

Joint Research Centre

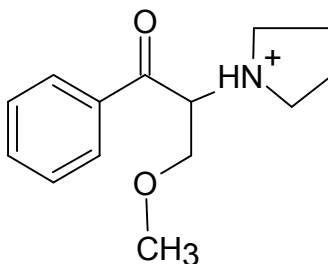
The European Commission's in-house science service

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 12/10/2016 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	16090003	Received on	20 September 2016
Name of customer	Bildungs- und Wissenschaftszentrum		
Customer's identification	SV 0618 B - 43128/2016-1		

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



Data of identified compound(s)

IUPAC Name	1-(3-methoxy-1-oxo-1-phenylpropan-2-yl)pyrrolidin-1-ium		
Formula	C ₁₄ H ₂₀ NO ₂ ⁺	FW	234.3136
Monoisotopic Mass	234.148855		
InChI	InChI=1S/C14H19NO2/c1-17-11-13(15-9-5-6-10-15)14(16)12-7-3-2-4-8-12/h2-4,7-8,13H,5-6,9-11H2,1H3/p+1		
InChI Key	TVBNCCGCI PGJQO-UHFFFAOYSA-O	SMILES	COCC([NH+](CCCC1)C(=O)c2ccccc2

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Directorate F

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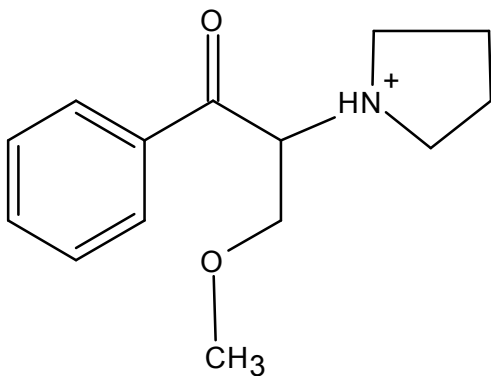
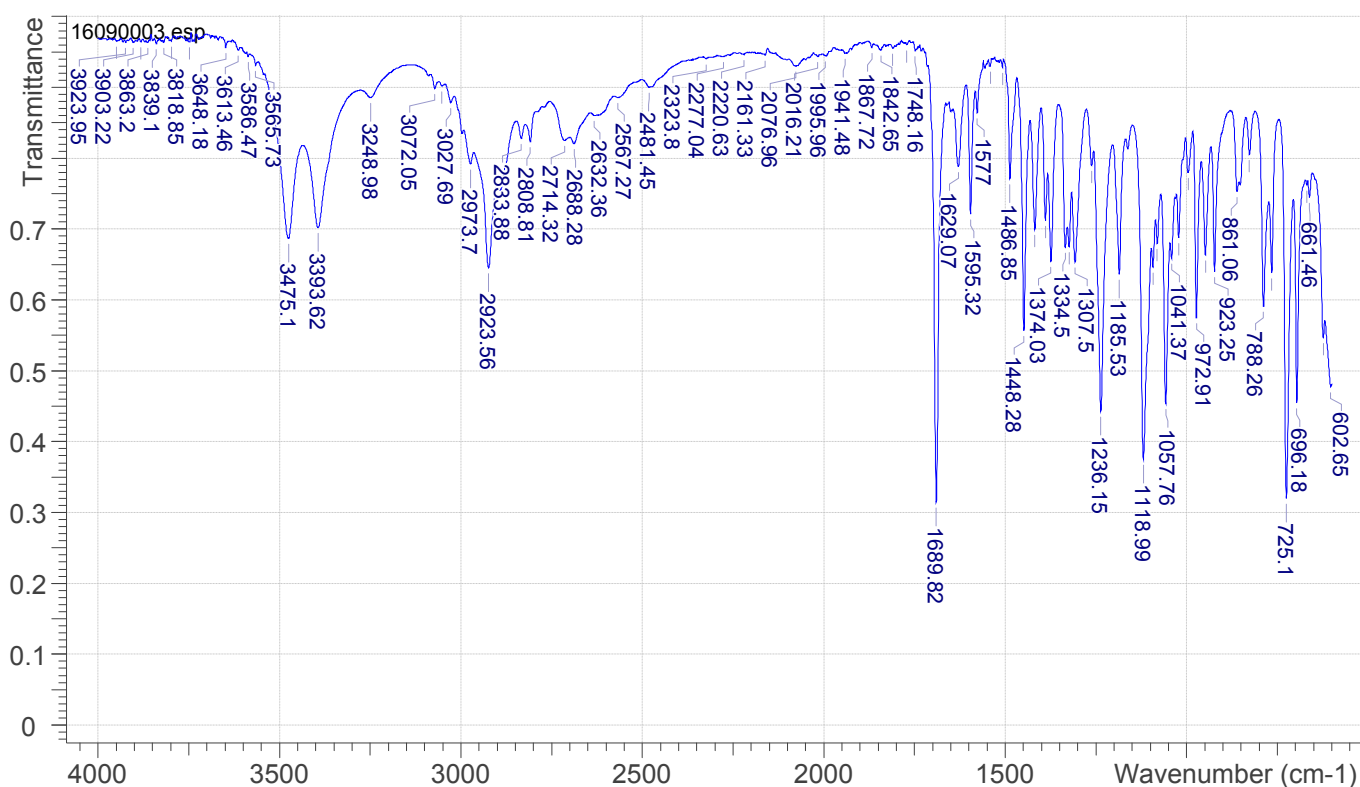
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Processing and interpretation based on data provided by:

Bildungs- und Wissenschaftszentrum

Title	43128-2016-1	Origin	TFS	Owner	Nicolet
File Name	\\139.191.6.82\ihcp\$\I01\BIO_CHEMICAL_INTERACTION_METABONOMICS\CLEN2SAND\EUCSI_DOWNLOAD\GERMAN CUSTOMS\43128-2016-1.JDX				
Date Stamp	14:29:10	Date	08 Sep 2016 11:28:54	Technique	Infrared
Instrument	Nicolet iS10	Spectral Region	IR	X Axis	Wavenumber (cm-1)
Y Axis	Absorbance	Spectrum Range	600.2354 - 4000.1221	Points Count	7053
Data Spacing	0.4821				



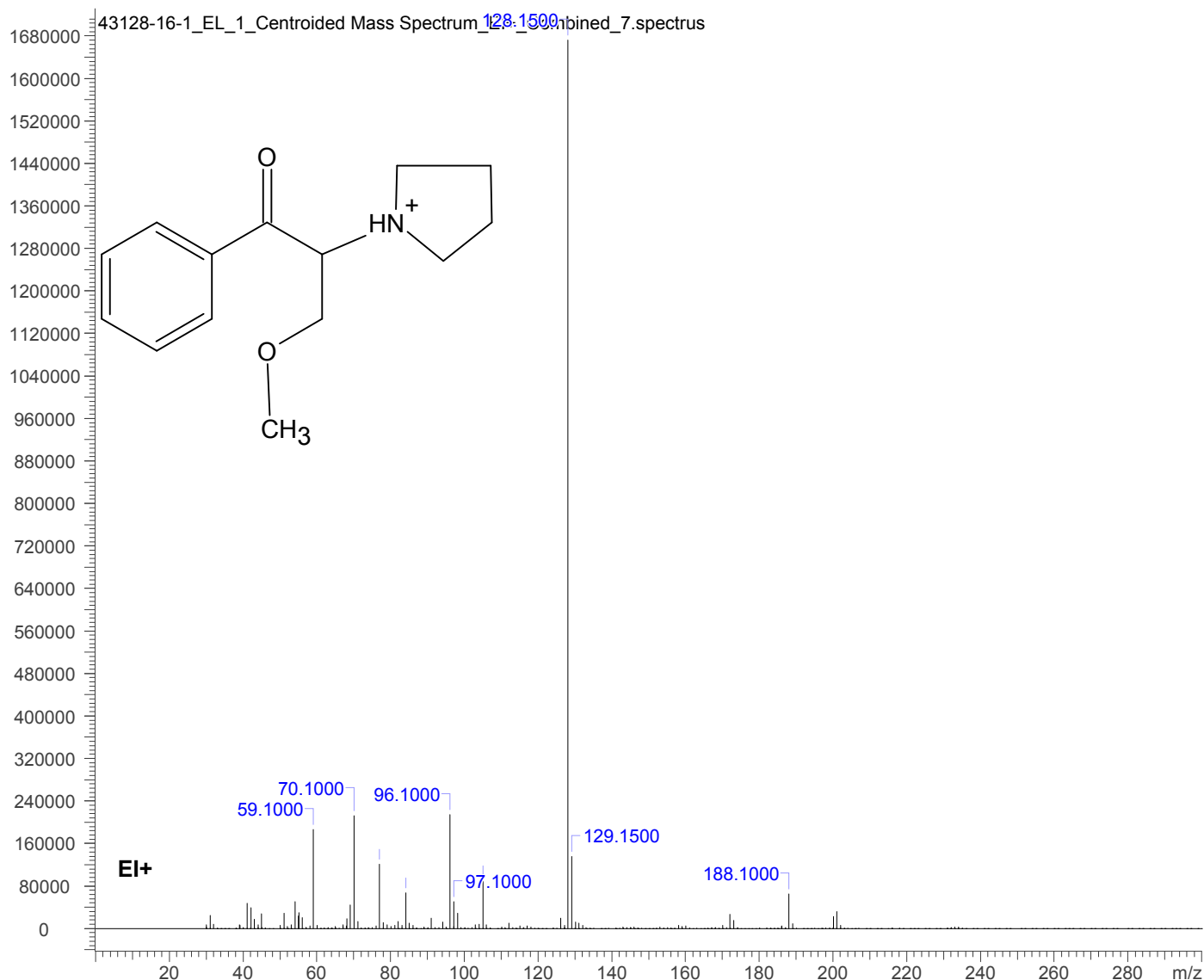
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Processing and interpretation based on data provided by:

Bildungs- und Wissenschaftszentrum

Combine	<1748-1761>	Comment	10 mg in 10 ml Ethanol, gelöst
Count	957	Data Source Name	43128-16-1_EL_1_Centroided Mass Spectrum_EI+
Data Type	Centroided Mass Spectrum	Date	11 Oct 2016 16:34:55
Date Stamp	24 Aug 2016 14:57:01	Estimated Molecular Ion	471.1
Inlet Model	Other Probe	Ion Mode	EI+
Plot Type	Stick	Retention Time	7.547
Scan	1755	Separation Type	Gas-Solid Chromatography
Spectrum Title	10 mg in 10 ml Ethanol, gelöst	Spectrum Type	MS
TIC	227.66	Total Signal	3806032.7857



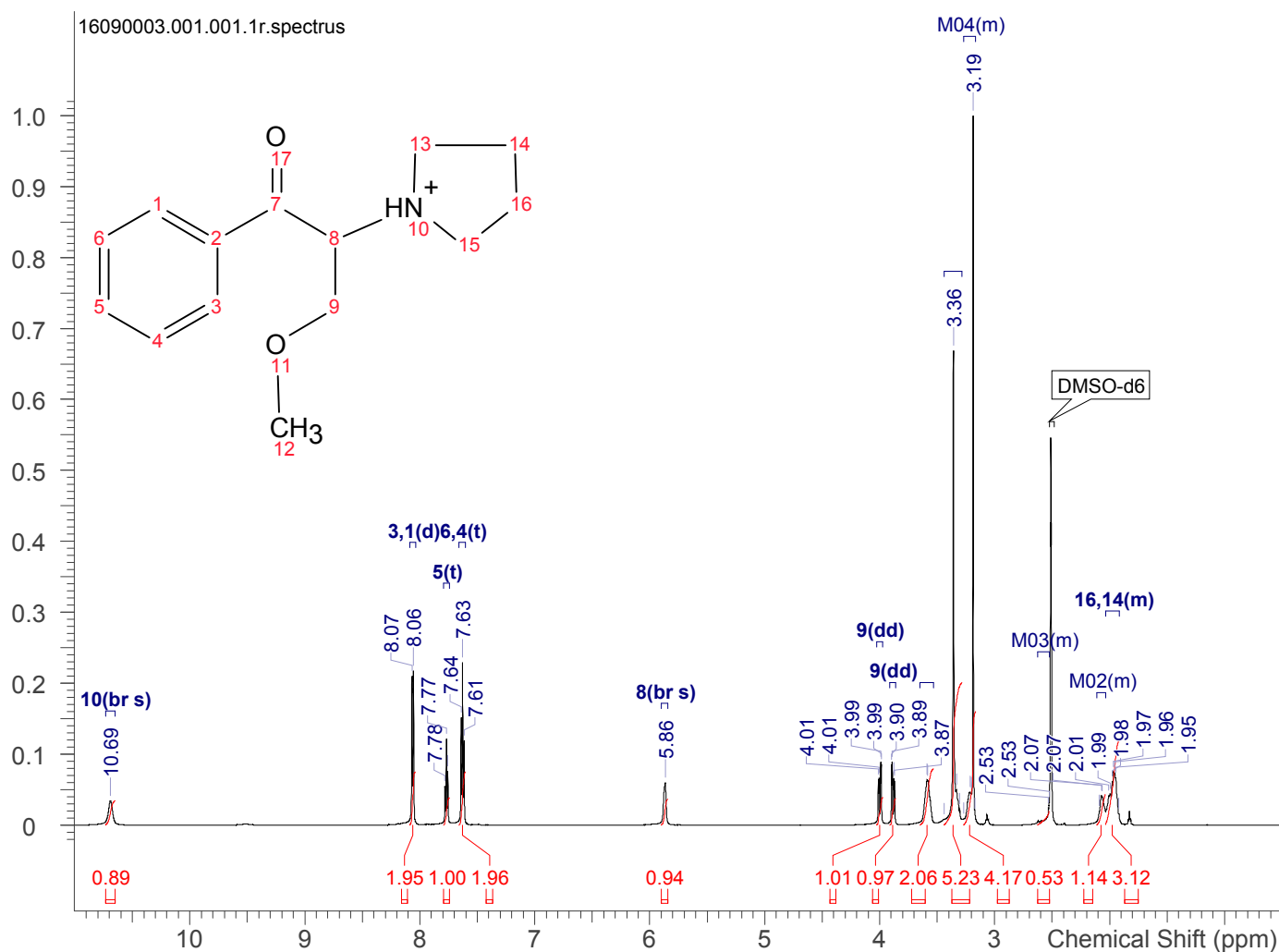
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Data from BCIM group at JRC, IHCP Ispra

NMR spectra

Acquisition Time (sec)	2.7263	Date	20 Sep 2016 14:31:52
Date Stamp	20 Sep 2016 14:31:52		
File Name	\\139.191.6.82\ihcp\$\I01\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure\BCIM_NAS\BCIM_600\16090003\1\PDATA\1\1r		
Frequency (MHz)	600.1300	Nucleus	¹ H
Original Points Count	32768	Owner	nrmrsu
Pulse Sequence	zg30	Receiver Gain	23.55
Solvent	DMSO-d ₆	Spectrum Offset (Hz)	3706.0515
Sweep Width (Hz)	12019.05	Temperature (degree C)	27.000
		Number of Transients	64
		Points Count	65536
		SW(cyclical) (Hz)	12019.23
		Spectrum Type	standard



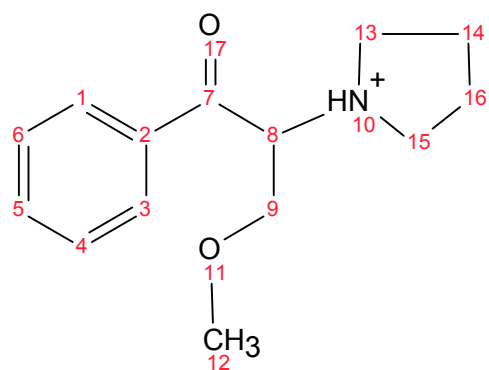
¹H NMR (600 MHz, DMSO-*d*₆) δ ppm 1.92 - 2.04 (m, 3 H) 2.04 - 2.11 (m, 1 H) 2.52 - 2.63 (m, 1 H) 3.16 - 3.27 (m, 4 H) 3.29 - 3.44 (m, 5 H) 3.53 - 3.65 (m, 2 H) 3.88 (dd, *J*=12.01, 3.21 Hz, 1 H) 4.00 (dd, *J*=12.01, 3.21 Hz, 1 H) 5.86 (br s, 1 H) 7.63 (t, *J*=7.79 Hz, 2 H) 7.77 (t, *J*=7.43 Hz, 1 H) 8.06 (d, *J*=7.67 Hz, 2 H) 10.69 (br s, 1 H)

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Table of assignments and zoomed parts:

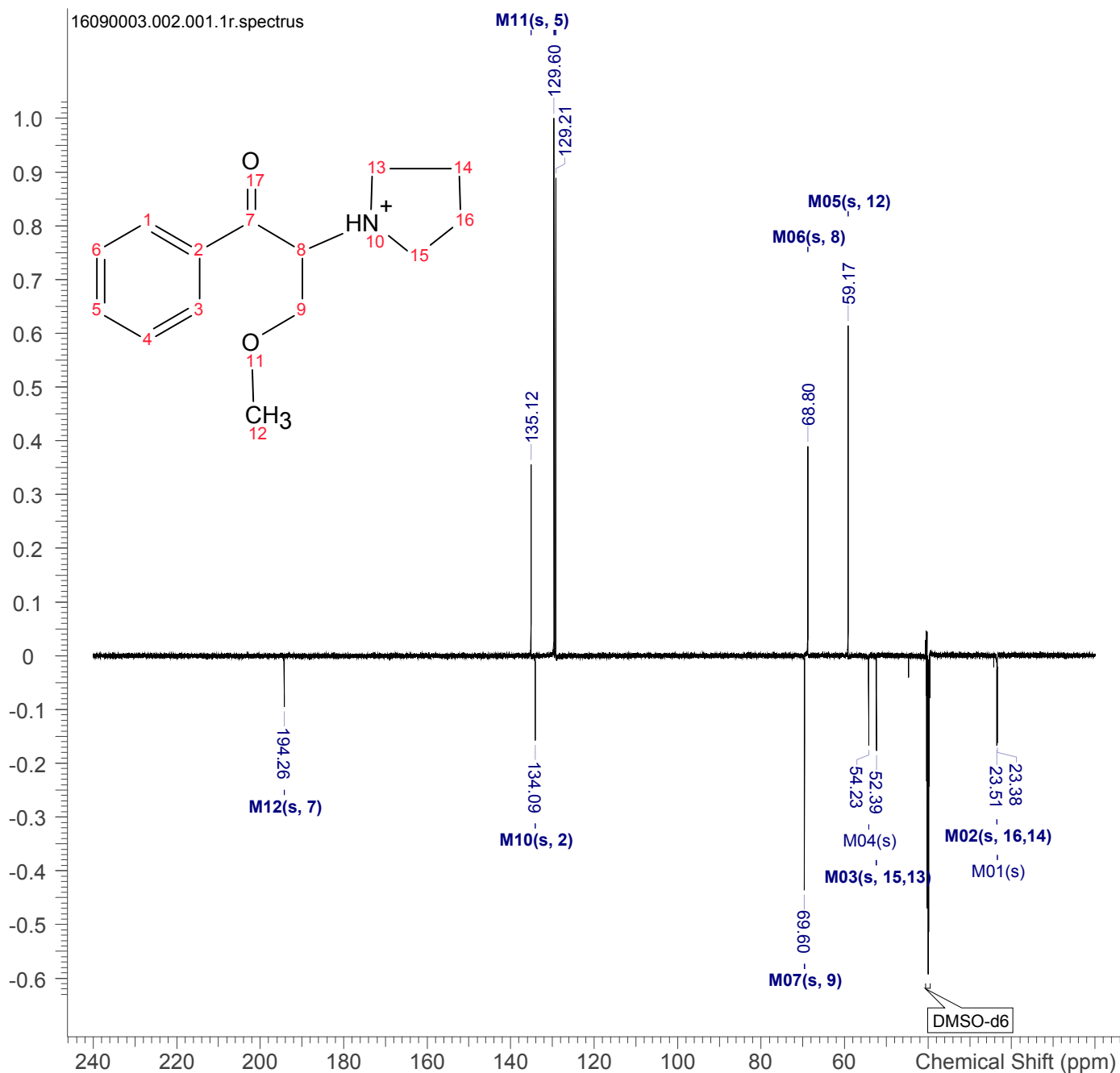
No.	Atom	Exp. Shift (ppm)	Multiplet
1	16	1.97	M01
2	14	1.97	M01
3	12	3.36	M05
4	15	3.36	M05
5	13	3.36	M05
6	15	3.58	M06
7	13	3.58	M06
8	9	3.88	M07
9	9	4.00	M08
10	8	5.86	M09
11	6	7.63	M10
12	4	7.63	M10
13	5	7.77	M11
14	3	8.06	M12
15	1	8.06	M12
16	10	10.69	M13



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Acquisition Time (sec)	0.9044	Comment	5 mm CPQCI 1H/19F-13C/15N/D Z-GRD Z114073/0012
Date	20 Sep 2016 14:44:46	Date Stamp	20 Sep 2016 14:44:46
File Name	\\139.191.6.82\ihcp\$\101\Bio_Chemical_Interaction_Metabonomics\CLEN2SAND\proposed-structure\BCIM_NAS\BCIM_600\16090003\2\PDATA\1\1r		
Frequency (MHz)	150.9028	Nucleus	13C
Number of Transients	256	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)	26.995		



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Table of assignments and zoomed parts:

No.	Atom	Exp. Shift (ppm)	Multiplet
1	16	23.51	M02
2	14	23.51	M02
3	15	52.39	M03
4	13	52.39	M03
5	12	59.17	M05
6	8	68.80	M06
7	9	69.60	M07
8	6	129.21	M08
9	4	129.21	M08
10	3	129.60	M09
11	1	129.60	M09
12	2	134.09	M10
13	5	135.12	M11
14	7	194.26	M12

