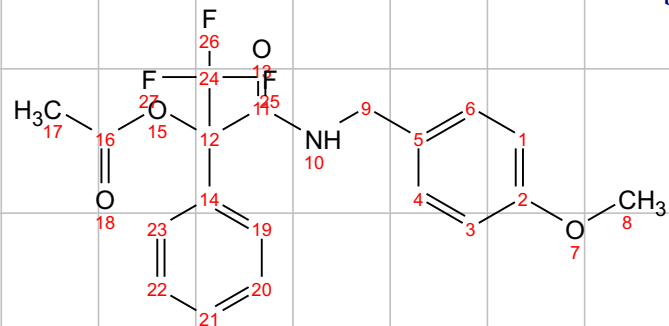
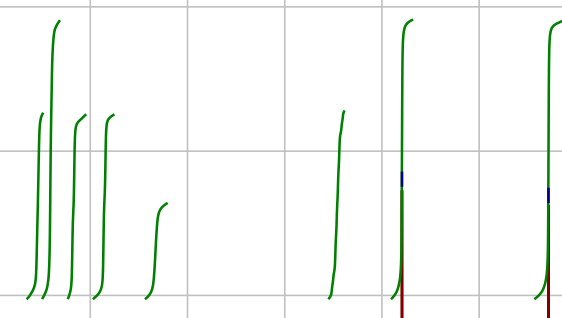


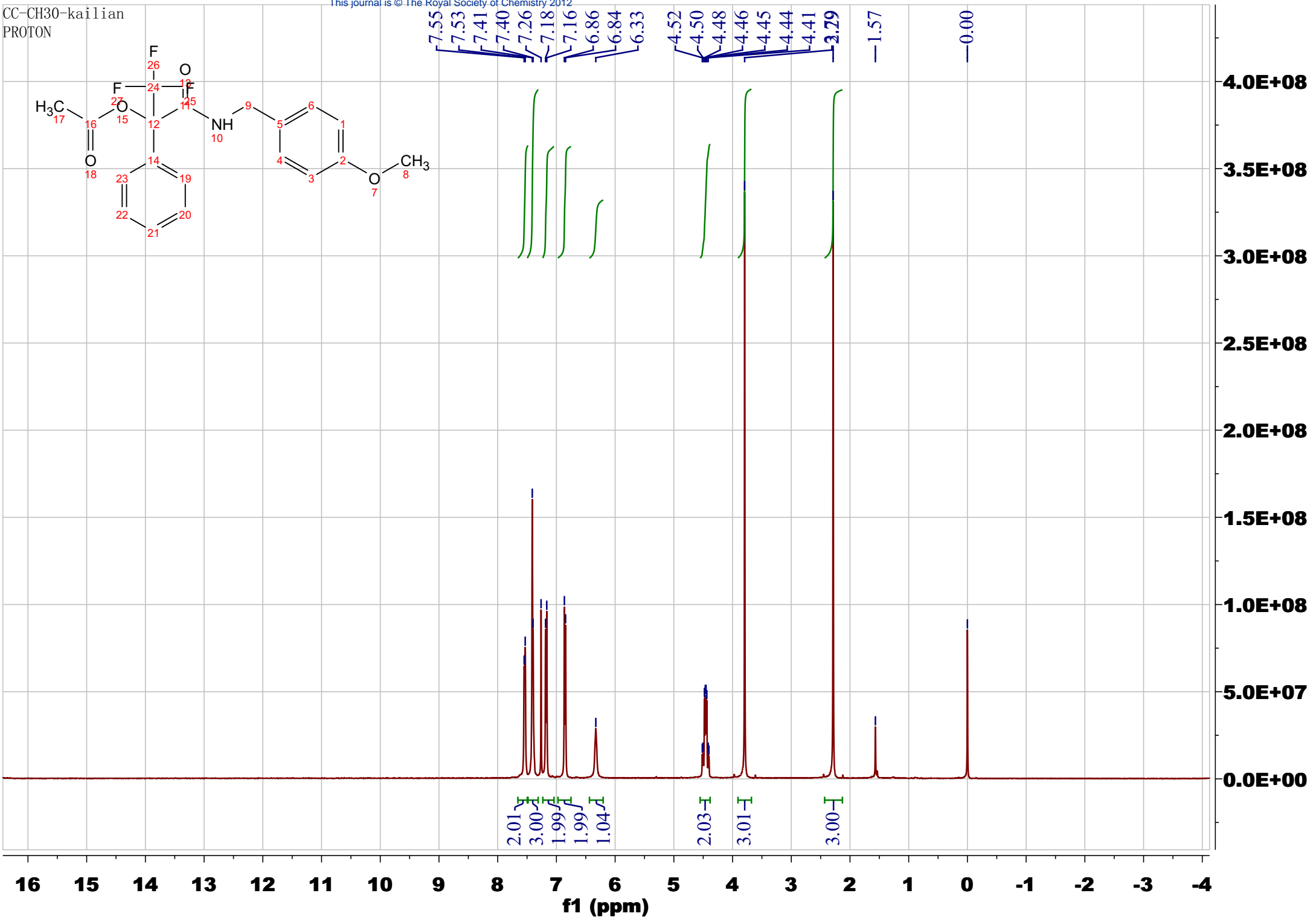
CC-CH30-kailian
PROTON



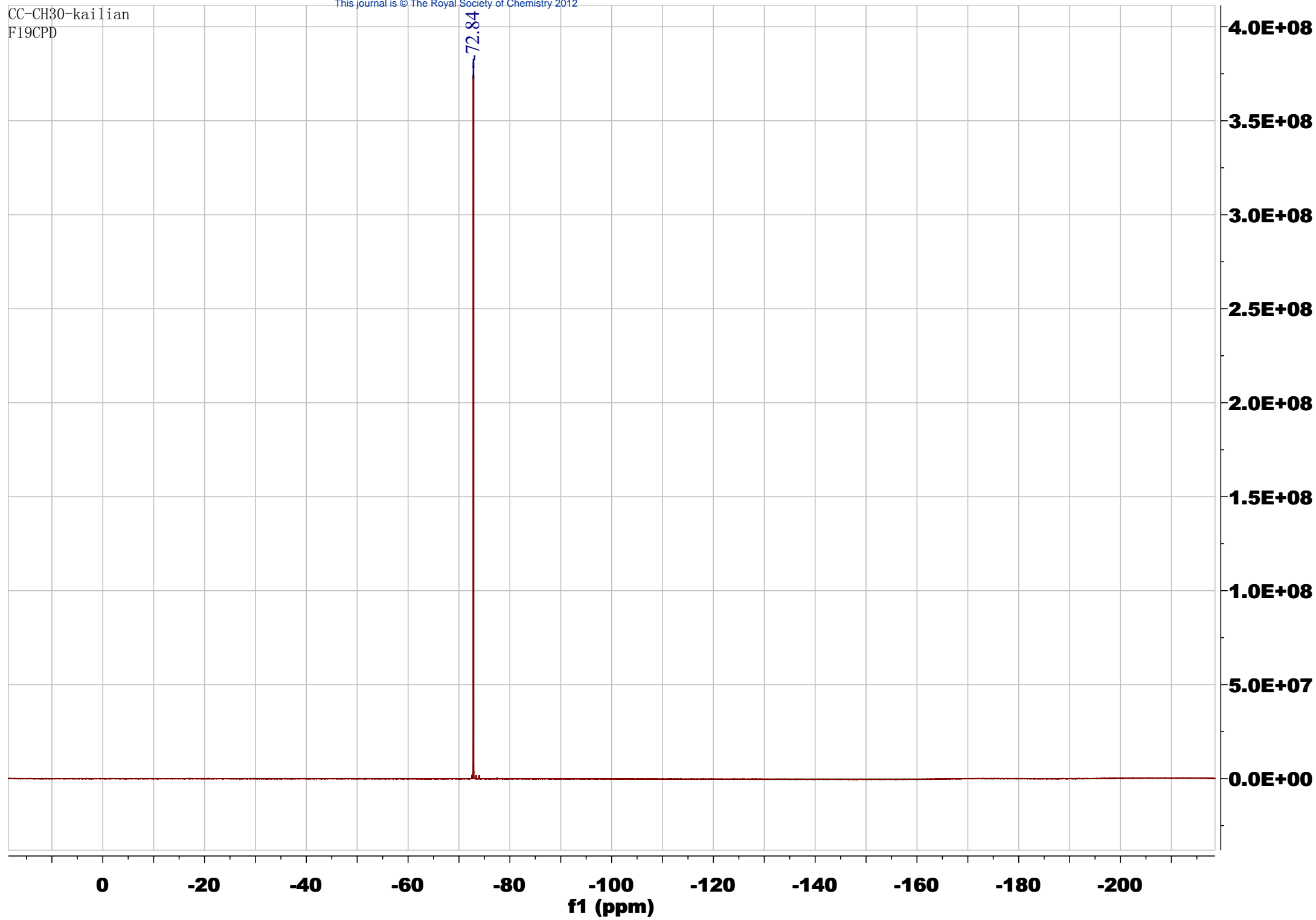
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7.40
7.26
7.18
7.16
6.86
6.84
6.33
4.52
4.50
4.48
4.46
4.45
4.44
4.41
3.79
1.57
0.00



2.01
3.00
1.99
1.99
1.04
2.03
3.01
3.00

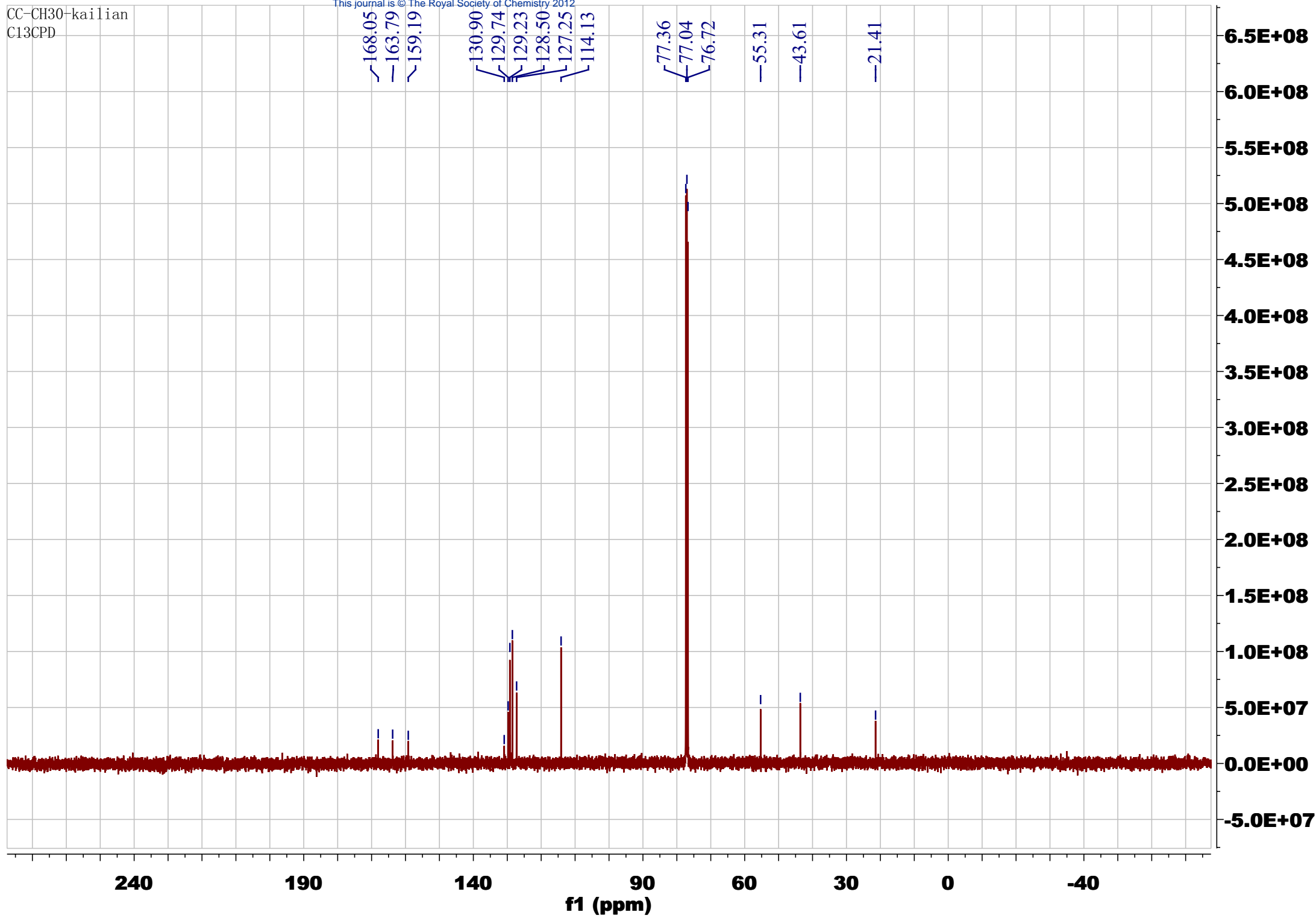


CC-CH30-kailian
F19CPD



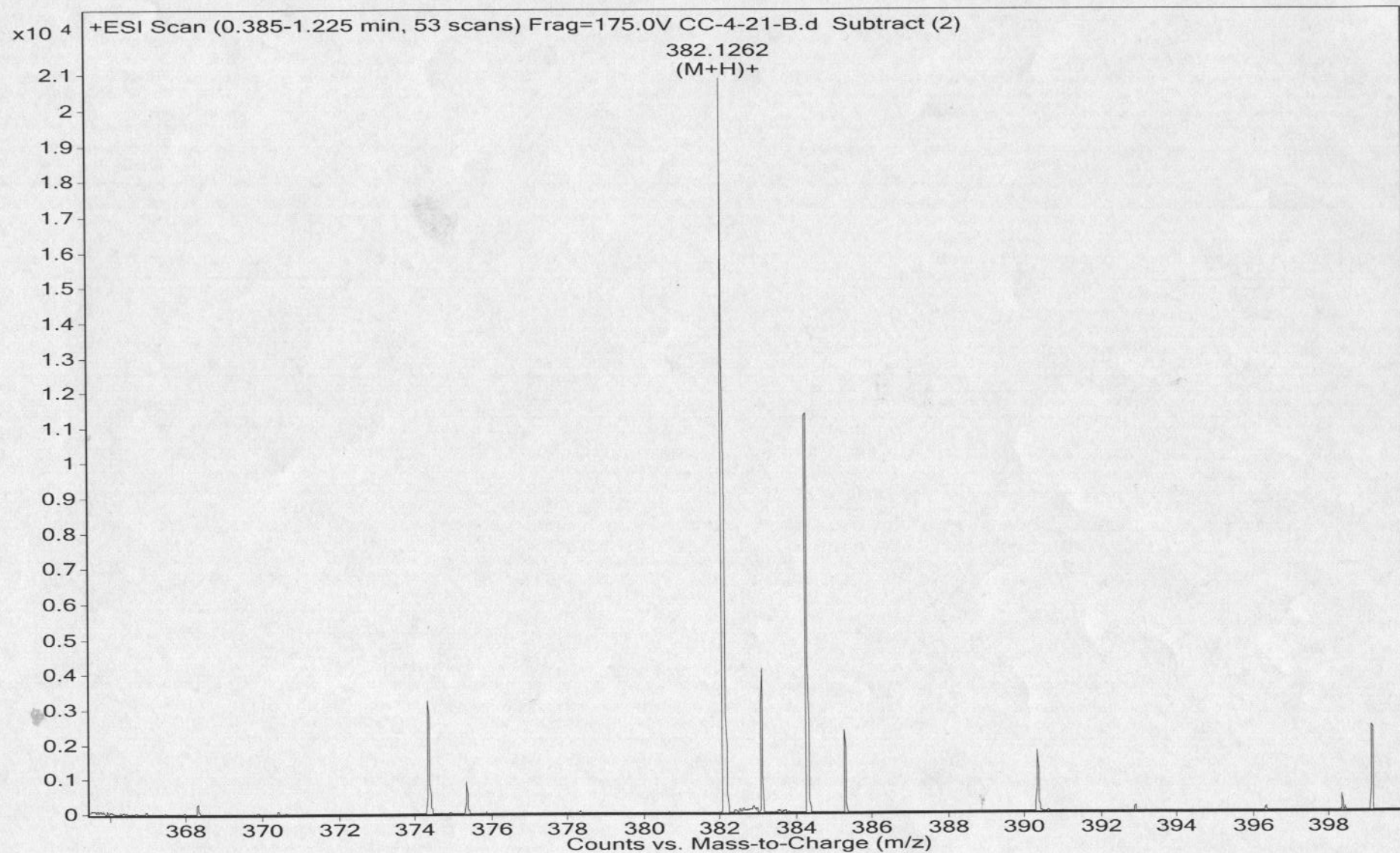
CC-CH30-kailian
C13CPD

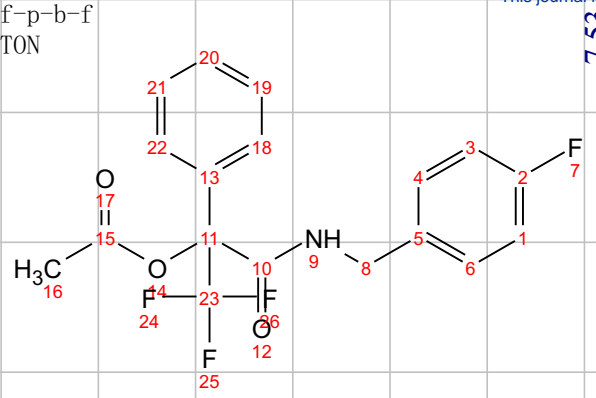
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382.1261

Sample Name	lc/ms	Position	Vial 5	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-4-21-B.d (4d)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 12:21:15 PM





7.53
7.52
7.42
7.40
7.26
7.24
7.22
7.20
7.03
7.01
6.99
6.42
4.55
4.53
4.51
4.49
4.48
4.46
4.44
2.29
1.62
1.56
1.53

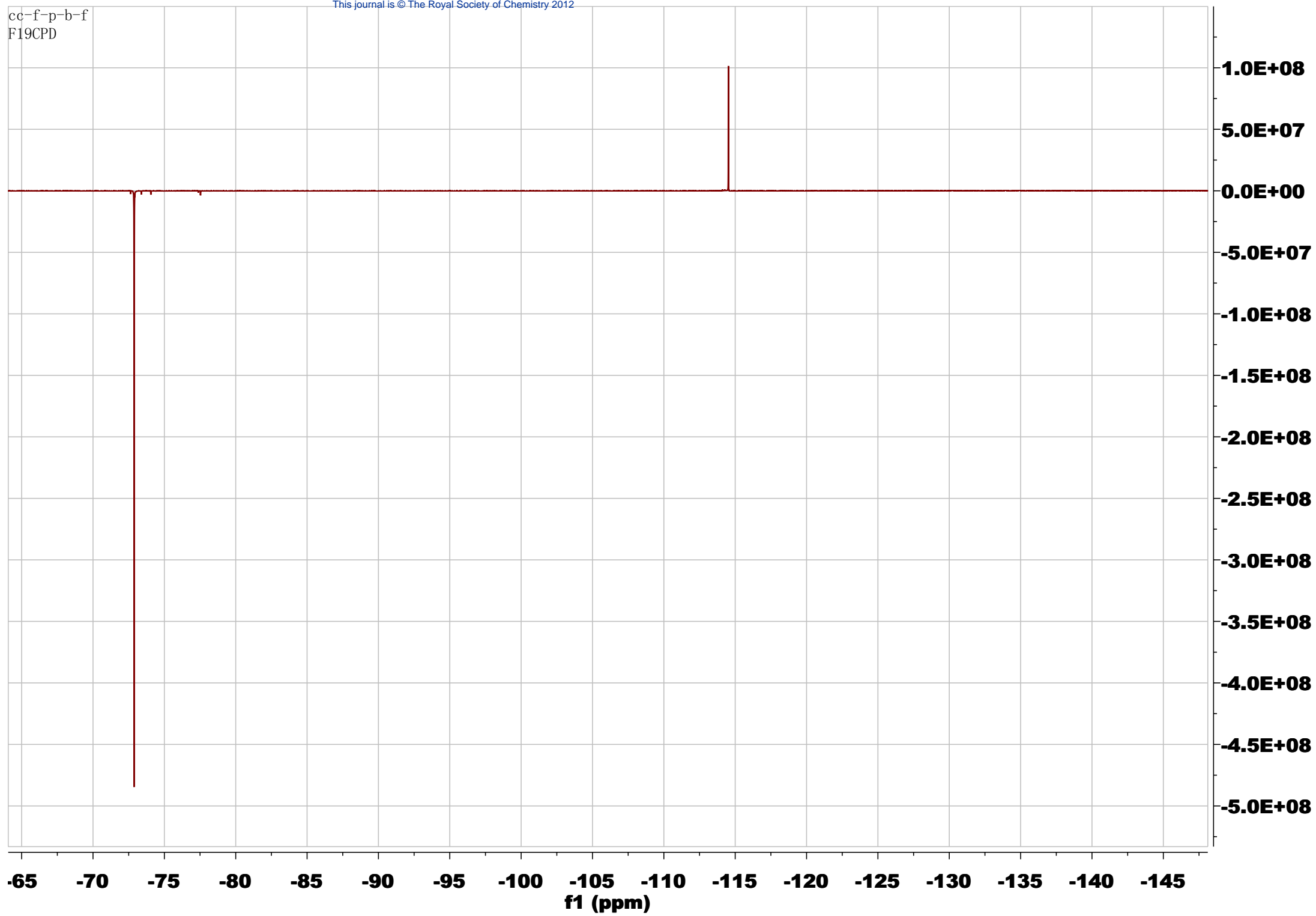


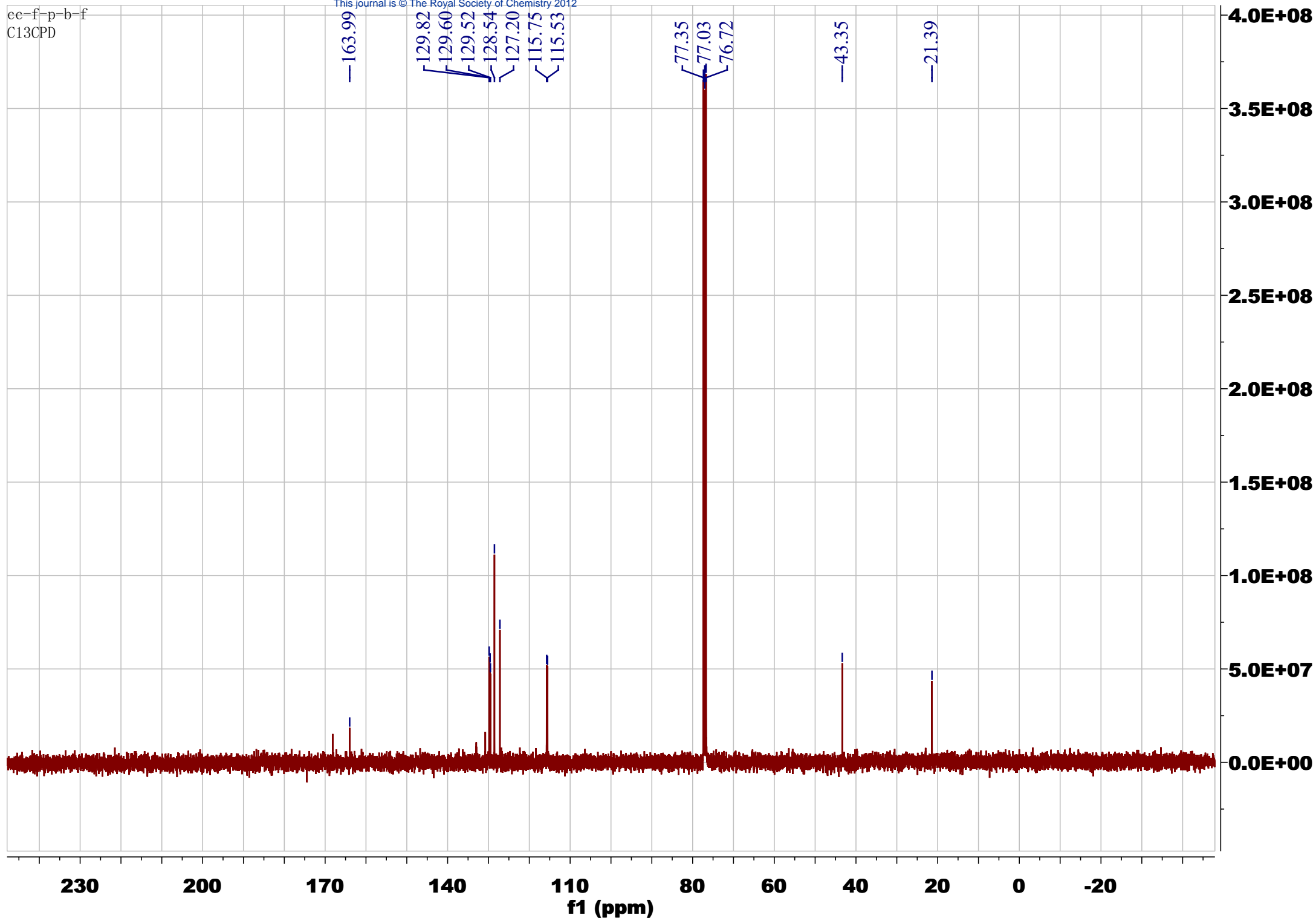
2.03
3.06
2.01
2.01
1.00

4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

cc-f-p-b-f
F19CPD

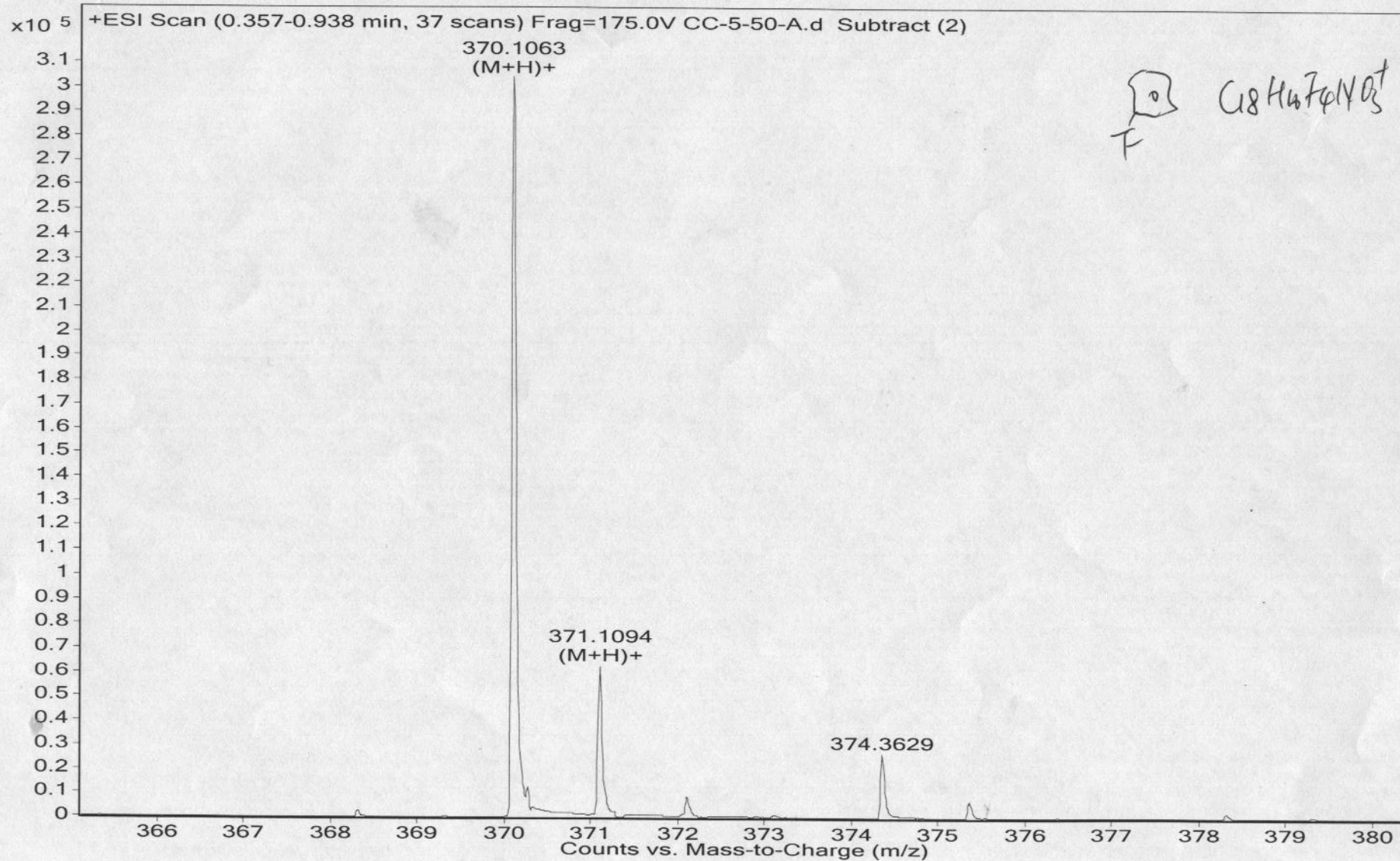


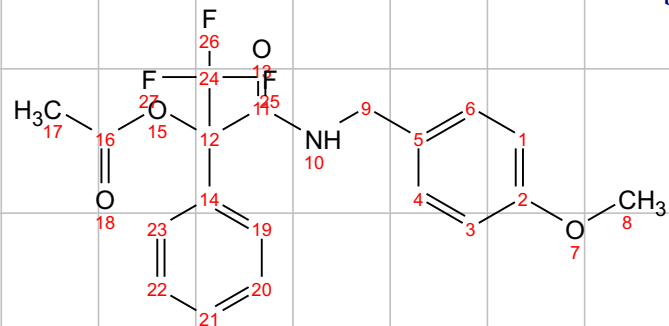


4e

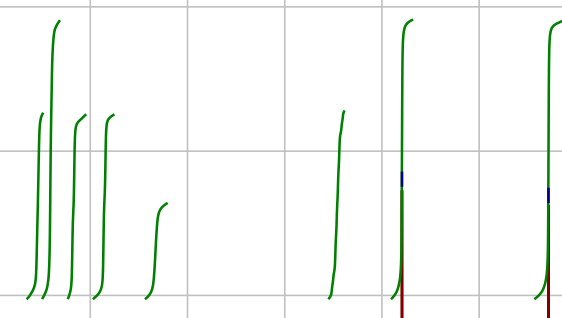
370.1064

Sample Name	lc/ms	Position	Vial 2	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-5-50-A.d	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 12:37:01 PM

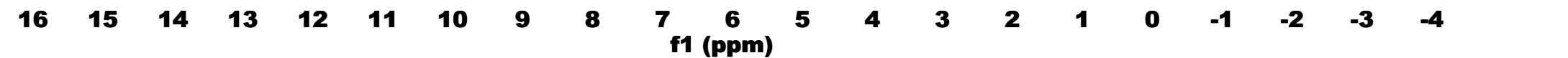




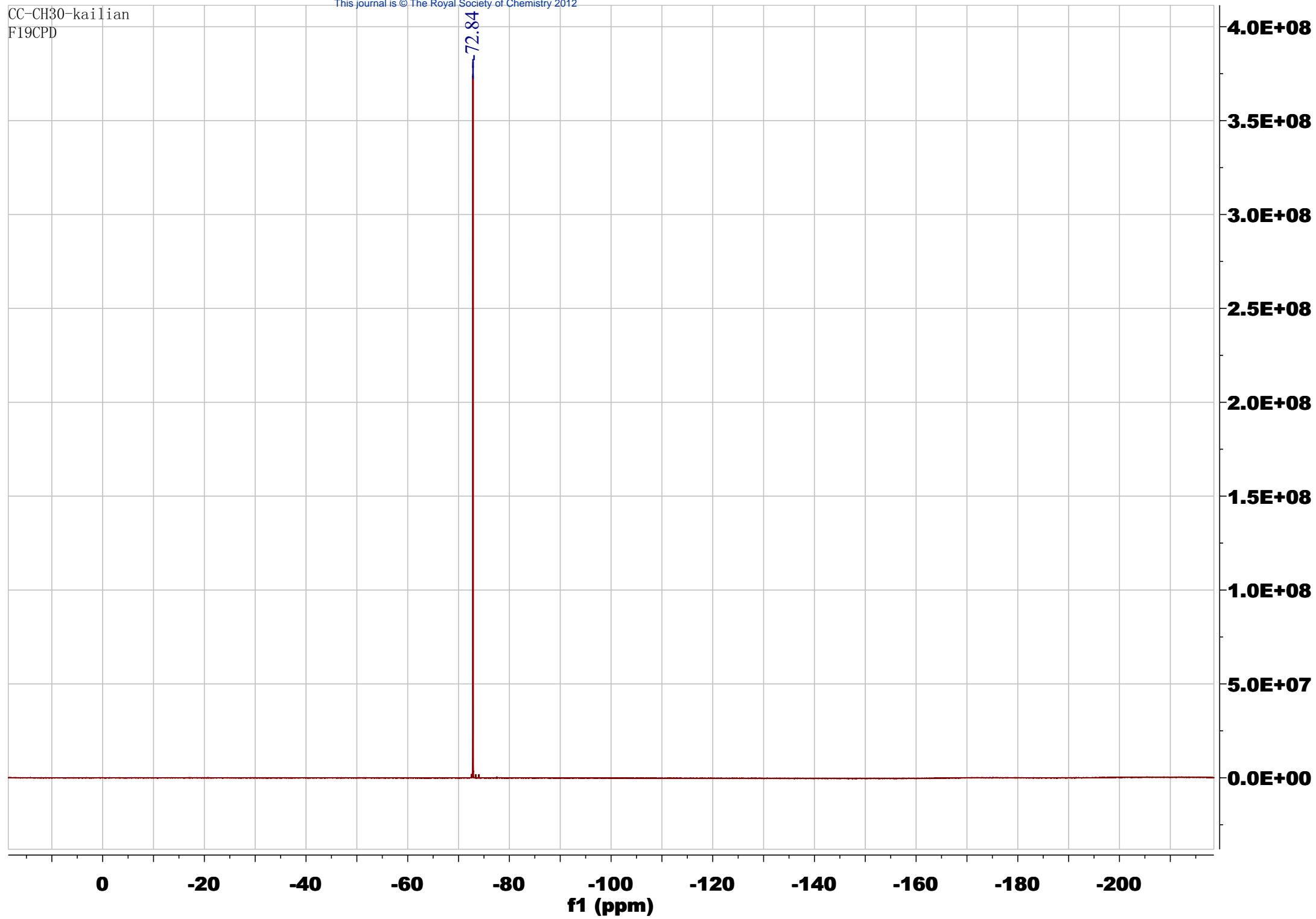
7.55
7.53
7.41
7.40
7.26
7.18
7.16
6.86
6.84
6.33
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4.50
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4.46
4.45
4.44
4.41
3.79
1.57
0.00

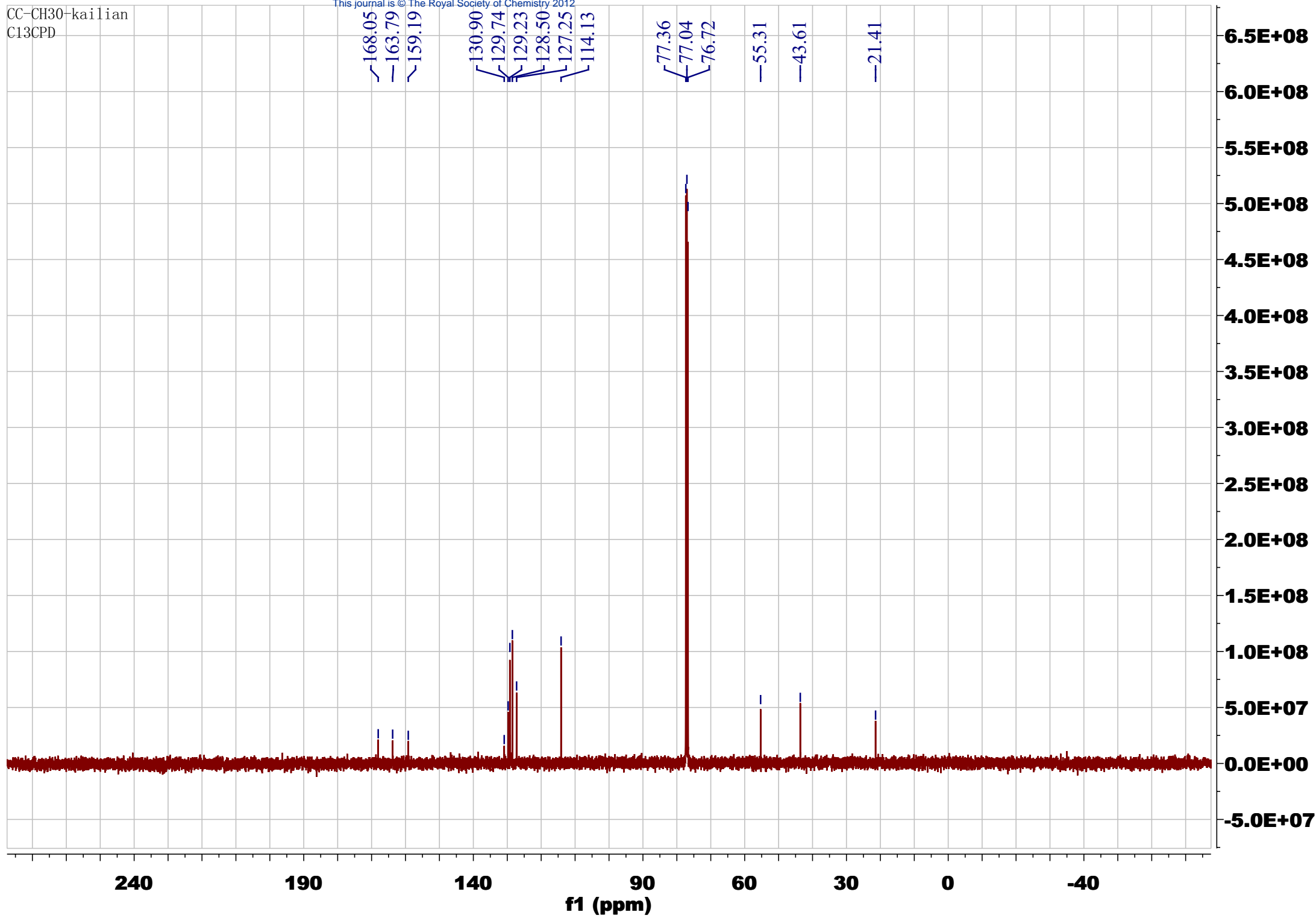


2.01
3.00
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1.99
1.04
2.03
3.01
3.00

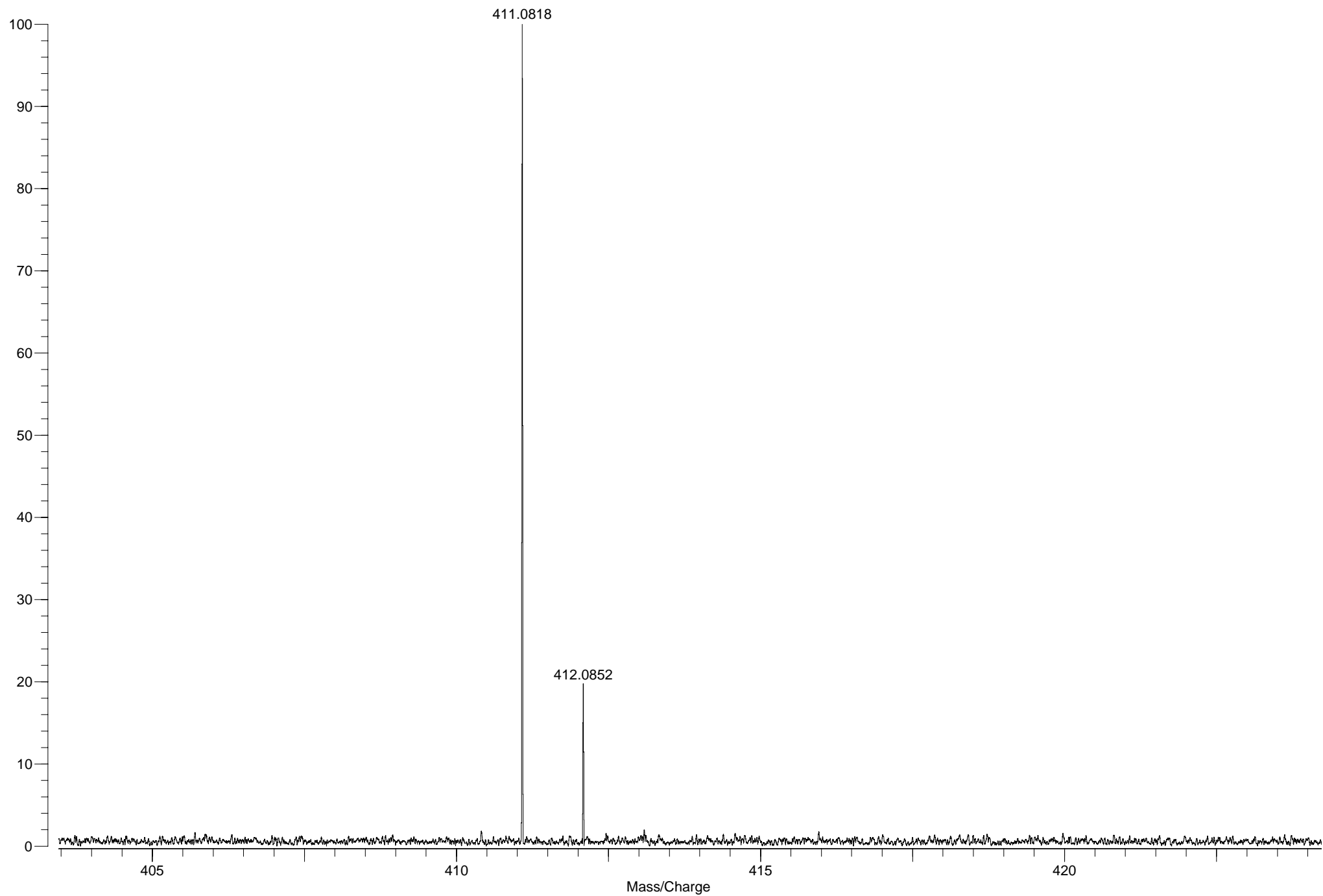


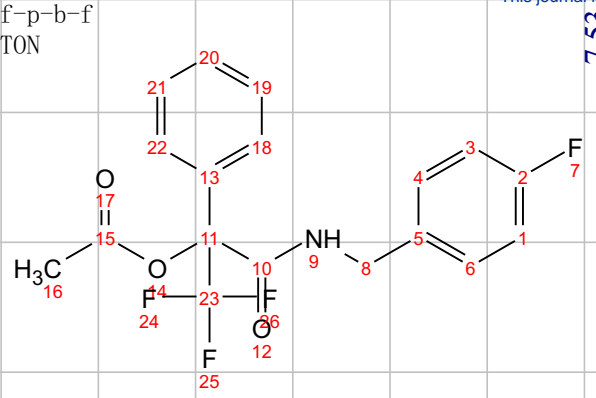
CC-CH30-kailian
F19CPD





Varian QFT-ESI
File: Zc-3-44_ESI.trans





7.53
7.52
7.42
7.40
7.26
7.24
7.22
7.20
7.03
7.01
6.99
6.42
4.55
4.53
4.51
4.49
4.48
4.46
4.44
2.29
1.62
1.56
1.53

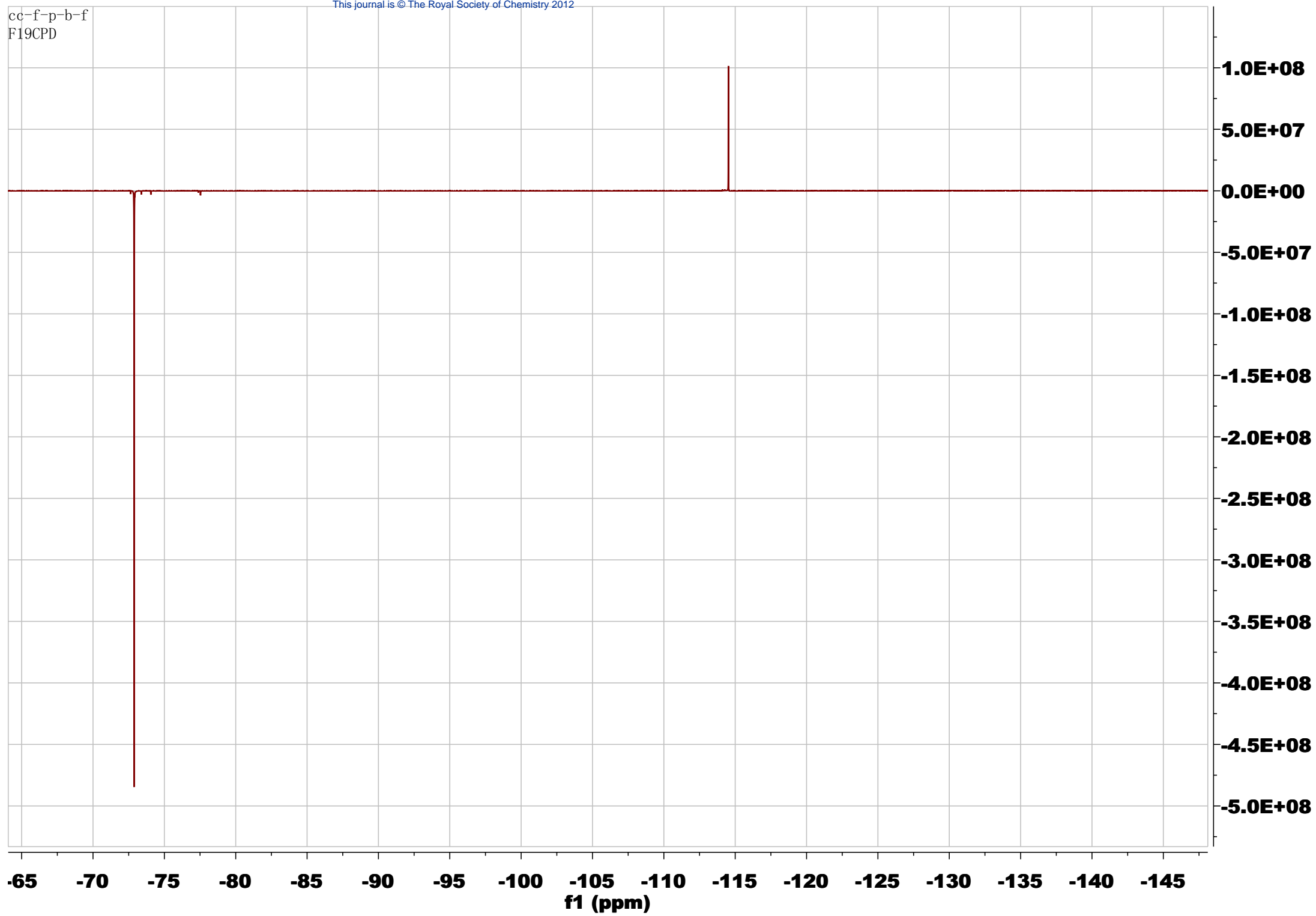


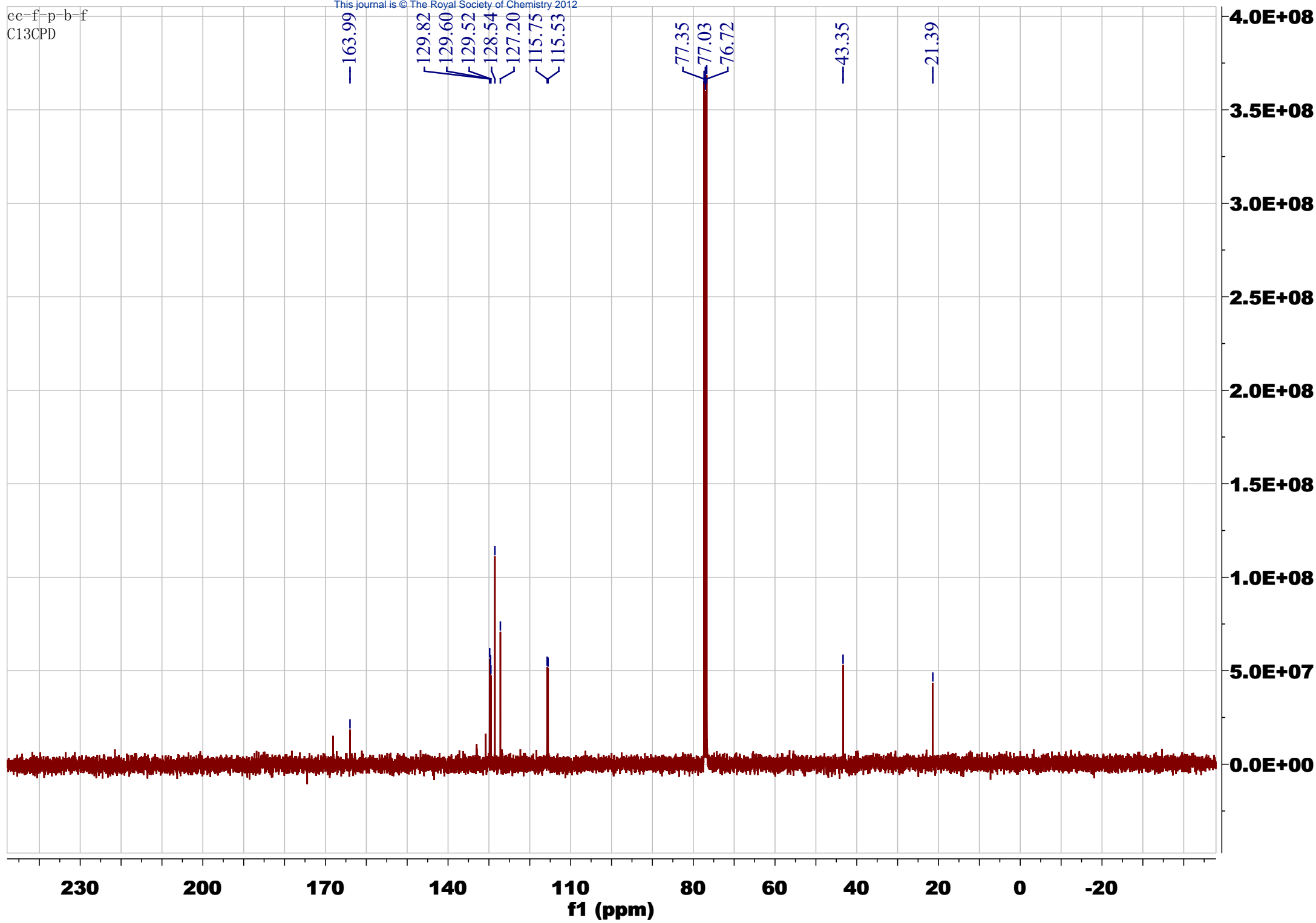
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2.01
2.01
1.00

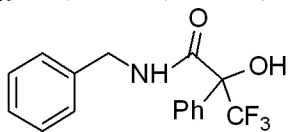
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

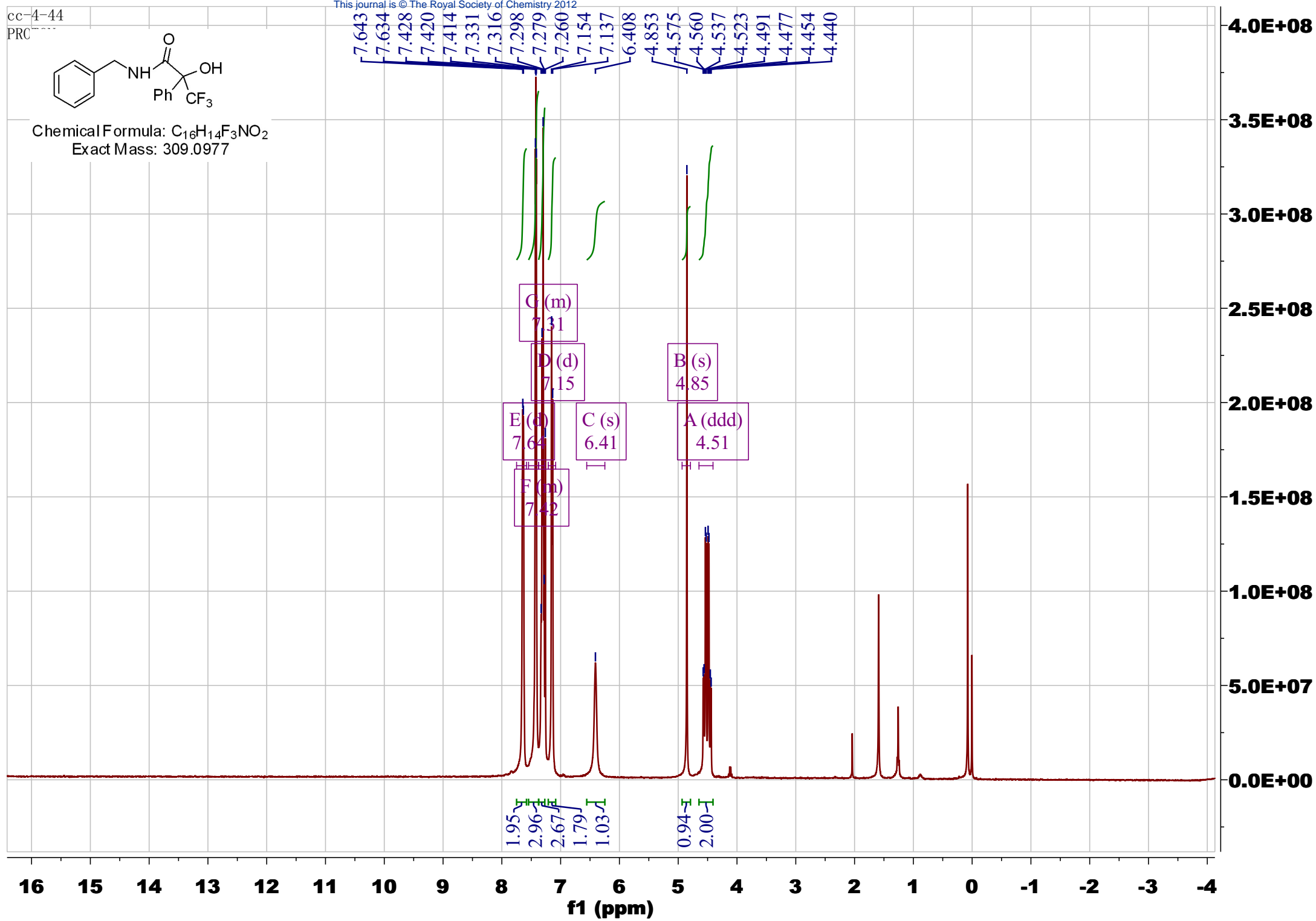
cc-f-p-b-f
F19CPD



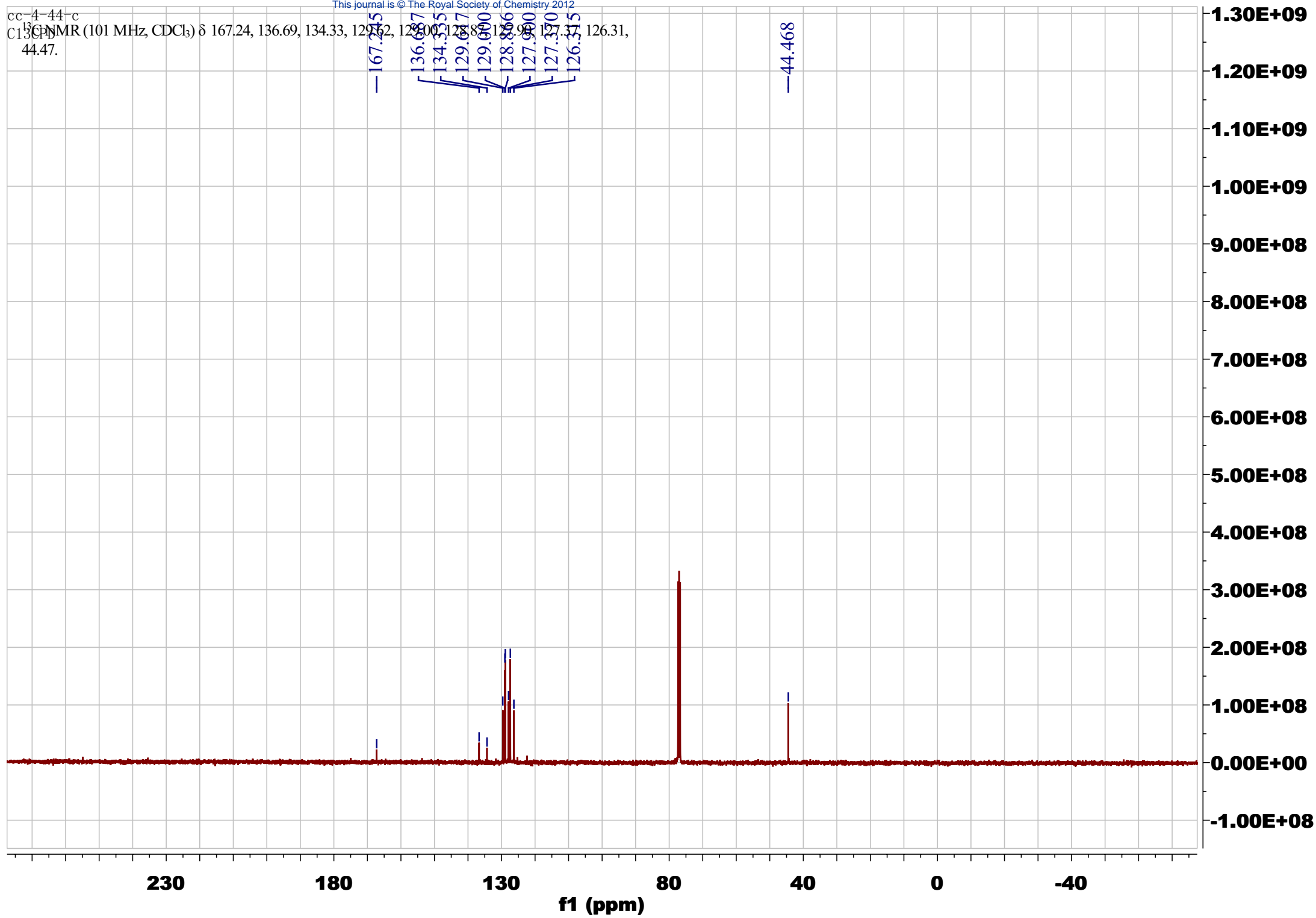




Chemical Formula: C₁₆H₁₄F₃NO₂
 Exact Mass: 309.0977

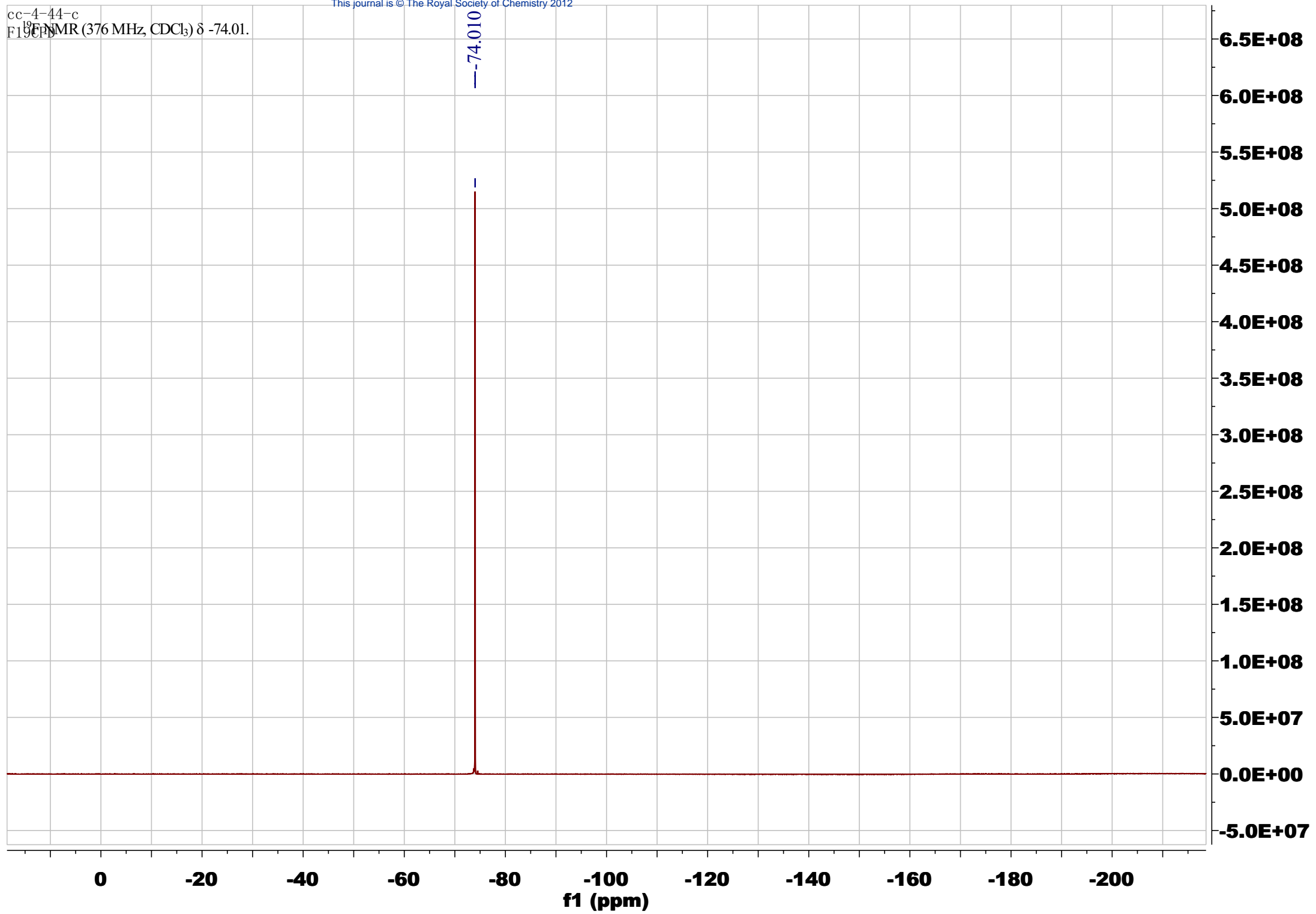


cc-4-44-c
C13CNMR (101 MHz, CDCl₃) δ 167.24, 136.69, 134.33, 129.62, 129.00, 128.88, 128.99, 127.37, 126.31, 44.47.



cc-4-44-c
F19F NMR (376 MHz, CDCl₃) δ -74.01.

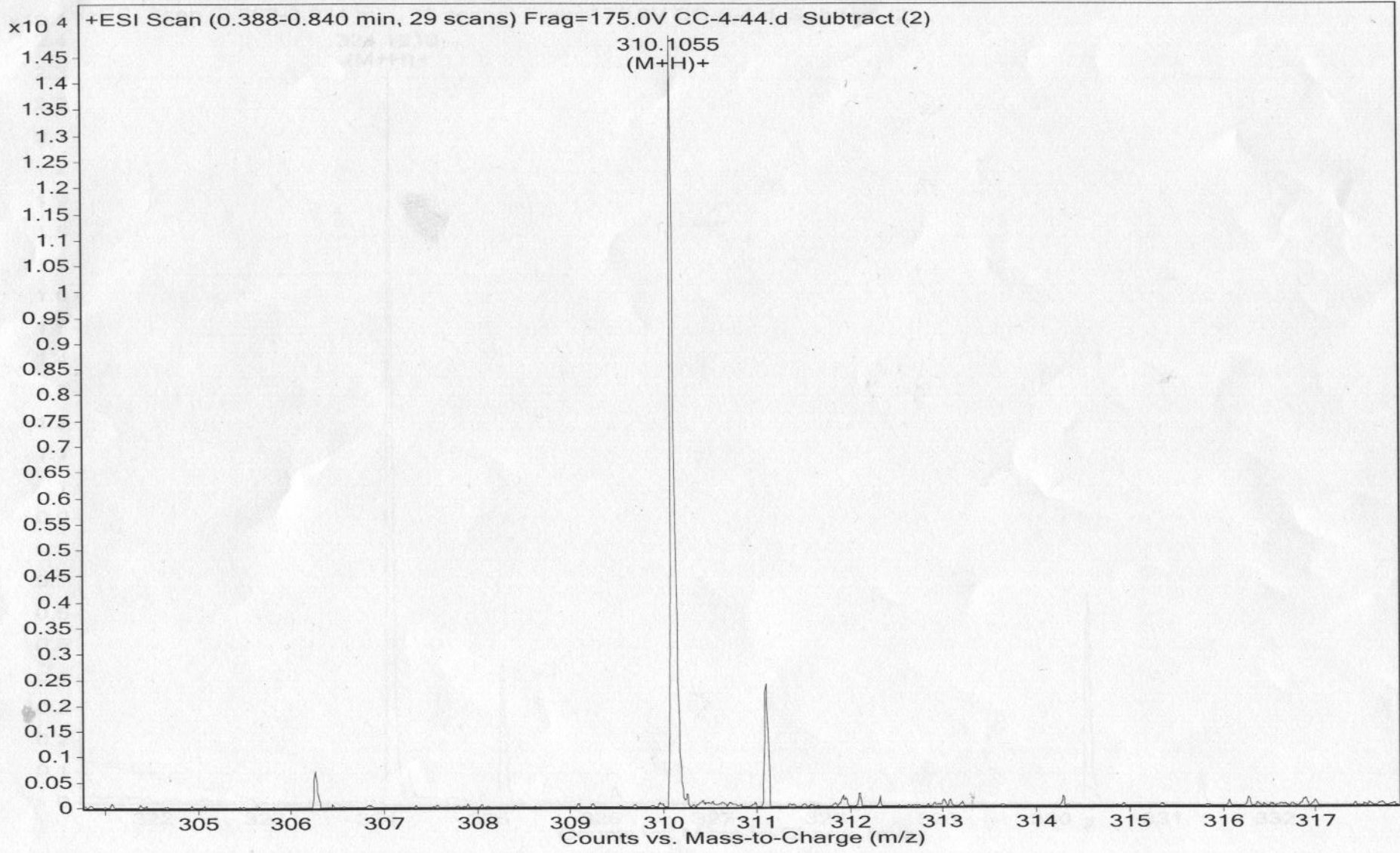
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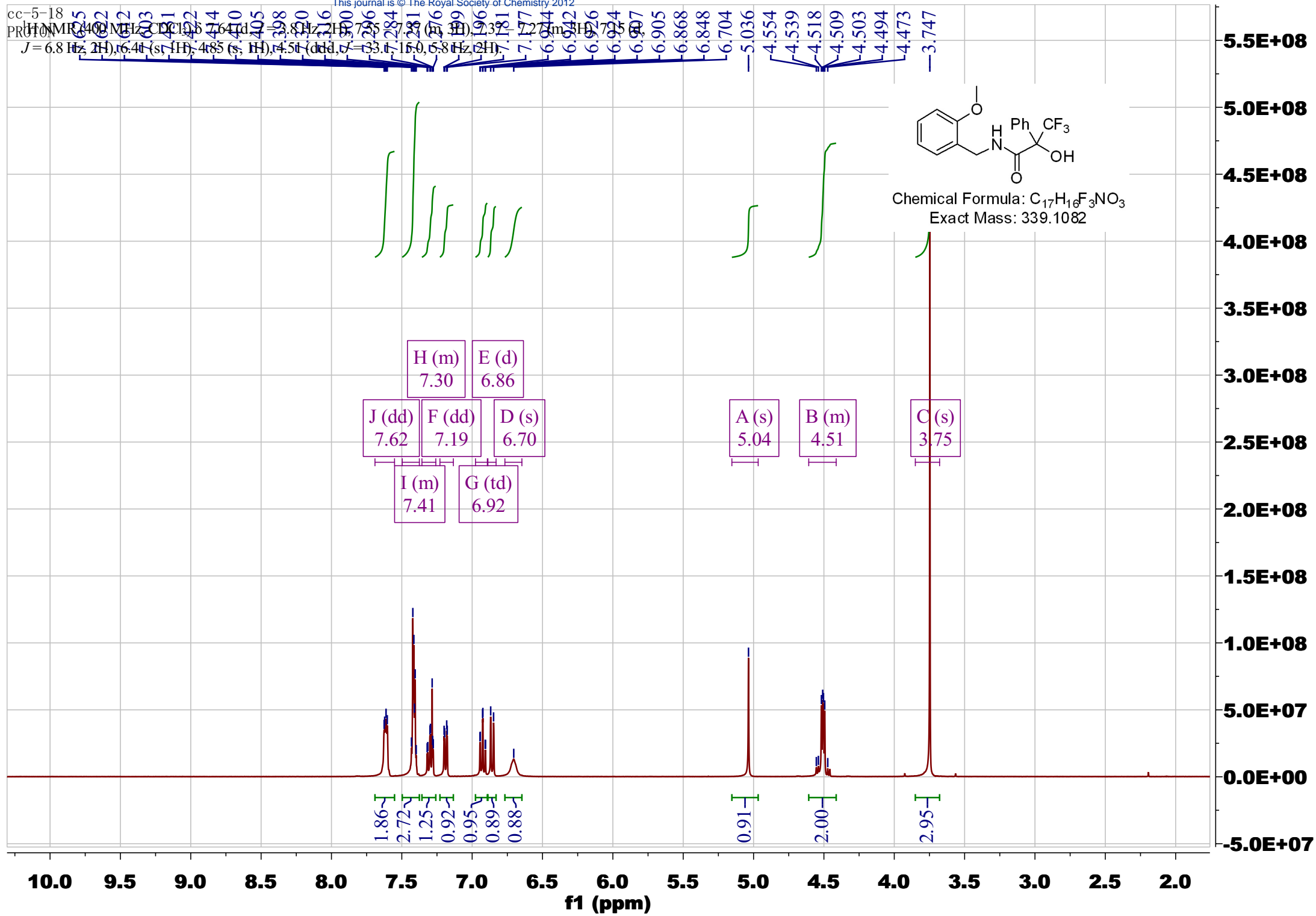


310.1049

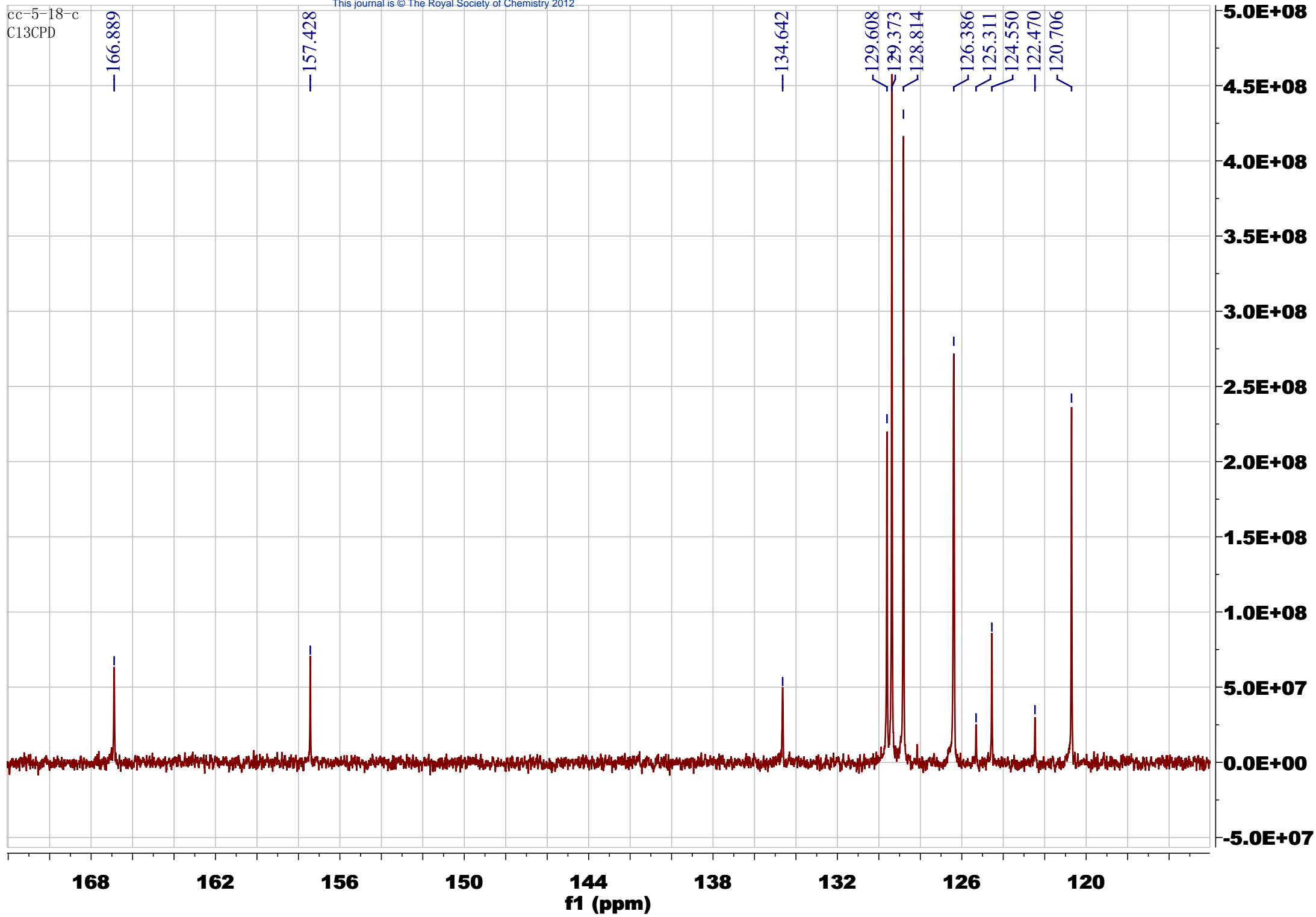
水解产物

Sample Name	lc/ms	Position	Vial 1	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-4-44.d (6a)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:20:48 AM

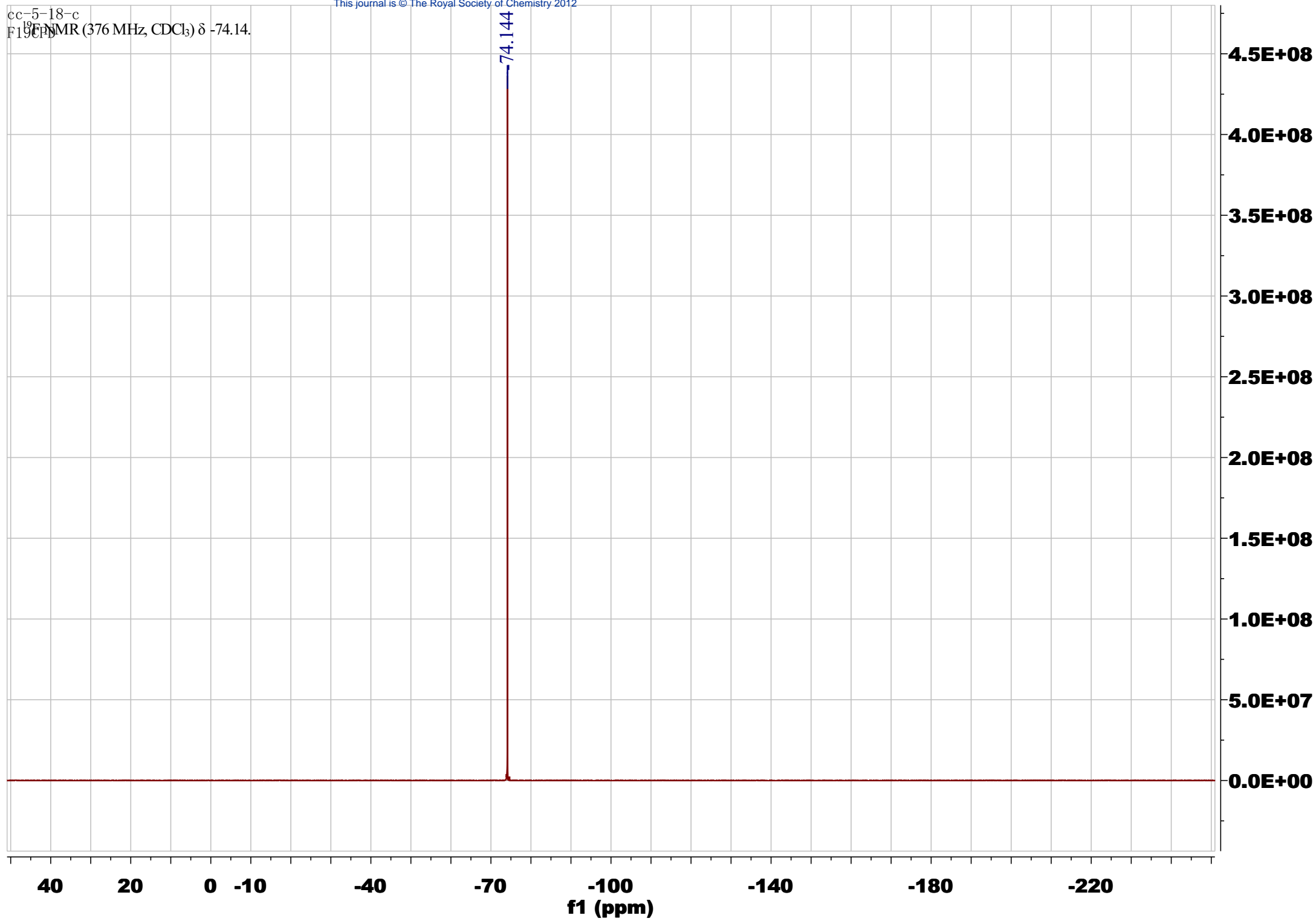




cc-5-18-c
C13CPD

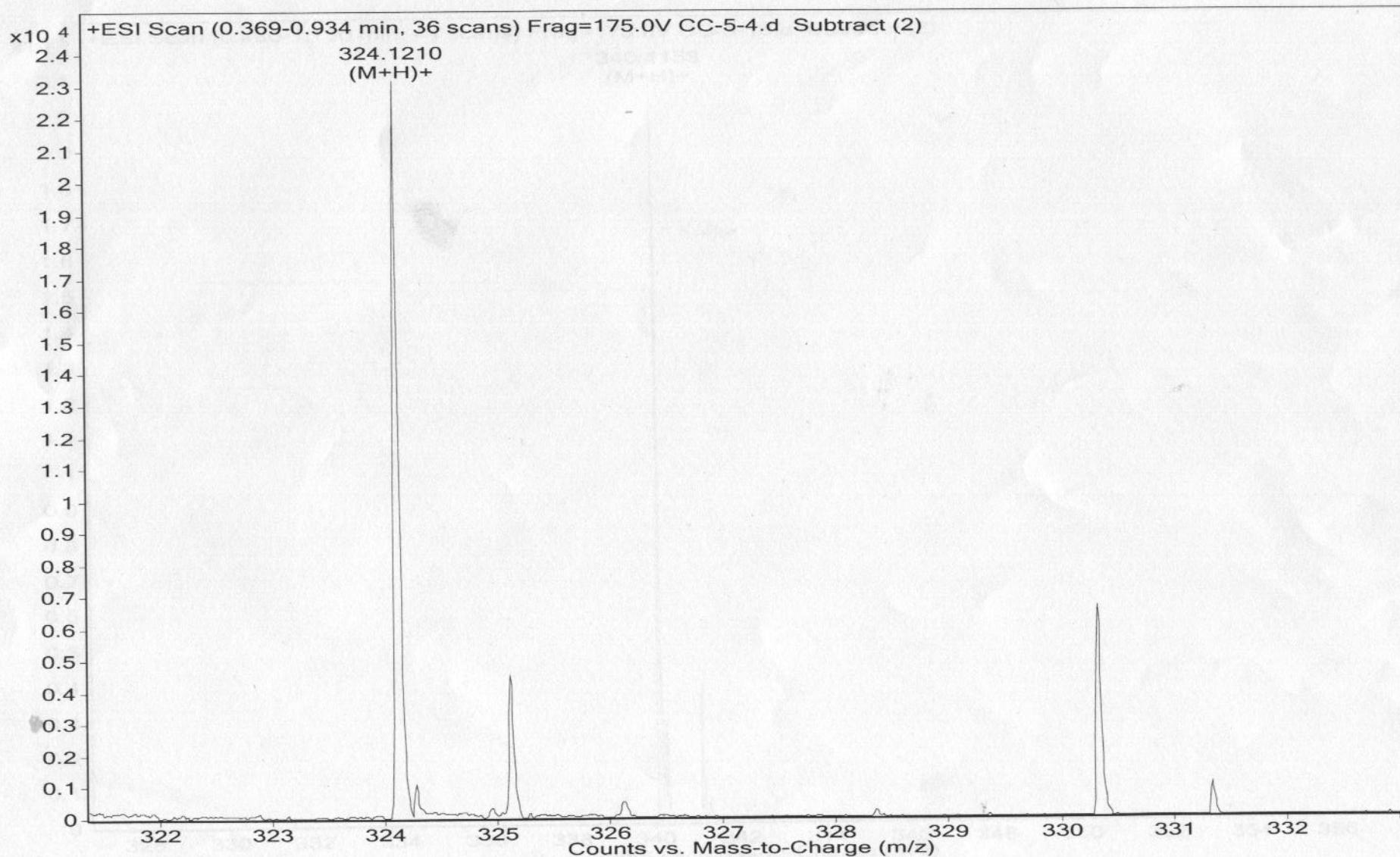


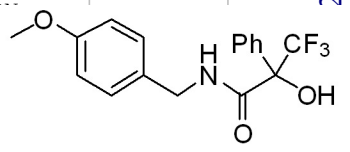
cc-5-18-c
F19C1NMR (376 MHz, CDCl₃) δ -74.14.



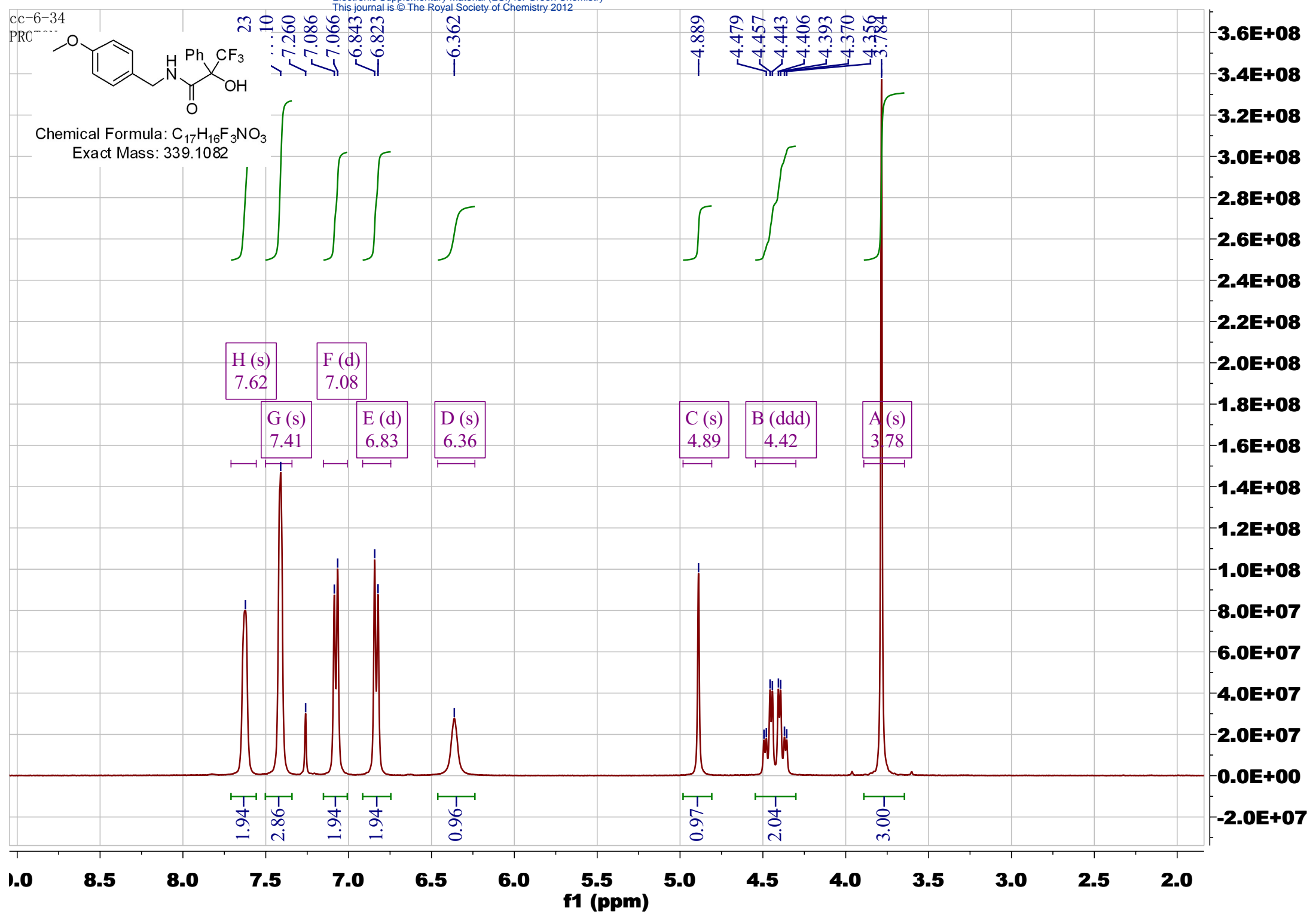
324.1206

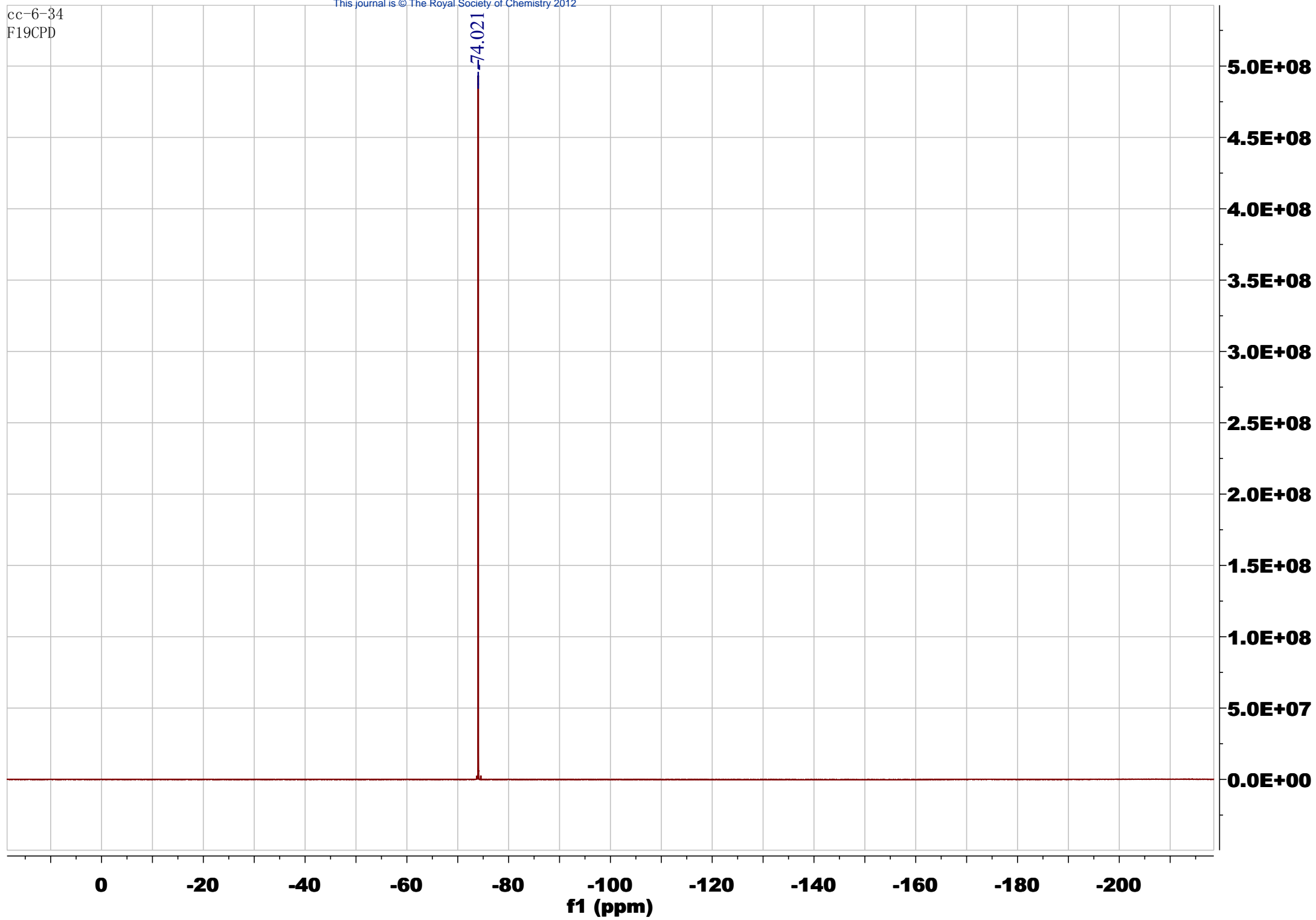
Sample Name	lc/ms	Position	Vial 2	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-5-4.d (6b)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:24:29 AM



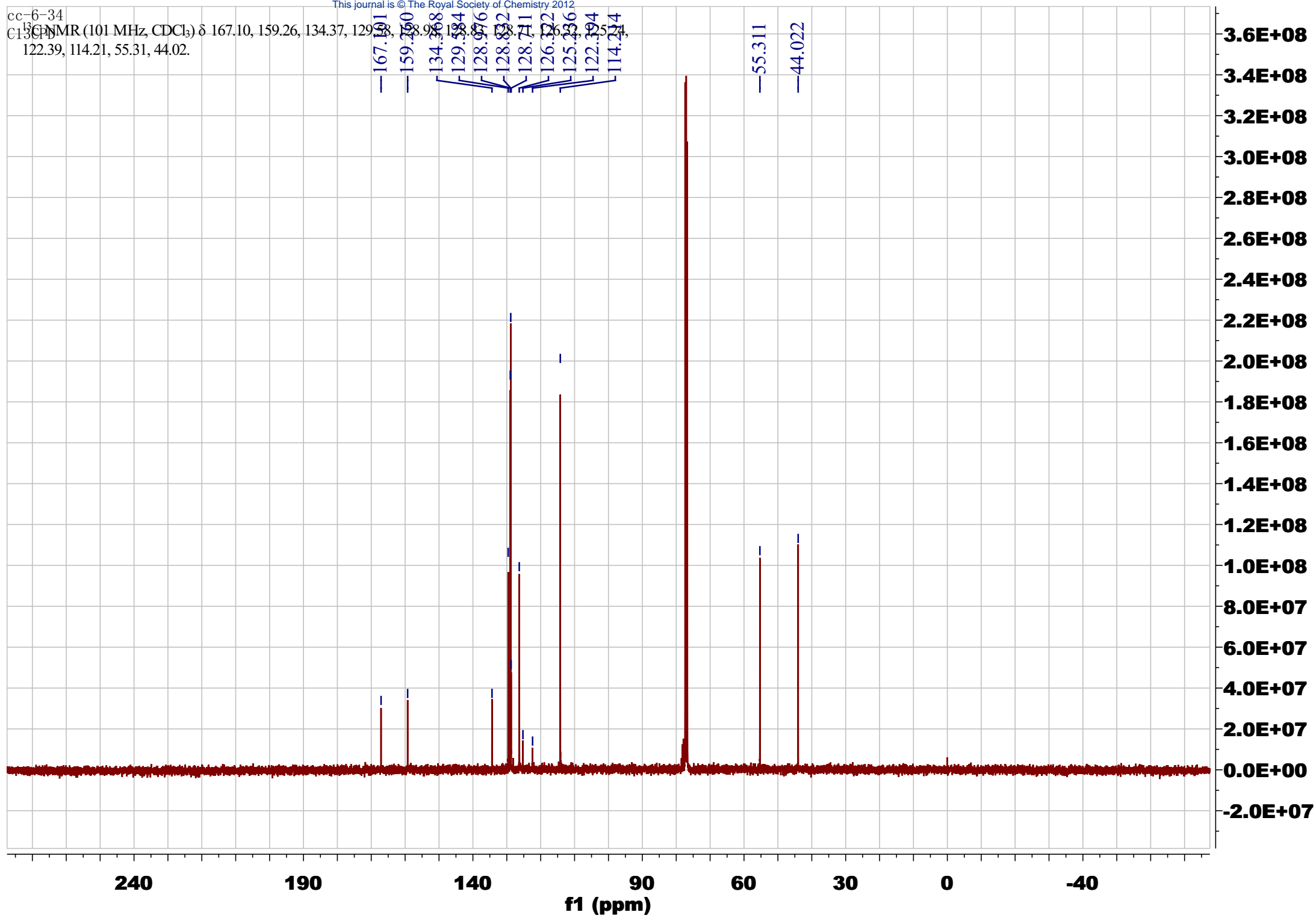


Chemical Formula: C₁₇H₁₆F₃NO₃
Exact Mass: 339.1082



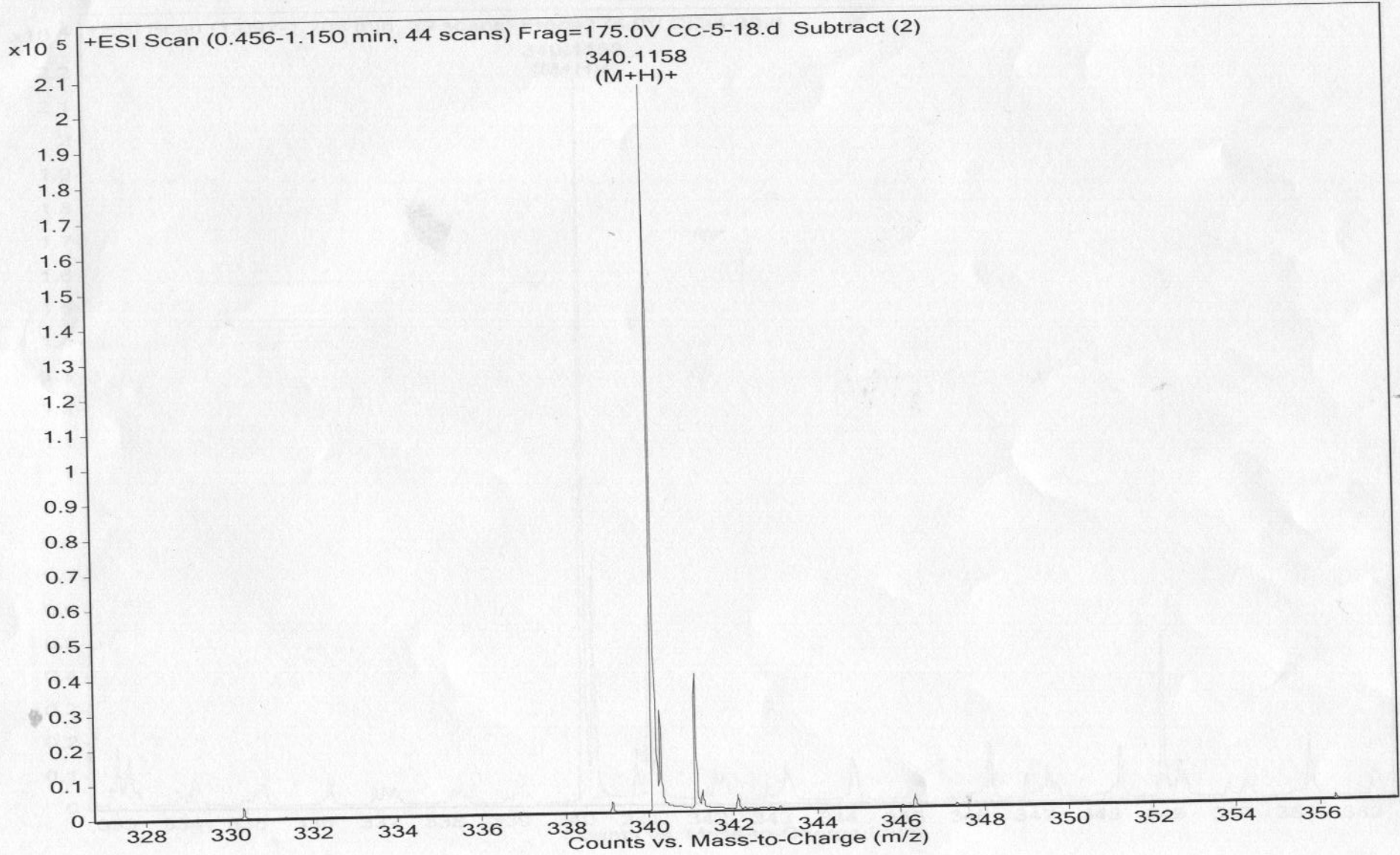


¹³C NMR (101 MHz, CDCl₃) δ 167.10, 159.26, 134.37, 129.58, 128.96, 128.88, 128.71, 126.52, 125.36, 122.19, 114.21, 55.31, 44.02.

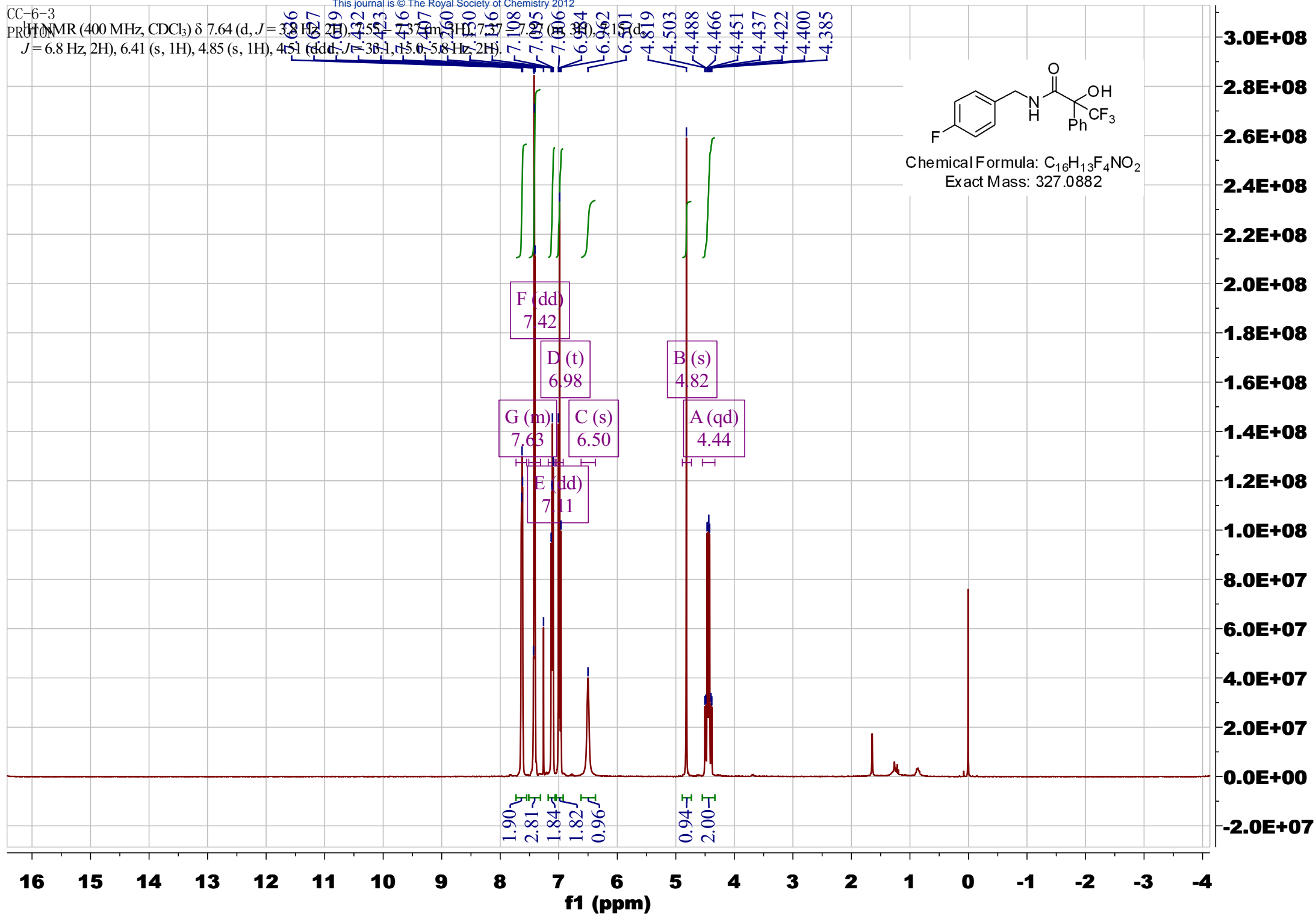
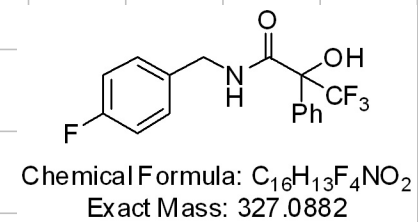


340.1155

Sample Name	lc/ms	Position	Vial 3	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-5-18.d (6C)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:28:12 AM

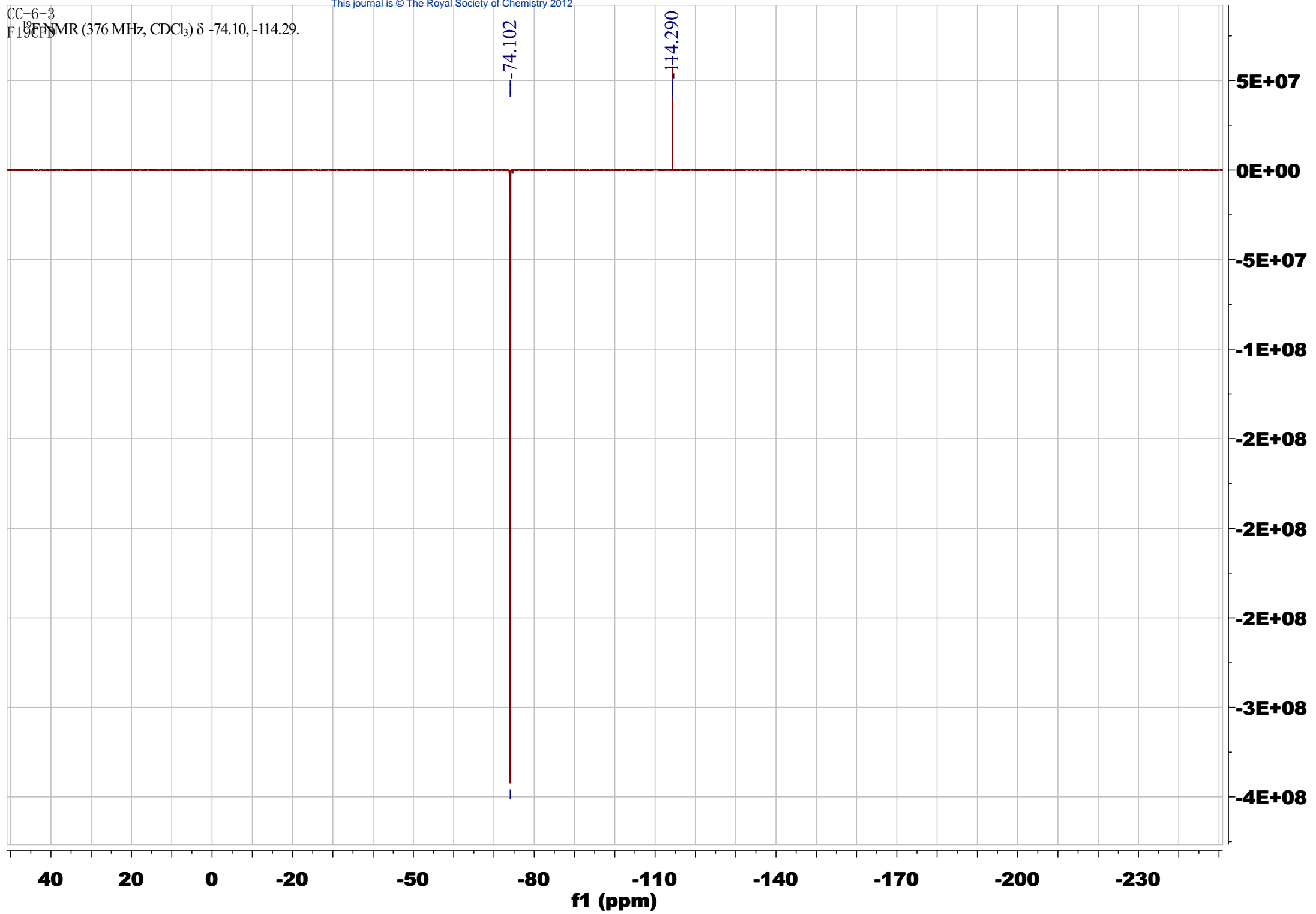


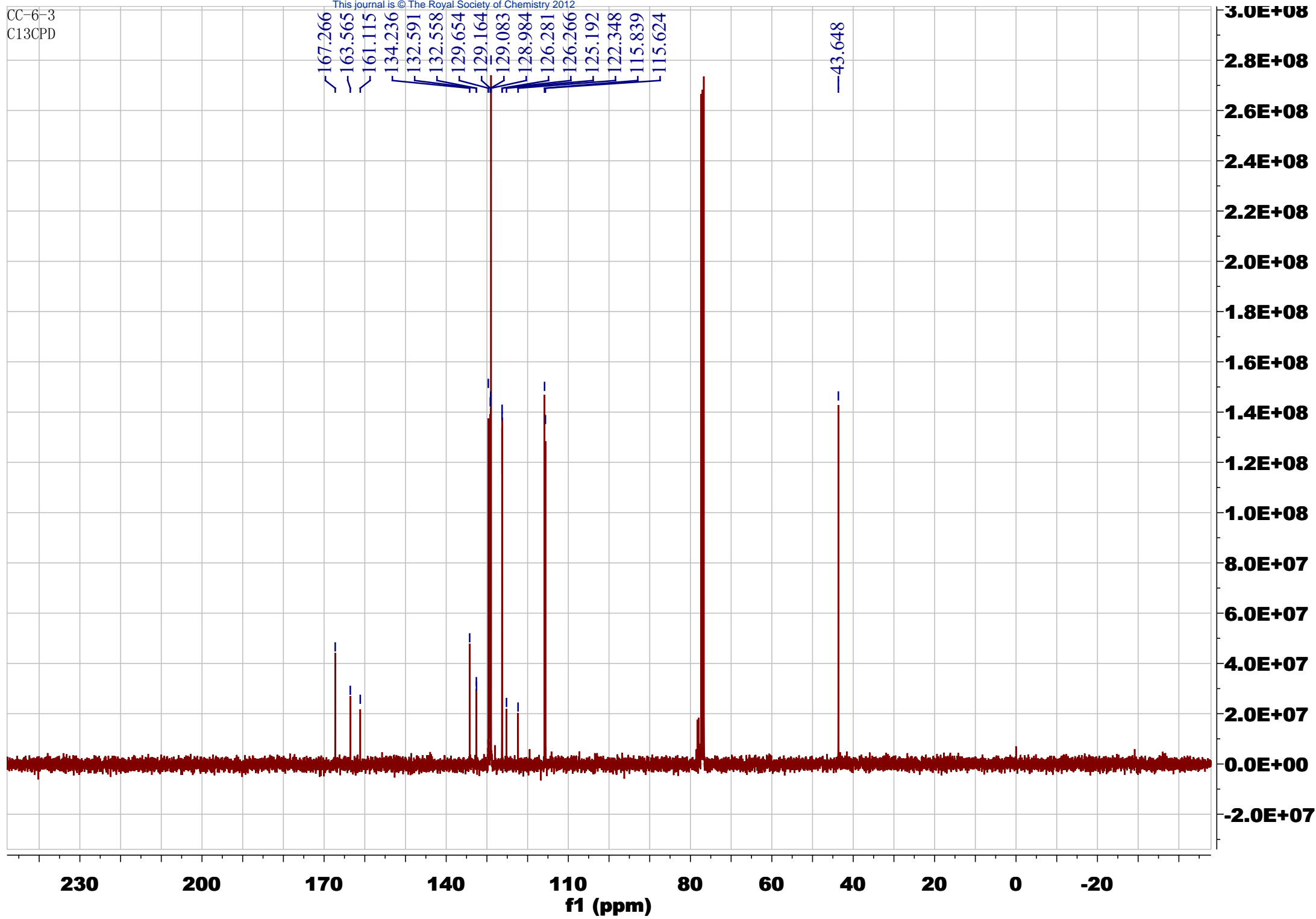
¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 3.8 Hz, 2H), 7.55 (d, *J* = 7.3 Hz, 2H), 7.37 (m, 2H), 7.37 (d, *J* = 6.8 Hz, 2H), 6.41 (s, 1H), 4.85 (s, 1H), 4.51 (dd, *J* = 3.8, 1.5 Hz, 2H), 4.46 (dd, *J* = 5.8 Hz, 2H).



CC-6-3
F19F NMR (376 MHz, CDCl₃) δ -74.10, -114.29.

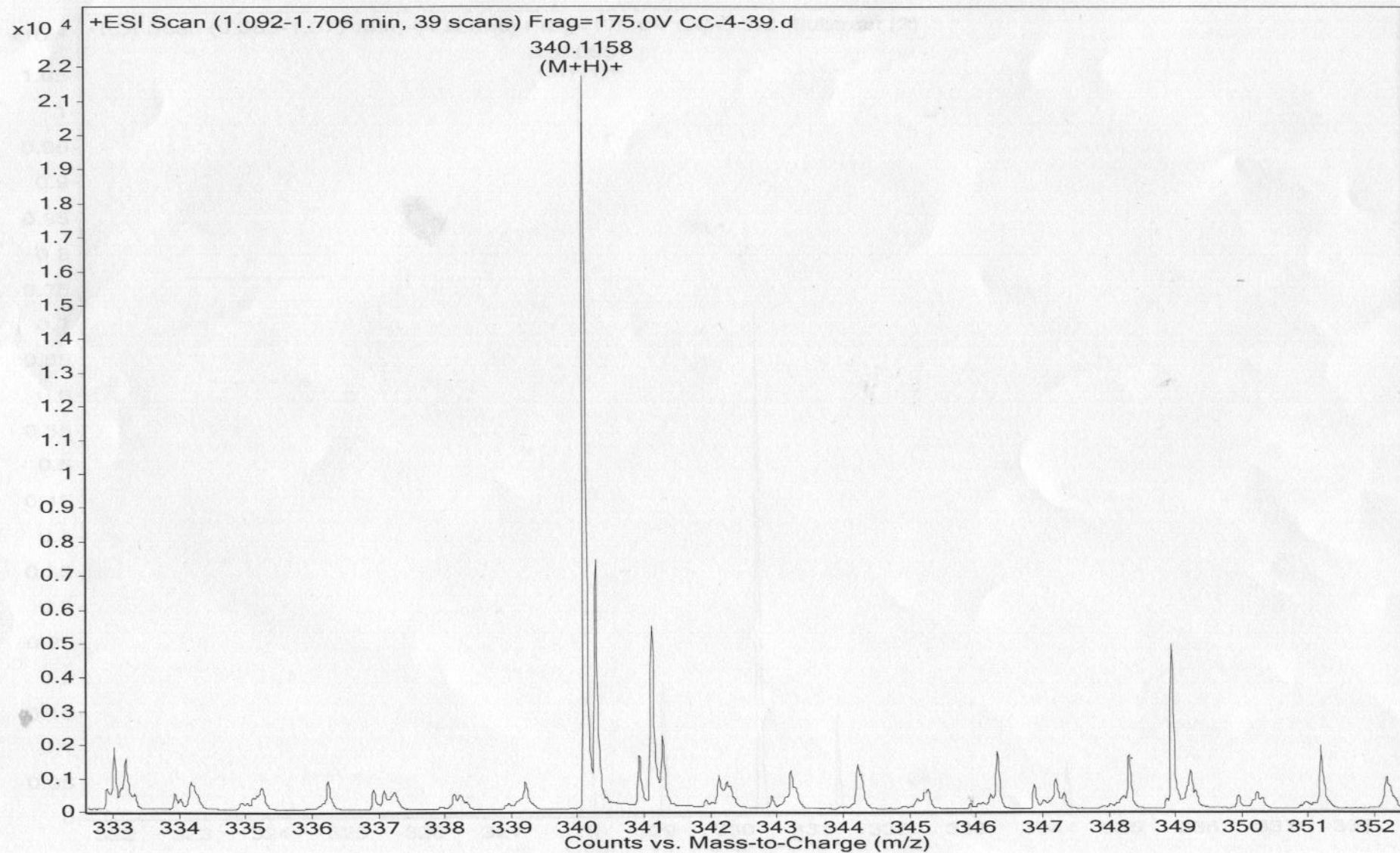
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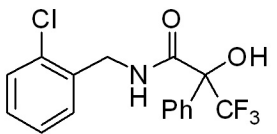




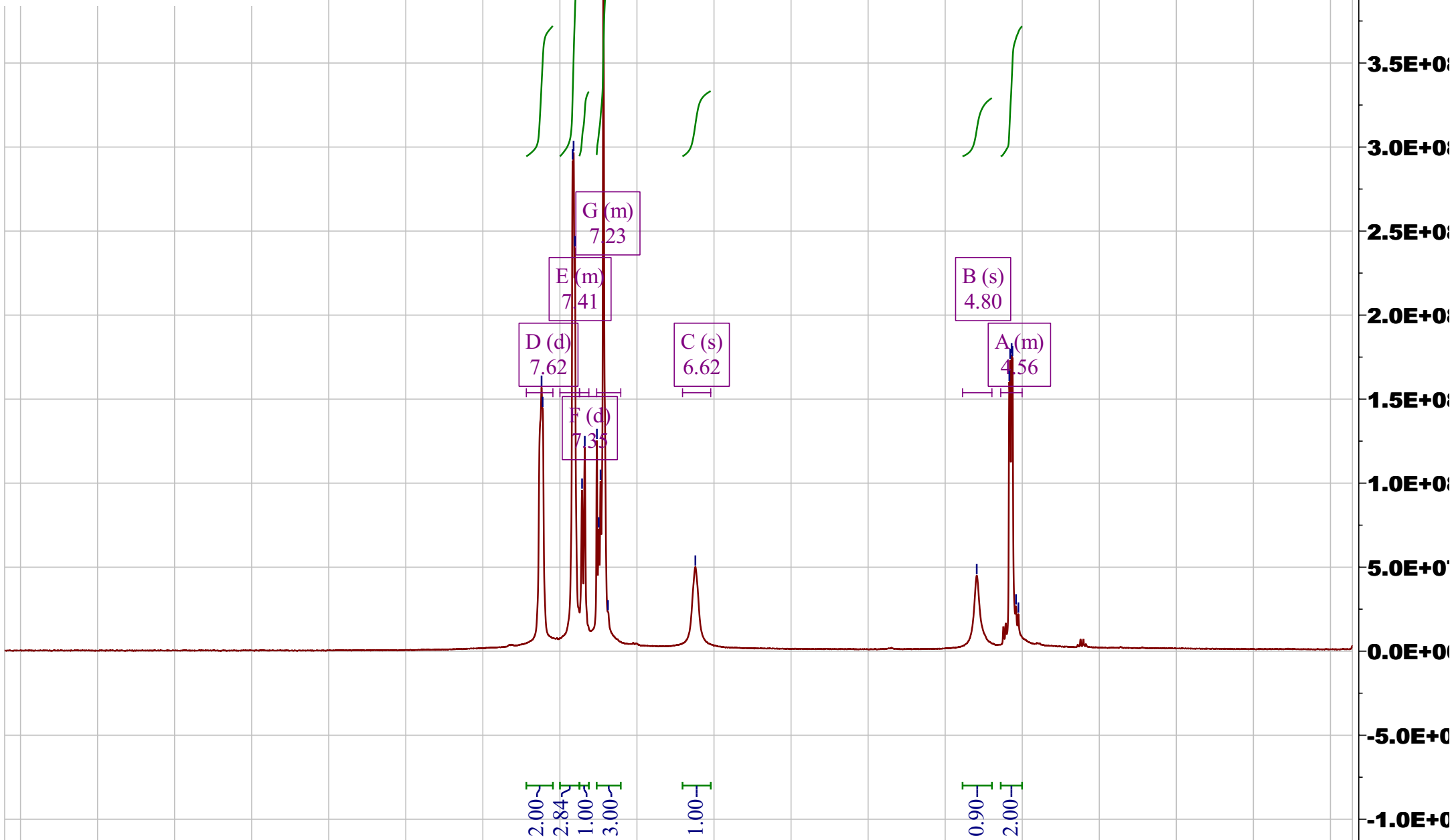
340.1155

Sample Name	lc/ms	Position	Vial 4	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-4-39.d (6d)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:31:53 AM

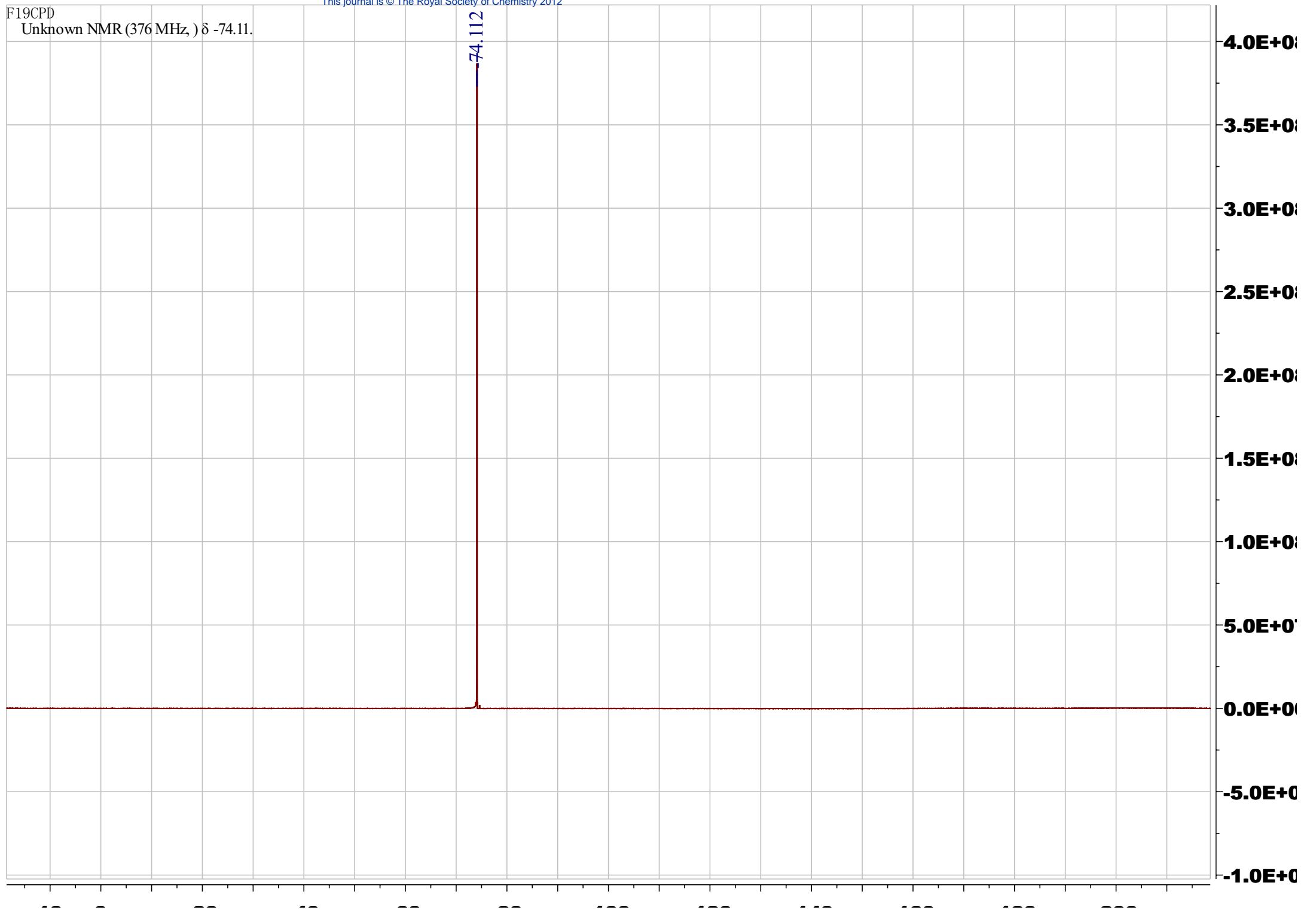




Chemical Formula: C₁₆H₁₃ClF₃NO₂
Exact Mass: 343.0587

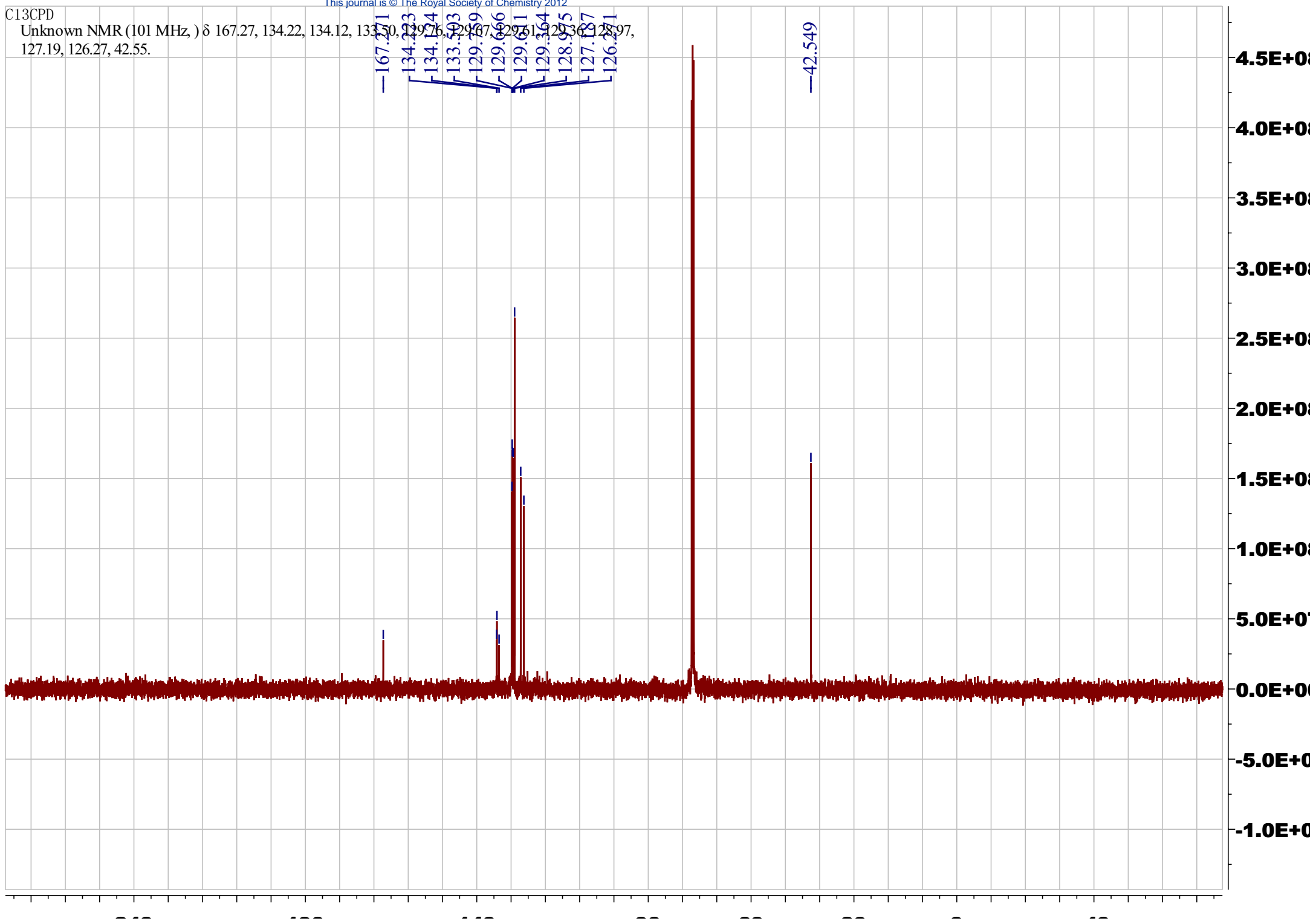


F19CPD
Unknown NMR (376 MHz,) δ -74.11.



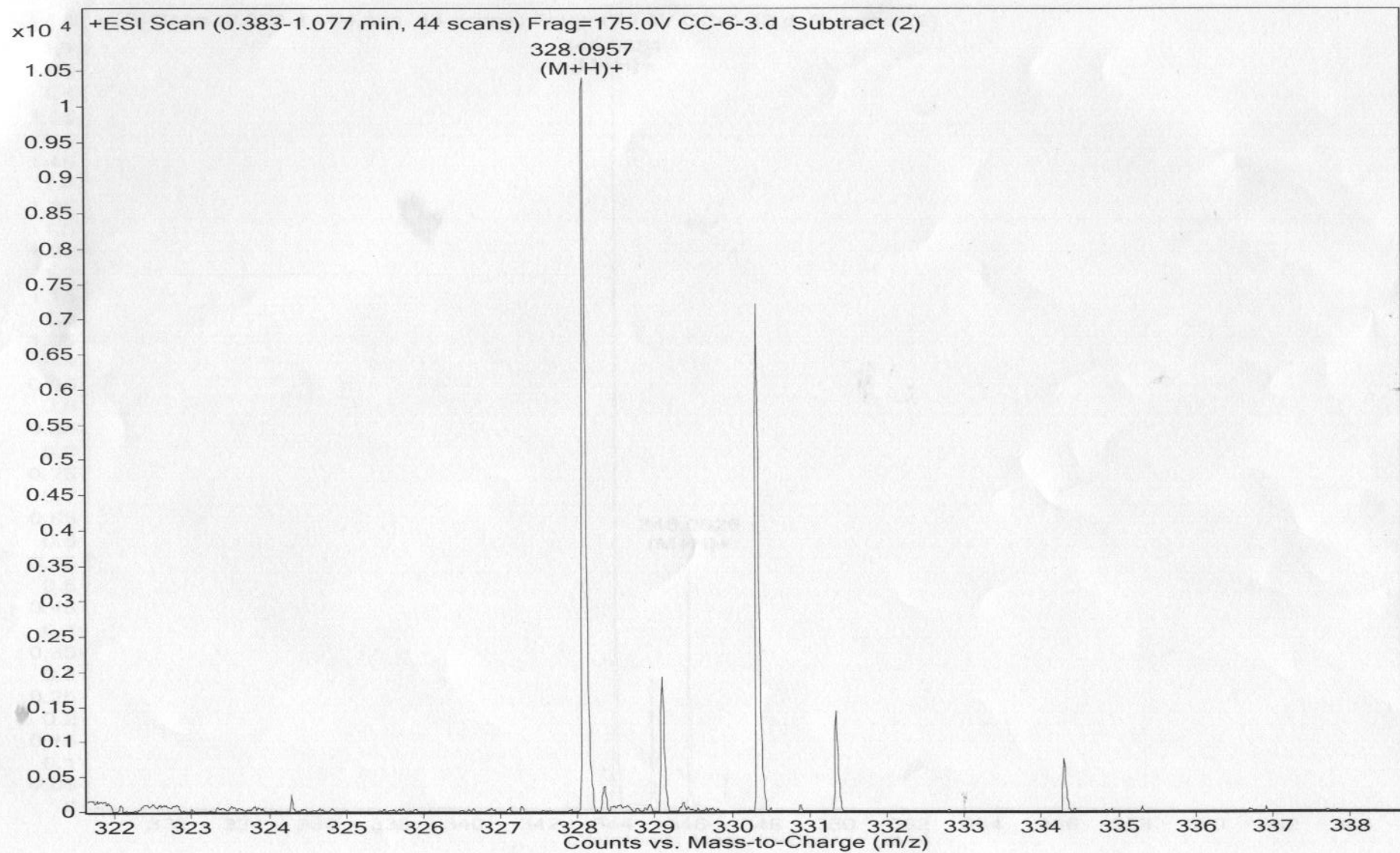
C13CPD

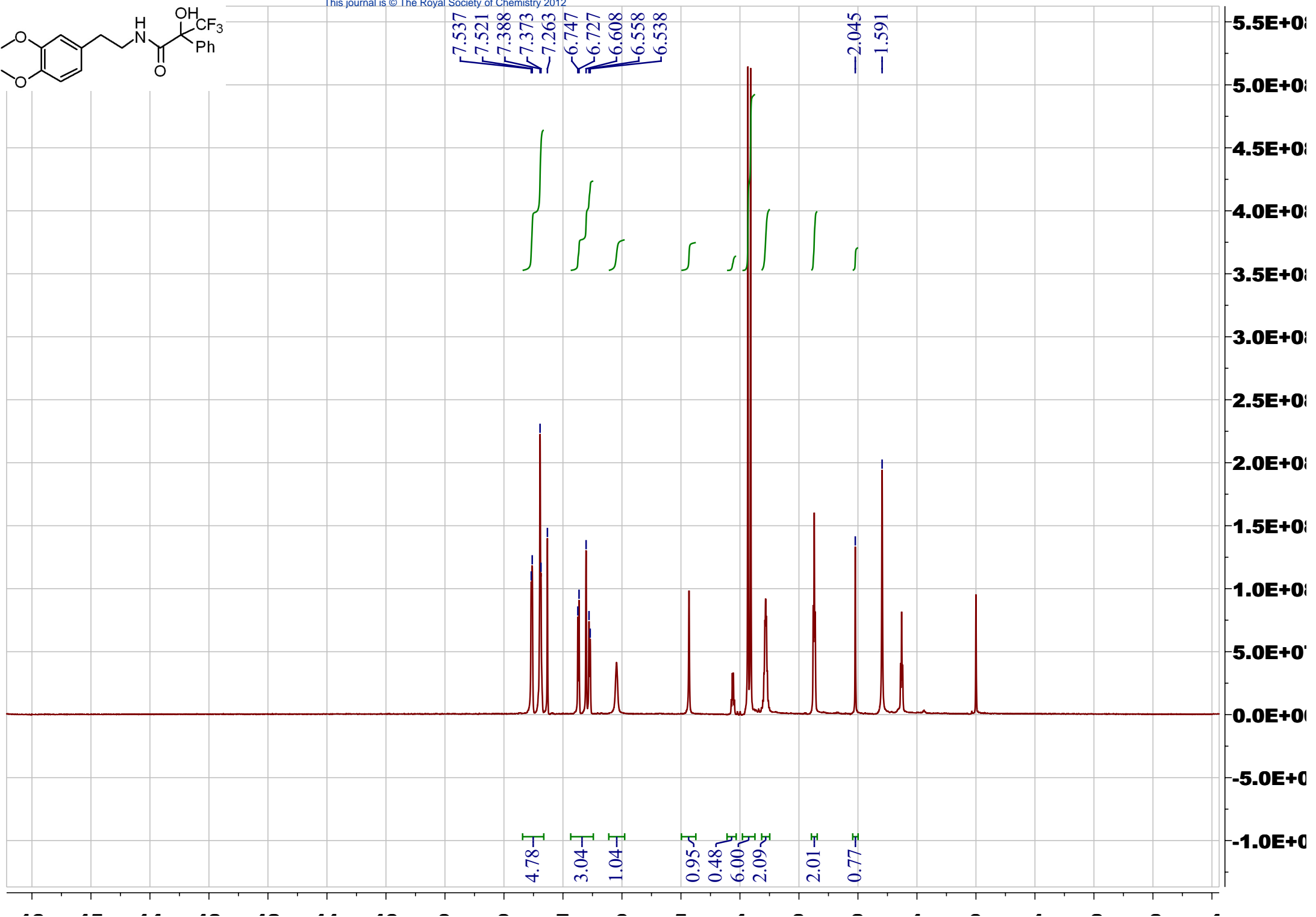
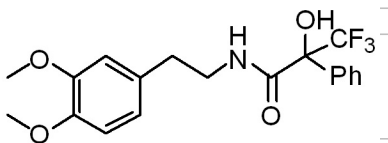
Unknown NMR (101 MHz,) δ 167.27, 134.22, 134.12, 133.50, 129.76, 129.67, 129.51, 129.36, 128.97, 127.19, 126.27, 42.55.



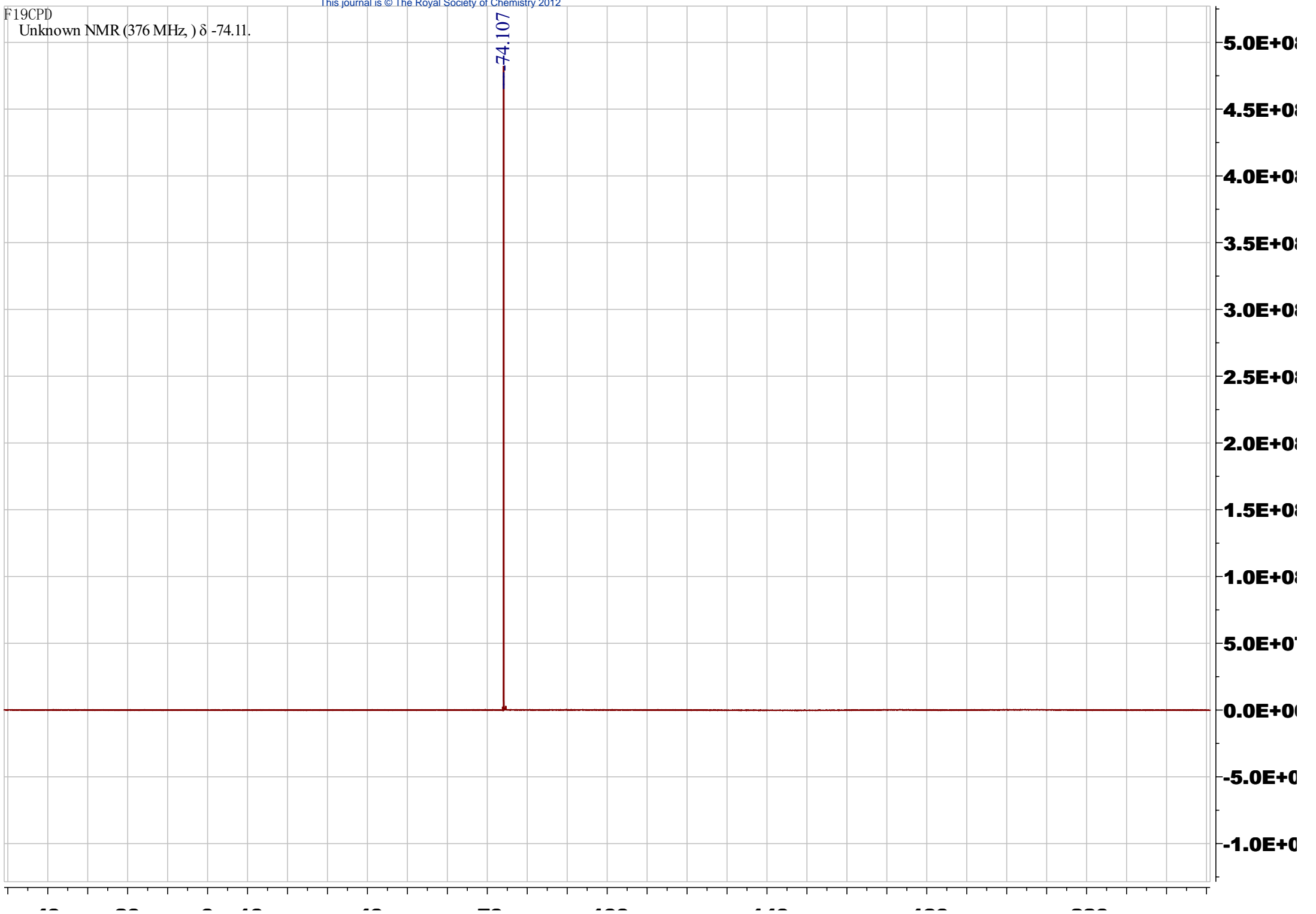
328.0953

Sample Name	lc/ms	Position	Vial 5	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-6-3.d (6e)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:35:34 AM





F19CPD
Unknown NMR (376 MHz,) δ -74.11.

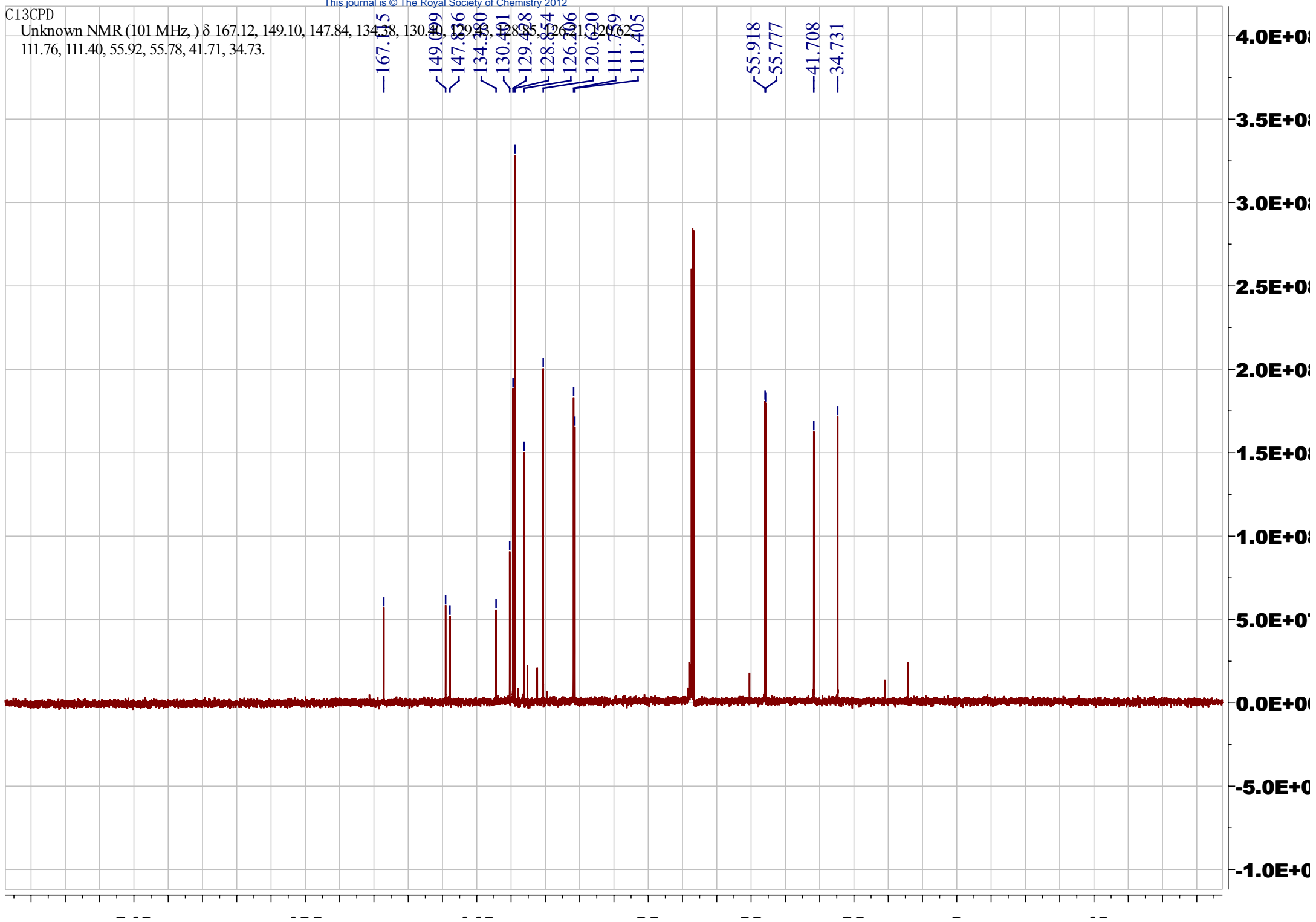


C13CPD

Unknown NMR (101 MHz,) δ 167.12, 149.10, 147.84, 134.58, 130.99, 129.99, 128.85, 126.26, 120.62, 111.76, 111.405, 55.92, 55.78, 41.71, 34.73.

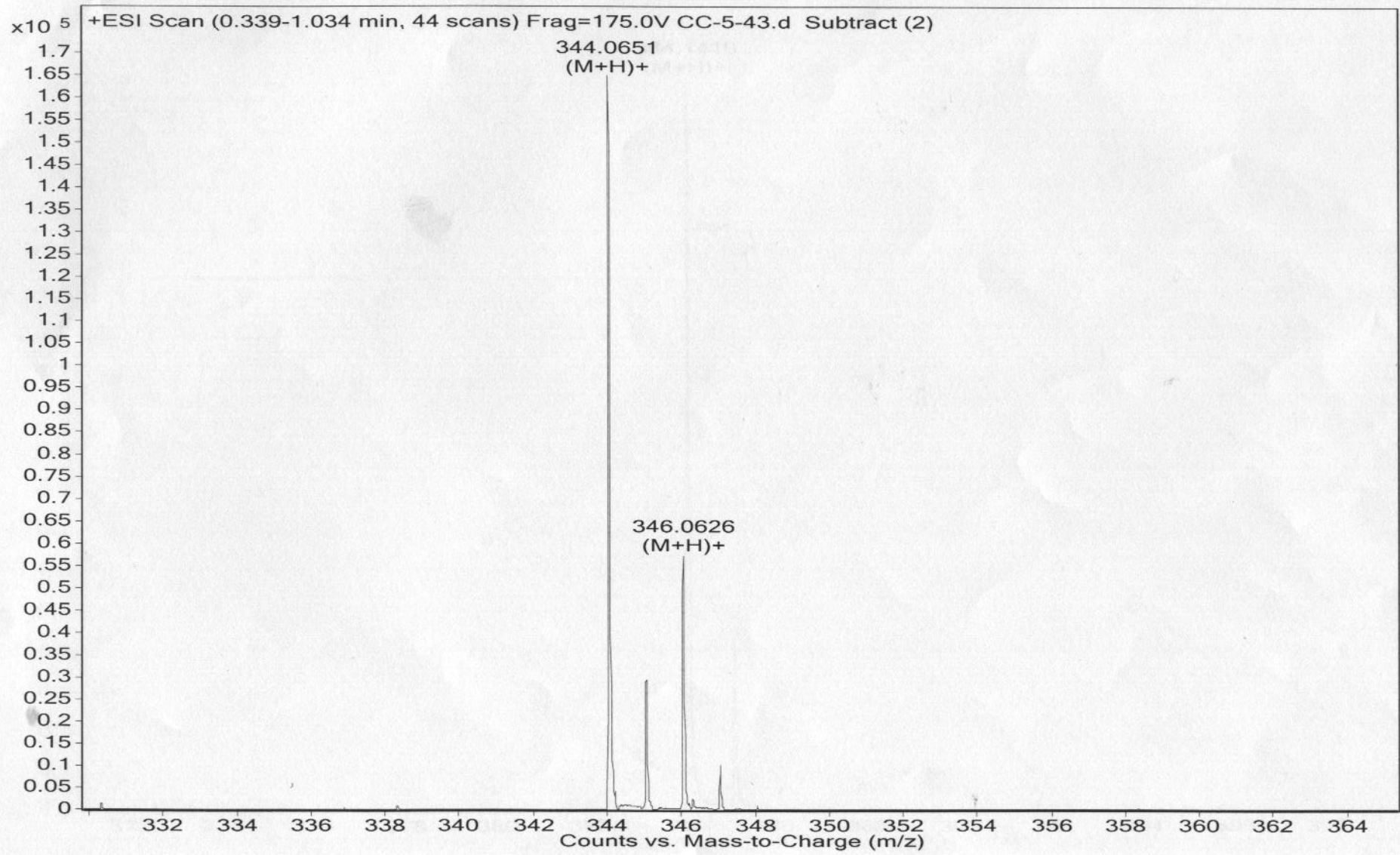
167.125
149.099
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134.580
130.991
129.988
128.854
126.206
120.620
111.769
111.405

55.918
55.777
41.708
34.731



344.0660

Sample Name	lc/ms	Position	Vial 6	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-5-43.d (6f)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 11:41:54 AM



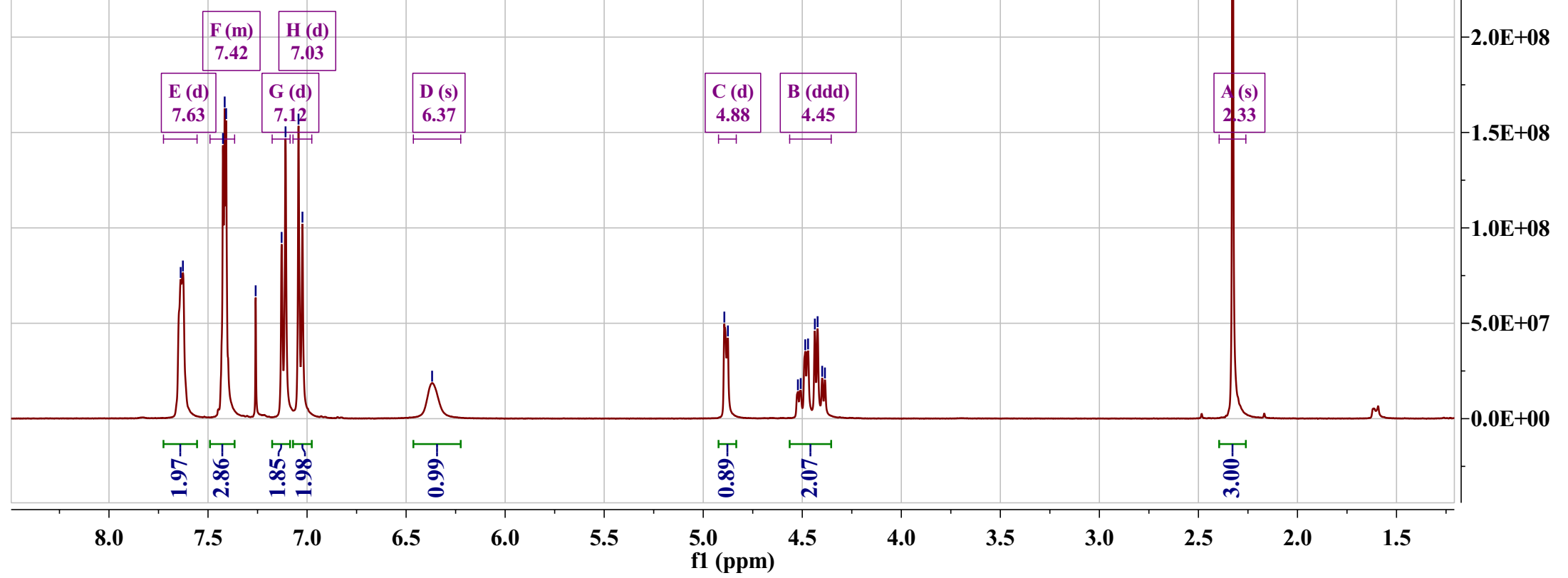
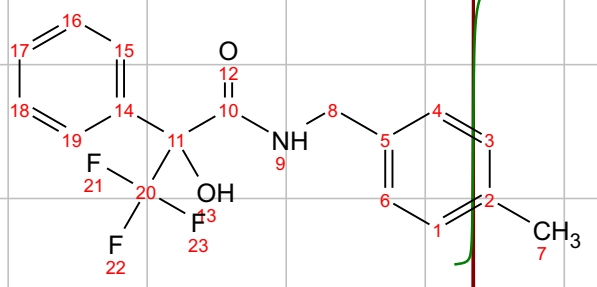
cc-5-4
PROTON

7.64
7.63
7.42
7.42
7.41
7.26
7.13
7.11
7.04
7.02

4.89
4.88
4.52
4.51
4.48
4.47
4.44
4.42
4.40
4.39

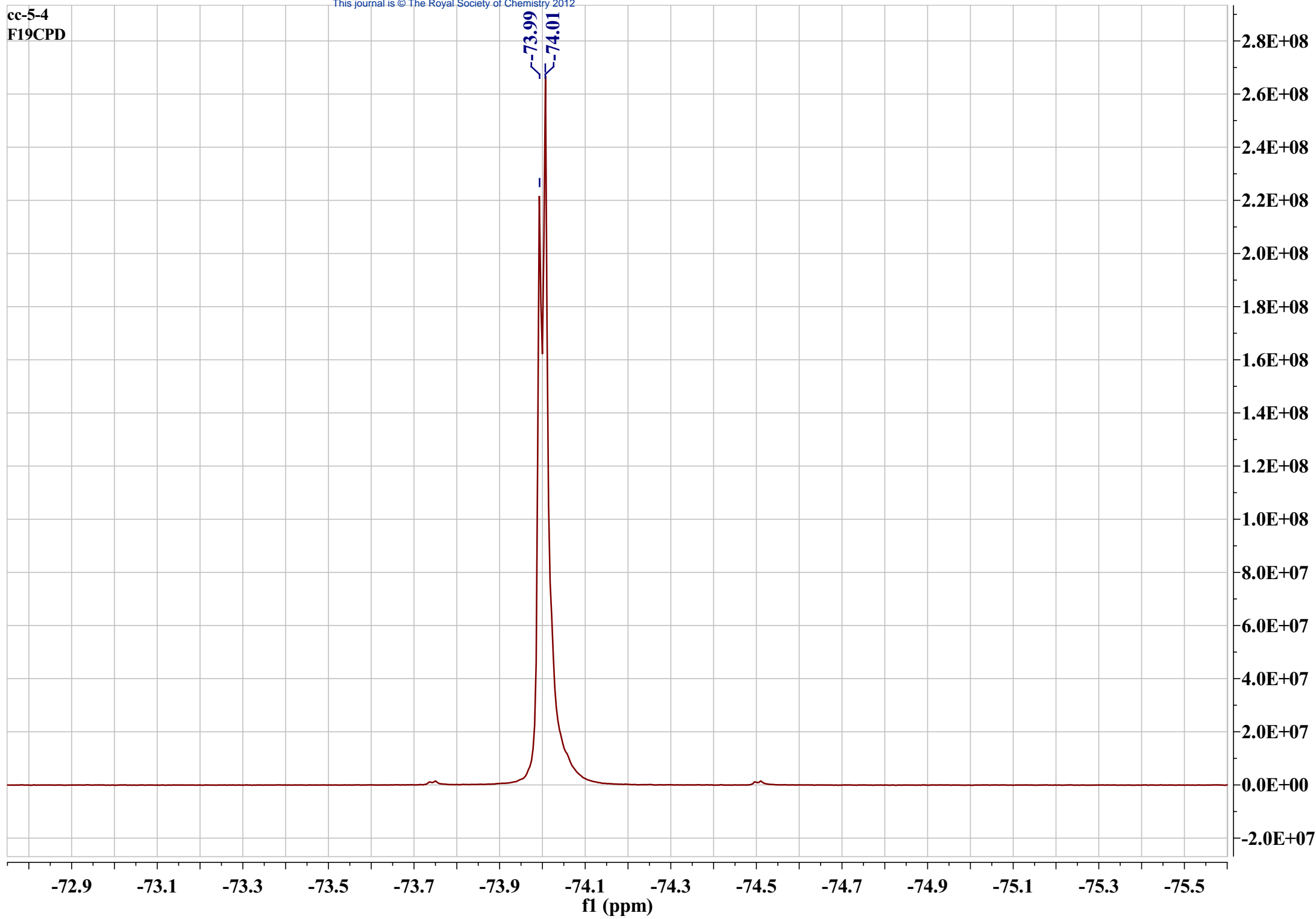
2.33

¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, *J* = 4.5 Hz, 2H), 7.49 – 7.37 (m, 3H), 7.12 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.37 (s, 1H), 4.88 (d, *J* = 7.2 Hz, 1H), 4.45 (ddd, *J* = 34.1, 14.8, 5.6 Hz, 2H), 2.33 (s, 3H).

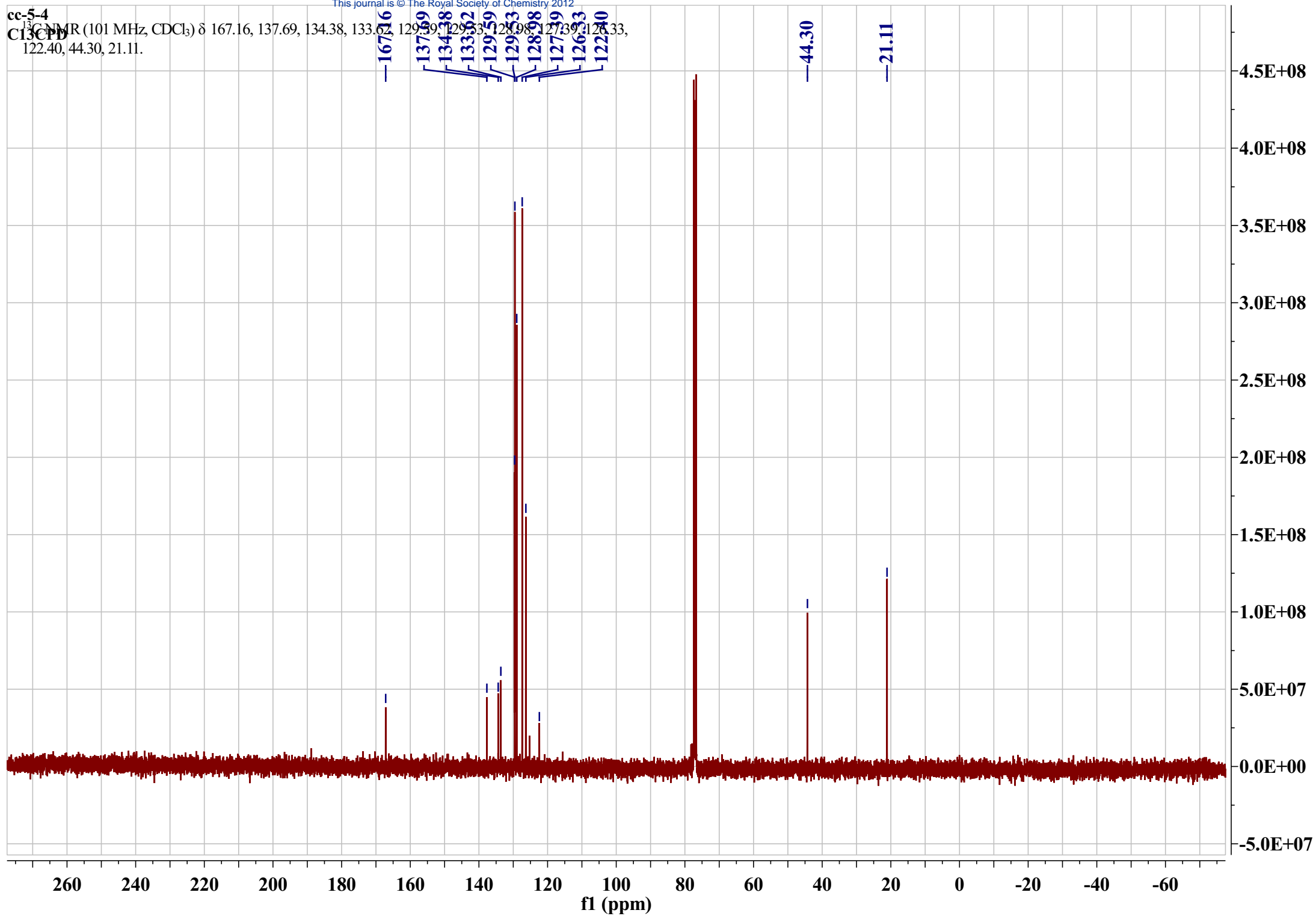


cc-5-4
F19CPD

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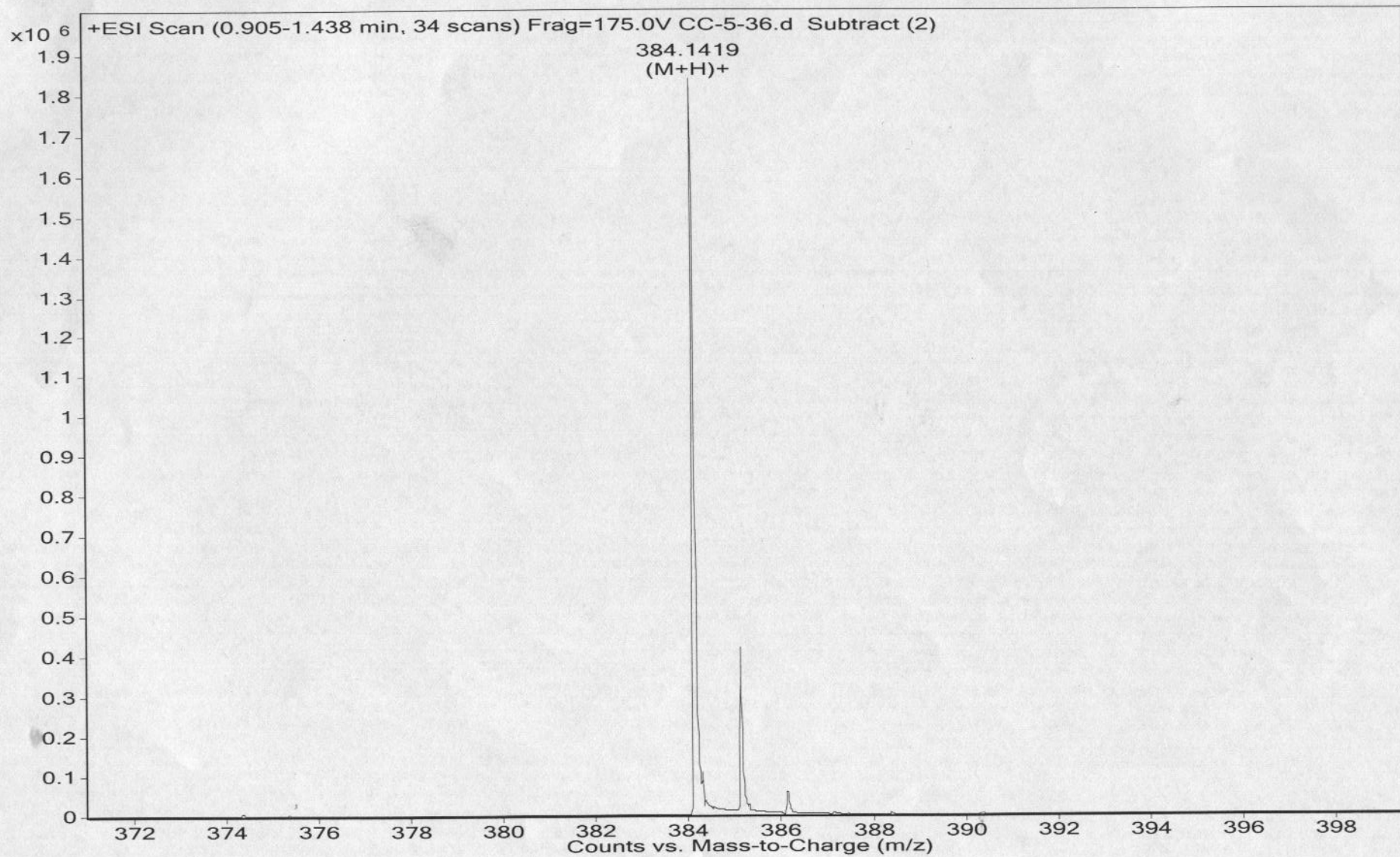


cc-5-4
¹³C NMR (101 MHz, CDCl₃) δ 167.16, 137.69, 134.38, 133.62, 129.59, 129.33, 128.98, 127.39, 126.33, 122.40, 44.30, 21.11.

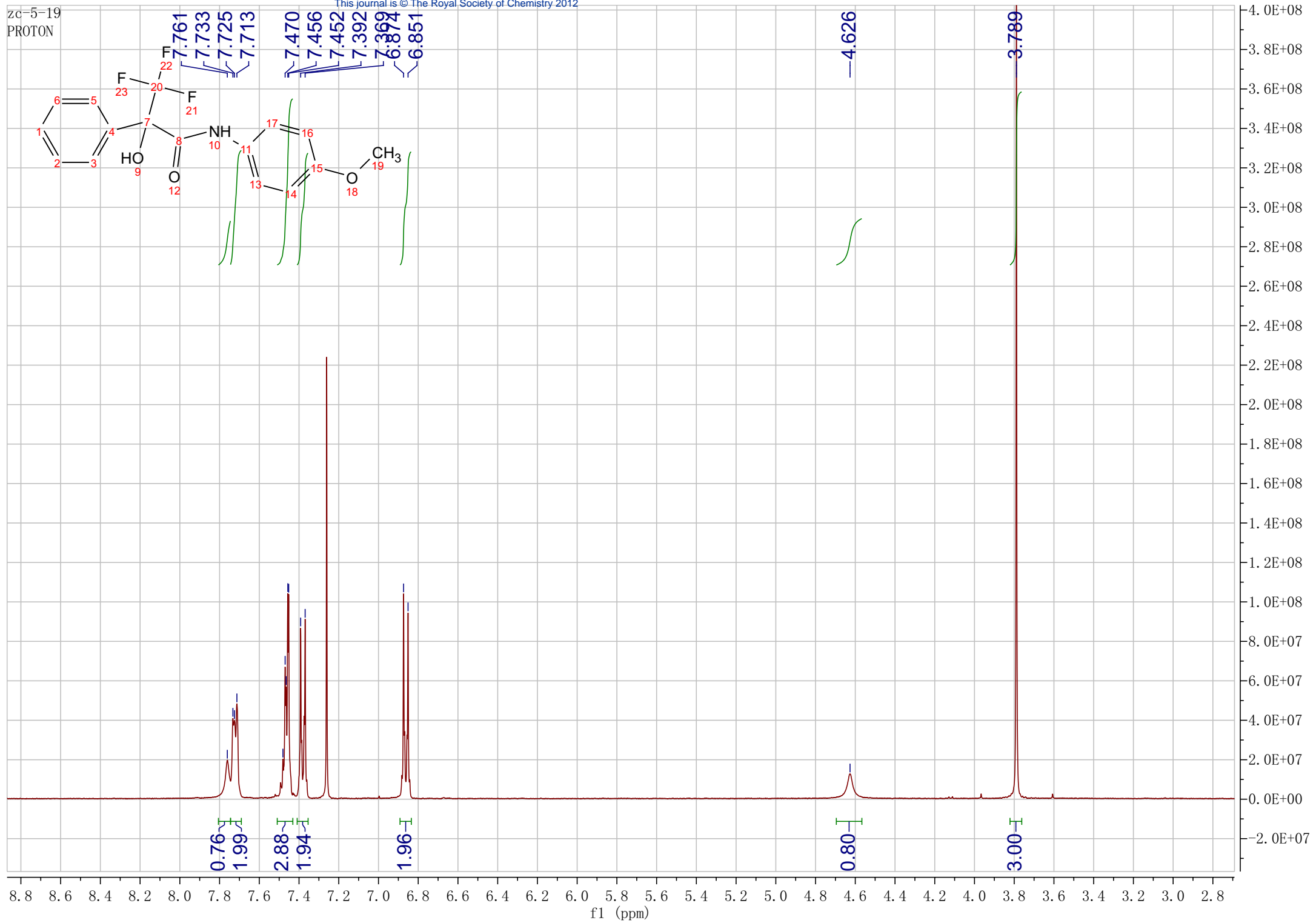


384.1417

Sample Name	lc/ms	Position	Vial 1	Instrument Name	Agilent_G6520_QTOF_L	User Name	Agilent FSE
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CC-5-36.d (69)	ACQ Method	chen-ms.m	Comment		Acquired Time	4/19/2012 12:06:29 PM

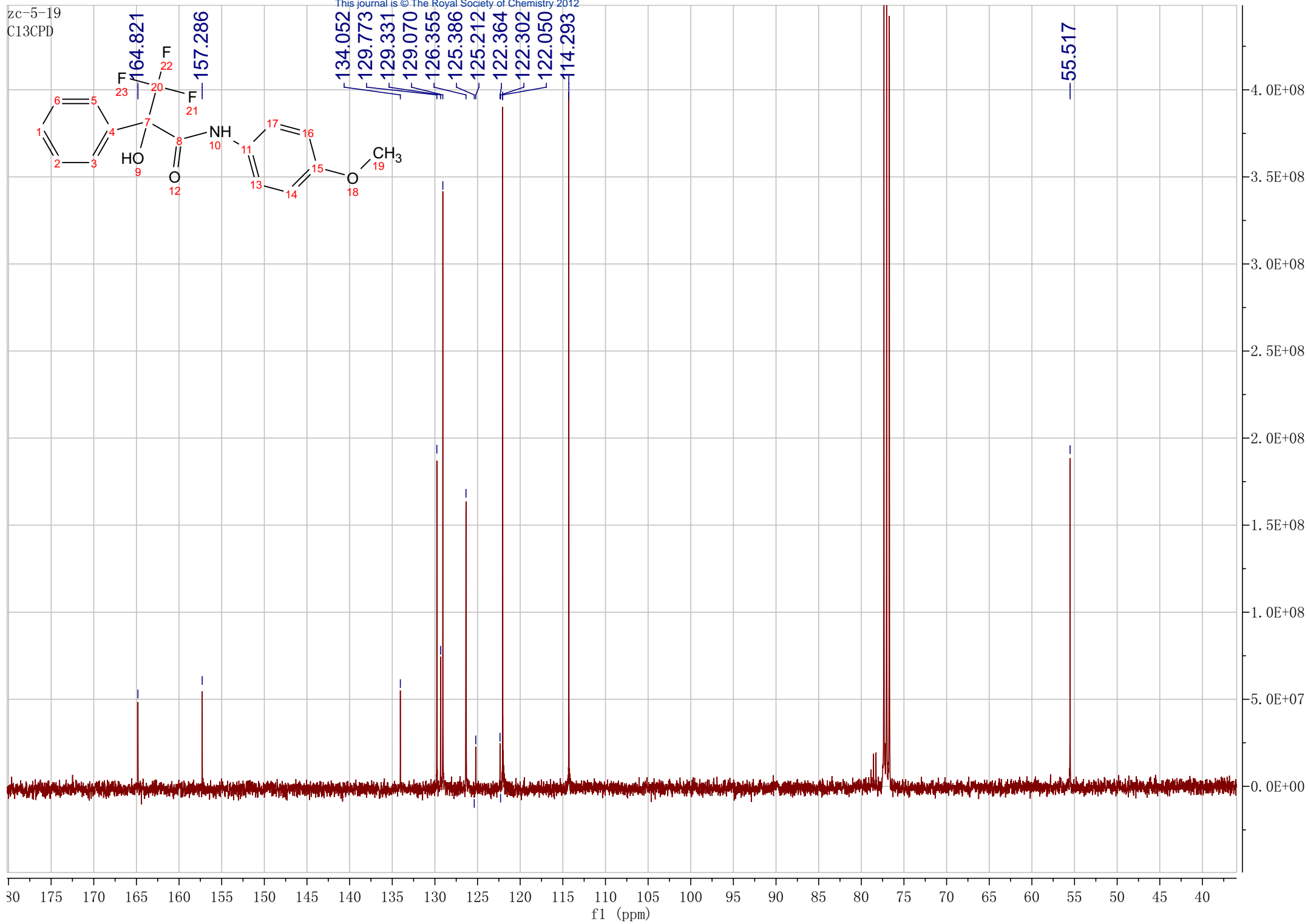


zc-5-19
PROTON

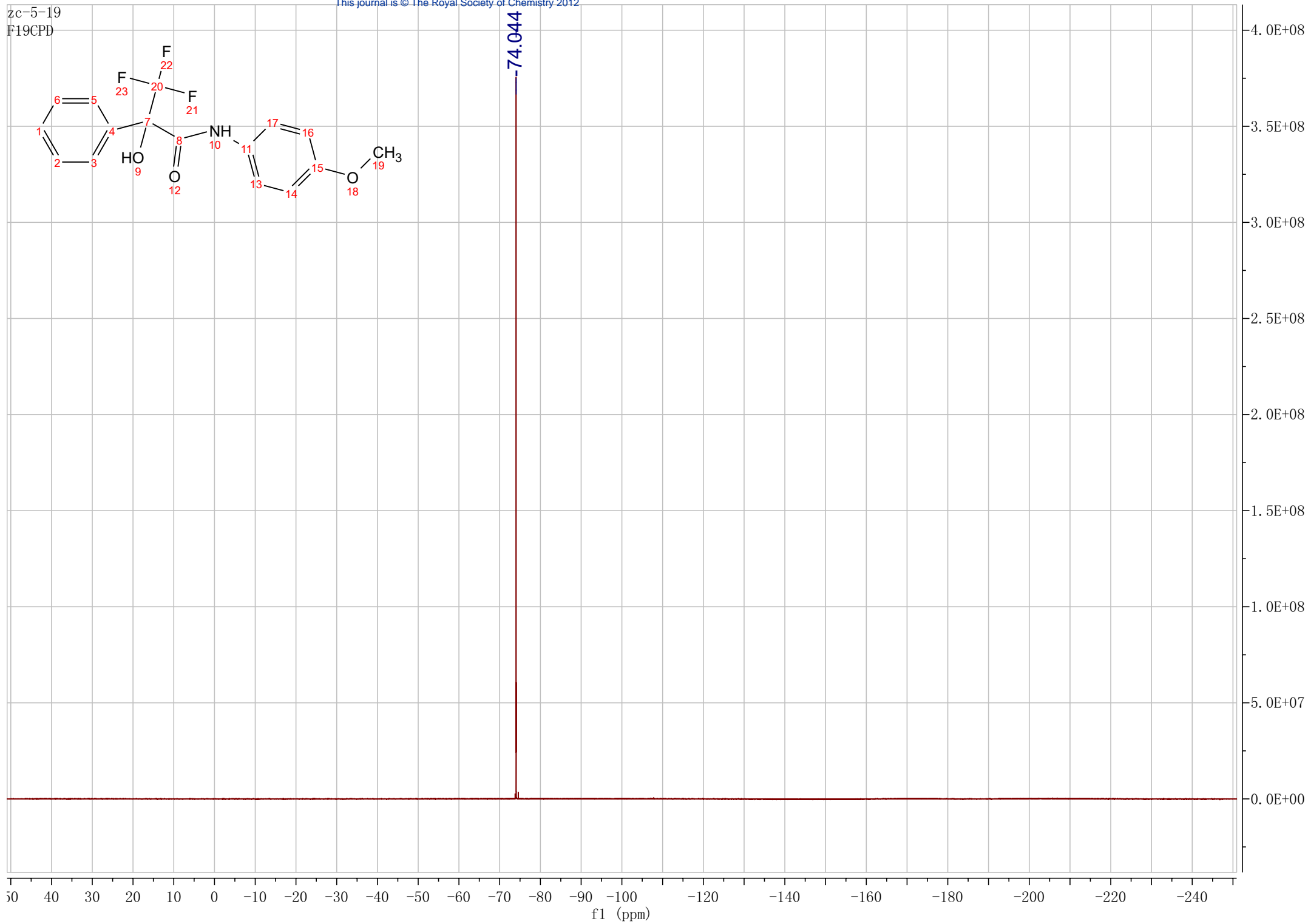
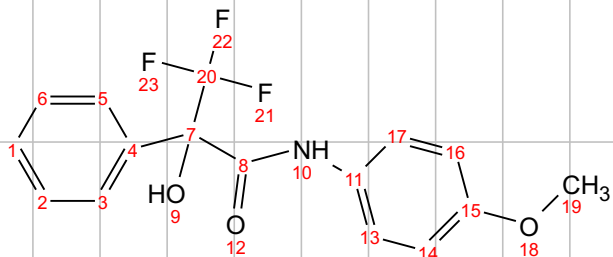


zc-5-19
C13CPD

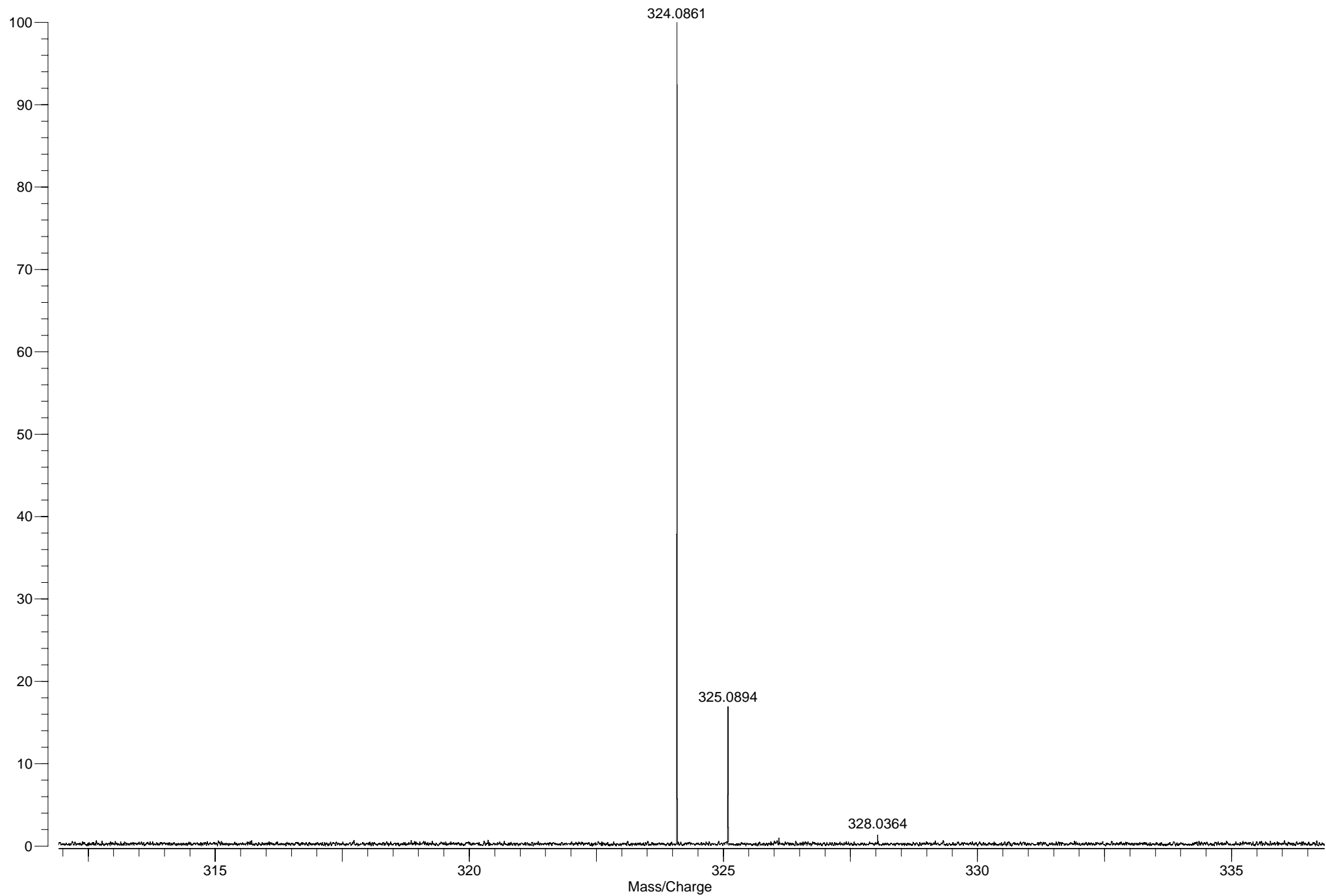
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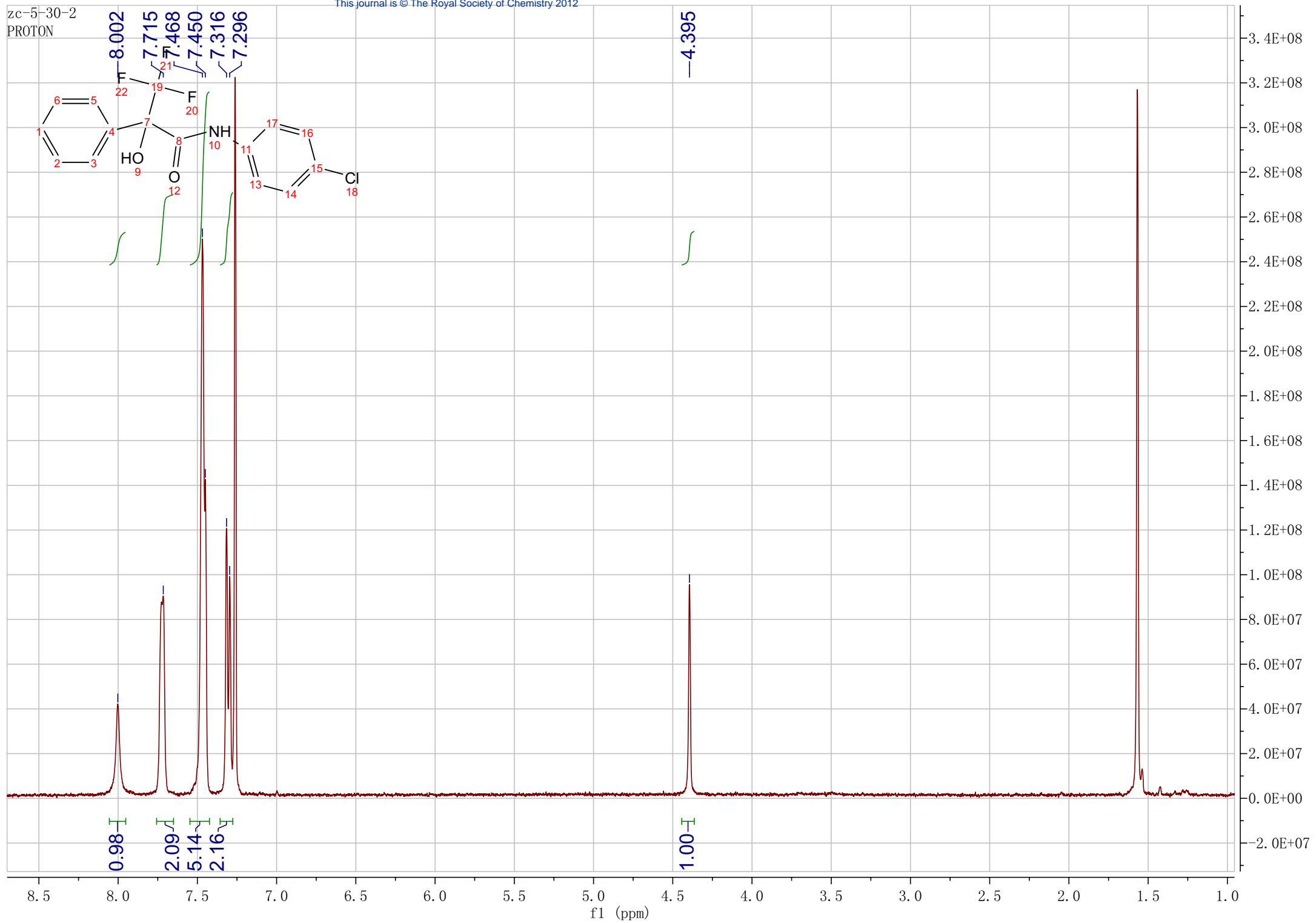
zc-5-19
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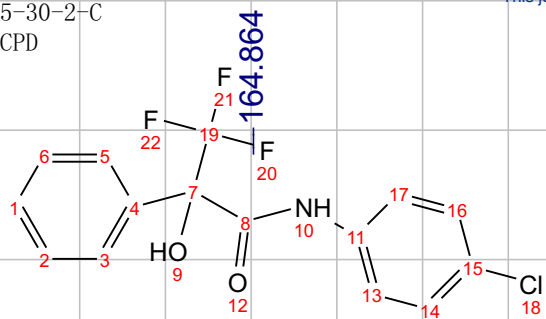


zc-5-30-2
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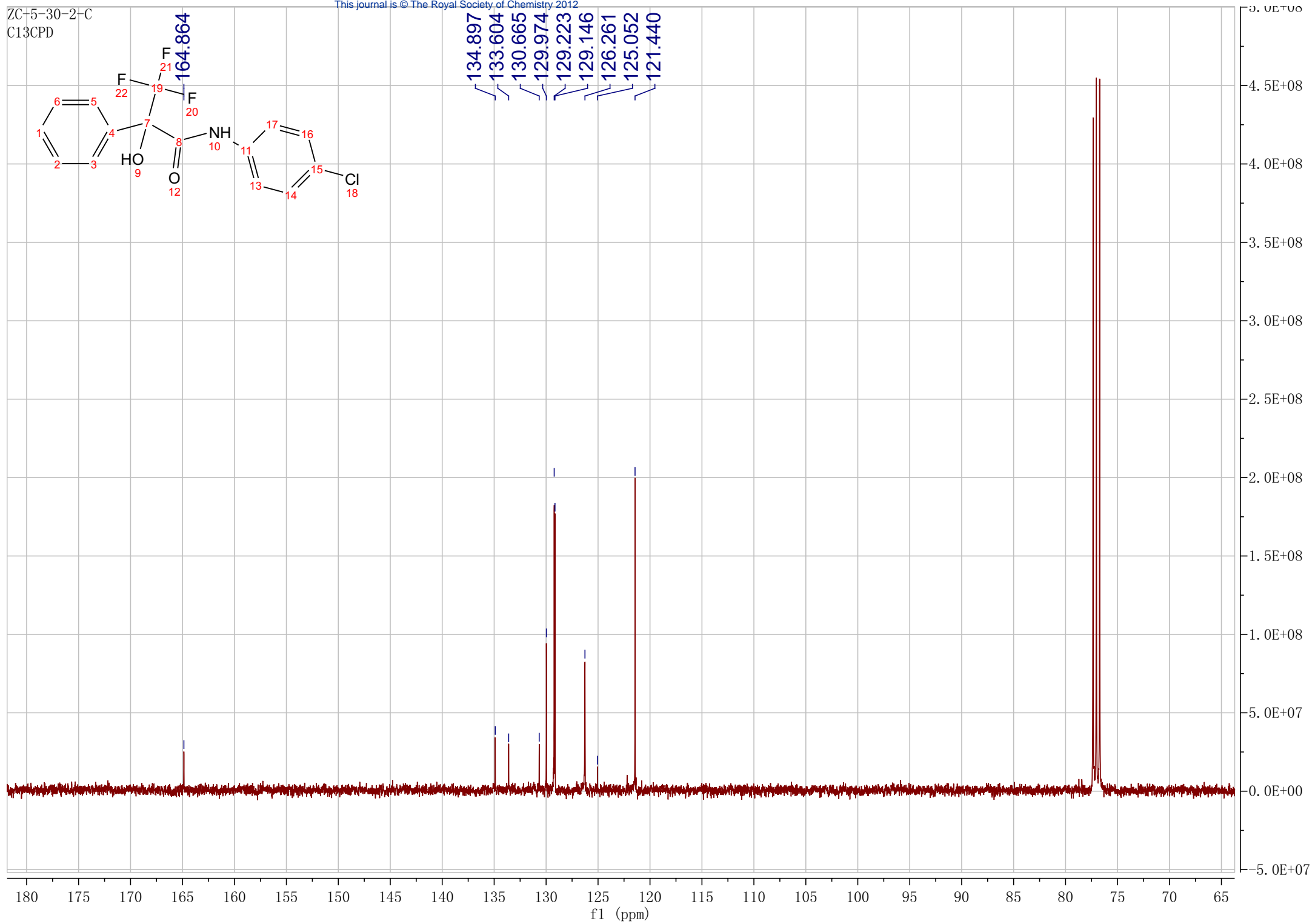


ZC-5-30-2-C
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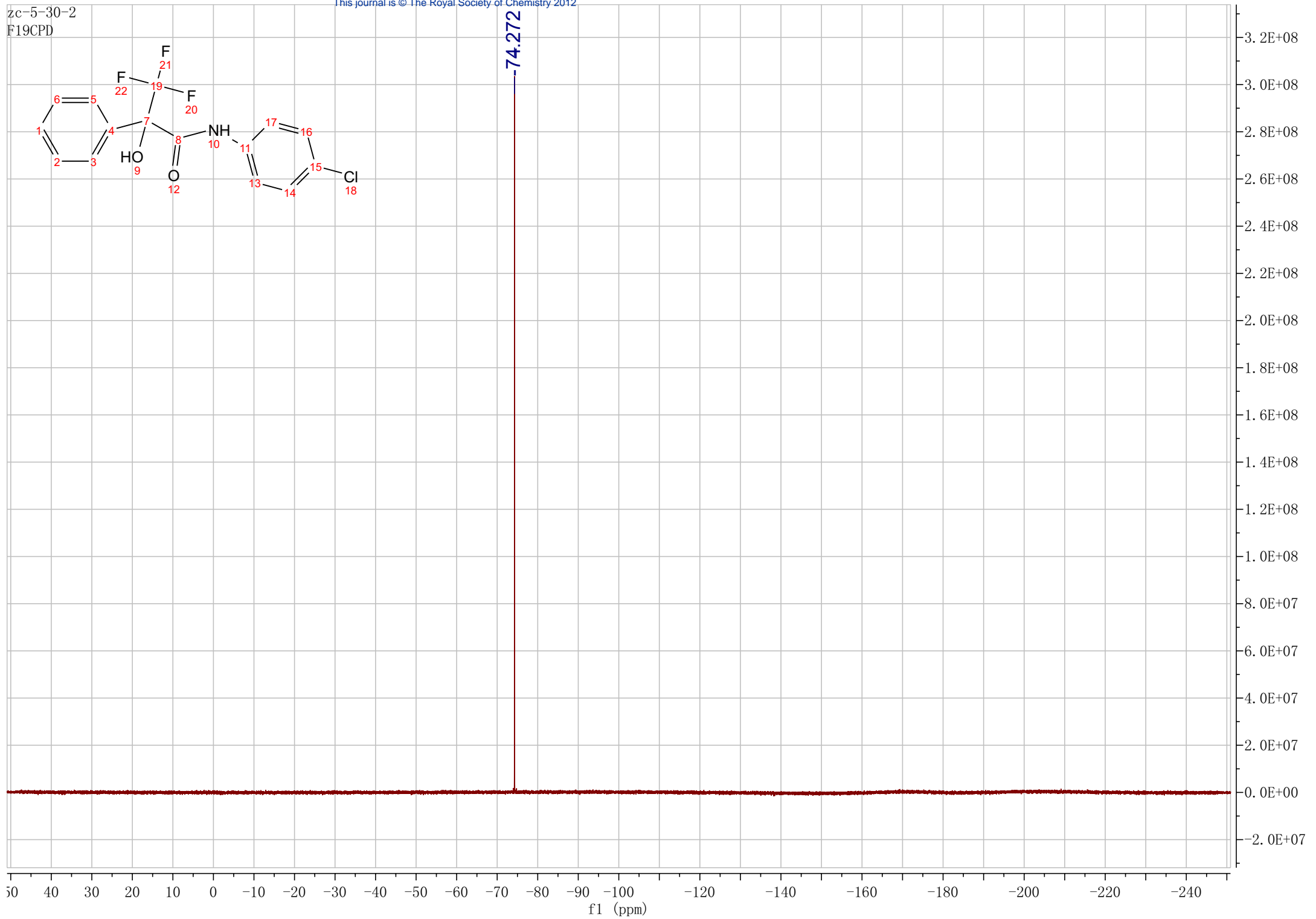
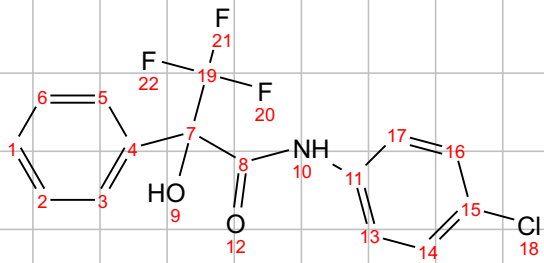


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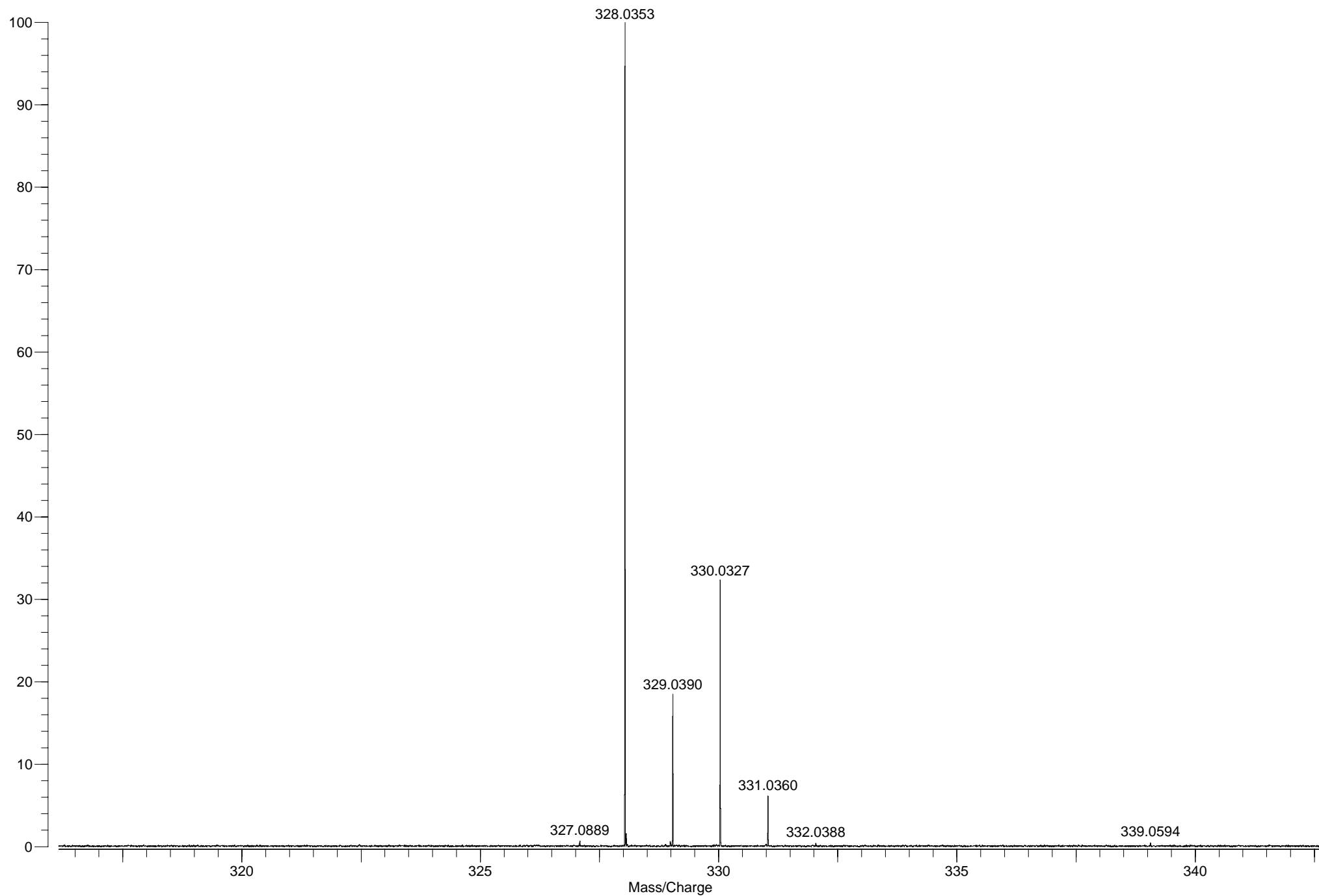


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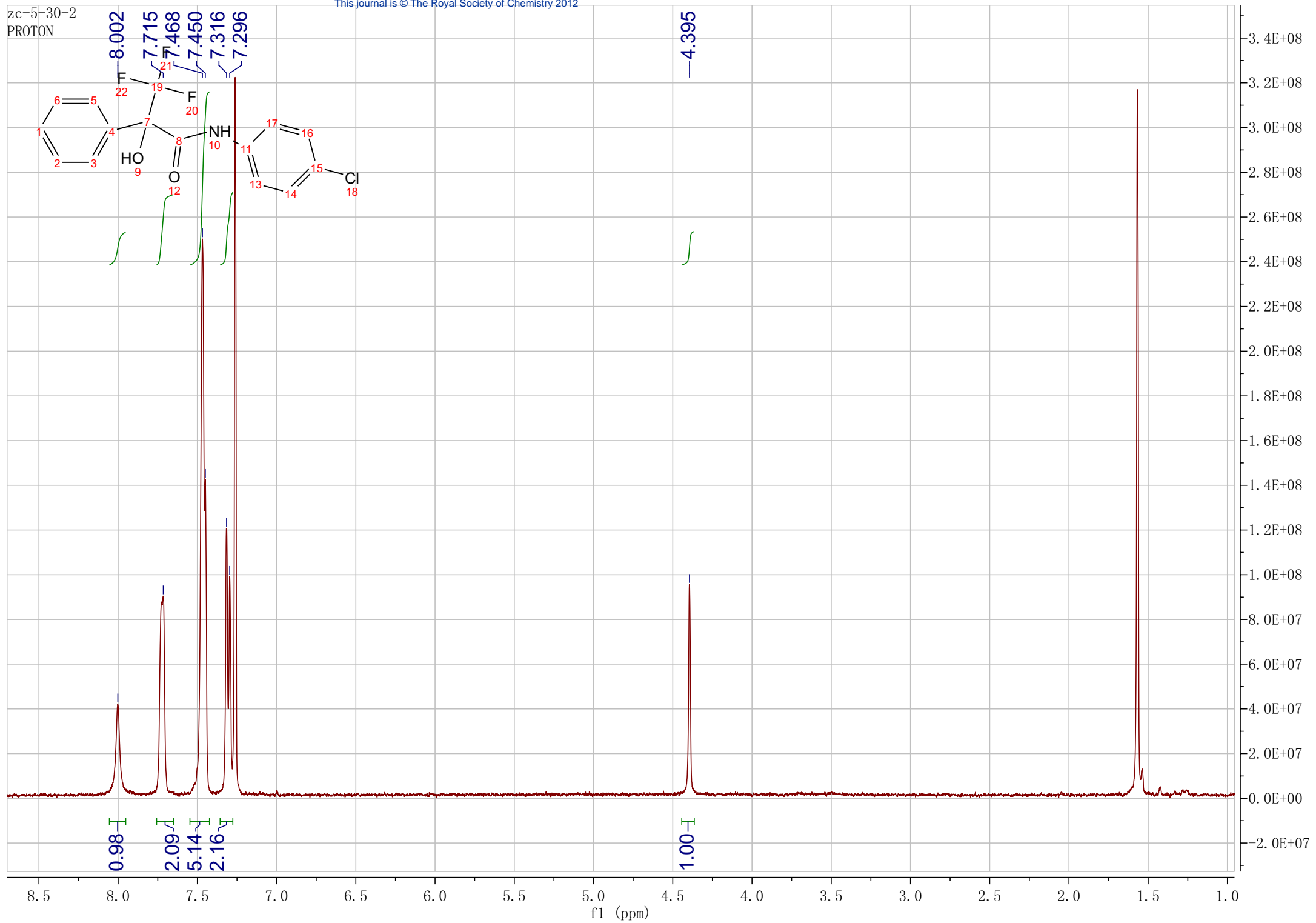
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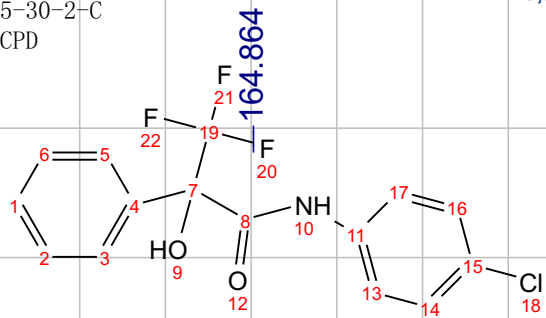


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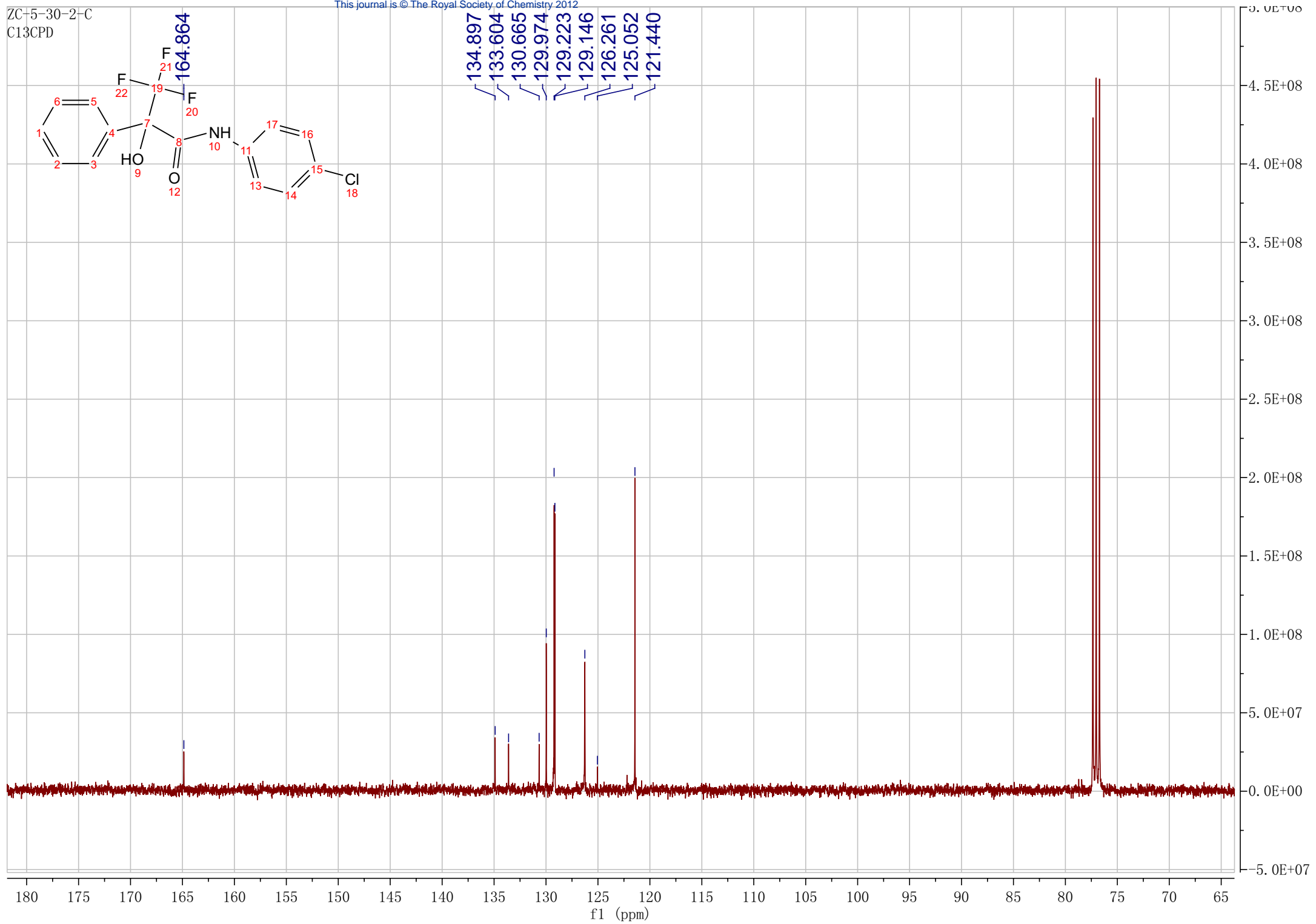


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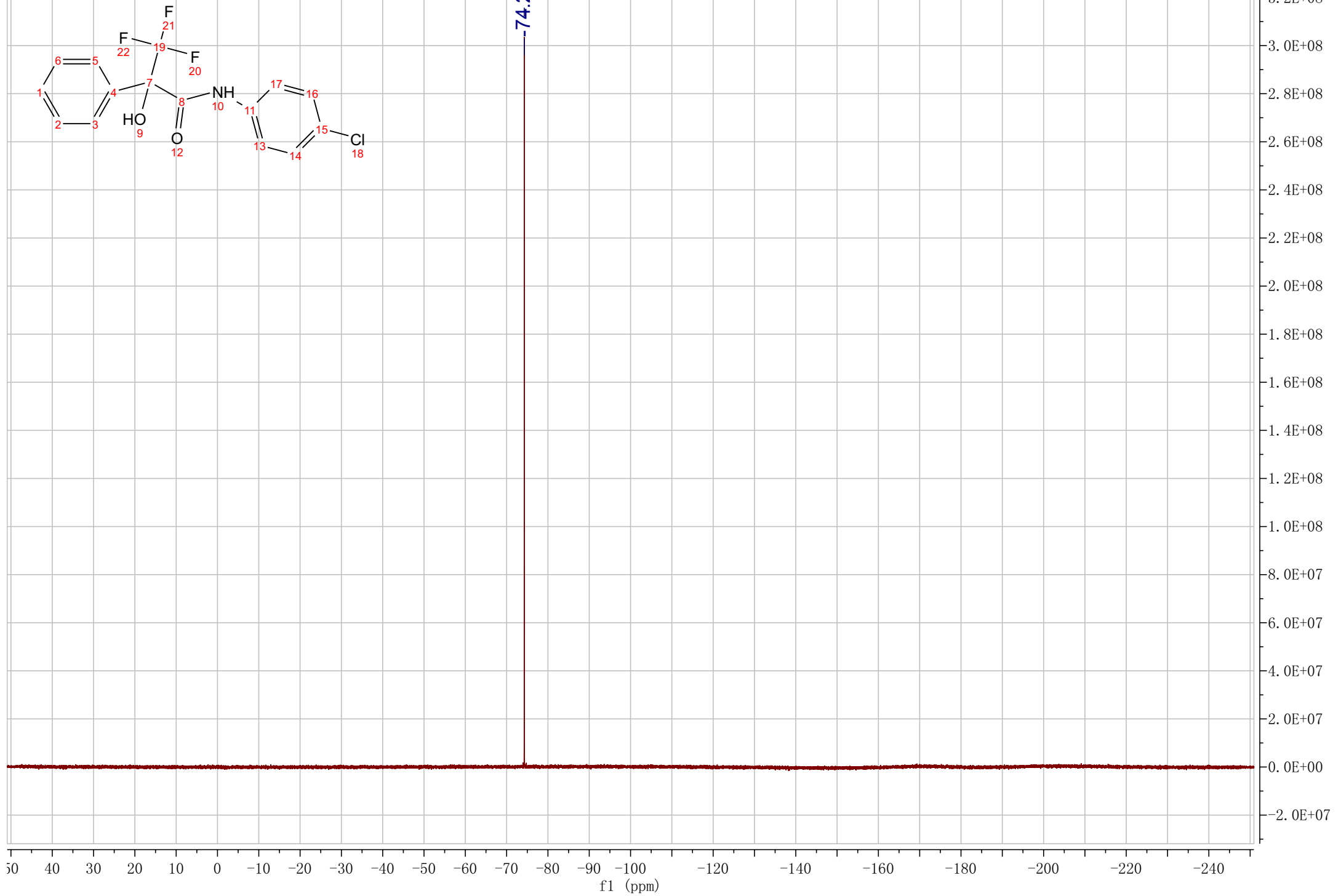


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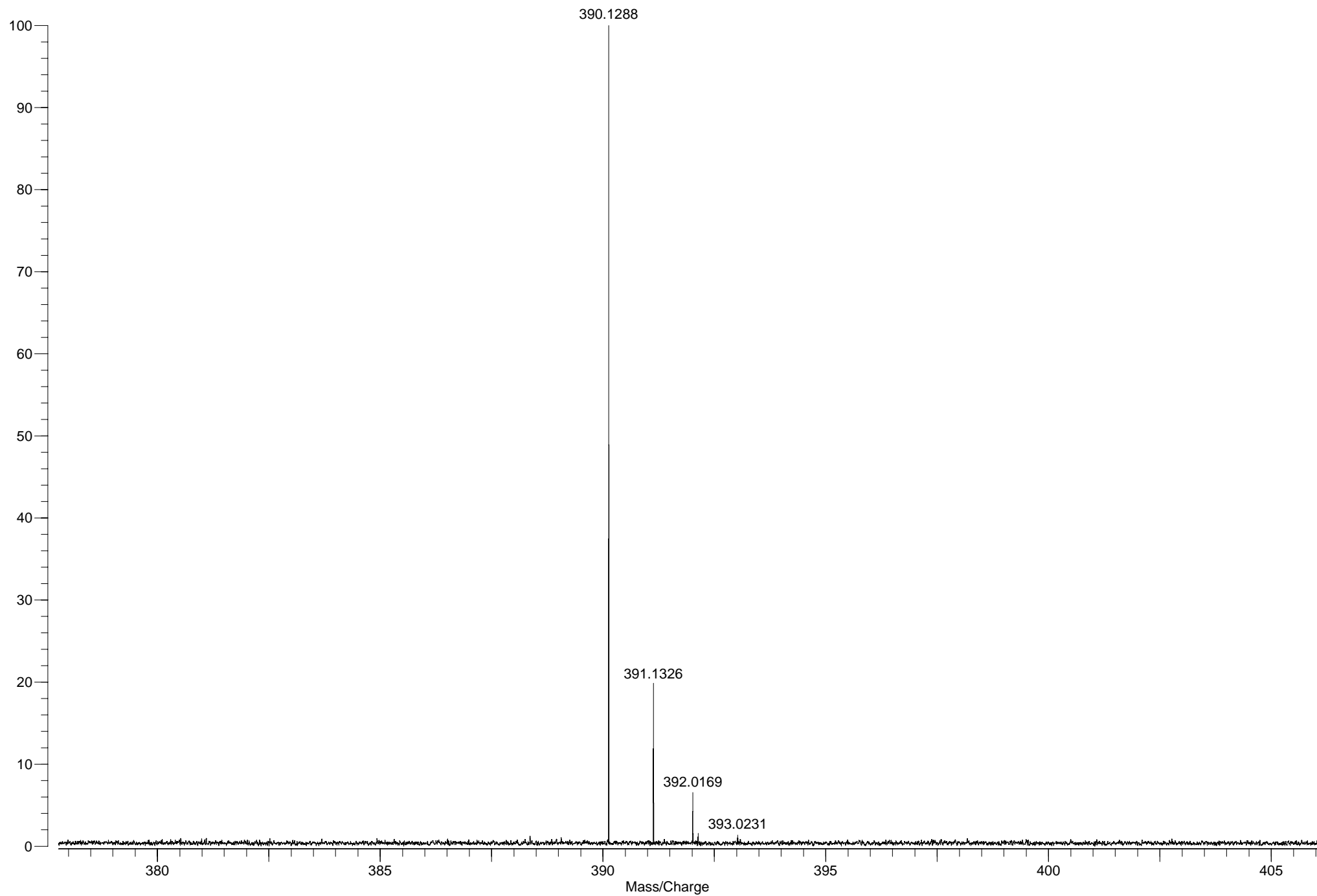


zc-5-30-2
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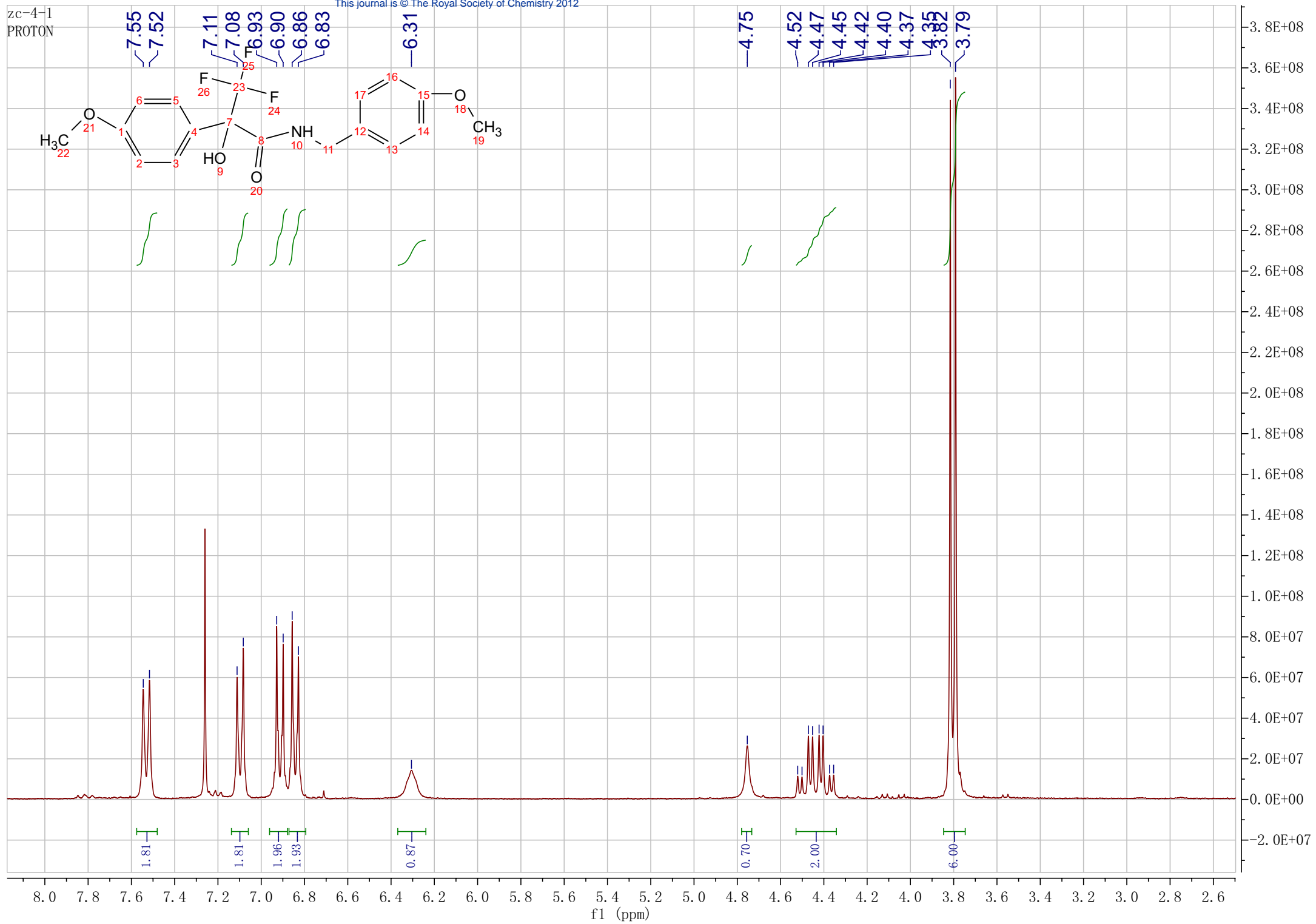


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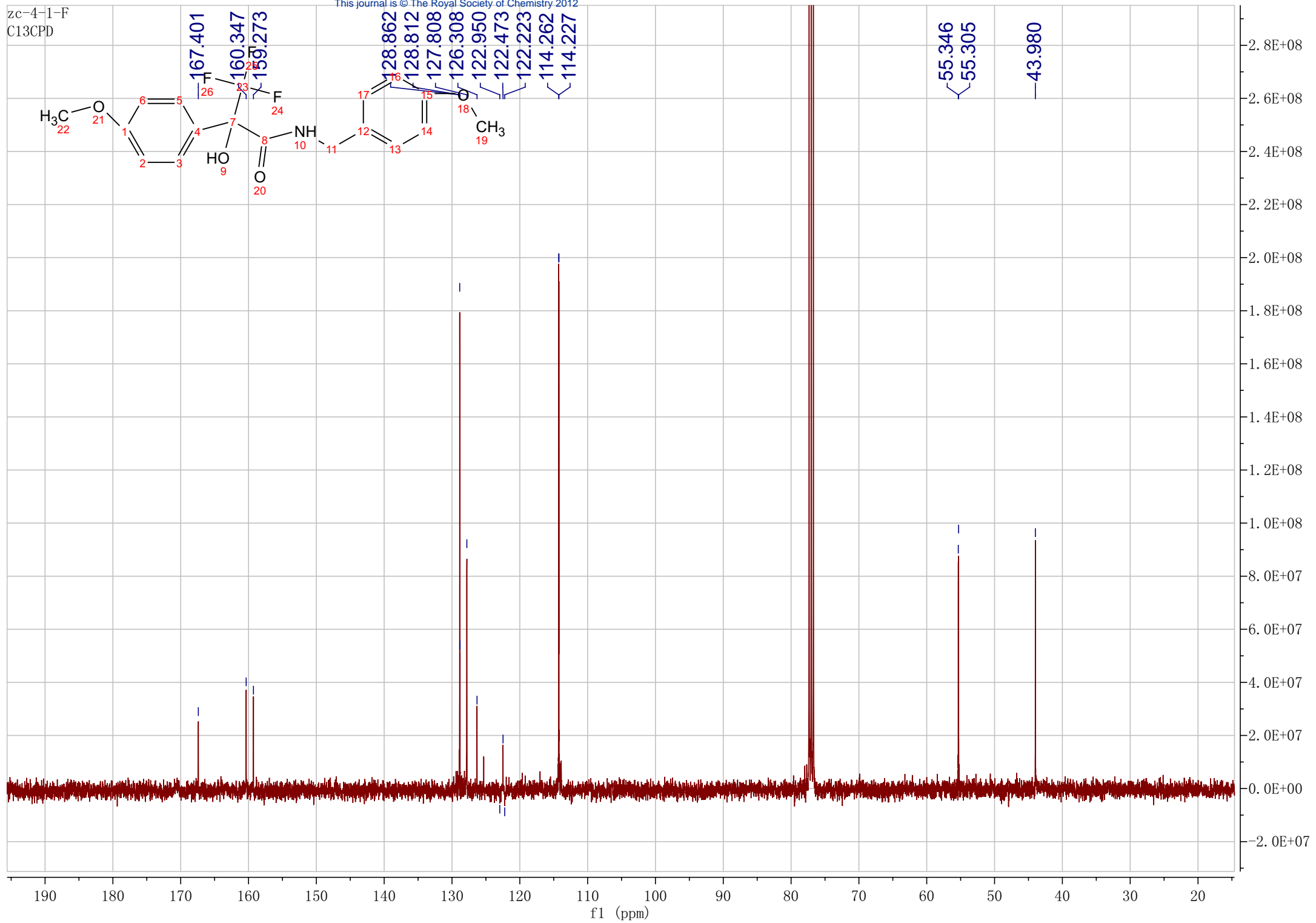
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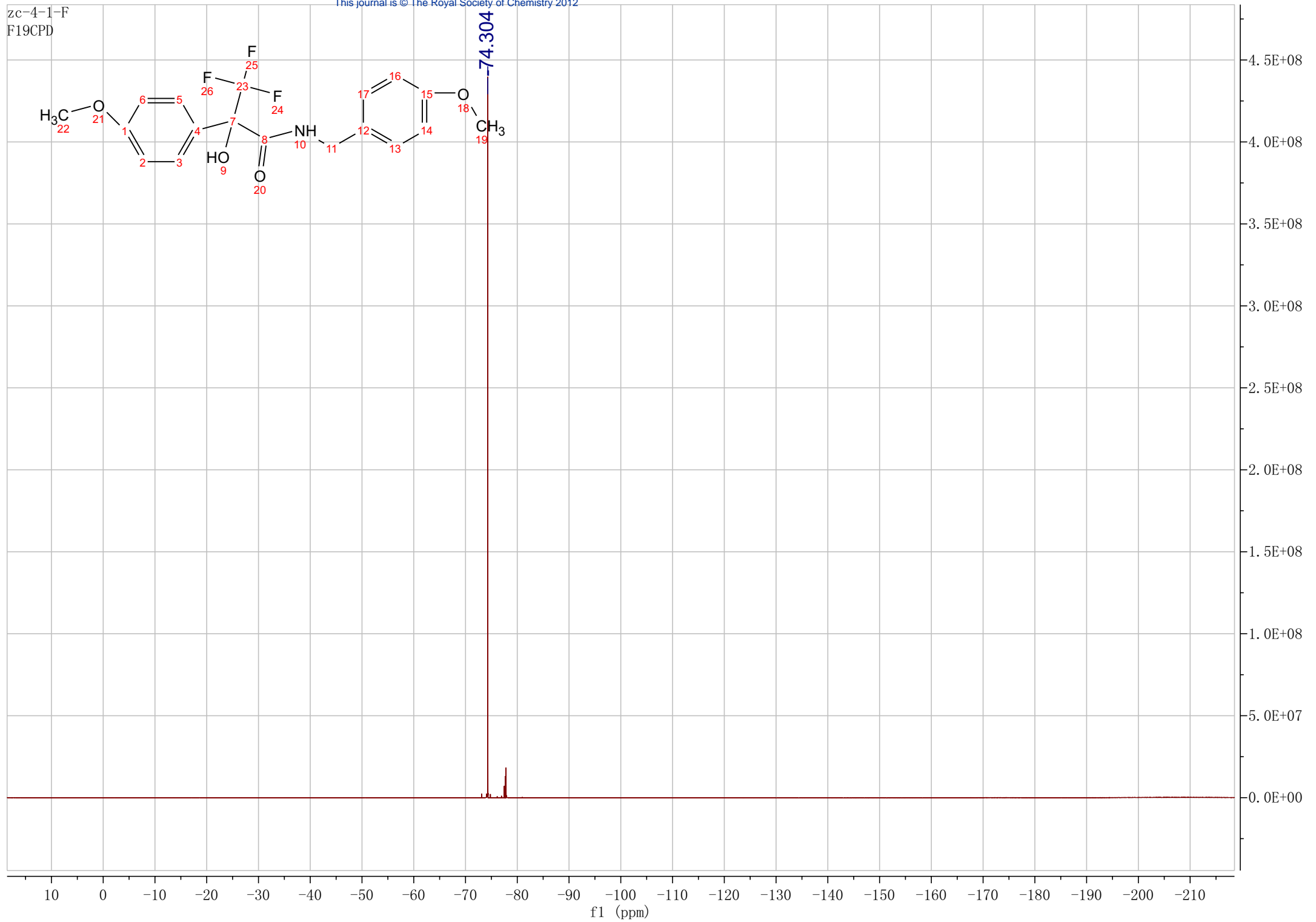
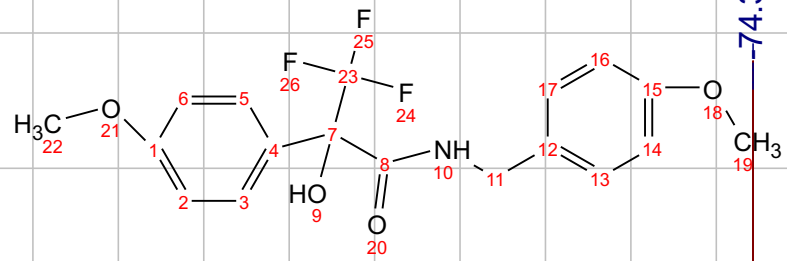
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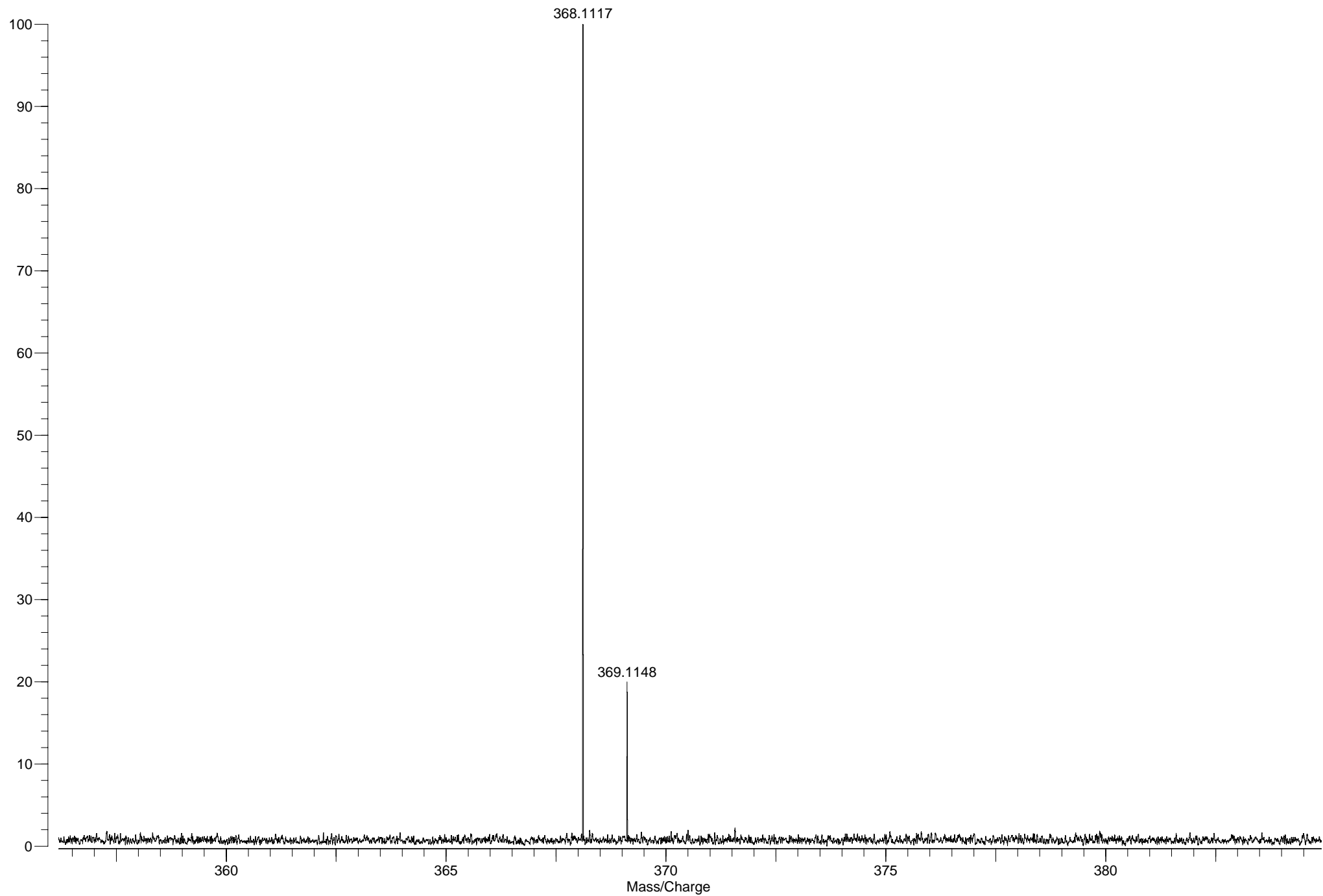


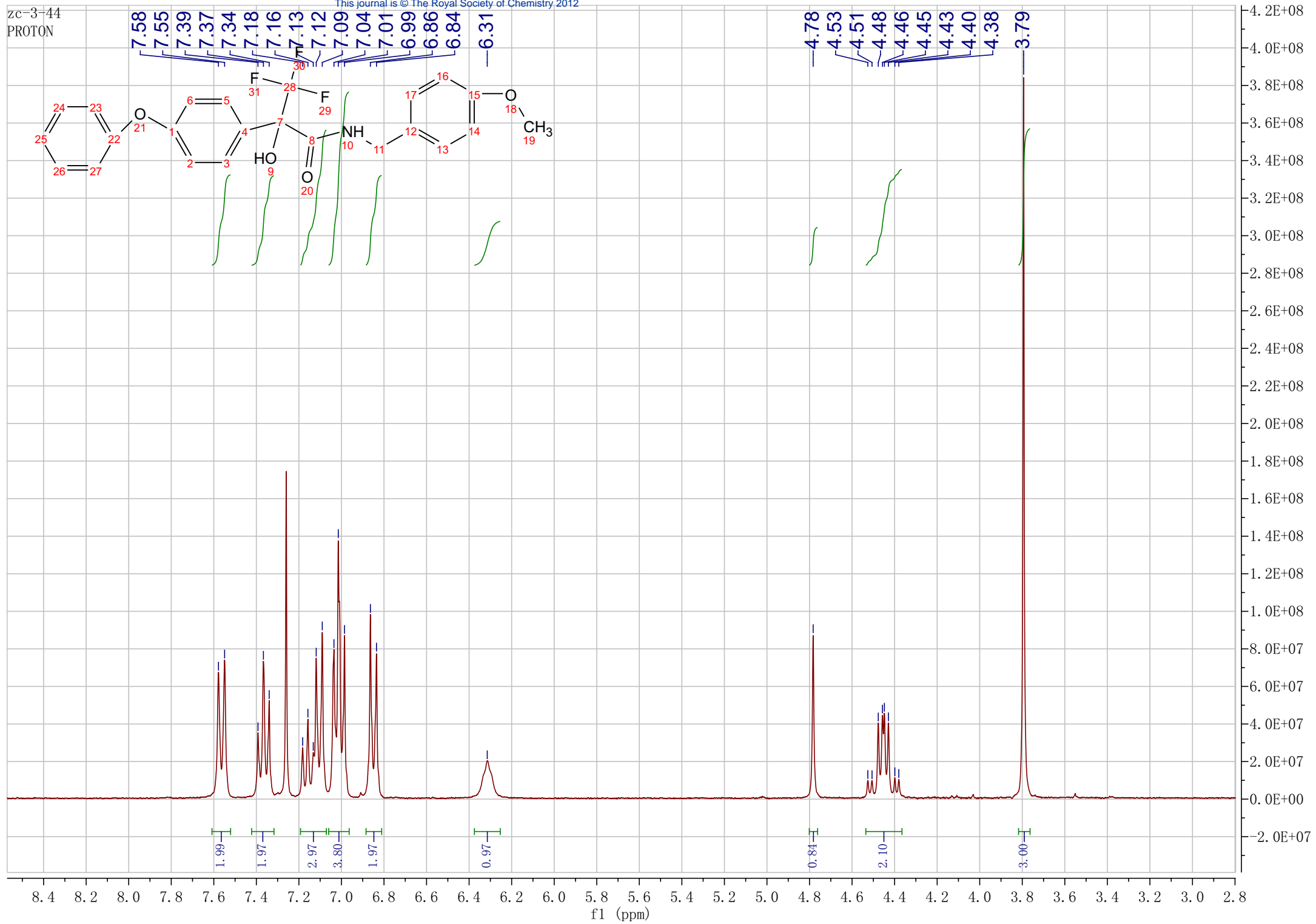
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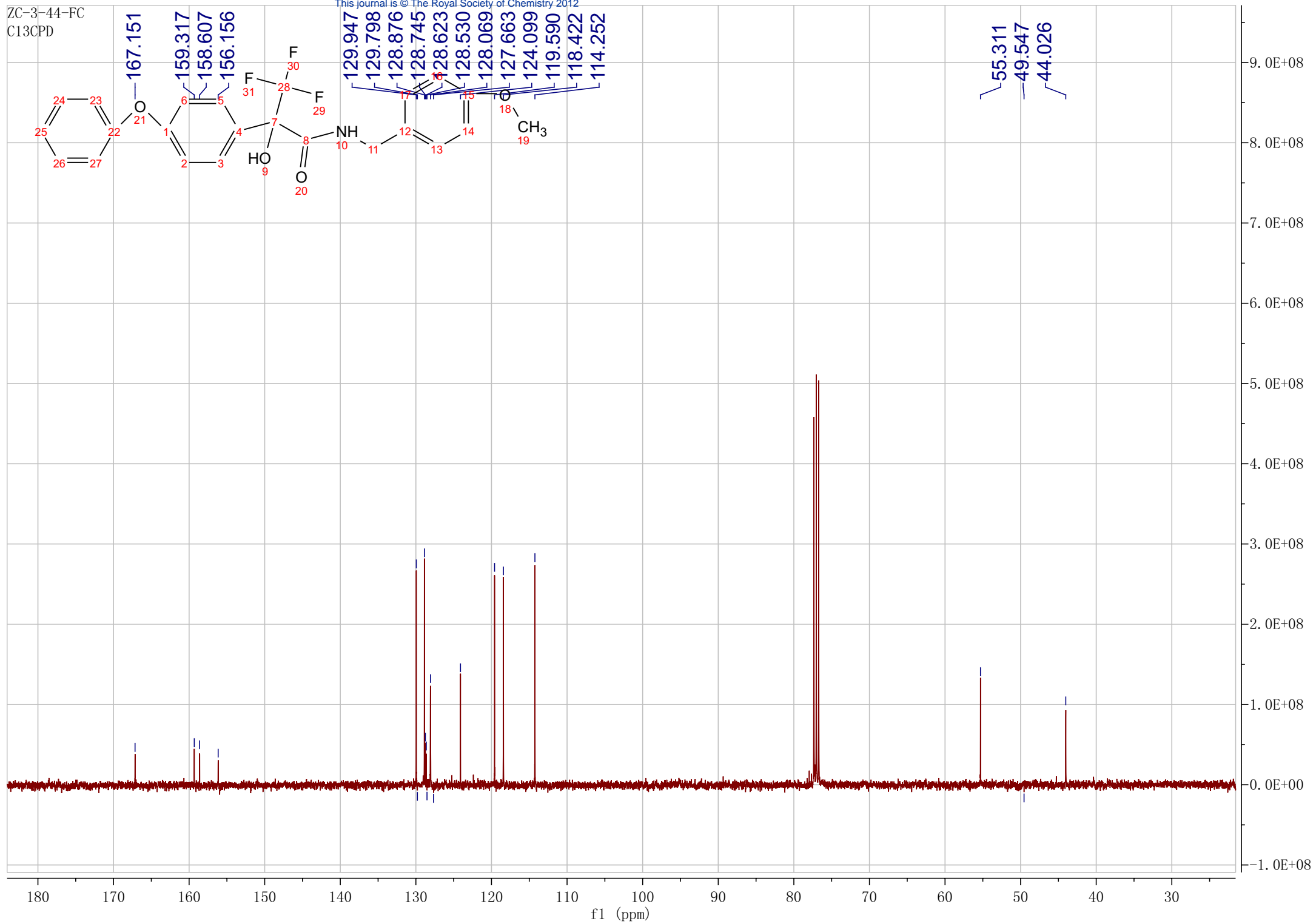
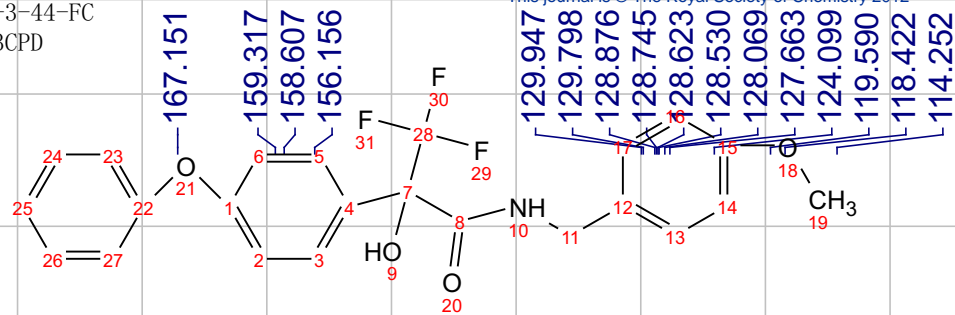
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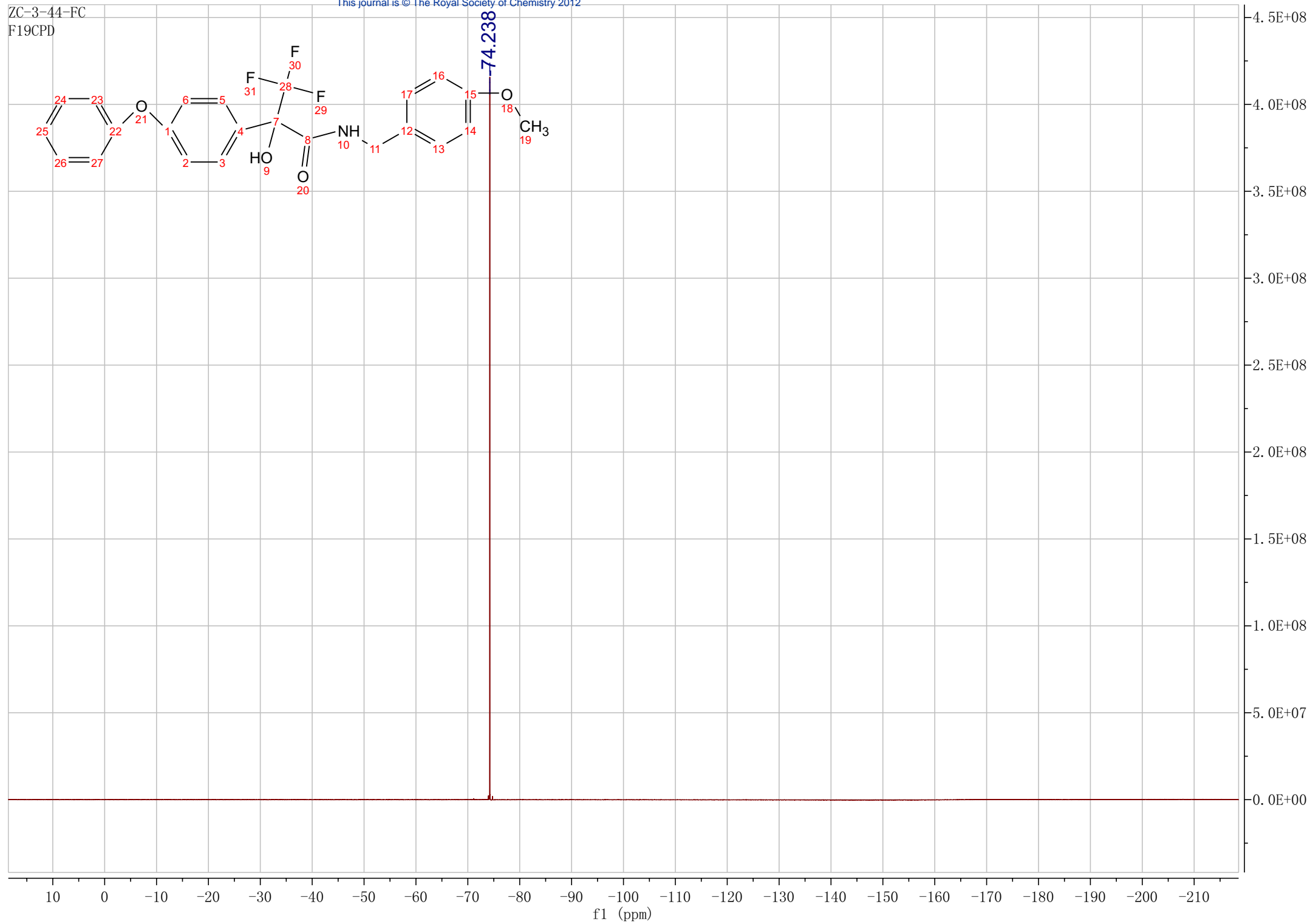
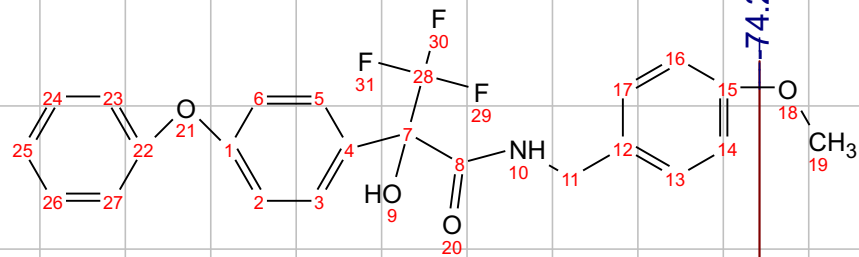


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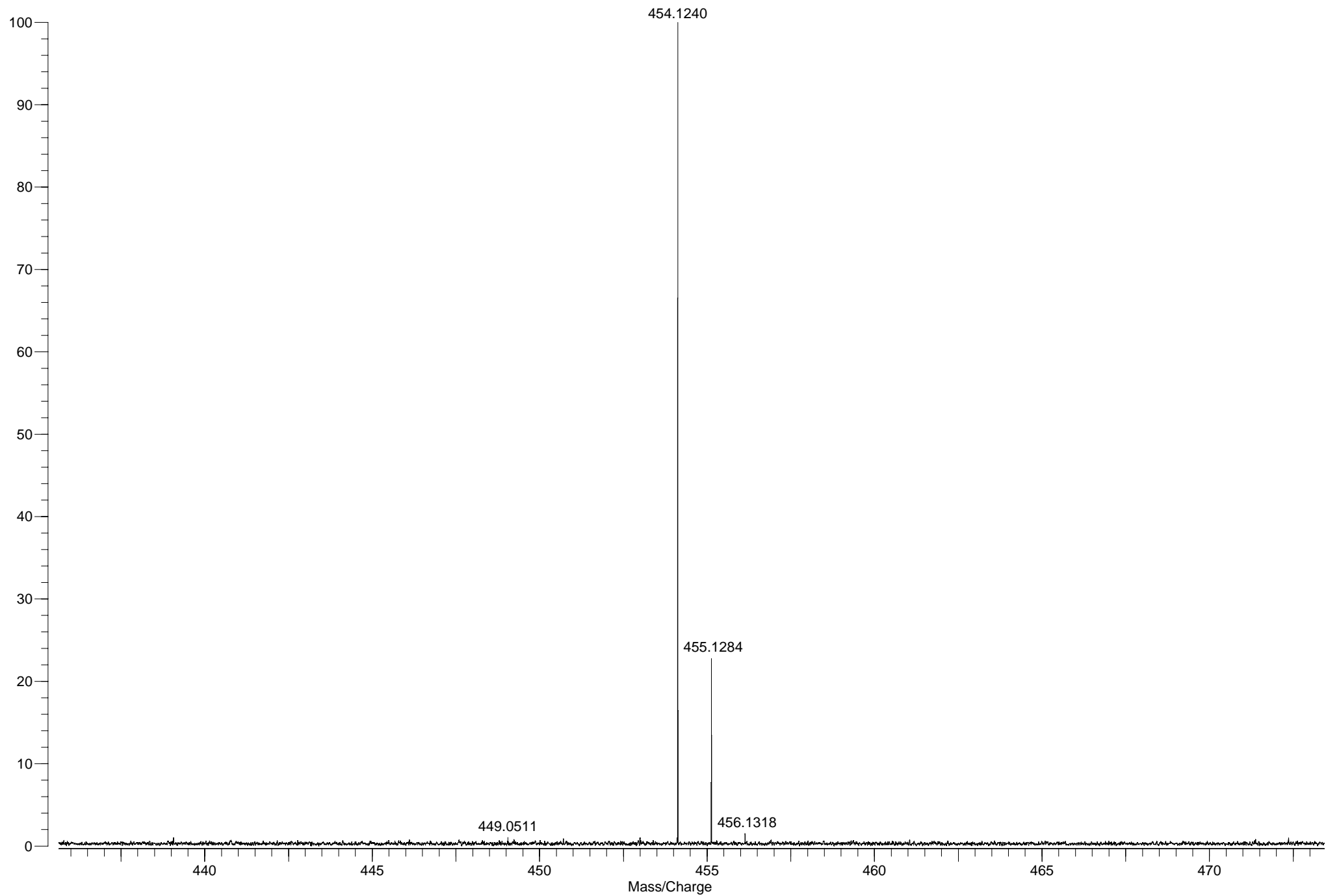
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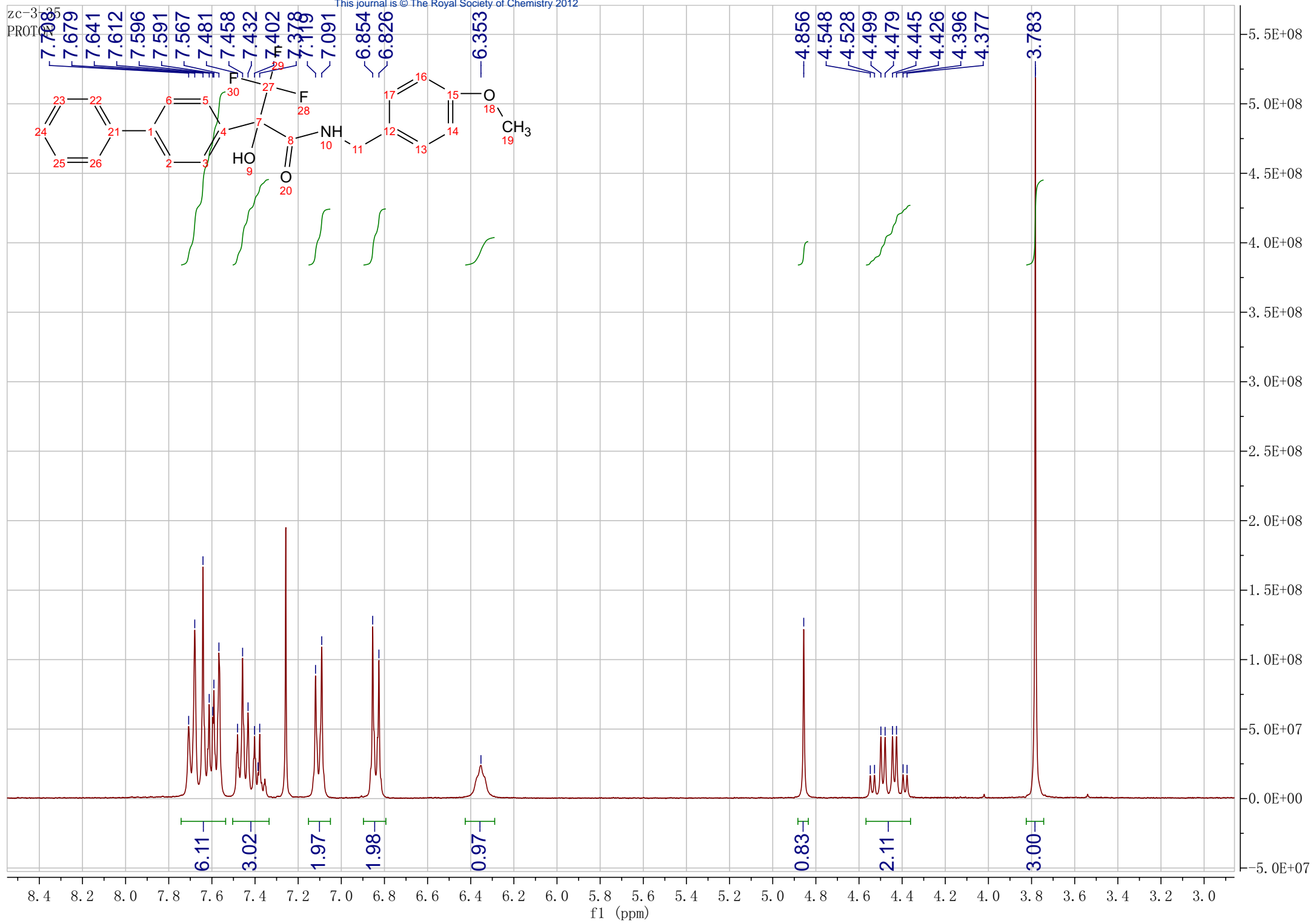
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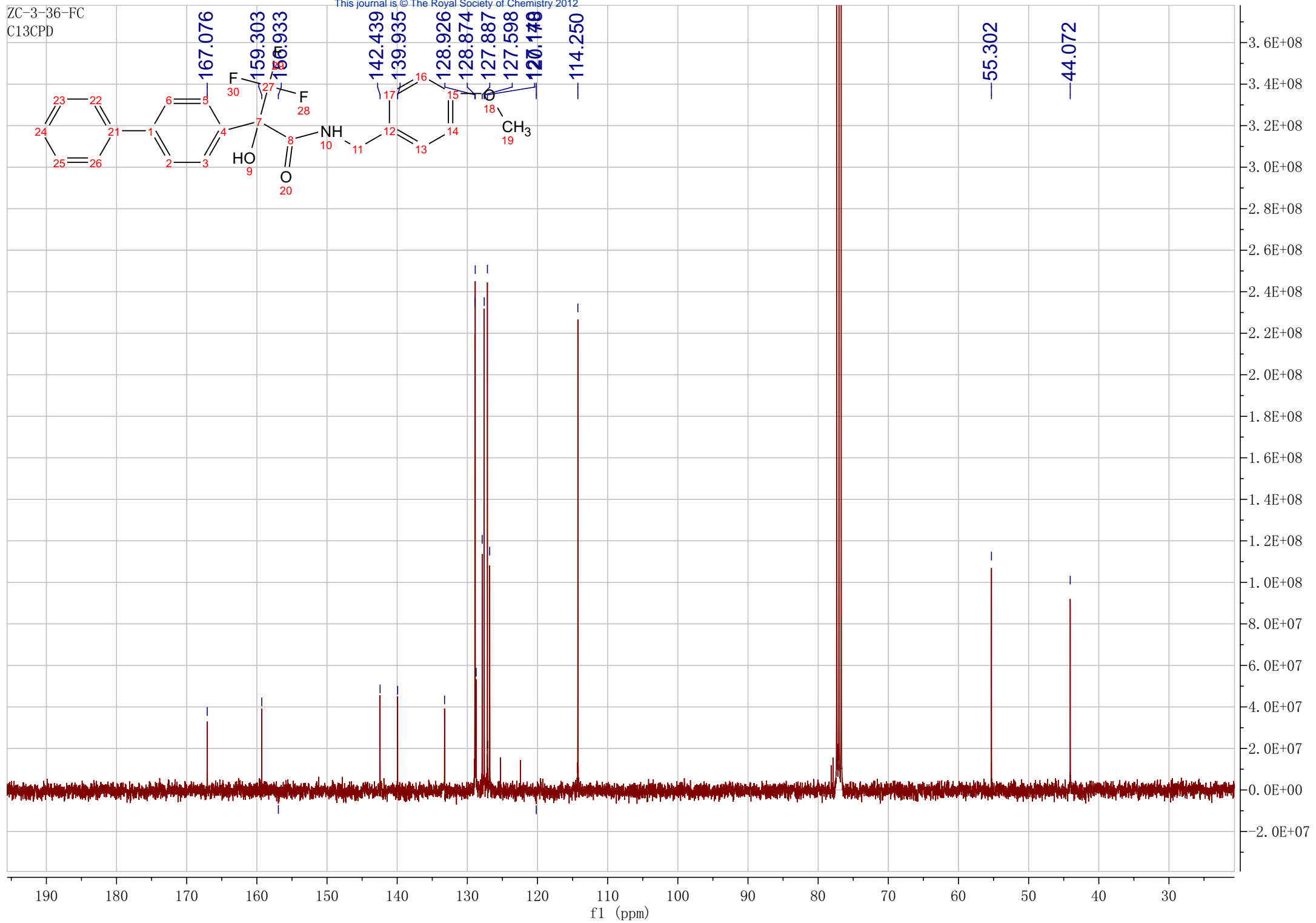


zc-3-35
PROT

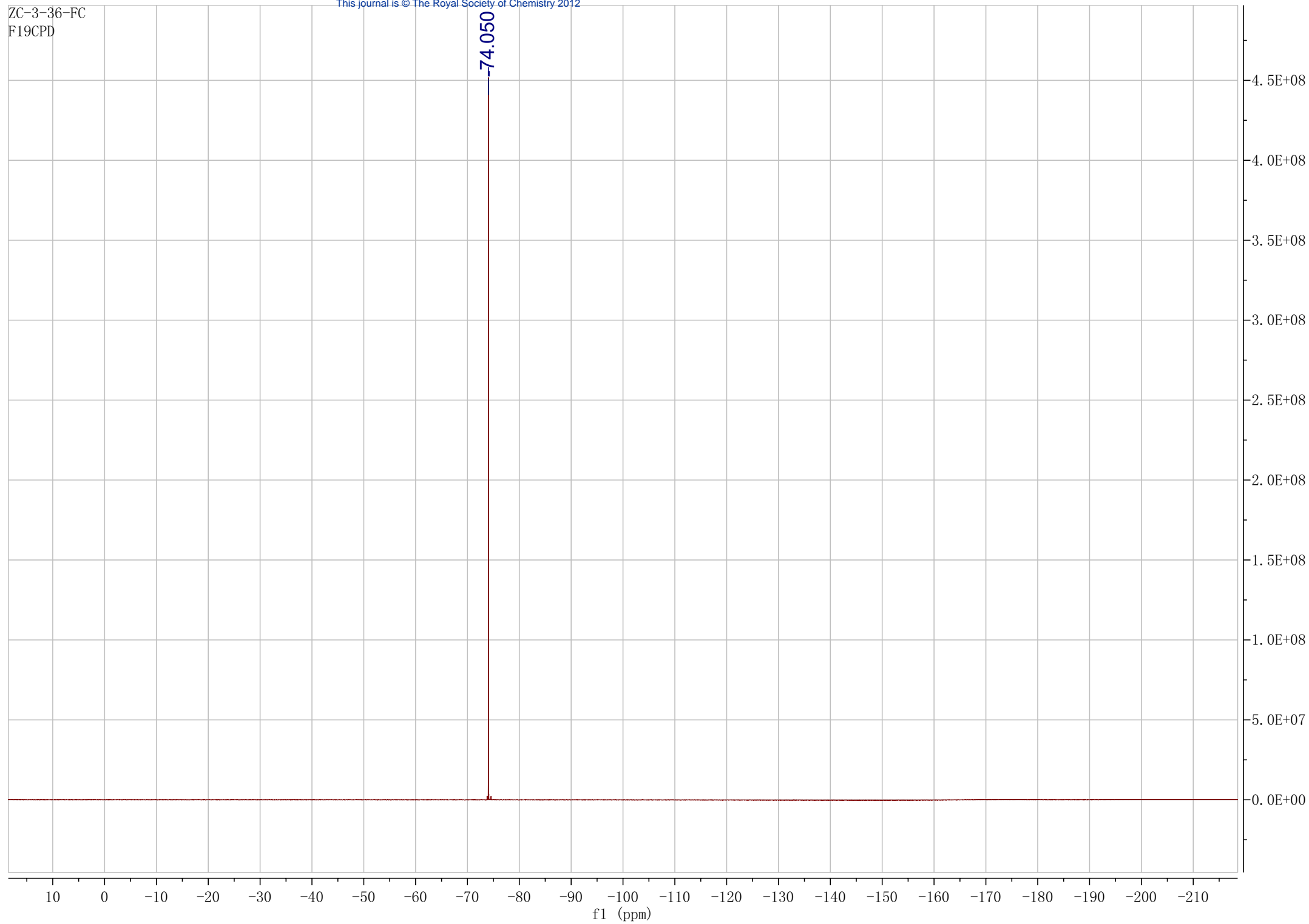


ZC-3-36-FC
C13CPD

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ZC-3-36-FC
F19CPD



Varian ProMALDI
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