

Supplementary Information

Amide-controlled, one-pot synthesis of tri-substituted purines generates structural diversity and analogues with trypanocidal activity

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^c *Unidad de Enfermedades Infecciosas, Hospital Universitario San Cecilio, Instituto de Investigación Biosanitaria de Granada, Dr. Azpitarte, 4, 18012 Granada, Spain*

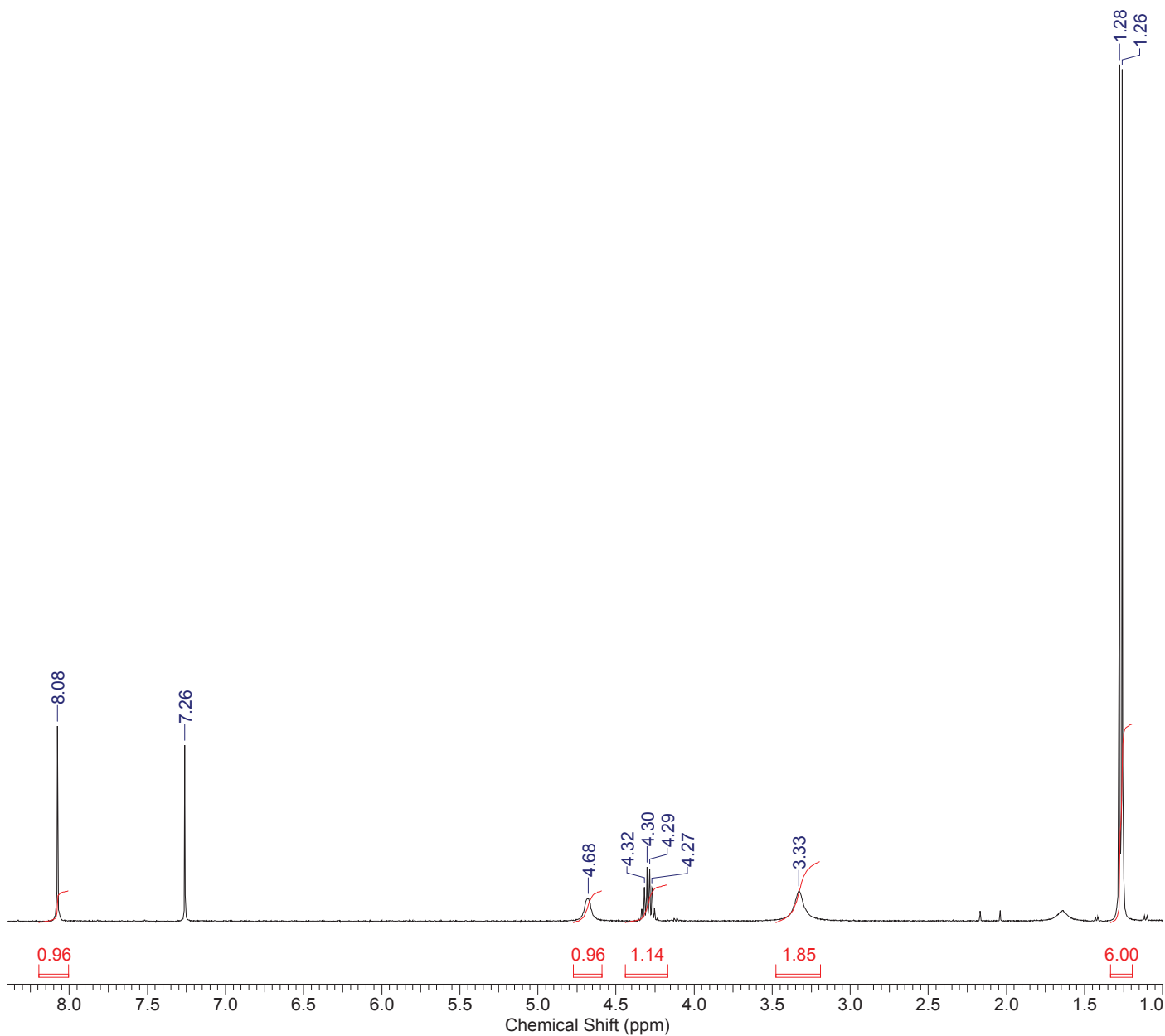
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8. 5-amino-6-chloro-4-isopropylaminopyrimidine (H-NMR)

17 Jul 2012

Acquisition Time (sec)	2.5559	Date	Jan 31 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\PRE-AM1	Frequency (MHz)	400.58
Nucleus	1H	Number of Transients	8
Points Count	16384	Pulse Sequence	s2pul
Sweep Width (Hz)	6410.26	Temperature (degree C)	25.000
		Original Points Count	16384
		Solvent	CHLOROFORM-D



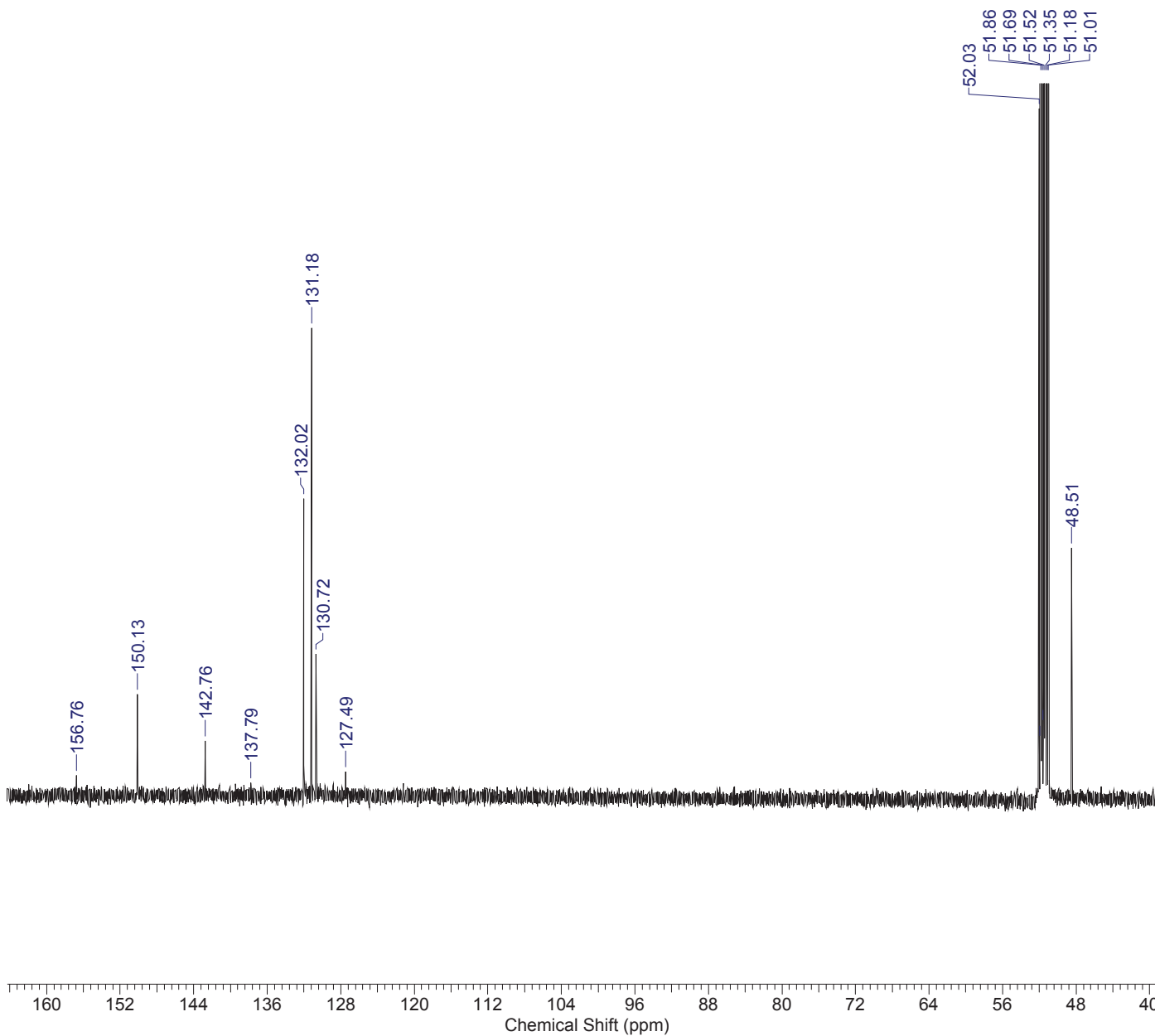
No.	(ppm)	(Hz)	Height
1	1.26	504.8	0.9945
2	1.28	511.1	1.0000
3	3.33	1333.5	0.0371
4	4.27	1710.0	0.0404
5	4.29	1716.6	0.0631
6	4.30	1723.3	0.0649
7	4.32	1729.9	0.0412
8	4.68	1873.9	0.0284
9	7.26	2908.4	0.2072
10	8.08	3235.1	0.2294

No.	(ppm)	Value	Absolute Value
1	[1.19 .. 1.34]	6.000	2.56874e+7
2	[3.19 .. 3.48]	1.853	7.93366e+6
3	[4.17 .. 4.44]	1.143	4.89318e+6
4	[4.59 .. 4.77]	0.960	4.11209e+6
5	[8.00 .. 8.20]	0.960	4.11063e+6

12. 5-Amino-4-benzylamino-6-chloropyrimidine (C-NMR)

8 Jul 2013

Acquisition Time (sec)	1.0486	Date	Mar 6 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-511_Pre-2\carbono		
Frequency (MHz)	125.68	Nucleus	¹³ C
Points Count	32768	Pulse Sequence	s2pul
Sweep Width (Hz)	31250.00	Temperature (degree C)	25.000
		Original Points Count	32768
		Solvent	CHLOROFORM-D

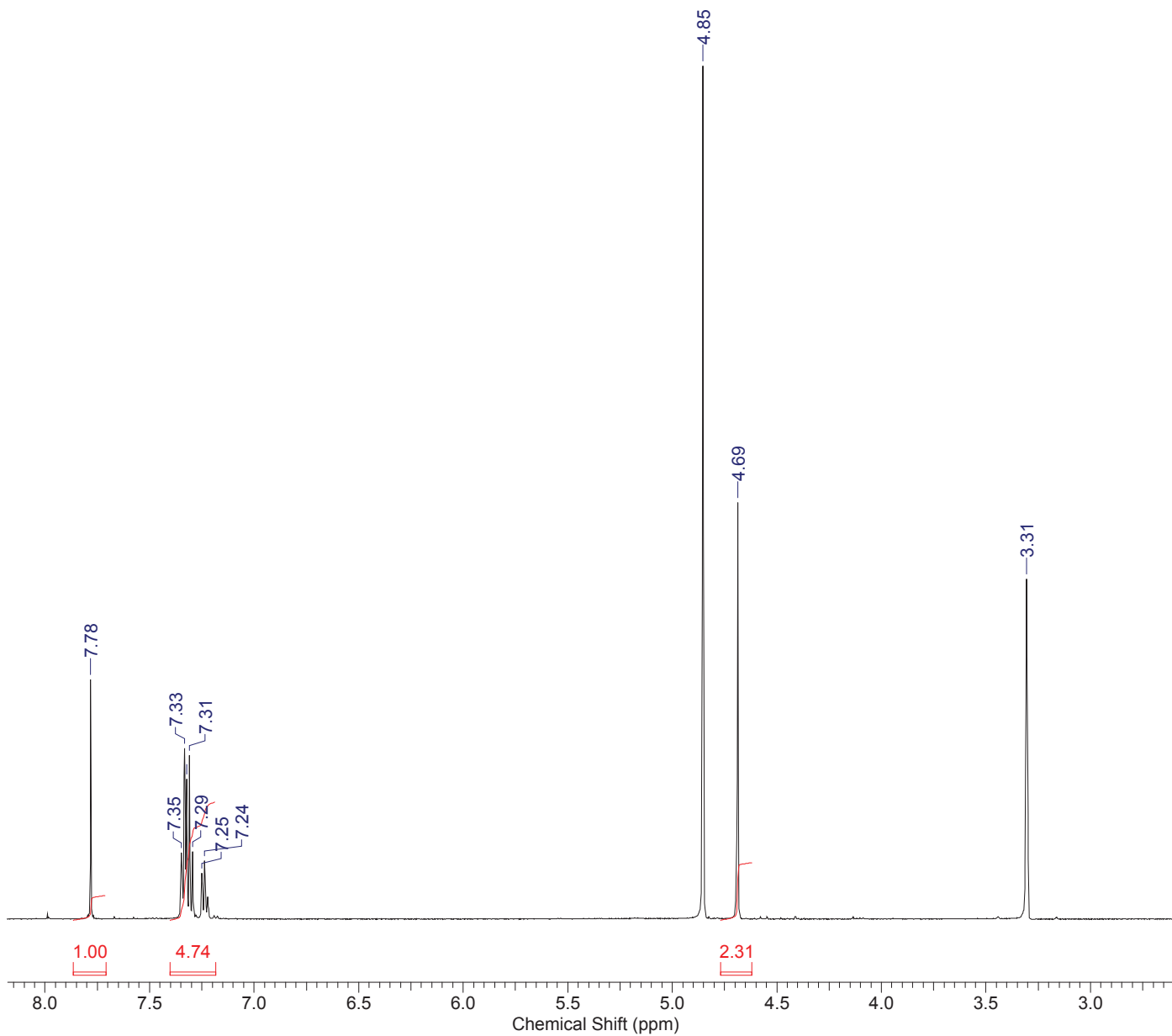


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	48.51	6096.4	0.0362	11	52.03	6539.9	0.1005
2	51.01	6411.1	0.1618	12	127.49	16023.5	0.0035
3	51.18	6432.1	0.3818	13	130.72	16429.8	0.0207
4	51.35	6454.0	0.8678	14	131.18	16487.0	0.0684
5	51.52	6475.0	1.0000	15	132.02	16592.8	0.0434
6	51.63	6489.3	0.0104	16	137.79	17318.6	0.0019
7	51.69	6496.9	0.7416	17	142.76	17943.3	0.0080
8	51.81	6511.3	0.0145	18	150.13	18869.3	0.0148
9	51.86	6517.9	0.4658	19	156.76	19701.9	0.0029
10	51.97	6532.2	0.0080				

12. 5-Amino-4-benzylamino-6-chloropyrimidine (H-NMR)

8 Jul 2013

Acquisition Time (sec)	1.7432	Date	Mar 6 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-511_Pre-2\proton				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	80
Original Points Count	13048	Points Count	16384	Pulse Sequence	s2pul
Solvent	METHANOL-D4		Sweep Width (Hz)	7485.03	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	3.31	1652.0	0.3992
2	4.69	2342.8	0.4889
3	4.85	2425.5	1.0000
4	7.24	3616.6	0.0695
5	7.25	3623.4	0.0555
6	7.29	3644.9	0.0804
7	7.31	3652.7	0.1928
8	7.32	3660.0	0.1651
9	7.33	3665.0	0.2014
10	7.35	3671.9	0.0790
11	7.78	3889.3	0.2820

No.	(ppm)	Value	Absolute Value
1	[4.62 .. 4.77]	2.308	5.89304e+7
2	[7.18 .. 7.40]	4.741	1.21016e+8
3	[7.71 .. 7.87]	1.000	2.55278e+7

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

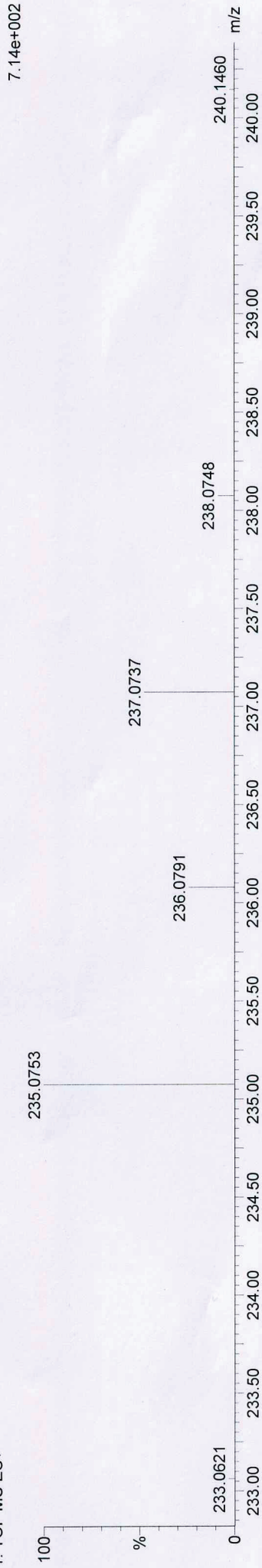
383 formula(e) evaluated with 7 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-11 H: 0-1000 N: 0-9 O: 0-20 Cl: 0-1

MJ-2 89 (1.975)

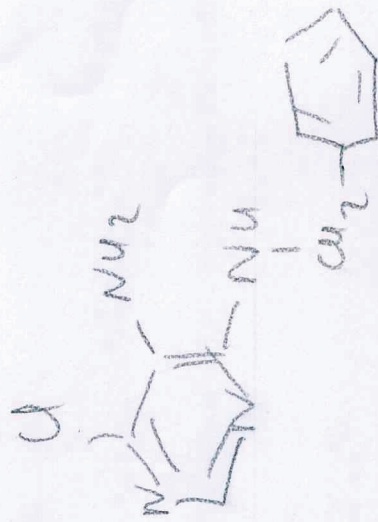
1: TOF MS ES+



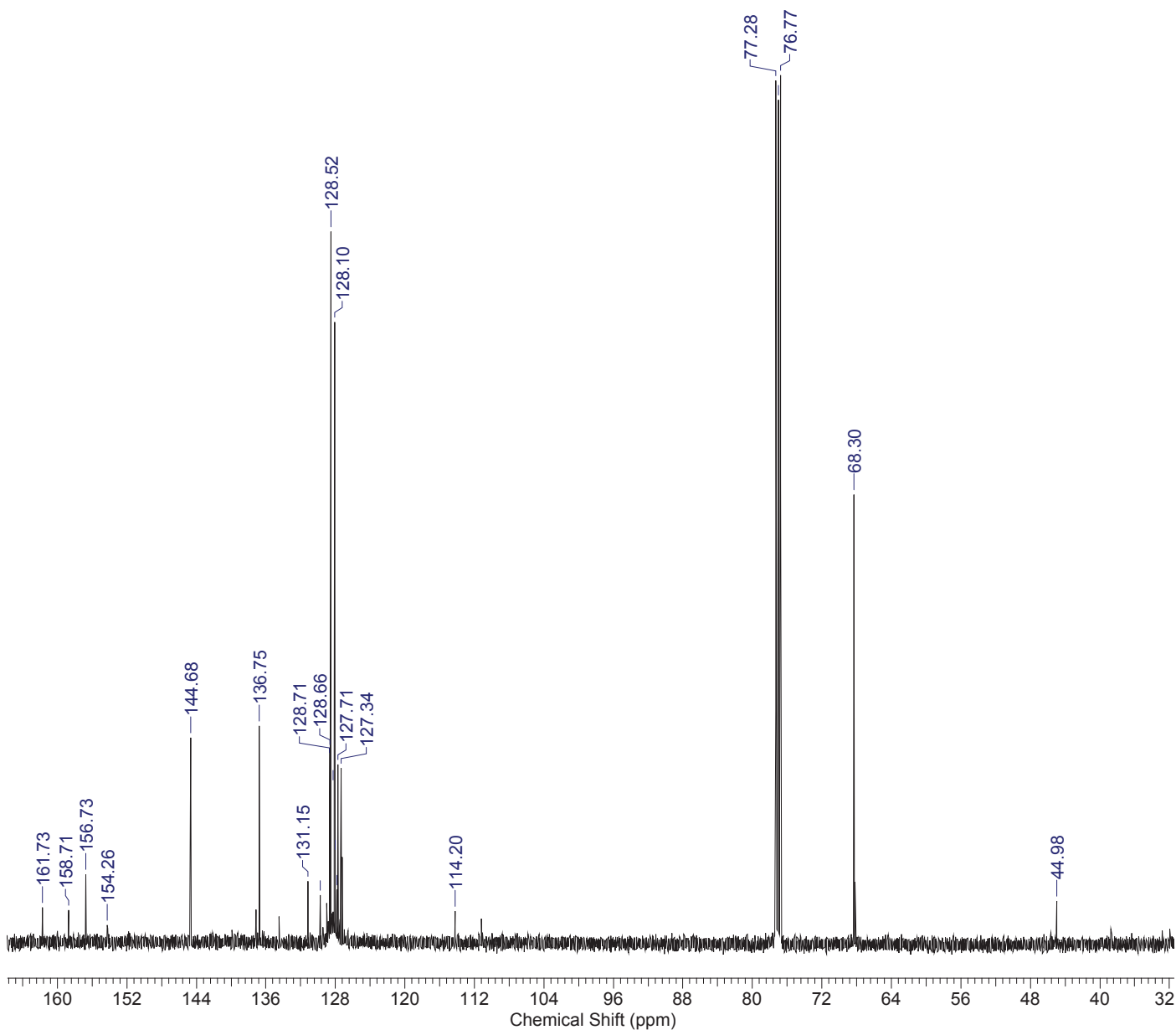
Minimum:
Maximum:

-1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.0753	235.0750	0.3	1.3	7.5	24.3	C11 H12 N4 Cl
	235.0737	1.6	6.8	2.5	31.4	C10 H16 O4 Cl
	235.0710	4.3	18.3	3.5	43.6	C6 H12 N6 O2 Cl
	235.0719	3.4	14.5	7.5	173.8	C11 H11 N2 O4
	235.0791	-3.8	-16.2	3.5	198.1	C5 H11 N6 O5
	235.0778	-2.5	-10.6	-1.5	205.2	C4 H15 N2 O9
	235.0751	0.2	0.9	-0.5	222.4	H11 N8 O7

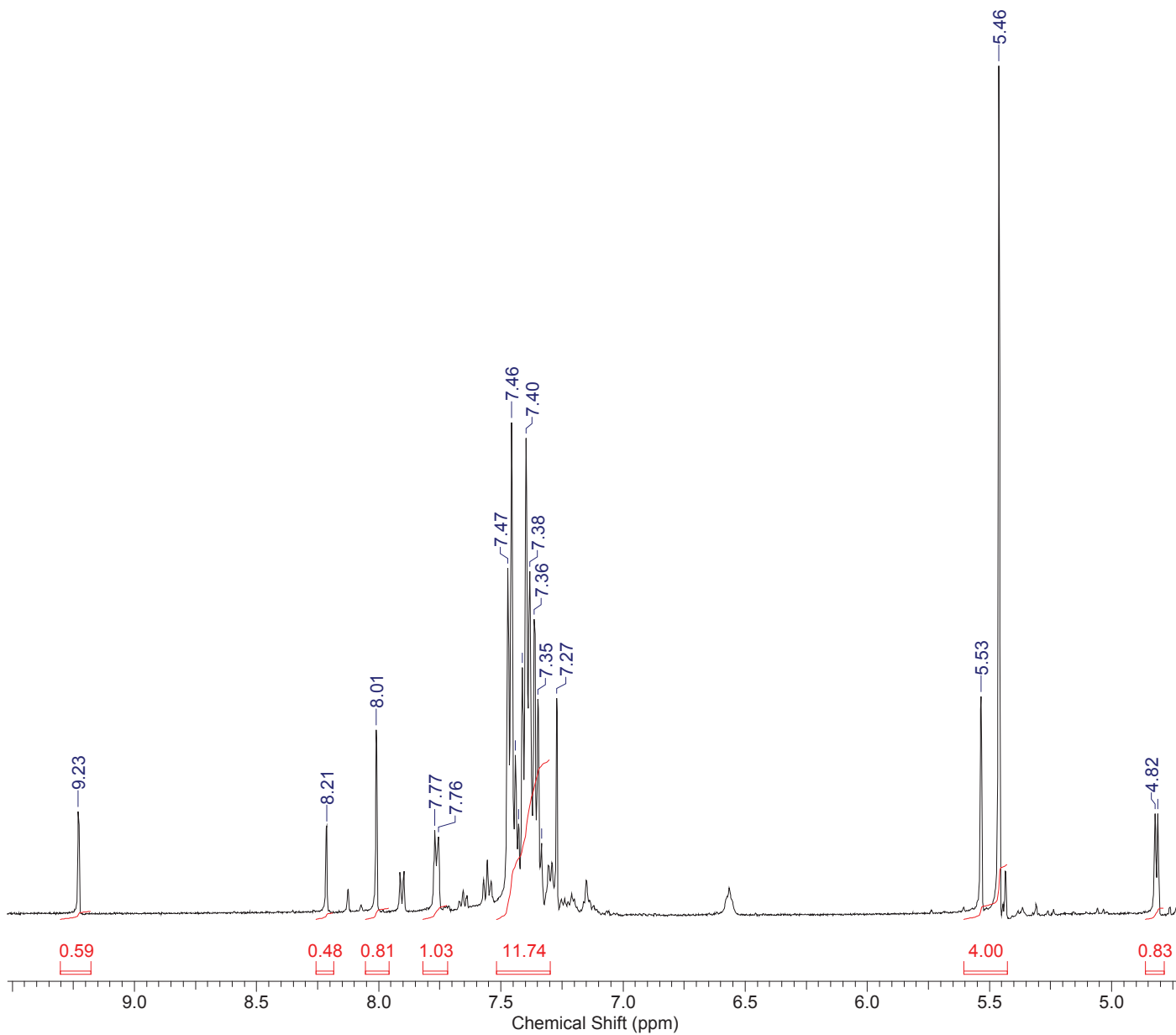


Acquisition Time (sec)	1.0486	Date	Nov 23 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-23752 ASIMJ-30-1\carbono				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	4800
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	31250.00		
Temperature (degree C)	25.000				



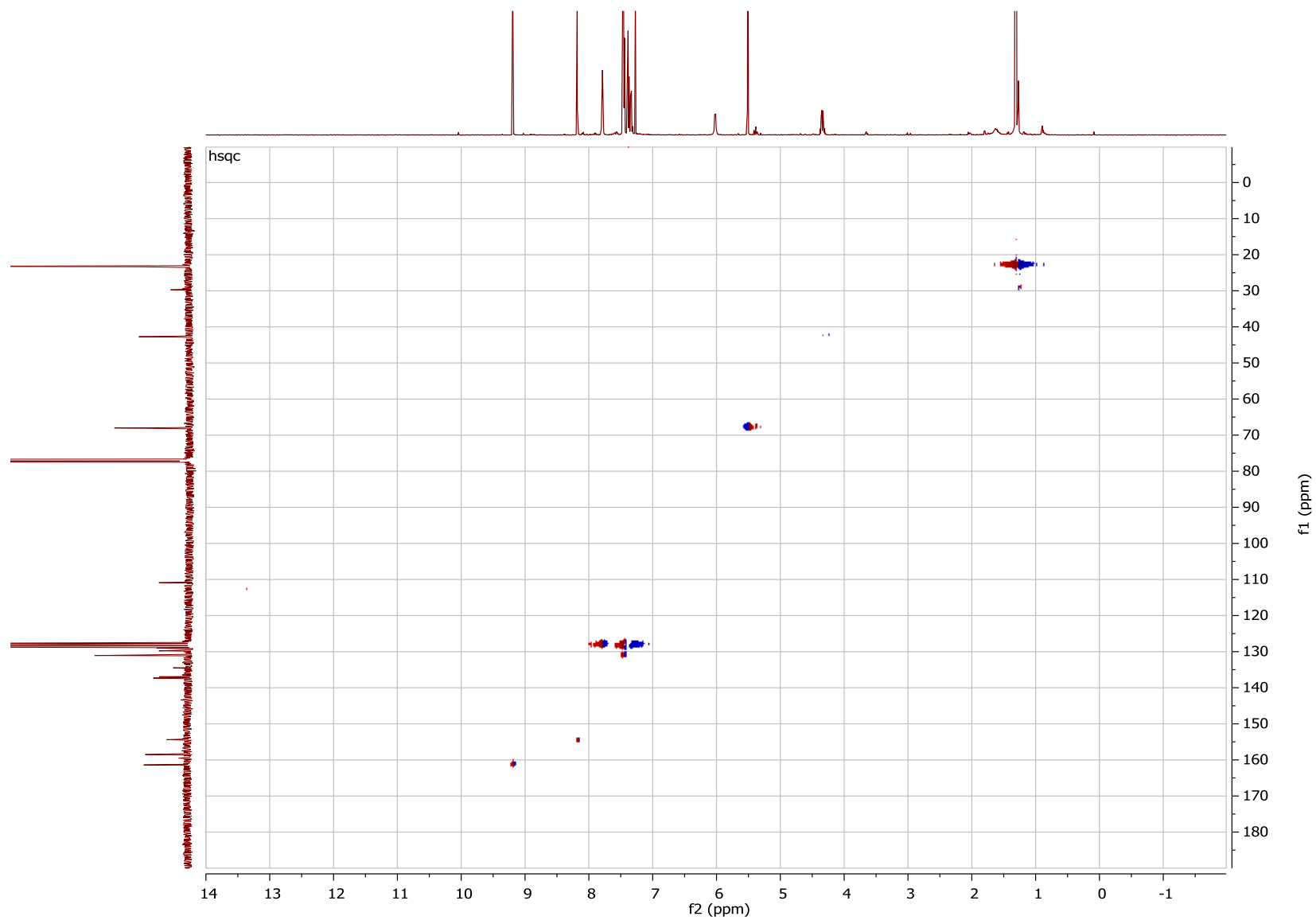
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	44.98	5652.9	0.0478	13	128.24	16117.9	0.1818
2	68.30	8583.6	0.5167	14	128.52	16153.2	0.8196
3	76.77	9648.9	1.0000	15	128.66	16170.4	0.2225
4	77.03	9681.4	0.9718	16	128.71	16177.0	0.2132
5	77.28	9712.8	0.9939	17	129.76	16308.6	0.0542
6	114.20	14353.6	0.0357	18	131.15	16483.2	0.0704
7	127.24	15992.0	0.0981	19	136.75	17187.0	0.2494
8	127.34	16004.4	0.2005	20	144.68	18184.6	0.2363
9	127.71	16051.1	0.2053	21	154.26	19388.2	0.0201
10	127.85	16069.3	0.0603	22	156.73	19698.1	0.0787
11	128.01	16088.3	0.1016	23	158.71	19948.0	0.0371
12	128.10	16099.8	0.7153	24	161.73	20326.6	0.0404

Acquisition Time (sec)	2.0447	Date	Nov 23 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-23752 ASIMJ-30-1\proton				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82		
Temperature (degree C)	25.000				

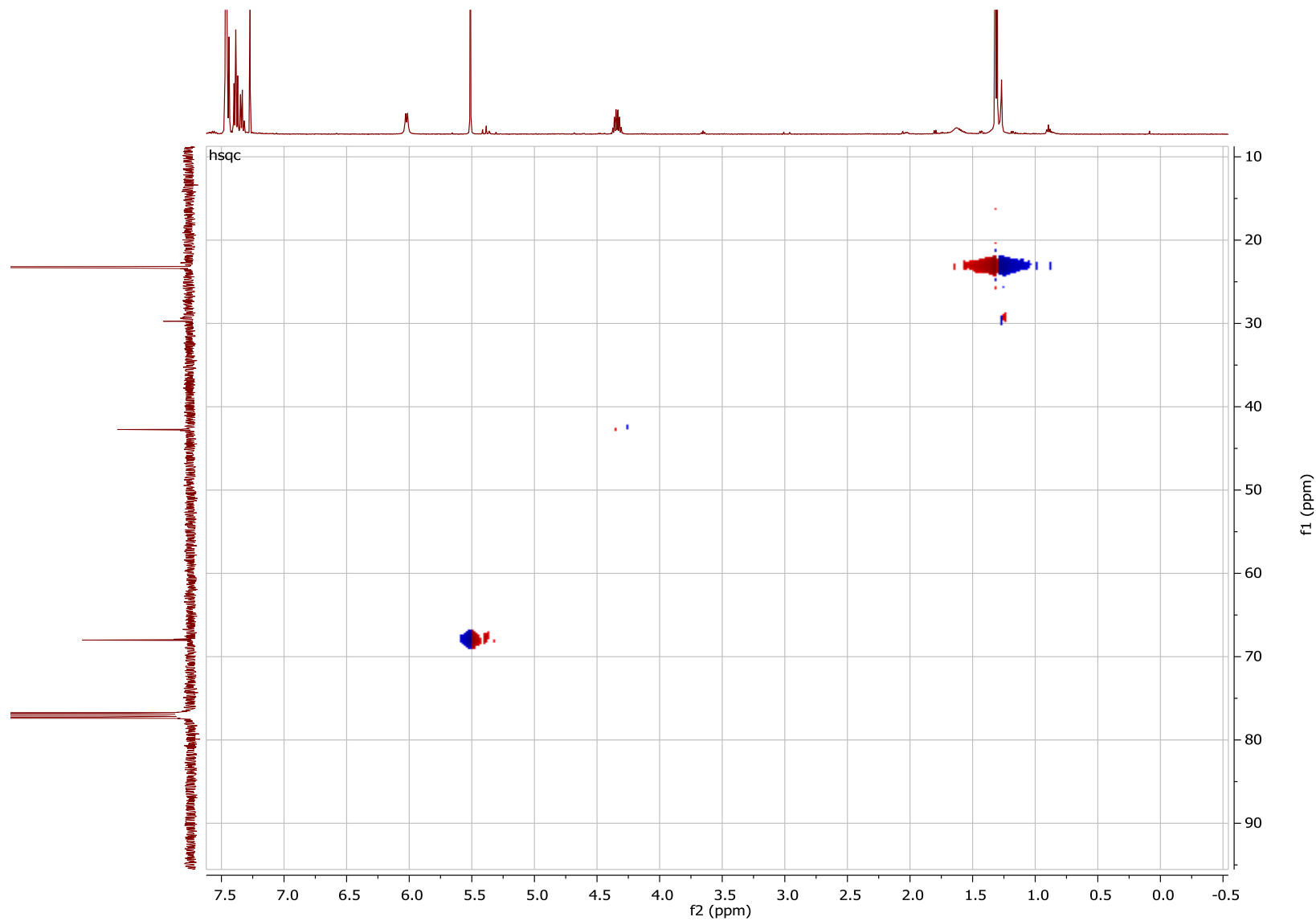


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	4.81	2404.2	0.1236	11	7.41	3704.2	0.2949	1	[4.79 .. 4.86]	0.828	2.78104e+6
2	4.82	2410.0	0.1237	12	7.43	3712.0	0.1116	2	[5.43 .. 5.61]	4.000	1.34299e+7
3	5.46	2729.4	1.0000	13	7.44	3718.4	0.1921	3	[7.30 .. 7.52]	11.745	3.94331e+7
4	5.53	2766.1	0.2609	14	7.46	3726.7	0.5819	4	[7.72 .. 7.82]	1.026	3.44435e+6
5	7.27	3634.7	0.2593	15	7.47	3734.5	0.4113	5	[7.96 .. 8.05]	0.815	2.73543e+6
6	7.33	3665.6	0.0892	16	7.76	3876.4	0.0969	6	[8.18 .. 8.26]	0.477	1.60142e+6
7	7.35	3672.9	0.2579	17	7.77	3883.7	0.1042	7	[9.18 .. 9.30]	0.590	1.98125e+6
8	7.36	3680.2	0.3517	18	8.01	4003.5	0.2218				
9	7.38	3689.5	0.4076	19	8.21	4104.8	0.1094				
10	7.40	3696.9	0.5635	20	9.23	4612.9	0.1266				

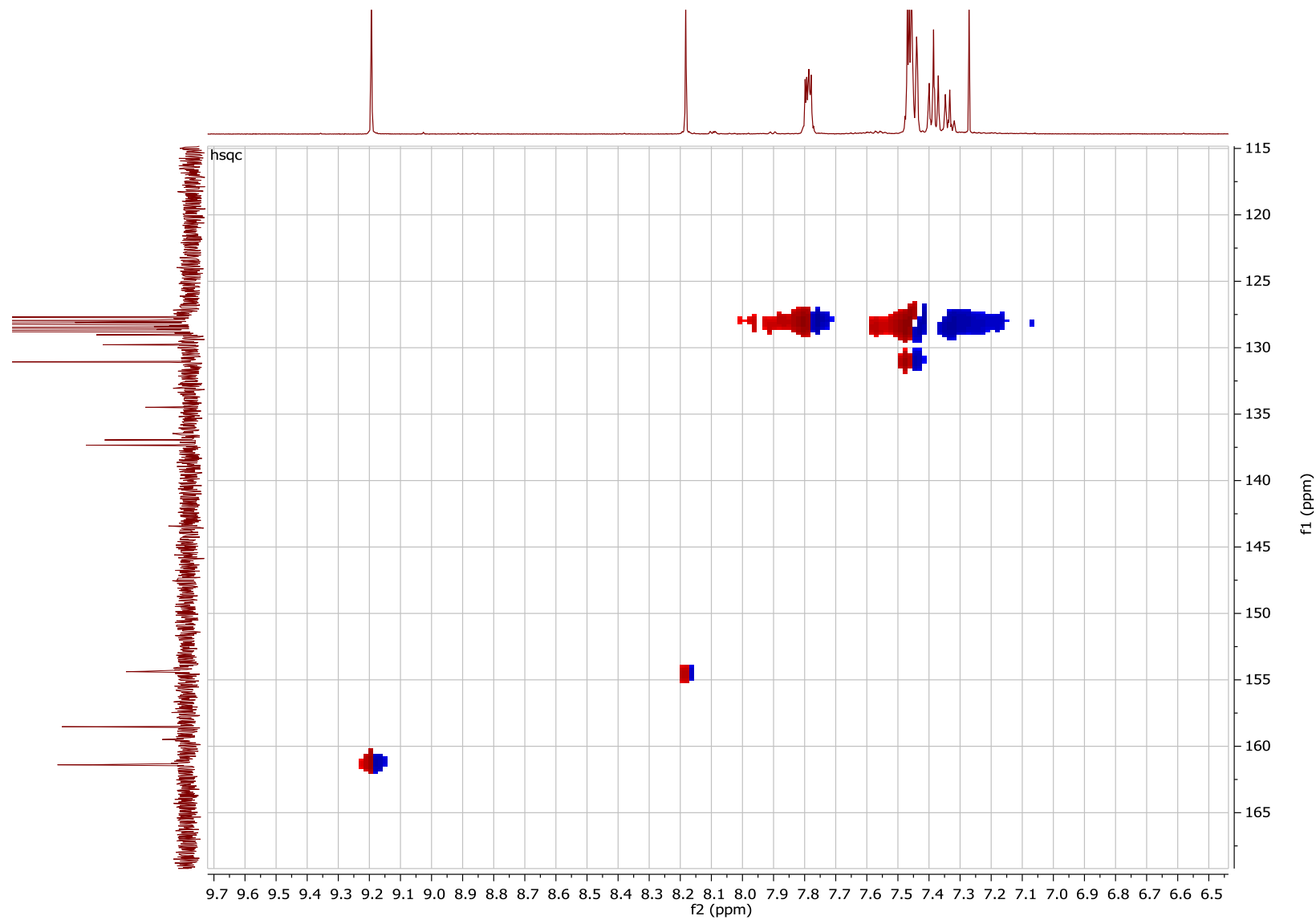
15. N5-benzylidene-6-(benzyloxy)-N4-isopropylpyrimidine-4,5-diamine HSQC



15. N5-benzylidene-6-(benzyloxy)-N4-isopropylpyrimidine-4,5-diamine HSQC Zoom in



15. N5-benzylidene-6-(benzyloxy)-N4-isopropylpyrimidine-4,5-diamine HSQC Zoom in



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

900 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)

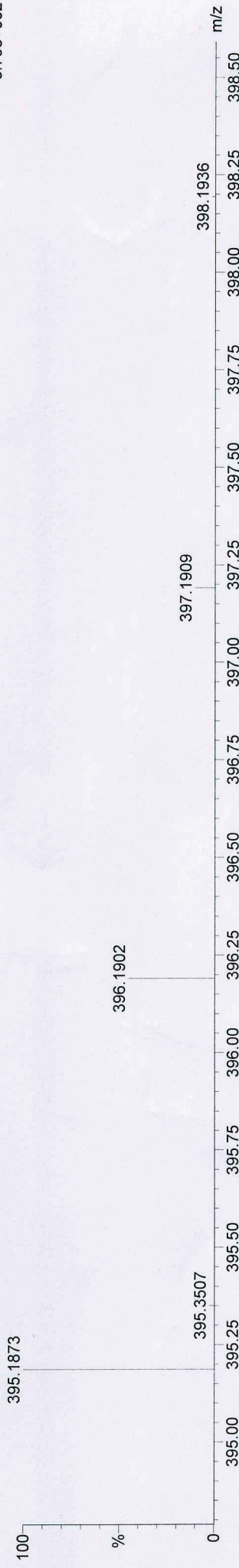
Elements Used:

C: 0-25 H: 0-1000 N: 0-10 O: 0-10 Na: 0-1

MJ-30-1 4 (0.087)

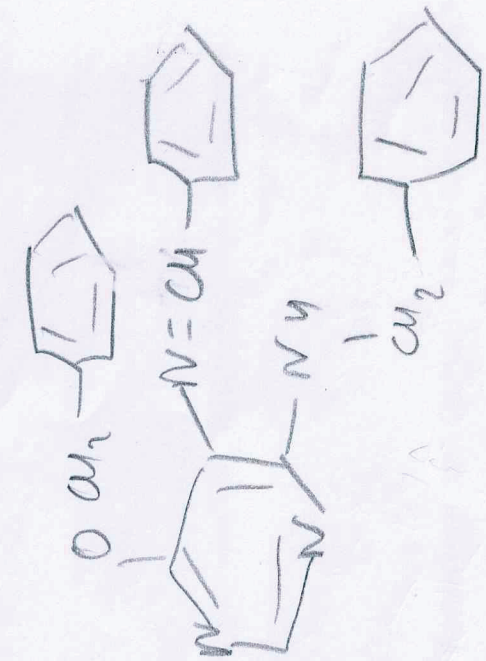
1: TOF MS ES+

8.79e+002



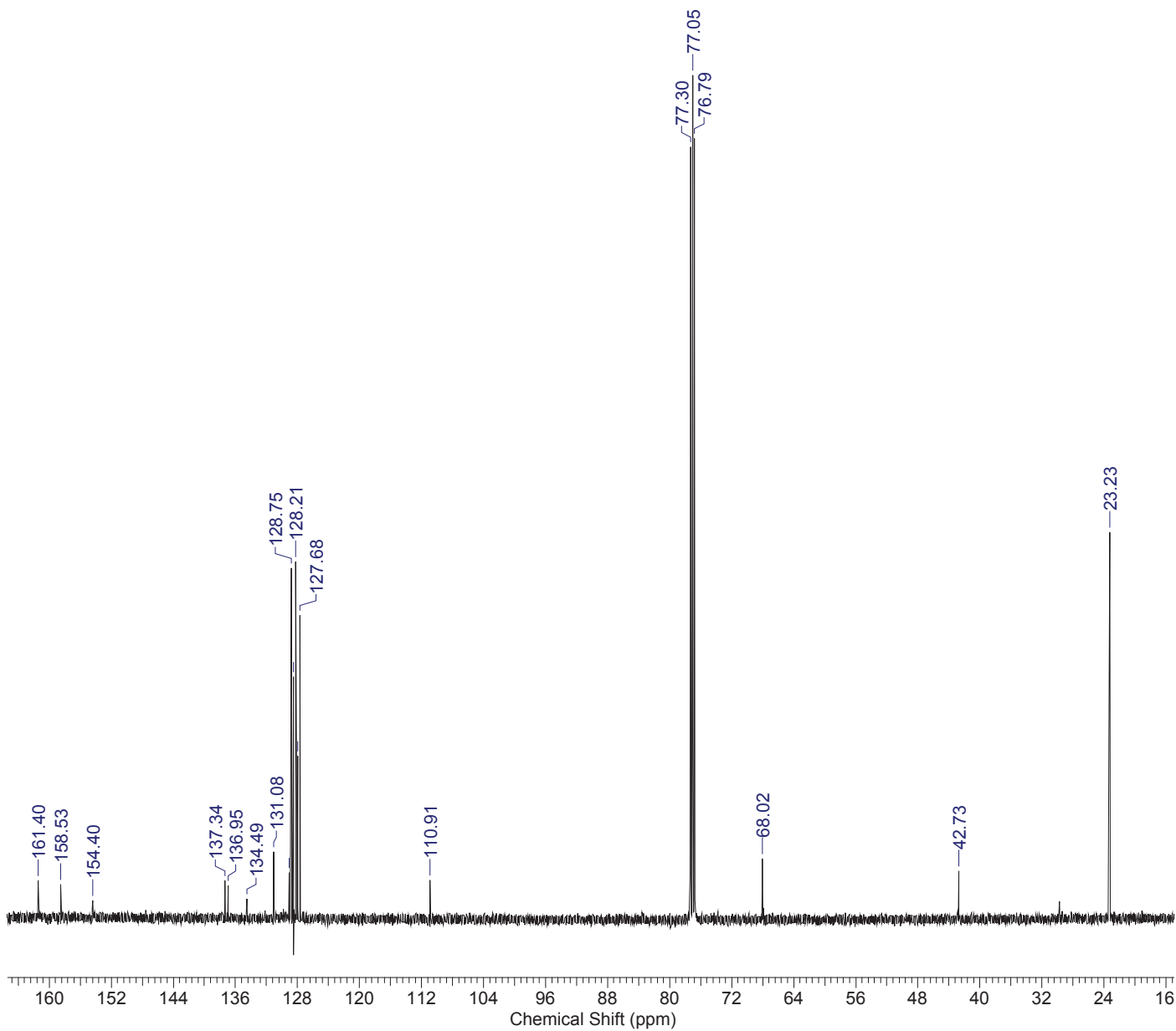
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
395.1873	395.1872	0.1	0.3	16.5	32.0	C25 H23 N4 O
	395.1858	1.5	3.8	11.5	38.3	C24 H27 O5
	395.1890	-1.7	-4.3	3.5	90.9	C13 H27 N6 O8
	395.1880	-0.7	-1.8	5.5	95.3	C12 H24 N10 O4 Na
	395.1866	0.7	1.8	0.5	106.1	C11 H28 N6 O8 Na

Minimum: -1.5
Maximum: 50.0



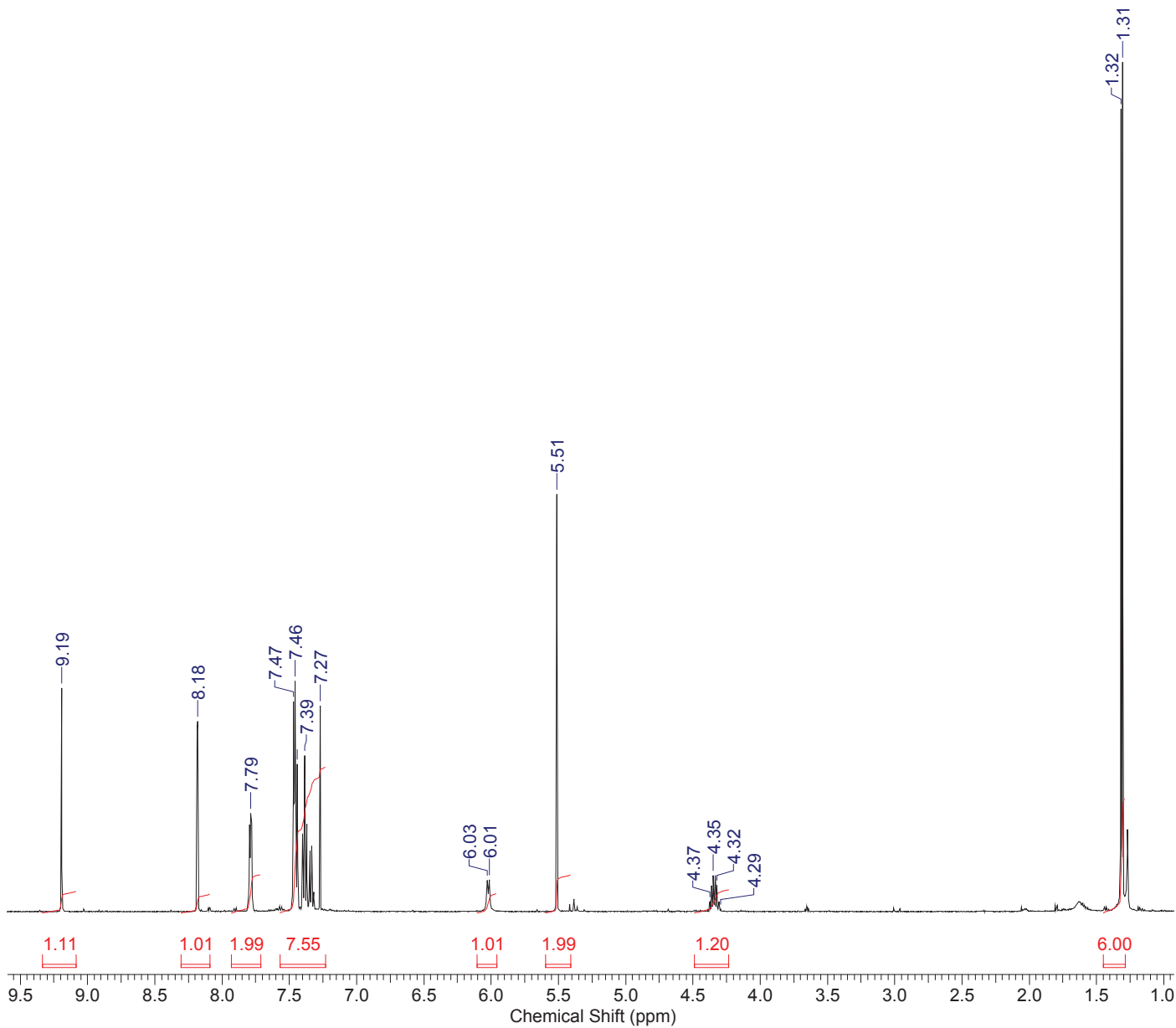
8 Jul 2013

Acquisition Time (sec)	1.0486	Comment	new experiment	Date	Jul 3 2013
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-15463 Benz-1\carbono				
Frequency (MHz)	125.68	Nucleus	¹³ C	Number of Transients	3200
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	31250.00
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.23	2919.2	0.4578	11	128.53	16154.6	0.2868
2	42.73	5371.1	0.0564	12	128.75	16182.3	0.4156
3	68.02	8548.9	0.0705	13	129.03	16217.6	0.0545
4	76.79	9651.3	0.9251	14	131.08	16474.1	0.0790
5	77.05	9683.8	1.0000	15	134.49	16903.3	0.0235
6	77.30	9715.2	0.9148	16	136.95	17212.3	0.0390
7	110.91	13939.2	0.0453	17	137.34	17260.9	0.0447
8	127.68	16047.8	0.3596	18	154.40	19405.8	0.0215
9	127.96	16082.2	0.1924	19	158.53	19924.6	0.0402
10	128.21	16113.6	0.4232	20	161.40	20285.1	0.0449

Acquisition Time (sec)	2.0447	Date	Jun 24 2013
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-15463_Benz-1\PROTON_01		
Frequency (MHz)	499.79	Nucleus	1H
Original Points Count	16384	Points Count	16384
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82
Temperature (degree C)	25.000		



No.	(ppm)	(Hz)	Height
1	1.31	652.2	1.0000
2	1.32	659.1	0.9448
3	4.29	2145.9	0.0044
4	4.32	2159.1	0.0327
5	4.35	2173.8	0.0440
6	4.37	2186.5	0.0131
7	5.51	2754.9	0.4921
8	6.01	3005.8	0.0392
9	6.03	3013.6	0.0388
10	7.27	3634.2	0.2440
11	7.39	3691.5	0.1852
12	7.44	3718.4	0.1749
13	7.46	3727.2	0.2726
14	7.46	3730.6	0.2329
15	7.47	3733.5	0.2488
16	7.79	3892.0	0.1170
17	8.18	4089.6	0.2253
18	9.19	4594.8	0.2644

No.	(ppm)	Value	Absolute Value
1	[1.29 .. 1.45]	6.000	3.44717e+8
2	[4.23 .. 4.49]	1.202	6.90548e+7
3	[5.41 .. 5.60]	1.992	1.14457e+8
4	[5.96 .. 6.11]	1.009	5.79428e+7
5	[7.23 .. 7.57]	7.548	4.33660e+8
6	[7.71 .. 7.93]	1.991	1.14368e+8
7	[8.09 .. 8.31]	1.008	5.79299e+7
8	[9.08 .. 9.33]	1.110	6.37490e+7

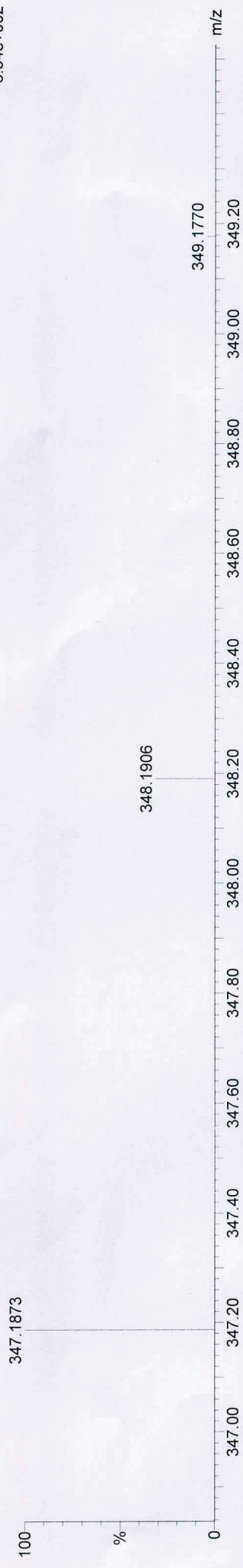
Elemental Composition Report

Single Mass Analysis

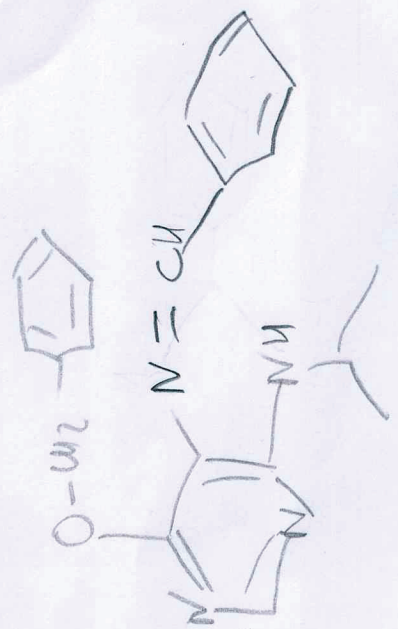
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 215 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:
 C: 0-21 H: 0-100 N: 0-5 O: 0-5 Na: 0-1

1: TOF MS ES+ 5.34e+002



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
347.1873	347.1872	0.1	0.3	12.5	3.2	C21 H23 N4 O
347.1858	347.1858	1.5	4.3	7.5	5.6	C20 H27 O5
347.1848	347.1848	2.5	7.2	9.5	6.4	C19 H24 N4 O Na



Minimum:
Maximum:

Elemental Composition Report

Single Mass Analysis

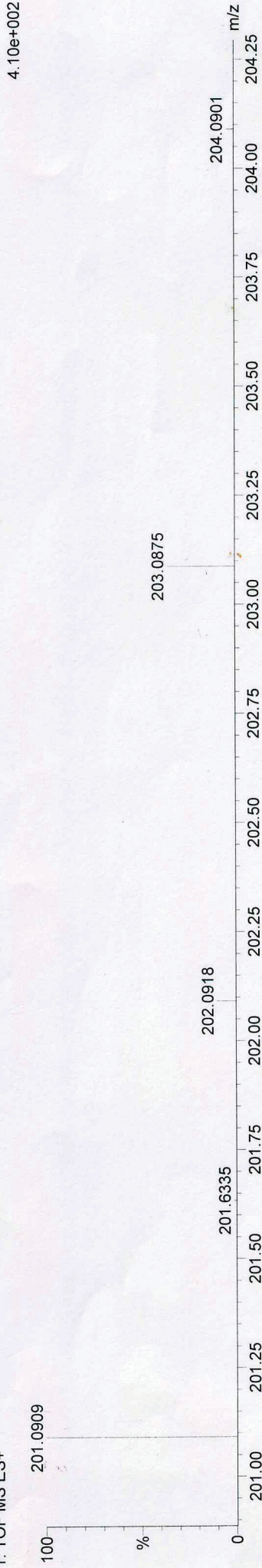
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 960 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
 Elements Used:

C: 0-17 H: 0-1000 N: 0-10 O: 0-10 Na: 0-1 S: 0-1 Cl: 0-1

PRE-TB-F dilu 9 (0.217)

1: TOF MS ES+



Minimum:
 Maximum:

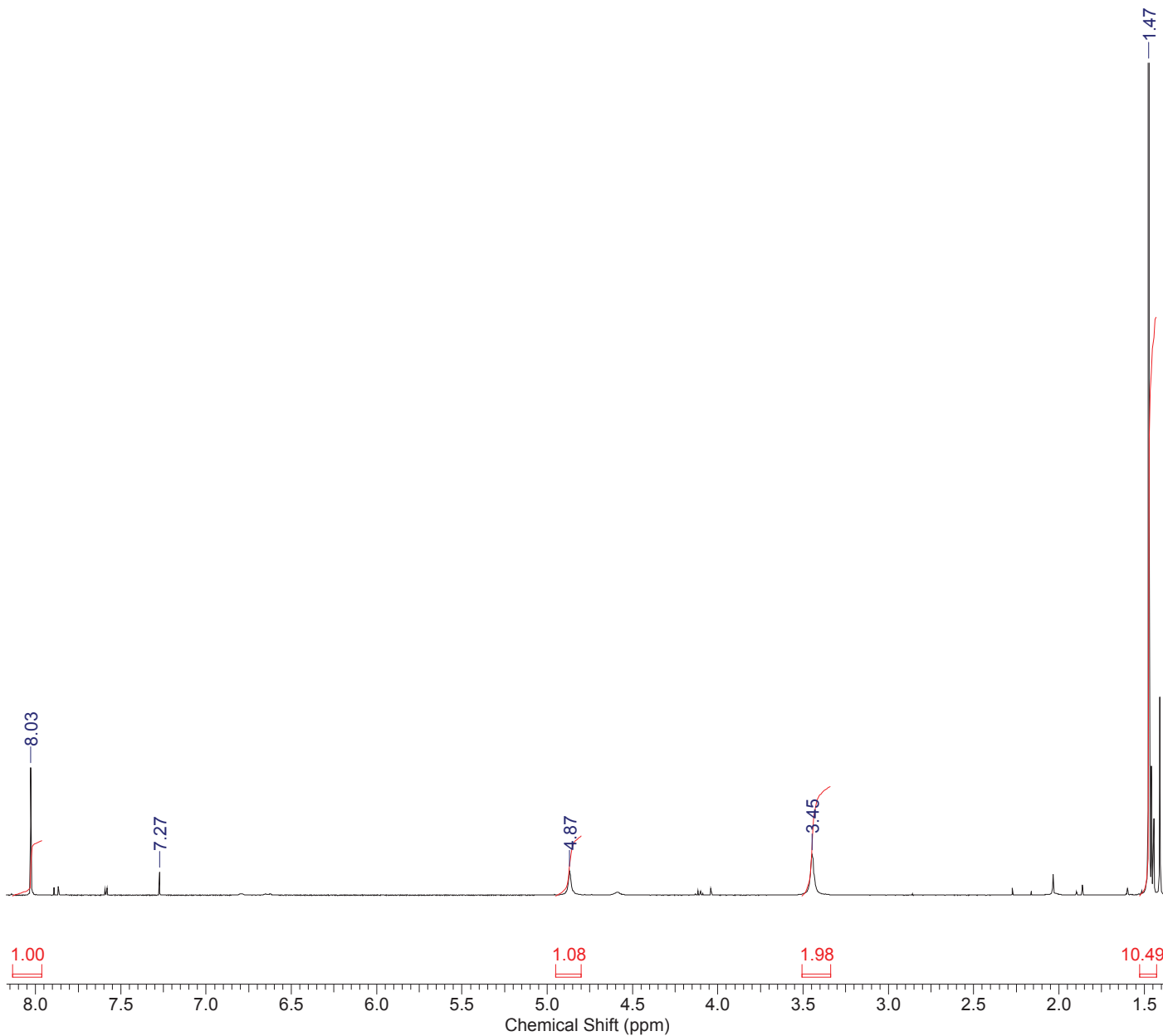
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
201.0909	201.0907	0.2	1.0	3.5	0.6	C8 H14 N4 Cl
201.0909	201.0909	0.0	0.0	-1.5	52.4	C5 H17 N2 O4 S
201.0916	201.0916	-0.7	-3.5	7.5	72.7	C13 H13 O2

4.10e+002

18. 5-amino-4-tert-butylamino-6-chloropyrimidine (H-NMR)

2 Jul 2013

Acquisition Time (sec)	2.0447	Date	Jun 19 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\Pre-TB-1	Frequency (MHz)	499.79
Nucleus	1H	Number of Transients	1
Points Count	16384	Pulse Sequence	s2pul
Sweep Width (Hz)	8012.82	Temperature (degree C)	25.000
		Original Points Count	16384
		Solvent	CHLOROFORM-D



No.	(ppm)	(Hz)	Height
1	1.47	736.5	1.0000
2	3.45	1722.5	0.0217
3	4.87	2433.1	0.0131
4	7.27	3635.3	0.0125
5	8.03	4011.9	0.0669

No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.53]	10.486	1.68216e+8
2	[3.34 .. 3.51]	1.981	3.17831e+7
3	[4.80 .. 4.95]	1.083	1.73672e+7
4	[7.96 .. 8.14]	1.000	1.60426e+7

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

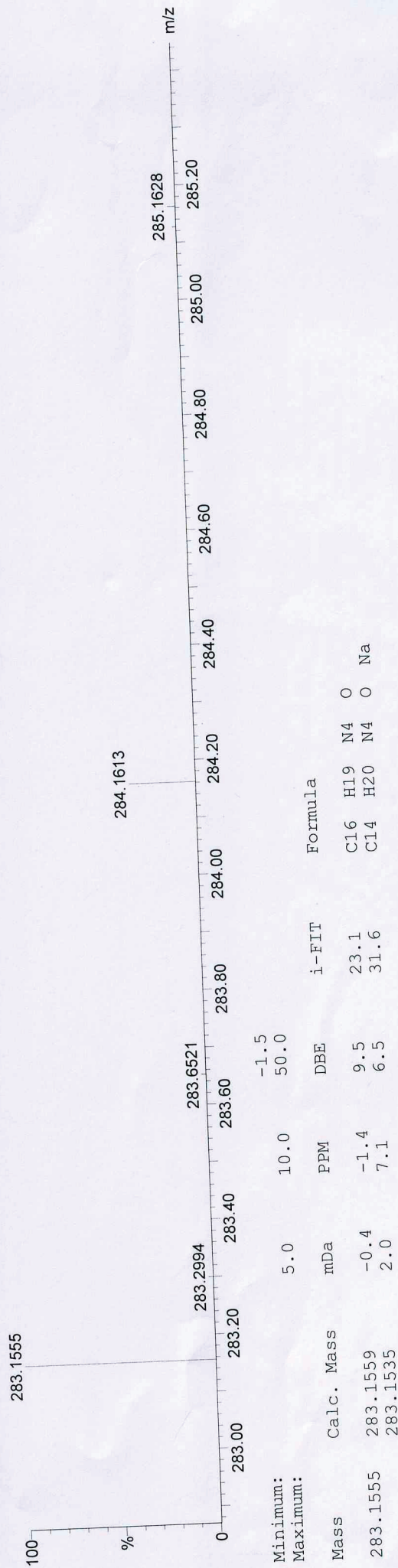
Monoisotopic Mass, Even Electron Ions
 44 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:
 C: 0-16 H: 0-1000 N: 0-5 O: 0-1 Na: 0-1

ASIMJ-5 12-04 9 (0.212)

6.64e+002

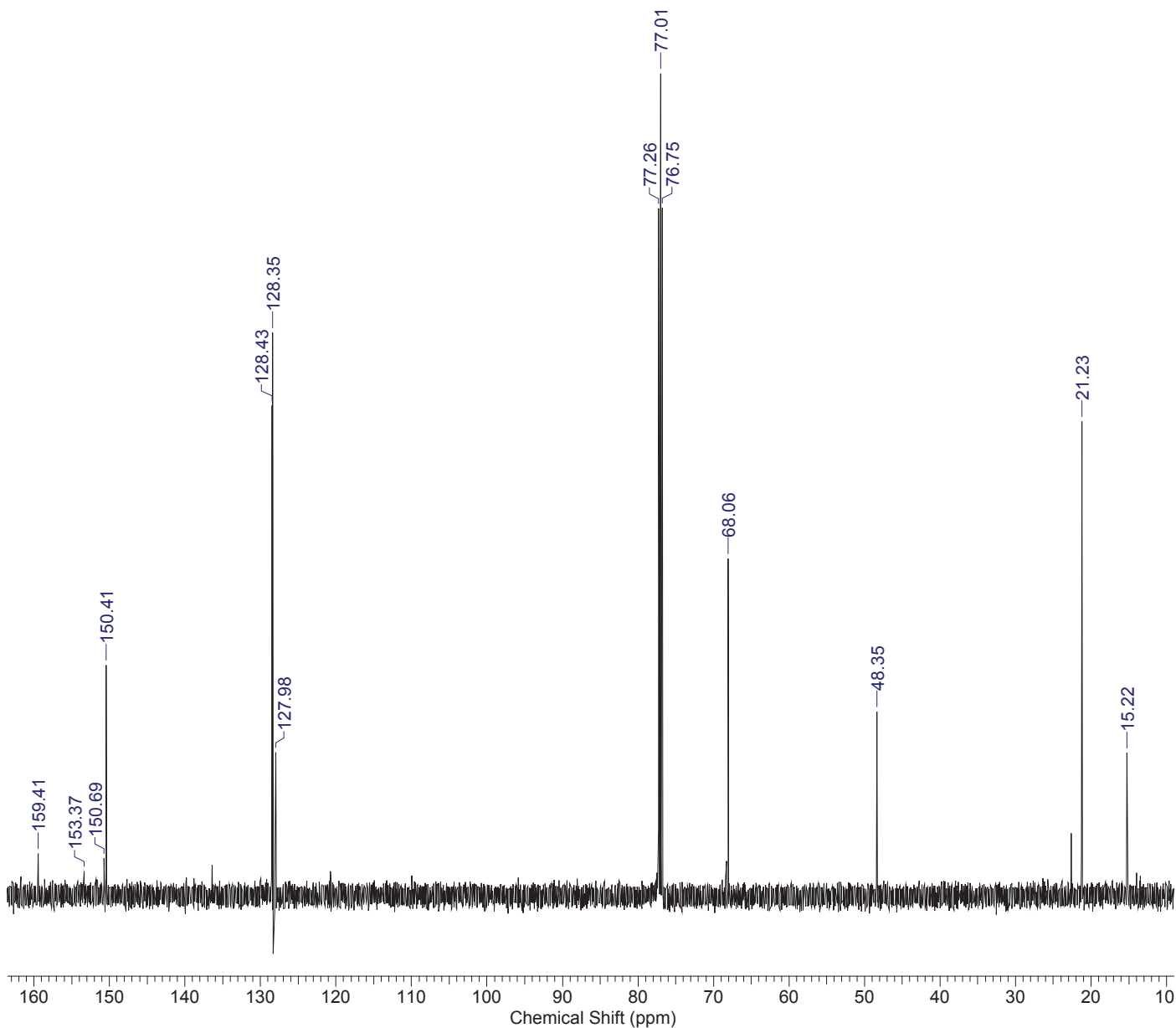
1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.1555	283.1559	-0.4	-1.4	9.5	23.1	C16 H19 N4 O
283.1535	283.1535	2.0	7.1	6.5	31.6	C14 H20 N4 O Na

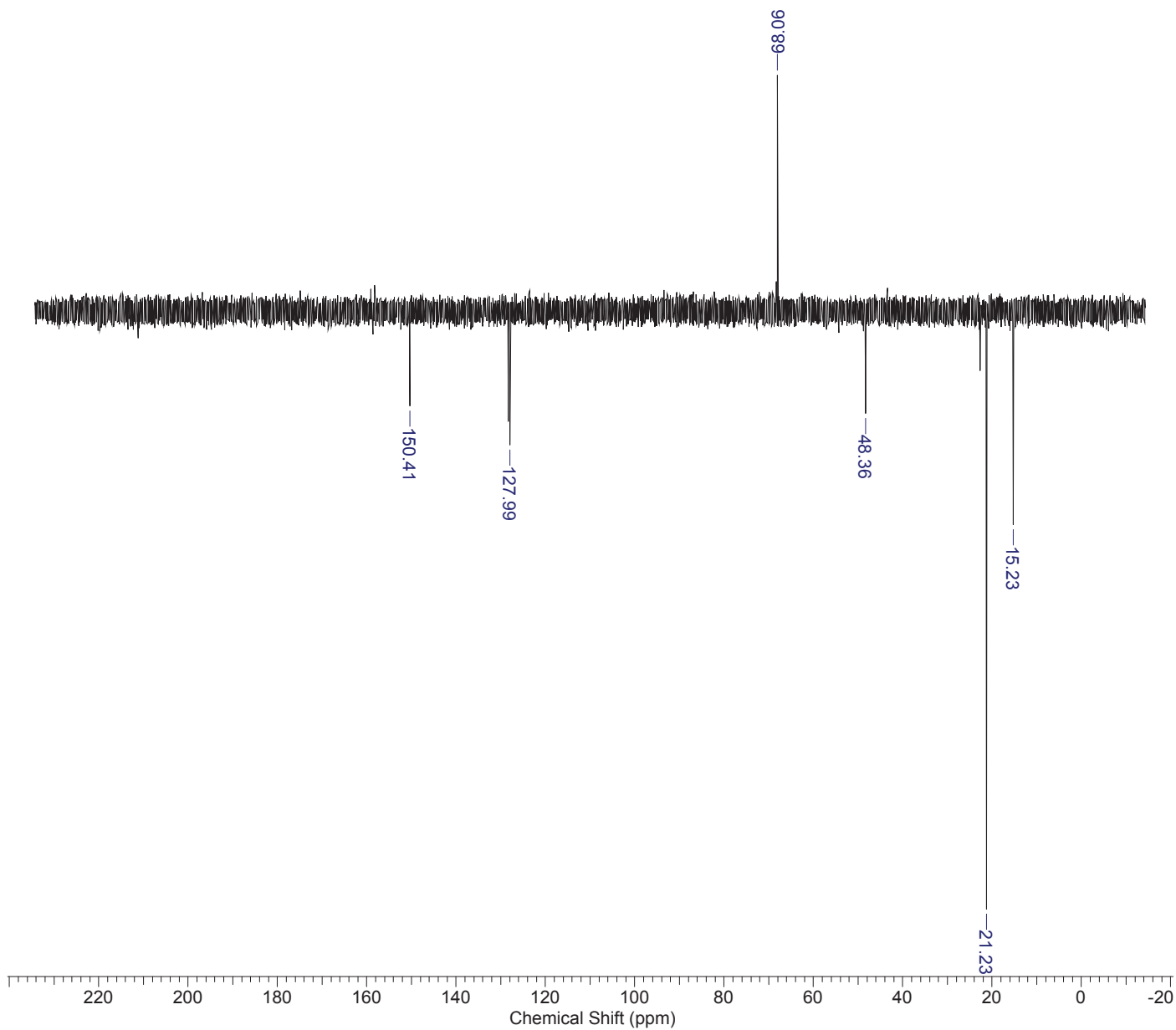
Minimum: -1.5
 Maximum: 50.0

Acquisition Time (sec)	1.0486	Date	Feb 22 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-158-12 ASIMJ-5\carbono				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	640
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	31250.00		
Temperature (degree C)	25.000				



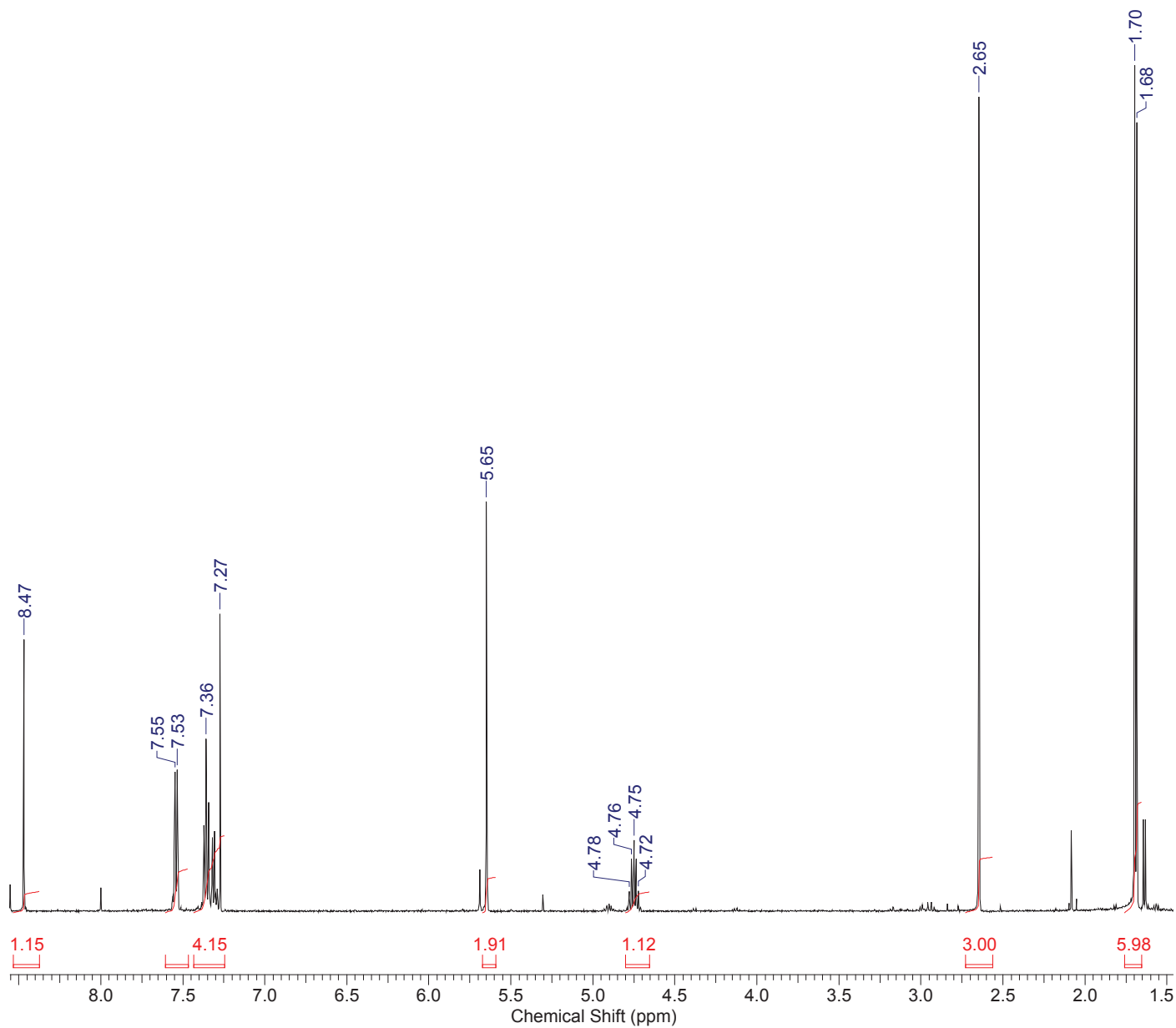
No.	(ppm)	(Hz)	Height
1	15.22	1913.4	0.1727
2	21.23	2667.8	0.5761
3	48.35	6077.3	0.2229
4	68.06	8554.1	0.4096
5	76.75	9646.1	0.8368
6	77.01	9678.5	1.0000
7	77.26	9710.0	0.8358
8	127.98	16085.5	0.1738
9	128.35	16132.2	0.6845
10	128.43	16141.7	0.5959
11	150.41	18903.7	0.2798
12	150.69	18939.9	0.0444
13	153.37	19276.6	0.0292
14	159.41	20035.7	0.0507

Acquisition Time (sec)	1.0486	Comment	new experiment	Date	Feb 22 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-158-12 ASIMJ-5\dept				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	2400
Original Points Count	32768	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D			Sweep Width (Hz)	31250.00
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	15.23	1914.4	-0.9040
2	21.23	2668.8	-2.5316
3	48.36	6078.3	-0.4334
4	68.06	8554.1	1.0000
5	127.99	16086.4	-0.5665
6	150.41	18903.7	-0.4006

Acquisition Time (sec)	1.9923	Date	Feb 22 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-158-12 ASIMJ-5\proton				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	1
Original Points Count	15964	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.68	841.9	0.9325
2	1.70	848.7	1.0000
3	2.65	1322.6	0.9626
4	4.72	2360.5	0.0255
5	4.75	2374.2	0.0857
6	4.76	2381.0	0.0634
7	4.78	2387.9	0.0253
8	5.65	2823.2	0.4849
9	7.27	3634.6	0.3526
10	7.36	3677.1	0.2053
11	7.53	3765.2	0.1687
12	7.55	3772.0	0.1659
13	8.47	4232.7	0.3220

No.	(ppm)	Value	Absolute Value
1	[1.66 .. 1.76]	5.985	2.44828e+6
2	[2.56 .. 2.73]	3.000	1.22724e+6
3	[4.65 .. 4.80]	1.124	4.59616e+5
4	[5.59 .. 5.67]	1.908	7.80710e+5
5	[7.25 .. 7.43]	4.154	1.69922e+6
6	[7.47 .. 7.61]	2.360	9.65603e+5
7	[8.37 .. 8.53]	1.147	4.69248e+5

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

525 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)

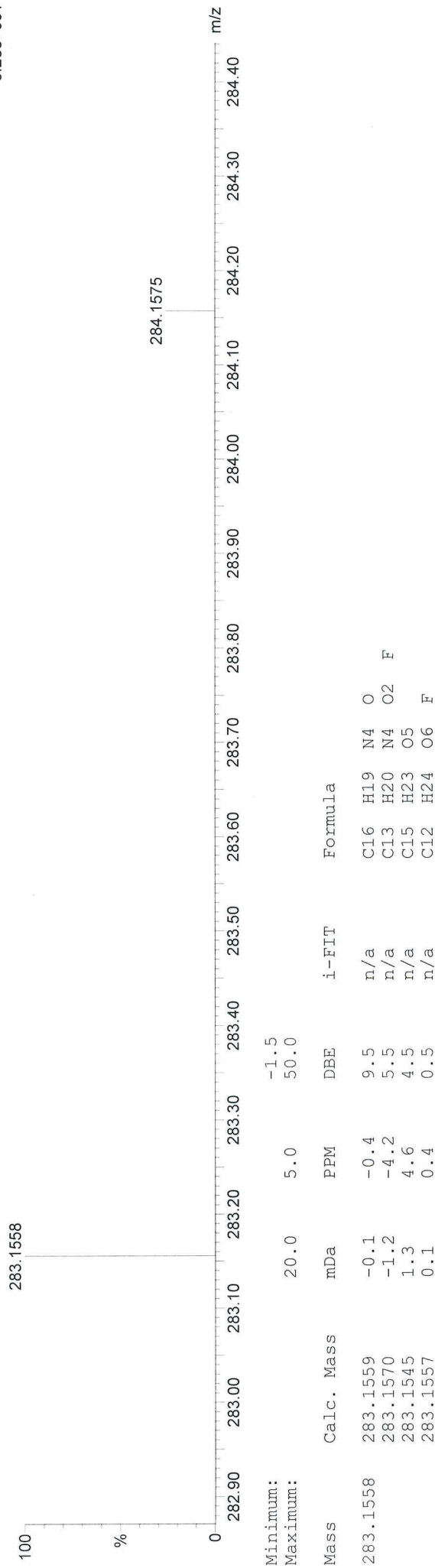
Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-6 F: 0-3

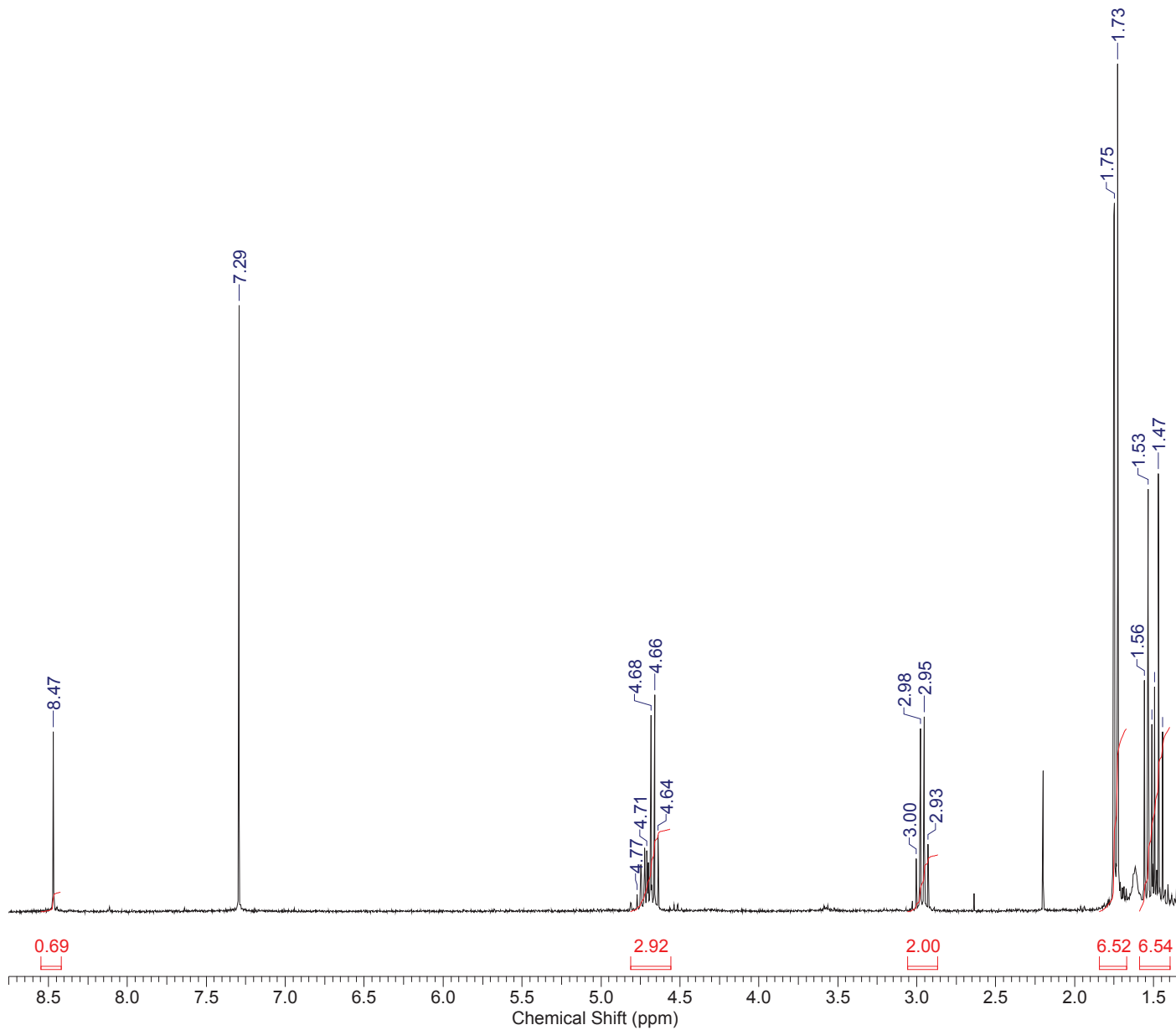
12/3293

ASIMJ-5 9 (0.217)

1: TOF MS ES+
9.28e+001



Acquisition Time (sec)	2.0484	Comment	ASI-MJ-2	Date	Feb 6 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\1H-ASI-MJ-2				
Frequency (MHz)	300.20	Nucleus	1H	Number of Transients	64
Original Points Count	7379	Points Count	8192	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	3602.31
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	1.44	433.4	0.2121
2	1.47	440.9	0.5167
3	1.49	448.4	0.2655
4	1.51	453.2	0.2214
5	1.53	460.7	0.4987
6	1.56	467.7	0.2730
7	1.73	518.7	1.0000
8	1.75	525.3	0.8356
9	2.93	878.9	0.0799
10	2.95	886.4	0.2303

No.	(ppm)	(Hz)	Height
11	2.98	893.9	0.2163
12	3.00	901.3	0.0624
13	4.64	1392.1	0.0903
14	4.66	1399.2	0.2558
15	4.68	1406.2	0.2320
16	4.71	1413.7	0.0724
17	4.77	1432.2	0.0207
18	7.29	2189.5	0.7151
19	8.47	2542.2	0.2124

No.	(ppm)	Value	Absolute Value
1	[1.39 .. 1.59]	6.536	2.20237e+8
2	[1.67 .. 1.84]	6.517	2.19591e+8
3	[2.87 .. 3.06]	2.000	6.73878e+7
4	[4.56 .. 4.81]	2.918	9.83286e+7
5	[8.42 .. 8.55]	0.693	2.33543e+7

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

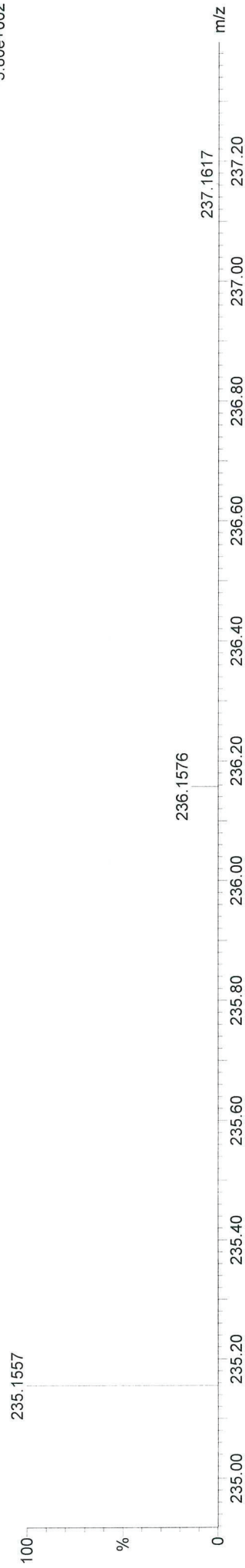
Monoisotopic Mass, Even Electron Ions
 427 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-6 F: 0-3

12/3290

1: TOF MS ES+
 5.80e+002

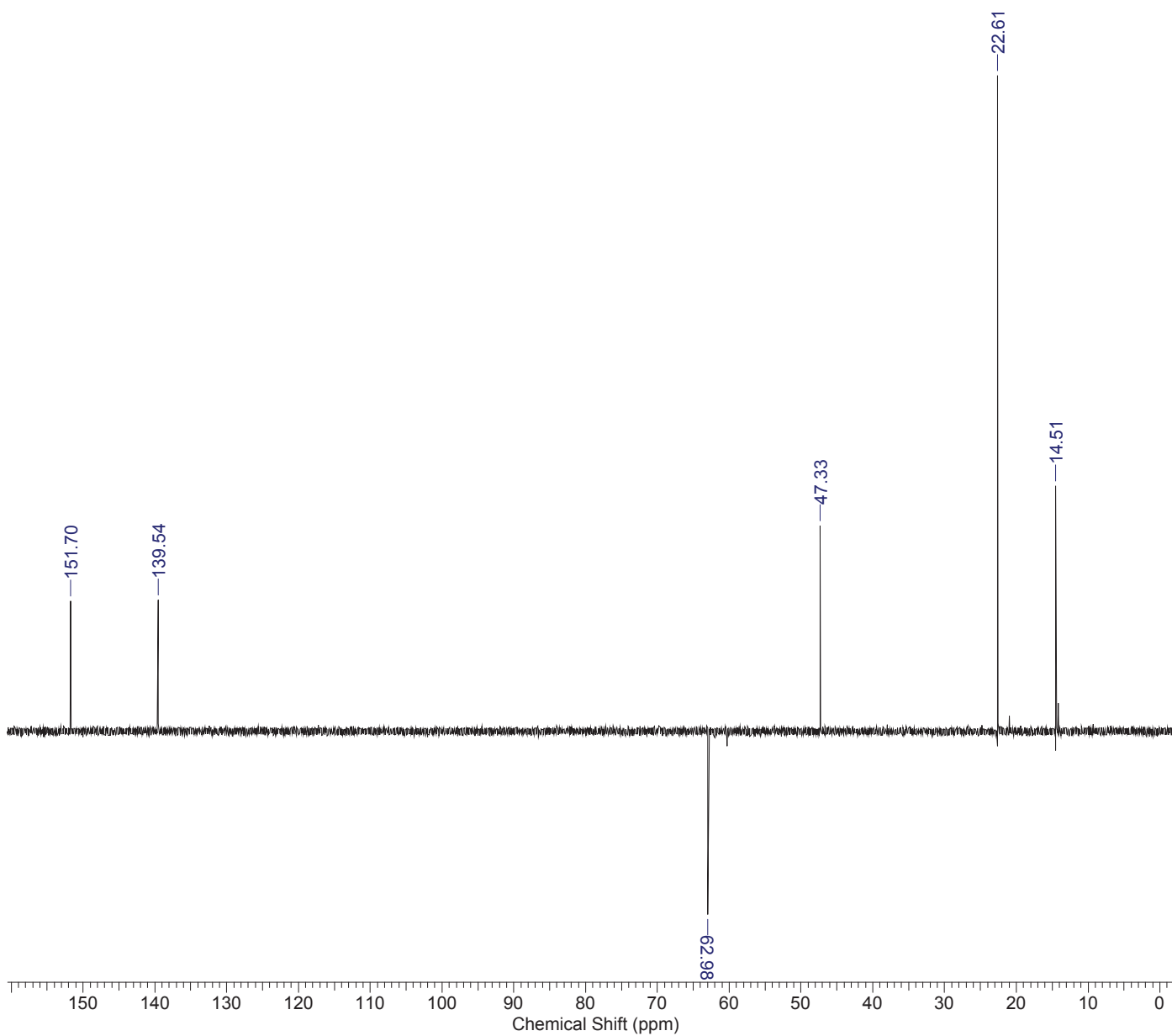
ASIMJ-2 9 (0.217)



Minimum: -1.5
 Maximum: 50.0

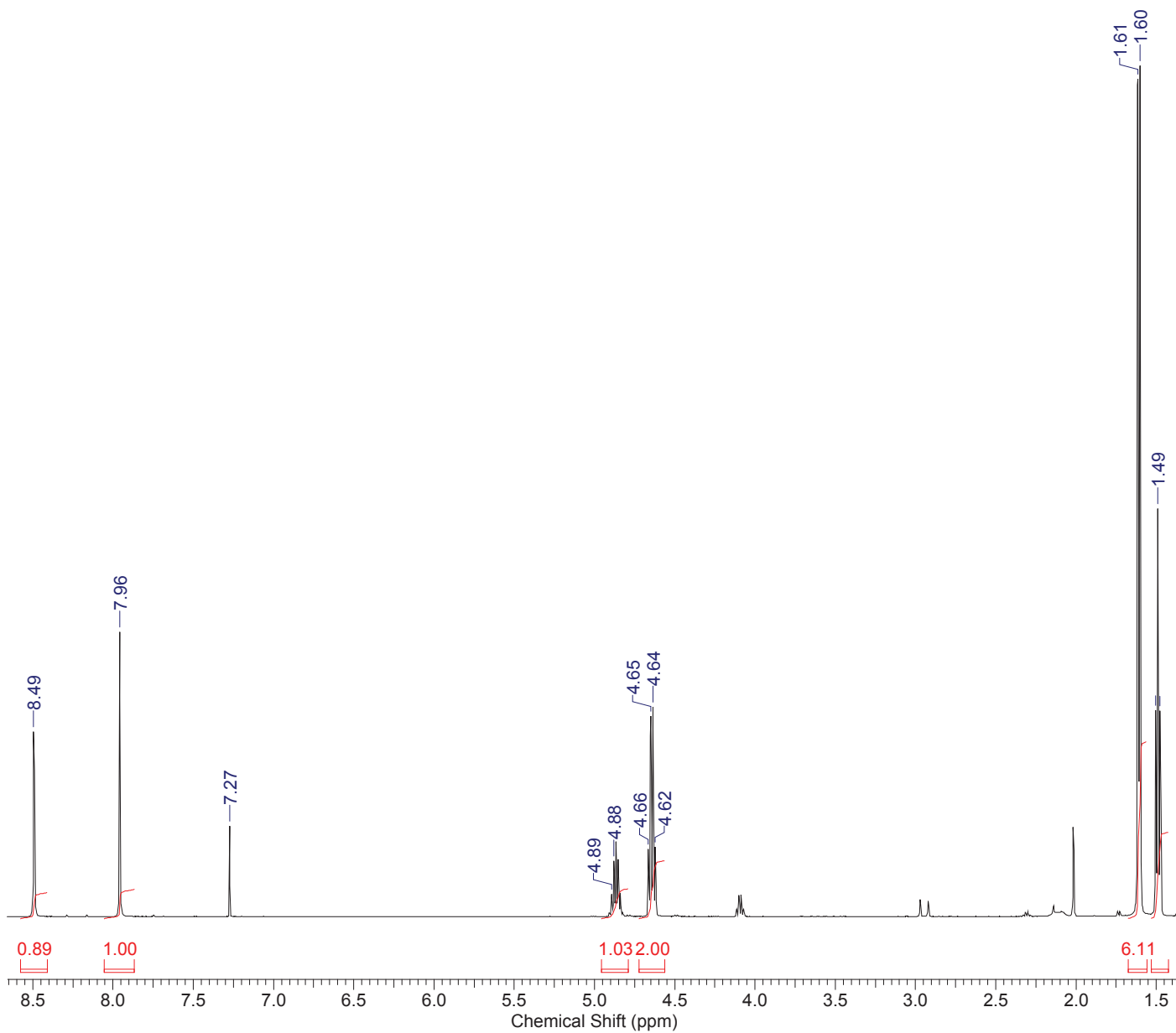
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.1557	235.1559	-0.2	-0.9	5.5	0.3	C12 H19 N4 O
	235.1545	1.2	5.1	0.5	1.0	C11 H23 O5

Acquisition Time (sec)	1.0486	Date	Feb 4 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-99-12_ASIMJ-1\DEPT_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D		Sweep Width (Hz)	31250.00	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	14.51	1823.8	0.3743
2	22.61	2841.4	1.0000
3	47.33	5948.6	0.3133
4	62.98	7915.1	-0.2795
5	139.54	17538.0	0.2003
6	151.70	19066.8	0.1987

Acquisition Time (sec)	2.0447	Date	Feb 4 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-99-12 ASIMJ-1\PROTON_01				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.48	738.3	0.2434
2	1.49	745.2	0.4809
3	1.51	752.5	0.2440
4	1.60	800.9	1.0000
5	1.61	806.8	0.9840
6	4.62	2309.8	0.0837
7	4.64	2317.1	0.2483
8	4.65	2323.5	0.2373
9	4.66	2331.3	0.0814
10	4.88	2439.4	0.0676
11	4.89	2446.2	0.0283
12	7.27	3635.2	0.1085
13	7.96	3977.6	0.3363
14	8.49	4245.6	0.2190

No.	(ppm)	Value	Absolute Value
1	[1.42 .. 1.53]	2.979	1.74678e+8
2	[1.56 .. 1.67]	6.113	3.58379e+8
3	[4.56 .. 4.72]	2.000	1.17260e+8
4	[4.79 .. 4.96]	1.030	6.03864e+7
5	[7.87 .. 8.06]	1.002	5.87716e+7
6	[8.41 .. 8.58]	0.894	5.24249e+7

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

369 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

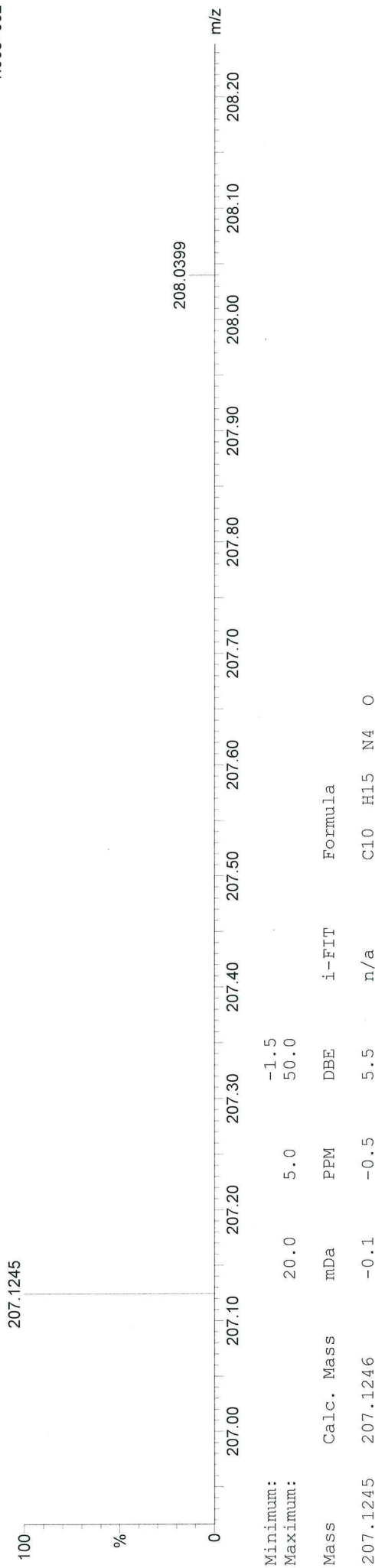
Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-6 F: 0-3

12/3289

ASIMJ-1 40 (0.885)

1: TOF MS ES+
1.90e+002

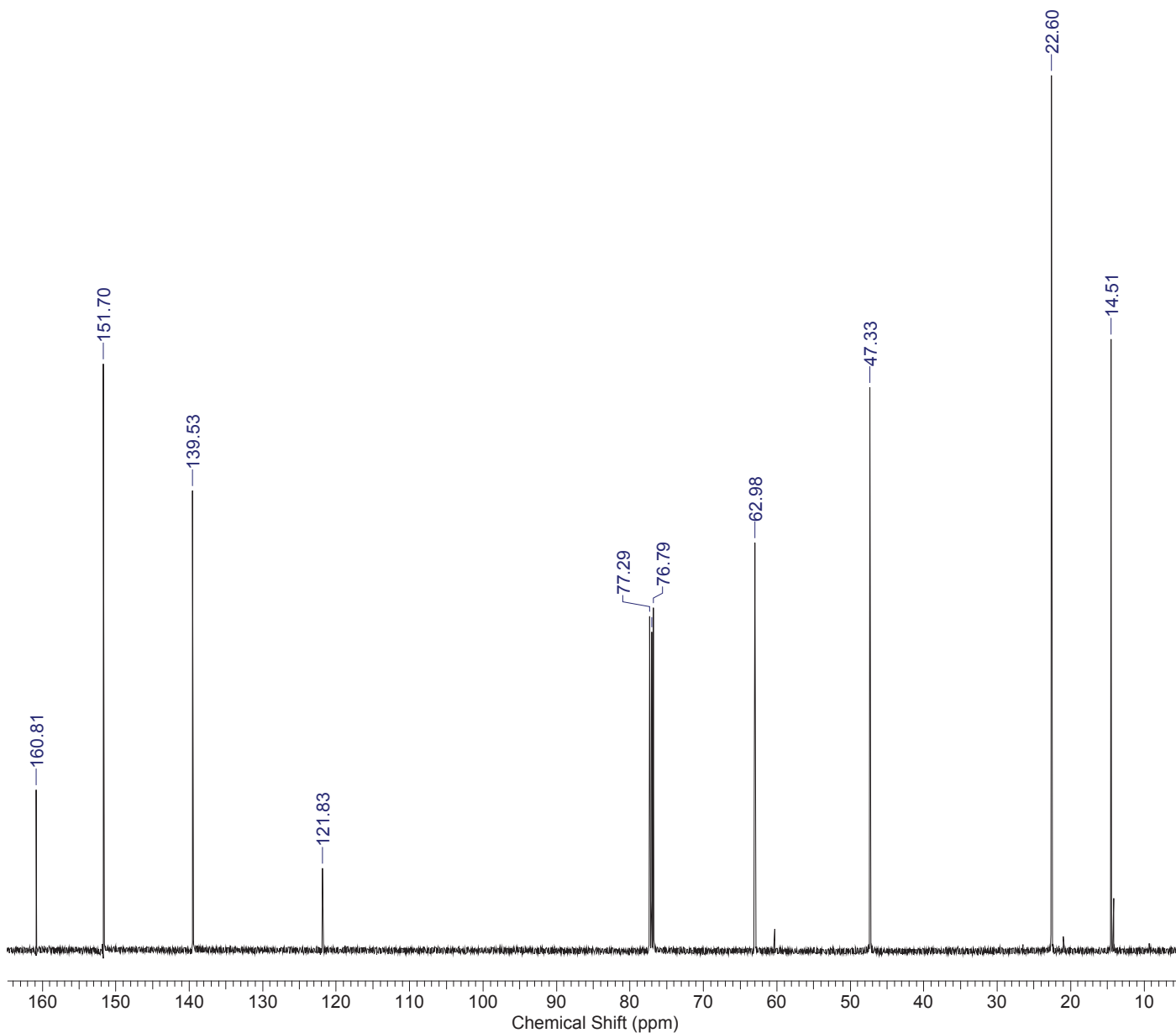


Minimum:
Maximum:

-1.5
50.0

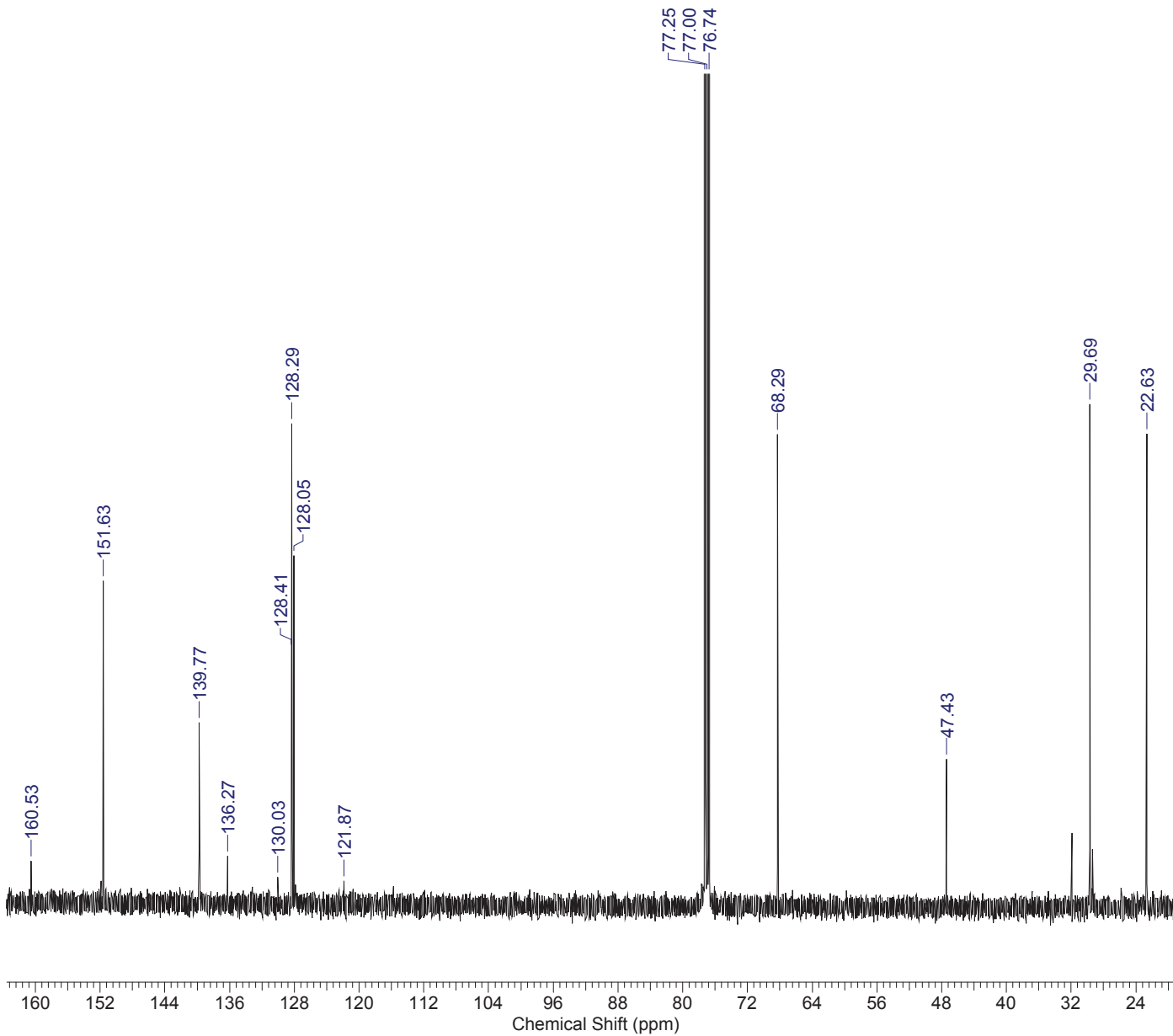
Mass Calc. Mass mDa DBE i-FIT Formula

Acquisition Time (sec)	1.0486	Date	Feb 4 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-99-12_ASIMJ-1\CARBON_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	3200
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	31250.00		
Temperature (degree C)	25.000				



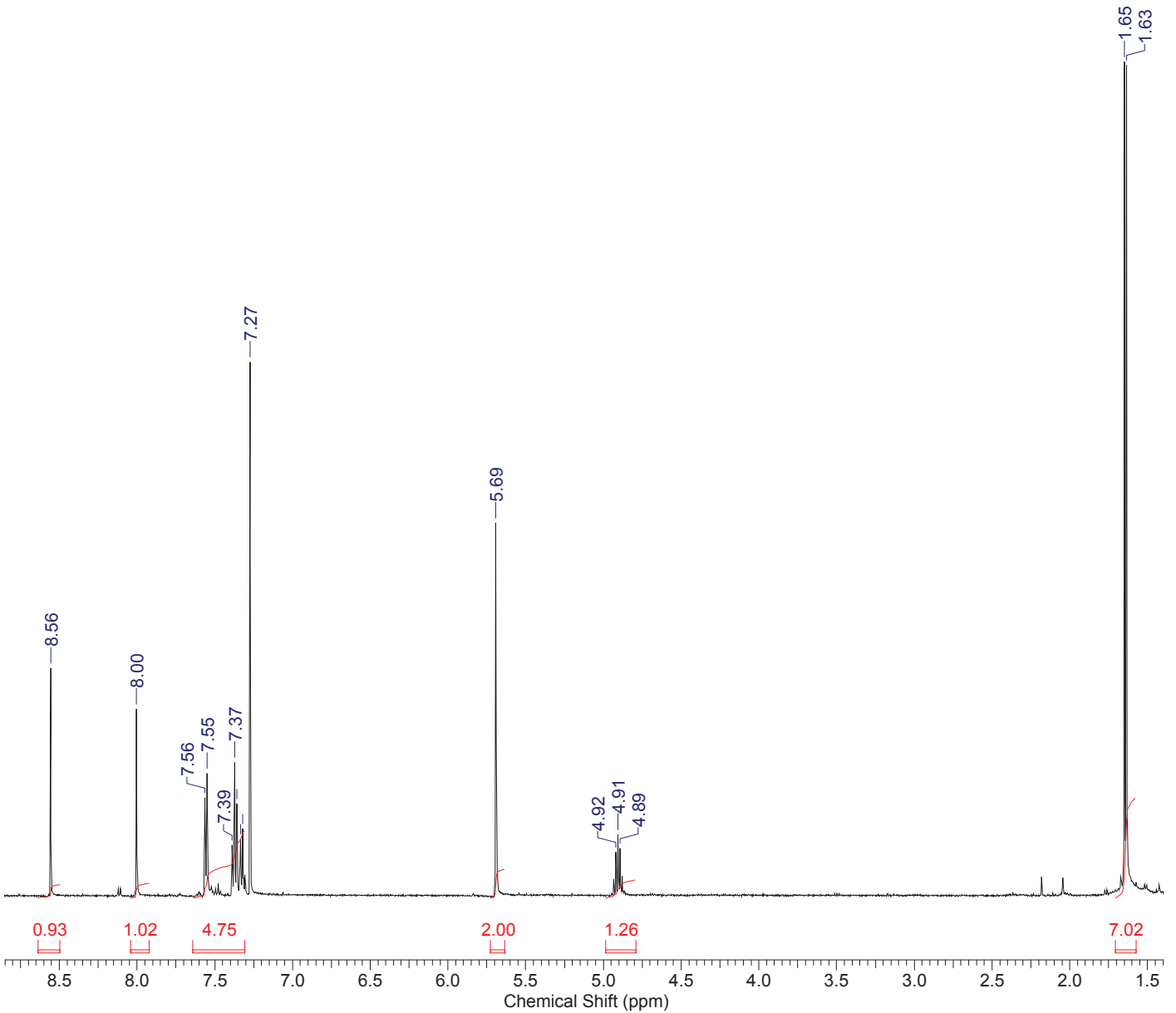
No.	(ppm)	(Hz)	Height
1	14.51	1823.8	0.6984
2	22.60	2840.4	1.0000
3	47.33	5948.6	0.6432
4	62.98	7915.1	0.4655
5	76.79	9650.8	0.3913
6	77.04	9683.3	0.3638
7	77.29	9714.7	0.3814
8	121.83	15312.0	0.0933
9	139.53	17537.0	0.5250
10	151.70	19066.8	0.6704
11	160.81	20211.2	0.1830

Acquisition Time (sec)	1.0486	Date	Feb 20 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-145-12 ASIMJ-4\carbono				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	32000
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	31250.00		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	22.63	2844.3	0.2148
2	29.69	3731.2	0.2284
3	47.43	5961.0	0.0663
4	68.29	8582.7	0.2146
5	76.74	9645.1	1.0000
6	77.00	9677.5	0.9472
7	77.25	9709.0	0.9887
8	121.87	15316.8	0.0107
9	128.05	16094.1	0.1592
10	128.29	16124.6	0.2194
11	128.41	16138.9	0.1165
12	130.03	16343.0	0.0125
13	136.27	17126.9	0.0220
14	139.77	17567.5	0.0830
15	151.63	19057.2	0.1476
16	160.53	20175.9	0.0197

Acquisition Time (sec)	1.9923	Date	Feb 20 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\RMN-145-12 ASIMJ-4\proton				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	8
Original Points Count	15964	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.63	816.9	0.9483
2	1.65	823.8	0.9517
3	4.89	2445.1	0.0564
4	4.91	2452.0	0.0723
5	4.92	2458.8	0.0524
6	5.69	2845.2	0.4268
7	7.27	3634.6	0.6098
8	7.32	3658.6	0.0785
9	7.33	3665.9	0.0672
10	7.36	3677.6	0.1072
11	7.37	3685.0	0.1544
12	7.39	3692.3	0.0603
13	7.55	3773.0	0.1416
14	7.56	3780.4	0.1137
15	8.00	4000.0	0.2149
16	8.56	4276.3	0.2617

No.	(ppm)	Value	Absolute Value
1	[1.57 .. 1.71]	7.019	9.08332e+6
2	[4.79 .. 4.98]	1.259	1.62902e+6
3	[5.64 .. 5.73]	2.000	2.58826e+6
4	[7.31 .. 7.64]	4.745	6.14069e+6
5	[7.92 .. 8.04]	1.024	1.32578e+6
6	[8.50 .. 8.64]	0.932	1.20635e+6

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

498 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)

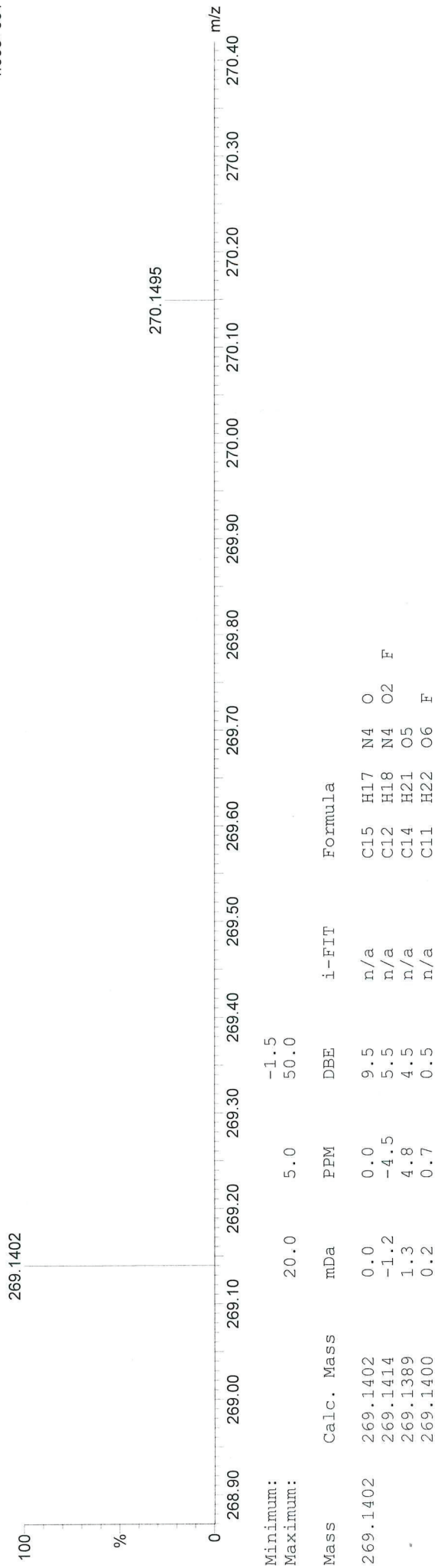
Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-6 F: 0-3

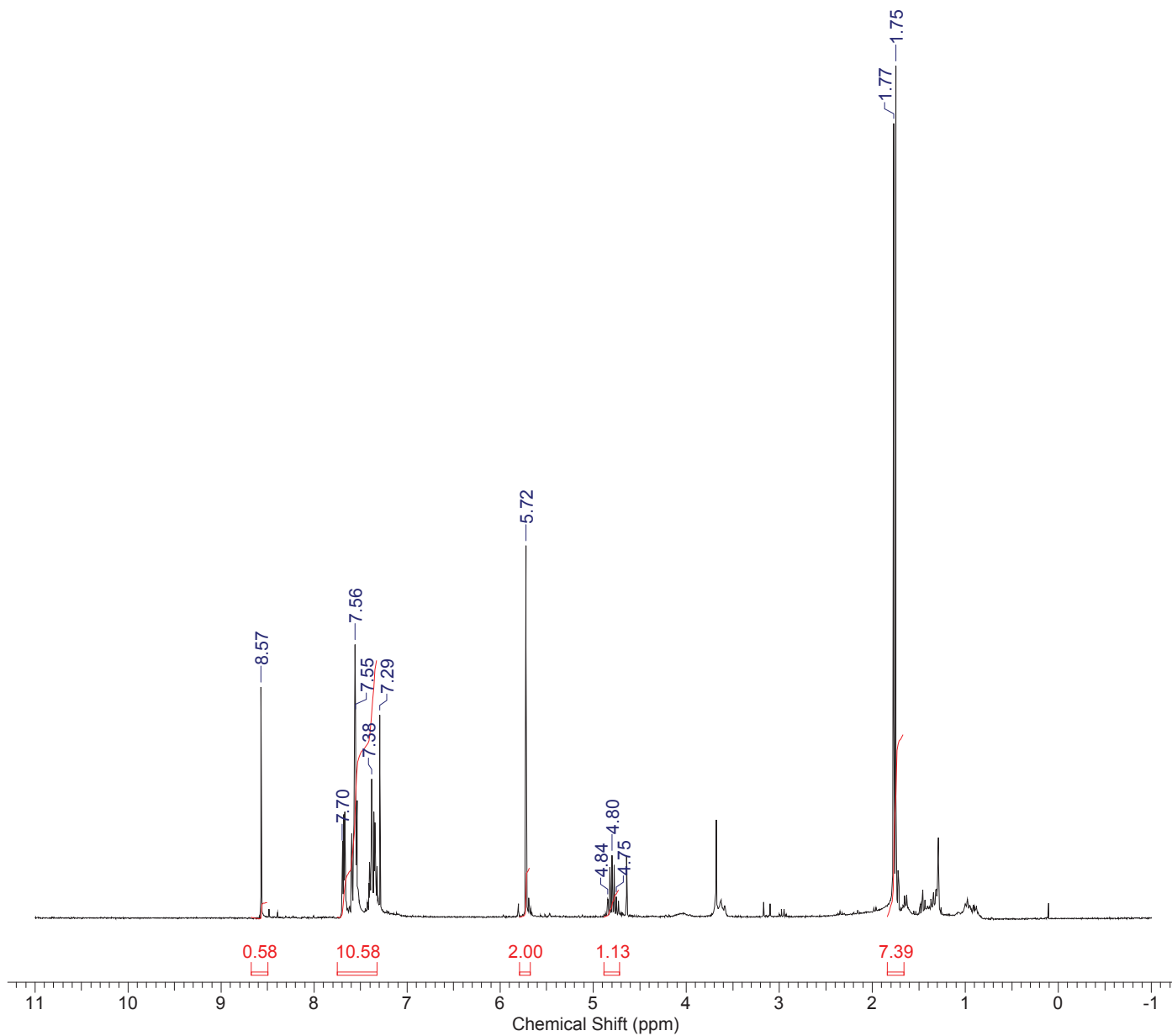
12/3292

ASIMJ-4.9 (0.217)

1: TOF MS ES+
4.60e+001



Acquisition Time (sec)	2.0487	Comment	ASIMJ-6p	Date	Apr 19 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-5265_ASIMJ-6p\1H-ASIMJ-6p				
Frequency (MHz)	300.20	Nucleus	1H	Number of Transients	64
Original Points Count	7380	Points Count	8192	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	3602.31		
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	1.75	524.4	1.0000
2	1.77	531.5	0.9324
3	4.75	1426.0	0.0237
4	4.80	1439.6	0.0729
5	4.84	1453.7	0.0214
6	5.72	1717.6	0.4364
7	7.29	2189.5	0.2378
8	7.38	2215.9	0.1621
9	7.55	2267.8	0.2390
10	7.56	2270.4	0.3199
11	7.70	2311.7	0.0844
12	8.57	2572.5	0.2705

No.	(ppm)	Value	Absolute Value
1	[1.66 .. 1.84]	7.393	2.72495e+8
2	[4.72 .. 4.88]	1.126	4.14961e+7
3	[5.68 .. 5.79]	2.000	7.37148e+7
4	[7.32 .. 7.75]	10.583	3.90054e+8
5	[8.50 .. 8.68]	0.582	2.14378e+7

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

136 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

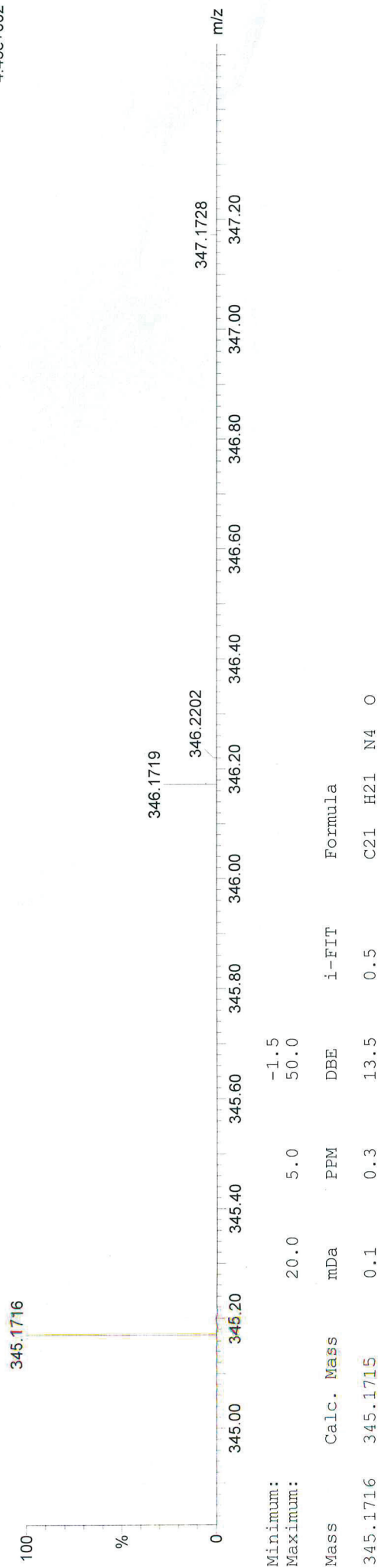
Elements Used:

C: 0-21 H: 0-1000 N: 0-4 O: 0-4 Na: 0-1

ASIMJ-6 4 (0.087)

12/5473

1: TOF MS ES+
4.45e+002

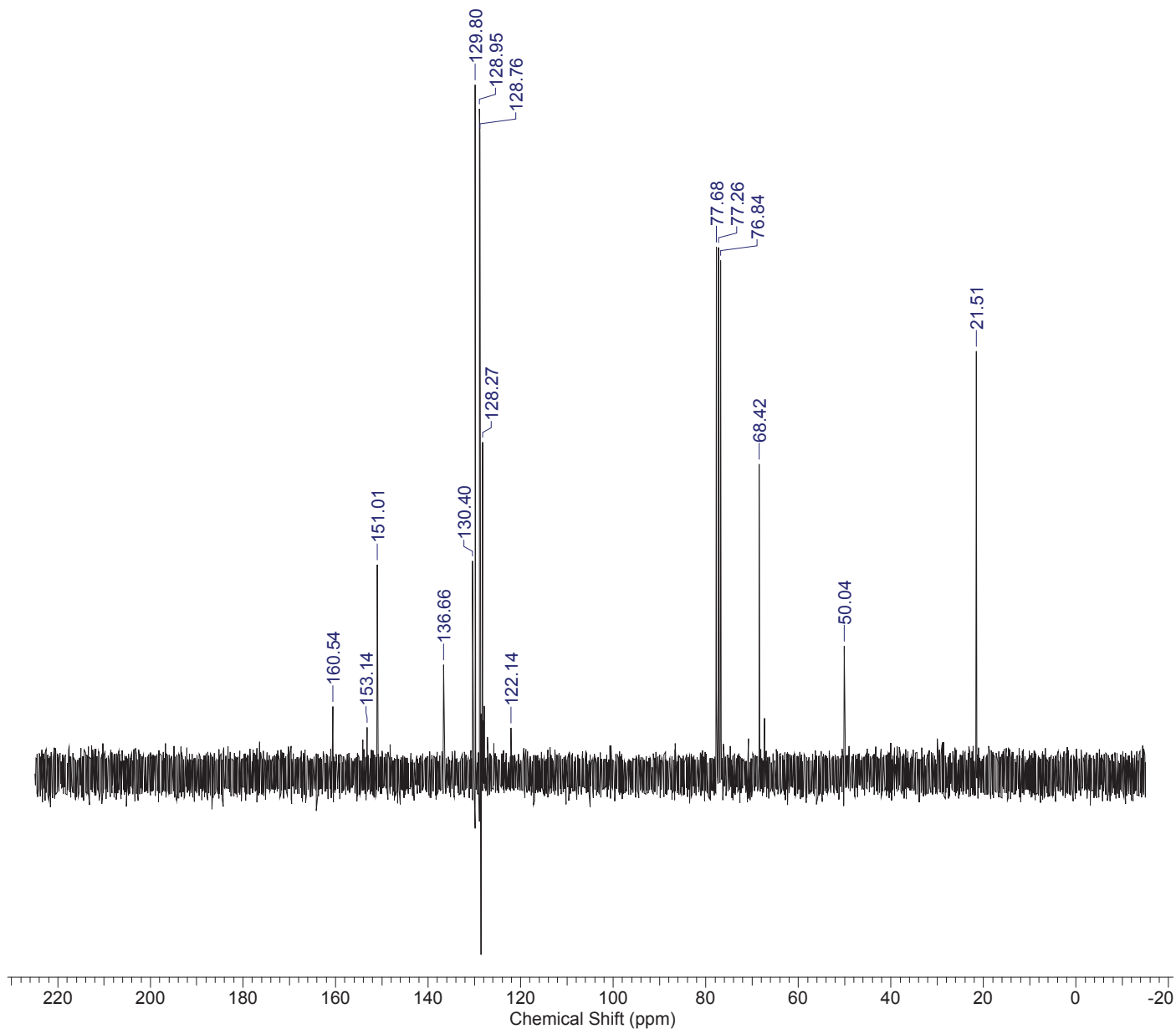


Minimum:
Maximum:

-1.5
50.0

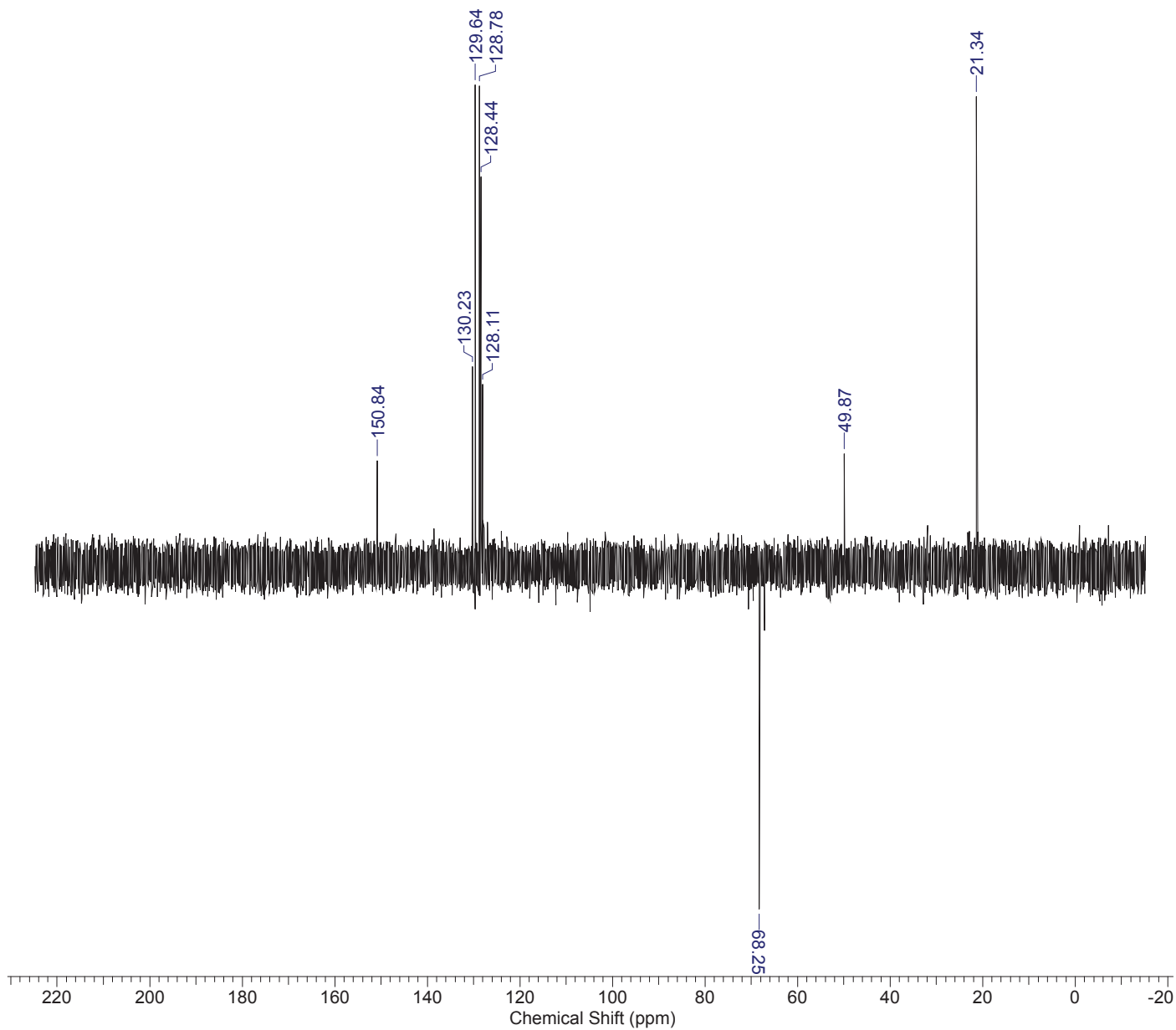
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
345.1716	345.1715	0.1	0.3	13.5	0.5	C21 H21 N4 O

Acquisition Time (sec)	1.3005	Comment	ASIMJ-6p	Date	Apr 19 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-5265_ASIMJ-6p\13C-ASIMJ-6p				
Frequency (MHz)	75.49	Nucleus	13C	Number of Transients	6400
Original Points Count	23559	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	18115.94		
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	21.51	1624.0	0.6139
2	50.04	3777.4	0.1866
3	68.42	5165.1	0.4500
4	76.84	5800.9	0.7455
5	77.26	5832.4	0.7640
6	77.68	5864.5	0.7647
7	122.14	9220.4	0.0674
8	128.27	9683.8	0.4819
9	128.61	9709.2	0.8357
10	128.76	9720.2	0.9293
11	128.95	9734.6	0.9649
12	129.80	9799.3	1.0000
13	130.40	9844.1	0.3097
14	136.66	10316.8	0.1588
15	151.01	11399.9	0.3044
16	153.14	11560.8	0.0682
17	160.54	12119.7	0.0983

Acquisition Time (sec)	1.0000	Comment	ASIMJ-6p	Date	Apr 19 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-5265_ASIMJ-6p\DEPT-ASIMJ-6p				
Frequency (MHz)	75.49	Nucleus	¹³ C	Number of Transients	4800
Original Points Count	18116	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D			Sweep Width (Hz)	18115.94
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	21.34	1611.3	0.9748
2	49.87	3764.7	0.2347
3	68.25	5152.5	-0.7110
4	128.11	9671.1	0.3783
5	128.44	9696.5	0.8089
6	128.59	9707.6	0.8026
7	128.78	9721.9	0.9972
8	129.64	9786.6	1.0000
9	130.23	9831.4	0.4147
10	150.84	11387.2	0.2201

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

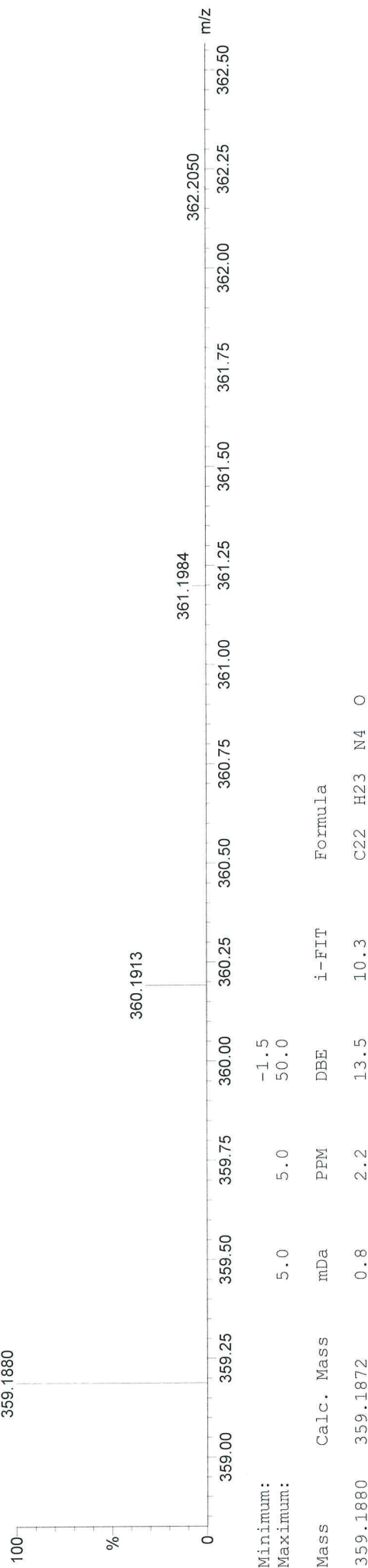
635 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-20 Na: 0-1

12/21702

ASIMJ-27P3 14 (0.317)

1: TOF MS ES+
8.90e+002

Minimum:

Maximum:

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

359.1880

359.1872

0.8

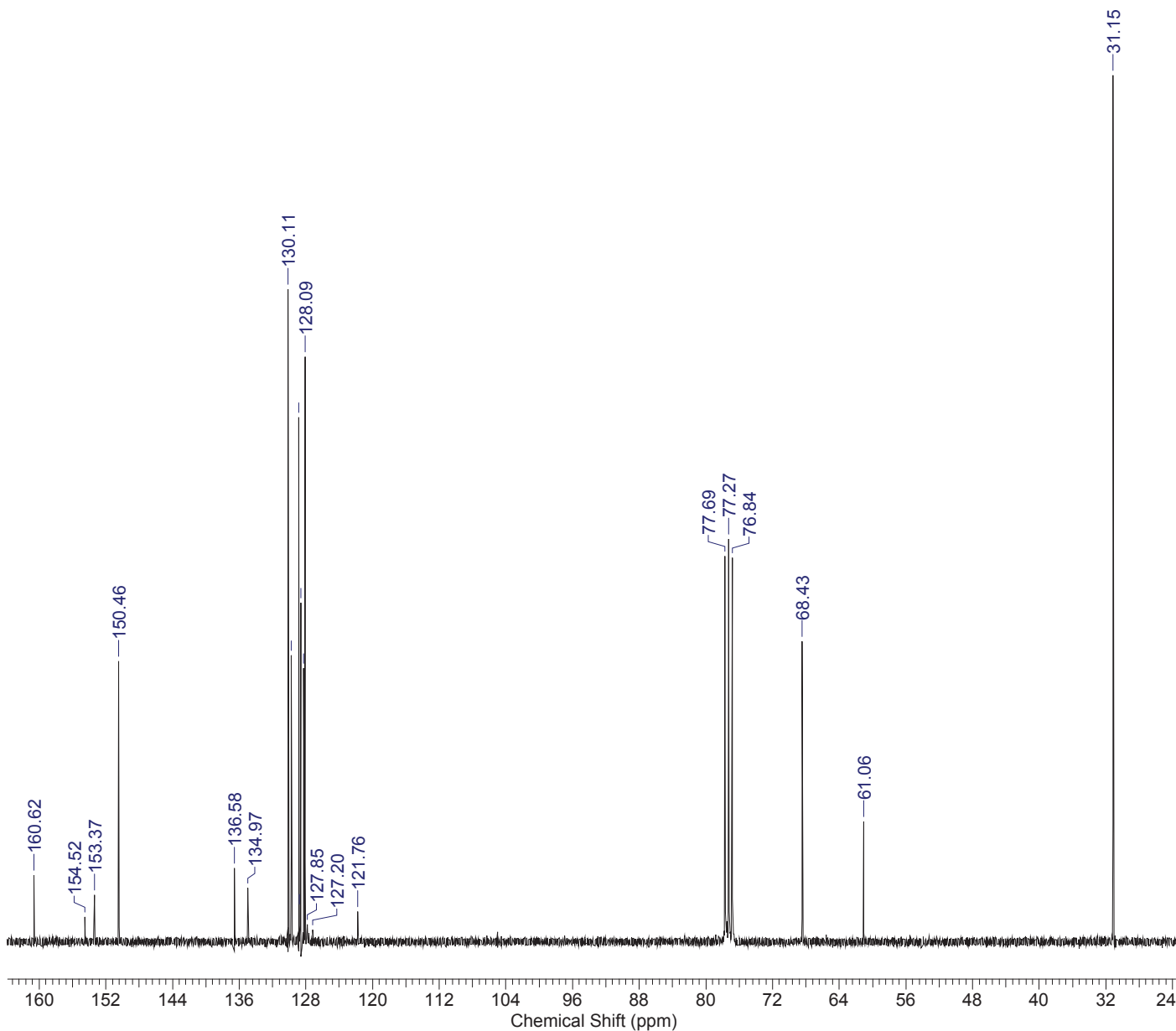
2.2

13.5

10.3

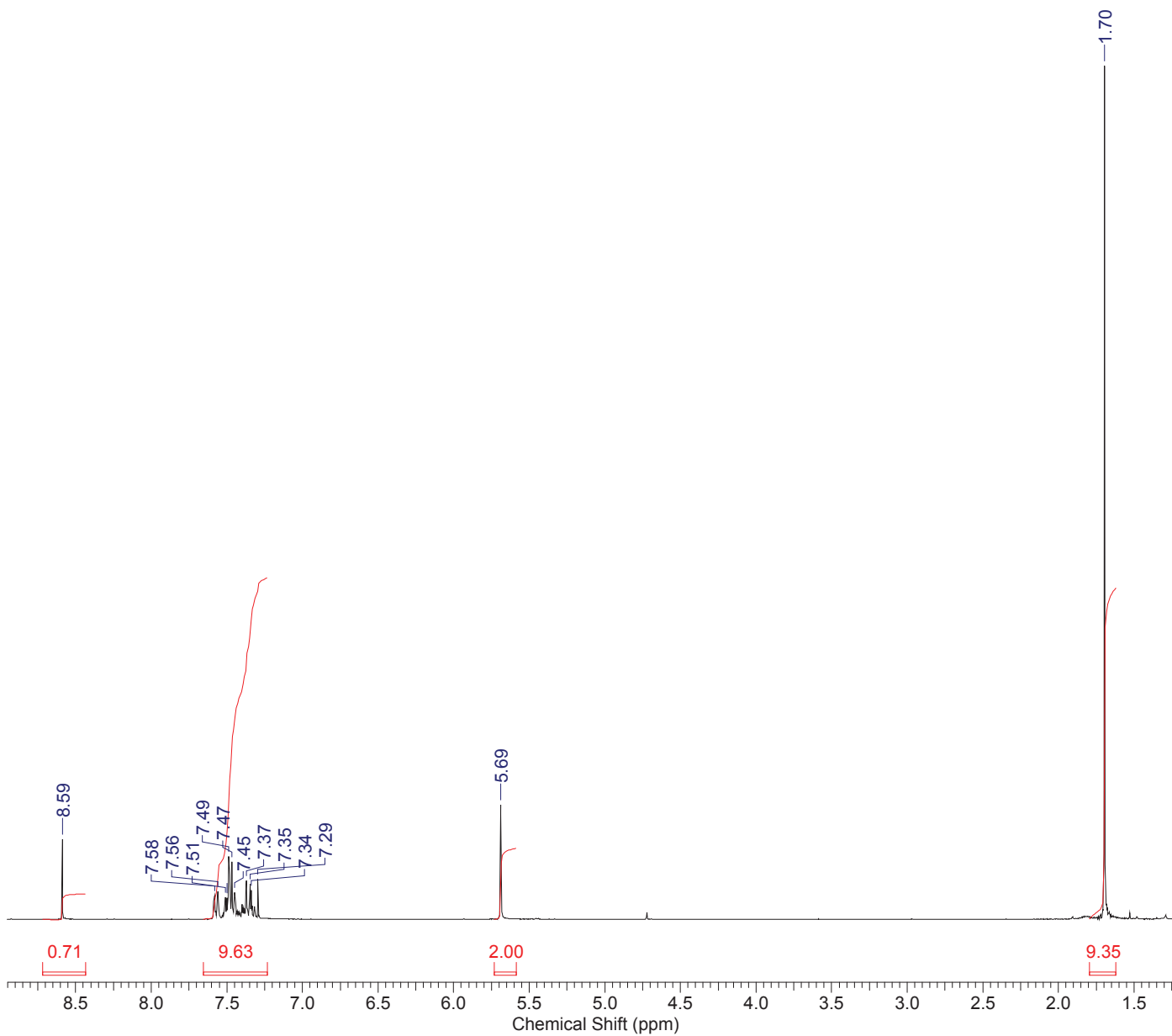
C22 H23 N4 O

Acquisition Time (sec)	1.3005	Comment	ASIMJ-27-P2-P	Date	Oct 22 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-21939 ASIMJ-27-P2-P\13C-ASIMJ-27-P2-P				
Frequency (MHz)	75.49	Nucleus	13C	Number of Transients	10000
Original Points Count	23559	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	18115.94
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	31.15	2351.6	1.0000	13	128.59	9707.5	0.3914
2	61.06	4609.5	0.1388	14	128.67	9713.6	0.0190
3	68.43	5166.3	0.3470	15	128.78	9721.9	0.0381
4	76.84	5800.9	0.4431	16	128.85	9727.4	0.6056
5	77.27	5833.0	0.4649	17	129.72	9793.2	0.3308
6	77.69	5865.1	0.4451	18	130.11	9822.5	0.7535
7	121.76	9192.3	0.0353	19	134.97	10189.6	0.0624
8	127.20	9602.5	0.0139	20	136.58	10310.7	0.0852
9	127.85	9651.7	0.0204	21	150.46	11358.4	0.3239
10	128.09	9669.9	0.6750	22	153.37	11578.5	0.0544
11	128.27	9683.8	0.3159	23	154.52	11665.3	0.0286
12	128.52	9702.6	0.0149	24	160.62	12125.8	0.0769

Acquisition Time (sec)	2.0487	Comment	ASIMJ-27-P2-P	Date	Oct 19 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-21939 ASIMJ-27-P2-P\1H-ASIMJ-27-P2-P				
Frequency (MHz)	300.20	Nucleus	1H	Number of Transients	64
Original Points Count	7380	Points Count	8192	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	3602.31		
Temperature (degree C)	30.000				

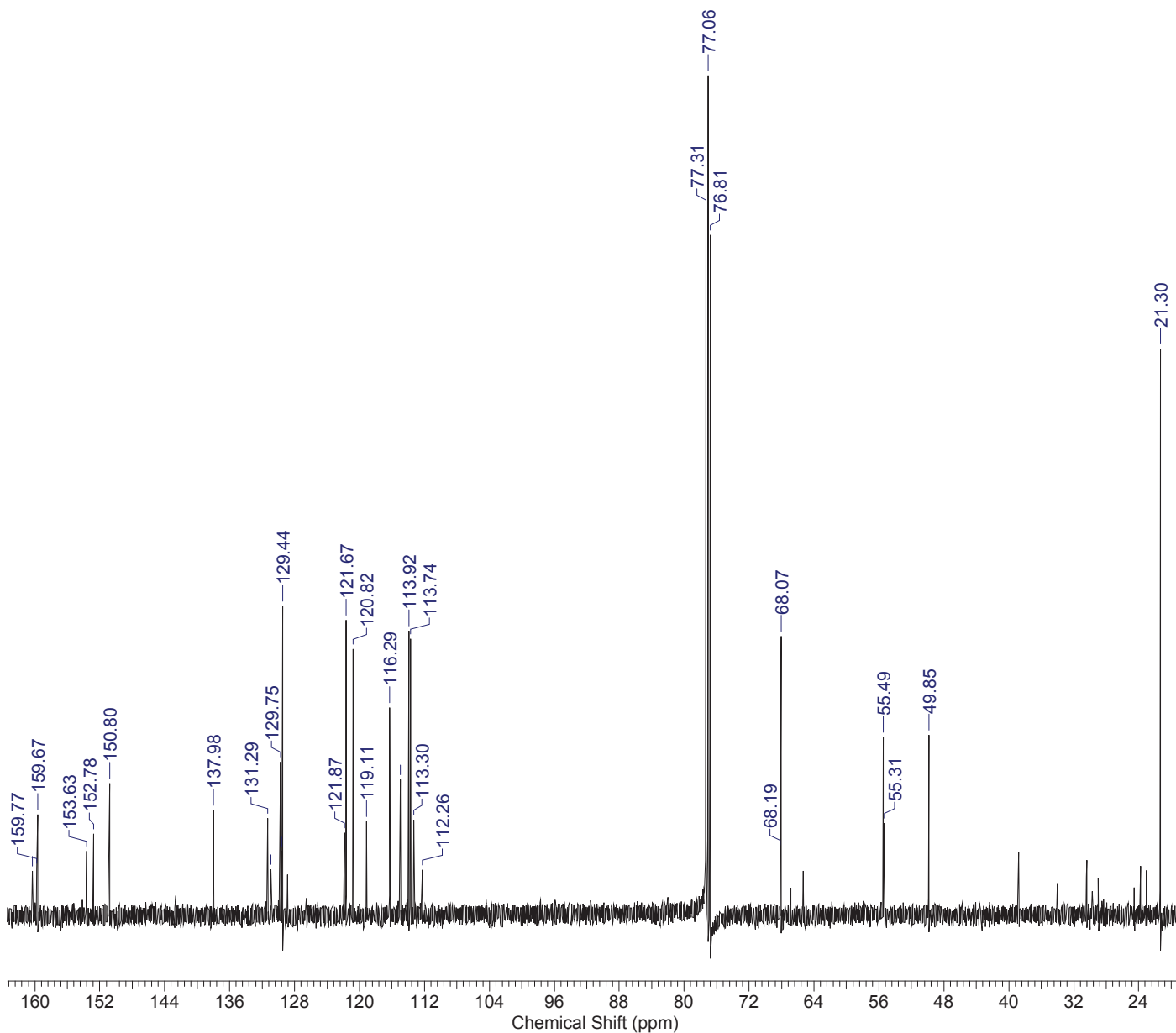


No.	(ppm)	(Hz)	Height
1	1.70	509.0	1.0000
2	5.69	1707.9	0.1344
3	7.29	2189.9	0.0470
4	7.34	2203.1	0.0338
5	7.35	2205.3	0.0415
6	7.37	2212.8	0.0455
7	7.45	2236.1	0.0317
8	7.47	2241.4	0.0675
9	7.49	2247.5	0.0736
10	7.50	2251.0	0.0253
11	7.51	2254.6	0.0254
12	7.56	2269.5	0.0329
13	7.58	2276.1	0.0273
14	8.59	2578.2	0.0940

No.	(ppm)	Value	Absolute Value
1	[1.62 .. 1.80]	9.348	7.90278e+8
2	[5.58 .. 5.73]	2.000	1.69088e+8
3	[7.23 .. 7.66]	9.629	8.14099e+8
4	[8.43 .. 8.72]	0.706	5.96692e+7

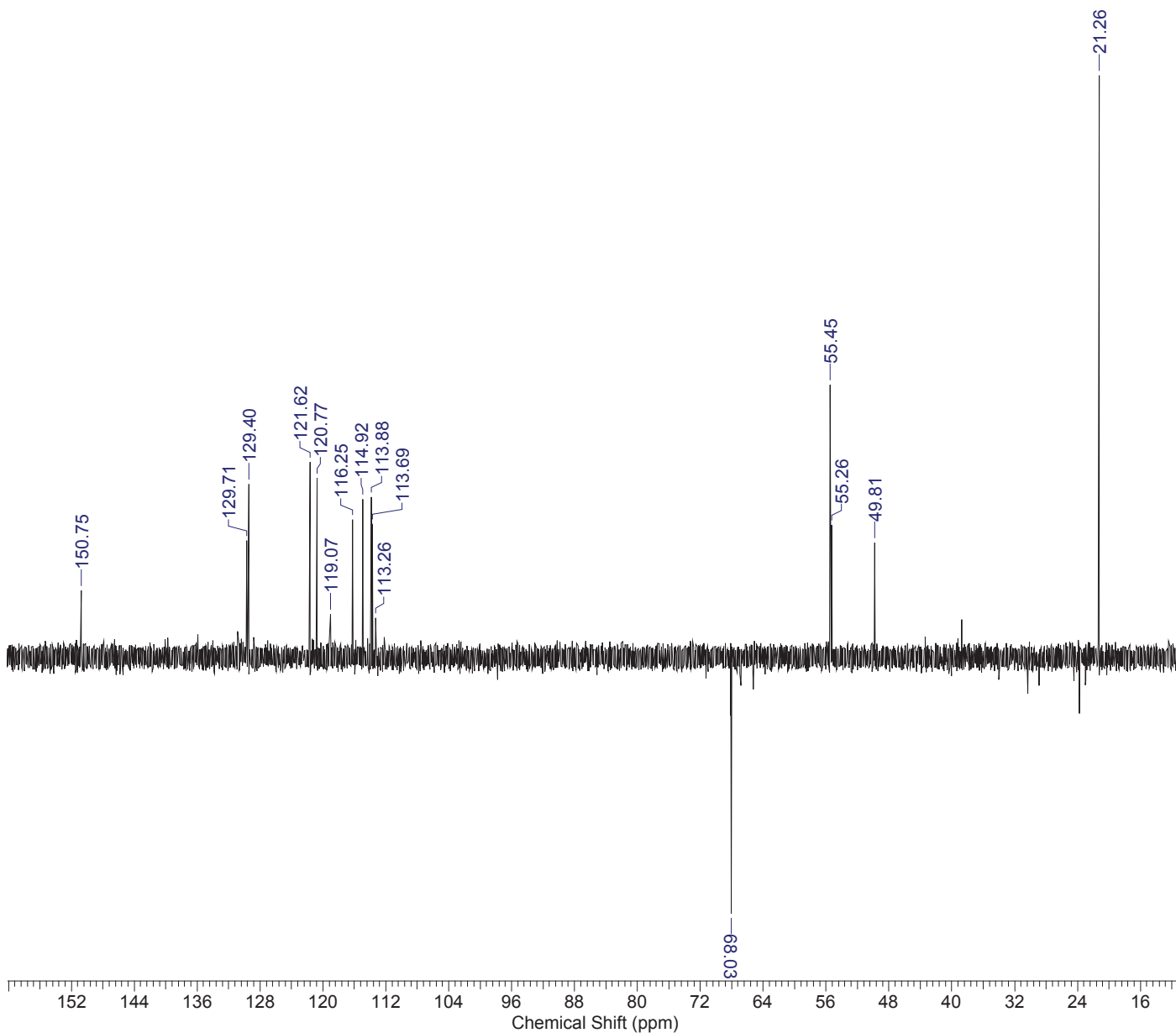
2 Jul 2013

Acquisition Time (sec)	1.0486	Comment	new experiment	Date	Jun 3 2013
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-13401		2G-ASIMJ-4\carbono		
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D		Sweep Width (Hz)		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.30	2676.9	0.6743	17	119.11	14970.1	0.1106
2	49.85	6265.7	0.2134	18	120.82	15184.7	0.3164
3	55.26	6945.7	0.0986	19	121.67	15291.5	0.3509
4	55.31	6951.4	0.1089	20	121.87	15317.3	0.0970
5	55.49	6974.3	0.2111	21	129.44	16269.1	0.3675
6	68.07	8555.5	0.3317	22	129.63	16292.0	0.0748
7	68.19	8570.8	0.0769	23	129.75	16308.2	0.1815
8	76.81	9653.3	0.8097	24	130.91	16453.2	0.0534
9	77.06	9684.7	1.0000	25	131.29	16500.8	0.1145
10	77.31	9717.1	0.8400	26	137.98	17342.0	0.1240
11	112.26	14109.9	0.0529	27	150.80	18953.8	0.1563
12	113.30	14240.6	0.1126	28	152.78	19202.7	0.0955
13	113.74	14294.9	0.3282	29	153.63	19308.5	0.0752
14	113.92	14317.8	0.3379	30	159.67	20068.6	0.1188
15	114.96	14448.5	0.1602	31	159.77	20081.0	0.0549
16	116.29	14616.3	0.2461	32	160.27	20144.0	0.0514

Acquisition Time (sec)	1.0486	Comment	new experiment	Date	Jun 3 2013
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-13401		2G-ASIMJ-4\dept		
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D		Sweep Width (Hz)	31250.00	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	21.26	2671.6	1.0000
2	49.81	6260.4	0.1963
3	55.22	6940.4	0.1545
4	55.26	6945.2	0.2267
5	55.45	6969.0	0.4680
6	68.03	8550.3	-0.4404
7	113.26	14235.3	0.0677
8	113.69	14289.7	0.2291
9	113.88	14312.5	0.2754
10	114.92	14443.2	0.2714
11	116.25	14611.1	0.2360
12	119.07	14964.9	0.0744
13	120.77	15179.5	0.3076
14	121.62	15286.3	0.3350
15	129.40	16263.8	0.2975
16	129.71	16302.9	0.1999
17	150.75	18947.5	0.1144

Elemental Composition Report

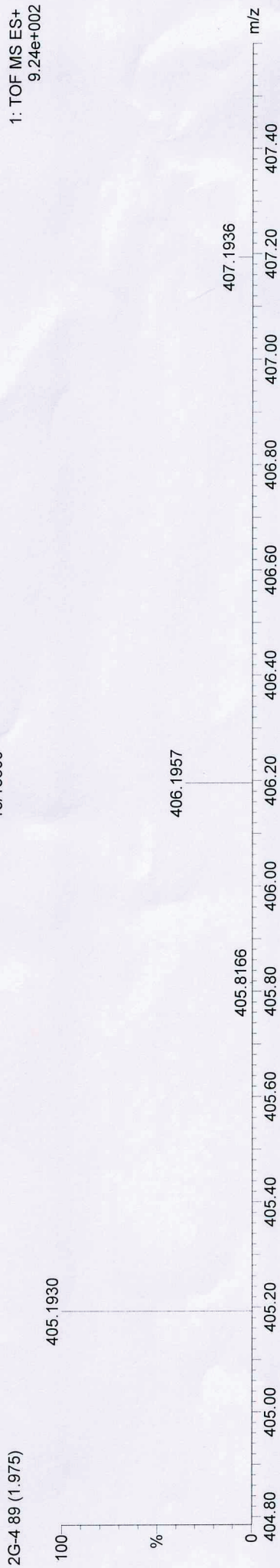
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 359 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:

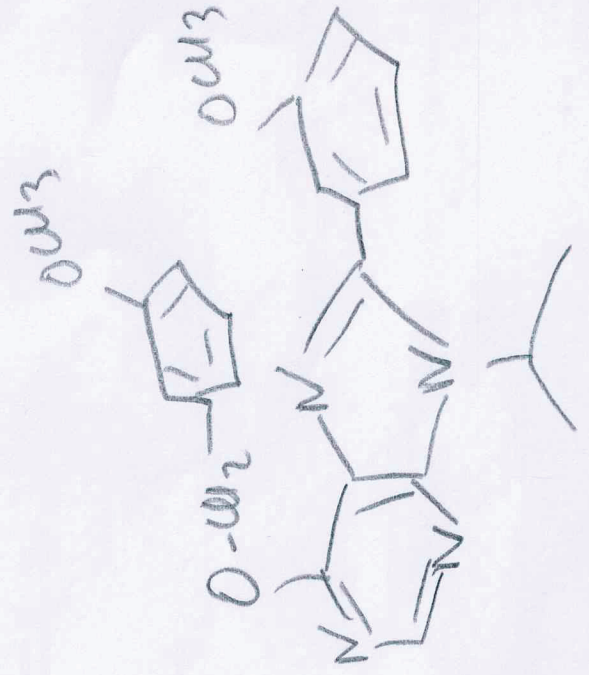
C: 0-23 H: 0-1000 N: 0-4 O: 0-4 Na: 0-1 I: 0-2

1: TOF MS ES+
 9.24e+002

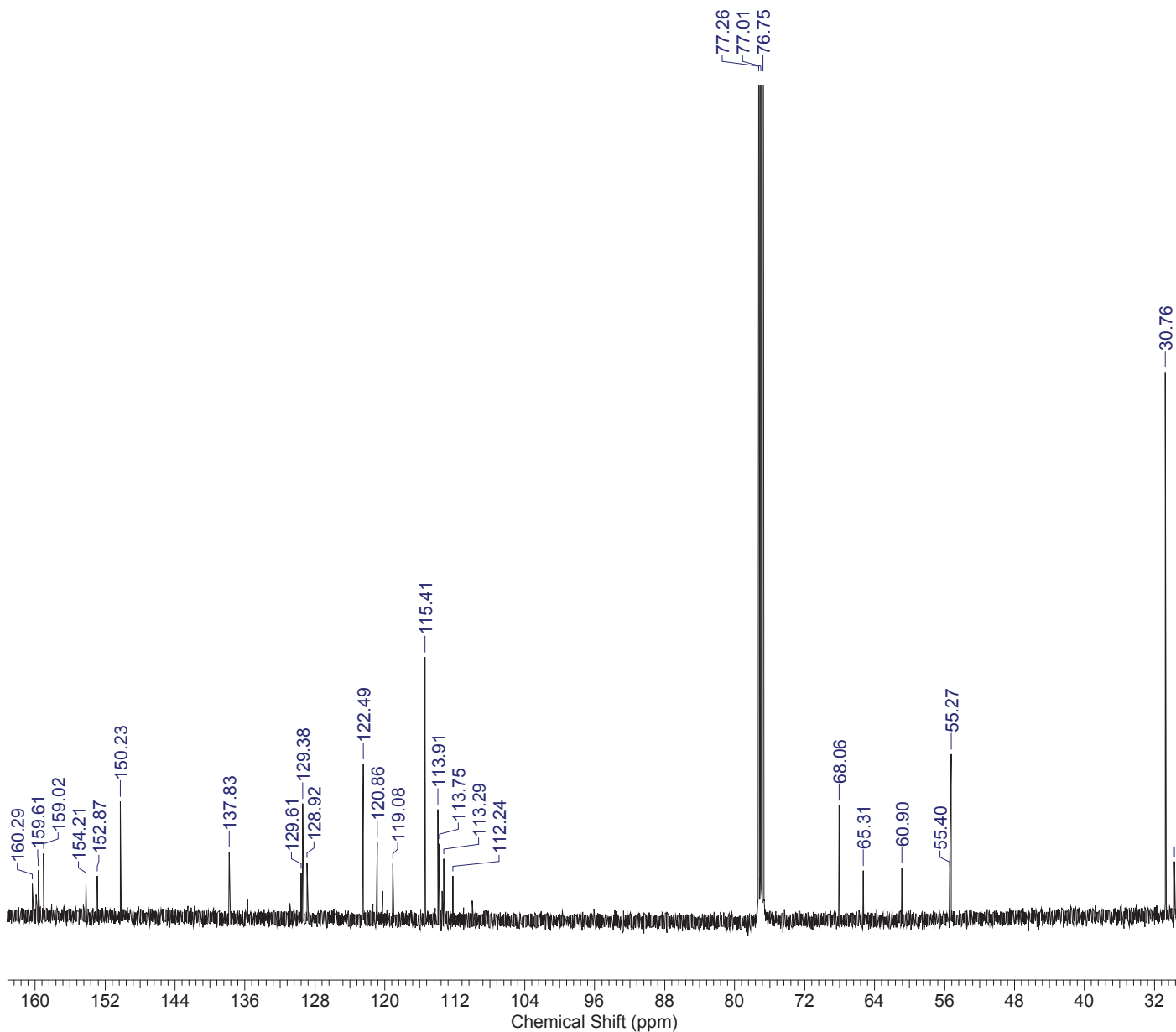


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.1930	405.1927	0.3	0.7	13.5	12.2	C23 H25 N4 O3
	405.1903	2.7	6.7	10.5	19.1	C21 H26 N4 O3 Na

Minimum: -1.5
 Maximum: 50.0

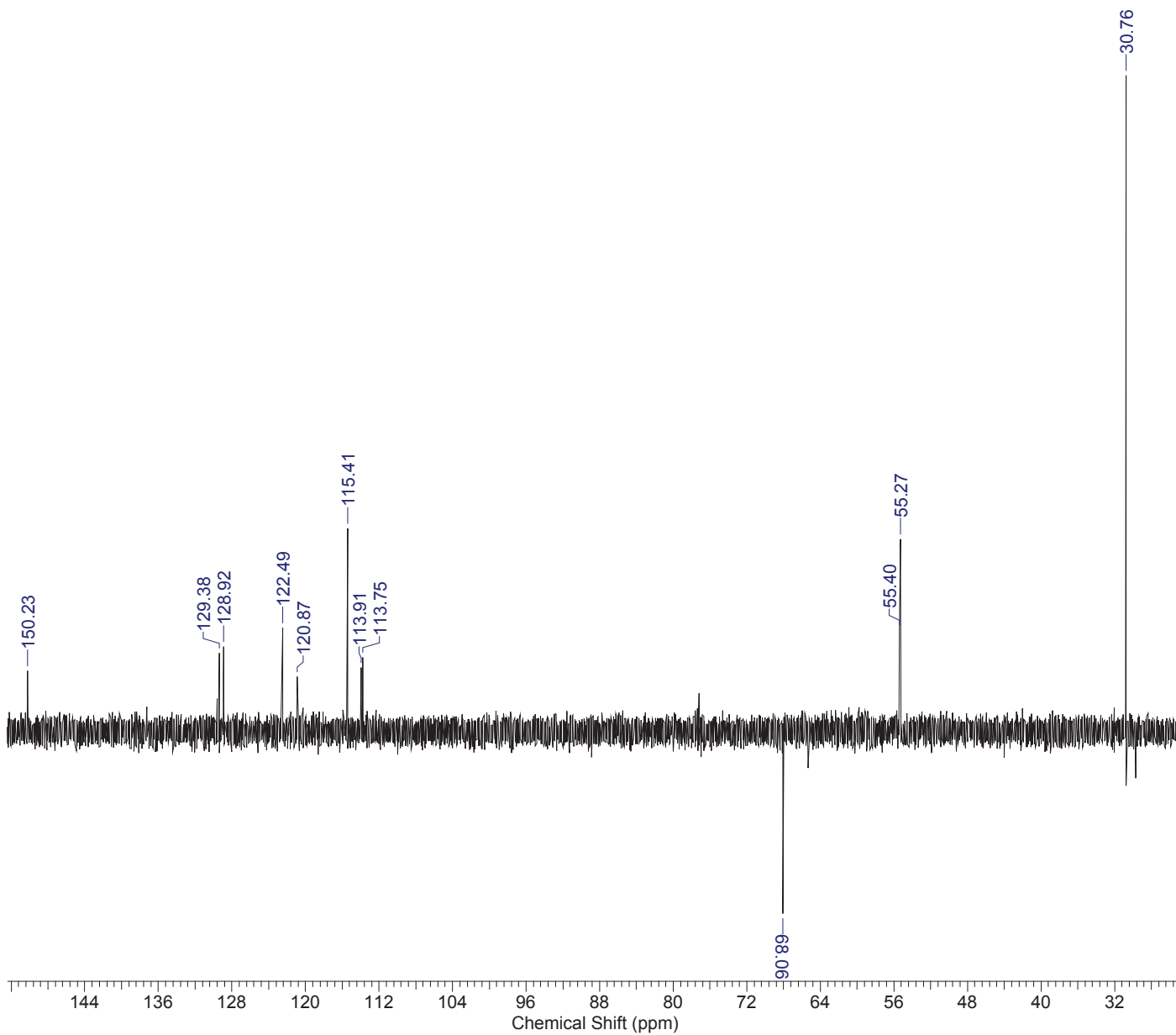


Acquisition Time (sec)	1.0486	Date	May 9 2013		
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-11181_2ASIMJ-1_500\CARBON_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	9600
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	31250.00		
Temperature (degree C)	25.000				



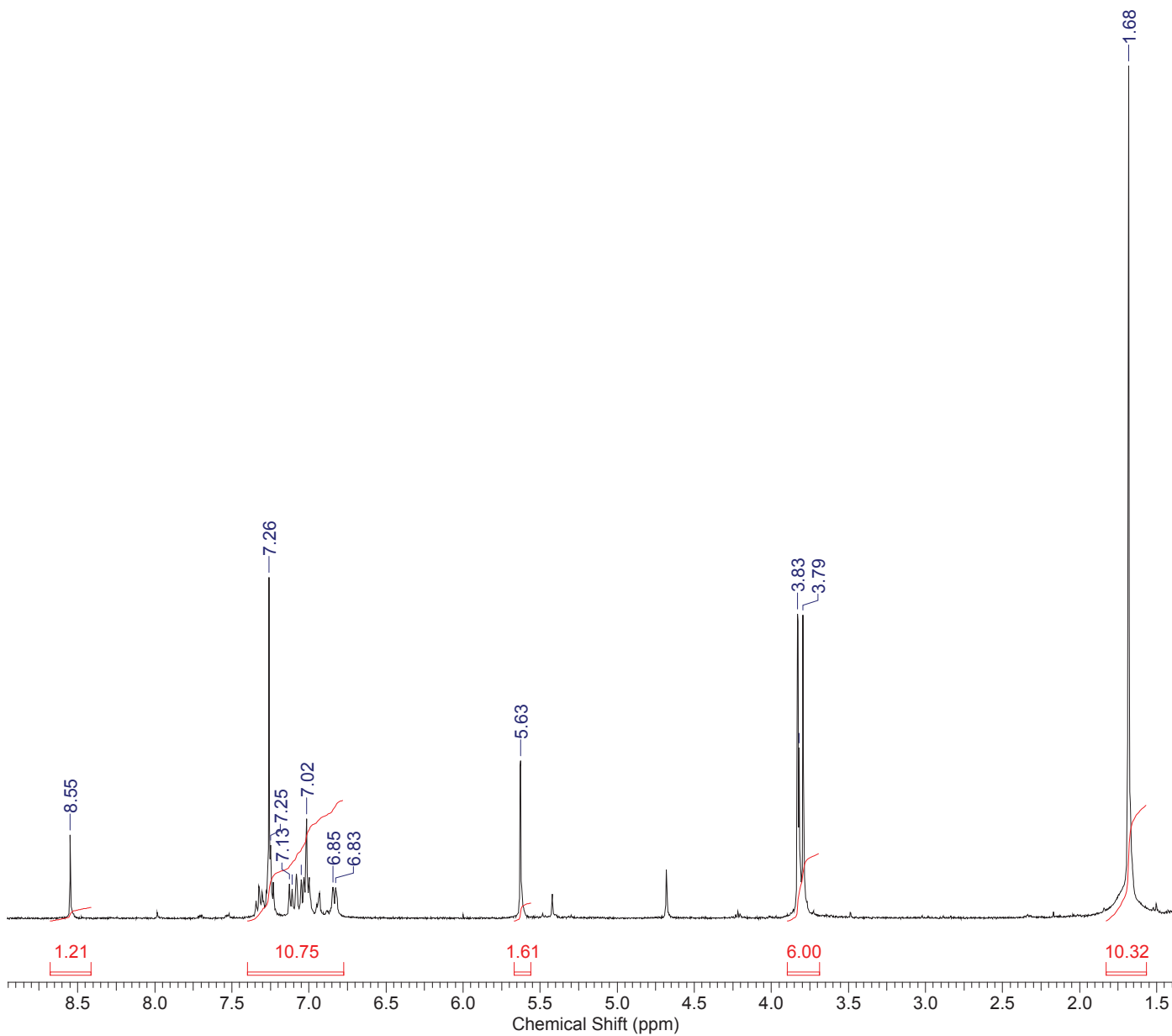
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	29.69	3732.2	0.0320	15	115.41	14505.2	0.1495
2	30.76	3865.7	0.3134	16	119.08	14966.8	0.0306
3	55.27	6946.1	0.0937	17	120.86	15190.0	0.0431
4	55.40	6963.3	0.0260	18	122.49	15395.0	0.0882
5	60.90	7653.8	0.0282	19	128.92	16203.7	0.0316
6	65.31	8207.9	0.0267	20	129.38	16261.0	0.0655
7	68.06	8554.1	0.0643	21	129.61	16289.6	0.0254
8	76.75	9646.1	0.9387	22	137.83	17323.4	0.0375
9	77.01	9678.5	1.0000	23	150.23	18881.7	0.0665
10	77.26	9710.0	0.9149	24	152.87	19213.6	0.0236
11	112.24	14106.5	0.0238	25	154.21	19381.5	0.0199
12	113.29	14239.1	0.0335	26	159.02	19986.1	0.0368
13	113.75	14296.3	0.0422	27	159.61	20060.5	0.0268
14	113.91	14317.3	0.0619	28	160.29	20146.3	0.0191

Acquisition Time (sec)	1.0486	Date	May 9 2013		
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-11181_2ASIMJ-1_500\DEPT_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	4800
Original Points Count	32768	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D		Sweep Width (Hz)	31250.00	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	30.76	3865.7	1.0000
2	55.27	6946.1	0.2925
3	55.40	6963.3	0.1543
4	68.06	8554.1	-0.2783
5	113.75	14296.3	0.1128
6	113.91	14317.3	0.0972
7	115.41	14505.2	0.3092
8	120.87	15190.9	0.0830
9	122.49	15395.0	0.1573
10	128.92	16203.7	0.1286
11	129.38	16261.0	0.1188
12	150.23	18881.7	0.0920

Acquisition Time (sec)	2.5559	Date	May 7 2013		
File Name	C:\Users\usuario\Documents\Espectros 2ª Gen-Asier\13-11181_2ASIMJ-1\proton				
Frequency (MHz)	400.57	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6410.26		
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	0.07	27.3	0.0985
2	1.68	674.1	1.0000
3	3.79	1519.7	0.3582
4	3.82	1529.8	0.2027
5	3.83	1533.7	0.3594
6	5.63	2254.1	0.1875
7	6.83	2734.2	0.0392
8	6.85	2742.0	0.0397
9	7.02	2810.1	0.1198
10	7.05	2824.2	0.0487
11	7.11	2846.9	0.0375
12	7.13	2854.7	0.0438
13	7.25	2903.6	0.0888
14	7.26	2907.9	0.4022
15	8.55	3424.4	0.1006

No.	(ppm)	Value	Absolute Value
1	[1.57 .. 1.83]	10.325	4.28525e+8
2	[3.69 .. 3.90]	6.000	2.49022e+8
3	[5.56 .. 5.67]	1.614	6.70018e+7
4	[6.77 .. 7.40]	10.753	4.46282e+8
5	[8.41 .. 8.68]	1.215	5.04239e+7

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

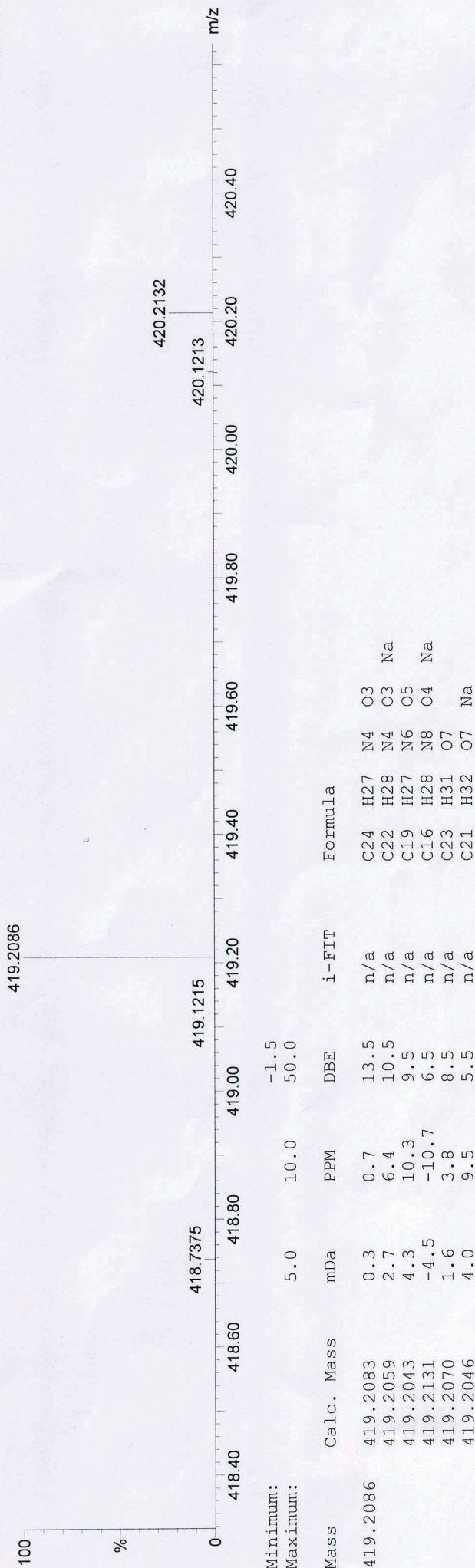
Monoisotopic Mass, Even Electron Ions
 468 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:

C: 0-24 H: 0-1000 N: 0-8 O: 0-7 Na: 0-1

1: TOF MS ES+

MJN 40 (0.880)

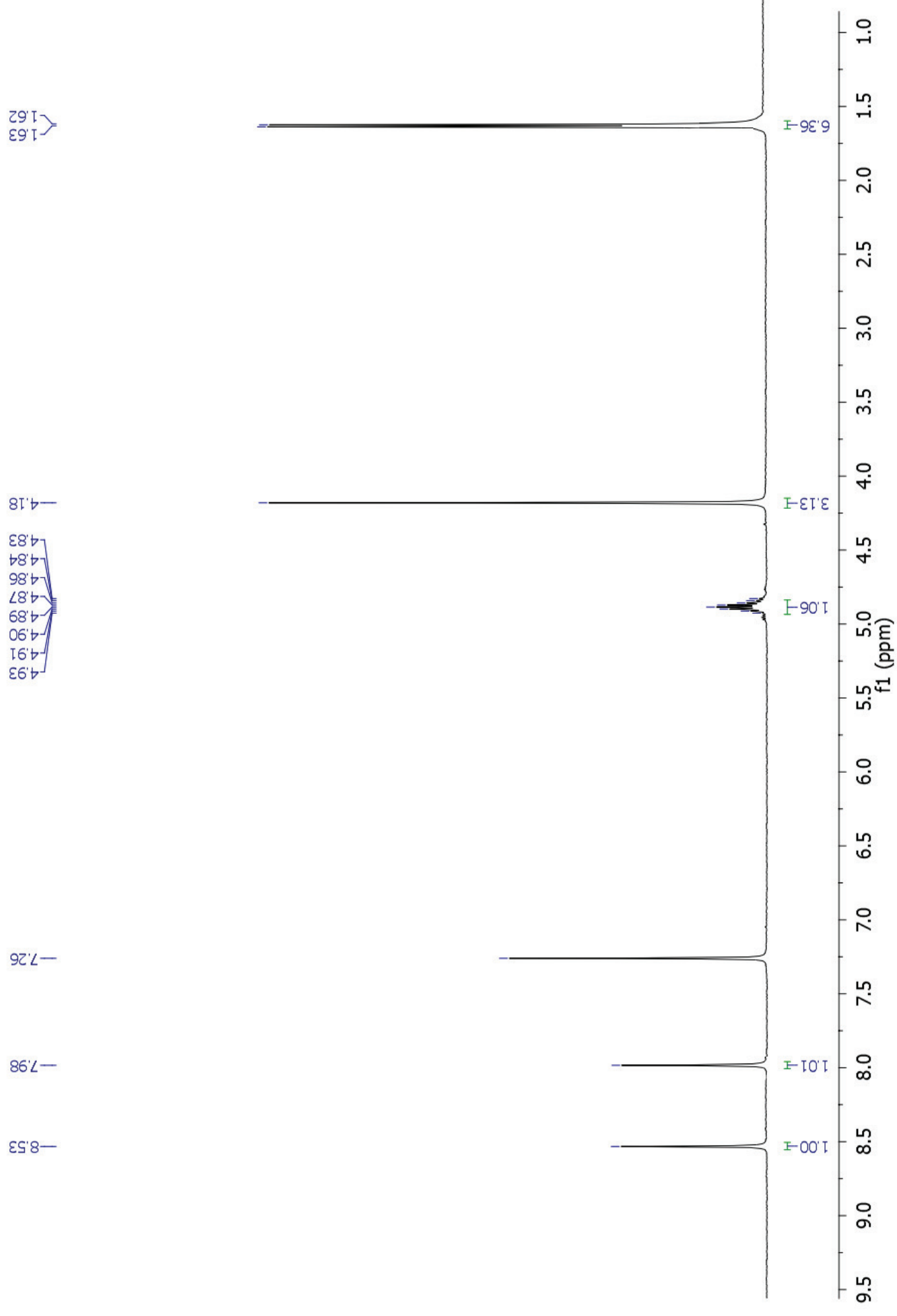
1.03e+002



Minimum:
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
419.2086	419.2083	0.3	0.7	13.5	n/a	C24 H27 N4 O3
	419.2059	2.7	6.4	10.5	n/a	C22 H28 N4 O3 Na
	419.2043	4.3	10.3	9.5	n/a	C19 H27 N6 O5
	419.2131	-4.5	-10.7	6.5	n/a	C16 H28 N8 O4 Na
	419.2070	1.6	3.8	8.5	n/a	C23 H31 O7
	419.2046	4.0	9.5	5.5	n/a	C21 H32 O7 Na

B5. 9-isopropyl-6-methoxy-9H-purine (H-NMR)



Elemental Composition Report

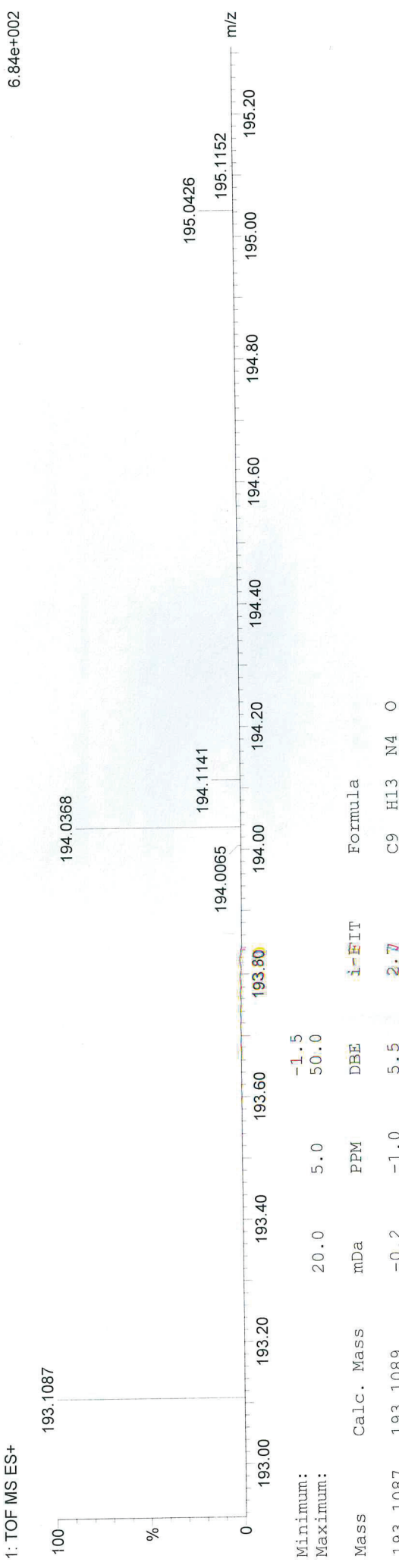
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 729 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:

C: 0-14 H: 0-1000 N: 0-5 O: 0-5 Na: 0-1 S: 0-1 Cl: 0-1 Br: 0-2

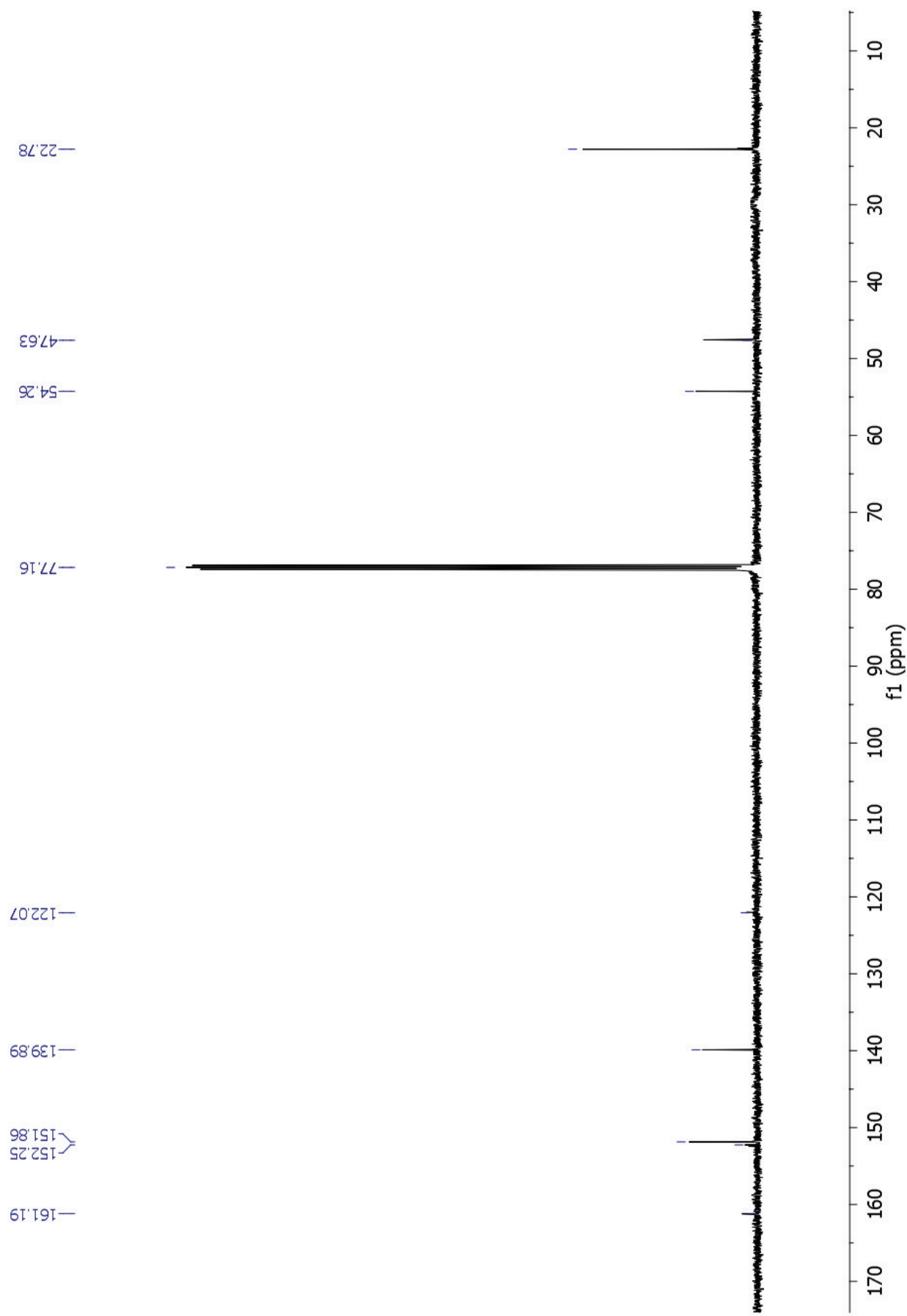
21 43 (0.951)



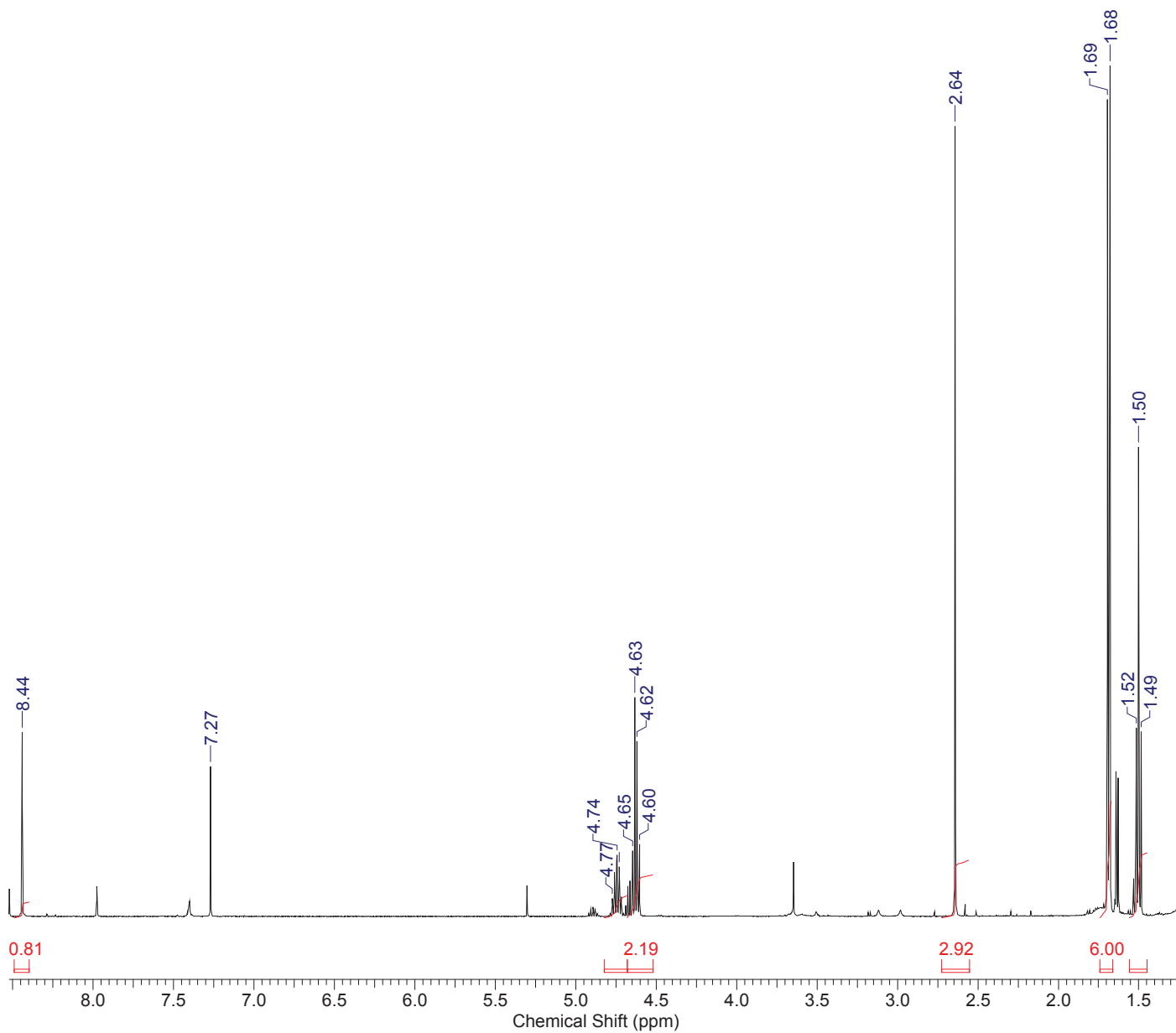
Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
193.1087	193.1089	-0.2	-1.0	5.5	2.7	C9 H13 N4 O

B5. 9-Isopropyl-6-methoxy-9H-purine (C-NMR)



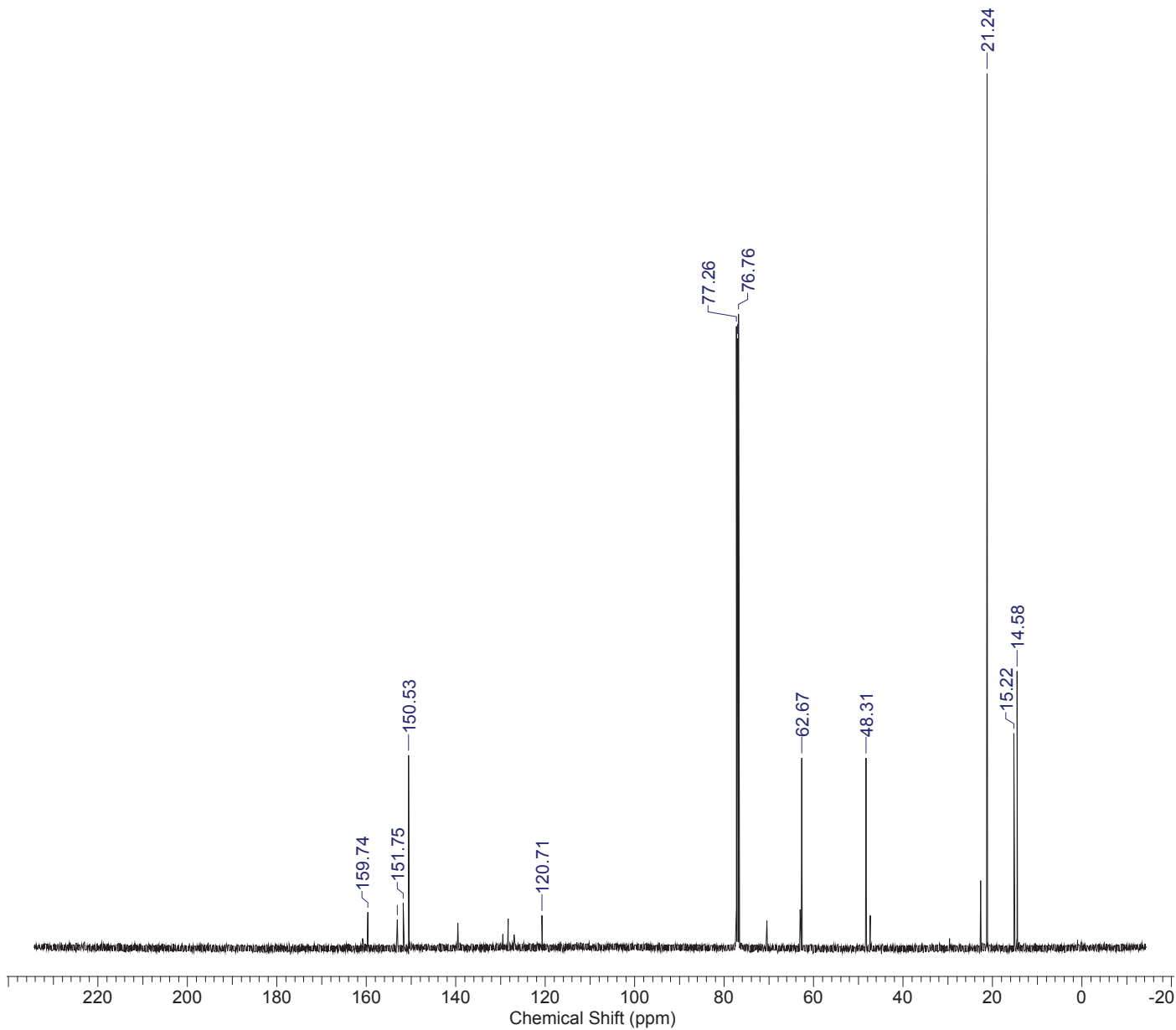
Acquisition Time (sec)	2.0447	Date	Jun 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-11090 ASIMJ-3NP\PROTON_01				
Frequency (MHz)	499.79	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	16384	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	8012.82		
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.49	742.7	0.2185
2	1.50	750.1	0.5522
3	1.52	757.4	0.2229
4	1.68	839.6	1.0000
5	1.69	846.4	0.9601
6	2.64	1320.8	0.9286
7	4.60	2301.0	0.0863
8	4.62	2308.3	0.2071
9	4.63	2315.2	0.2585
10	4.65	2322.5	0.0785
11	4.73	2364.1	0.0599
12	4.74	2370.9	0.0736
13	4.77	2385.1	0.0228
14	7.27	3634.2	0.1774
15	8.44	4218.7	0.2174

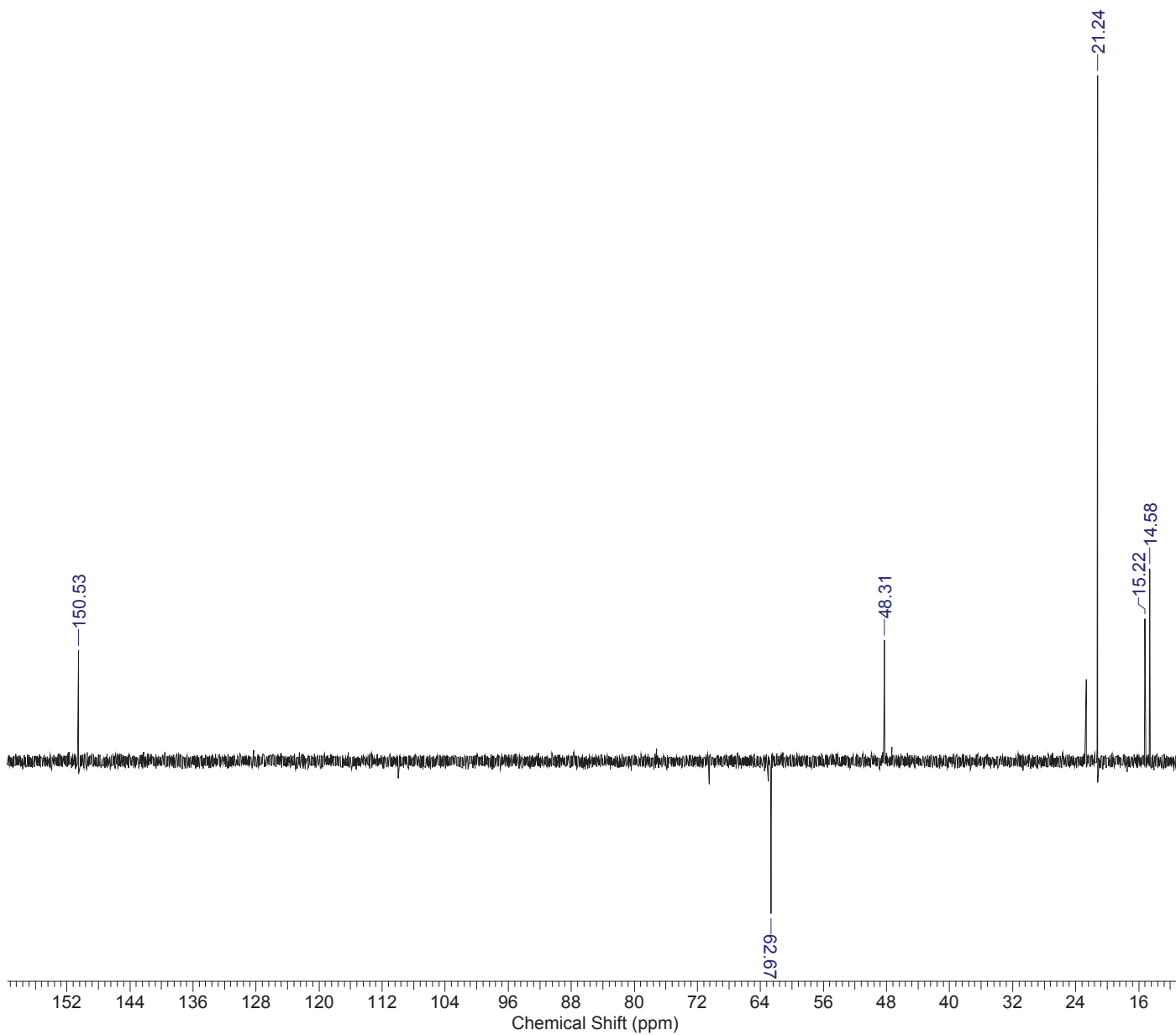
No.	(ppm)	Value	Absolute Value
1	[1.45 .. 1.56]	3.311	1.98984e+8
2	[1.66 .. 1.74]	6.000	3.60639e+8
3	[2.55 .. 2.72]	2.923	1.75698e+8
4	[4.52 .. 4.68]	2.188	1.31488e+8
5	[4.68 .. 4.82]	1.122	6.74613e+7
6	[8.40 .. 8.49]	0.805	4.83939e+7

Acquisition Time (sec)	1.0486	Date	Jun 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-11090 ASIMJ-3NP\CARBON_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	9600
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D		Sweep Width (Hz)	31250.00	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	14.58	1832.4	0.3162
2	15.22	1912.5	0.2453
3	21.24	2669.7	1.0000
4	48.31	6071.6	0.2170
5	62.67	7877.0	0.2167
6	76.76	9647.0	0.7249
7	77.01	9678.5	0.6964
8	77.26	9710.9	0.7109
9	120.71	15171.8	0.0363
10	150.53	18918.9	0.2196
11	151.75	19072.5	0.0509
12	153.15	19248.9	0.0315
13	159.74	20076.7	0.0403

Acquisition Time (sec)	1.0486	Date	Jun 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-11090 ASIMJ-3NP\DEPT_01				
Frequency (MHz)	125.68	Nucleus	13C	Number of Transients	4800
Original Points Count	32768	Points Count	32768	Pulse Sequence	DEPT135
Solvent	CHLOROFORM-D		Sweep Width (Hz)	31250.00	
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	14.58	1832.4	0.2804
2	15.22	1913.4	0.2078
3	21.24	2669.7	1.0000
4	48.31	6071.6	0.1761
5	62.67	7877.0	-0.2224
6	150.53	18918.9	0.1615

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

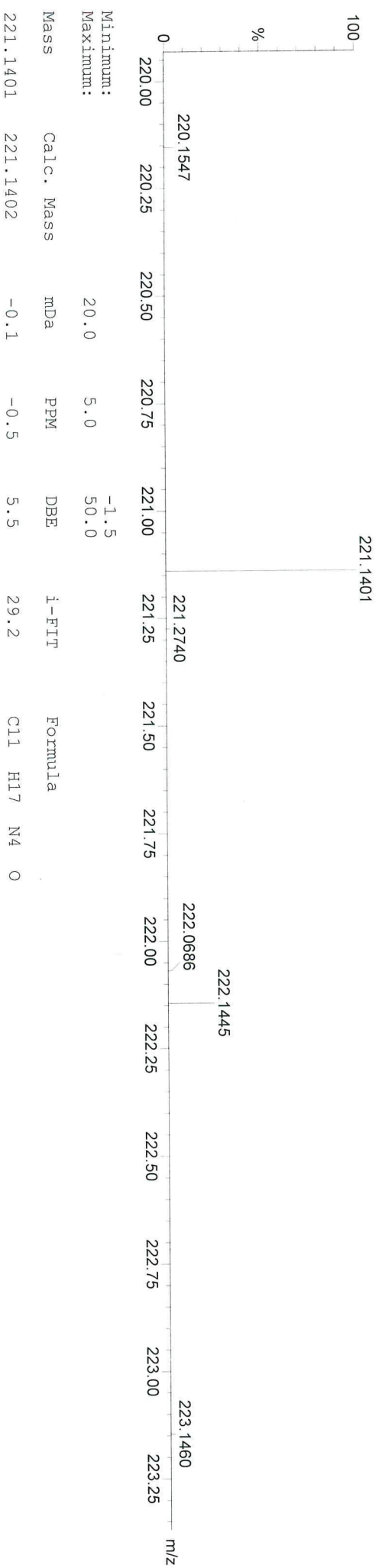
279 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-1000 N: 0-6 O: 0-7 Na: 0-1

MJ-3NP 6 (0.141)

1: TOF MS ES+
1.31e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1401	221.1402	-0.1	-0.5	5.5	29.2	C11 H17 N4 O

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

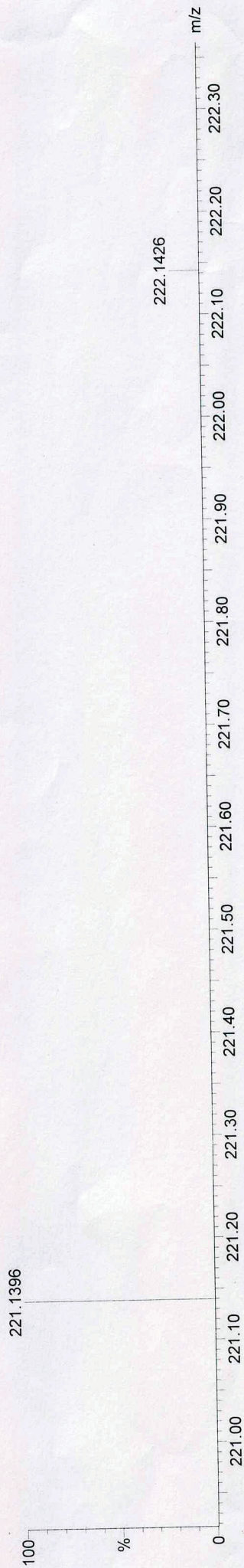
Monoisotopic Mass, Even Electron Ions
 398 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:

C: 0-22 H: 0-1000 N: 0-5 O: 0-6 F: 0-3

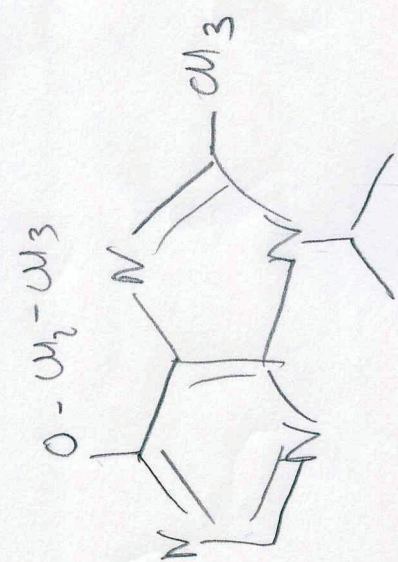
12/3291

1: TOF MS ES+
 4.26e+002

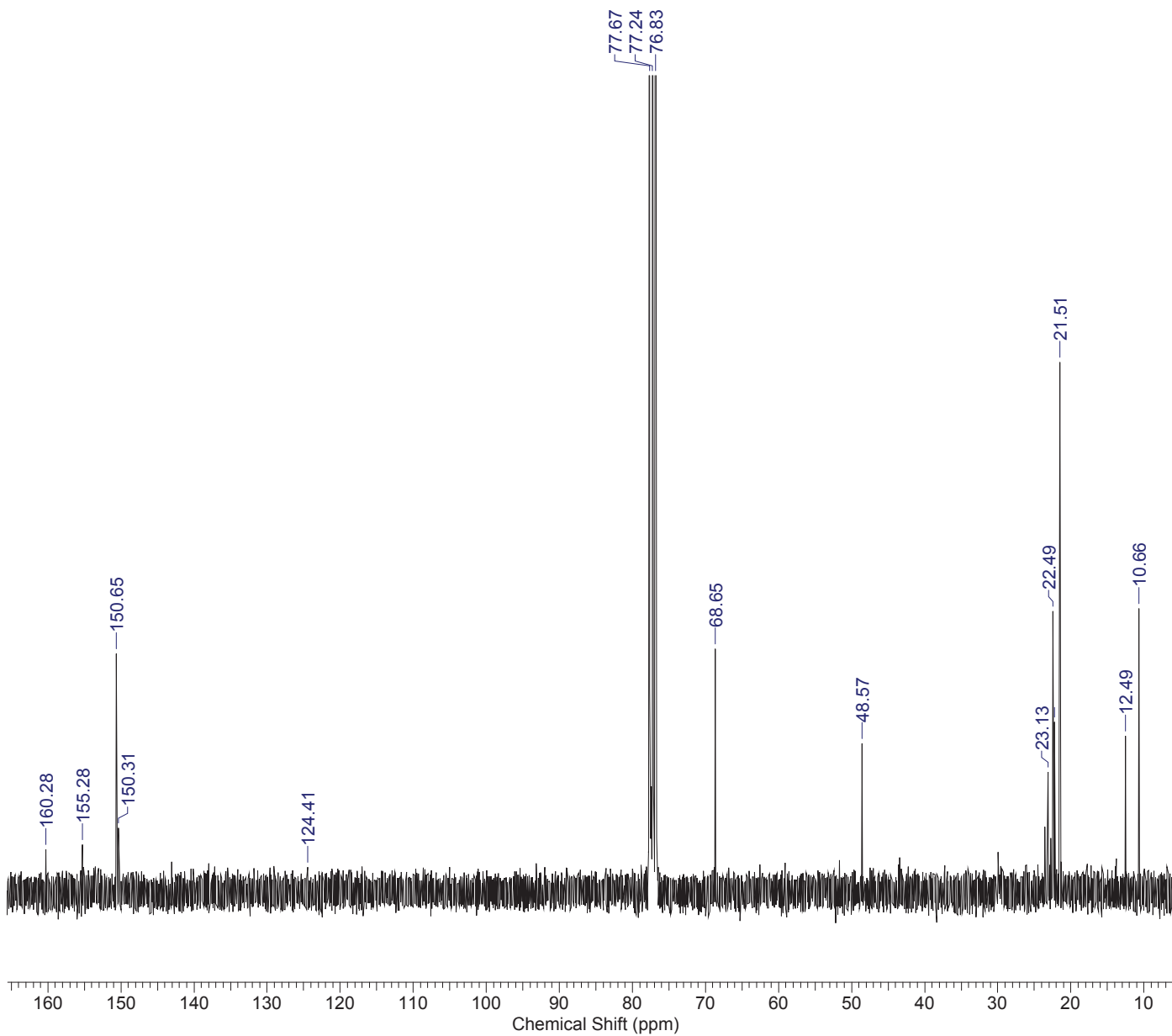
ASIMJ-3 7 (0.163)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1396	221.1402	-0.6	-2.7	5.5	n/a	C11 H17 N4 O
221.1389	221.1389	0.7	3.2	0.5	n/a	C10 H21 O5



Acquisition Time (sec)	1.3005	Comment	MJ-A2	Date	Sep 20 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-20186 MJ-A2\13C-MJ-A2				
Frequency (MHz)	75.49	Nucleus	13C	Number of Transients	16000
Original Points Count	23559	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	18115.94		
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	10.66	804.6	0.1251
2	12.49	942.9	0.0691
3	21.51	1624.0	0.2337
4	22.20	1676.0	0.0753
5	22.49	1697.5	0.1240
6	23.13	1746.2	0.0532
7	48.57	3666.9	0.0657
8	68.65	5182.8	0.1075
9	76.83	5799.8	0.9759
10	77.24	5831.4	0.9895
11	77.67	5863.4	1.0000
12	124.41	9391.8	0.0113
13	150.31	11347.4	0.0285
14	150.65	11372.8	0.1053
15	155.28	11722.8	0.0213
16	160.28	12099.8	0.0190

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 933 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

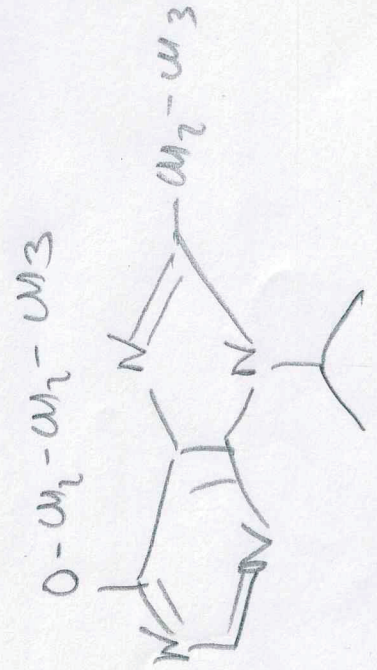
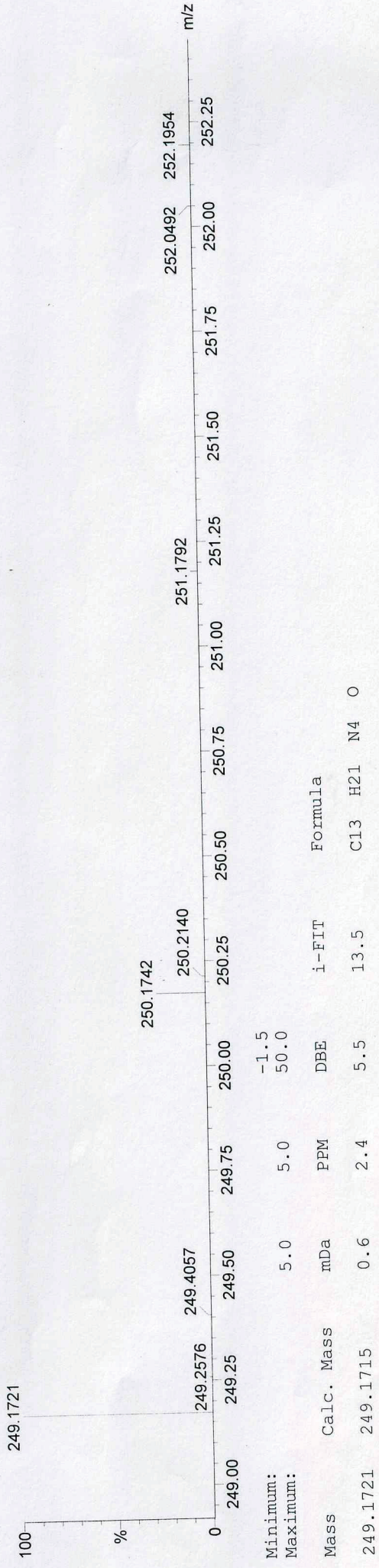
Elements Used:

C: 0-20 H: 0-1000 N: 0-10 O: 0-20 S: 0-1 Cl: 0-1

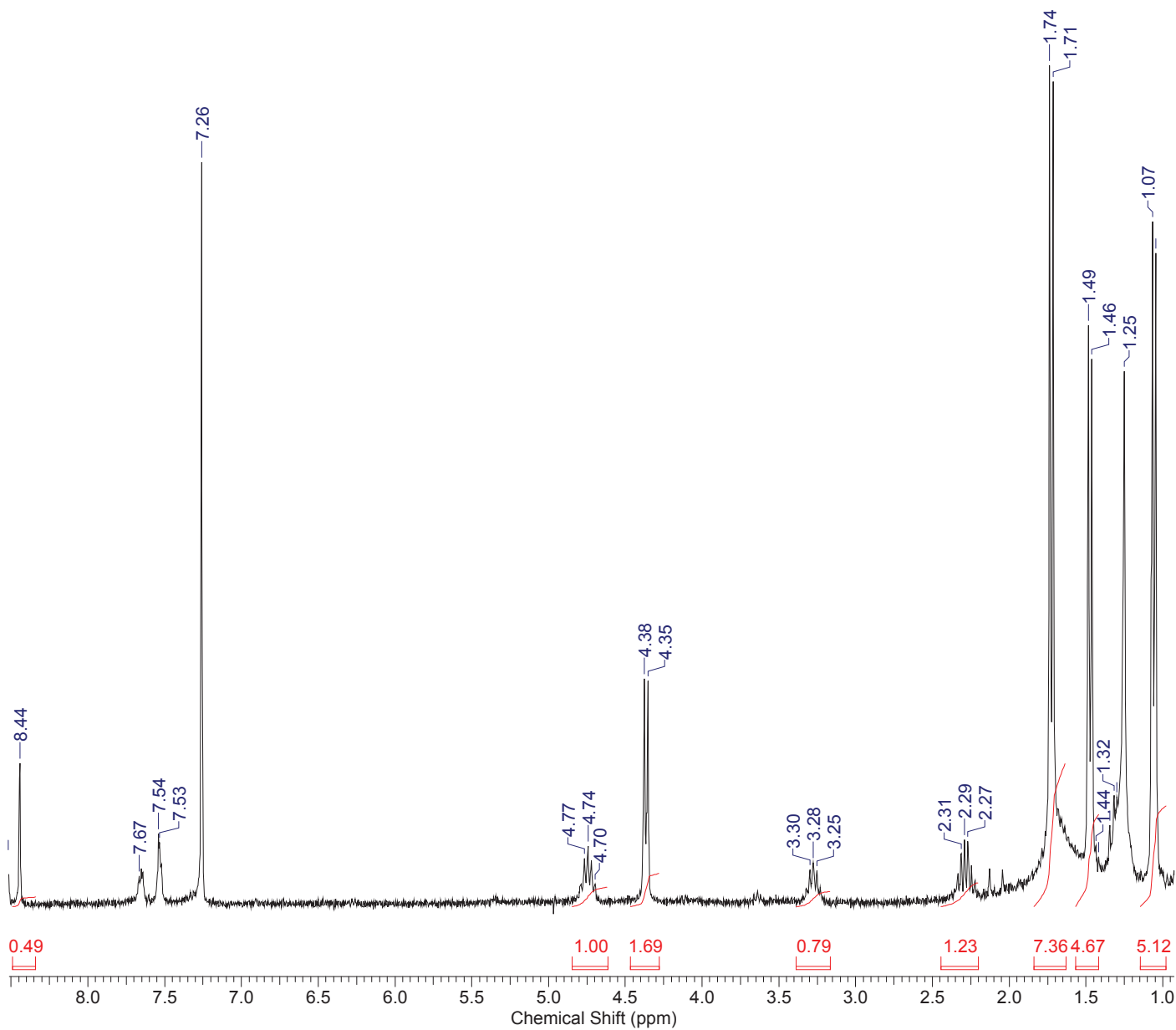
12/20093

1: TOF MS ES+
 6.28e+002

A3 72 (1.585)



Acquisition Time (sec)	2.0487	Comment	ASIMJ-28	Date	Nov 8 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-22927 ASIMJ-28\1H-ASIMJ-28				
Frequency (MHz)	300.20	Nucleus	1H	Number of Transients	64
Original Points Count	7380	Points Count	8192	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	3602.31		
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	0.90	270.8	0.0616
2	1.05	313.9	0.7765
3	1.07	320.5	0.8141
4	1.25	375.9	0.6365
5	1.30	390.4	0.1307
6	1.32	395.2	0.1323
7	1.35	404.0	0.0966
8	1.42	426.0	0.0595
9	1.44	431.3	0.0728
10	1.46	438.8	0.6506
11	1.49	445.8	0.6911
12	1.71	514.4	0.9806
13	1.74	521.4	1.0000
14	2.27	681.1	0.0776
15	2.29	687.7	0.0800

No.	(ppm)	(Hz)	Height
16	2.31	694.3	0.0634
17	3.25	976.6	0.0428
18	3.28	983.7	0.0524
19	3.30	990.3	0.0439
20	4.35	1306.5	0.2686
21	4.38	1313.5	0.2709
22	4.70	1410.3	0.0271
23	4.74	1423.9	0.0719
24	4.77	1430.5	0.0572
25	7.26	2179.5	0.8846
26	7.53	2261.3	0.0765
27	7.54	2263.9	0.0865
28	7.67	2301.3	0.0365
29	8.44	2534.8	0.1705
30	8.52	2557.2	0.0618

No.	(ppm)	Value	Absolute Value
1	[0.98 .. 1.15]	5.125	3.00038e+8
2	[1.42 .. 1.57]	4.671	2.73462e+8
3	[1.63 .. 1.84]	7.357	4.30721e+8
4	[2.20 .. 2.44]	1.231	7.20844e+7
5	[3.16 .. 3.39]	0.786	4.60005e+7
6	[4.28 .. 4.47]	1.692	9.90542e+7
7	[4.61 .. 4.85]	1.000	5.85494e+7
8	[8.34 .. 8.49]	0.490	2.86777e+7

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

910 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

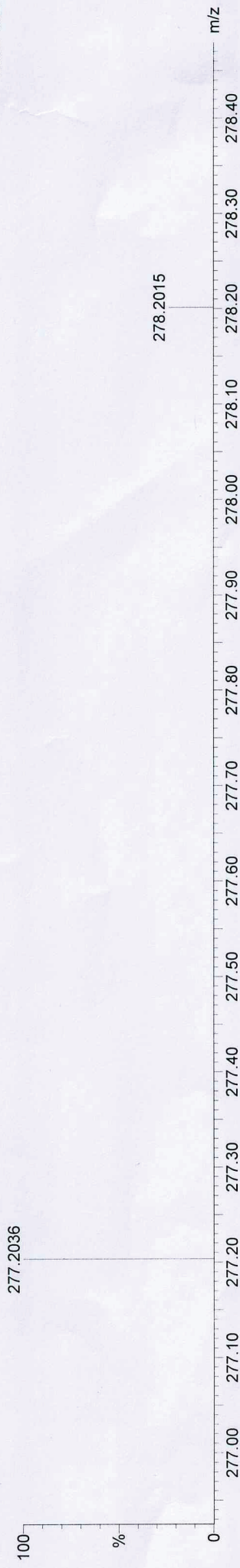
Elements Used:

C: 0-23 H: 0-1000 N: 0-10 O: 0-10 Cl: 0-1 Br: 0-1

12/22452

MJ-28 96 (2.120)

1: TOF MS ES+
1.15e+002



Minimum:
Maximum:

-1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
277.2036	277.2028	0.8	2.9	5.5	n/a	C15 H25 N4 O
	277.2047	-1.1	-4.0	0.5	n/a	C14 H30 N2 O Cl

