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EUROPEAN PROJECT RESPONSE 2 to challenges in forensic drugs analyses
Co-funded by the Internal Security Found of the European Union

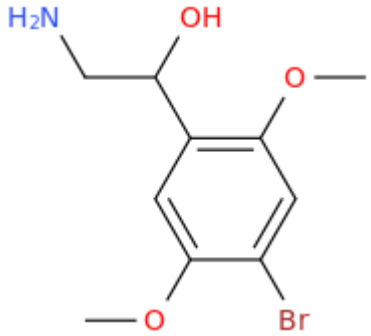
ANALYTICAL REPORT

BOH-2C-B (C10H14BrNO3)

2-amino-1-(4-bromo-2,5-dimethoxyphenyl)ethan-1-ol

Remark – other NPS detected: unidentified impurities

Sample ID:	2193-20
Sample description:	powder
Sample type:	test purchase /ISF projekt (NFL-SI)
Date of entry (DD/MM/YYYY) into NFL database:	28/09/2020
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure[1] (base form)	
Systematic name	2-amino-1-(4-bromo-2,5-dimethoxyphenyl)ethan-1-ol
Other names	2-Amino-1-(4-bromo-2,5-dimethoxy-phenyl)-ethanol; BOHB; α-(aminomethyl)-4-bromo-2,5-dimethoxy-benzenemethanol; β-hydroxy 2C-B
Formula (per base form)	C10H14BrNO3
M_w (g/mol)	276,13
Salt form/anions detected	HCl
StdInChIKey (per base form)	PCSKDXWCLQXURQ-UHFFFAOYSA-N
Other NPS detected	unidentified impurities
Additional info (purity..)	

[1] 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 µl and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 7.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 6.1 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, 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 µl and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).** Split MS : IR = 1: 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (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 KOH 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

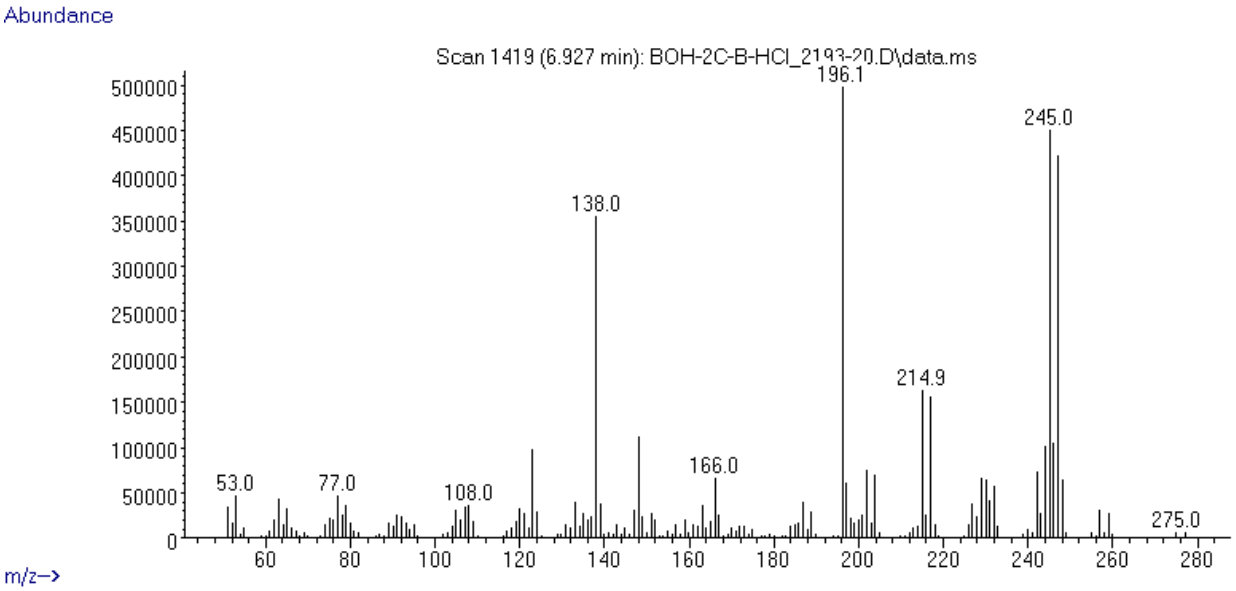
Supporting information

Solubility in	result/remark
CH_2Cl_2	not soluble
MeOH	soluble
H_2O	soluble

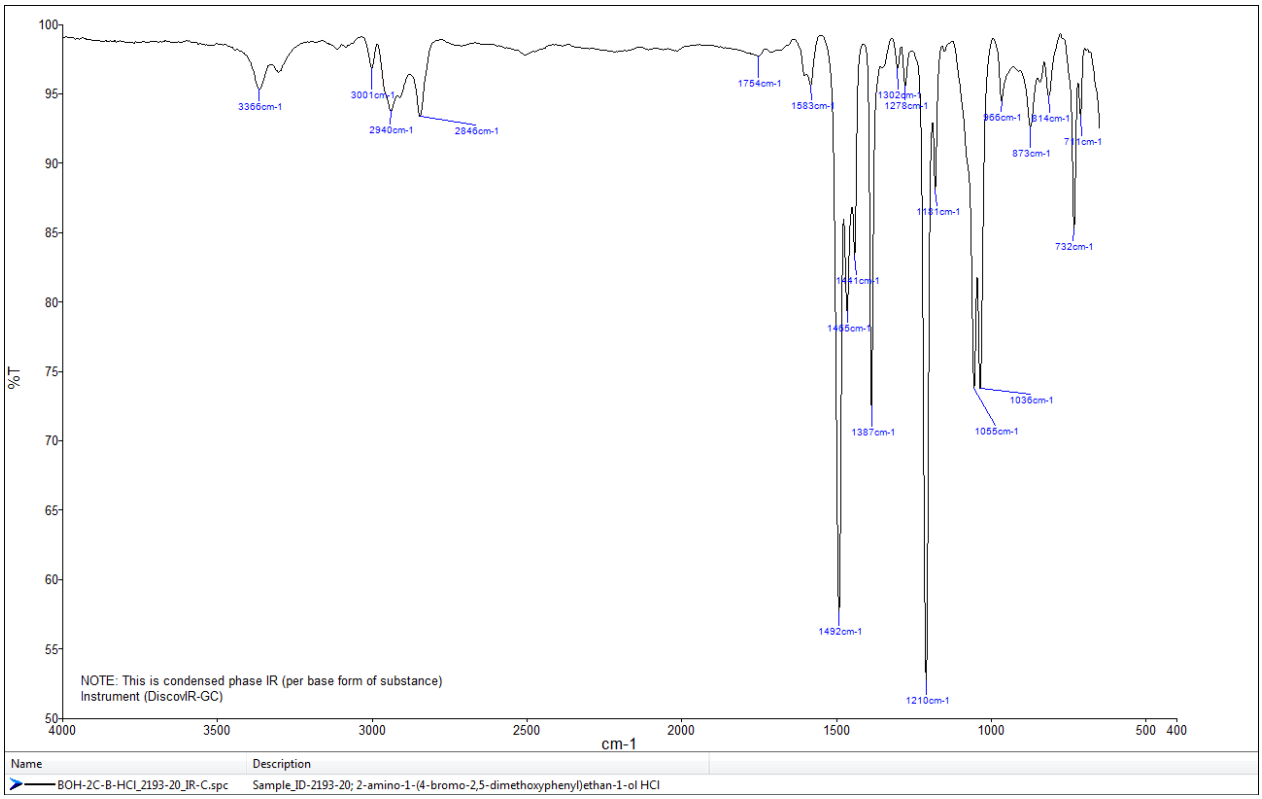
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,93 BP(1): 196; BP(2): 245,BP(3) :247,
HPLC-TOF	+	Exact mass (theoretical): 275,0157; measured value Δppm:1,56; formula:C10H14BrNO3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		MS -EI, IR-ATR and IR-C spectra in good agreement with spectra of BOH-2C-B compound (confirmed in ADEBAR project) published in EDND2 database.
other		

ANALYTICAL RESULTS

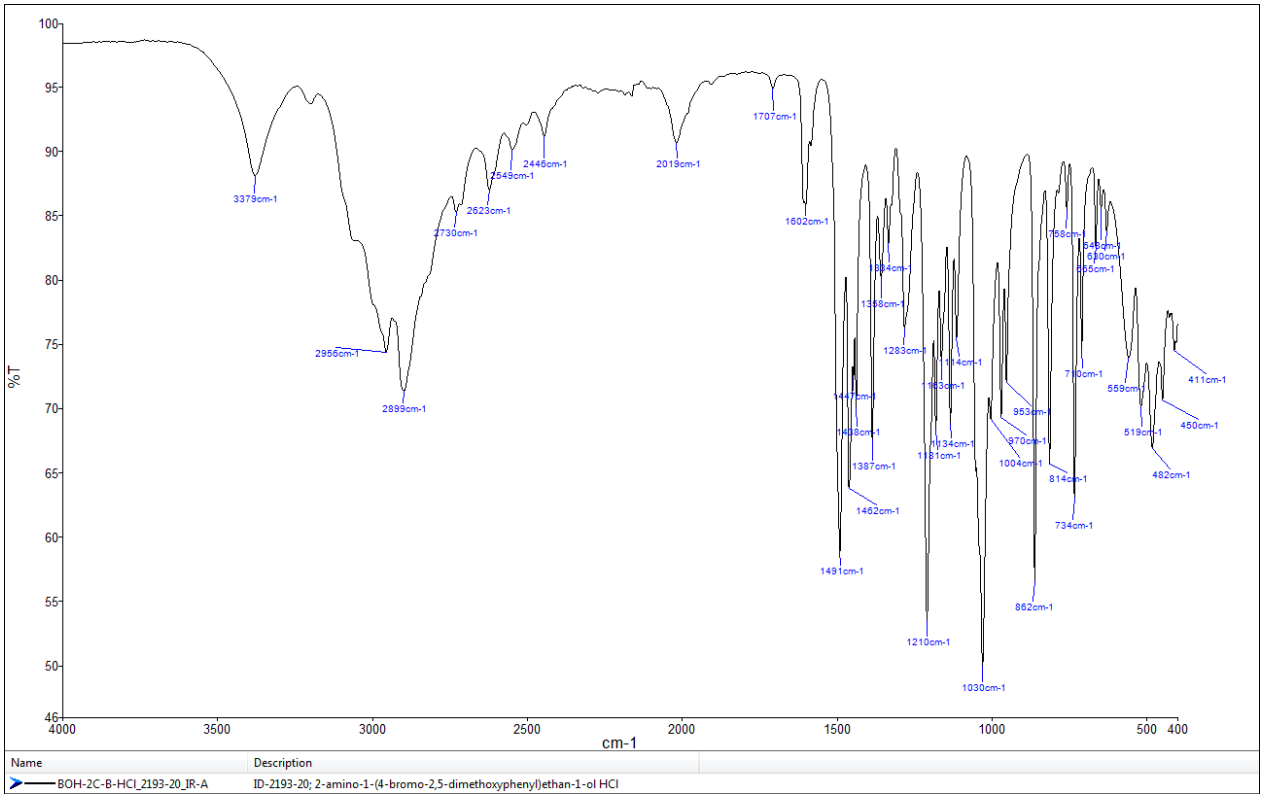
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



TOF REPORT

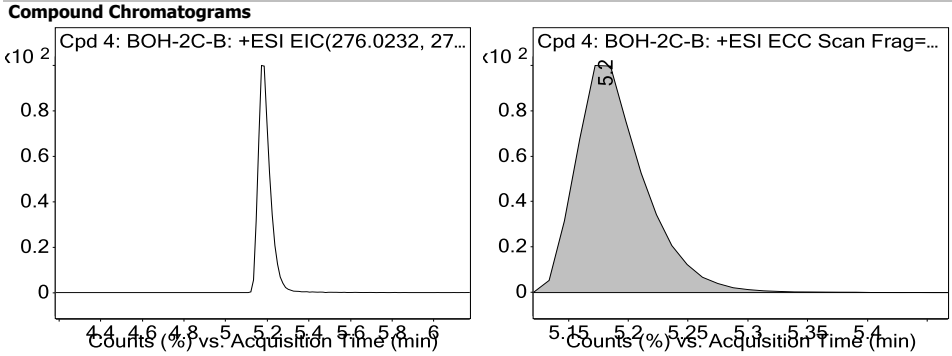
Data File	BOH-2C-B_2193-2020.d	**Sample Name**	ID-2193-20
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-15_01_2020-XDB-C18-ESI+.m	**Acquired Time**	9/24/2020 9:15:53 AM
IRM Calibration Status	Success	**DA Method**	a-Drugs_NFL.m
Comment	MeOH		

Compound Table

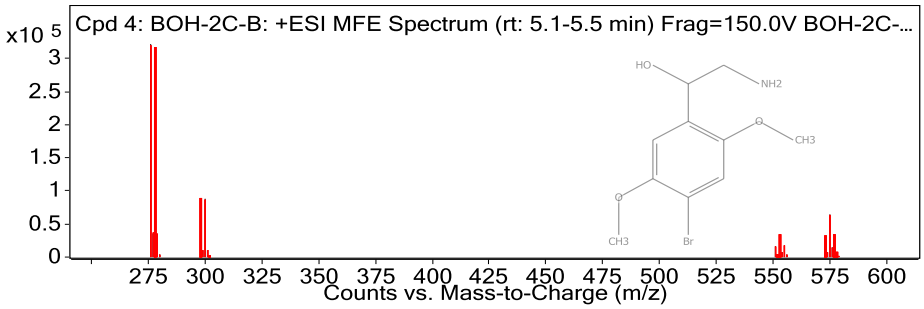
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 4: BOH-2C-B	BOH-2C-B	C10 H14 Br N O3	5.2	275.0153
Cpd 5: C11 H16 Br N O3		C11 H16 Br N O3	5.3	289.0313

Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
BOH-2C-B	276.0222	5.2	275.0153	5.2	C10 H14 Br N O3	275.0157	1.56

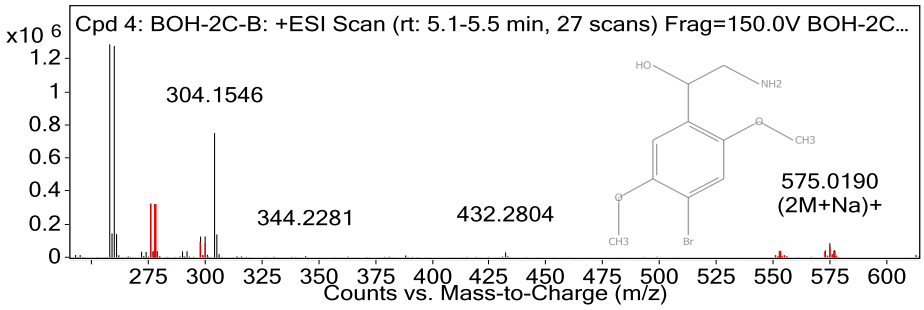
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



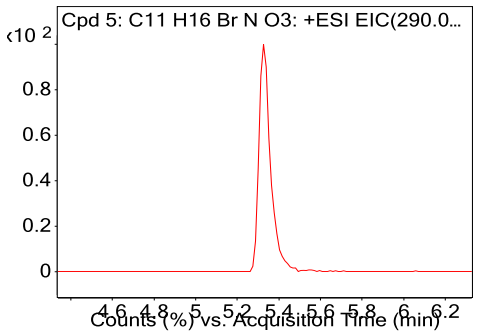
MS Spectrum Peak List

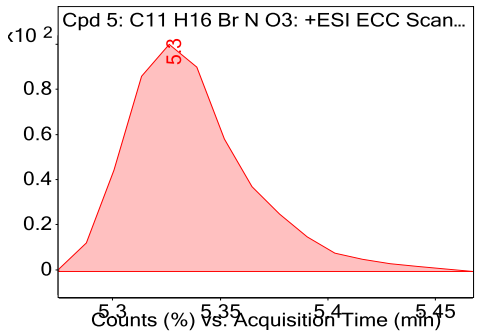
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
276.0222	1	322004.06	C10 H14 Br N O3	(M+H)+
277.0252	1	35566.99	C10 H14 Br N O3	(M+H)+
278.0202	1	317590.1	C10 H14 Br N O3	(M+H)+
279.0232	1	34967.69	C10 H14 Br N O3	(M+H)+
298.0041	1	87038.9	C10 H14 Br N O3	(M+Na)+
300.0023	1	88195.29	C10 H14 Br N O3	(M+Na)+
553.0358	1	33592	C10 H14 Br N O3	(2M+H)+
573.0203	1	31703.75	C10 H14 Br N O3	(2M+Na)+
575.0184	1	64514.5	C10 H14 Br N O3	(2M+Na)+
577.0165	1	32799.44	C10 H14 Br N O3	(2M+Na)+

Obs. m/z	Obs. RT	Obs. Mass
290.0386	5.3	289.0313

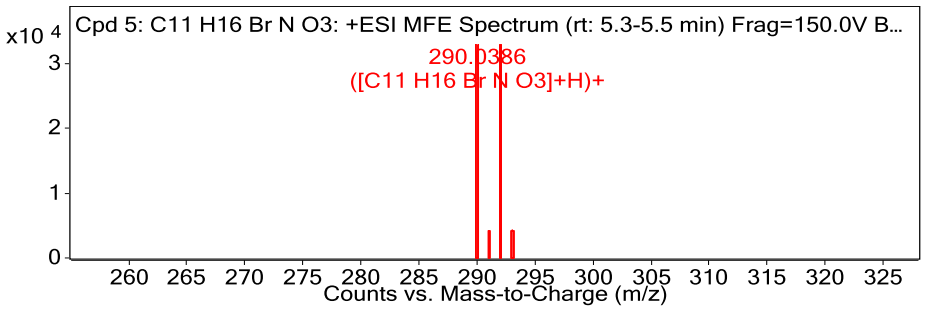
Compound Chromatograms

TOF REPORT

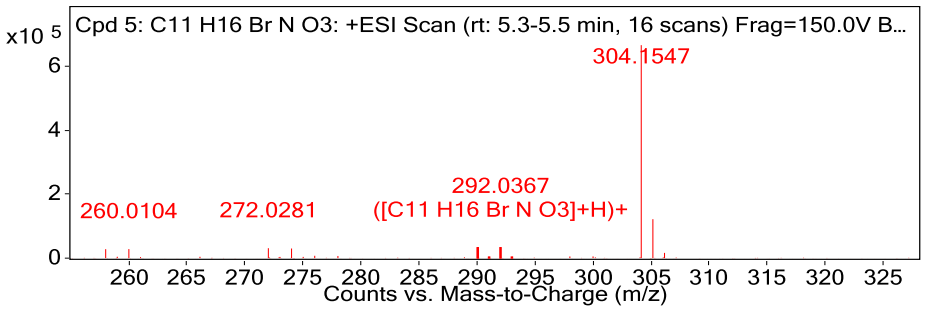




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
290.0386	1	32883.56	C11 H16 Br N O3	(M+H)+
291.0419	1	4264.97	C11 H16 Br N O3	(M+H)+
292.0367	1	32784.23	C11 H16 Br N O3	(M+H)+
293.04	1	4437.88	C11 H16 Br N O3	(M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**2193_IC**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Program:	**ANIONI**	*Operator:*	**kemija**
Inj. Date / Time:	**25-sep-2020 / 08:46**	*Run Time:*	**43,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1	8,61	**Chloride**	BMB	45,304	211,577	n.a.
		TOTAL:		45,30	211,58	0,0