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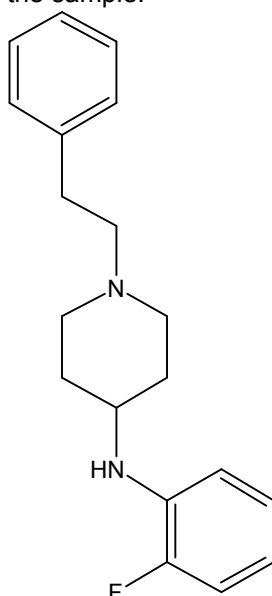
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ADMINISTRATIVE ARRANGEMENT JRC-Nr 33619-CLEN2SAND-DG TAXUD-Nr TAXUD/2014/DE/315 BETWEEN DG TAXATION AND CUSTOMS UNION (DG TAXUD) AND THE JOINT RESEARCH CENTRE (JRC) for fast recognition of New Psychoactive Substances (NPS) and identification of unknown chemicals

This report was generated on 22/03/2016 based on data from the European Customs laboratories and the Joint Research Centre. This report includes sample and molecular information, spectral data and associated tables and figures. The chemical structure(s) was/were identified by Bio-chemical interactions & metabolomics (BCIM) group chemists on the basis of analytical data available. NMR assignments proposed below were performed by ACD labs tools in agreement with the chemical structure identified by analytical experts. Reported data are related to the sample in the following table:

Eurodat number	15010007	Received on	16 January 2015
PACKAGING	Plastic sachet	Registration date	16 January 2015
Name of customer	Service commun des laboratoires France		
Customer's identification	2014-23818		

The following structure(s) was/were identified in the sample:



Data of identified compound(s)

IUPAC Name	<i>N</i> -(2-fluorophenyl)-1-(2-phenylethyl)piperidin-4-amine		
NAME	Despropionyl o-Fluoro Fentanyl	SYNONYMS	Despropionyl-2-fluoro fentanyl
Formula	C ₁₉ H ₂₃ FN ₂	FW	298.3977
Monoisotopic Mass	298.184527		
InChI	InChI=1S/C19H23FN2/c20-18-8-4-5-9-19(18)21-17-11-14-22(15-12-17)13-10-16-6-2-1-3-7-16/h1-9,17,21H,10-15H2		
InChI Key	WUNLGTOLOUTCPE-UHFFFAOYSA-N	SMILES	Fc3ccccc3NC2CCN(CCc1ccccc1)CC2
Chemspider link	http://www.chemspider.com/Chemical-Structure.22493203.html		
Pubchem link	https://pubchem.ncbi.nlm.nih.gov/compound/40515645		

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<https://ec.europa.eu/jrc/en/institutes/ihcp>

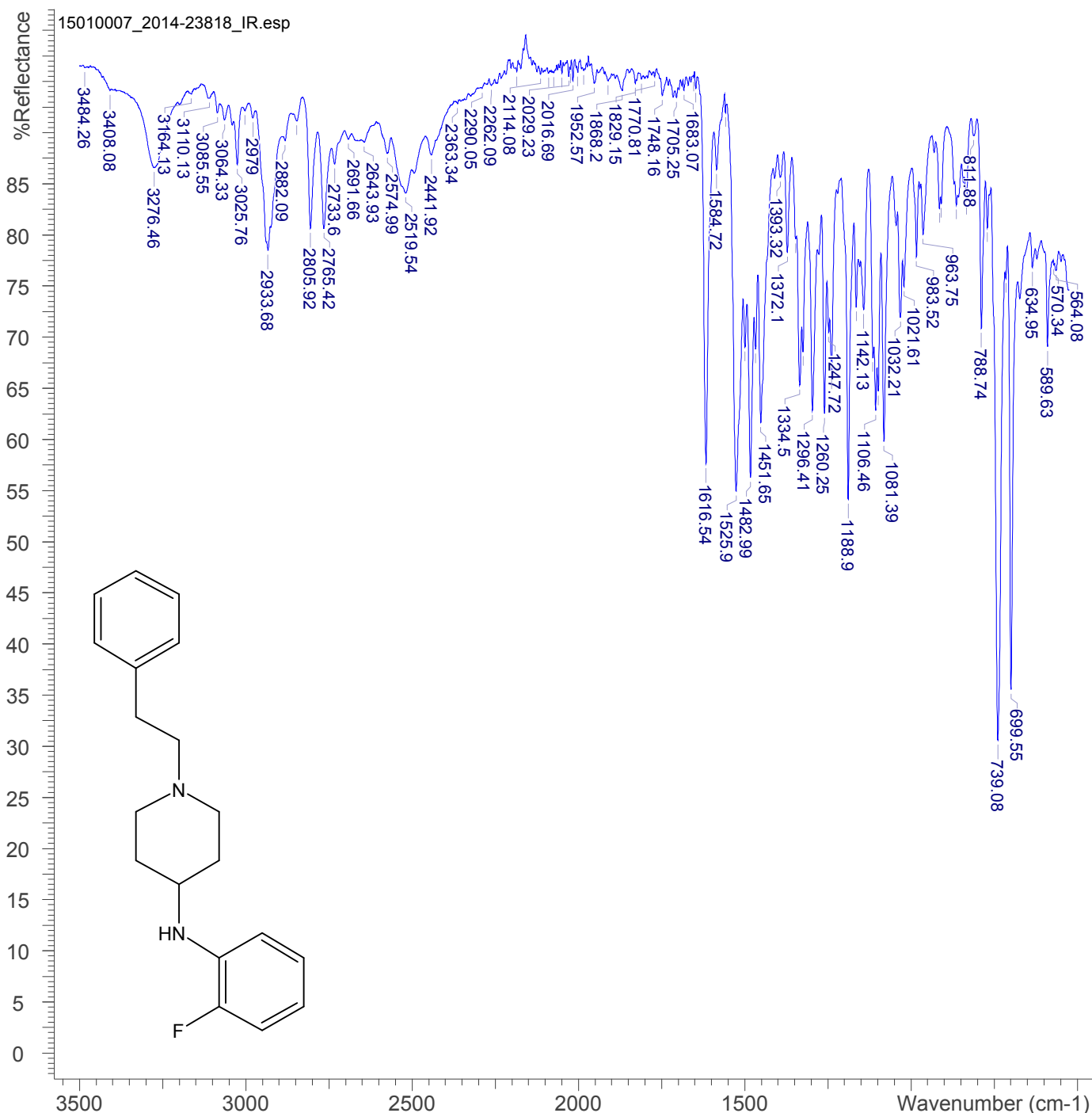
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Processing and interpretation based on data provided by:

Service commun des laboratoires France

Title	23818		
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Date Stamp	02 Jan 2015 12:44:04	Date	02 Jan 2015 14:45:28
Technique	Infrared	Spectral Region	IR
X Axis	Wavenumber (cm-1)	Y Axis	%Reflectance
Spectrum Range	525.0251 - 3500.1670	Points Count	6172
Data Spacing	0.4821		



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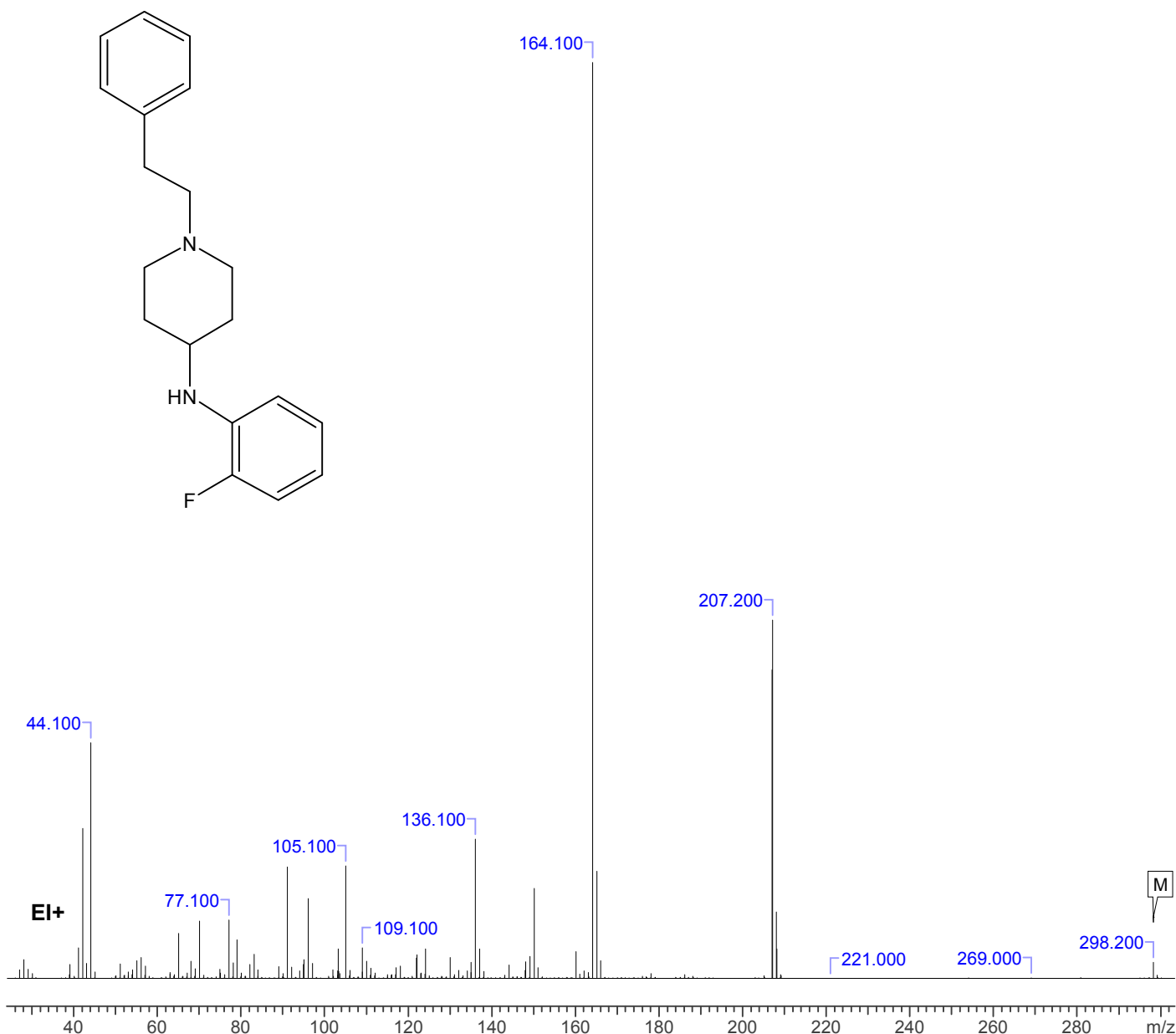
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Processing and interpretation based on data provided by:

Service commun des laboratoires France

Combine	<1811-1818>	Comment	NL/FB
Count	574	Data Source Name	2014-23818_Centroid_EI+
Data Type	Condensed	Date	9:34:22 AM
Date Stamp	30 Dec 14 8:09 am		
File Name	\\139.191.6.82\ihcp\$\101\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure_SAND-DB\Results\15010007_2014-23818\15010007_2014-23818_EI+_7.768.esp		
Inlet Model	GC	Ion Mode	EI+
Mass Spec Model	STUP1	Plot Type	Stick
Retention Time	7.768	Sample	Ds CH2Cl2/MeOH : 2014-23818
Scan	1818	Scan Mode	Centroid
Spectrum Assigned	52.6% [25-363/0-100]	Spectrum Type	MS
TIC	435.17	Total Signal	6128410.75

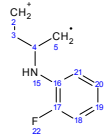
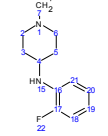
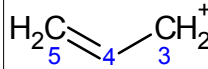
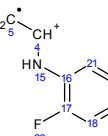
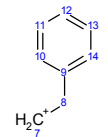
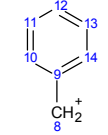
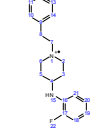
15010007_2014-23818_EI+_7.768.esp



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Table of fragments

No.	Fragment	Structure	Formula	Label	<i>m/z</i> Calc.	TIC Calc. (%)	Difference (Da)	<i>m/z</i> Exp.	RI Exp. (%)	TIC Exp. (%)
1	2-5,15-22(-H)		C10H11FN	M - C9H12N	164.087	25.789	0.013	164.100	100.000	25.789
2	1-7,15-22		C12H16FN2	M - C7H7	207.129	10.356	0.071	207.200	39.112	10.356
3	3-5(+H3)		C3H8	M - C16H15FN2	44.062	6.116	0.038	44.100	25.723	6.082
4	4-5,15-22(-H)		C8H7FN	M - C11H16N	136.056	3.835	0.044	136.100	15.212	3.835
5	7-14		C8H9	M - C11H14FN2	105.070	3.086	0.030	105.100	12.283	3.086
6	8-14		C7H7	M - C12H16FN2	91.054	3.011	0.046	91.100	12.119	3.011
7	M		C19H23FN2	M	298.184	0.494	0.016	298.200	1.725	0.494

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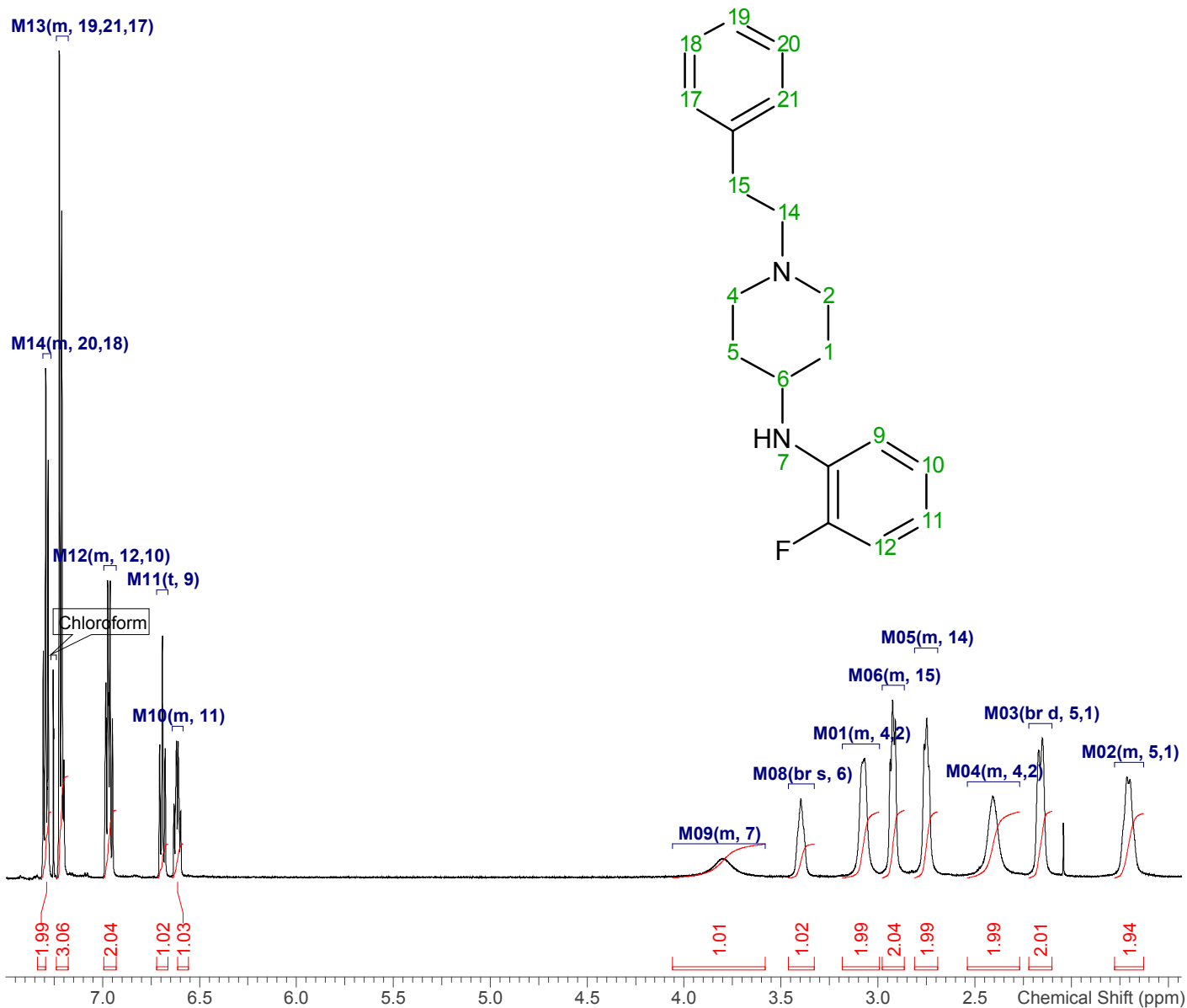
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Data from BCIM group at JRC, IHCP Ispra

NMR spectra

Acquisition Time (sec)	2.7263	Comment	15010007 - Paris 23818		
Date	22 Jan 2015 14:39:07	Date Stamp	22 Jan 2015 14:39:07		
File Name	\\s-jrciprna004p-fs-vihcp.jrc.it\ihcp\$\N01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure\BCIM_NAS\BCIM_600\15010007\30\PDATA\1\1r				
Frequency (MHz)	600.1300	Nucleus	1H	Number of Transients	16
Origin	spect	Original Points Count	32768	Owner	nmrsu
Points Count	65536	Pulse Sequence	zg30	Receiver Gain	1.91
SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3688.0654
Spectrum Type	standard	Sweep Width (Hz)	12019.05	Temperature (degree C)	27.000

15010007.030.001.1r.esp



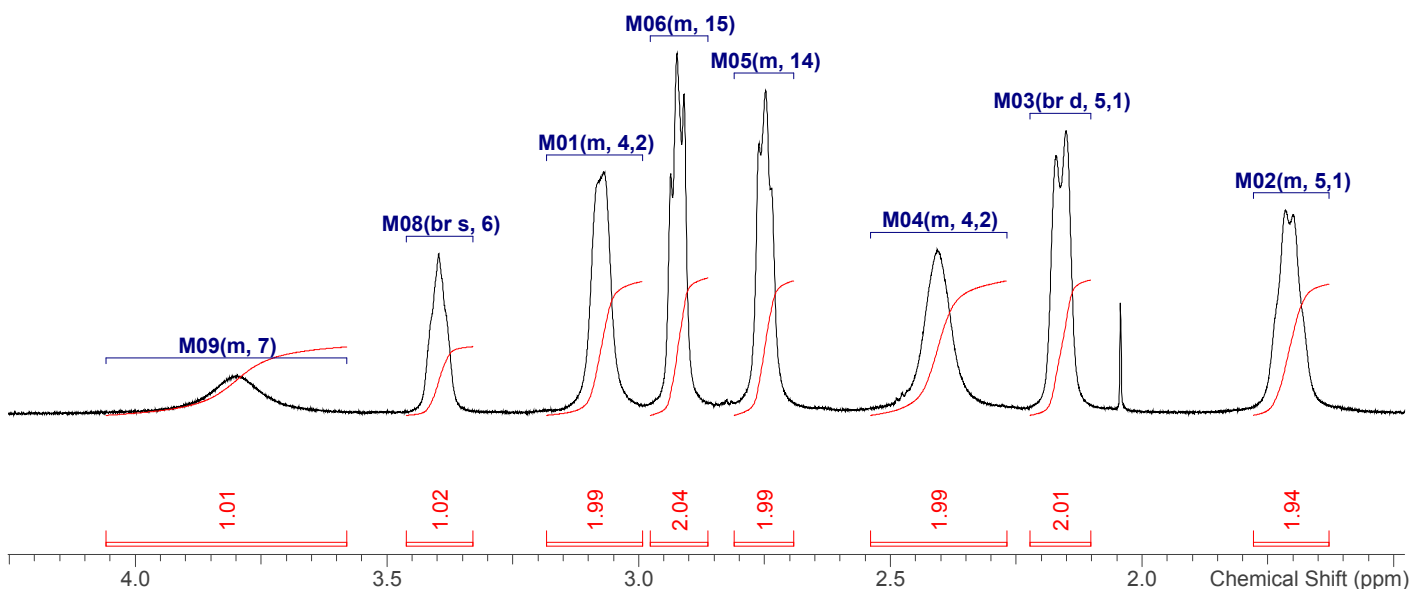
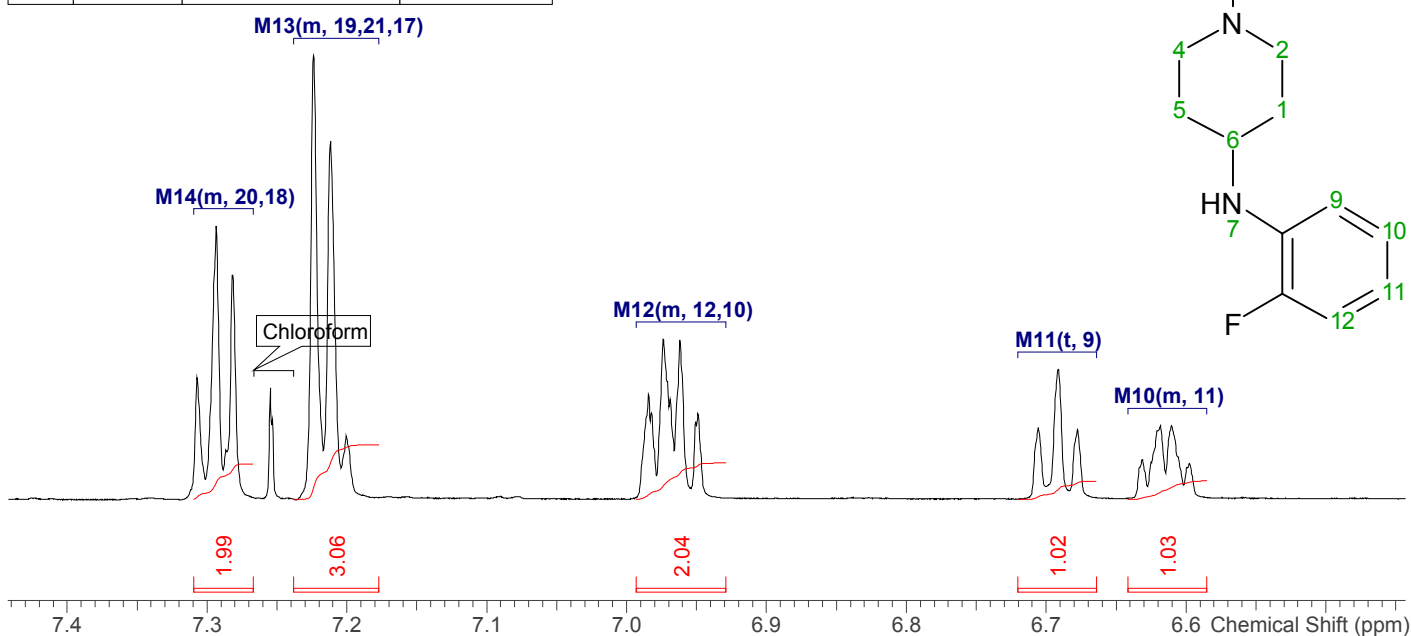
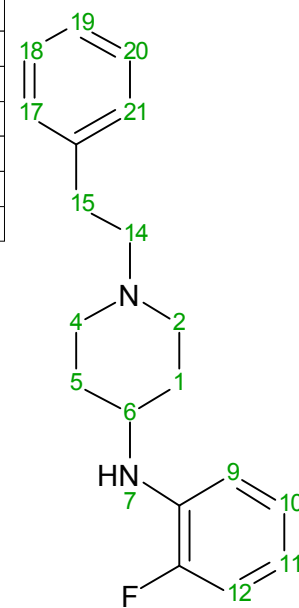
¹H NMR (600 MHz, CHLOROFORM-*d*) δ ppm 1.63 - 1.78 (m, 2 H) 2.16 (br d, *J*=11.74 Hz, 2 H) 2.27 - 2.54 (m, 2 H) 2.69 - 2.81 (m, 2 H) 2.86 - 2.98 (m, 2 H) 2.99 - 3.18 (m, 2 H) 3.40 (br s, 1 H) 3.58 - 4.06 (m, 1 H) 6.59 - 6.64 (m, 1 H) 6.69 (t, *J*=8.44 Hz, 1 H) 6.93 - 6.99 (m, 2 H) 7.18 - 7.24 (m, 3 H) 7.27 - 7.31 (m, 1 H)

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Table of assignments and zoomed parts:

No.	Atom	Exp. Shift (ppm)	Multiplet	No.	Atom	Exp. Shift (ppm)	Multiplet
1	5	1.71	M02	12	7	3.80	M09
2	1	1.71	M02	13	11	6.62	M10
3	5	2.16	M03	14	9	6.69	M11
4	1	2.16	M03	15	12	6.97	M12
5	4	2.42	M04	16	10	6.97	M12
6	2	2.42	M04	17	19	7.22	M13
7	14	2.75	M05	18	21	7.22	M13
8	15	2.92	M06	19	17	7.22	M13
9	4	3.08	M01	20	20	7.29	M14
10	2	3.08	M01	21	18	7.29	M14
11	6	3.40	M08				

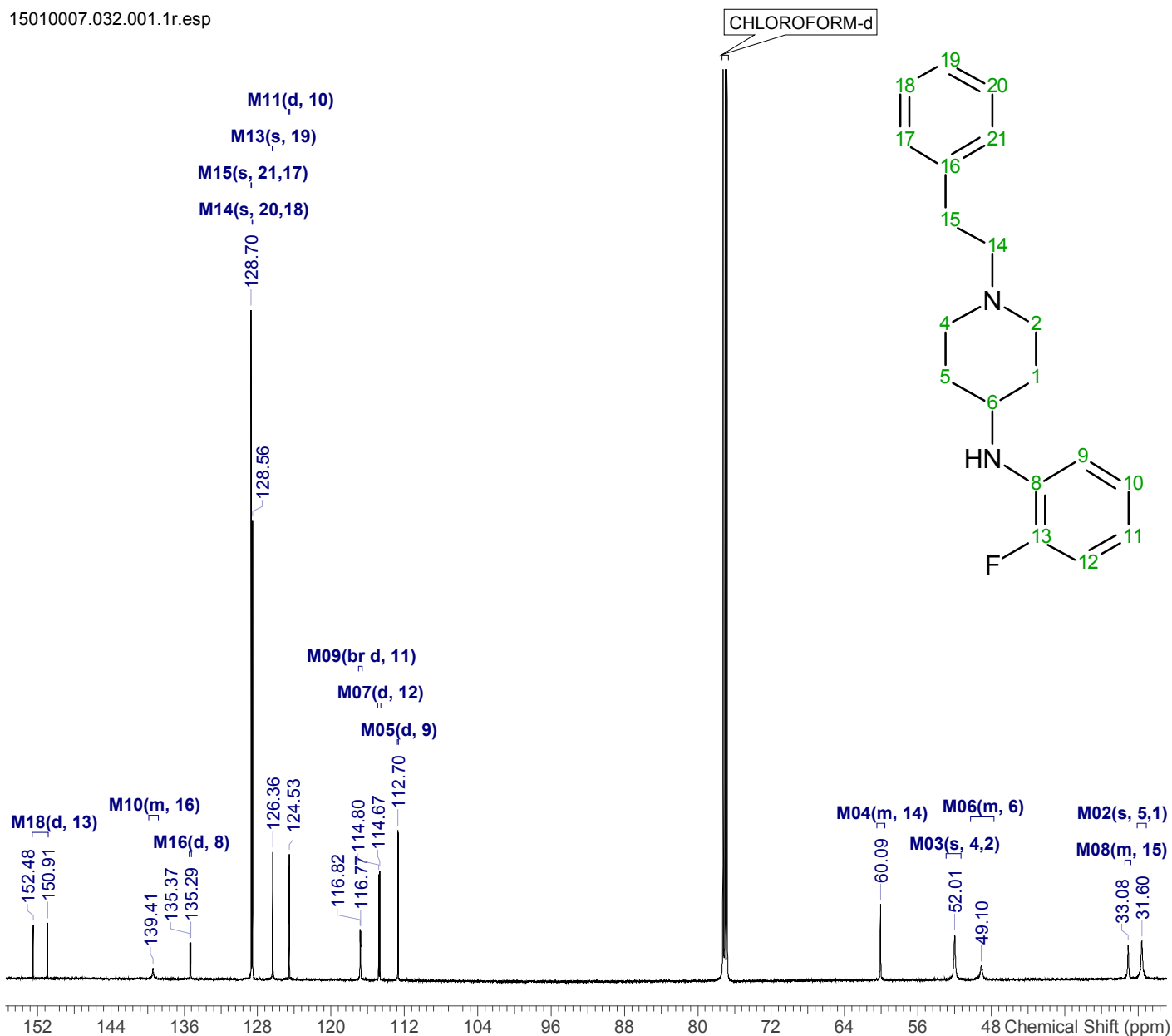


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Acquisition Time (sec)	0.9088	Comment	5 mm CPQCI 1H/19F-13C/15N/D Z-GRD Z114073/0012
Date	22 Jan 2015 12:07:09	Date Stamp	22 Jan 2015 12:07:09
File Name	\\s-jrciprna004p-fs-vihcp.jrc.it\ihcp\$\101\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure\BCIM_NAS\BCIM_600\15010007\32\pdata\1\1r		
Frequency (MHz)	150.9028	Nucleus	13C
Number of Transients	2048	Origin	spect
Original Points Count	32768	Owner	nmsu
Points Count	32768	Pulse Sequence	zpgg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	36057.69
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	15089.0967
Spectrum Type	standard	Sweep Width (Hz)	36056.59
Temperature (degree C)	27.002		

15010007.032.001.1r.esp



¹³C NMR (151 MHz, CHLOROFORM-*d*) δ ppm 31.60 (s, 1 C) 32.83 - 33.43 (m, 1 C) 47.70 - 50.26 (m, 1 C) 52.01 (s, 1 C) 59.61 - 60.48 (m, 1 C) 112.69 (d, *J*=3.30 Hz, 1 C) 114.74 (d, *J*=18.71 Hz, 1 C) 116.80 (br d, *J*=6.60 Hz, 1 C) 124.54 (d, *J*=3.30 Hz, 1 C) 126.36 (s, 1 C) 128.56 (s, 1 C) 128.70 (s, 1 C) 135.33 (d, *J*=12.10 Hz, 1 C) 138.84 - 139.85 (m, 1 C) 151.70 (d, *J*=237.69 Hz, 1 C)

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Table of assignments and zoomed parts:

No.	Atom	Exp. Shift (ppm)	Multiplet	No.	Atom	Exp. Shift (ppm)	Multiplet
1	5	31.60	M02	11	10	124.54	M11
2	1	31.60	M02	12	19	126.36	M13
3	15	33.10	M08	13	20	128.56	M14
4	6	49.14	M06	14	18	128.56	M14
5	4	52.01	M03	15	21	128.70	M15
6	2	52.01	M03	16	17	128.70	M15
7	14	60.04	M04	17	8	135.33	M16
8	9	112.69	M05	18	16	139.38	M10
9	12	114.74	M07	19	13	151.70	M18
10	11	116.80	M09				

