

Electronic Supplementary Information for

Unusual Constituents from the Medicinal Mushroom

Ganoderma lingzhi

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Contents

1 Crystal data of compounds 2 and 5	4
Table 1S. Crystal data and structure refinement for Cu_2_0m.....	4
Table 2S. Crystal data and structure refinement for Cu_5_0m.....	5
2. Supplementary Figures.....	6
Figure 1S. ¹ H NMR spectrum of 1 (600 MHz, CD ₃ OD).....	6
Figure 2S. ¹³ C NMR and DEPT spectra of 1 (150 MHz, CD ₃ OD).....	7
Figure 3S. HSQC spectrum of 1 (CD ₃ OD).....	8
Figure 4S. ¹ H- ¹ H COSY spectrum of 1 (CD ₃ OD).....	9
Figure 5S. HMBC spectrum of 1 (CD ₃ OD).....	10
Figure 6S. ROESY spectrum of 1 (CD ₃ OD).....	11
Figure 7S. HREIMS (+) report of 1	12
Figure 8S. ¹ H NMR spectrum of 2 (600 MHz, CDCl ₃).....	13
Figure 9S. ¹³ C NMR and DEPT spectra of 2 (150 MHz, CDCl ₃).....	14
Figure 10S. HSQC spectrum of 2 (CDCl ₃).....	15
Figure 11S. ¹ H- ¹ H COSY spectrum of 2 (CDCl ₃).....	16
Figure 12S. HMBC spectrum of 2 (CDCl ₃).....	17
Figure 13S. ROESY spectrum of 2 (CDCl ₃).....	18
Figure 14S. HREIMS (+) report of 2	19
Figure 15S. ¹ H NMR spectrum of 3 (600 MHz, CDCl ₃).....	20
Figure 16S. ¹³ C NMR and DEPT spectra of 3 (150 MHz, CDCl ₃).....	21
Figure 17S. HSQC spectrum of 3 (CDCl ₃).....	22
Figure 18S. ¹ H- ¹ H COSY spectrum of 3 (CDCl ₃).....	23
Figure 19S. HMBC spectrum of 3 (CDCl ₃).....	24
Figure 20S. ROESY spectrum of 3 (CDCl ₃).....	25
Figure 21S. HRESIMS (+) report of 3	26
Figure 22S. ¹ H NMR spectrum of 4 (600 MHz, CD ₃ OD).....	27
Figure 23S. ¹³ C NMR and DEPT spectra of 4 (150 MHz, CD ₃ OD).....	28
Figure 24S. HSQC spectrum of 4 (CD ₃ OD).....	29
Figure 25S. ¹ H- ¹ H COSY spectrum of 4 (CD ₃ OD).....	31
Figure 26S. HMBC spectrum of 4 (CD ₃ OD).....	32
Figure 27S. ROESY spectrum of 4 (CD ₃ OD).....	33
Figure 28S. HRESIMS (+) report of 4	34
Figure 29S. ¹ H NMR spectrum of 5 (600 MHz, CD ₃ OD).....	35
Figure 30S. ¹³ C NMR and DEPT spectra of 5 (150 MHz, CD ₃ OD).....	36
Figure 31S. HSQC spectrum of 5 (CD ₃ OD).....	37
Figure 32S. ¹ H- ¹ H COSY spectrum of 5 (CD ₃ OD).....	38
Figure 33S. HMBC spectrum of 5 (CD ₃ OD).....	39
Figure 34S. ROESY spectrum of 5 (CD ₃ OD).....	40
Figure 35S. HRESIMS (+) report of 5	41
Figure 36S. ¹ H NMR spectrum of 6 and 7 (600 MHz, CDCl ₃).....	41
Figure 37S. ¹³ C NMR and DEPT spectra of 6 and 7 (150 MHz, CDCl ₃).....	43
Figure 38S. HSQC spectrum of 6 and 7 (CDCl ₃).....	44

Figure 39S. ^1H - ^1H COSY spectrum of 6 and 7 (CDCl_3).....	45
Figure 40S. HMBC spectrum of 6 and 7 (CDCl_3)	46
Figure 41S. ROESY spectrum of 6 and 7 (CDCl_3).....	47
Figure 42S. HREIMS (+) report of 6	48
Figure 43S. HRESIMS (+) report of 7	49
Figure 44S. ^1H NMR spectrum of 8 (600 MHz, CDCl_3)	50
Figure 45S. ^{13}C NMR and DEPT spectra of 8 (150 MHz, CDCl_3).....	51
Figure 46S. HSQC spectrum of 8 (CDCl_3)	52
Figure 47S. ^1H - ^1H COSY spectrum of 8 (CDCl_3)	53
Figure 48S. HMBC spectrum of 8 (CDCl_3)	54
Figure 49S. HREIMS (+) report of 8	55
Figure 50S. ^1H NMR spectrum of 9 (500 MHz, CDCl_3)	56
Figure 51S. ^{13}C NMR and DEPT spectra of 9 (125 MHz, CDCl_3).....	57
Figure 52S. ^1H NMR spectrum of 9a (800 MHz, CDCl_3)	58
Figure 53S. ^{13}C NMR and DEPT spectra of 9a (200 MHz, CDCl_3).....	59
3. Computational details for 8	60
Table 3S. Important thermodynamic parameters (a. u.) of the optimized 8 at B3LYP/6-31G(d,p) level in the gas phase.	61
Table 4S. Conformational analysis of 8 (^a Relative energy; ^b Conformational distribution)	61
References	61

1. Crystal data of compounds 1 and 5

Table 1S. Crystal data and structure refinement for Cu_1_0m

Identification code	Cu_1_0m	
Empirical formula	C ₁₅ H ₂₂ O ₂	
Formula weight	234.32	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 7.70800(10) Å	α = 90°.
	b = 12.5490(2) Å	β = 90°.
	c = 13.1278(2) Å	γ = 90°.
Volume	1269.82(3) Å ³	
Z	4	
Density (calculated)	1.226 mg/m ³	
Absorption coefficient	0.621 mm ⁻¹	
F(000)	512	
Crystal size	0.850 x 0.220 x 0.190 mm ³	
Theta range for data collection	4.875 to 70.187°.	
Index ranges	-8<=h<=9, -15<=k<=14, -15<=l<=14	
Reflections collected	8045	
Independent reflections	2306 [R(int) = 0.0442]	
Completeness to theta = 67.679°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2306 / 0 / 161	
Goodness-of-fit on F ²	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0513, wR2 = 0.1314	
R indices (all data)	R1 = 0.0513, wR2 = 0.1315	
Absolute structure parameter	0.09(6)	
Extinction coefficient	0.0064(17)	
Largest diff. peak and hole	0.292 and -0.319 e.Å ⁻³	

Table 2S. Crystal data and structure refinement for Cu_5_0m

Identification code	Cu_5_0m		
Empirical formula	C ₁₆ H ₂₄ O ₄		
Formula weight	280.35		
Temperature	100(2) K		
Wavelength	1.54178 Å		
Crystal system	Monoclinic		
Space group	P2 ₁		
Unit cell dimensions	a = 6.4948(2) Å	α = 90°.	
	b = 7.4524(3) Å	β = 101.0040(10)°.	
	c = 15.2812(6) Å	γ = 90°.	
Volume	726.04(5) Å ³		
Z	2		
Density (calculated)	1.282 mg/m ³		
Absorption coefficient	0.736 mm ⁻¹		
F(000)	304		
Crystal size	0.640 x 0.420 x 0.100 mm ³		
Theta range for data collection	2.946 to 70.141°.		
Index ranges	-7<=h<=7, -8<=k<=8, -15<=l<=17		
Reflections collected	7540		
Independent reflections	2510 [R(int) = 0.0263]		
Completeness to theta = 67.679°	94.8 %		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	2510 / 1 / 191		
Goodness-of-fit on F ²	1.056		
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0844		
R indices (all data)	R1 = 0.0327, wR2 = 0.0845		
Absolute structure parameter	0.17(3)		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.217	and	-0.260 e.Å ⁻³

2. Supplementary Figures

Figure 1S. ^1H NMR spectrum of **1** (600 MHz, CDCl_3)

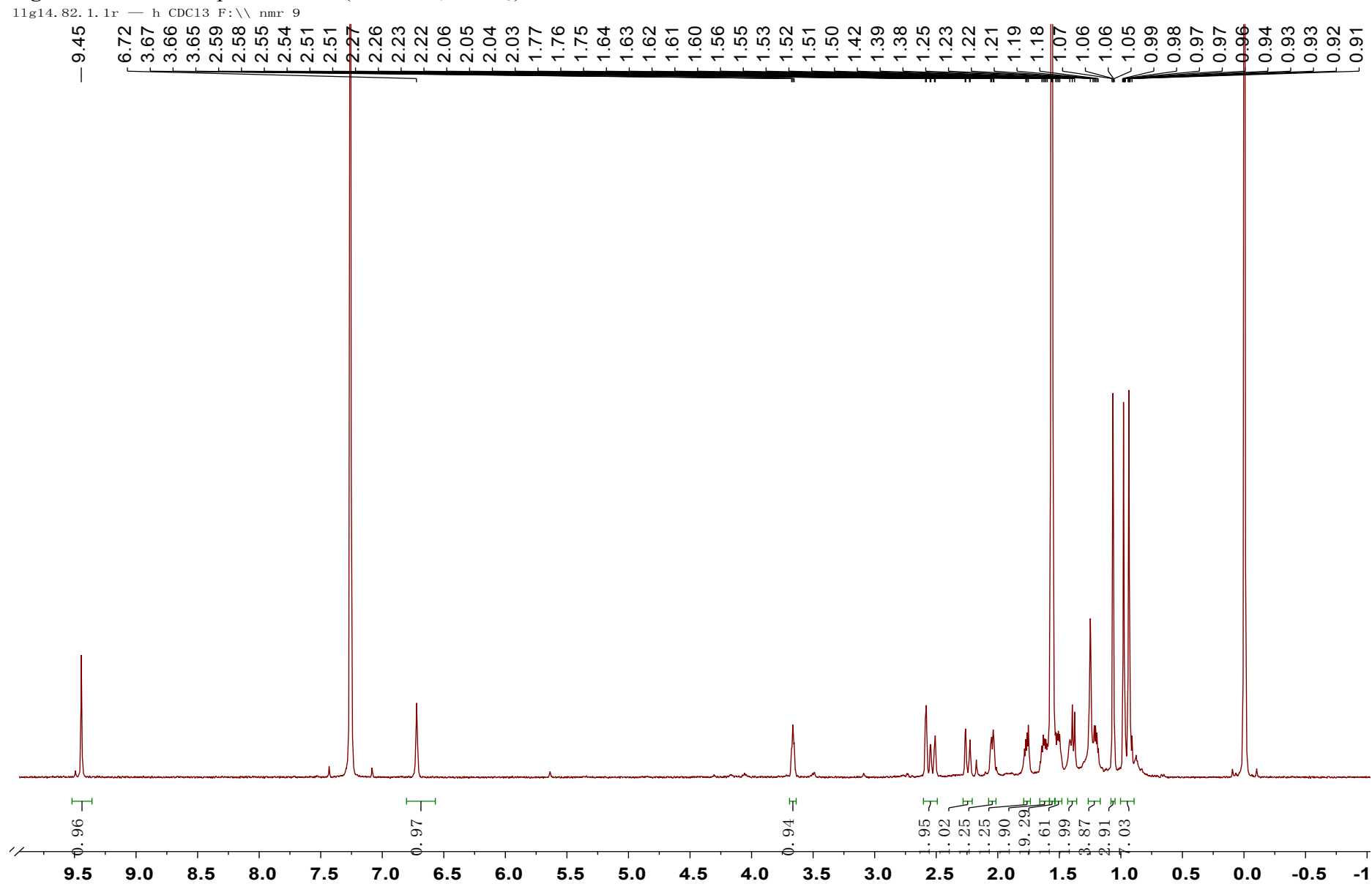


Figure 2S. ^{13}C NMR and DEPT spectra of **1** (150 MHz, CDCl_3)

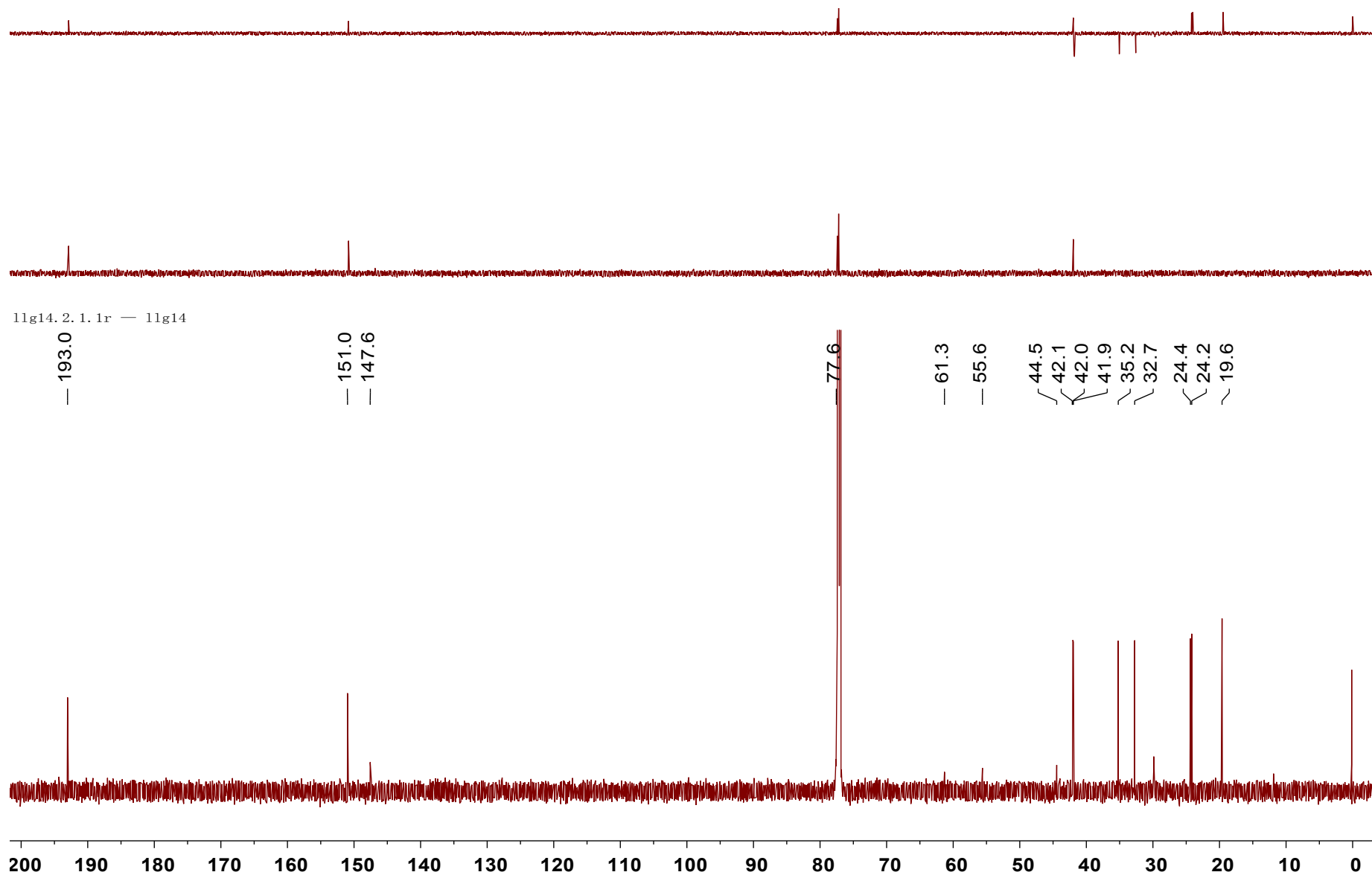


Figure 3S. HSQC spectrum of **1** (CDCl₃)

11g14.86.1.2rr — hsqc CDC13 av600

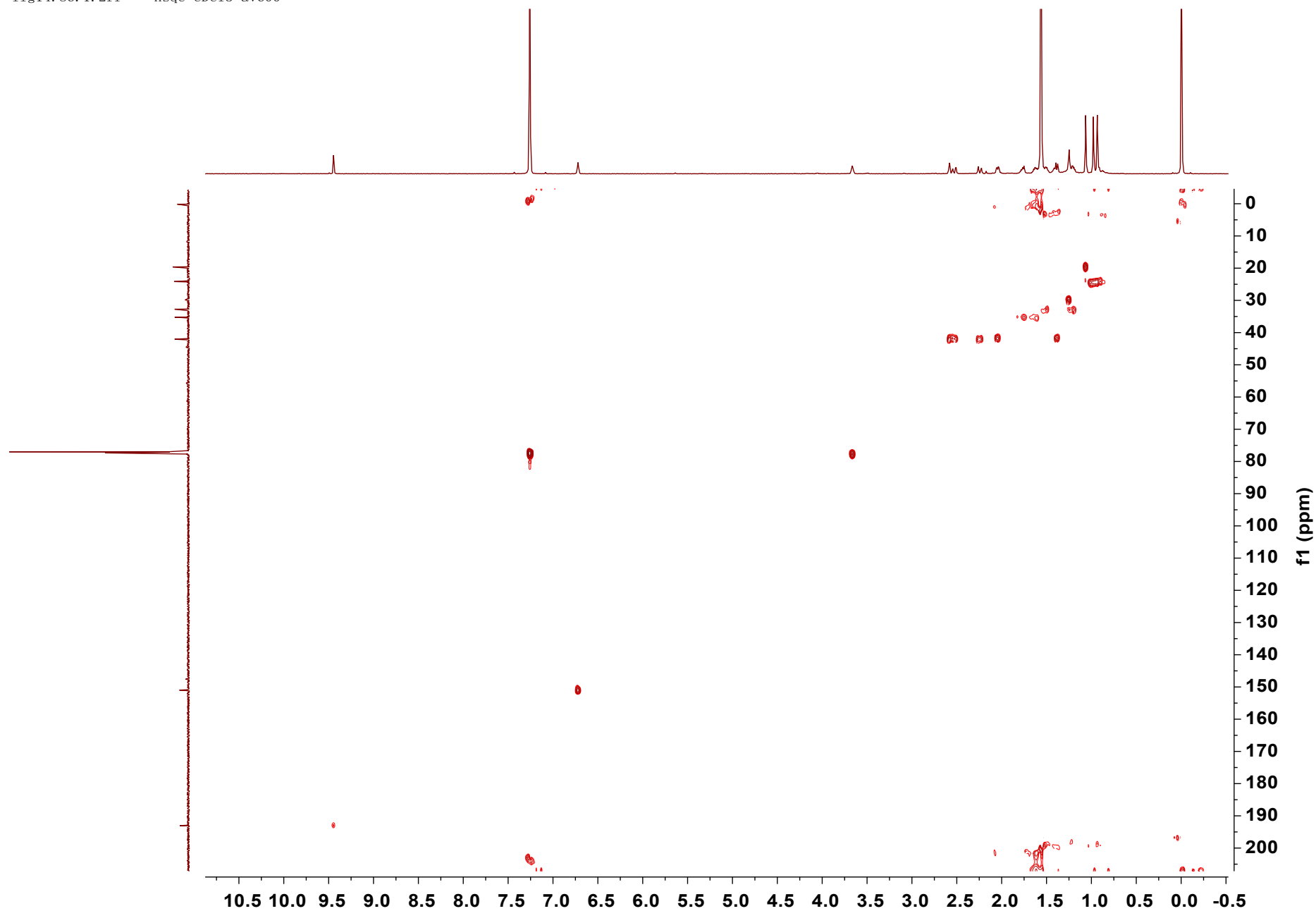


Figure 4S. ^1H - ^1H COSY spectrum of **1** (CDCl_3)

11g14.84.1.2rr — cosy CDC13 av600

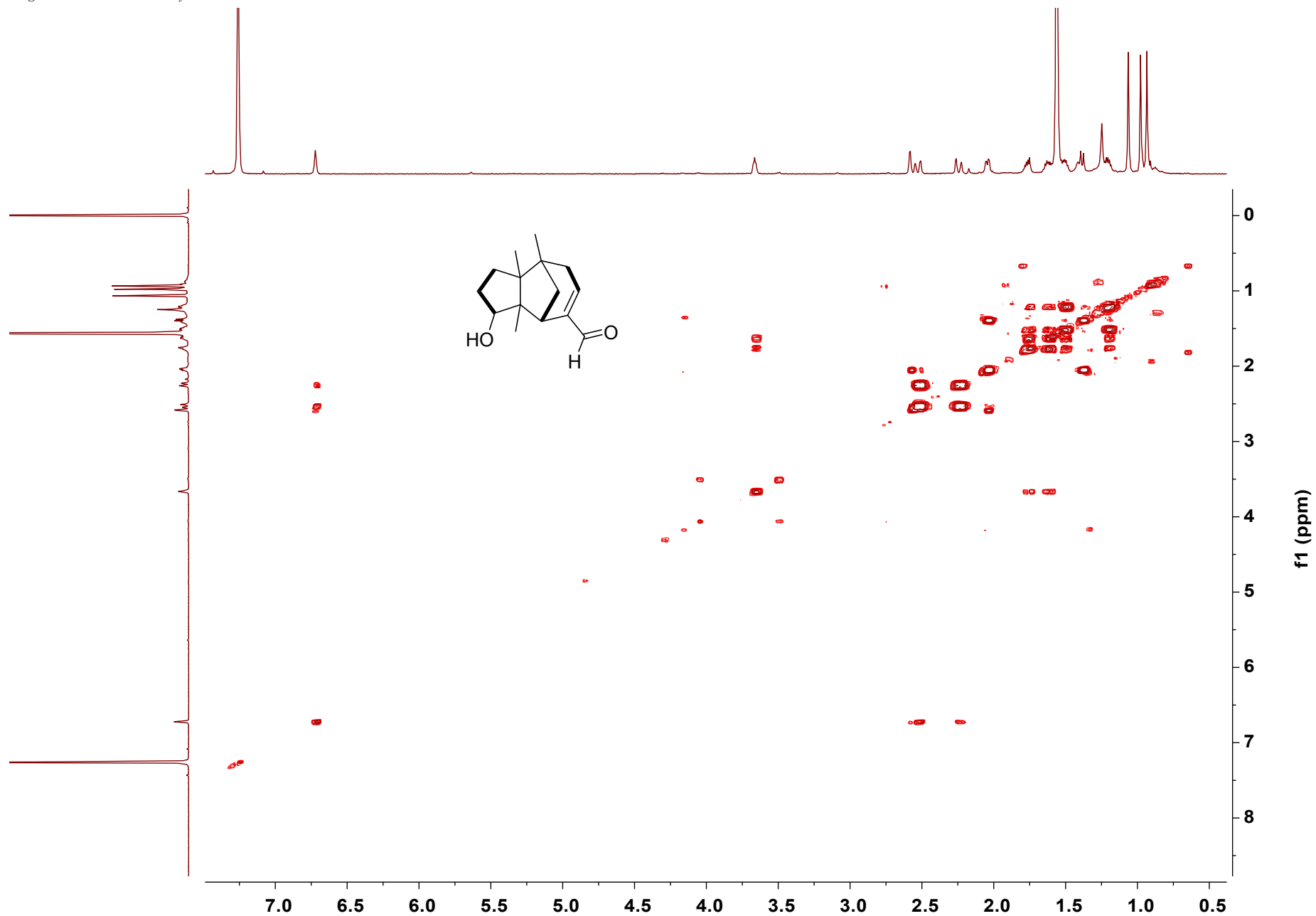


Figure 5S. HMBC spectrum of **1** (CDCl₃)

11g14.85.1.2rr — hmbe CDC13 av600

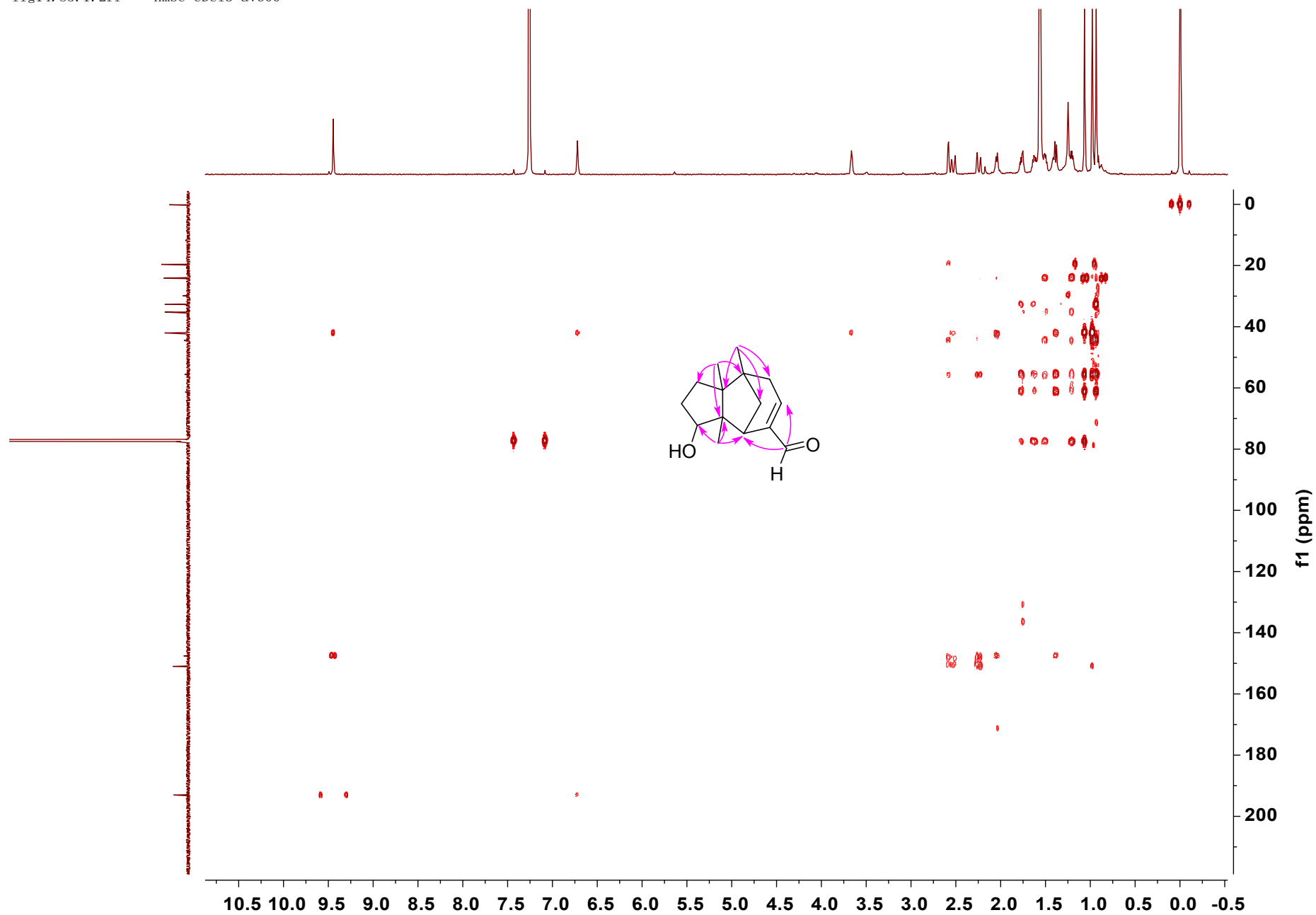


Figure 6S. ROESY spectrum of **1** (CDCl₃)

11g14.83.1.2rr — roesy CDC13 av600

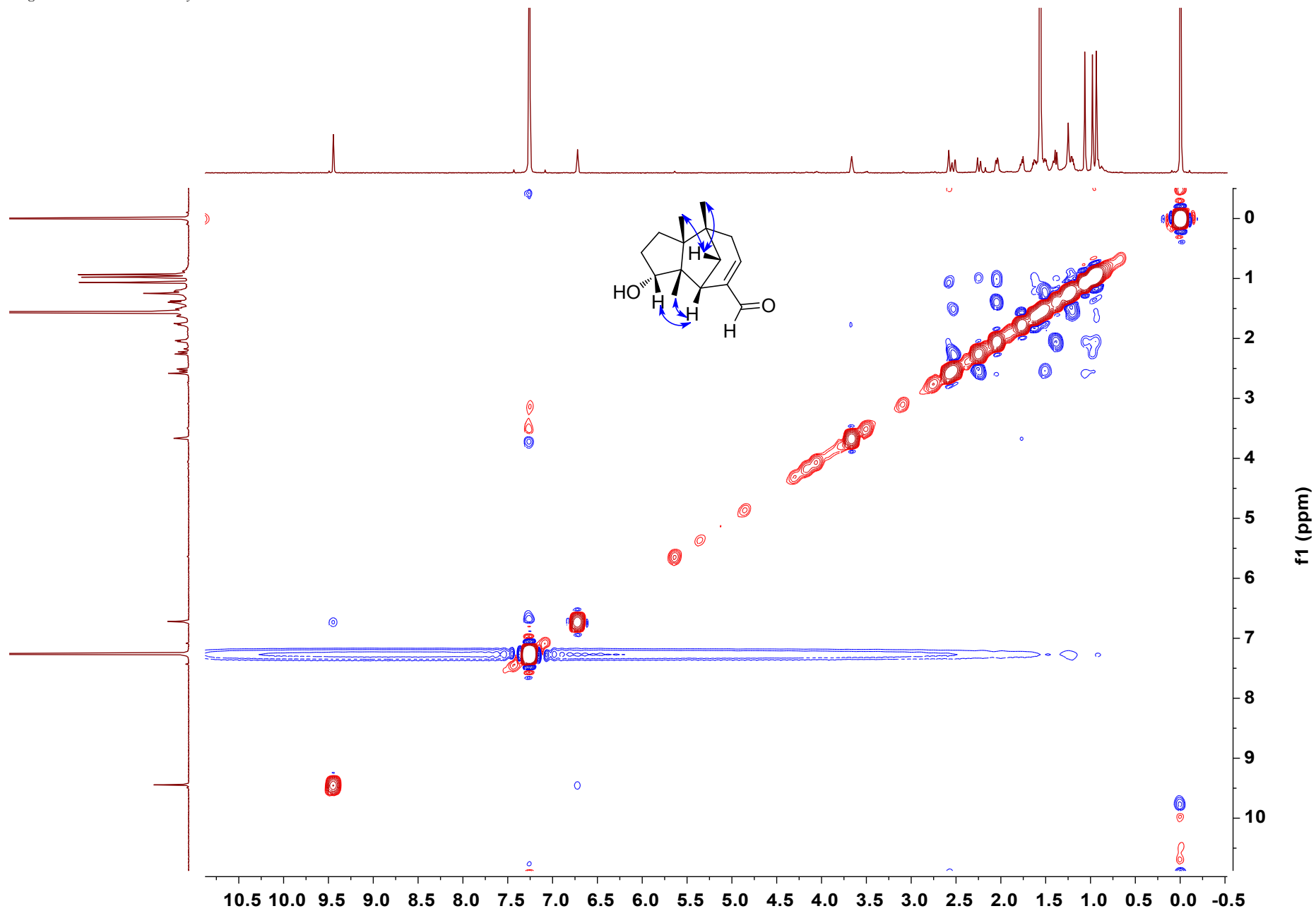


Figure 7S. HREIMS (+) report of 1

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-3

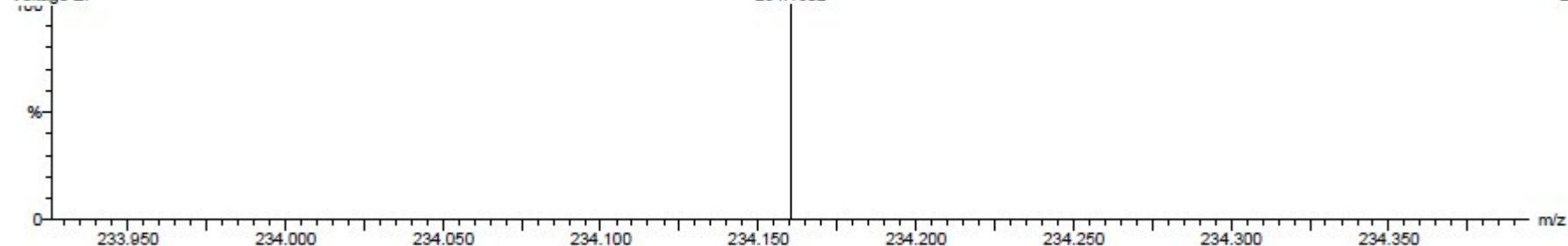
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17:13:11 14-Apr-2017

Voltage EI+

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234.1602

Autospec Premier
P778
2



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
234.1602	234.1620	-1.8	-7.7	5.0	5546025.5	C15 H22 O2

Figure 8S. ¹H NMR spectrum of **2** (600 MHz, CD₃OD)

11g7.82.1.1r - h MeOD F:\ nmr 21

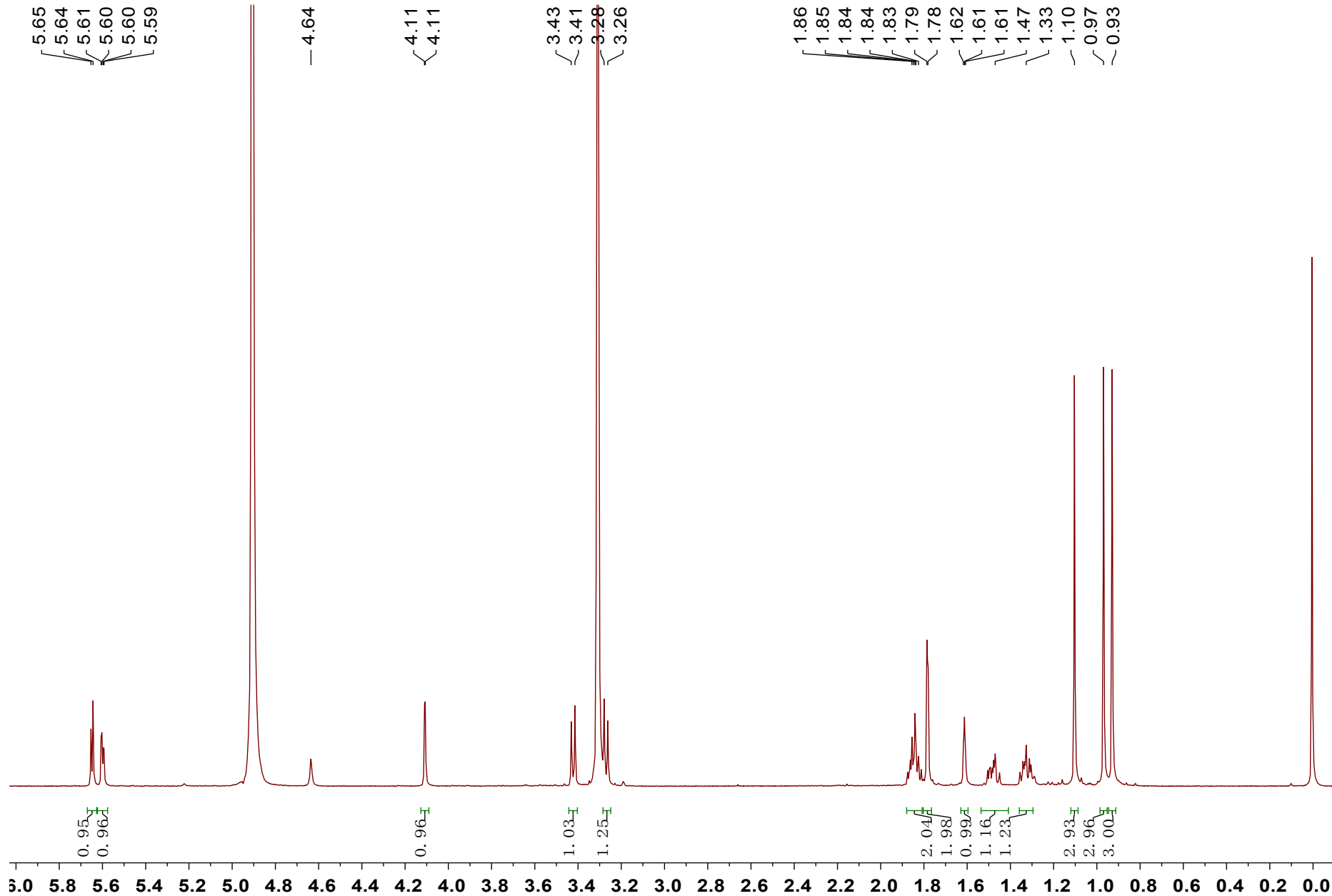


Figure 9S. ^{13}C NMR and DEPT spectra of **2** (150 MHz, CD_3OD)

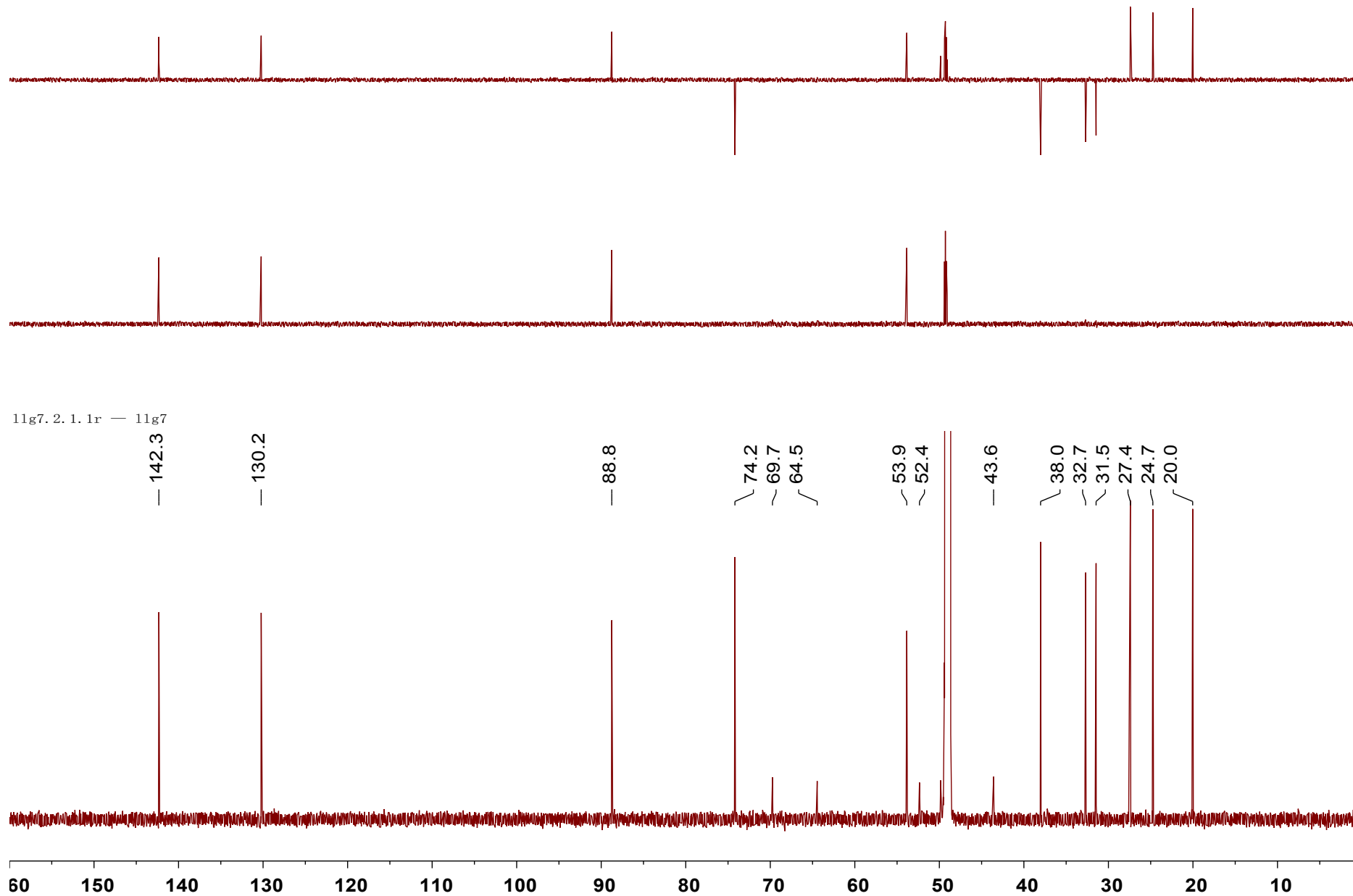


Figure 10S. HSQC spectrum of **2** (CD₃OD)

pdata/1 — hsqc MeOD av600

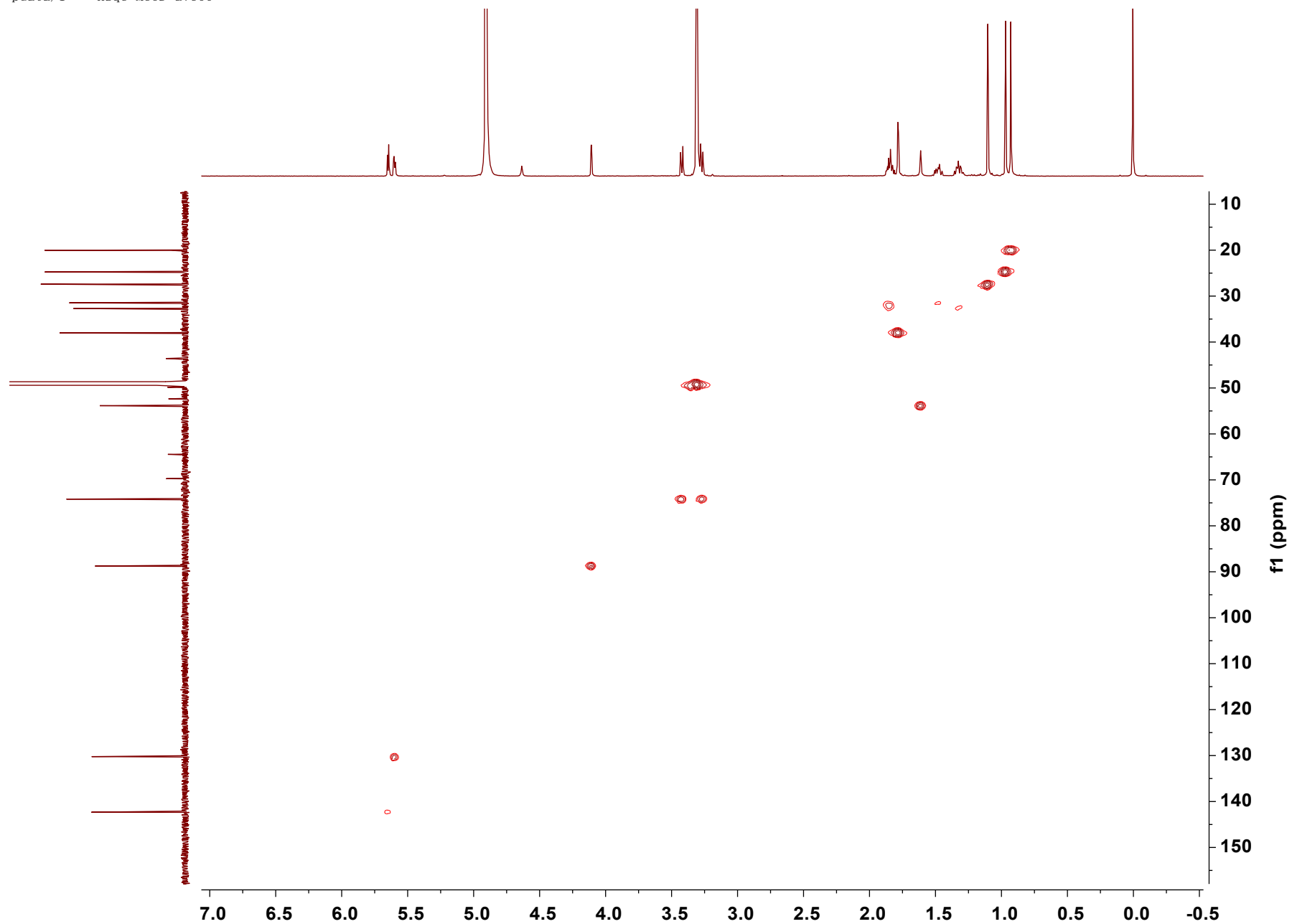


Figure 11S. ^1H - ^1H COSY spectrum of **2** (CD_3OD)

11g7.84.1.2rr — cosy MeOD av600

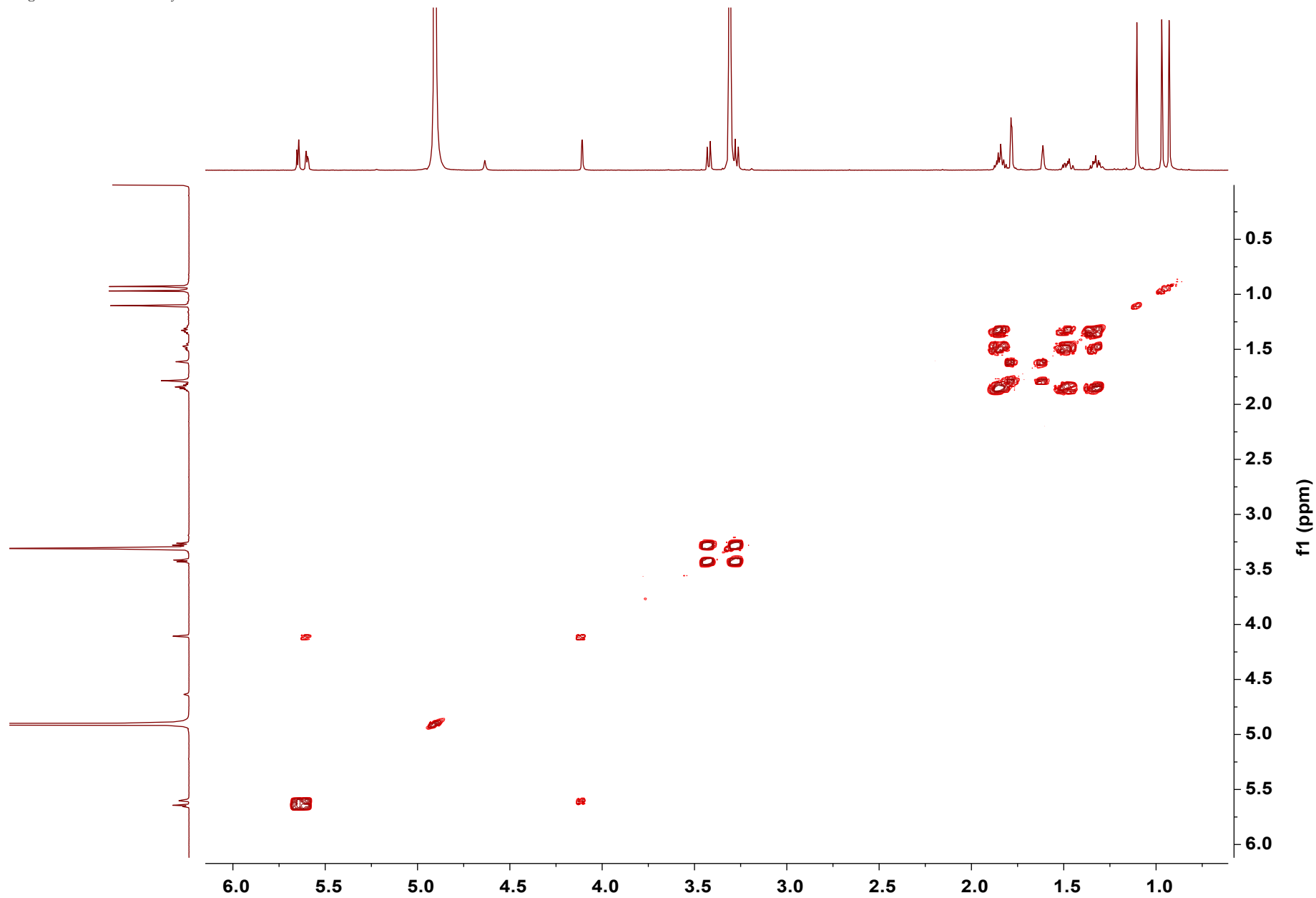


Figure 12S. HMBC spectrum of **2** (CD₃OD)

11g7.85.1.2rr — hmbc MeOD av600

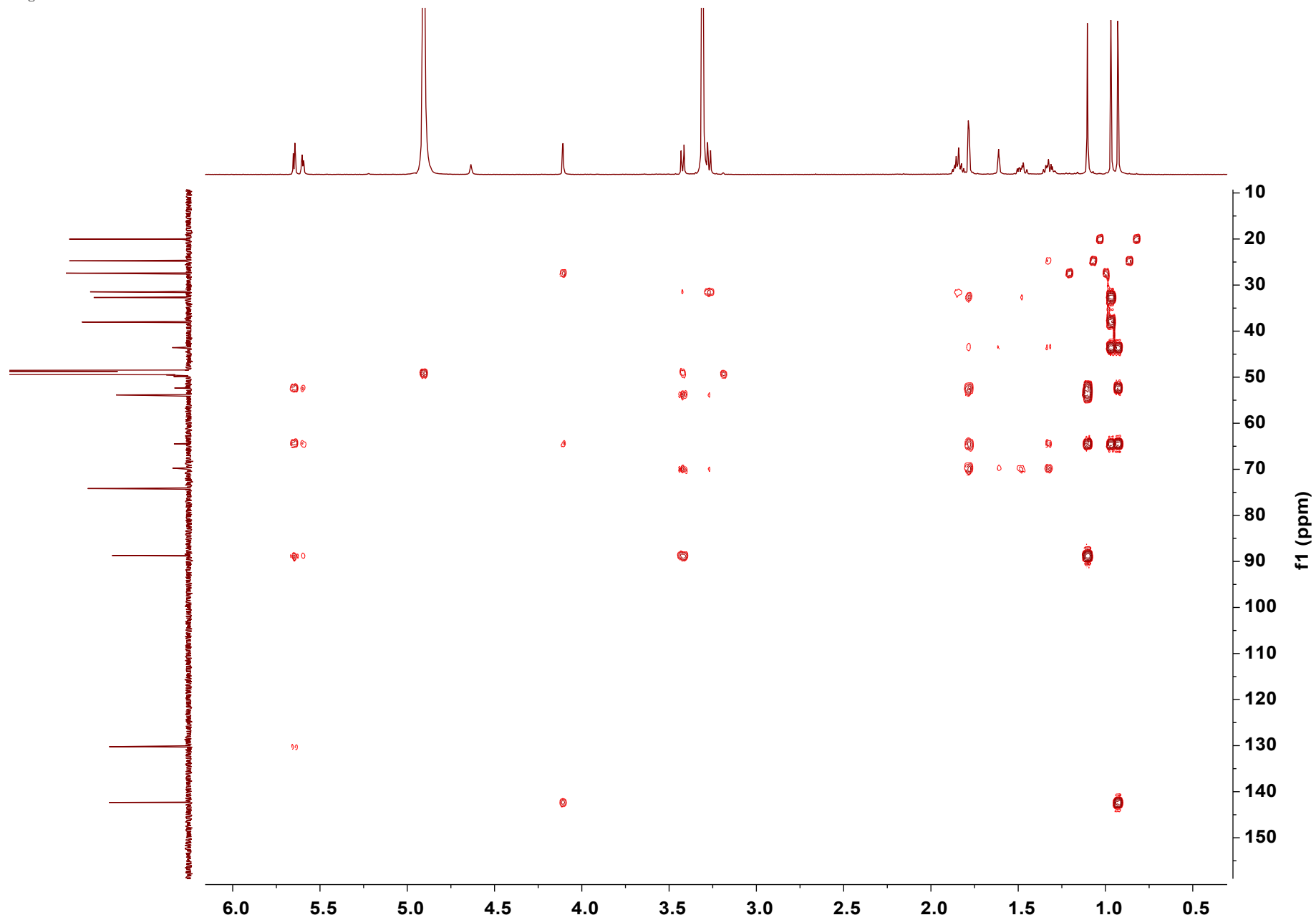


Figure 13S. ROESY spectrum of **2** (CD₃OD)

11g7.83.1.2rr — roesy_pr MeOD av600

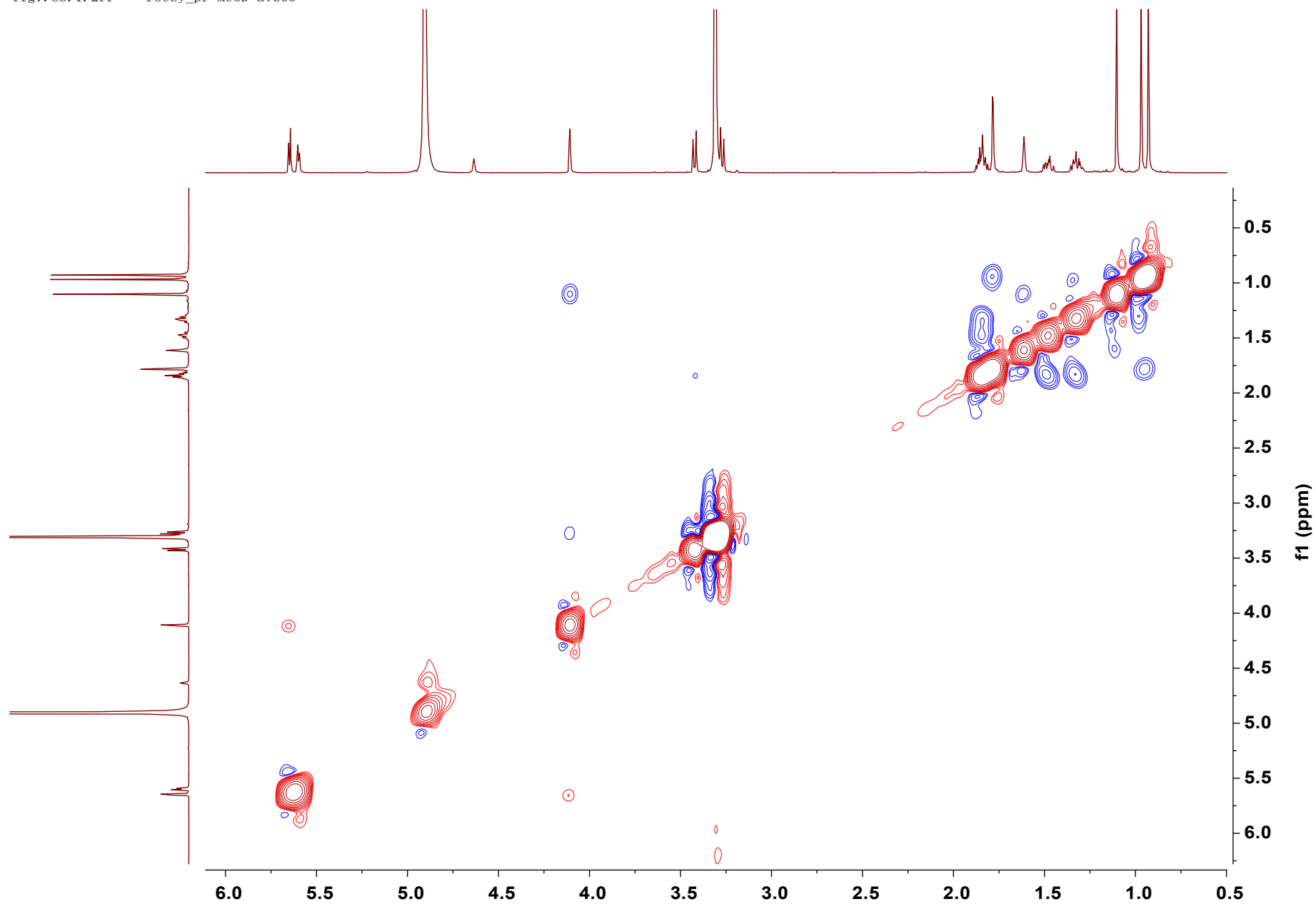


Figure 14S. HREIMS (+) report of 2.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-3

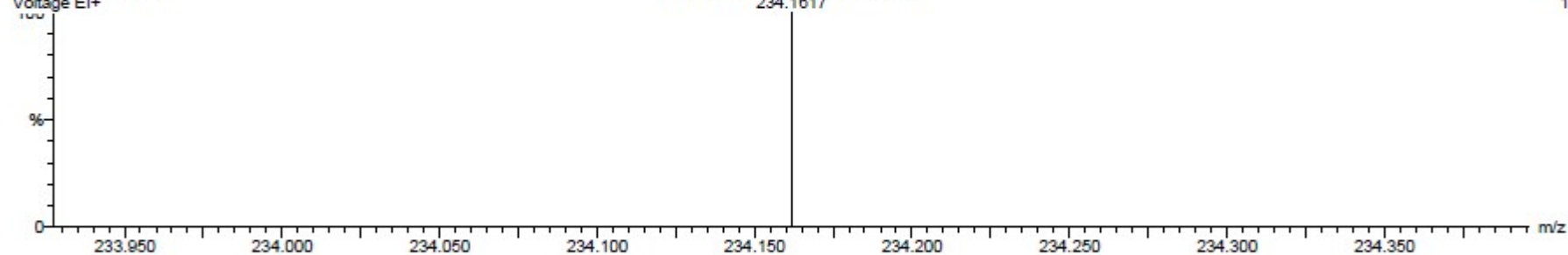
Ilg7

17:22:56 14-Apr-2017

Voltage EI+

KIB
M170414EA-01AFAMM 14 (1.286)
234.1617

Autospec Premier
P776
1



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
234.1617	234.1620	-0.3	-1.3	5.0	5546026.0	C15 H22 O2

Figure 15S. ^1H NMR spectrum of **3** (600 MHz, CDCl_3)

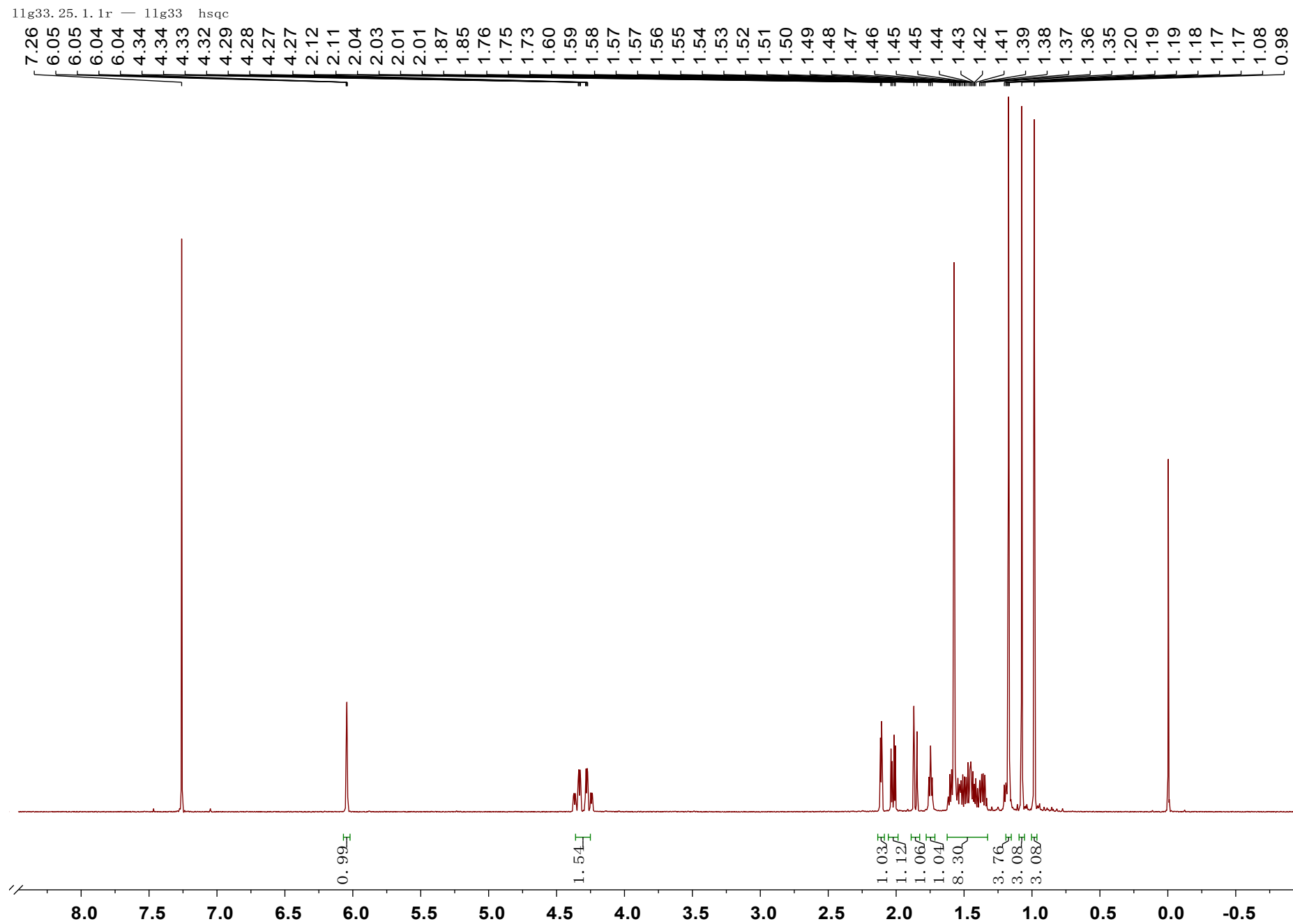


Figure 16S. ^{13}C NMR and DEPT spectra of **3** (150 MHz, CDCl_3)

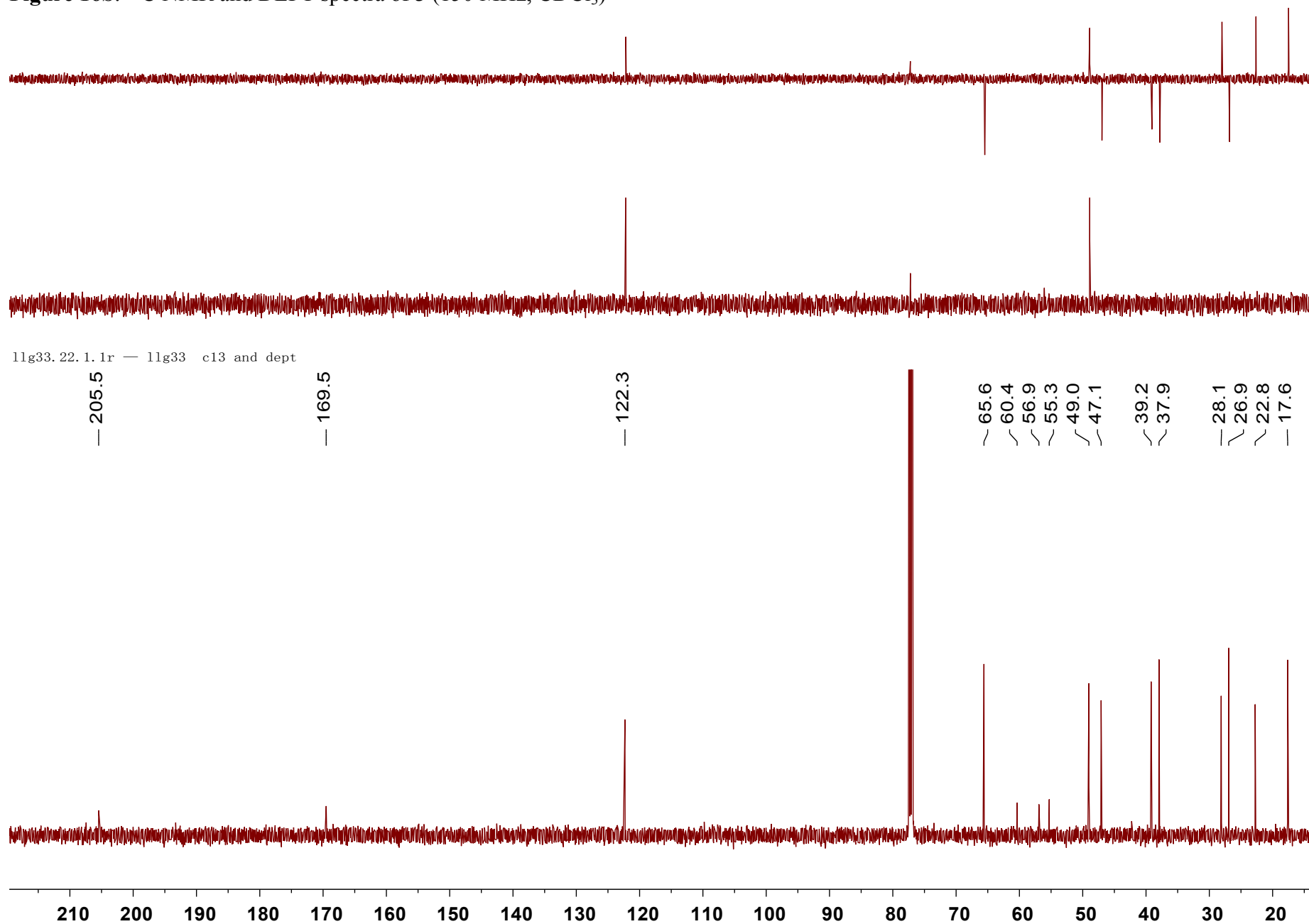


Figure 17S. HSQC spectrum of **3** (CDCl₃)

11g33.27.1.2rr — 11g33 hsqc

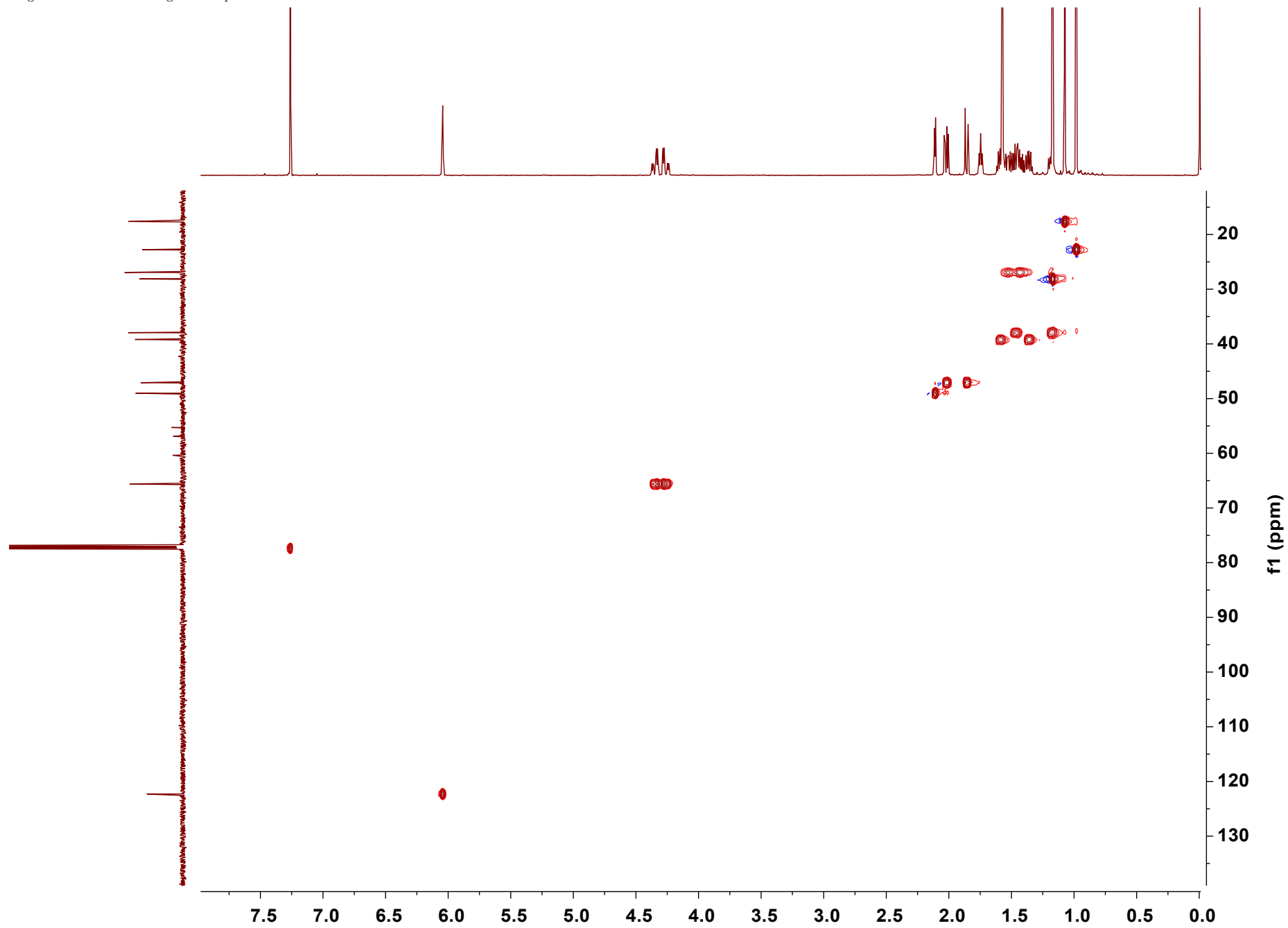


Figure 18S. ^1H - ^1H COSY spectrum of **3** (CDCl_3)

11g33.26.1.2rr — 11g33 cosy

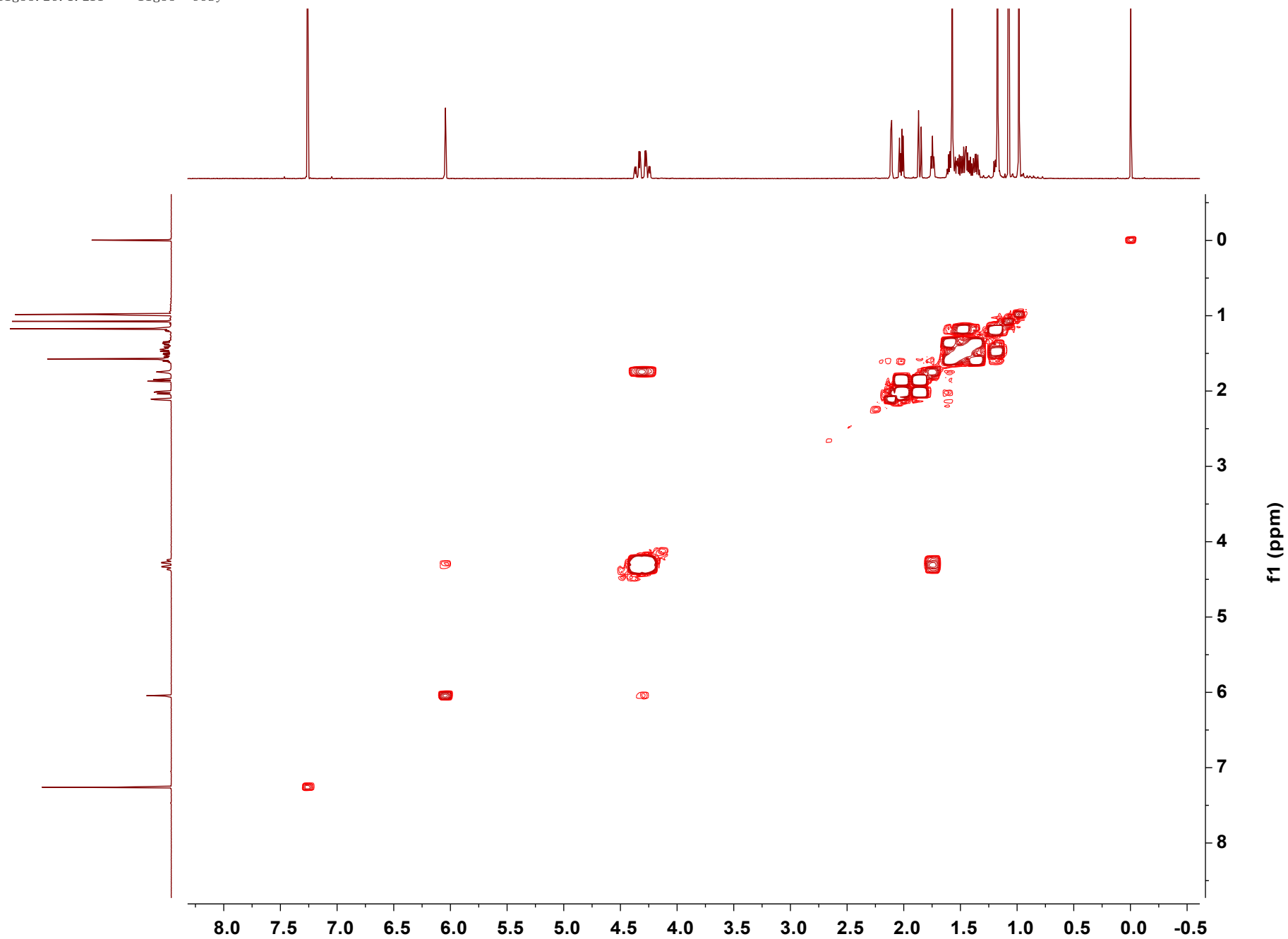


Figure 19S. HMBC spectrum of **3** (CDCl₃)

11g33.28.1.2rr — 11g33 hmbc

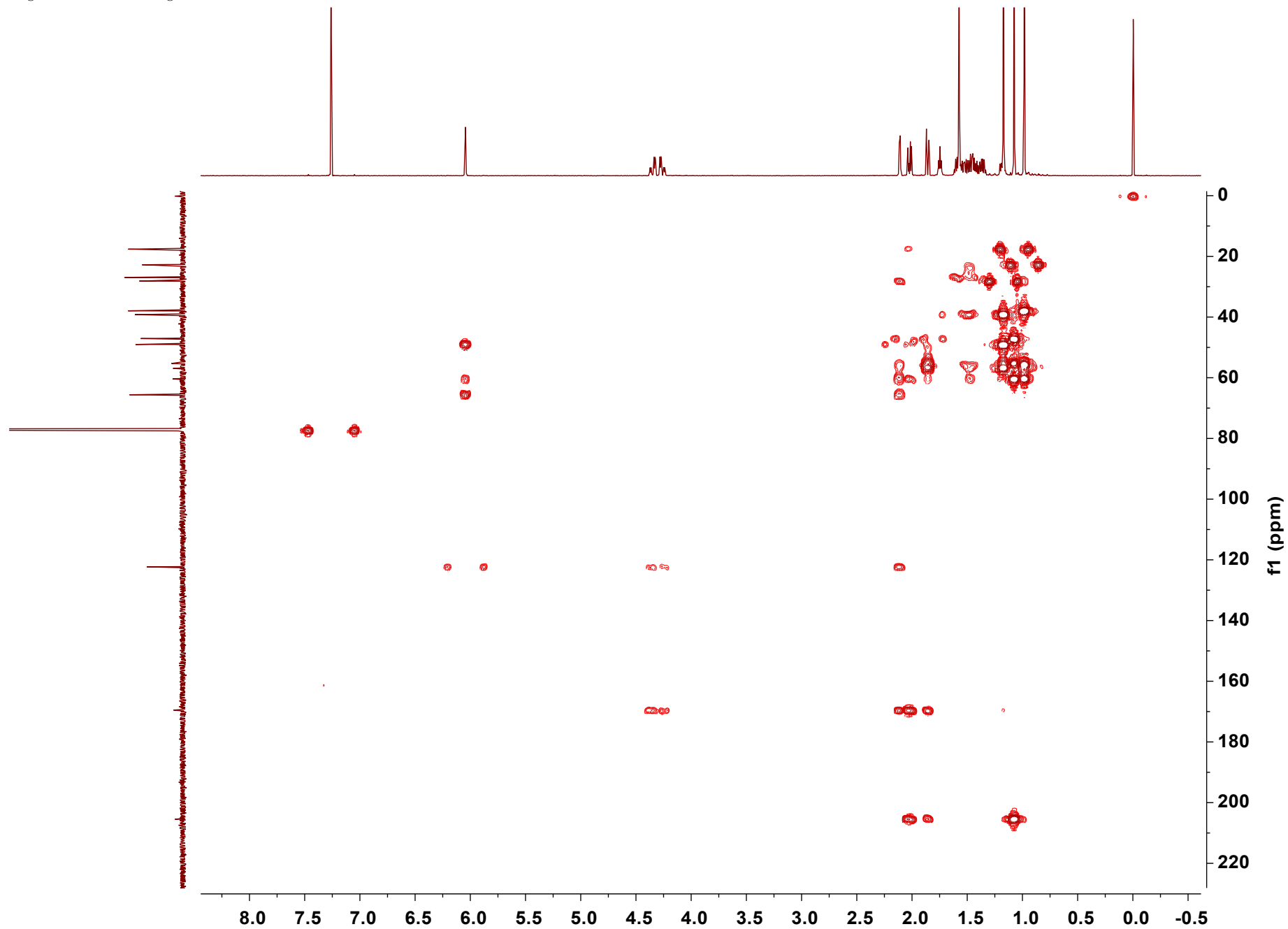


Figure 20S. ROESY spectrum of **3** (CDCl₃)

11g33.29.1.2rr — 11g33 roesy

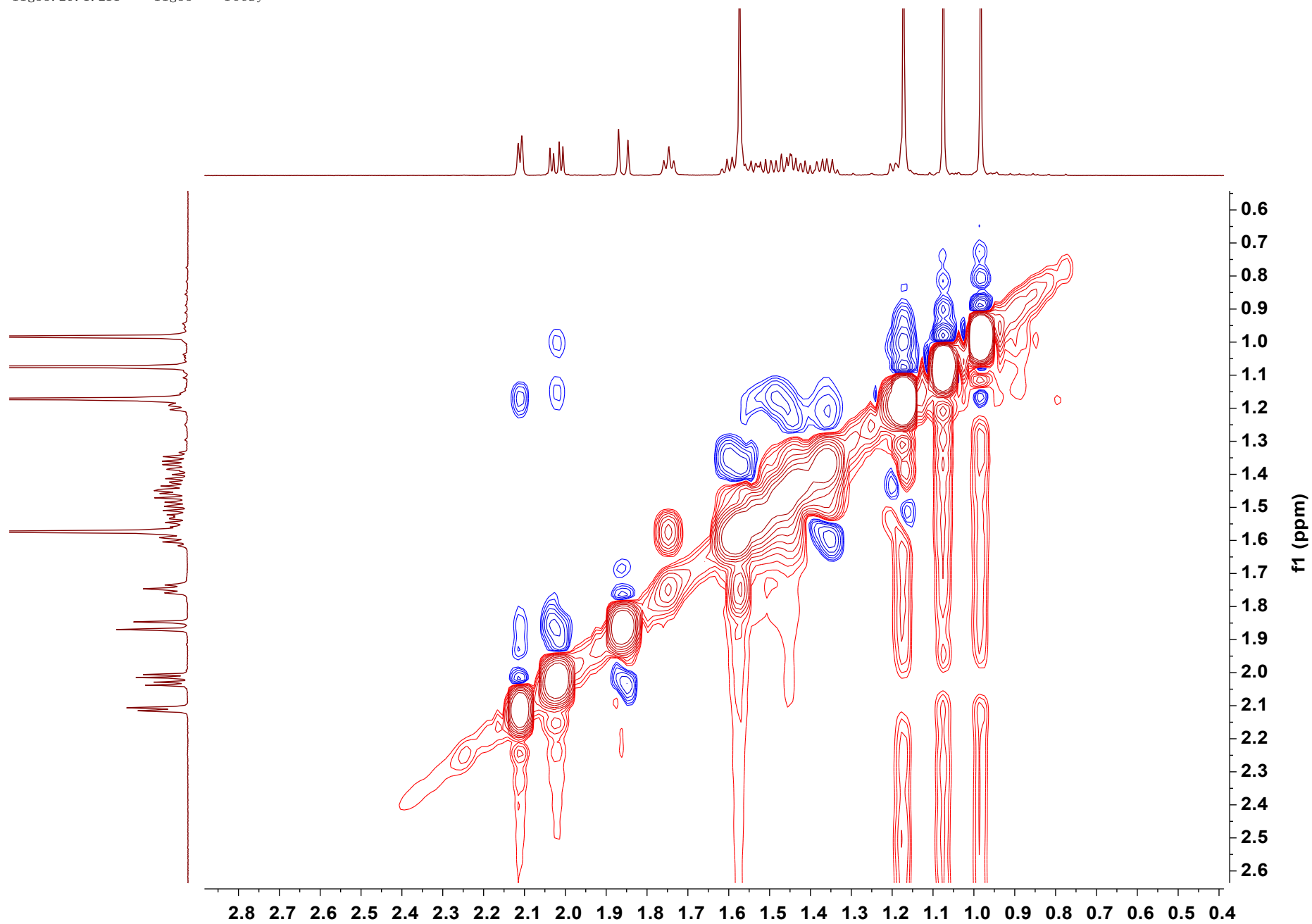


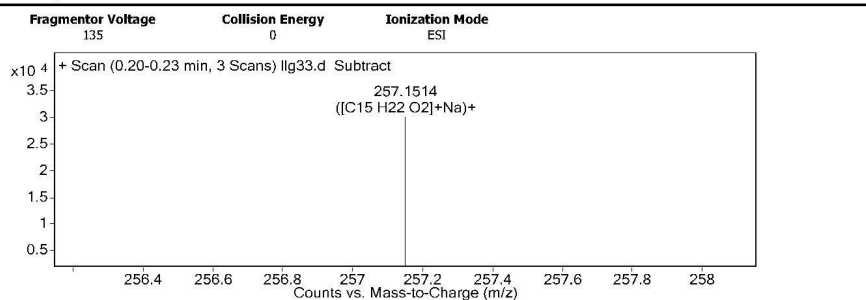
Figure 21S. HRESIMS (+) report of 3

Qualitative Analysis Report

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Acq Method	s-HRp.m	Acquired Time	3/9/2017 4:47:34 PM
IRM Calibration Status	Success	DA Method	sibu.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (85125.2)

User Spectra



m/z	z	Abund	Formula	Ion
122.0814	1	9480.3		
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258.1545	1	4738.96	C15 H22 O2	(M+Na)+
273.1274	1	7475.14		
317.1736	1	6282.44		
471.1962	1	13362.15		
472.2004	1	3624.74		
1122.4535	1	4067.84		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O2	234.1620	257.1512	257.1514	-0.4	-1.6	5.0000

--- End Of Report ---

Figure 22S. ¹H NMR spectrum of 4 (600 MHz, CD₃OD)

11gal4a.1.1.1r - 11gal4a

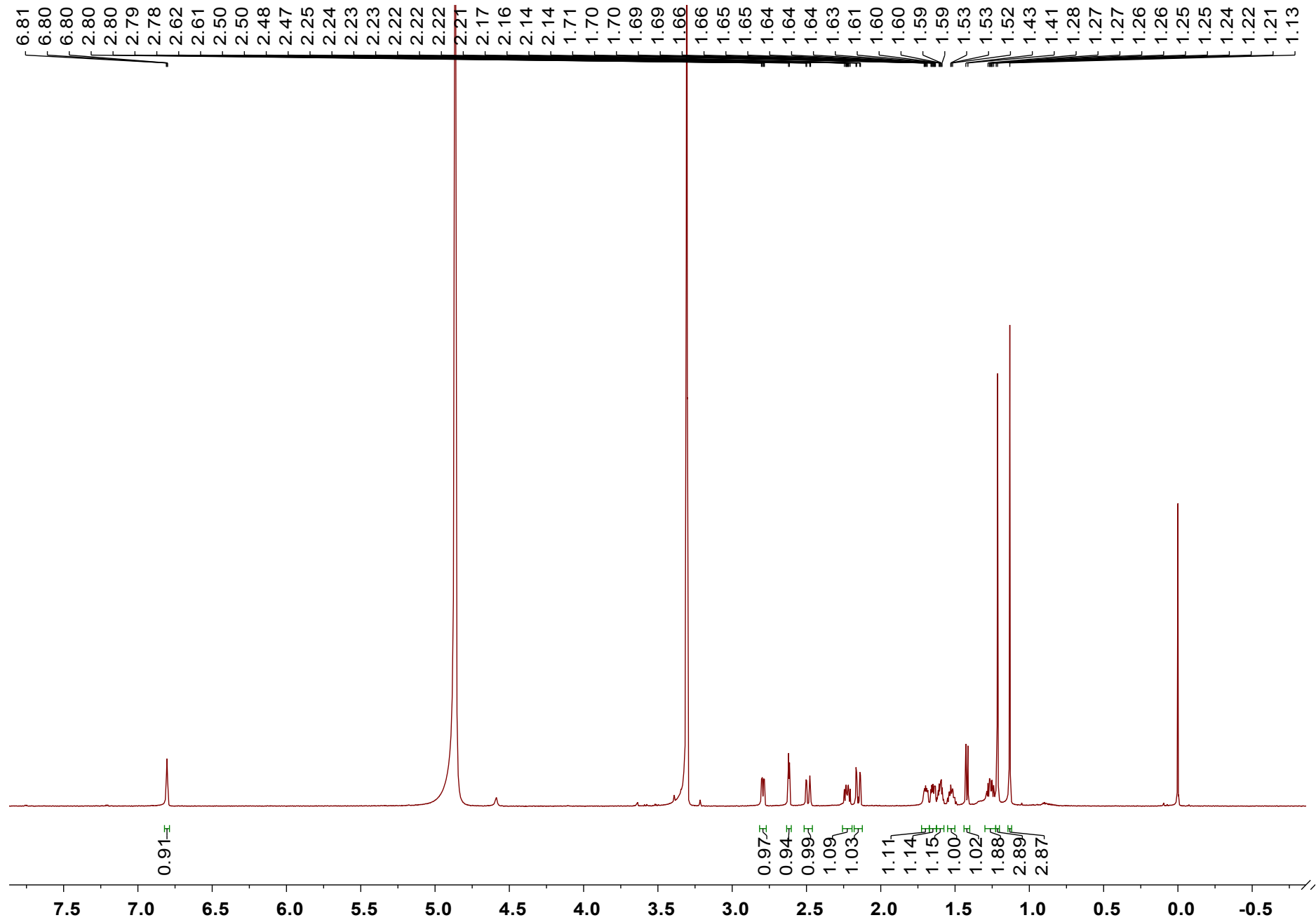
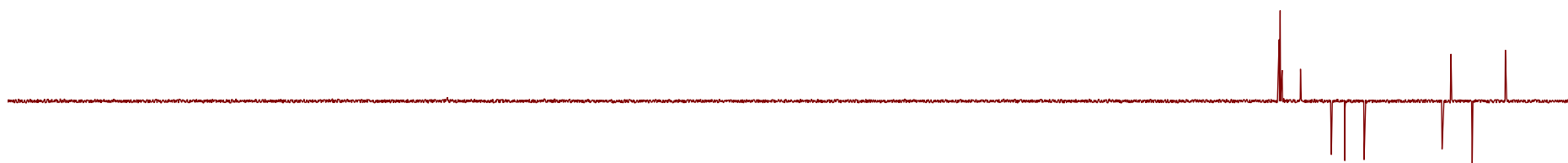


Figure 23S. ^{13}C NMR and DEPT spectra of **4** (150 MHz, CD_3OD)

1lga14a. 3. 1. 1r — 1lga14a



1lga14a. 2. 1. 1r — 1lga14a

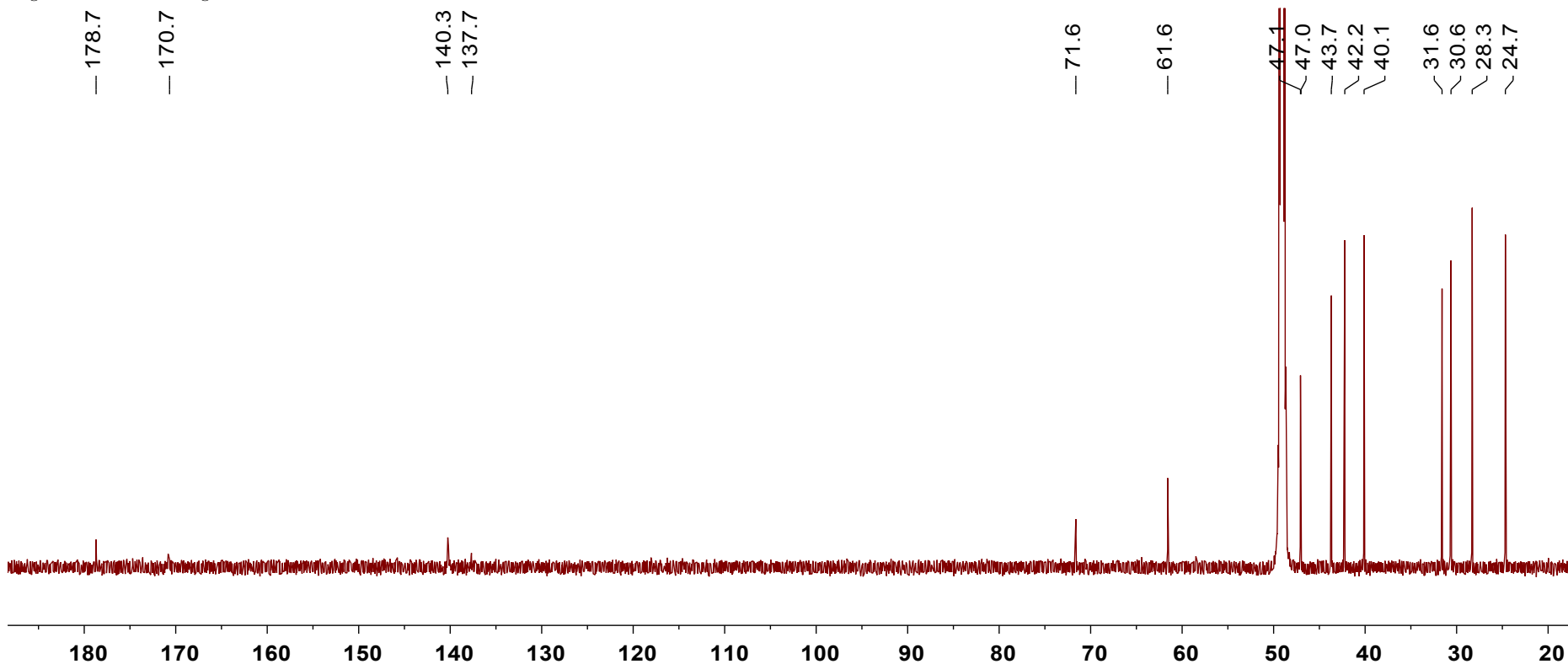


Figure 24S. HSQC spectrum of 4 (CD₃OD)

11ga14a.40.1.2rr — HSQGP-sxhuo MeOD D:\\ root 9

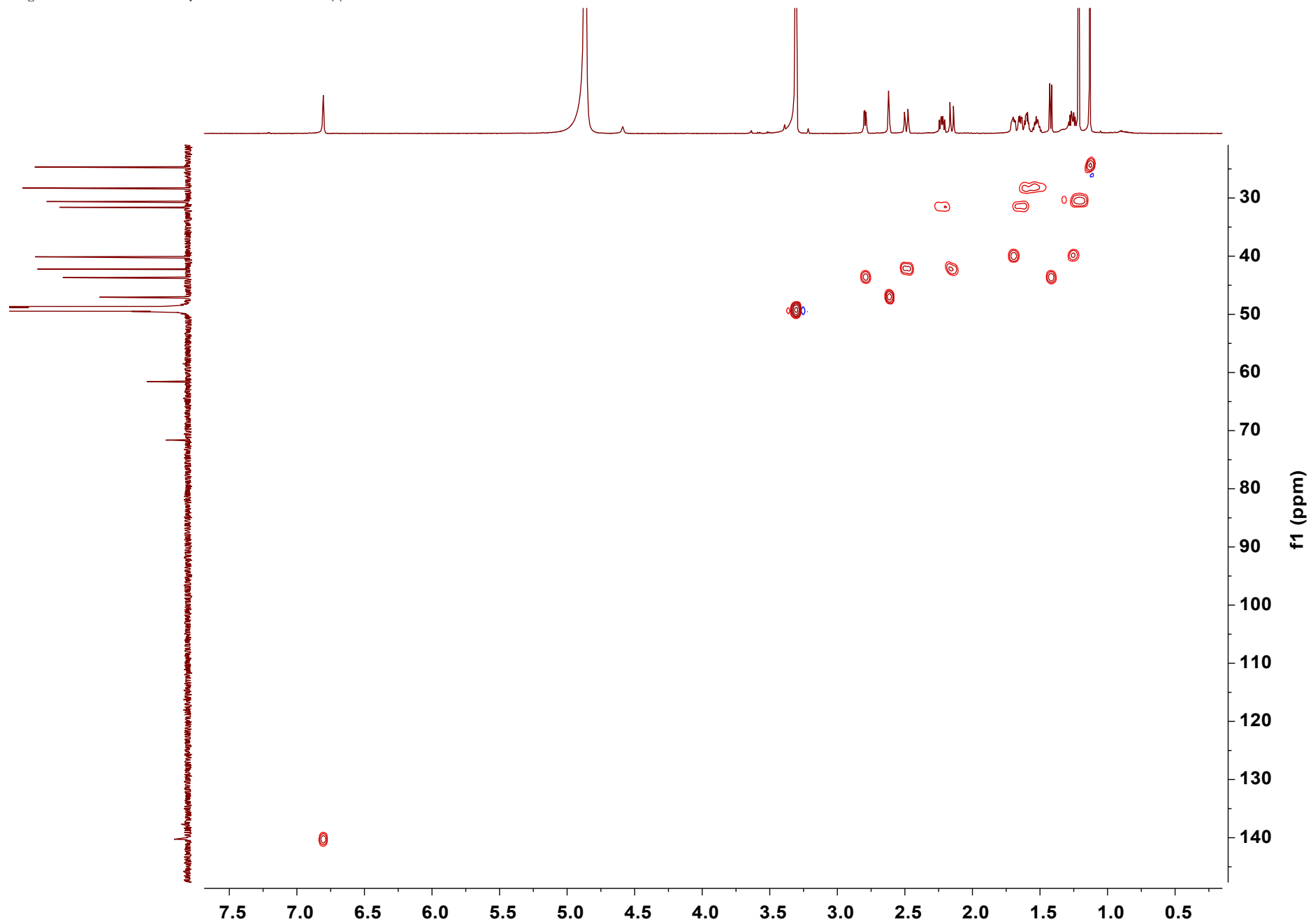


Figure 25S. ^1H - ^1H COSY spectrum of **4** (CD_3OD)

1lga14a.10.1.1.2rr — COSY-sxhuo MeOD D:\ root 9

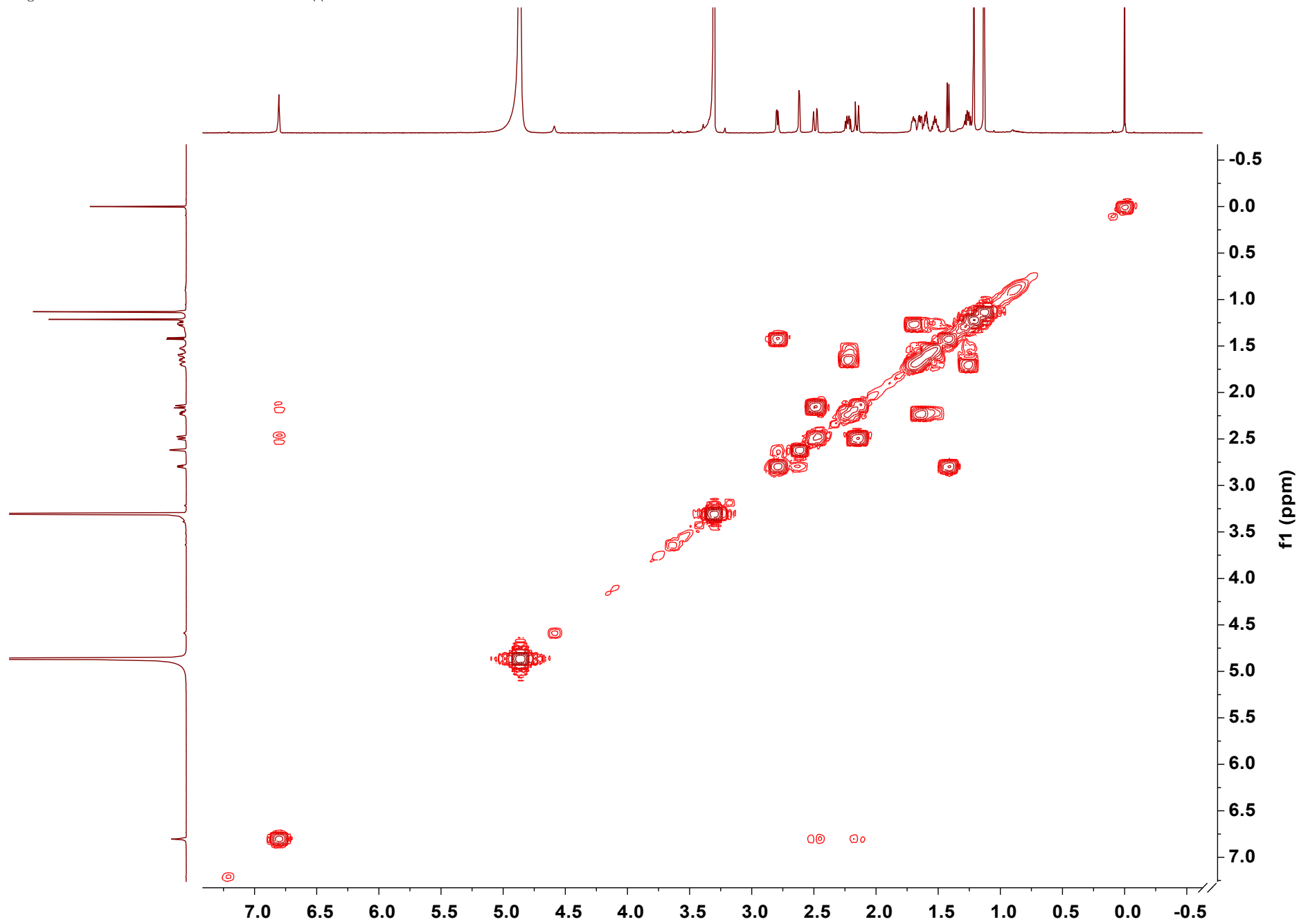


Figure 26S. HMBC spectrum of 4 (CD₃OD)

11ga14a.10.1.2rr — 11ga14a

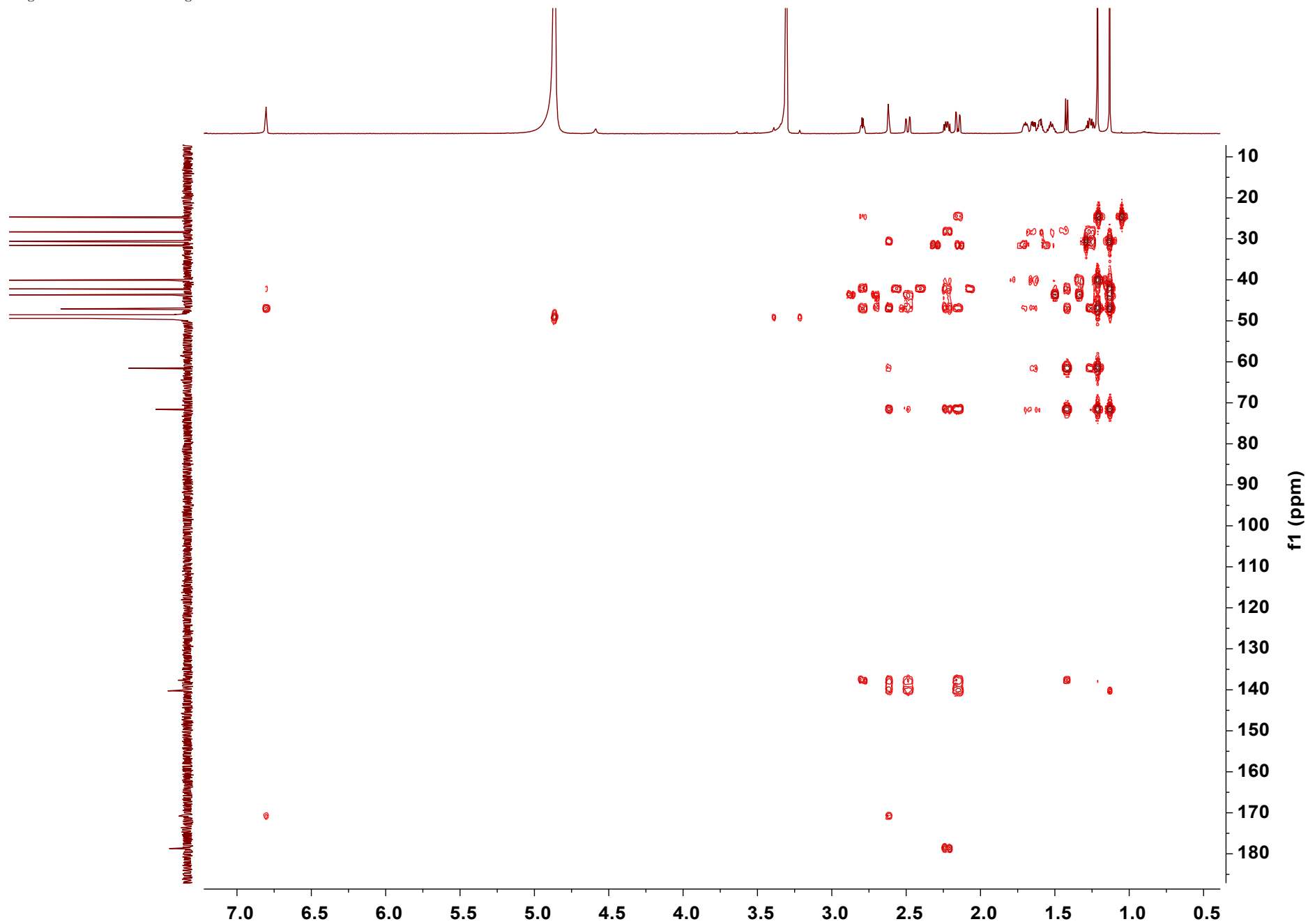


Figure 27S. ROESY spectrum of **4** (CD₃OD)

11ga14a.14.1.2rr — ROESYPHPR-sxhuo MeOD D:\ \ root 9

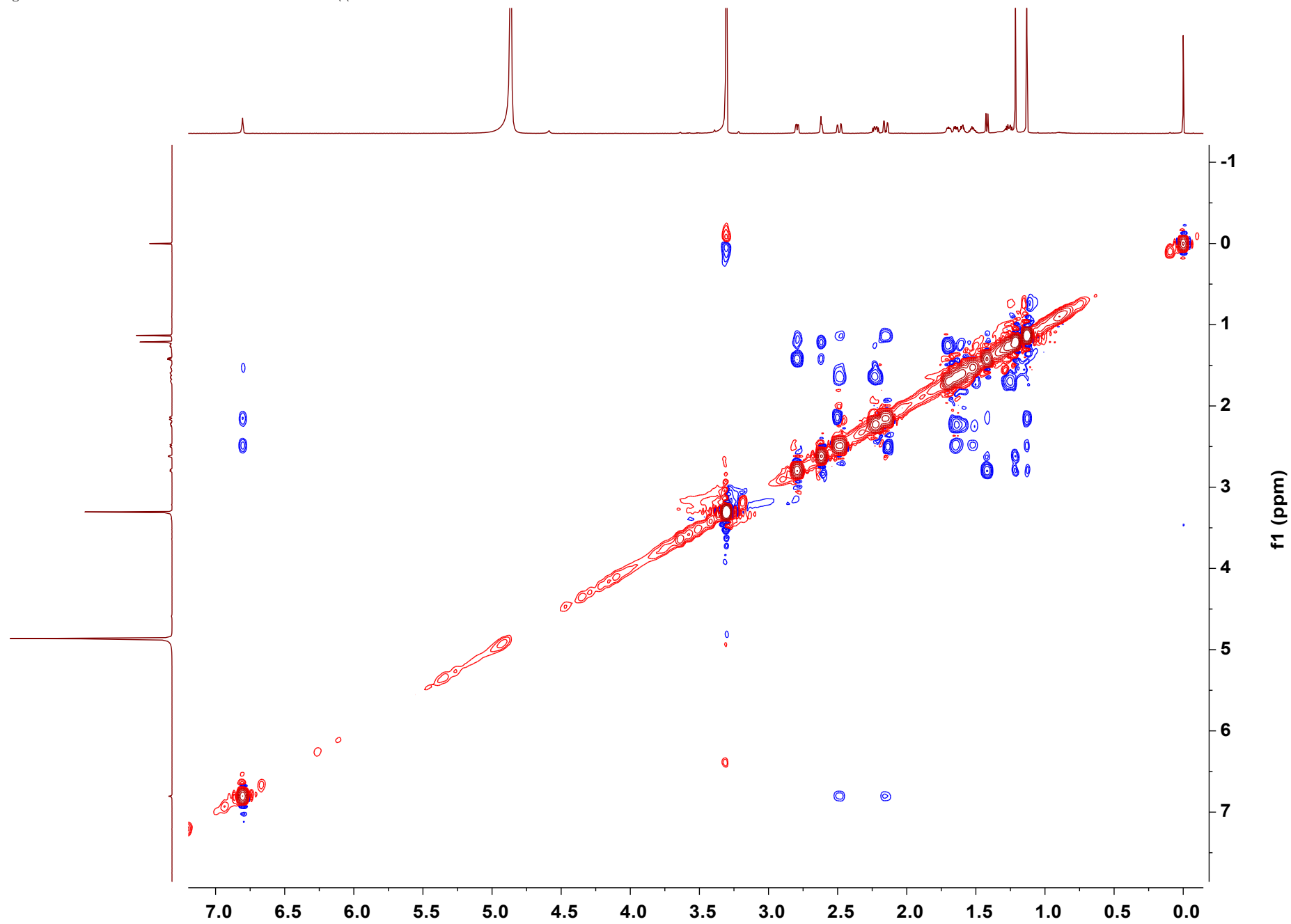


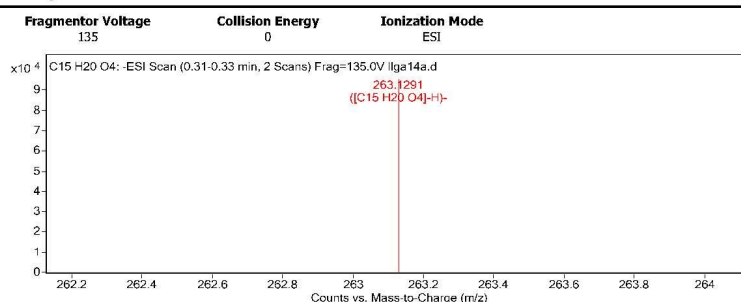
Figure 28S. HRESIMS (+) report of 4

Qualitative Analysis Report

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Sample Type	Sample	Position	P2-A2
Instrument Name	Instrument 1	User Name	
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IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (85125.2)	

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
119.0364	1	17871.06		
263.1291	1	95318.84	C15 H20 O4	(M-H)-
264.1324	1	15007.87	C15 H20 O4	(M-H)-
966.0011	1	8760.39		
982.9916	1	85130.63		
983.994	1	14735.99		
996.012	1	50640.63		
997.0147	1	10217.79		
1033.9889	1	71822.22		
1034.9913	1	13631.42		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O4	264.1362	263.1289	263.1291	-0.3	-0.9	6.0000

--- End Of Report ---

Figure 29S. ¹H NMR spectrum of 5 (600 MHz, CD₃OD)

ecg485.21.1.1r — ecg485 H

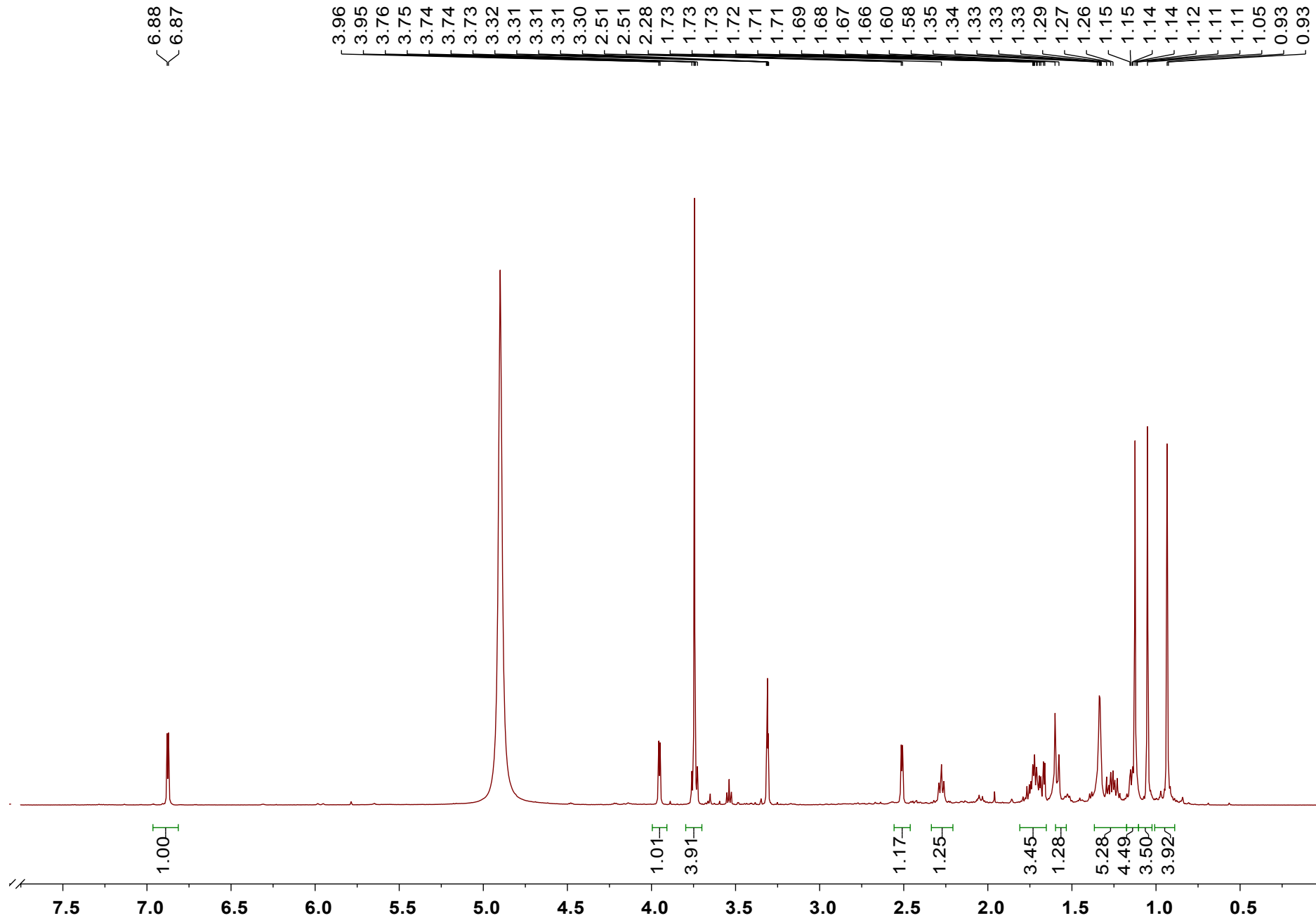
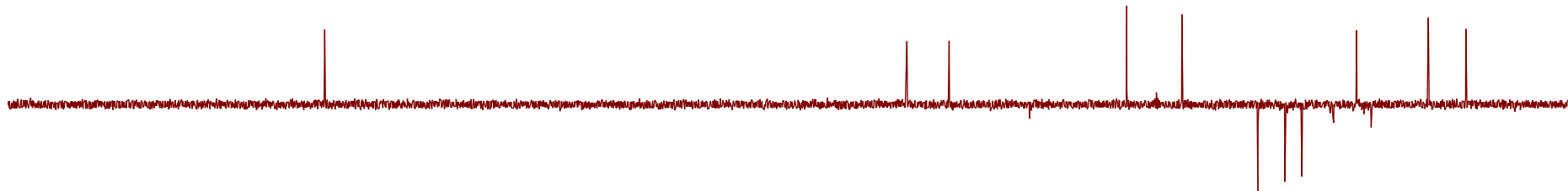
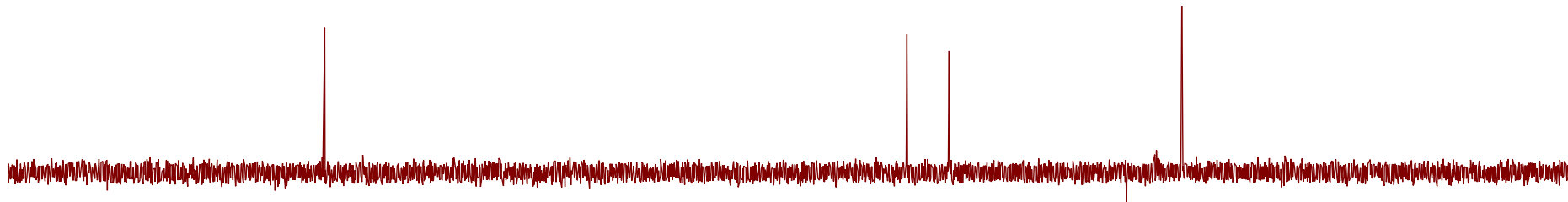


Figure 30S. ^{13}C NMR and DEPT spectra of **5** (150 MHz, CD_3OD)

t. 24. 1. 1r —



t. 23. 1. 1r —



llgc1. 22. 1. 1r — llgc1

c13 and dept

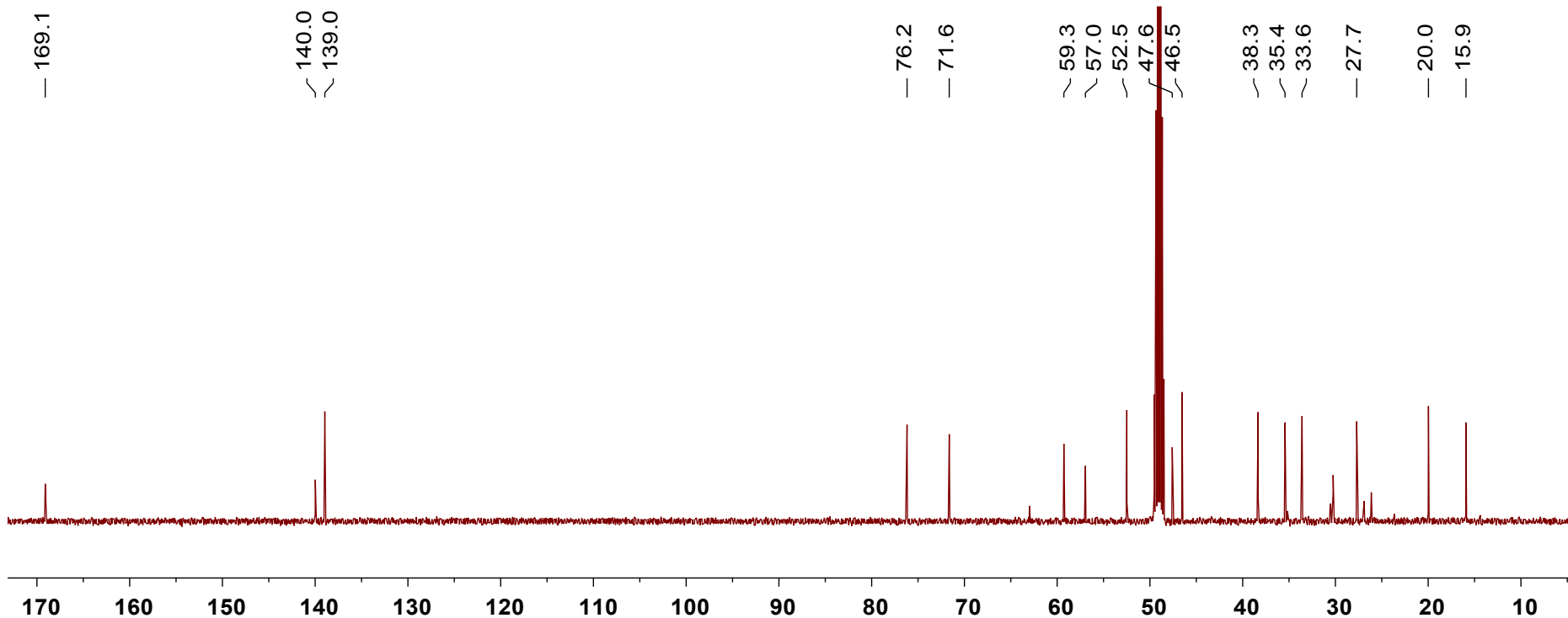


Figure 31S. HSQC spectrum of **5** (CD₃OD)

11gc1.26.1.2rr — 11gc1_hsqc

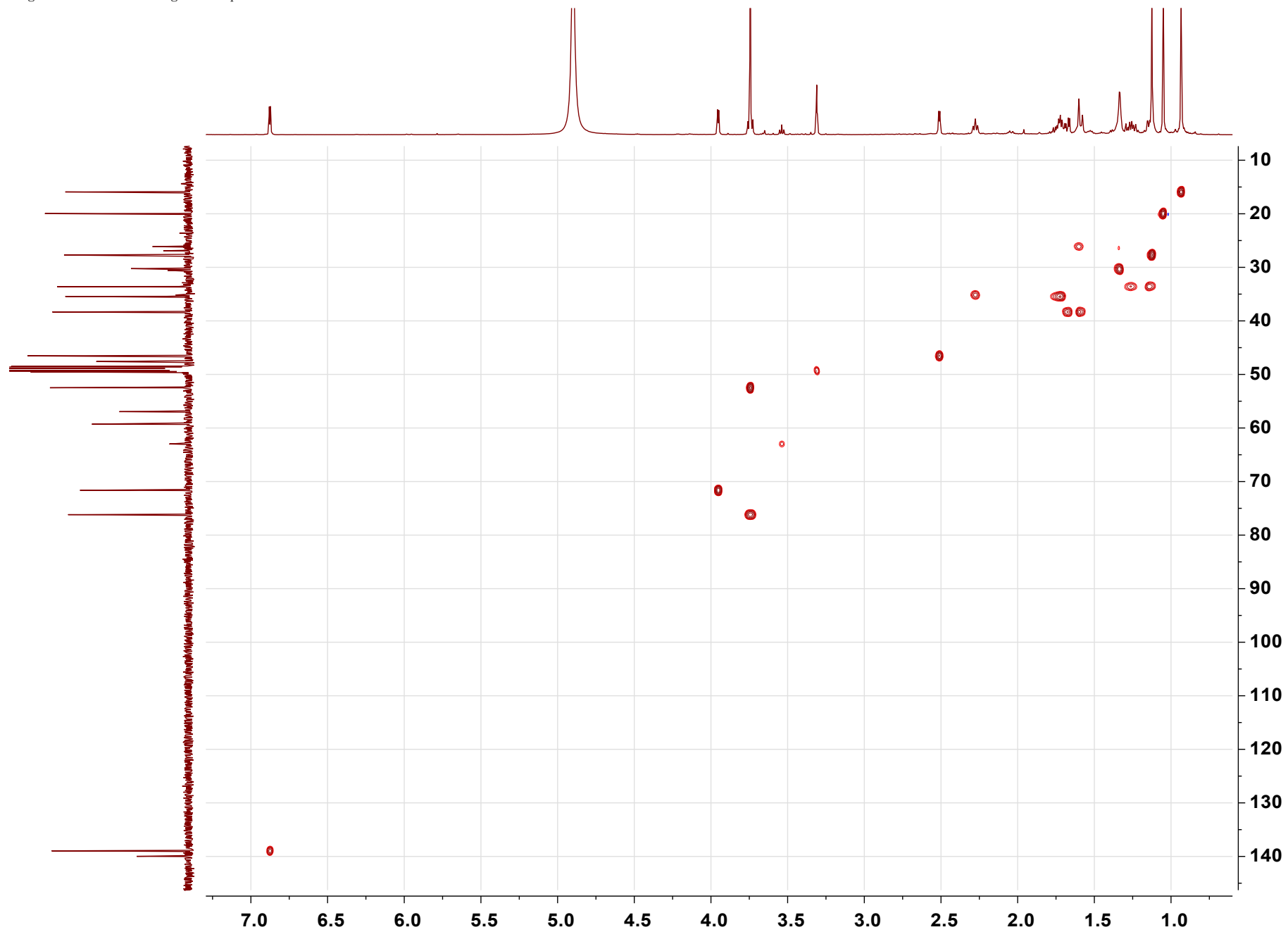


Figure 32S. ^1H - ^1H COSY spectrum of **5** (CD_3OD)

11gc1.25.1.2rr — 11gc1 cosy

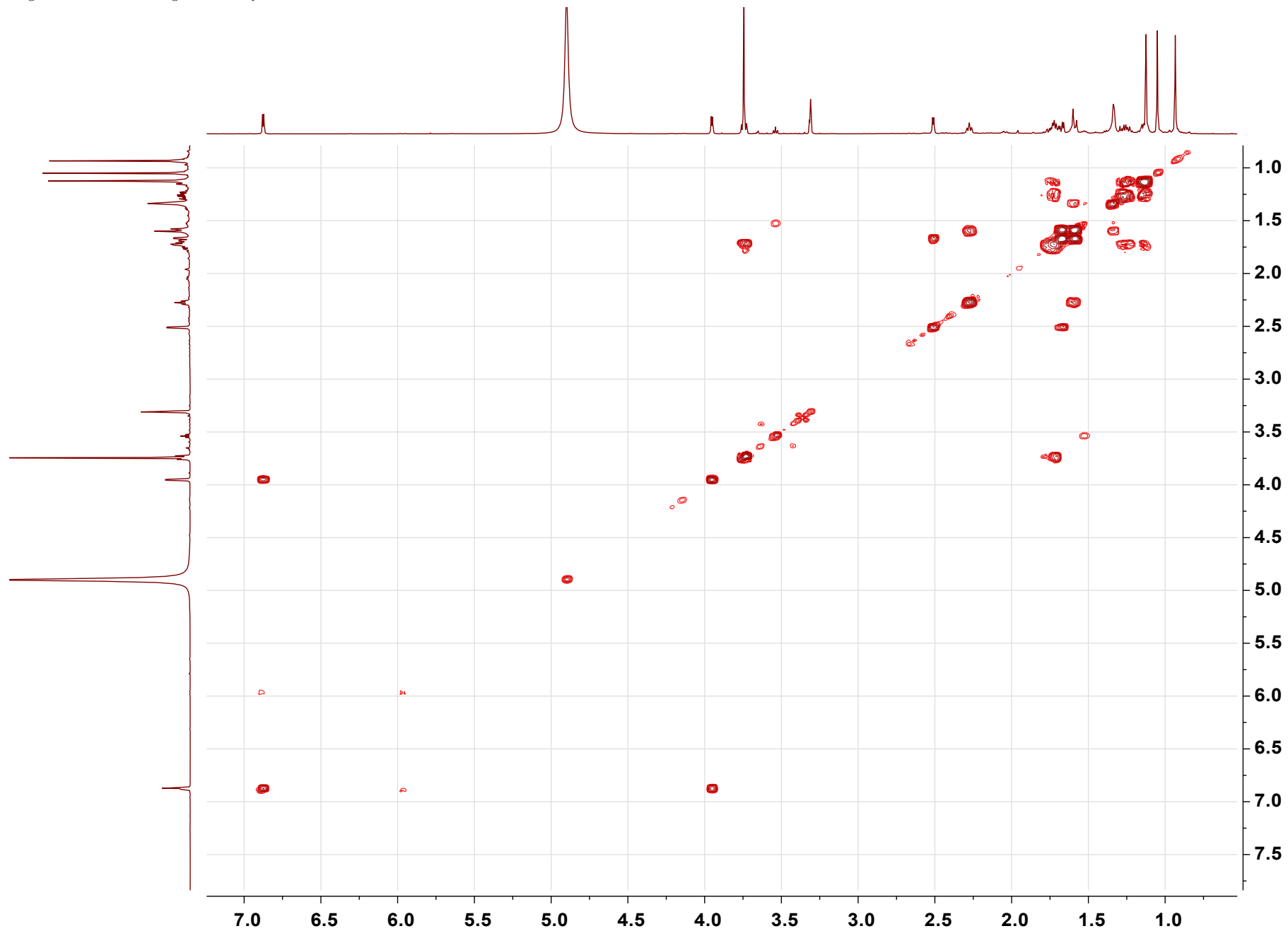


Figure 33S. HMBC spectrum of 5 (CD₃OD)

11gc1.27.1.2rr — 11gc1 hmbc

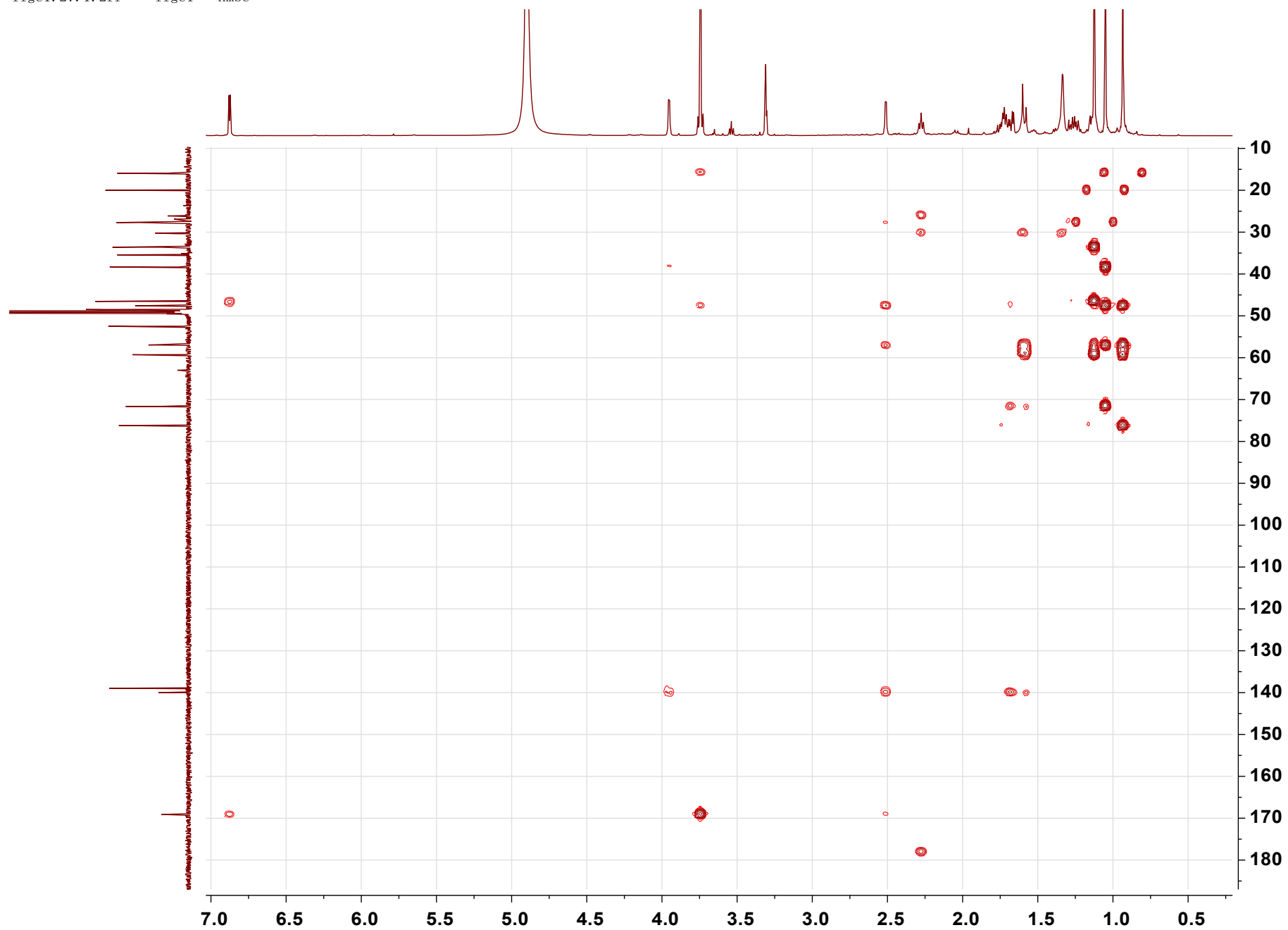


Figure 34S. ROESY spectrum of **5** (CD₃OD)

11gc1.28.1.2rr — 11gc1 roesy

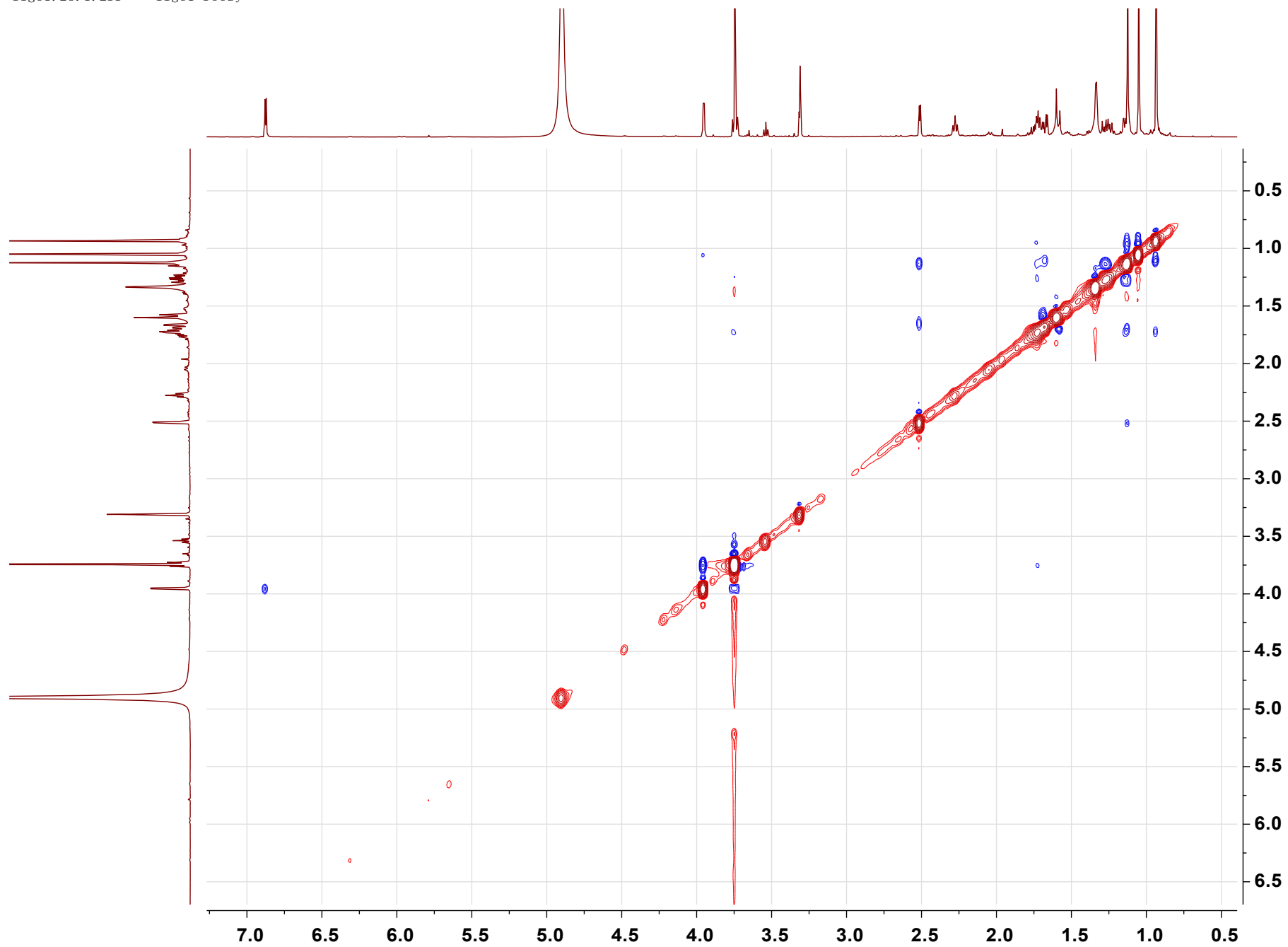


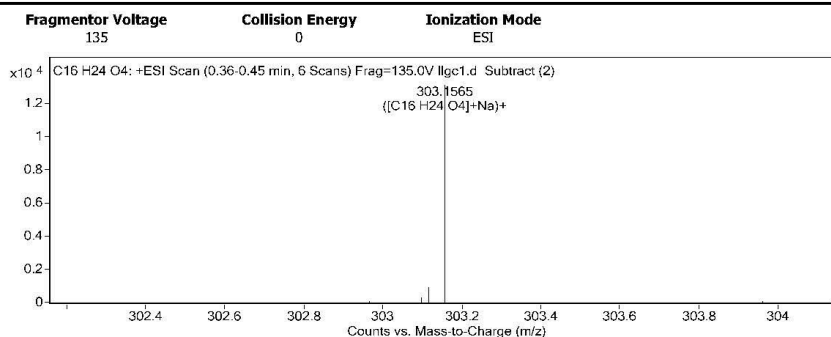
Figure 35S. HRESIMS (+) report of 5

Qualitative Analysis Report

Data Filename	llgc1.d	Sample Name	llgc1
Sample Type	Sample	Position	P2-A3
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	11/27/2017 10:16:11 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
273.146	1	16040.5		
275.1618	1	11812.88		
289.1199	1	5606.91		
289.1395	1	4961.16		
303.1565	1	13069.8	C16 H24 O4	(M+Na)+
319.1309	1	9919.51		
331.1505	1	12196.29		
333.1672	1	7356.92		
347.1255	1	4758.05		
401.1549	1	6929.66		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C16 H24 O4	280.1675	303.1567	303.1565	0.0	0.1	5.0000

--- End Of Report ---

Figure 36S. ^1H NMR spectrum of **6** and **7** (600 MHz, CDCl_3)

11gf4b.21.1.1r — 11gf4b_hsqc

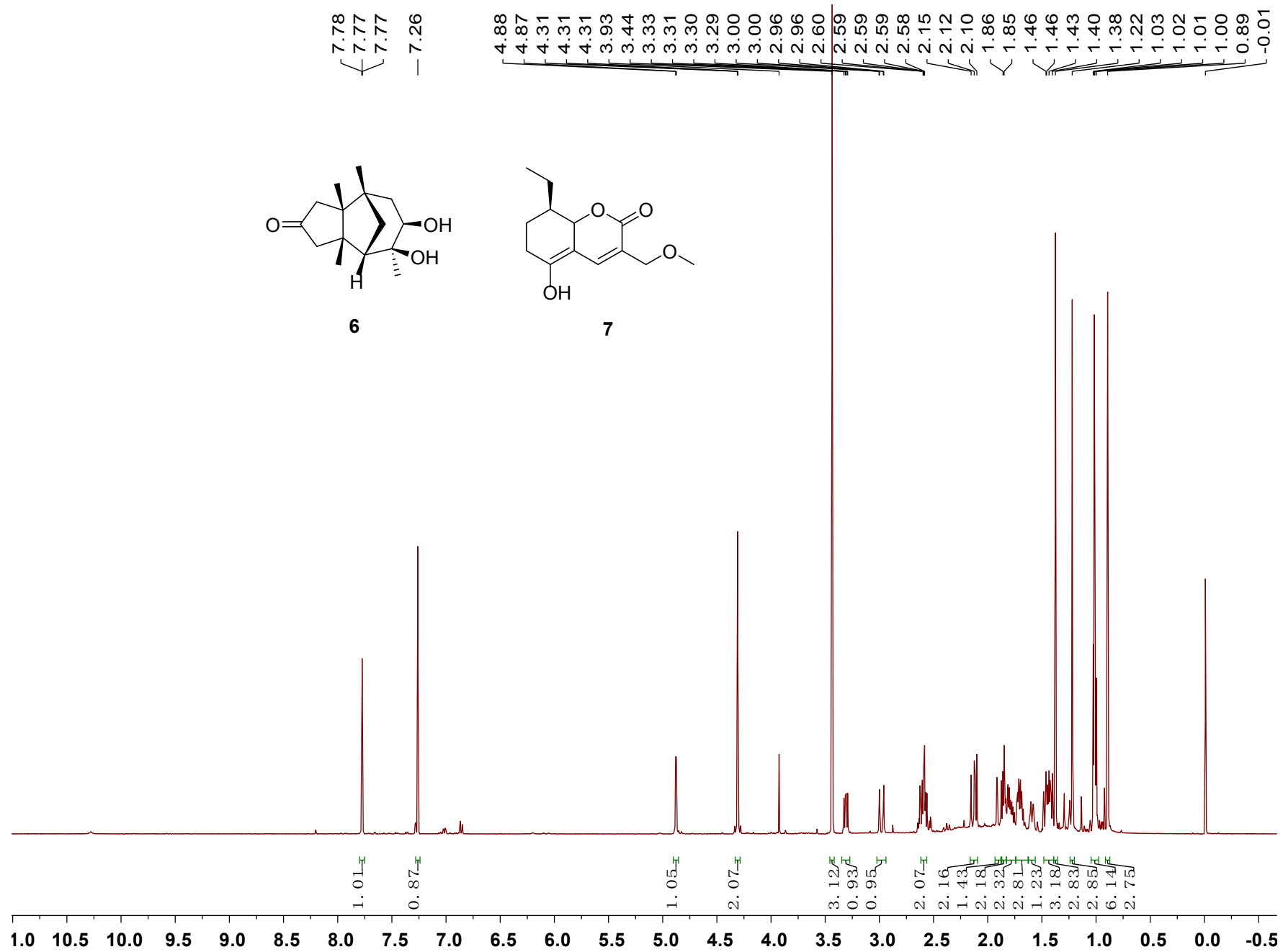


Figure 37S. ^{13}C NMR and DEPT spectra of **6** and **7** (150 MHz, CDCl_3)

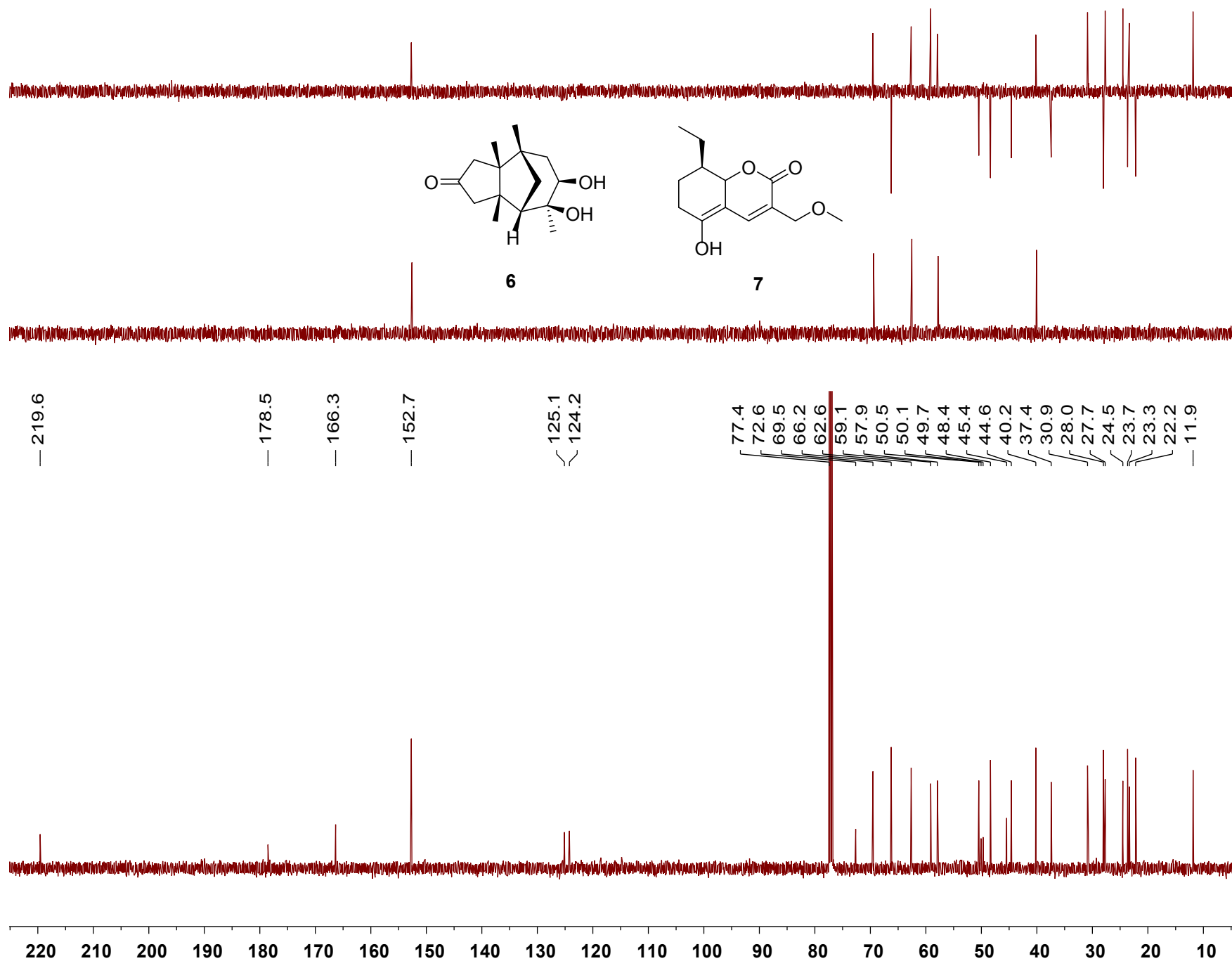


Figure 38S. HSQC spectrum of **6** and **7** (CDCl₃)

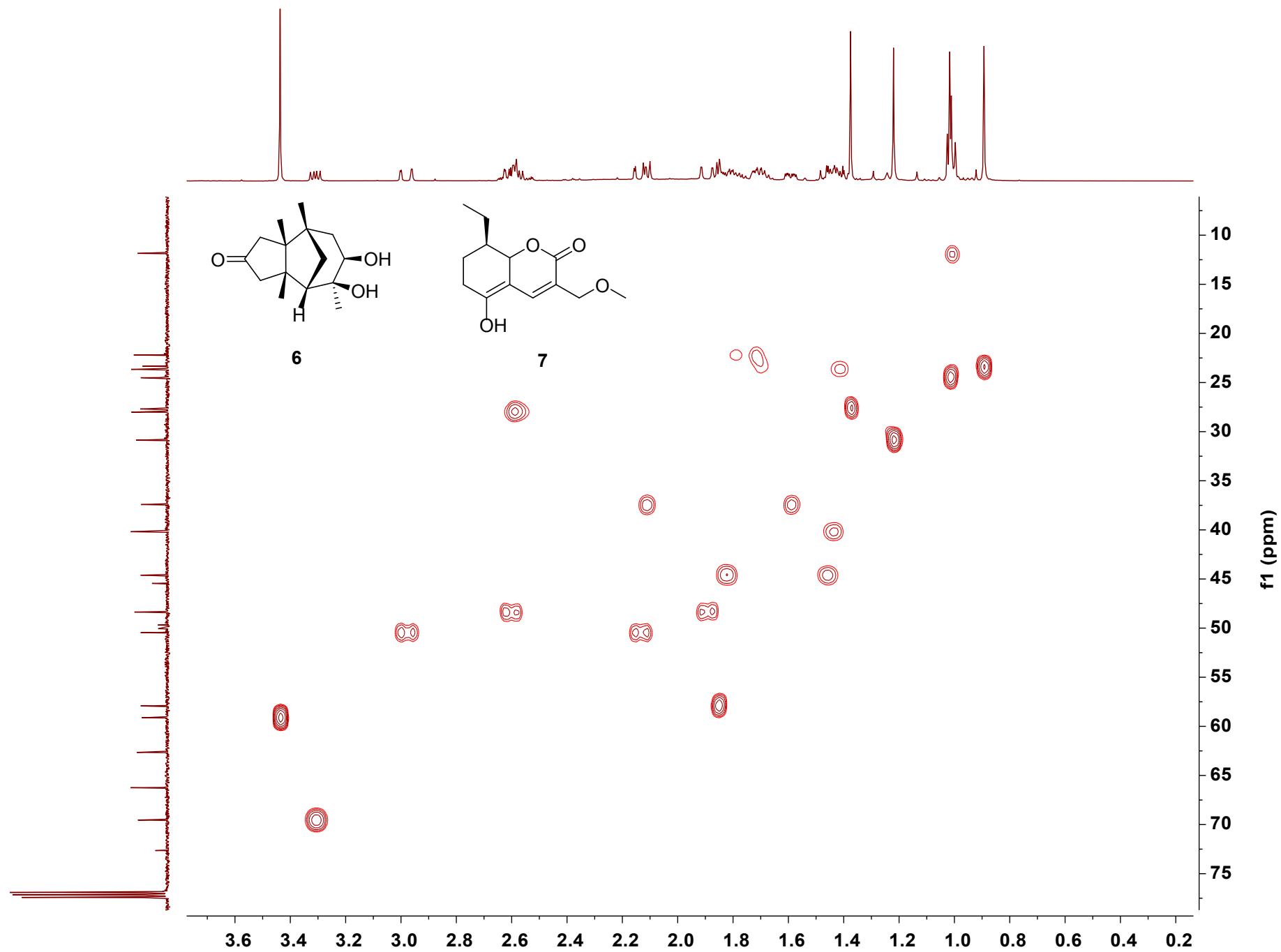


Figure 39S. ^1H - ^1H COSY spectrum of **6** and **7** (CDCl_3)

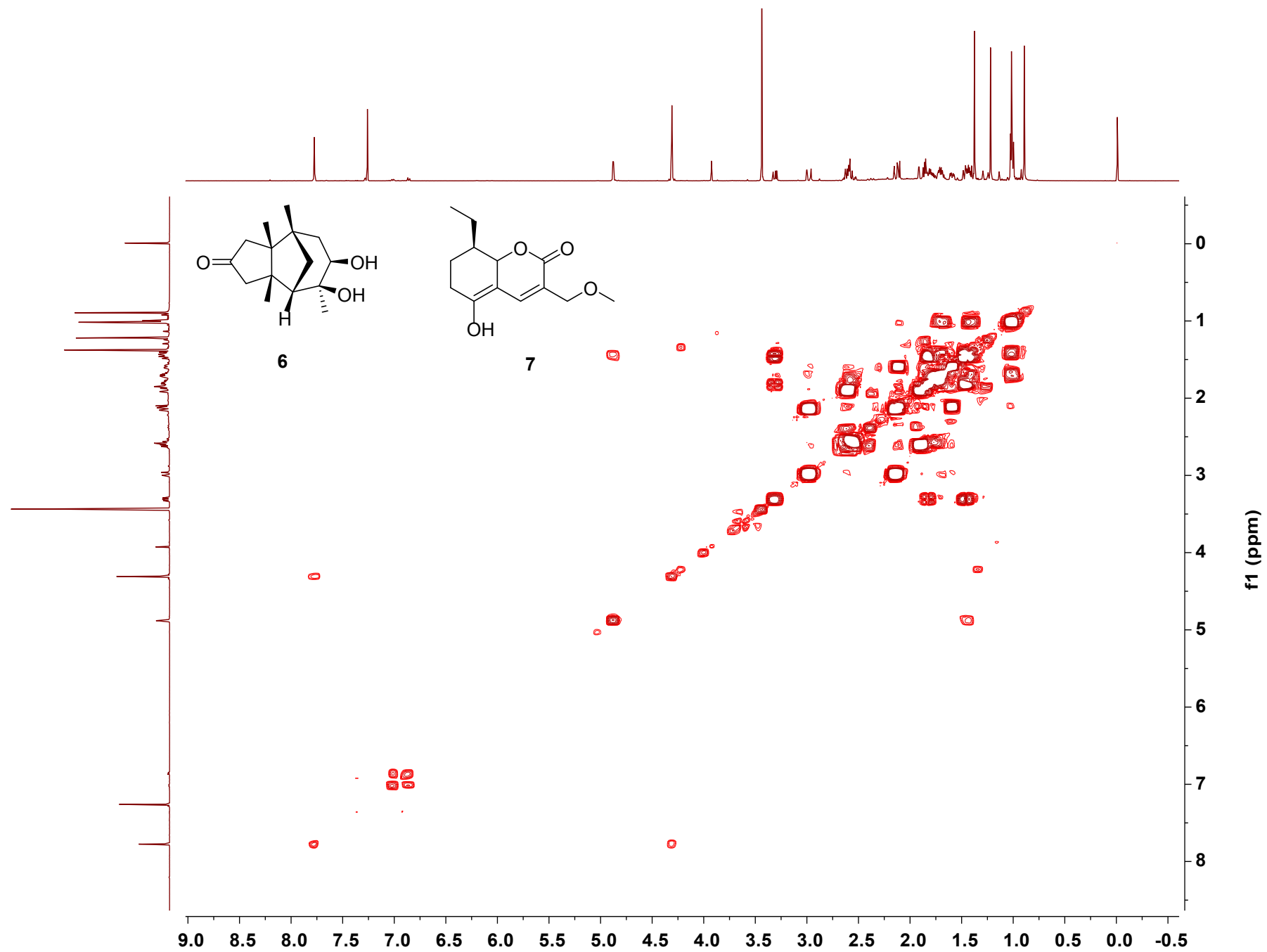


Figure 40S. HMBC spectrum of **6** and **7** (CDCl₃)

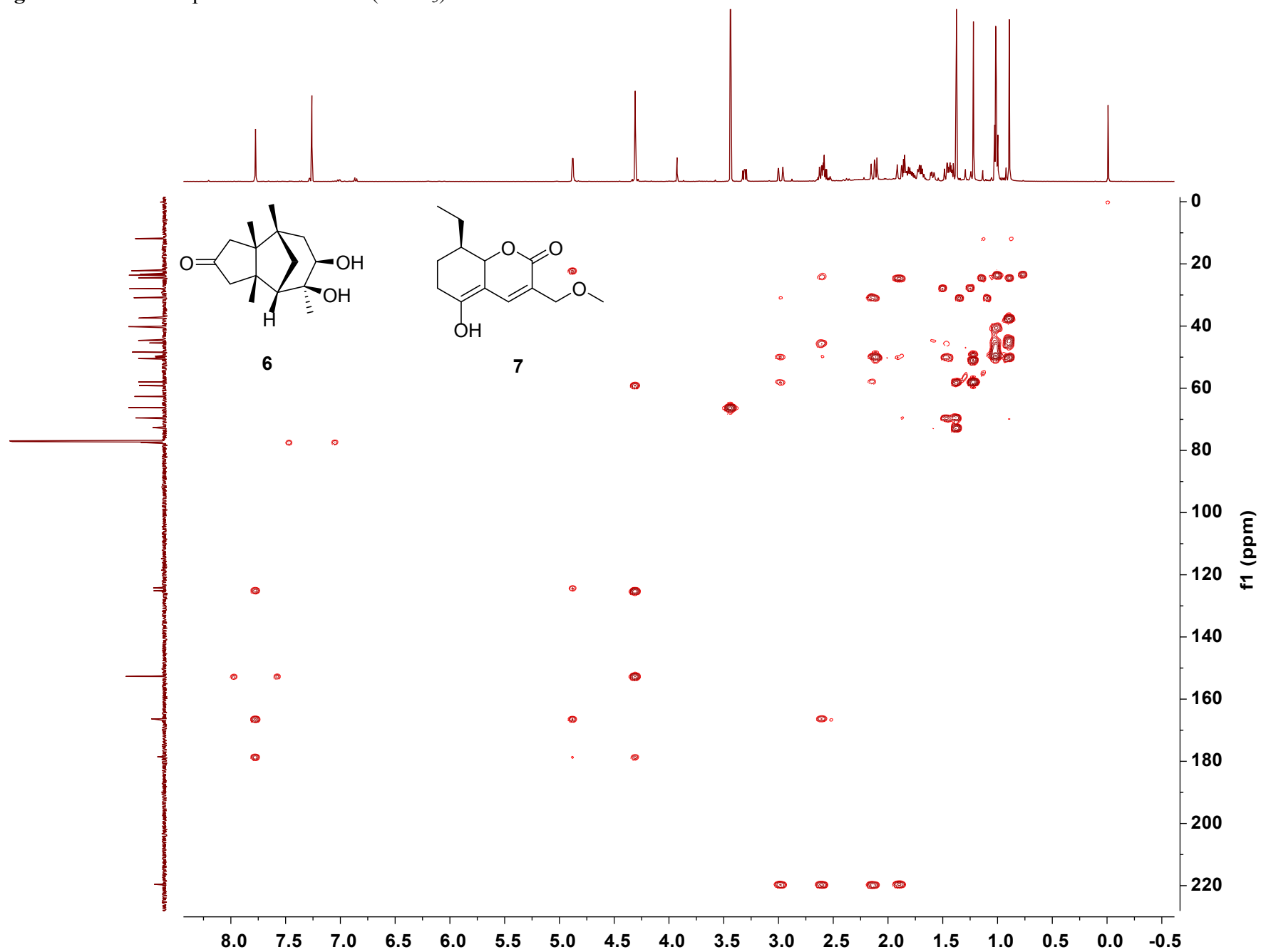


Figure 41S. ROESY spectrum of **6** and **7** (CDCl₃)

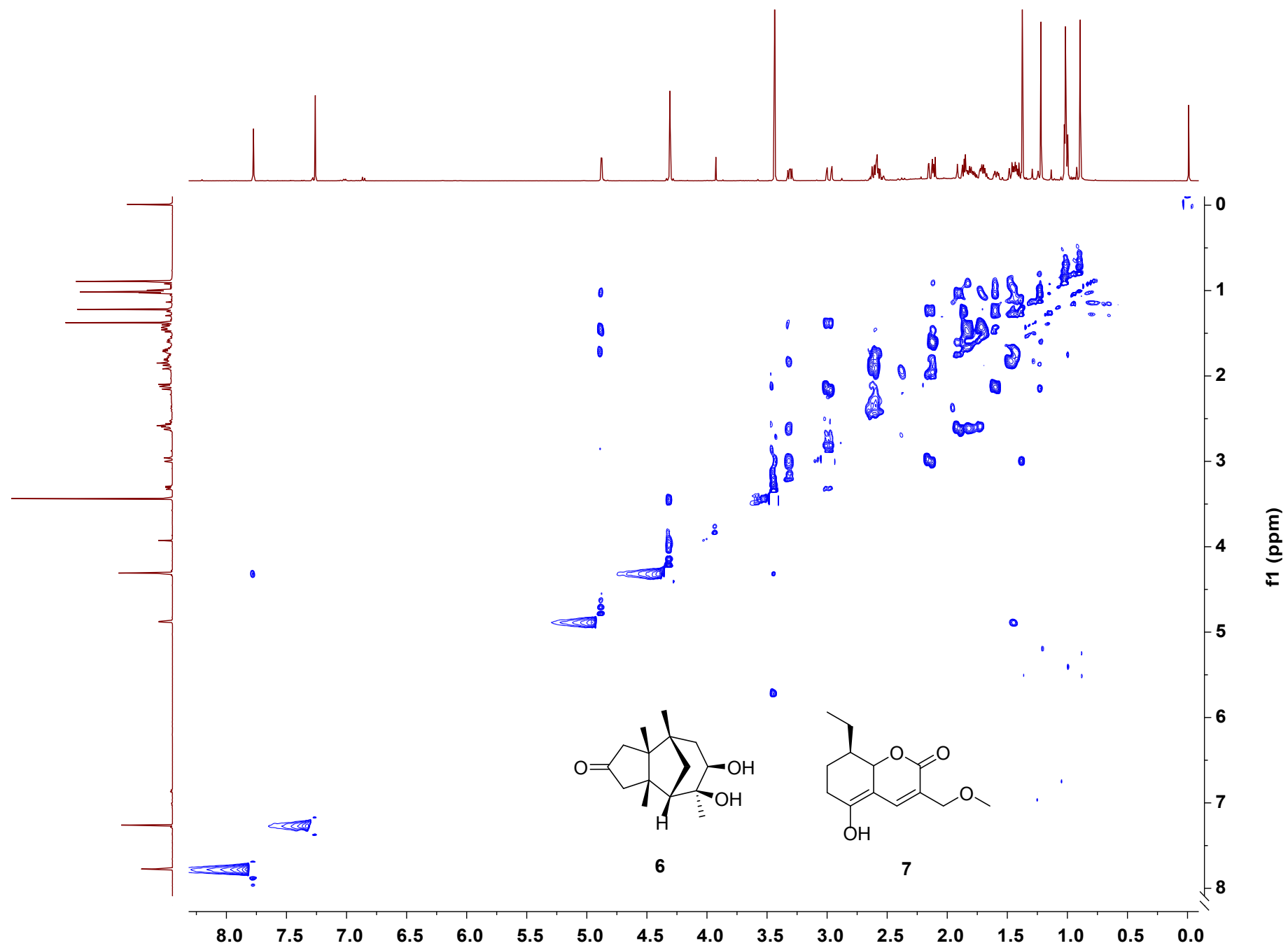


Figure 42S. HREIMS (+) report of 6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

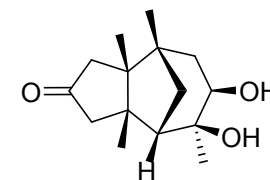
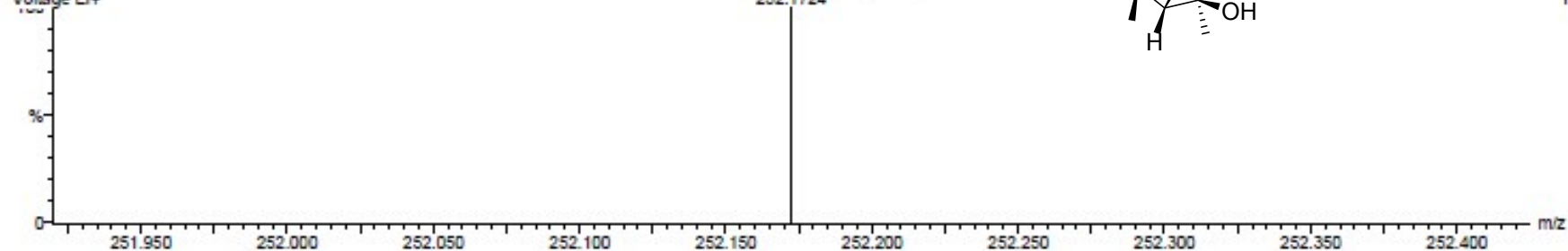
Elements Used:

C: 0-200 H: 0-400 O: 1-4

Ilqf4b

15:48:58 23-Mar-2017

Voltage EI+



Autospec Premier
P776
1

Minimum: 200.0 10.0 -10.0
Maximum: 200.0 10.0 120.0

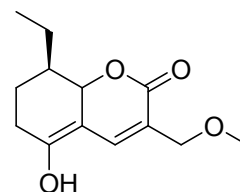
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.1724	252.1725	-0.1	-0.4	4.0	5546026.0	C15 H24 O3

Figure 43S. HRESIMS (+) report of 7

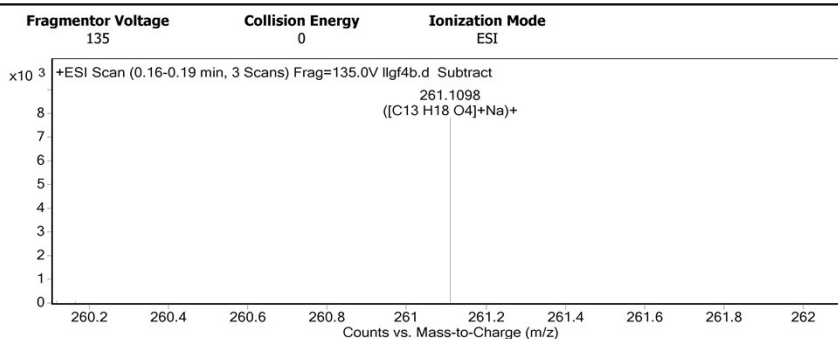
Qualitative Analysis Report

Data Filename	llgf4b.d	Sample Name	llgf4b
Sample Type	Sample	Position	P1-C4
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	4/13/2017 5:06:25 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)	



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
140.0685		946.86		
189.0908	1	1526.56		
221.1168		1220.66		
261.1098	1	7823.98	C13 H18 O4	(M+Na)+
262.1145	1	1280.33	C13 H18 O4	(M+Na)+
277.0841	1	1696.94		
281.173	1	1670.97		
675.2618	1	1245.27		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C13 H18 O4	238.1205	261.1097	261.1098	-0.5	-2.0	5.0000

--- End Of Report ---

Figure 44S. ¹H NMR spectrum of **8** (600 MHz, CDCl₃)

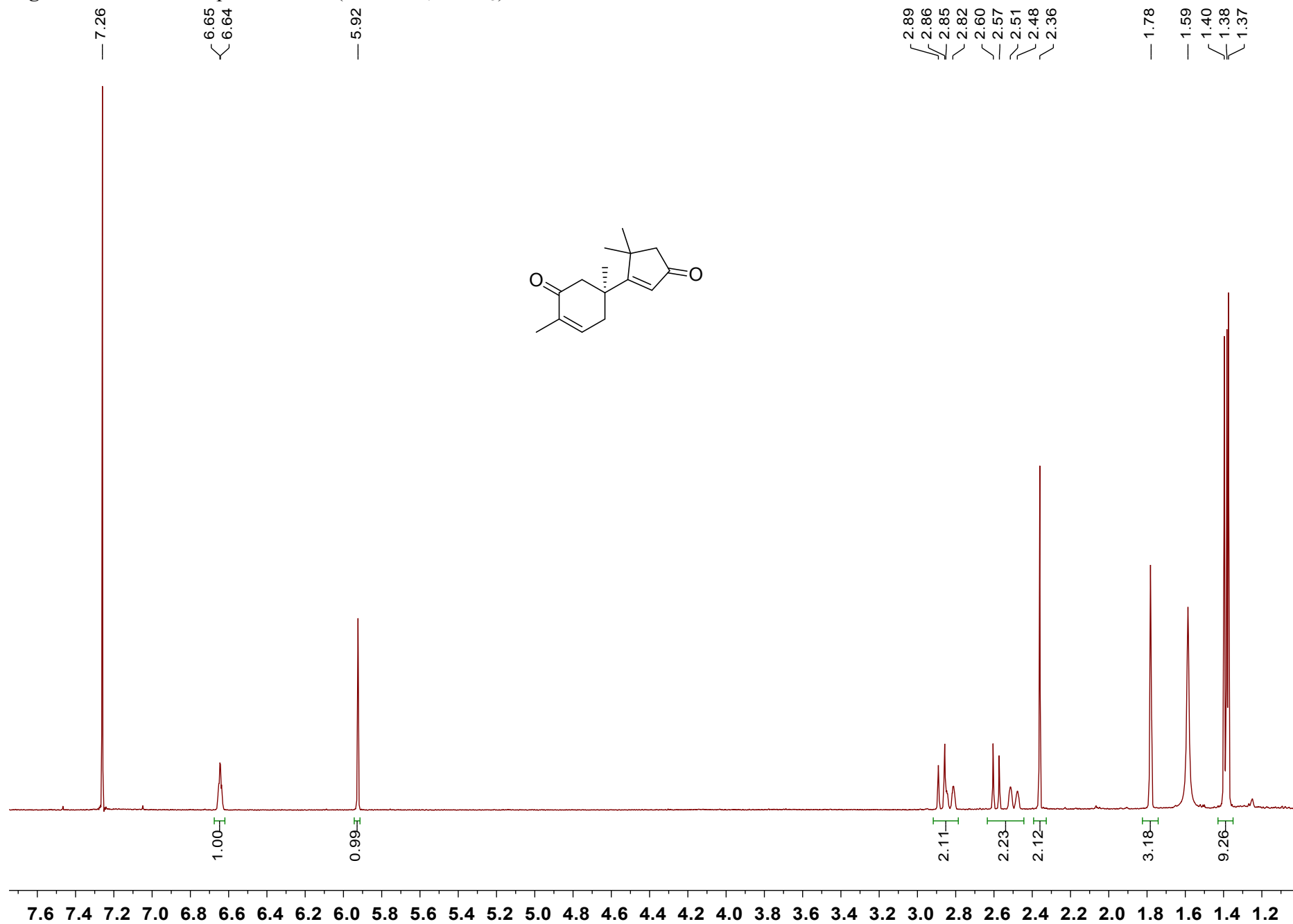


Figure 45S. ^{13}C NMR and DEPT spectra of **8** (150 MHz, CDCl_3)

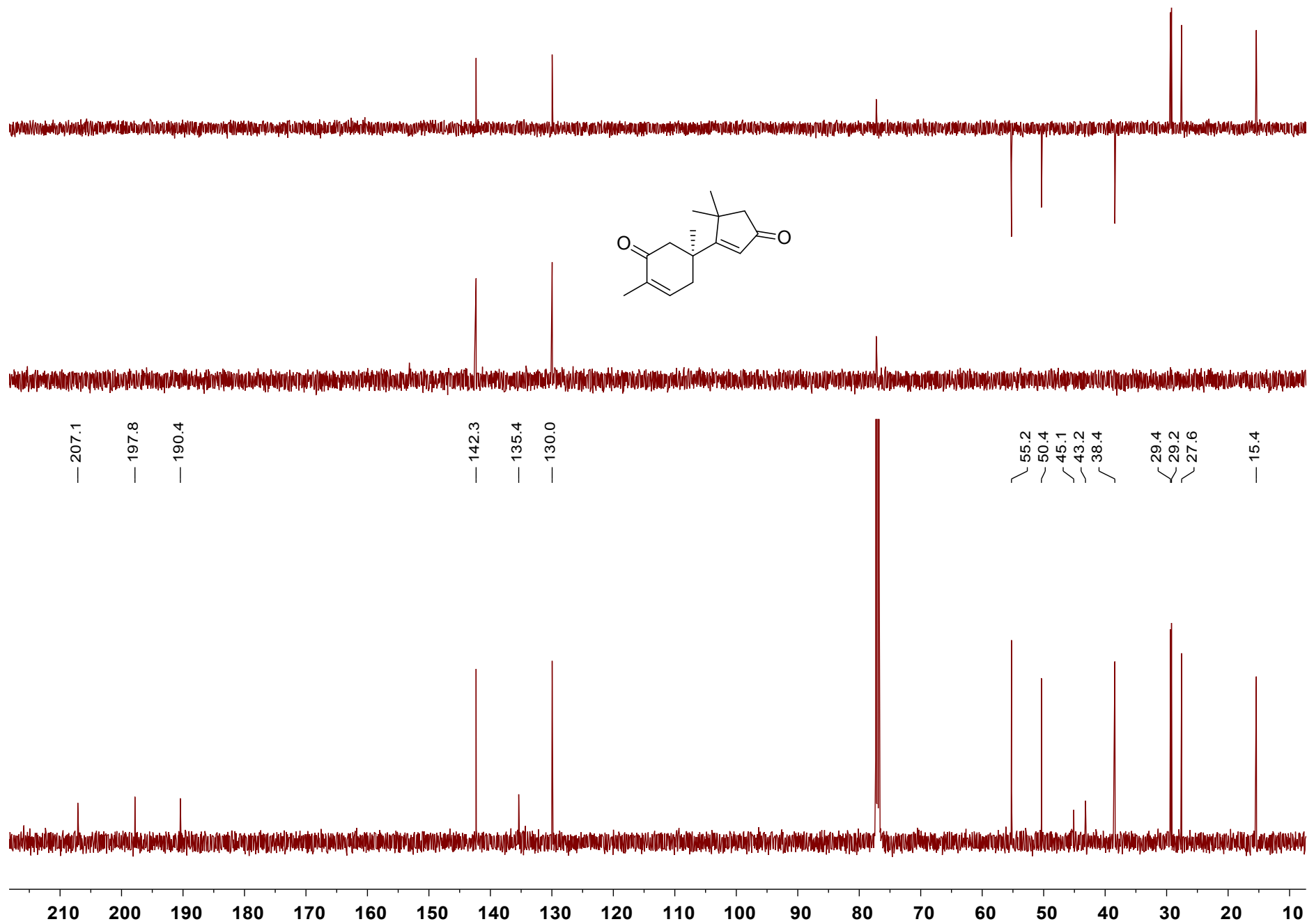


Figure 46S. HSQC spectrum of **8** (CDCl₃)

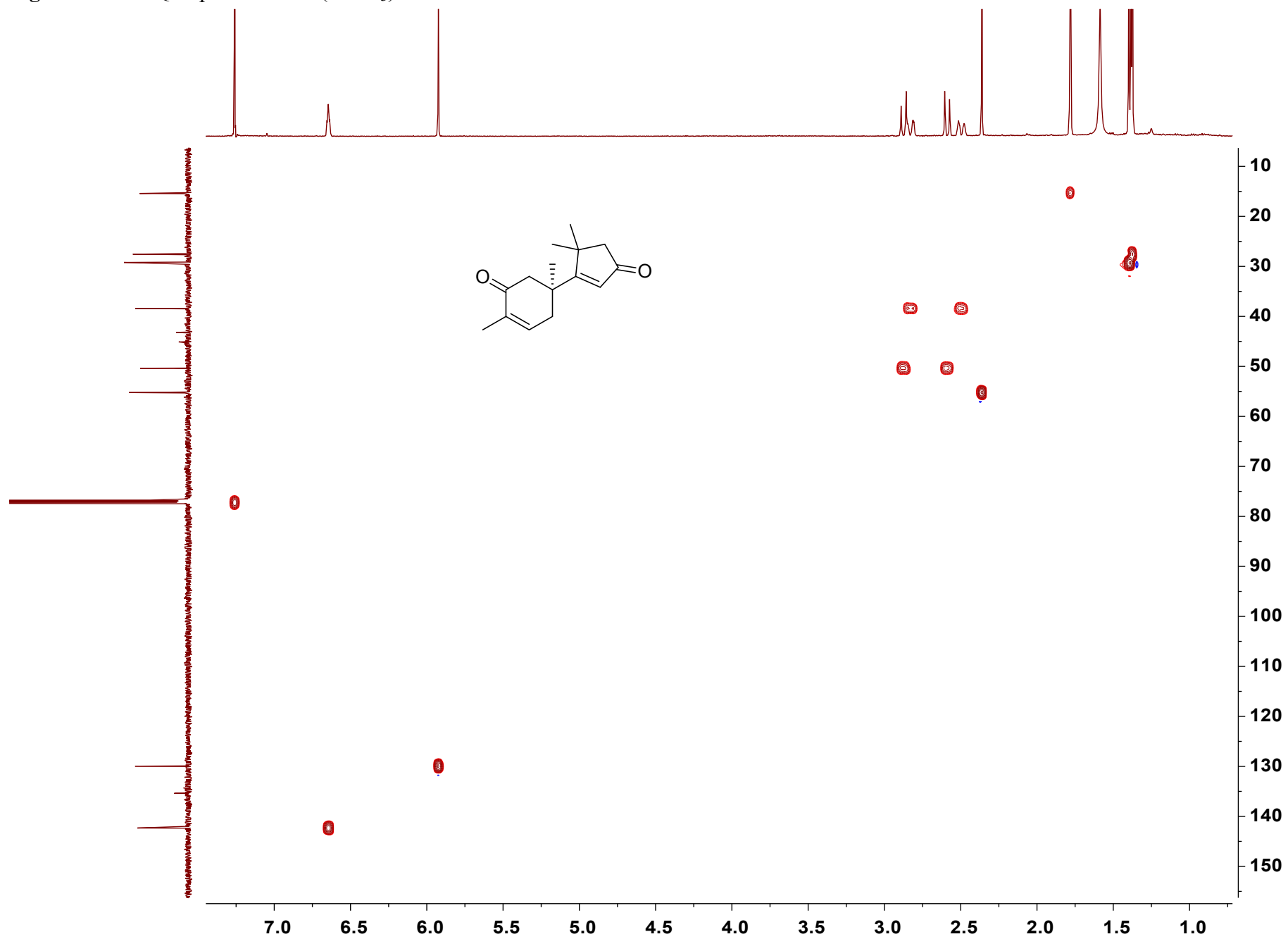


Figure 47S. ^1H - ^1H COSY spectrum of **8** (CDCl_3)

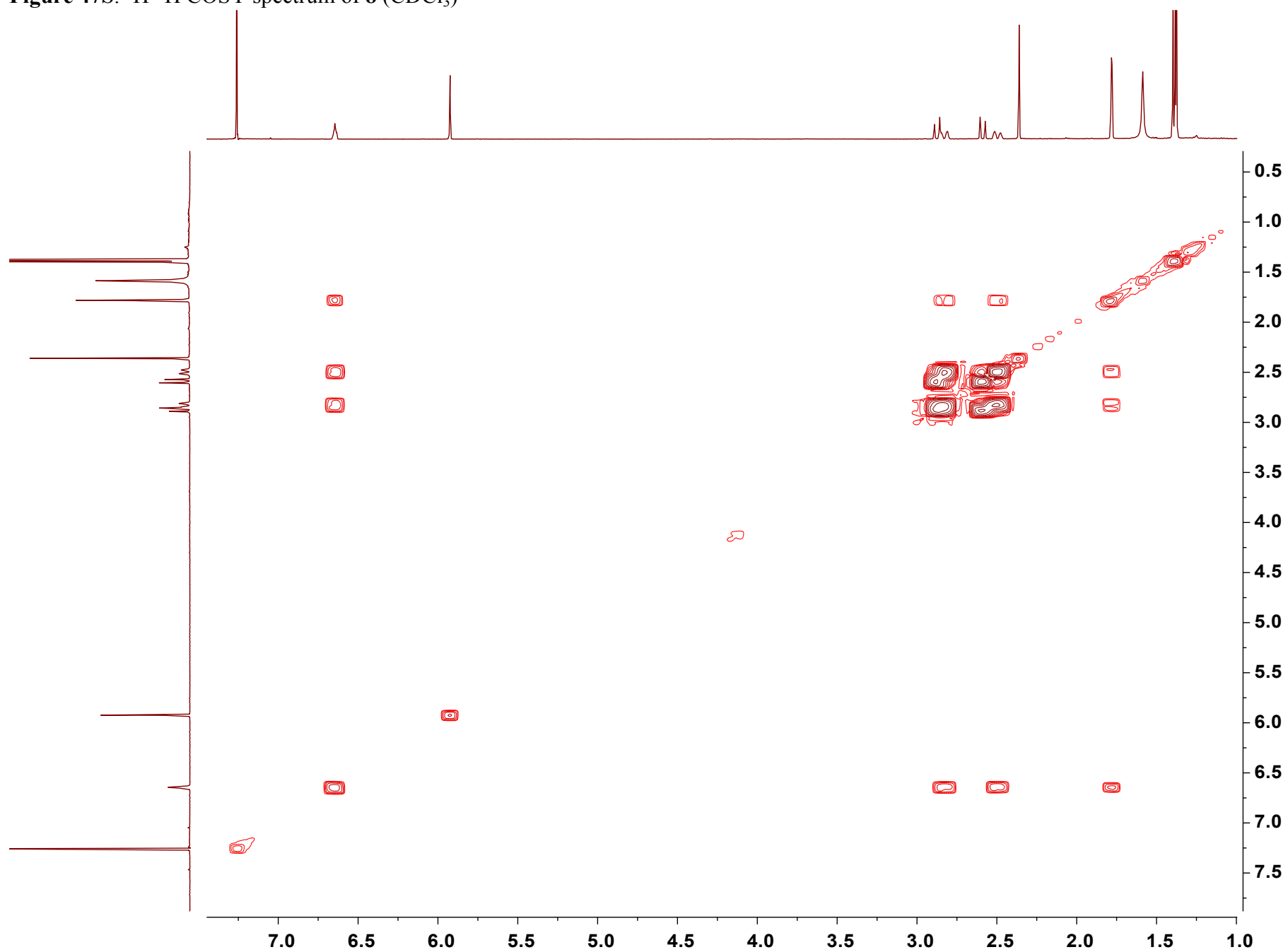


Figure 48S. HMBC spectrum of **8** (CDCl₃)

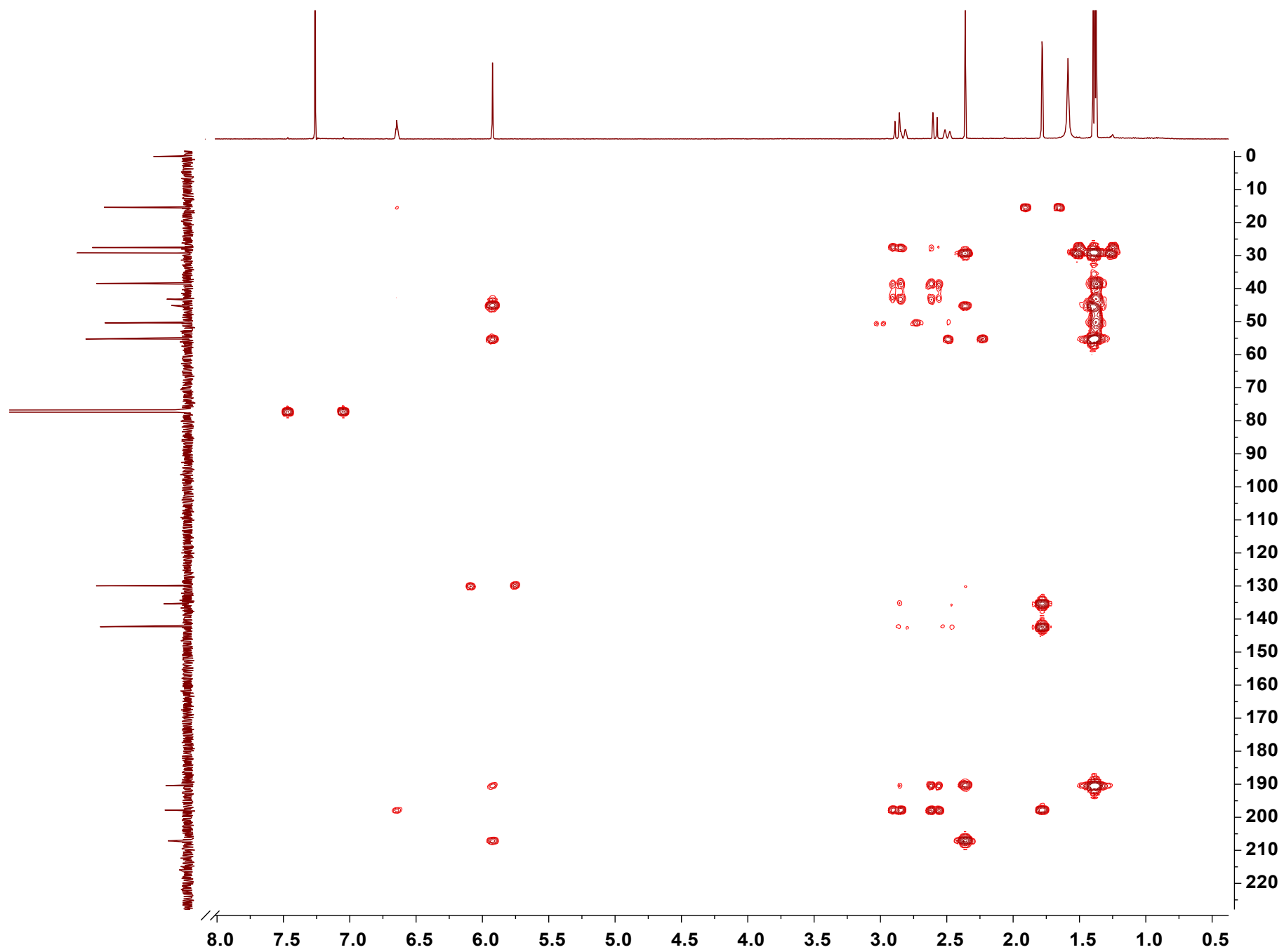


Figure 49S. HREIMS (+) report of 8

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-3

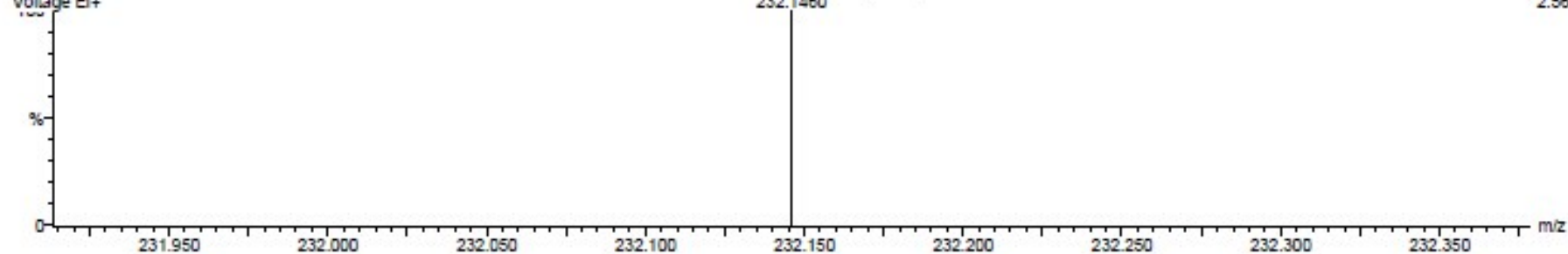
Ilq18

14:22:55 16-Feb-2017

Voltage EI+

K1B
M170217EA-01AFAMM 15 (1.378)
232.1460

Autospec Premier
P776
2.56



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
232.1460	232.1463	-0.3	-1.3	6.0	5546025.5	C15 H20 O2

Figure 50S. ¹H NMR spectrum of **9** (500 MHz, CDCl₃)

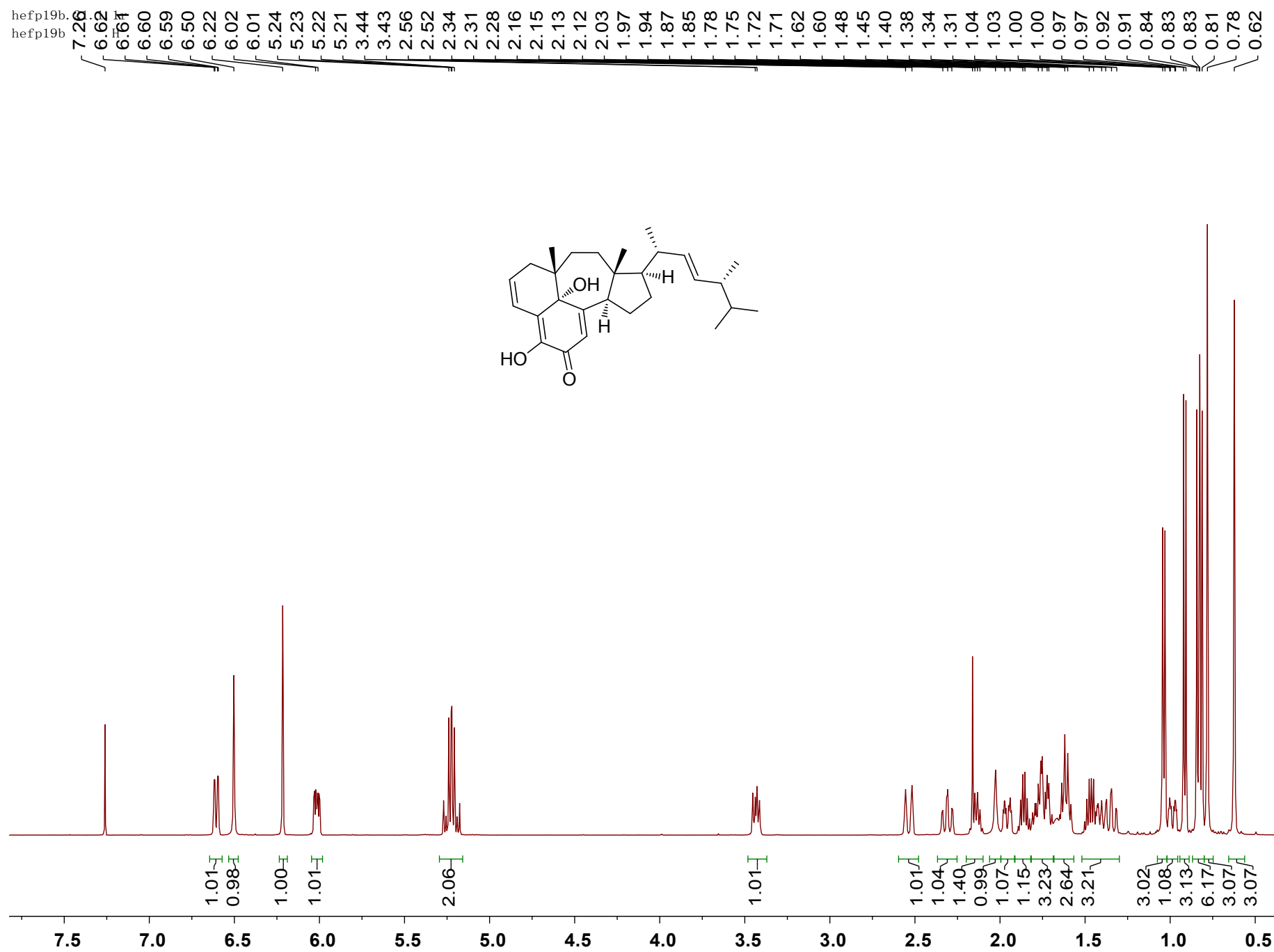


Figure 51S. ^{13}C NMR and DEPT spectra of **9** (125 MHz, CDCl_3)

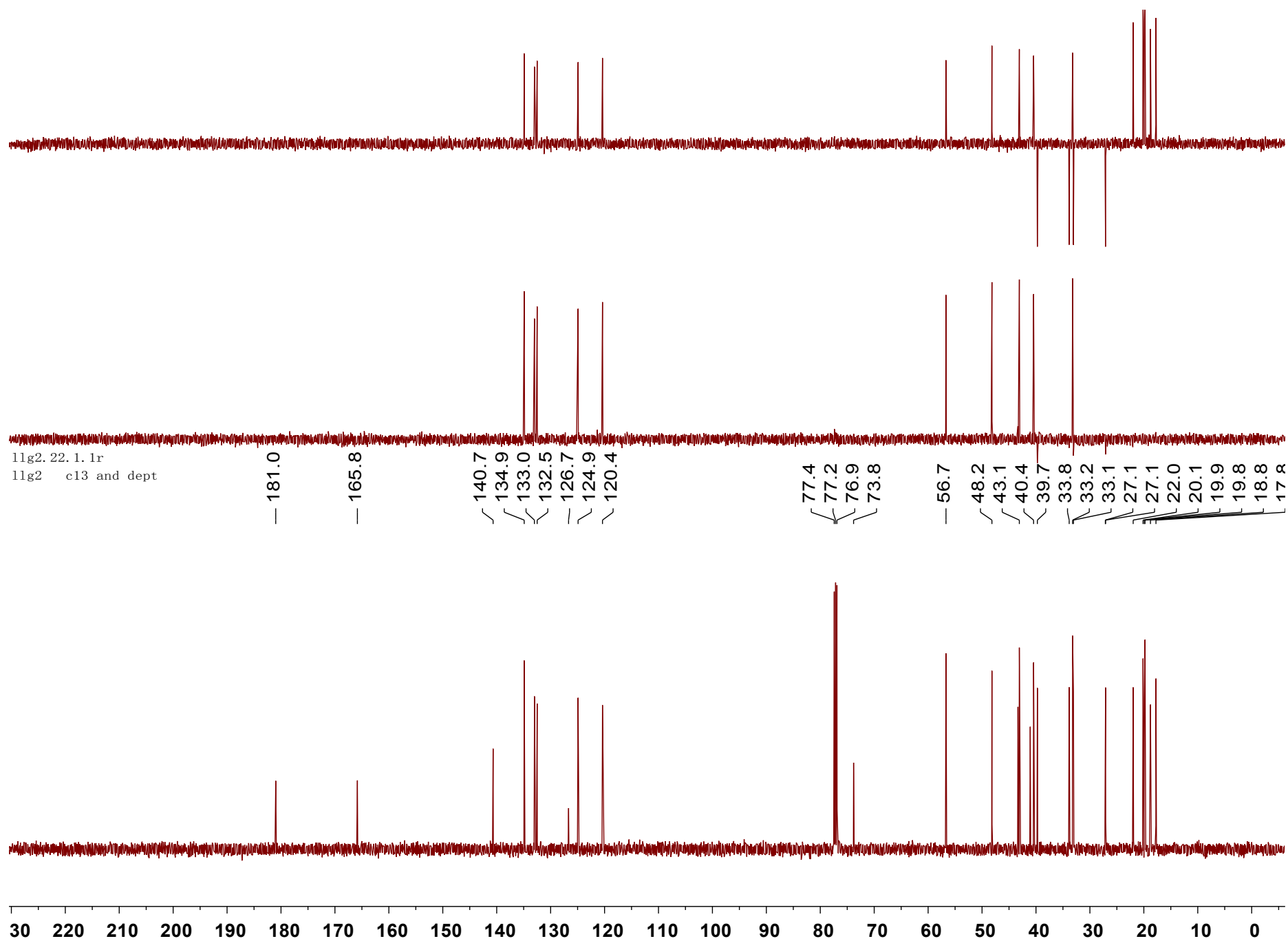


Figure 52S. ¹H NMR spectrum of 9a (500 MHz, CDCl₃)

11g2ac.21.1.1r - Bruker AViii-500MHz; 11g2ac H

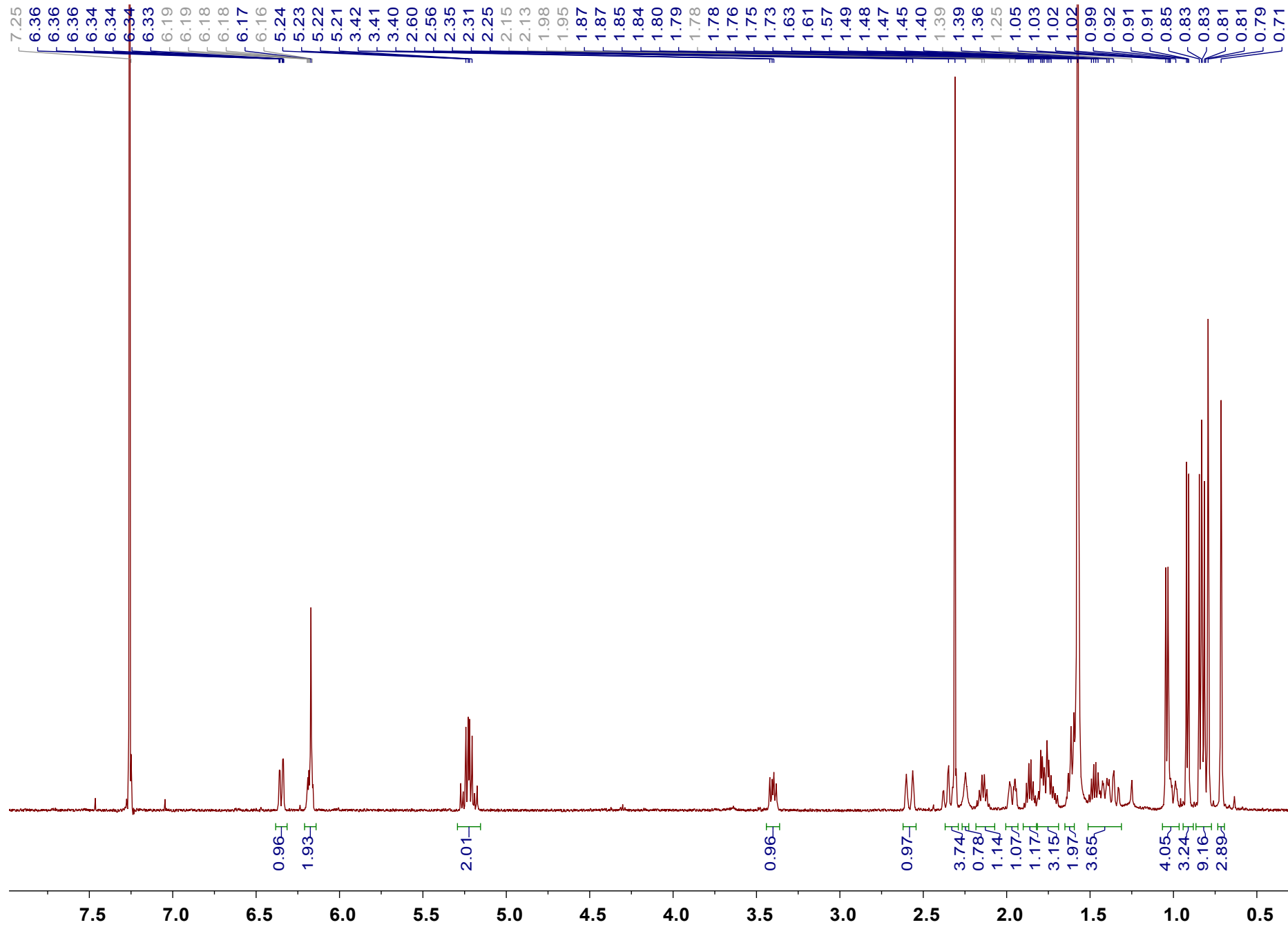
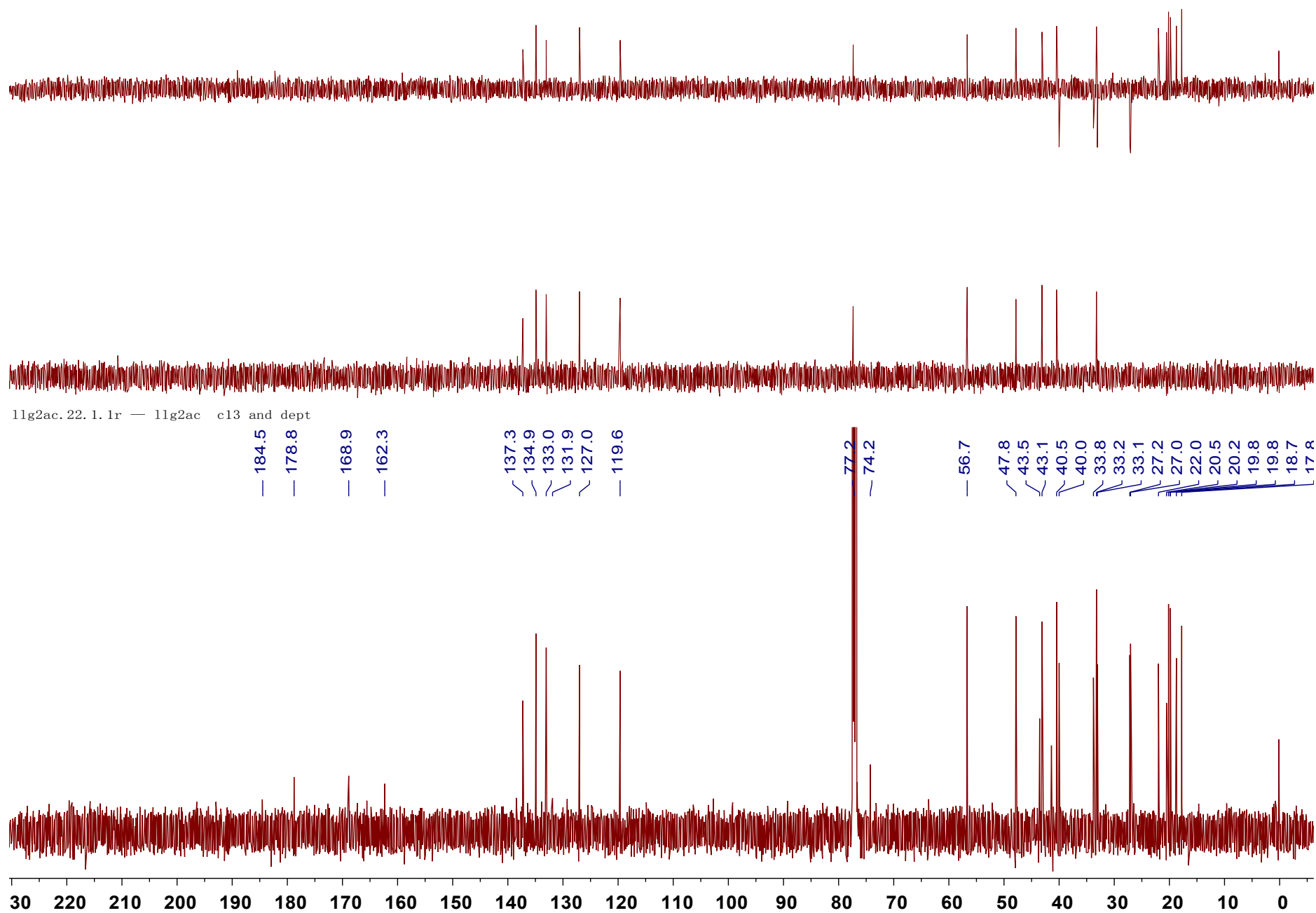
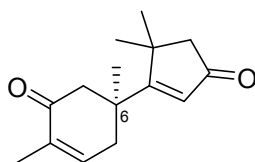


Figure 53S. ^{13}C NMR and DEPT spectra of **9a** (125 MHz, CDCl_3)



3. Computational details for **8**



A conformation search based on molecular mechanics with MMFF94s force fields were performed for (6*S*)-**8** gave 10 stable conformers with distributions higher than 1%.^{1,2} All these conformers were further optimized by the density functional theory method at the B3LYP/6-31G(d,p) level in Gaussian 09 program package,³ led to six ((6*S*)-**8a**–(6*S*)-**8f**) conformers within 3 kcal/mol energy threshold from global minimum, respectively. The predominant conformers were subjected to theoretical calculation of ECD using time-dependent density functional theory (TDDFT) at B3LYP/6-31G(d,p) level with IEFPCM model in air based on B3LYP/6-31G(d,p) optimized conformers. The calculated ECD curves for (6*S*)-**8** were weighted using SpecDis 1.71 with $\sigma = 0.2$ eV, and UV shift 11 nm, respectively.⁴ The ECD curve of the enantiomer (6*R*)-**8** was generated by SpecDis by the function “enantiomeric ECD”.

Table S1. Energy analysis for conformers of (6*S*)-**8a**–(6*S*)-**8f** at B3LYP/6-31G(d,p) level in the gas phase.

Species	$E'=E+ZPE$	E	H	G	ΔE (kcal/mol)	$P_E\%$
(6 <i>S</i>)- 8a	-733.761789	-733.778874	-733.760845	-733.822524	0.00	50.7
(6 <i>S</i>)- 8b	-733.760472	-733.777482	-733.759528	-733.820998	0.96	9.2
(6 <i>S</i>)- 8c	-733.760548	-733.777528	-733.759603	-733.820912	1.01	5.1
(6 <i>S</i>)- 8d	-733.761192	-733.778096	-733.760248	-733.821357	0.73	13.3
(6 <i>S</i>)- 8e	-733.761144	-733.778017	-733.760200	-733.821137	0.87	10.1
(6 <i>S</i>)- 8f	-733.760329	-733.777416	-733.759384	-733.821258	0.79	11.7

E, E', H, G : total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy

Standard orientation of (6*S*)-**8a**

Atom	X	Y	Z
C(1)	0.595	-0.102	1.871
C(2)	0.371	-0.265	0.341
C(3)	0.981	-1.622	-0.107
C(4)	1.135	0.847	-0.420
C(5)	2.484	-1.644	-0.150
C(6)	3.279	-0.560	-0.211

C(7)	2.651	0.784	-0.260
C(8)	4.782	-0.614	-0.228
O(9)	3.321	1.807	-0.232
C(10)	-3.477	0.407	0.033
C(11)	-3.314	-1.096	-0.165
C(12)	-1.875	-1.378	-0.041
C(13)	-1.141	-0.251	0.081
C(14)	-2.046	1.010	-0.044
O(15)	-4.207	-1.902	-0.357
C(16)	-1.849	2.064	1.062
C(17)	-1.871	1.680	-1.431
H(18)	0.029	-0.858	2.422
H(19)	1.654	-0.225	2.116
H(20)	0.284	0.882	2.224
H(21)	0.639	-2.425	0.556
H(22)	0.600	-1.883	-1.106
H(23)	0.934	0.753	-1.497
H(24)	0.829	1.851	-0.120
H(25)	2.945	-2.632	-0.136
H(26)	5.142	-1.645	-0.185
H(27)	5.178	-0.139	-1.131
H(28)	5.198	-0.057	0.618
H(29)	-4.174	0.829	-0.696
H(30)	-3.917	0.564	1.026
H(31)	-1.507	-2.397	-0.050
H(32)	-0.866	2.541	1.021
H(33)	-1.978	1.629	2.058
H(34)	-2.598	2.855	0.947
H(35)	-2.029	0.958	-2.239
H(36)	-2.612	2.479	-1.544
H(37)	-0.886	2.129	-1.562

Standard orientation of (6*S*)-**8b**

Atom	X	Y	Z
C(1)	-0.637	-1.700	-1.193
C(2)	-0.342	-0.526	-0.228
C(3)	-0.874	-0.896	1.192
C(4)	-1.134	0.706	-0.732
C(5)	-2.373	-0.872	1.313
C(6)	-3.211	-0.231	0.477
C(7)	-2.650	0.537	-0.666
C(8)	-4.708	-0.241	0.616
O(9)	-3.376	1.070	-1.493

C(10)	3.354	0.579	0.501
C(11)	3.457	-0.818	-0.101
C(12)	2.080	-1.259	-0.372
C(13)	1.172	-0.291	-0.125
C(14)	1.883	1.034	0.284
O(15)	4.482	-1.449	-0.290
C(16)	1.856	2.053	-0.884
C(17)	1.344	1.699	1.567
H(18)	-0.214	-2.640	-0.831
H(19)	-1.713	-1.852	-1.300
H(20)	-0.224	-1.499	-2.186
H(21)	-0.499	-1.890	1.466
H(22)	-0.461	-0.215	1.947
H(23)	-0.911	1.587	-0.120
H(24)	-0.878	0.957	-1.765
H(25)	-2.791	-1.417	2.159
H(26)	-5.022	-0.832	1.480
H(27)	-5.096	0.777	0.725
H(28)	-5.177	-0.652	-0.283
H(29)	3.592	0.500	1.569
H(30)	4.093	1.253	0.060
H(31)	1.880	-2.260	-0.733
H(32)	0.852	2.414	-1.112
H(33)	2.272	1.611	-1.795
H(34)	2.467	2.924	-0.623
H(35)	1.383	1.012	2.419
H(36)	1.966	2.565	1.816
H(37)	0.317	2.059	1.466

Standard orientation of (6S)-**8c**

Atom	X	Y	Z
C(1)	0.243	-1.930	-2.028
C(2)	-0.353	-1.008	-0.934
C(3)	-1.054	-1.871	0.148
C(4)	-1.476	-0.162	-1.581
C(5)	-1.943	-1.073	1.067
C(6)	-2.482	0.122	0.761
C(7)	-2.238	0.705	-0.587
C(8)	-3.344	0.922	1.697
O(9)	-2.675	1.804	-0.899
C(10)	2.895	0.626	0.515
C(11)	2.181	1.752	-0.226
C(12)	0.952	1.167	-0.788

C(13)	0.765	-0.109	-0.384
C(14)	1.855	-0.520	0.651
O(15)	2.576	2.897	-0.352
C(16)	1.285	-0.485	2.092
C(17)	2.525	-1.884	0.400
H(18)	0.969	-2.637	-1.623
H(19)	-0.557	-2.508	-2.502
H(20)	0.739	-1.338	-2.803
H(21)	-1.666	-2.626	-0.370
H(22)	-0.330	-2.444	0.733
H(23)	-1.119	0.469	-2.398
H(24)	-2.206	-0.858	-2.021
H(25)	-2.158	-1.513	2.040
H(26)	-3.475	0.410	2.654
H(27)	-2.901	1.906	1.881
H(28)	-4.329	1.108	1.257
H(29)	3.746	0.311	-0.102
H(30)	3.300	0.972	1.470
H(31)	0.308	1.746	-1.437
H(32)	0.530	-1.253	2.270
H(33)	0.835	0.487	2.312
H(34)	2.098	-0.654	2.807
H(35)	2.951	-1.945	-0.606
H(36)	3.344	-2.021	1.114
H(37)	1.838	-2.725	0.532

Standard orientation of (6*S*)-**8d**

Atom	X	Y	Z
C(1)	0.617	-0.260	1.829
C(2)	0.390	-0.052	0.305
C(3)	0.951	-1.261	-0.492
C(4)	1.199	1.194	-0.137
C(5)	2.454	-1.343	-0.507
C(6)	3.289	-0.308	-0.305
C(7)	2.714	1.036	-0.042
C(8)	4.788	-0.416	-0.324
O(9)	3.429	1.999	0.197
C(10)	-3.524	-0.106	0.075
C(11)	-3.125	1.341	-0.192
C(12)	-1.658	1.393	-0.096
C(13)	-1.111	0.169	0.065
C(14)	-2.211	-0.935	-0.001
O(15)	-3.882	2.270	-0.412

C(16)	-2.181	-1.673	-1.365
C(17)	-2.165	-1.973	1.136
H(18)	0.114	-1.153	2.201
H(19)	1.684	-0.366	2.047
H(20)	0.241	0.602	2.388
H(21)	0.550	-2.201	-0.100
H(22)	0.607	-1.200	-1.534
H(23)	0.969	1.427	-1.186
H(24)	0.941	2.079	0.450
H(25)	2.876	-2.325	-0.720
H(26)	5.111	-1.441	-0.523
H(27)	5.215	0.244	-1.087
H(28)	5.211	-0.091	0.632
H(29)	-3.958	-0.150	1.082
H(30)	-4.297	-0.440	-0.622
H(31)	-1.131	2.337	-0.152
H(32)	-1.299	-2.305	-1.484
H(33)	-2.211	-0.963	-2.197
H(34)	-3.059	-2.322	-1.444
H(35)	-2.201	-1.495	2.120
H(36)	-3.035	-2.635	1.058
H(37)	-1.274	-2.605	1.094

Standard orientation of (6*S*)-**8e**

Atom	X	Y	Z
C(1)	0.653	-1.118	1.420
C(2)	0.395	-0.186	0.213
C(3)	0.923	-0.854	-1.097
C(4)	1.223	1.108	0.416
C(5)	2.425	-0.896	-1.201
C(6)	3.278	-0.126	-0.502
C(7)	2.728	0.879	0.447
C(8)	4.776	-0.215	-0.606
O(9)	3.457	1.538	1.174
C(10)	-3.458	-0.064	-0.465
C(11)	-3.012	1.394	-0.473
C(12)	-1.557	1.383	-0.239
C(13)	-1.095	0.145	0.041
C(14)	-2.277	-0.864	0.151
O(15)	-3.717	2.367	-0.669
C(16)	-2.081	-2.195	-0.597
C(17)	-2.615	-1.152	1.637
H(18)	0.147	-2.080	1.313

H(19)	1.721	-1.325	1.520
H(20)	0.317	-0.653	2.351
H(21)	0.535	-1.873	-1.191
H(22)	0.526	-0.306	-1.965
H(23)	1.046	1.794	-0.422
H(24)	0.939	1.633	1.332
H(25)	2.830	-1.619	-1.909
H(26)	5.080	-0.980	-1.325
H(27)	5.202	0.747	-0.911
H(28)	5.217	-0.449	0.368
H(29)	-4.404	-0.190	0.067
H(30)	-3.631	-0.362	-1.507
H(31)	-0.981	2.297	-0.298
H(32)	-1.295	-2.815	-0.157
H(33)	-1.841	-2.034	-1.653
H(34)	-3.009	-2.775	-0.555
H(35)	-2.798	-0.222	2.184
H(36)	-3.526	-1.759	1.692
H(37)	-1.825	-1.699	2.153

Standard orientation of (6*S*)-**8f**

Atom	X	Y	Z
C(1)	0.653	0.775	1.652
C(2)	0.387	-0.092	0.398
C(3)	1.039	-1.484	0.619
C(4)	1.100	0.534	-0.837
C(5)	2.544	-1.464	0.608
C(6)	3.299	-0.535	-0.008
C(7)	2.624	0.574	-0.729
C(8)	4.802	-0.536	-0.015
O(9)	3.261	1.470	-1.264
C(10)	-3.382	0.293	-0.585
C(11)	-3.139	-1.210	-0.559
C(12)	-1.718	-1.393	-0.217
C(13)	-1.113	-0.228	0.103
C(14)	-2.159	0.930	0.132
O(15)	-3.952	-2.083	-0.806
C(16)	-2.575	1.256	1.590
C(17)	-1.736	2.228	-0.580
H(18)	0.131	0.371	2.524
H(19)	1.721	0.792	1.882
H(20)	0.334	1.810	1.509
H(21)	0.679	-1.923	1.557

H(22)	0.722	-2.175	-0.174
H(23)	0.859	-0.064	-1.727
H(24)	0.771	1.553	-1.040
H(25)	3.039	-2.288	1.122
H(26)	5.202	-1.386	0.544
H(27)	5.185	-0.575	-1.040
H(28)	5.193	0.389	0.422
H(29)	-3.422	0.603	-1.637
H(30)	-4.344	0.553	-0.135
H(31)	-1.274	-2.380	-0.238
H(32)	-1.765	1.701	2.170
H(33)	-2.915	0.355	2.111
H(34)	-3.404	1.972	1.579
H(35)	-1.444	2.044	-1.618
H(36)	-2.583	2.923	-0.594
H(37)	-0.911	2.738	-0.076

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