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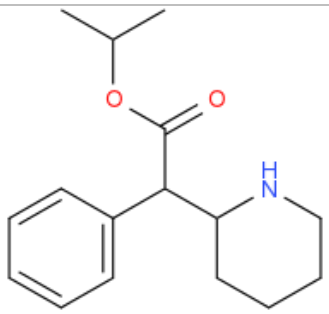
ANALYTICAL REPORT

Isopropylphenidate,C16H23NO2)

isopropyl 2-phenyl-2-(piperidin-2-yl)acetate

Remark – other NPS detected: none

Sample ID:	1171-15
Sample description:	powder - white
Sample type:	P- purchased
Date of entry:	4/17/2015

Substance identified-structure[i] (base form)	 *HCL
Systematic name	isopropyl 2-phenyl-2-(piperidin-2-yl)acetate
Other names	propan-2-yl 2-phenyl-2-(piperidin-2-yl)acetate
Formula (per base form)	C16H23NO2
M_w (g/mol)	261.36
Salt form	HCl
Smiles	C1(=CC=CC=C1)C(C(=O)OC(C)C)C1NCCCC1
Compound Class	Piperidines & pyrrolidines
Other NPS detected	none
Add.info (purity..)	trace amounts of impurities detected by NMR

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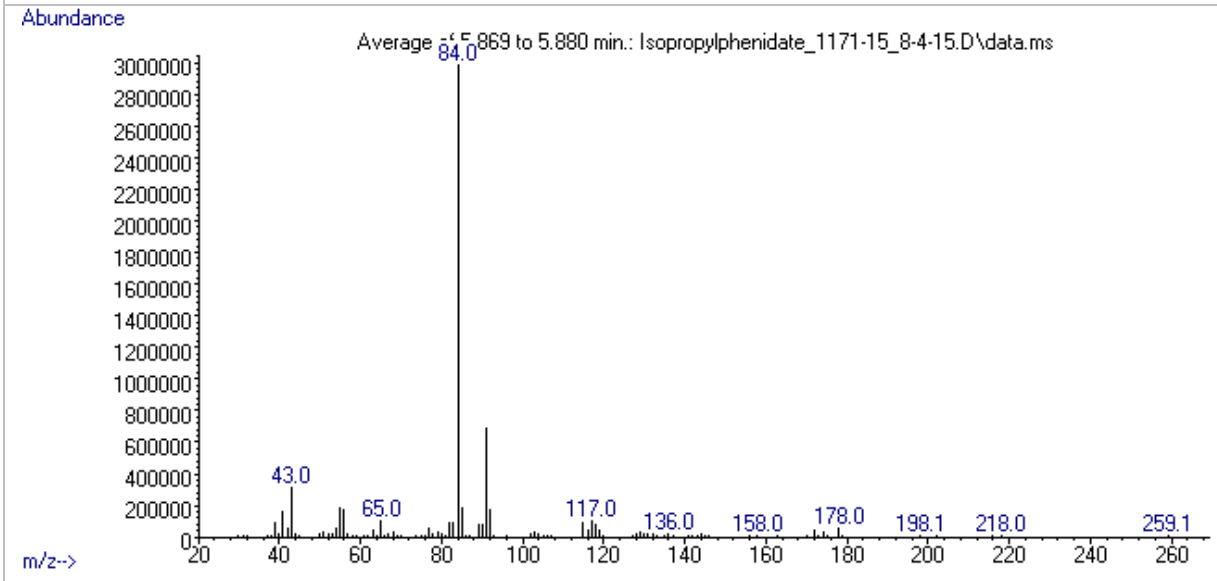
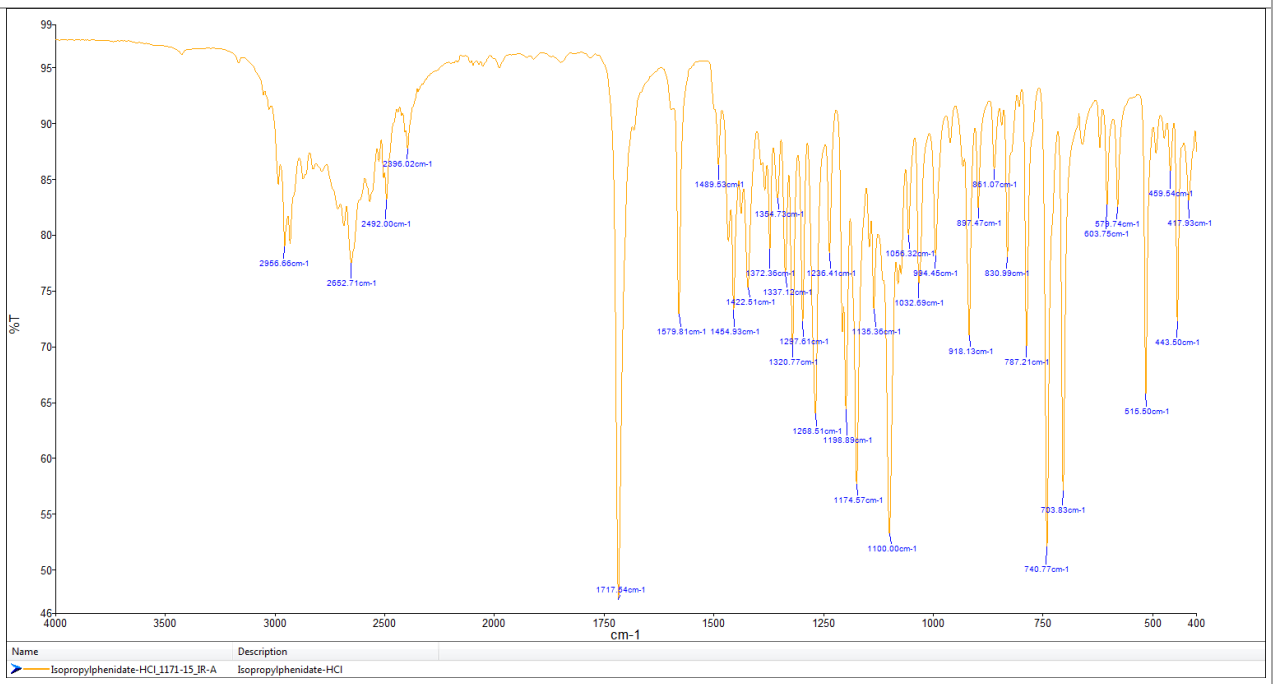
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 84; BP(2): 91,BP(3) :43,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	pending
HPLC-TOF	+	Exact mass: 261.1729, measured/ Δppm:-2.01; formula:C16H23NO2
NMR-confirmed	+	
validation		
other		

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

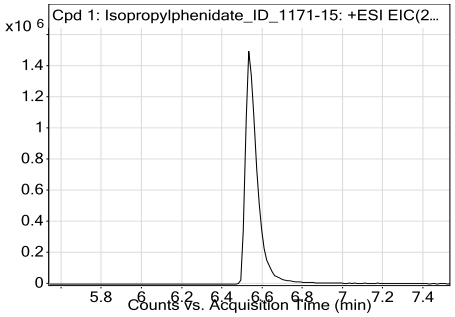
Data File	Isopropylphenidate_ID_1171-15_TOF.d	**Sample Name**	Isopropylphenidate
Sample Type	Sample	**Position**	P1-F4
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-2-4-2015-XDB-C18-ESI-poz.m	**Acquired Time**	4/10/2015 9:19:51 AM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	white powder, extract in MeOH		

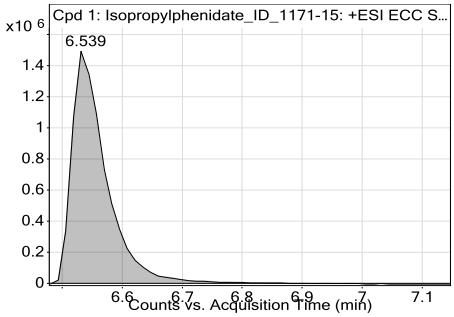
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: Isopropylphenidate_ID_1171-15	Isopropylphenidate_ID_1171-15	C16 H23 N O2	C16 H23 N O2	6.539	261.1734

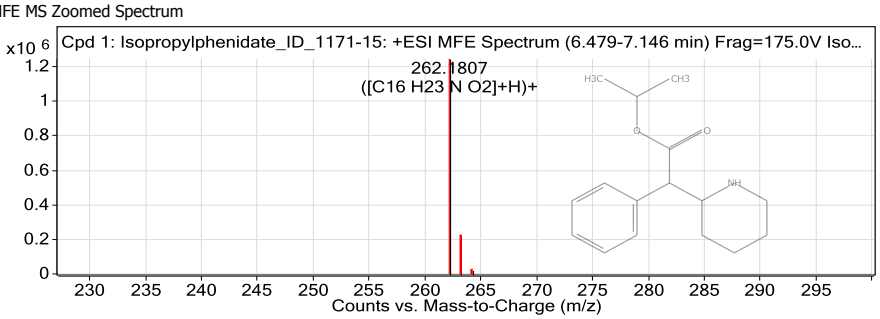
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
Isopropylphenidate_ID_1171-15	262.1807	6.539	261.1734	6.506	C16 H23 N O2	261.1729	-2.01	C16 H23 N O2	Find by Molecular Feature

Compound Chromatograms

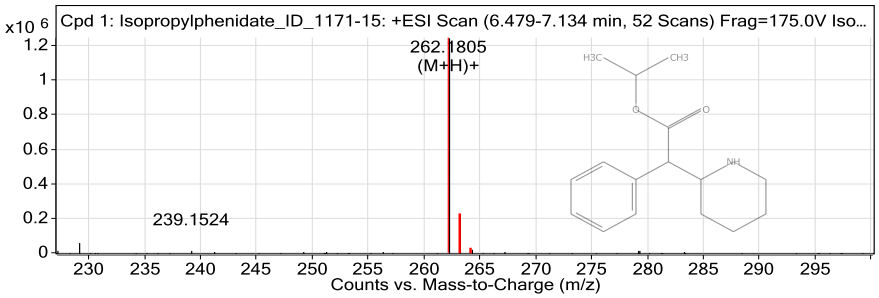




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
262.1807	1	1245881.75	C16 H23 N O2	(M+H)+
263.1837	1	220356.88	C16 H23 N O2	(M+H)+
264.1862	1	24458.61	C16 H23 N O2	(M+H)+
265.1844	1	2397.19	C16 H23 N O2	(M+H)+

--- End Of Report ---

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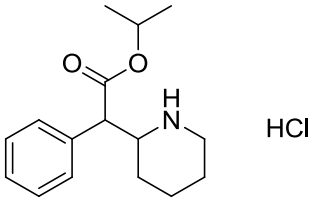
REPORT

Sample ID:	**1171-15**
Our notebook code:	P-1171-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^1H, ^{13}C, ^1H–^1H *gs*-COSY, ^1H–^{13}C *gs*-HSQC, ^1H–^{13}C *gs*-HMBC, ^1H–^{15}N *gs*-HMBC
Proposed structure with chemical name:	 HCl isopropyl 2-phenyl-2-(piperidin-2-yl)acetate hydrochloride
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Trace amounts of impurities are detected ^1H and ^{13}C NMR spectra
Supporting information:	Copies of ^1H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	April 30, 2015

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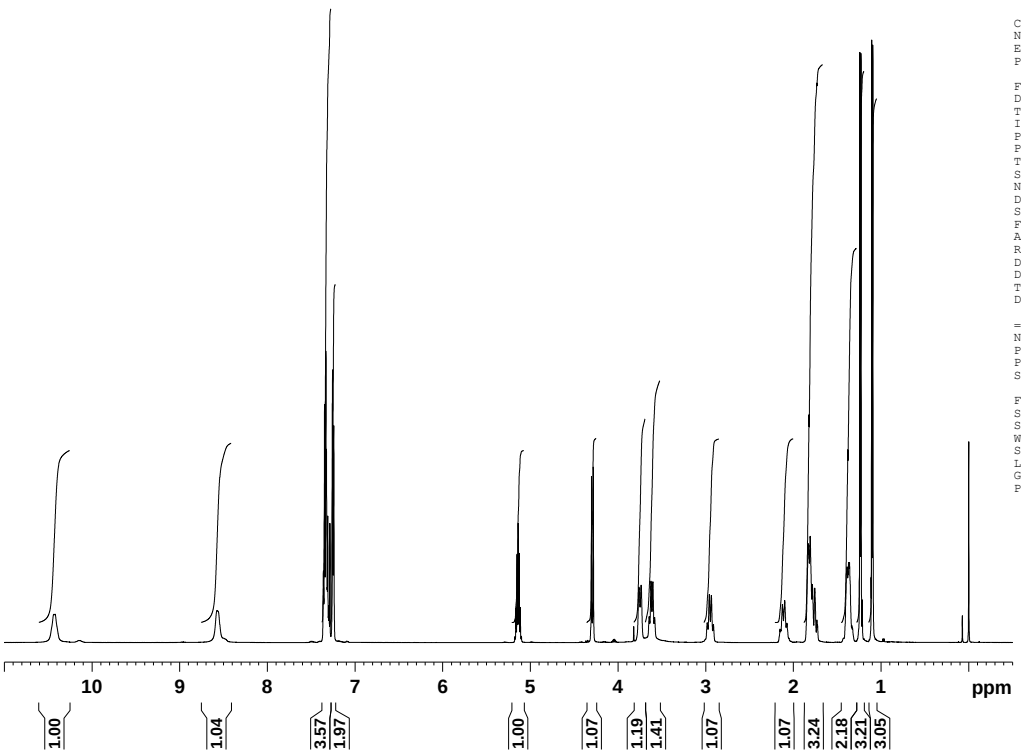
P-1171-15
1H



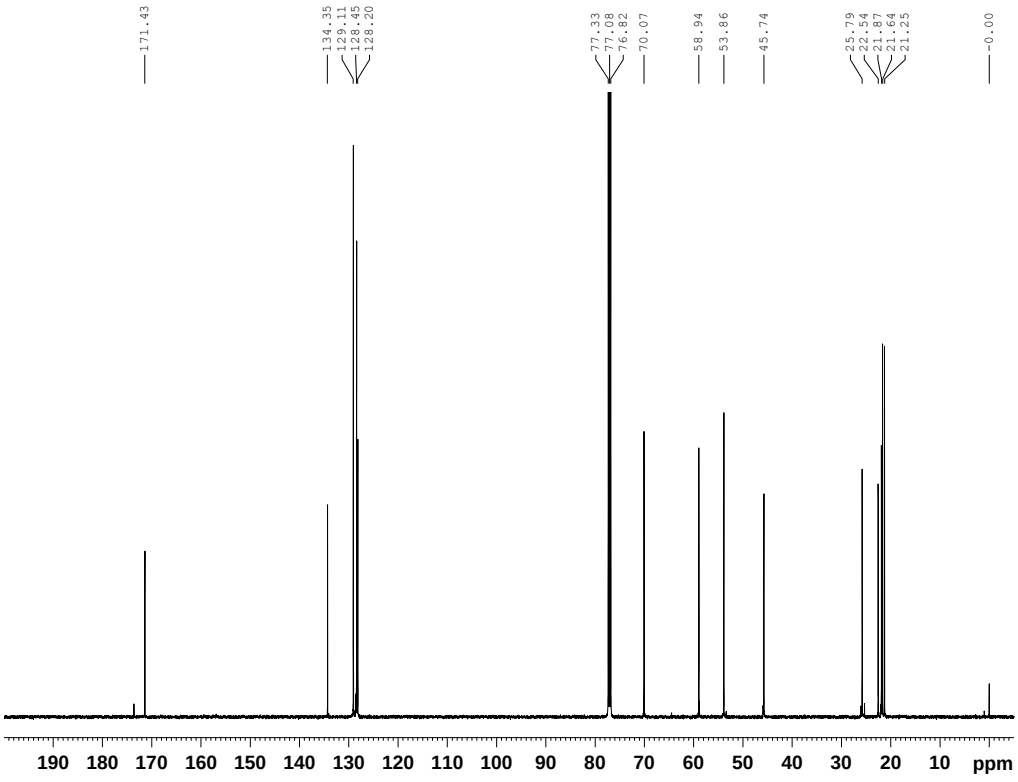

```
Current Data Parameters
NAME                  P-1171-15
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150424
Time                       2.49
INSTRUM                   spect
PROBHD   5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           16
DS                            2
SWH                10330.578 Hz
FIDRES              0.157632 Hz
AQ                  3.1719923 sec
RG                           57
DW                      48.400 usec
DE                       6.50 usec
TE                      296.0 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                500.1299996 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

P-1171-15
13C




```
Current Data Parameters
NAME                  P-1171-15
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150424
Time                       5.18
INSTRUM                   spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         4096
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                125.7577887 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```