Electronic Supplementary Information (ESI)

Synthesis, Cu(II) complexation, ^{64}Cu-labeling and biological evaluation of cross-bridged cyclam chelators with phosphonate pendant arms

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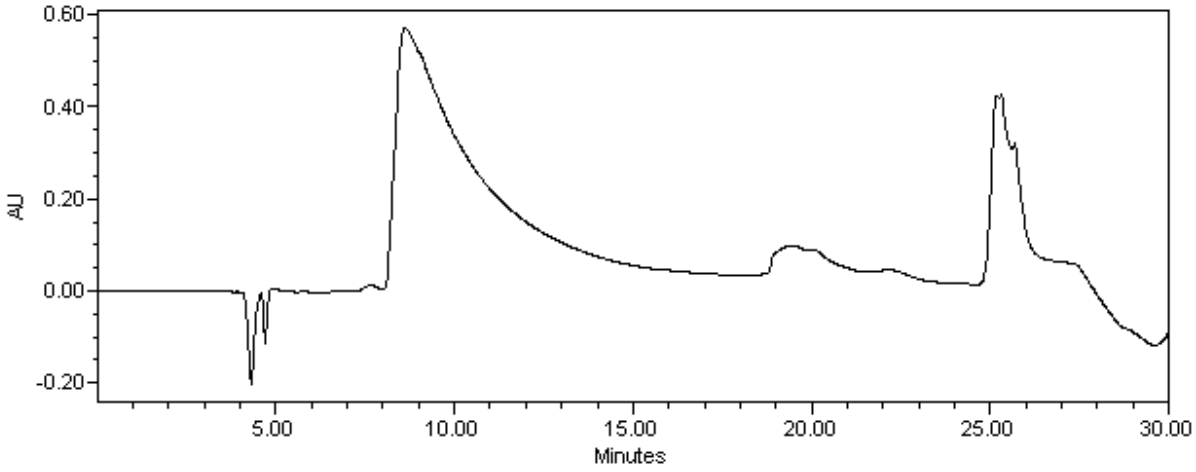
1. Details of HPLC Purification of CB-TE1A1P (**2**)

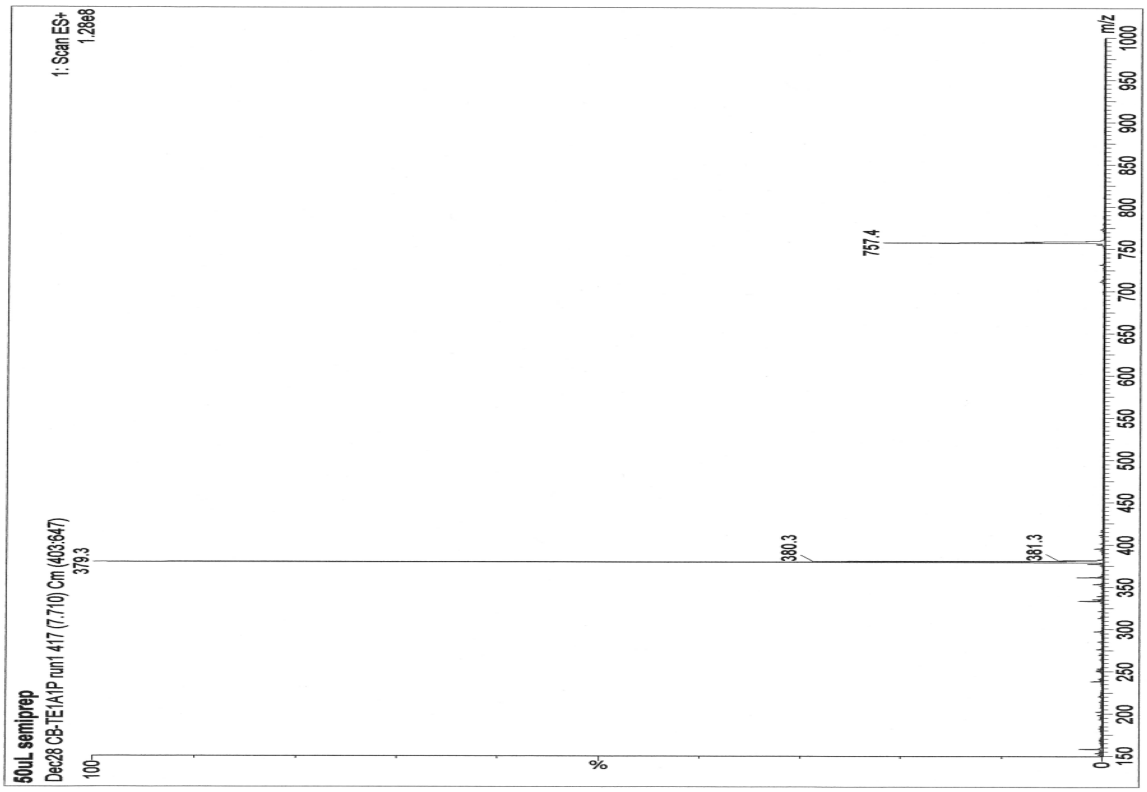
A batch of CB-TE1A1P that contained some impurities was purified by HPLC using a C_{18} semipreparative column with a 3 mL/min flow rate and the following gradient:

Time (min)	% 0.1% TFA in water	% 0.1% TFA in acetonitrile
0	100	0
10	100	0
20	90	10
21	50	50
23	50	50
24	80	20
25	100	0
30	100	0

The compound eluted with a broad peak starting at 8.0 minutes. The collection was stopped after minute 15.0. A UV chromatogram at 210 nm is shown in the figure below.



LC-MS was used to make sure that no impurity eluted in the 8.0-15.0 minute range. The only peaks visible in the MS chromatogram of the collected fractions are M^*H^+ (m/z= 379.3) and $2M^*H^+$ (m/z=757.4).



2. List of X-ray Crystallographic Software Employed

APEX2 Version 2.2 /SHELXTL (Bruker AXS Inc., 2007)
SAINT Version 7.34a (Bruker AXS Inc., 2007)
SADABS Version 2007/2 (Sheldrick, Bruker AXS Inc.)
XPREP Version 2005/2 (Sheldrick, Bruker AXS Inc.)

Bruker suite of programs APEX2/SHELXTL, SAINT, SADABS, XPREP may be obtained from Bruker AXS.Inx, 5467 East Cheryl Parkway, Madison WI 53711

XS Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) **A64**, 112-122.)
XL Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) **A64**, 112-122.)

X-ray crystal structure figures were prepared using CrystalMaker 8.5 for Mac (CrystalMaker Software Ltd., Centre for Innovation & Enterprise, Oxford University Begbroke Science Park, Sandy Lane, Yarnton, Oxfordshire, OX5 1PF, UK; http://www.crystalmaker.com)

3. Detailed Energetic Results for DFT Calculations

Cu-CBTE2P

Method	Conformer	E (kcal/mol)	ZPE (kcal/mol)	ZPE-corr E (kcal/mol)	Hº (kcal/mol)	Sº (cal/mol K)	Gº (kcal/mol)
B3LYP/6-31G*	[2233]/[2233]	-2224578.459	303.547	-2224274.912	-2224259.710	151.315	-2224304.824
B3LYP/6-31G*	[2323]/[2323]	-2224577.968	303.065	-2224274.903	-2224259.624	152.192	-2224305.000
	Delta (1st-2nd)	-0.491		-0.009	-0.086		0.176
M06/6-31G*	[2233]/[2233]	-2224057.804	302.986	-2223754.818	-2223739.849	149.505	-2223784.424
M06/6-31G*	[2323]/[2323]	-2224056.887	302.769	-2223754.118	-2223739.125	149.999	-2223783.847
	Delta (1st-2nd)	-0.917		-0.700	-0.724		-0.577
M06/6-31+G**	[2233]/[2233]	-2224119.778					
M06/6-31+G**	[2323]/[2323]	-2224118.92					
		-0.858					

Cu-CBTE1A1P

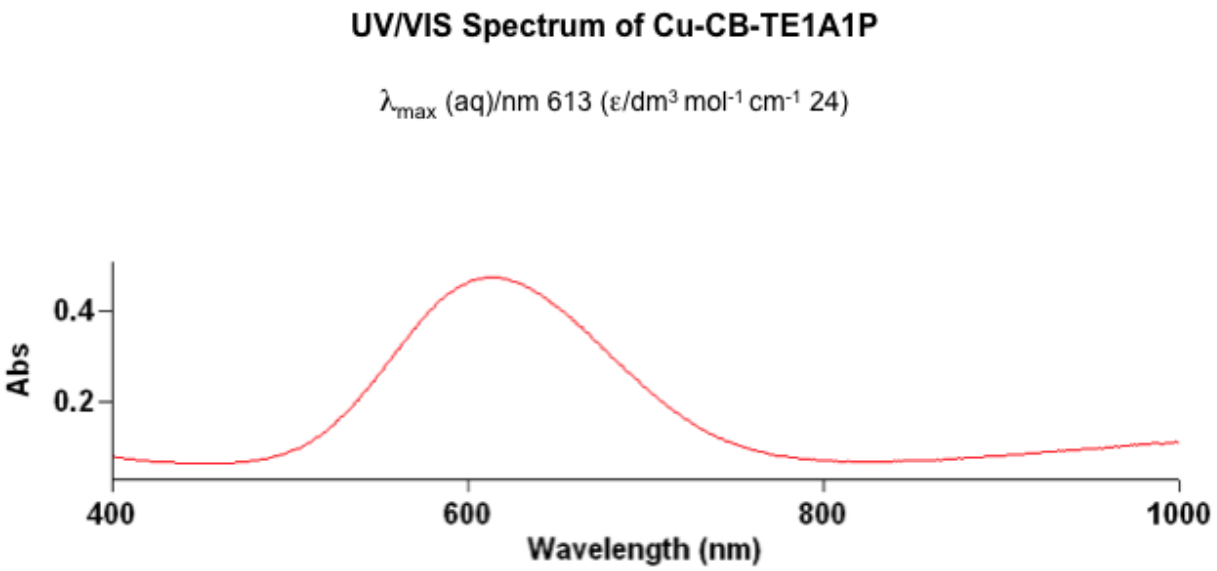
Method	Conformer	E (kcal/mol)	ZPE (kcal/mol)	ZPE-corr E (kcal/mol)	Hº (kcal/mol)	Sº (cal/mol K)	Gº (kcal/mol)
B3LYP/6-31G*	[2233]/[2233]	-1986668.793	296.081	-1986372.713	-1986358.562	144.926	-1986401.771
B3LYP/6-31G*	[2323]/[2323]	-1986669.104	296.320	-1986372.784	-1986358.654	144.825	-1986401.833
	Delta (1st-2nd)	0.311		0.071	0.092		0.062
M06/6-31G*	[2233]/[2233]	-1986163.941	295.292	-1985868.649	-1985854.737	142.918	-1985897.348
M06/6-31G*	[2323]/[2323]	-1986163.415	295.461	-1985867.954	-1985854.048	143.092	-1985896.711
	Delta (1st-2nd)	-0.526		-0.695	-0.689		-0.637
M06/6-31+G**	[2233]/[2233]	-1986219.083					

M06/6-31+G**	[2323]/[2323]	-1986218.413					
		-0.67					

Cu-CBTE2A

Method	Conformer	E (kcal/mol)	ZPE (kcal/mol)	ZPE-corrected E (kcal/mol)	Hº (kcal/mol)	Sº (cal/mol K)	Gº (kcal/mol)
B3LYP/6-31G*	[2233]/[2233]	-1748754.253	289.366	-1748464.887	-1748451.890	137.475	-1748492.879
B3LYP/6-31G*	[2323]/[2323]	-1748755.612	289.171	-1748466.441	-1748453.402	138.029	-1748494.555
	Delta (1st-2nd)	1.359		1.554	1.512		1.676
M06/6-31G*	[2233]/[2233]	-1748265.280	287.683	-1747977.597	-1747964.701	136.644	-1748005.442
M06/6-31G*	[2323]/[2323]	-1748266.435	288.257	-1747978.179	-1747965.361	136.448	-1748006.043
	Delta (1st-2nd)	1.155		0.582	0.660		0.601
M06/6-31+G**	[2233]/[2233]	-1748313.884					
M06/6-31+G**	[2323]/[2323]	-1748314.563					
	Delta (1st-2nd)	0.679					

4. UV/VIS Spectrum of Cu-CB-TE1A1P



5. NMR spectra of ligand **2** and precursor **6**

(Note that NMR spectra for ligand **1** and its precursor **4** may be found in the ESI of reference 55 (D. J. Stigers, R. Ferdani, G. R. Weisman, E. H. Wong, C. J. Anderson, J. A. Golen, C. Moore and A. L. Rheingold, *Dalton Trans.*, 2010, **39**, 1699-1701; doi: 10.1039/b920871b).

1	Data File Name	RF-CB-TE1A1P_1H
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5	Receiver Gain	28
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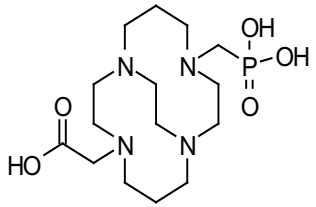
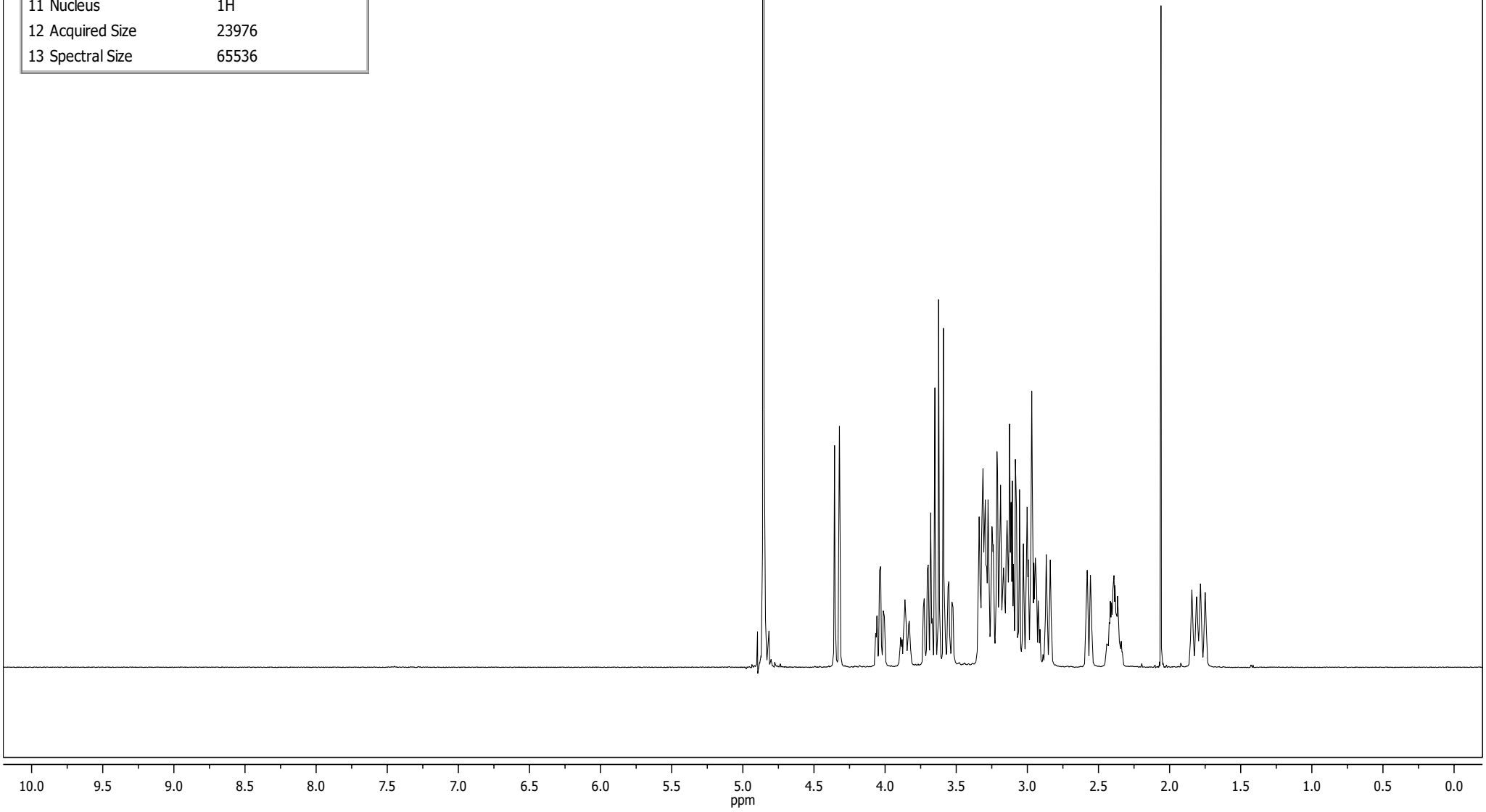
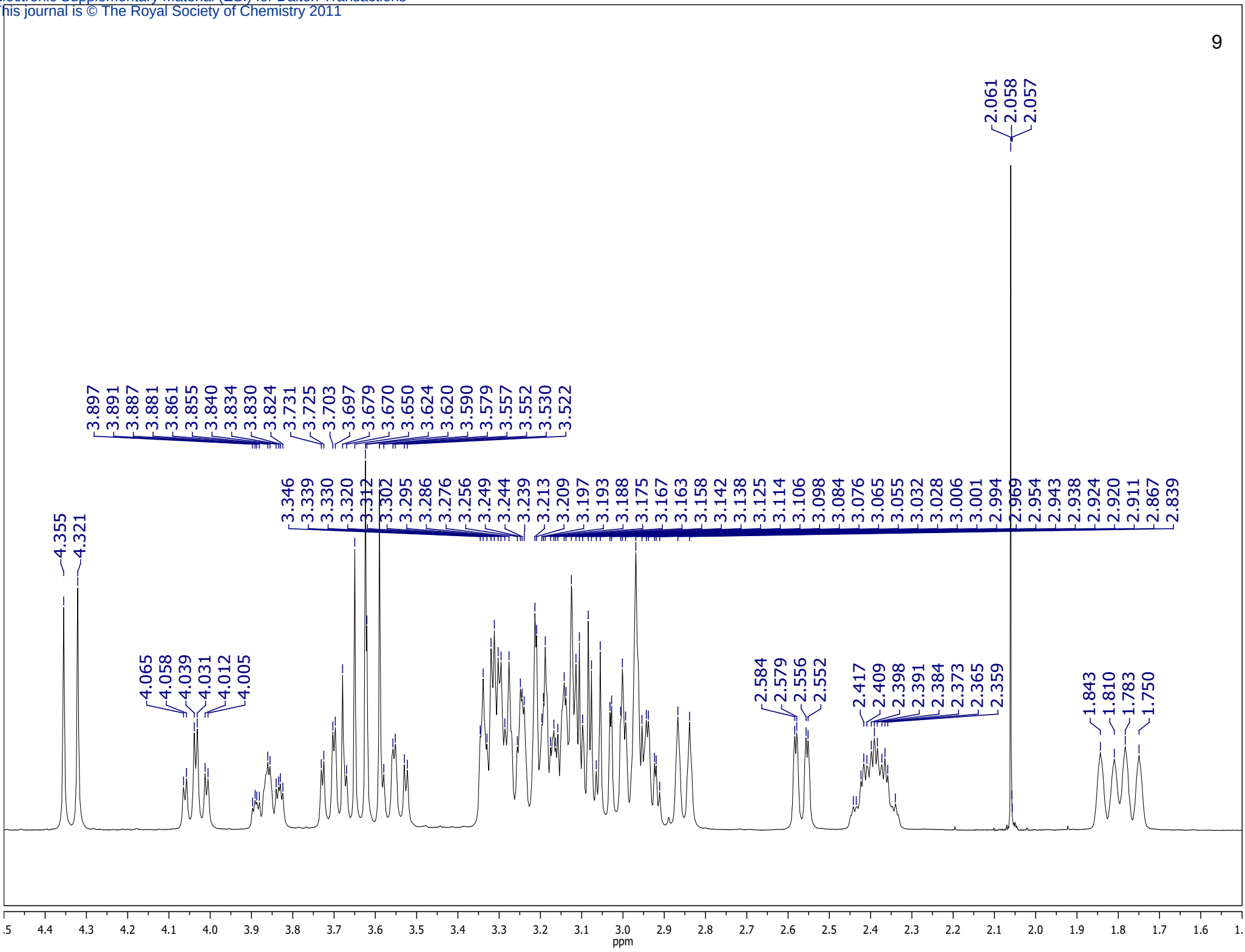
7	Acquisition Date	2011-01-21T10:51:45
8	Spectrometer Frequency	499.77707
9	Spectral Width	7992.0
10	Lowest Frequency	-1419.1
11	Nucleus	1H
12	Acquired Size	23976
13	Spectral Size	65536

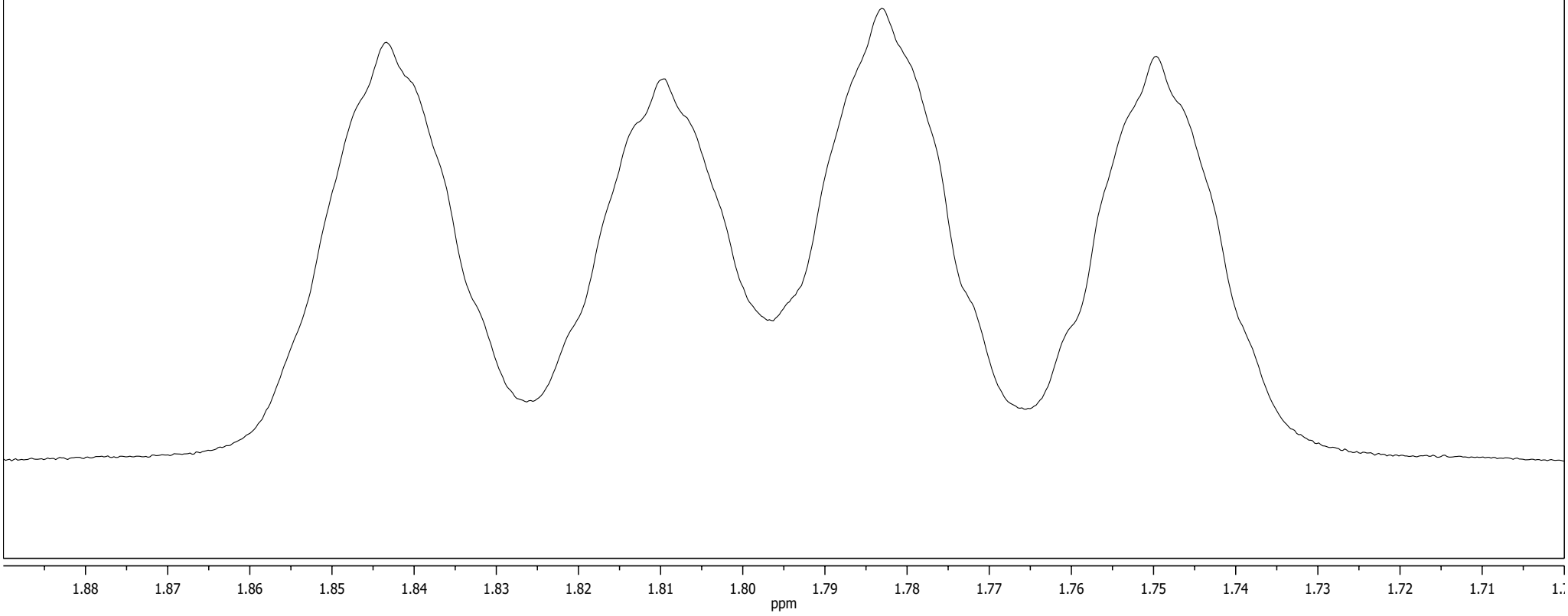


D_2O, 499.78 MHz, internal reference
with MeCN set at δ 2.06



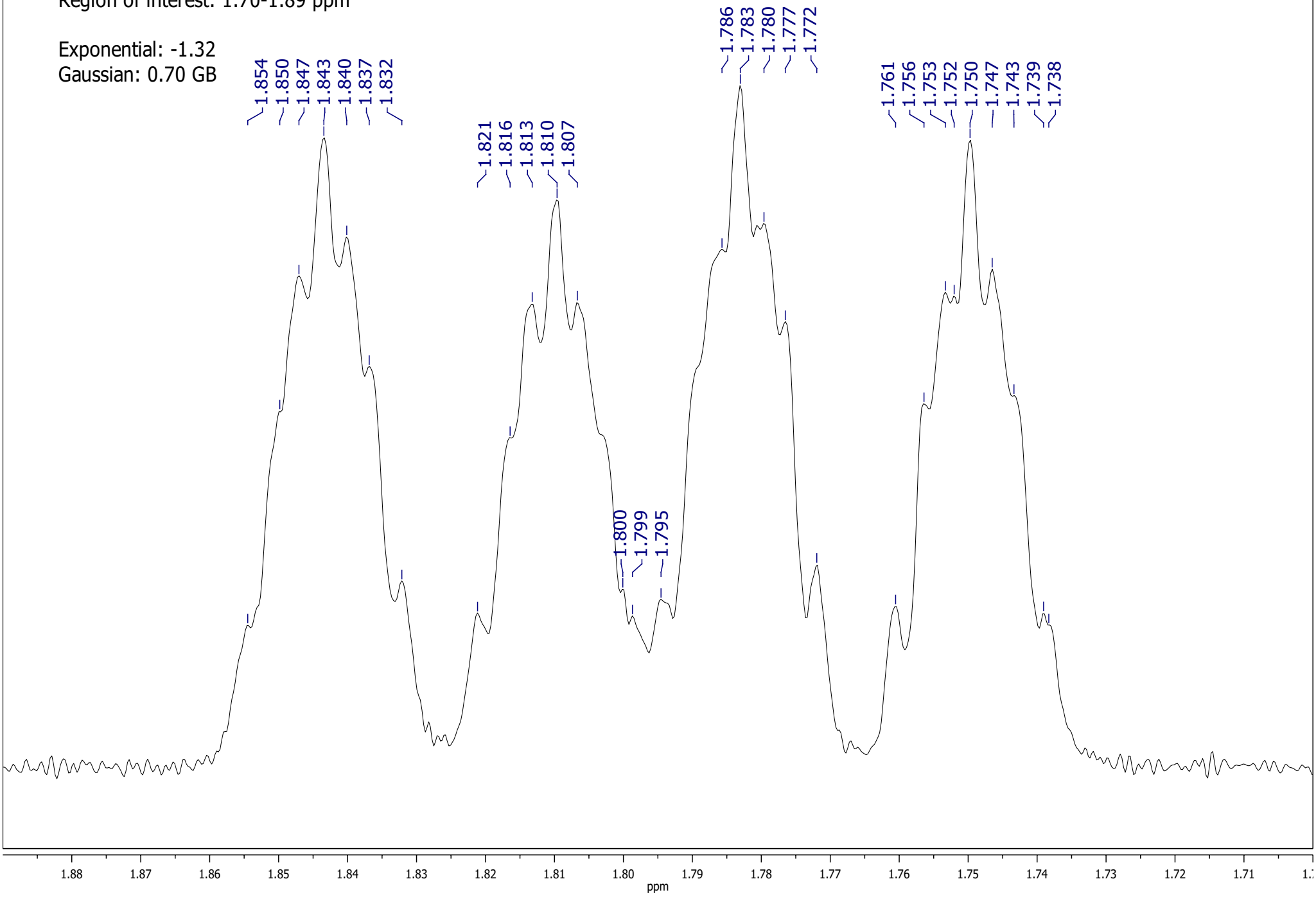


Region of interest: 1.70-1.89 ppm



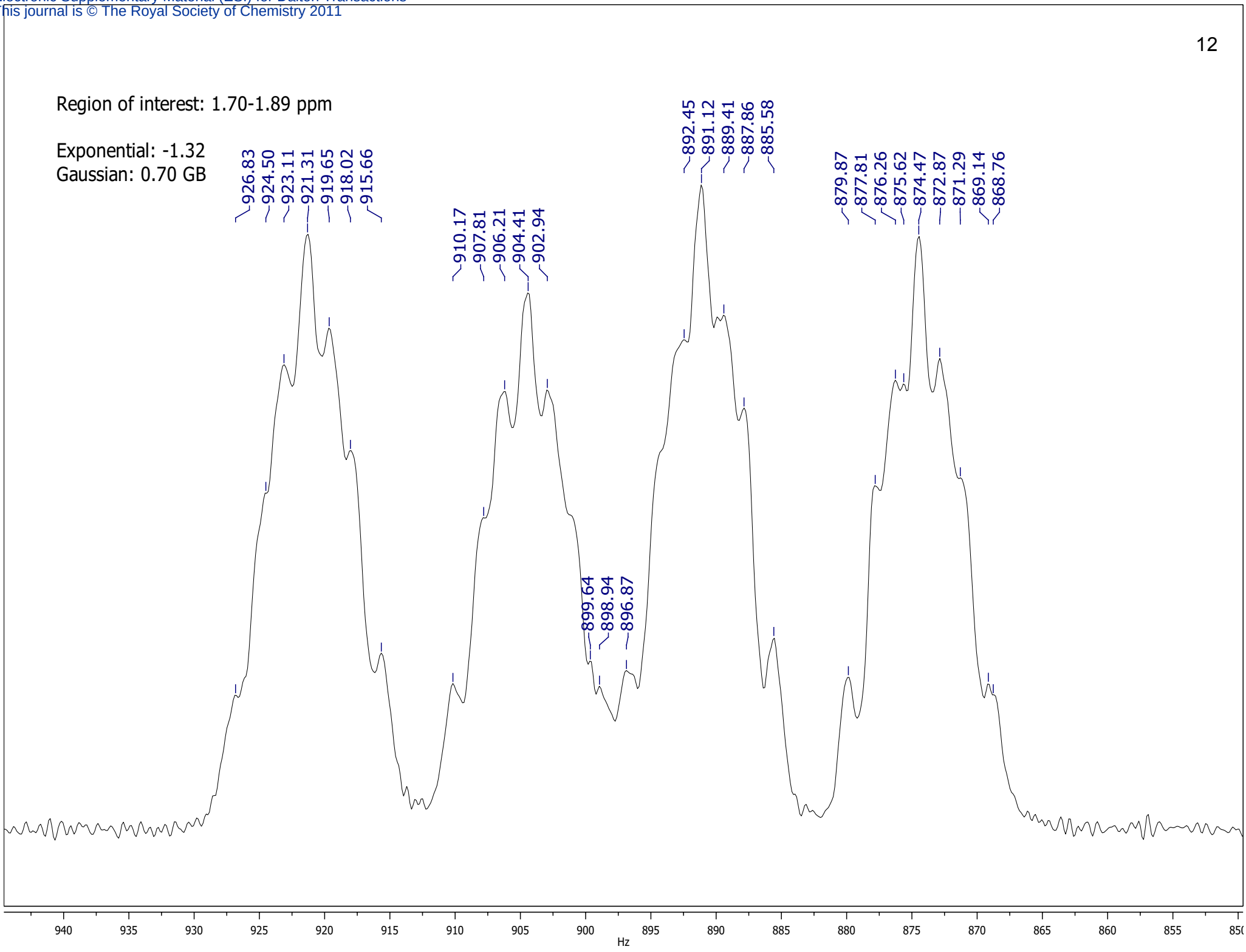
Region of interest: 1.70-1.89 ppm

Exponential: -1.32
Gaussian: 0.70 GB

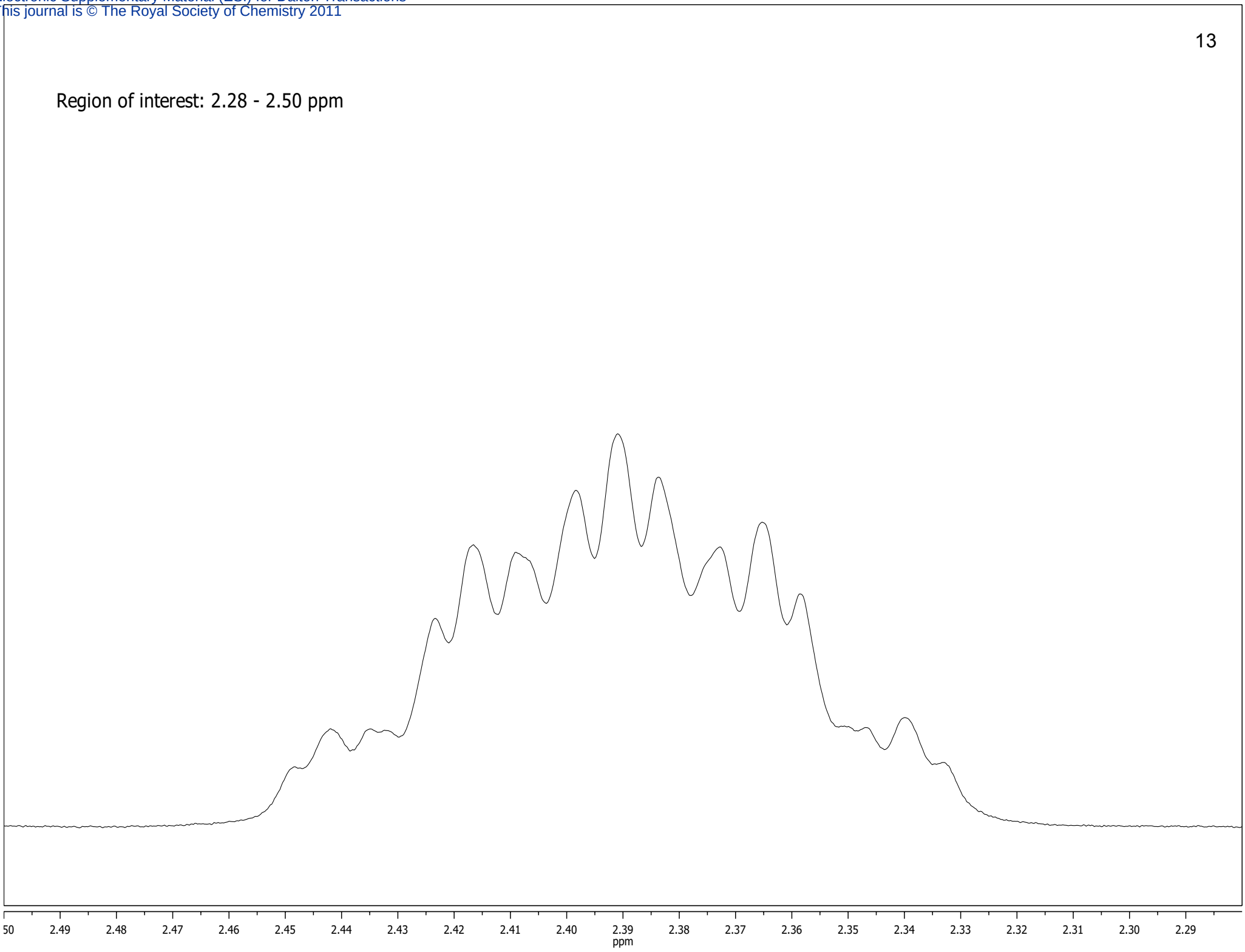


Region of interest: 1.70-1.89 ppm

Exponential: -1.32
Gaussian: 0.70 GB

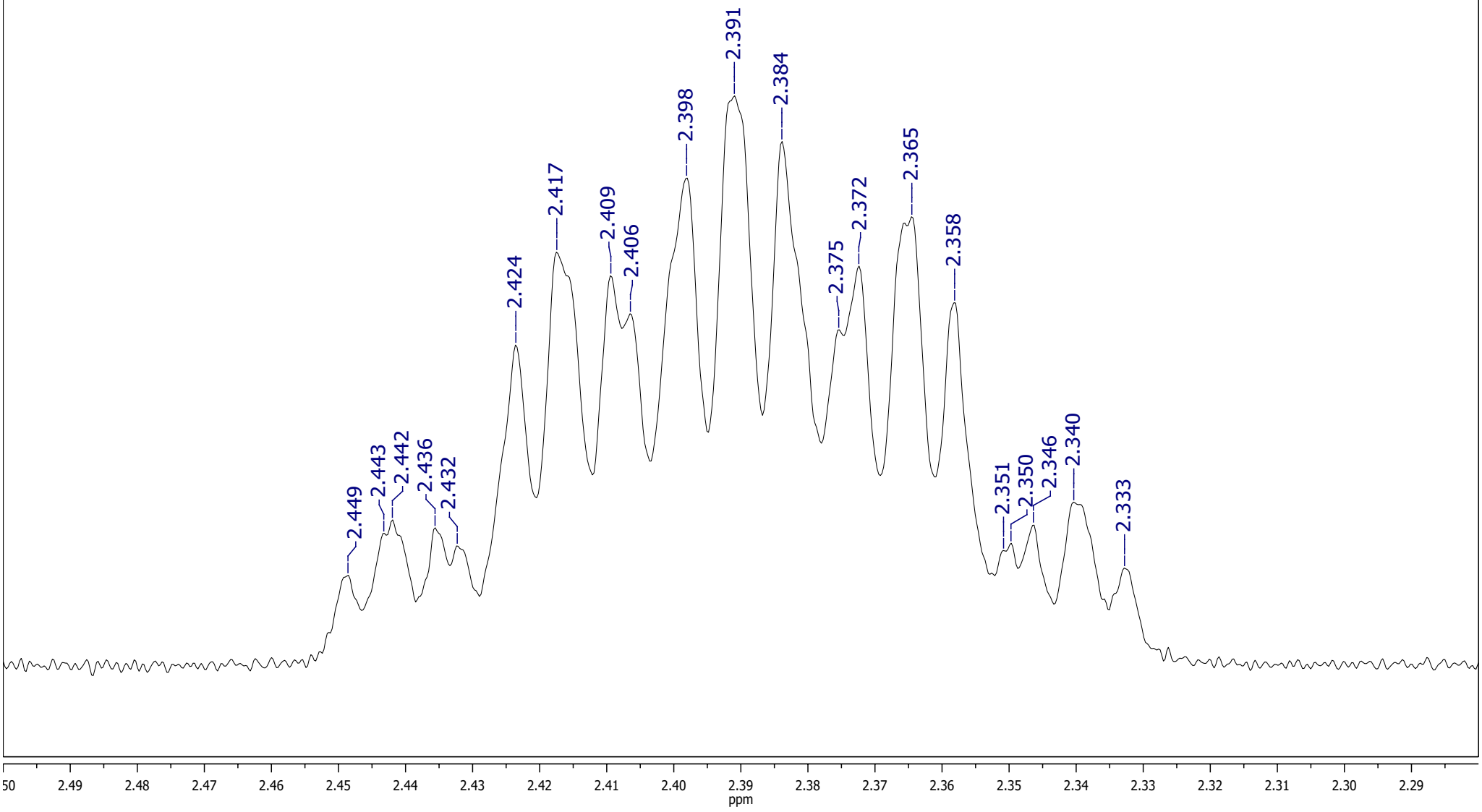


Region of interest: 2.28 - 2.50 ppm



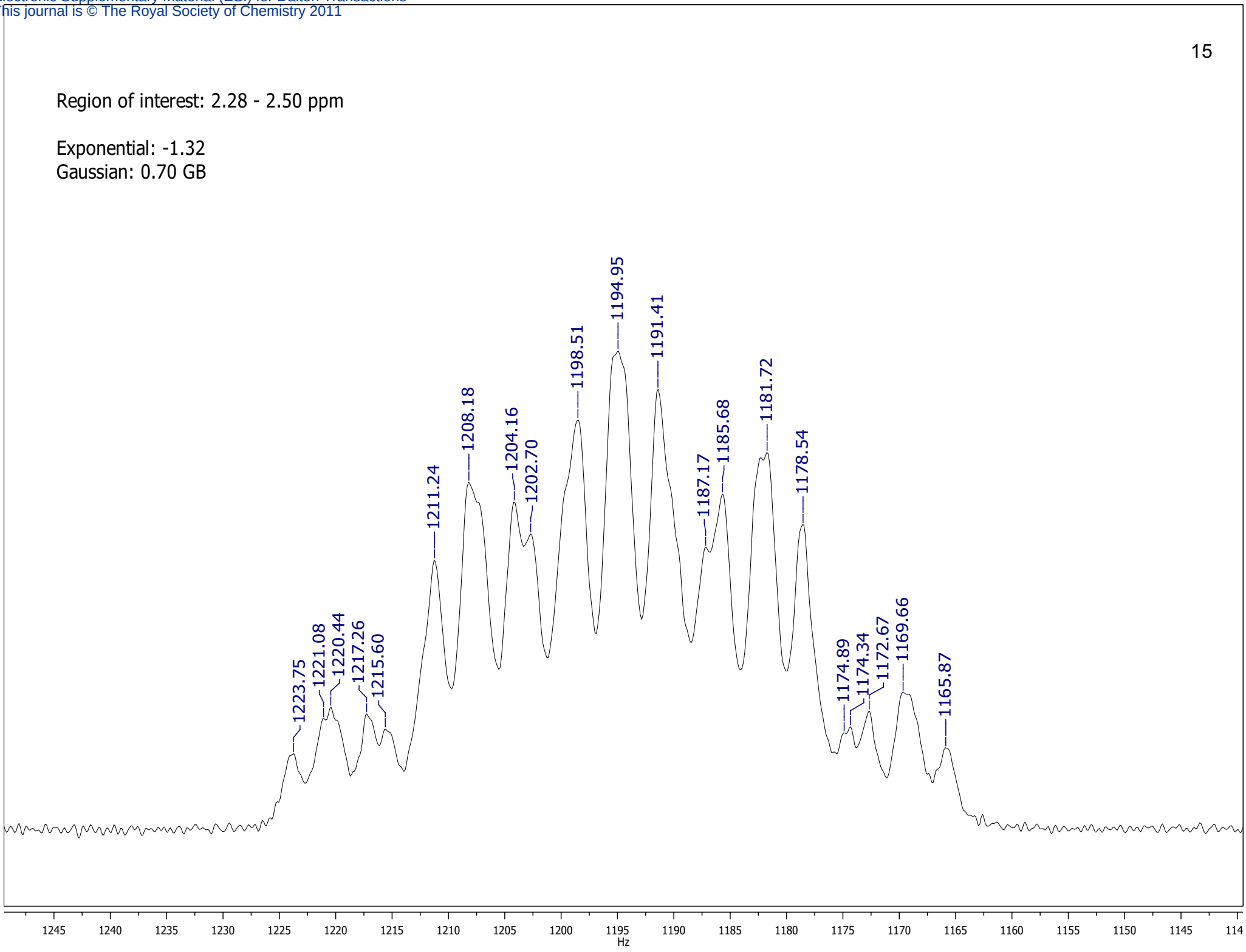
Region of interest: 2.28 - 2.50 ppm

Exponential: -1.32
Gaussian: 0.70 GB



Region of interest: 2.28 - 2.50 ppm

Exponential: -1.32
Gaussian: 0.70 GB



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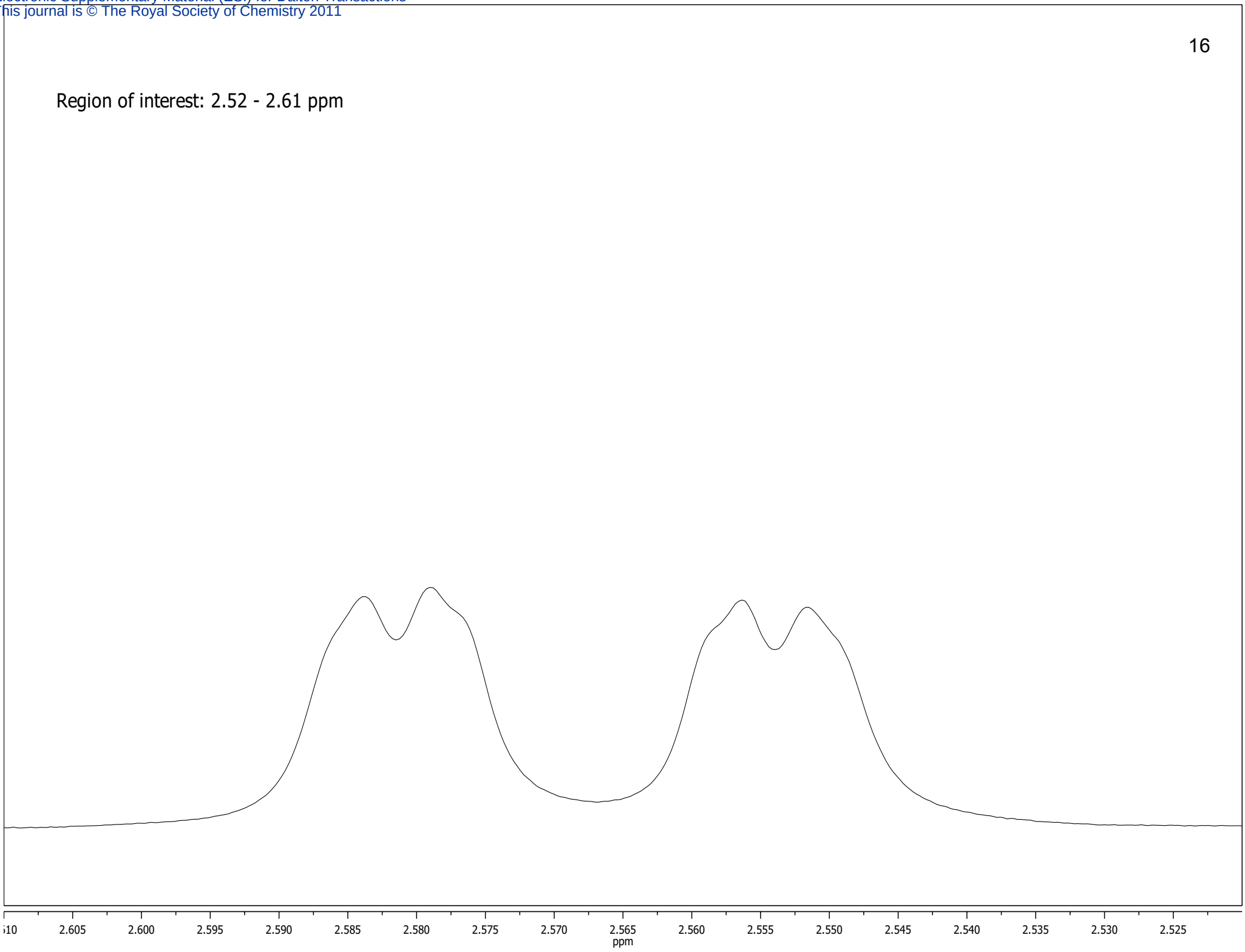

Region of interest: 2.52 - 2.61 ppm

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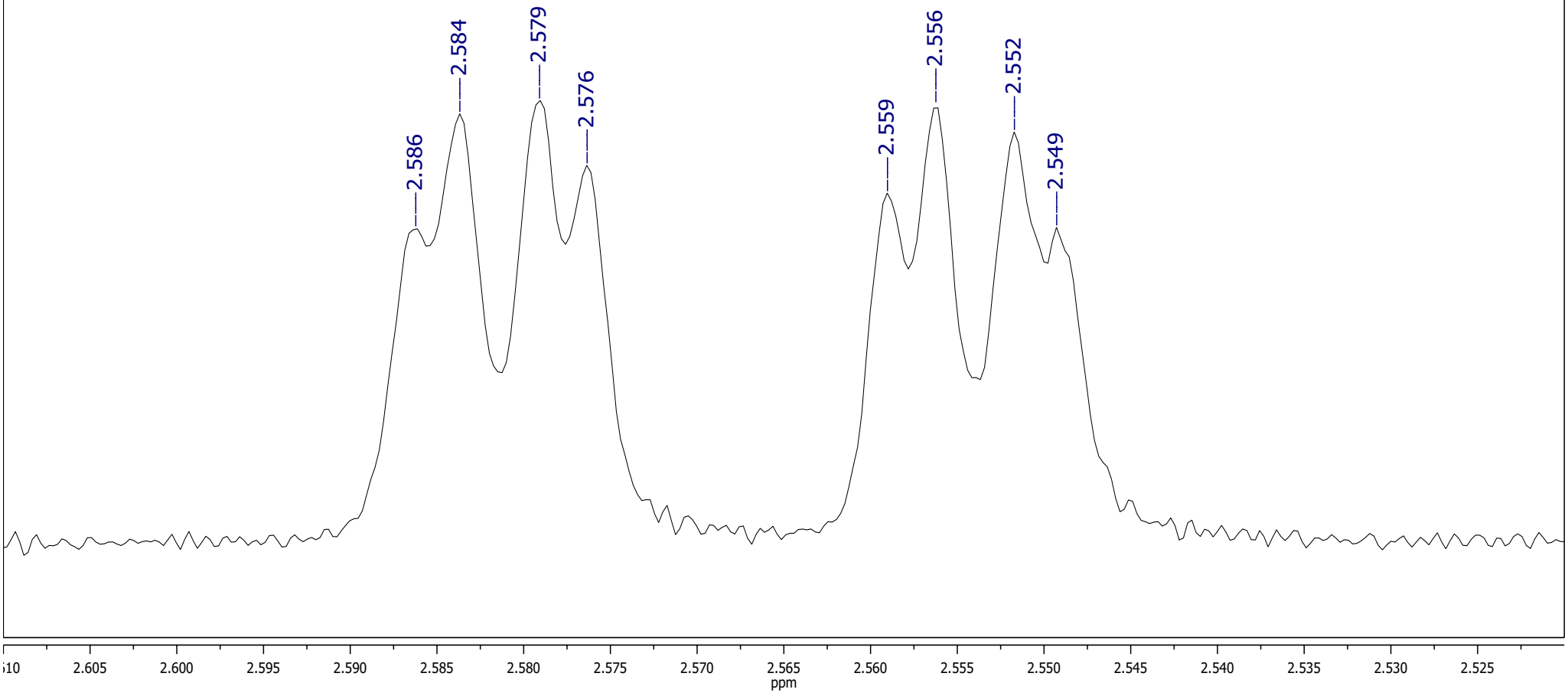
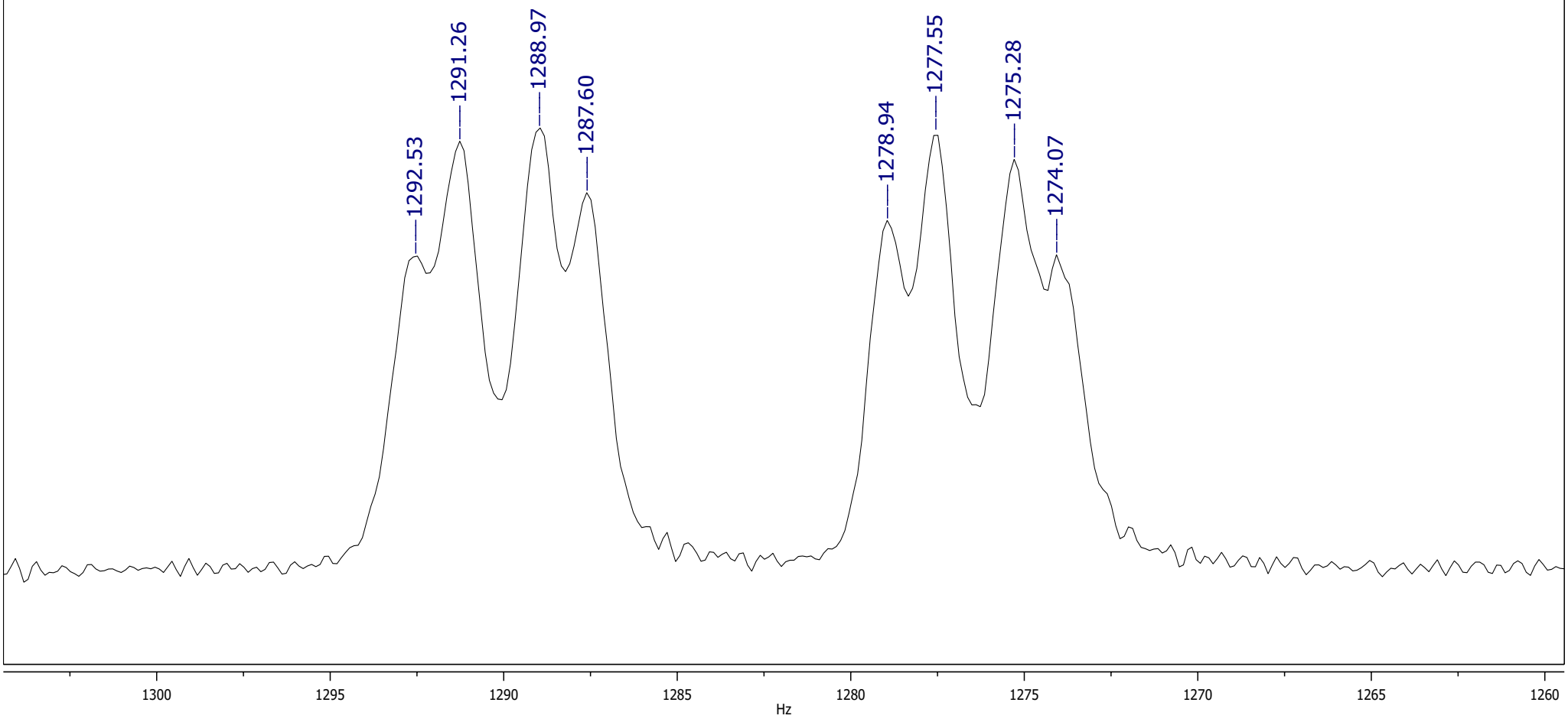


Region of interest: 2.52 - 2.61 ppm

Exponential: -1.32
Gaussian: 0.60 GB



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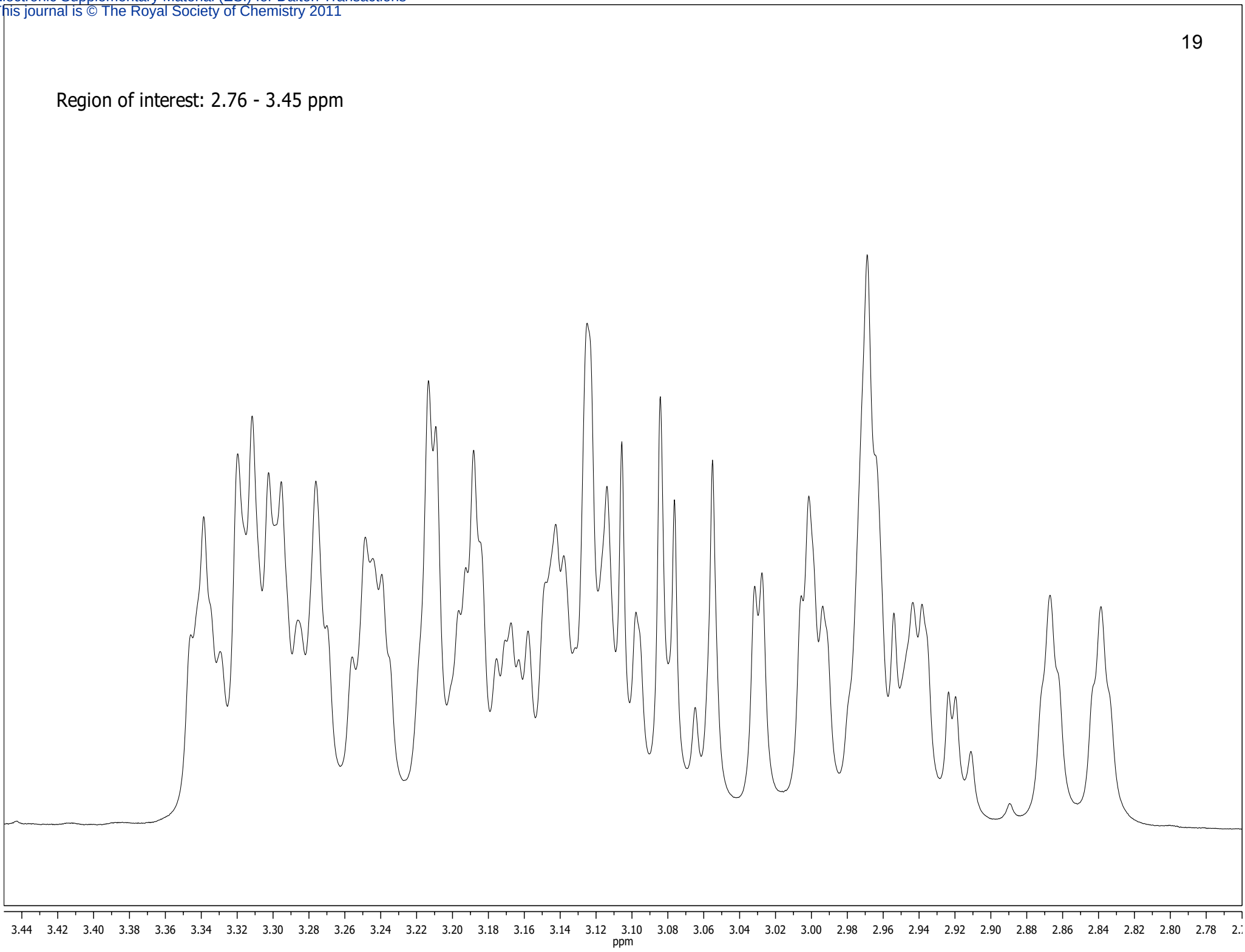
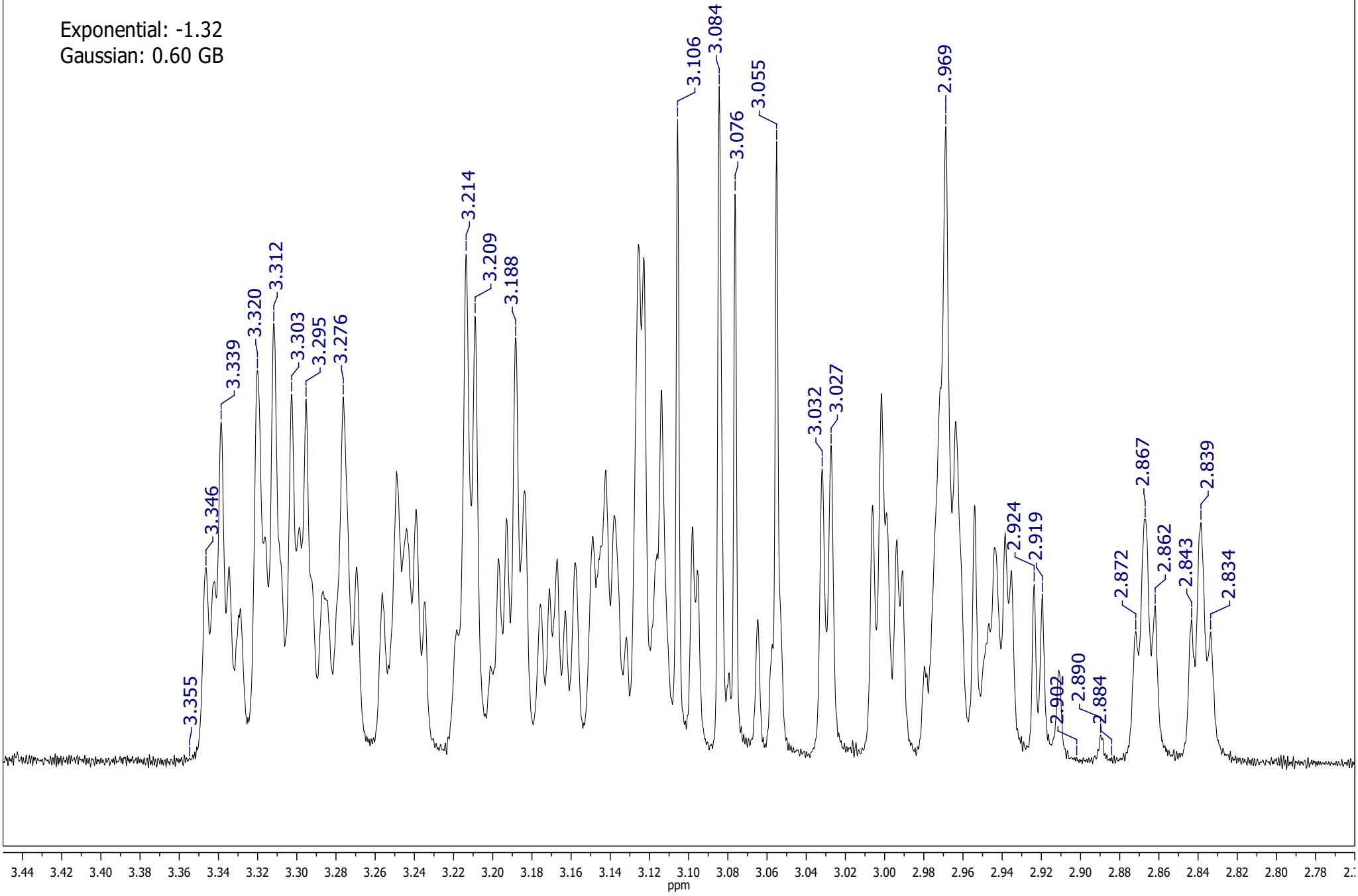


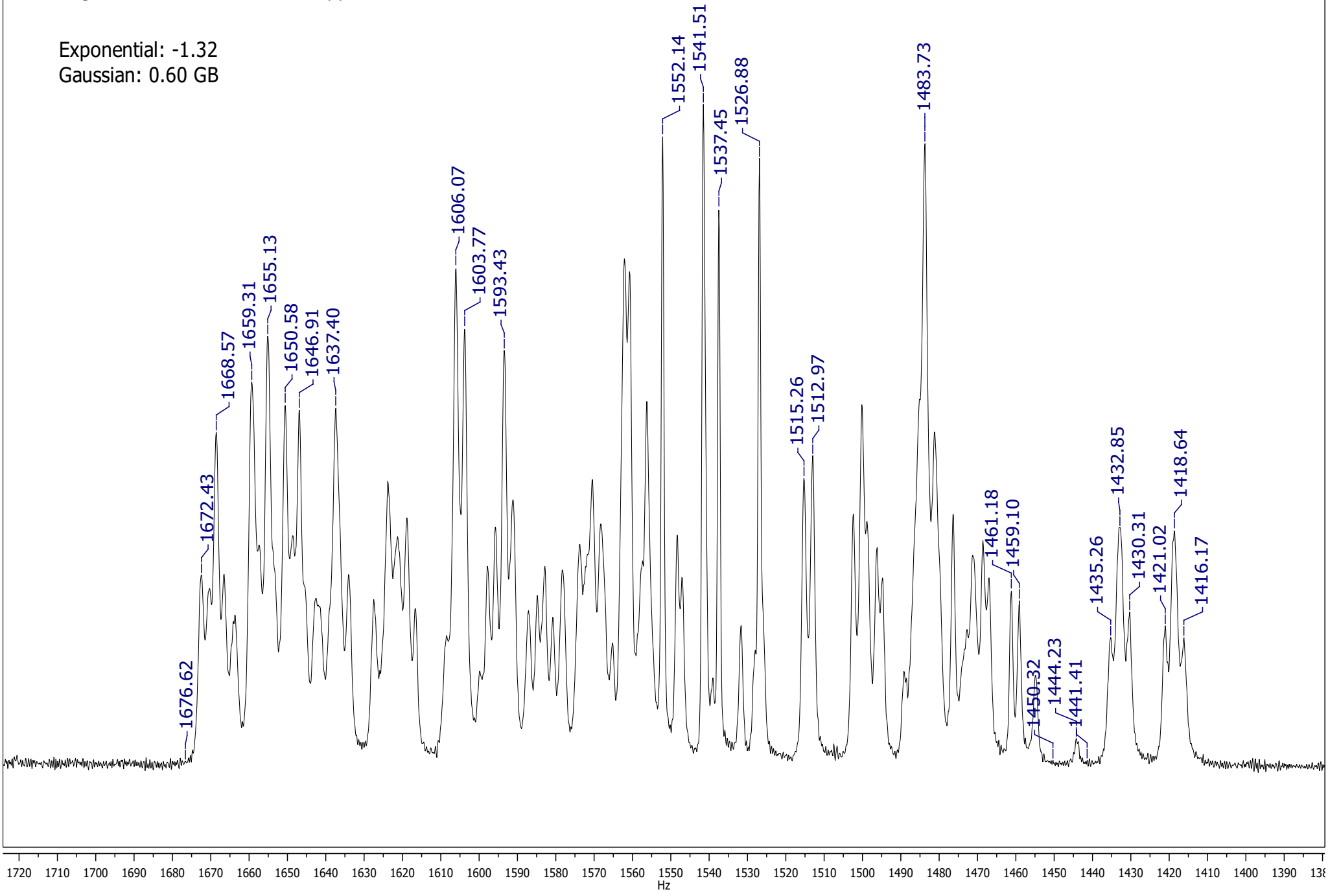
Region of interest: 2.76 - 3.45 ppm

Exponential: -1.32
Gaussian: 0.60 GB

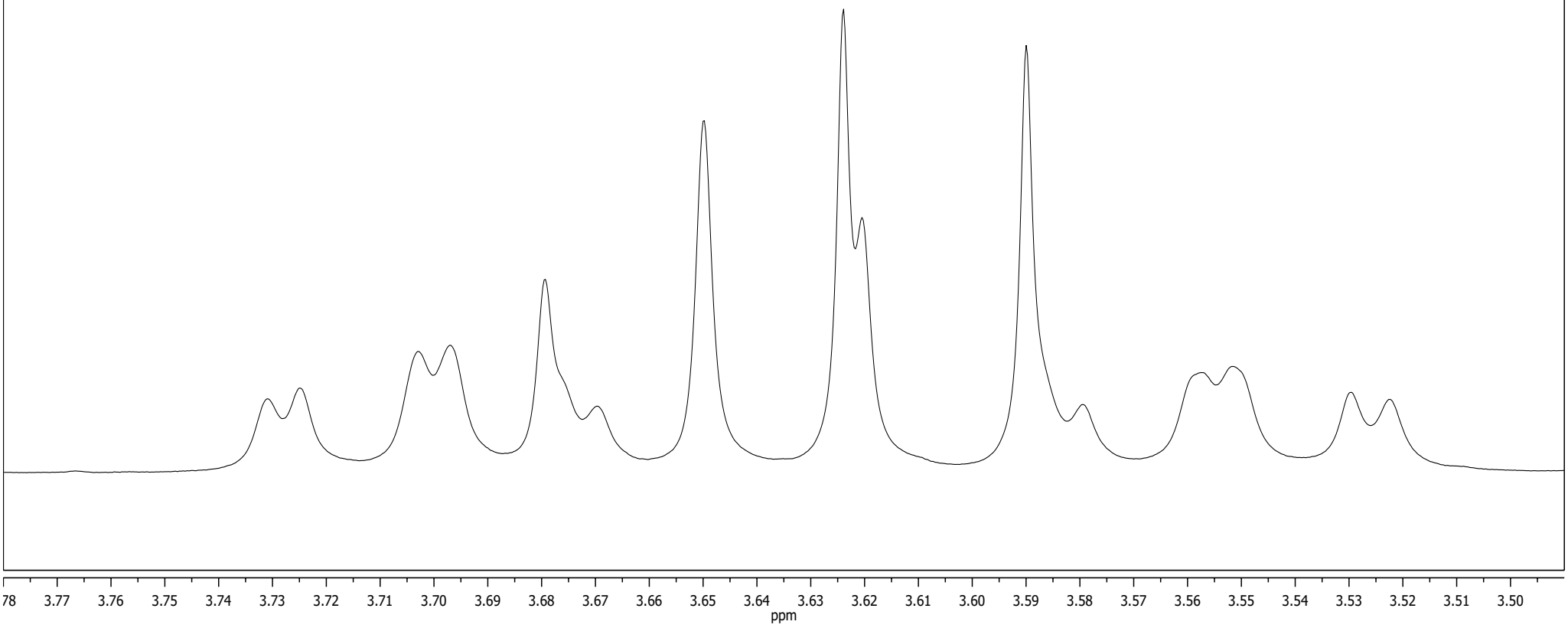


Region of interest: 2.76 - 3.45 ppm

Exponential: -1.32
Gaussian: 0.60 GB



Region of interest: 3.49 - 3.78 ppm



Region of interest: 3.49 - 3.78 ppm

Exponential: -1.32
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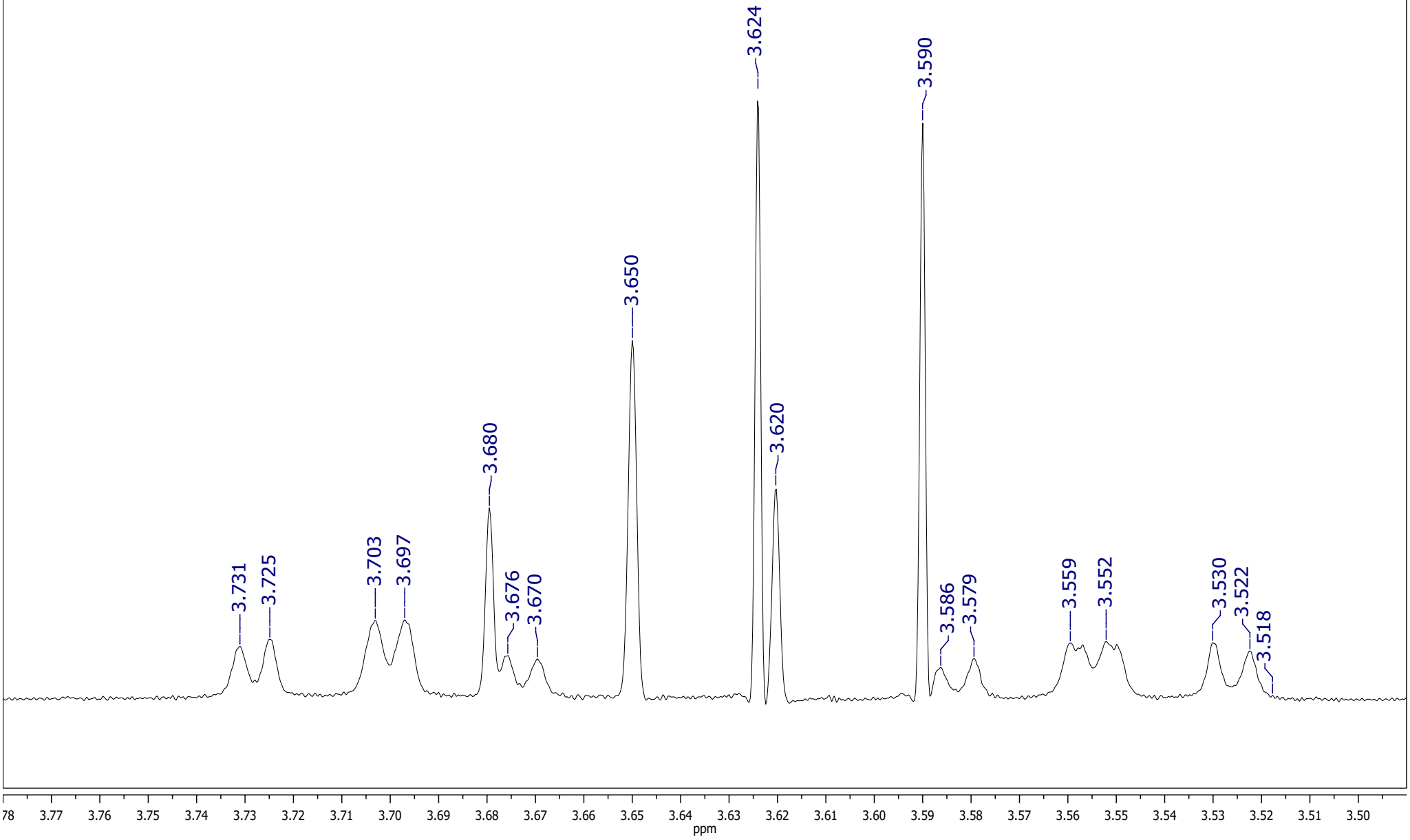

Region of interest: 3.49 - 3.78 ppm

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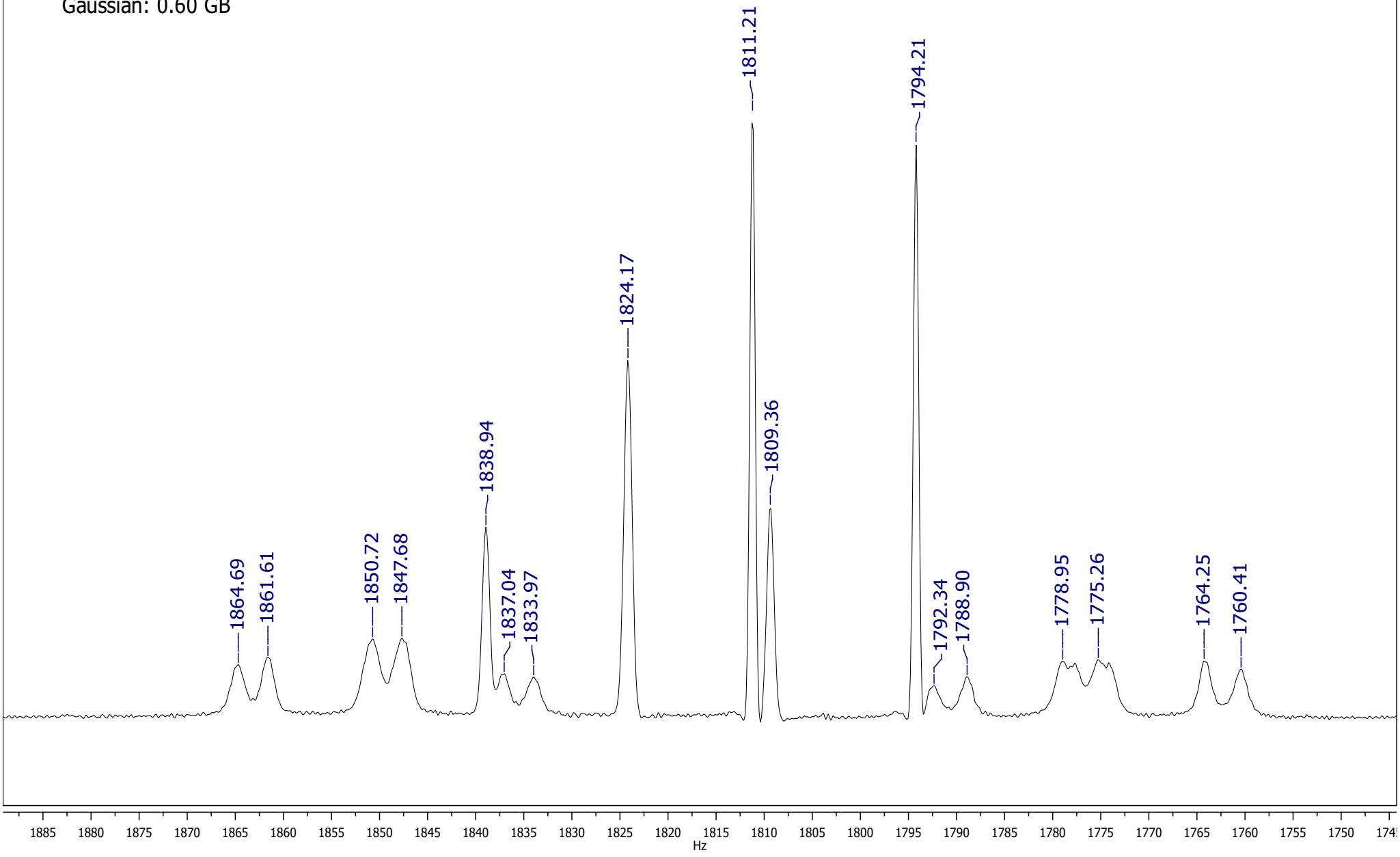

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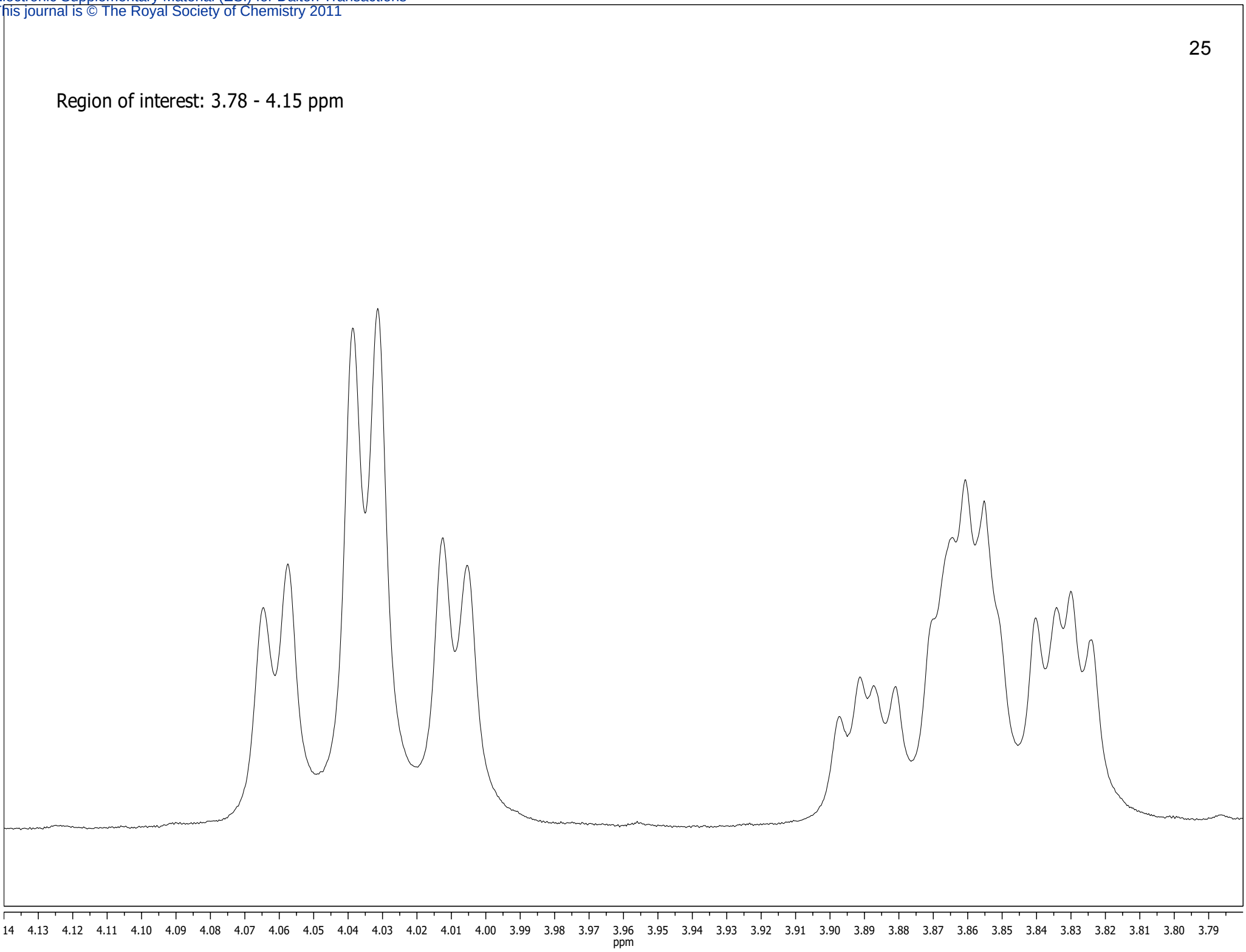
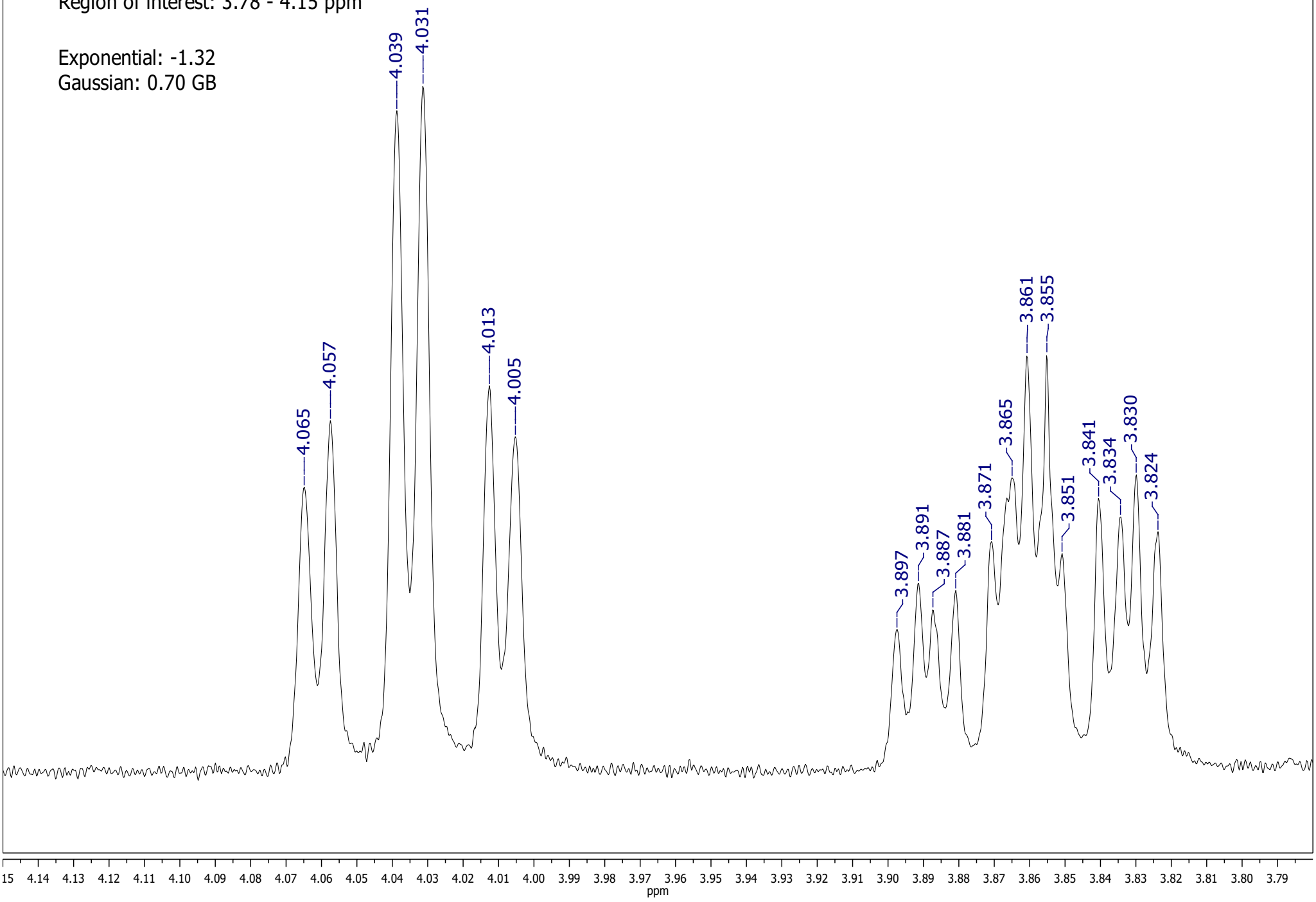


Region of interest: 3.78 - 4.15 ppm

Exponential: -1.32
Gaussian: 0.70 GB



Region of interest: 3.78 - 4.15 ppm

Exponential: -1.32
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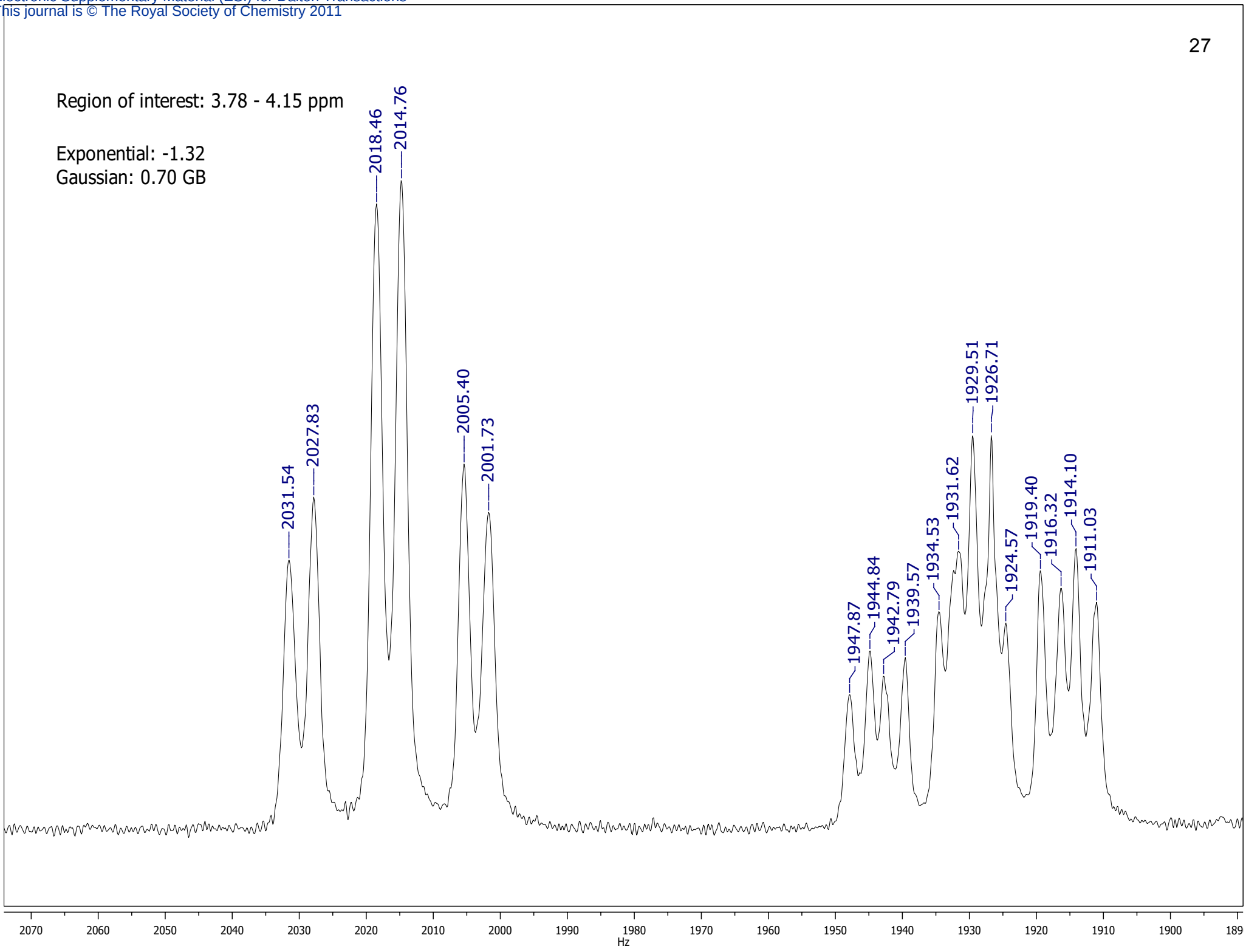

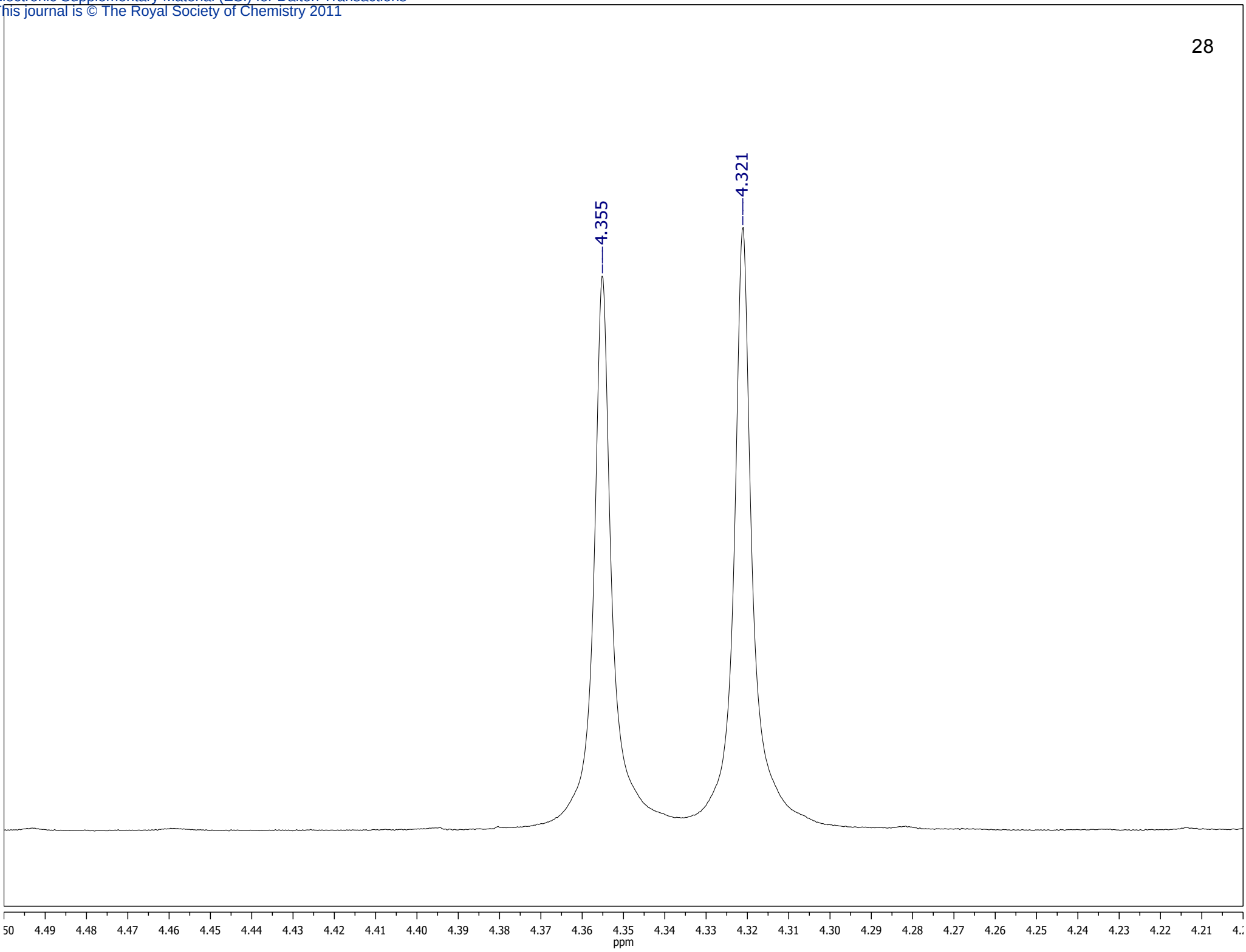

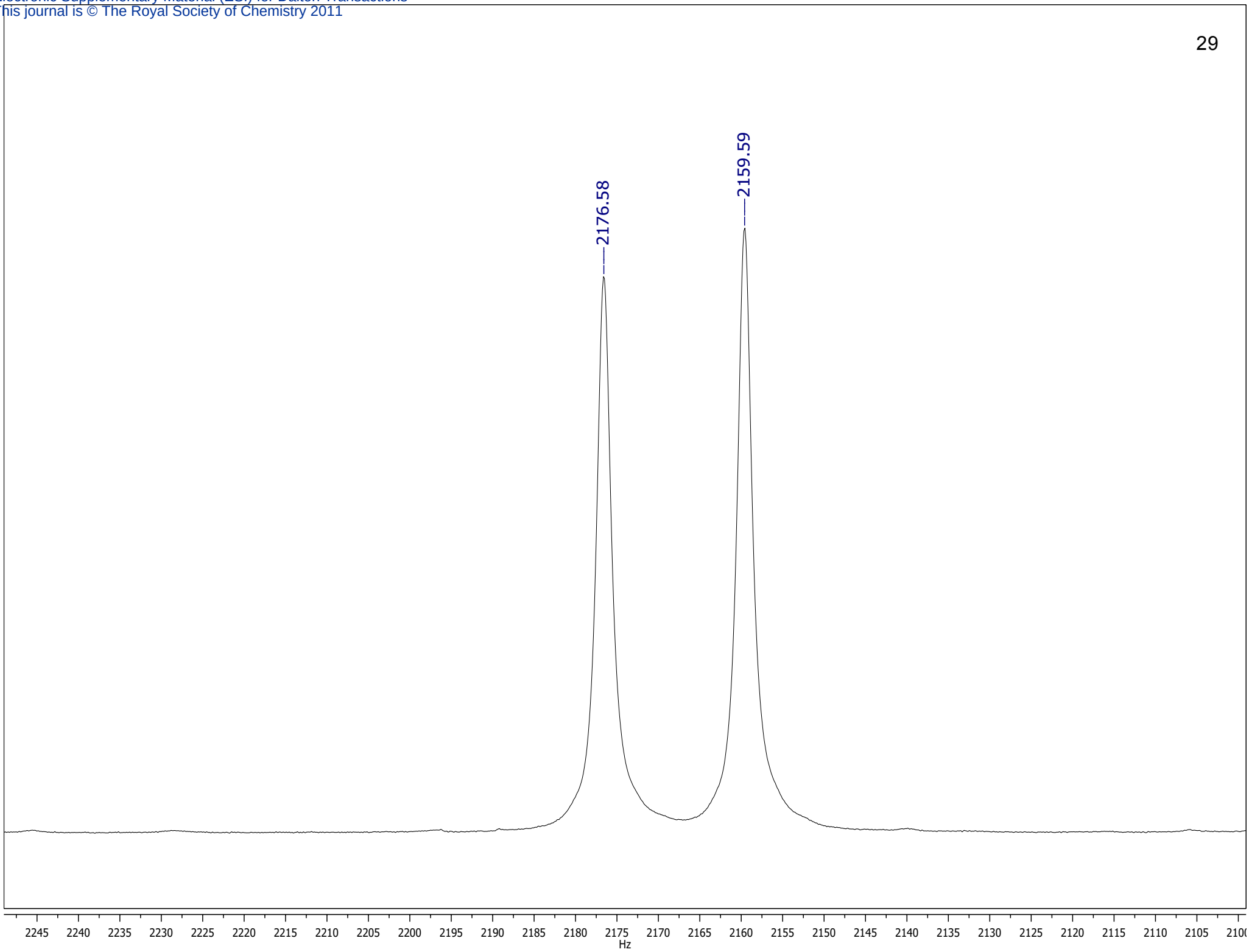

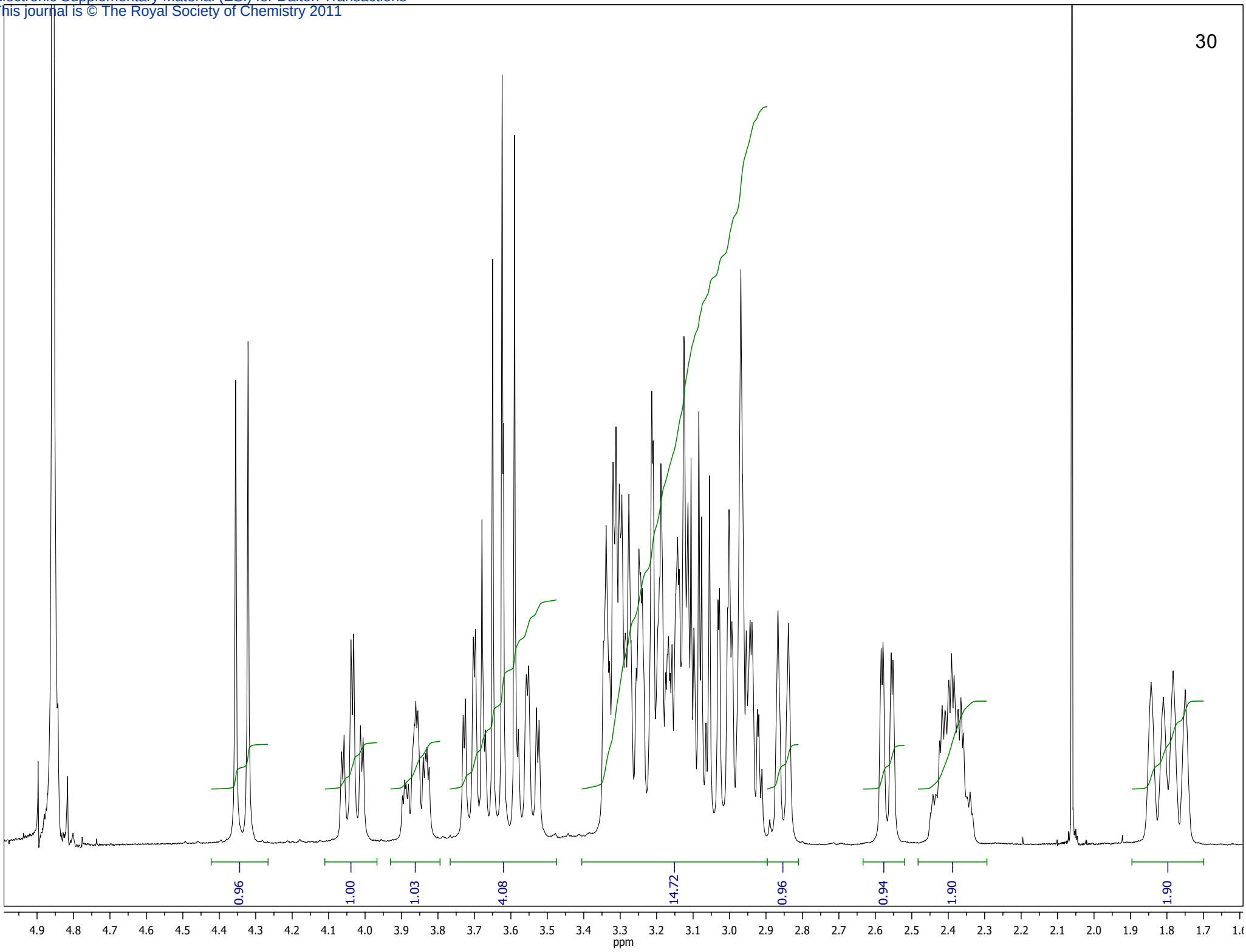

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11	Acquired Size	23976
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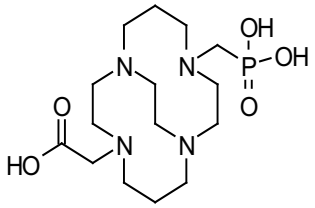
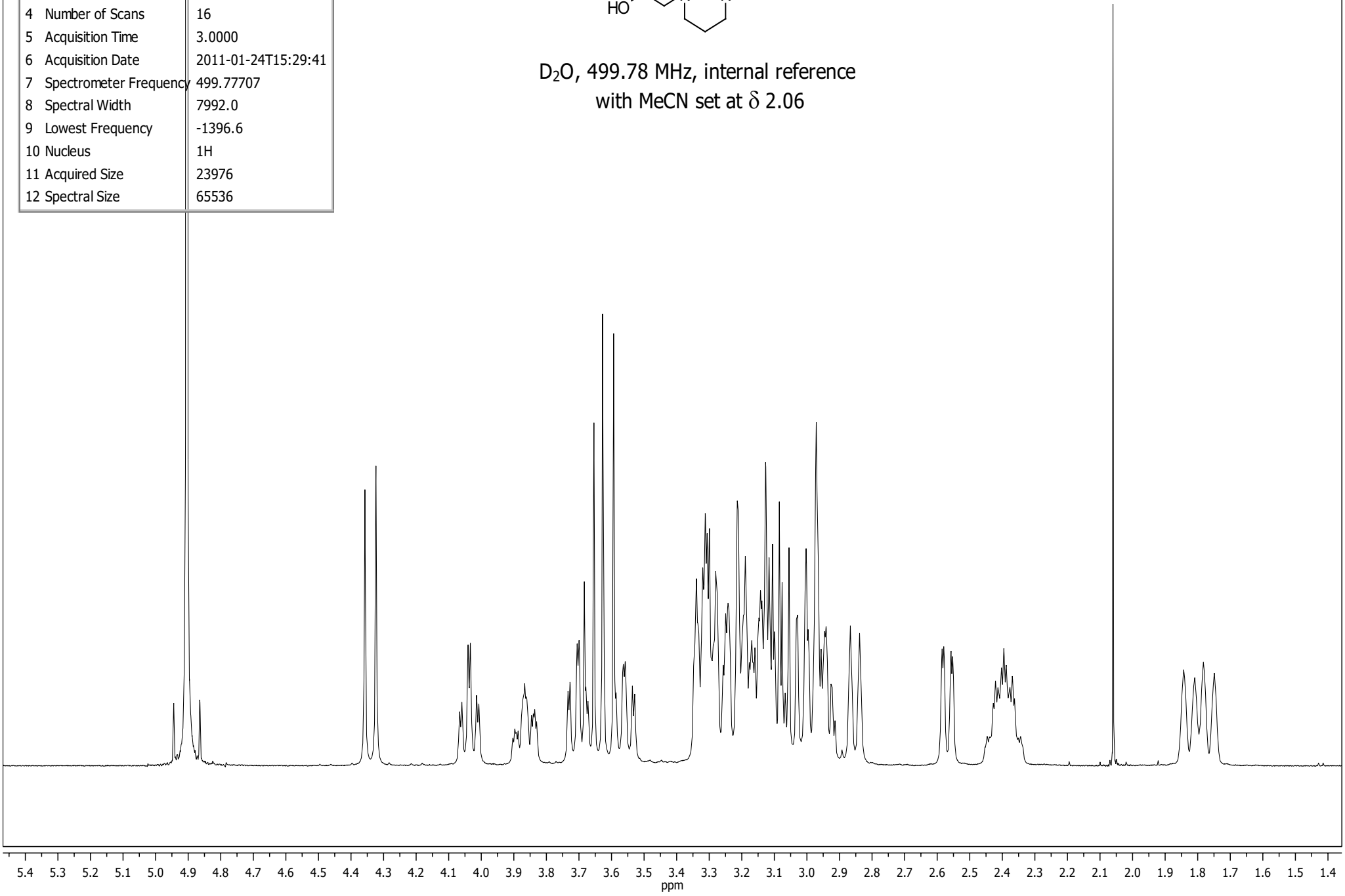


D_2O, 499.78 MHz, internal reference
with MeCN set at δ 2.06



(See previous page for details of 1D proton spectrum.)

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Nucleus	(1H, 1H)
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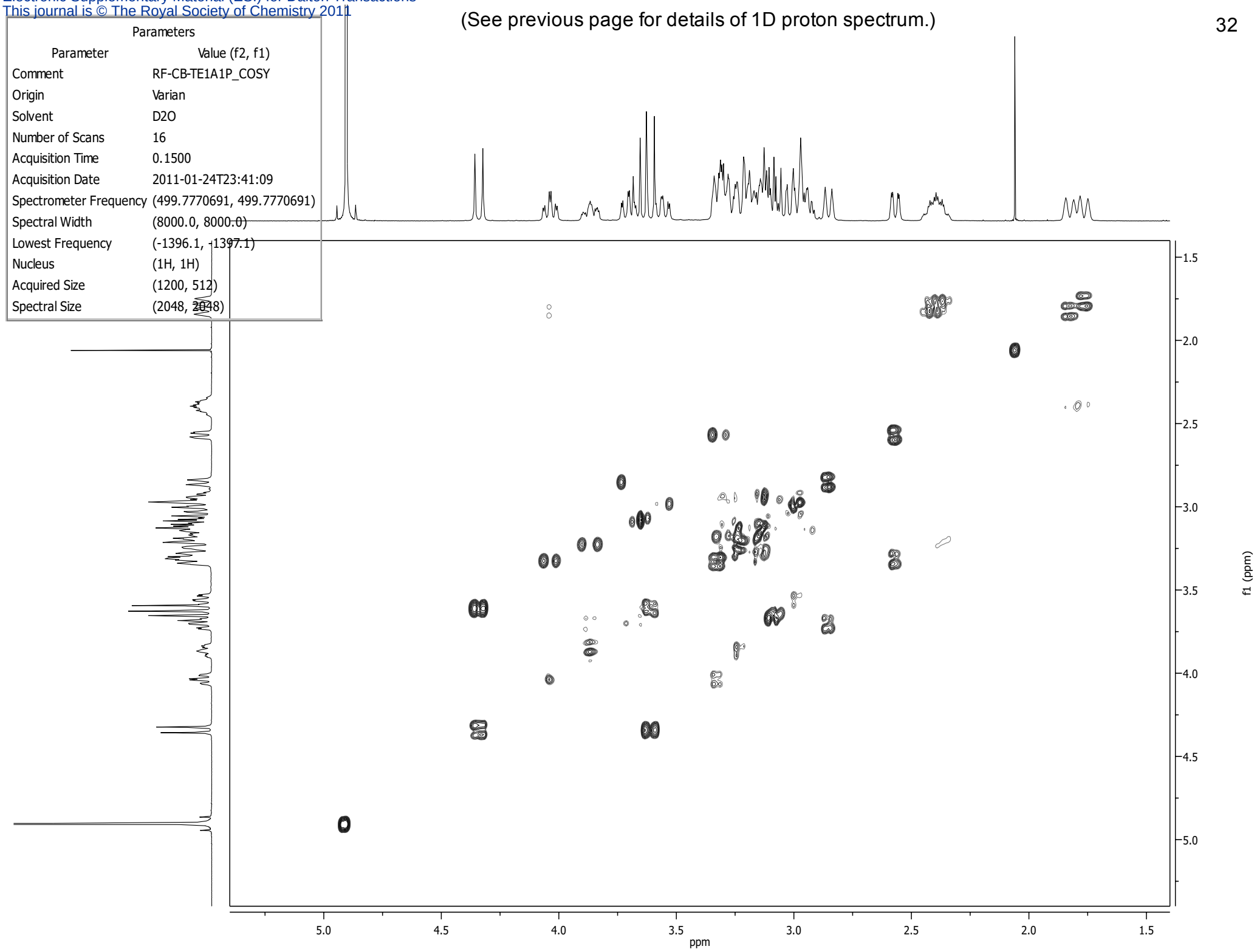

Parameters	
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Solvent	D2O
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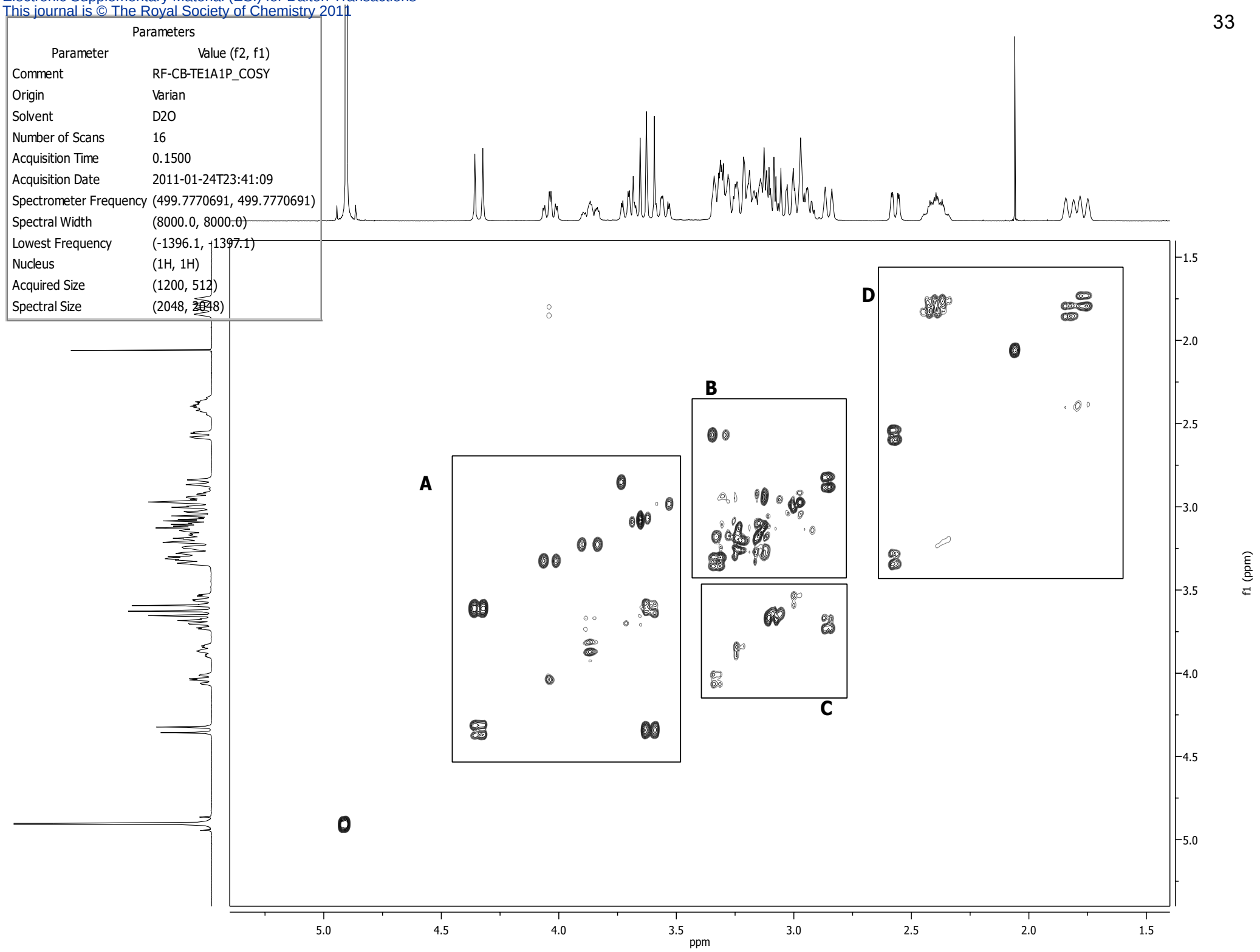
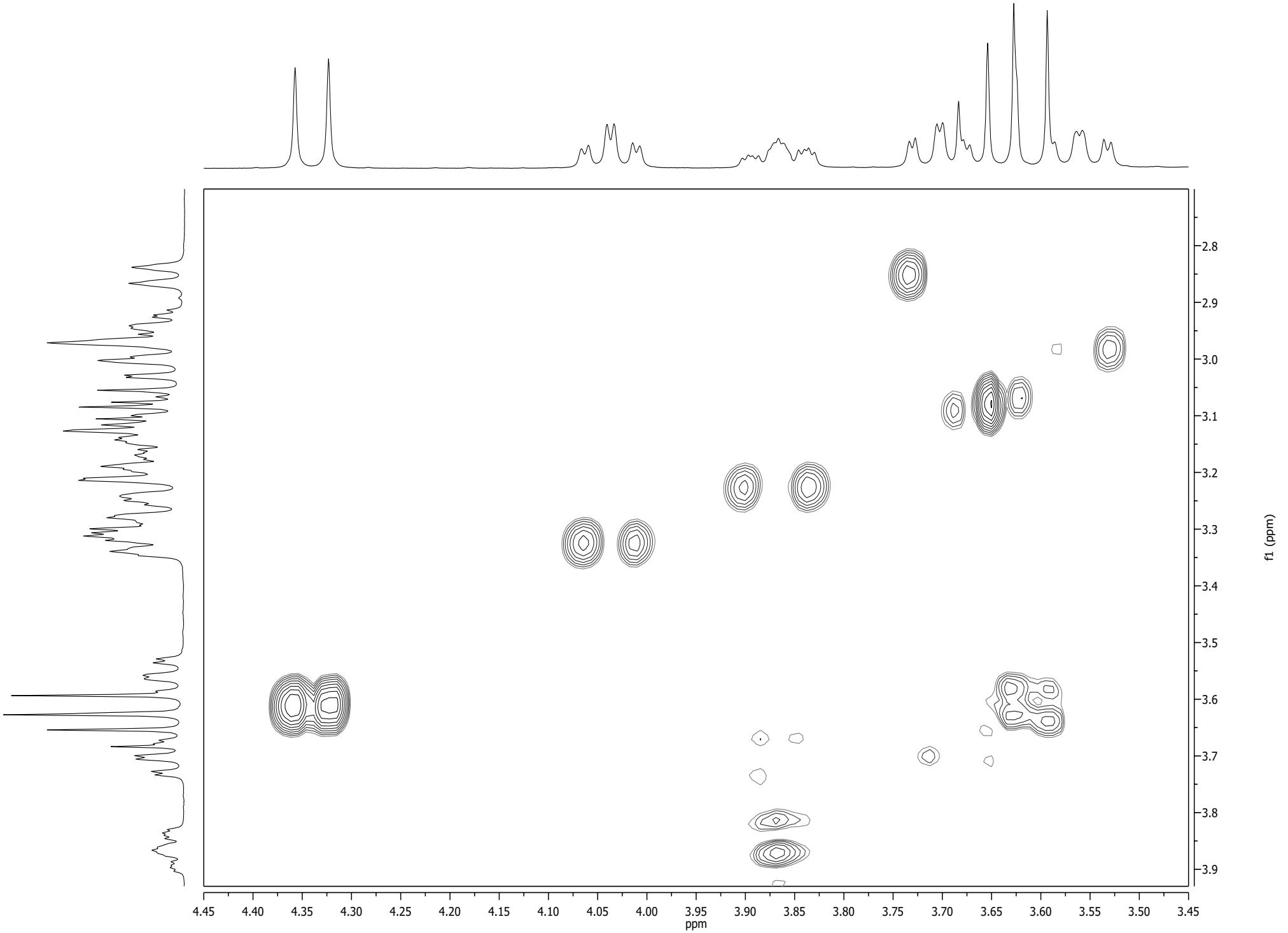
Acquisition Time	0.1500
Acquisition Date	2011-01-24T23:41:09
Spectrometer Frequency	(499.7770691, 499.7770691)
Spectral Width	(8000.0, 8000.0)
Lowest Frequency	(-1396.1, -1397.1)
Nucleus	(1H, 1H)
Acquired Size	(1200, 512)
Spectral Size	(2048, 2048)




4.45
4.40
4.35
4.30
4.25
4.20
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3.85
3.80
3.75
3.70
3.65
3.60
3.55
3.50
3.45
ppm
2.8
2.9
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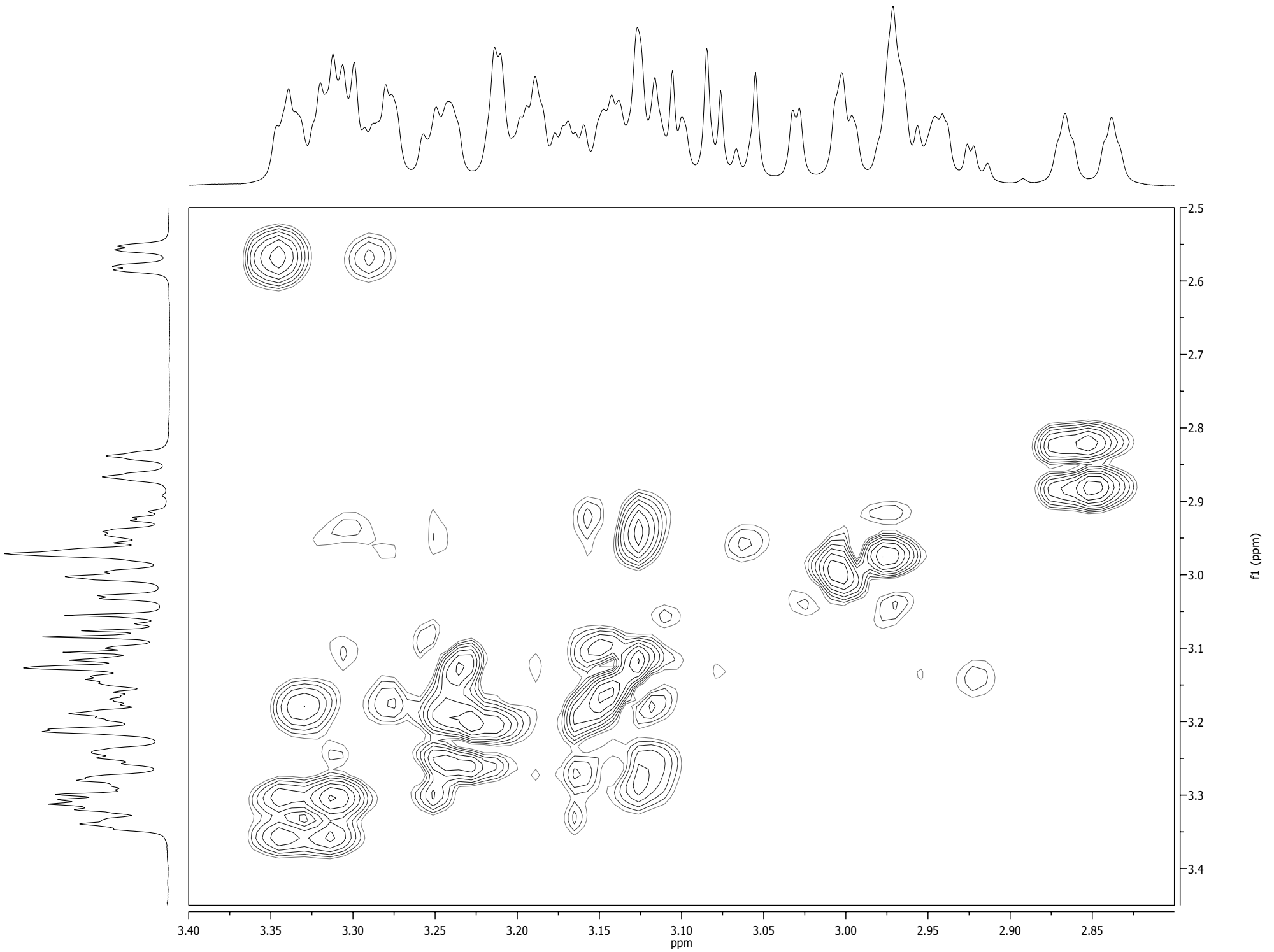
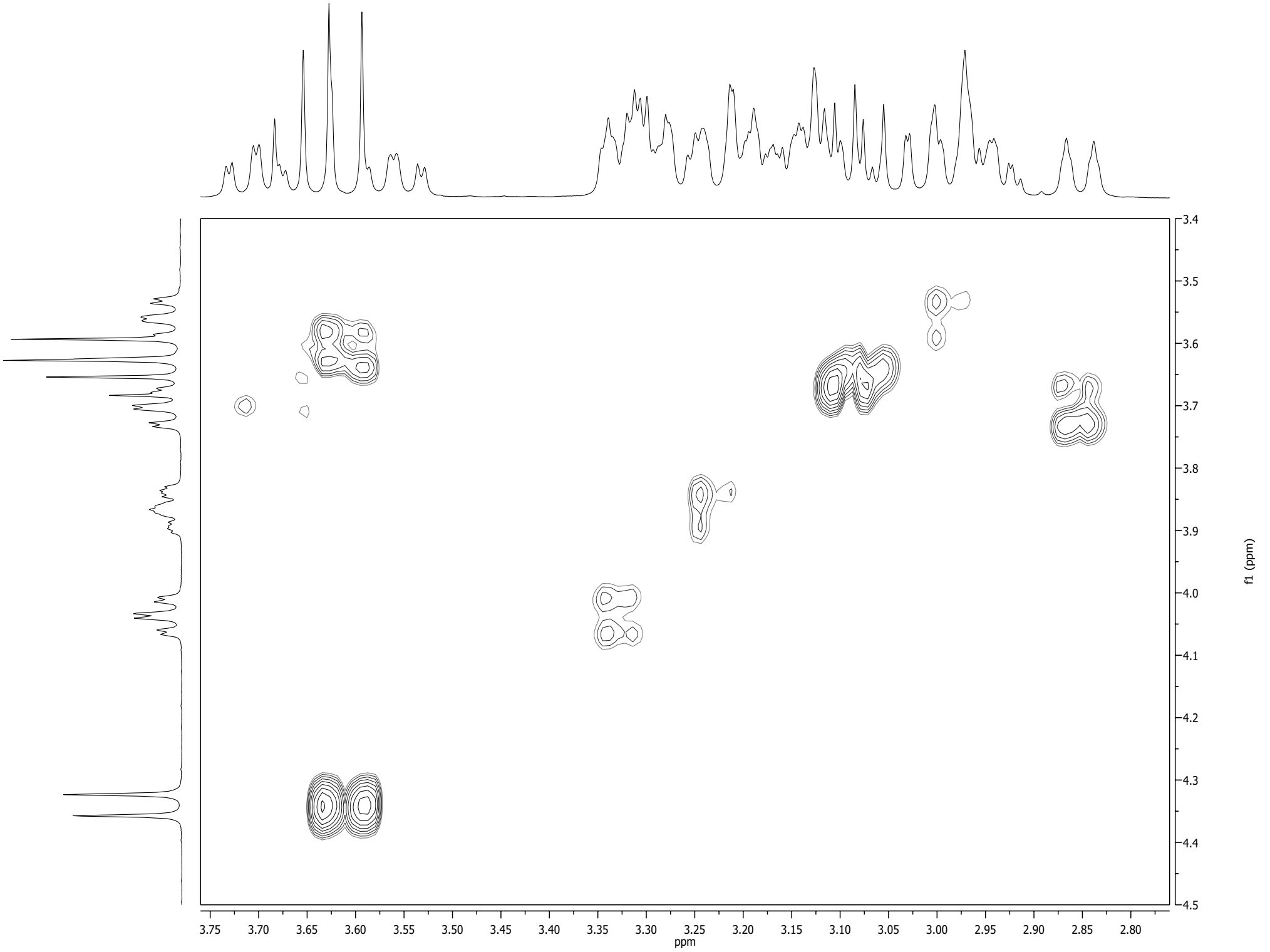
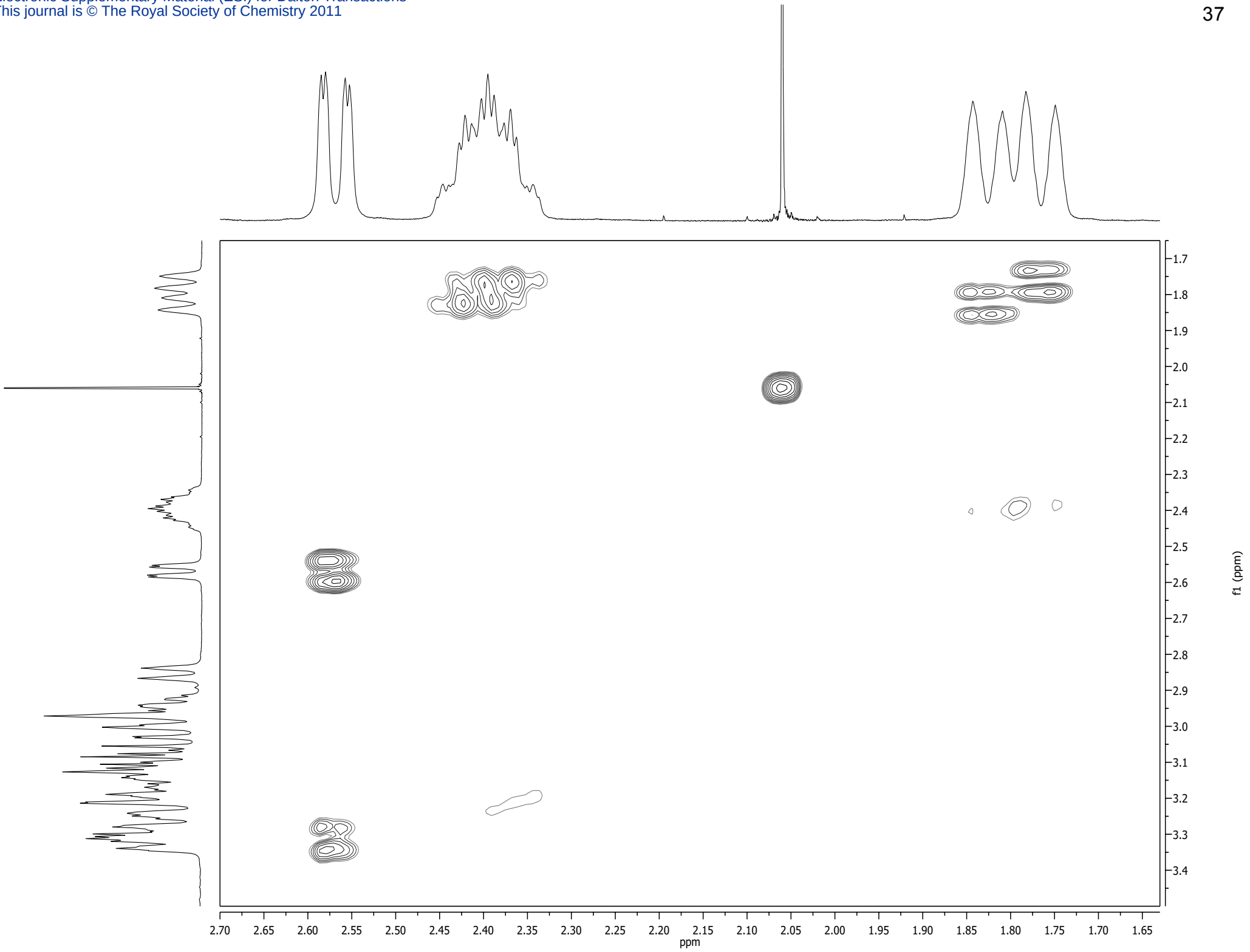
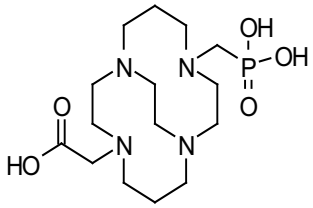
3.4
3.5
3.6
3.7
3.8
3.9
f1 (ppm)



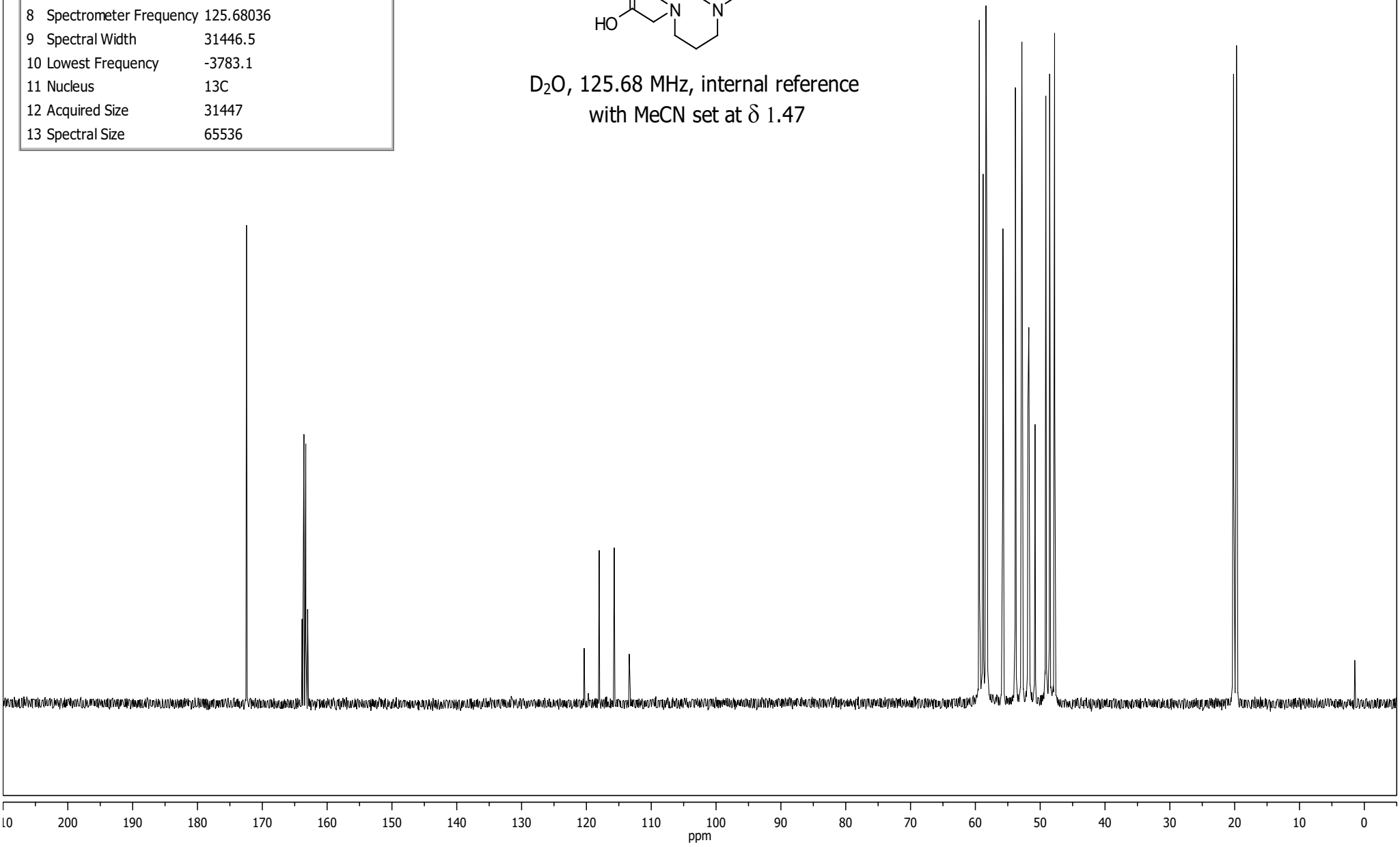


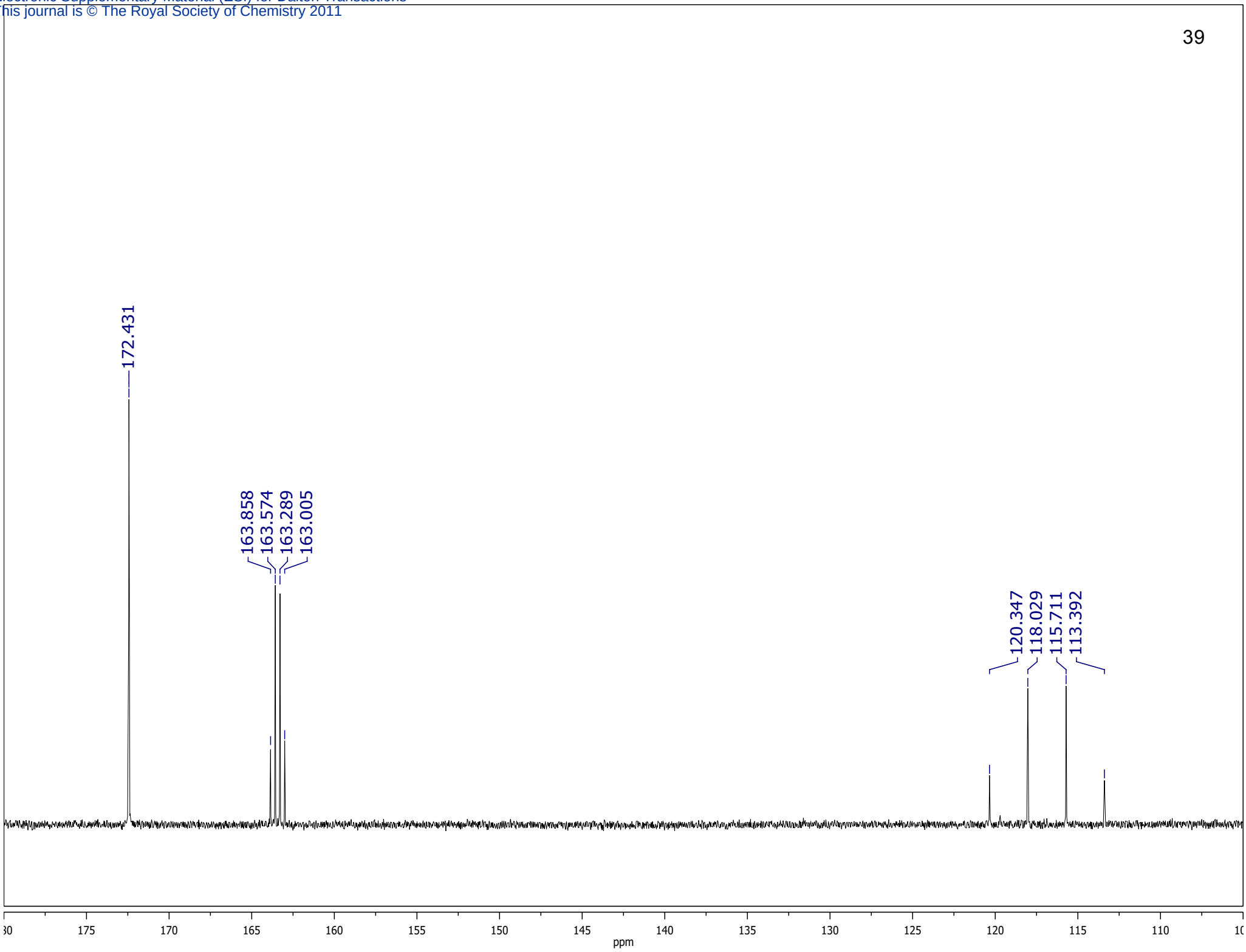

2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20
2.15
2.10
2.05
2.00
1.95
1.90
1.85
1.80
1.75
1.70
1.65
ppm
1.7
1.8
1.9
2.0
2.1
2.2
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
3.2
3.3
3.4
f1 (ppm)

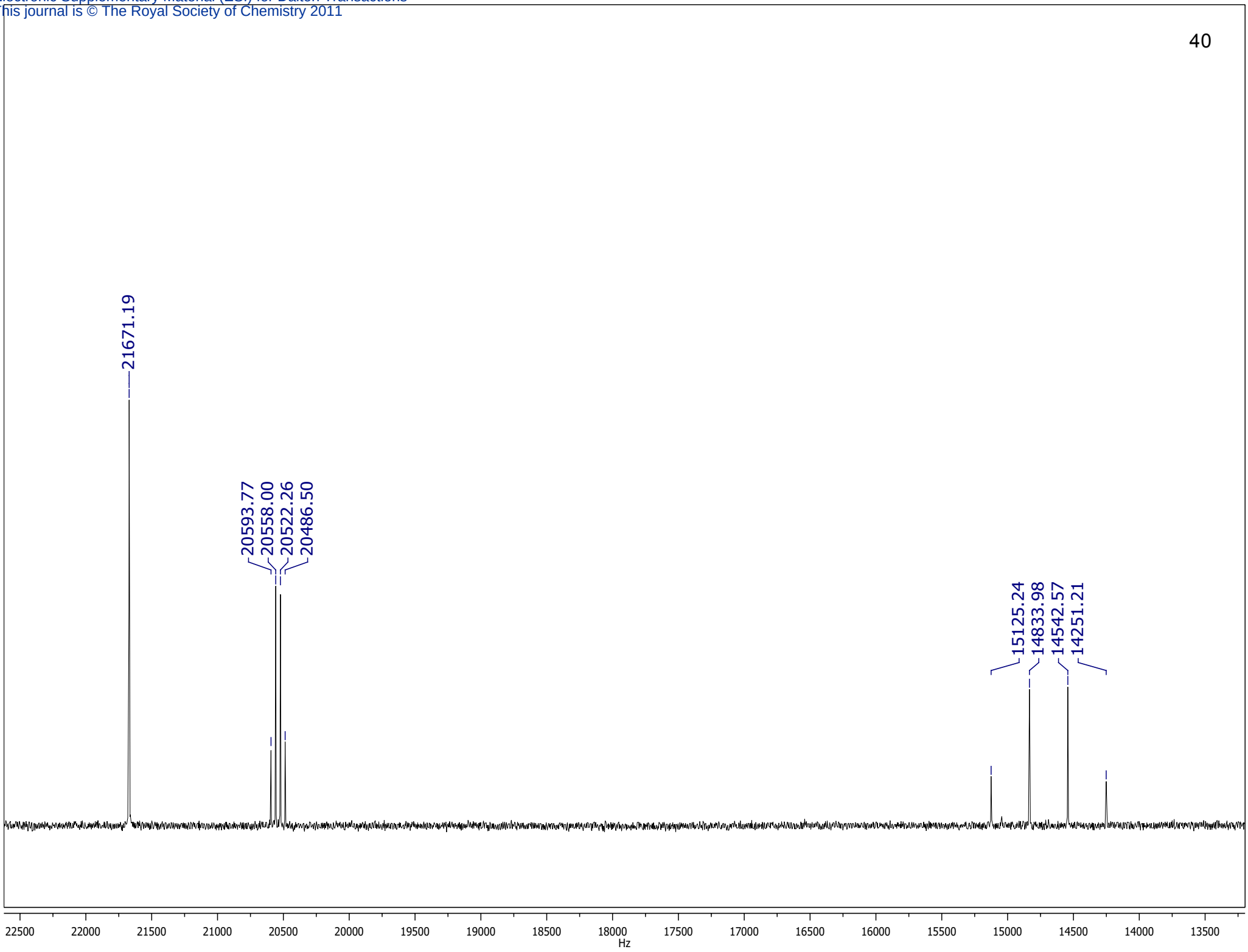
1	Data File Name	RF-CB-TE1A1P_13C_125MHz
2	Origin	Varian
3	Solvent	D2O
4	Number of Scans	38000
5	Receiver Gain	40
6	Acquisition Time	1.0000
7	Acquisition Date	2011-01-22T08:03:16
8	Spectrometer Frequency	125.68036
9	Spectral Width	31446.5
10	Lowest Frequency	-3783.1
11	Nucleus	13C
12	Acquired Size	31447
13	Spectral Size	65536

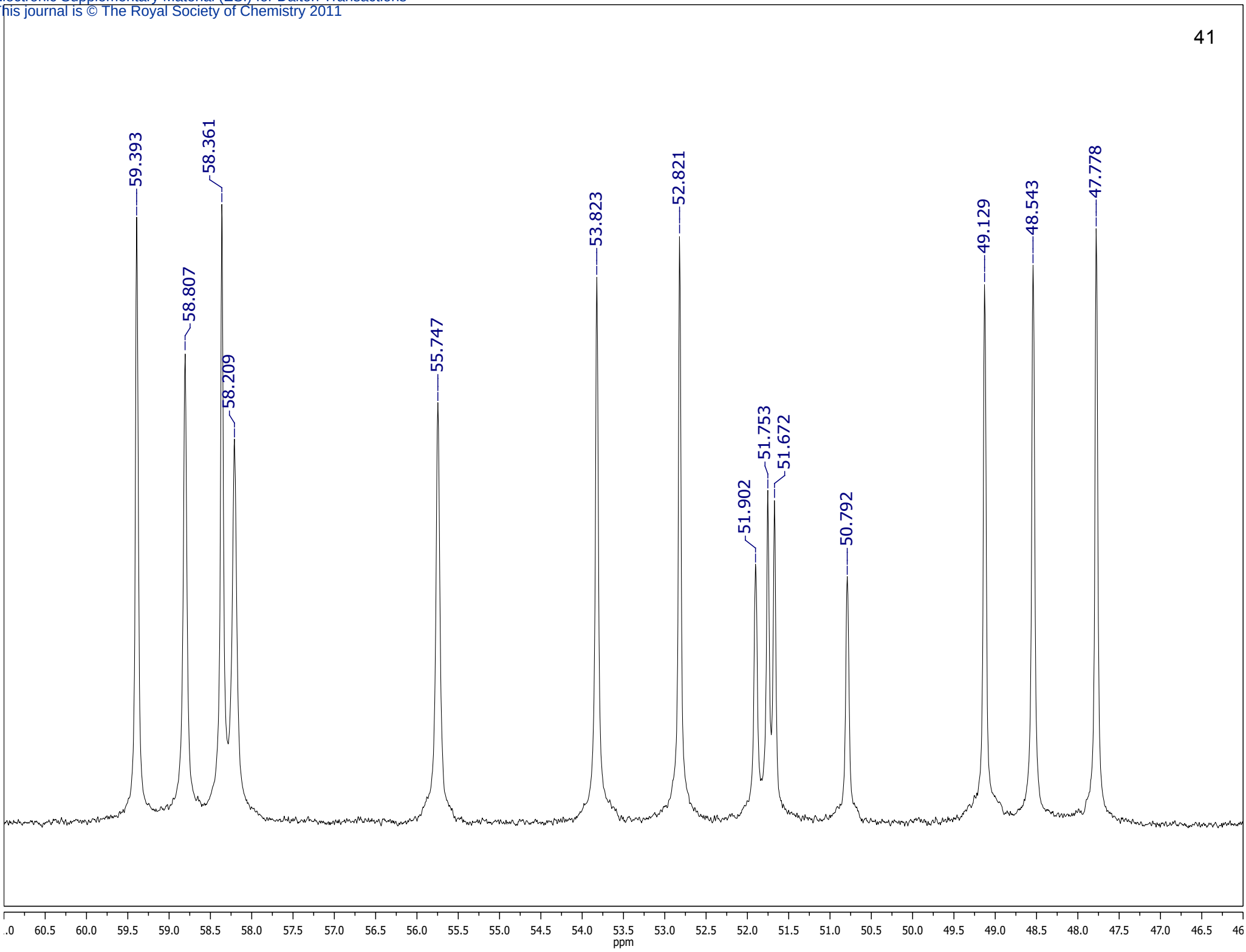


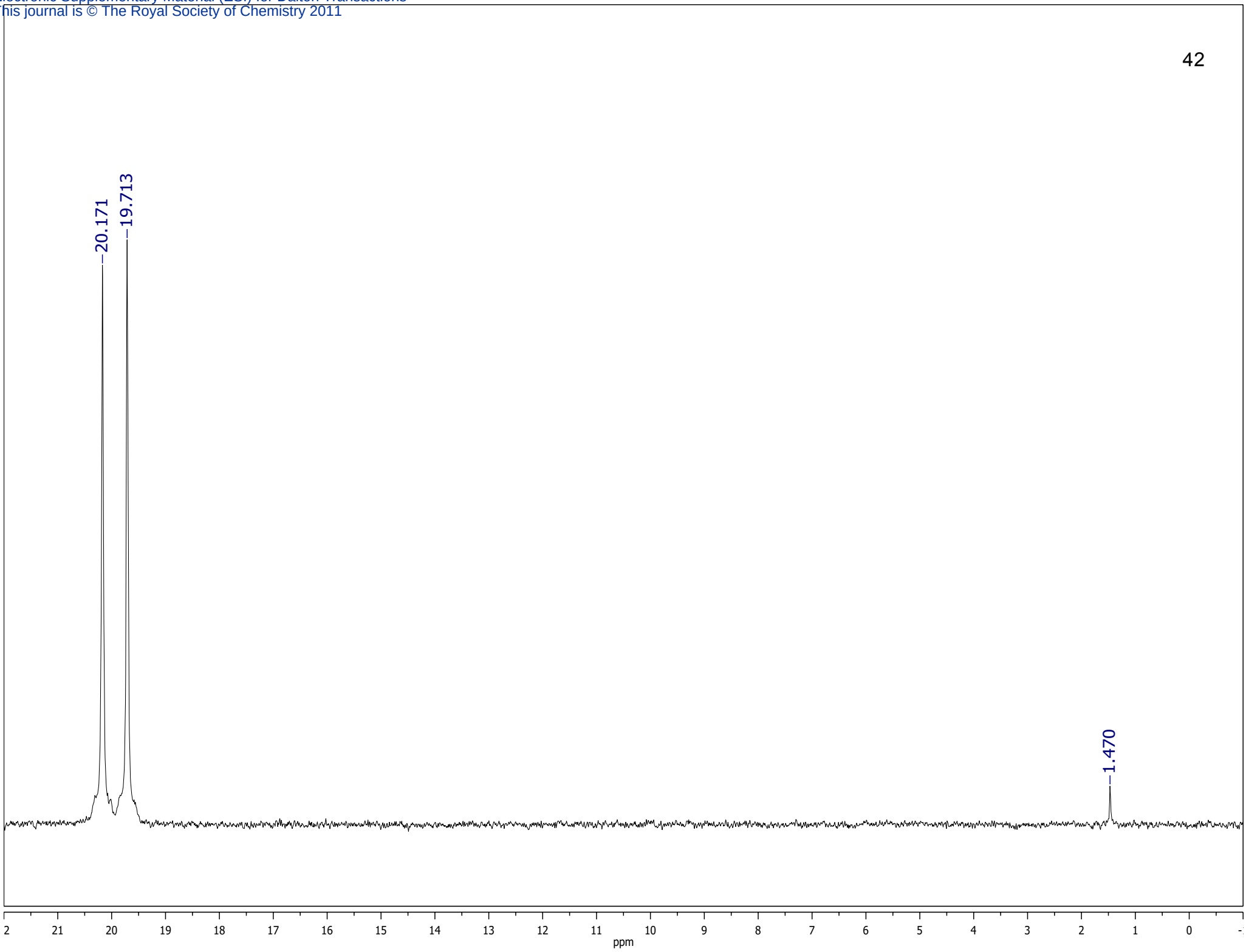
D_2O, 125.68 MHz, internal reference
with MeCN set at δ 1.47



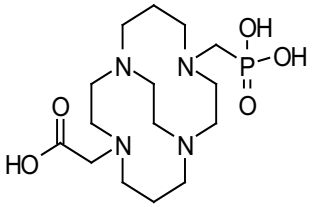






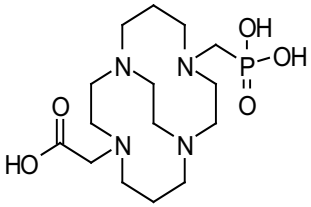


	Parameter	Value
1	Comment	RF-CB-TE1A1P-125 MHz
2	Origin	Varian
3	Solvent	D2O
4	Number of Scans	38000
5	Acquisition Time	1.0000
6	Acquisition Date	2011-01-22T08:03:16
7	Spectrometer Frequency	125.68036
8	Spectral Width	31446.5
9	Lowest Frequency	-3692.7
10	Nucleus	13C
11	Acquired Size	31447
12	Spectral Size	65536

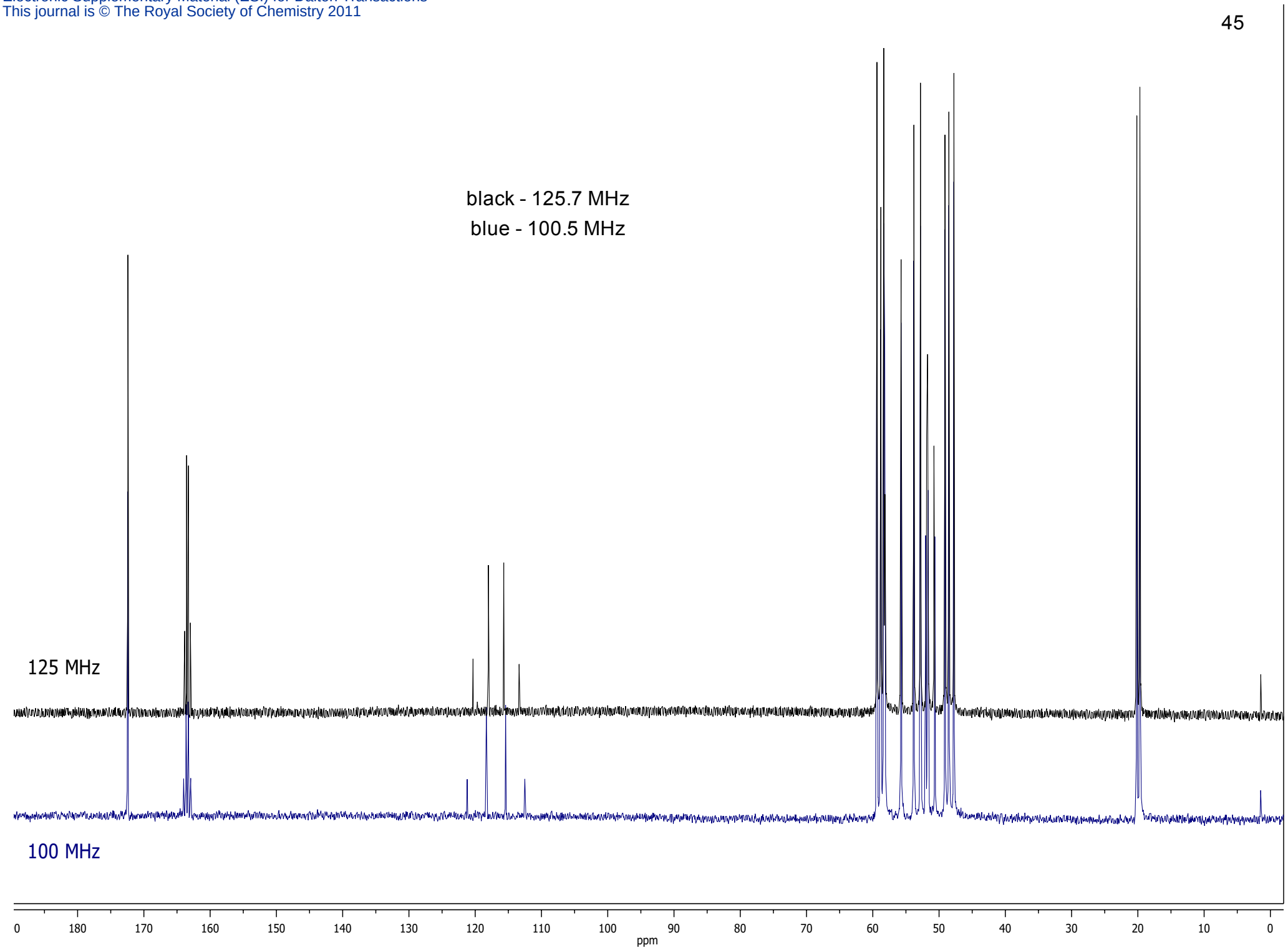


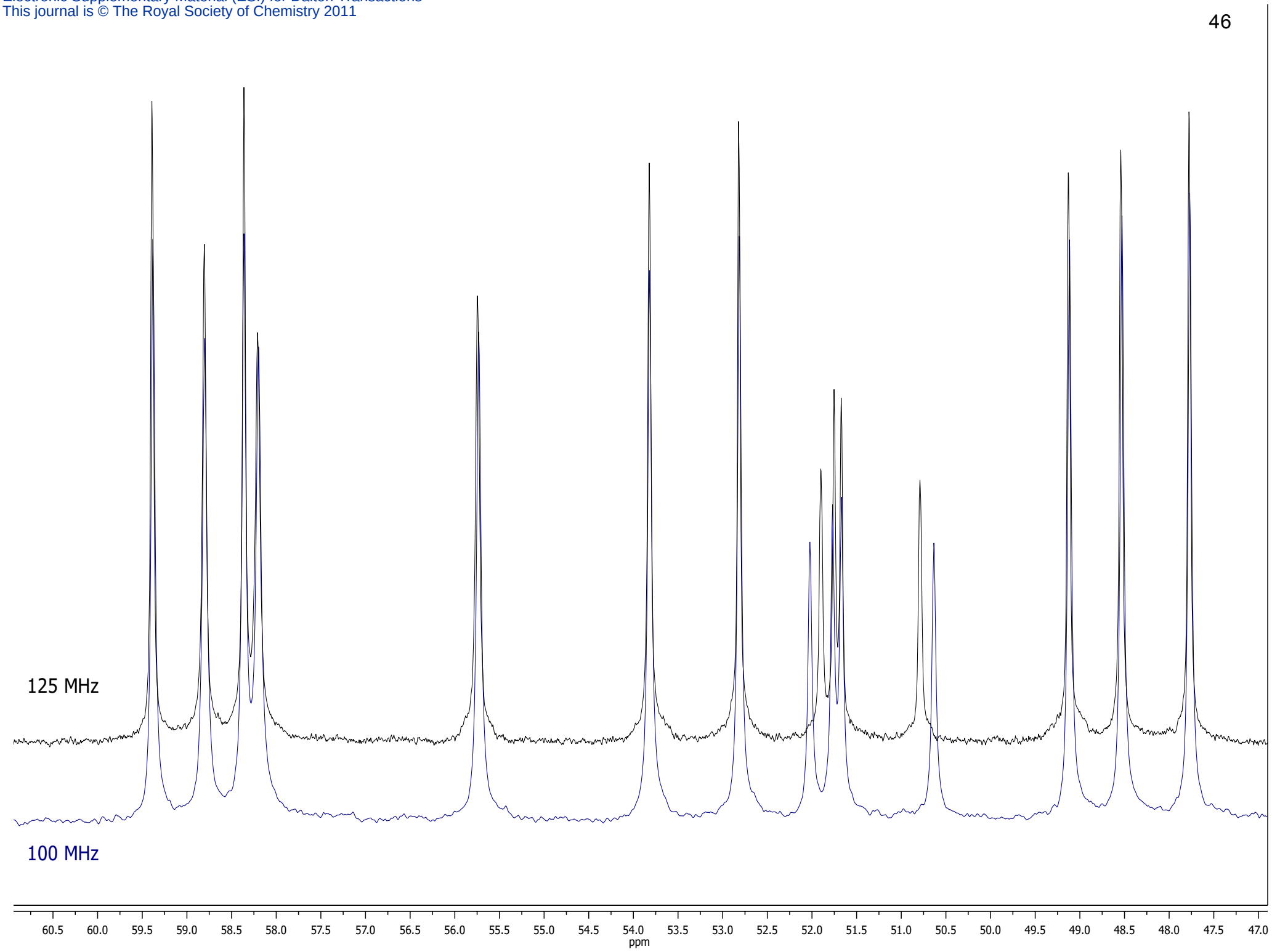
D_2O, 125.68 MHz,
MeCN as internal interference, set at δ 1.47

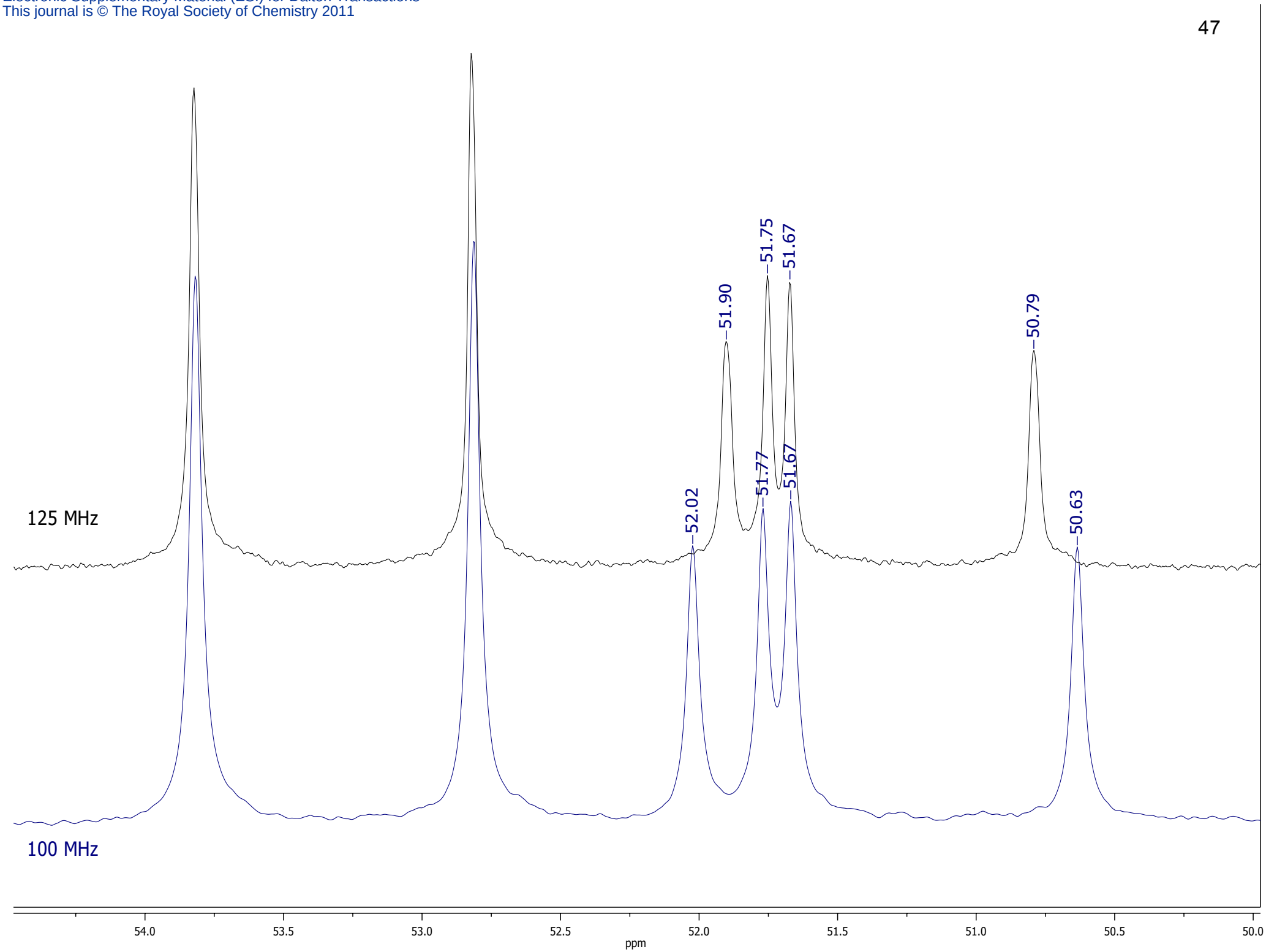
	Parameter	Value
1	Comment	RF-CB-TE1A1P-100 MHz
2	Origin	Varian
3	Solvent	D2O
4	Number of Scans	26560
5	Acquisition Time	1.0025
6	Acquisition Date	2011-01-25T18:03:03
7	Spectrometer Frequency	100.52657
8	Spectral Width	25062.7
9	Lowest Frequency	-1418.1
10	Nucleus	13C
11	Acquired Size	25126
12	Spectral Size	65536

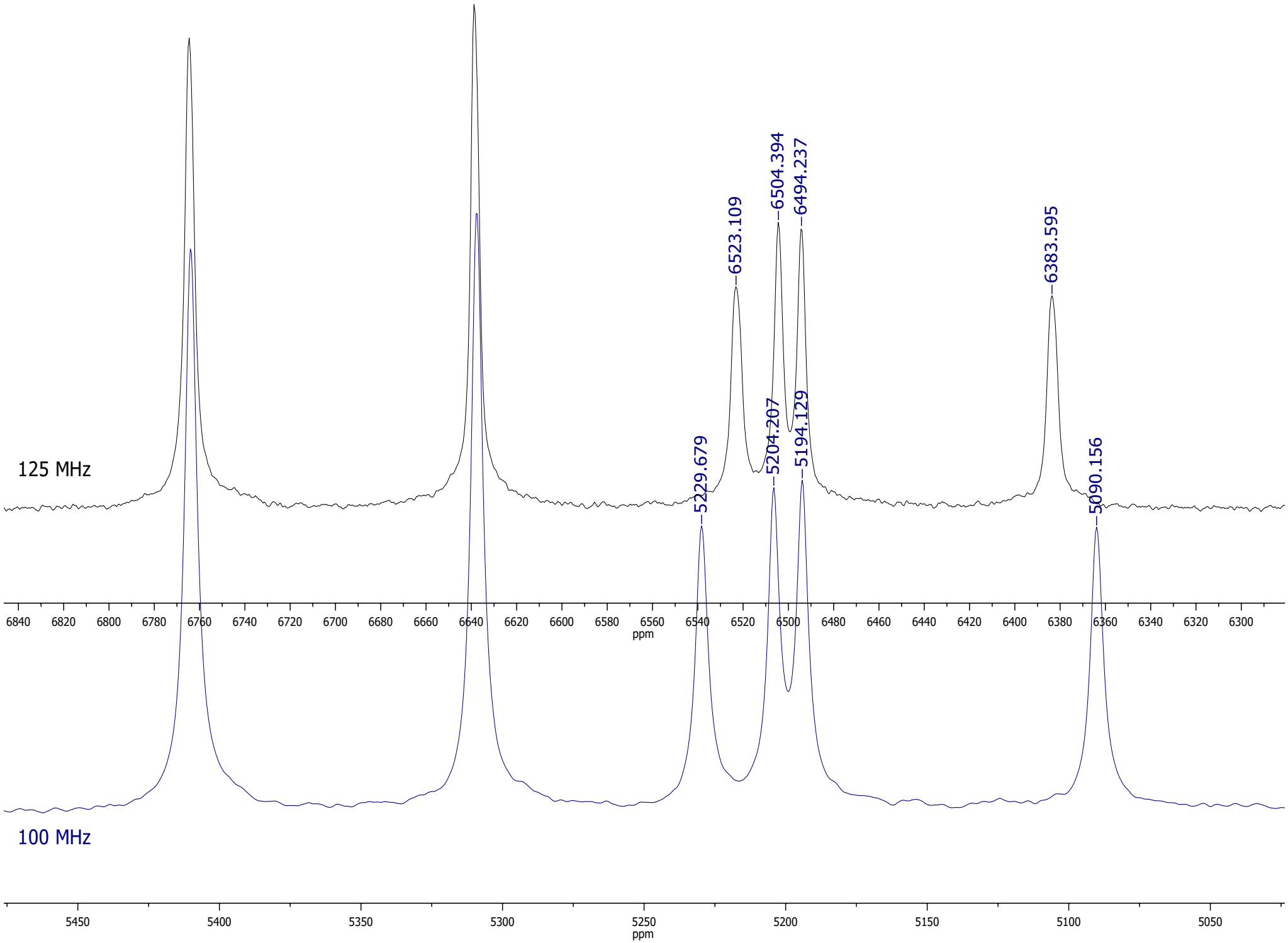


D_2O, 100.53 MHz,
MeCN as internal interference, set at δ 1.47

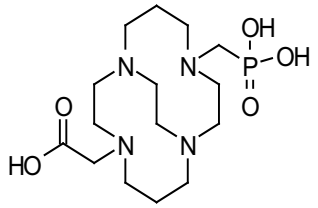






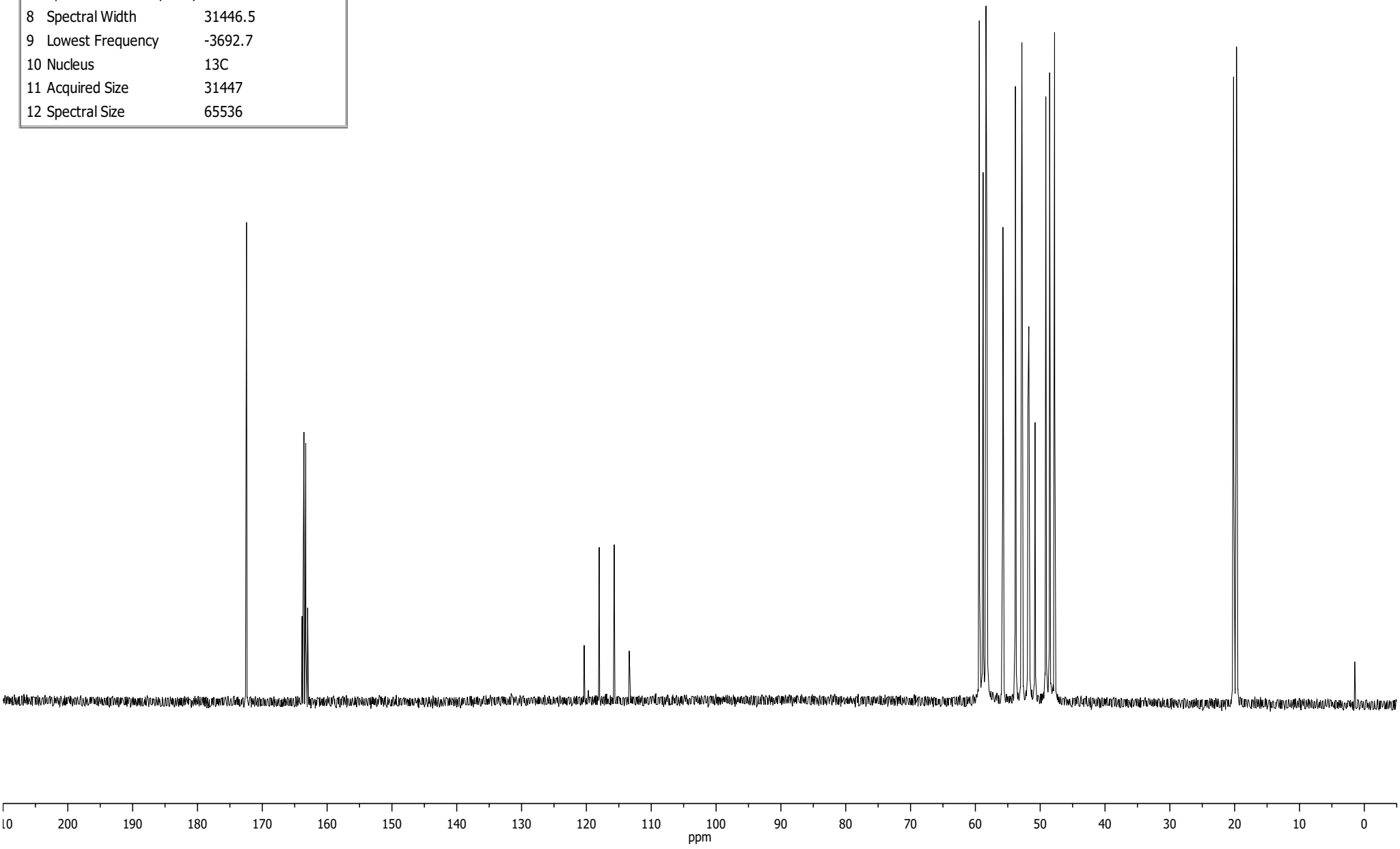


1	Origin	RF-CB-TE1A1P
2	Solvent	D2O
3	Temperature	25.0
4	Number of Scans	16
5	Acquisition Time	3.0000
6	Acquisition Date	2011-01-24T15:29:41
7	Spectrometer Frequency	499.77707
8	Spectral Width	7992.0
9	Lowest Frequency	-1396.6
10	Nucleus	1H
11	Acquired Size	23976
12	Spectral Size	65536

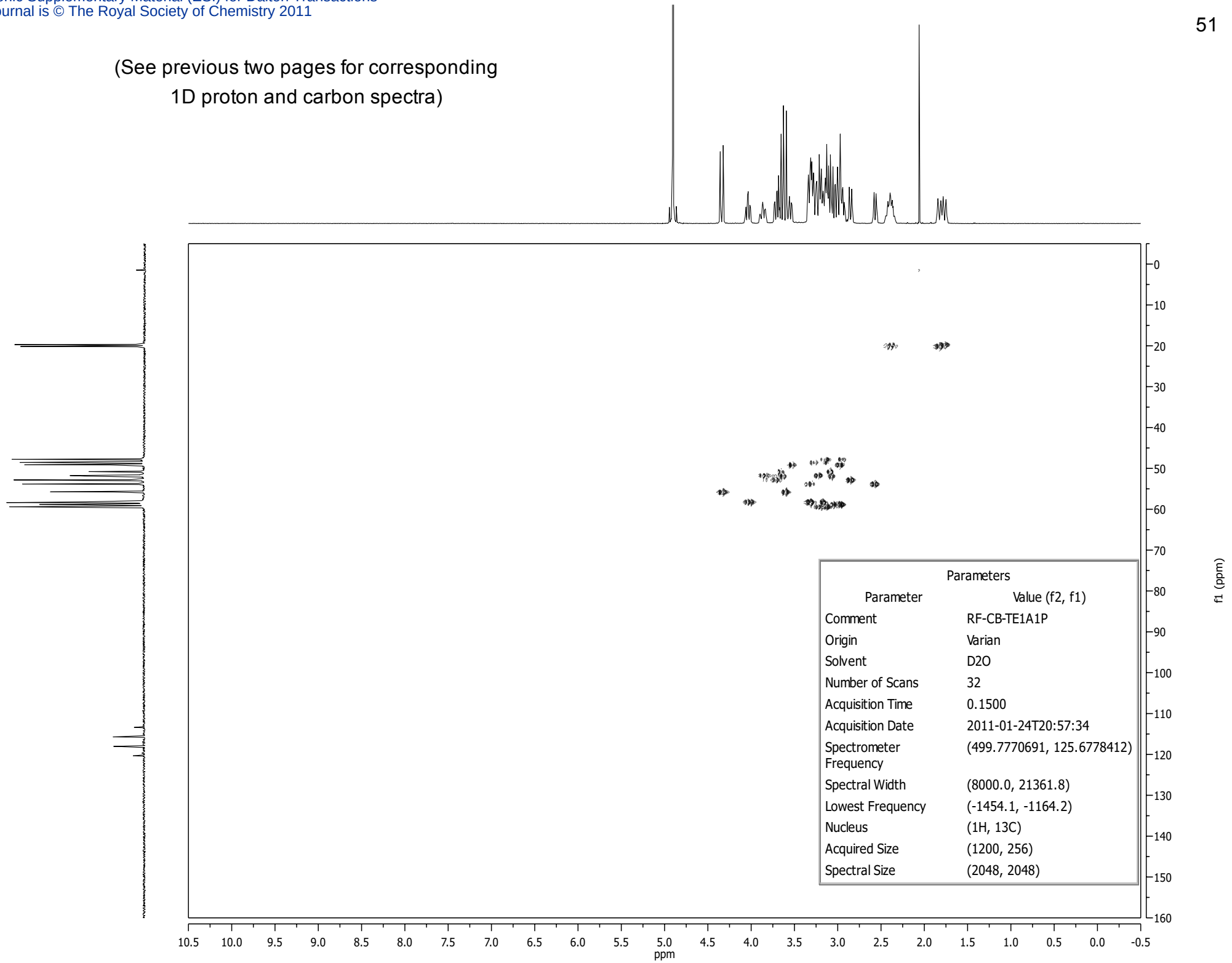


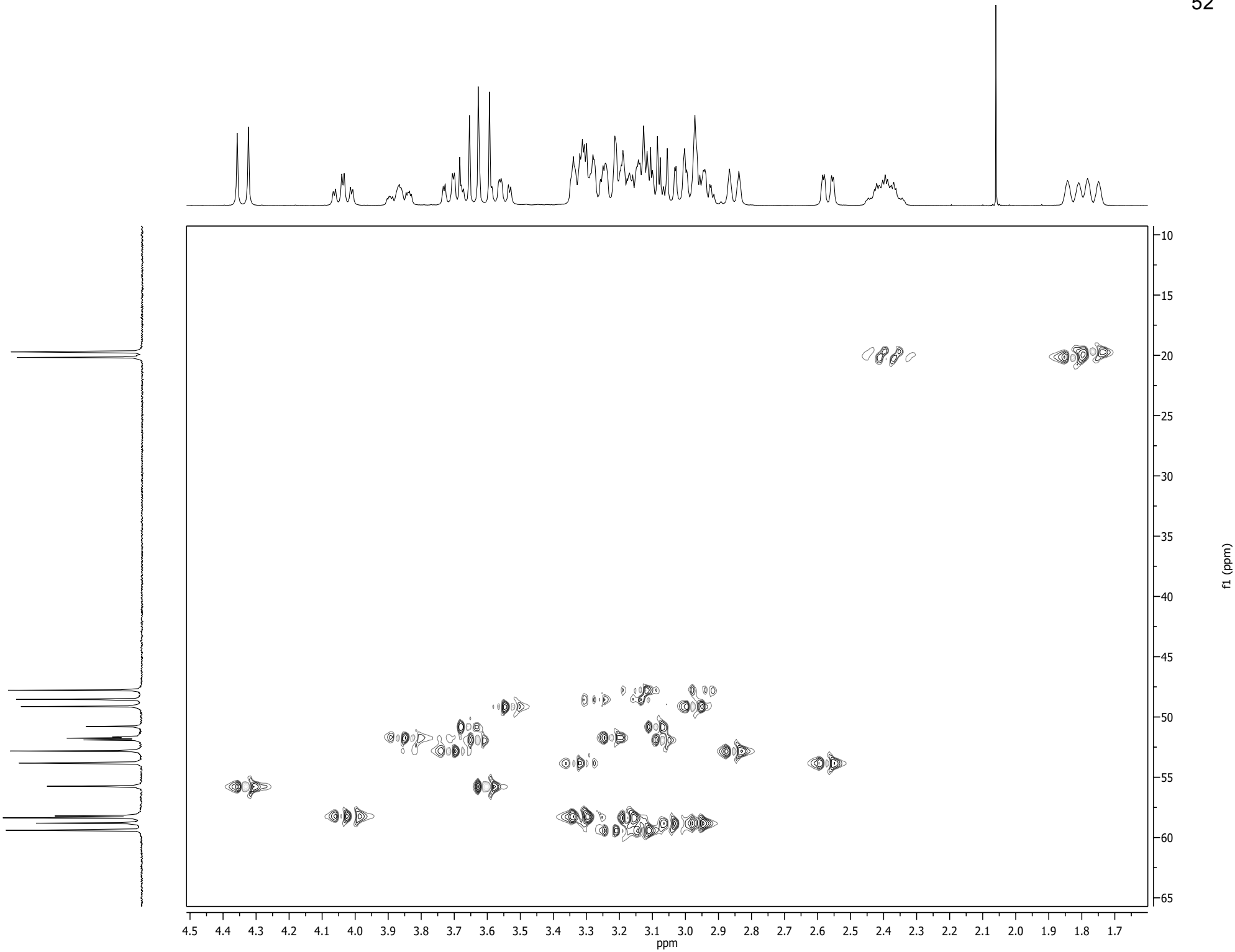
D_2O, 499.78 MHz, internal reference
with MeCN set at δ 2.06

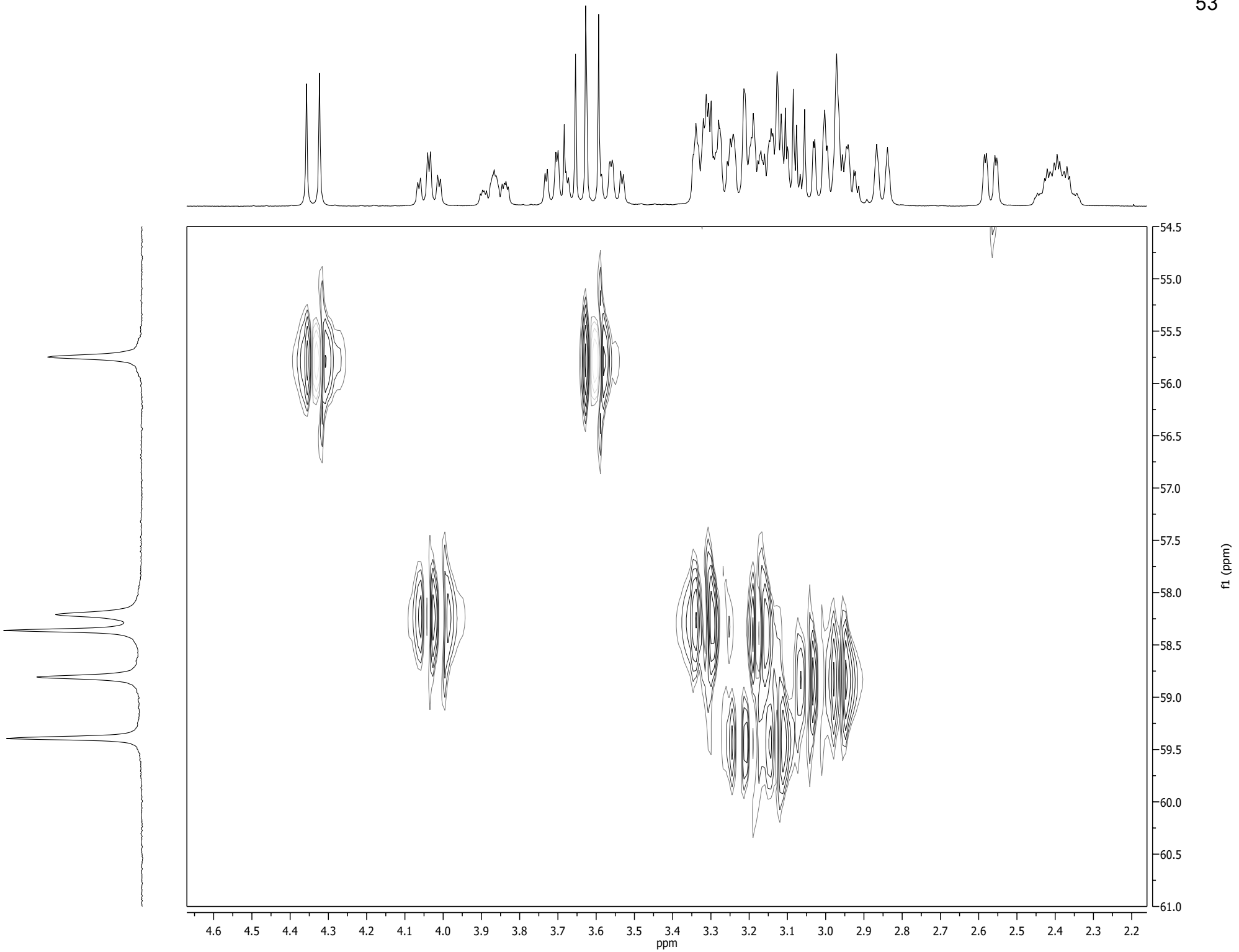
1	Origin	RF-CB-TE1A1P
2	Solvent	D2O
3	Temperature	25.0
4	Number of Scans	38000
5	Acquisition Time	1.0000
6	Acquisition Date	2011-01-22T08:03:16
7	Spectrometer Frequency	125.68036
8	Spectral Width	31446.5
9	Lowest Frequency	-3692.7
10	Nucleus	13C
11	Acquired Size	31447
12	Spectral Size	65536

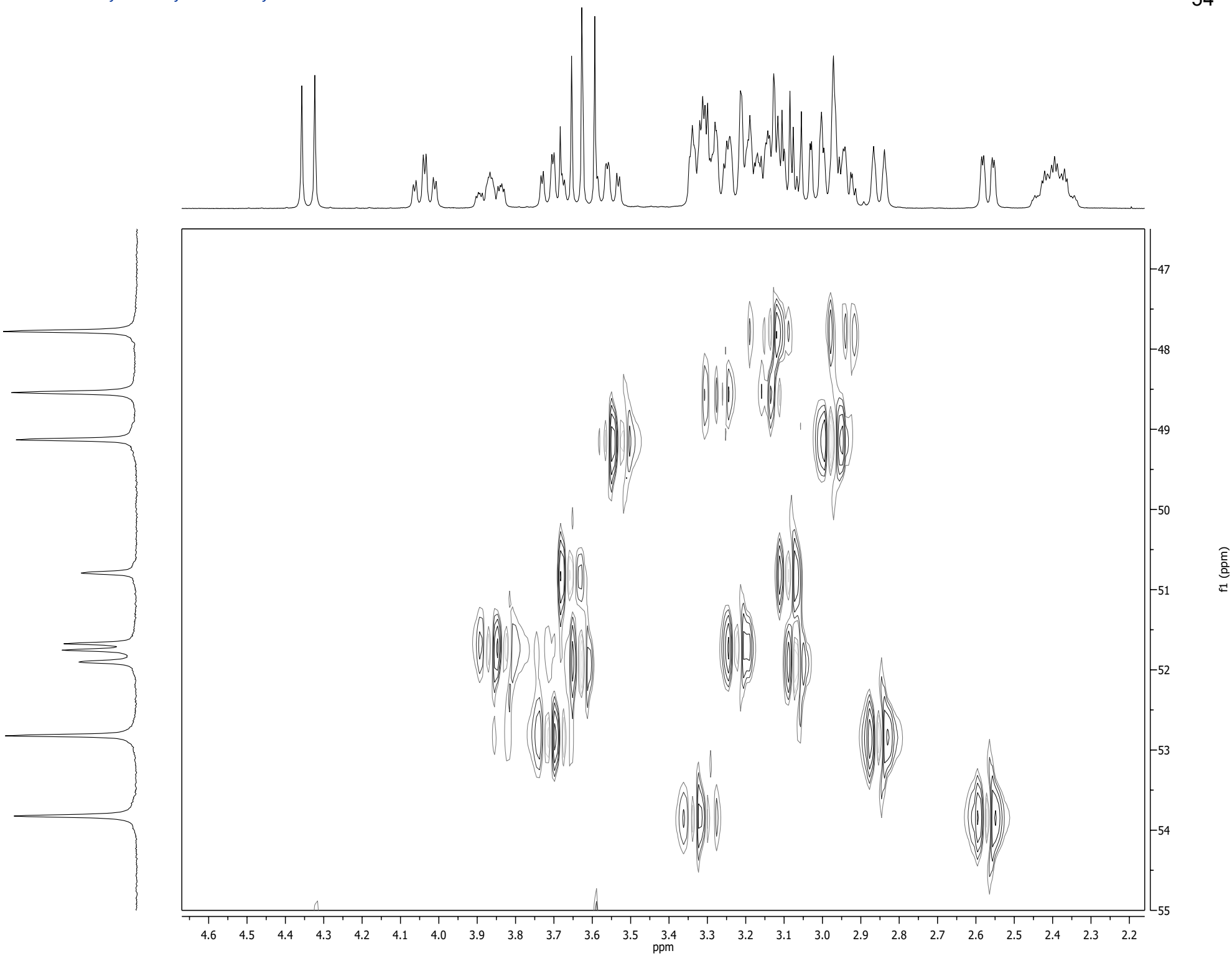


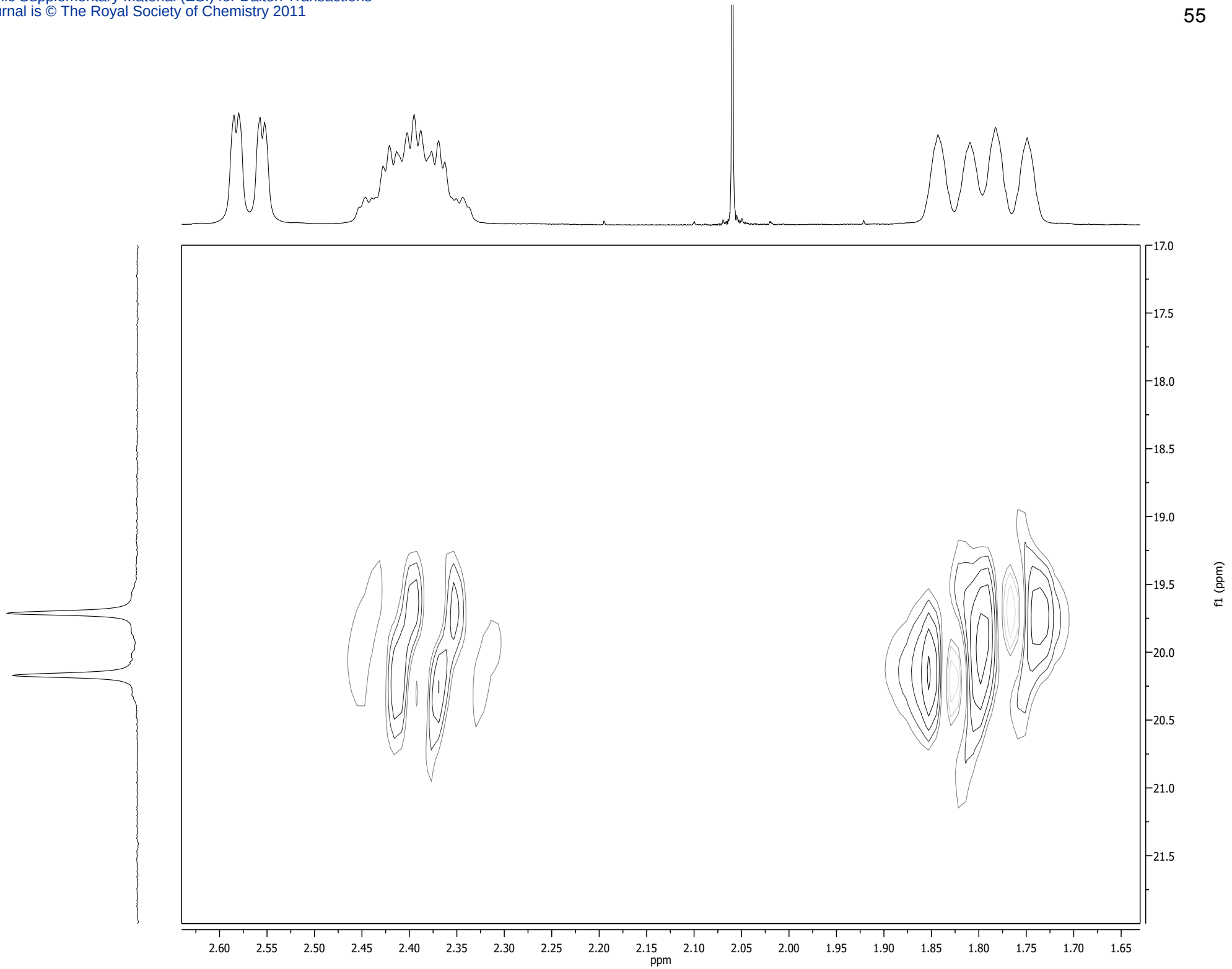
(See previous two pages for corresponding 1D proton and carbon spectra)



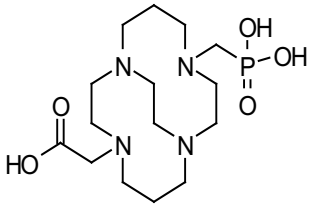

4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7
ppm
10 15 20 25 30 35 40 45 50 55 60 65
f1 (ppm)




4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
ppm
47
48
49
50
51
52
53
54
55
f1 (ppm)

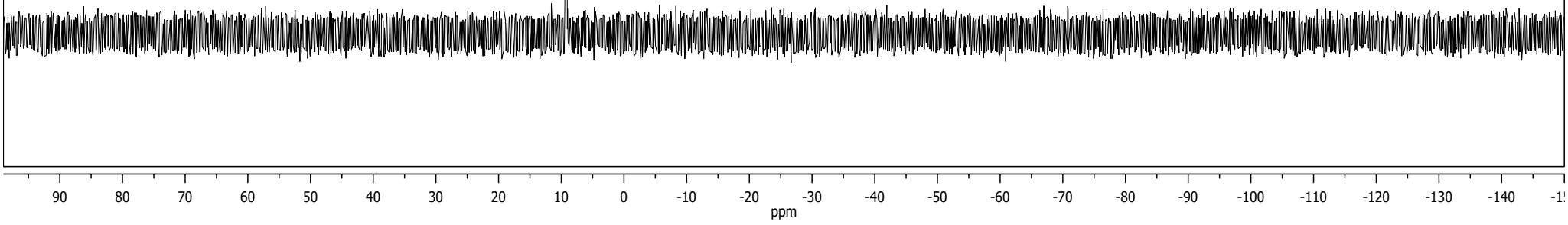

17.0
17.5
18.0
18.5
19.0
19.5
20.0
20.5
21.0
21.5
f1 (ppm)
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20
2.15
2.10
2.05
2.00
1.95
1.90
1.85
1.80
1.75
1.70
1.65
ppm

1	Data File Name	RF-CB-TE1A1P_31P
2	Origin	Varian
3	Solvent	D2O
4	Number of Scans	512
5	Receiver Gain	60
6	Acquisition Time	1.6000
7	Acquisition Date	2011-01-22T10:13:04
8	Spectrometer Frequency	202.30717
9	Spectral Width	50600.9
10	Lowest Frequency	-30548.5
11	Nucleus	31P
12	Acquired Size	80961
13	Spectral Size	262144

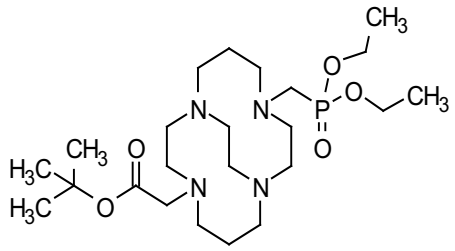


9.240

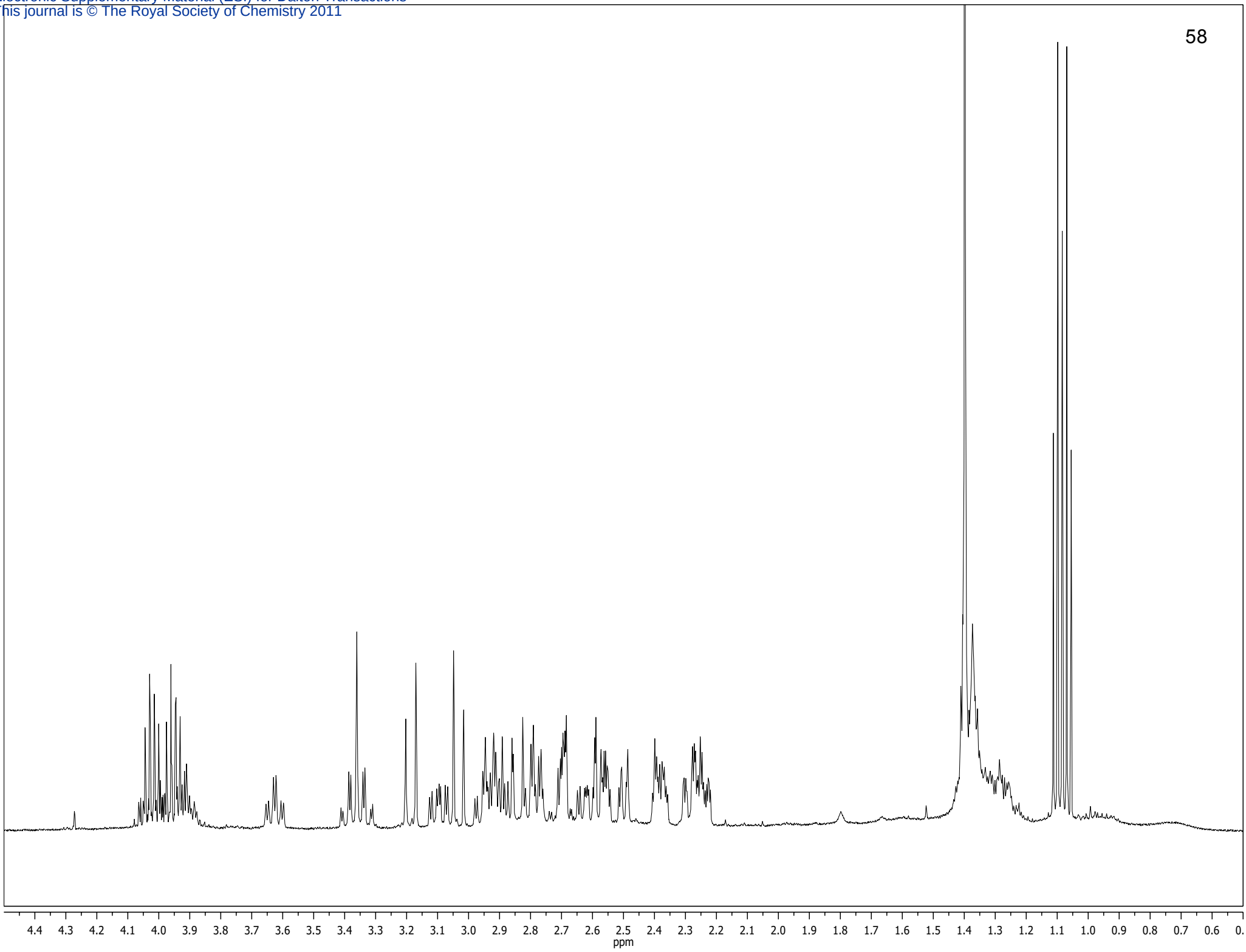
D_2O, 202.31 MHz, external reference with 85% phosphoric acid set at δ 0.00

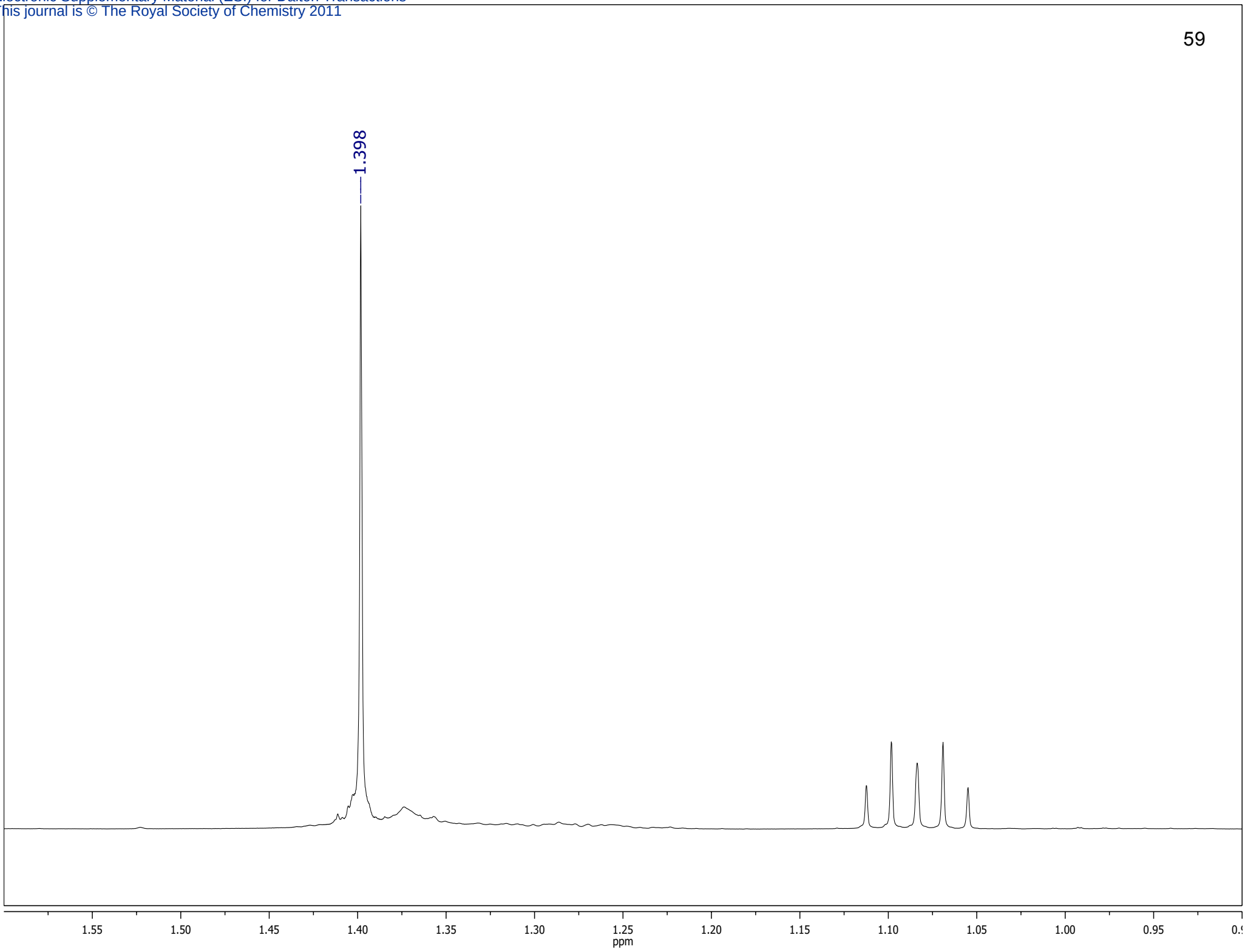


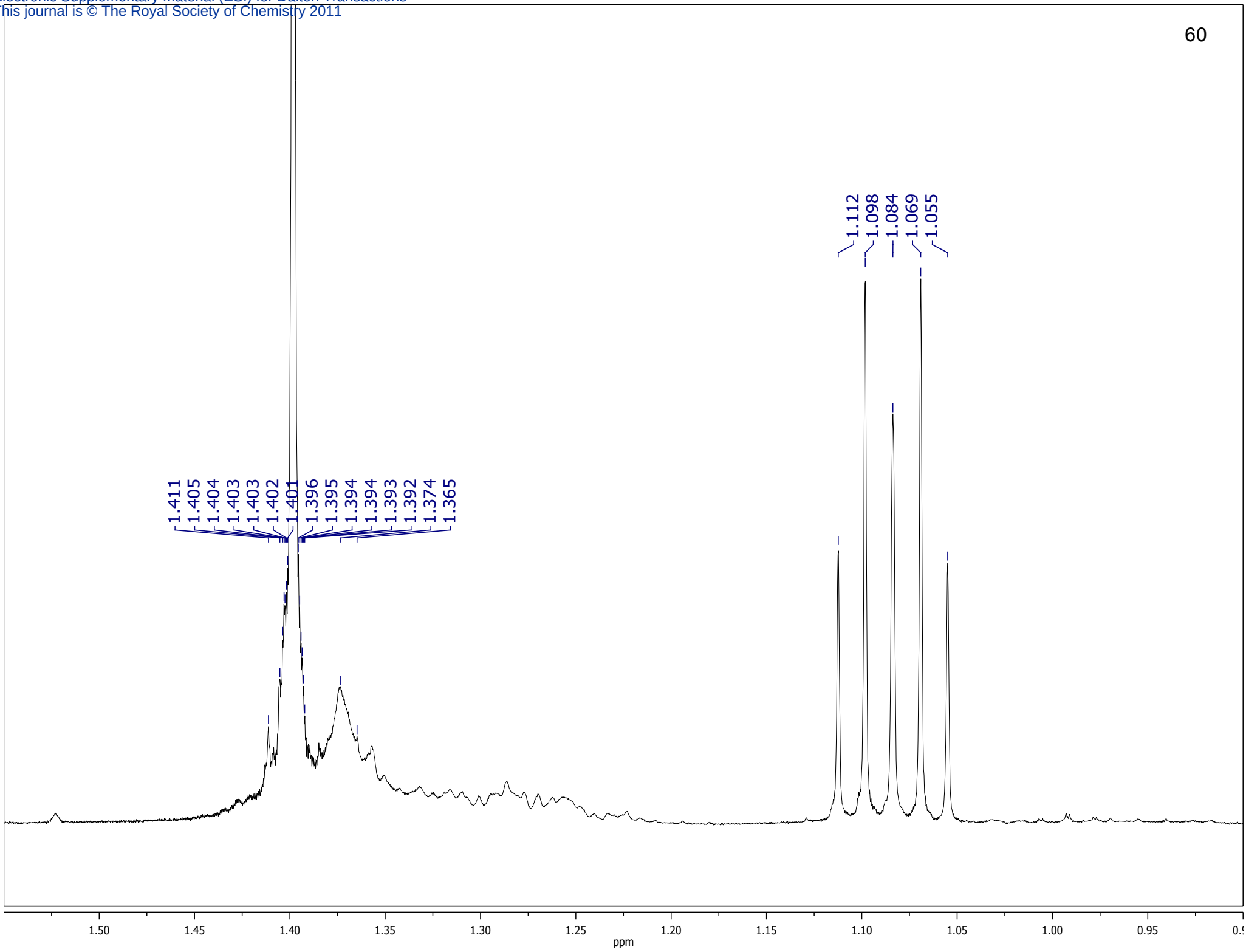
1	Data File Name	RF-CB-TE1A1P_protected_CH2Cl2 extracts_2011-02-16/ PROTON
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	32
5	Receiver Gain	34
6	Acquisition Time	3.0000
7	Acquisition Date	2011-02-16T15:28:30
8	Spectrometer Frequency	499.77585
9	Spectral Width	7992.0
10	Lowest Frequency	-1498.0
11	Nucleus	1H
12	Acquired Size	23976
13	Spectral Size	65536

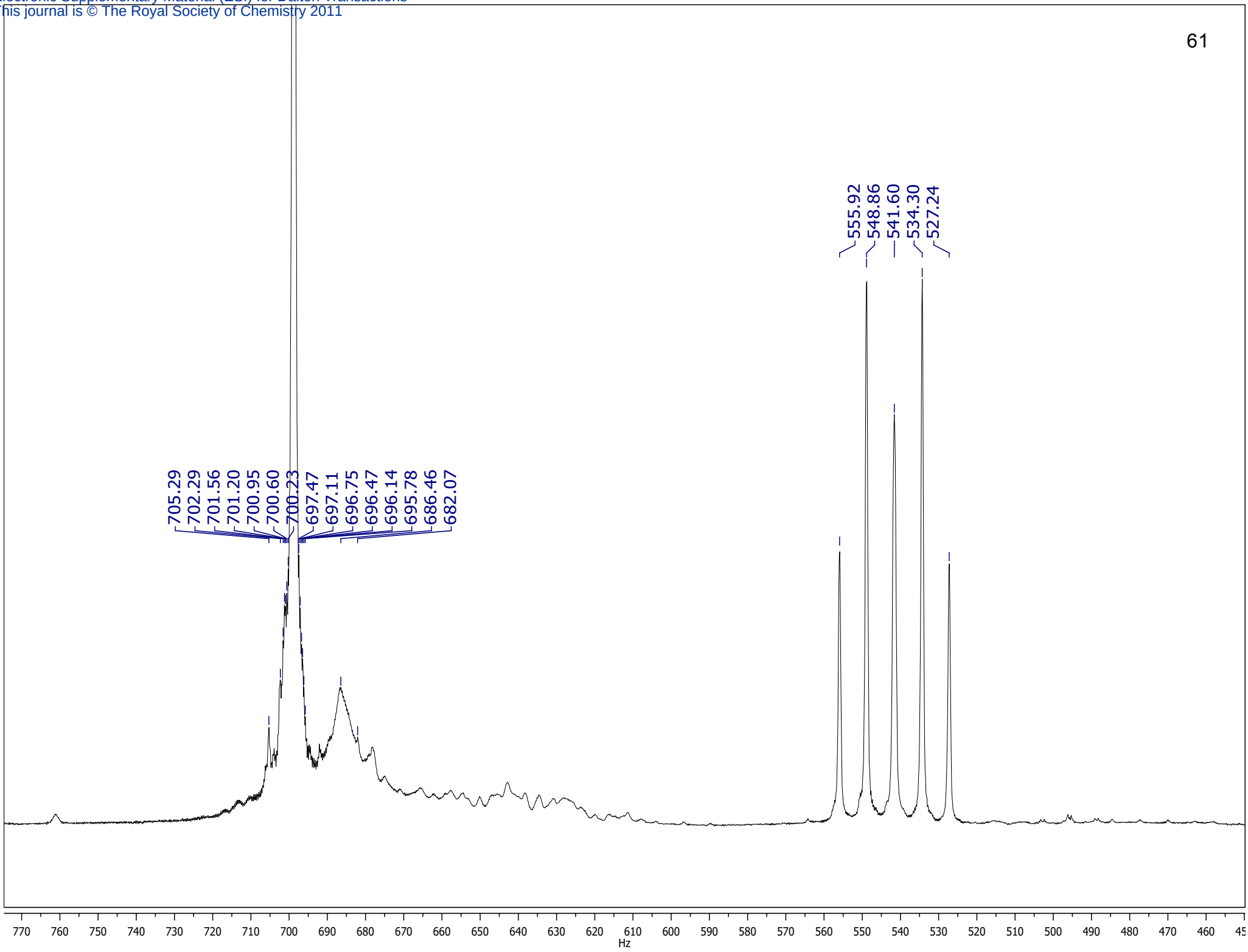


RF-CB-TE1A1P_protected (CH_2Cl_2 extracts)
C_6D_6, 499.78 MHz, internal reference set to TMS at δ 0.00
Sample was dried over Na_2SO_4 prior to running NMR

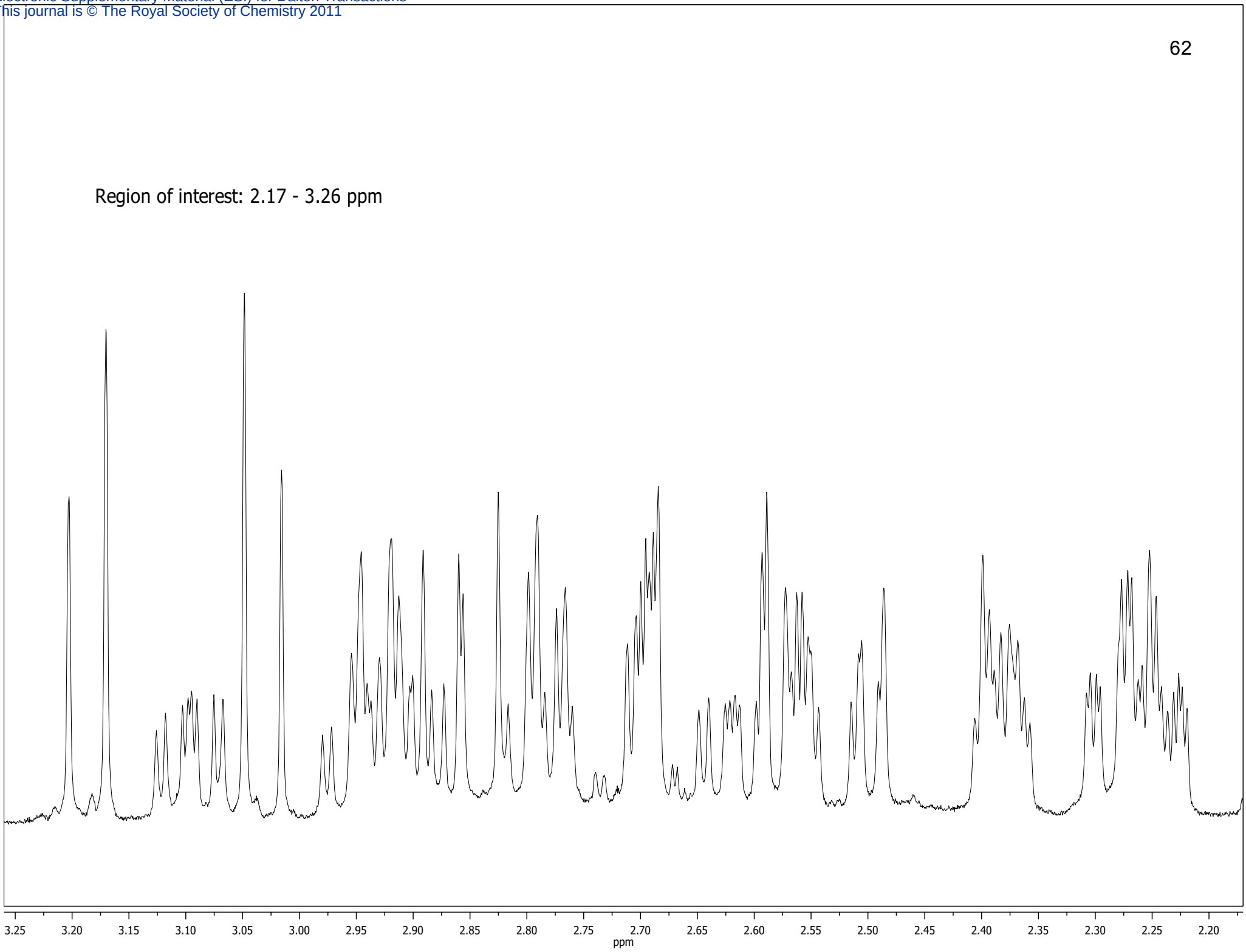




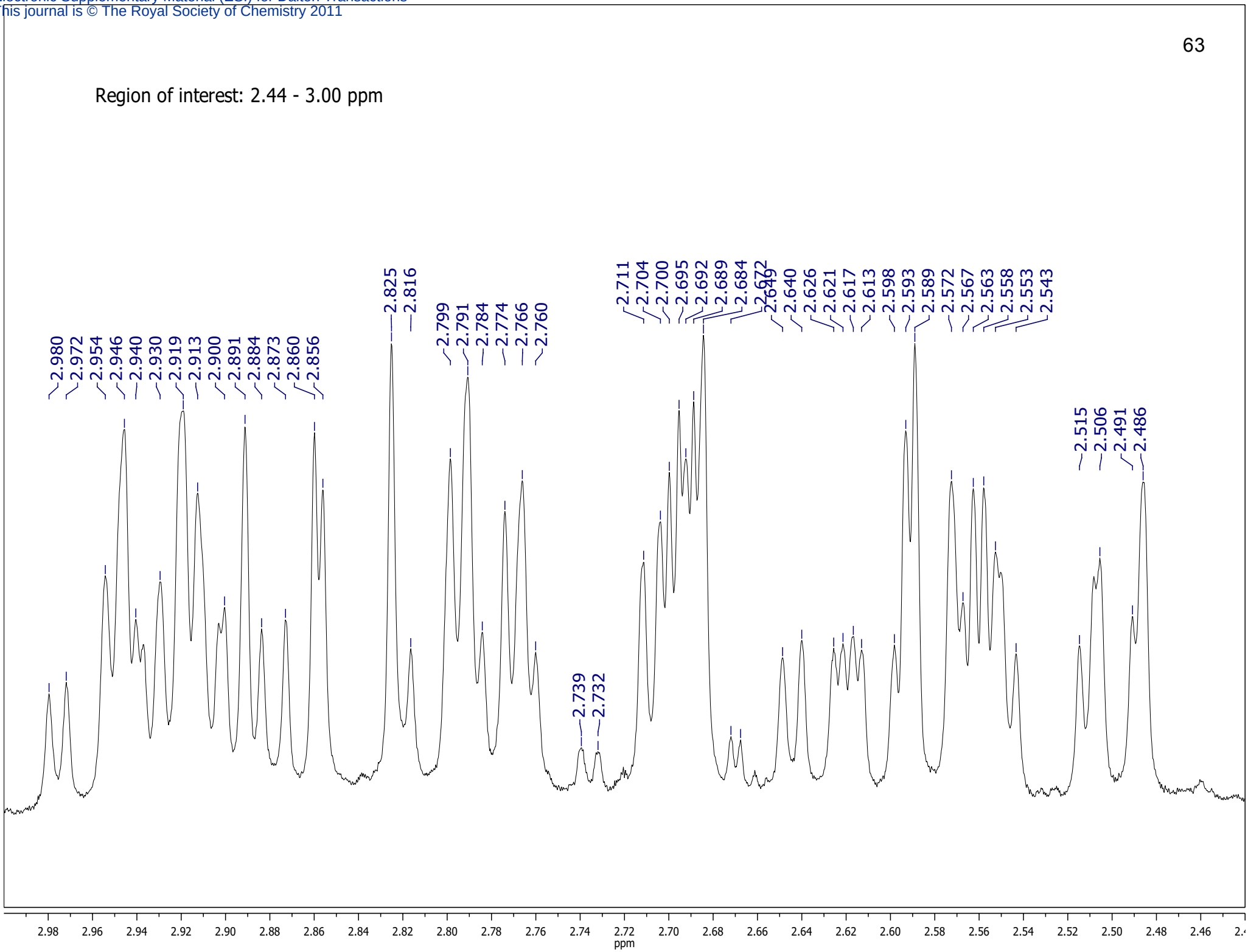




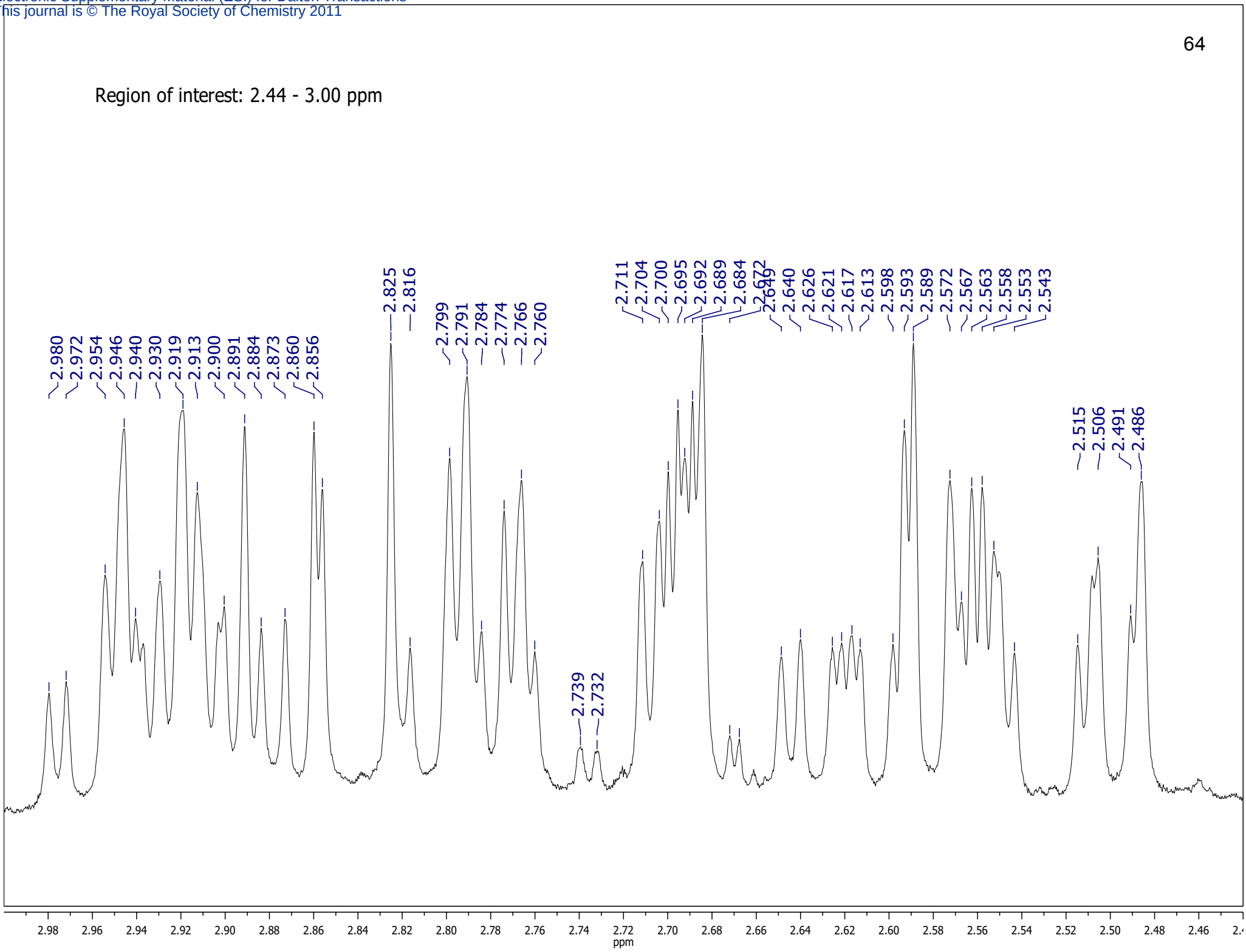
Region of interest: 2.17 - 3.26 ppm



Region of interest: 2.44 - 3.00 ppm

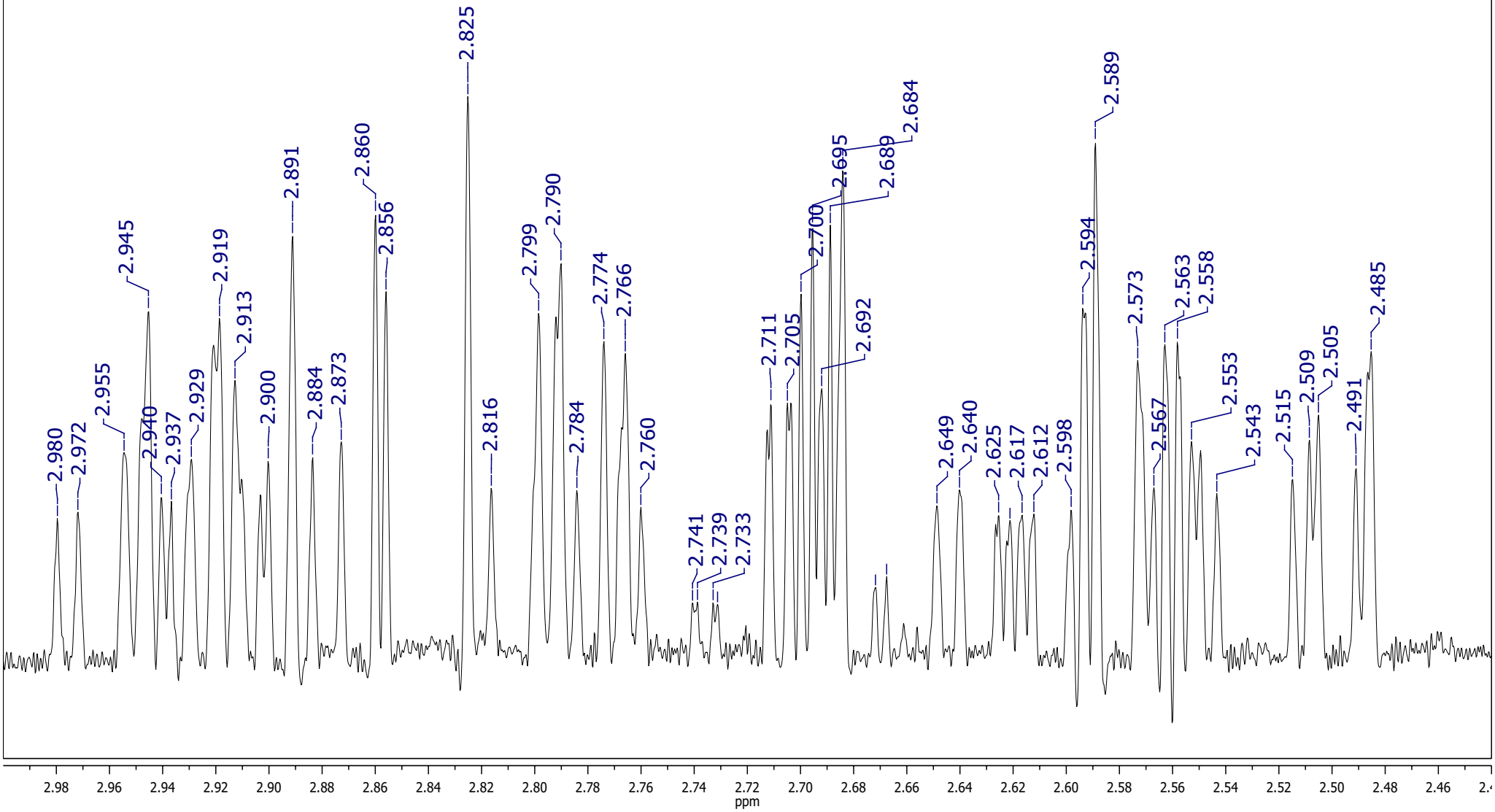


Region of interest: 2.44 - 3.00 ppm



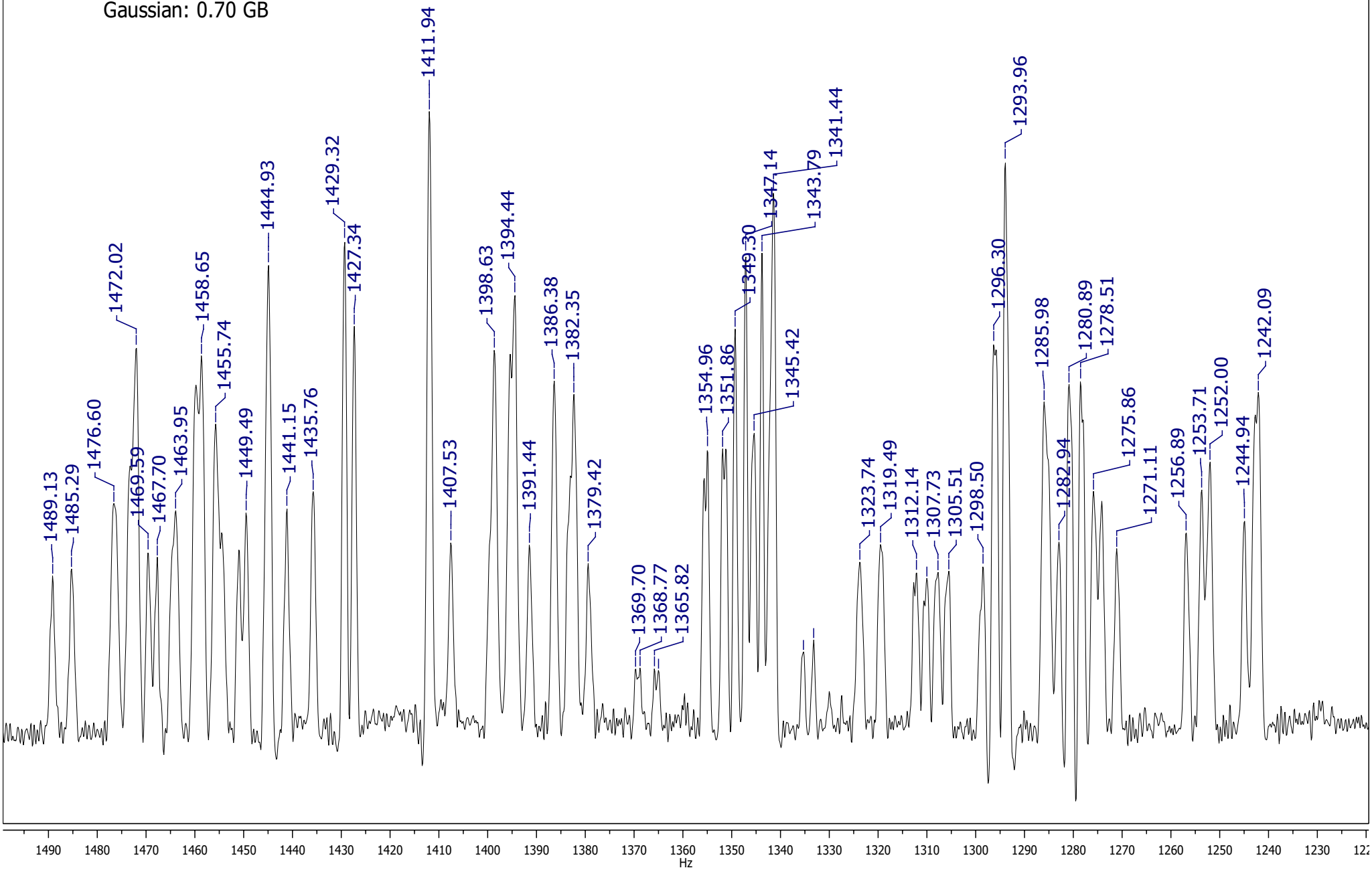
Region of interest: 2.44- 3.00 ppm

Exponential: -1.32
Gaussian: 0.70 GB



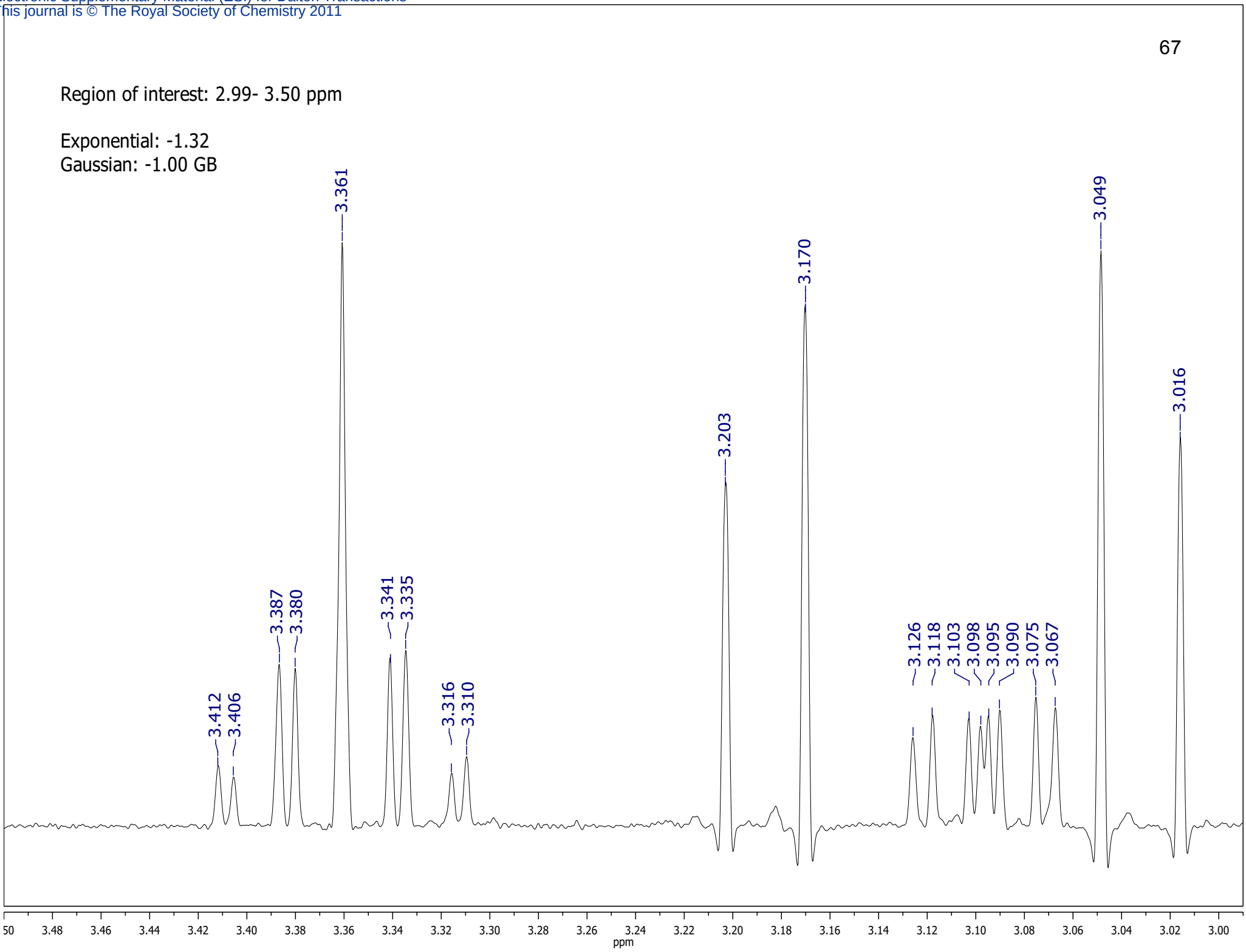
Region of interest: 2.44- 3.00 ppm

Exponential: -1.32
Gaussian: 0.70 GB



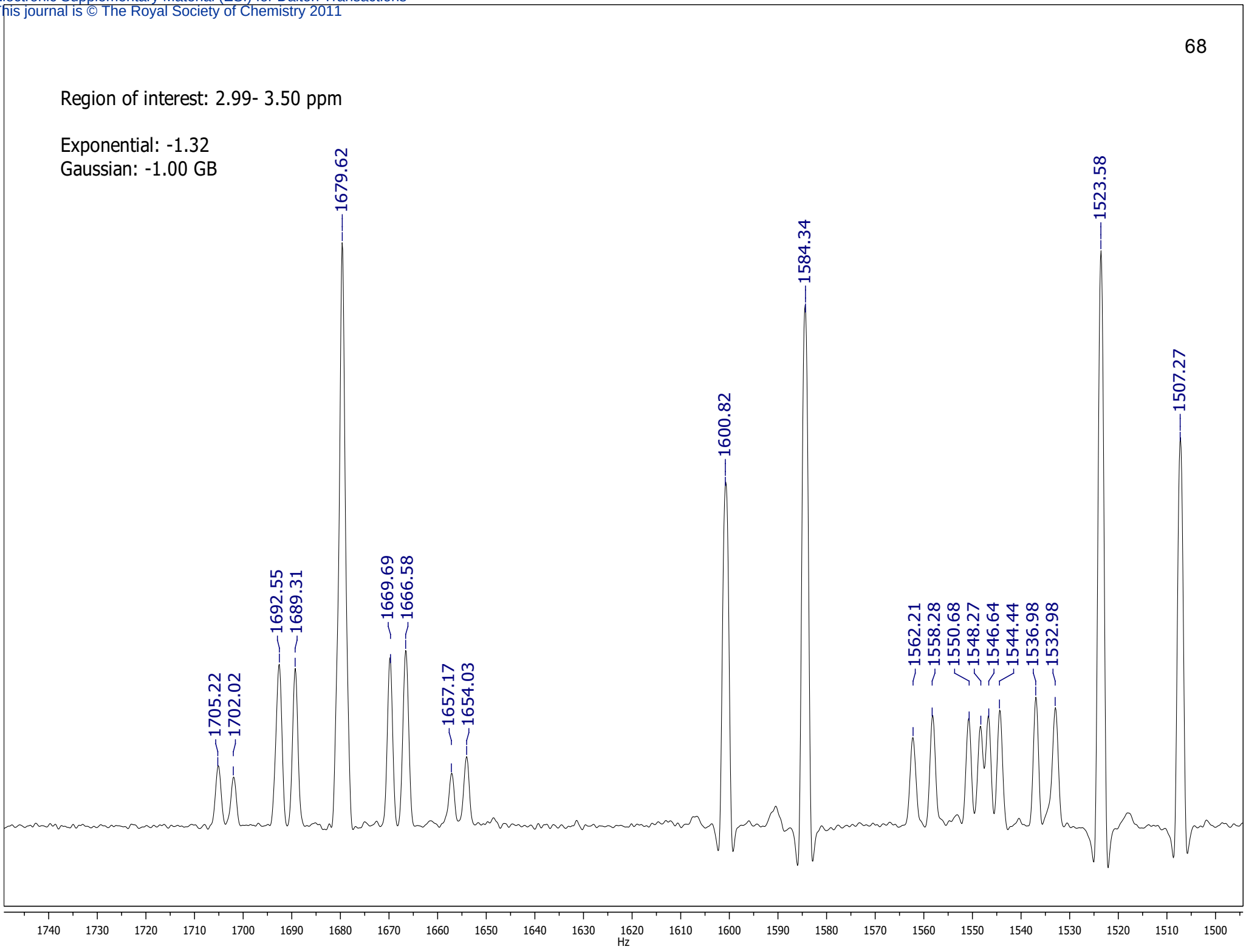
Region of interest: 2.99- 3.50 ppm

Exponential: -1.32
Gaussian: -1.00 GB

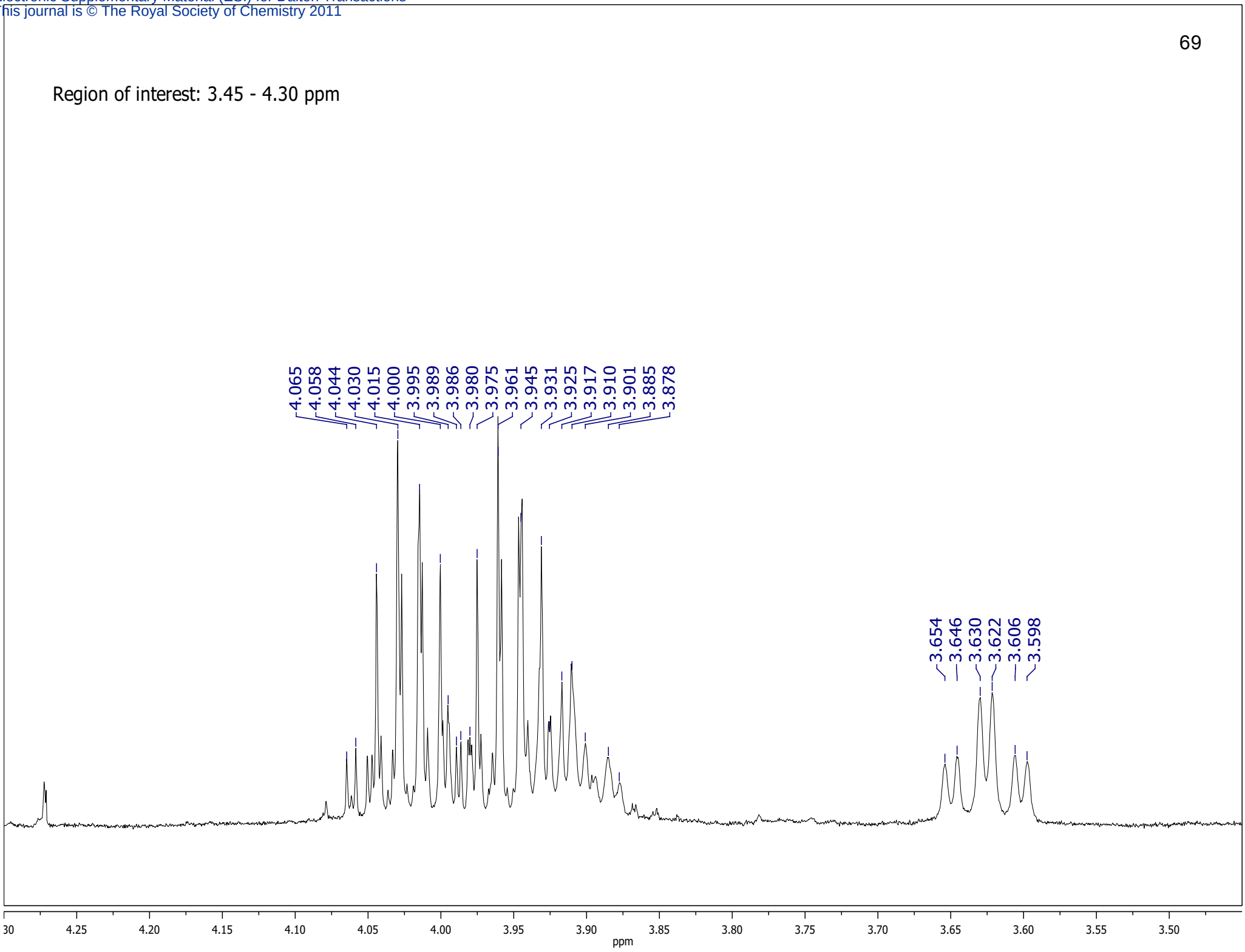


Region of interest: 2.99- 3.50 ppm

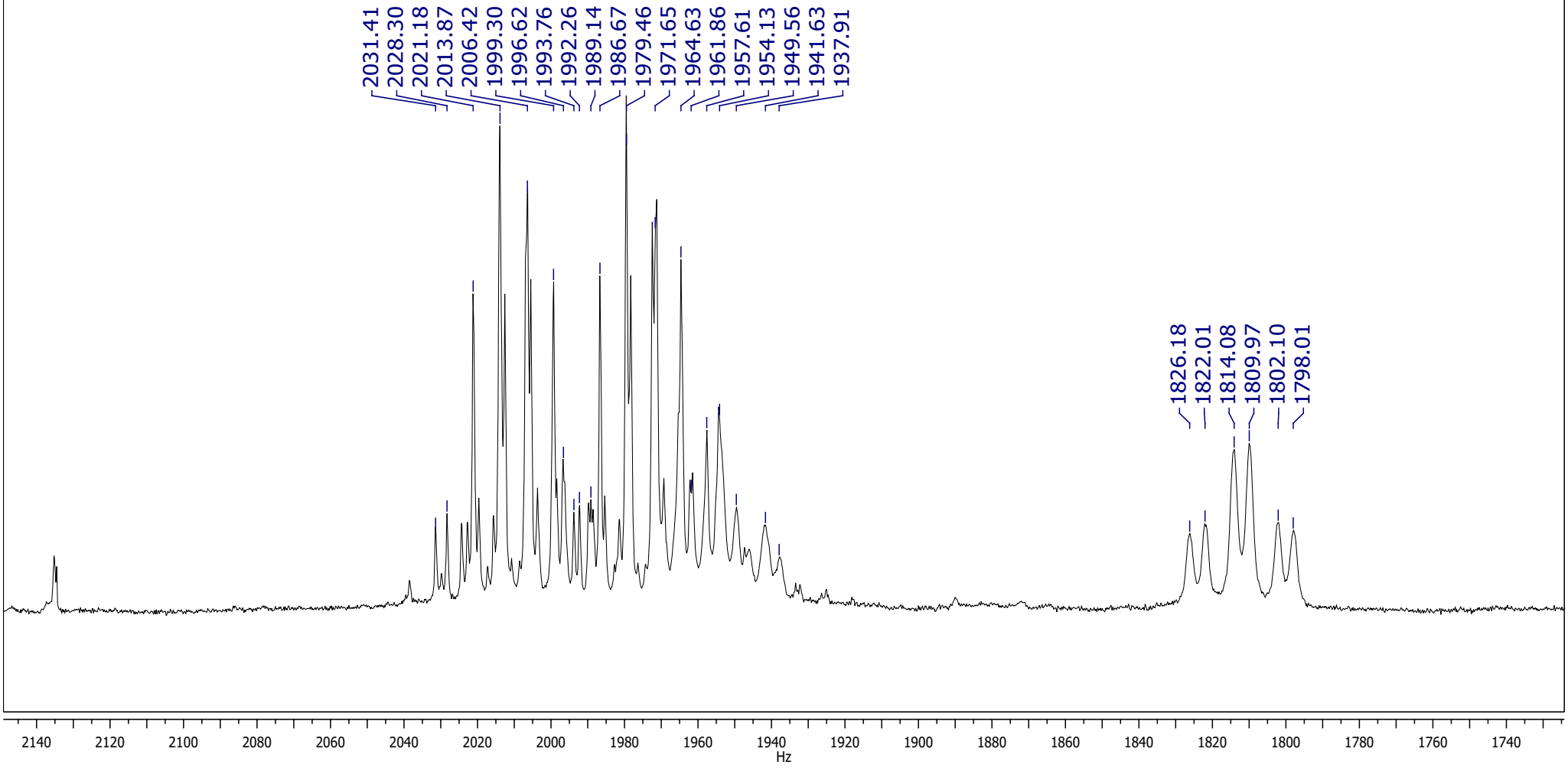
Exponential: -1.32
Gaussian: -1.00 GB

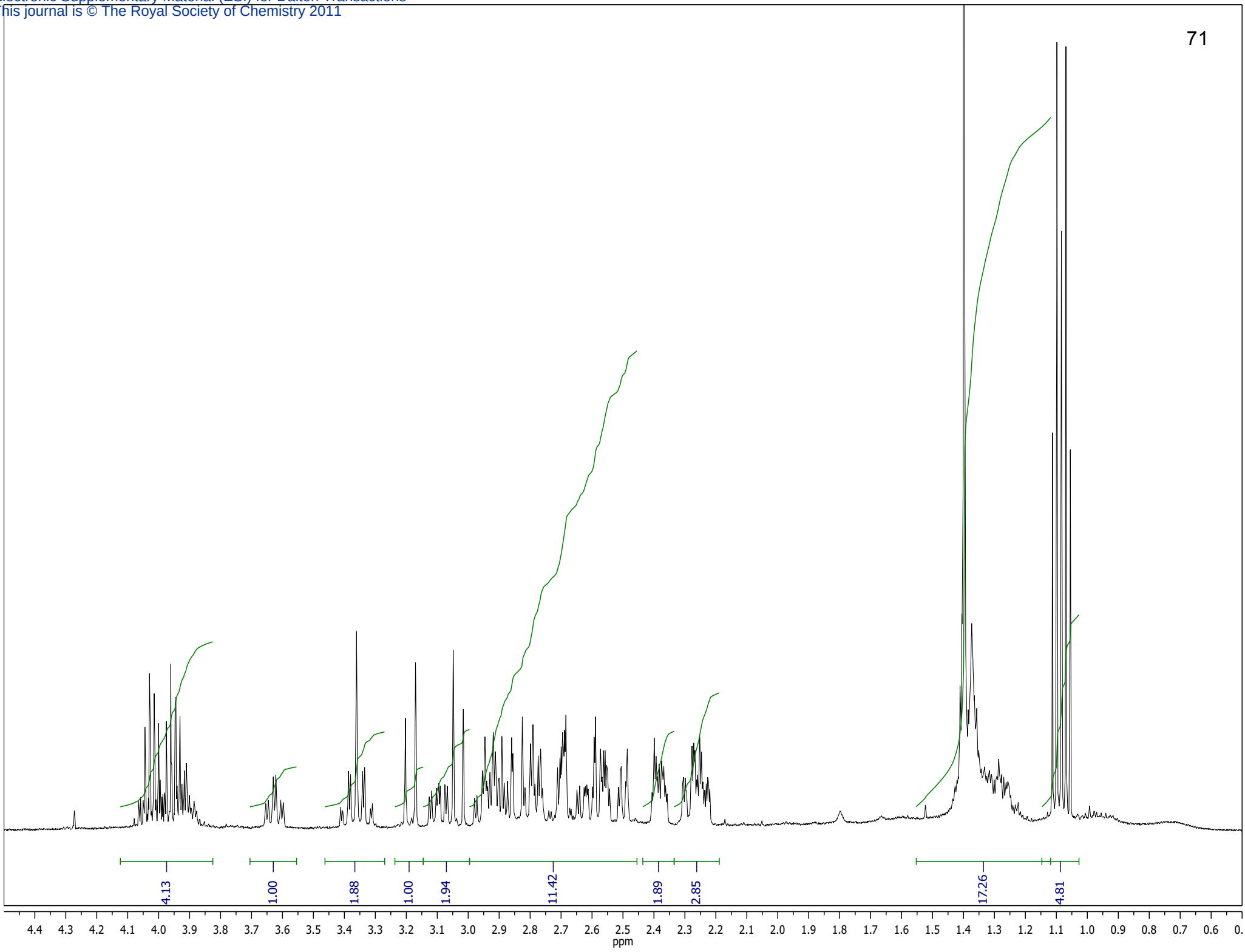


Region of interest: 3.45 - 4.30 ppm



Region of interest: 3.45 - 4.30 ppm

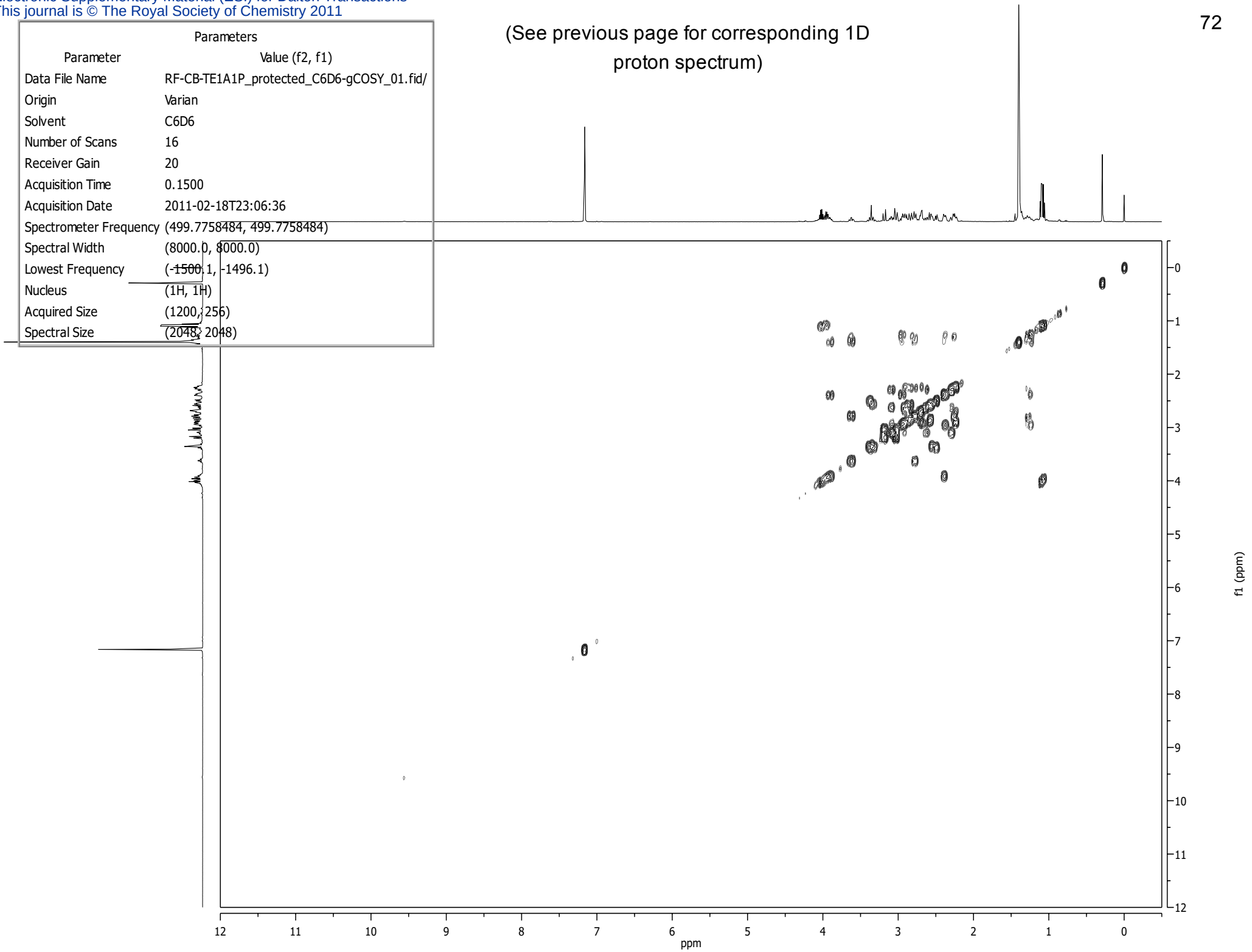


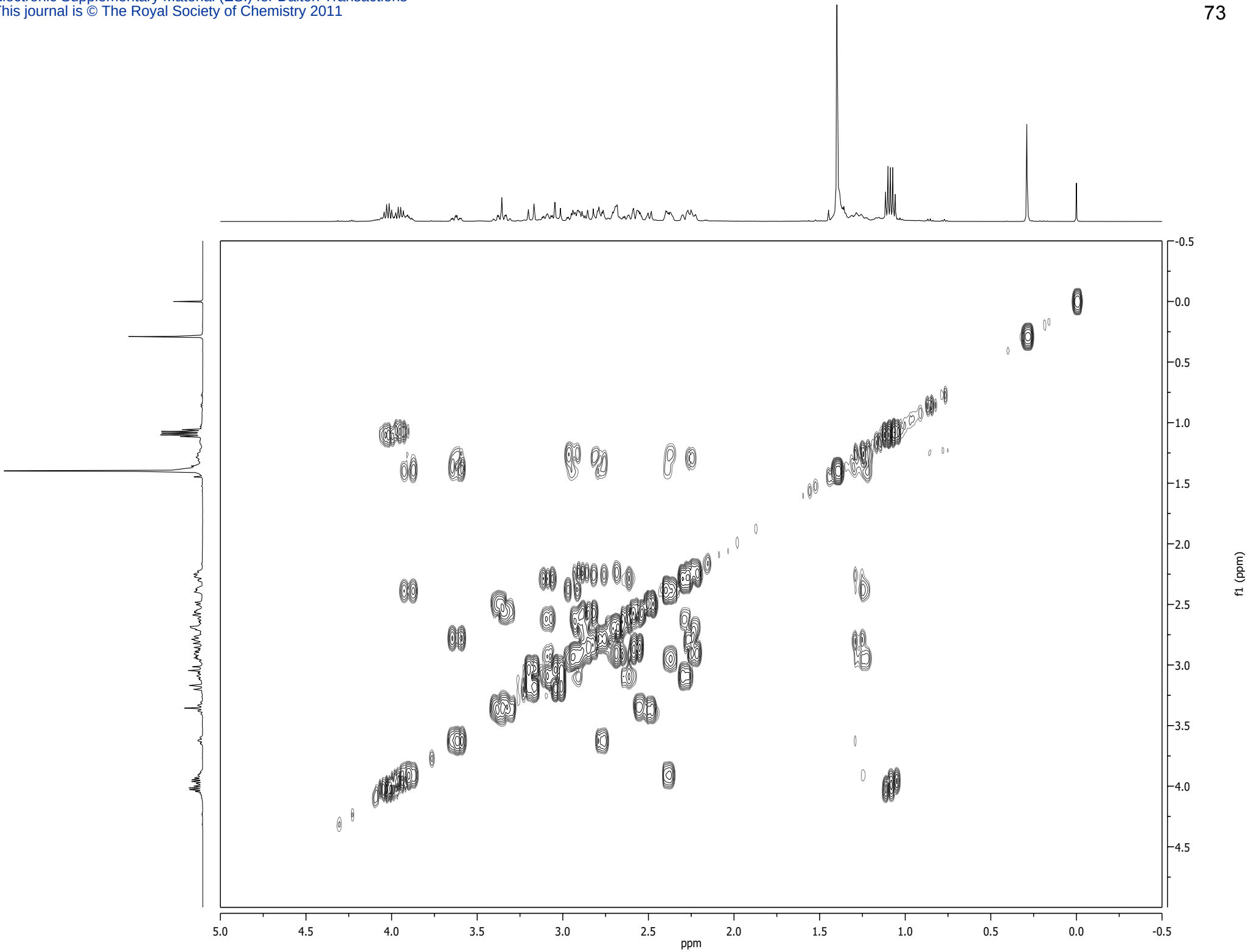


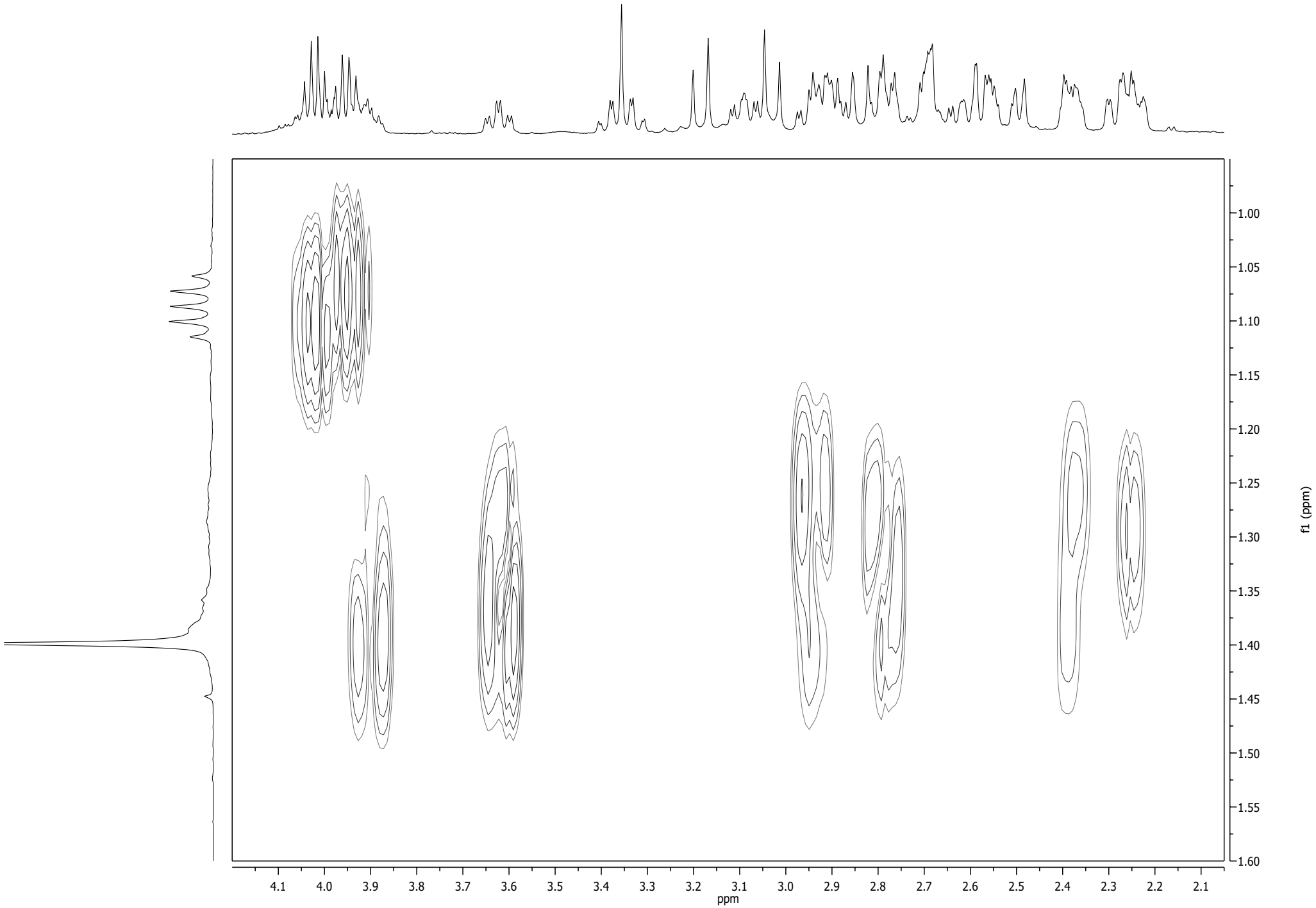
(See previous page for corresponding 1D proton spectrum)

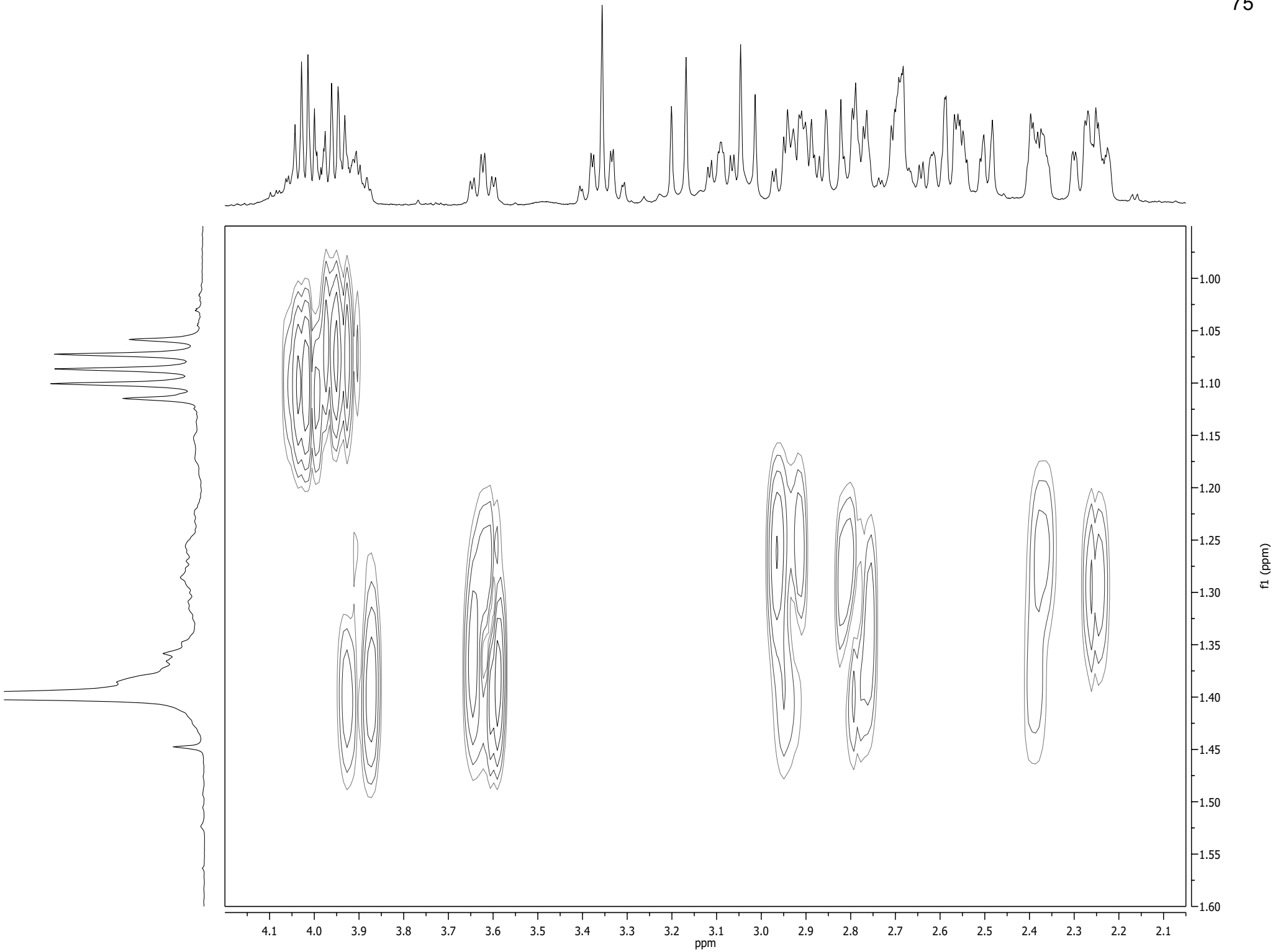
Parameters

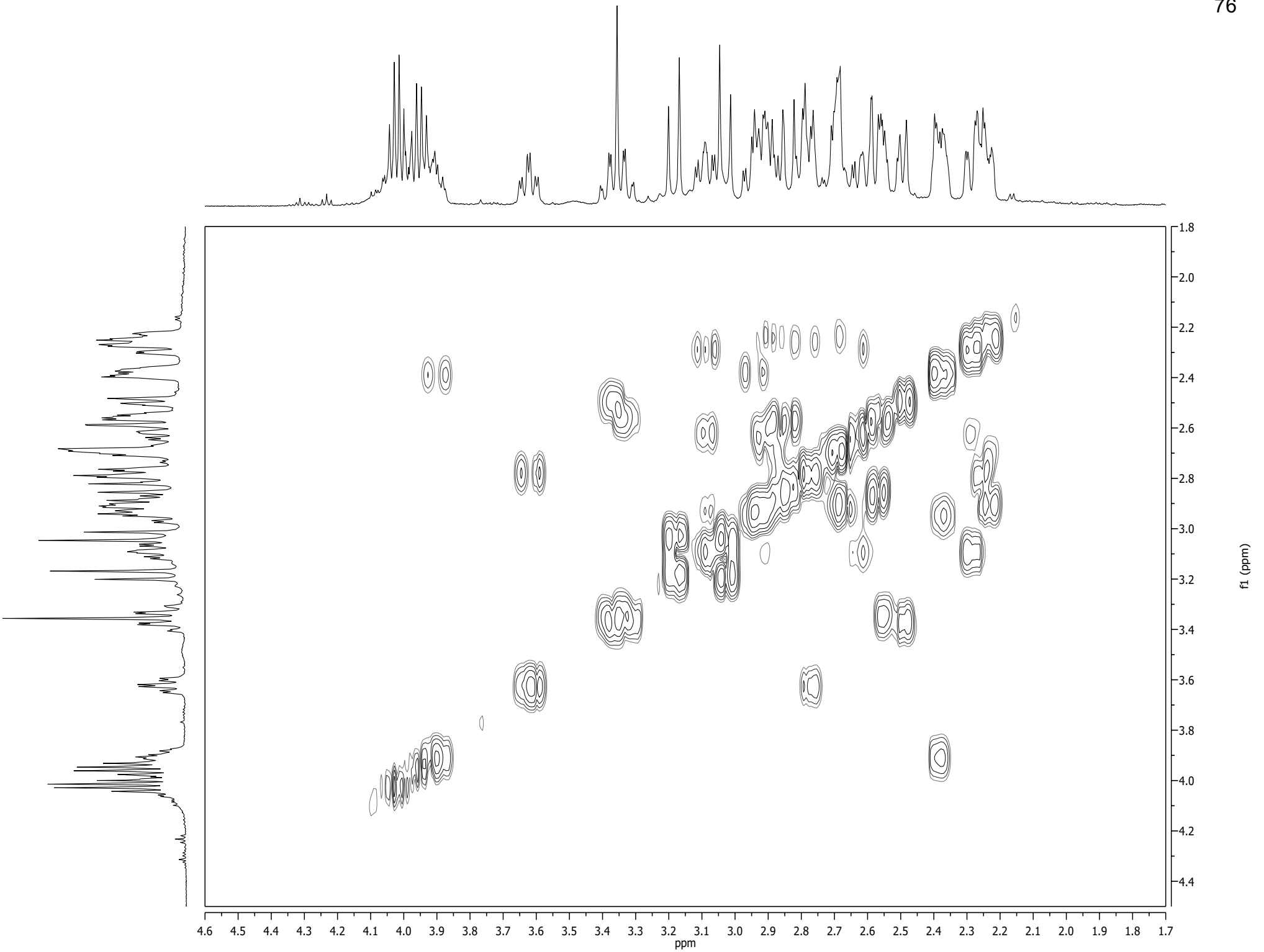
Parameter	Value (f2, f1)
Data File Name	RF-CB-TE1A1P_protected_C6D6-gCOSY_01.fid/
Origin	Varian
Solvent	C6D6
Number of Scans	16
Receiver Gain	20
Acquisition Time	0.1500
Acquisition Date	2011-02-18T23:06:36
Spectrometer Frequency	(499.7758484, 499.7758484)
Spectral Width	(8000.0, 8000.0)
Lowest Frequency	(-1500.1, -1496.1)
Nucleus	(1H, 1H)
Acquired Size	(1200, 256)
Spectral Size	(2048, 2048)

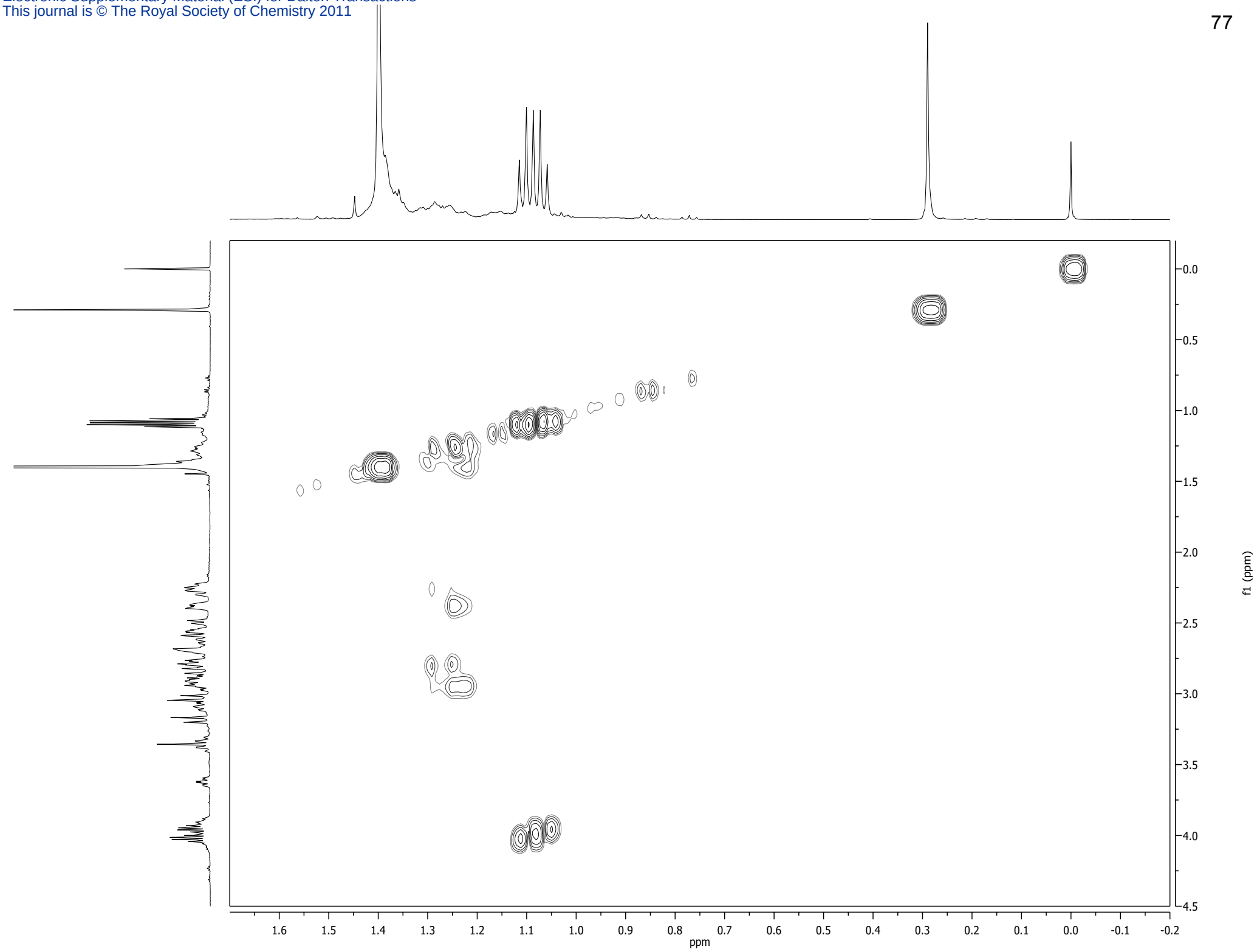


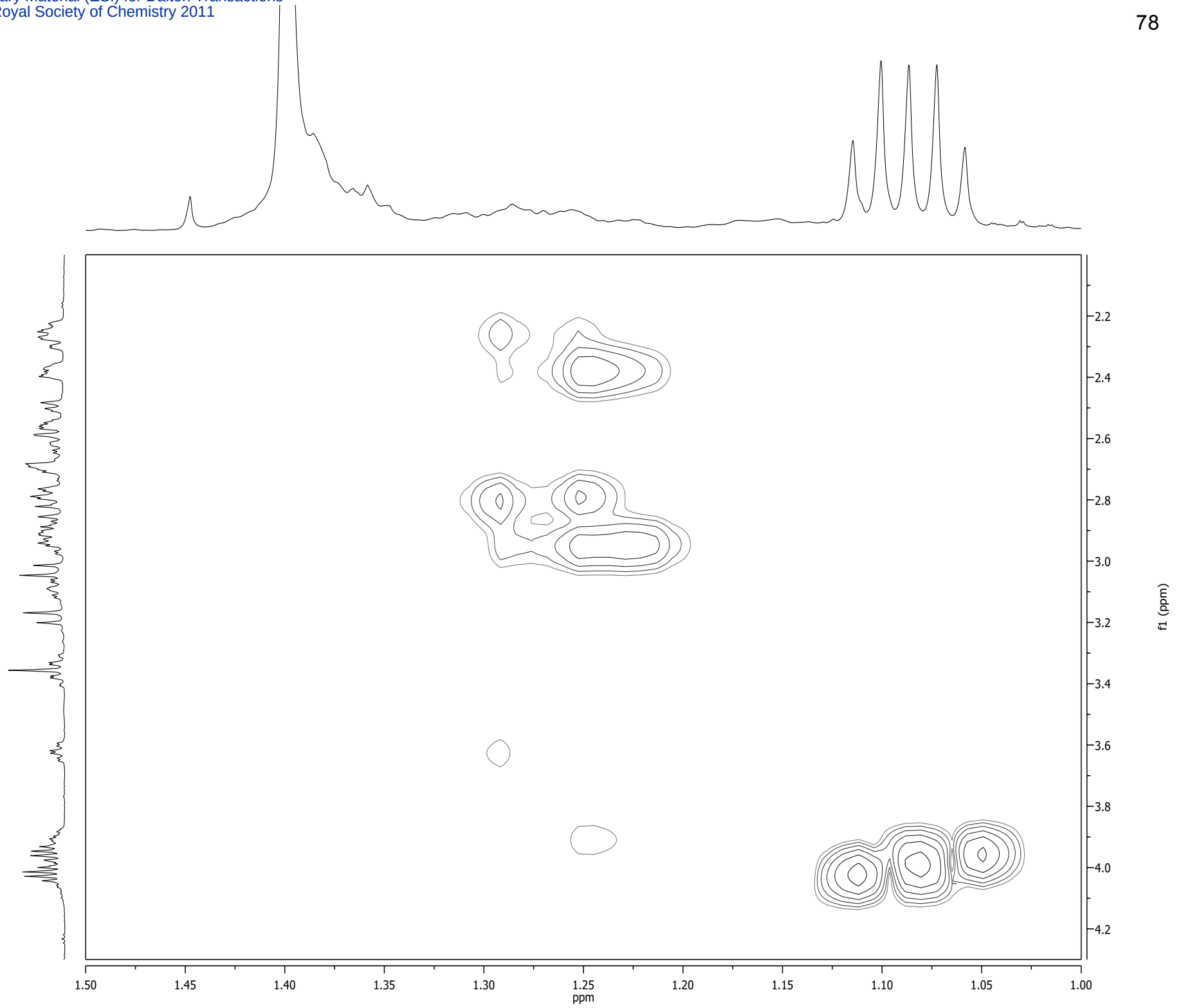

5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
f1 (ppm)


4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
ppm
1.00
1.05
1.10
1.15
1.20
1.25
1.30
1.35
1.40
1.45
1.50
1.55
1.60
f1 (ppm)

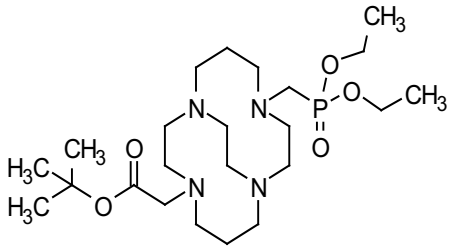




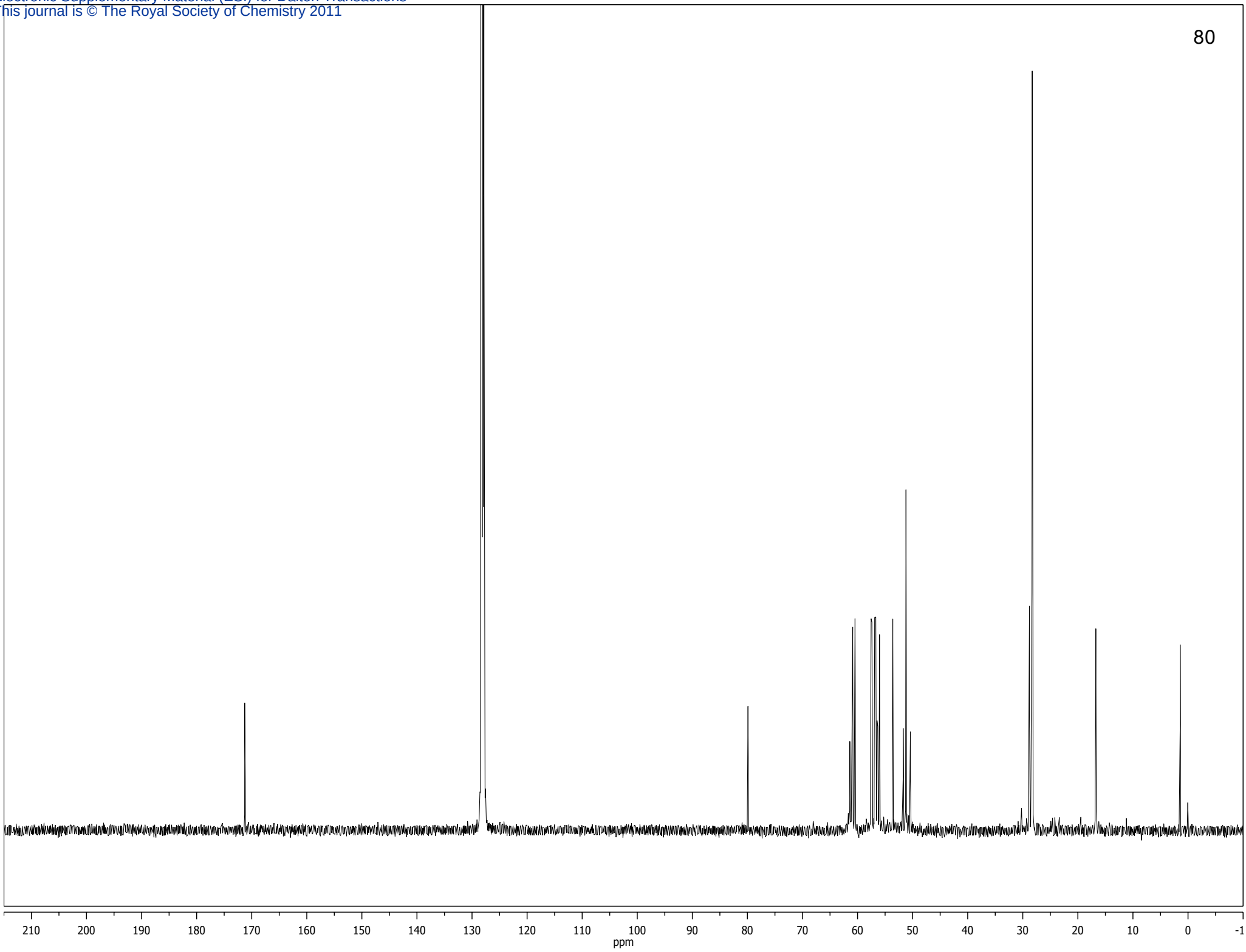


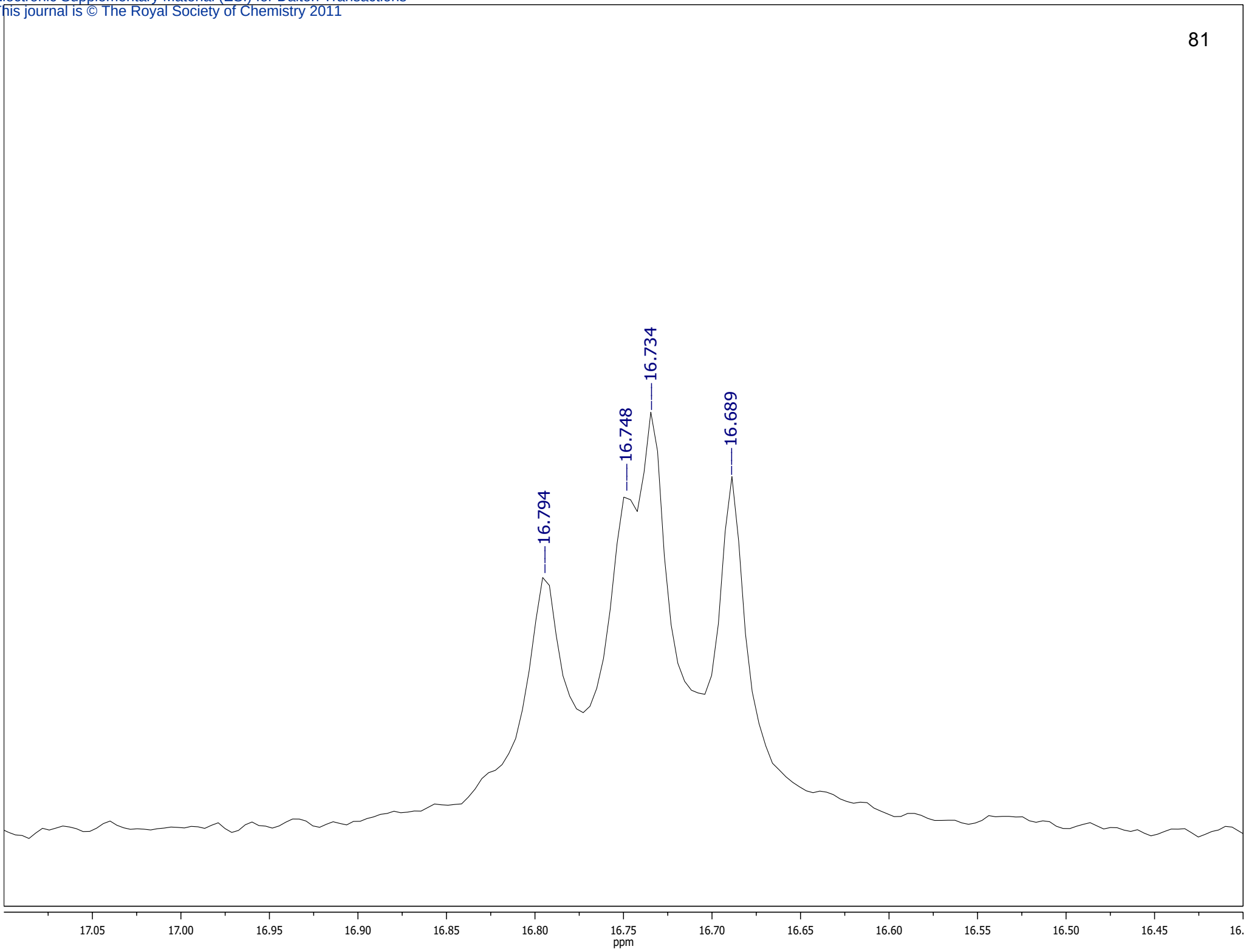


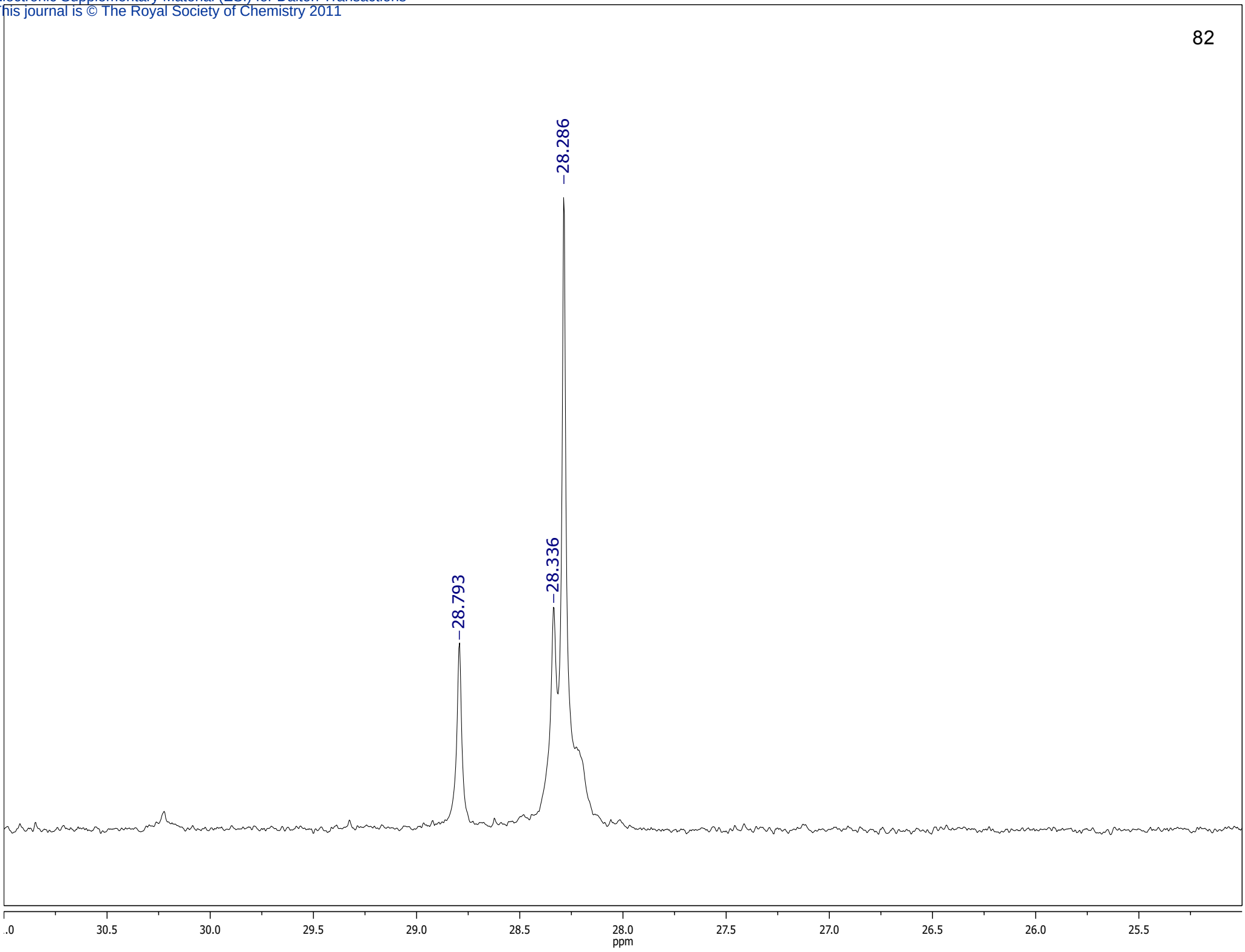
1	Data File Name	RF-CB-TE1A1P_protected_PhMe_13C_2011-02-17/ CARBON
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	5000
5	Receiver Gain	40
6	Acquisition Time	1.0000
7	Acquisition Date	2011-02-17T11:00:46
8	Spectrometer Frequency	125.68005
9	Spectral Width	31446.5
10	Lowest Frequency	-3735.5
11	Nucleus	13C
12	Acquired Size	31447
13	Spectral Size	65536

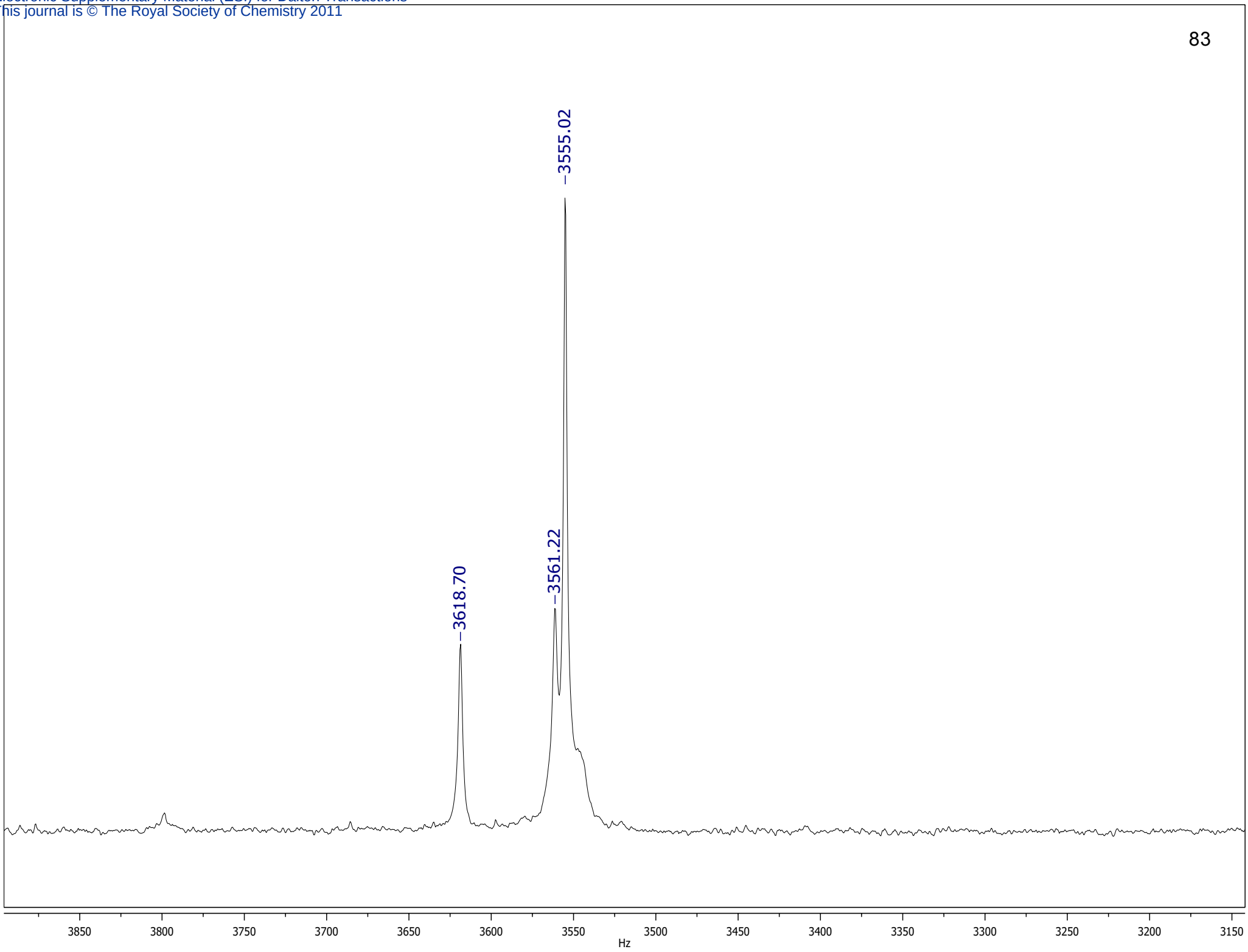


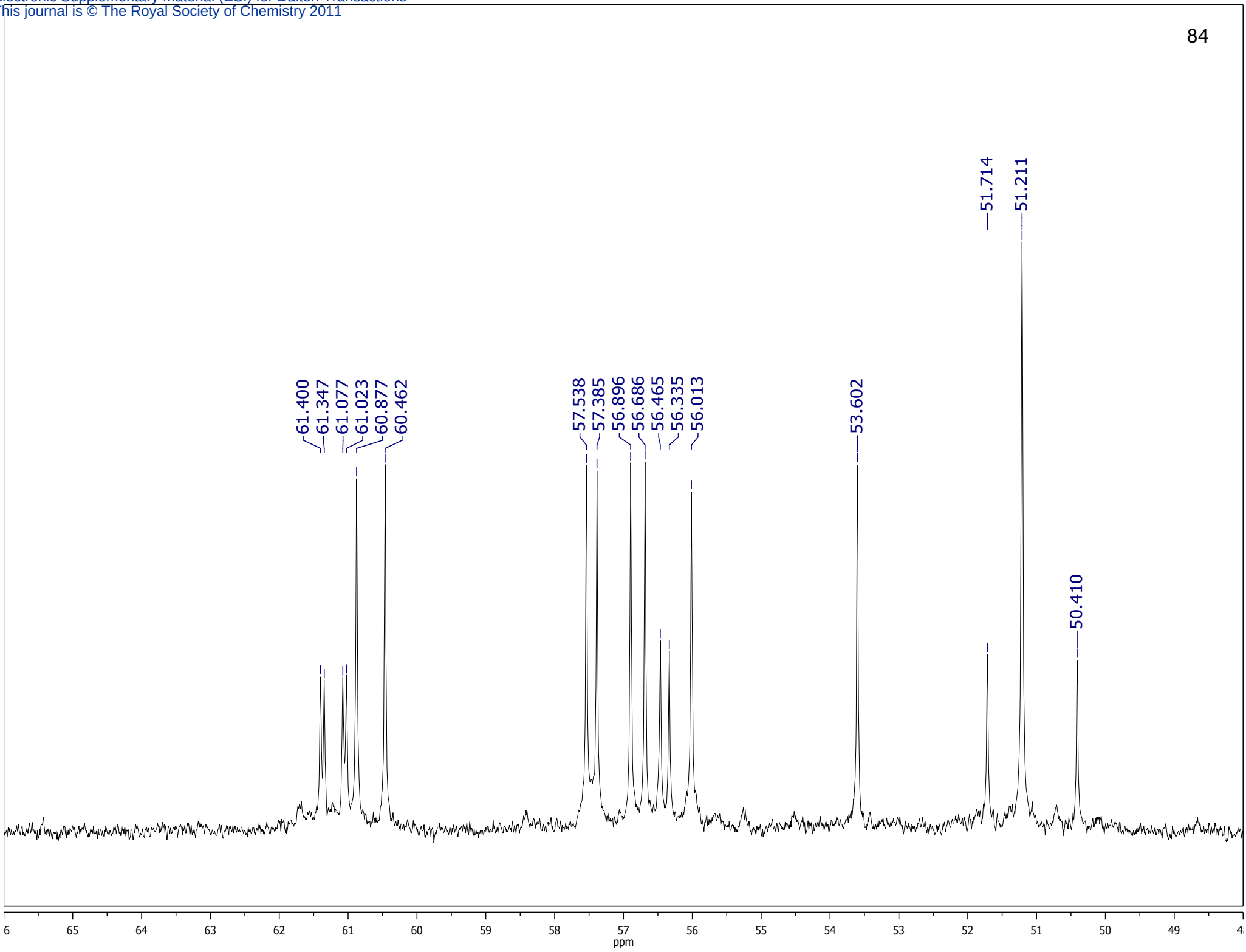
RF-CB-TE1A1P_protected_PhMe extracts
^{13}C NMR, 125.68 MHz, C_6D_6 with reference peak
set at δ 128.06 (central peak)

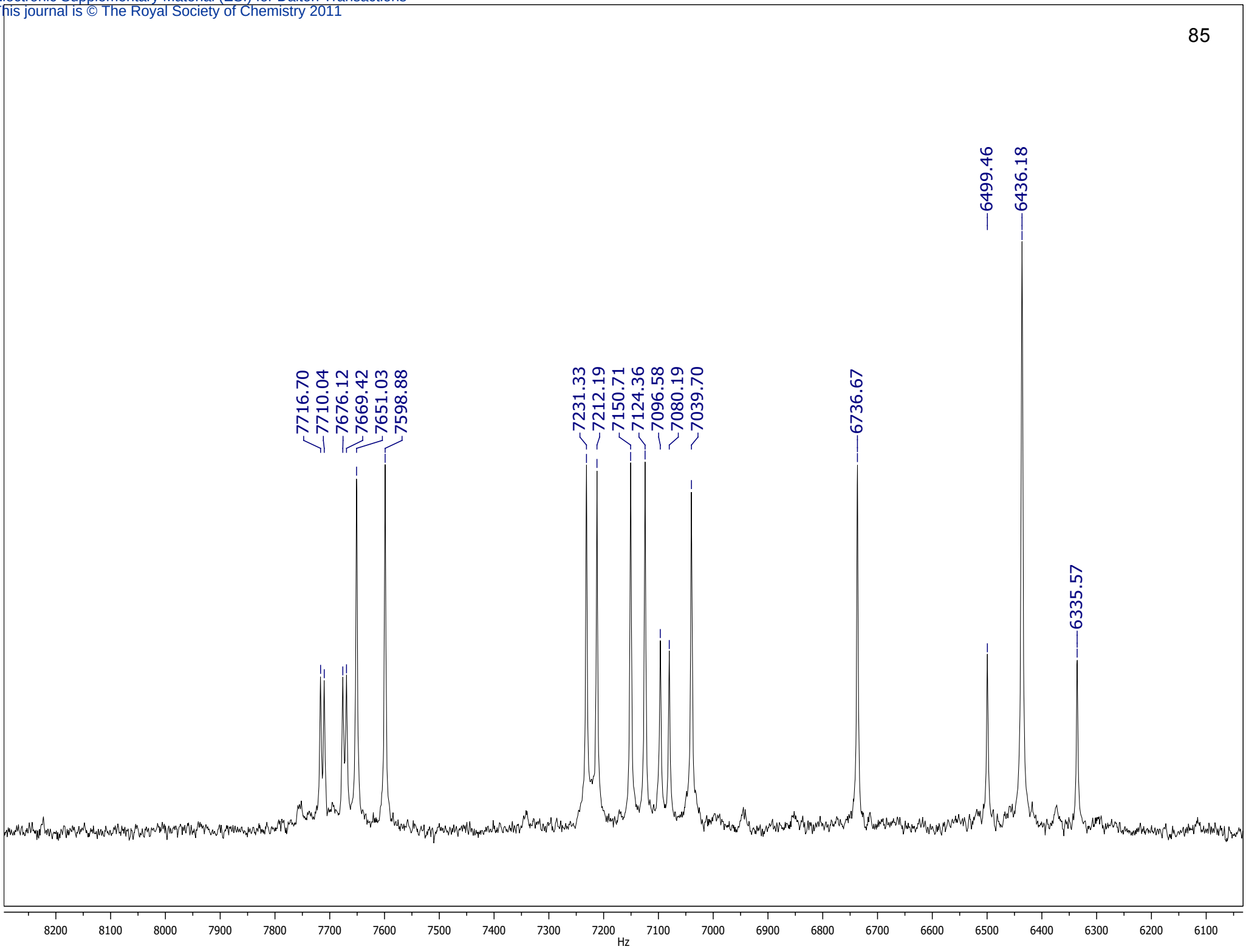


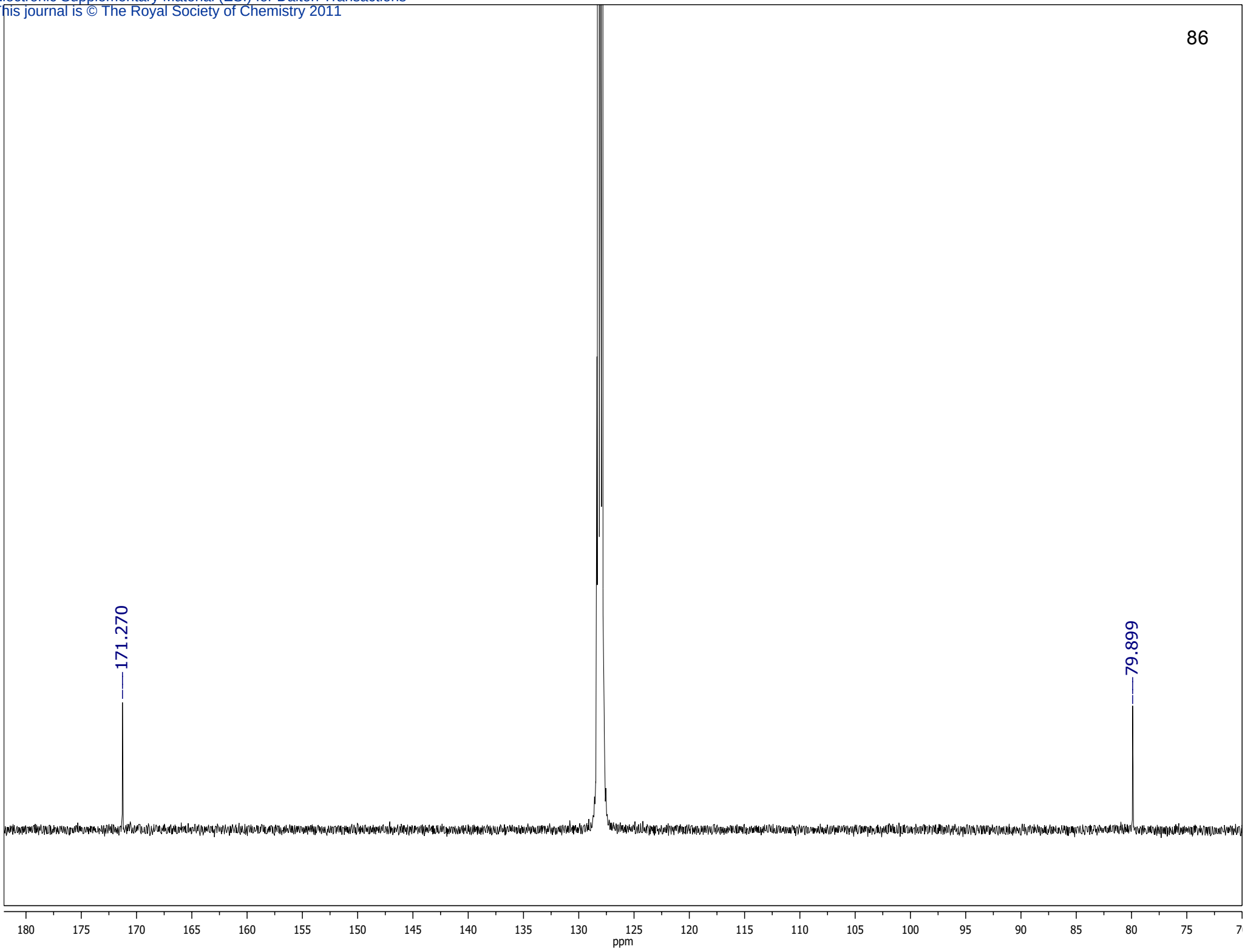




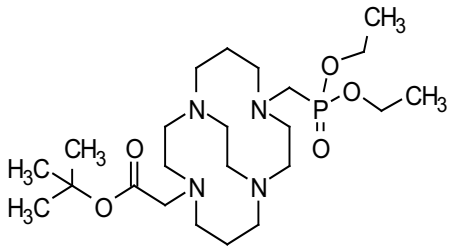






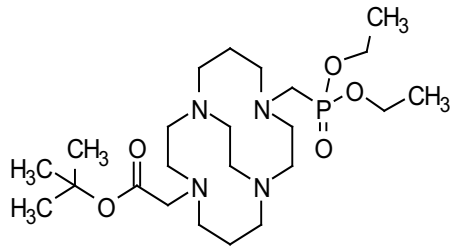


1	Data File Name	RF-CB-TE1A1P_protected_PhMe_13C_2011-02-17/ CARBON
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	5000
5	Receiver Gain	40
6	Acquisition Time	1.0000
7	Acquisition Date	2011-02-17T11:00:46
8	Spectrometer Frequency	125.68005
9	Spectral Width	31446.5
10	Lowest Frequency	-3735.5
11	Nucleus	13C
12	Acquired Size	31447
13	Spectral Size	65536

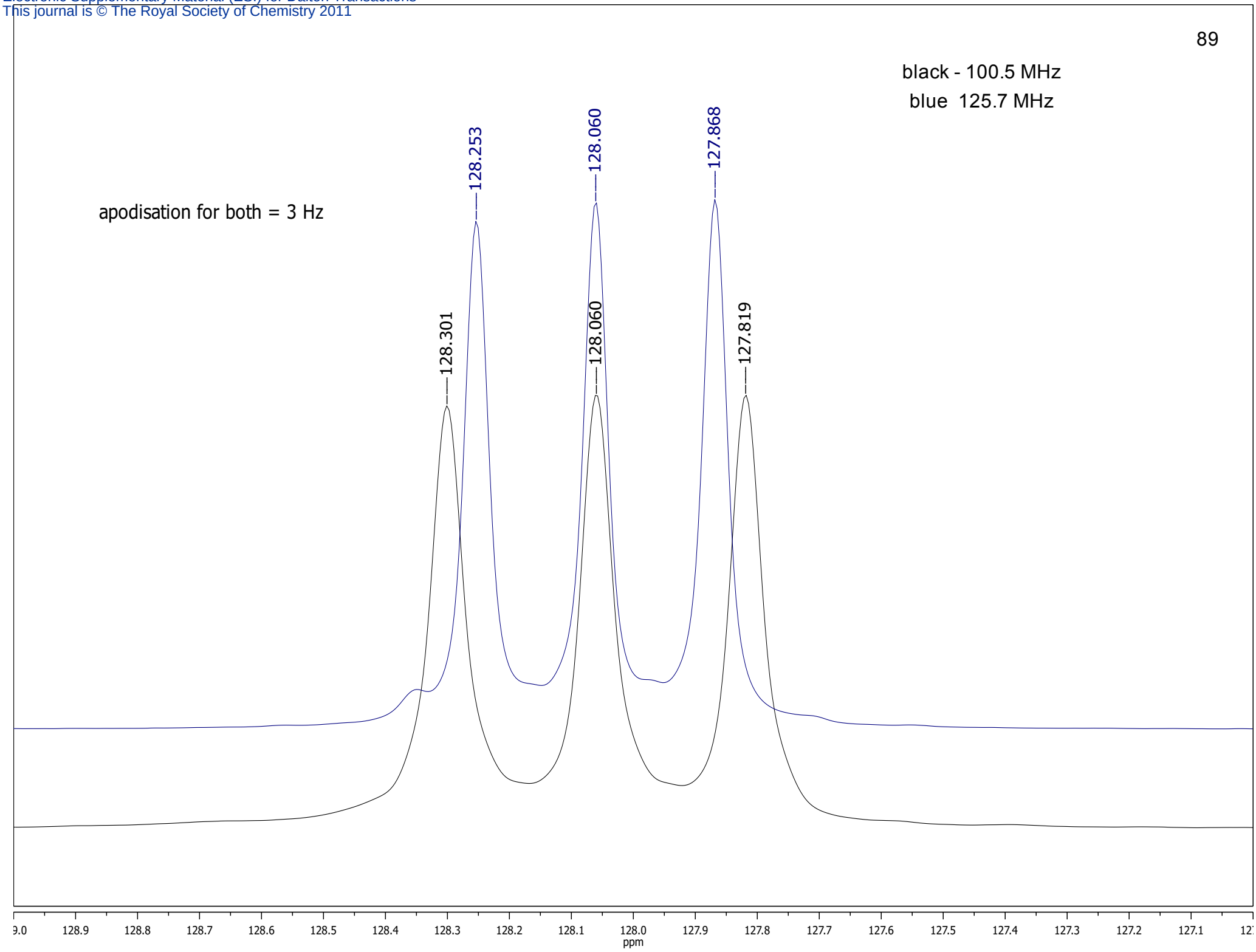


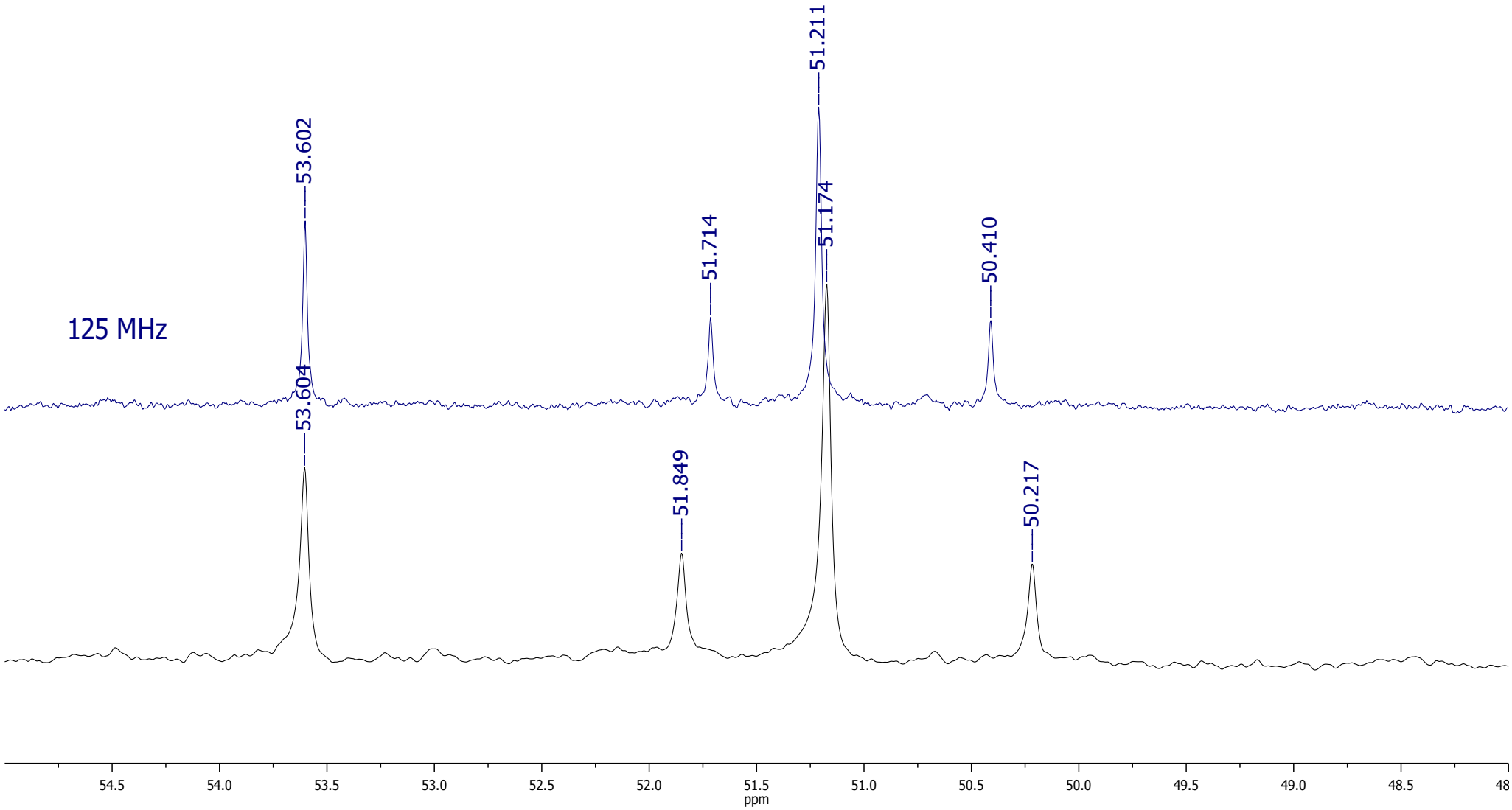
RF-CB-TE1A1P_protected_PhMe extracts
^{13}C NMR, 125.68 MHz, C_6D_6 with reference peak set at
128.06 ppm (central peak)

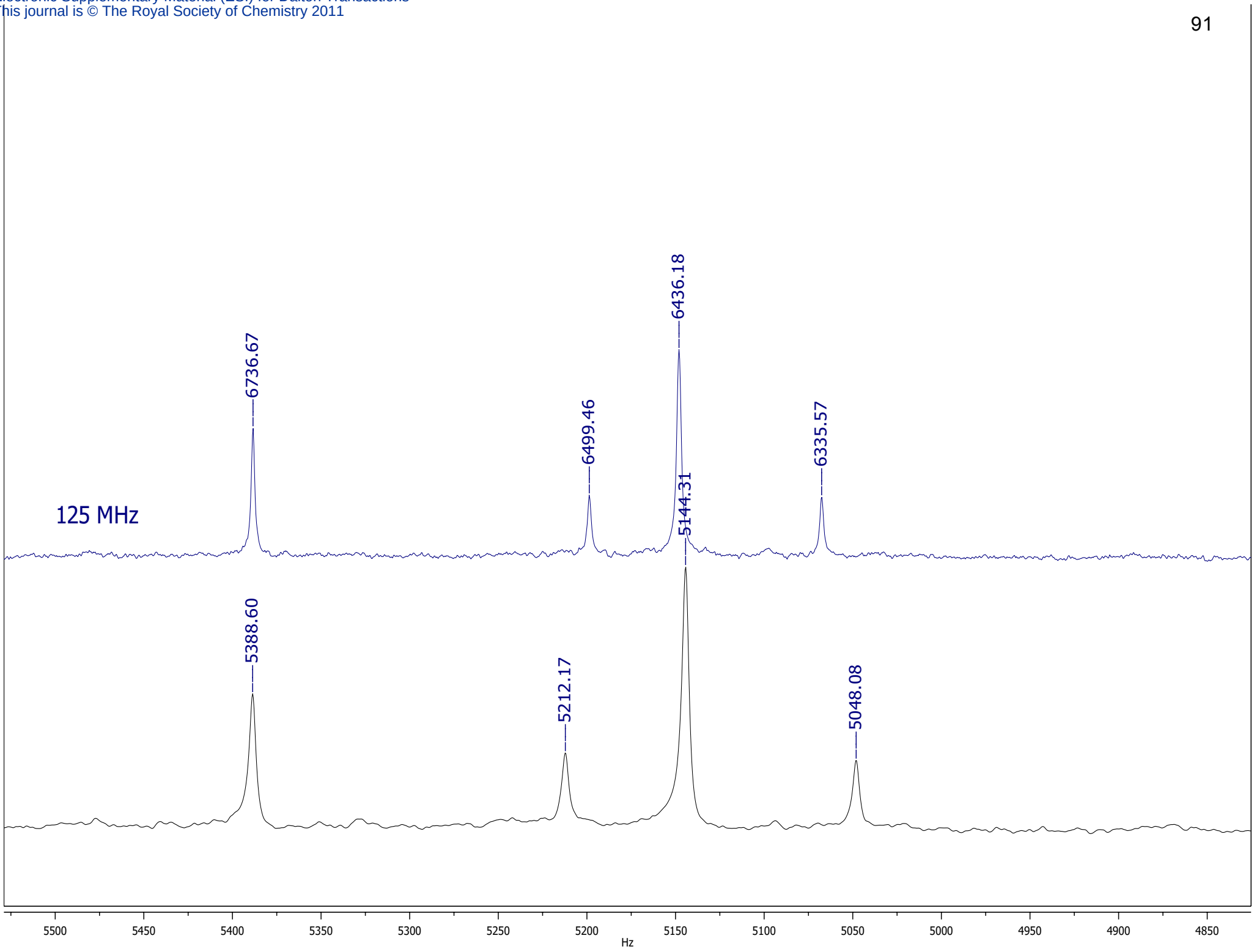
1	Data File Name	RF-CB-TE1A1P_protected_400_13C_17Feb2011/ CARBON.fid
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	5000
5	Receiver Gain	24
6	Acquisition Time	1.0025
7	Acquisition Date	1969-11-13T03:20:24
8	Spectrometer Frequency	100.52631
9	Spectral Width	25062.7
10	Lowest Frequency	-1402.7
11	Nucleus	13C
12	Acquired Size	25126
13	Spectral Size	65536

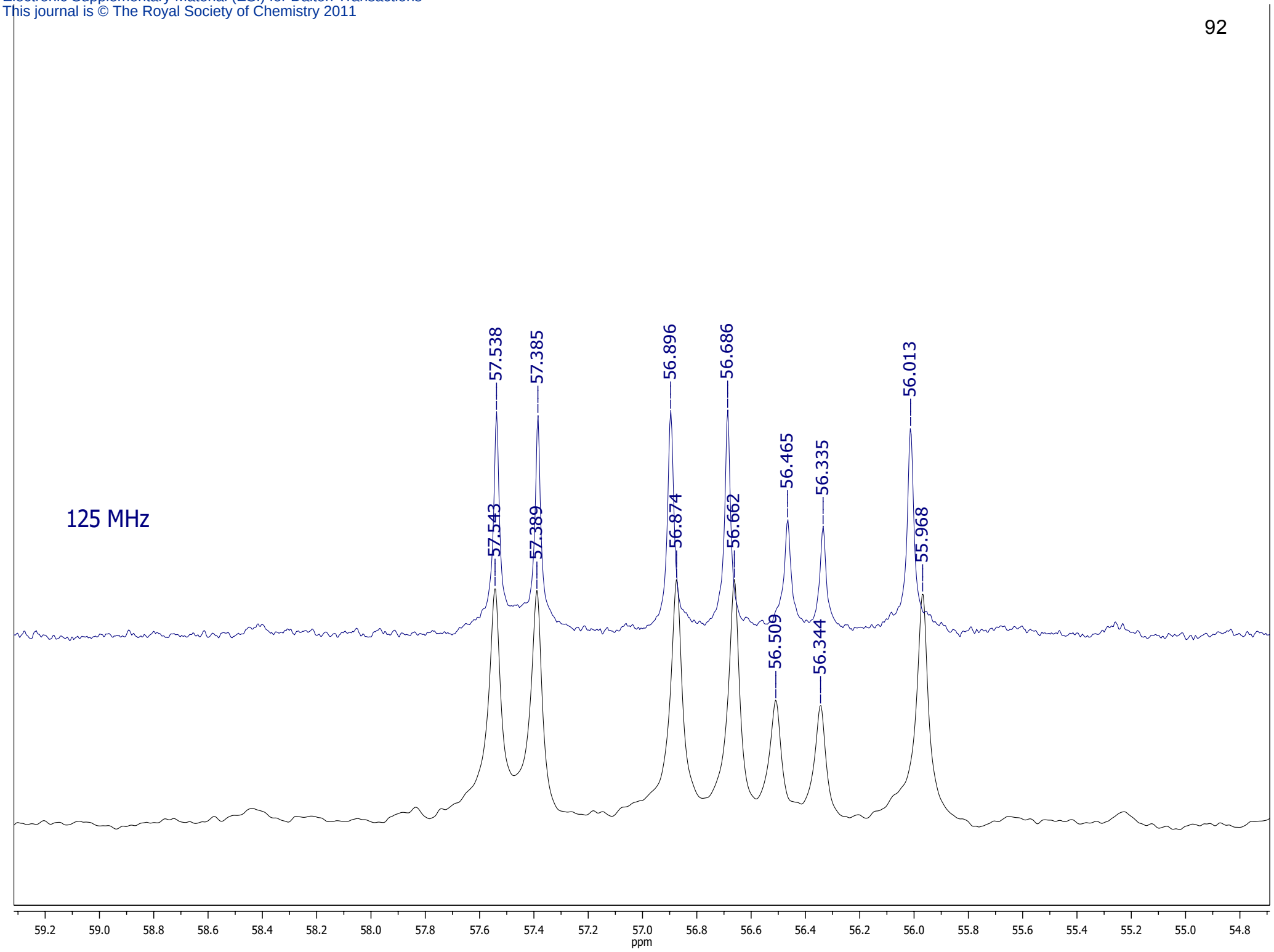


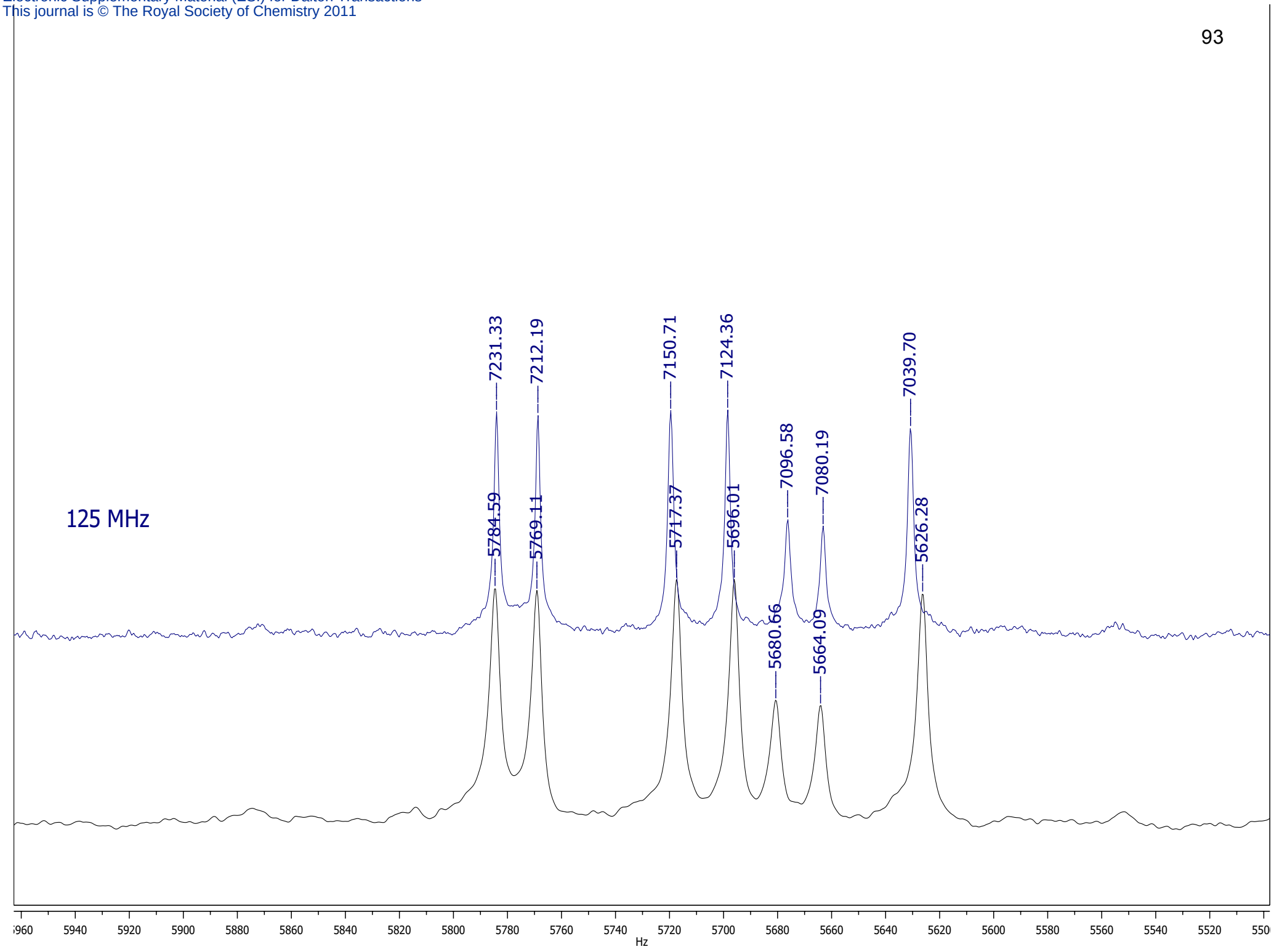
RF-CB-TE1A1P_protected_PhMe extracts
^{13}C NMR, 100.52 MHz, C_6D_6 with reference peak set at 128.06 ppm (central peak)

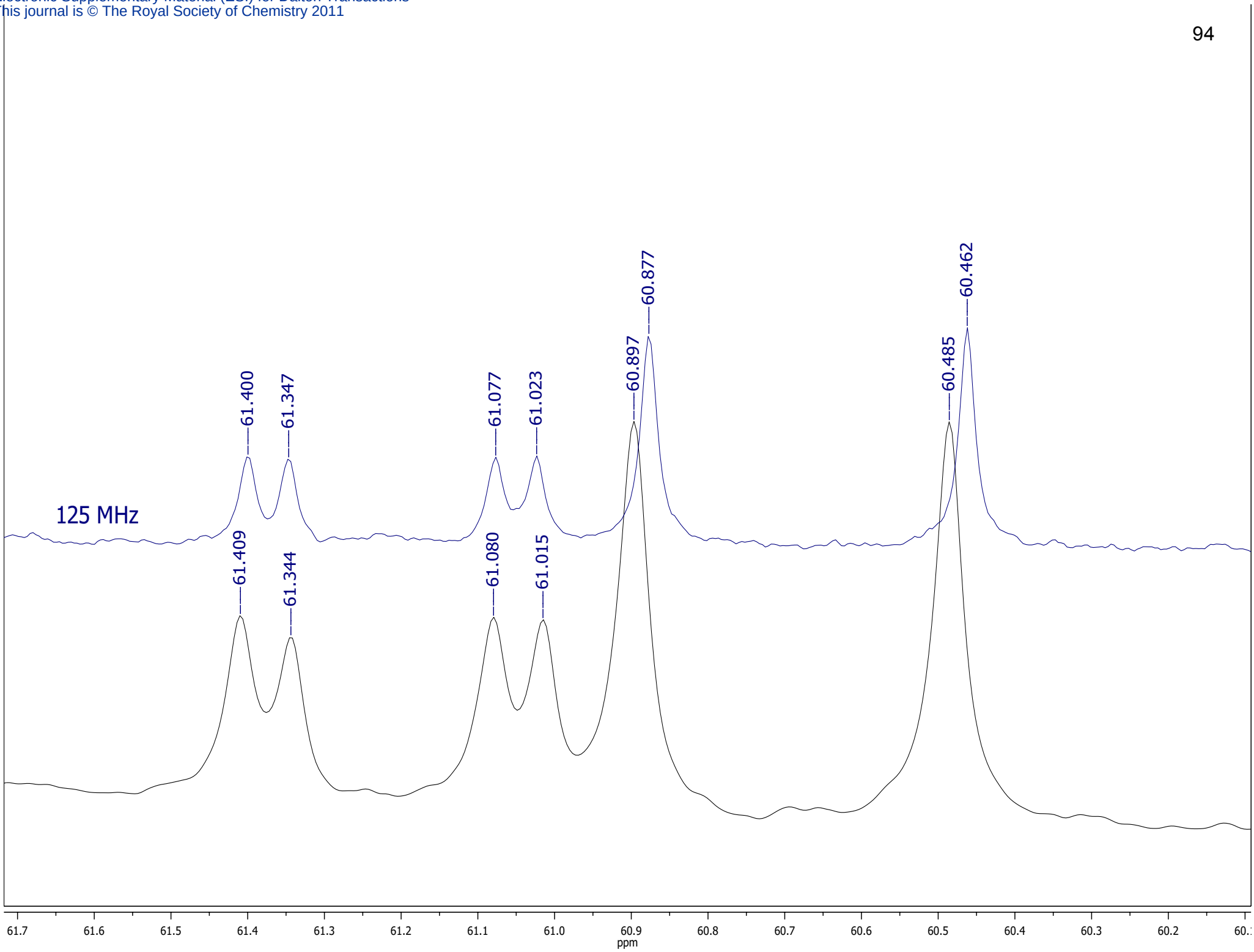


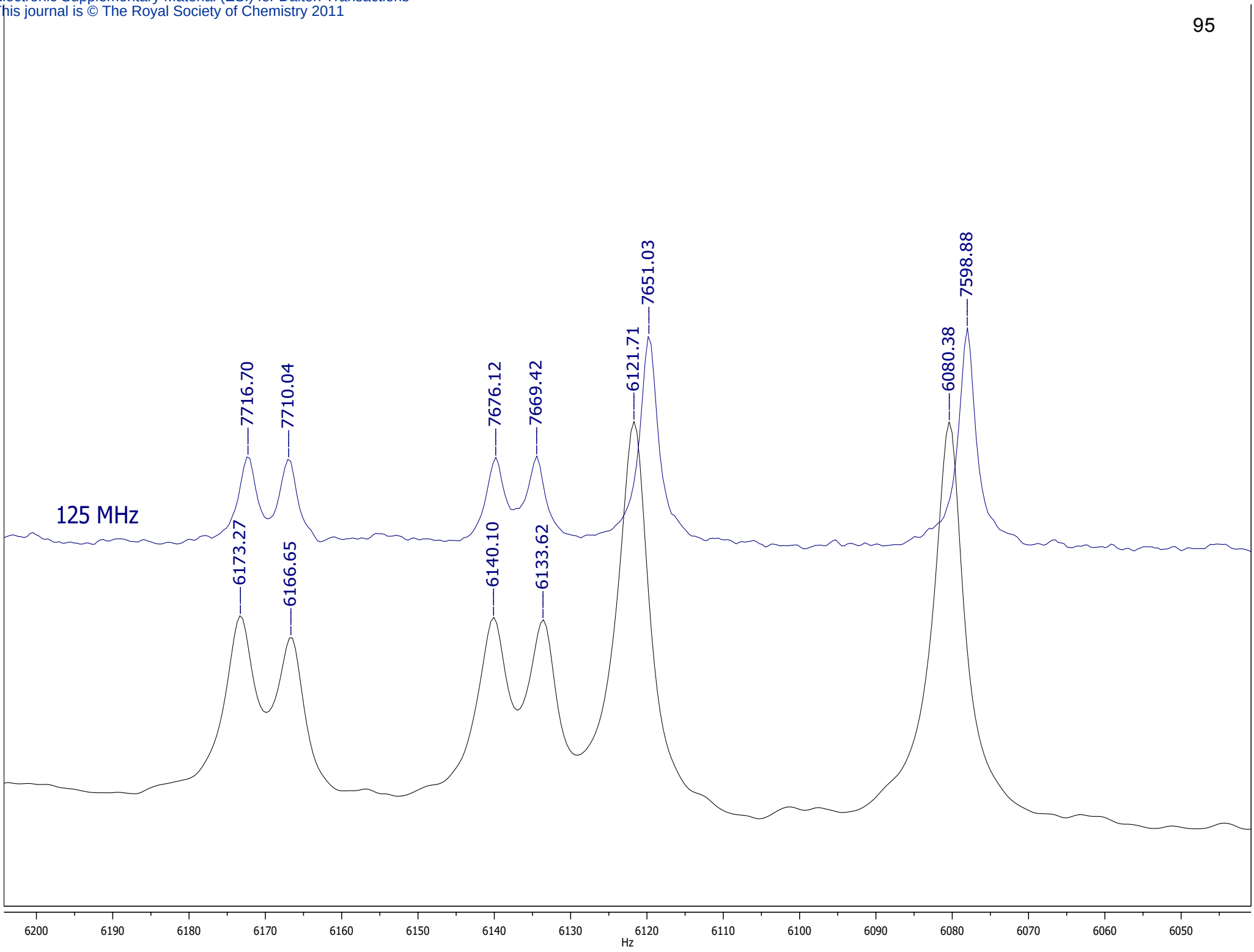




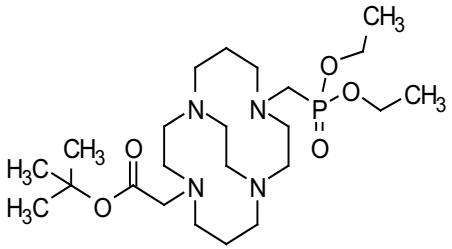






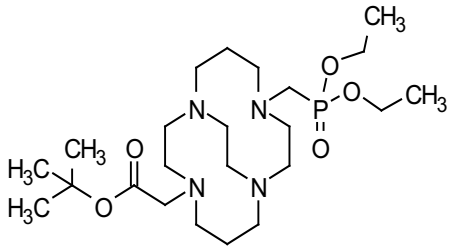


1	Data File Name	RF-CB-TE1A1P_protected_PhMe extracts_C6D6-PROTON
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	16
5	Receiver Gain	24
6	Acquisition Time	3.0000
7	Acquisition Date	2011-02-18T16:17:15
8	Spectrometer Frequency	499.77585
9	Spectral Width	7992.0
10	Lowest Frequency	-1496.1
11	Nucleus	1H
12	Acquired Size	23976
13	Spectral Size	65536

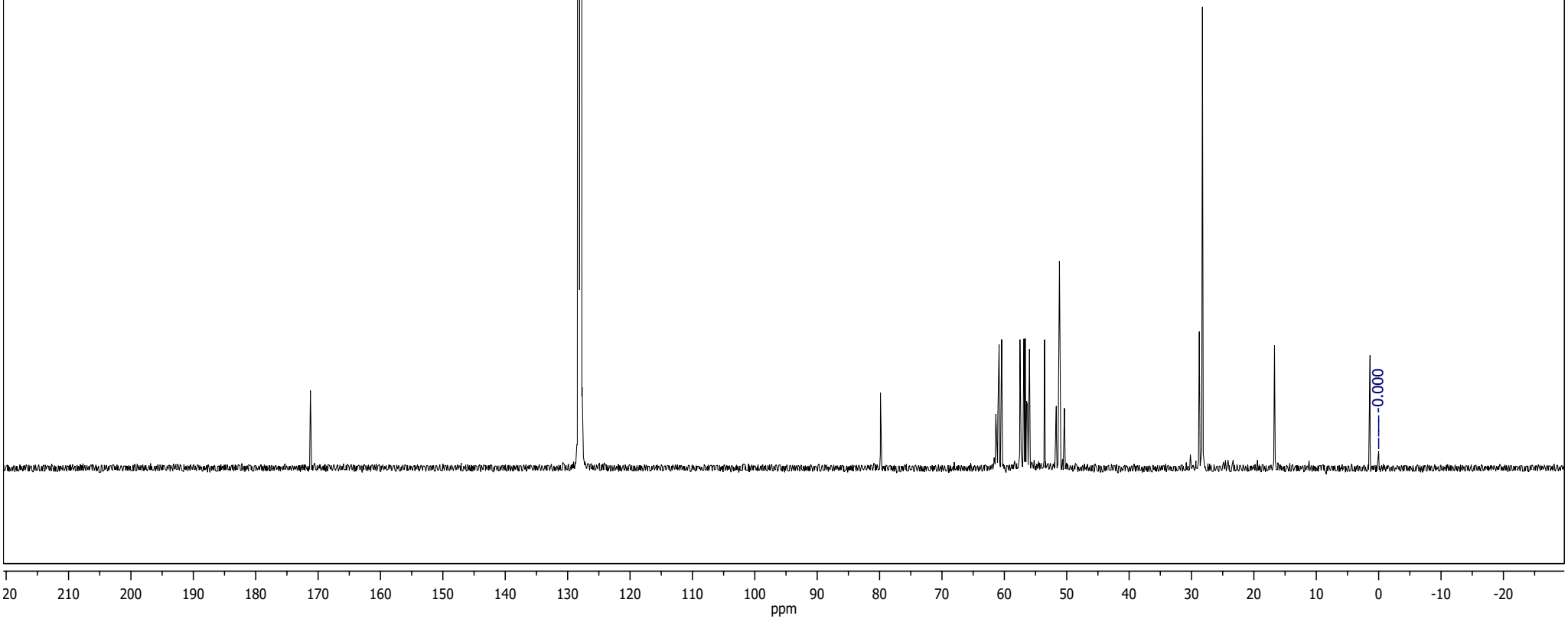


C_6D_6, 499.78 MHz, internal reference set to TMS at δ 0.00

1	Data File Name	RF-CB-TE1A1P_protected_PhMe extracts_13C
2	Origin	Varian
3	Solvent	C6D6
4	Number of Scans	5000
5	Receiver Gain	40
6	Acquisition Time	1.0000
7	Acquisition Date	2011-02-17T11:00:46
8	Spectrometer Frequency	125.68005
9	Spectral Width	31446.5
10	Lowest Frequency	-3735.5
11	Nucleus	13C
12	Acquired Size	31447
13	Spectral Size	65536



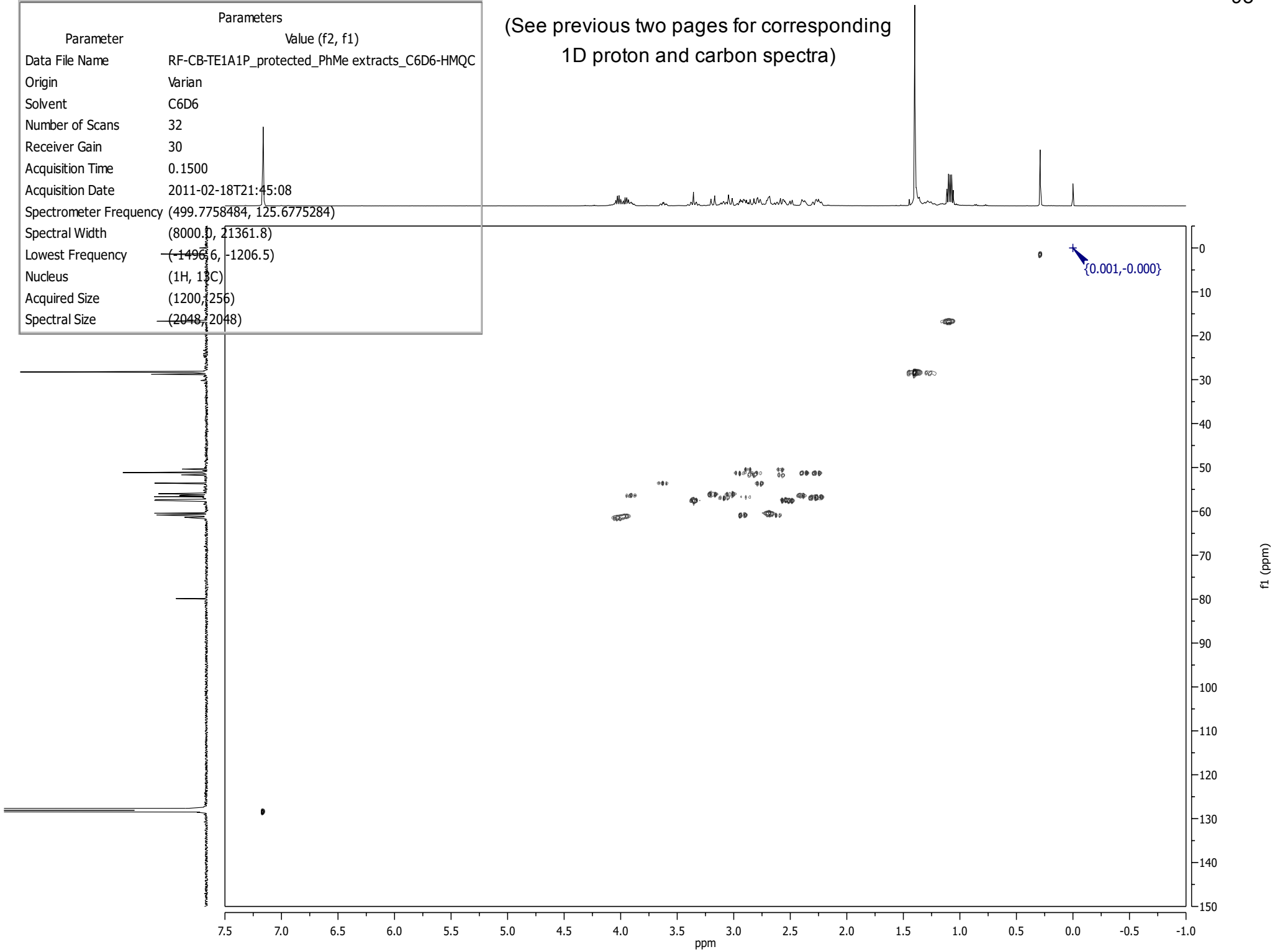
C_6D_6, 125.68 MHz, internal reference set to TMS at δ 0.00

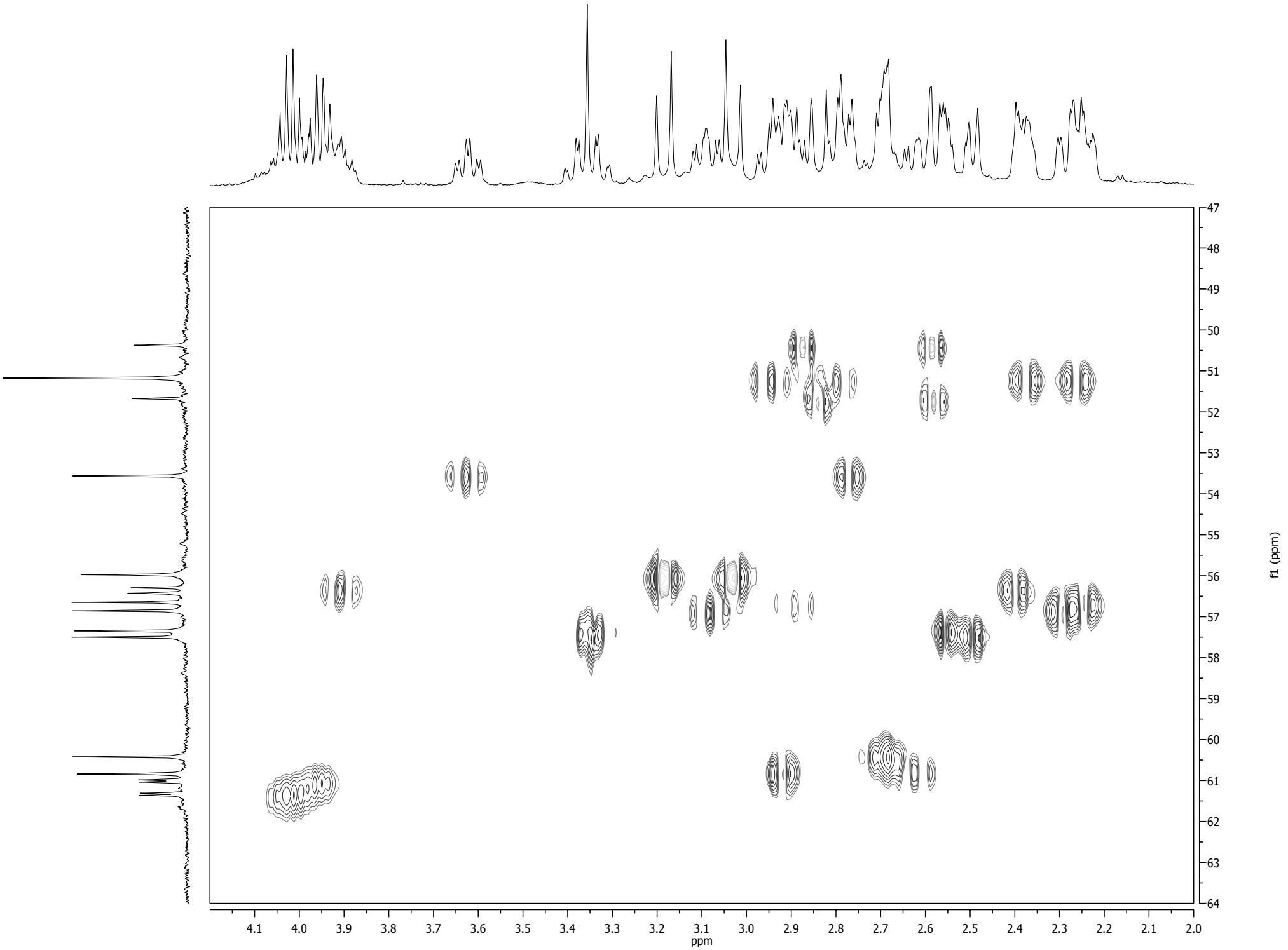


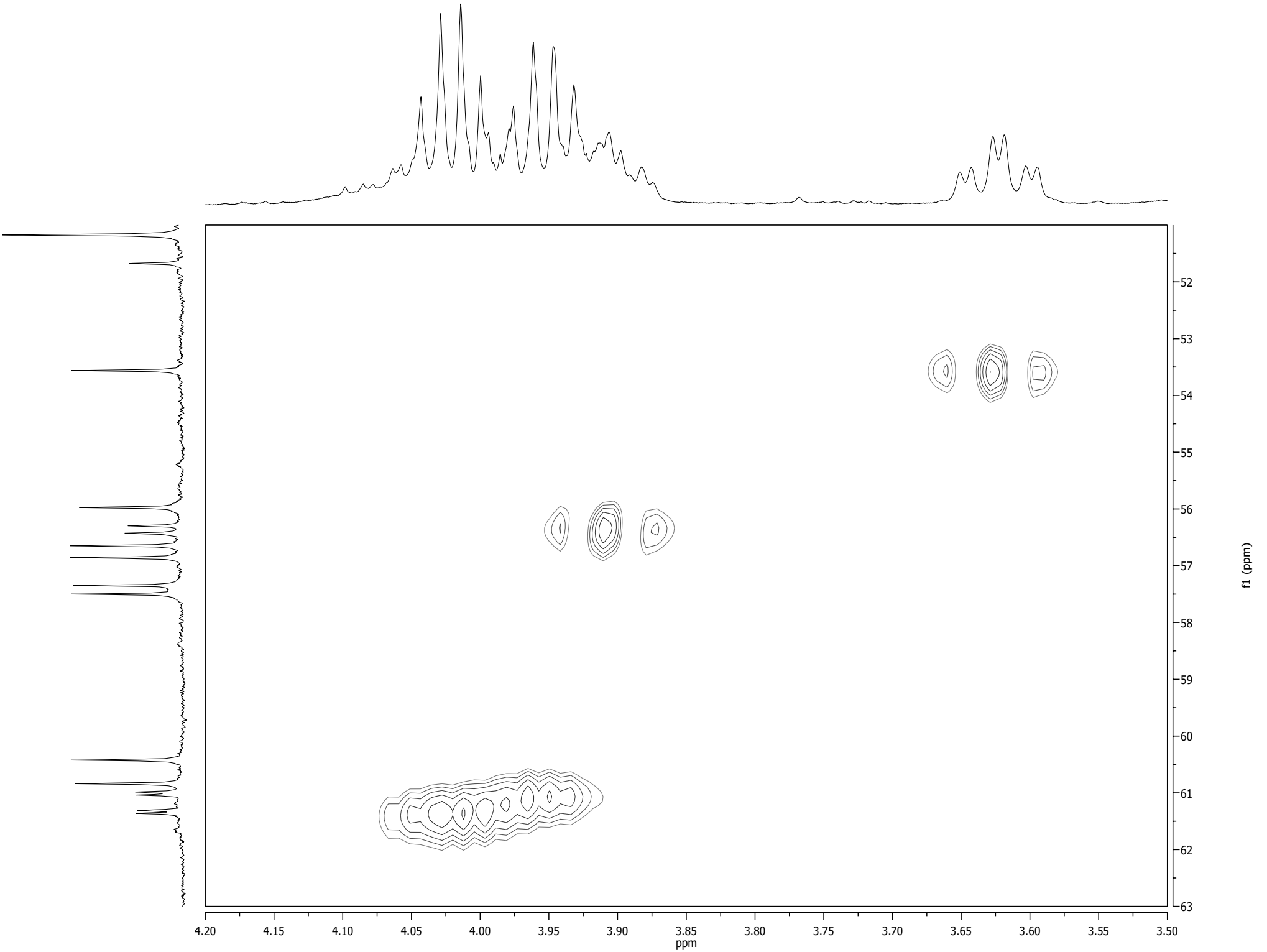
Parameters

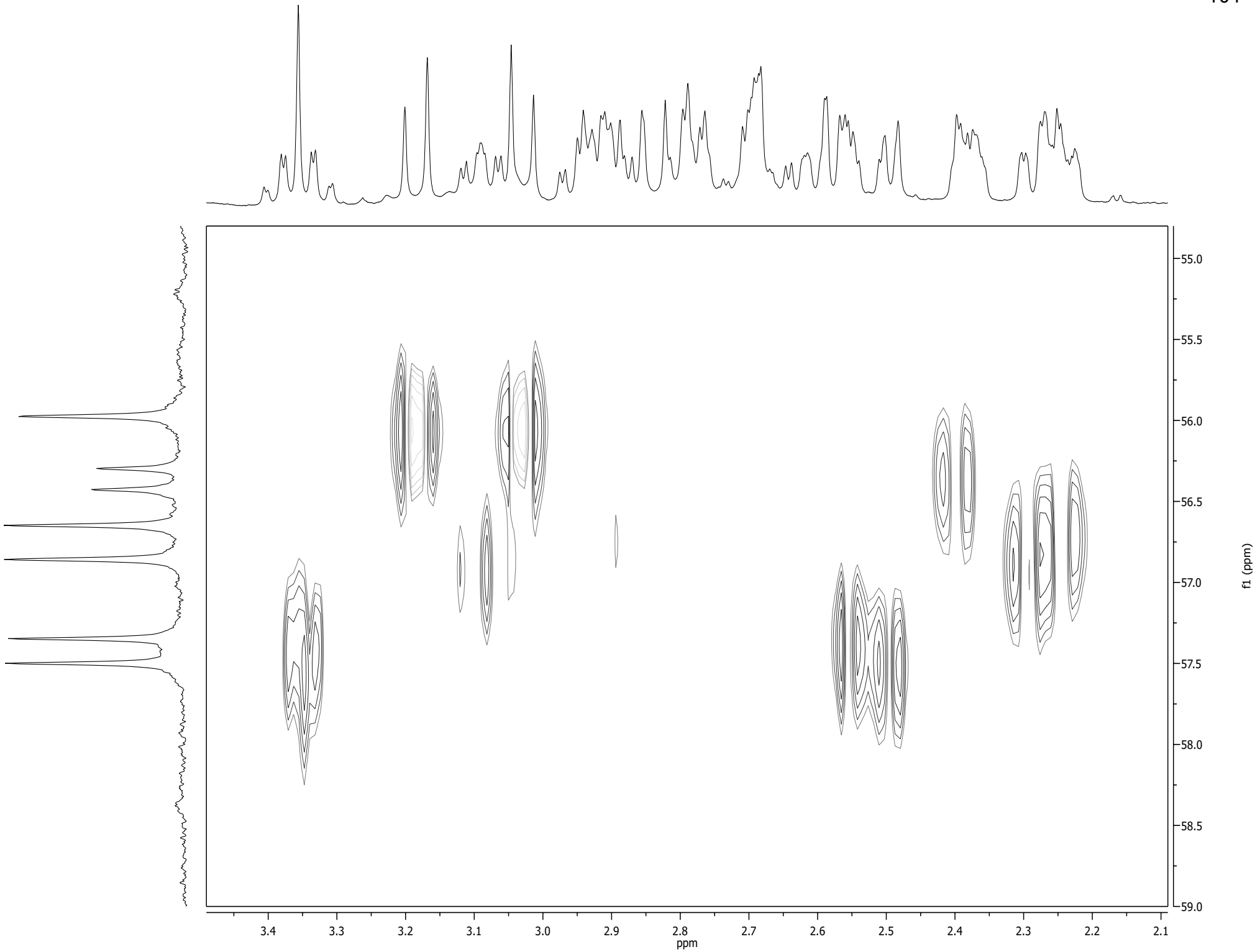
Parameter	Value (f2, f1)
Data File Name	RF-CB-TE1A1P_protected_PhMe extracts_C6D6-HMQC
Origin	Varian
Solvent	C6D6
Number of Scans	32
Receiver Gain	30
Acquisition Time	0.1500
Acquisition Date	2011-02-18T21:45:08
Spectrometer Frequency	(499.7758484, 125.6775284)
Spectral Width	(8000.0, 21361.8)
Lowest Frequency	(-1496.6, -1206.5)
Nucleus	(1H, 13C)
Acquired Size	(1200, 256)
Spectral Size	(2048, 2048)

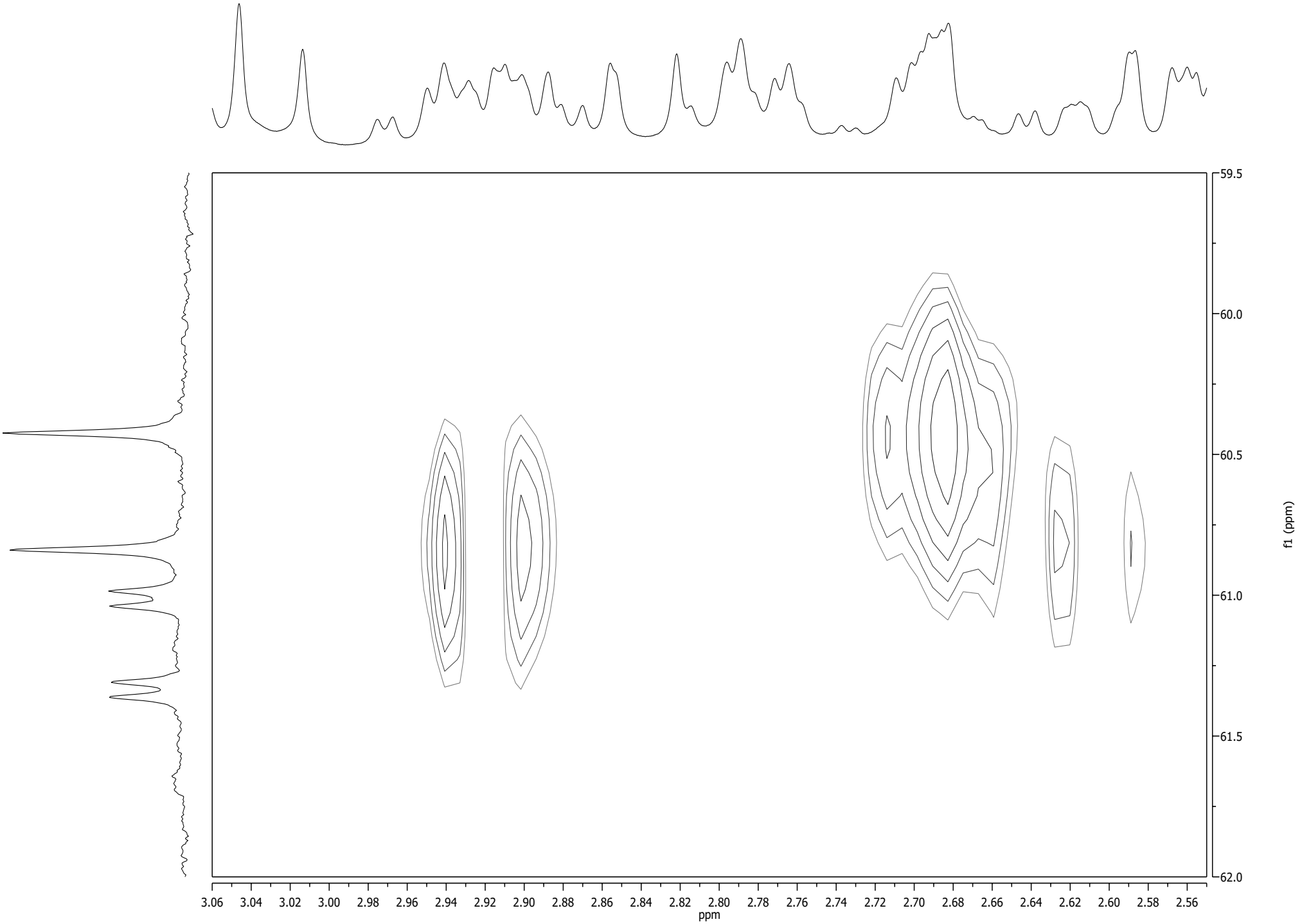
(See previous two pages for corresponding 1D proton and carbon spectra)

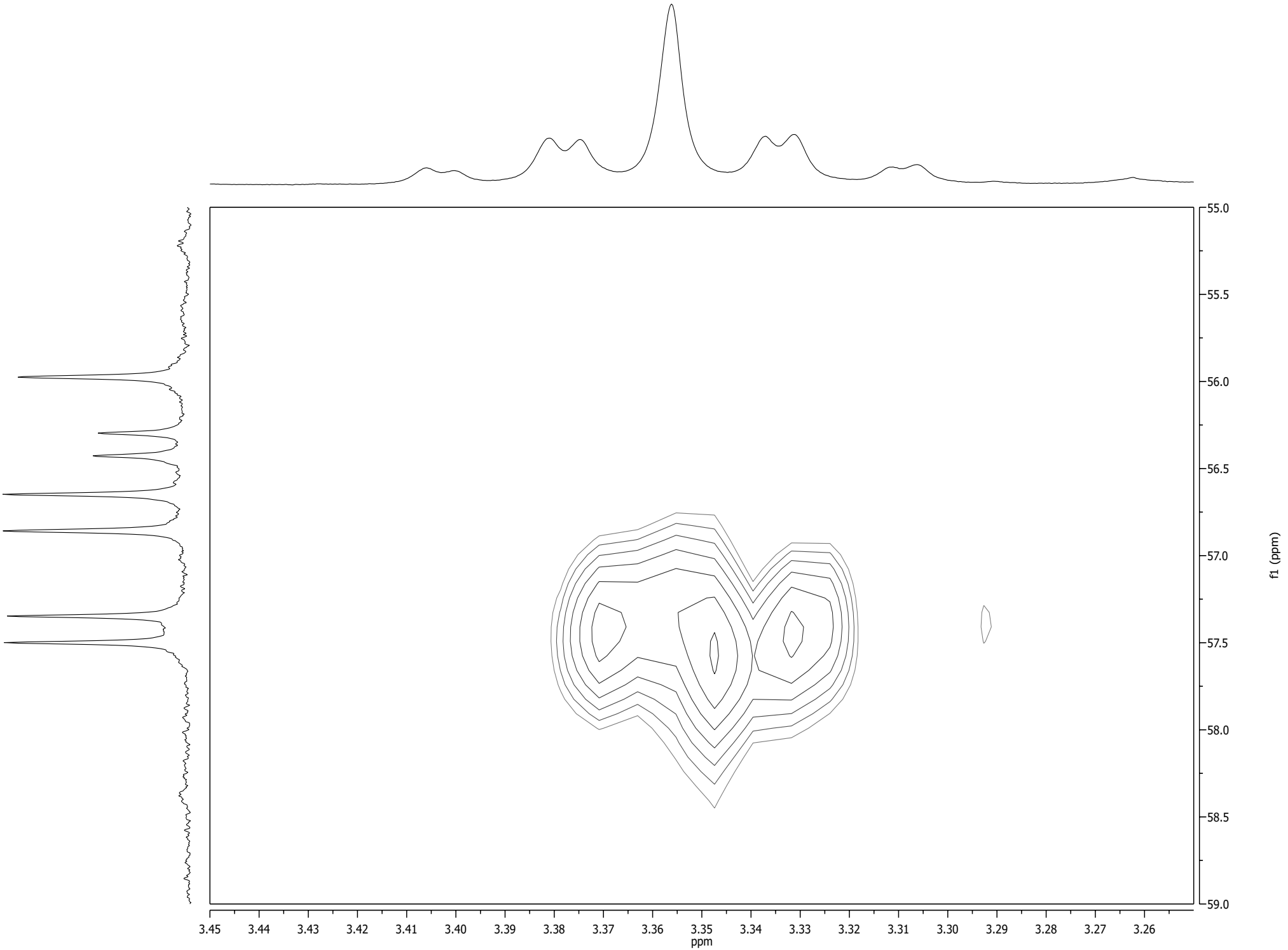


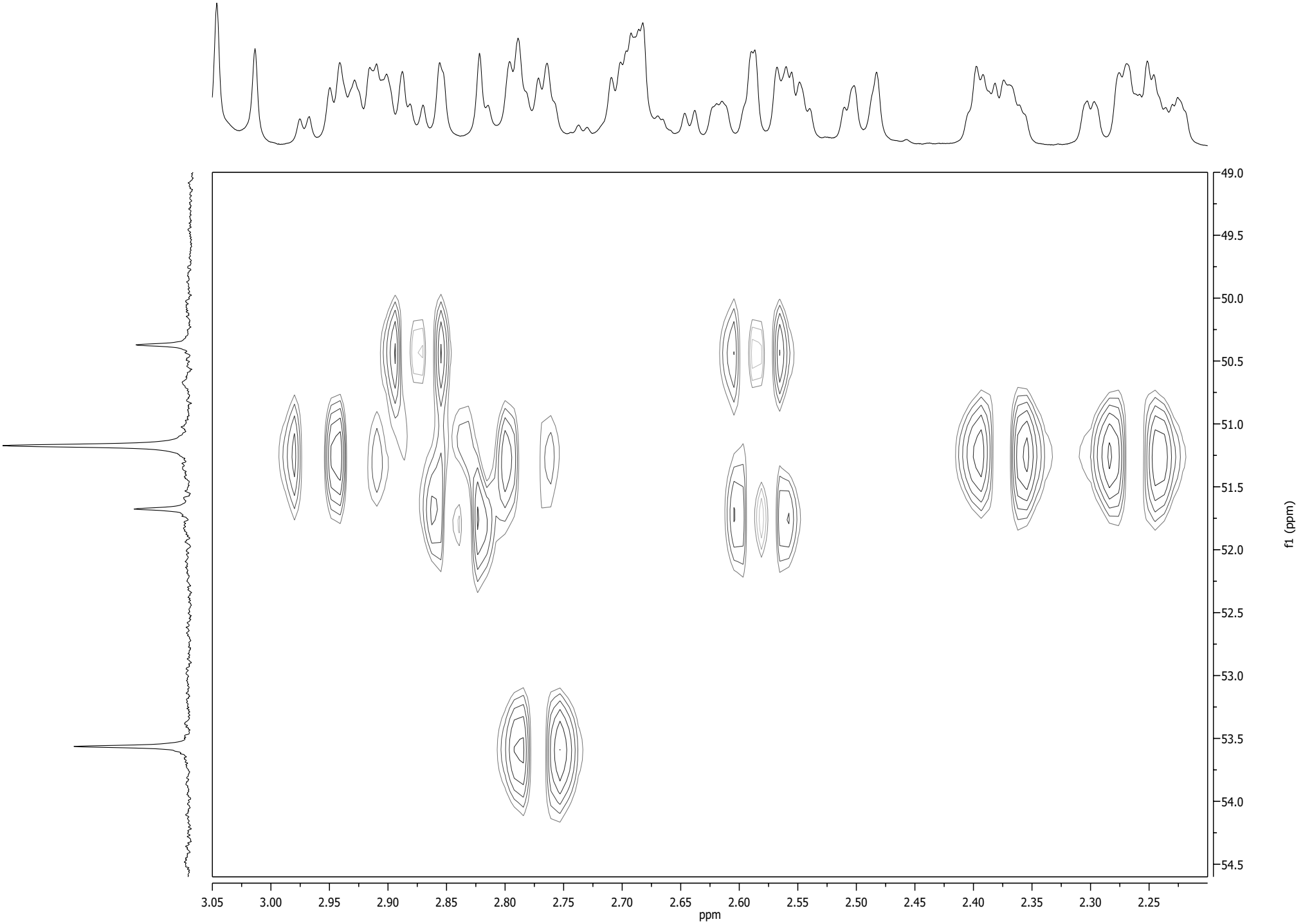

4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
ppm
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
f1 (ppm)

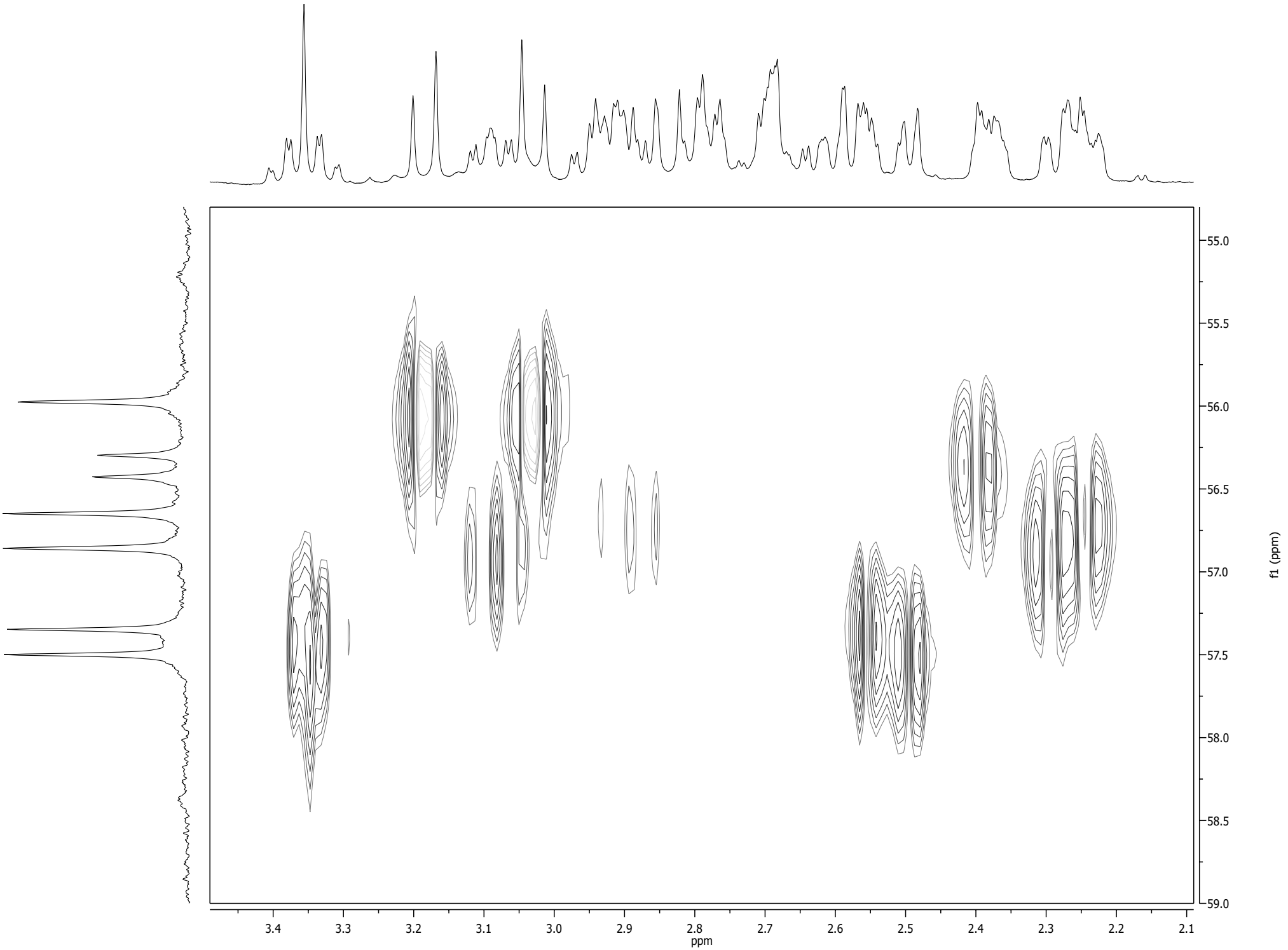

4.20
4.15
4.10
4.05
4.00
3.95
3.90
3.85
3.80
3.75
3.70
3.65
3.60
3.55
3.50
ppm
52
53
54
55
56
57
58
59
60
61
62
63
f1 (ppm)

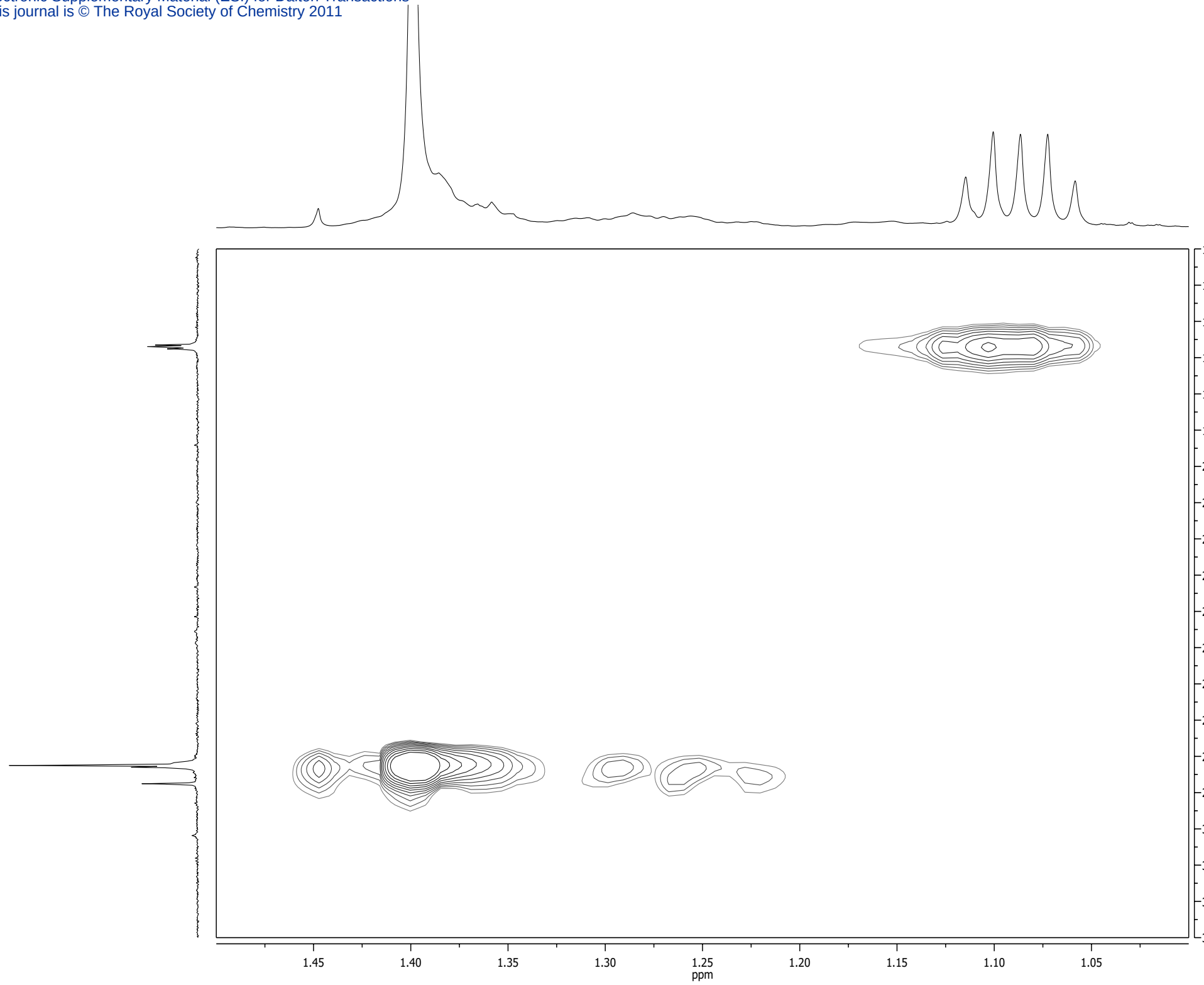

55.0
55.5
56.0
56.5
57.0
57.5
58.0
58.5
59.0
f1 (ppm)
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
ppm


59.5
60.0
60.5
61.0
61.5
62.0
f1 (ppm)
3.06
3.04
3.02
3.00
2.98
2.96
2.94
2.92
2.90
2.88
2.86
2.84
2.82
2.80
2.78
2.76
2.74
2.72
2.70
2.68
2.66
2.64
2.62
2.60
2.58
2.56
ppm

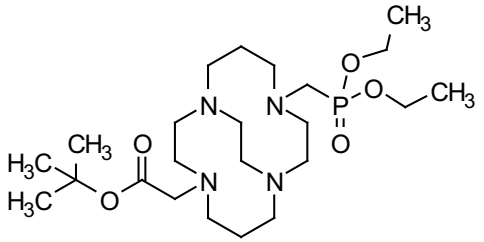



49.0
49.5
50.0
50.5
51.0
51.5
52.0
52.5
53.0
53.5
54.0
54.5
f1 (ppm)
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
ppm


55.0
55.5
56.0
56.5
57.0
57.5
58.0
58.5
59.0
f1 (ppm)
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
ppm



	Parameter	Value
1	Title	RF-CB-TE1A1P_protected-31P
2	Solvent	C6D6
3	Temperature	25.0
4	Number of Scans	32
5	Spectrometer Frequency	202.31
6	Spectral Width	50600.9
7	Lowest Frequency	-30527.2
8	Nucleus	31P
9	Acquired Size	80961
10	Spectral Size	262144



RF-CB-TE1A1P_protected_PhMe extracts
^{31}P NMR, 202.31 MHz, C_6D_6, external reference with
85% phosphoric acid set to δ 0.00