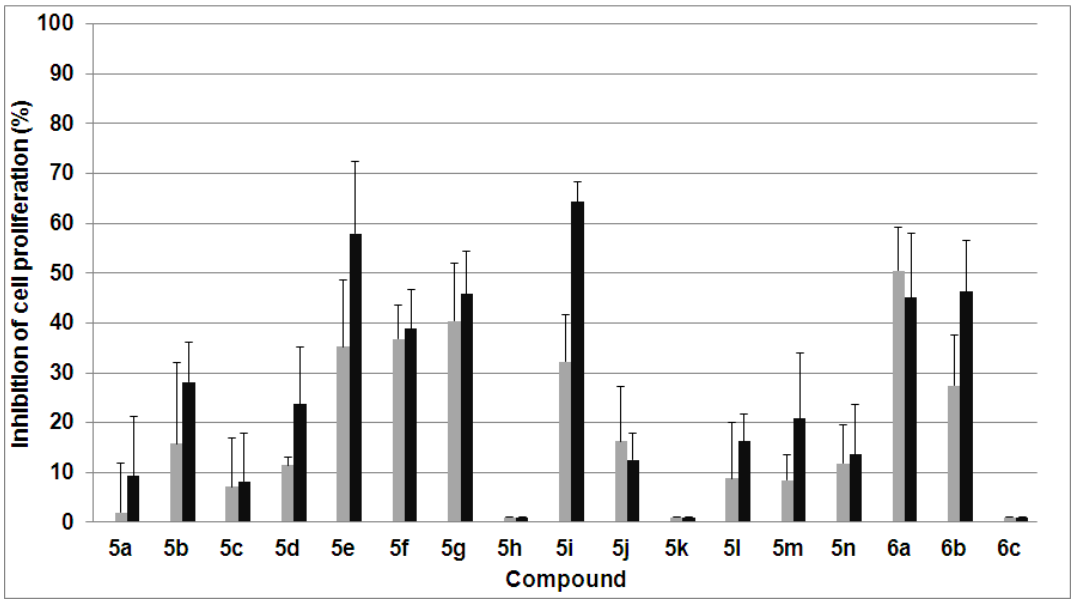
Supporting Information

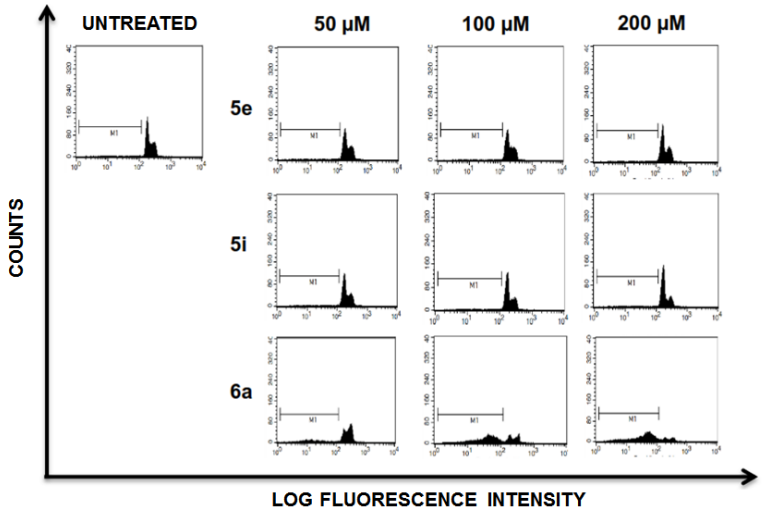
Synthesis of a Novel Purine Analogue Library as Pro-Apoptotic Inducers of Human Leukemic Lymphocytes and DAPK-1 Inhibitors.

AUTHORS: Maria J. Pineda de las Infantas[†,*] Sara Torres-Rusillo[§], Juan Diego Unciti-Broceta[‡], Pablo Fernandez-Rubio[§], Maria Angelica Luque Gonzalez, Miguel A. Gallo[†], Ignacio J. Molina[§,*], Asier Unciti-Broceta[¥] and Juan J. Diaz-Mochon[†,‡,*]

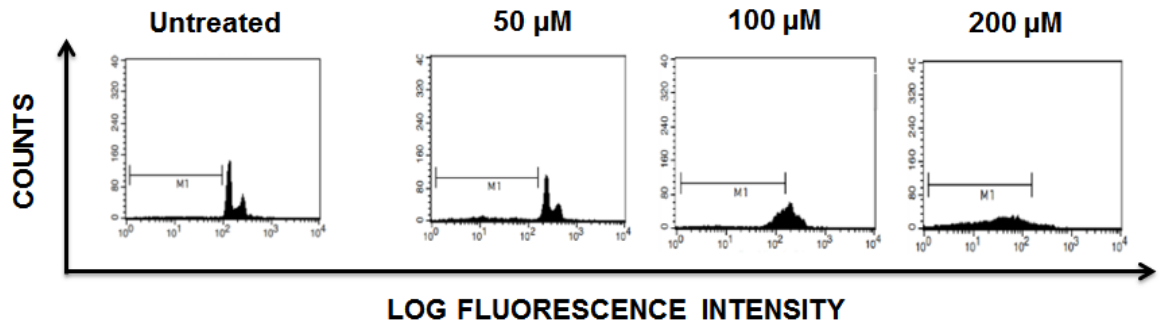
AFFILIATIONS: [†]Departamento de Química Farmacéutica y Orgánica. Facultad de Farmacia, Universidad de Granada, Campus de Cartuja s/n, 18011 Granada, Spain; [§] Instituto de Biopatología y Medicina Regenerativa, Centro de Investigación Biomédica, Universidad de Granada, Parque Tecnológico de Ciencias de la Salud (PTS), Avda. del Conocimiento s/n, 18016 Armilla, Granada, Spain; [¥]Edinburgh Cancer Research UK Centre, MRC Institute of Genetics and Molecular Medicine, University of Edinburgh, Crewe Road South, Edinburgh EH4 2XR, UK; [‡] Centro Pfizer - Universidad de Granada - Junta de Andalucía de Genómica e Investigación Oncológica (GENYO), Parque Tecnológico de Ciencias de la Salud (PTS), Avenida de la Ilustración 114, 18016 Granada, Spain.



SI Fig. 1. Antiproliferative effect of novel analogues on Jurkat cells after 48 h treatment at 50 μM (grey bars) and 100 μM (solid bars). Proliferation was determined by the MTT assay, results analyzed by spectrocolorimetry and expressed as percentage of inhibition relative to the untreated cells control. Equivalent amounts of DMSO was used for all doses and controls to exclude non-specific growth inhibition due to the drug solvent. Error bars (SEM).



SI Fig. 2. Effect of compounds, **5e**, **5i** and **6a** on cell cycle. K562 cells were incubated for 24h in the presence of indicated compounds and doses or their equivalent amounts of DMSO used as vehicle. Cell cycle subpopulations were analyzed by flow cytometry after permeabilization and staining of cells with propidium iodide. The percentages of cells gated within the sub-G1 peak are indicated in the figure.



SI Fig. 3. Effect of **6d** on the cell cycle of K562 cells. K562 cells were treated for 24 h with **6d** at indicated concentrations or their equivalent amounts of DMSO used as vehicle. Numbers indicate the percentage of cells contained within the sub-G1 region.

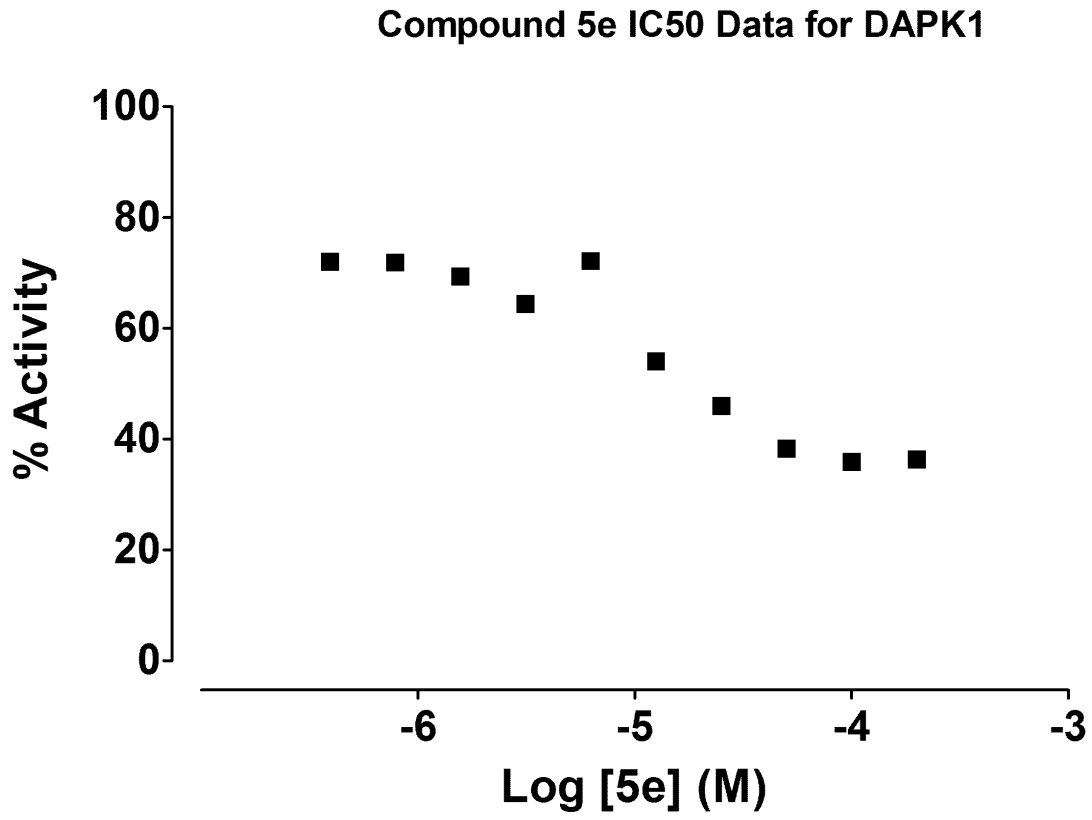
Kinase assay:

Originally, compound **5e** is encoded as **ASIMJ-5, 5i** as **ASIMJ-11**, **6a** as **ASIMJ-6** and **6d** as **ASIMJ-27.** Therefore, in raw data files compounds are named with their original codes.

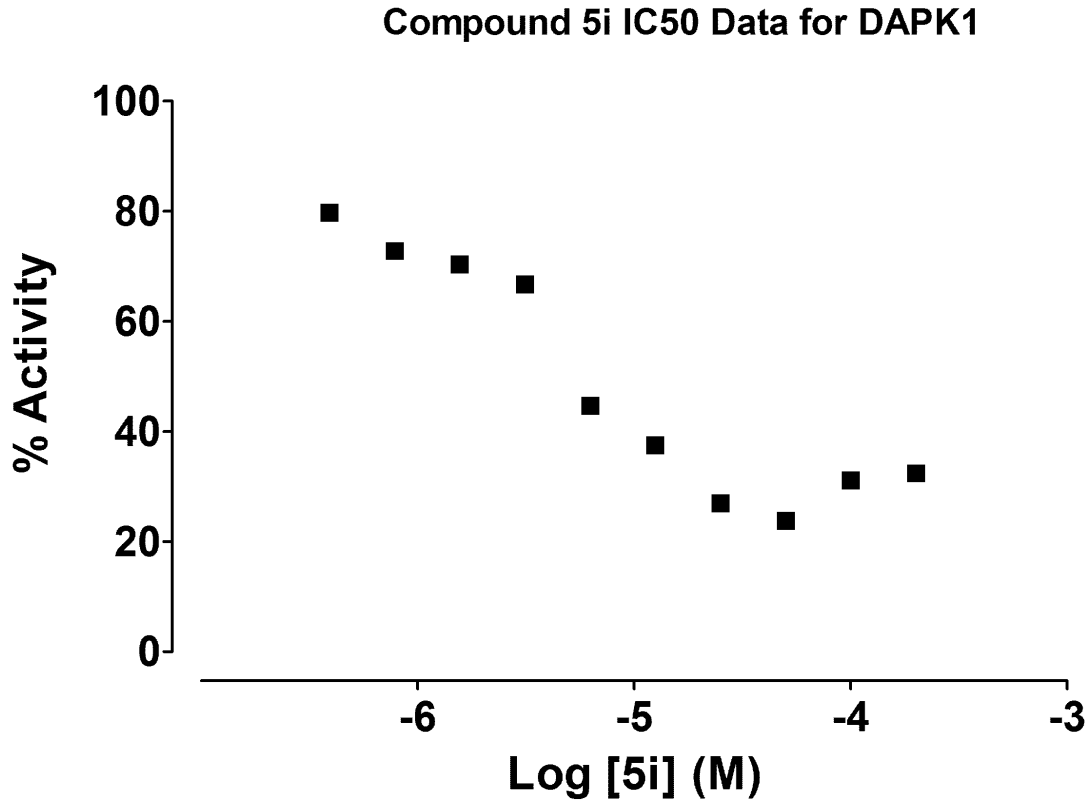
File *Cambridge BioSci_REPORT_20121003-CBL-UK-96KP-2cpds-RV01.xlsx* contains list of 96-kinases used and single-dose (10 µM) mode P^{33} kinase radiolabeled assay raw data using **5e** and **6a**.

File *Cambridge Bioscience_REPORT_20130220-CBL-UK-ASIMJ-11-27.xlsx* contains IC_{50} mode P^{33} radiolabeled DAPK1 assay raw data using **5i** and **6d**

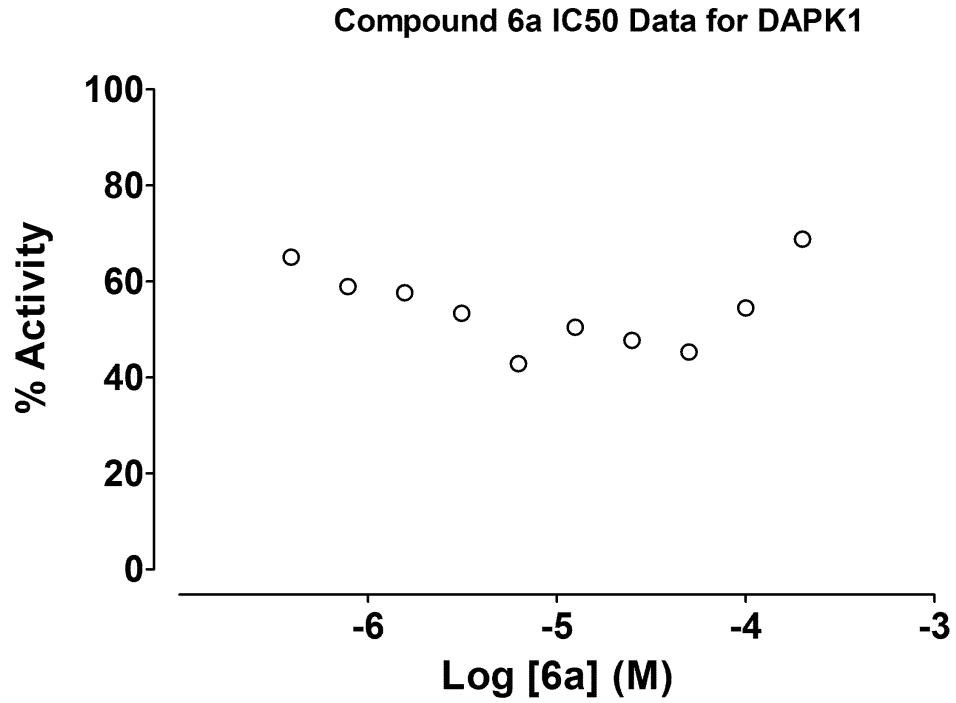
File *CBL_Report_20121115-CBL-UK-UGR.xls* contains IC_{50} mode P^{33} radiolabeled DAPK1 and DAPK2 assay raw data using **5e** and **6a**



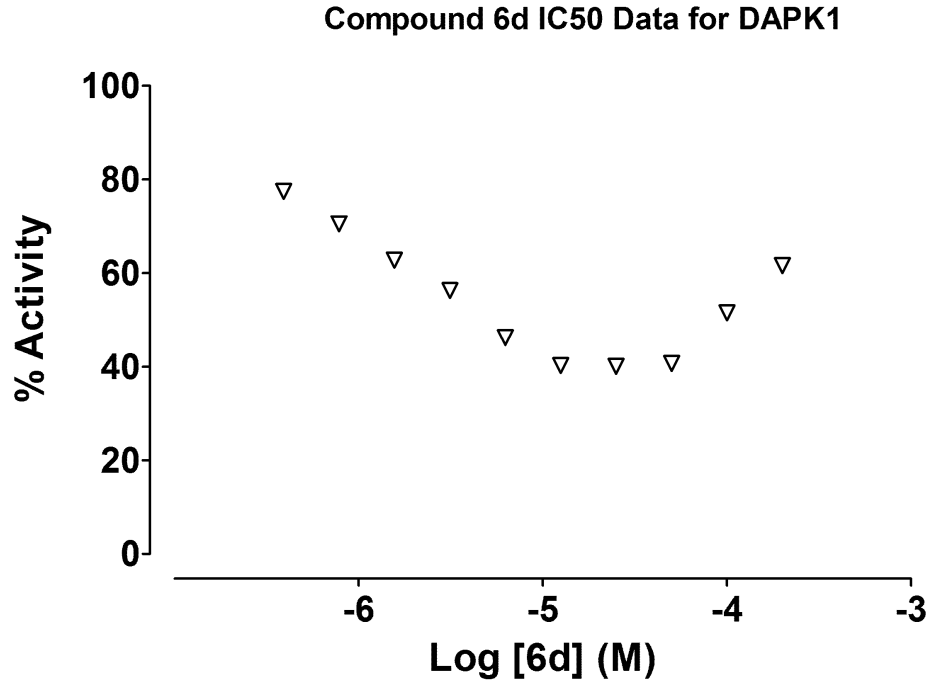
SI Fig.4 Dose-response curve of **5e** against DAPK1. IC_{50} = 2.301e-005M HILL SLOPE = -0.3121



SI Fig.5 Dose-response curve of **5i** against DAPK1. IC_{50} = 5.979e-006 M HILL SLOPE = -0.4186



SI Fig.6 Dose-response curve of **6a** against DAPK1. IC_{50} = ND



SI Fig.7 Dose-response curve of **6d** against DAPK1. IC_{50} = 2.54e-006 M HILL SLOPE = -0.147

4a 5-Amino-6-chloro-4-isopropylaminopyrimidine (H_NMR)

16 Jul 2012

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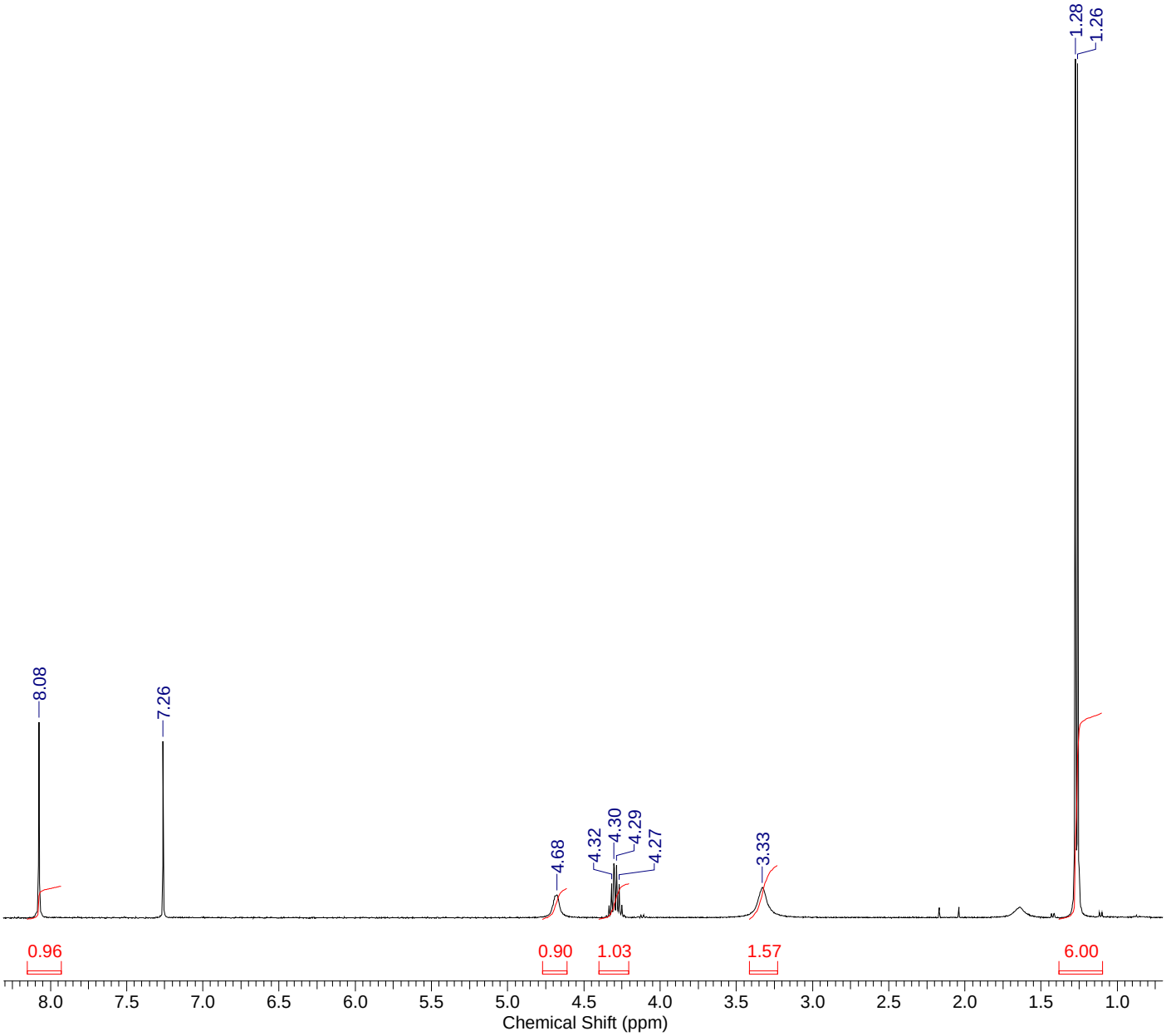
Points Count	16384	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	6410.26	***Temperature (degree C)***	25.000		



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	[1.10 .. 1.38]	6.000	2.66850e+7
2	[3.23 .. 3.41]	1.565	6.96065e+6
3	[4.21 .. 4.40]	1.026	4.56130e+6
4	[4.61 .. 4.77]	0.895	3.98062e+6
5	[7.93 .. 8.15]	0.964	4.28633e+6

Elemental Composition Report

Single Mass Analysis

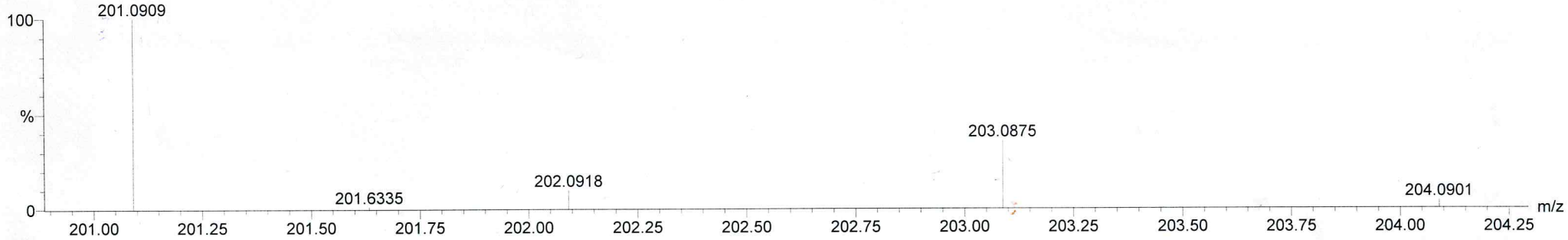
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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+

4.10e+002

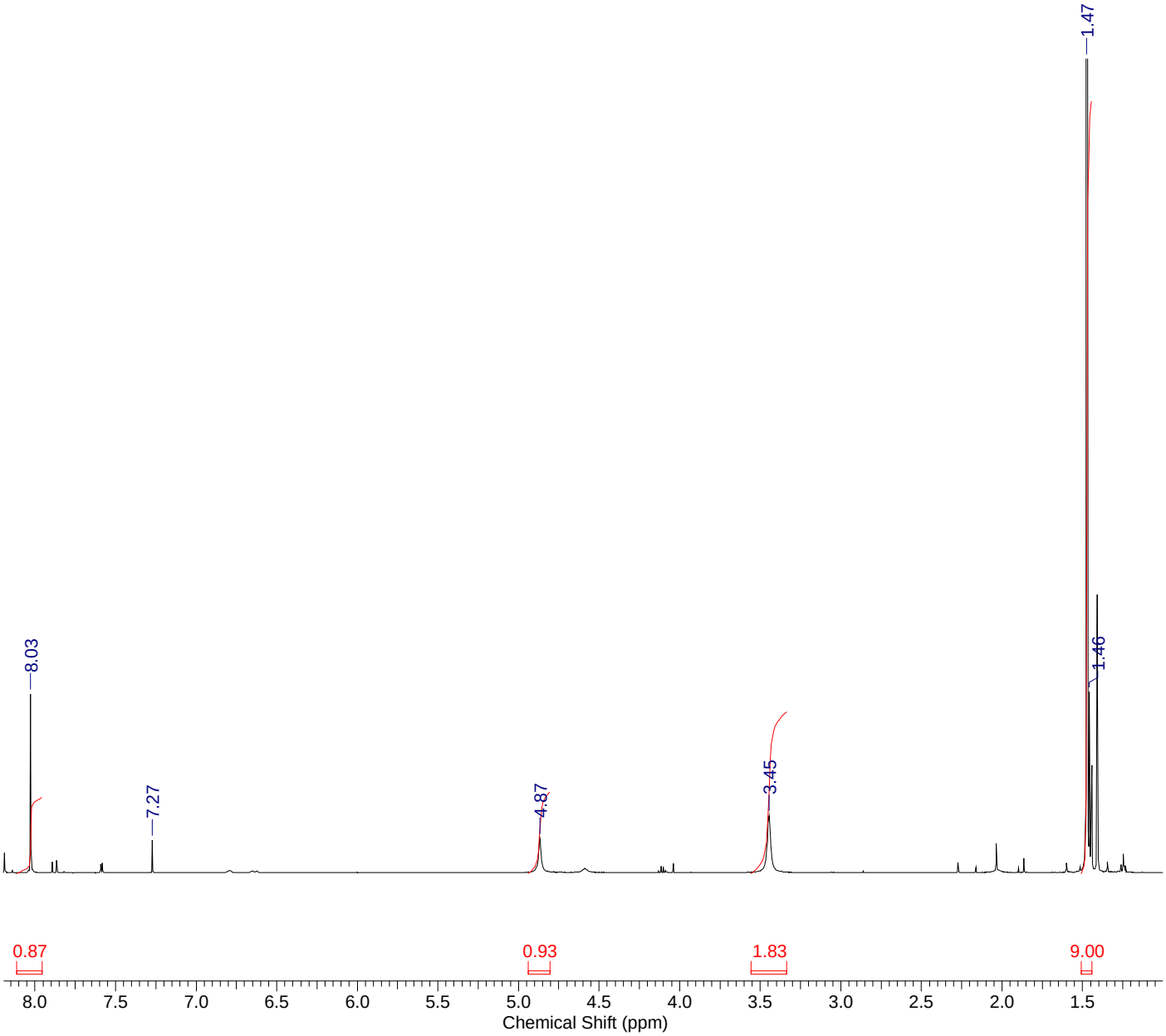


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
201.0909	201.0907	0.2	1.0	3.5	0.6	C8 H14 N4 Cl
	201.0909	0.0	0.0	-1.5	52.4	C5 H17 N2 O4 S
	201.0916	-0.7	-3.5	7.5	72.7	C13 H13 O2

4b 5-Amino-4-tert-butylamino-6-chloropyrimidine (H-NMR)

11 Mar 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	***Original Points Count***	16384
Points Count	16384	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	8012.82	***Temperature (degree C)***	25.000		



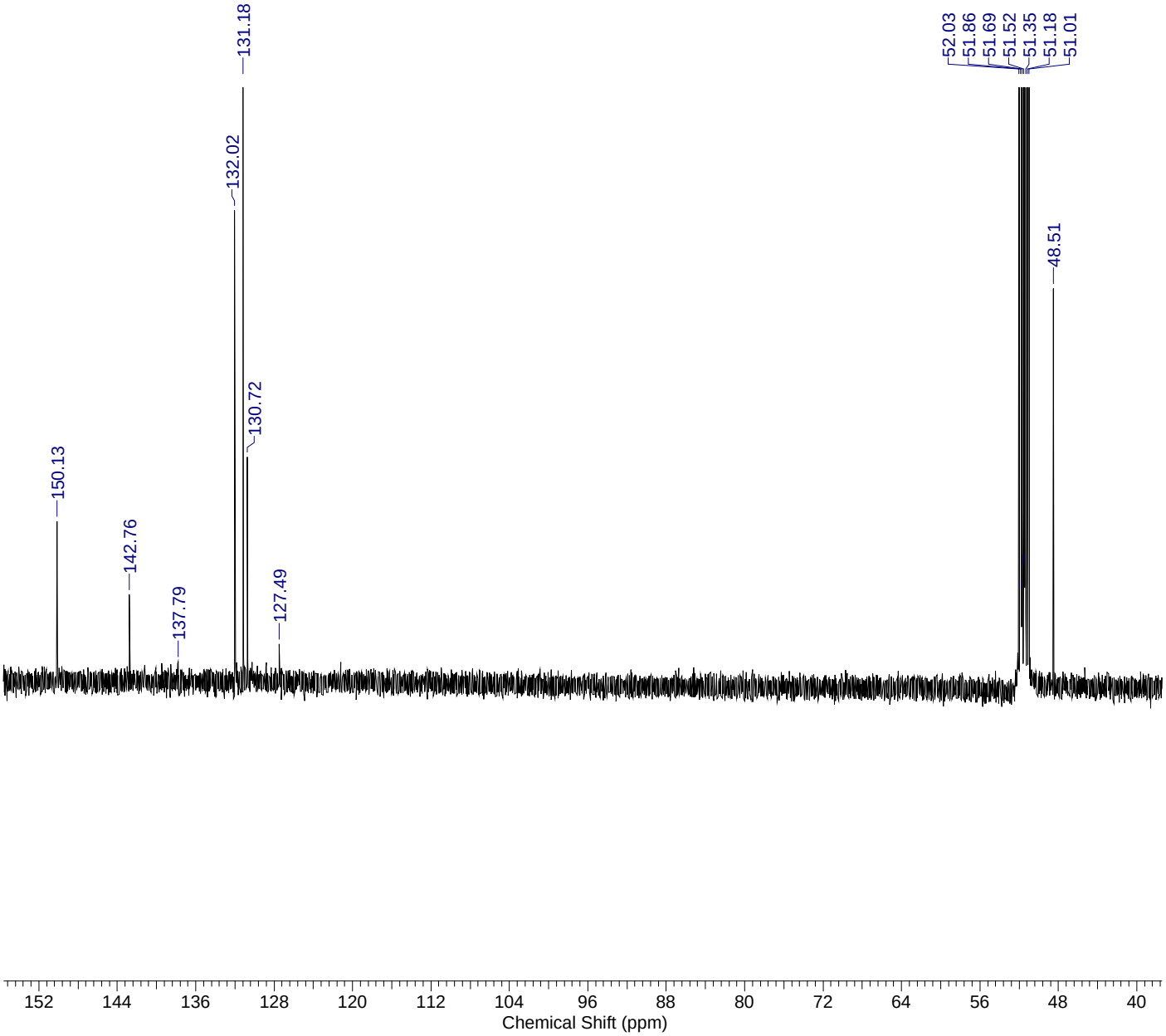
No.	(ppm)	(Hz)	Height
1	1.46	728.2	0.0677
2	1.47	736.5	1.0000
3	3.45	1722.5	0.0217
4	4.87	2433.1	0.0131
5	7.27	3635.3	0.0125
6	8.03	4011.9	0.0669

No.	(ppm)	Value	Absolute Value
1	[1.44 .. 1.51]	9.000	1.64609e+8
2	[3.34 .. 3.56]	1.831	3.34978e+7
3	[4.80 .. 4.94]	0.930	1.70182e+7
4	[7.95 .. 8.11]	0.867	1.58596e+7

4c 5-amino-4-benzilamino-6-chloropyrimidine (C-NMR)

16 Jul 2012

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***	13C	***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	48.51	6096.4	0.0362
2	51.01	6411.1	0.1618
3	51.18	6432.1	0.3818
4	51.35	6454.0	0.8678
5	51.52	6475.0	1.0000
6	51.63	6489.3	0.0104
7	51.69	6496.9	0.7416
8	51.81	6511.3	0.0145
9	51.86	6517.9	0.4658
10	51.97	6532.2	0.0080
11	52.03	6539.9	0.1005
12	127.49	16023.5	0.0035
13	130.72	16429.8	0.0207
14	131.18	16487.0	0.0684
15	132.02	16592.8	0.0434
16	137.79	17318.6	0.0019
17	142.76	17943.3	0.0080
18	150.13	18869.3	0.0148

4c 5-amino-4-benzilamino-6-chloropyrimidine (H-NMR)

16 Jul 2012

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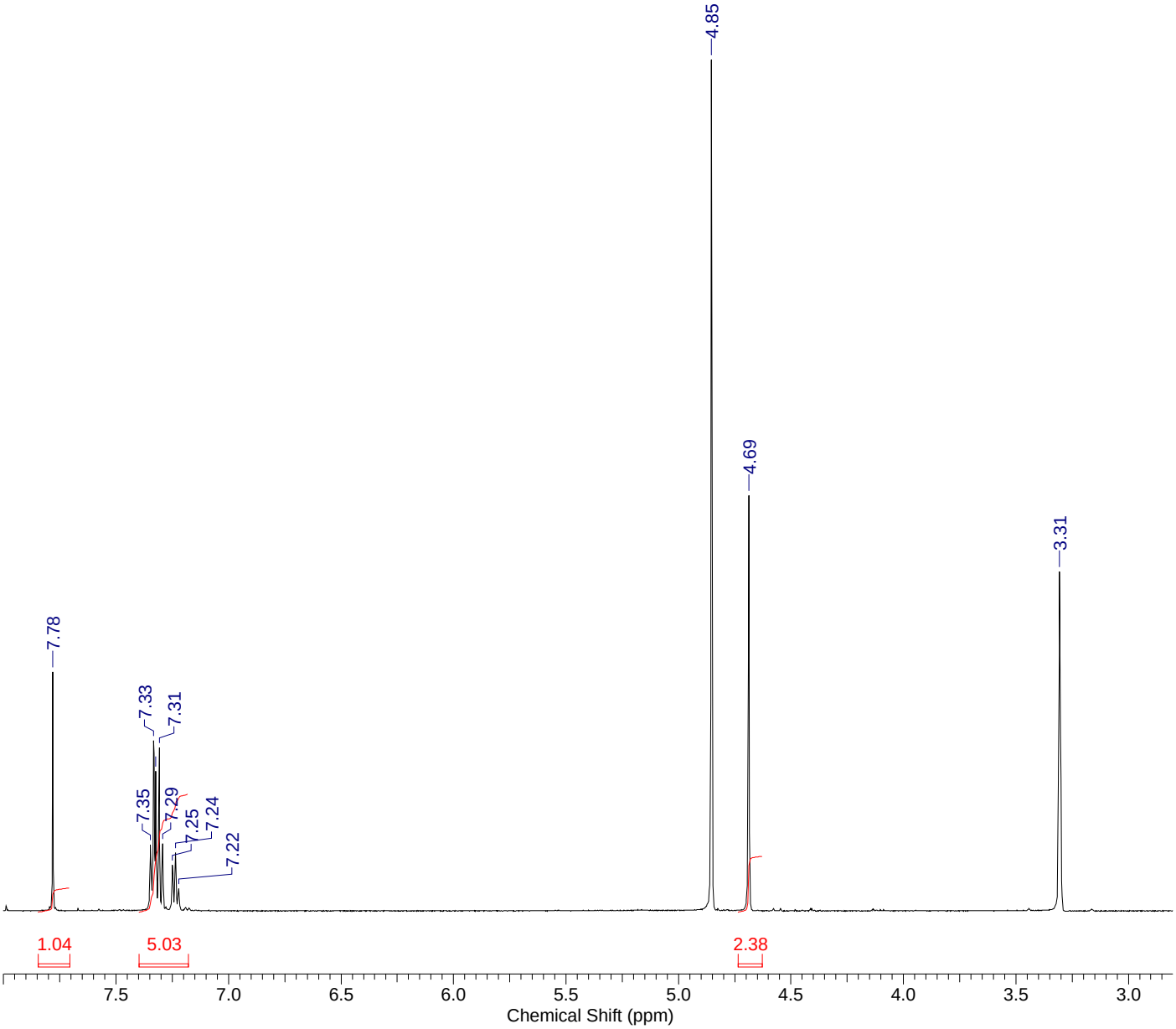
Original Points Count	13048	***Points Count***	16384	***Pulse Sequence***	s2pul
Solvent	METHANOL-D4			***Sweep Width (Hz)***	7485.03
Temperature (degree C)	25.000				



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	7.22	3609.3	0.0275
5	7.24	3616.6	0.0695
6	7.25	3623.4	0.0555
7	7.29	3644.9	0.0804
8	7.31	3652.7	0.1928
9	7.32	3660.0	0.1651
10	7.33	3665.0	0.2014
11	7.35	3671.9	0.0790
12	7.78	3889.3	0.2820

No.	(ppm)	Value	Absolute Value
1	[4.63 .. 4.74]	2.382	5.73421e+7
2	[7.18 .. 7.40]	5.029	1.21055e+8
3	[7.71 .. 7.85]	1.037	2.49540e+7

4c 5-amino-4-benzilamino-6-chloropyrimidine (MS)

Elemental Composition Report

Single Mass Analysis

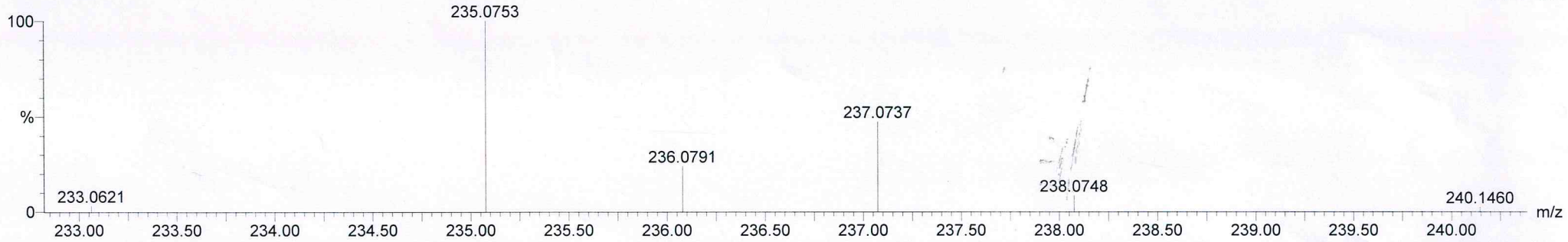
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

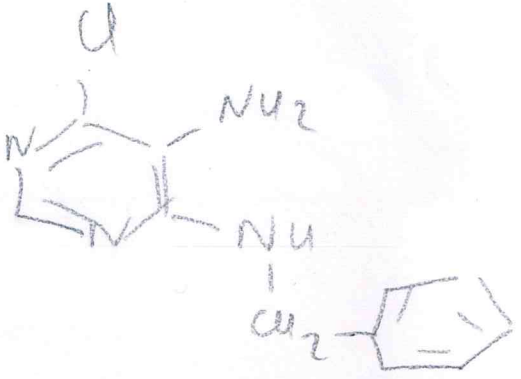
MJ-2 89 (1.975)

1: TOF MS ES+

7.14e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	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



5a. - 6-Ethoxy-9-isopropyl-9H-purine

Elemental Composition Report

Single Mass Analysis

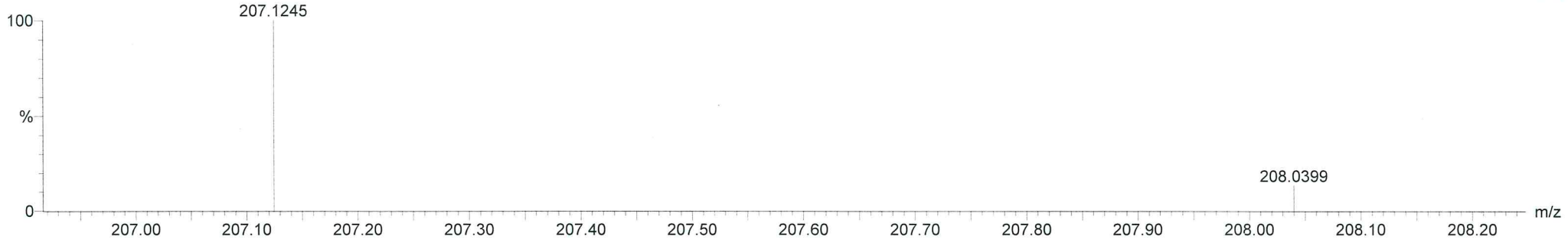
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
207.1245	207.1246	-0.1	-0.5	5.5	n/a	C10 H15 N4 O

5a .- 6-Ethoxy-9-isopropyl-9H-purine (H-NMR)

11 Jul 2012

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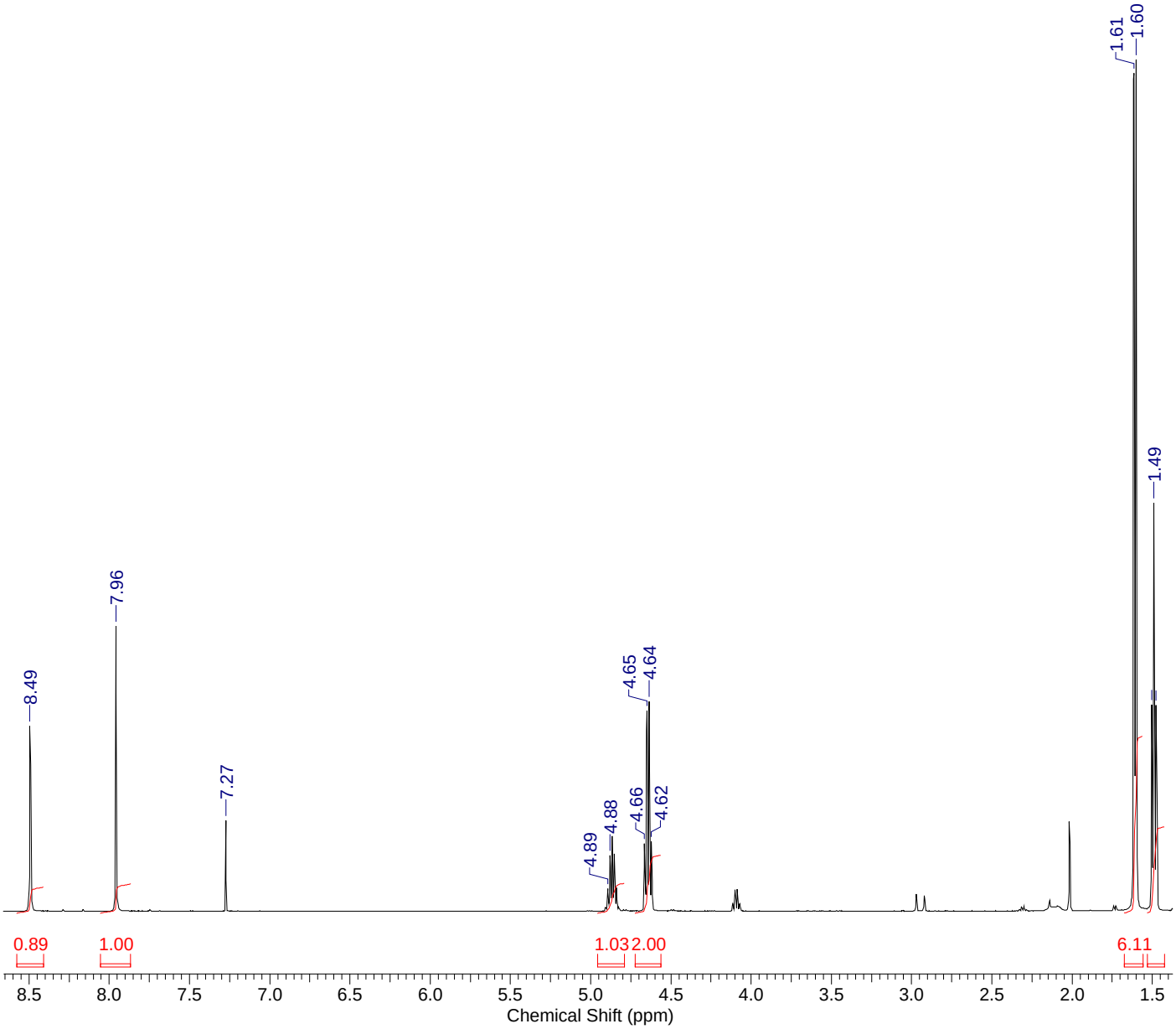
Original Points Count	16384	***Points Count***	16384	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	8012.82
Temperature (degree C)	25.000				



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

5a. - 6-Ethoxy-9-isopropyl-9H-purine (C-NMR)

11 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Feb 4 2012		
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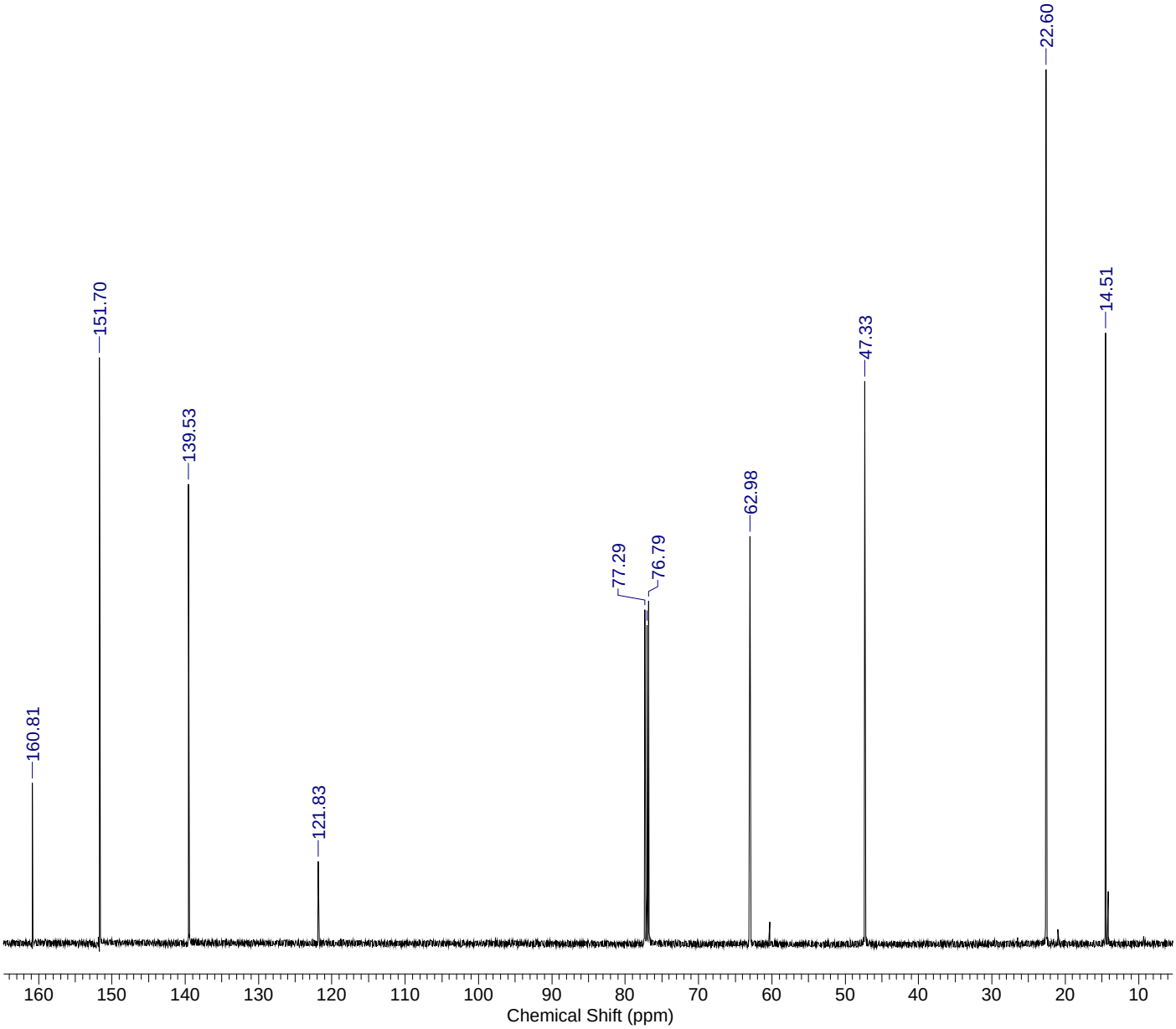
Original Points Count	32768	***Points Count***	32768	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	31250.00
Temperature (degree C)	25.000				



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

5a. - 6-Ethoxy-9-isopropyl-9H-purine DEPT

11 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Feb 4 2012		
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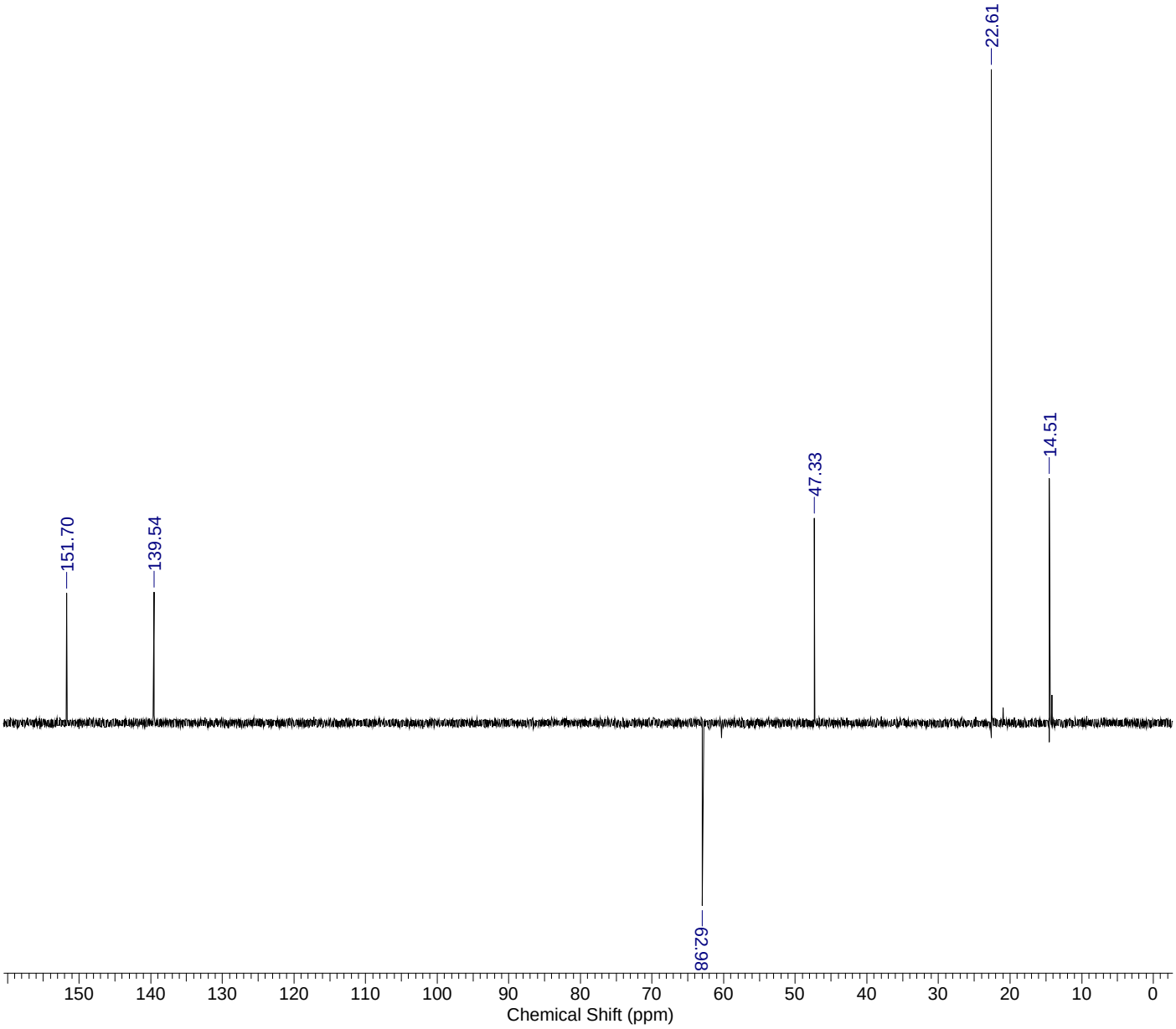
Frequency (MHz)	125.68	***Nucleus***	13C	***Number of Transients***	1200
Original Points Count	32768	***Points Count***	32768	***Pulse Sequence***	DEPT135
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	31250.00
Temperature (degree C)	25.000				



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

5b. - 6-Ethoxy-8-ethyl-9-isopropyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

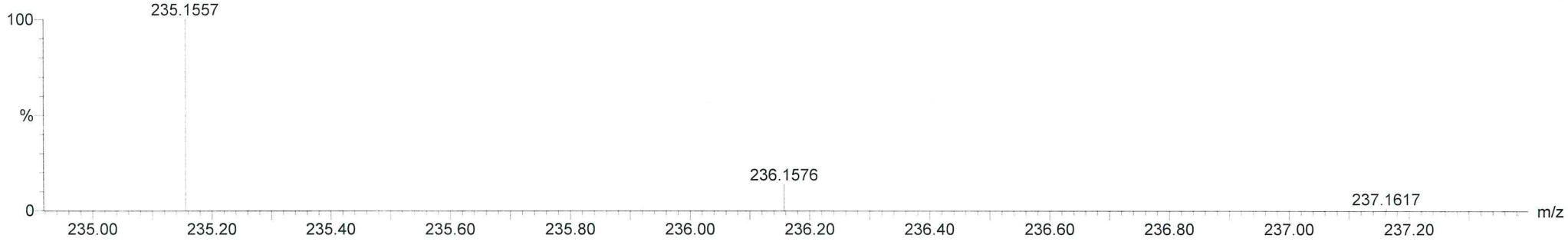
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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

ASIMJ-2 9 (0.217)

1: TOF MS ES+
5.80e+002

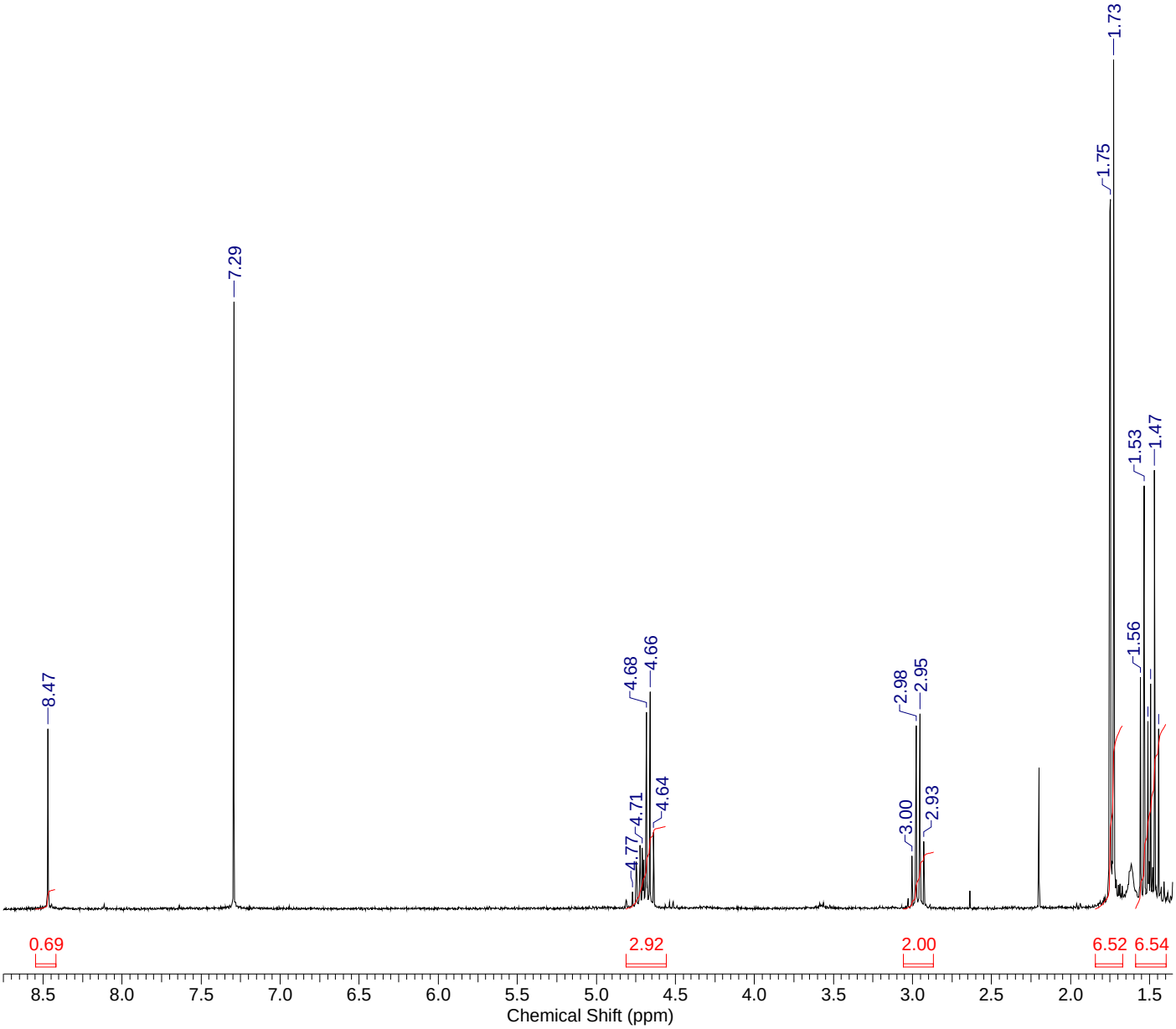


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.1557	235.1559	-0.2	-0.9	5.5	0.3	C12 H19 N4 O
	235.1545	1.2	5.1	0.5	1.0	C11 H23 O5

5b. - 6-Ethoxy-8-ethyl-9-isopropyl-9H-purine (H-NMR)

11 Jul 2012

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

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

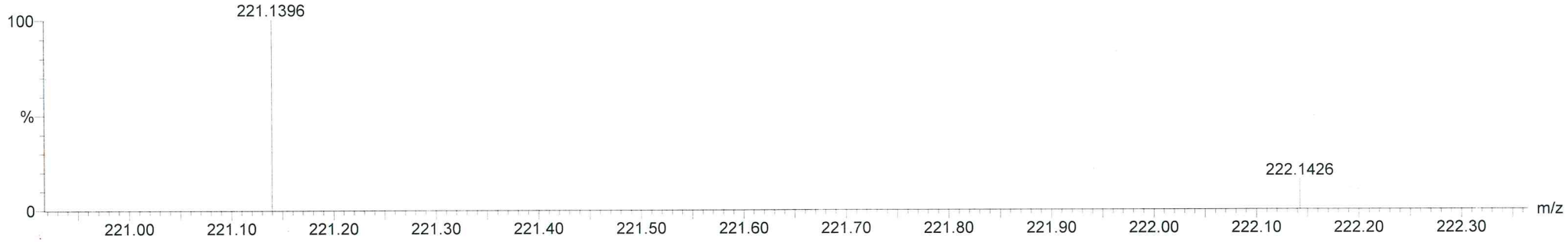
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

ASIMJ-3 7 (0.163)

1: TOF MS ES+
4.26e+002

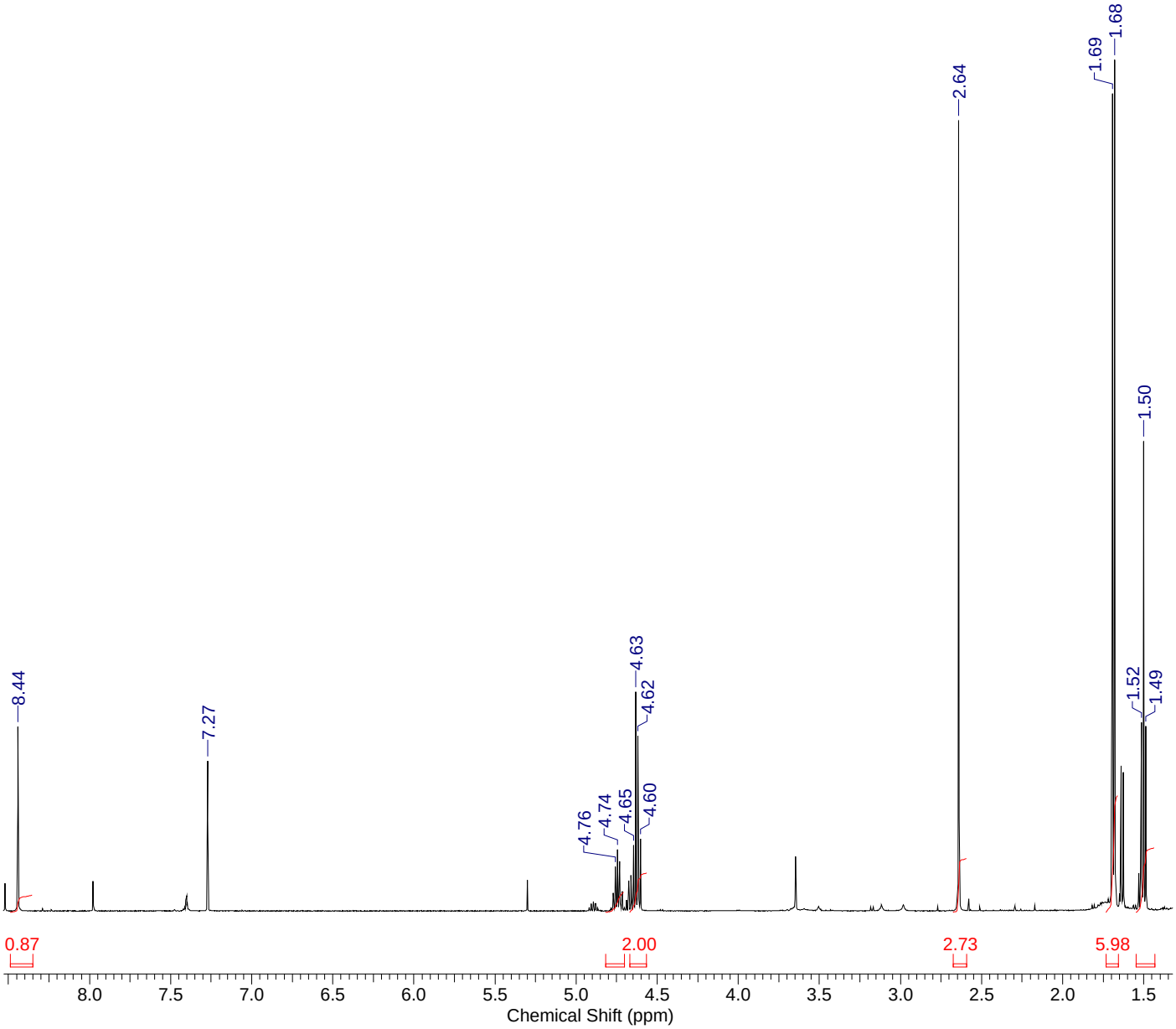


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1396	221.1402	-0.6	-2.7	5.5	n/a	C11 H17 N4 O
	221.1389	0.7	3.2	0.5	n/a	C10 H21 O5

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (H-NMR)

11 Jul 2012

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				



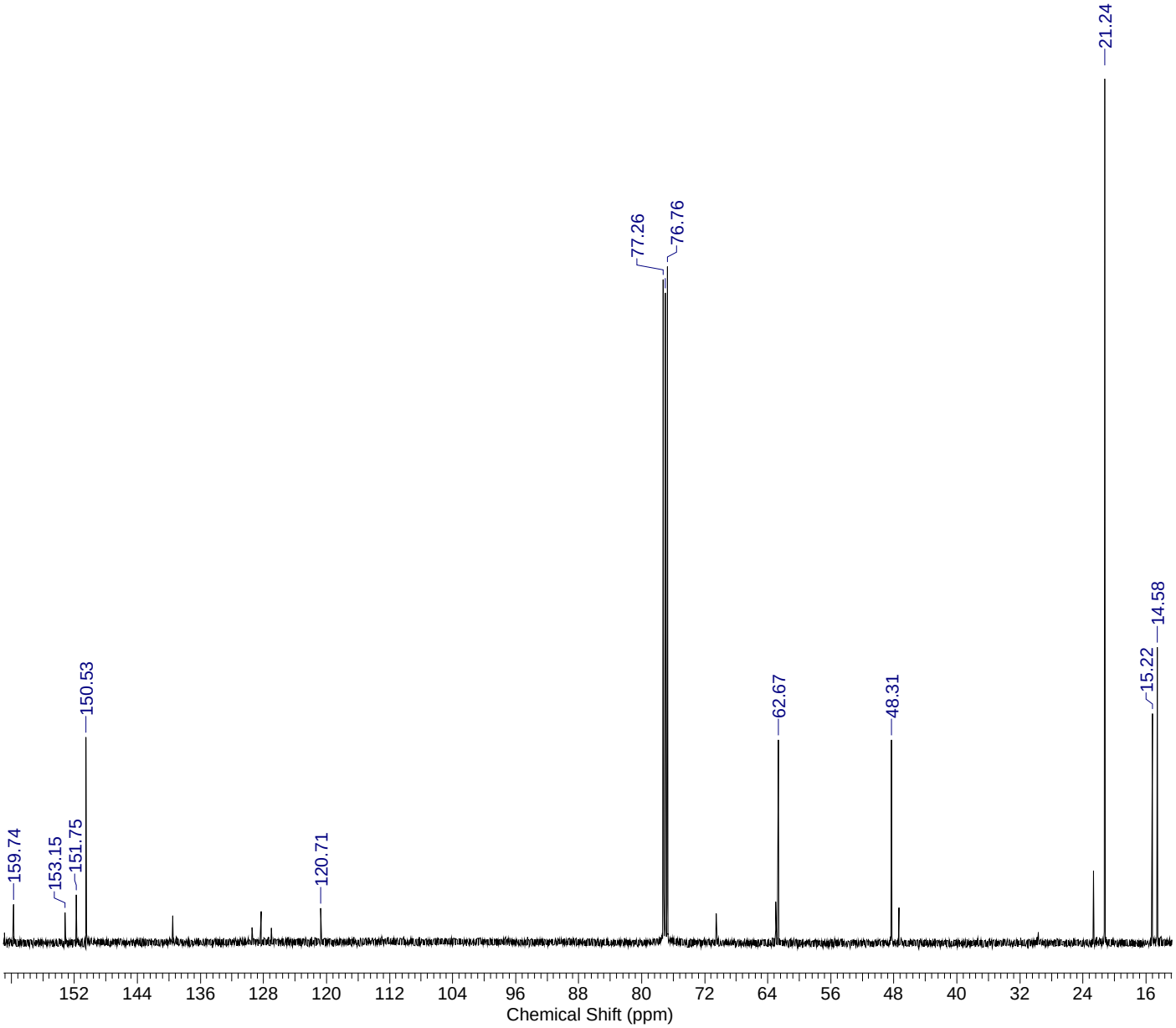
No.	(ppm)	(Hz)	Height
1	1.49	742.7	0.2185
2	1.50	750.1	0.5522
3	1.52	757.4	0.2229
4	1.68	839.6	1.0000
5	1.69	846.4	0.9601
6	2.64	1320.8	0.9286
7	4.60	2301.0	0.0863
8	4.62	2308.3	0.2071
9	4.63	2315.2	0.2585
10	4.65	2322.5	0.0785
11	4.74	2370.9	0.0736
12	4.76	2378.3	0.0532
13	7.27	3634.2	0.1774
14	8.44	4218.7	0.2174

No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.55]	3.299	1.98237e+8
2	[1.66 .. 1.73]	5.976	3.59083e+8
3	[2.59 .. 2.68]	2.732	1.64127e+8
4	[4.57 .. 4.67]	2.000	1.20171e+8
5	[4.70 .. 4.82]	1.034	6.21041e+7
6	[8.35 .. 8.49]	0.871	5.23202e+7

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (C-NMR)

11 Jul 2012

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				

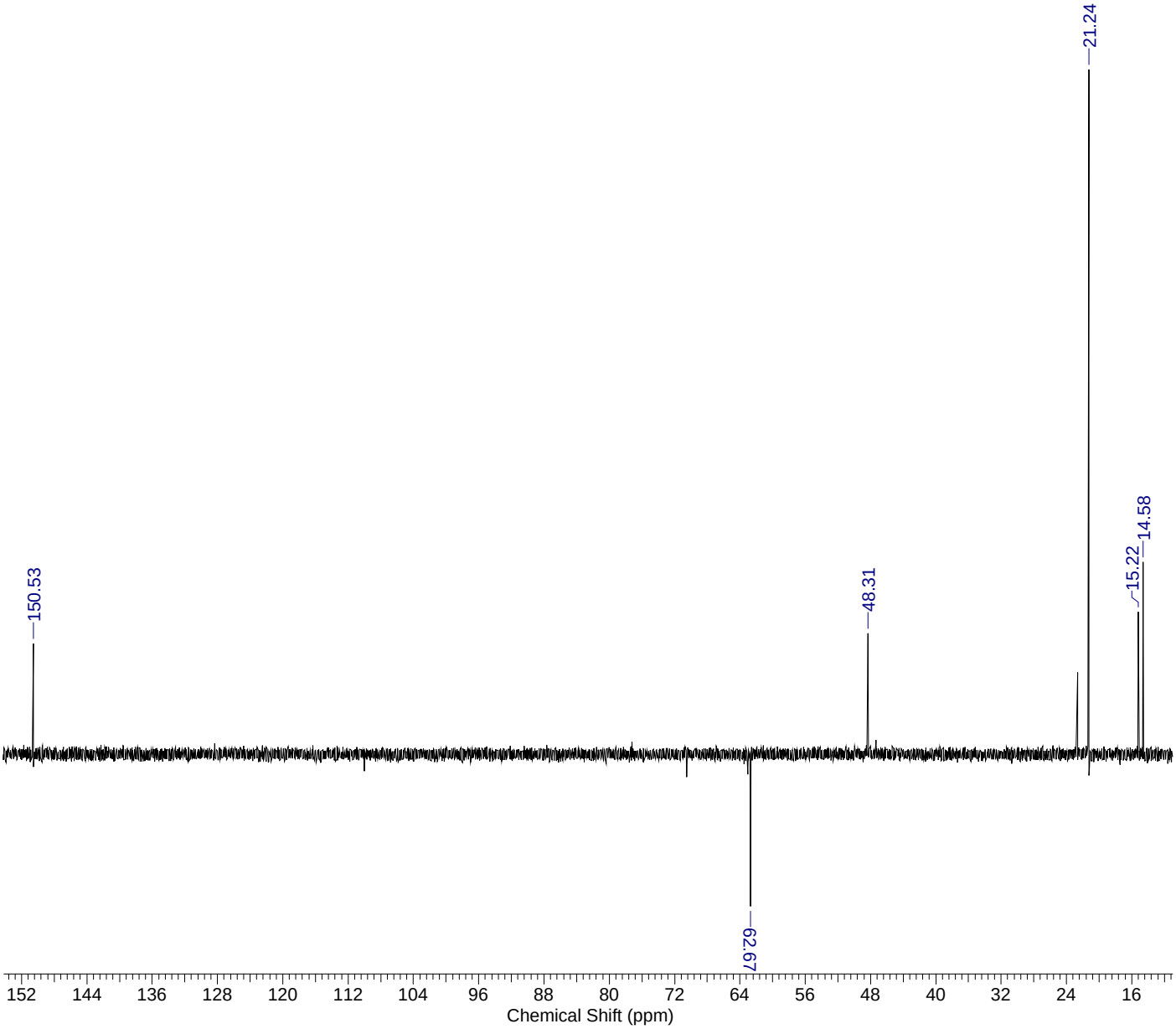


No.	(ppm)	(Hz)	Height
1	14.58	1832.4	0.3162
2	15.22	1912.5	0.2453
3	21.24	2669.7	1.0000
4	48.31	6071.6	0.2170
5	62.67	7877.0	0.2167
6	76.76	9647.0	0.7249
7	77.01	9678.5	0.6964
8	77.26	9710.9	0.7109
9	120.71	15171.8	0.0363
10	150.53	18918.9	0.2196
11	151.75	19072.5	0.0509
12	153.15	19248.9	0.0315
13	159.74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

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (DEPT)

11 Jul 2012

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				

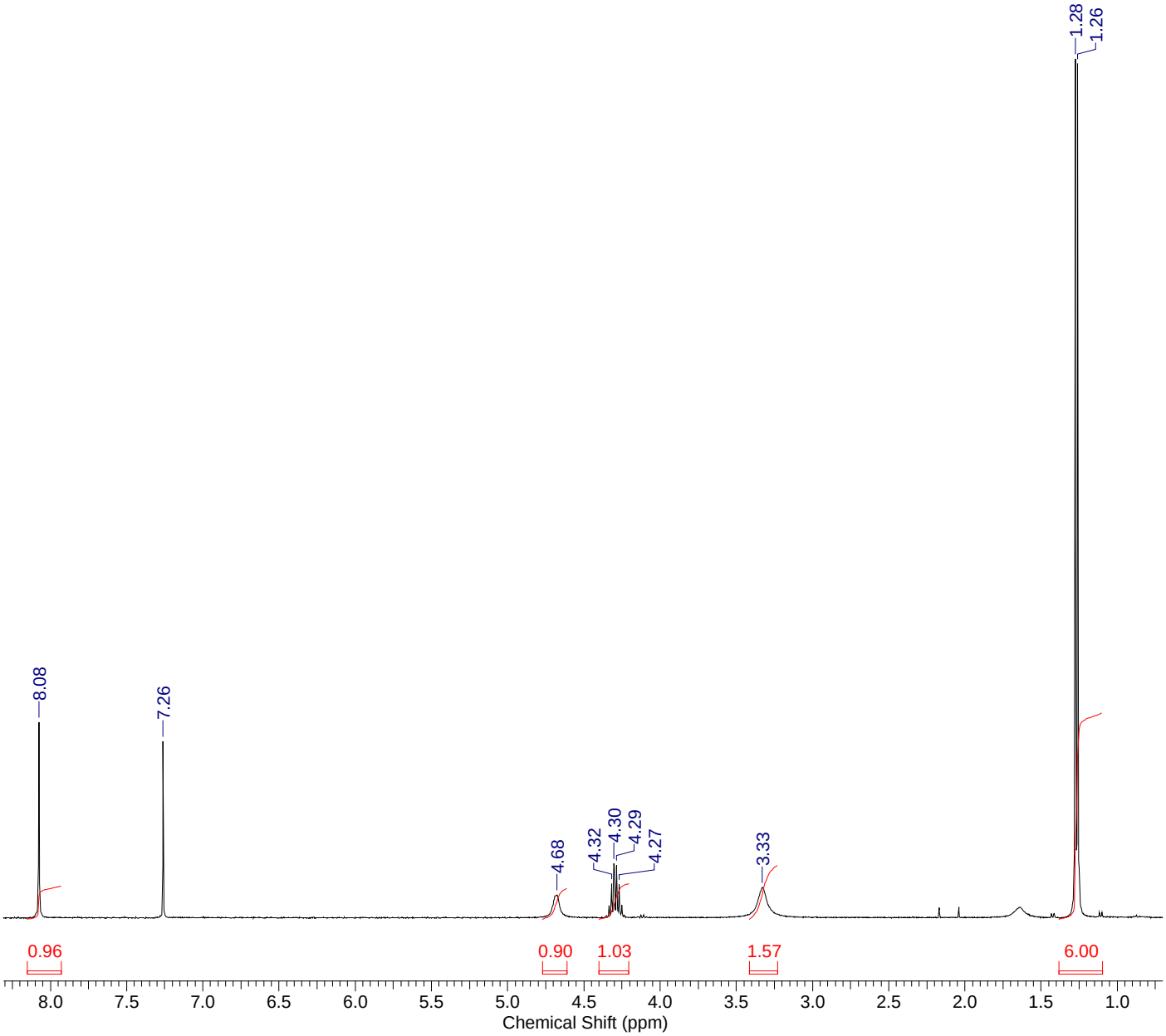


No.	(ppm)	(Hz)	Height
1	14.58	1832.4	0.2804
2	15.22	1913.4	0.2078
3	21.24	2669.7	1.0000
4	48.31	6071.6	0.1761
5	62.67	7877.0	-0.2224
6	150.53	18918.9	0.1615

4a 5-Amino-6-chloro-4-isopropylaminopyrimidine (H_NMR)

16 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	***Original Points Count***	16384
Points Count	16384	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	6410.26	***Temperature (degree C)***	25.000		



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	[1.10 .. 1.38]	6.000	2.66850e+7
2	[3.23 .. 3.41]	1.565	6.96065e+6
3	[4.21 .. 4.40]	1.026	4.56130e+6
4	[4.61 .. 4.77]	0.895	3.98062e+6
5	[7.93 .. 8.15]	0.964	4.28633e+6

Elemental Composition Report

Single Mass Analysis

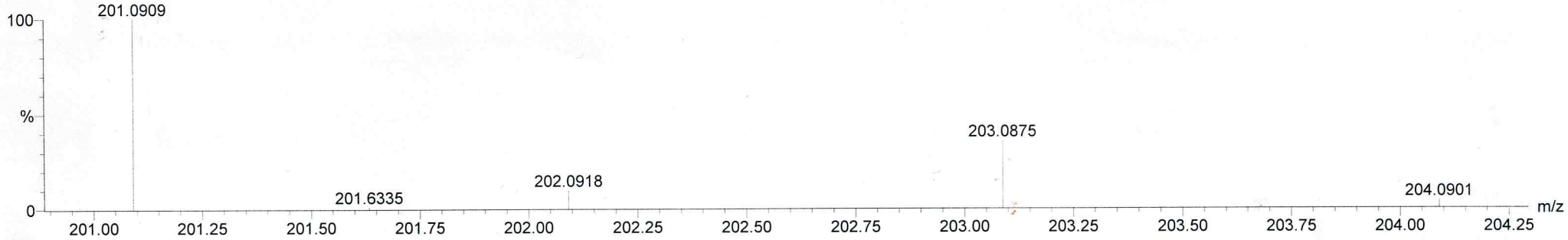
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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+

4.10e+002

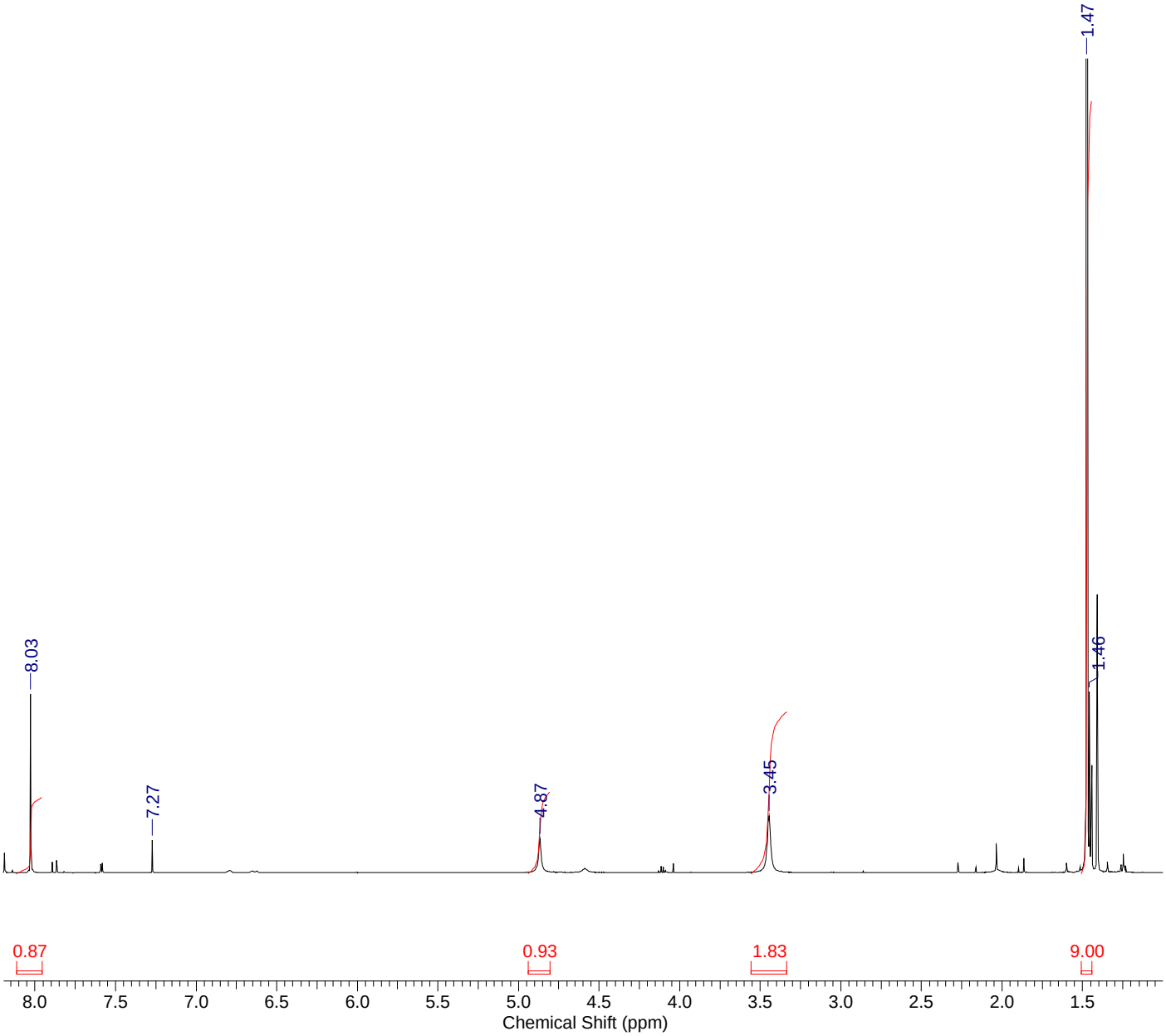


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
201.0909	201.0907	0.2	1.0	3.5	0.6	C8 H14 N4 Cl
	201.0909	0.0	0.0	-1.5	52.4	C5 H17 N2 O4 S
	201.0916	-0.7	-3.5	7.5	72.7	C13 H13 O2

4b 5-Amino-4-tert-butylamino-6-chloropyrimidine (H-NMR)

11 Mar 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	***Original Points Count***	16384
Points Count	16384	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	8012.82	***Temperature (degree C)***	25.000		



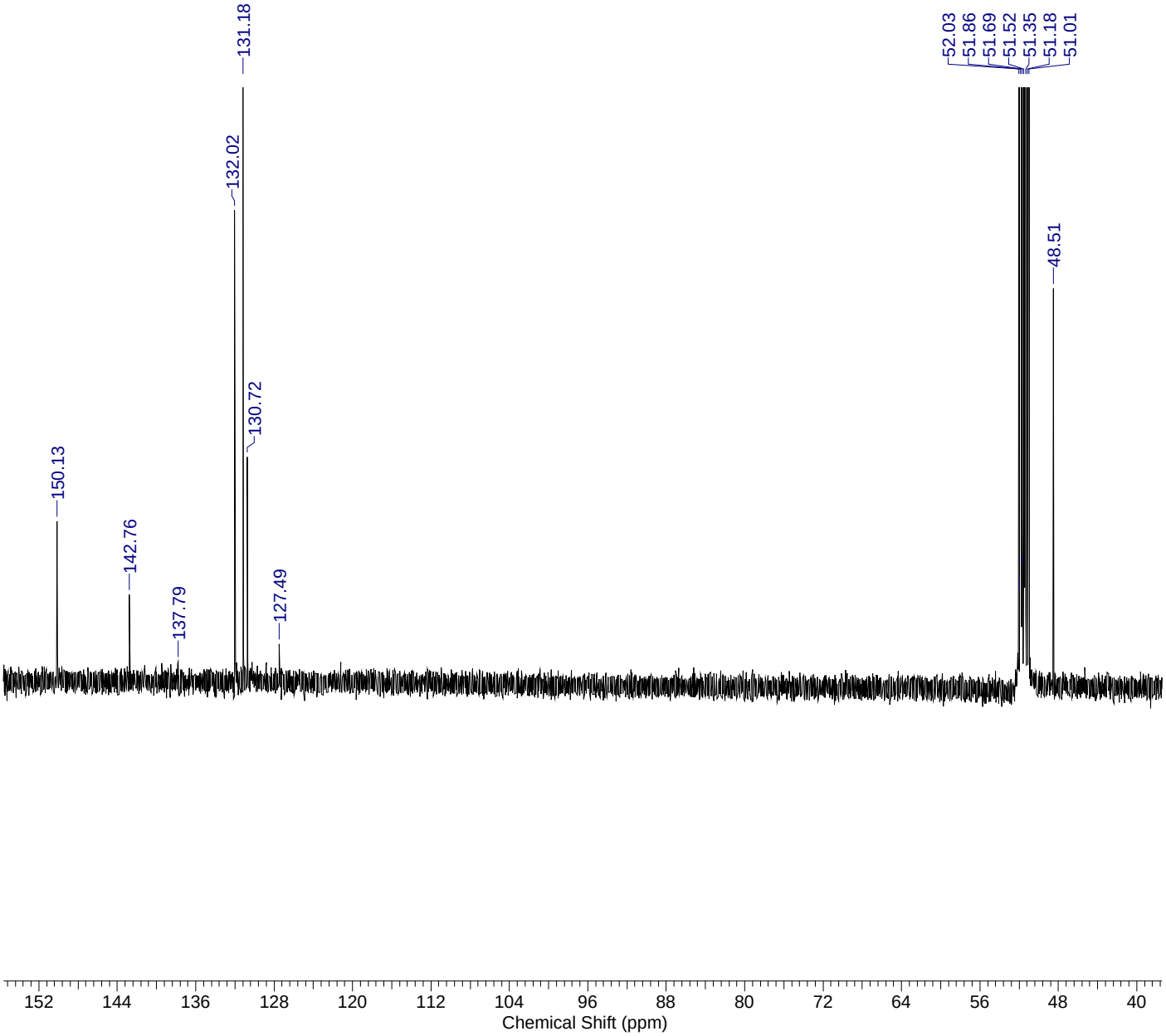
No.	(ppm)	(Hz)	Height
1	1.46	728.2	0.0677
2	1.47	736.5	1.0000
3	3.45	1722.5	0.0217
4	4.87	2433.1	0.0131
5	7.27	3635.3	0.0125
6	8.03	4011.9	0.0669

No.	(ppm)	Value	Absolute Value
1	[1.44 .. 1.51]	9.000	1.64609e+8
2	[3.34 .. 3.56]	1.831	3.34978e+7
3	[4.80 .. 4.94]	0.930	1.70182e+7
4	[7.95 .. 8.11]	0.867	1.58596e+7

4c 5-amino-4-benzilamino-6-chloropyrimidine (C-NMR)

16 Jul 2012

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***	13C	***Original Points Count***	32768
Points Count	32768	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	31250.00	***Temperature (degree C)***	25.000		

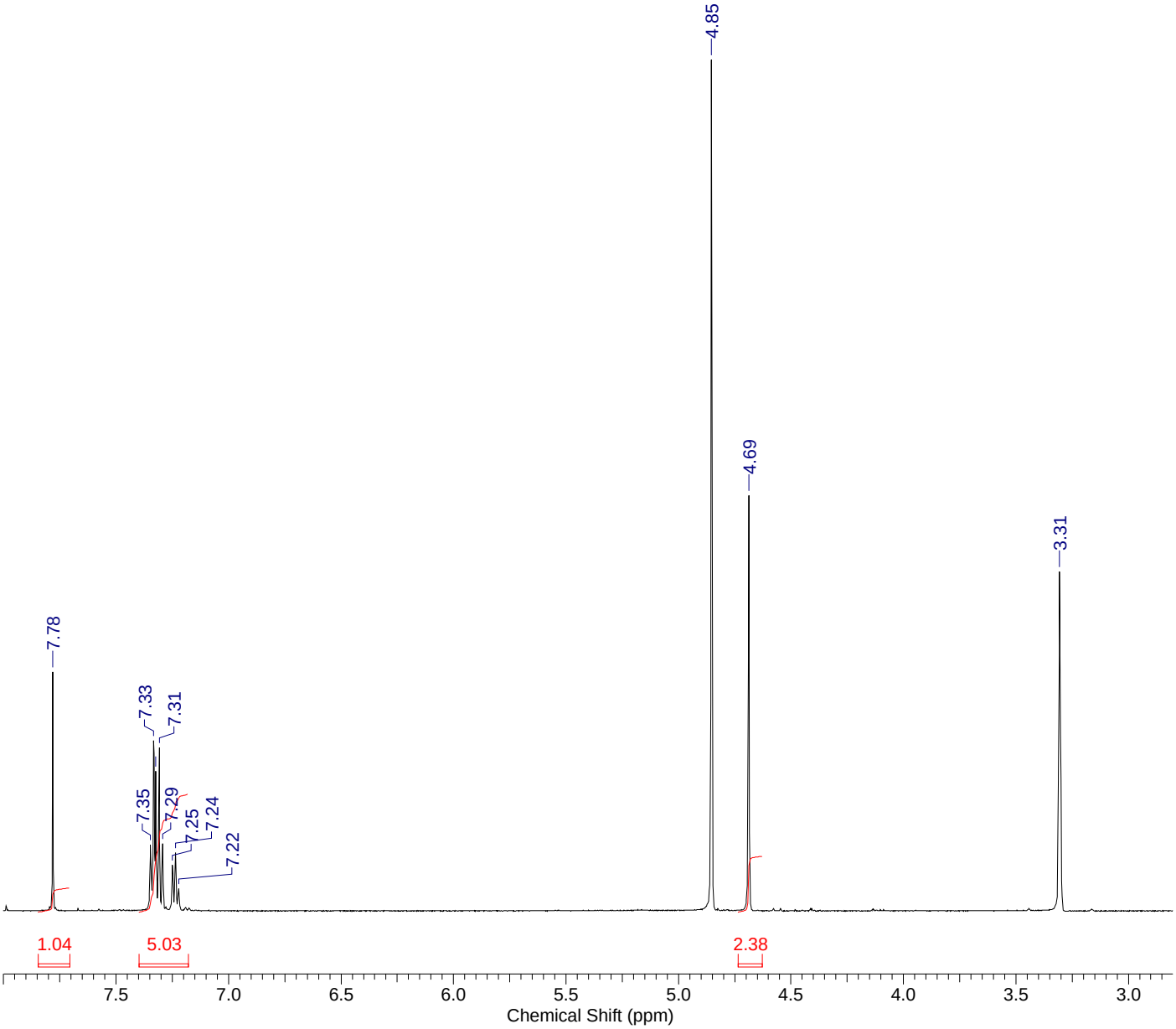


No.	(ppm)	(Hz)	Height
1	48.51	6096.4	0.0362
2	51.01	6411.1	0.1618
3	51.18	6432.1	0.3818
4	51.35	6454.0	0.8678
5	51.52	6475.0	1.0000
6	51.63	6489.3	0.0104
7	51.69	6496.9	0.7416
8	51.81	6511.3	0.0145
9	51.86	6517.9	0.4658
10	51.97	6532.2	0.0080
11	52.03	6539.9	0.1005
12	127.49	16023.5	0.0035
13	130.72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

4c 5-amino-4-benzilamino-6-chloropyrimidine (H-NMR)

16 Jul 2012

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	7.22	3609.3	0.0275
5	7.24	3616.6	0.0695
6	7.25	3623.4	0.0555
7	7.29	3644.9	0.0804
8	7.31	3652.7	0.1928
9	7.32	3660.0	0.1651
10	7.33	3665.0	0.2014
11	7.35	3671.9	0.0790
12	7.78	3889.3	0.2820

No.	(ppm)	Value	Absolute Value
1	[4.63 .. 4.74]	2.382	5.73421e+7
2	[7.18 .. 7.40]	5.029	1.21055e+8
3	[7.71 .. 7.85]	1.037	2.49540e+7

4c 5-amino-4-benzilamino-6-chloropyrimidine (MS)

Elemental Composition Report

Single Mass Analysis

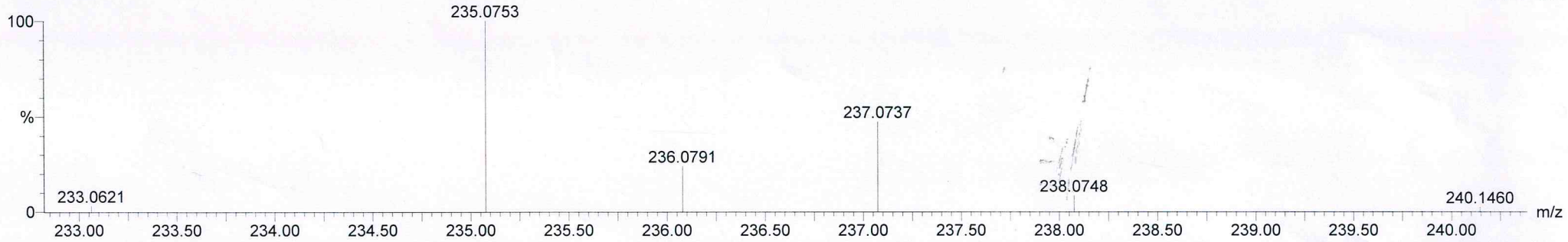
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

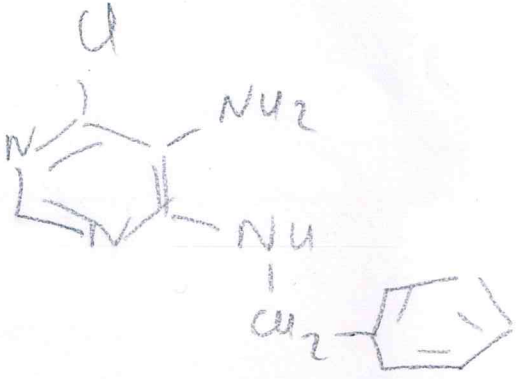
MJ-2 89 (1.975)

1: TOF MS ES+

7.14e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	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



5a. - 6-Ethoxy-9-isopropyl-9H-purine

Elemental Composition Report

Single Mass Analysis

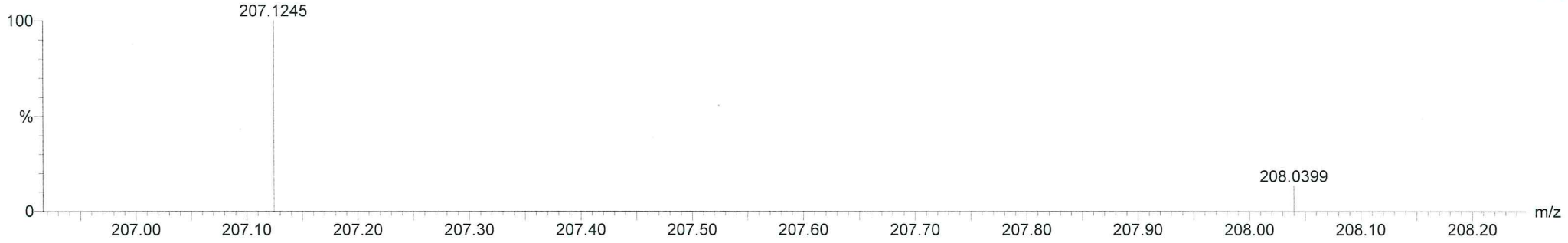
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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

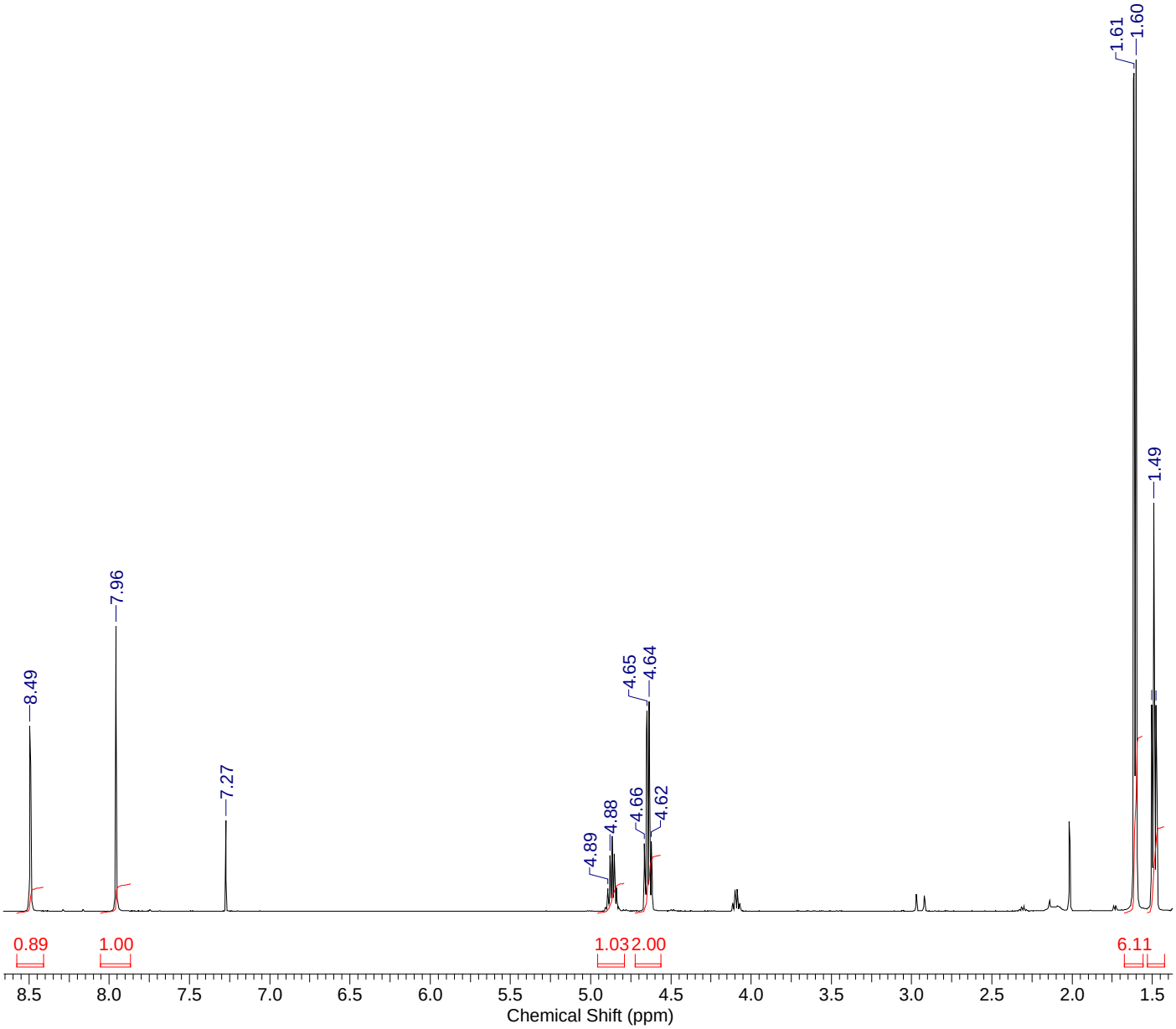


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
207.1245	207.1246	-0.1	-0.5	5.5	n/a	C10 H15 N4 O

5a .- 6-Ethoxy-9-isopropyl-9H-purine (H-NMR)

11 Jul 2012

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				



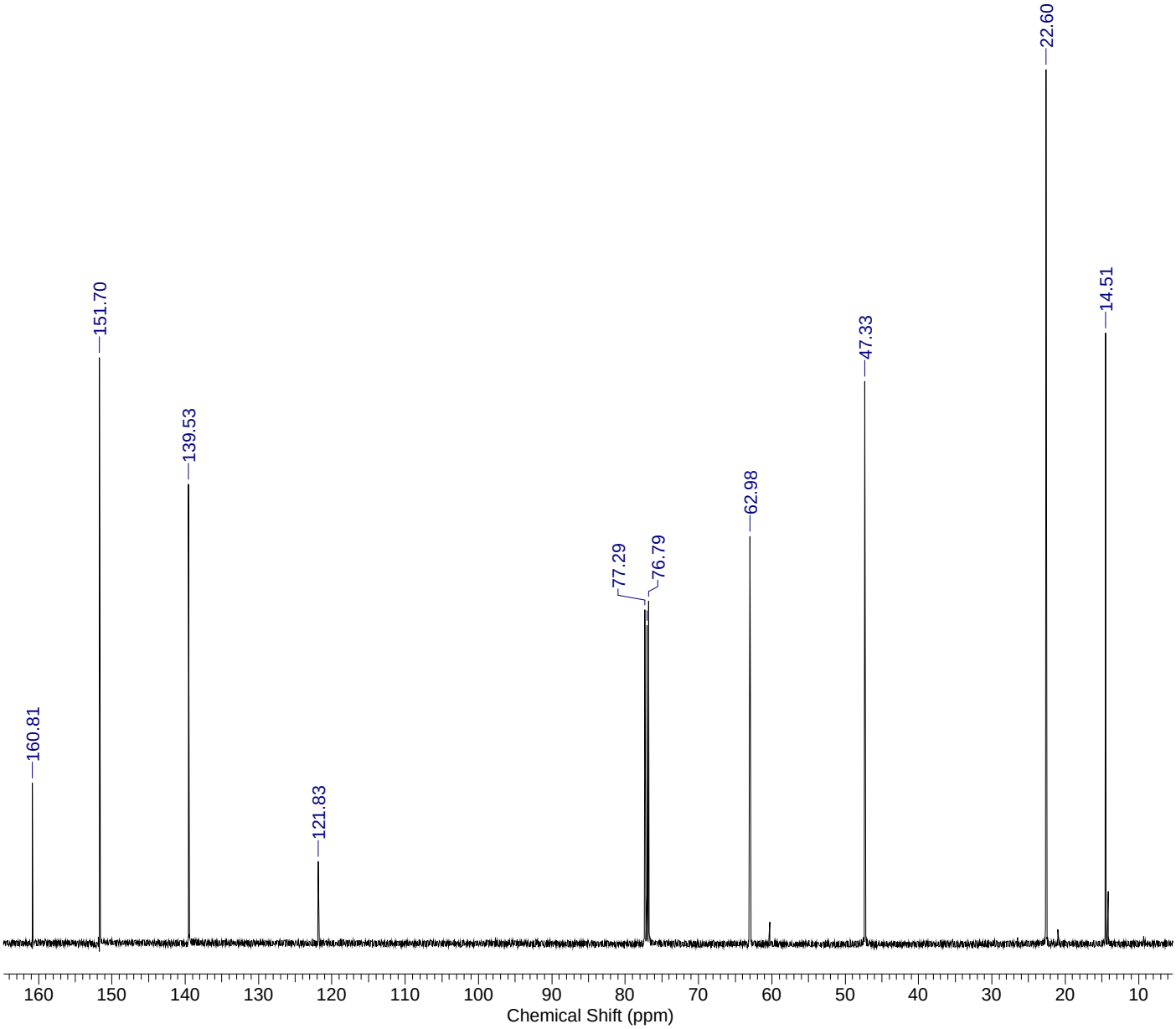
No.	(ppm)	(Hz)	Height
1	1.48	738.3	0.2434
2	1.49	745.2	0.4809
3	1.51	752.5	0.2440
4	1.60	800.9	1.0000
5	1.61	806.8	0.9840
6	4.62	2309.8	0.0837
7	4.64	2317.1	0.2483
8	4.65	2323.5	0.2373
9	4.66	2331.3	0.0814
10	4.88	2439.4	0.0676
11	4.89	2446.2	0.0283
12	7.27	3635.2	0.1085
13	7.96	3977.6	0.3363
14	8.49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

5a. - 6-Ethoxy-9-isopropyl-9H-purine (C-NMR)

11 Jul 2012

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				

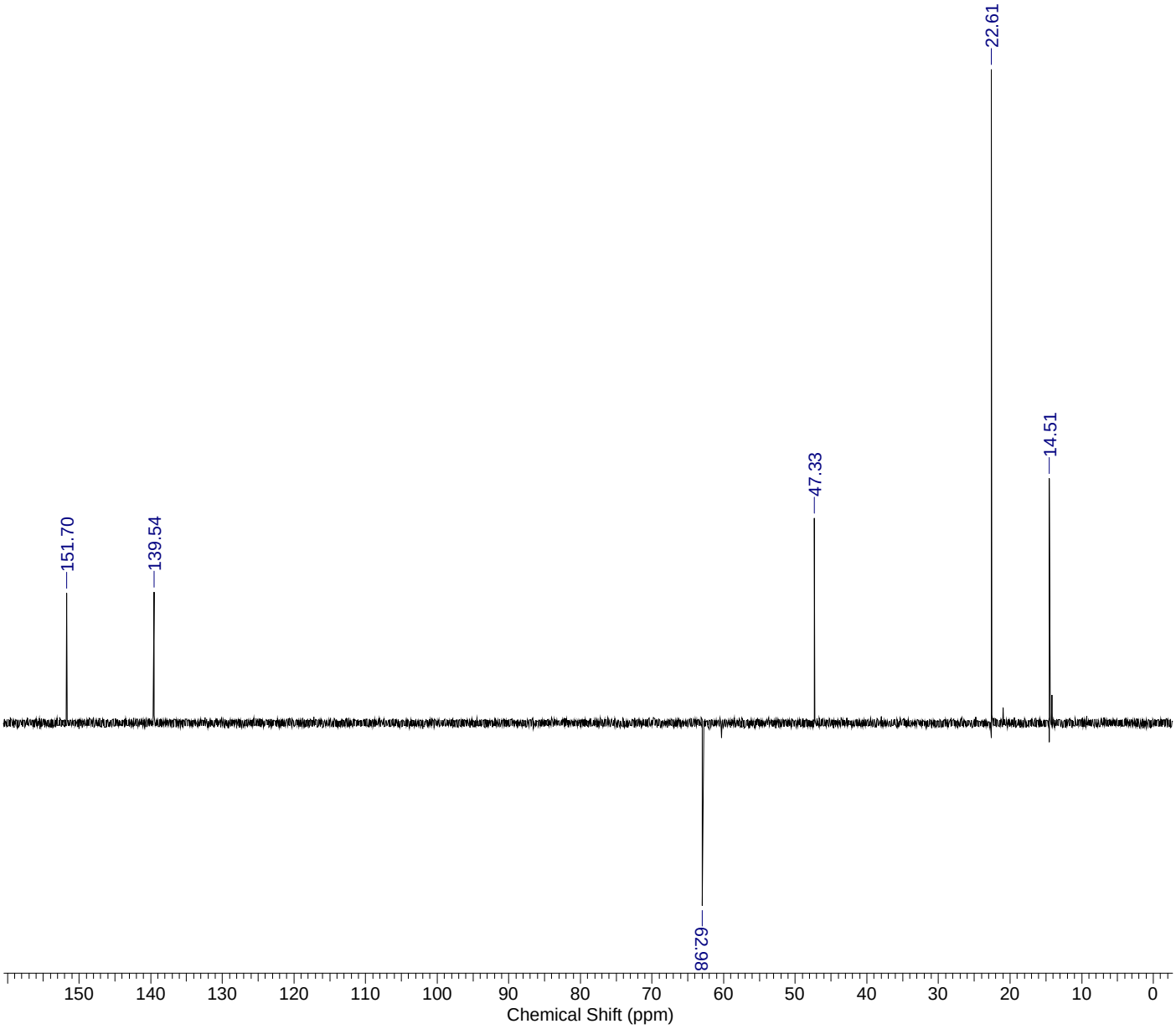


No.	(ppm)	(Hz)	Height
1	14.51	1823.8	0.6984
2	22.60	2840.4	1.0000
3	47.33	5948.6	0.6432
4	62.98	7915.1	0.4655
5	76.79	9650.8	0.3913
6	77.04	9683.3	0.3638
7	77.29	9714.7	0.3814
8	121.83	15312.0	0.0933
9	139.53	17537.0	0.5250
10	151.70	19066.8	0.6704
11	160.81	20211.2	0.1830

5a. - 6-Ethoxy-9-isopropyl-9H-purine DEPT

11 Jul 2012

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

5b. - 6-Ethoxy-8-ethyl-9-isopropyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

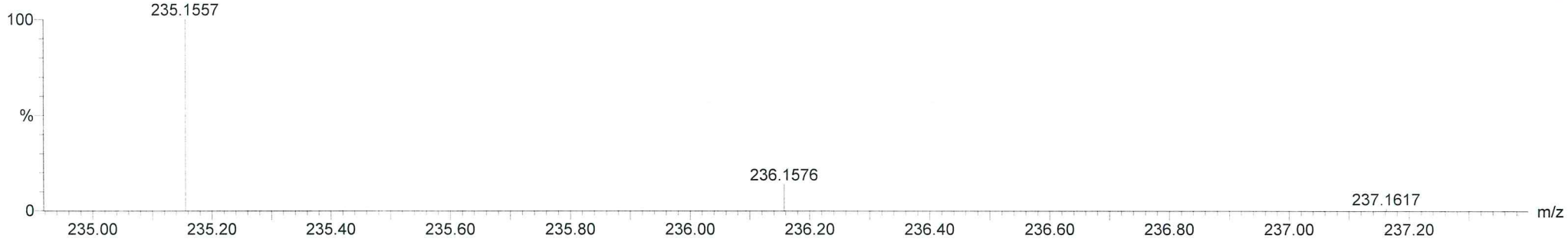
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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

ASIMJ-2 9 (0.217)

1: TOF MS ES+
5.80e+002

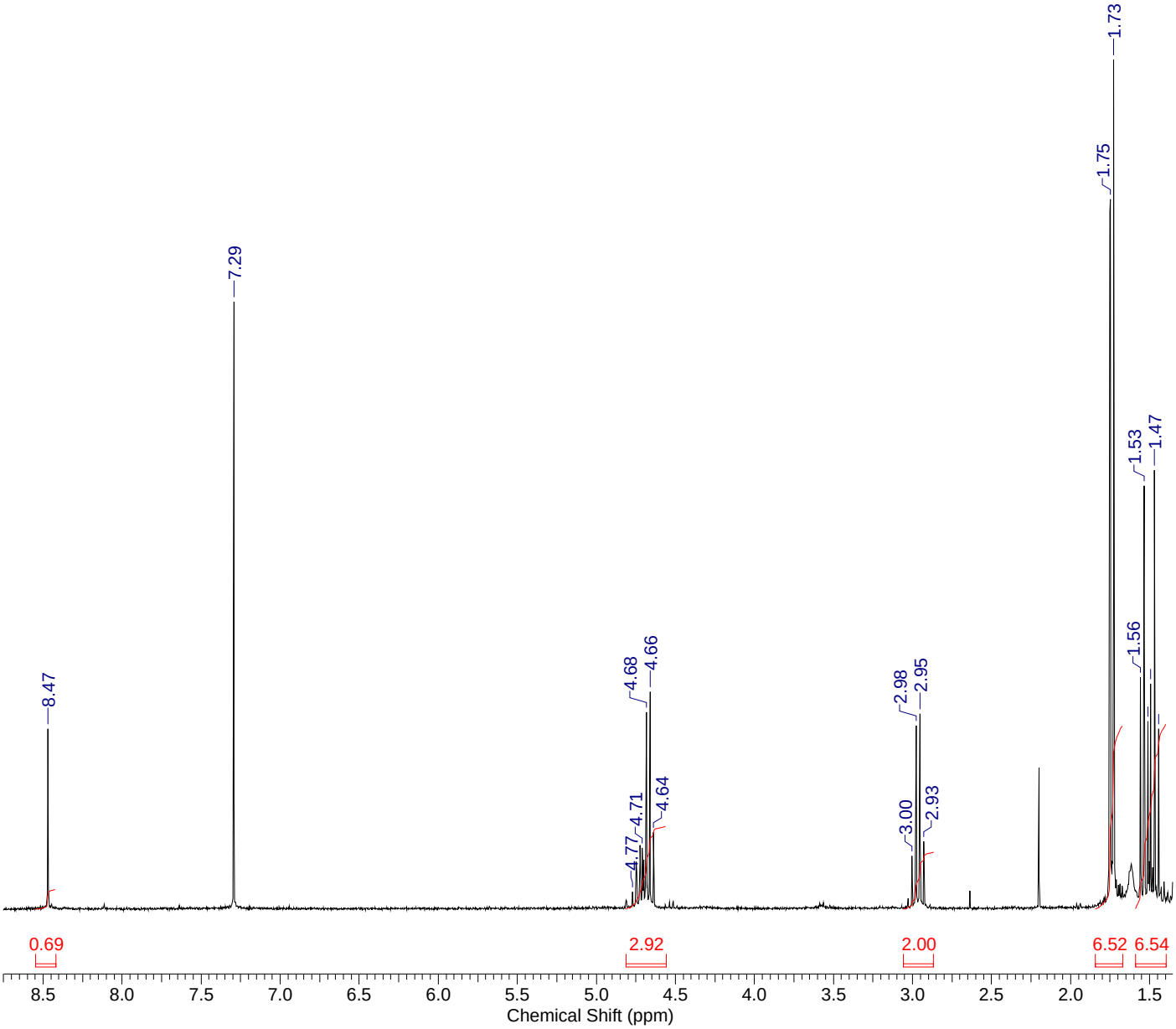


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.1557	235.1559	-0.2	-0.9	5.5	0.3	C12 H19 N4 O
	235.1545	1.2	5.1	0.5	1.0	C11 H23 O5

5b. - 6-Ethoxy-8-ethyl-9-isopropyl-9H-purine (H-NMR)

11 Jul 2012

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

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

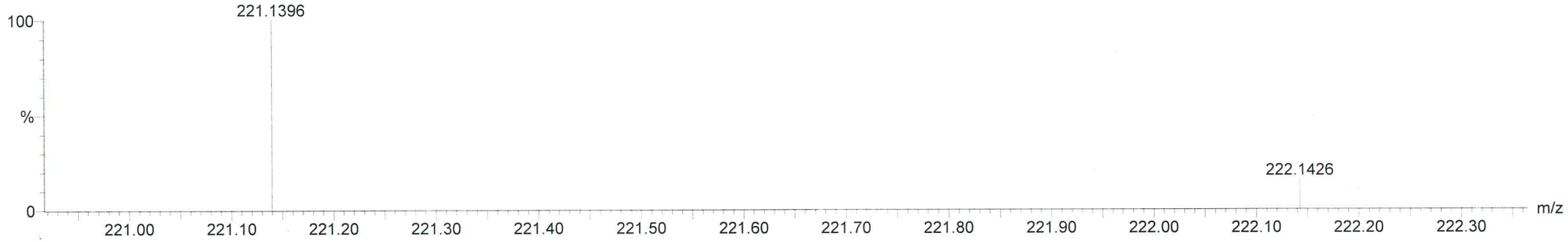
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

ASIMJ-3 7 (0.163)

1: TOF MS ES+
4.26e+002

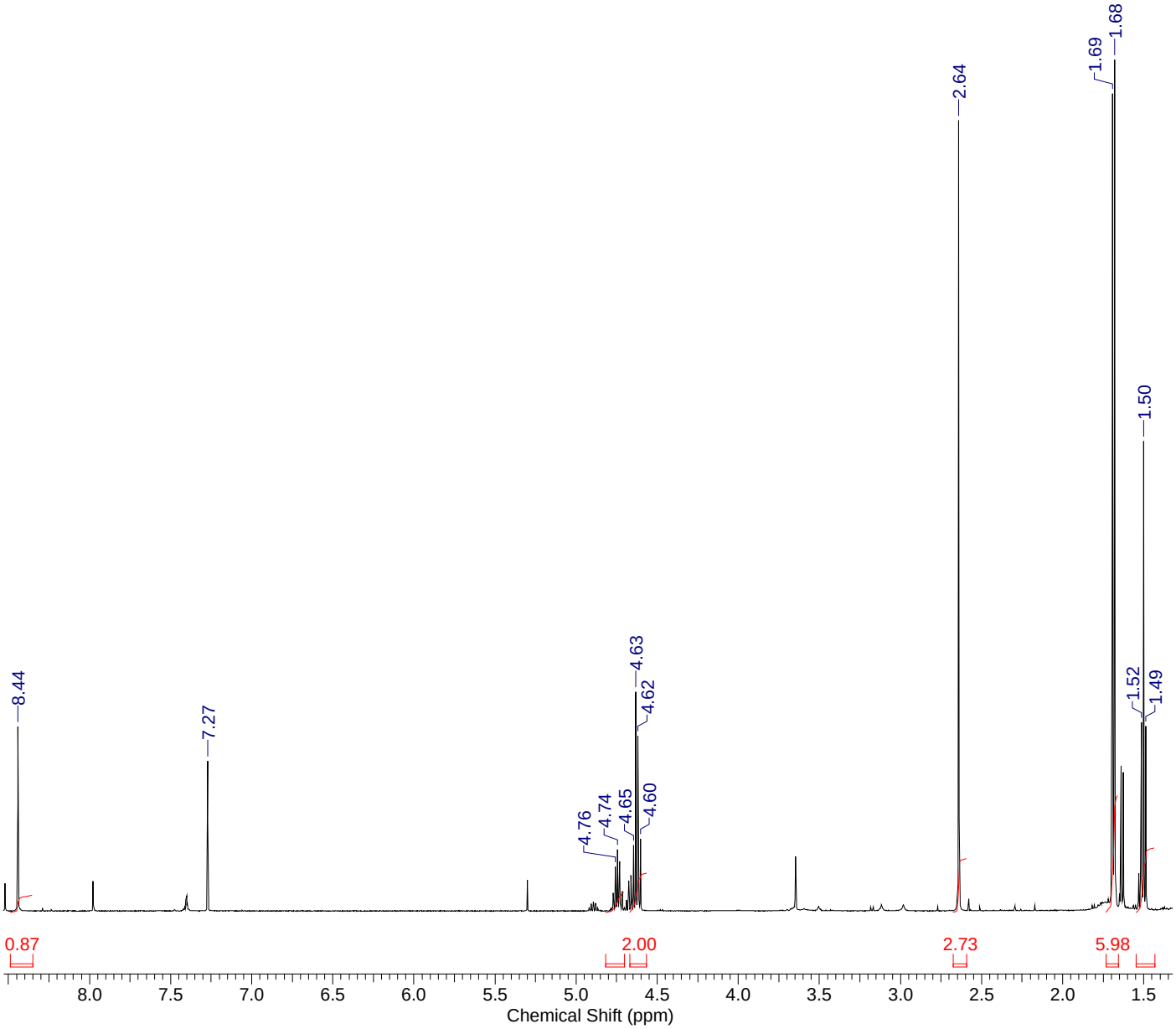


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1396	221.1402	-0.6	-2.7	5.5	n/a	C11 H17 N4 O
	221.1389	0.7	3.2	0.5	n/a	C10 H21 O5

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (H-NMR)

11 Jul 2012

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				



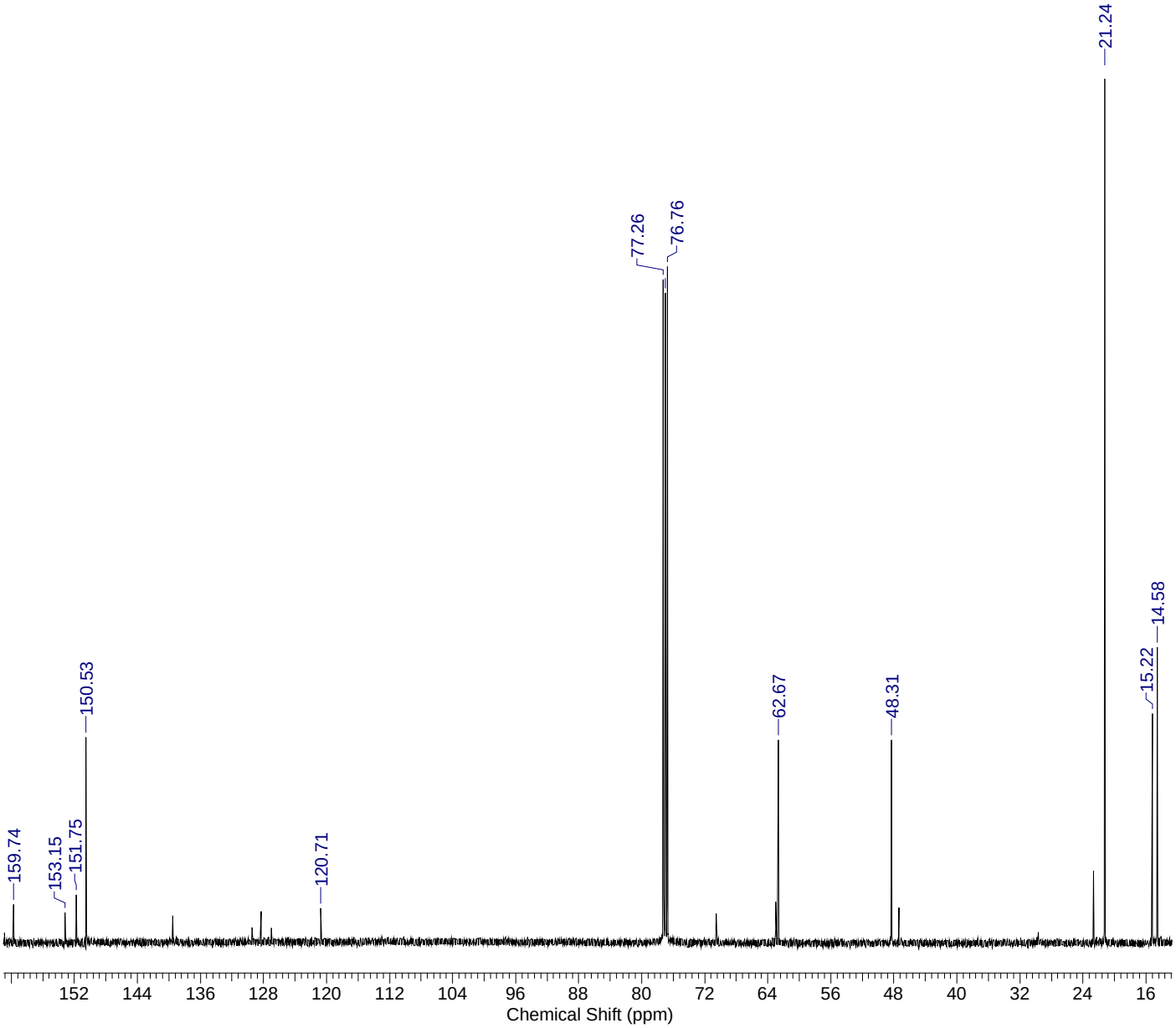
No.	(ppm)	(Hz)	Height
1	1.49	742.7	0.2185
2	1.50	750.1	0.5522
3	1.52	757.4	0.2229
4	1.68	839.6	1.0000
5	1.69	846.4	0.9601
6	2.64	1320.8	0.9286
7	4.60	2301.0	0.0863
8	4.62	2308.3	0.2071
9	4.63	2315.2	0.2585
10	4.65	2322.5	0.0785
11	4.74	2370.9	0.0736
12	4.76	2378.3	0.0532
13	7.27	3634.2	0.1774
14	8.44	4218.7	0.2174

No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.55]	3.299	1.98237e+8
2	[1.66 .. 1.73]	5.976	3.59083e+8
3	[2.59 .. 2.68]	2.732	1.64127e+8
4	[4.57 .. 4.67]	2.000	1.20171e+8
5	[4.70 .. 4.82]	1.034	6.21041e+7
6	[8.35 .. 8.49]	0.871	5.23202e+7

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (C-NMR)

11 Jul 2012

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				

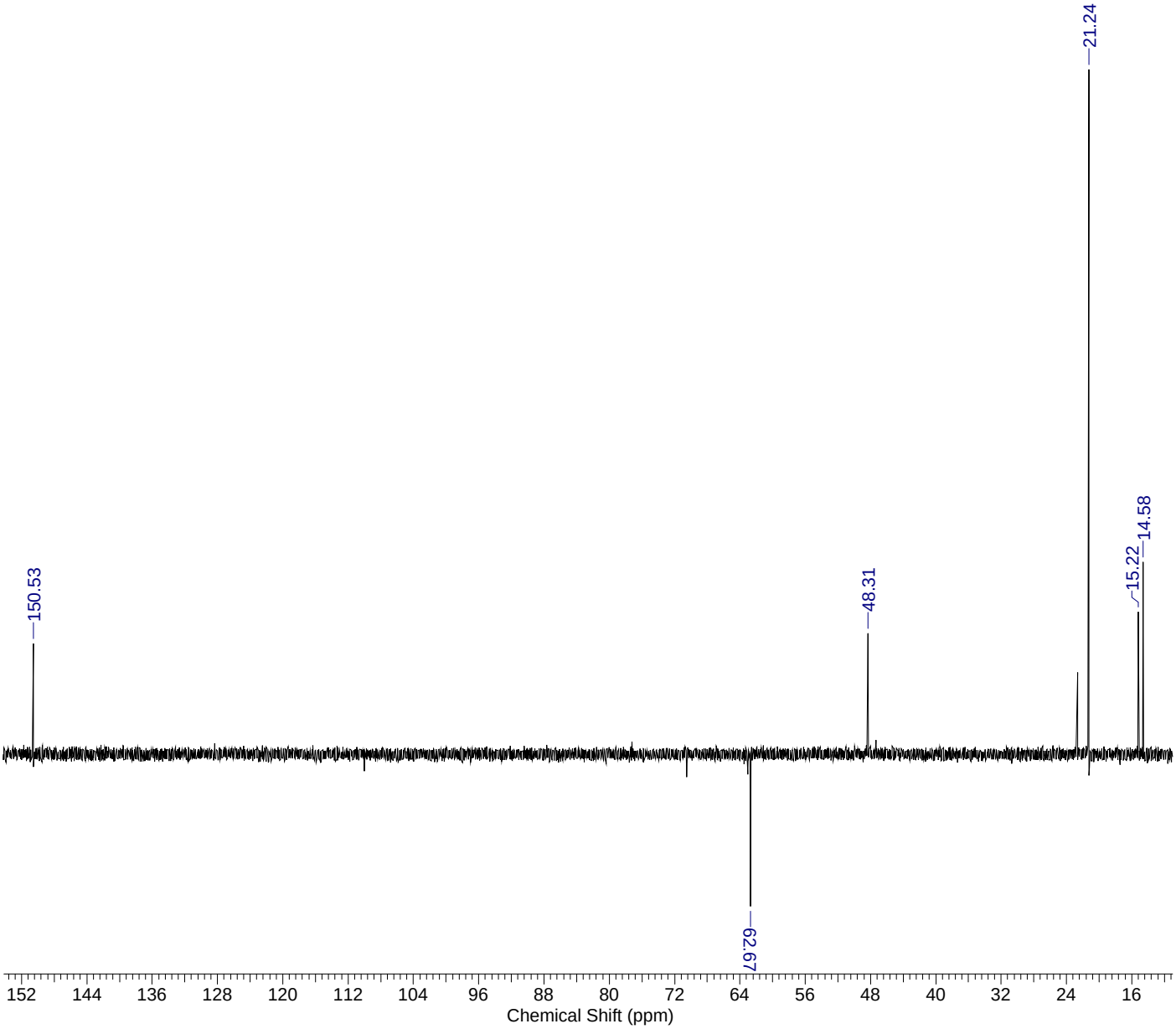


No.	(ppm)	(Hz)	Height
1	14.58	1832.4	0.3162
2	15.22	1912.5	0.2453
3	21.24	2669.7	1.0000
4	48.31	6071.6	0.2170
5	62.67	7877.0	0.2167
6	76.76	9647.0	0.7249
7	77.01	9678.5	0.6964
8	77.26	9710.9	0.7109
9	120.71	15171.8	0.0363
10	150.53	18918.9	0.2196
11	151.75	19072.5	0.0509
12	153.15	19248.9	0.0315
13	159.74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

5b. - 6-Ethoxy-9-isopropyl-8-methyl-9H-purine (DEPT)

11 Jul 2012

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

5d. - 6-(Benzyloxy)-9-isopropyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

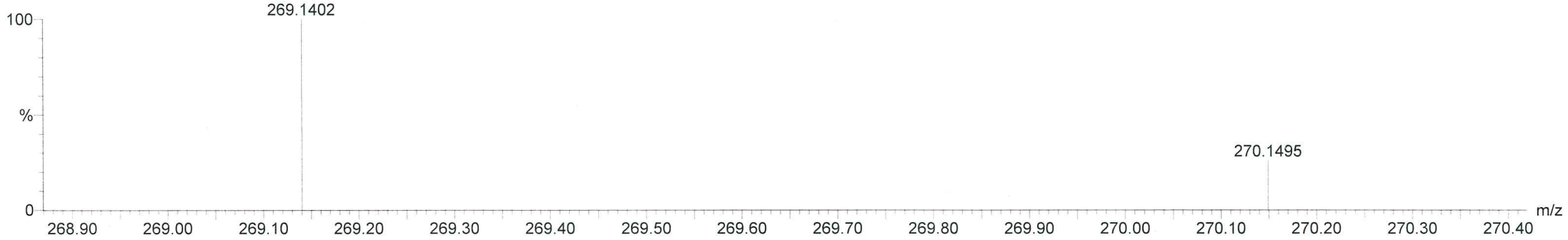
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

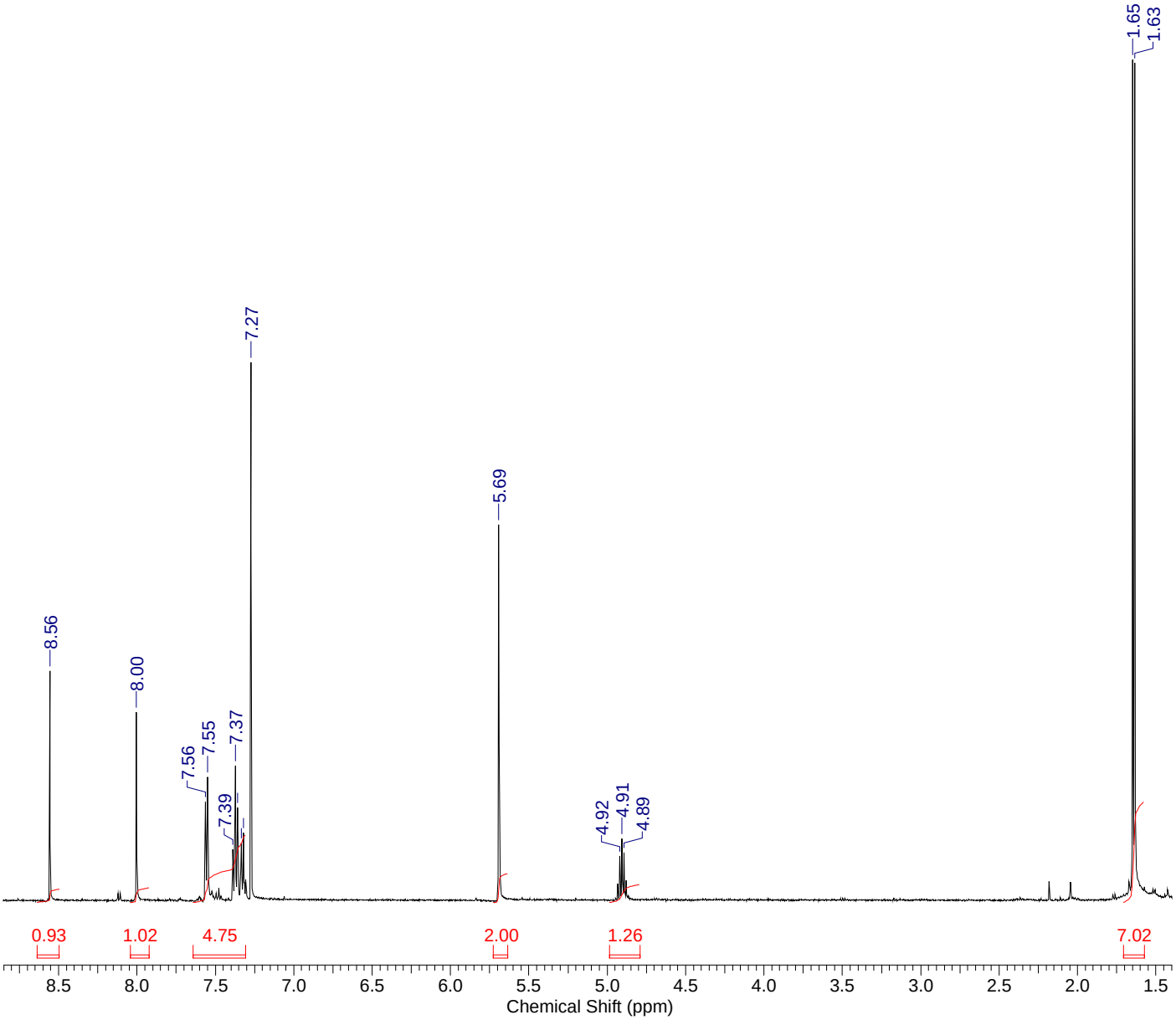


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.1402	269.1402	0.0	0.0	9.5	n/a	C15 H17 N4 O
	269.1414	-1.2	-4.5	5.5	n/a	C12 H18 N4 O2 F
	269.1389	1.3	4.8	4.5	n/a	C14 H21 O5
	269.1400	0.2	0.7	0.5	n/a	C11 H22 O6 F

5d. - 6-(Benzyloxy)-9-isopropyl-9H-purine (H-NMR)

12 Jul 2012

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				



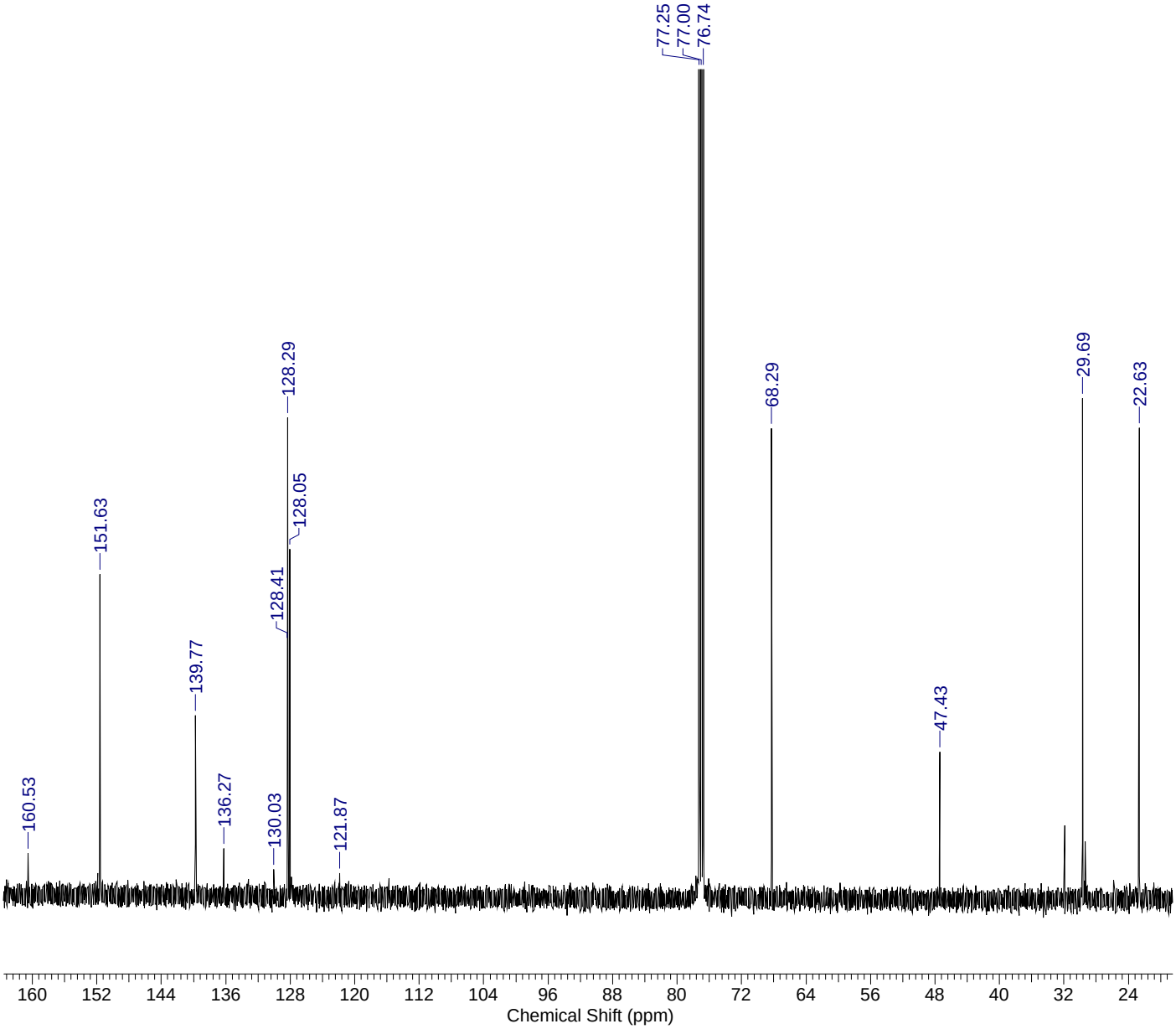
No.	(ppm)	(Hz)	Height
1	1.63	816.9	0.9483
2	1.65	823.8	0.9517
3	4.89	2445.1	0.0564
4	4.91	2452.0	0.0723
5	4.92	2458.8	0.0524
6	5.69	2845.2	0.4268
7	7.27	3634.6	0.6098
8	7.32	3658.6	0.0785
9	7.33	3665.9	0.0672
10	7.36	3677.6	0.1072
11	7.37	3685.0	0.1544
12	7.39	3692.3	0.0603
13	7.55	3773.0	0.1416
14	7.56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

5b.- 6-(Benzyloxy)-9-isopropyl-9H-purine (C-NMR)

12 Jul 2012

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

5e- 6-(Benzyloxy)-9-isopropyl-8-methyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

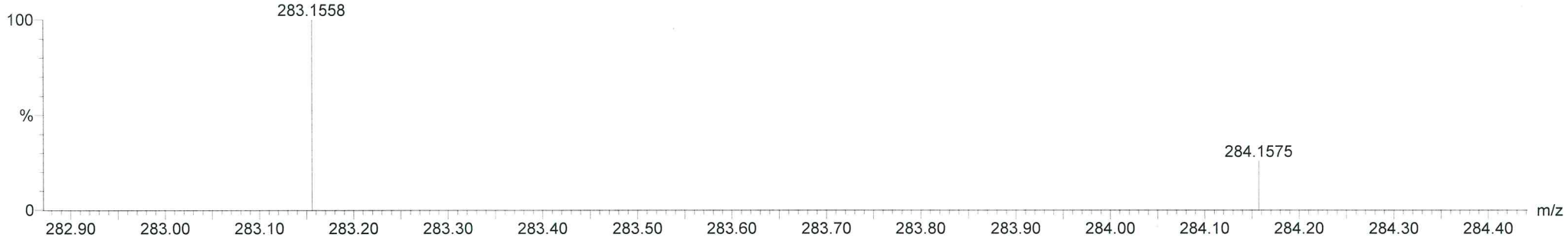
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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

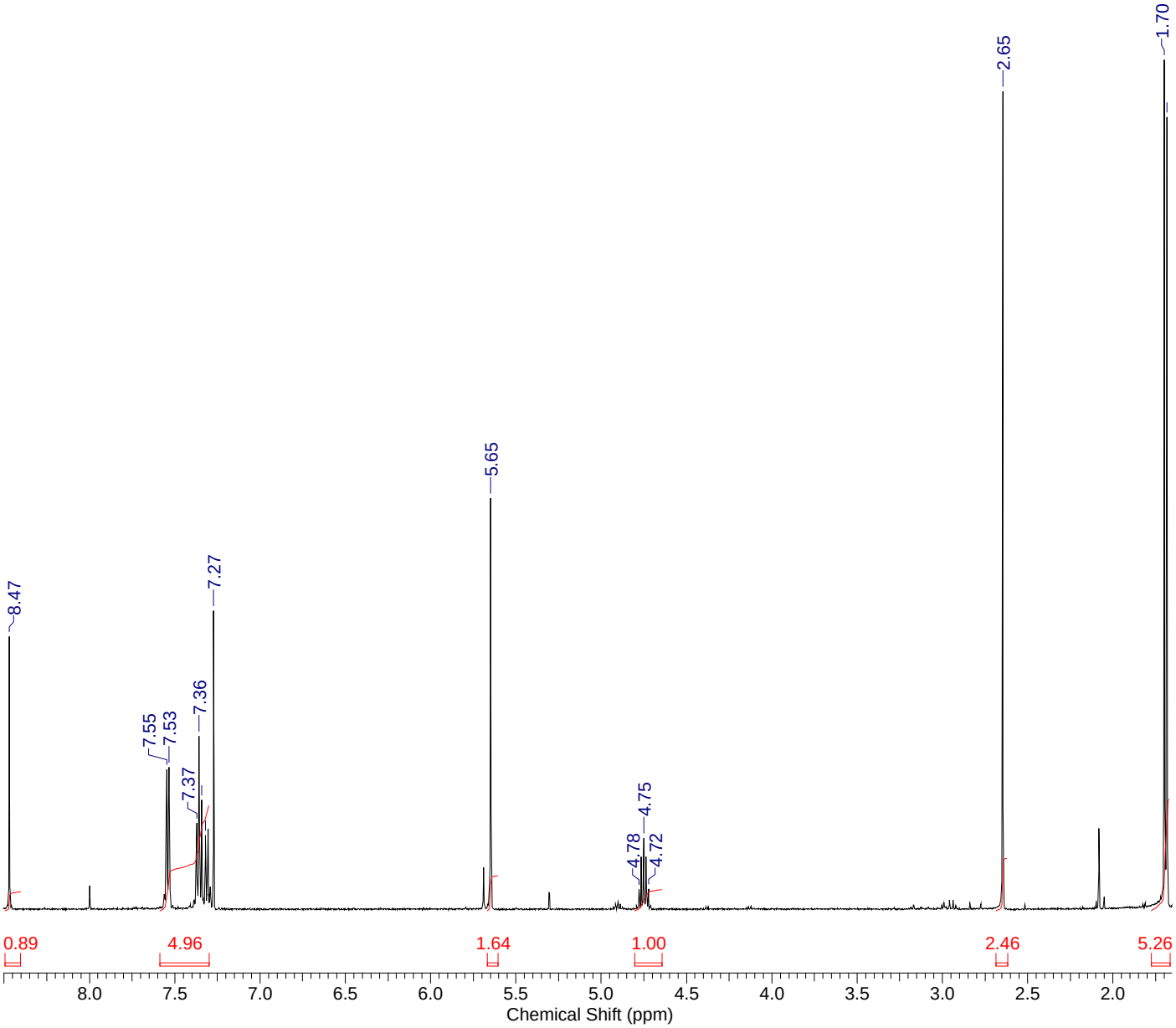


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.1558	283.1559	-0.1	-0.4	9.5	n/a	C16 H19 N4 O
	283.1570	-1.2	-4.2	5.5	n/a	C13 H20 N4 O2 F
	283.1545	1.3	4.6	4.5	n/a	C15 H23 O5
	283.1557	0.1	0.4	0.5	n/a	C12 H24 O6 F

5e- 6-(Benzyloxy)-9-isopropyl-8-methyl-9H-purine (H-NMR)

12 Jul 2012

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				



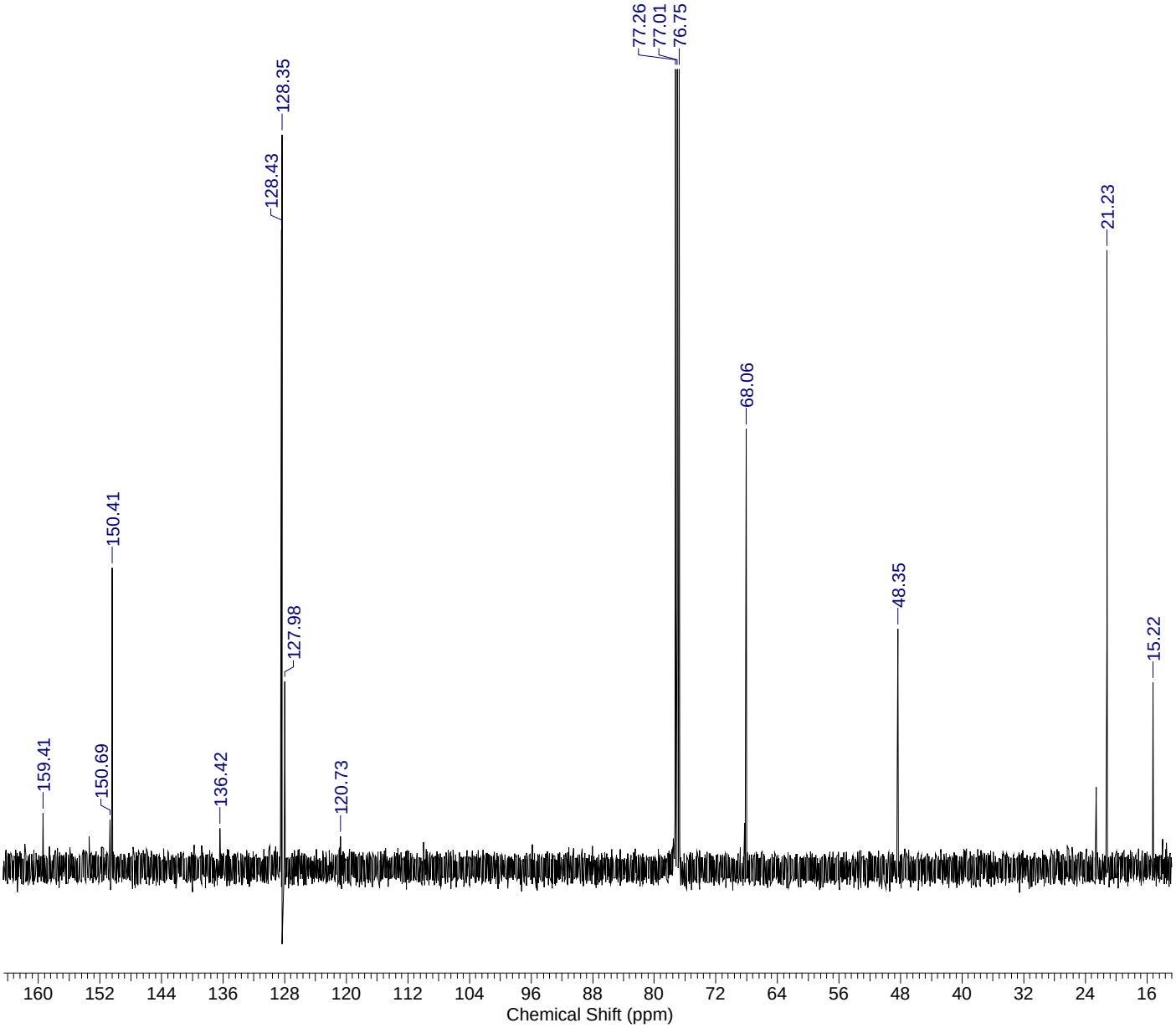
No.	(ppm)	(Hz)	Height
1	1.68	841.9	0.9325
2	1.70	848.7	1.0000
3	2.65	1322.6	0.9626
4	4.72	2360.5	0.0255
5	4.75	2374.2	0.0857
6	4.78	2387.9	0.0253
7	5.65	2823.2	0.4849
8	7.27	3634.6	0.3526
9	7.32	3658.6	0.0886
10	7.34	3669.3	0.1299
11	7.36	3677.1	0.2053
12	7.37	3684.0	0.1032
13	7.53	3765.2	0.1687
14	7.55	3772.0	0.1659
15	8.47	4232.7	0.3220

No.	(ppm)	Value	Absolute Value
1	[1.67 .. 1.77]	5.257	2.46703e+6
2	[2.62 .. 2.69]	2.457	1.15307e+6
3	[4.64 .. 4.80]	1.000	4.69325e+5
4	[5.61 .. 5.67]	1.637	7.68287e+5
5	[7.30 .. 7.59]	4.958	2.32686e+6
6	[8.41 .. 8.49]	0.894	4.19388e+5

5e- 6-(Benzyloxy)-9-isopropyl-8-methyl-9H-purine (C-NMR)

12 Jul 2012

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				

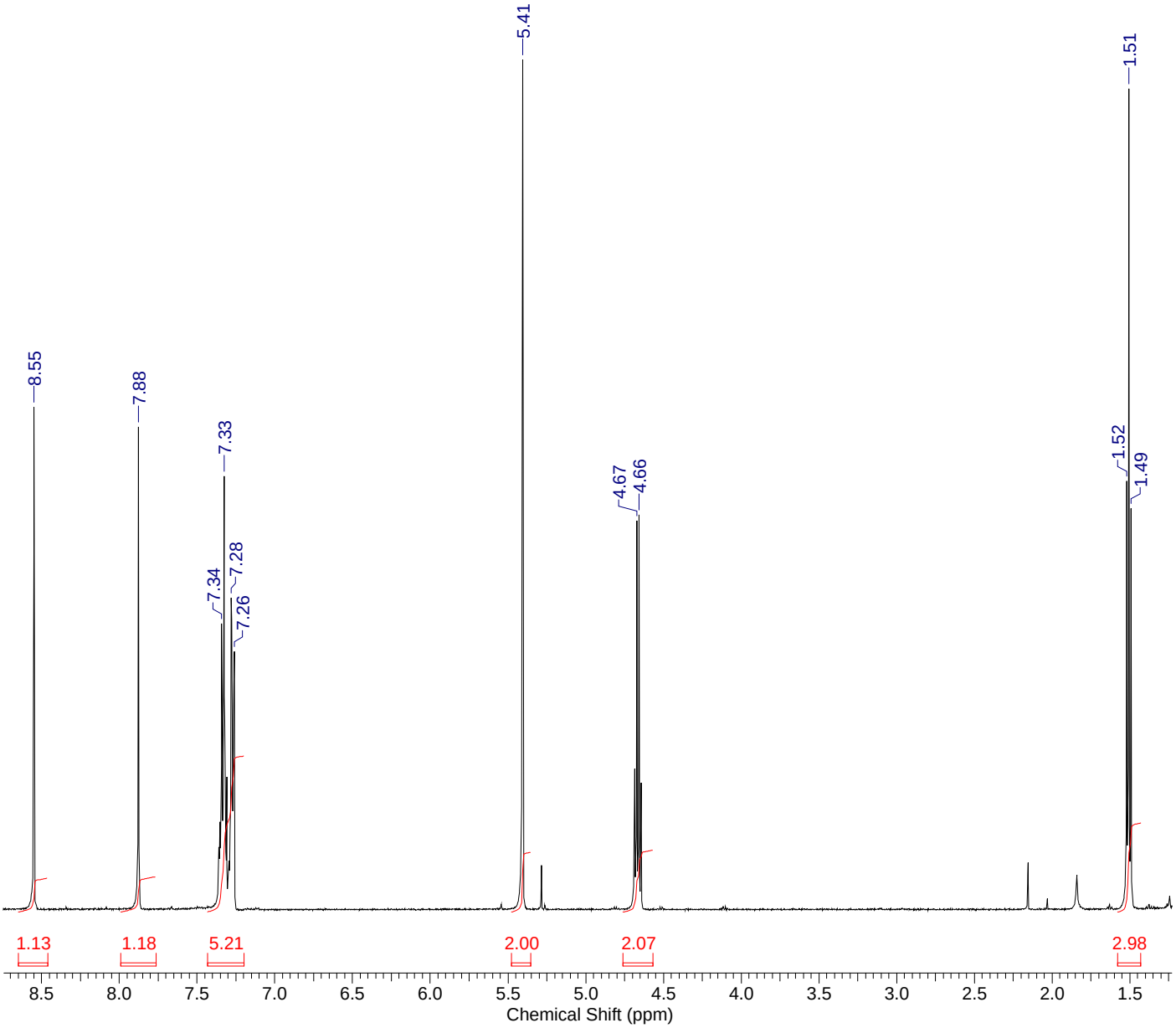


No.	(ppm)	(Hz)	Height
1	15.22	1913.4	0.1727
2	21.23	2667.8	0.5761
3	48.35	6077.3	0.2229
4	68.06	8554.1	0.4096
5	76.75	9646.1	0.8368
6	77.01	9678.5	1.0000
7	77.26	9710.0	0.8358
8	120.73	15173.7	0.0292
9	127.98	16085.5	0.1738
10	128.35	16132.2	0.6845
11	128.43	16141.7	0.5959
12	136.42	17146.0	0.0365
13	150.41	18903.7	0.2798
14	150.69	18939.9	0.0444
15	159.41	20035.7	0.0507

5f. - 9-Benzyl-6-ethoxy-9H-purine (H-NMR)

12 Jul 2012

Acquisition Time (sec)	1.7432	***Date***	Mar 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-776_ASIMJ-7\proton				
Frequency (MHz)	499.79	***Nucleus***	1H	***Number of Transients***	1
Original Points Count	13048	***Points Count***	16384	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	7485.03
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.49	745.6	0.4736
2	1.51	752.9	0.9656
3	1.52	759.8	0.5060
4	4.66	2327.8	0.4660
5	4.67	2334.6	0.4591
6	5.41	2701.5	1.0000
7	7.26	3629.0	0.3060
8	7.28	3639.0	0.3686
9	7.33	3661.9	0.5110
10	7.34	3669.2	0.3384
11	7.88	3936.0	0.5694
12	8.55	4272.3	0.5924

No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.58]	2.977	1.96327e+7
2	[4.57 .. 4.76]	2.071	1.36568e+7
3	[5.35 .. 5.48]	2.000	1.31902e+7
4	[7.20 .. 7.43]	5.210	3.43629e+7
5	[7.76 .. 7.99]	1.182	7.79846e+6
6	[8.46 .. 8.65]	1.134	7.47657e+6

5f. - 9-Benzyl-6-ethoxy-9H-purine (MS)

Elemental Composition Report

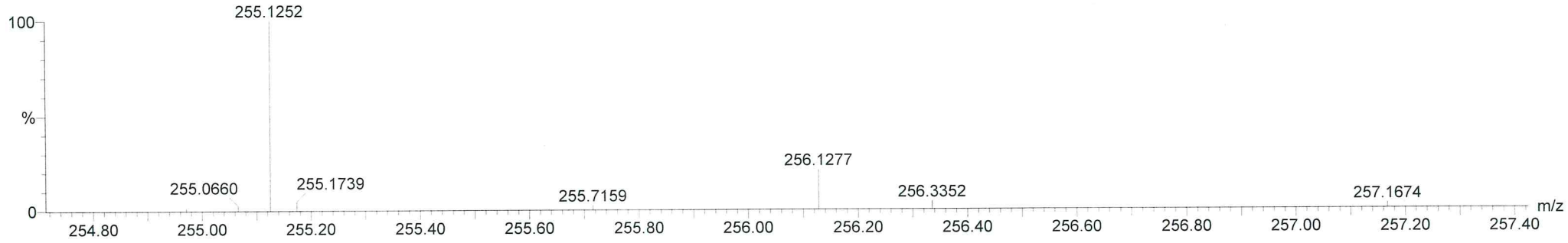
Single Mass Analysis

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

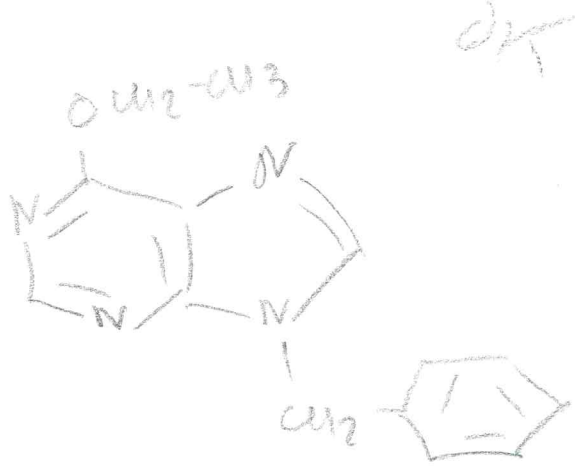
Monoisotopic Mass, Even Electron Ions
1456 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-1000 N: 0-5 O: 0-6 Na: 0-1 S: 0-1 Cl: 0-4

7 173 (3.827)

1: TOF MS ES+
8.63e+001



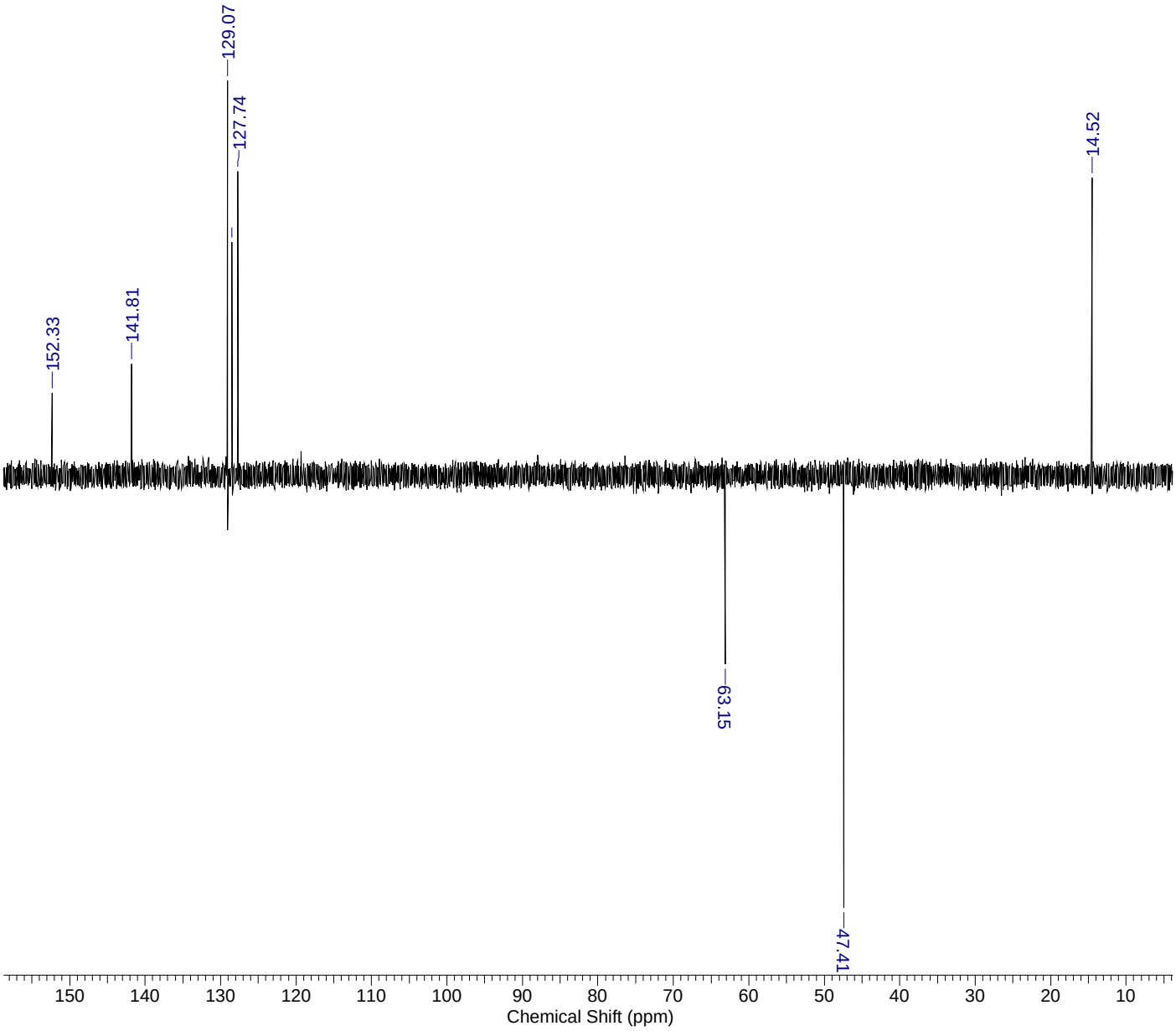
Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
255.1252	255.1246	0.6	2.4	9.5	n/a	C14 H15 N4 O
	255.1256	-0.4	-1.6	1.5	n/a	C9 H20 N4 O Na S
	255.1264	-1.2	-4.7	4.5	n/a	C13 H20 N2 O Cl
	255.1240	1.2	4.7	1.5	n/a	C11 H21 N2 O Na Cl



5f. - 9-Benzyl-6-ethoxy-9H-purine (DEPT)

12 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Mar 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-776_ASIMJ-7\dept				
Frequency (MHz)	125.68	***Nucleus***	13C	***Number of Transients***	16000
Original Points Count	32768	***Points Count***	32768	***Pulse Sequence***	DEPT135
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	31250.00
Temperature (degree C)	25.000				

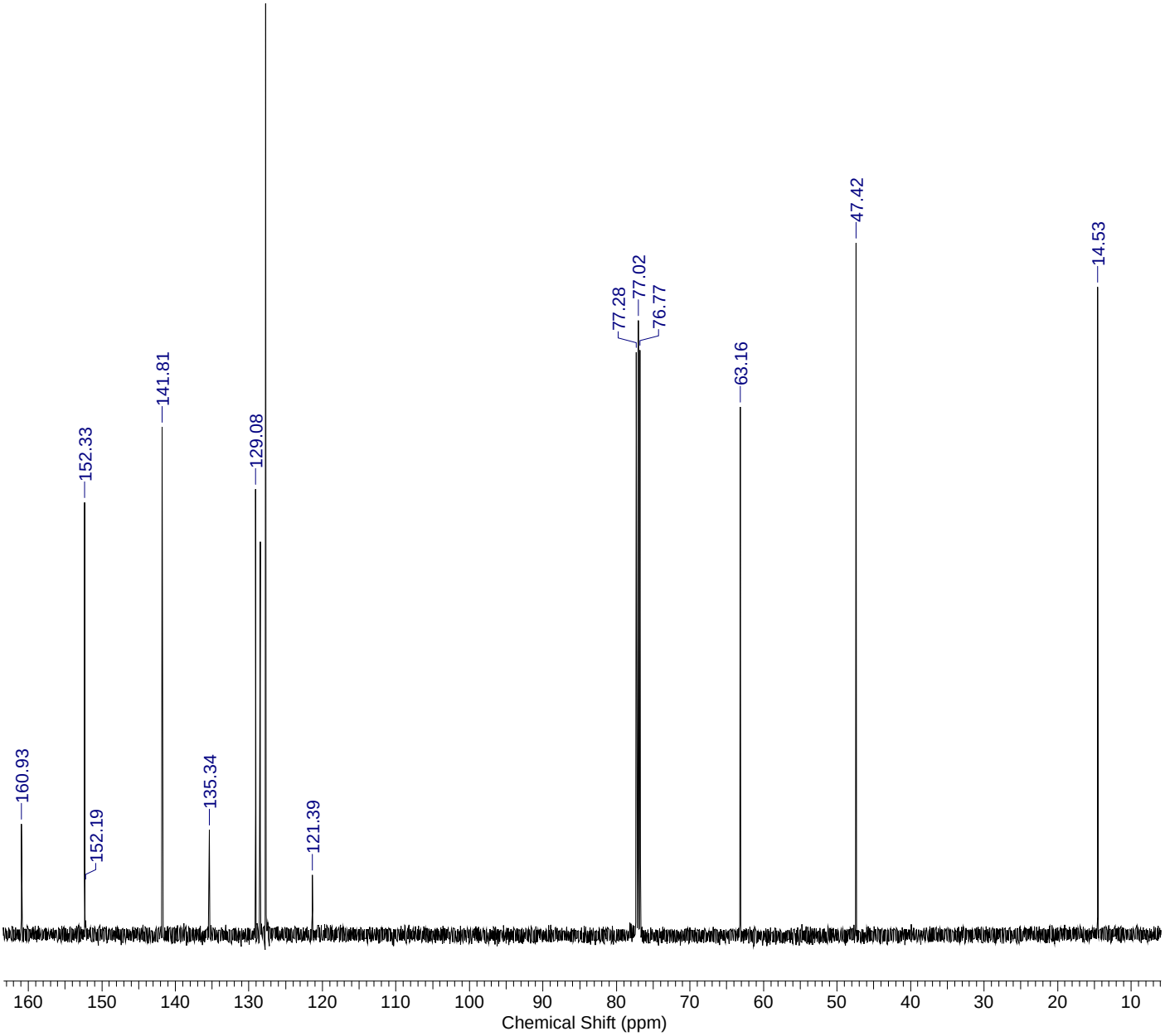


No.	(ppm)	(Hz)	Height
1	14.52	1825.4	0.7533
2	47.41	5958.7	-1.0949
3	63.15	7936.7	-0.4780
4	127.74	16054.6	0.7700
5	128.47	16147.1	0.5904
6	129.07	16222.5	1.0000
7	141.81	17822.8	0.2828
8	152.33	19145.6	0.2094

5f. - 9-Benzyl-6-ethoxy-9H-purine (C-NMR)

12 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Mar 8 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-776_ASIMJ-7\carbono				
Frequency (MHz)	125.68	***Nucleus***	13C	***Original Points Count***	32768
Points Count	32768	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	31250.00	***Temperature (degree C)***	25.000		

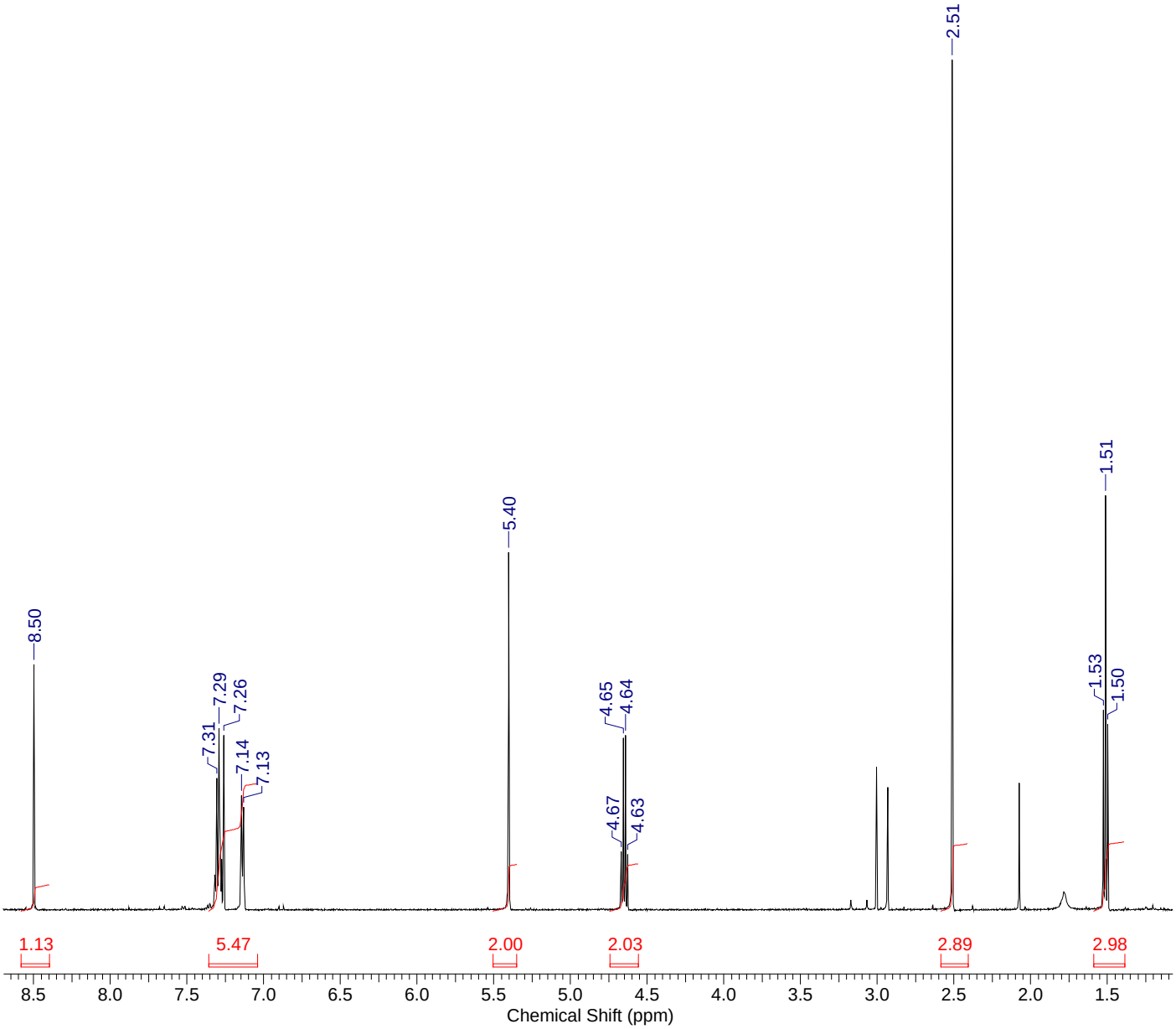


No.	(ppm)	(Hz)	Height
1	14.53	1825.7	0.5283
2	47.42	5960.0	0.5640
3	63.16	7938.0	0.4304
4	76.77	9648.9	0.4766
5	77.02	9680.4	0.5011
6	77.28	9712.8	0.4751
7	121.39	15256.7	0.0480
8	129.08	16223.8	0.3630
9	135.34	17010.6	0.0852
10	141.81	17823.1	0.4137
11	152.19	19127.8	0.0409
12	152.33	19145.9	0.3521
13	160.93	20226.5	0.0896

5g.- 9-Benzyl-6-ethoxy-8-methyl-9H-purine (H-NMR)

12 Jul 2012

Acquisition Time (sec)	1.7432	***Comment***	12-932_ASIMJ-8		
Date	Mar 9 2012	***File Name***	C:\Users\usuario\Documents\Espectros Asier\12-932_ASIMJ-8\proton		
Frequency (MHz)	499.79	***Nucleus***	1H	***Number of Transients***	1
Original Points Count	13048	***Points Count***	16384	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	7485.03
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	1.50	748.4	0.2200
2	1.51	755.2	0.4884
3	1.53	762.5	0.2364
4	2.51	1255.0	1.0000
5	4.63	2312.7	0.0667
6	4.64	2319.6	0.2066
7	4.65	2326.4	0.2036
8	4.67	2333.7	0.0700
9	5.40	2700.6	0.4217
10	7.13	3564.1	0.1221
11	7.14	3570.9	0.1359
12	7.26	3629.0	0.2067
13	7.29	3644.0	0.2149
14	7.31	3651.4	0.1564
15	8.50	4247.1	0.2897

No.	(ppm)	Value	Absolute Value
1	[1.39 .. 1.59]	2.976	8.15960e+6
2	[2.41 .. 2.59]	2.892	7.92848e+6
3	[4.56 .. 4.74]	2.033	5.57444e+6
4	[5.35 .. 5.51]	2.000	5.48381e+6
5	[7.04 .. 7.36]	5.470	1.49981e+7
6	[8.40 .. 8.58]	1.129	3.09530e+6

5g.- 9-Benzyl-6-ethoxy-8-methyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

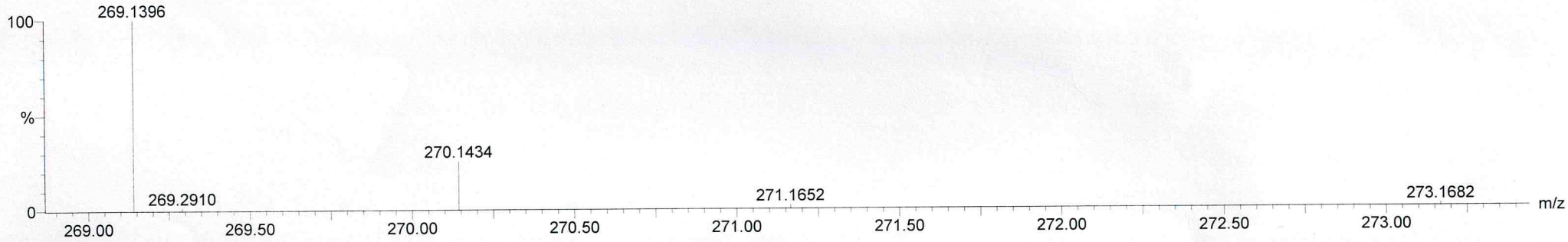
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1585 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-1000 N: 0-5 O: 0-6 Na: 0-1 S: 0-1 Cl: 0-4

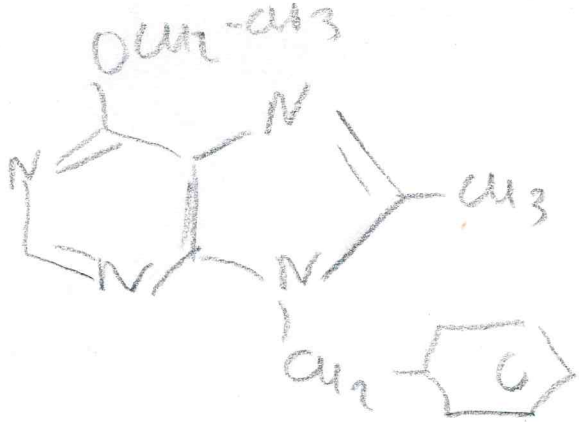
12/932 8

8 9 (0.212)

1: TOF MS ES+
6.73e+002



Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.1396	269.1402	-0.6	-2.2	9.5	6.0	C15 H17 N4 O
	269.1389	0.7	2.6	4.5	11.4	C14 H21 O5
	269.1397	-0.1	-0.4	1.5	n/a	C12 H23 N2 O Na Cl

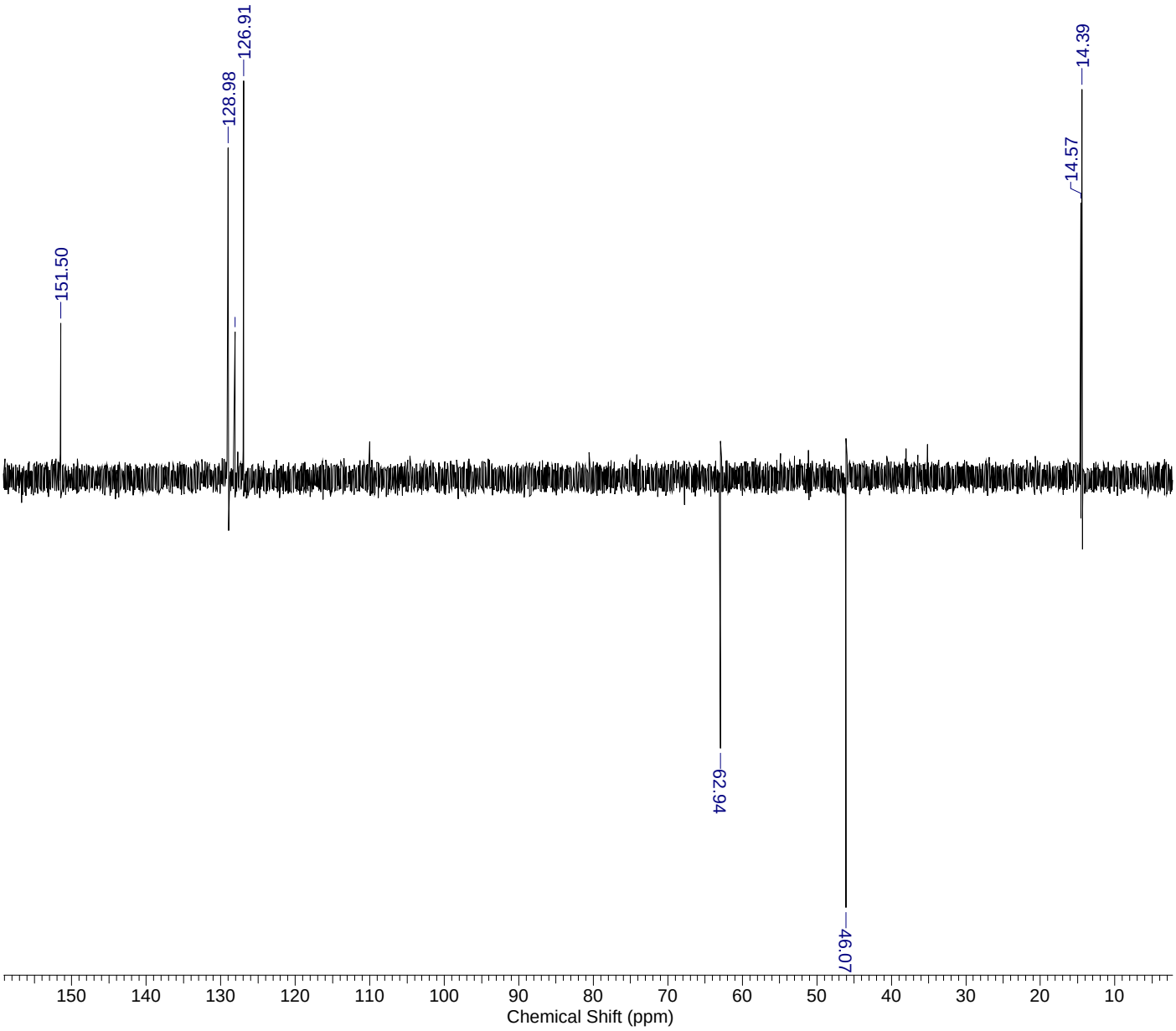


OK!

5g.- 9-Benzyl-6-ethoxy-8-methyl-9H-purine (DEPT)

13 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Mar 9 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-932_ASIMJ-8\dept				
Frequency (MHz)	125.68	***Nucleus***	13C	***Number of Transients***	16000
Original Points Count	32768	***Points Count***	32768	***Pulse Sequence***	DEPT135
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	31250.00
Temperature (degree C)	25.000				

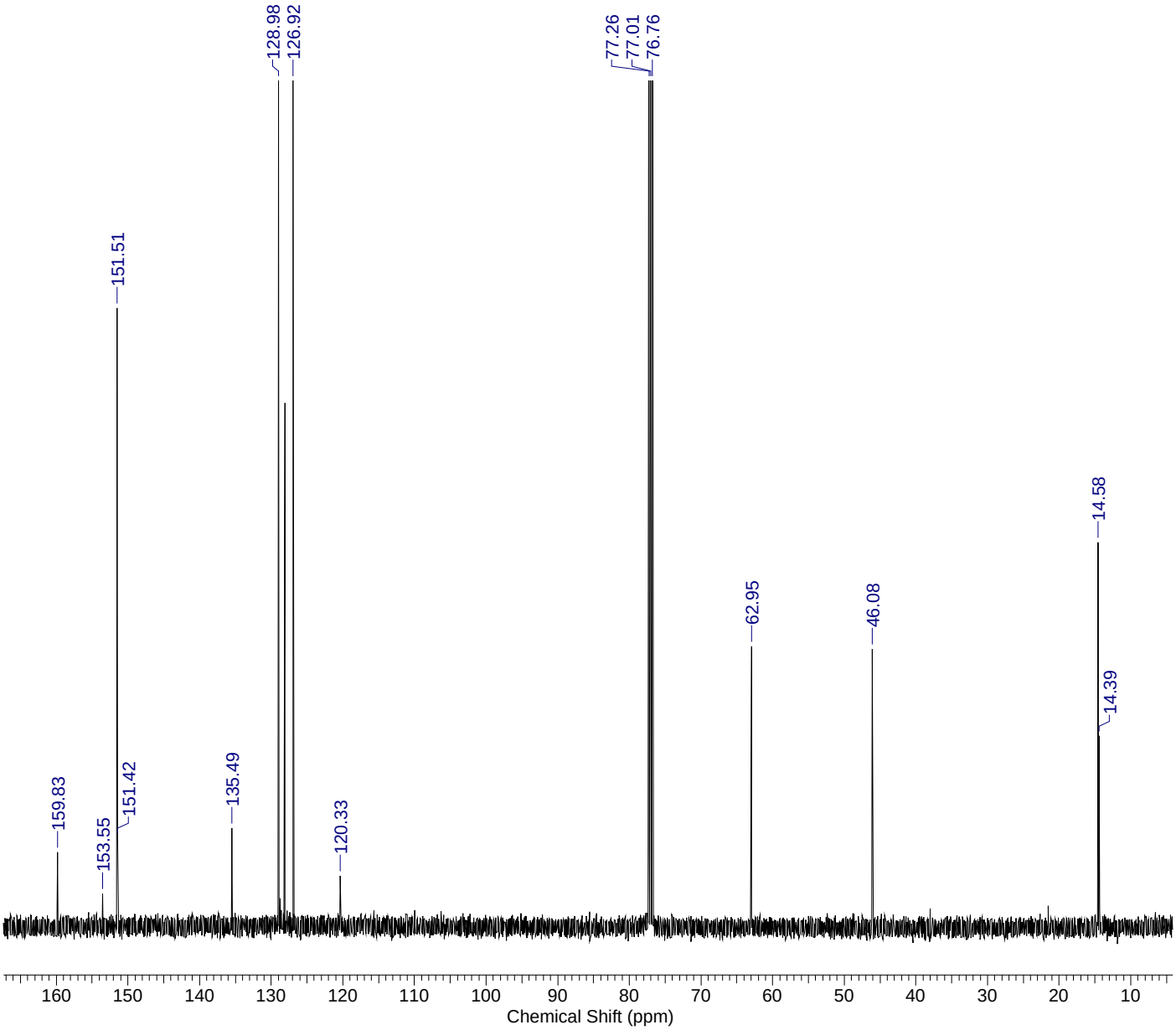


No.	(ppm)	(Hz)	Height
1	14.39	1808.2	0.9785
2	14.57	1831.1	0.6915
3	46.07	5790.8	-1.0822
4	62.94	7910.9	-0.6801
5	126.91	15950.7	1.0000
6	128.10	16100.4	0.3679
7	128.98	16211.0	0.8309
8	151.50	19040.7	0.3892

5g.- 9-Benzyl-6-ethoxy-8-methyl-9H-purine (C-NMR)

13 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Mar 9 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-932_ASIMJ-8\carbono				
Frequency (MHz)	125.68	***Nucleus***	13C	***Number of Transients***	24000
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	14.39	1808.5	0.1595
2	14.58	1832.4	0.3217
3	46.08	5791.2	0.2324
4	62.95	7911.3	0.2345
5	76.76	9647.0	0.9961
6	77.01	9678.5	0.9284
7	77.26	9710.9	0.9758
8	120.33	15124.1	0.0419
9	126.92	15952.0	0.8726
10	128.98	16211.4	1.0000
11	135.49	17029.6	0.0823
12	151.42	19031.5	0.0738
13	151.51	19042.0	0.5181
14	153.55	19299.5	0.0270
15	159.83	20088.2	0.0619

5h. - 9-Benzyl-6-ethoxy-8-ethyl-9H-purine(MS)

Elemental Composition Report

Single Mass Analysis

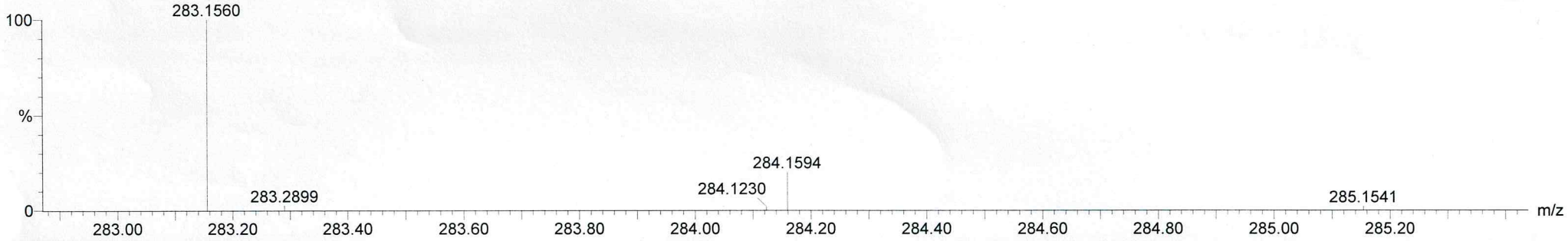
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1687 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-1000 N: 0-5 O: 0-6 Na: 0-1 S: 0-1 Cl: 0-4

9-2 9 (0.212)

1: TOF MS ES+

2.55e+002

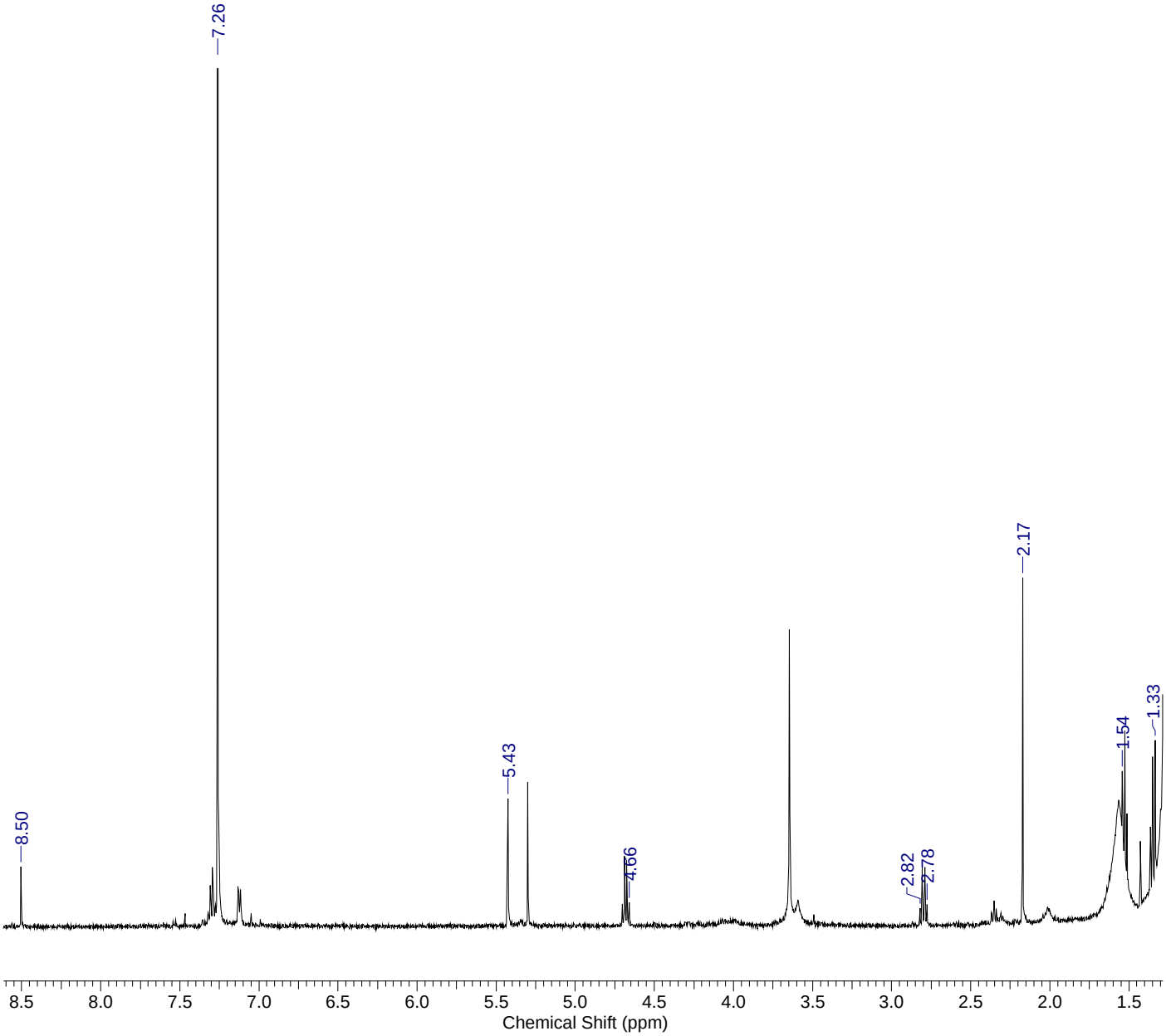


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.1560	283.1559	0.1	0.4	9.5	0.0	C16 H19 N4 O
	283.1569	-0.9	-3.2	1.5	10.1	C11 H24 N4 O Na S
	283.1553	0.7	2.5	1.5	113.7	C13 H25 N2 O Na Cl

5h. - 9-Benzyl-6-ethoxy-8-ethyl-9H-purine(H-NMR)

13 Jul 2012

Acquisition Time (sec)	1.7432	***Date***	Mar 16 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\ASIMJ-9-b			***Frequency (MHz)***	499.79
Nucleus	1H	***Number of Transients***	80	***Original Points Count***	13048
Points Count	16384	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	7485.03	***Temperature (degree C)***	25.000		

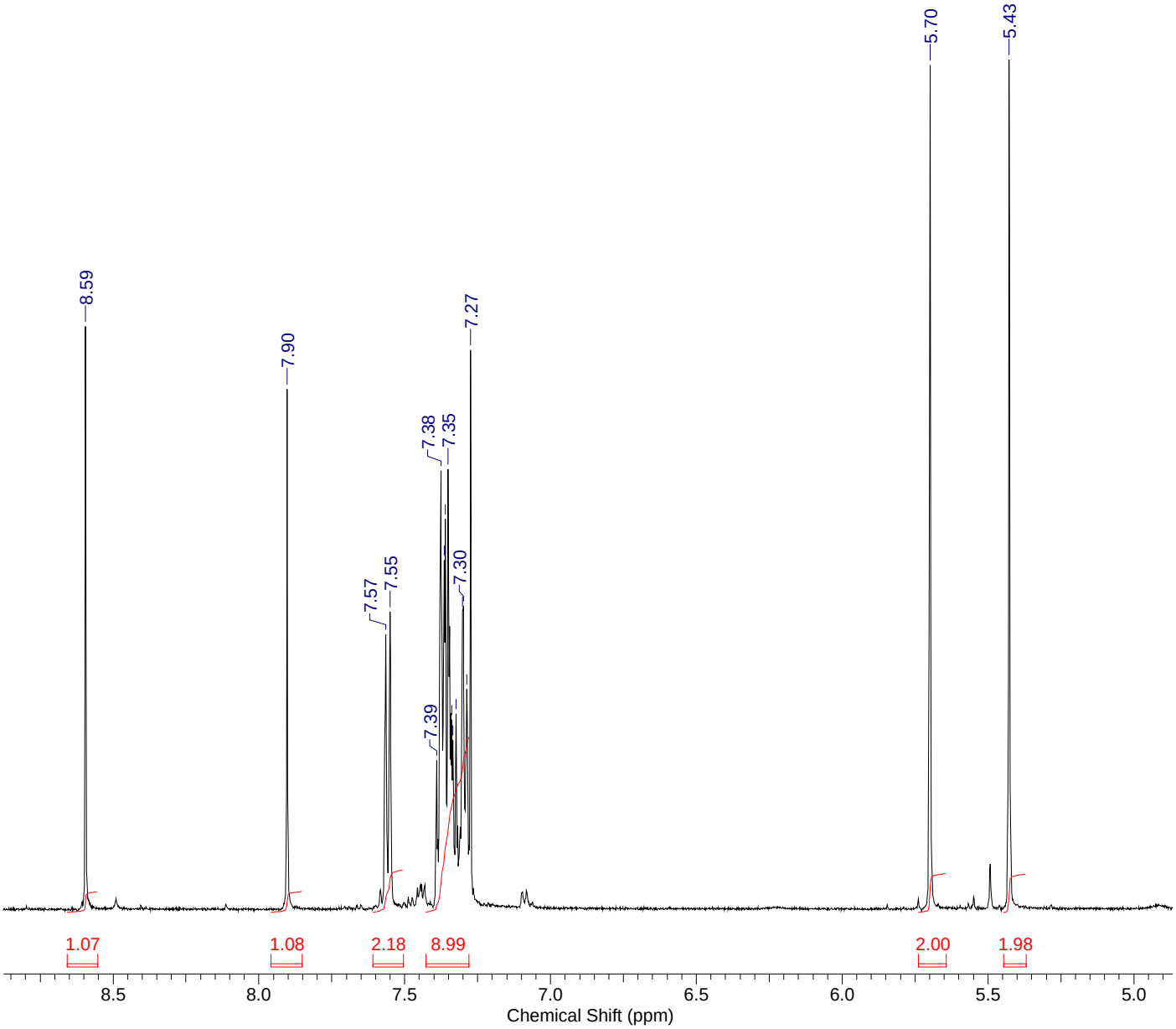


No.	(ppm)	(Hz)	Height
1	1.33	666.6	0.0980
2	1.54	770.3	0.0824
3	2.17	1085.5	0.1798
4	2.78	1387.1	0.0154
5	2.82	1409.5	0.0133
6	4.66	2328.7	0.0164
7	5.43	2712.0	0.0685
8	7.26	3629.0	1.0000
9	8.50	4250.3	0.0342

5i- 9-Benzyl-6-(benzyloxy)-9H-purine (H-NMR)

13 Jul 2012

Acquisition Time (sec)	1.7432	***Date***	Mar 22 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-2550_ASIMJ-11\proton				
Frequency (MHz)	499.79	***Nucleus***	1H	***Number of Transients***	1
Original Points Count	13048	***Points Count***	16384	***Pulse Sequence***	s2pul
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	7485.03
Temperature (degree C)	25.000				



No.	(ppm)	(Hz)	Height
1	5.43	2712.3	1.0000
2	5.70	2848.0	0.9935
3	7.27	3635.2	0.6594
4	7.29	3642.1	0.2619
5	7.30	3648.0	0.3593
6	7.30	3649.8	0.3531
7	7.32	3660.8	0.2326
8	7.33	3665.8	0.2023
9	7.34	3668.1	0.2262
10	7.35	3674.1	0.5198
11	7.36	3679.1	0.4614
12	7.36	3680.9	0.4127
13	7.38	3686.4	0.5180
14	7.39	3693.2	0.1784
15	7.55	3773.7	0.3524
16	7.57	3781.0	0.3259
17	7.90	3950.0	0.6136
18	8.59	4295.4	0.6872

No.	(ppm)	Value	Absolute Value
1	[5.37 .. 5.45]	1.977	1.29501e+6
2	[5.64 .. 5.74]	2.000	1.30998e+6
3	[7.28 .. 7.43]	8.993	5.89047e+6
4	[7.50 .. 7.61]	2.181	1.42841e+6
5	[7.85 .. 7.96]	1.076	7.04517e+5
6	[8.55 .. 8.66]	1.066	6.97998e+5

5i- 9-Benzyl-6-(benzyloxy)-9H-purine (MS)

Elemental Composition Report

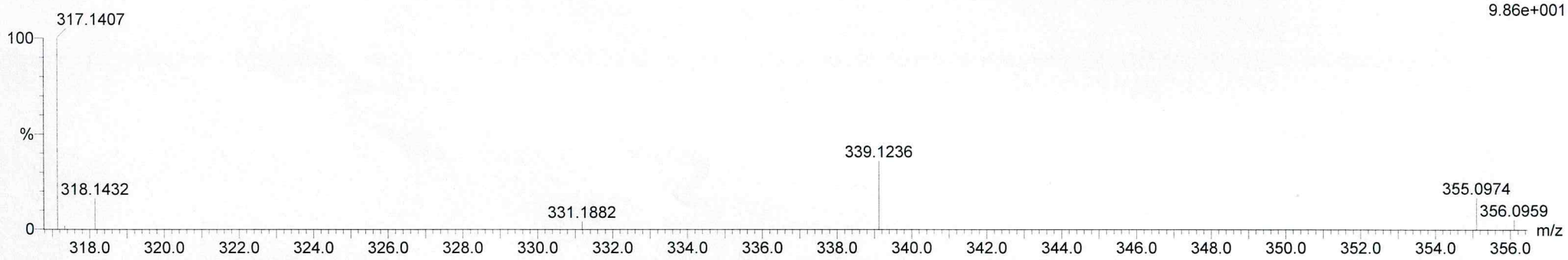
Single Mass Analysis

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
573 formula(e) evaluated with 3 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

ASIMJ-11 9 (0.217)

1: TOF MS ES+

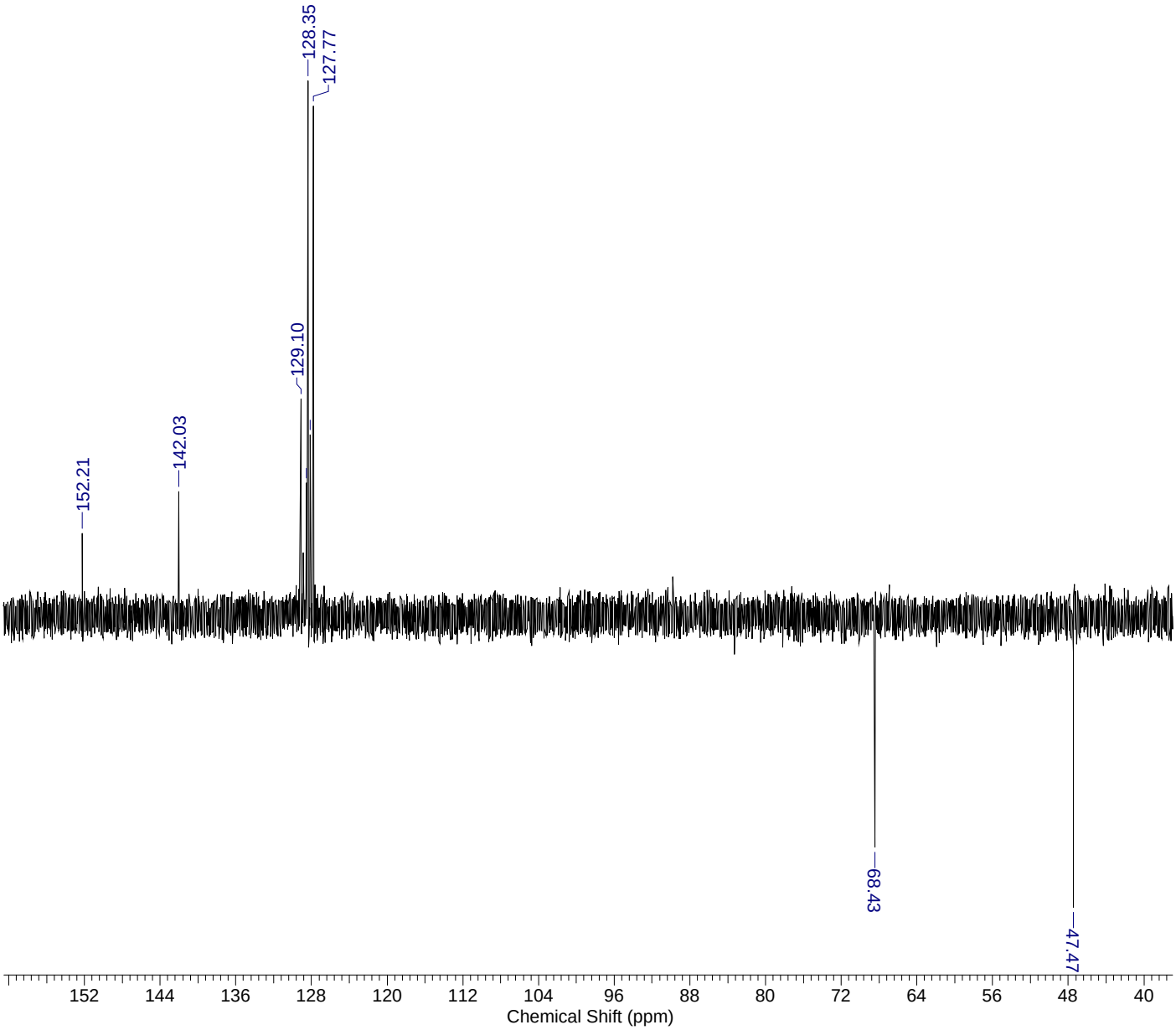


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
317.1407	317.1414	-0.7	-2.2	9.5	n/a	C16 H18 N4 O2 F
	317.1400	0.7	2.2	4.5	n/a	C15 H22 O6 F
	317.1402	0.5	1.6	13.5	n/a	C19 H17 N4 O

5i- 9-Benzyl-6-(benzyloxy)-9H-purine (DEPT)

13 Jul 2012

Acquisition Time (sec)	1.0486	***Date***	Mar 22 2012		
File Name	C:\Users\usuario\Documents\Espectros Asier\12-2550_ASIMJ-11\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				

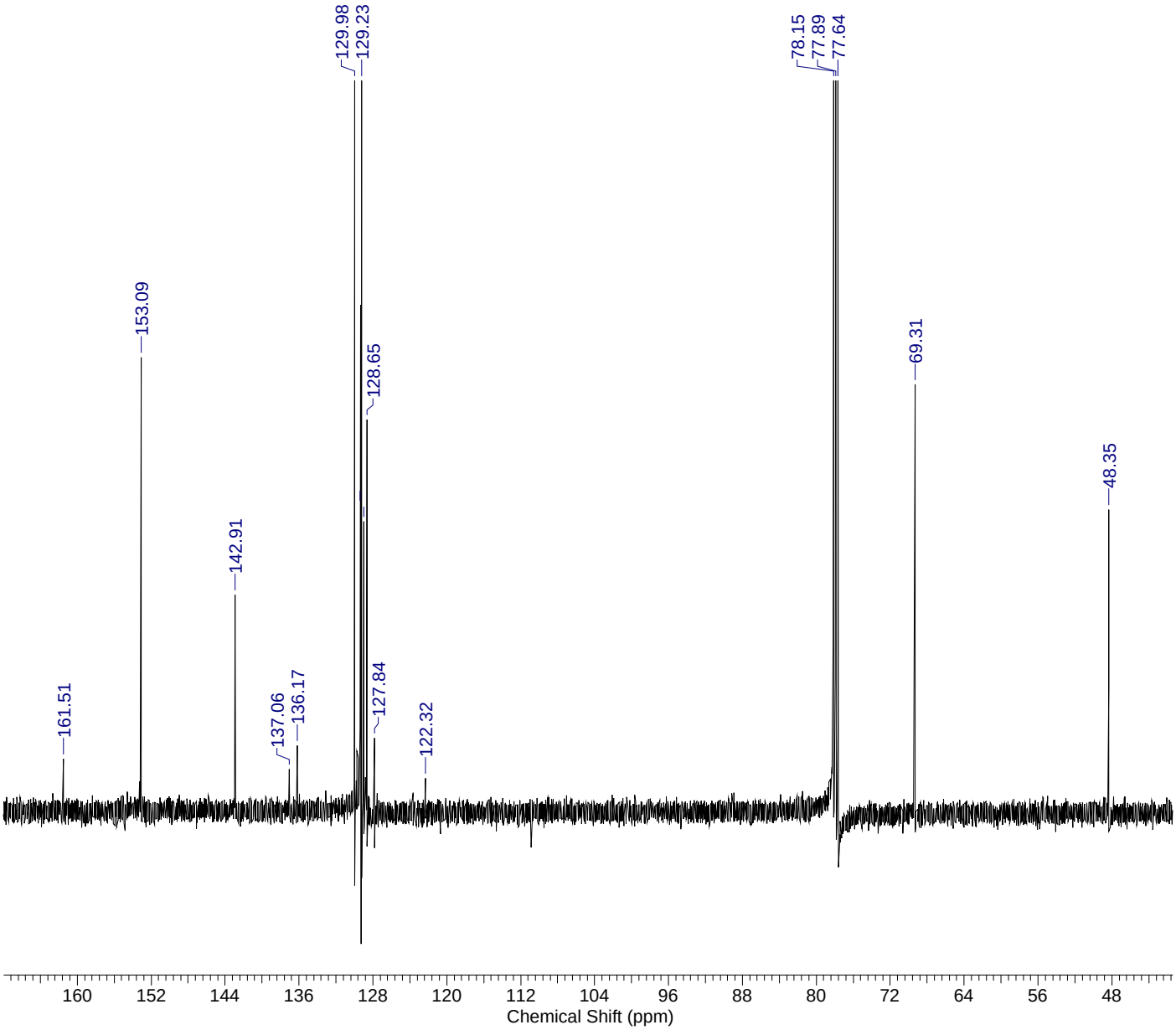


No.	(ppm)	(Hz)	Height
1	47.47	5966.3	-0.5445
2	68.43	8600.5	-0.4322
3	127.77	16058.4	0.9520
4	128.11	16101.3	0.3392
5	128.35	16131.9	1.0000
6	128.42	16140.4	0.3473
7	128.51	16151.9	0.2487
8	129.10	16226.3	0.4056
9	142.03	17850.4	0.2332
10	152.21	19130.3	0.1543

5i- 9-Benzyl-6-(benzyloxy)-9H-purine (C-NMR)

13 Jul 2012

Acquisition Time (sec)	1.0486	***Comment***	12-2283_P-1192-2		
Date	Mar 22 2012	***File Name***	C:\Users\usuario\Documents\Espectros Asier\12-2550_ASIMJ-11\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				

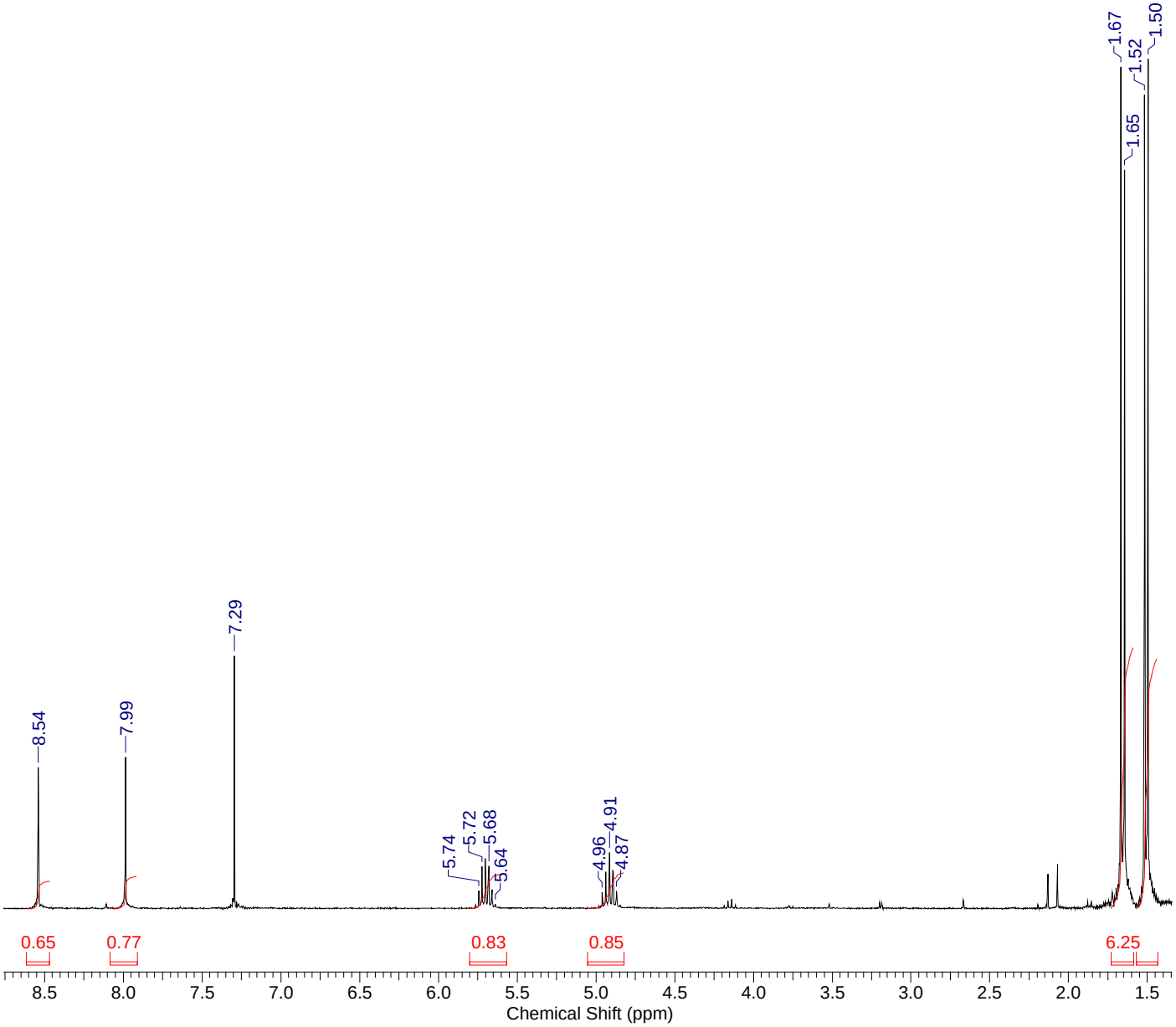


No.	(ppm)	(Hz)	Height
1	48.35	6076.9	0.2799
2	69.31	8711.0	0.3954
3	77.64	9758.2	0.9398
4	77.89	9789.7	1.0000
5	78.15	9822.1	0.9750
6	122.32	15373.6	0.0301
7	127.84	16067.9	0.0676
8	128.65	16170.0	0.3631
9	128.99	16211.9	0.2688
10	129.23	16242.4	0.7733
11	129.31	16252.0	0.4697
12	129.40	16263.4	0.2837
13	129.98	16336.9	0.6977
14	136.17	17115.1	0.0606
15	137.06	17226.7	0.0387
16	142.91	17961.0	0.2006
17	153.09	19240.9	0.4209
18	161.51	20299.5	0.0482

5j. - 6-Isopropoxy-9-isopropyl-9H-purine (H-NMR)

13 Jul 2012

Acquisition Time (sec)	2.0487	***Comment***	ASIMJ-16	***Date***	May 2 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-7088_ASIMJ-16\1H-ASI-MJ-16				
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	1.50	449.2	1.0000
2	1.52	455.4	0.9576
3	1.65	494.1	0.8691
4	1.67	500.7	0.9903
5	4.87	1461.6	0.0207
6	4.91	1475.3	0.0659
7	4.96	1488.9	0.0192
8	5.64	1693.0	0.0050
9	5.68	1705.3	0.0499
10	5.72	1718.0	0.0497
11	5.74	1724.2	0.0212
12	7.29	2189.5	0.2972
13	7.99	2397.5	0.1783
14	8.54	2563.3	0.1663

No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.57]	6.000	3.31244e+8
2	[1.59 .. 1.73]	6.250	3.45021e+8
3	[4.82 .. 5.05]	0.853	4.70811e+7
4	[5.57 .. 5.80]	0.833	4.59729e+7
5	[7.91 .. 8.08]	0.767	4.23590e+7
6	[8.47 .. 8.61]	0.650	3.58623e+7

5j. - 6-Isopropoxy-9-isopropyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

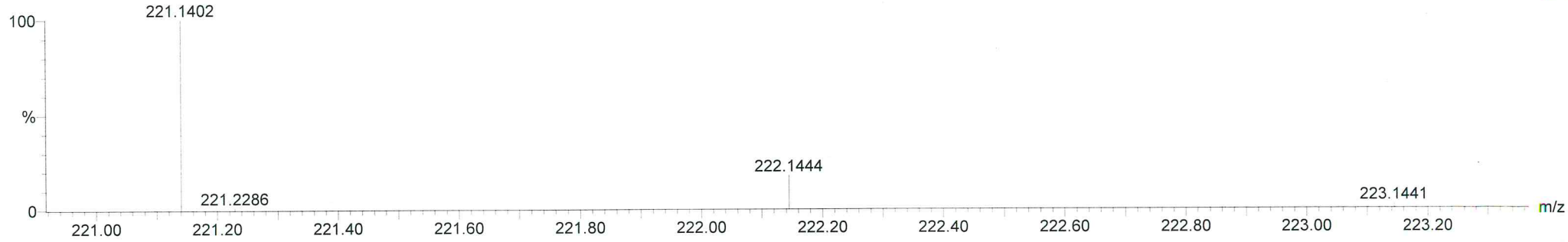
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
422 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-15 H: 0-1000 N: 0-10 O: 0-10 Na: 0-1

12/7270

ASIMJ-16 69 (1.534)

1: TOF MS ES+
3.64e+002

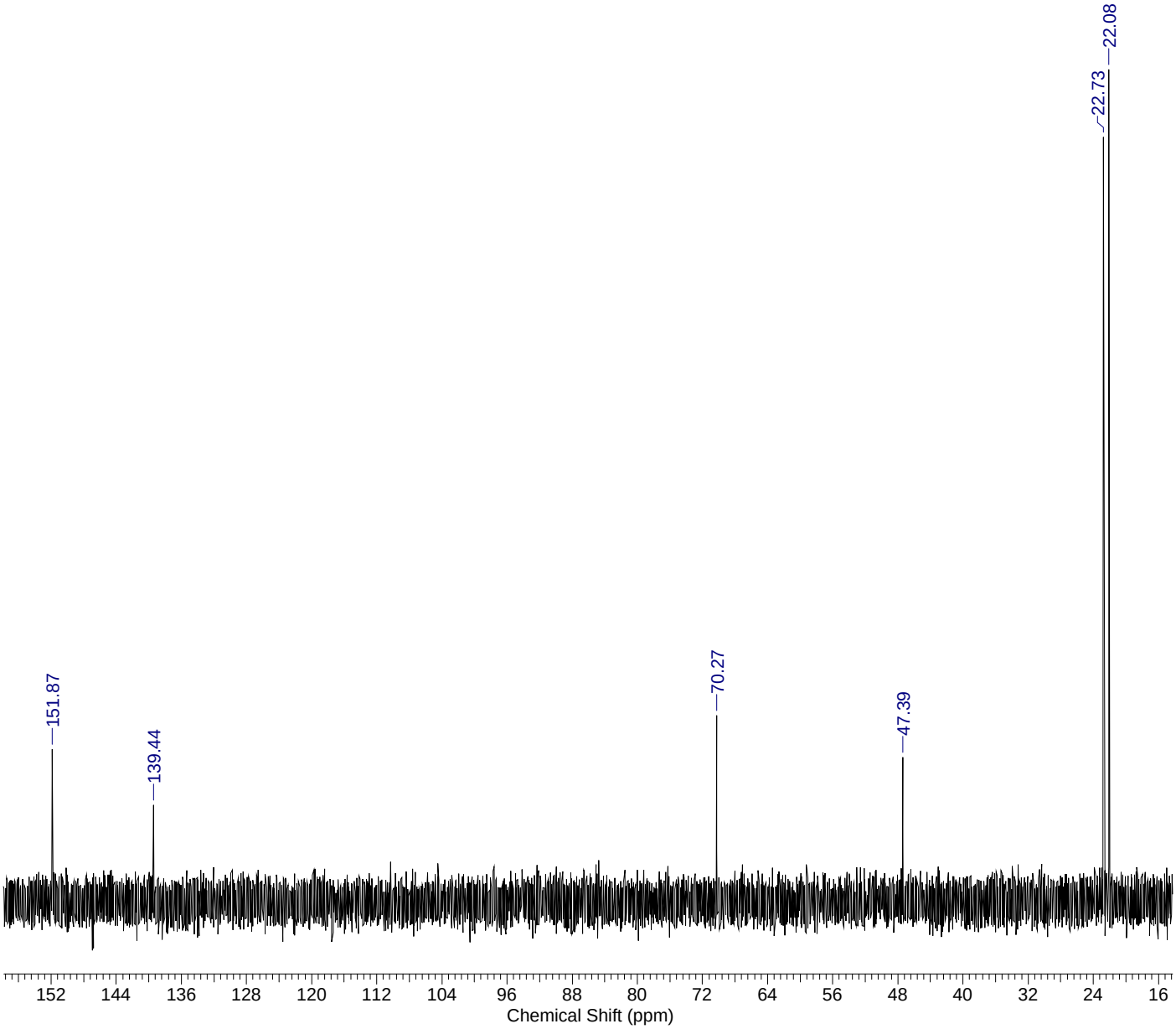


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1402	221.1402	0.0	0.0	5.5	2.0	C11 H17 N4 O

5j. - 6-Isopropoxy-9-isopropyl-9H-purine (DEPT)

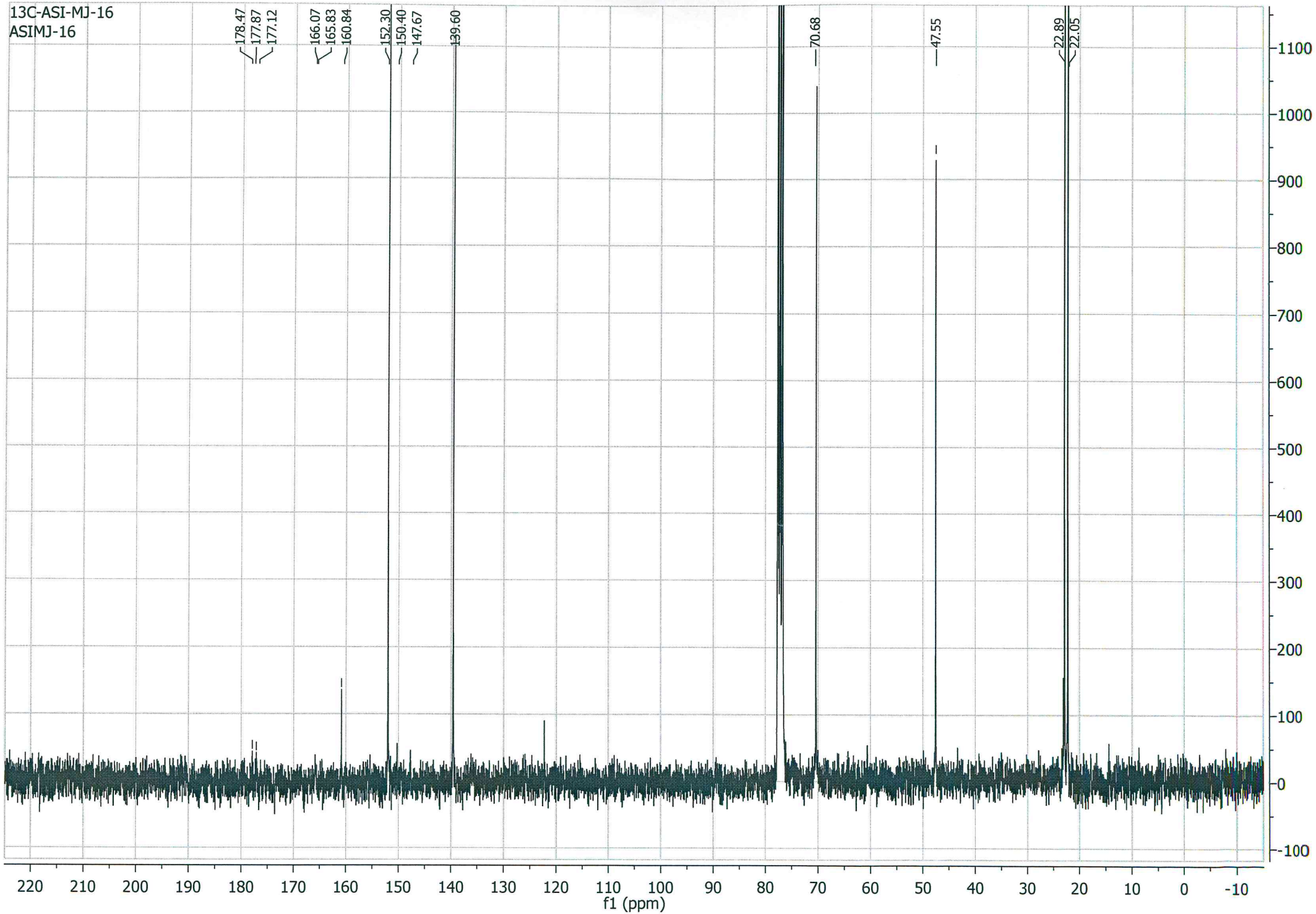
13 Jul 2012

Acquisition Time (sec)	1.0000	***Comment***	ASIMJ-16	***Date***	May 2 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-7088_ASIMJ-16\DEPT-ASI-MJ-16				
Frequency (MHz)	75.49	***Nucleus***	13C	***Number of Transients***	2000
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	22.08	1667.2	1.0000
2	22.73	1715.8	0.9186
3	47.39	3577.3	0.1738
4	70.27	5305.0	0.2243
5	139.44	10526.9	0.1162
6	151.87	11465.1	0.1832

5j. - 6-Isopropoxy-9-isopropyl-9H-purine (C-NMR)



5k. - 6-Isopropoxy-9-isopropyl-8-methyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

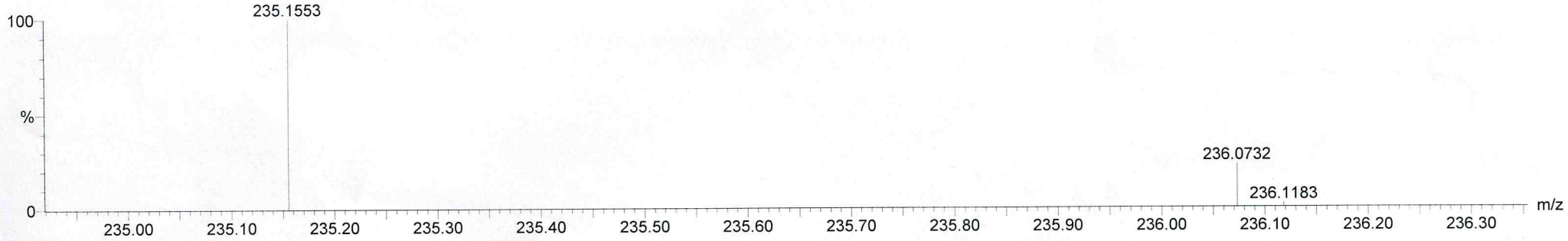
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
463 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-15 H: 0-1000 N: 0-10 O: 0-10 Na: 0-1

ASIMJ-17conc 243 (5.361)

1: TOF MS ES+

3.70e+002

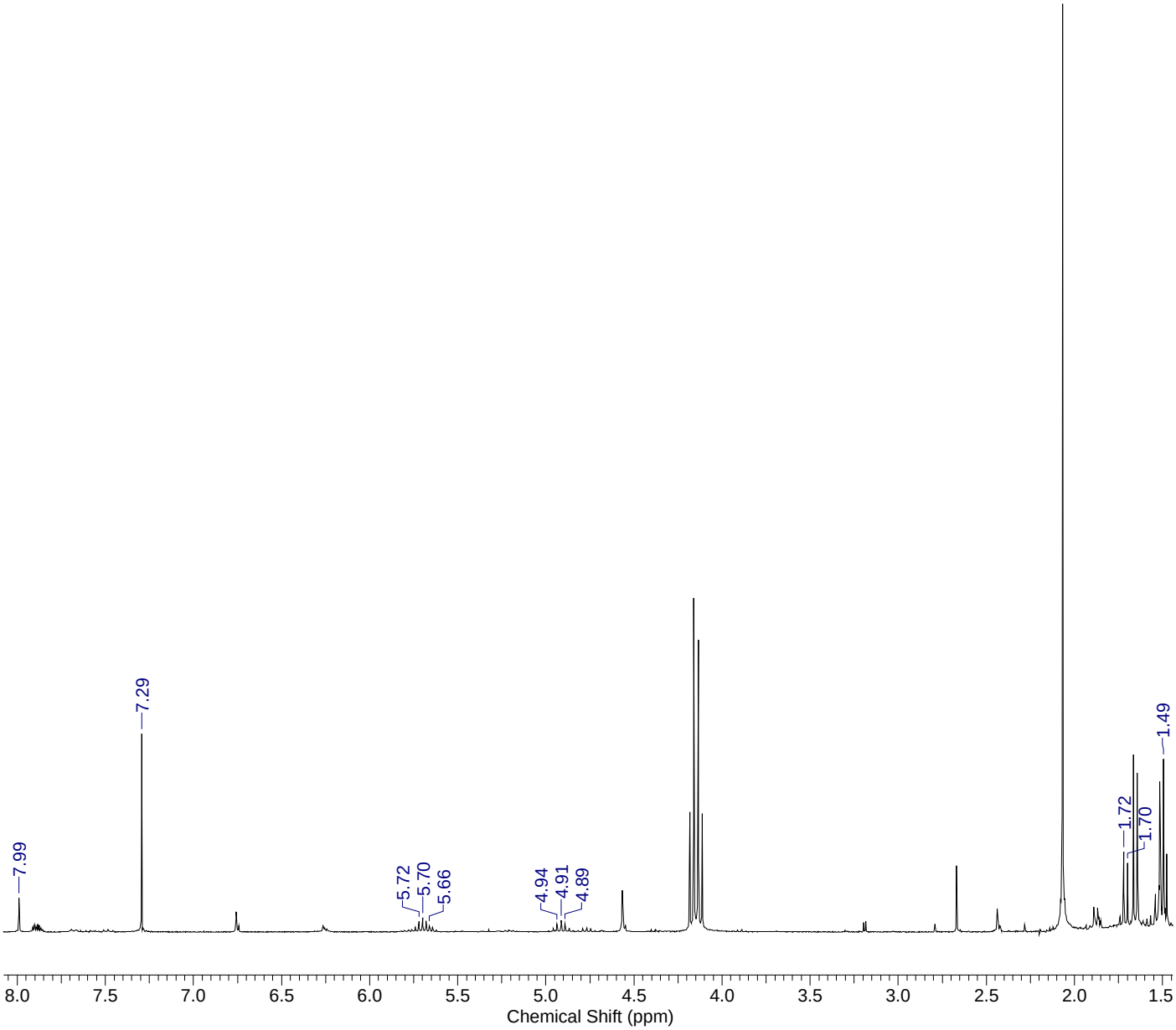


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.1553	235.1559	-0.6	-2.6	5.5	n/a	C12 H19 N4 O
	235.1545	0.8	3.4	0.5	n/a	C11 H23 O5

5k. - 6-Isopropoxy-9-isopropyl-8-methyl-9H-purine (H-NMR)

19 Jul 2012

Acquisition Time (sec)	2.0487	***Comment***	ASIMJ-17	***Date***	May 4 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\1H-ASI-MJ-17				
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	1.49	448.4	0.1083
2	1.70	509.5	0.0433
3	1.72	516.5	0.0502
4	4.89	1468.2	0.0054
5	4.91	1474.8	0.0075
6	4.94	1481.9	0.0049
7	5.66	1700.0	0.0038
8	5.70	1711.0	0.0091
9	5.72	1717.1	0.0065
10	7.29	2189.5	0.1243
11	7.99	2398.4	0.0213

5l. - 6-tert-butoxy-9-isopropyl-9H-purine

Elemental Composition Report

Single Mass Analysis

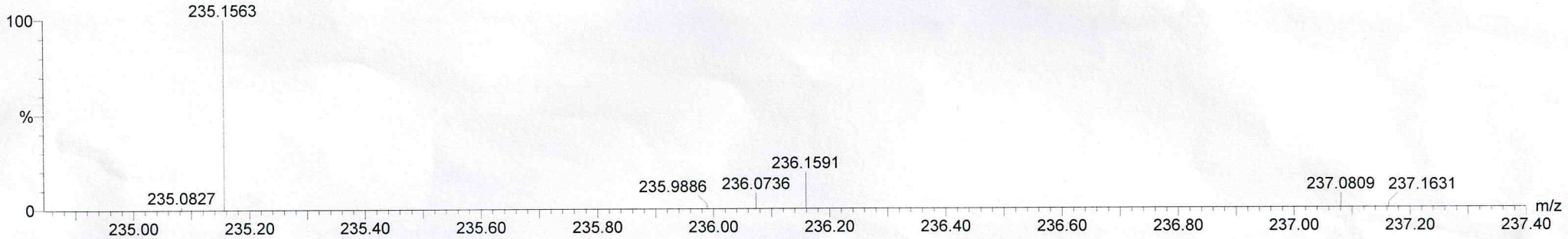
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
618 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 Br: 0-2

ASIMJ-19 62 (1.375)

1: TOF MS ES+

6.92e+002

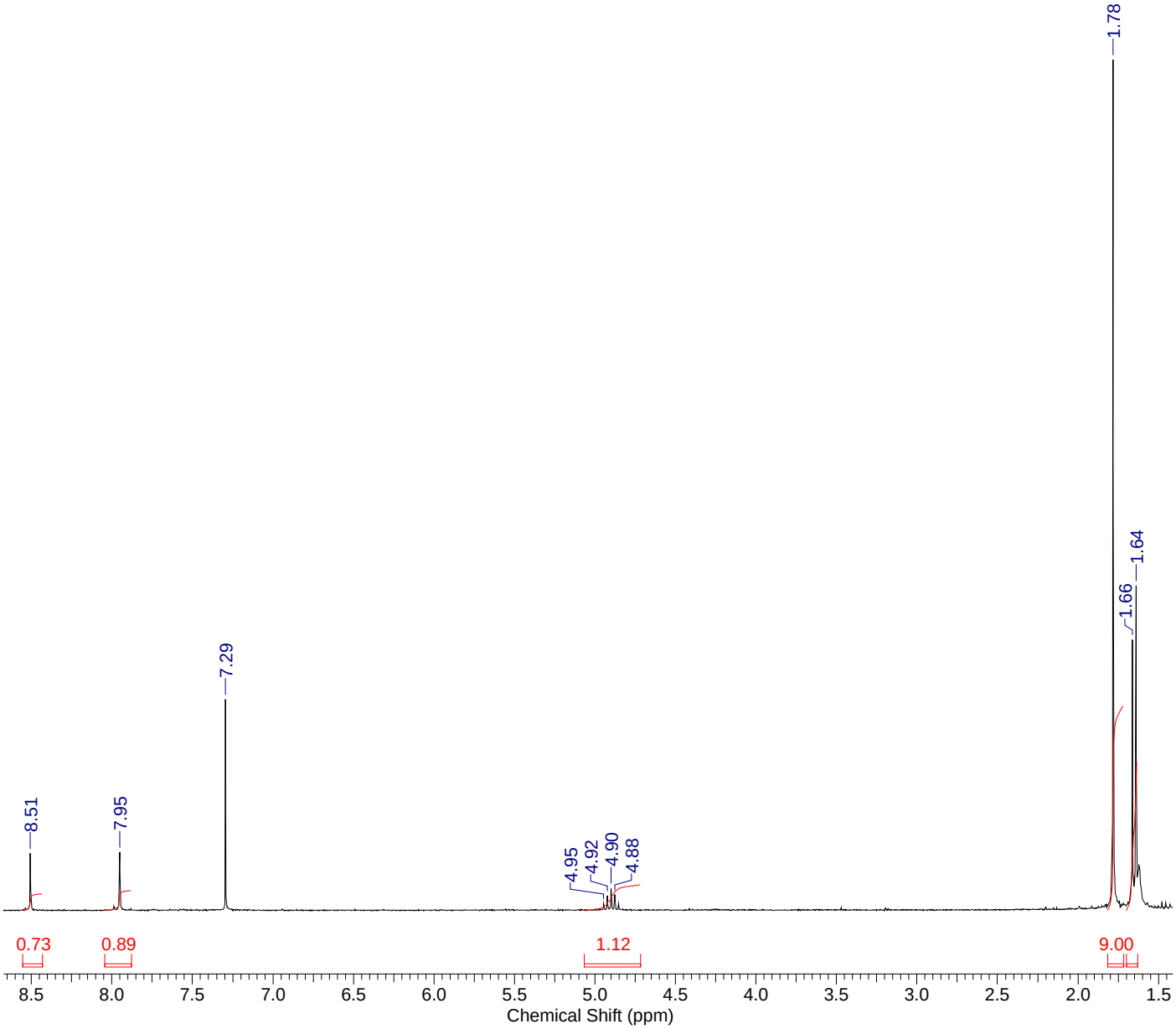


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.1563	235.1559	0.4	1.7	5.5	3.8	C12 H19 N4 O

5l. - 6-tert-butoxy-9-isopropyl-9H-purine (H-NMR)

16 Jul 2012

Acquisition Time (sec)	2.0487	***Comment***	ASIMJ-19	***Date***	May 10 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\1H-ASI-MJ-19				
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	1.64	492.3	0.3819
2	1.66	499.4	0.3184
3	1.78	535.0	1.0000
4	4.88	1464.3	0.0184
5	4.90	1470.9	0.0260
6	4.92	1477.9	0.0176
7	4.95	1484.5	0.0081
8	7.29	2189.5	0.2480
9	7.95	2387.4	0.0686
10	8.51	2554.1	0.0673

No.	(ppm)	Value	Absolute Value
1	[1.63 .. 1.70]	6.904	3.95374e+8
2	[1.72 .. 1.82]	9.000	5.15413e+8
3	[4.72 .. 5.07]	1.118	6.40499e+7
4	[7.88 .. 8.04]	0.889	5.09284e+7
5	[8.43 .. 8.55]	0.728	4.16779e+7

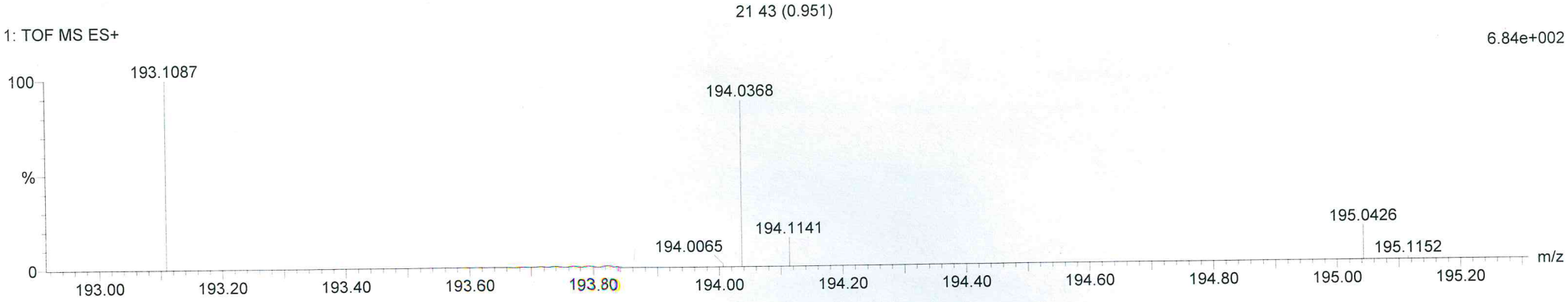
5m. - 9-isopropyl-6-methoxy-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

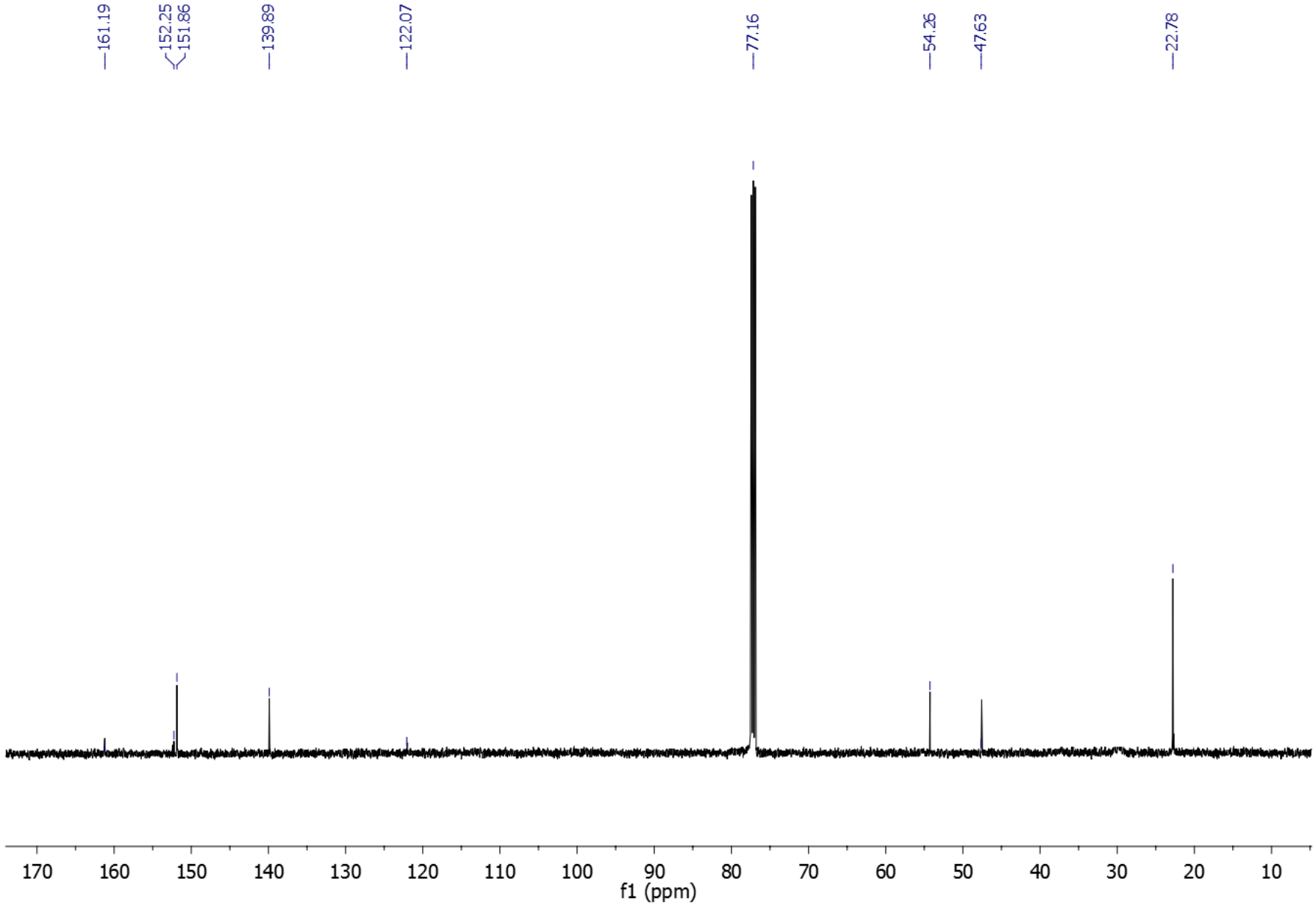
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

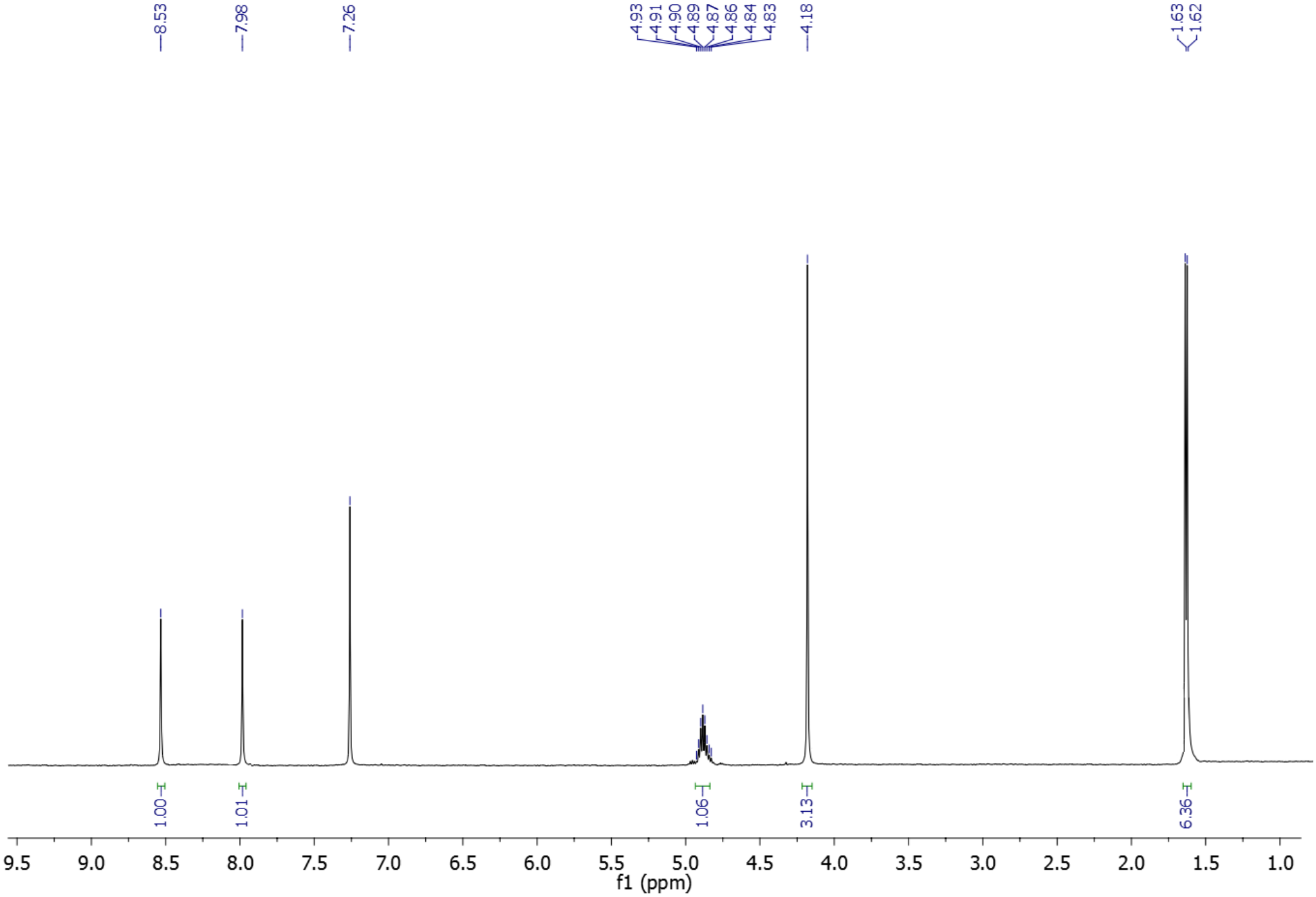


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
193.1087	193.1089	-0.2	-1.0	5.5	2.7	C9 H13 N4 O

5m. - 9-isopropyl-6-methoxy-9H-purine (C-NMR)



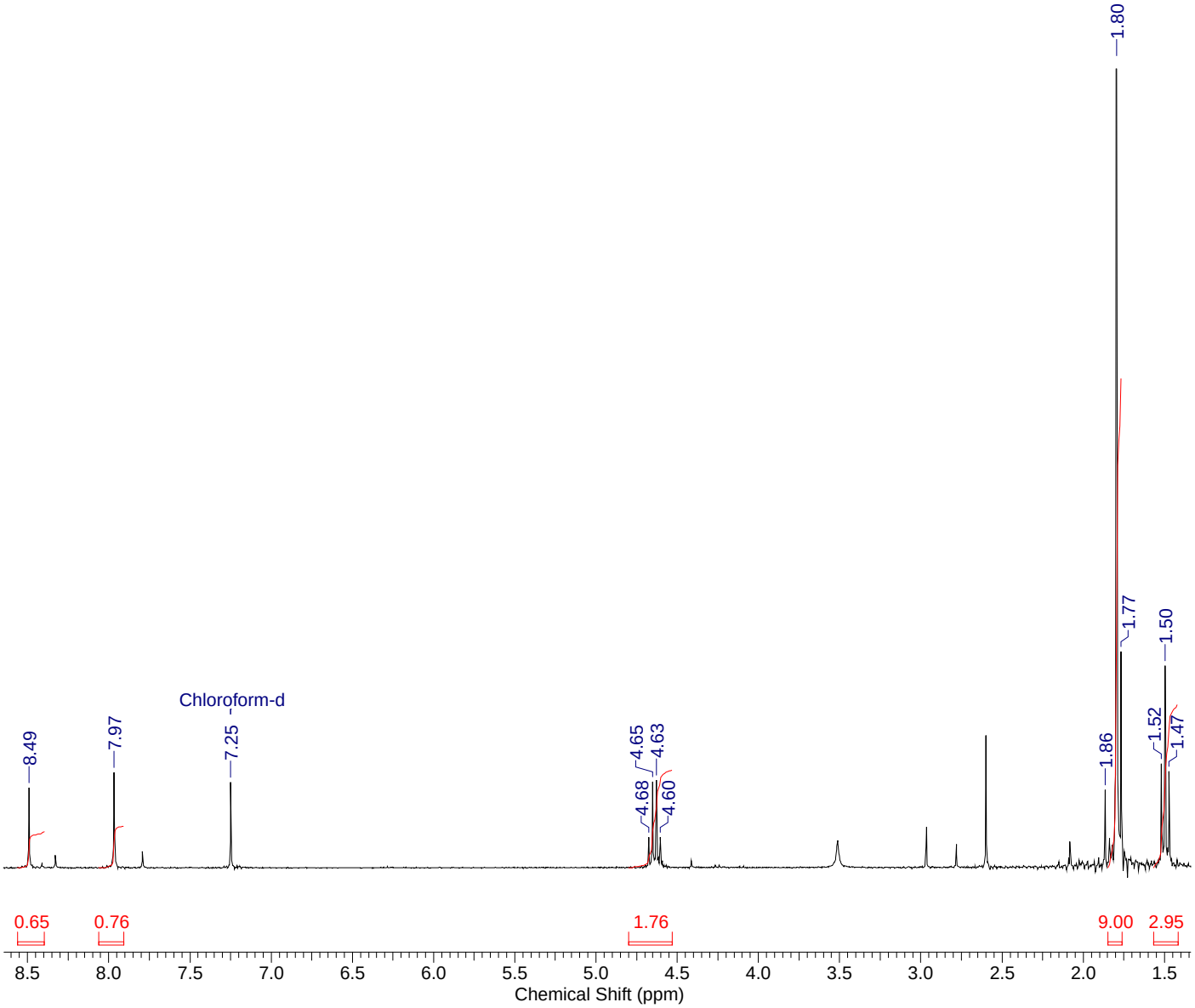
5m. - 9-isopropyl-6-methoxy-9H-purine (H-NMR)



5n. - 9-tert-butyl-6-ethoxy-9H-purine (H-NMR)

11 Mar 2013

Acquisition Time (sec)	2.0486	***Comment***	ASIMJ-24	***Date***	Jul 2 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-14413_ASIMJ-24\1H-ASIMJ-24				
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)***	3602.47
Temperature (degree C)	30.000				



No.	(ppm)	(Hz)	Height
1	1.47	441.8	0.0741
2	1.50	448.9	0.1551
3	1.52	455.9	0.0800
4	1.77	530.7	0.1656
5	1.80	539.0	1.0000
6	1.86	559.7	0.0599
7	4.60	1382.2	0.0235
8	4.63	1389.2	0.0674
9	4.65	1396.7	0.0659
10	4.68	1403.7	0.0234
11	7.25	2176.4	0.0657
12	7.97	2392.0	0.0729
13	8.49	2549.0	0.0616

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value	Absolute Value
1	[1.42 .. 1.57]	2.952	1.25818e+8
2	[1.76 .. 1.85]	9.000	3.83645e+8
3	[4.53 .. 4.80]	1.761	7.50525e+7
4	[7.91 .. 8.06]	0.756	3.22197e+7
5	[8.40 .. 8.56]	0.653	2.78490e+7

5n. - 9-tert-butyl-6-ethoxy-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

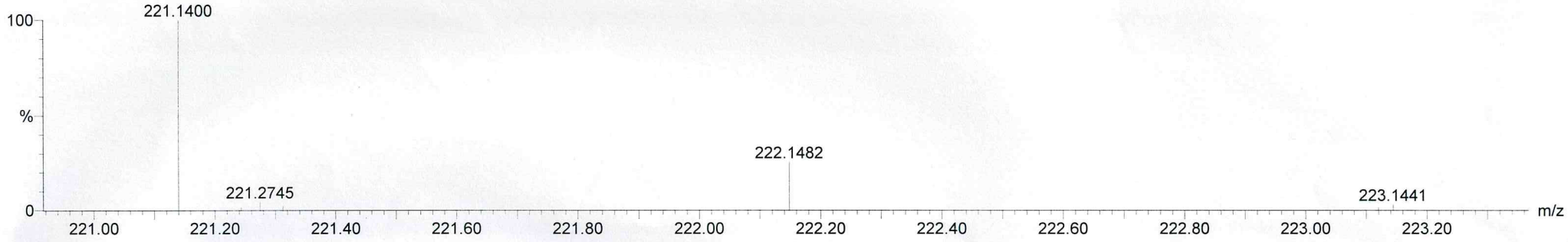
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
362 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-56 H: 0-1000 N: 0-4 O: 0-10 Na: 0-1 Br: 0-1

ASIMJ-24 8 (0.175)

1: TOF MS ES+

2.36e+003

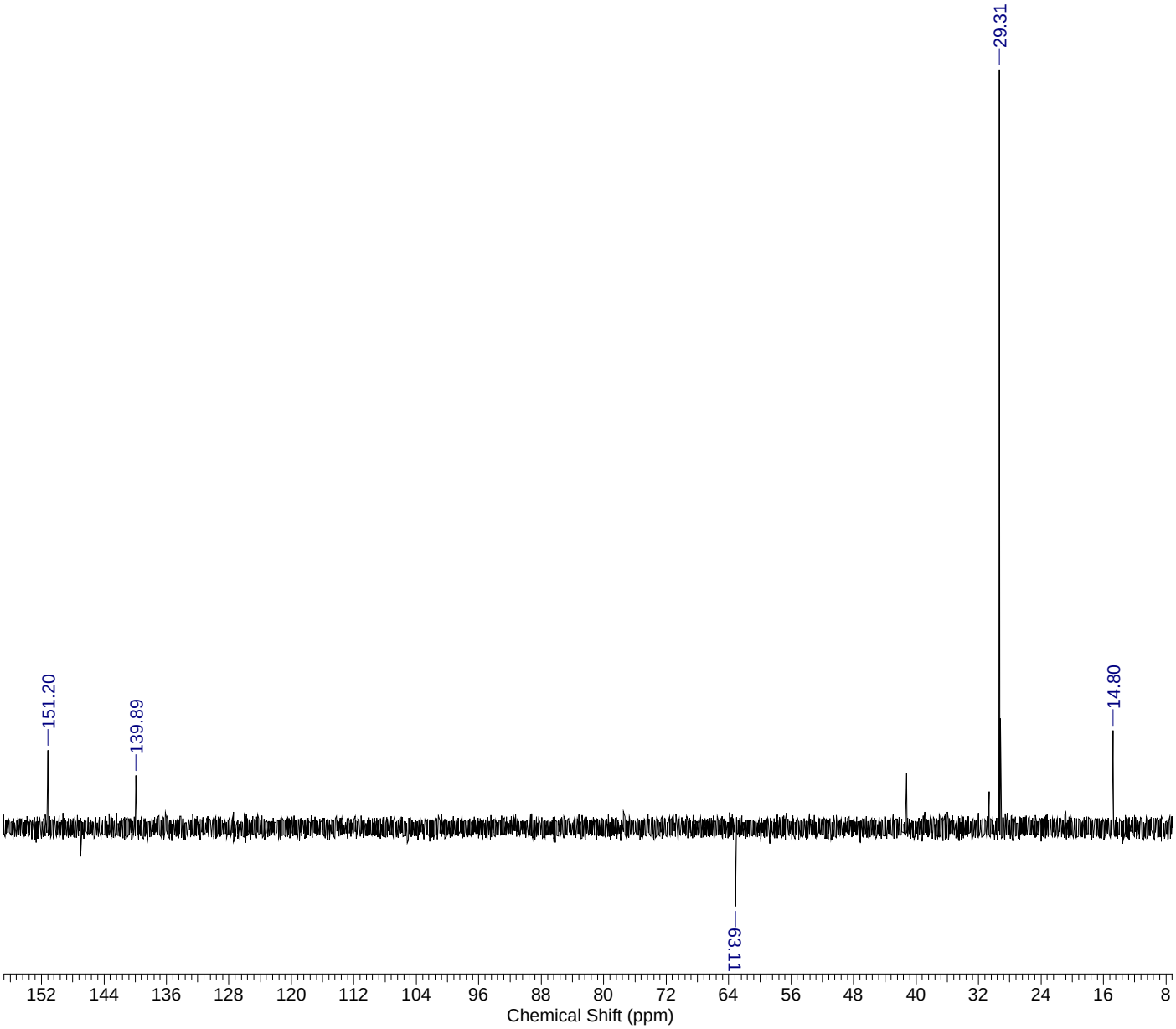


Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.1400	221.1402	-0.2	-0.9	5.5	66.8	C11 H17 N4 O
	221.1389	1.1	5.0	0.5	88.4	C10 H21 O5

5n. - 9-tert-butyl-6-ethoxy-9H-purine (DEPT)

11 Mar 2013

Acquisition Time (sec)	1.0000	***Comment***	ASIMJ-24	***Date***	Jul 2 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-14413_ASIMJ-24\DEPT-ASIMJ-24				
Frequency (MHz)	75.49	***Nucleus***	13C	***Number of Transients***	3200
Original Points Count	18116	***Points Count***	32768	***Pulse Sequence***	DEPT135
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	18115.94
Temperature (degree C)	30.000				

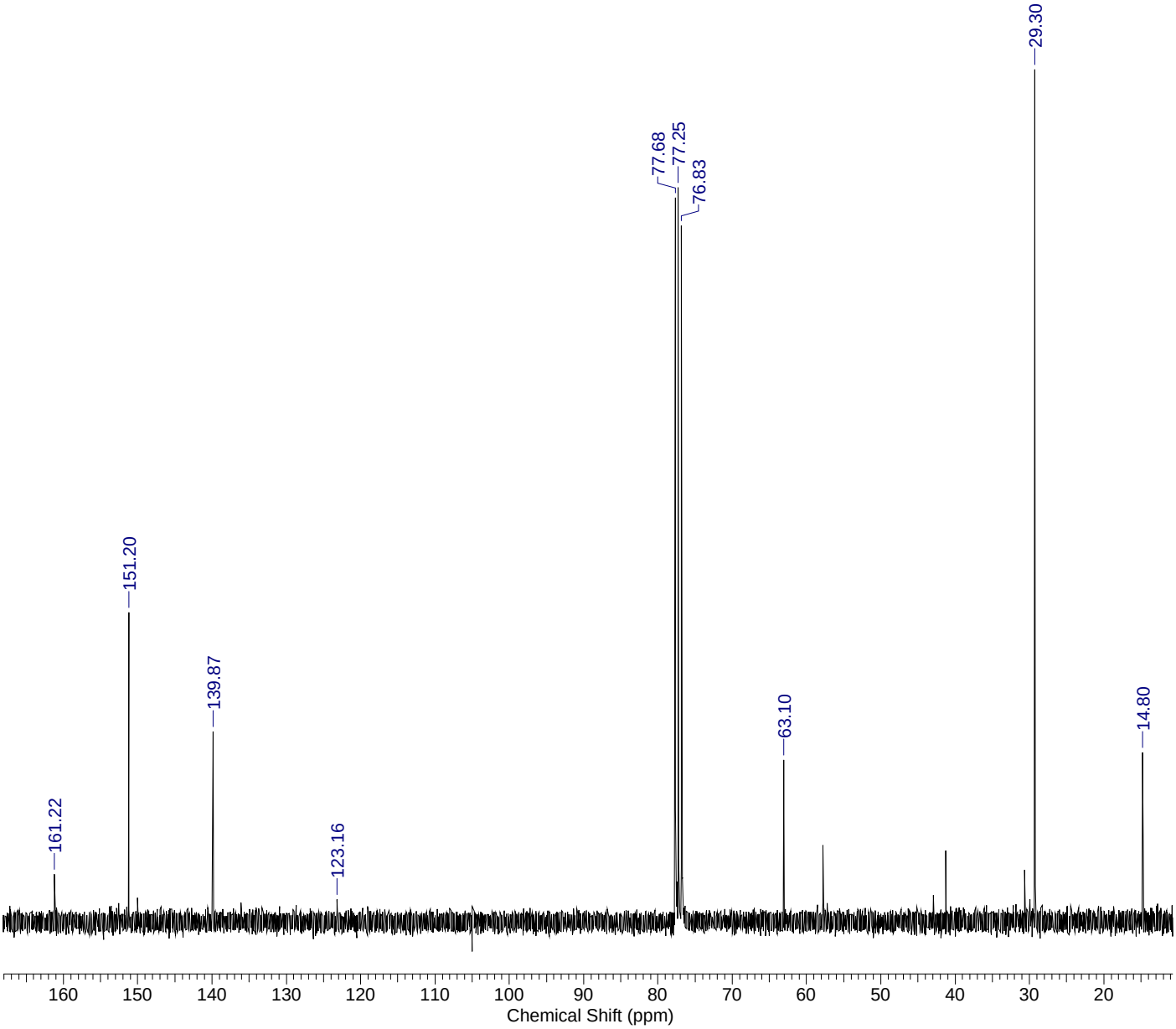


No.	(ppm)	(Hz)	Height
1	14.80	1117.3	0.1283
2	29.31	2212.5	1.0000
3	63.11	4764.0	-0.1038
4	139.89	10560.3	0.0691
5	151.20	11414.5	0.1018

5n. - 9-tert-butyl-6-ethoxy-9H-purine (C-NMR)

11 Mar 2013

Acquisition Time (sec)	1.3005	***Comment***	ASIMJ-24	***Date***	Jul 2 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-14413_ASIMJ-24\13C-ASIMJ-24				
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				

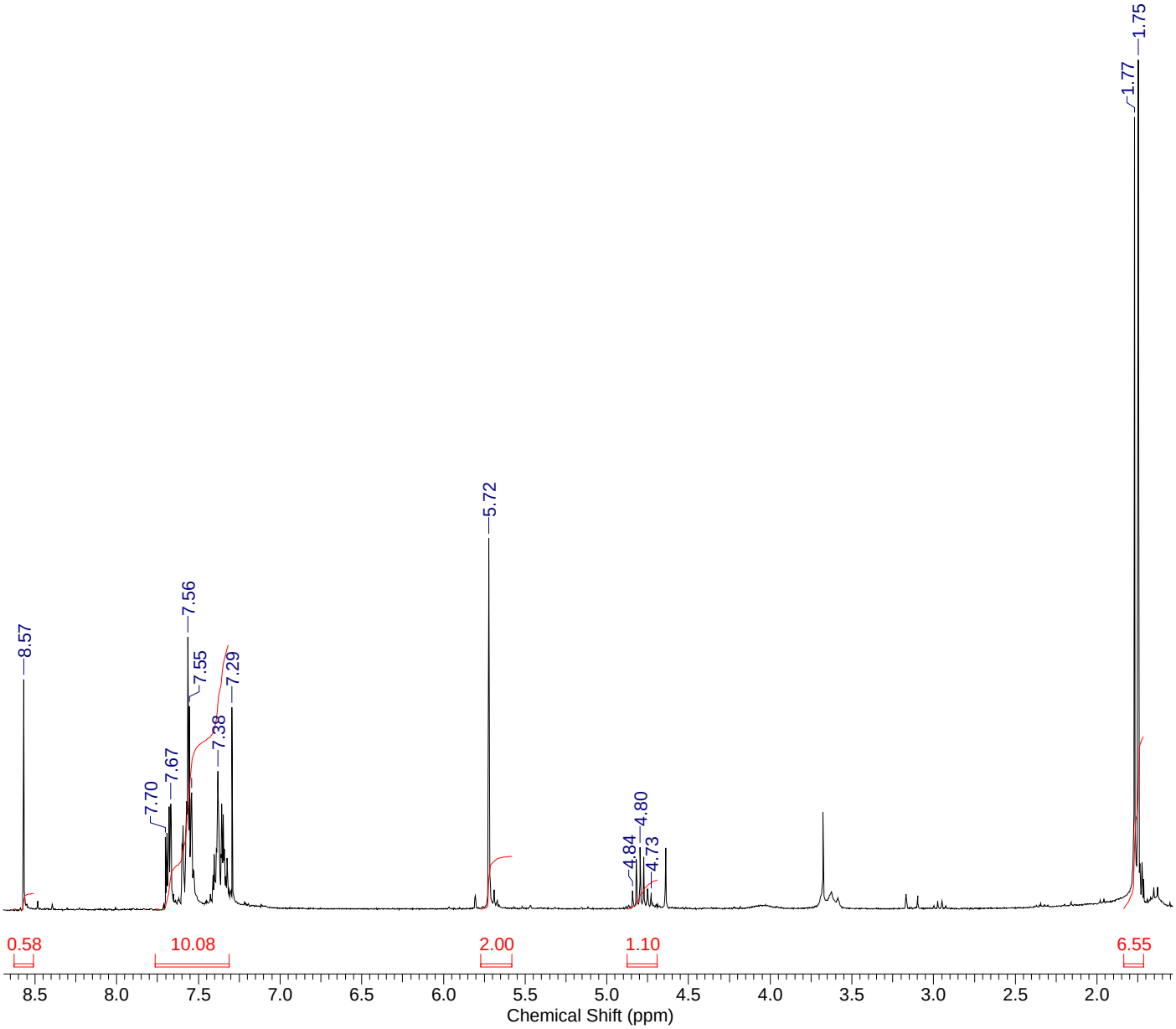


No.	(ppm)	(Hz)	Height
1	14.80	1117.1	0.1996
2	29.21	2205.1	0.1902
3	29.30	2212.3	1.0000
4	63.10	4763.8	0.1907
5	76.83	5799.9	0.8168
6	77.25	5832.0	0.8619
7	77.68	5864.0	0.8498
8	123.16	9297.9	0.0274
9	139.87	10559.6	0.2236
10	151.20	11414.3	0.3633
11	161.22	12170.6	0.0567

6a. - 6-Benzyloxy-9-isopropyl-8-phenyl-9H-purine (H-NMR)

12 Jul 2012

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	4.73	1419.4	0.0187
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	7.54	2263.4	0.1369
10	7.55	2267.8	0.2390
11	7.56	2270.4	0.3199
12	7.67	2302.1	0.1240
13	7.70	2311.7	0.0844
14	8.57	2572.5	0.2705

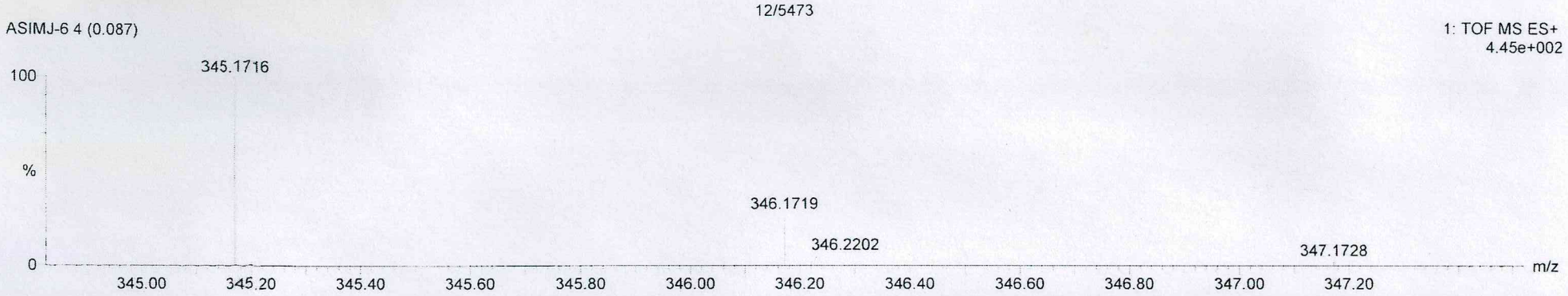
No.	(ppm)	Value	Absolute Value
1	[1.72 .. 1.84]	6.555	2.56480e+8
2	[4.69 .. 4.88]	1.098	4.29797e+7
3	[5.58 .. 5.77]	2.000	7.82552e+7
4	[7.31 .. 7.76]	10.078	3.94315e+8
5	[8.51 .. 8.63]	0.583	2.28139e+7

6a. - 6-Benzyloxy-9-isopropyl-8-phenyl-9H-purine (MS)

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

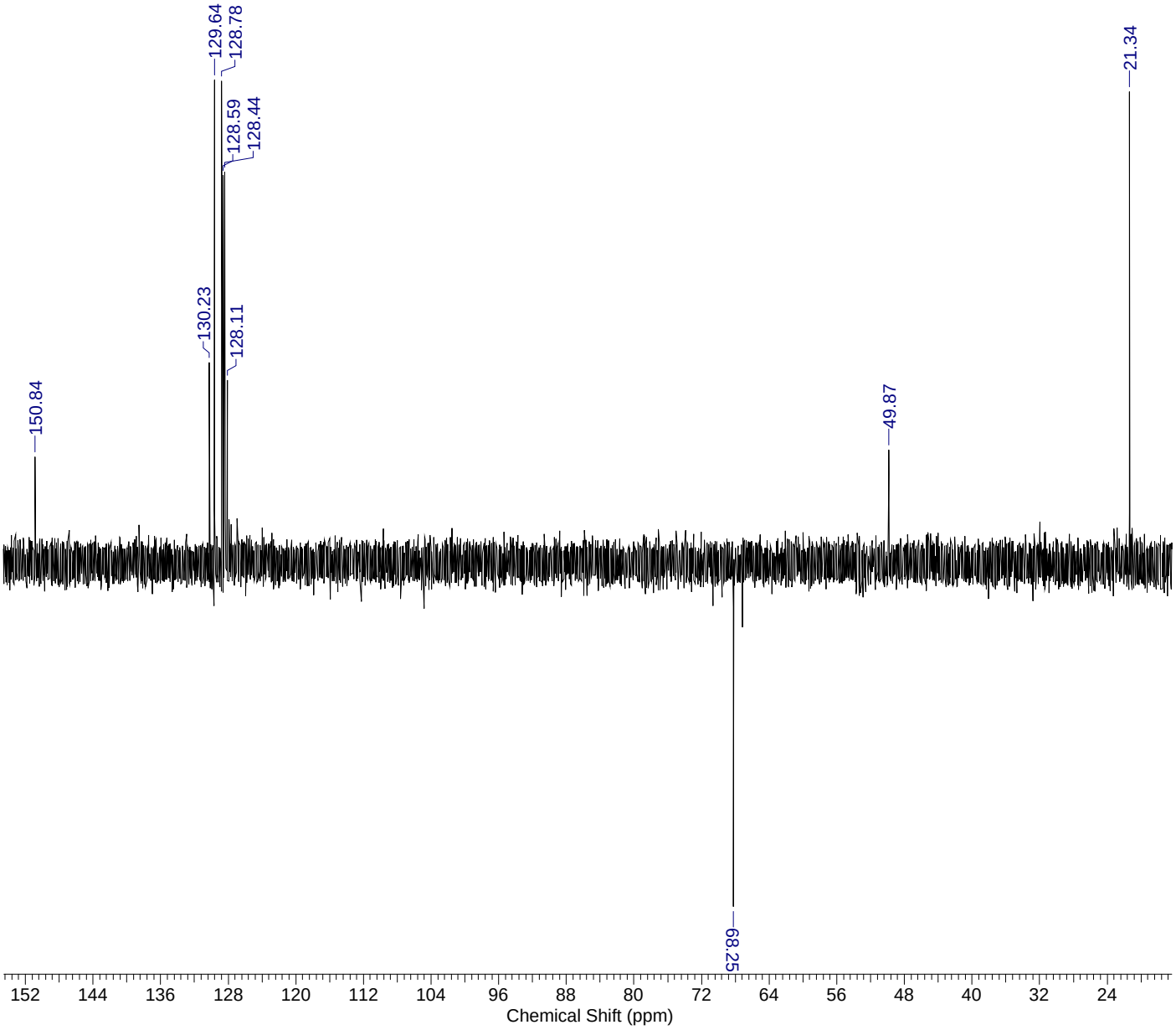


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
345.1716	345.1715	0.1	0.3	13.5	0.5	C21 H21 N4 O

6a. - 6-Benzyloxy-9-isopropyl-8-phenyl-9H-purine (DEPT)

12 Jul 2012

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***	13C	***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				

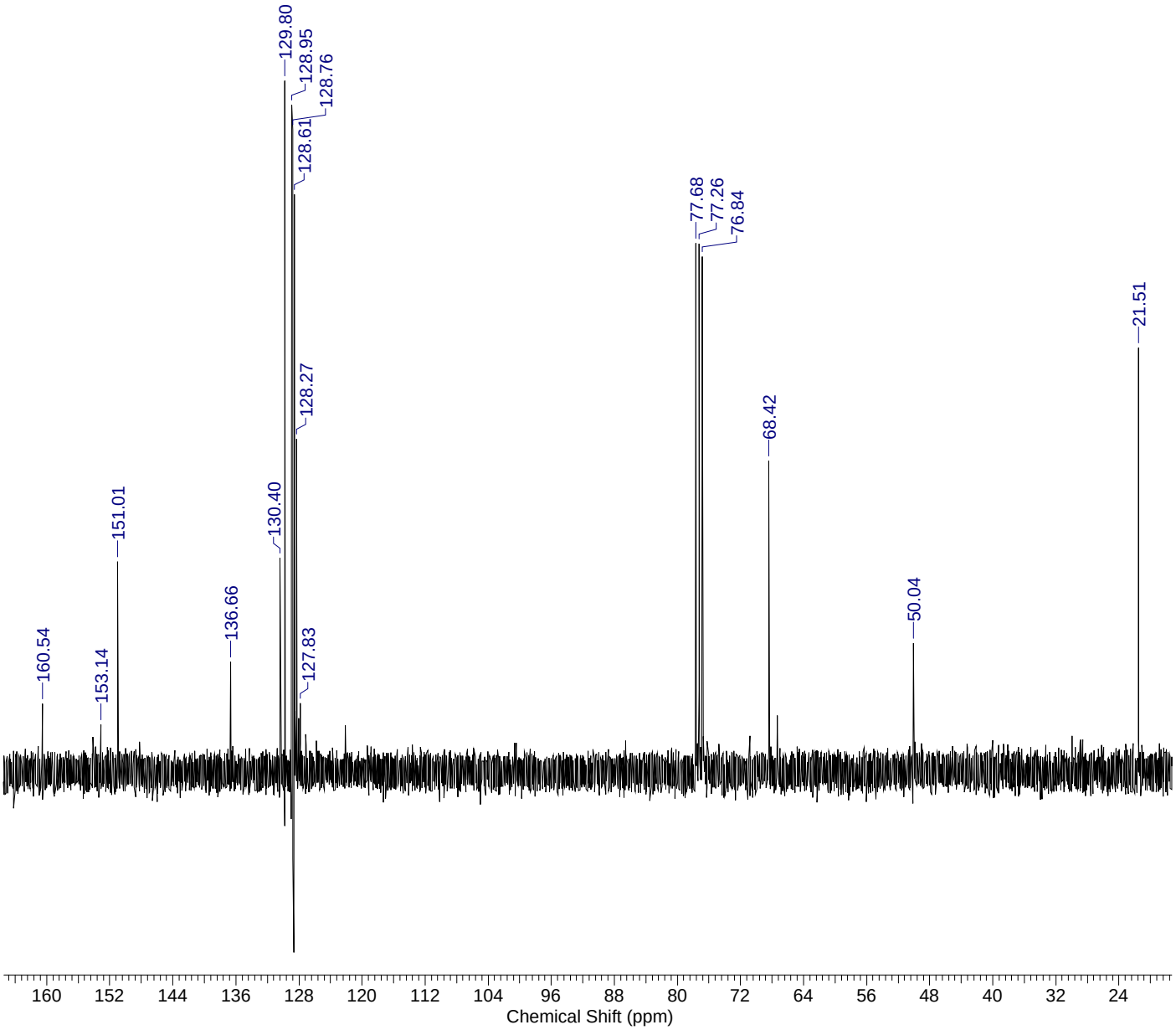


No.	(ppm)	(Hz)	Height
1	21.34	1611.3	0.9748
2	49.87	3764.7	0.2347
3	68.25	5152.5	-0.7110
4	128.11	9671.1	0.3783
5	128.44	9696.5	0.8089
6	128.47	9698.7	0.1493
7	128.59	9707.6	0.8026
8	128.78	9721.9	0.9972
9	129.64	9786.6	1.0000
10	130.23	9831.4	0.4147
11	150.84	11387.2	0.2201

6a. - 6-Benzyloxy-9-isopropyl-8-phenyl-9H-purine (C-NMR)

12 Jul 2012

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				

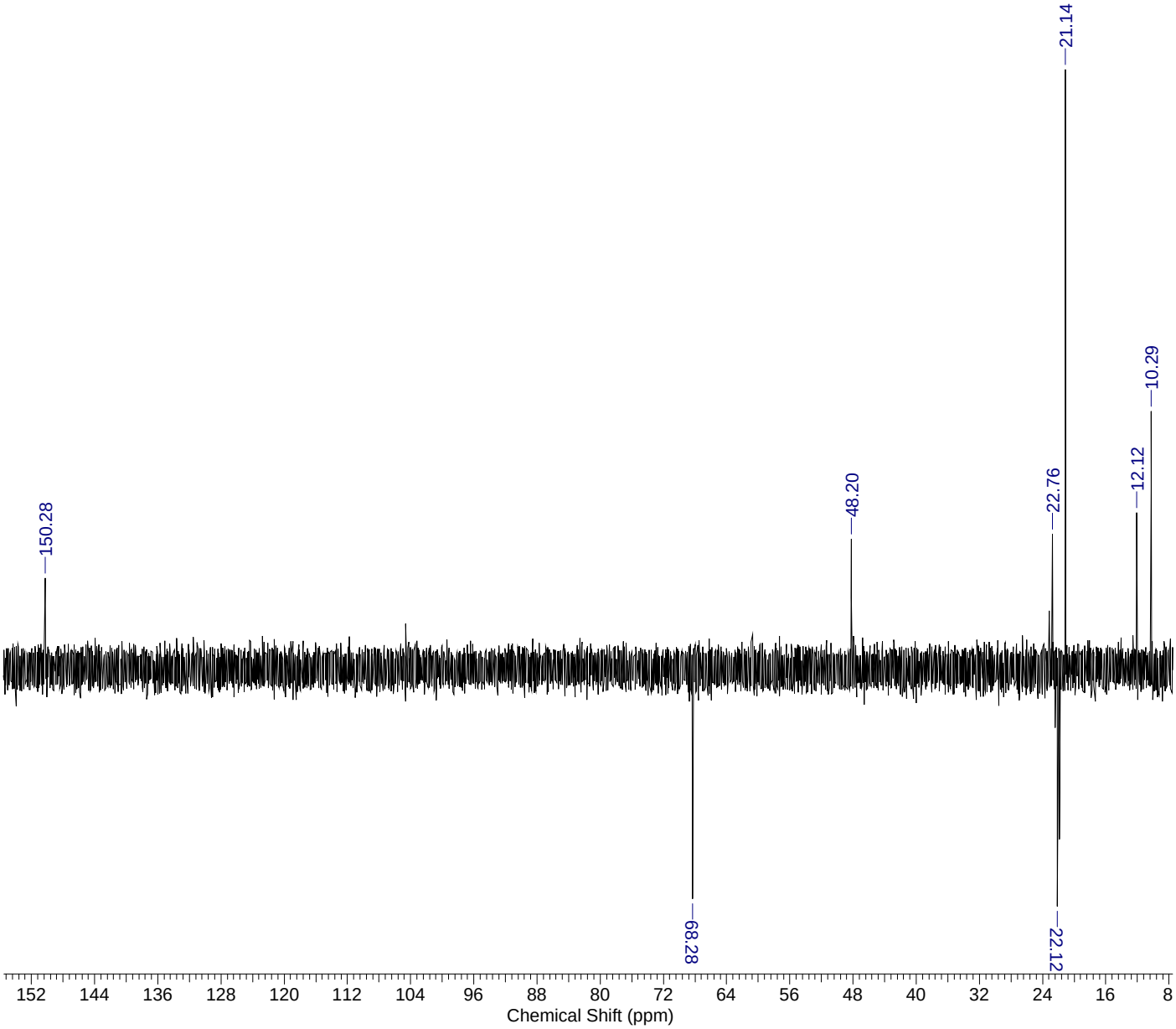


No.	(ppm)	(Hz)	Height
1	21.51	1624.0	0.6139
2	50.04	3777.4	0.1866
3	68.42	5165.1	0.4500
4	76.84	5800.9	0.7455
5	77.26	5832.4	0.7640
6	77.68	5864.5	0.7647
7	127.83	9650.0	0.0998
8	128.27	9683.8	0.4819
9	128.61	9709.2	0.8357
10	128.76	9720.2	0.9293
11	128.95	9734.6	0.9649
12	129.80	9799.3	1.0000
13	130.40	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

6b. - 8-Ethyl-9-isopropyl-6-propoxy-9H-purine (DEPT)

12 Nov 2012

Acquisition Time (sec)	1.0000	***Comment***	MJ-A2	***Date***	Sep 20 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-20186_MJ-A2\DEPT-MJ-A2				
Frequency (MHz)	75.49	***Nucleus***	13C	***Number of Transients***	8000
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	10.29	776.7	0.4301
2	12.12	914.9	0.2606
3	21.14	1596.0	1.0000
4	22.12	1669.6	-0.3966
5	22.76	1718.2	0.2249
6	48.20	3638.9	0.2167
7	68.28	5154.9	-0.3837
8	150.28	11344.8	0.1510

6b. - 8-Ethyl-9-isopropyl-6-propoxy-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

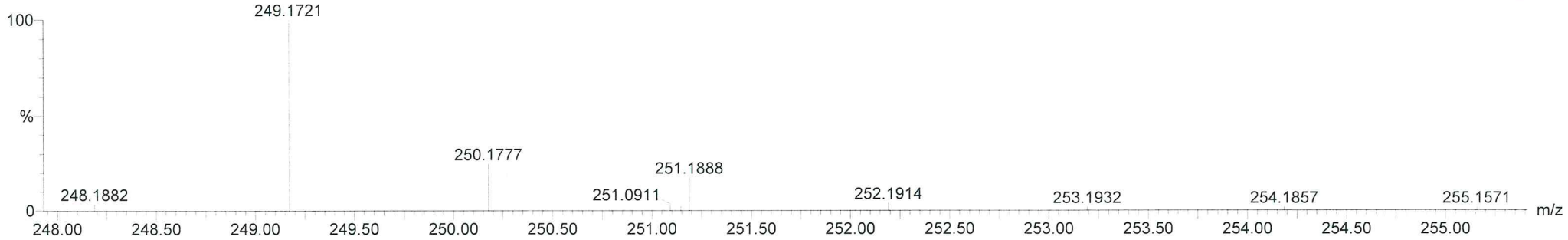
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
875 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: 0-10 O: 0-20 S: 0-1 Cl: 0-1

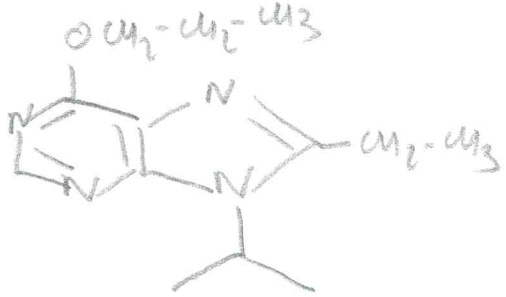
MJ-P4 8 (0.175)

1: TOF MS ES+

1.40e+003



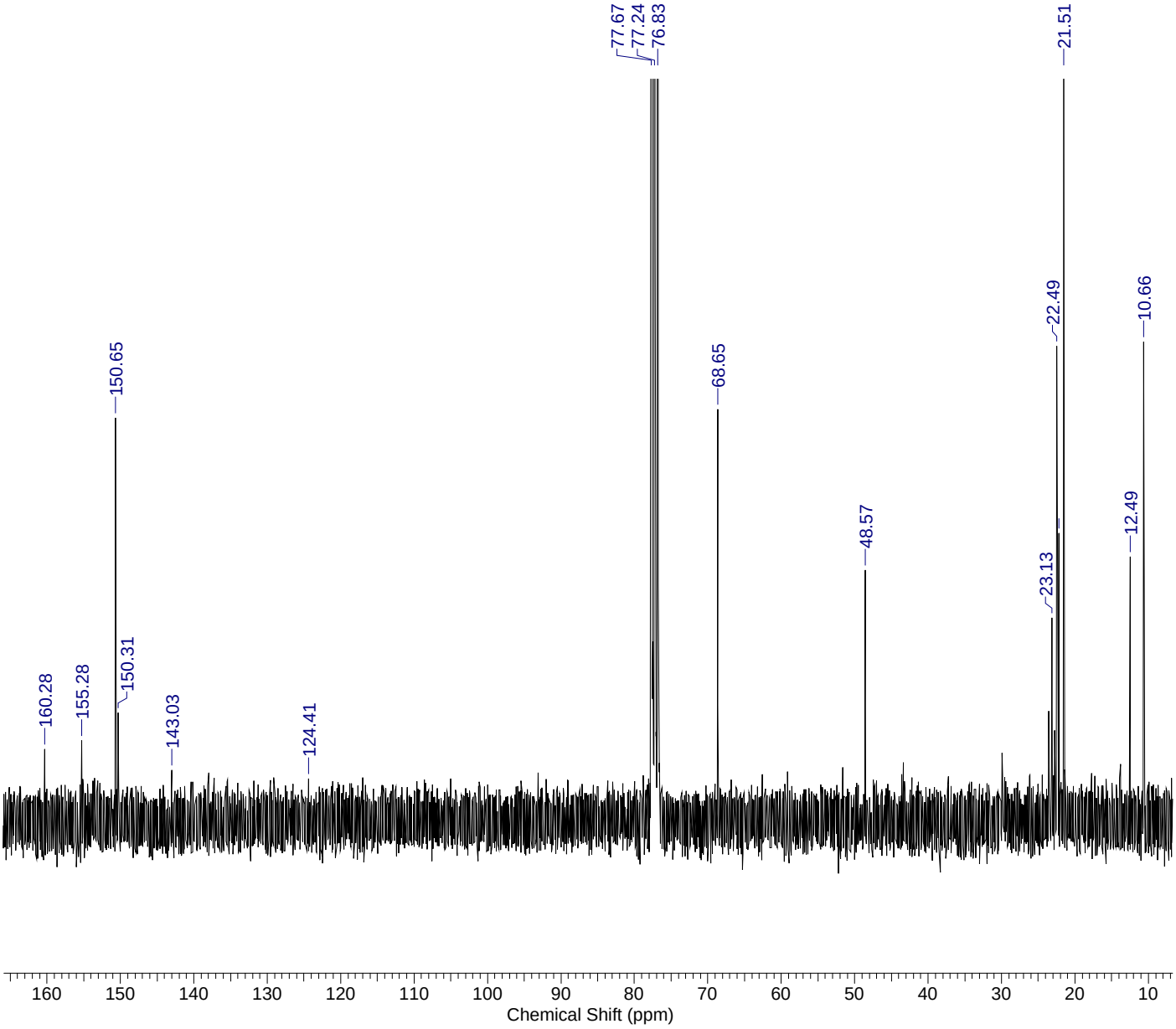
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
249.1721	249.1715	0.6	2.4	5.5	119.6	C13 H21 N4 O



6b. - 8-Ethyl-9-isopropyl-6-propoxy-9H-purine (C-NMR)

12 Nov 2012

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				

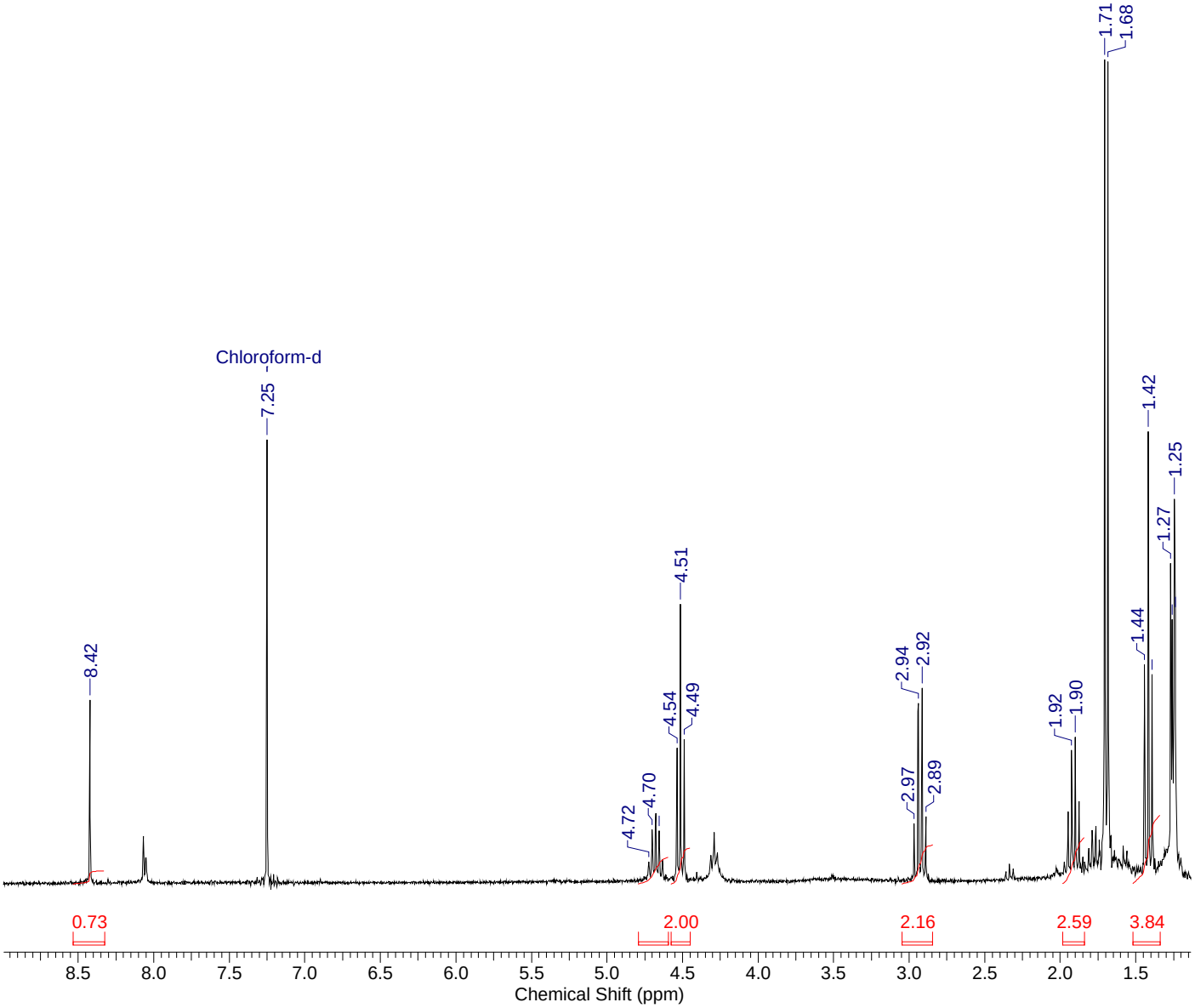


No.	(ppm)	(Hz)	Height
1	10.66	804.6	0.1251
2	12.49	942.9	0.0691
3	21.51	1624.0	0.2337
4	22.20	1676.0	0.0753
5	22.49	1697.5	0.1240
6	23.13	1746.2	0.0532
7	48.57	3666.9	0.0657
8	68.65	5182.8	0.1075
9	76.83	5799.8	0.9759
10	77.24	5831.4	0.9895
11	77.67	5863.4	1.0000
12	124.41	9391.8	0.0113
13	143.03	10797.8	0.0137
14	150.31	11347.4	0.0285
15	150.65	11372.8	0.1053
16	155.28	11722.8	0.0213
17	160.28	12099.8	0.0190

6b. - 8-Ethyl-9-isopropyl-6-propoxy-9H-purine (H-NMR)

11 Mar 2013

Acquisition Time (sec)	2.0487	***Comment***	MJ-A2	***Date***	Sep 20 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-20186_MJ-A2\1H-MJ-A2				
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	1.24	371.6	0.3303
2	1.25	374.2	0.4666
3	1.26	378.2	0.3208
4	1.27	380.8	0.3891
5	1.39	417.7	0.2539
6	1.42	425.2	0.5489
7	1.44	432.7	0.2663
8	1.68	505.7	0.9972
9	1.71	512.3	1.0000
10	1.90	570.3	0.1781
11	1.92	577.8	0.1624
12	2.89	867.6	0.0819

No.	(ppm)	(Hz)	Height
13	2.92	875.1	0.2377
14	2.94	882.6	0.2192
15	2.97	890.5	0.0735
16	4.49	1347.9	0.1756
17	4.51	1354.9	0.3394
18	4.54	1362.0	0.1647
19	4.66	1397.6	0.0647
20	4.70	1411.2	0.0661
21	4.72	1417.8	0.0268
22	7.25	2176.4	0.5389
23	8.42	2528.3	0.2231

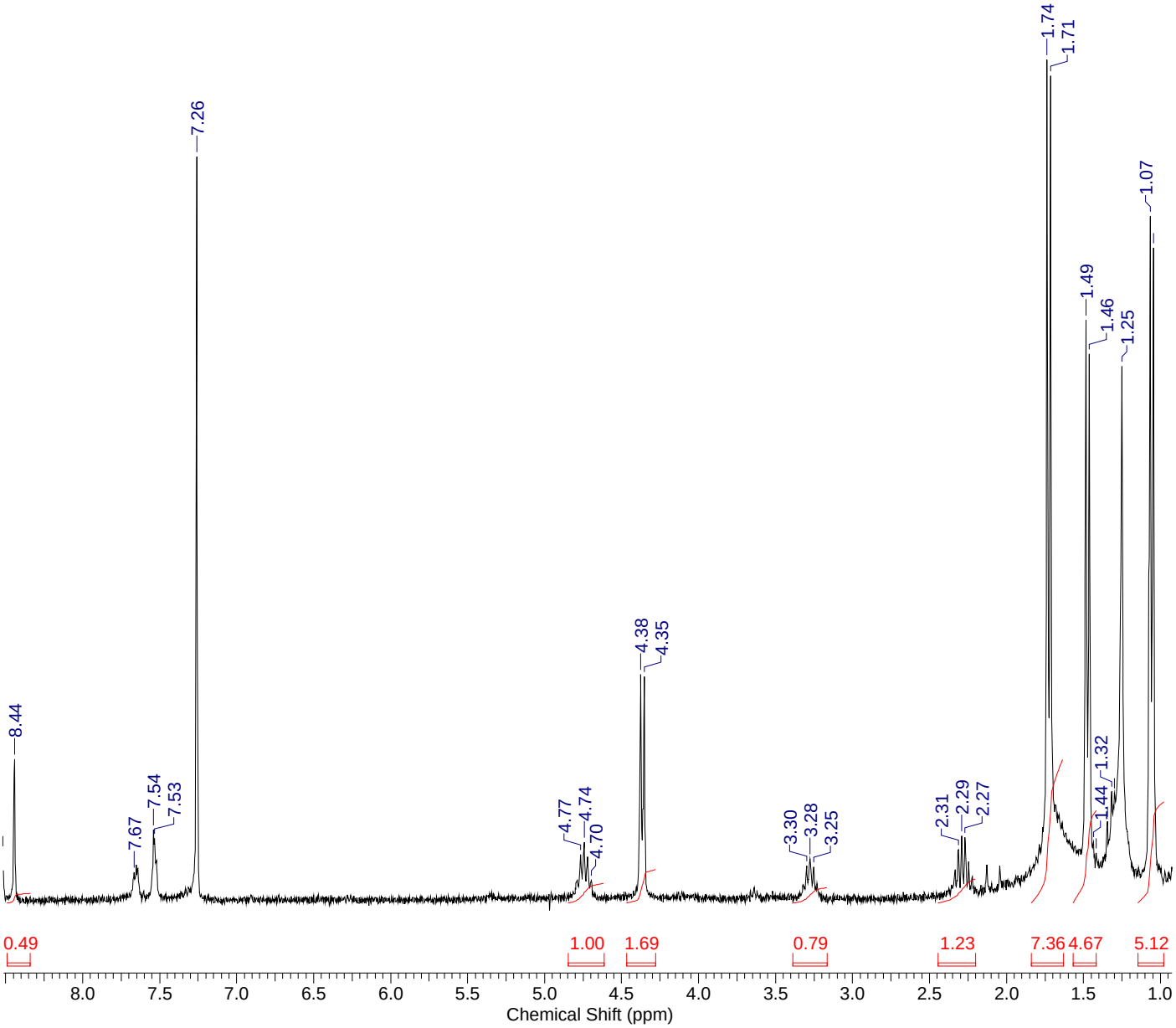
No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value	Absolute Value
1	[1.34 .. 1.52]	3.843	7.82922e+7
2	[1.84 .. 1.98]	2.592	5.28076e+7
3	[2.84 .. 3.05]	2.161	4.40219e+7
4	[4.45 .. 4.58]	2.000	4.07425e+7
5	[4.59 .. 4.79]	1.505	3.06523e+7
6	[8.33 .. 8.53]	0.735	1.49725e+7

6c. - 6-Isobutoxy-8,9-diisopropyl-9H-purine (H-NMR)

2 Jul 2013

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

6c. - 6-Isobutoxy-8,9-diisopropyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

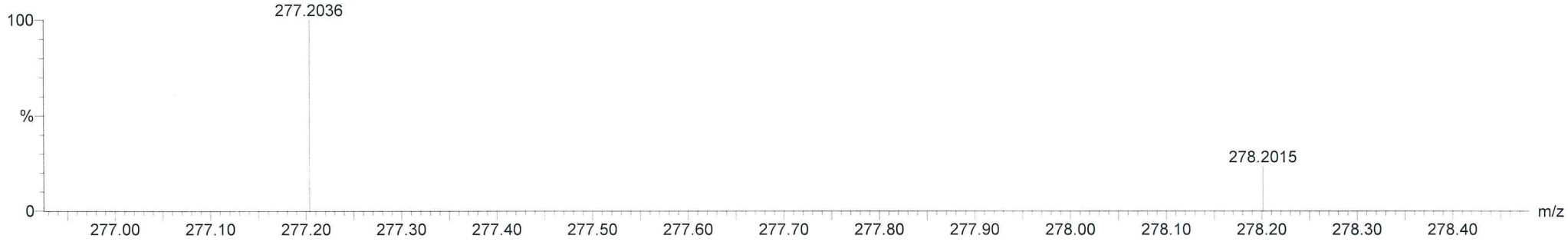
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

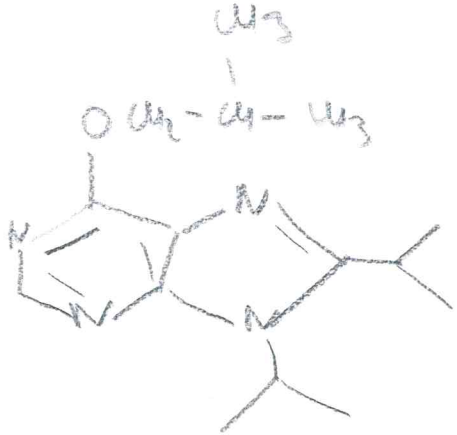
12/22452

MJ-28 96 (2.120)

1: TOF MS ES+
1.15e+002



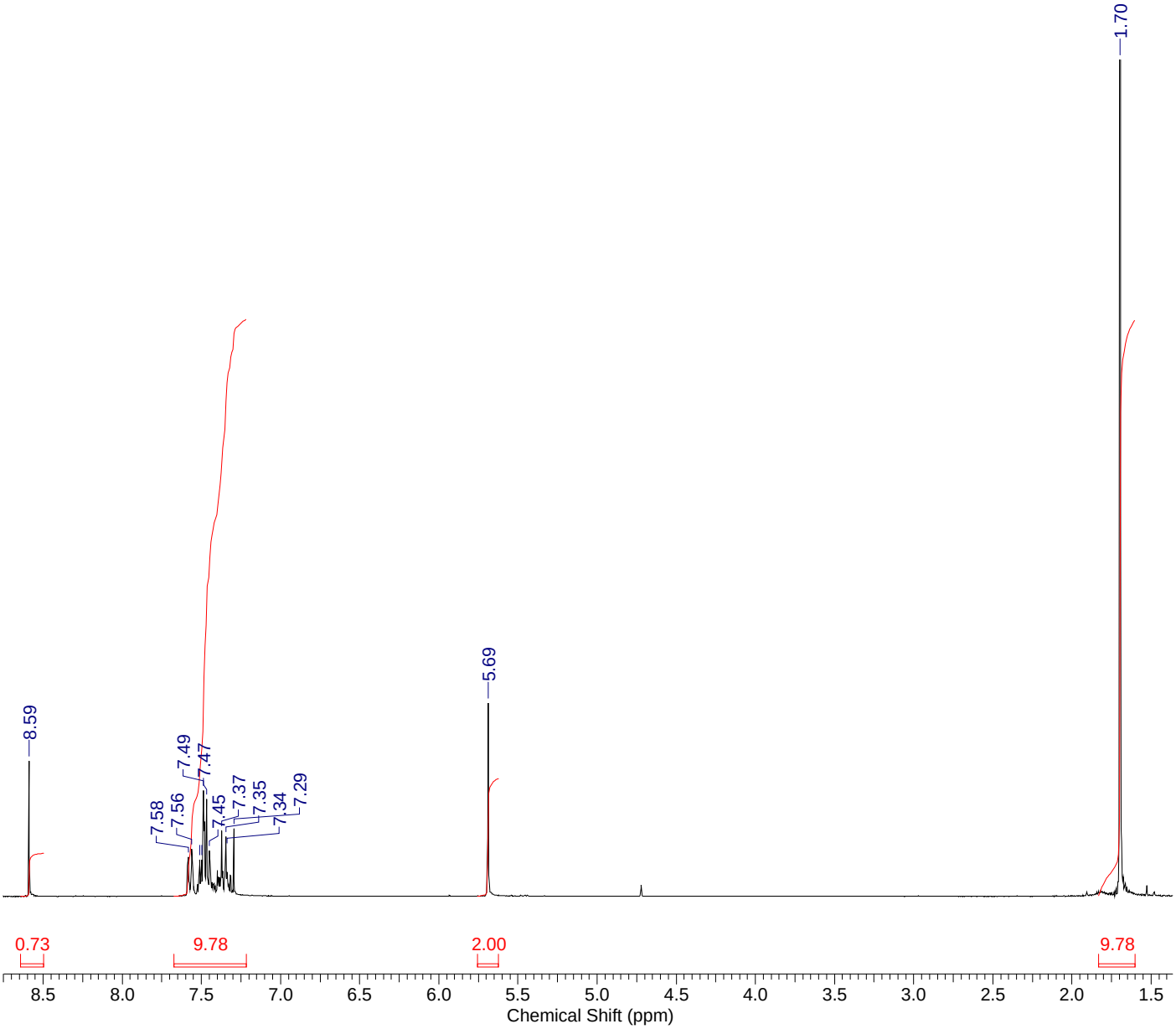
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
277.2036	277.2028	0.8	2.9	5.5	n/a	C15 H25 N4 O
	277.2047	-1.1	-4.0	0.5	n/a	C14 H30 N2 O Cl



6d. - 9-tert-butyl-6-(benzyloxy)-8-phenyl-9H-purine (H-NMR)

12 Mar 2013

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	[1.60 .. 1.83]	9.778	8.16565e+8
2	[5.62 .. 5.76]	2.000	1.67019e+8
3	[7.22 .. 7.67]	9.780	8.16722e+8
4	[8.50 .. 8.64]	0.727	6.07282e+7

6d. - 9-tert-butyl-6-(benzyloxy)-8-phenyl-9H-purine (MS)

Elemental Composition Report

Single Mass Analysis

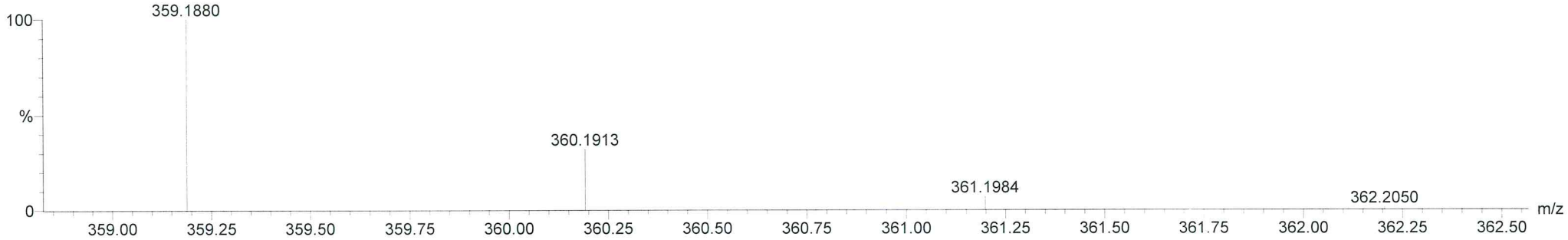
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
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

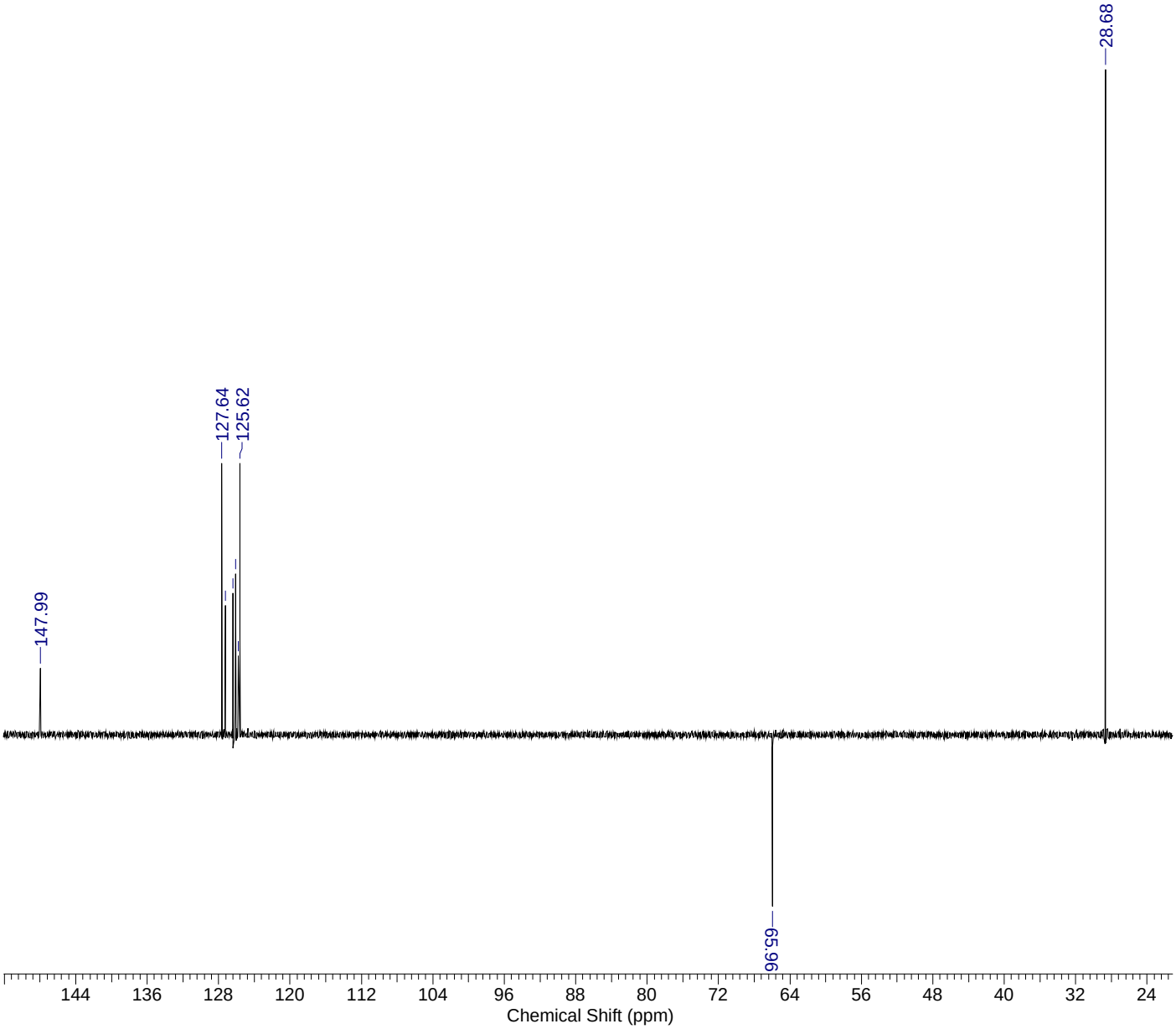


Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
359.1880	359.1872	0.8	2.2	13.5	10.3	C22 H23 N4 O

6d. - 9-tert-butyl-6-(benzyloxy)-8-phenyl-9H-purine (DEPT)

12 Nov 2012

Acquisition Time (sec)	1.0000	***Comment***	ASIMJ-27-P2-P	***Date***	Oct 22 2012
File Name	C:\Users\usuario\Documents\Espectros Asier\12-21939_ASIMJ-27-P2-P\DEPT-ASIMJ-27-P2-P				
Frequency (MHz)	75.49	***Nucleus***	13C	***Number of Transients***	5000
Original Points Count	18116	***Points Count***	32768	***Pulse Sequence***	DEPT135
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	18115.94
Temperature (degree C)	30.000				

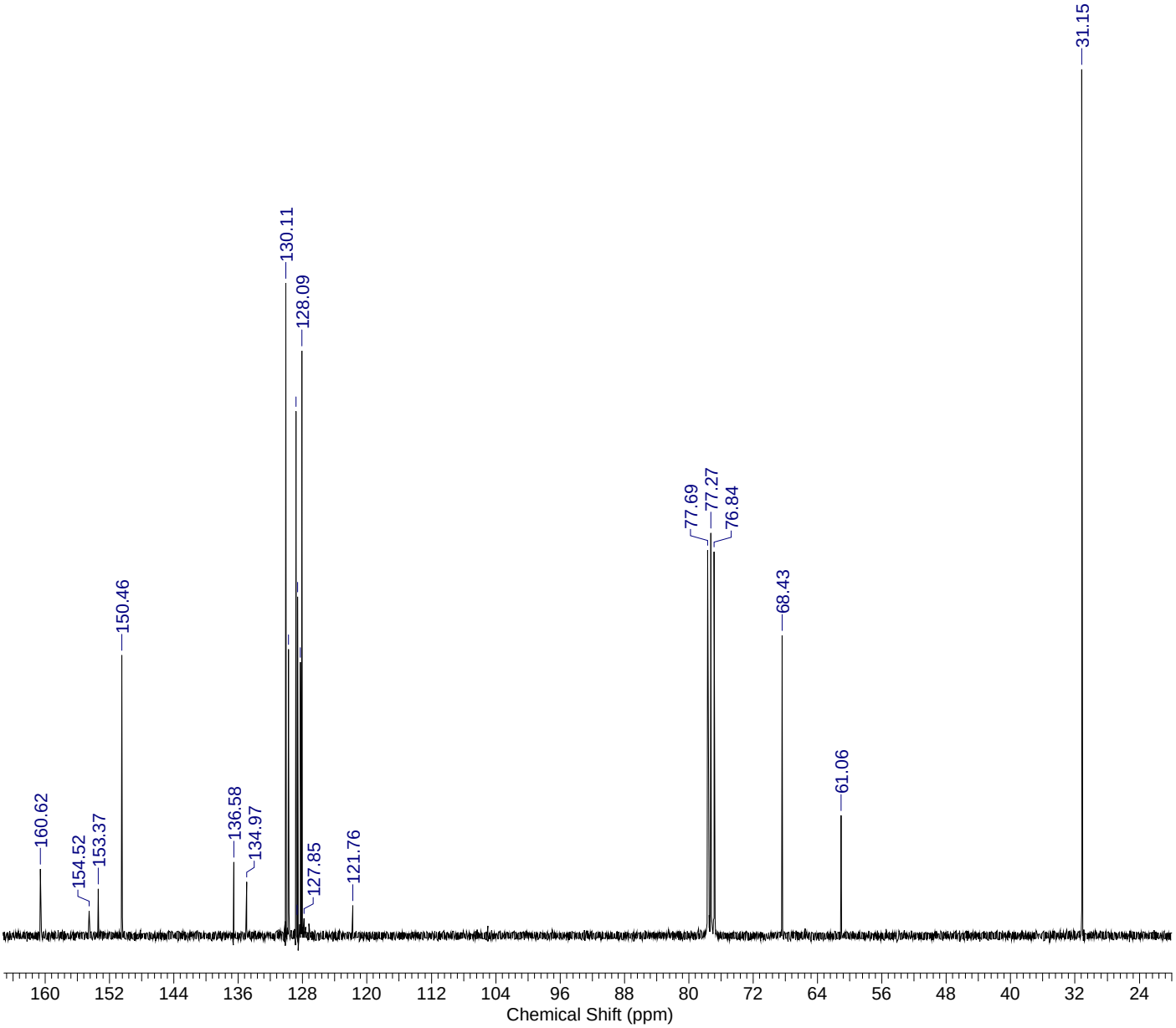


No.	(ppm)	(Hz)	Height
1	28.68	2165.1	1.0000
2	65.96	4979.8	-0.2578
3	125.62	9483.5	0.4080
4	125.81	9497.8	0.1184
5	126.12	9521.1	0.2422
6	126.38	9541.0	0.2129
7	127.25	9606.8	0.1947
8	127.64	9636.1	0.4085
9	147.99	11171.9	0.1000

6d. - 9-tert-butyl-6-(benzyloxy)-8-phenyl-9H-purine (C-NMR)

12 Mar 2013

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
1	31.15	2351.6	1.0000
2	61.06	4609.5	0.1388
3	68.43	5166.3	0.3470
4	76.84	5800.9	0.4431
5	77.27	5833.0	0.4649
6	77.69	5865.1	0.4451
7	121.76	9192.3	0.0353
8	127.85	9651.7	0.0204
9	128.09	9669.9	0.6750
10	128.27	9683.8	0.3159
11	128.59	9707.5	0.3914

No.	(ppm)	(Hz)	Height
12	128.67	9713.6	0.0190
13	128.78	9721.9	0.0381
14	128.85	9727.4	0.6056
15	129.72	9793.2	0.3308
16	130.11	9822.5	0.7535
17	134.97	10189.6	0.0624
18	136.58	10310.7	0.0852
19	150.46	11358.4	0.3239
20	153.37	11578.5	0.0544
21	154.52	11665.3	0.0286
22	160.62	12125.8	0.0769