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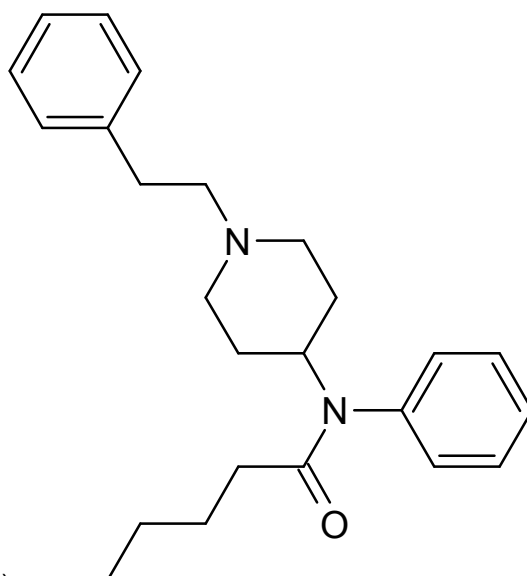
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ADMINISTRATIVE ARRANGEMENT JRC-Nr 33619-CLEN2SAND-DG TAXUD-Nr TAXUD/2014/DE/315 BETWEEN DG TAXATION AND CUSTOMS UNION (DG TAXUD) AND THE JOINT RESEARCH CENTRE (JRC) for fast recognition of New Psychoactive Substances (NPS) and identification of unknown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

This report was generated on 27/01/2016 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	16010001	Received on	08 January 2016
PACKAGING	1 glass vial white powder (30 mg)		
Registration date	08 January 2016	Name of customer	Service commun des laboratoires France
Customer's identification	2015-30772		

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



Data of identified compound(s)

Formula	C ₂₄ H ₃₂ N ₂ O
FW	364.5237
Monoisotopic Mass	364.2515
Chemicalize IUPAC name	N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]pentanamide
InChI (v.1.04)	InChI=1S/C24H32N2O/c1-2-3-14-24(27)26(22-12-8-5-9-13-22)23-16-19-25(20-17-23)18-15-21-10-6-4-7-11-21/h4-13,23H,2-3,14-20H2,1H3
InChI Key (v.1.04)	VCCPXHWAJYWQMR-UHFFFAOYSA-N
SMILES (v.14.01)	CCCCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3

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)

via E. Fermi, 2749

TP 281 I-21027 Ispra (VA) - Italy

Phone: +39 0332 785678

Fax: +39 0332 789453

claude.guillou@ec.europa.eu

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

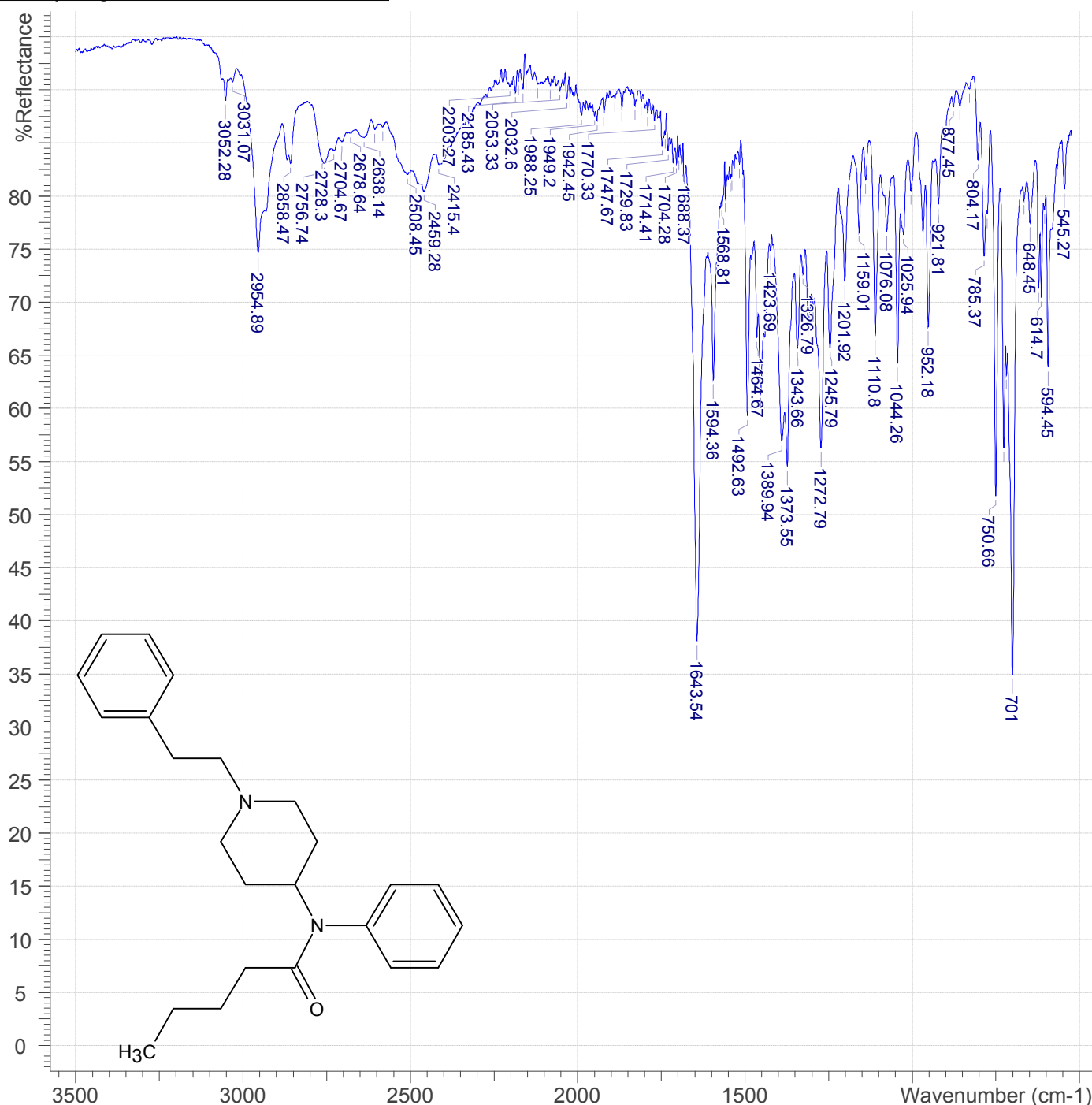
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Processing and interpretation based on data provided by:

Service commun des laboratoires France

Title	30772		
File Name	\\139.191.6.82\ihcp\101\BIO_CHEMICAL_INTERACTION_METABONOMICS\CLEN2SAND\PROPOSED-STRUCTURE\CLEN_NAS\16010001_2015-30772\30772.SPA		
Date Stamp	24 Nov 2015 13:51:25	Date	24 Nov 2015 14:51:38
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		



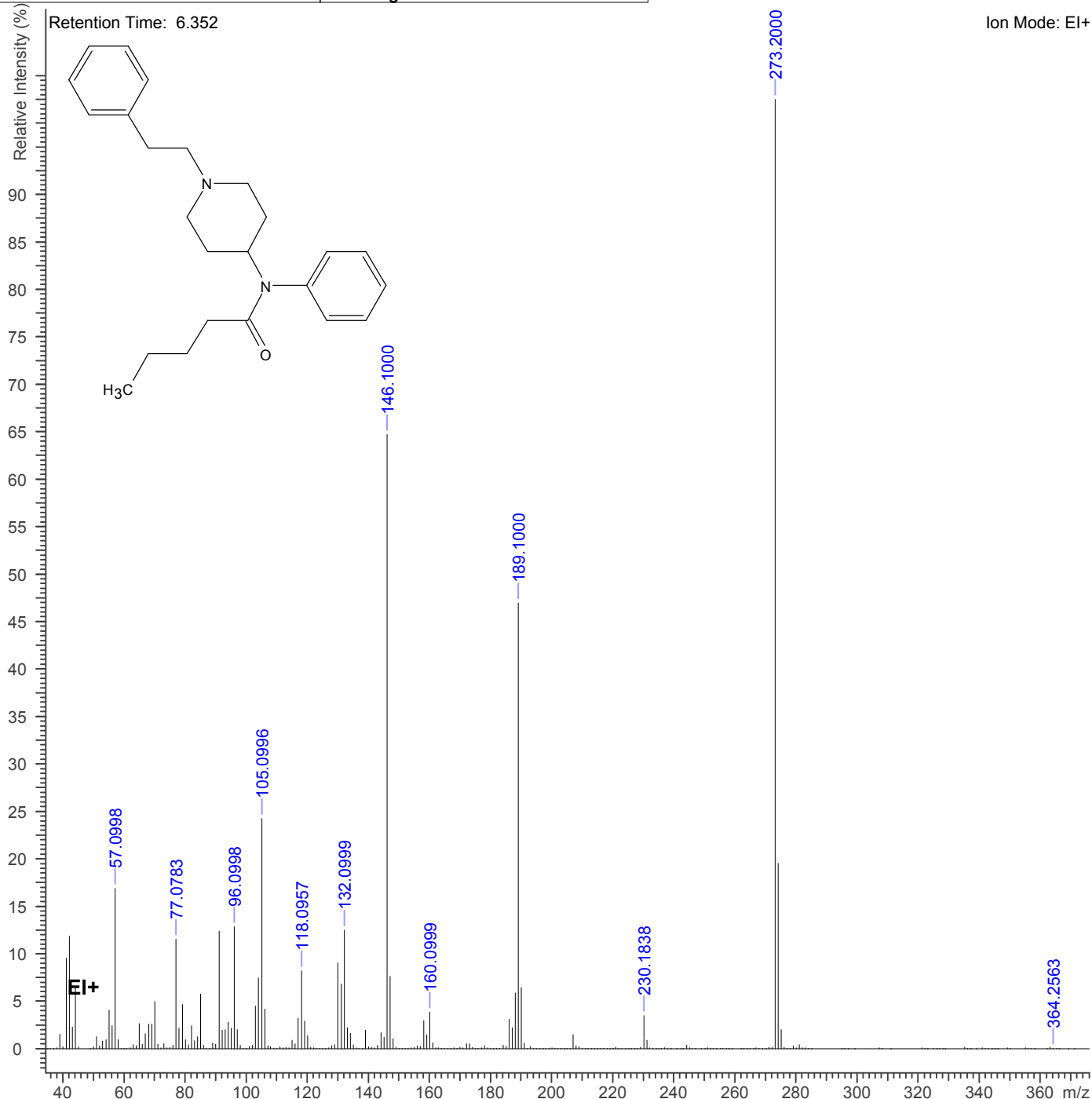
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Processing and interpretation based on data provided by:

Service commun des laboratoires France

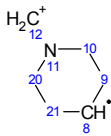
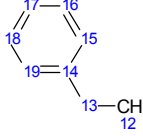
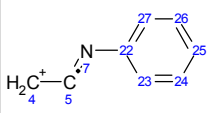
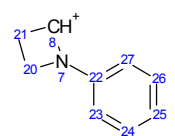
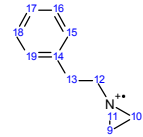
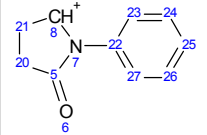
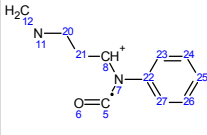
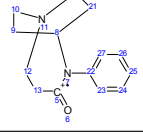
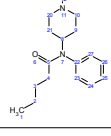
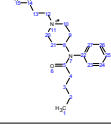
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Data Type	Condensed	Date	24 Nov 2015 18:54:48		
Date Stamp	24 Nov 15 06:42 pm				
File Name	2015-30772 Centroid EI+			Ion Mode	EI+
Mass Spec Model	GCMS	Plot Type	Stick	Retention Time	6.352
Sample	Ds CH ₂ Cl ₂ /MeOH : 2015-30772			Scan	858
Scan Mode	Centroid	Spectrum Assigned	0.0% [35-503/0-100]		
TIC	529.31	Total Signal	7190323.5		



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Table of fragments

No.	Fragment	Structure	Formula	Label	m/z Calc.	TIC Calc. (%)	Difference (Da)	m/z Exp.	RI Exp. (%)	TIC Ex (%)	Origin
1	8-12,20-21(-H)		C ₆ H ₁₀ N	M - C ₁₈ H ₂₂ NO	96.081	2.604	0.019	96.100	12.837	2.604	Manual
2	12-19		C ₈ H ₉	M - C ₁₆ H ₂₃ N ₂ O	105.070	5.012	0.030	105.100	24.260	5.012	Manual
3	4-5,7,22-27(+H)		C ₈ H ₈ N	M - C ₁₆ H ₂₄ NO	118.065	1.702	0.031	118.096	8.209	1.702	Manual
4	7-8,20-27		C ₉ H ₁₀ N	M - C ₁₅ H ₂₂ NO	132.081	2.613	0.019	132.100	12.464	2.613	Manual
5	9-19(-H)		C ₁₀ H ₁₂ N	M - C ₁₄ H ₂₀ NO	146.096	13.718	0.004	146.100	64.697	13.718	Manual
6	5-8,20-27		C ₁₀ H ₁₀ NO	M - C ₁₄ H ₂₂ N	160.076	0.819	0.024	160.100	3.854	0.819	Manual
7	5-8,11-12,20-27(+H)		C ₁₁ H ₁₃ N ₂ O	M - C ₁₃ H ₁₉	189.102	10.133	-0.002	189.100	46.973	10.133	Manual
8	5-13,20-27		C ₁₄ H ₁₈ N ₂ O	M - C ₁₀ H ₁₄	230.141	0.774	0.042	230.184	3.471	0.774	Manual
9	1-12,20-27		C ₁₇ H ₂₅ N ₂ O	M - C ₇ H ₇	273.196	23.081	0.004	273.200	100.000	23.081	Manual
10	M		C ₂₄ H ₃₂ N ₂ O	M	364.251	0.012	0.005	364.256	0.047	0.012	Manual

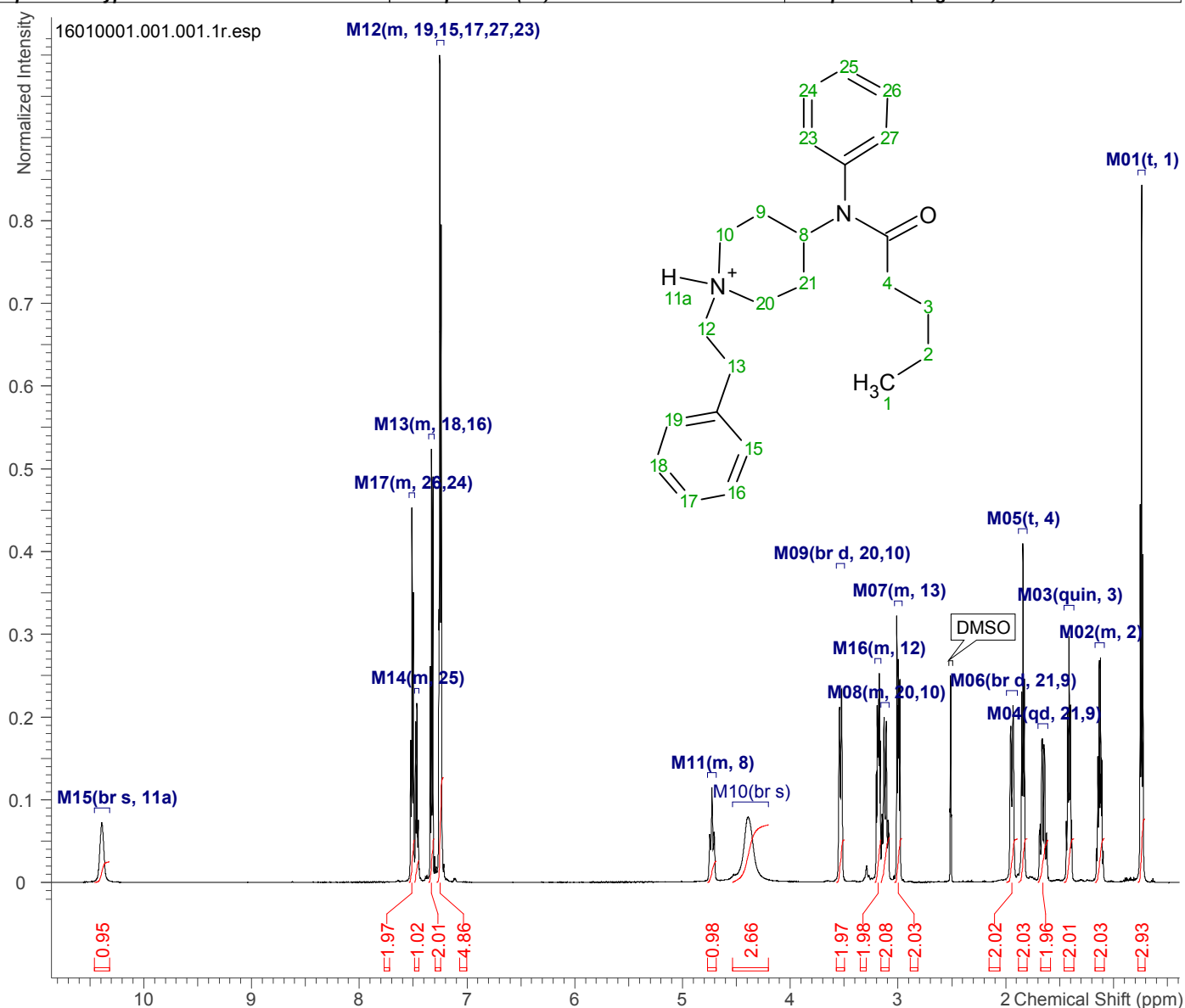
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Data from BCIM group at JRC, IHCP Ispra

NMR spectra

Acquisition Time (sec)	2.7263	Comment	2015-30772 10 mg in 600 uL DMSO-d6 Paris 01/ 2016	
Date	08 Jan 2016 15:17:51		Date Stamp	08 Jan 2016 15:17:51
File Name	\\139.191.6.82\ihcp-101\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure\BCIM_NAS\BCIM_600\16010001\1\PDATA\1\1r			
Frequency (MHz)	600.13	Nucleus	1H	Number of Transients 128
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) 26.998



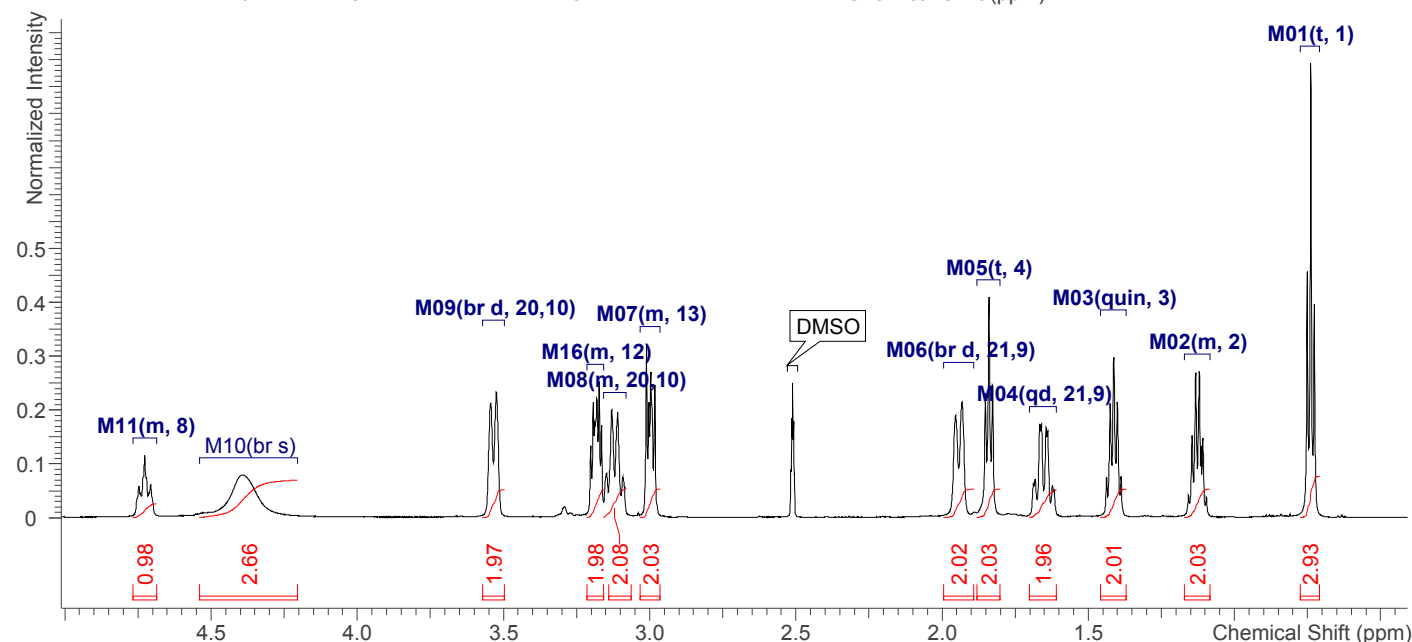
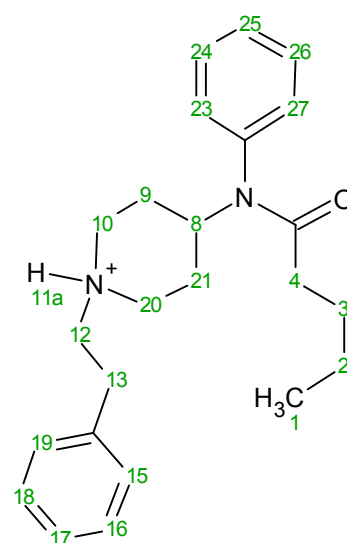
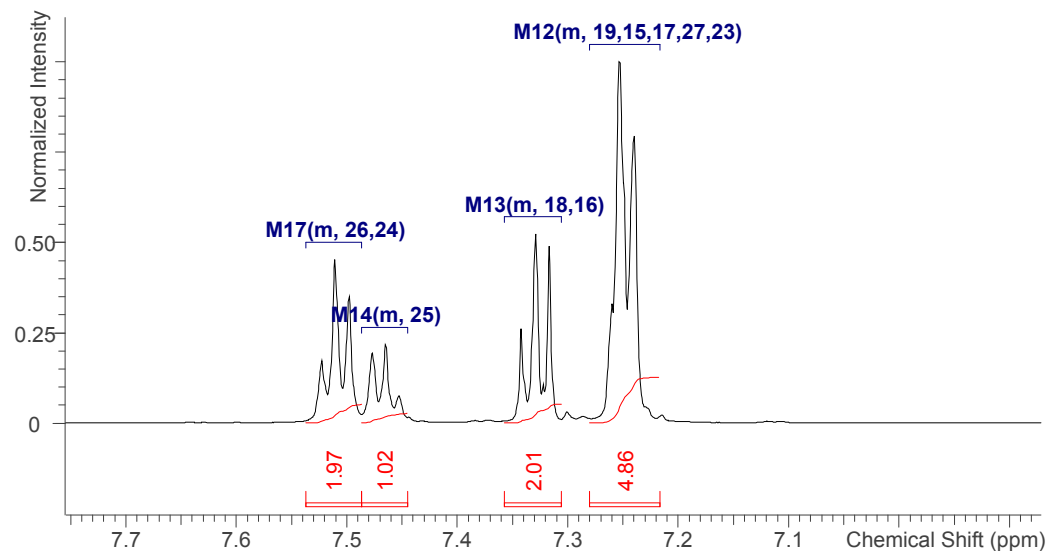
δ_H (DMSO- d_6): 10.39 (1H, br s, M15), 7.49-7.54 (2H, m, M17), 7.44-7.49 (1H, m, M14), 7.31-7.36 (2H, m, M13), 7.22-7.28 (5H, m, M12), 4.69-4.77 (1H, m, M11), 4.39 (3H, br s, M10), 3.53 (2H, br d, $J=11$ Hz, M09), 3.16-3.21 (2H, m, M16), 3.08-3.16 (2H, m, M08), 2.96-3.03 (2H, m, M07), 1.94 (2H, br d, $J=13$ Hz, M06), 1.84 (2H, t, $J=7$ Hz, M05), 1.65 (2H, qd, $J=13$ and 3 Hz, M04), 1.41 (2H, quin, $J=7$ Hz, M03), 1.08-1.17 (2H, m, M02), 0.74 (3H, t, $J=7$ Hz, M01)

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Table of assignments and zoomed parts:

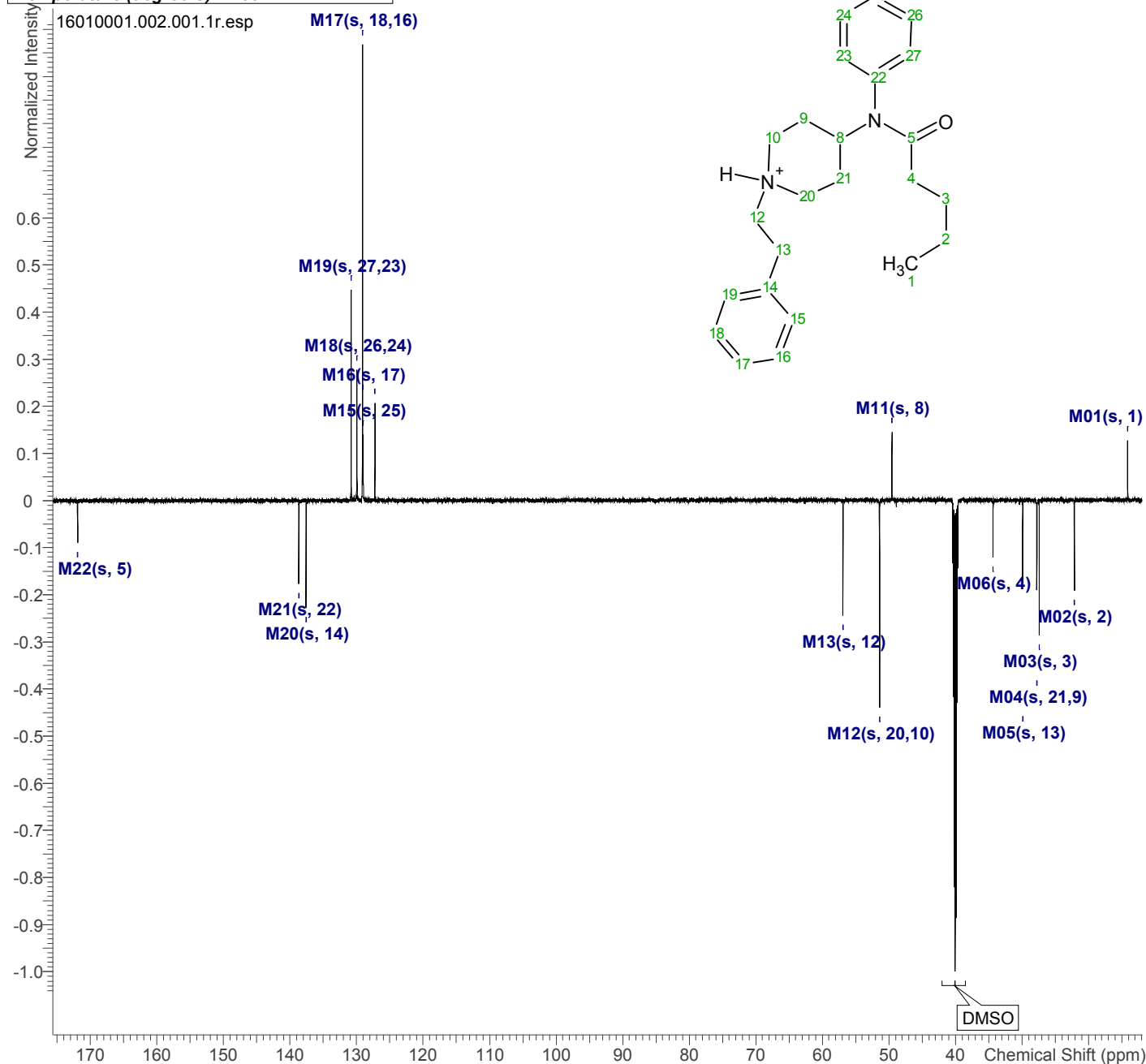
No.	Atom	Exp. Shift (ppm)	Multiplet	No.	Atom	Exp. Shift (ppm)
1	1	0.74	M01	14	10	3.53
2	2	1.12	M02	15	8	4.73
3	3	1.41	M03	16	19	7.25
4	21	1.65	M04	17	15	7.25
5	9	1.65	M04	18	17	7.25
6	4	1.84	M05	19	27	7.25
7	21	1.94	M06	20	23	7.25
8	9	1.94	M06	21	18	7.33
9	13	3.00	M07	22	16	7.33
10	20	3.12	M08	23	25	7.47
11	10	3.12	M08	24	26	7.51
12	12	3.18	M16	25	24	7.51
13	20	3.53	M09	26	11a	10.39



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Acquisition Time (sec)	0.9044	Comment	5 mm CPQCI 1H/19F-13C/15N/D Z-GRD Z114073/0012
Date	08 Jan 2016 15:30:45	Date Stamp	08 Jan 2016 15:30:45
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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)	27.002		



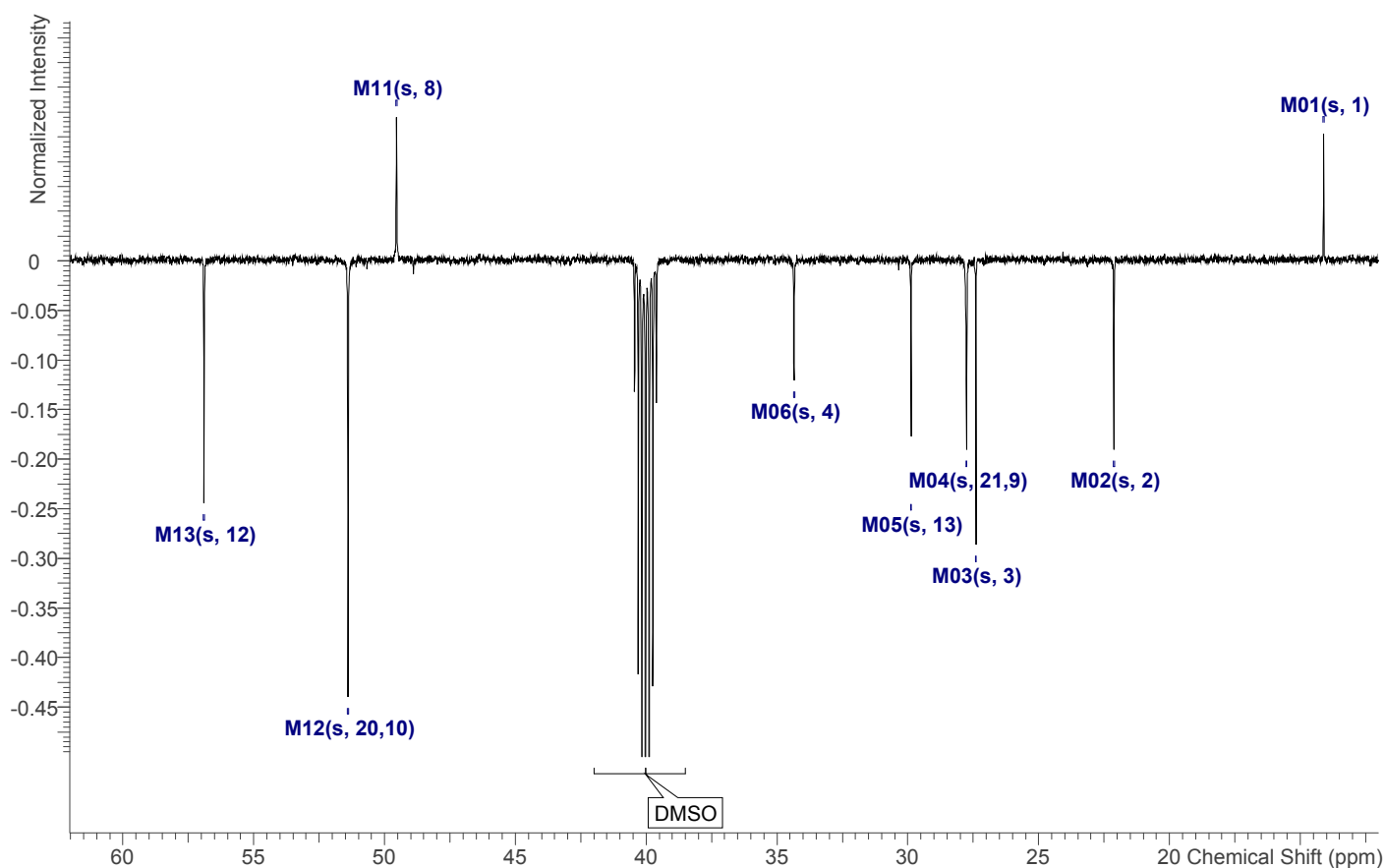
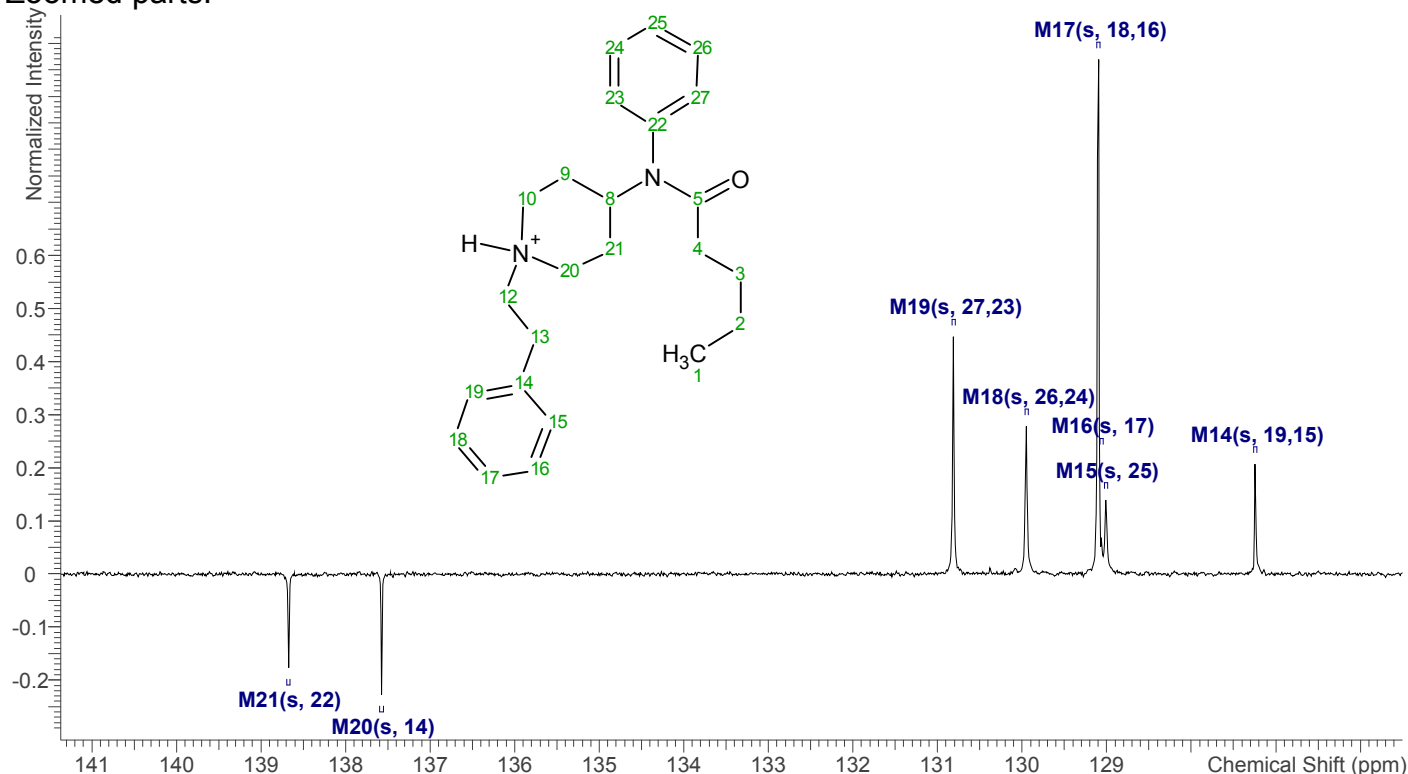
δ_c (DMSO- d_6): 171.9 (C-5), 138.7 (C-22), 137.6 (C-14), 130.8 (C-23, 27), 129.9 (C-24, 26), 129.1 (C-16, 18), 129.1 (C-17), 129.0 (C-25), 127.2 (C-15, 19), 56.9 (C-12), 51.4 (C-10, 20), 49.5 (C-8), 34.3 (C-4), 29.9 (C-13), 27.8 (C-9, 21), 27.4 (C-3), 22.1 (C-2), 14.1 (C-1)

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

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Zoomed parts:

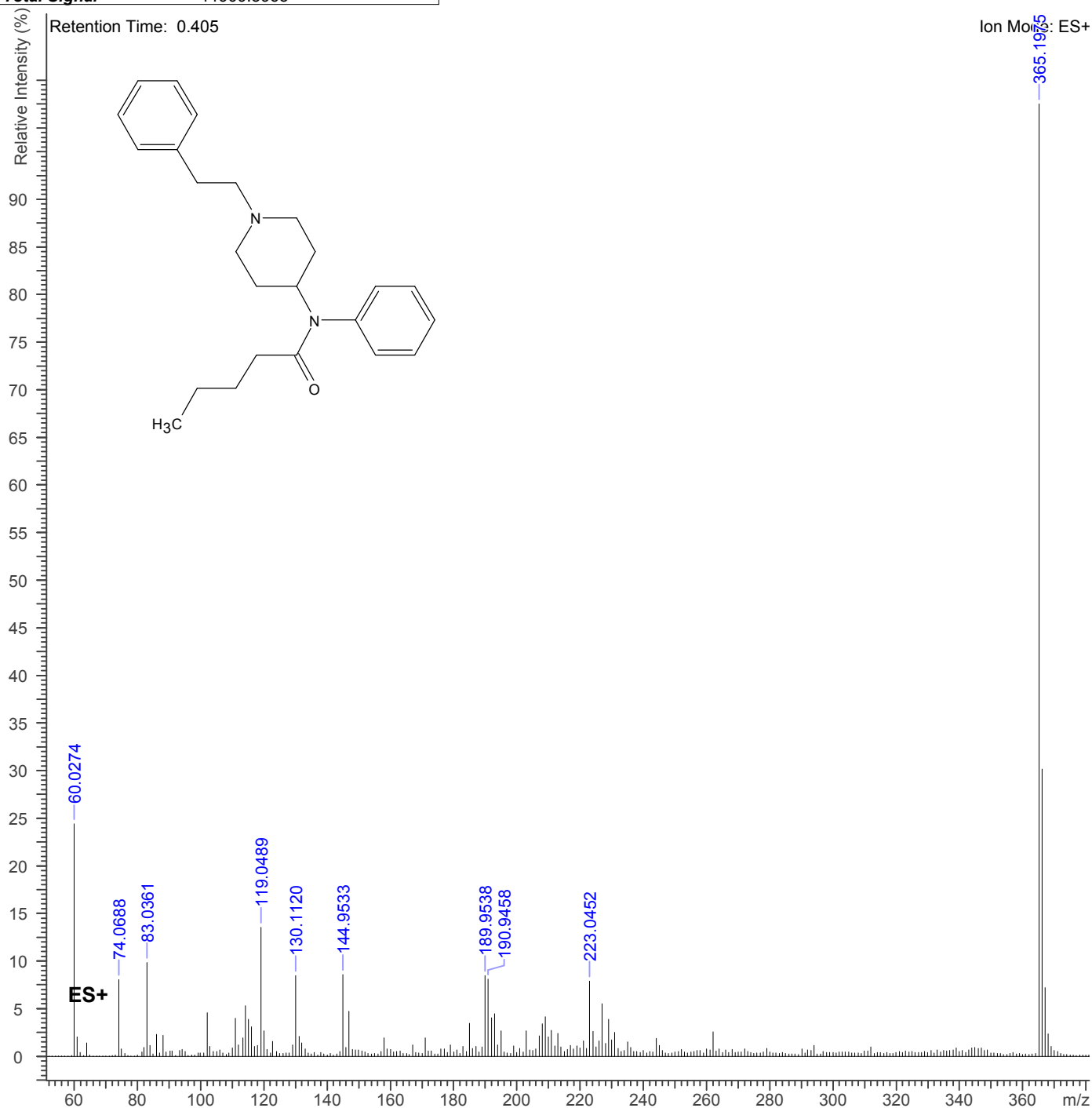


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MS spectra

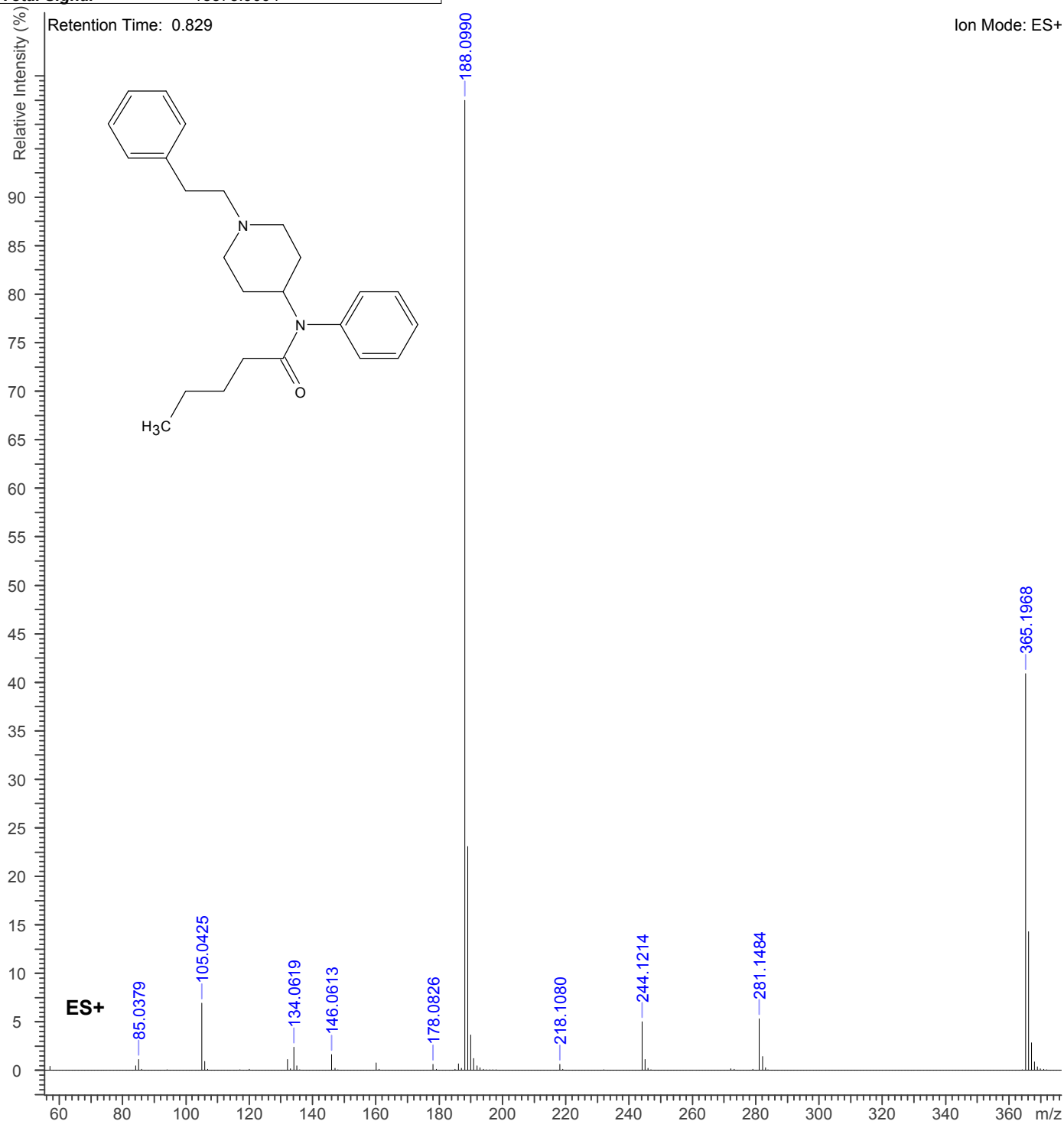
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Date Stamp	19 Jan 2016 16:45:45	Estimated Molecular Ion	365.198
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Inlet Model	Electrospray Inlet	Ion Mode	ES+
Plot Type	Stick	Retention Time	0.405
Scan	22	Separation Type	No Chromatography
Spectrum Assigned	27.5% [50-400/0-100]	TIC	479.63
Total Signal	11909.3965		



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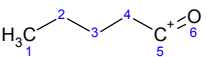
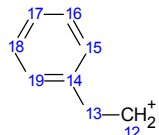
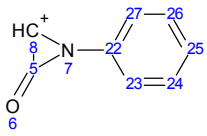
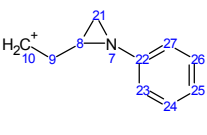
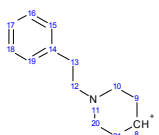
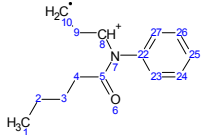
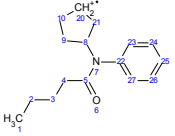
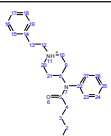
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Inlet Model	Electrospray Inlet	Ion Mode	ES+
Plot Type	Stick	Retention Time	0.829
Scan	45	Separation Type	No Chromatography
Spectrum Assigned	87.5% [50-400/0-100]	TIC	225.77
Total Signal	18373.9004		



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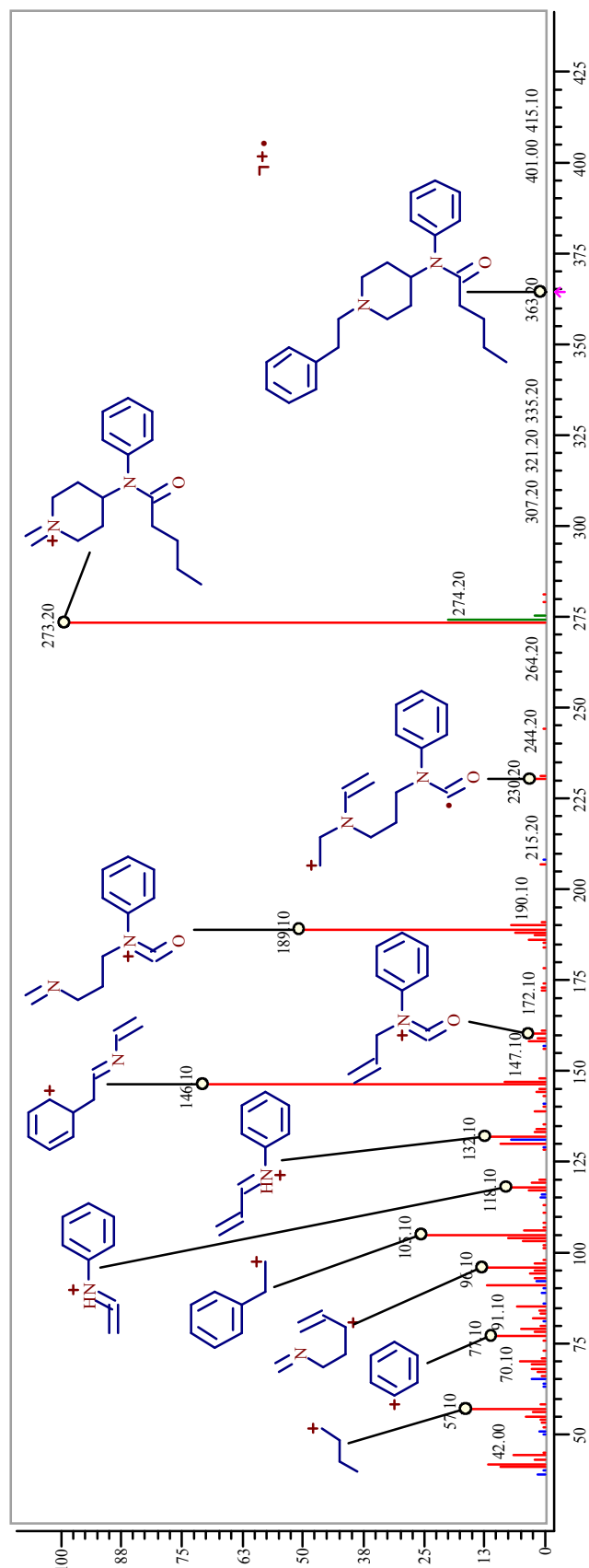
Table of fragments

No.	Fragment	Structure	Formula	Label	m/z Calc.	TIC Calc. (%)	Difference (Da)	m/z Exp.	RI Exp. (%)	TIC Exp. (%)	Origin
1	1-6		C5H9O	M - C19H23N2	85.065	0.540	-0.027	85.038	1.149	0.540	Manual
2	12-19		C8H9	M - C16H23N2O	105.070	3.350	-0.027	105.043	6.917	3.350	Manual
3	5-8,22-27(+H2)		C8H8NO	M - C16H24N	134.060	1.165	0.002	134.062	2.392	1.165	Manual
4	7-10,21-27		C10H12N	M - C14H20NO	146.096	0.819	-0.035	146.061	1.648	0.819	Manual
5	1-7,22-27(+H2)		C11H16NO	M - C13H16N	178.123	0.312	-0.040	178.083	0.619	0.312	Manual
6	8-21		C13H18N	M - C11H14NO	188.143	51.427	-0.044	188.099	100.000	51.427	Manual
7	1-10,22-27(+H)		C14H20NO	M - C10H12N	218.154	0.316	-0.046	218.108	0.605	0.316	Manual
8	1-10,20-27(-H)		C16H22NO	M - C8H10N	244.170	2.672	-0.048	244.121	5.013	2.672	Manual
9	7-27(+H2)		C19H25N2	M - C5H7O	281.201	2.943	-0.053	281.148	5.331	2.943	Manual
10	M(+H)		C24H33N2O	M + H	365.259	23.922	-0.062	365.197	40.879	23.922	Manual

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



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

