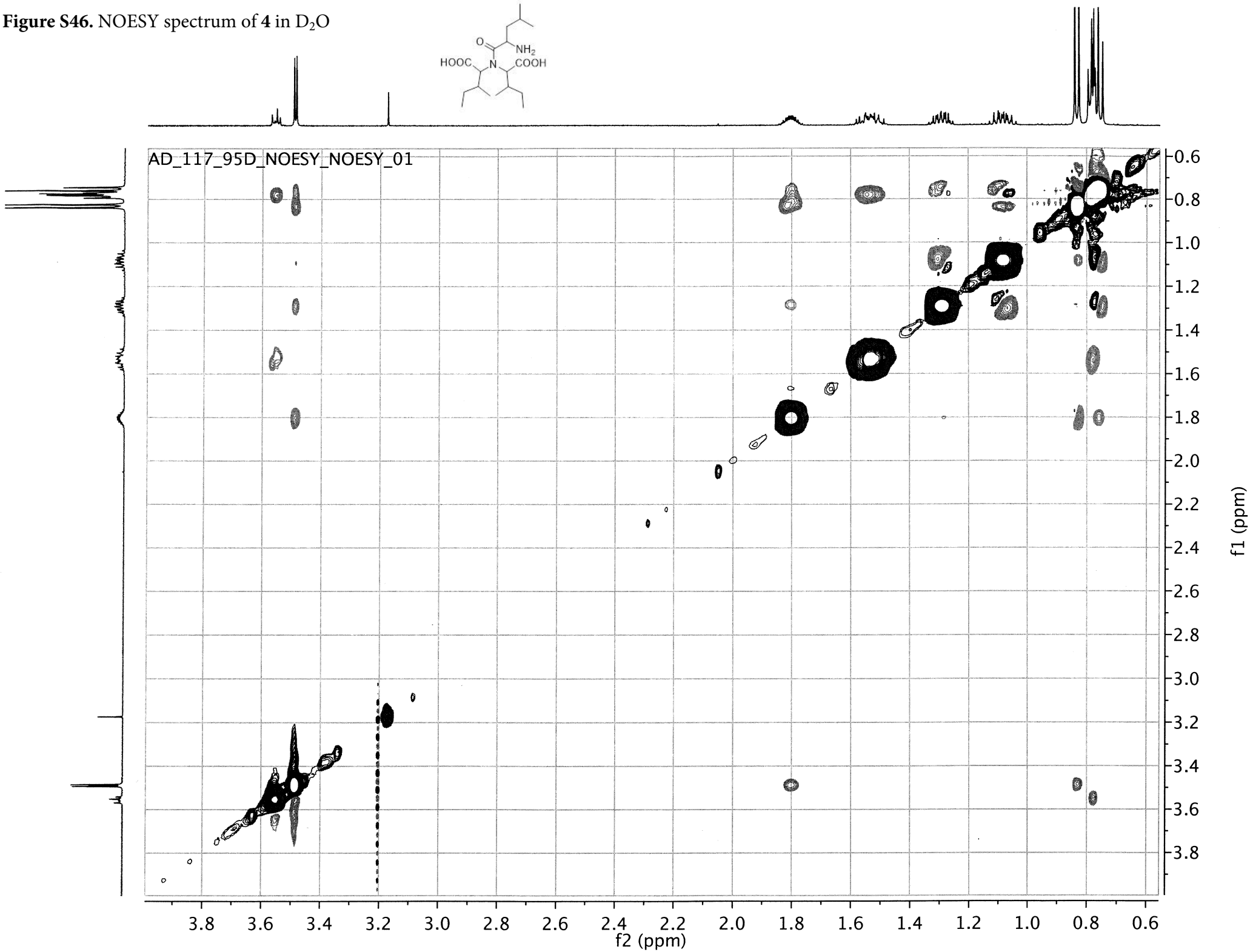
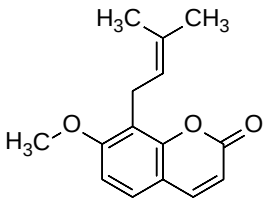


Table 1. MTT, LPO and COX assay results for compounds **1**-**4** isolated from *P. haussknechtii*

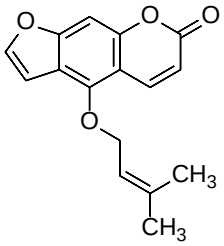
	Concentration	MTT [a,b] (absorbance)	LPO [a,c] (fluorescence)	COX-1 [a,d] (Inhibition %)	COX-2 [a,d] (Inhibition %)
1	146.2 µM	0.605 ± 0.02	ND [e]	ND [e]	ND [e]
	73.1 µM	0.251 ± 0.03	53.6 ± 2.1	63.7 ± 3.0	60.1 ± 0.9
	36.5 µM	0.134 ± 0.01	37.4 ± 1.6	49.4 ± 0.4	42.1 ± 0.3
	18.3 µM	0.065 ± 0.01	22.4 ± 0.8	28.6 ± 0.4	29.8 ± 0.3
	9.12 µM	ND [e]	15.9 ± 2.2	10.8 ± 2.7	14.1 ± 2.8
2	145.3 µM	0.528 ± 0.04	62.6 ± 2.4	ND [e]	ND [e]
	72.6 µM	0.259 ± 0.02	46.2 ± 1.8	55.8 ± 0.8	53.9 ± 3.7
	36.3 µM	0.160 ± 0.03	24.7 ± 1.6	45.2 ± 2.7	40.7 ± 0.3
	18.2 µM	0.081 ± 0.03	17.9 ± 0.9	24.6 ± 0.1	33.7 ± 1.3
	9.07 µM	ND [e]	ND [e]	21.1 ± 1.4	23.9 ± 0.6
3	178.6 µM	ND [e]	60.3 ± 2.2	ND [e]	ND [e]
	89.3 µM	0.651 ± 0.02	42.5 ± 1.5	18.2 ± 0.3	4.8 ± 1.7
	44.6 µM	0.328 ± 0.05	26.1 ± 1.4	ND [e]	ND [e]
	22.3 µM	0.166 ± 0.03	19.5 ± 0.8	ND [e]	ND [e]
	11.1 µM	0.054 ± 0.01	ND [e]	ND [e]	ND [e]
4	139.6 µM	ND [e]	ND [e]	ND [e]	ND [e]
	69.8 µM	0.680 ± 0.04	61.5 ± 3.1	46.1 ± 0.3	75.5 ± 3.6
	34.9 µM	0.370 ± 0.05	44.5 ± 2.7	37.4 ± 2.7	49.1 ± 0.2
	17.5 µM	0.217 ± 0.05	29.5 ± 0.8	21.1 ± 0.3	33.6 ± 1.1
	8.71 µM	0.127 ± 0.06	19.2 ± 1.4	14.9 ± 0.1	22.2 ± 1.5

[a]Values are expressed as mean ± SEM (n = 2). [b]Positive controls vitamin C and TBHQ gave absorbance values of 0.49 and 0.50 at 142.1 and 150.4 µM, respectively. [c]Commercial antioxidants BHT, BHA and TBHQ with IC_{50} values of 10 µM, 6.9 µM and 5 µM, respectively. [d]The standards aspirin, ibuprofen and naproxen with IC_{50} values of 600 µM, 72.8 µM and 52.2 µM, respectively for the inhibition of COX-1 enzyme activity and Celebrex® and naproxen with IC_{50} values of 1.3 µM and 52.2 µM, respectively for the inhibition of COX-2 enzyme activity. [e]Data not available.

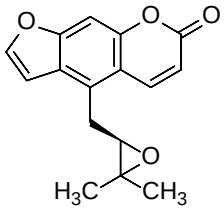
Figure S47. Chemical structures of known compounds



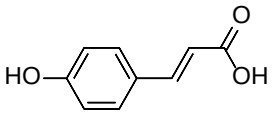
Osthol



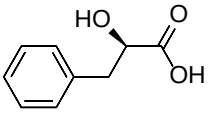
Isoimperatorin



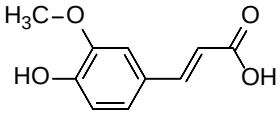
Oxypeucedanin



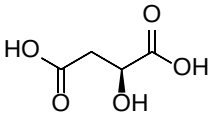
p-coumaric acid



3-phenyllacetic acid

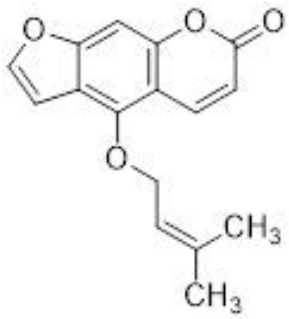


ferulic acid



malic acid

Figure S48. ^{1}H NMR spectrum of isoimperatorin in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	4083.5	8.172	28.3
2	4073.7	8.152	28.9
3	3797.8	7.600	35.9
4	3795.4	7.595	39.2
5	3632.0	7.269	18.7
6	3573.4	7.151	36.4
7	3479.5	6.963	26.5
8	3478.5	6.961	26.4
9	3477.0	6.958	27.7
10	3476.0	6.956	23.9
11	3138.6	6.281	38.9
12	3128.8	6.261	38.2
13	2776.7	5.557	4.7
14	2775.2	5.554	5.8
15	2769.8	5.543	9.3
16	2768.4	5.540	12.1
17	2766.9	5.537	9.2
18	2762.5	5.528	5.0
19	2761.5	5.526	5.8
20	2464.2	4.931	36.7
21	2456.8	4.917	35.7
22	902.1	1.805	96.7
23	851.2	1.704	97.2
24	810.6	1.622	6.5

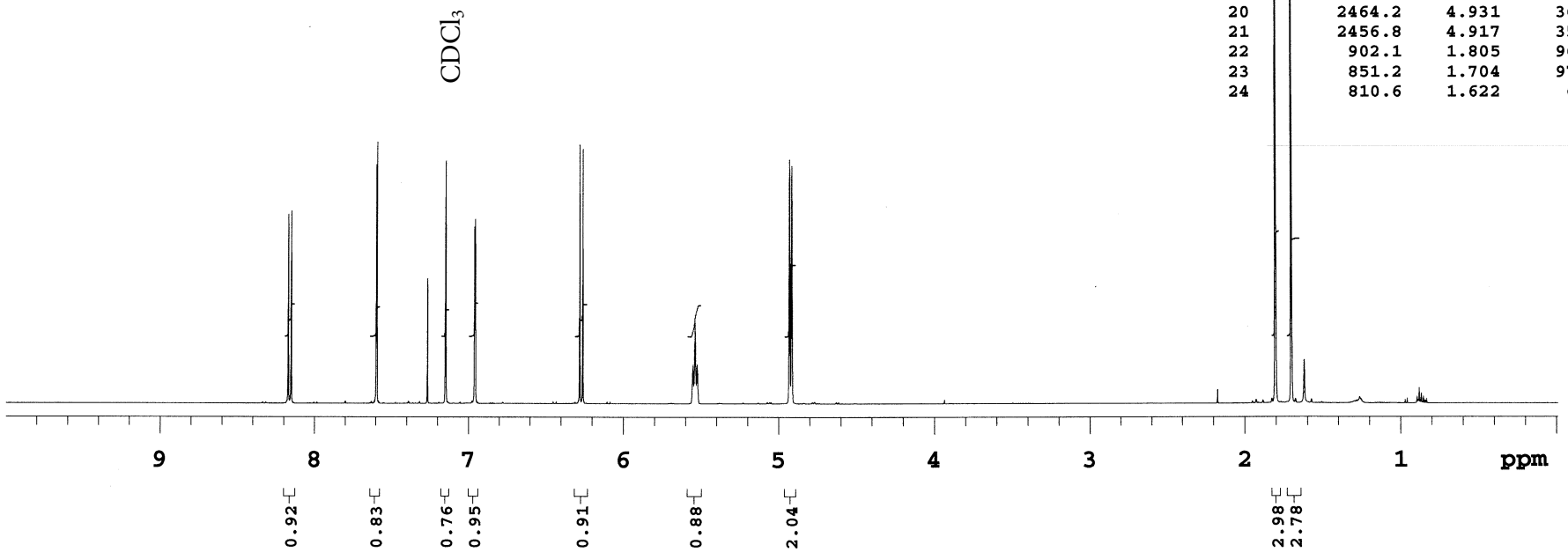


Figure S49. ^{13}C NMR spectrum of isoimperatorin in $CDCl_3$

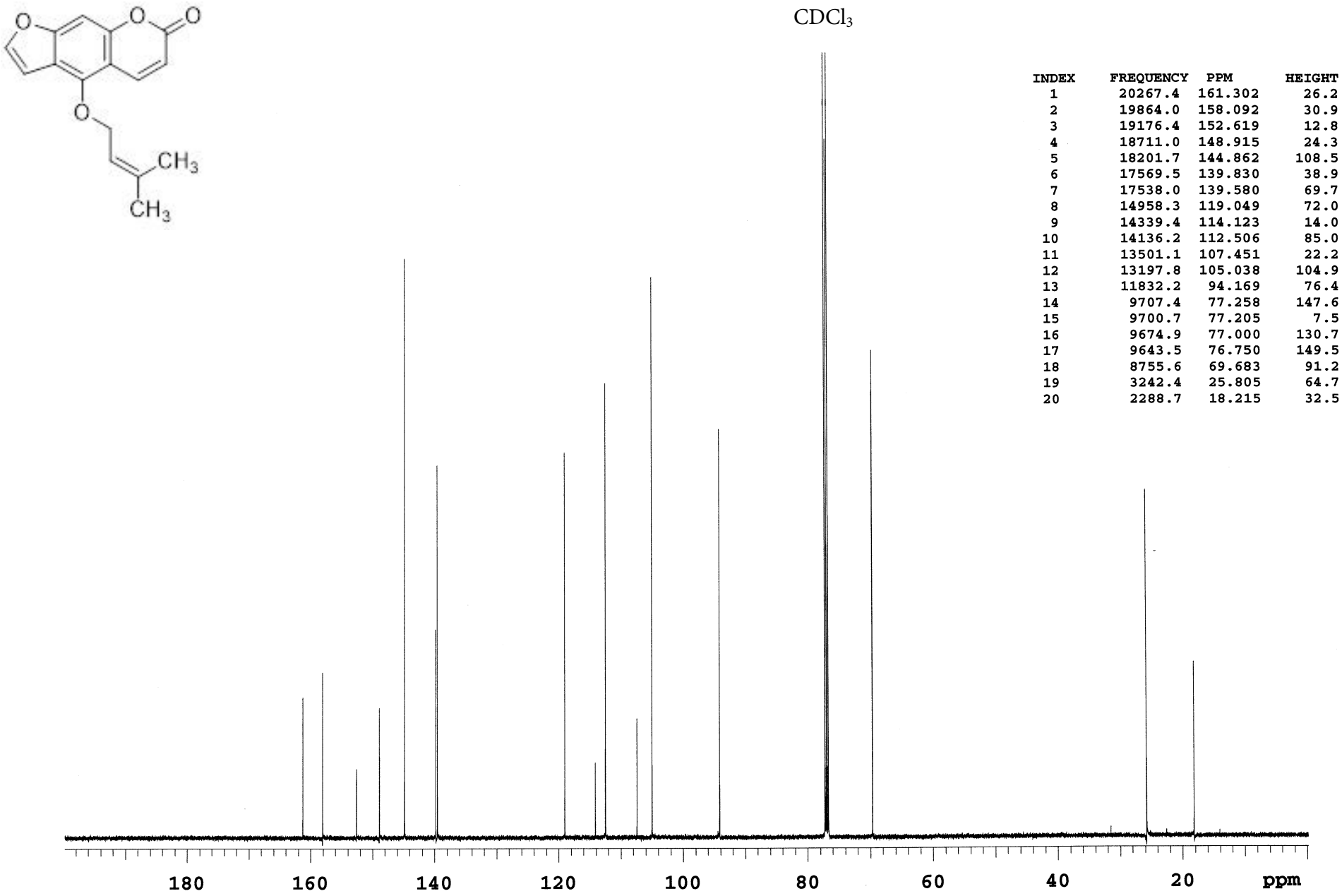


Figure S50. HSQC spectrum of isoimperatorin in $CDCl_3$

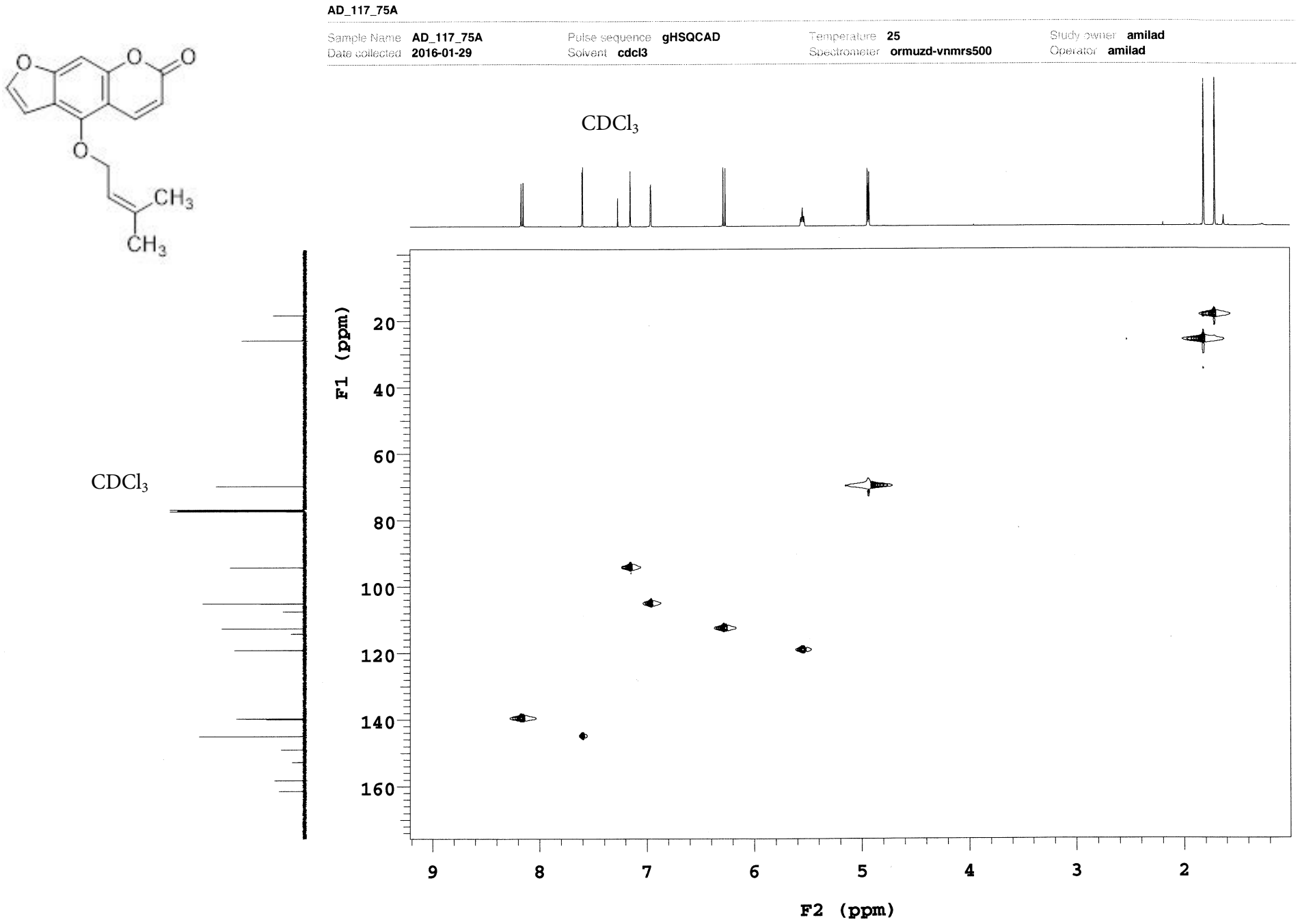
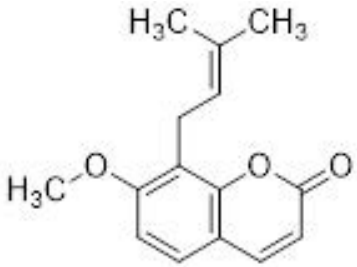


Figure S51. ^{1}H NMR spectrum of osthol in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	3796.8	7.598	16.1
2	3787.5	7.580	16.5
3	3634.4	7.273	13.9
4	3625.6	7.256	14.4
5	3617.8	7.240	7.6
6	3407.0	6.818	14.9
7	3398.7	6.802	13.6
8	3107.7	6.219	15.4
9	3098.4	6.201	14.4
10	2598.1	5.199	5.5
11	1946.7	3.896	99.0
12	1757.9	3.518	15.6
13	1750.6	3.503	15.2
14	907.4	1.816	50.6
15	820.8	1.643	47.9

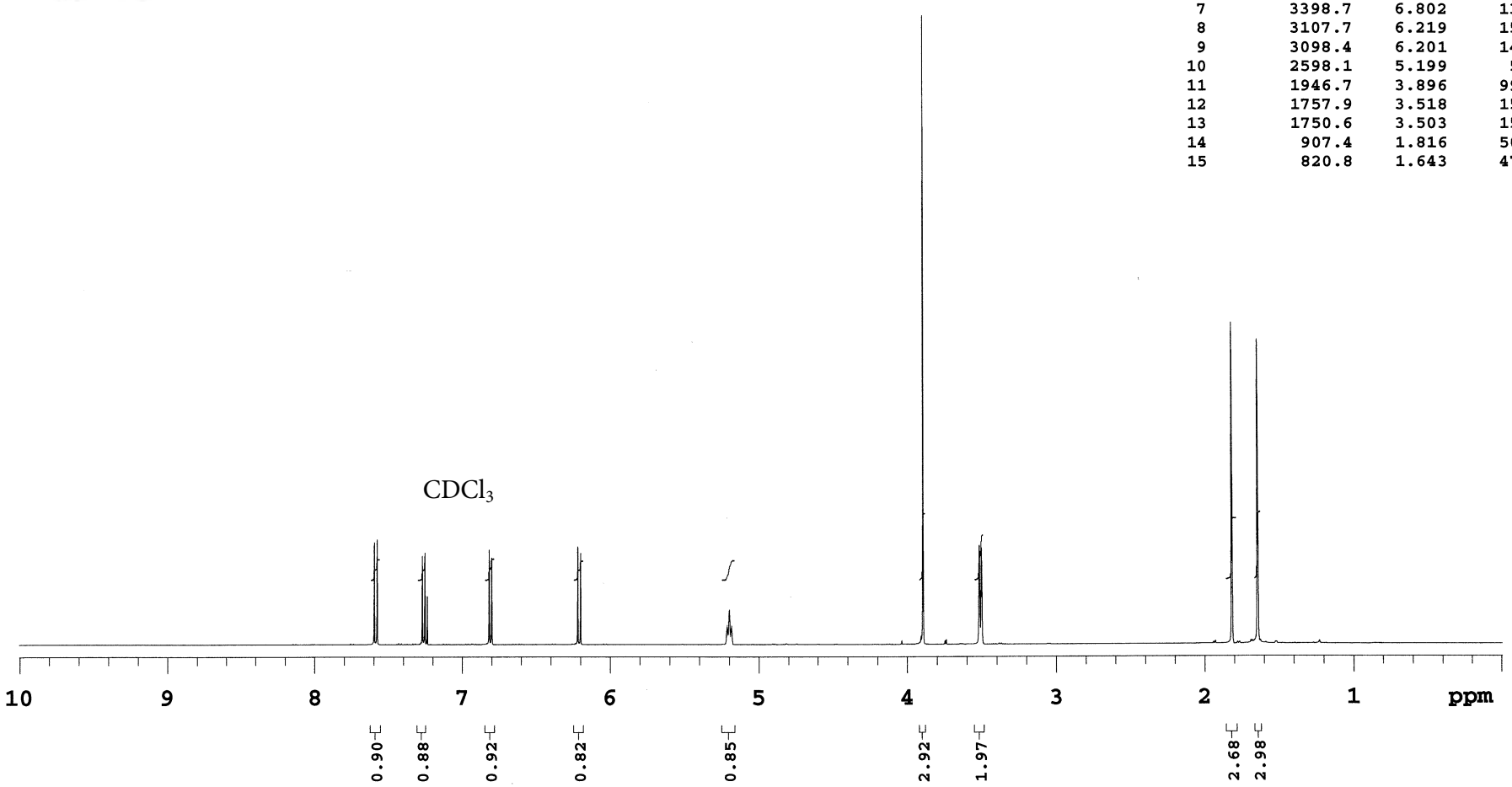


Figure S52. ^{13}C NMR spectrum of osthol in $CDCl_3$

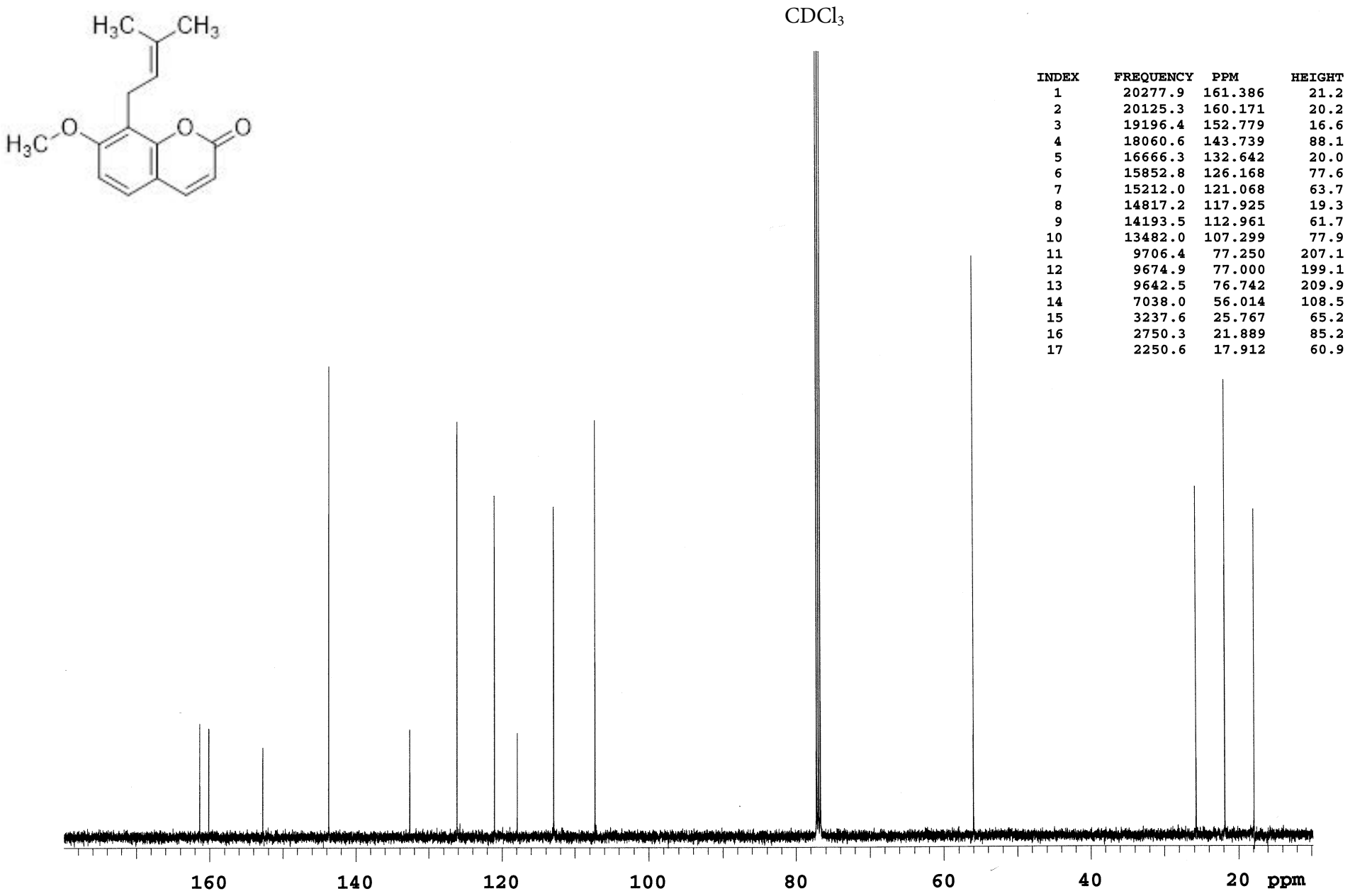
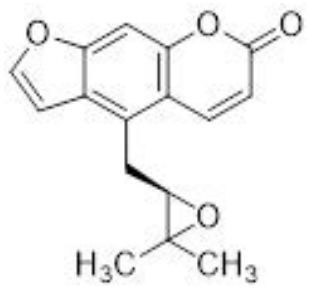


Figure S53. 1H NMR spectrum of oxypeucedanin in $CDCl_3$



Sample Name:
AD_117_73D
Data Collected on:
ahriman-vnmrs500
Archive directory:
/home/walkup/vnmrsys/data/amilad
Sample directory:
AD_117_73D_20160122_01
FidFile: AD_117_73D_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 22 2016

INDEX	FREQUENCY	PPM	HEIGHT
1	4094.7	8.191	14.2
2	4084.9	8.171	14.2
3	3795.4	7.593	125.0
4	3792.9	7.588	14.5
5	3619.3	7.240	14.4
6	3583.1	7.168	20.9
7	3464.7	6.931	12.9
8	3463.8	6.929	12.9
9	3462.8	6.927	12.3
10	3149.3	6.300	22.0
11	3139.5	6.280	21.7
12	2296.9	4.595	11.0
13	2292.5	4.586	10.4
14	2286.1	4.573	14.3
15	2281.7	4.564	14.1
16	2213.2	4.427	13.0
17	2206.9	4.415	13.0
18	2202.5	4.406	10.6
19	2196.1	4.393	9.6
20	1610.7	3.222	7.6
21	1606.3	3.213	8.3
22	1603.9	3.208	8.6
23	1599.5	3.200	7.6
24	693.7	1.388	100.8
25	655.1	1.310	97.9
26	611.5	1.223	9.9

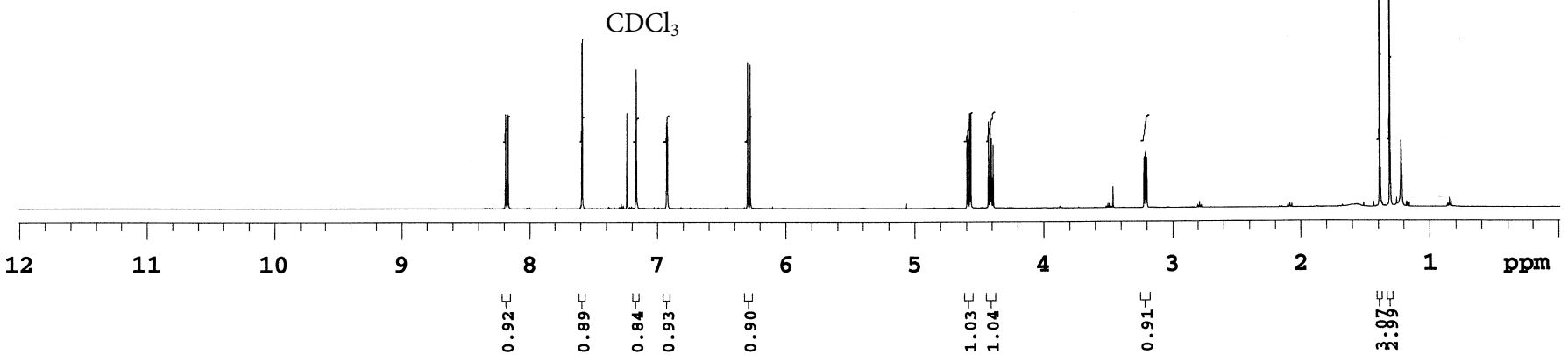
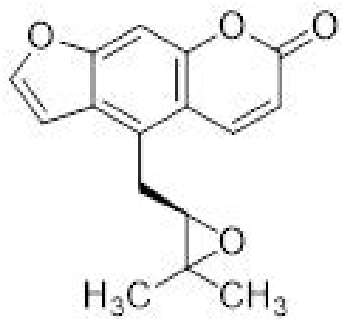


Figure S54. ^{13}C NMR spectrum of oxypeucedanin in $CDCl_3$



INDEX	FREQUENCY	PPM	HEIGHT
1	20234.0	161.037	9.2
2	19853.5	158.008	16.7
3	19164.0	152.521	13.0
4	18636.6	148.323	13.7
5	18256.1	145.295	39.6
6	17465.5	139.003	42.8
7	14345.1	114.168	9.3
8	14215.4	113.136	29.6
9	13495.4	107.406	14.2
10	13127.2	104.476	36.0
11	11918.9	94.859	48.0
12	9707.4	77.258	117.0
13	9674.9	77.000	105.8
14	9643.5	76.750	117.9
15	9082.7	72.287	45.0
16	7675.1	61.084	40.8
17	7328.9	58.329	25.4
18	3728.8	29.676	9.5
19	3088.9	24.583	60.2
20	2387.9	19.005	27.5

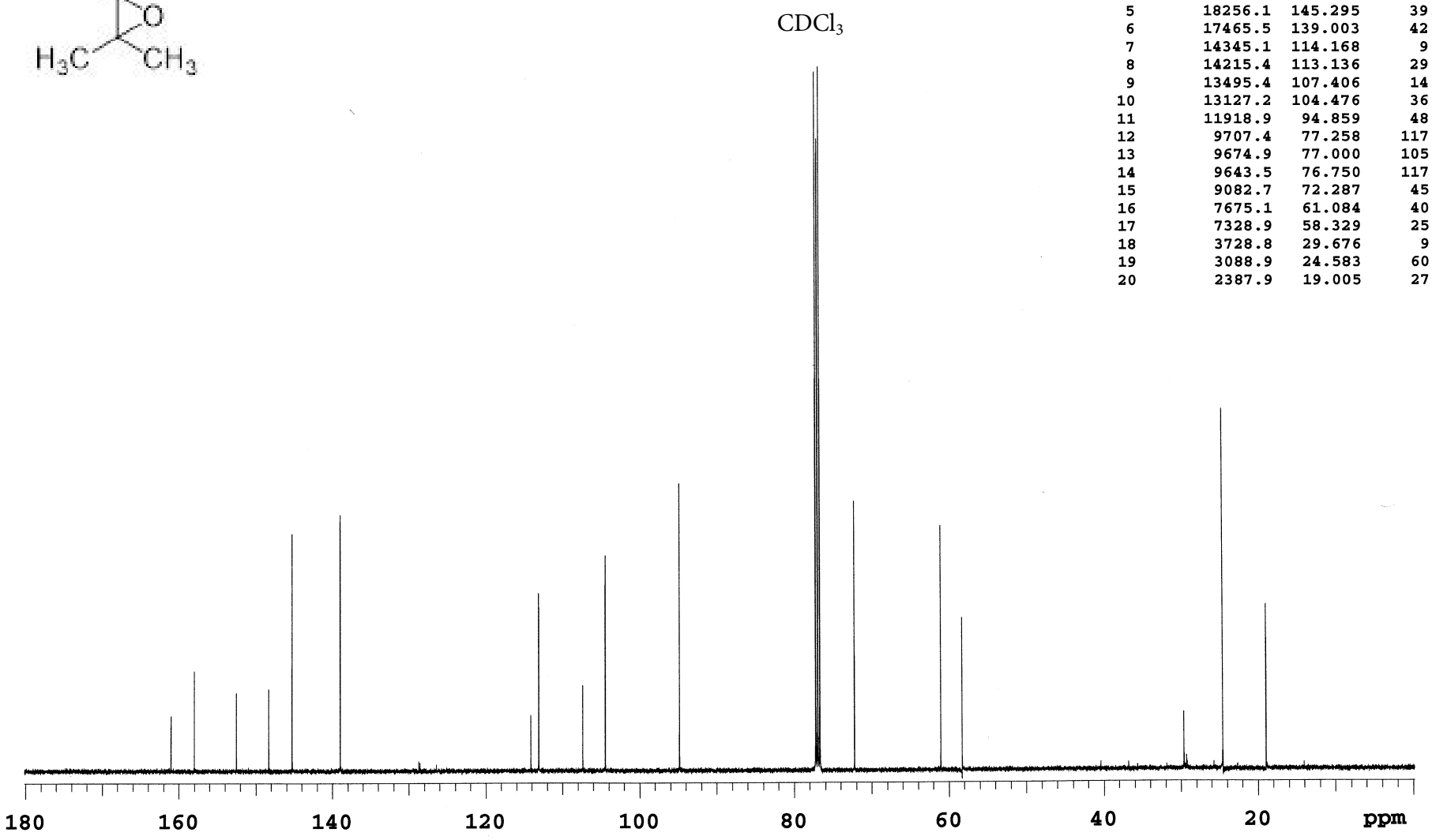


Figure S55. ^{1}H NMR spectrum of malic acid in CD_3OD

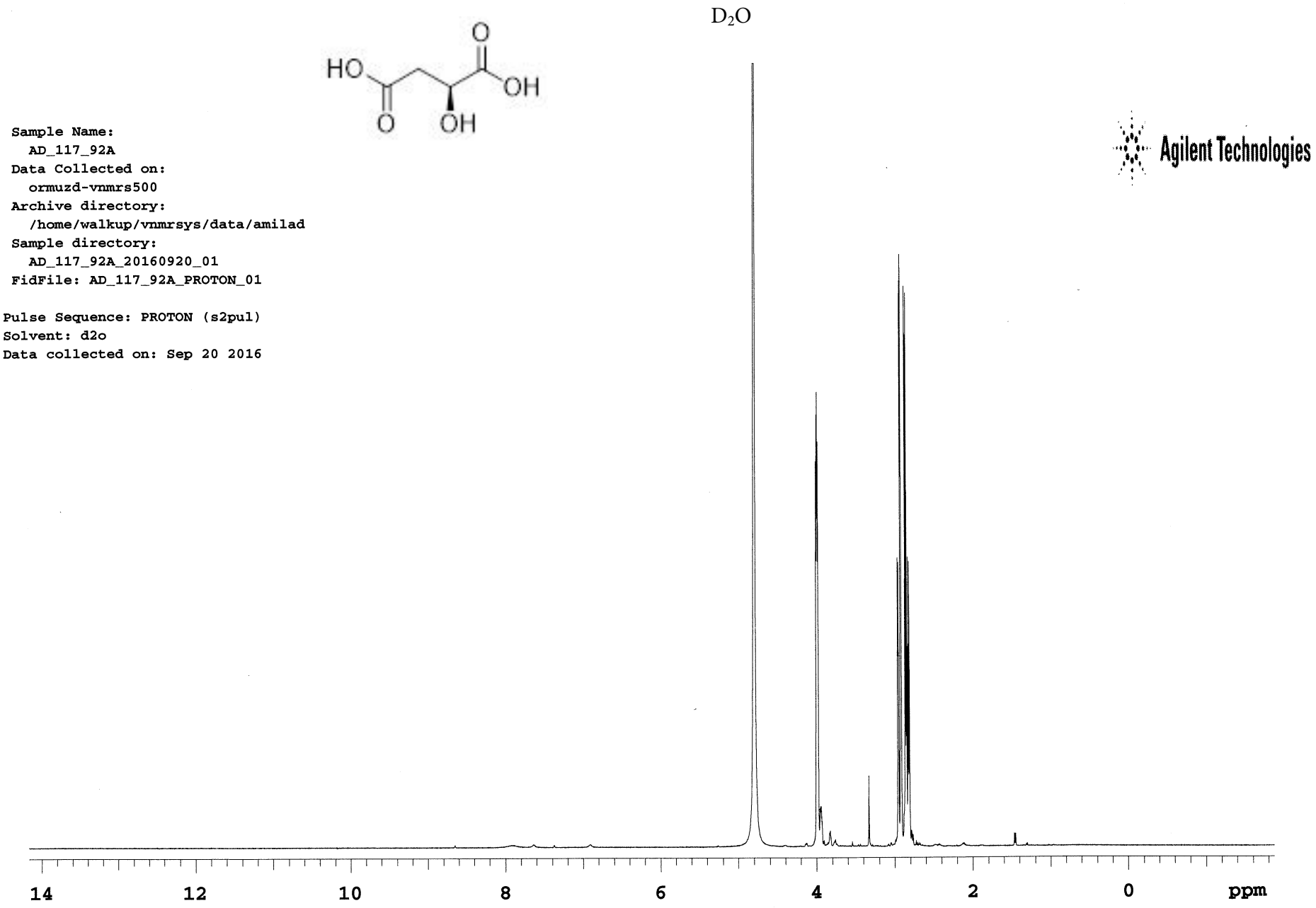


Figure S56. ^{13}C NMR spectrum of malic acid in CD_3OD

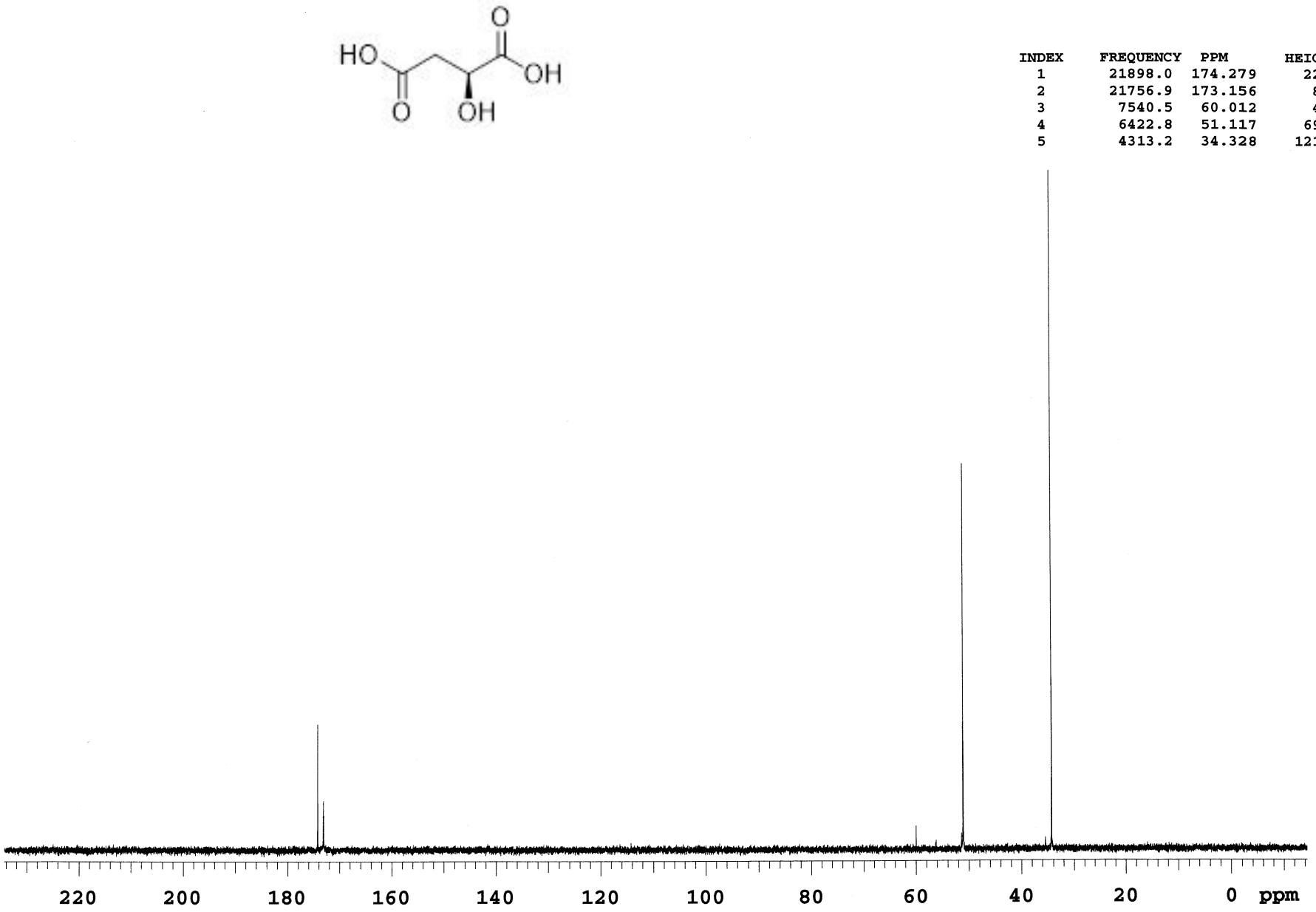


Figure S57. ^{1}H NMR spectrum of *p*-coumaric acid in CD_3OD

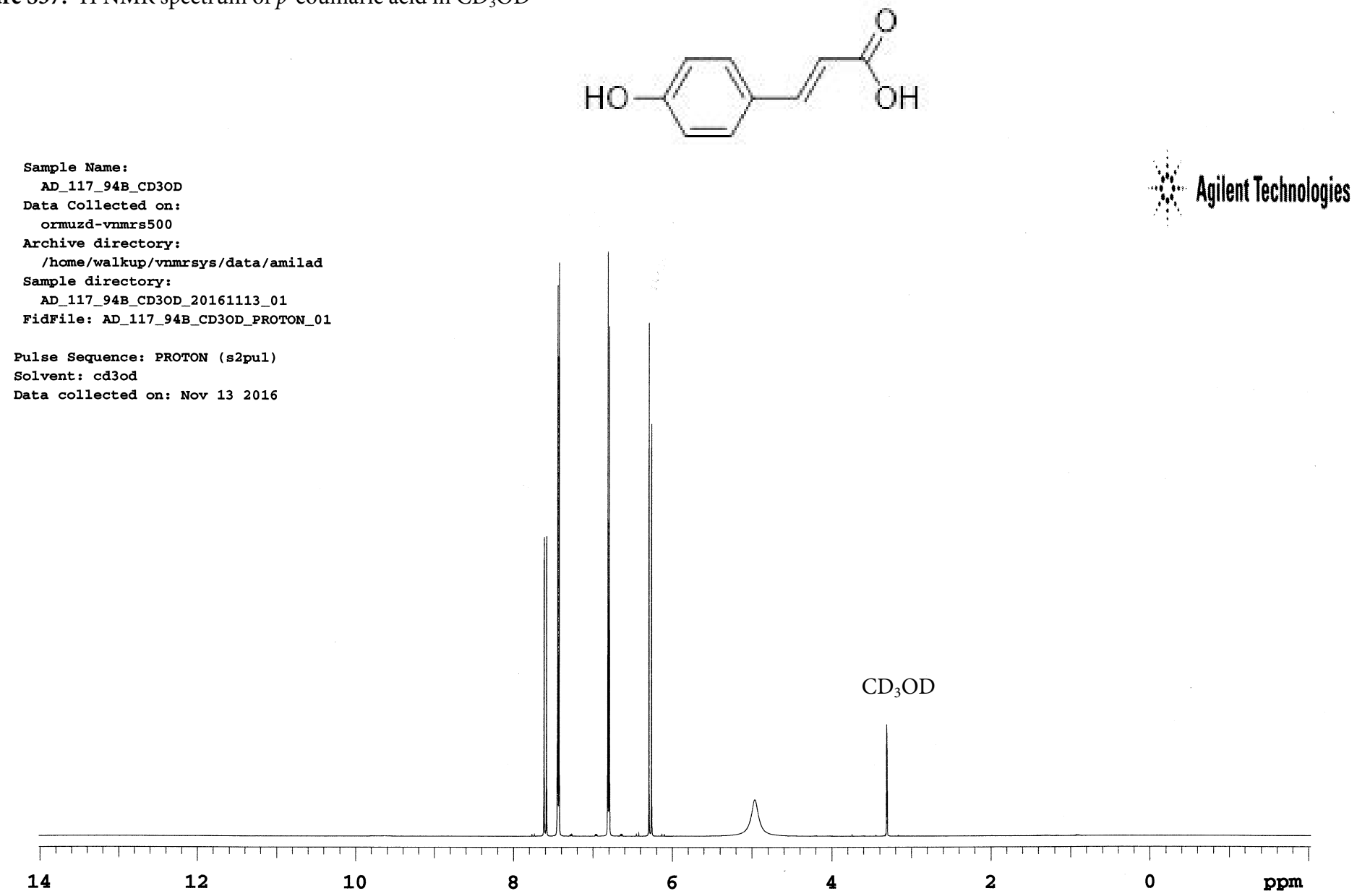


Figure S58. ^{13}C NMR spectrum of *p*-coumaric acid in CD_3OD

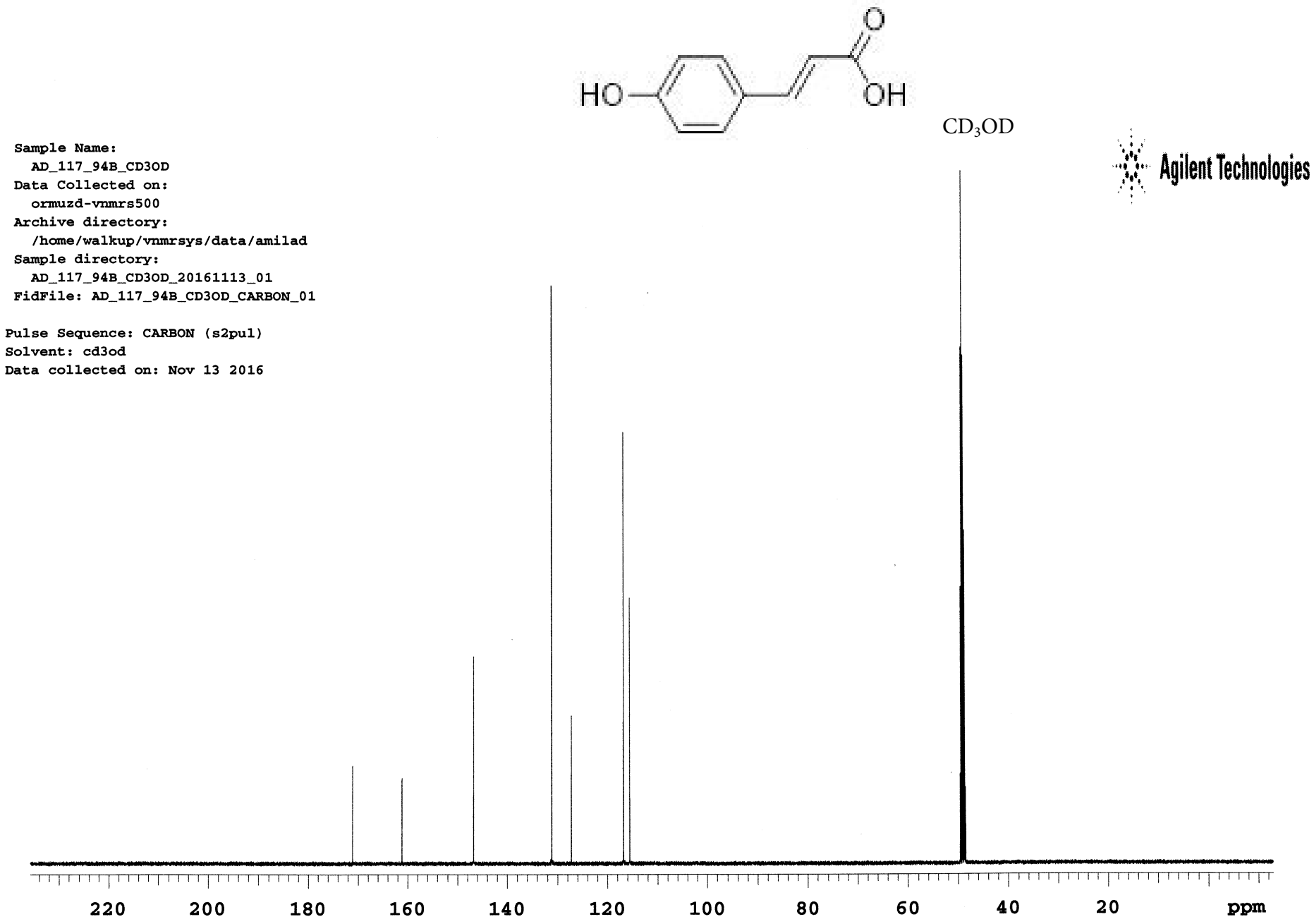


Figure S59. ^{1}H NMR spectrum of 3-phenyllactic acid in D_2O

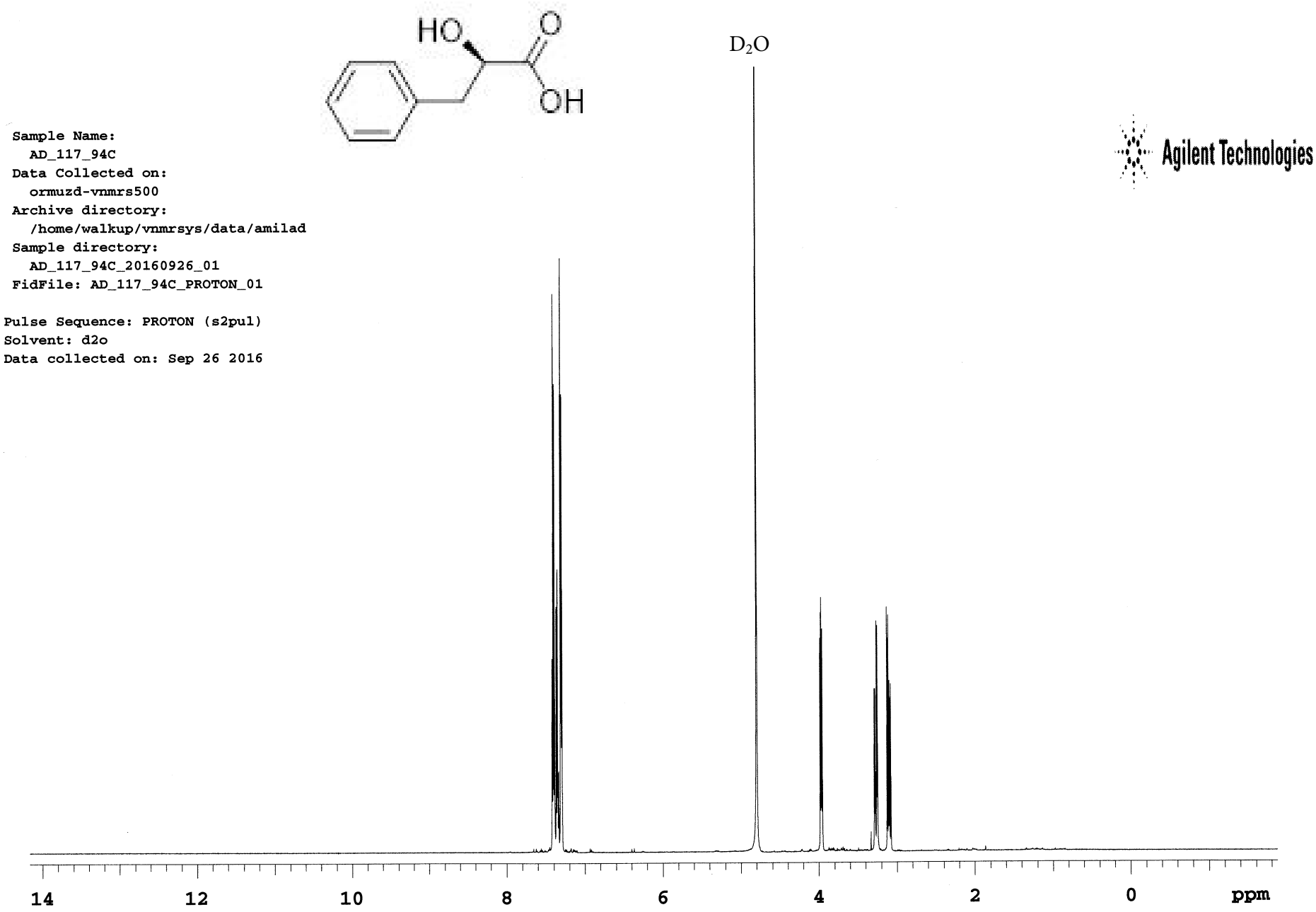
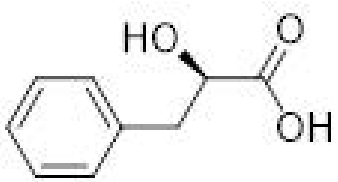


Figure S60. 13C NMR spectrum of 3-phenyllactic acid in D_2O



INDEX	FREQUENCY	PPM	HEIGHT
1	21842.7	173.839	9.8
2	16957.0	134.956	14.7
3	16239.9	129.248	94.1
4	16209.4	129.005	108.5
5	16032.0	127.593	41.9
6	7026.4	55.921	28.7
7	4552.6	36.233	45.8

Sample Name:
AD_117_94C
Data Collected on:
ormuzd-vnmrs500
Archive directory:
/home/walkup/vnmrsys/data/amilad
Sample directory:
AD_117_94C_20160926_02
FidFile: AD_117_94C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: d2o
Data collected on: Sep 26 2016

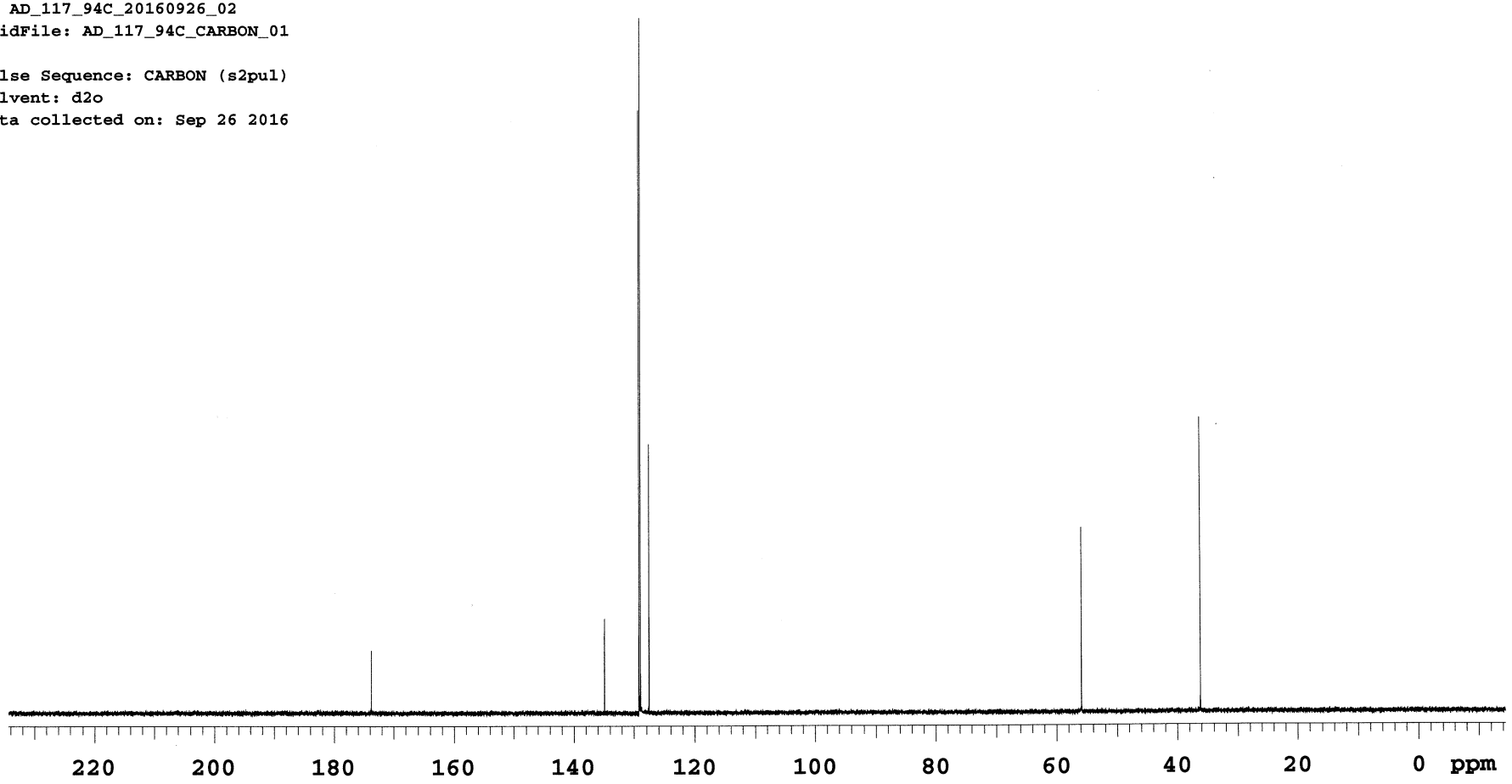


Figure S61. DEPT spectrum of 3-phenyllactic acid in D_2O

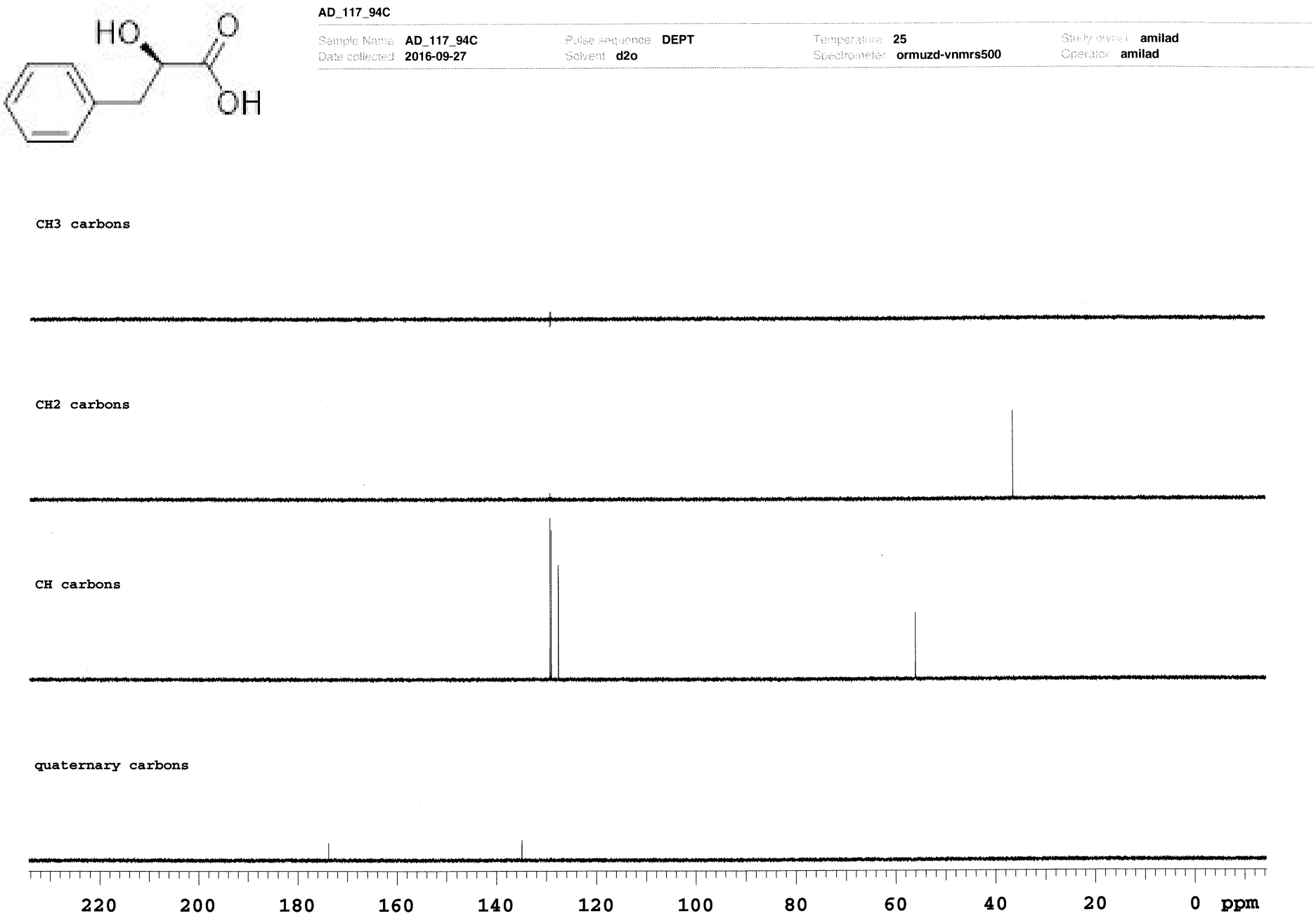


Figure S62. HMBC spectrum of 3-phenyllactic acid in D_2O

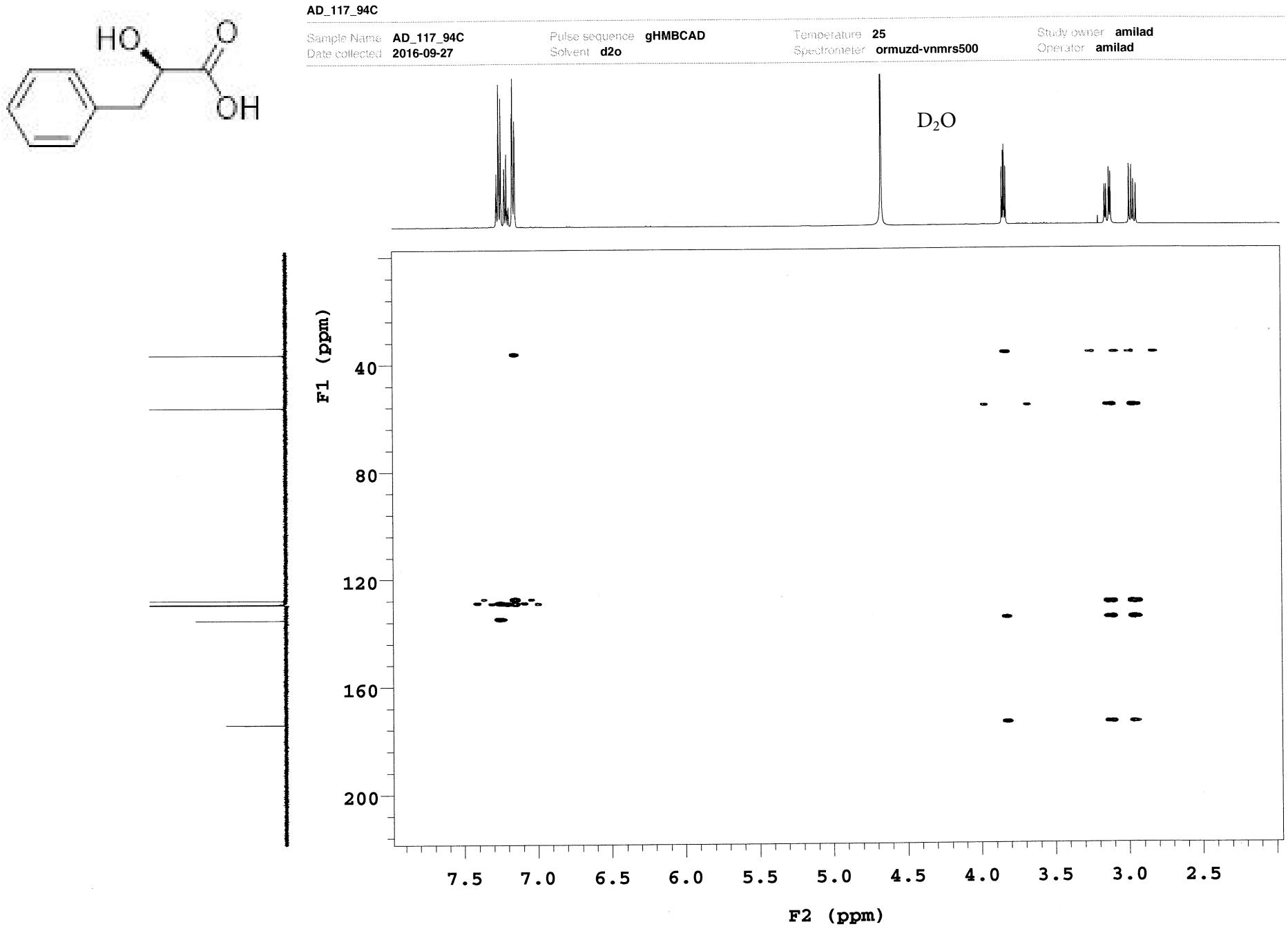
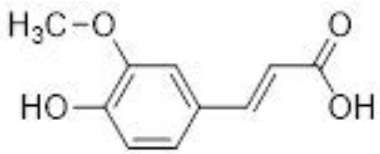


Figure S63. 1H NMR spectrum of ferulic acid in CD_3OD



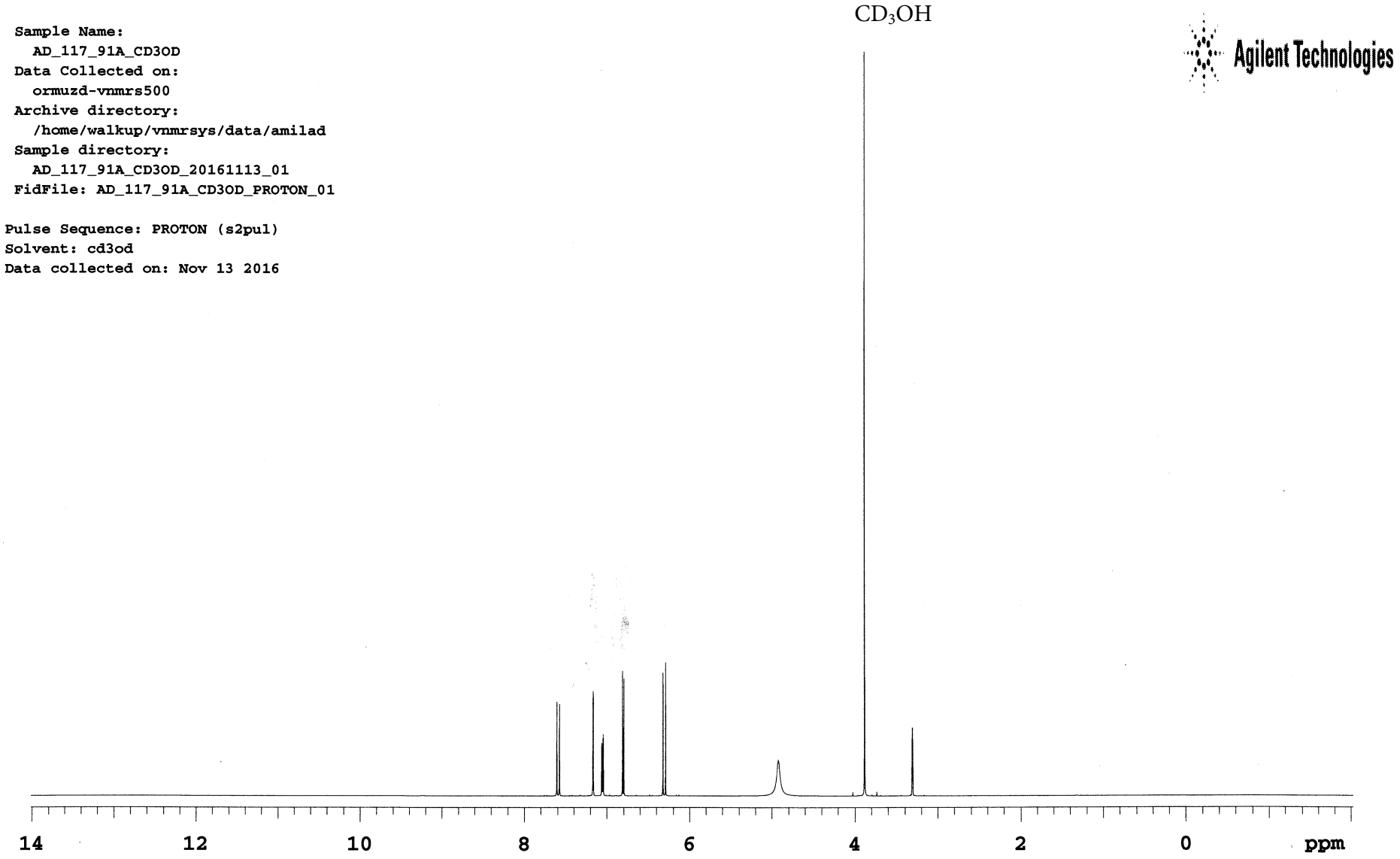


Figure S64. ^{13}C NMR spectrum of ferulic acid in CD_3OD

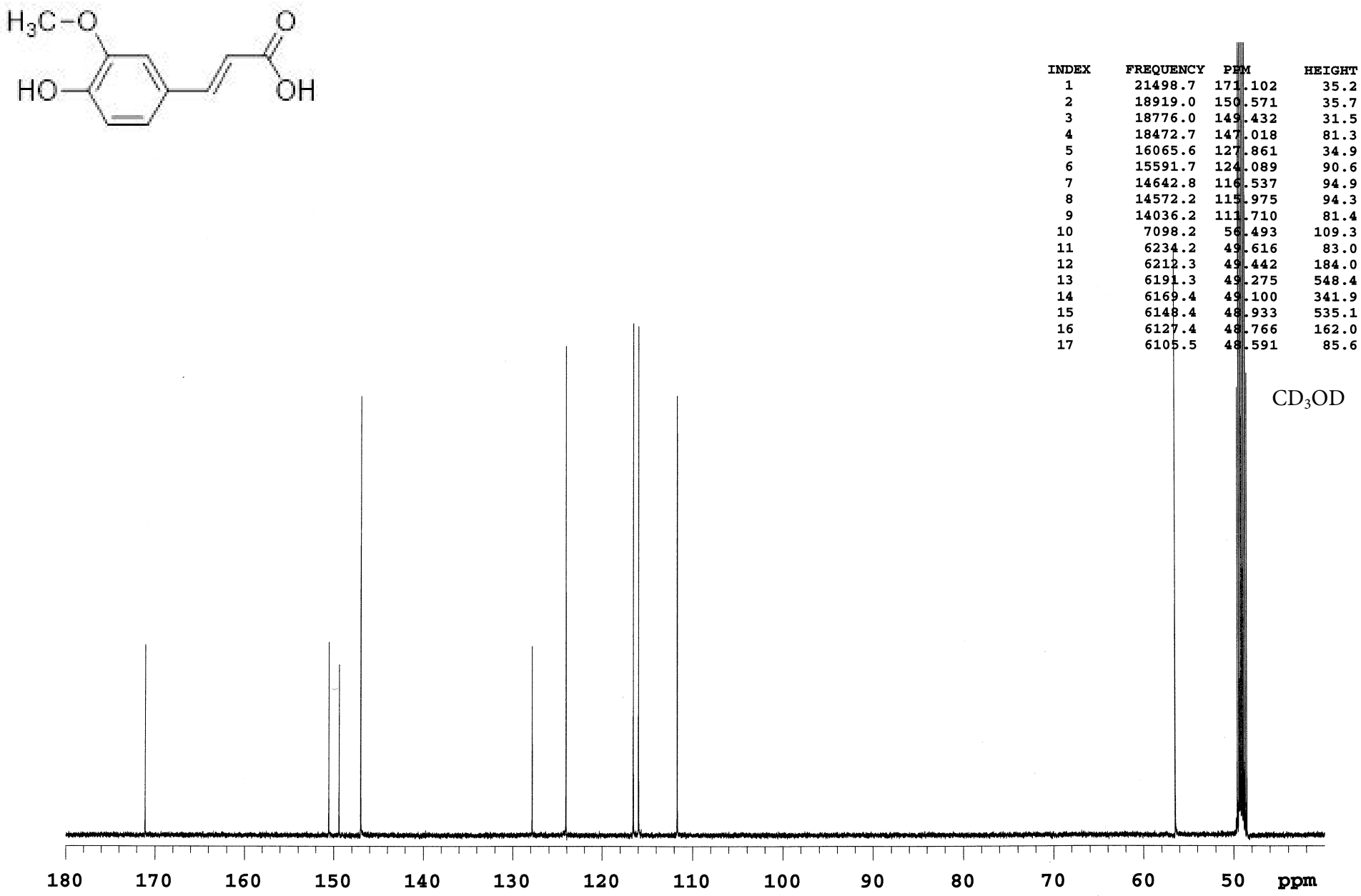


Figure S65. DEPT spectrum of ferulic acid in CD_3OD

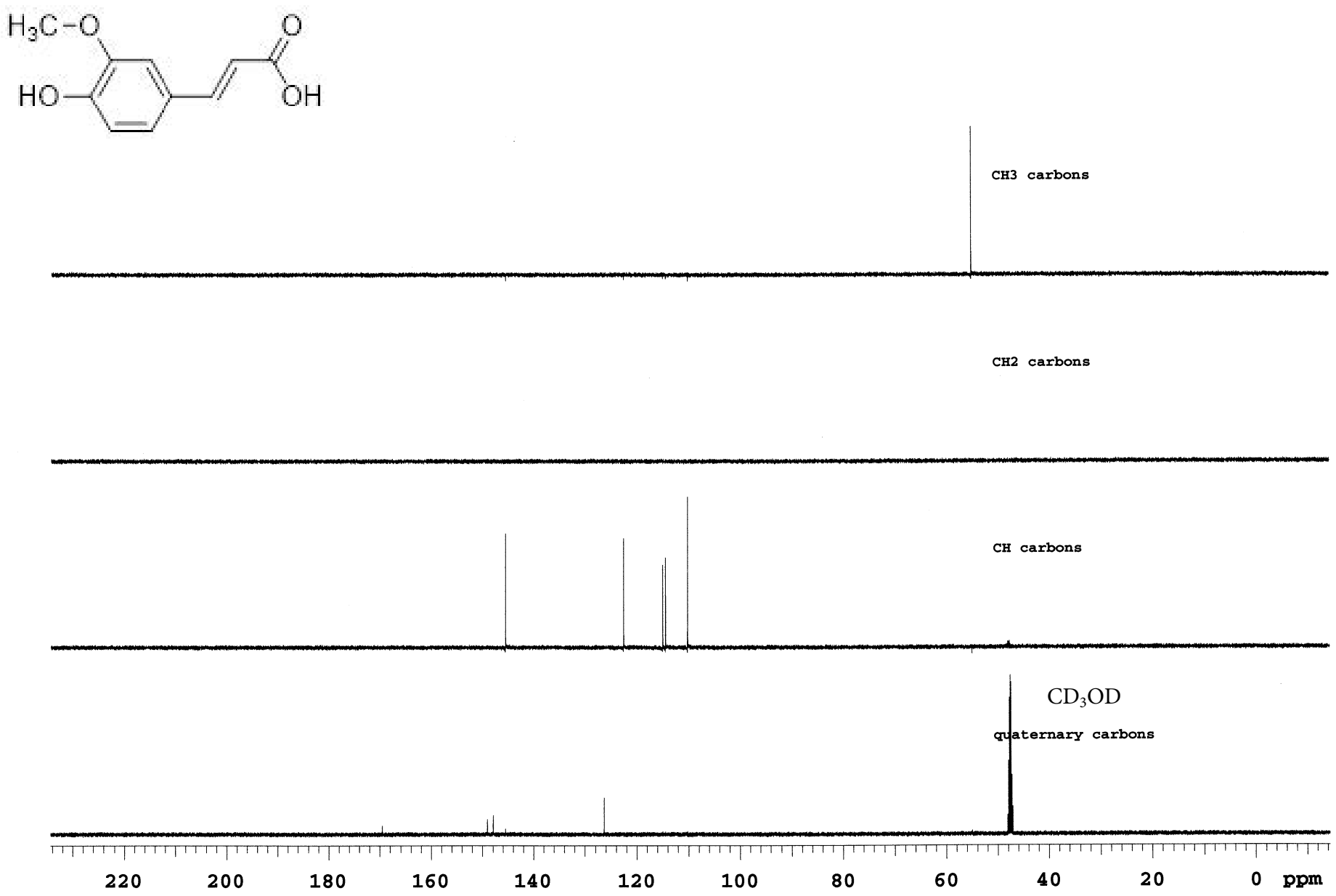


Table 2. LPO and COX assay results for known compounds isolated from *P. haussknechtii*

Compound	Concentration	LPO [a,b] (fluorescence)	COX-1 [a,c] (Inhibition %)	COX-2 [a,c] (Inhibition %)
isoimperatorin	92.6 µM	65.5 ± 0.7	25.0 ± 4.7	16.1 ± 1.8
osthol	102.5 µM	56.0 ± 0.5	58.7 ± 0.1	57.0 ± 3.1
	51.2 µM	ND [d]	46.7 ± 5.7	39.8 ± 0.2
	25.6 µM	ND [d]	35.8 ± 0.6	21.0 ± 0.2
	12.8 µM	ND [d]	19.6 ± 1.9	10.5 ± 0.2
oxypeucedanin	87.4 µM	38.5 ± 0.4	20.5 ± 0.6	29.7 ± 1.8
malic acid	186.5 µM	73.0 ± 0.8	12.2 ± 1.1	13.5 ± 1.8

[a]Values are expressed as mean ± SEM (n = 2). [b]Commercial antioxidants BHT, BHA and TBHQ with IC_{50} values of 10 µM, 6.9 µM and 5 µM, respectively. [c]The standards aspirin, ibuprofen and naproxen with IC_{50} values of 600 µM, 72.8 µM and 52.2 µM, respectively for the inhibition of COX-1 enzyme activity and Celebrex® and naproxen with IC_{50} values of 1.3 µM and 52.2 µM, respectively for the inhibition of COX-2 enzyme activity.