FACT SHEET

N-ethyl hexedrone

March 2016

For more information, please contact:
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The information contained in this document is also available on the BEWSD-website (with corresponding pdf-files and analytical data).
This part of the website is not accessible for the general public.
A login can be requested by contacting ews.drugs@wiv-isp.be.

A. General information

Recent collected sample in Belgium

Substance: N-ethylhexedrone

Date of seizure: 1 case October 2015, 2 cases November 2015

Date of analysis: February 2nd, 2016

Product type: Cathinone

Region: Bierset Airport

Total weight: 50 g

Created

March

Type

Psychotropic substances

Group

Cathinones

Name

N-ethylhexedrone

Nature of substance

N-ethylhexedrone is a cathinone and is the N-ethyl derivative of the previously notified cathinone hexedrone (β-propylmethcathinone). It is also bears structural similarity to alpha-PHP (α-pyrrolidinohexanophenone), differing by the presence of an N-ethyl moiety in place of the pyrrolidine moiety. N-ethylbuphedrone and N-ethylnorpentedrone are similar derivatives. NEH was created after the wide ban on NPS in China (dating 1.10.2015)

Systematic chemical name

2-(ethylamino)-1-phenylhexan-1-one

Other names

1-phenyl-2-ethylamino-hexanone

Common name

NEH

Other names

HEX-EN; Ethyl-hexedrone and Ethyl-Hex

B. Alerts

Alerts

No alerts.

Reports to EMCDDA

Belgium: On 2 March 2016 the Belgian FP reported 3 seizures totalizing 50g white powder, by the Customs department, 3 shipments total, 1 in October 2015, 2 in November 2015, at Bierset Airport. Analysis done by JRC. Parcels coming from China.

Czech Republic: On 1 March 2016 the Czech FP reported a seizure of 1 bag with white powder, 1 g- sent by mail (probably from Poland), seized on 16.02.2016 by the Police at Prague. It was analytically confirmed by GC-MS and FTIR at Institute of Criminalistics in Prague.

Germany: On 18 February 2016 the German FP reported a collected sample of 10 grams of white powder (bought as Hex-Pentedron) by the Forensic Toxicology Department, Institute of Forensic Medicine at the University Medical Center Freiburg (Germany) in November 2015. The substance was analytically confirmed by GC-EI-MS and by 1H- and 13C-NMR. The substance was collected from a Chniese Onlineshop.

Not country-specific or non-EU country: Formal notification of 2-(ethylamino)-1-phenylhexan-1-one (N-ethylhexedrone) by Hungary as a new psychoactive substance under the terms of Council Decision 2005/387/JHA, 16 February 2016

Netherlands: On 15 February 2016 the Dutch FP reported a seizure of 3 kilograms of white powder by Dutch Customs in Heerenveen on 22 December 2015. The circumstances of the seizure were reported as a case of distribution. The substance was analytically confirmed by GC-MS, FT-IR and NMR.

Slovenia: On 7 February 2016 the Slovenian FP reported a collected sample of 0.14 grams of white powder by Police/Slovenian EWS in the frame of the EU project 1-SEE in Ljubljana on 8 January 2016. The substance was analytically confirmed by GC-MS, HPLC-TOF, FTIR-ATR, Ion Chromatography and NMR.

Hungary: On 4 February 2016 the Hungarian FP reported a seizure of 2.57 grams of white powder by Hungarian Police at Heves in January 2016. The substance was analytically confirmed by ATR-FT-IR, GC/MS, H NMR and C NMR.

Belgium: During October 2015 and November 2015, 3 shipments were seized, totalling 50 g of NEH. Since initial analysis was unsuccesful, the compound was analysed by JRC, spectra can be found in attachment.

C. Pictures

None available.

D. Clinical information

Usage

Just like the close derivative cathinons, such as N-ethylbuphedrone (NEB), NEH is being sold on the internet, and is being used as a stimulant, mostly as a replacement for mephedrone. Specific information is not available.

Health risks

Pharmacology and Toxicology

N-ethylhexedrone was originally mentioned in a patent on Aminoketone Derivatives by Boehringer Ingelheim 1964. The patent described novel α-secondary-amino-ketones having valuable pharmacological properties and N-ethylhexedrone was reported as example 32 therein. Online vendors selling N-ethylhexedrone are marketing the substance as having similar effects as pentedrone, 4-CMC and 3-CMC.

Other uses

None known.

E. Legal status

Not controlled.

F. Chemistry

Systematic chemical name

2-(ethylamino)-1-phenylhexan-1-one

Chemical names

1-phenyl-2-ethylamino-hexanone

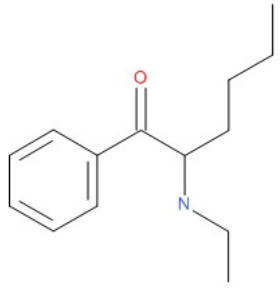
Common name

NEH

Other names

HEX-EN; Ethyl-hexedrone and Ethyl-Hex

Molecular structure



Molecular formula: C14H21NO

Molecular weight: 219.32

Identification and analytical profile can be found at the end of this document and were kindly provided by the Belgian FP (data from JRC).

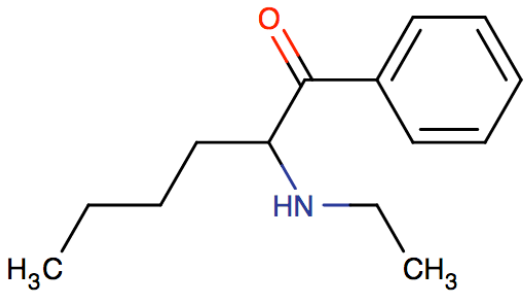
- 16010002.zip
- SCL 2015-30611-JRC-106010002.docx
- 15110016_report01.pdf
- 16010002_report01.pdf

G. References

Patent: GB1069797, 1964; Chem.Abstr., 1968, vol. 68, # 95537w

Sample SCL 2015-30611 (JRC Eurodat sample number: 106010002)

The interpretation of NMR results leads to the following molecular structure:



Obtained after drawing this molecule in http://cactus.nci.nih.gov/cgi-bin/lookup/search

the SMILES identified is: CCCCC(NCC)C(=O)c1ccccc1

Chemicalize.org

Input of SMILES (CCCCC(NCC)C(=O)c1ccccc1) in Chemicalize.org :

http://www.chemicalize.org/structure/#!mol=CCCCC%28NCC%29C%28%3DO%29c1ccccc1&source=calculate

IUPAC: 2-(ethylamino)-1-phenylhexan-1-one

Smiles: CCCCC(NCC)C(=O)c1ccccc1
InChI: 1/C14H21NO/c1-3-5-11-13(15-4-2)14(16)12-9-7-6-8-10-12/h6-10,13,15H,3-5,11H2,1-2H3
InChI key: CWNKMHIETKEBCA-UHFFFAOYNA-N

No URLs found for this structure

OPSIN:

http://opsin.ch.cam.ac.uk/

InChI:

InChI=1/C14H21NO/c1-3-5-11-13(15-4-2)14(16)12-9-7-6-8-10-12/h6-10,13,15H,3-5,11H2,1-2H3

StdInChIKey:

CWNKMHIETKEBCA-UHFFFAOYSA-N (Click to search the internet for this structure)

SMILES:

C(C)NC(C(=O)C1=CC=CC=C1)CCCC

The search CWNKMHIETKEBCA-UHFFFAOYSA-N (Click to search the internet for this structure) returns nothing:

Aucun document ne correspond aux termes de recherche spécifiés (**CWNKMHIETKEBCA-UHFFFAOYSA-N**).

But we found it on sale here:

http://chemicalcowboys.org/?wpsc_product_category=ethyl-hexedrone&view_type=default

Ethyl-Hexedrone 10g

Other Names: N-Ethyl-Hexedrone, Ethyl-Hex, NEH

IUPAC: 2-(ethylamino)-1-phenylhexan-1-one

CAS: N/A

Purity (HPLC): 98%

Strictly not for human consumption!

European Commission

Joint Research Centre

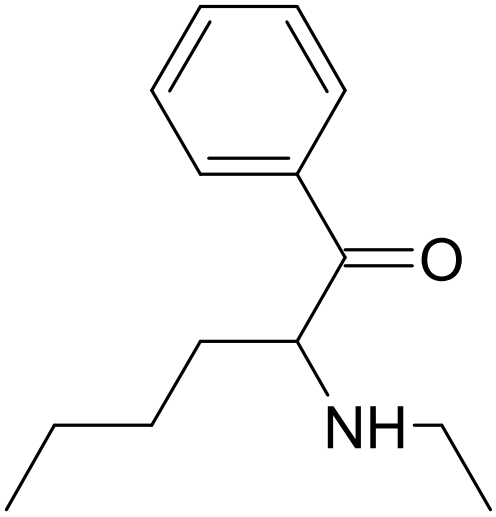
The European Commission's in-house science service

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 01/02/2016 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	16010002	***Received on***	08 January 2016
PACKAGING	1 glass vial beige powder (50 mg)		
Registration date	08 January 2016	***Name of customer***	Service commun des laboratoires France
Customer's identification	2015-30611		

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



Data of identified compound(s)

Formula	$C_{14}H_{21}NO$	***FW***	219.3226
Monoisotopic Mass	219.1623	***IUPAC Name (v.14.01)***	2-(ethylamino)-1-phenylhexan-1-one
InChI (v.1.04)	InChI=1S/C14H21NO/c1-3-5-11-13(15-4-2)14(16)12-9-7-6-8-10-12/h6-10,13,15H,3-5,11H2,1-2H3		
InChI Key (v.1.04)	CWNKMHIETKEBCA-UHFFFAOYSA-N		
SMILES (v.14.01)	O=C(C(CCCC)NCC)c1ccccc1		

Claude Guillou, Fabiano Reniero, Hubert Chassaigne, Joana Lobo Vicente, Veronica Holland, Salvatore Tirendi, Kamil Kolar

European Commission, Joint Research Centre

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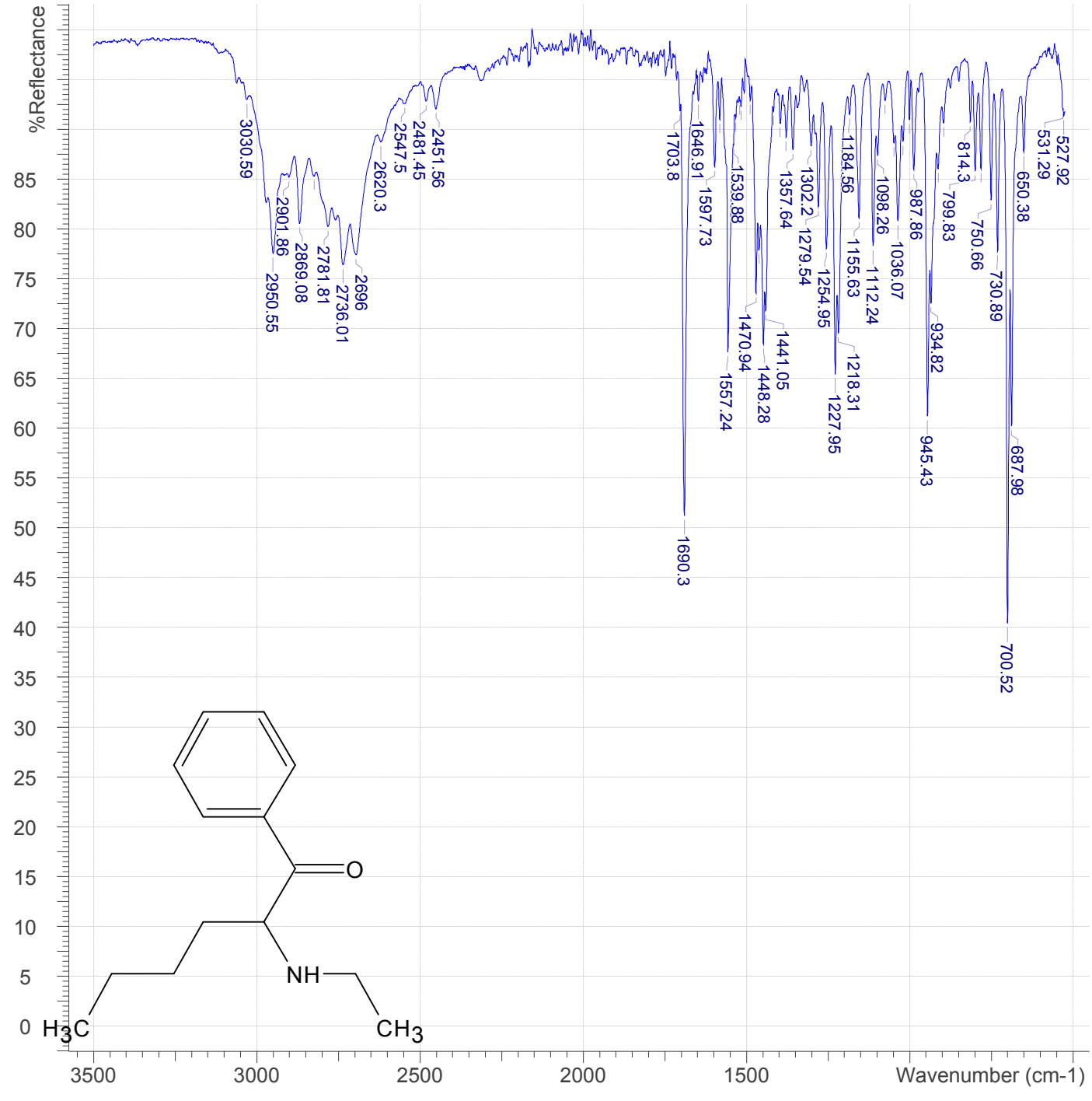
http://ihcp.jrc.ec.europa.eu

Processing and interpretation based on data provided by:

Service commun des laboratoires France

Title	30611		
File Name	\\139.191.6.82\ihcp-I01\BIO_CHEMICAL_INTERACTION_METABONOMICS\CLEN2SAND\!PROPOSED-STRUCTURE\CLEN_NAS\16010002_2015-30611\30611.SPA		
Date Stamp	13 Nov 2015 15:24:22	***Date***	13 Nov 2015 16:24:50
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		



Processing and interpretation based on data provided by:

Service commun des laboratoires France

Comment	vcr/eb	***Count***	195	***Data Type***	Condensed
Date	13 Nov 2015 18:27:22			***Date Stamp***	13 Nov 15 6:15 pm
Estimated Molecular Ion	543.500	***File Name***	2015-30611_Centroid_EI+		
Inlet Model	GC	***Ion Mode***	EI+	***Mass Spec Model***	STUP1
Plot Type	Stick	***Retention Time***	3.387		
Sample	Dans CH2Cl2/ CH3OH : 2015-30611			***Scan***	561
Scan Mode	Centroid	***Spectrum Assigned***	77.3% [34-546/0-100]		
TIC	187.44	***Total Signal***	1955715		

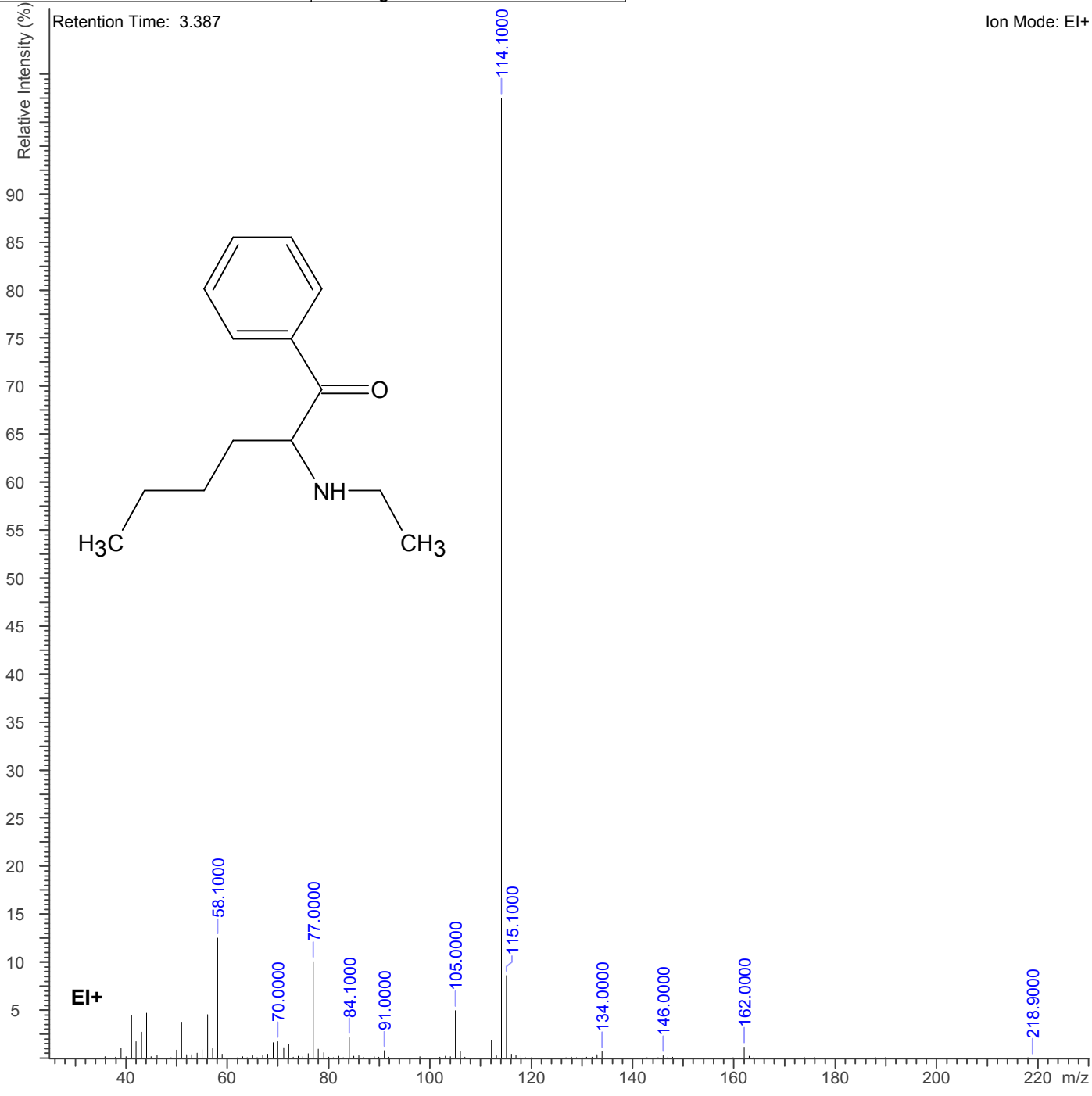
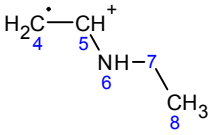
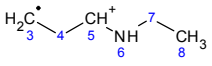
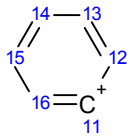
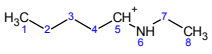
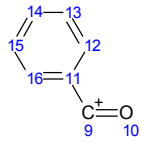
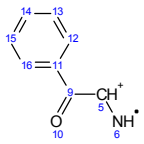
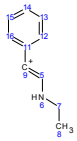
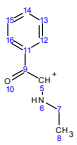
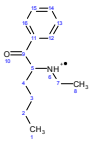
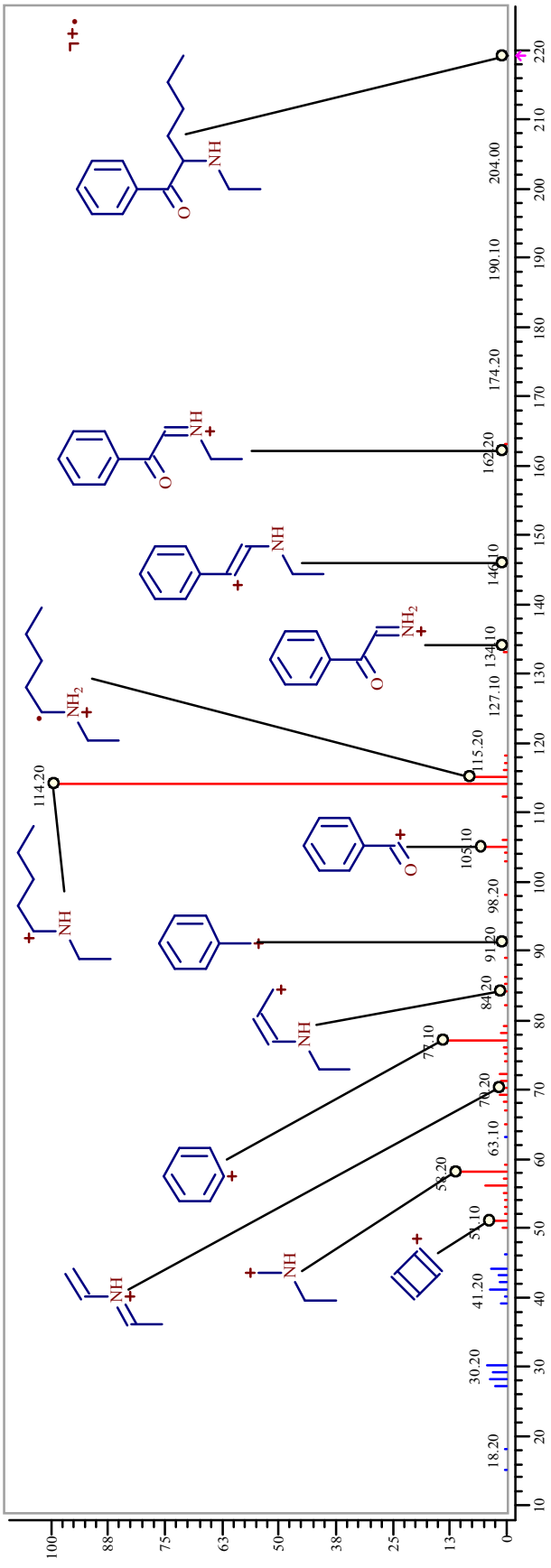


Table of fragments

No.	Fragment	Structure	Formula	Label	*m/z* Calc.	TIC Calc. (%)	Difference (Da)	*m/z* Exp.	RI Exp. (%)	TIC Exp. (%)	Origin
1	5-8(+H)		C3H8N	M - C11H13O	58.065	6.924	0.035	58.100	12.497	6.924	Manual
2	4-8(-H)		C4H8N	M - C10H13O	70.065	0.978	-0.065	70.000	1.745	0.978	Manual
3	3-8(-H)		C5H10N	M - C9H11O	84.081	1.208	0.019	84.100	2.132	1.208	Manual
4	11-16		C6H5	M - C8H16NO	77.039	5.740	-0.039	77.000	10.063	5.740	Manual
5	9,11-16(+H2)		C7H7	M - C7H14NO	91.054	0.450	-0.054	91.000	0.779	0.450	Manual
6	1-8		C7H16N	M - C7H5O	114.128	57.960	-0.028	114.100	100.000	57.960	Manual
7	9-16		C7H5O	M - C7H16N	105.033	2.858	-0.033	105.000	4.944	2.858	Manual
8	5-6,9-16(+H)		C8H8NO	M - C6H13	134.060	0.383	-0.060	134.000	0.652	0.382	Manual
9	5-9,11-16		C10H12N	M - C4H9O	146.096	0.153	-0.096	146.000	0.256	0.153	Manual
10	5-16		C10H12NO	M - C4H9	162.091	0.692	-0.091	162.000	1.153	0.692	Manual
11	M		C14H21NO	M	219.162	0.009	-0.262	218.900	0.014	0.009	Manual

Fragmentation of the observed molecule and the virtual MS (EI+) spectrum predicted by Thermo Scientific Mass Frontier



Processing and interpretation based on data provided by:

Service commun des laboratoires France

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File Name	30611mrm_BB5_01_9030_2_MS2_Positive			***Instrument***	impact HD
Ion Mode	Positive	***Operator***	SCL	***Parent Ion Mass (Da)***	220
Plot Type	Stick	***Retention Time***	6.127	***Sample ID***	30611mrm
Scan	674	***Scan Mode***	MS2	***Spectrum Assigned***	82.1% [45-964/0-100]
TIC	503.12	***Total Signal***	2282845.25		

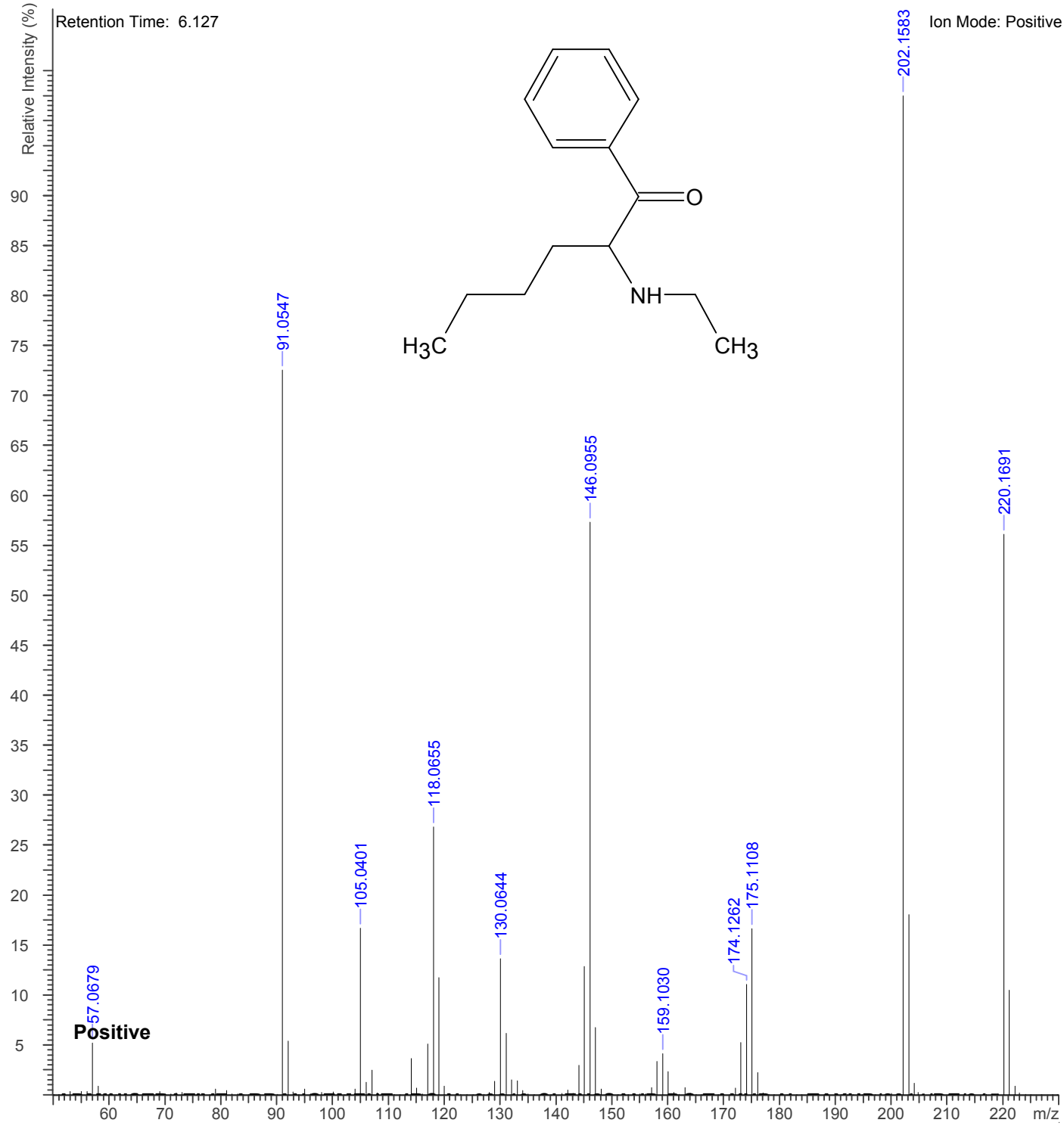
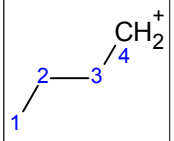
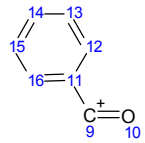
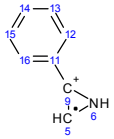
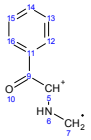
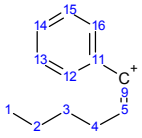
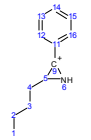
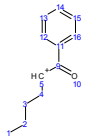
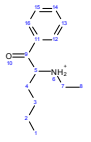


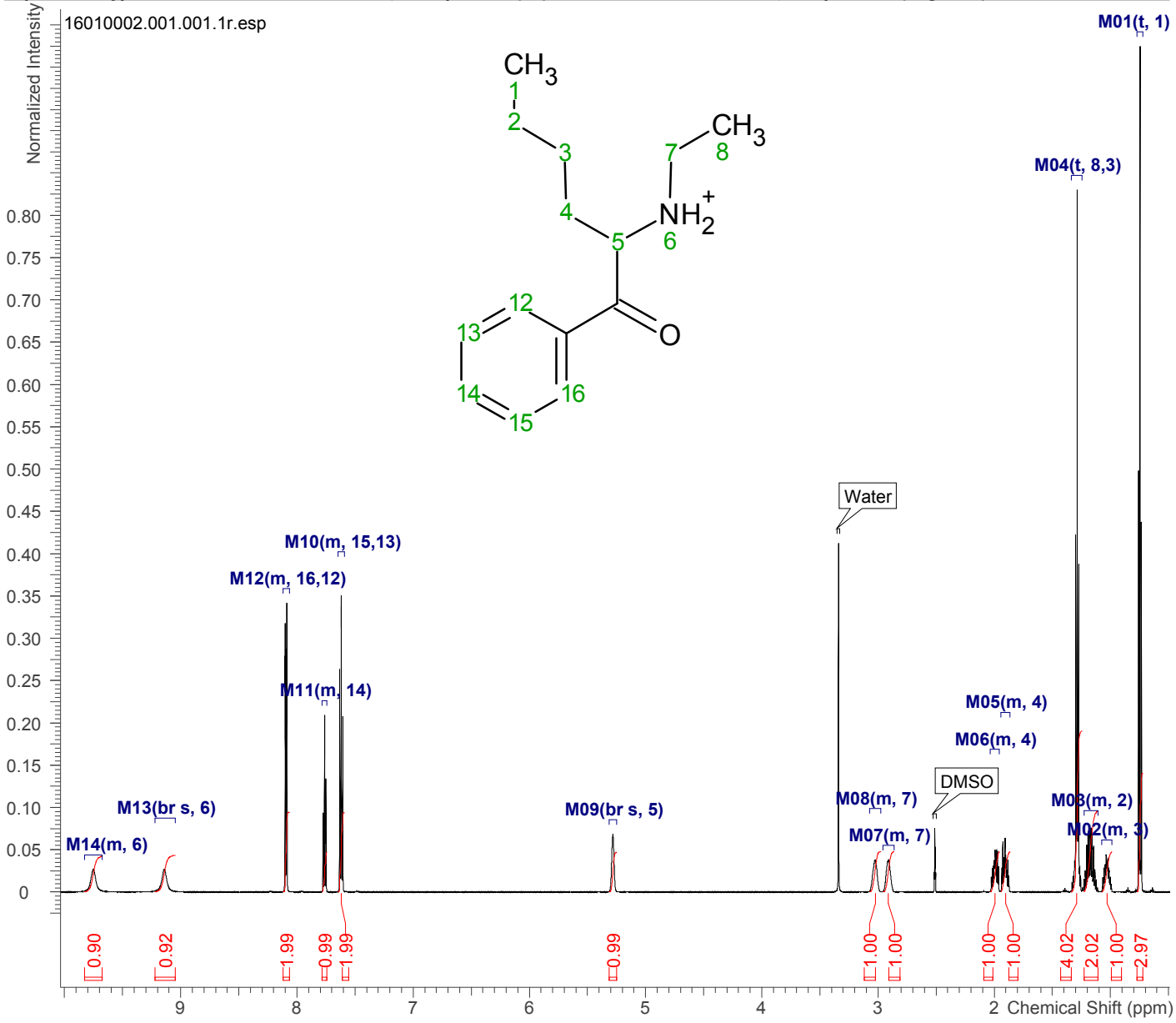
Table of fragments

No.	Fragment	Structure	Formula	Label	*m/z* Calc.	TIC Calc. (%)	Difference (Da)	*m/z* Exp.	RI Exp. (%)	TIC Exp. (%)	Origin
1	1-4(-H) [+H]		C4H9	M - C10H12NO	57.070	1.081	-0.002	57.068	5.197	1.081	Manual
2	9,11-16(+H) [+H]		C7H7	M - C7H14NO	91.054	15.586	0.000	91.055	72.523	15.535	Manual
3	9-16(-H) [+H]		C7H5O	M - C7H16N	105.033	3.597	0.007	105.040	16.703	3.586	Manual
4	5-6,9,11-16 [+H]		C8H8N	M - C6H13O	118.065	5.853	0.000	118.066	26.837	5.853	Manual
5	5-7,9-16(-H2) [+H]		C9H8NO	M - C5H13	146.060	12.670	0.035	146.095	57.319	12.670	Manual
6	1-5,9,11-16(-H) [+H]		C12H15	M - C2H6NO	159.117	0.934	-0.014	159.103	4.108	0.934	Manual
7	1-6,9,11-16(-H) [+H]		C12H16N	M - C2H5O	174.128	2.527	-0.002	174.126	11.073	2.527	Manual
8	1-5,9-16(-H) [+H]		C12H15O	M - C2H6N	175.112	3.790	-0.001	175.111	16.633	3.790	Manual
9	1-9,11-16(-H2) [+H]		C14H20N	M - HO	202.159	23.338	-0.001	202.158	100.000	23.338	Manual
10	M [+H]		C14H22NO	M + H	220.170	13.125	-0.001	220.169	56.097	13.125	Manual

Data from BCIM group at JRC, IHCP Ispra

NMR spectra

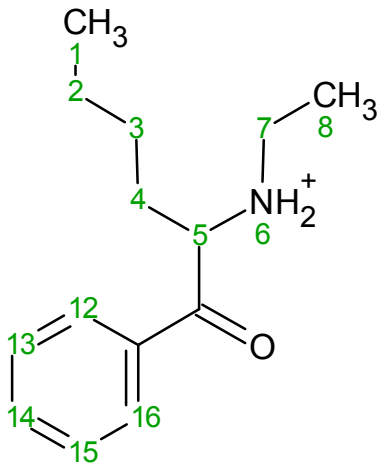
Acquisition Time (sec)	2.7263	***Comment***	2015-30611 10 mg in 600 uL DMSO-d6 Paris 01/ 2016		
Date	08 Jan 2016 19:16:41			***Date Stamp***	08 Jan 2016 19:16:41
File Name	\\139.191.6.82\ihcp-.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_600\16010002\1\PDATA\1\1r				
Frequency (MHz)	600.13	***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***	DMSO-d6	***Spectrum Offset (Hz)***	3706.0515
Spectrum Type	standard	***Sweep Width (Hz)***	12019.05	***Temperature (degree C)***	27.001

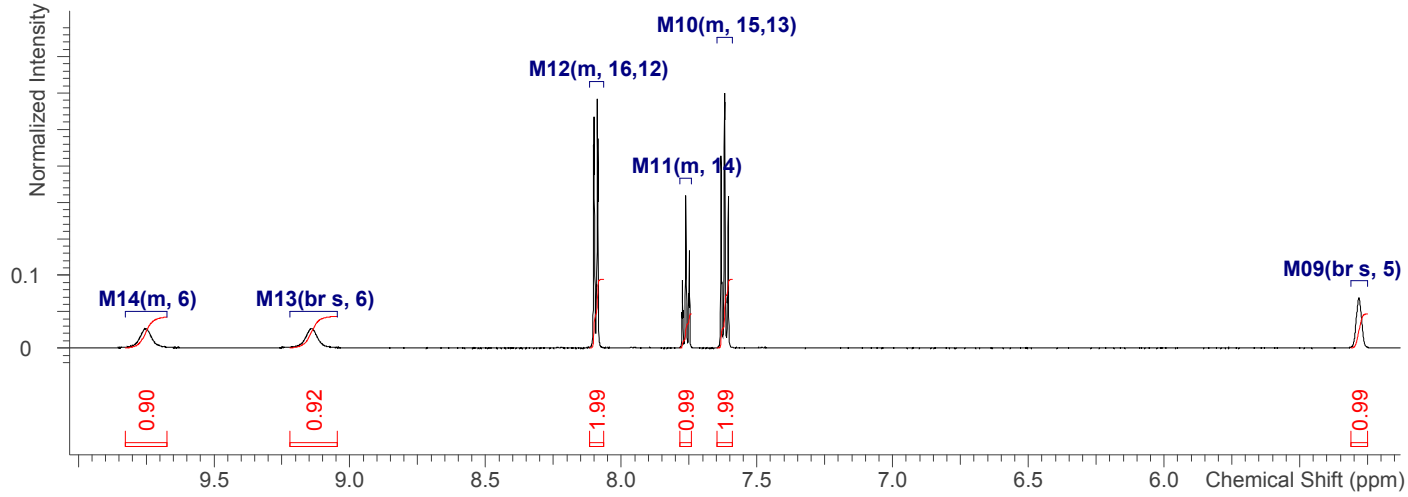


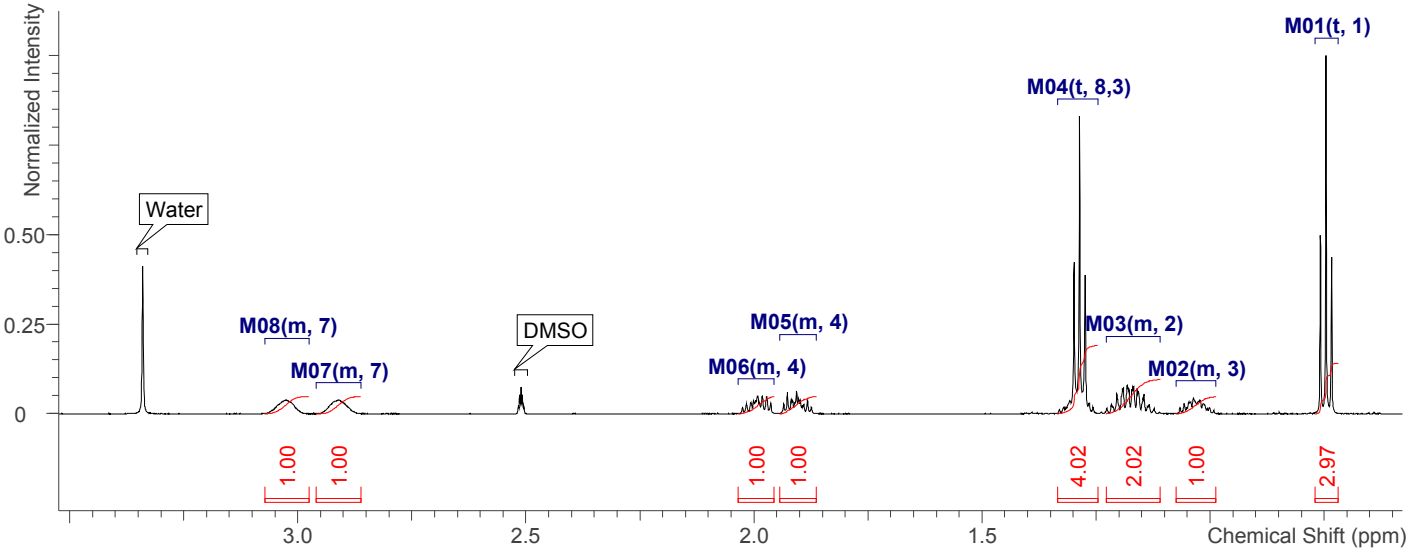
δ_H (DMSO-d_6): 9.67-9.83 (1H, m, M14), 9.14 (1H, br s, M13), 8.07-8.12 (2H, m, M12), 7.74-7.78 (1H, m, M11), 7.59-7.65 (2H, m, M10), 5.28 (1H, br s, M09), 2.98-3.07 (1H, m, M08), 2.86-2.96 (1H, m, M07), 1.96-2.03 (1H, m, M06), 1.86-1.94 (1H, m, M05), 1.29 (4H, t, *J*=7 Hz, M04), 1.11-1.23 (2H, m, M03), 0.99-1.07 (1H, m, M02), 0.75 (3H, t, *J*=7 Hz, M01)

Table of assignments and zoomed parts:

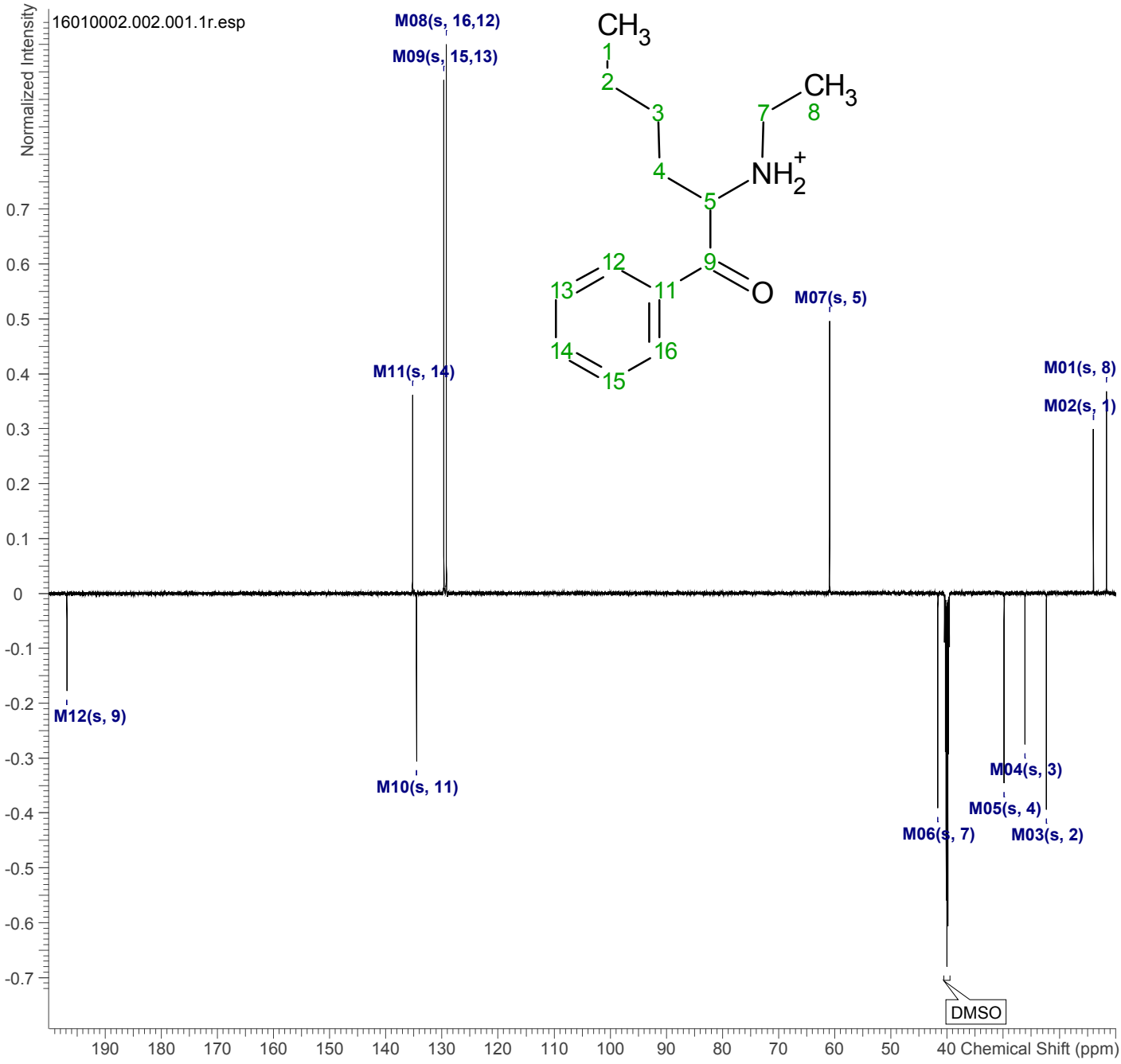
No.	Atom	Exp. Shift (ppm)	Multiplet
1	1	0.75	M01
2	3	1.03	M02
3	2	1.17	M03
4	8	1.29	M04
5	3	1.29	M04
6	4	1.91	M05
7	4	1.99	M06
8	7	2.91	M07
9	7	3.03	M08
10	5	5.28	M09
11	13	7.62	M10
12	15	7.62	M10
13	14	7.76	M11
14	12	8.09	M12
15	16	8.09	M12
16	6	9.14	M13
17	6	9.75	M14





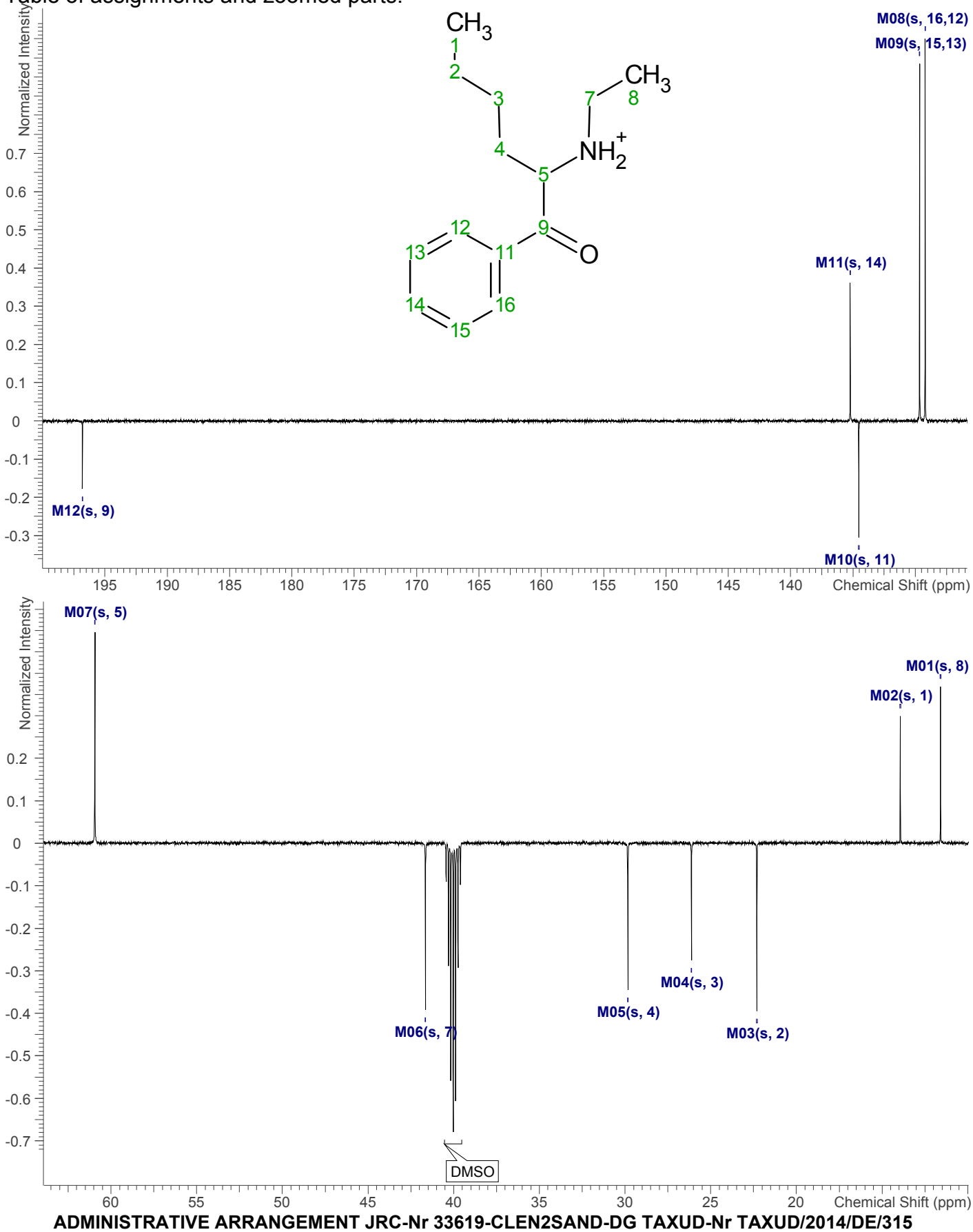


Acquisition Time (sec)	0.9044	***Comment***	5 mm CPQCI 1H/19F-13C/15N/D Z-GRD Z114073/0012
Date	08 Jan 2016 19:22:01	***Date Stamp***	08 Jan 2016 19:22:01
File Name	\\139.191.6.82\ihcp·.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_600\16010002_2015-30611\2\PDATA\1\1r		
Frequency (MHz)	150.90	***Nucleus***	13C
Number of Transients	256	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu
Points Count	32768	***Pulse Sequence***	jmod
Receiver Gain	183.05	***SW(cyclical) (Hz)***	36231.88
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	18108.3359
Spectrum Type	APT	***Sweep Width (Hz)***	36230.78
Temperature (degree C)	26.996		



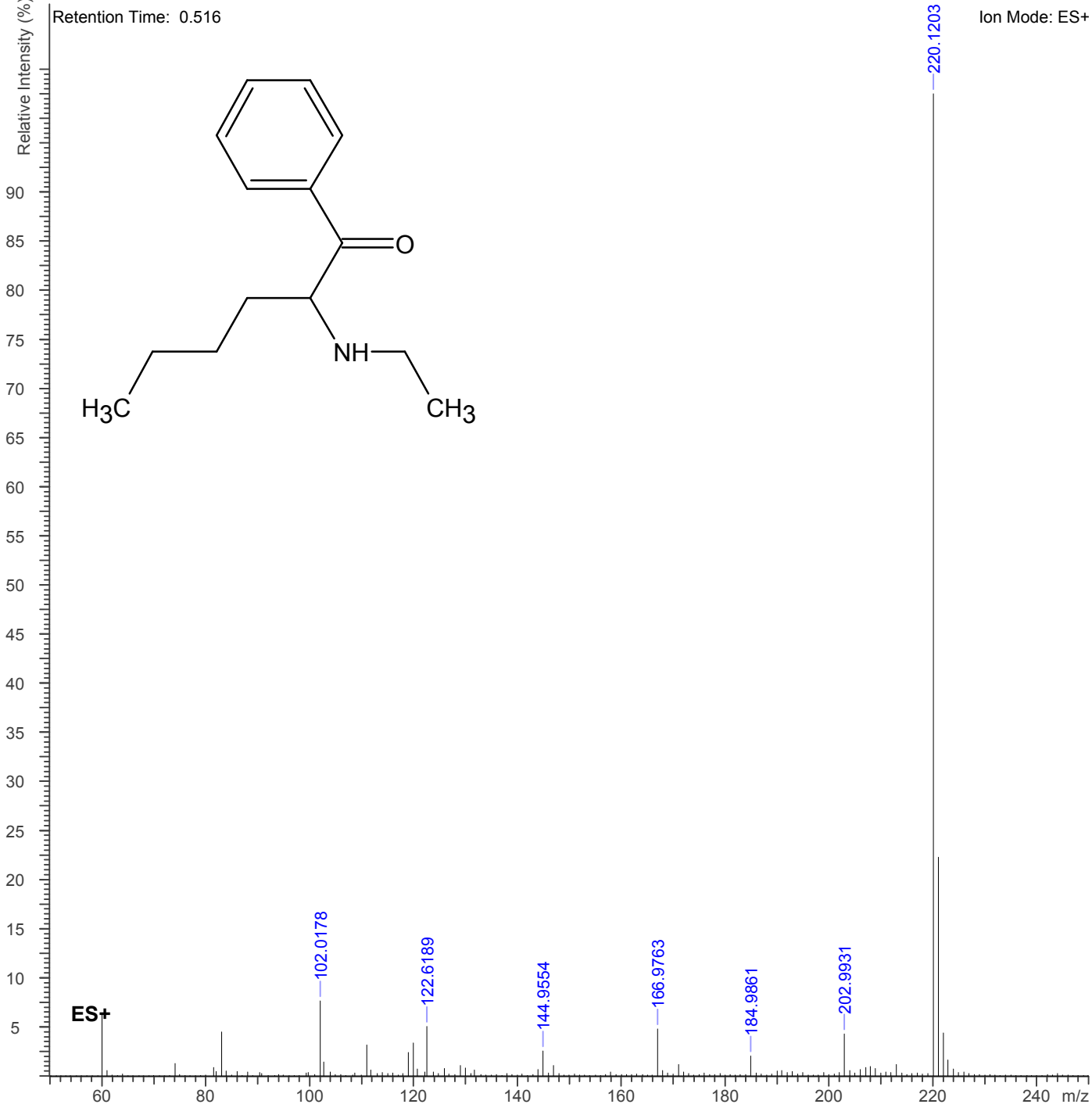
δ_C (DMSO-d_6): 196.8 (C-9), 135.2 (C-14), 134.5 (C-11), 129.7 (C-13, 15), 129.2 (C-16, 12), 60.9 (C-5), 41.7 (C-7), 29.8 (C-4), 26.1 (C-3), 22.3 (C-2), 13.9 (C-1), 11.6 (C-8)

Table of assignments and zoomed parts:



MS spectra

Combine	<2-55>	***Count***	201
Data Source Name	16010002_2015-30611_MS_50-250_1_Centroided Mass Spectrum_ES+		
Data Type	Centroided Mass Spectrum	***Date***	19 Jan 2016 17:26:41
Date Stamp	19 Jan 2016 16:53:02		
File Name	\\139.191.6.82\ihcp:·.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_QTOF\16010002_2015-30611\16010002_2015-30611_MS_50-250.CDF		
Inlet Model	Electrospray Inlet	***Ion Mode***	ES+
Plot Type	Stick	***Retention Time***	0.516
Scan	28	***Separation Type***	No Chromatography
Spectrum Assigned	53.5% [50-250/0-100]	***TIC***	219.87
Total Signal	18088.2031		



Combine	<3-51>	***Count***	201
Data Source Name	16010002_2015-30611_MSMS_220_15EV_50-250_1_Centroided Mass Spectrum_ES+		
Data Type	Centroided Mass Spectrum	***Date***	19 Jan 2016 17:26:41
Date Stamp	19 Jan 2016 16:54:48		
File Name	\\139.191.6.82\ihcp:.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_QTOF\16010002_2015-30611\16010002_2015-30611_MSMS_220_15EV_50-250.CDF		
Inlet Model	Electrospray Inlet	***Ion Mode***	ES+
Plot Type	Stick	***Retention Time***	0.811
Scan	44	***Separation Type***	No Chromatography
Spectrum Assigned	75.9% [50-250/0-100]	***TIC***	570.04
Total Signal	68643.875		

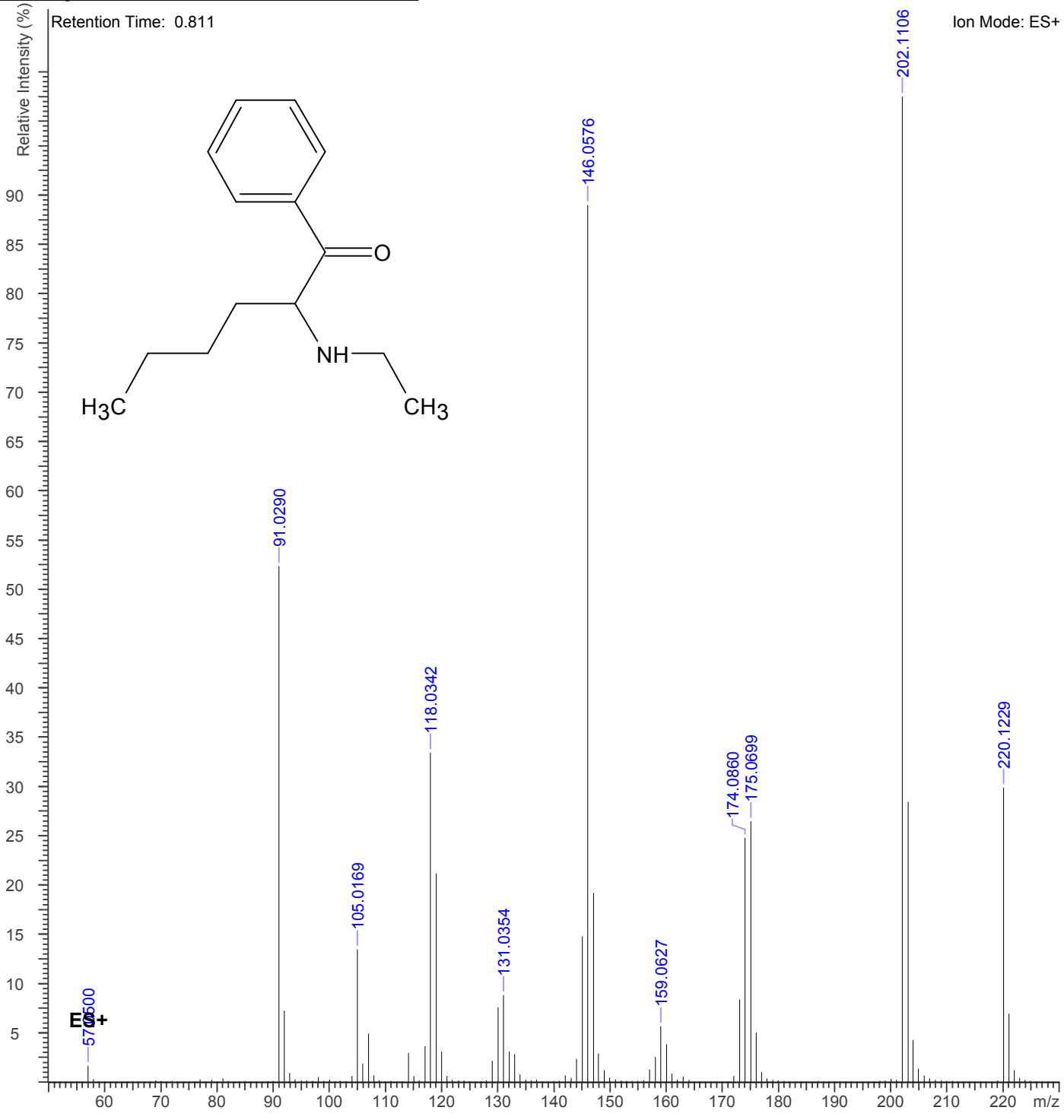
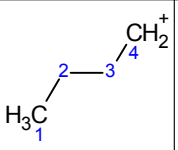
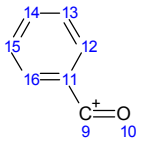
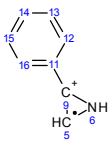
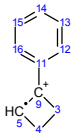
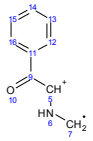
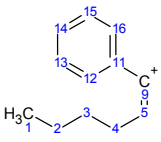
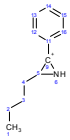
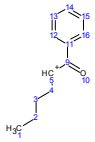
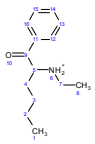
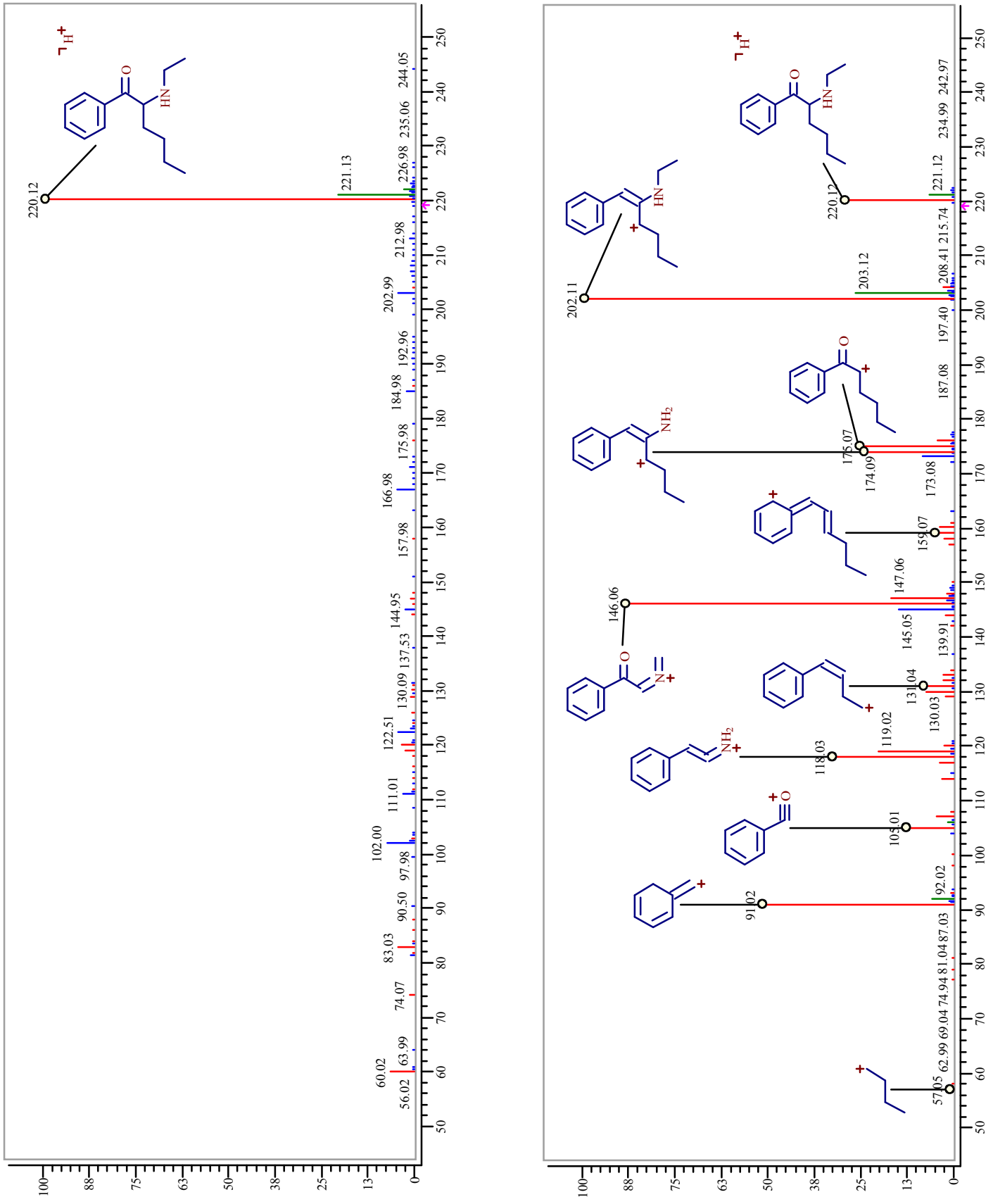


Table of fragments

No.	Fragment	Structure	Formula	Label	*m/z* Calc.	TIC Calc. (%)	Difference (Da)	*m/z* Exp.	RI Exp. (%)	TIC Exp. (%)	Origin
1	1-4		C4H9	M - C10H12NO	57.070	0.301	-0.020	57.050	1.640	0.301	Manual
2	9,11-16(+H2)		C7H7	M - C7H14NO	91.054	9.926	-0.025	91.029	52.331	9.926	Manual
3	9-16		C7H5O	M - C7H16N	105.033	2.550	-0.017	105.017	13.414	2.550	Manual
4	5-6,9,11-16(+H)		C8H8N	M - C6H13O	118.065	6.430	-0.031	118.034	33.399	6.430	Manual
5	3-5,9,11-16(+H)		C10H11	M - C4H10NO	131.086	1.725	-0.050	131.035	8.795	1.725	Manual
6	5-7,9-16(-H)		C9H8NO	M - C5H13	146.060	17.358	-0.002	146.058	88.973	17.358	Manual
7	1-5,9,11-16		C12H15	M - C2H6NO	159.117	1.128	-0.054	159.063	5.623	1.128	Manual
8	1-6,9,11-16		C12H16N	M - C2H5O	174.128	4.986	-0.042	174.086	24.755	4.986	Manual
9	1-5,9-16		C12H15O	M - C2H6N	175.112	5.314	-0.042	175.070	26.422	5.314	Manual
10	1-9,11-16(-H)		C14H20N	M - HO	202.159	20.599	-0.048	202.111	100.000	20.599	Manual
11	M(+H)		C14H22NO	M + H	220.170	6.160	-0.047	220.123	29.831	6.160	Manual

Fragmentation of the observed molecule and the virtual MS and MSMS spectra predicted by Thermo Scientific Mass Frontier



European Commission

Joint Research Centre

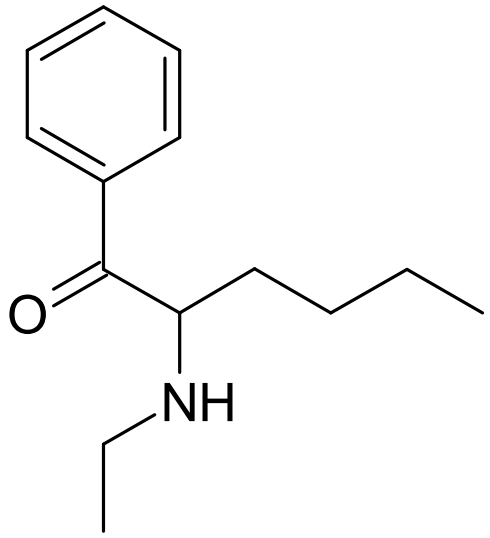
The European Commission's in-house science service

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 02/12/2015 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	15110016	***Received on***	27 November 2015
PACKAGING	50 mg white powder in glass vial		
Registration date	27 November 2015	***Name of customer***	Belgian Customs Laboratory
Customer's identification	15BD-00426-01		

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



Data of identified compound(s)

Formula	$C_{14}H_{21}NO$	***FW***	219.3226
Monoisotopic Mass	219.1623	***IUPAC Name (v.14.01)***	2-(ethylamino)-1-phenylhexan-1-one
InChI (v.1.04)	InChI=1S/C14H21NO/c1-3-5-11-13(15-4-2)14(16)12-9-7-6-8-10-12/h6-10,13,15H,3-5,11H2,1-2H3		
InChI Key (v.1.04)	CWNKMHIETKEBCA-UHFFFAOYSA-N		
SMILES (v.14.01)	O=C(C(CCCC)NCC)c1ccccc1		

Claude Guillou, Fabiano Reniero, Hubert Chassaigne, Joana Lobo Vicente, Veronica Holland, Salvatore Tirendi, Kamil Kolar

European Commission, Joint Research Centre

Institute for Health and Consumer Protection (IHCP)
Chemical Assessment and Testing Unit
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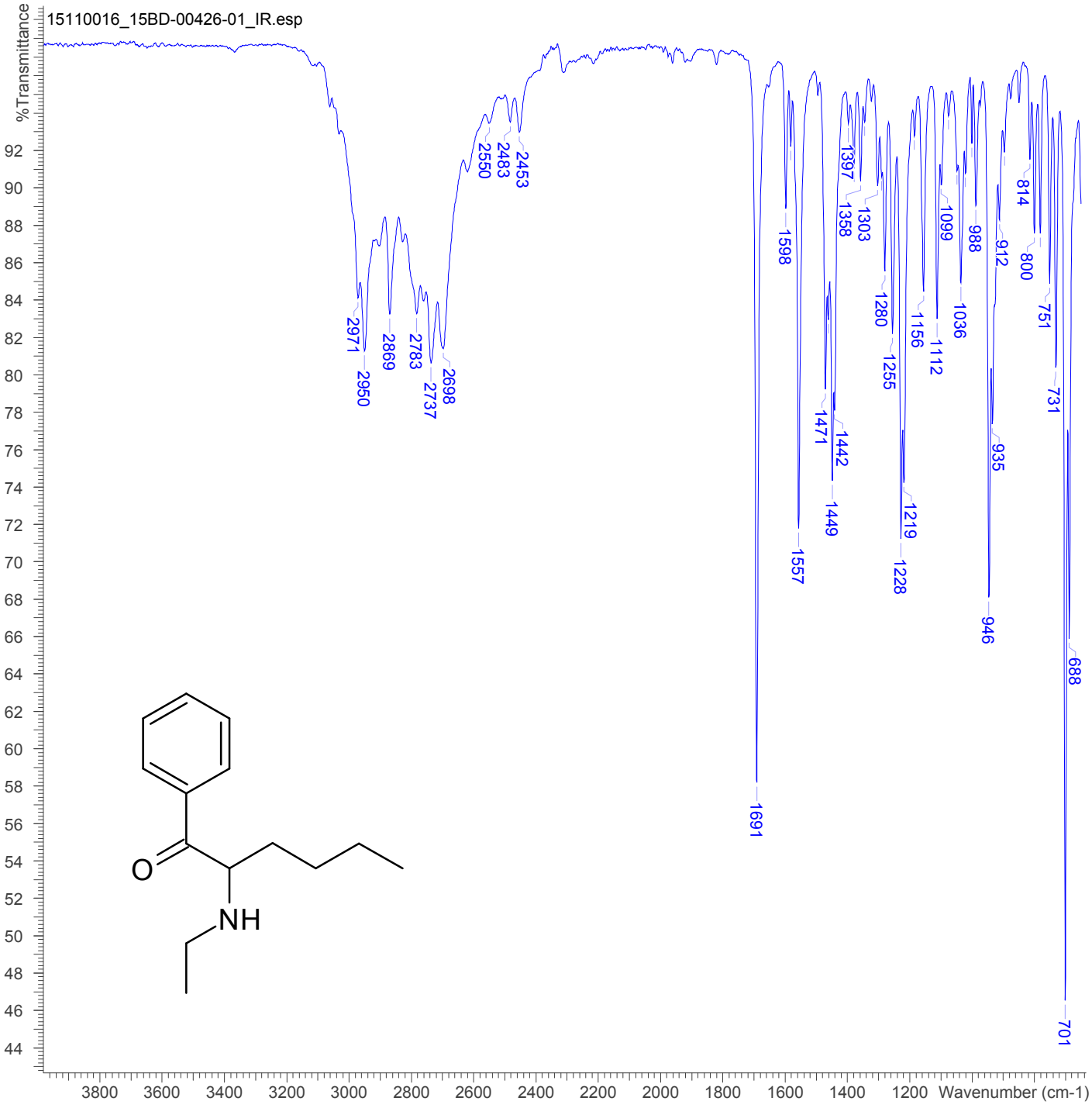
claude.guillou@jrc.ec.europa.eu
http://ihcp.jrc.ec.europa.eu

Processing and interpretation based on data provided by:

Belgian Customs Laboratory

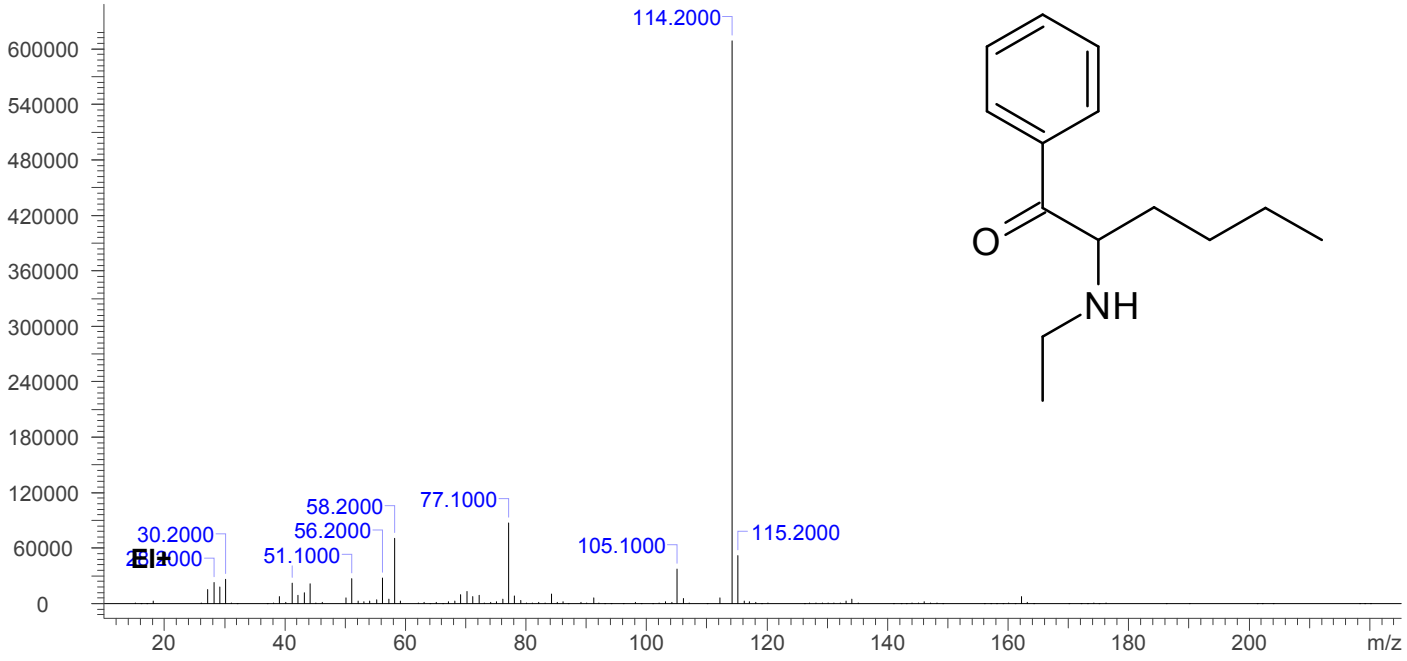
Comment	POEDER		
File Name	\\139.191.6.82\ihcp·I01\BIO_CHEMICAL_INTERACTION_METABONOMICS\CLEN2SAND\!PROPOSED-STRUCTURE\CLEN_NAS\15110016_15BD-00426-01\15BD-00426-01.SP		
Date Stamp	wed oct 28 14:44:18 2015	***Date***	wed oct 28 14:44:18 2015
Technique	Infrared	***Spectral Region***	IR
X Axis	Wavenumber (cm-1)	***Y Axis***	%Transmittance
Spectrum Range	650.0000 - 4000.0000	***Points Count***	3351
Data Spacing	1.0000		

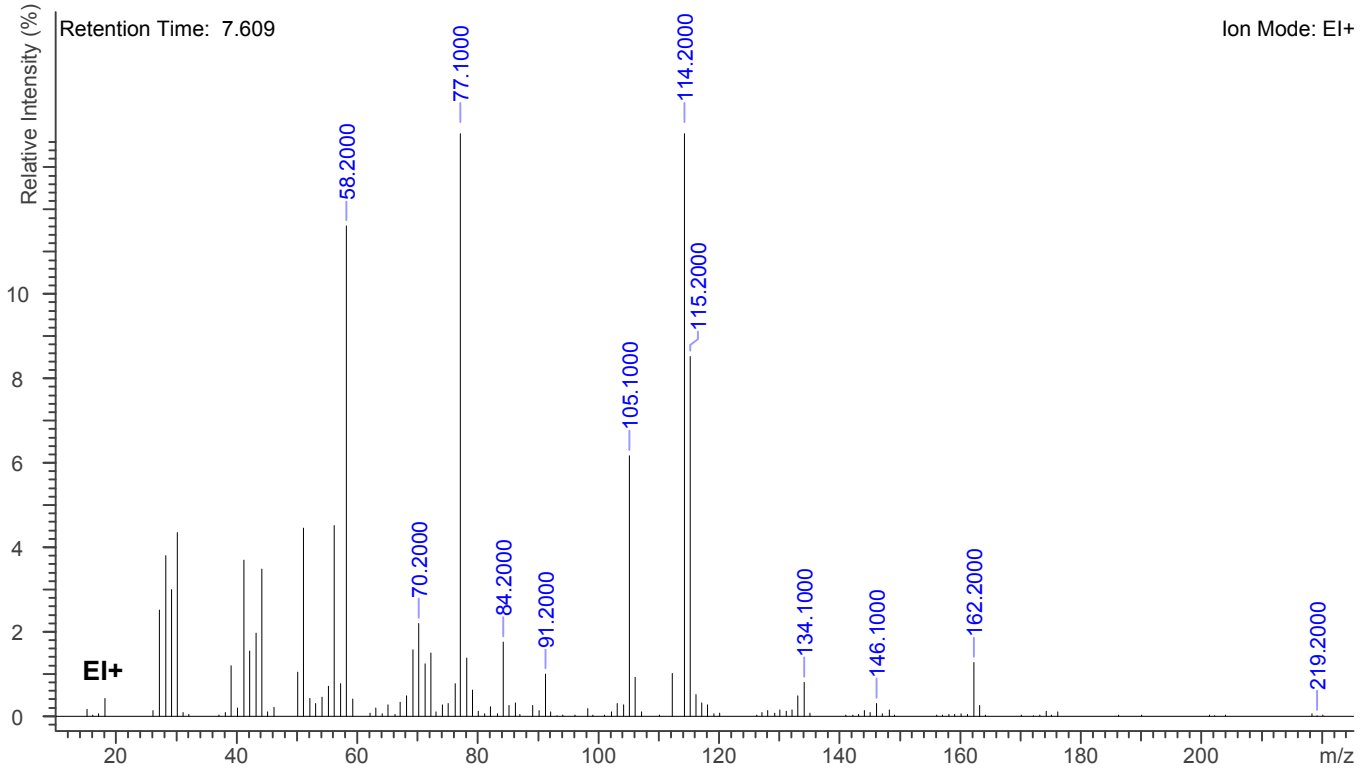


Processing and interpretation based on data provided by:

Belgian Customs Laboratory

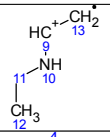
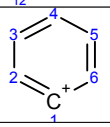
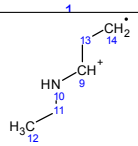
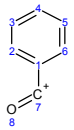
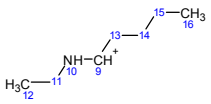
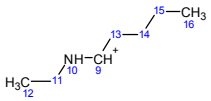
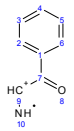
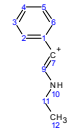
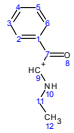
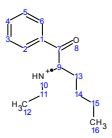
Comment	MTOH/DCM	***Count***	124	***Data Type***	Condensed
Date	28 Oct 2015 20:31:00			***Date Stamp***	28 Oct 15 8:01 pm
File Name	15BD-00426-01_1_Centroid_EI+			***Inlet Model***	GC
Ion Mode	EI+	***Mass Spec Model***	Instrumen	***Operator***	DL
Plot Type	Stick	***Retention Time***	7.609	***Sample***	15BD-00426-01
Scan	718	***Scan Mode***	Centroid	***Spectrum Assigned***	73.3% [15-220/0-100]
TIC	206.05	***Total Signal***	1254386		





ADMINISTRATIVE ARRANGEMENT JRC-Nr 33619-CLEN2SAND-DG TAXUD-Nr TAXUD/2014/DE/315

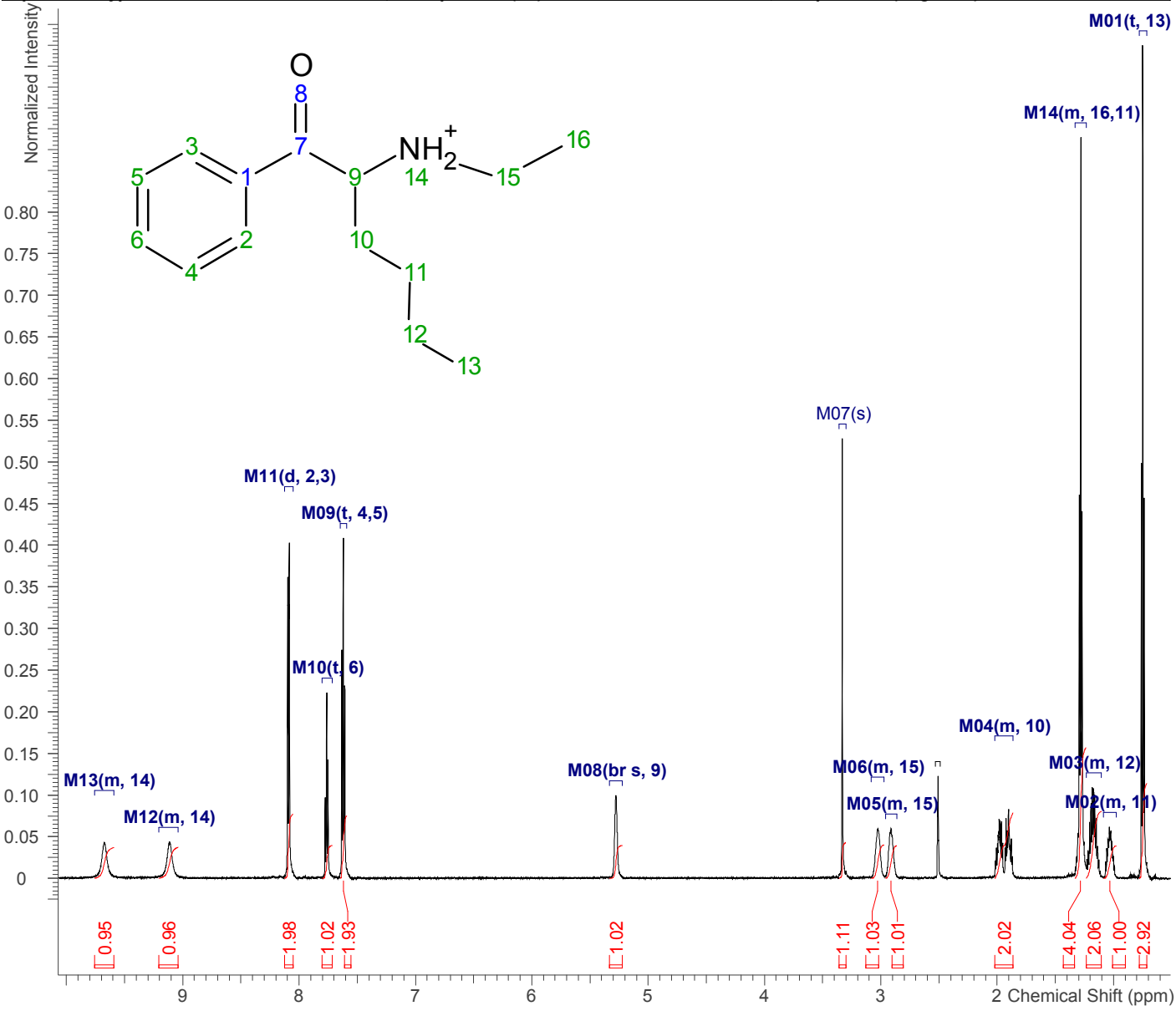
Table of fragments

No.	Fragment	Structure	Formula	Label	*m/z* Calc.	TIC Calc. (%)	Difference (Da)	*m/z* Exp.	RI Exp. (%)	TIC Exp. (%)	Origin
1	9-12(+H)		C3H8N	M - C11H13O	58.065	5.853	0.135	58.200	11.614	5.851	Manual
2	9-13(-H)		C4H8N	M - C10H13O	70.065	1.117	0.135	70.200	2.192	1.117	Manual
3	1-6		C6H5	M - C8H16NO	77.039	7.463	0.061	77.100	14.383	7.463	Manual
4	9-14(-H)		C5H10N	M - C9H11O	84.081	0.902	0.119	84.200	1.751	0.902	Manual
5	1-7(+H2)		C7H7	M - C7H14NO	91.054	0.525	0.146	91.200	1.001	0.525	Manual
6	1-8		C7H5O	M - C7H16N	105.033	3.244	0.067	105.100	6.169	3.243	Manual
7	9-16		C7H16N	M - C7H5O	114.128	52.724	0.072	114.200	100.000	52.724	Manual
8	9-16(+H)		C7H17N	M - C7H4O	115.136	4.492	0.064	115.200	8.518	4.419	Manual
9	1-10(+H)		C8H8NO	M - C6H13	134.060	0.424	0.040	134.100	0.795	0.422	Manual
10	1-7,9-12		C10H12N	M - C4H9O	146.096	0.165	0.004	146.100	0.302	0.165	Manual
11	1-12		C10H12NO	M - C4H9	162.091	0.694	0.109	162.200	1.270	0.693	Manual
12	M		C14H21NO	M	219.162	0.010	0.038	219.200	0.017	0.010	Manual

Data from BCIM group at JRC, IHCP Ispra

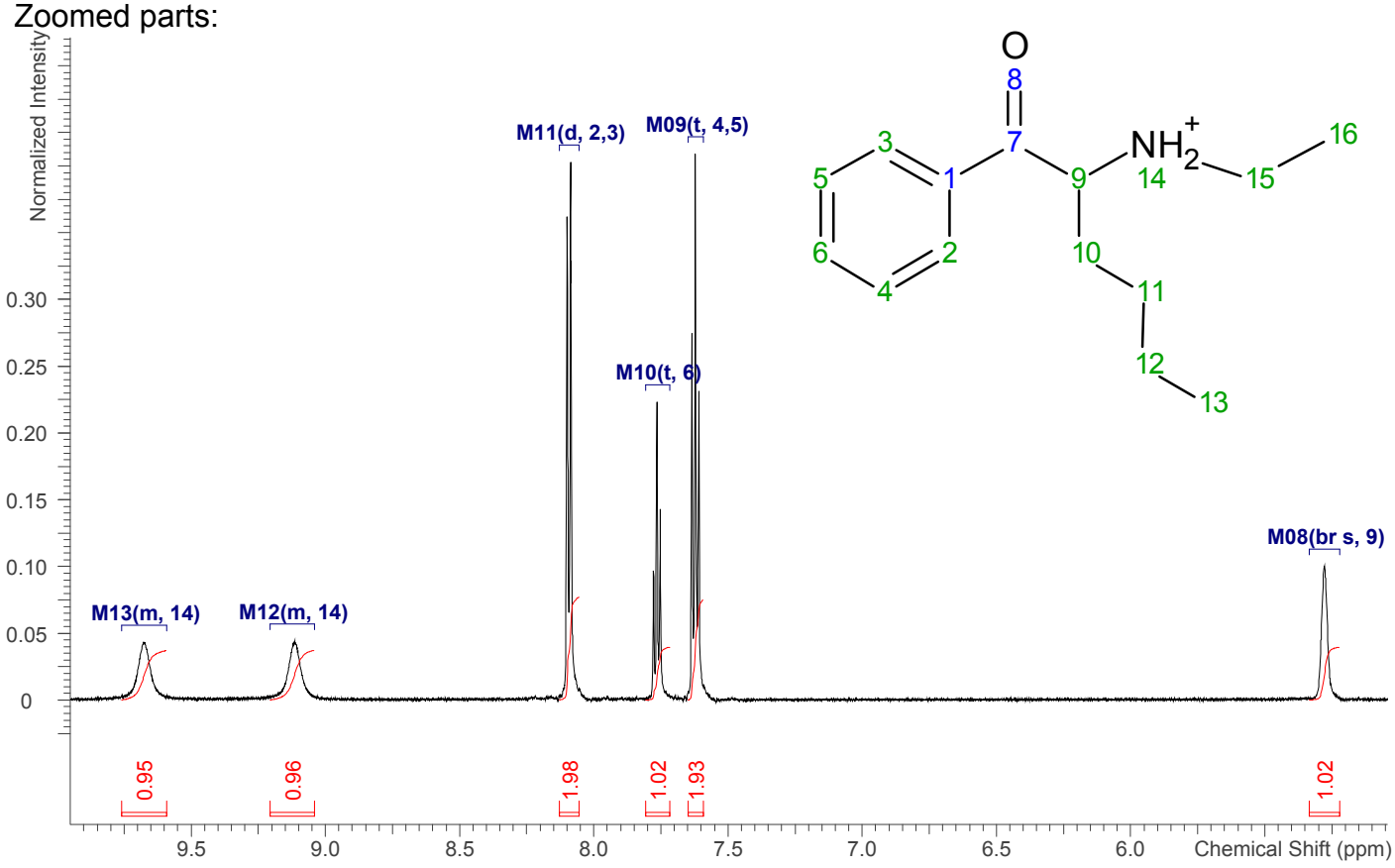
NMR spectra

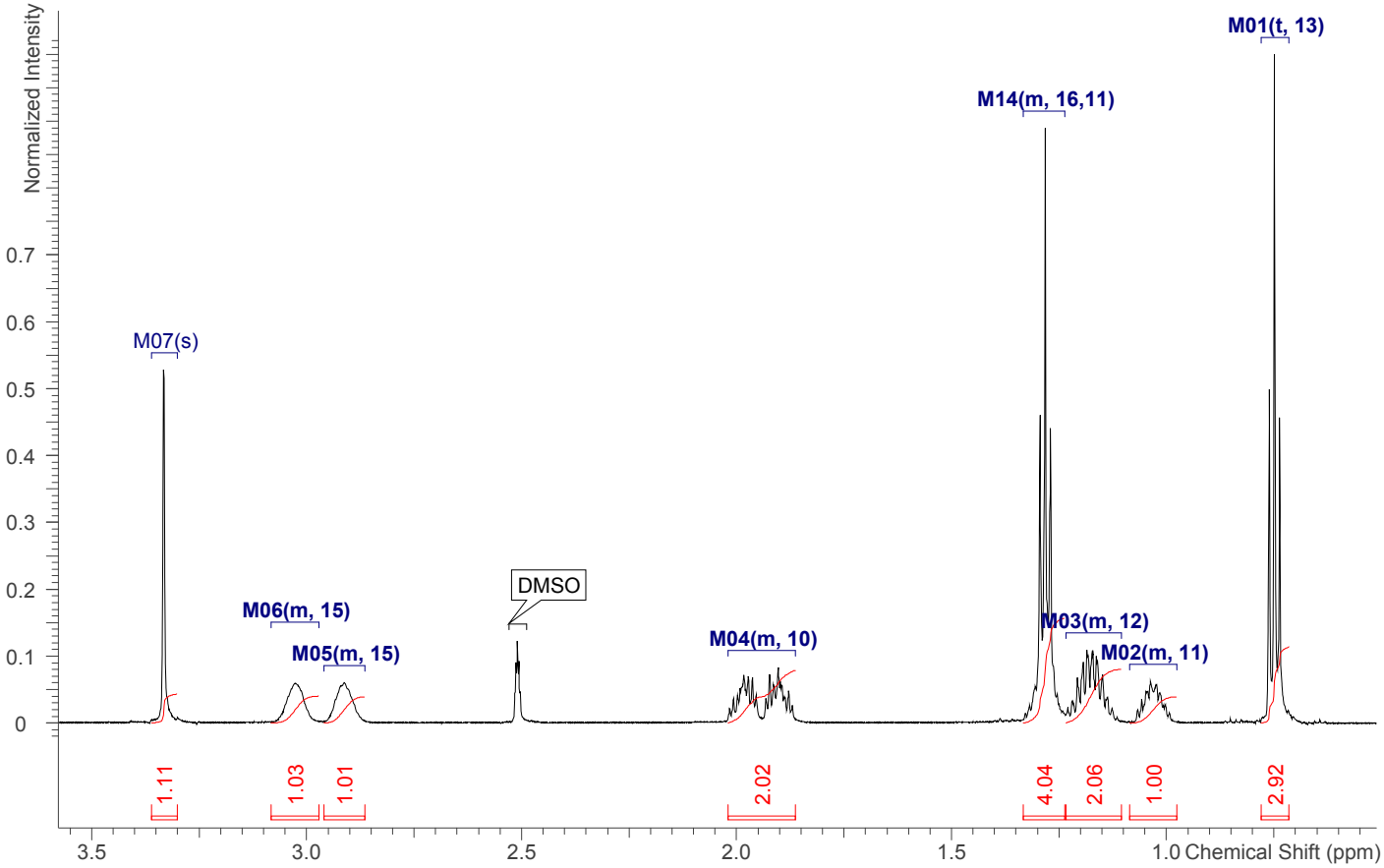
Acquisition Time (sec)	3.6351	***Comment***	15BD-00426-01 sample Belgium Customs		
Date	27 Nov 2015 17:58:49			***Date Stamp***	27 Nov 2015 17:58:49
File Name	\\139.191.6.82\ihcp-.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_600\15BD-00426-01\1\PDATA\1\1r				
Frequency (MHz)	600.13	***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)	9014.42	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3000.6492
Spectrum Type	standard	***Sweep Width (Hz)***	9014.29	***Temperature (degree C)***	27.000



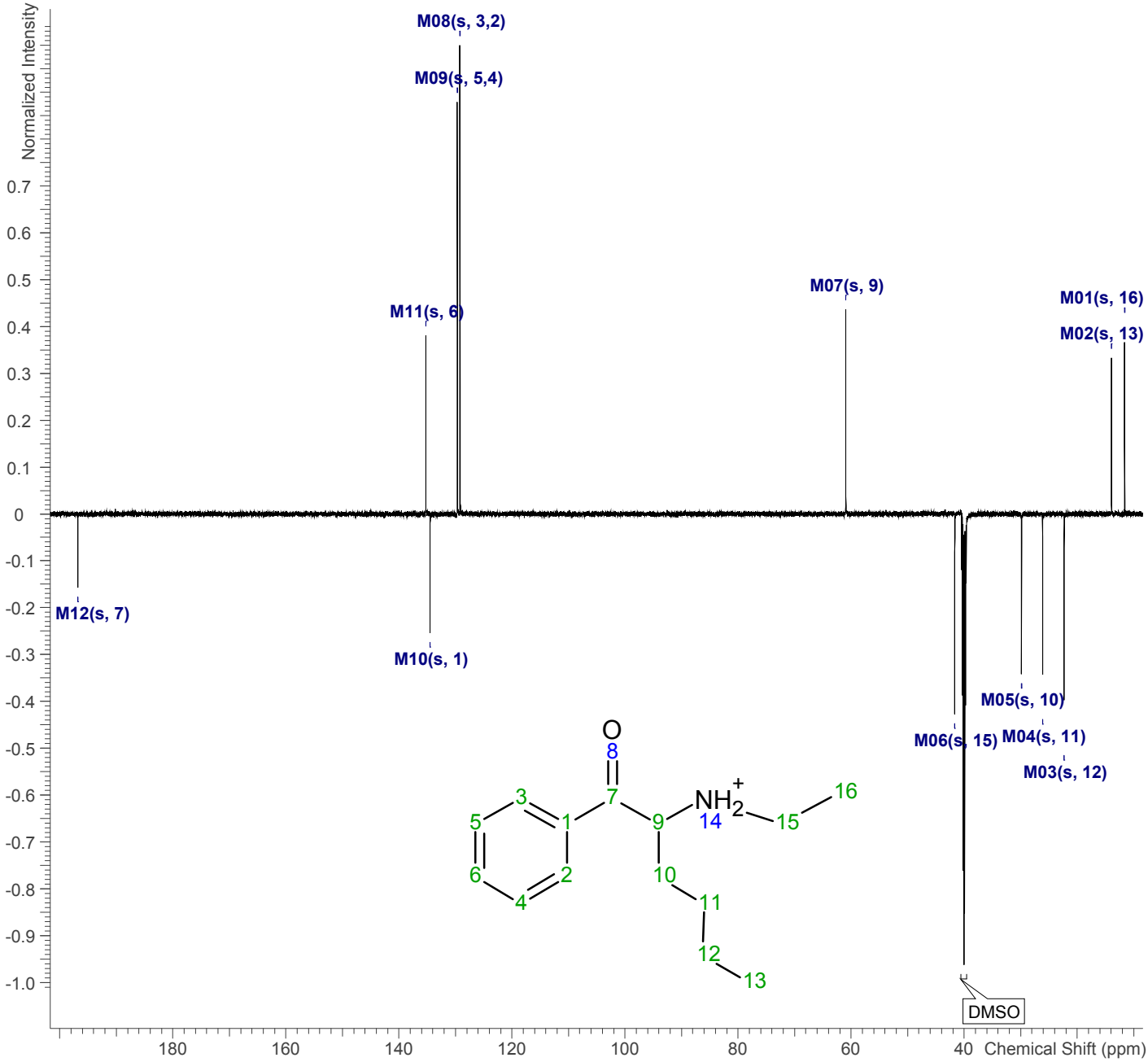
δ_H (DMSO-d_6): 9.59-9.76 (1H, m, M13, atom 14), 9.04-9.21 (1H, m, M12, atom 14), 8.09 (2H, d, *J*=8 Hz, M11, atom 2,3), 7.76 (1H, t, *J*=7 Hz, M10, atom 6), 7.62 (2H, t, *J*=7 Hz, M09, atom 4,5), 5.28 (1H, br s, M08, atom 9), 2.97-3.08 (1H, m, M06, atom 15), 2.86-2.96 (1H, m, M05, atom 15), 1.86-2.02 (2H, m, M04, atom 10), 1.24-1.33 (4H, m, M14, atom 11, 16), 1.10-1.23 (2H, m, M03, atom 12), 0.98-1.08 (1H, m, M02, atom 11), 0.75 (3H, t, *J*=7 Hz, M01, atom 13)

Zoomed parts:



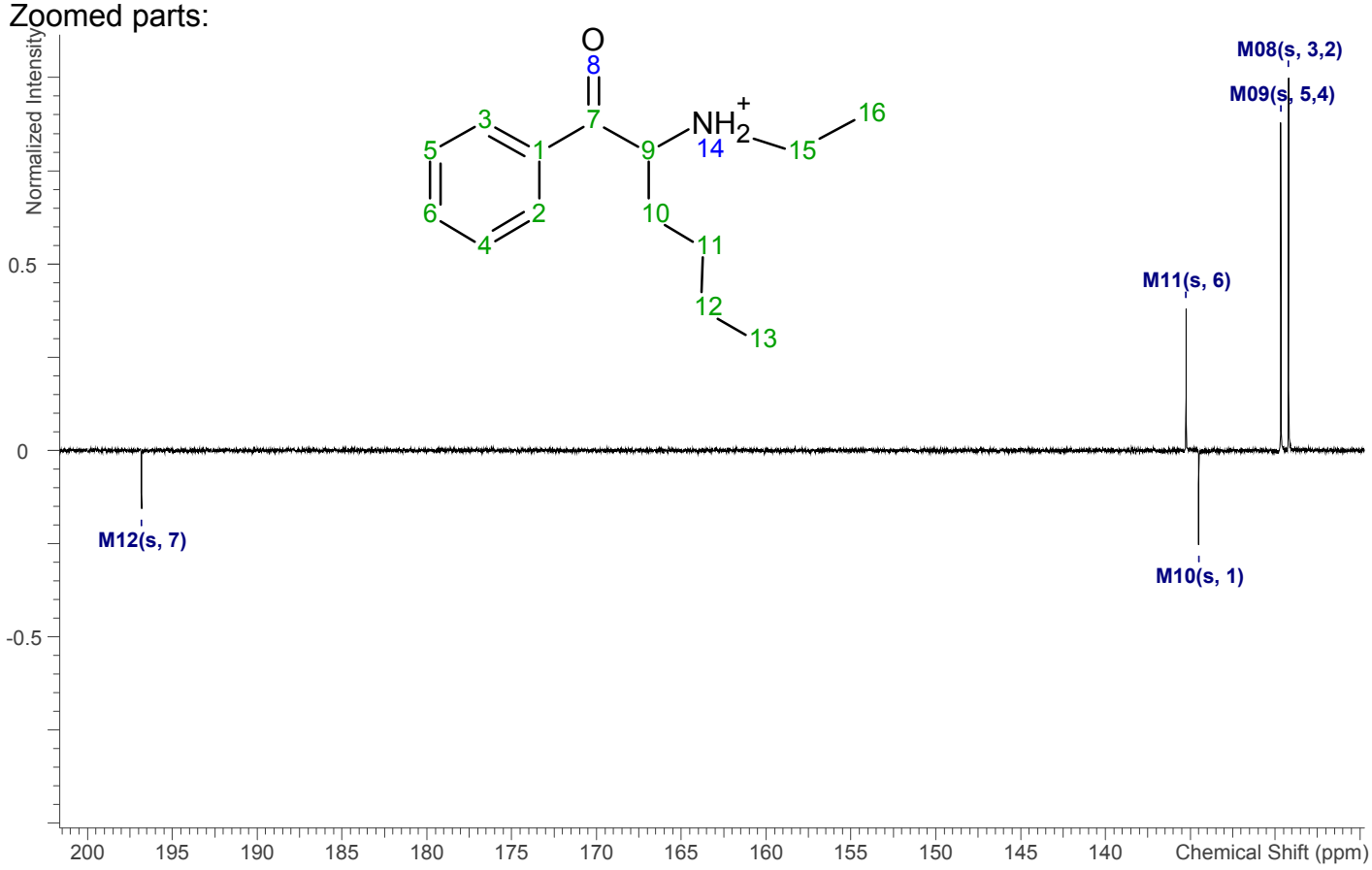


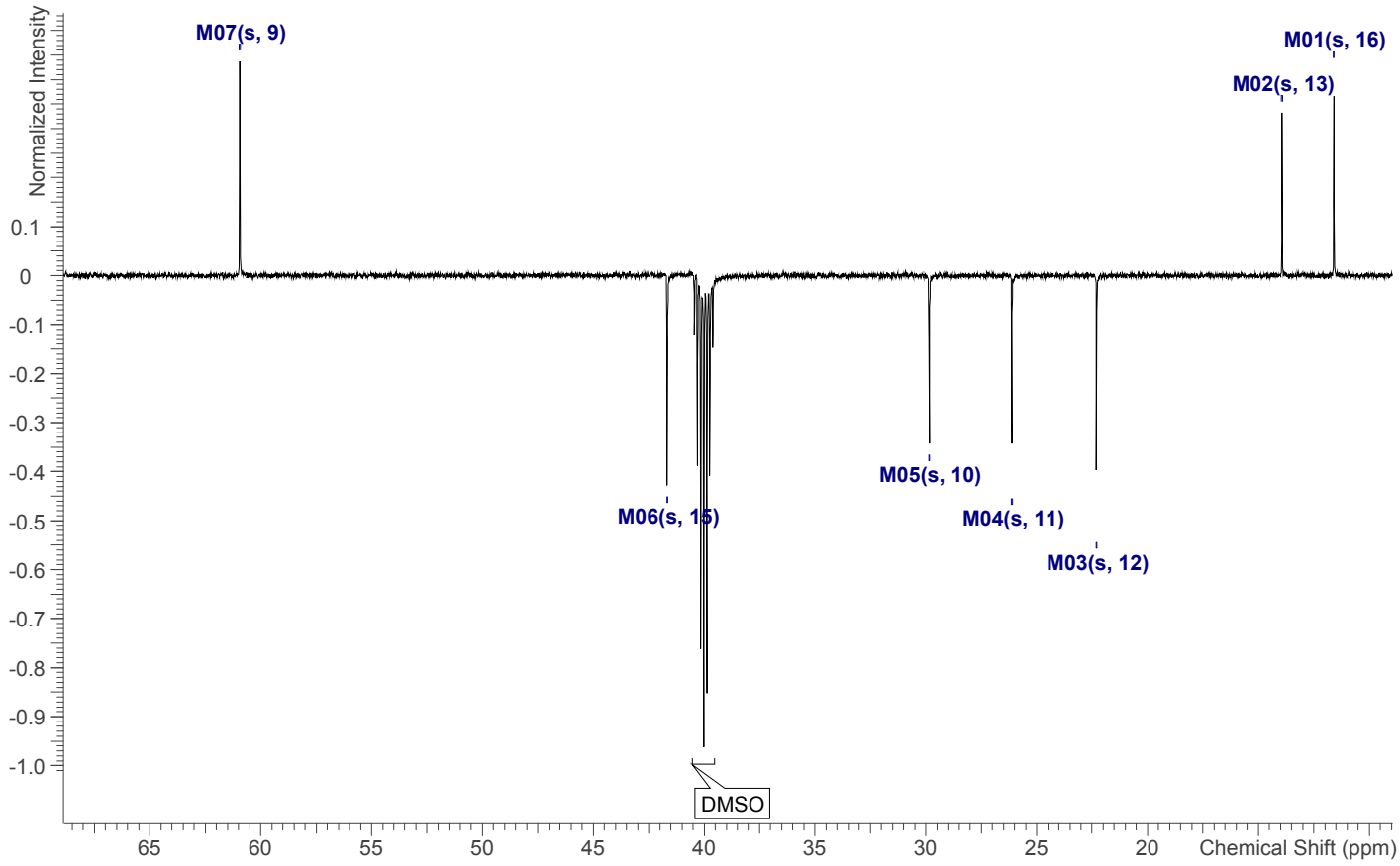
Acquisition Time (sec)	0.9044	***Comment***	5 mm CPQCI 1H/19F-13C/15N/D Z-GRD Z114073/0012
Date	27 Nov 2015 18:07:07		
Date Stamp	27 Nov 2015 18:07:07		
File Name	\\139.191.6.82\ihcp-.I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_600\15BD-00426-01\2\PDATA\1\1r		
Frequency (MHz)	150.90	***Nucleus***	13C
Number of Transients	256	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu
Points Count	32768	***Pulse Sequence***	jmod
Receiver Gain	183.05	***SW(cyclical) (Hz)***	36231.88
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	18108.3359
Spectrum Type	APT	***Sweep Width (Hz)***	36230.78
Temperature (degree C)	26.999		



δ_C (DMSO-d_6): 196.8 (C-7), 135.2 (C-6), 134.5 (C-1), 129.7 (C-5, 4), 129.2 (C-3, 2), 60.9 (C-9), 41.7 (C-15), 29.8 (C-10), 26.1 (C-11), 22.3 (C-12), 13.9 (C-13), 11.6 (C-16)

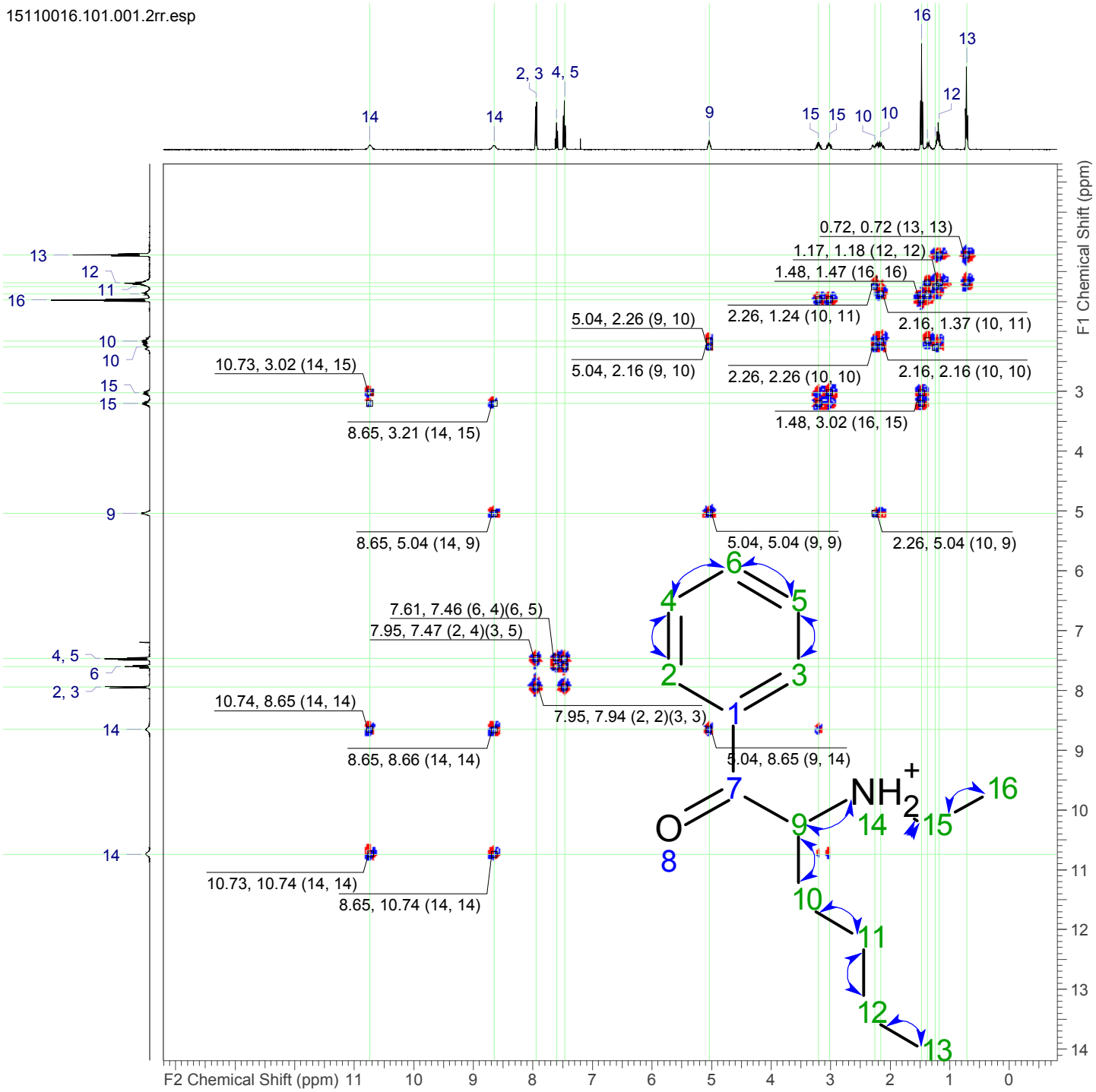
Zoomed parts:





Acquisition Time (sec)	(0.3408, 0.0426)	***Comment***	5 mm PABBO BB/19F-1H/D Z-GRD Z108618/0446
Date	01 Dec 2015 17:26:46		
File Name	\\139.191.6.82\ihcp~I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\!proposed-structure\BCIM_NAS\BCIM_400\15110016_15BD-00426-01\101\PDATA\1\2rr		
Frequency (MHz)	(400.1281, 400.1281)	***Nucleus***	(1H, 1H)
Number of Transients	4	***Origin***	spect
Original Points Count	(2048, 256)	***Owner***	nmrsu
Points Count	(1024, 1024)	***Pulse Sequence***	cosygpmfphpp
Solvent	CDCl3	***Spectrum Type***	COSY
Sweep Width (Hz)	(6003.75, 5996.54)	***Temperature (degree C)***	27.008
Title	151		

15110016.101.001.2rr.esp



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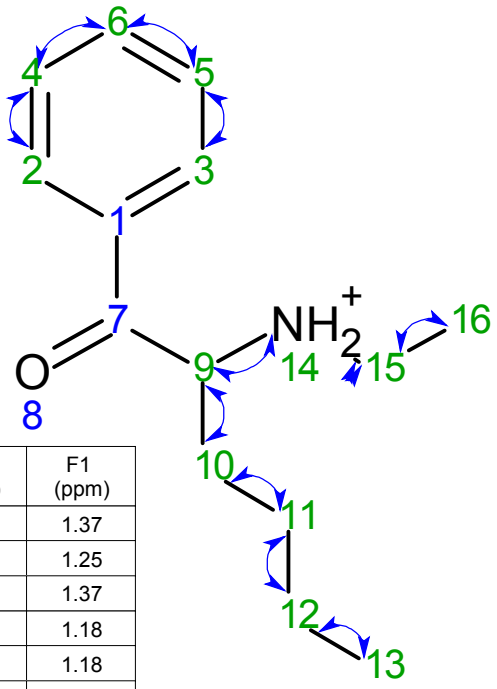

No.	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	2	7.95	7.94
2	4	2	7.47	7.94
3	3	3	7.95	7.94
4	5	3	7.47	7.94
5	2	4	7.95	7.47
6	4	4	7.47	7.47
7	6	4	7.61	7.46
8	3	5	7.95	7.47
9	5	5	7.47	7.47
10	6	5	7.61	7.46
11	4	6	7.46	7.60
12	5	6	7.46	7.60
13	6	6	7.61	7.61
14	9	9	5.04	5.04
15	10	9	2.26	5.04
16	14	9	8.65	5.04
17	9	10	5.04	2.16
18	9	10	5.04	2.26
19	10	10	2.16	2.16
20	10	10	2.26	2.26
21	11	10	1.37	2.15
22	11	10	1.24	2.26
23	10	11	2.26	1.24

No.	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
24	10	11	2.16	1.37
25	11	11	1.24	1.25
26	11	11	1.37	1.37
27	11	12	1.37	1.18
28	12	12	1.17	1.18
29	13	12	0.72	1.18
30	12	13	1.18	0.72
31	13	13	0.72	0.72
32	9	14	5.04	8.65
33	14	14	10.74	8.65
34	14	14	8.65	8.66
35	14	14	10.73	10.74
36	14	14	8.65	10.74
37	14	15	10.73	3.02
38	14	15	10.74	3.20
39	14	15	8.65	3.21
40	15	15	3.02	3.02
41	15	15	3.20	3.20
42	16	15	1.48	3.02
43	16	15	1.47	3.20
44	15	16	3.02	1.47
45	15	16	3.20	1.47
46	16	16	1.48	1.47

Fragmentation of the observed molecule and the virtual MS (EI+) spectrum predicted by Thermo Scientific Mass Frontier