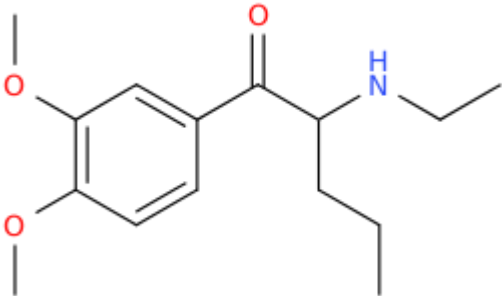


ANALYTICAL REPORT¹DL-4662 (C₁₅H₂₃N₃O₃)

1-(3,4-dimethoxyphenyl)-2-(ethylamino)pentan-1-one

Remark – other NPS detected: none

Sample ID:	1857-17
Sample description:	powder - white
Sample type:	collected /FSI Zurich, Switzerland
Date of sample receipt (M/D/Y):	10/11/2017
Date of entry (M/D/Y) into NFL database:	10/20/2017
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ² (base form)	
Systematic name	1-(3,4-dimethoxyphenyl)-2-(ethylamino)pentan-1-one
Other names	3,4-Dimethoxy-N-ethylnorpentedrone, DL 4662; 3',4'-Dimethoxy-alpha-(ethylamino)valerophenone
Formula (per base form)	C ₁₅ H ₂₃ N ₃ O ₃
M _w (g/mol)	265,35
Salt form/anions detected	HCl
StdInChIKey (for base form)	WZVCLFAACAERMB-UHFFFAOYSA-N
Other NPS detected	none
Add.info (purity..)	>96 % (FSI Zurich data)

¹ Acknowledgement: Sample (NMR confirmed) was kindly provided by FSI Zurich, Switzerland. Measurements shown in this report were done in NFL.

² Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N₂) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

4. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1: 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

5. IC (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30 °C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

Supporting information

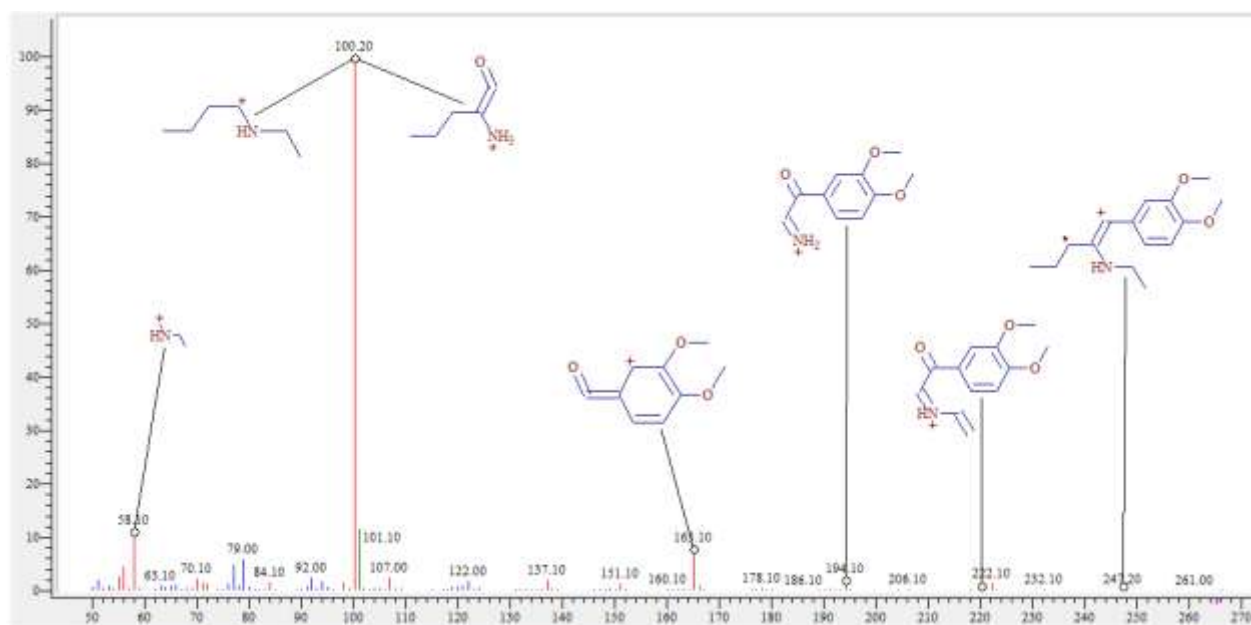
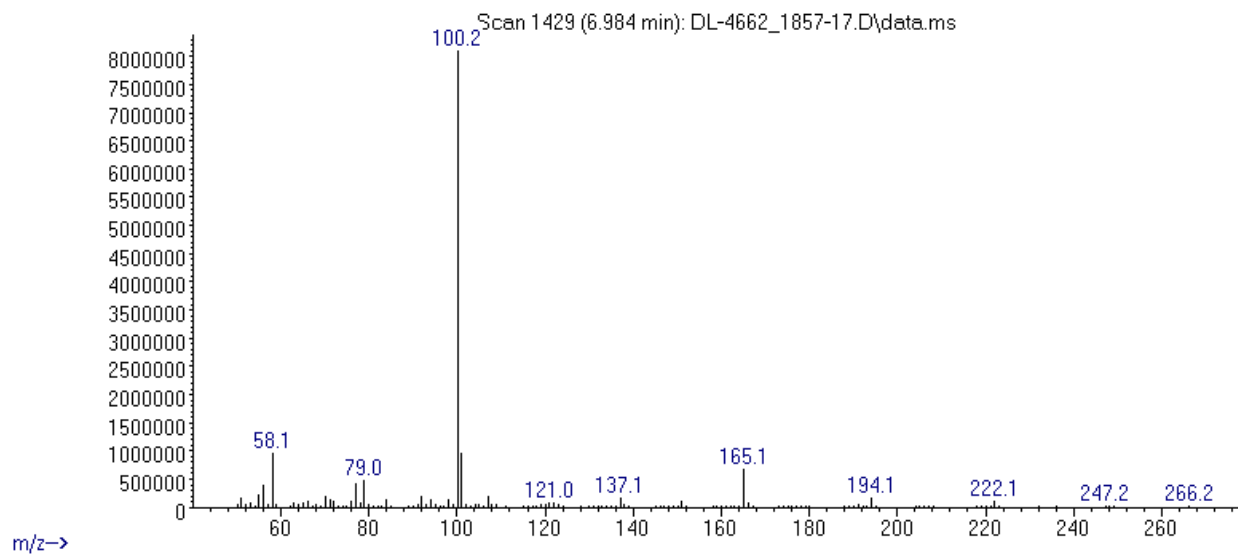
Solubility in	result/remark
CH ₂ Cl ₂	partially
MeOH	soluble
H ₂ O	soluble

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,98 BP(1): 100; BP(2): 101,BP(3) :58,
HPLC-TOF	+	Exact mass (theoretical): 265,1678; measured value Δppm:-2,58; formula:C15H23NO3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		
other		

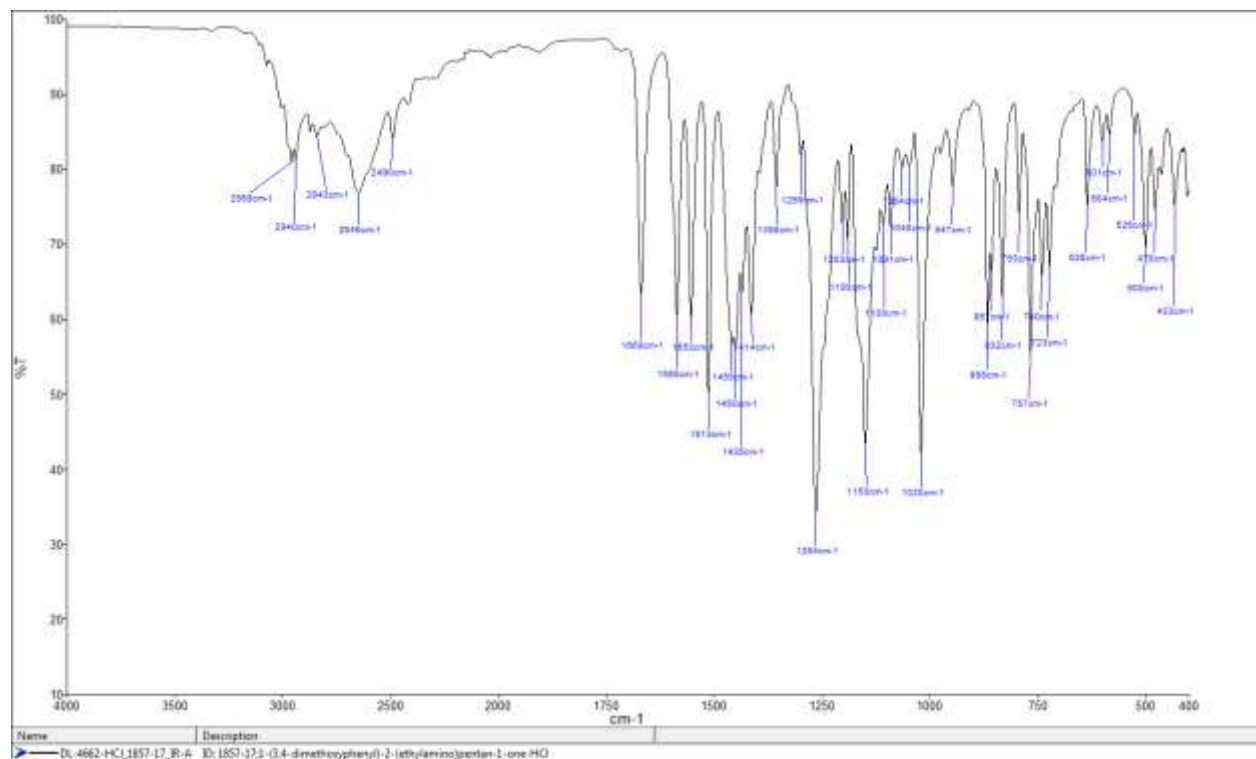
ANALYTICAL RESULTS

MS (EI)

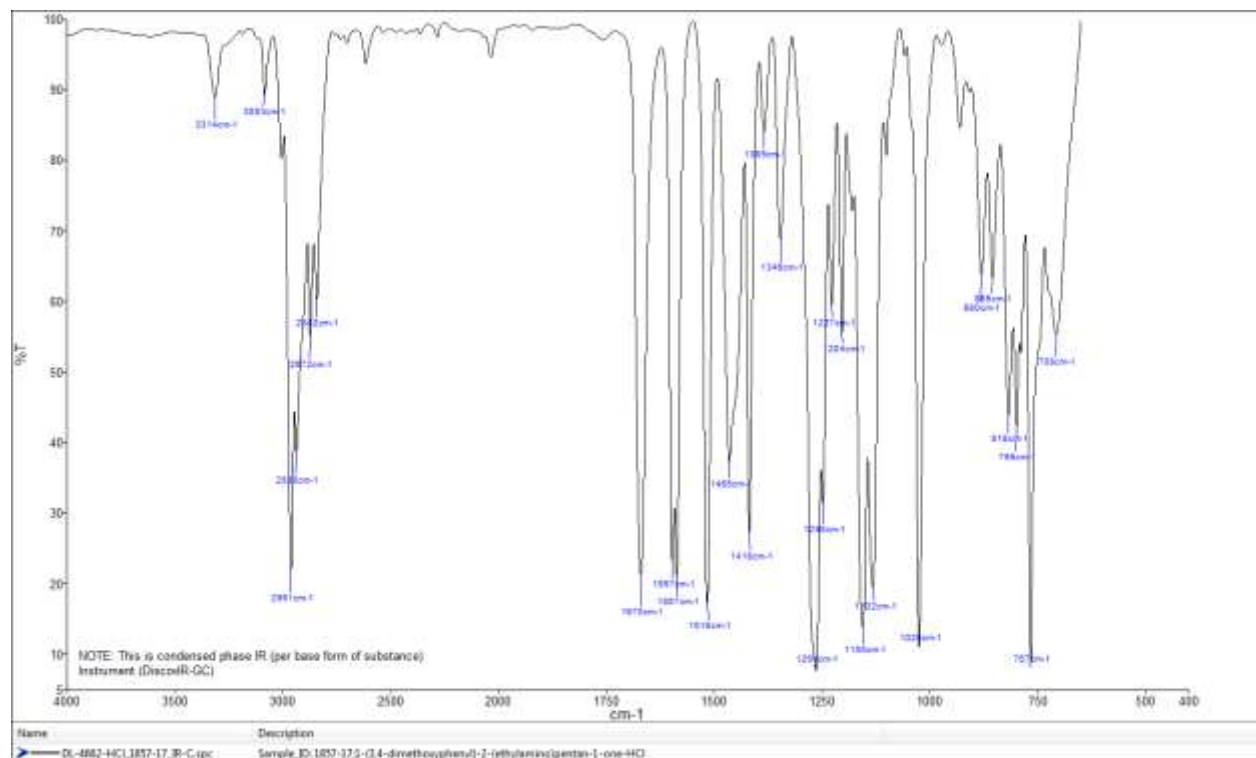
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

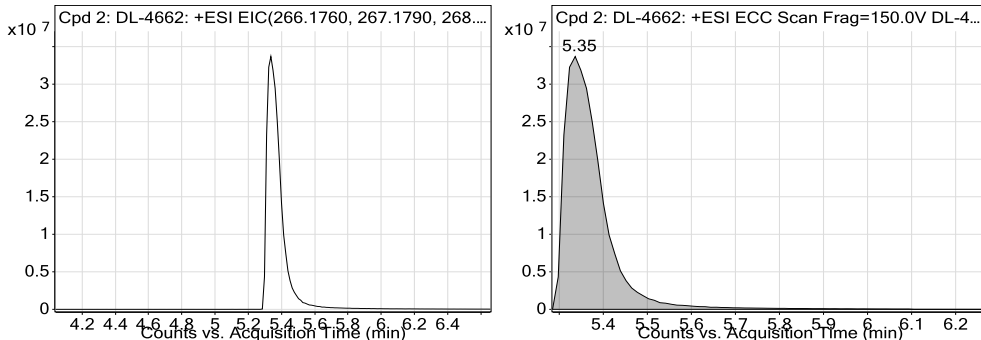
Data File	DL-4662_1857-17.d	Sample Name	1857-17
Sample Type	Sample	Position	P1-A7
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-19_07_2017-XDB-C18-ESI-final.m	Acquired Time	10/17/2017 2:19:19 PM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	MeOH		

Compound Table

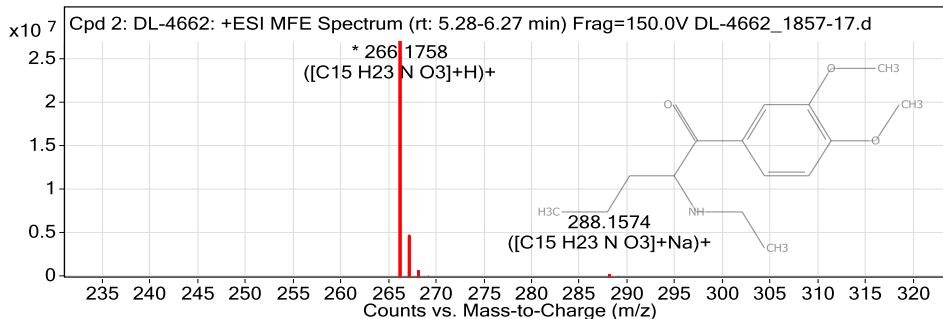
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: DL-4662	DL-4662	C15 H23 N O3	5.35	265.1685

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
DL-4662	266.1758	5.35	265.1685	5.35	C15 H23 N O3	265.1678	-2.58

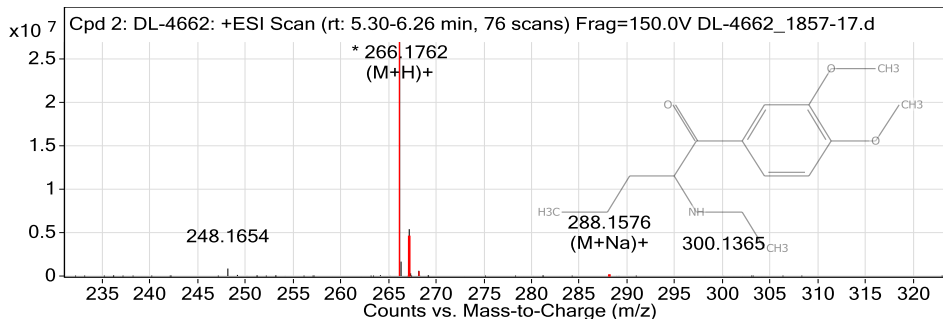
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
266.1758	1	26889304	C15 H23 N O3	(M+H)+
267.1789	1	4751792.22	C15 H23 N O3	(M+H)+
268.182	1	492015.78	C15 H23 N O3	(M+H)+
269.1841	1	43183.08	C15 H23 N O3	(M+H)+
270.1868	1	2399.08	C15 H23 N O3	(M+H)+
288.1574	1	122285.73	C15 H23 N O3	(M+Na)+
289.1605	1	19311.81	C15 H23 N O3	(M+Na)+

--- End Of Report ---

Peak Integration Report

Sample Name:	1857-17	Inj. Vol.:	25,00
Injection Type:	Unknown	Dilution Factor:	1,0000
Program:	ANIONI	Operator:	kemija
Inj. Date / Time:	17-okt-2017 / 17:10	Run Time:	42,00

No.	Time min	Peak Name	Peak Type	Area $\mu\text{S} \cdot \text{min}$	Height μS	Amount mg/L
1,00	9,46	Chloride	BMB	69,09	289,85	n.a.
		TOTAL:		69,09	289,85	0,00

