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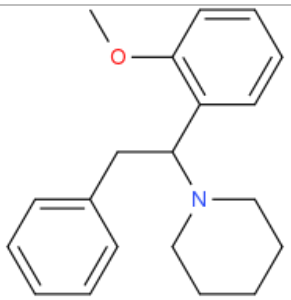
ANALYTICAL REPORT

2-MeO-diphenidine (C20H25NO)

1-(1-(2-methoxyphenyl)-2-phenylethyl)piperidine

Remark – other NPS detected: none

Sample ID:	1163-15A (corresponds to sample 3400-14-3E)
Sample description:	powder - white
Sample type:	seized
Comments:	LJ
Date of entry:	7/17/2014

Substance identified-structure[i] (base form)	
Systematic name	1-(1-(2-methoxyphenyl)-2-phenylethyl)piperidine
Other names	
Formula (per base form)	C20H25NO
M_w (g/mol)	295,42
Salt form	HCl
Smiles	COC1=C(C=CC=C1)C(CC1=CC=CC=C1)N1CCCCC1
Compound Class	Others
Other NPS detected	none
Add.info (purity..)	pure by GC-MS, HPLC, NMR (not detected impurities are possible)

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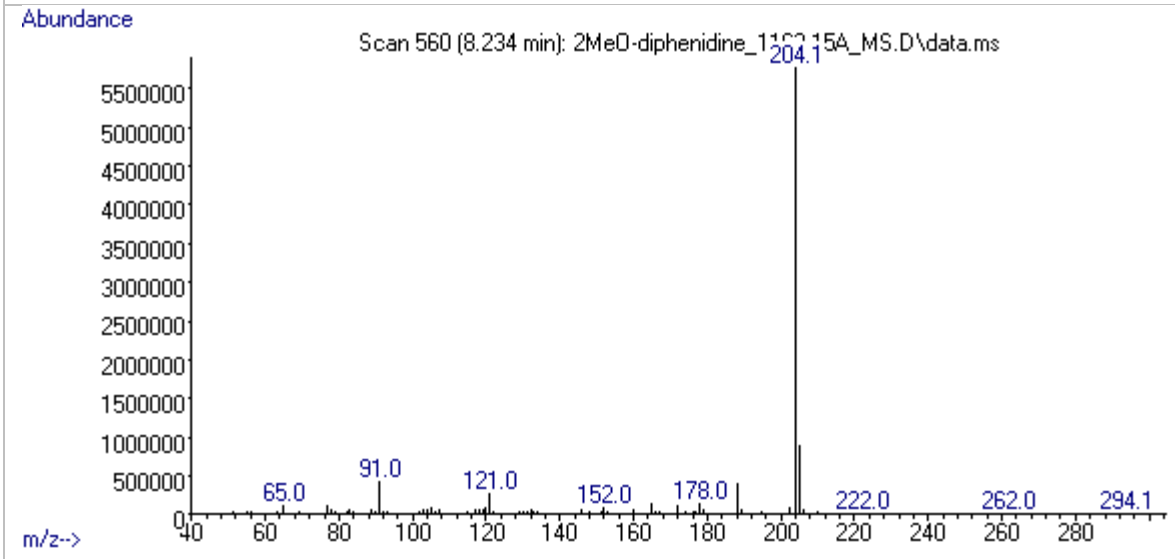
Supporting information

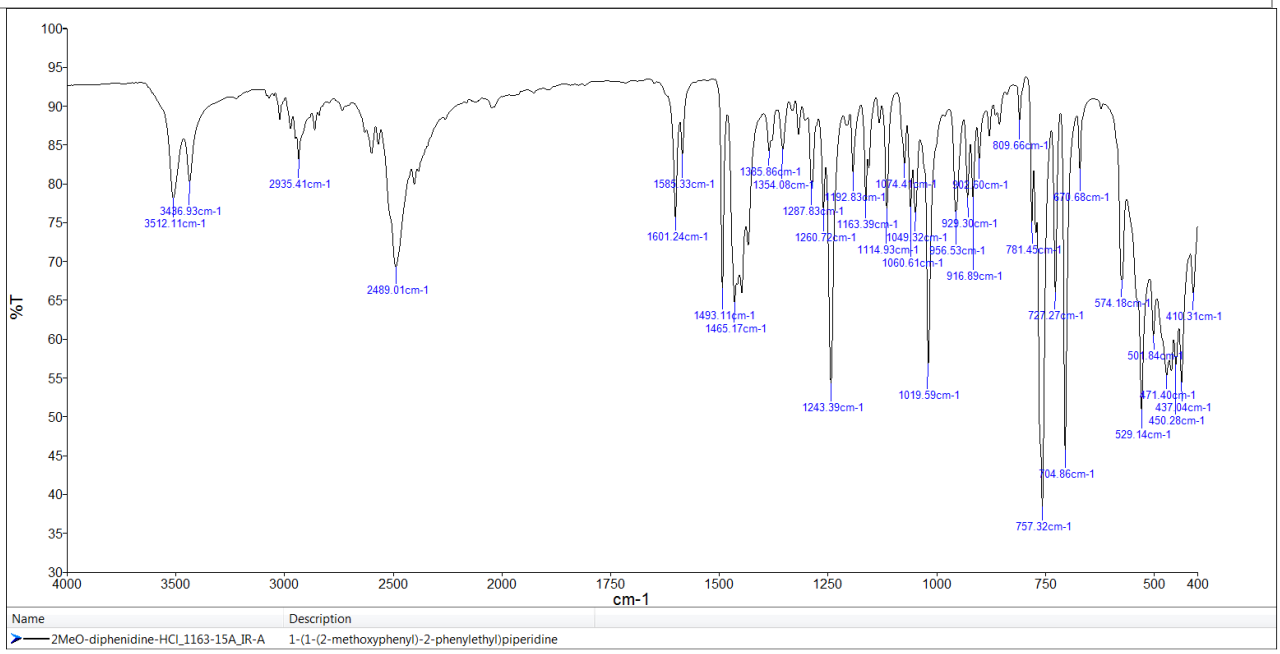
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): BP(1): 204; BP(2): 205,BP(3) :91,
FTIR-ATR	+	direct measurement
FTIR (condensed phase) always as base form	-	
HPLC-TOF	+	Exact mass (theoretical): 295,1936; measured value Δppm:-0,61; formula:C20H25NO
NMR-confirmed	+	
validation		
other		completely soluble in CH2Cl2 and in MeOH

GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50)for GC-MS instruments and 1:5 for GC-MS-FTIR(condensed phase). Injector temperature: 280 ^{0}C. Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C. m/z scan range: from 50 (40) to 550 amu.
FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1
FTIR (Spectra analyses-Danny): scan range 4000 to 600, resolution 4cm-1

MS spectrum (EI)



FTIR - ATR



[i] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Target Compound Screening Report

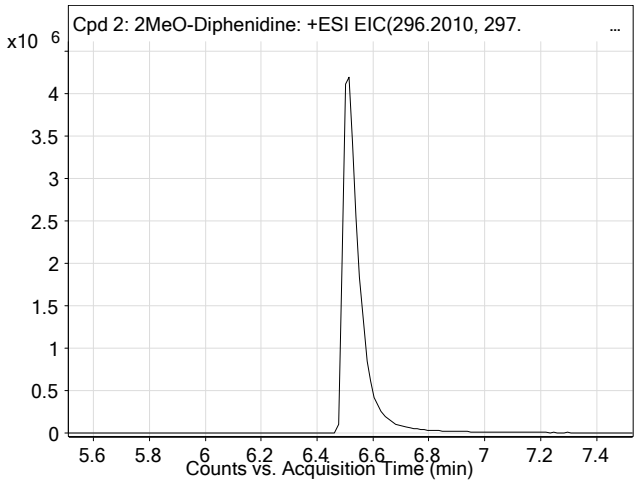
Data File	kben-233-3400_2014_1e.d	**Sample Name**	vzorec 1e
Sample Type	Sample	**Position**	P2-E7
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-17-9-2014-XDB-C18-ESI-poz.m	**Acquired Time**	9/18/2014 2:07:55 PM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment			

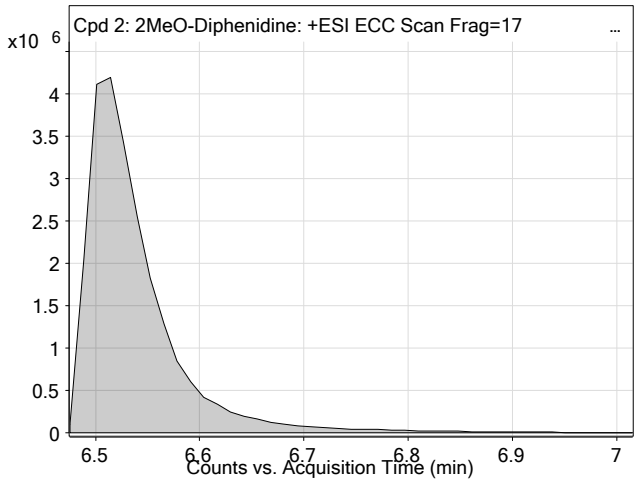
Compound Table

Label	Tgt Name	Obs. RT	Obs. Mass
Cpd 2: 2MeO-Diphenidine	2MeO-Diphenidine	6.515	295.1938

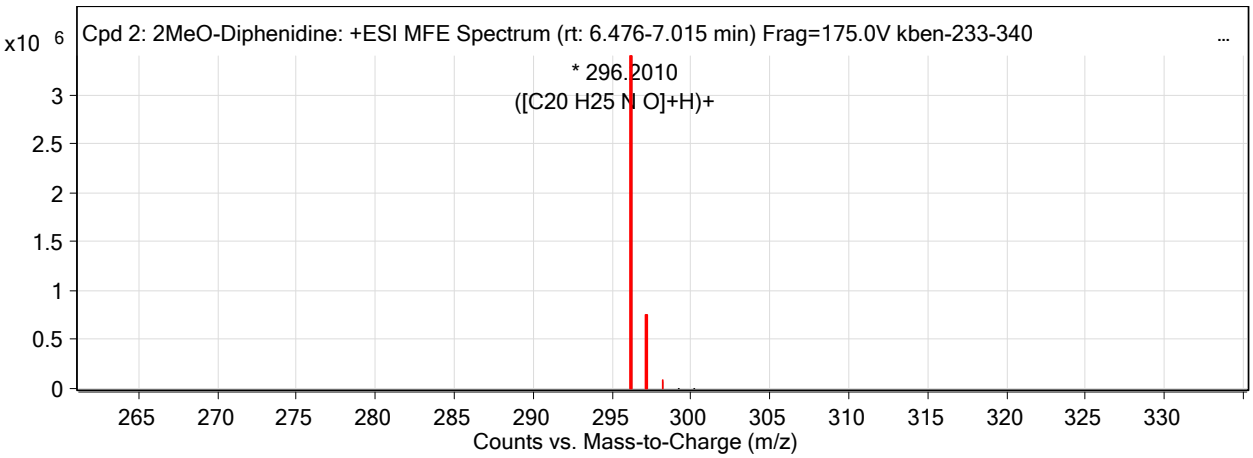
Name	Obs. *m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)	Find Cpds Algorithm
2MeO-Diphenidine	296.201	6.515	295.1938	6.545	C20 H25 N O	295.1936	-0.61	Find by Molecular Feature

Compound Chromatograms





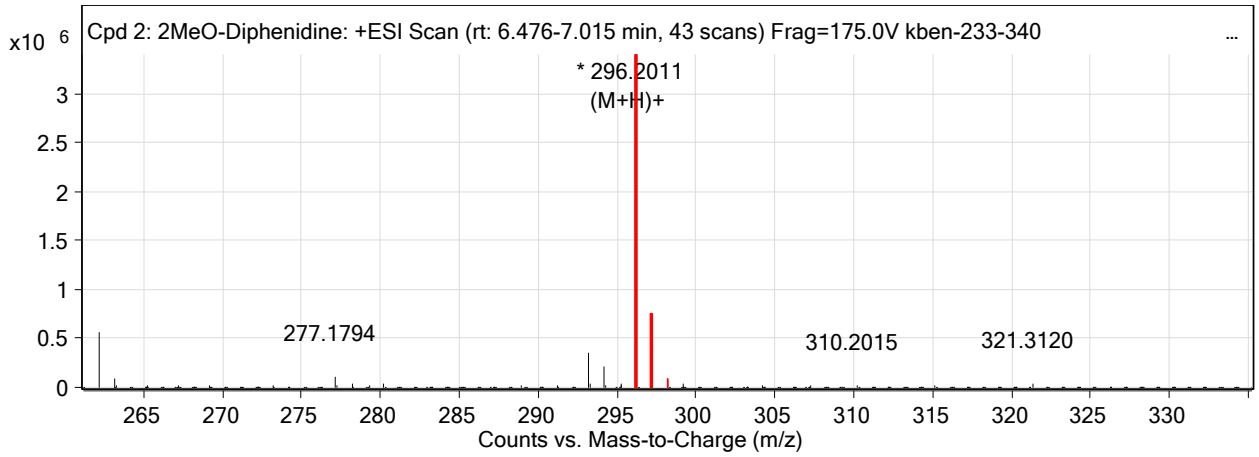
MFE MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Formula	Ion/Isotope
296.201	1	3394337	C20 H25 N O	(M+H)+
297.2048	1	706808.43	C20 H25 N O	(M+H)+
298.2072	1	67544.2	C20 H25 N O	(M+H)+
299.2089	1	4820.21	C20 H25 N O	(M+H)+
300.2072	1	341.62	C20 H25 N O	(M+H)+

MS Zoomed Spectrum



--- End Of Report ---

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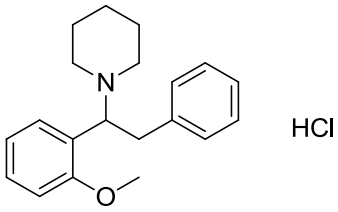
REPORT

Sample ID:	**233-3400-14-1E**
Our notebook code:	P-233-3400-14-1E
NMR sample preparation:	15 mg dissolved in 0.7 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC
Proposed structure with chemical name:	 HCl 1-(1-(2-methoxyphenyl)-2-phenylethyl)piperidine hydrochloride
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Compound is pure by NMR
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	April 30, 2015

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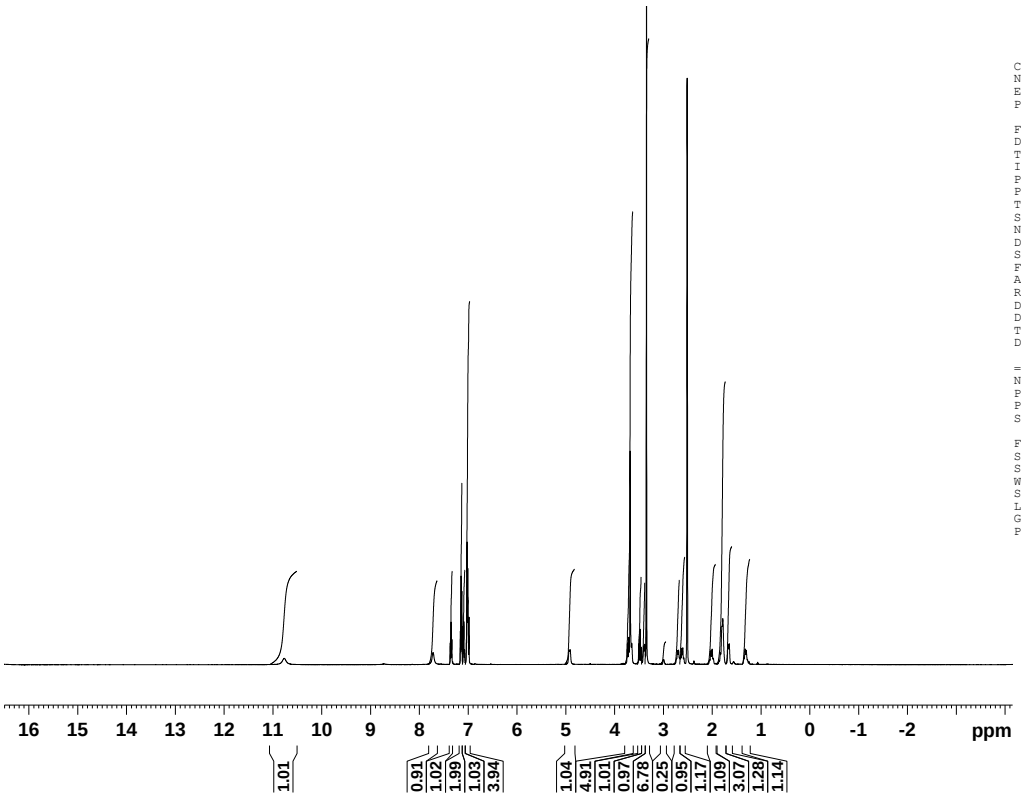
P-233-3400-14-1E
1H



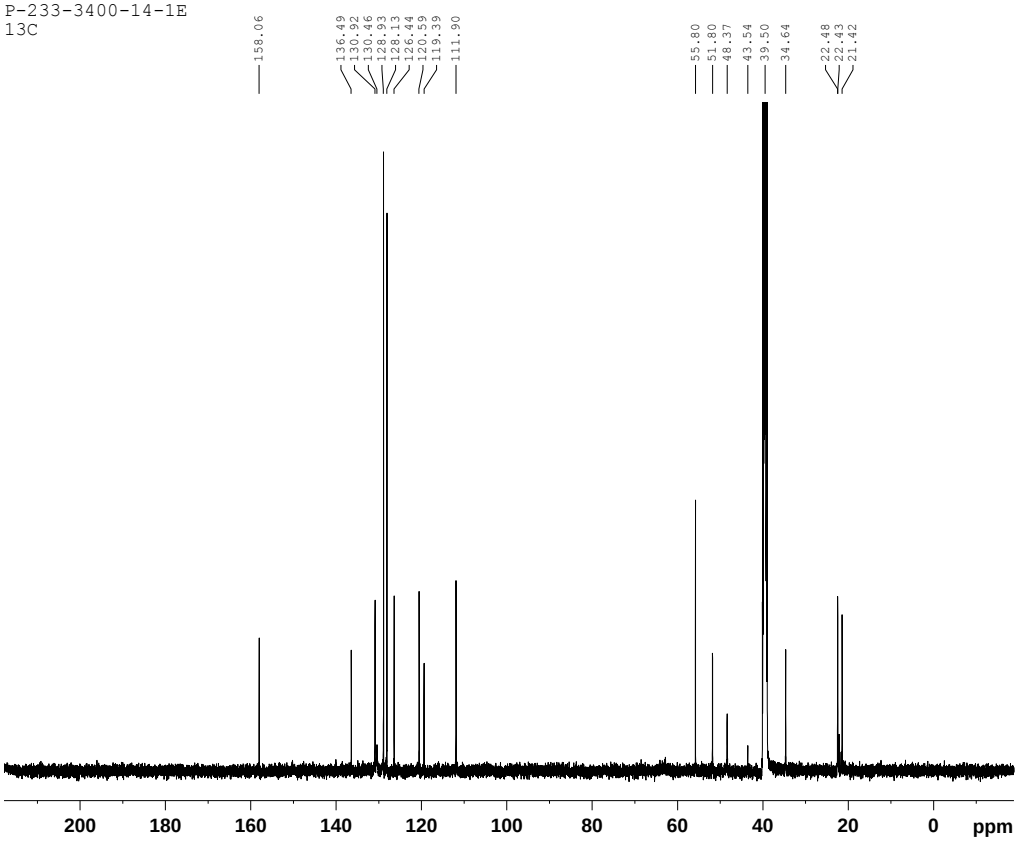

```
Current Data Parameters
NAME      P-233-3400-14-1E
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150131
Time                 15.37
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719923 sec
RG                   114
DW                48.400 usec
DE                 6.50 usec
TE                297.5 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  8.90 usec
PLW1        26.00000000 W
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                  65536
SF          500.1300000 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

P-233-3400-14-1E
13C




```
Current Data Parameters
NAME      P-233-3400-14-1E
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150131
Time                 18.44
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                   5120
DS                      4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                  2050
DW                16.800 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.00 usec
PLW1       122.00000000 W
SFO1        125.7703637 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PLW2        26.00000000 W
PLW12        0.32179001 W
PLW13        0.20595001 W
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF          125.7578493 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```