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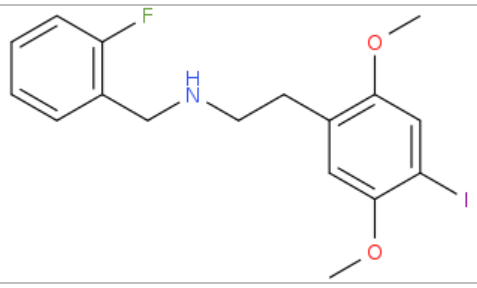
ANALYTICAL REPORT[1]

25I-NBF (C17H19FINO2)

N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine, monohydrochloride

Remark – other NPS detected: 25C-NBF and 25-NBF (<1%)

Sample ID:	1386-15
Sample description:	powder - white
Sample type:	test purchase /RESPONSE -purchasing
Date of sample receipt (M/D/Y):	12/9/2016
Date of entry (M/D/Y) into NFL database:	3/9/2016
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	N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine, monohydrochloride
Other names	25I-NB2F, 2C-I-NBF, NBF-2C-I, Cimbi-21
Formula (per base form)	C17H19FINO2
M_w (g/mol)	415.24
Salt form/anions detected	HCl
StdInChIKey	LPBKNBHMWRBPHT-UHFFFAOYSA-N
Compound Class	Phenethylamines
Other NPS detected	25C-NBF and 25-NBF (<1%)
Add.info (purity..)	traces of 25C-NBF and 25-NBF + unidentified non soluble impurities

[1] This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

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

Report updates

date	comments (explanation)
13 April 2018	compound class corrected

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50) . Injector temperature: 280 ^{0}C. Chromatographic separation: on 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 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) 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 ^{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 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

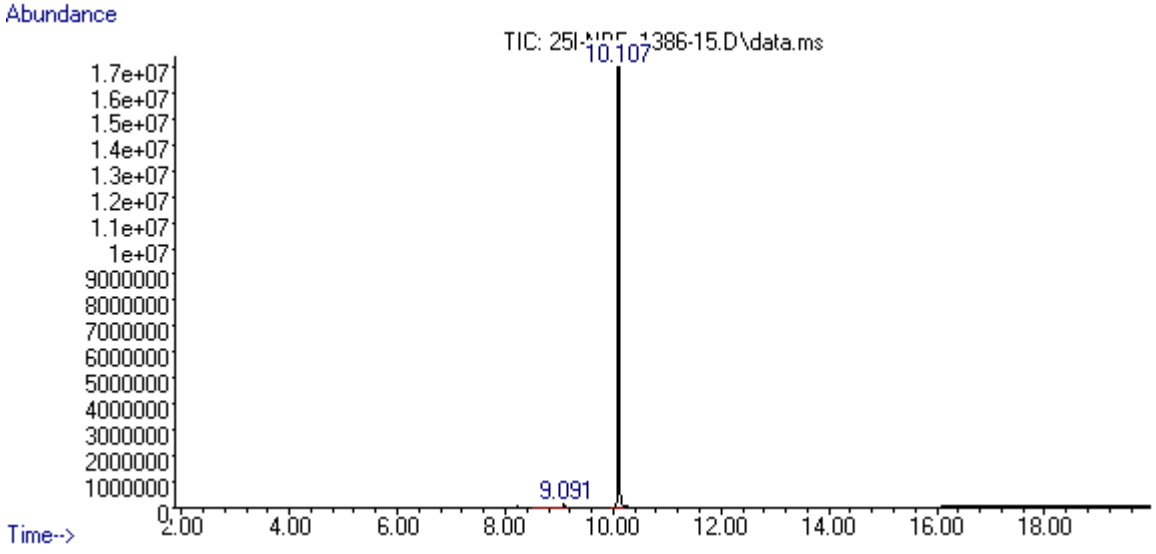
Supporting information

Solubility in	result/remark
CH_2Cl_2	partially
MeOH	partially
H_2O	partially

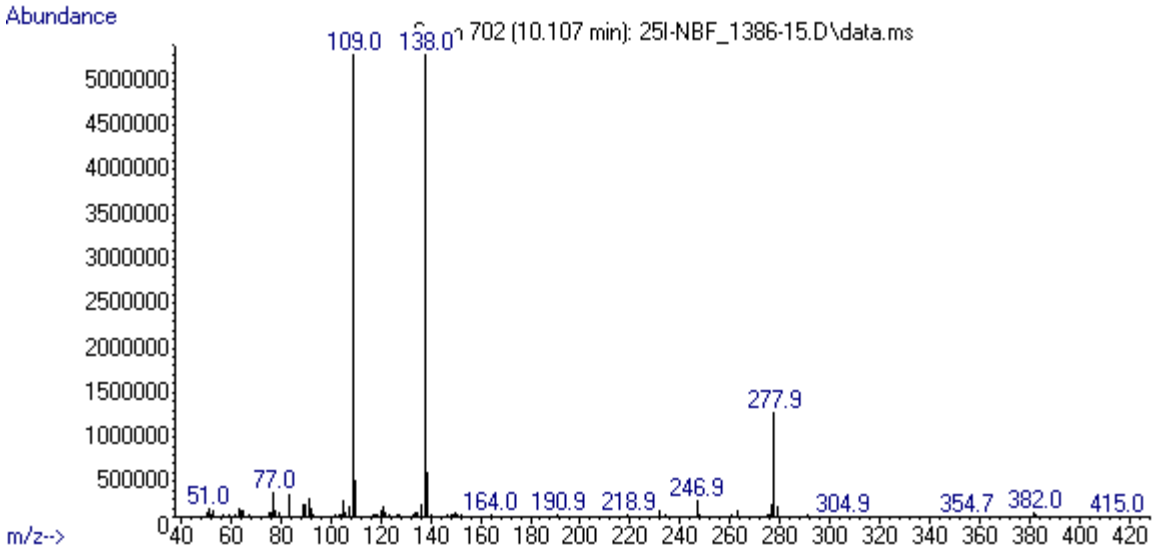
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 10.11 BP(1): 109; BP(2): 138,BP(3) :278,
HPLC-TOF	+	Exact mass (theoretical): 415.0445; measured value Δppm:0.04; formula:C17H19FINO2
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		MS spectrum confirmed by RM, GC-IR condensed phase spectrum match with RM, IR-ATR differences have been observed with comparison to RM (note-the test purchased sample was not pure)
other		

ANALYTICAL RESULTS

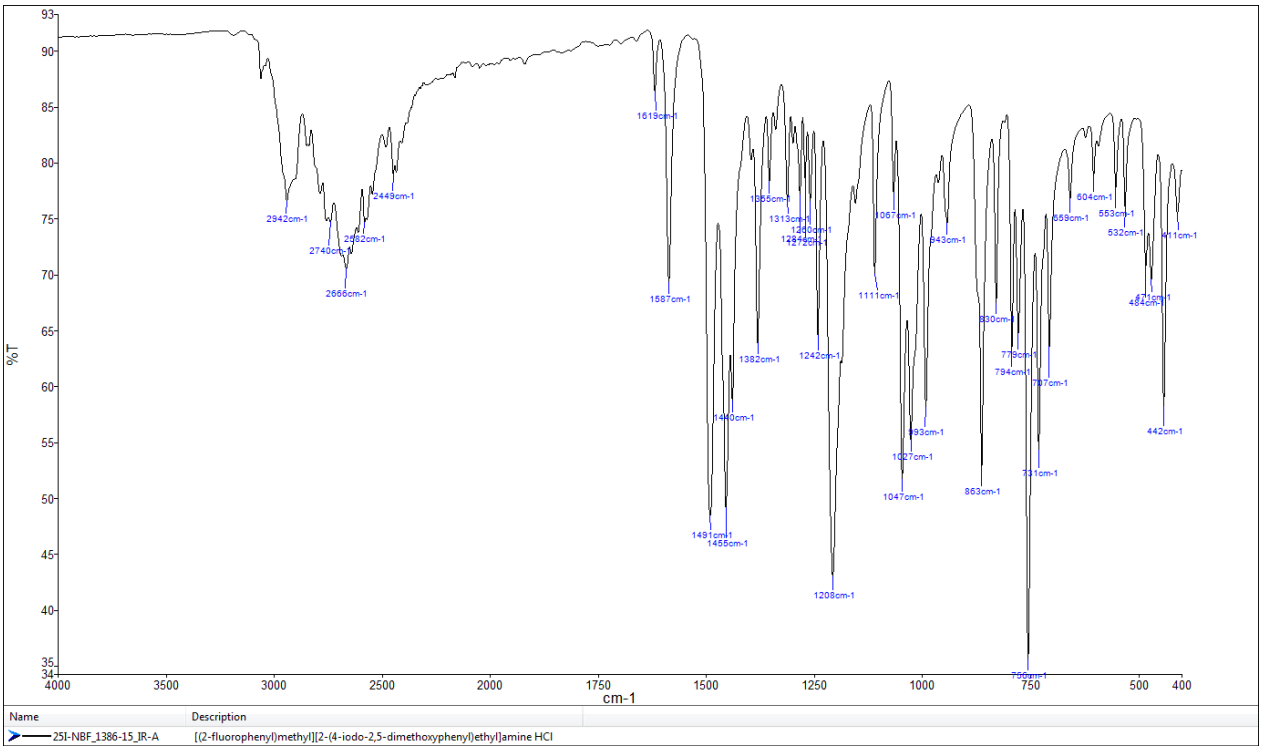
GC-MS (EI)



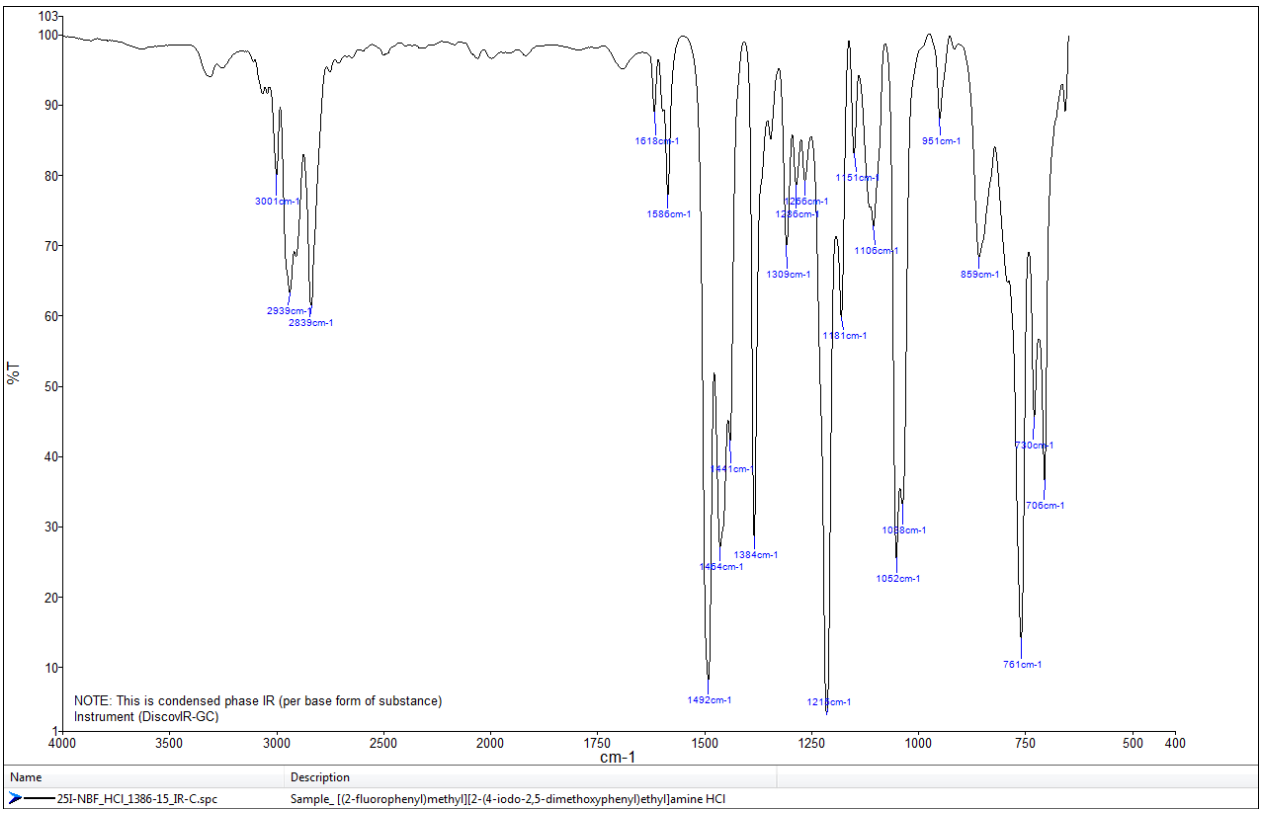
MS(EI)-25I-NBF



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



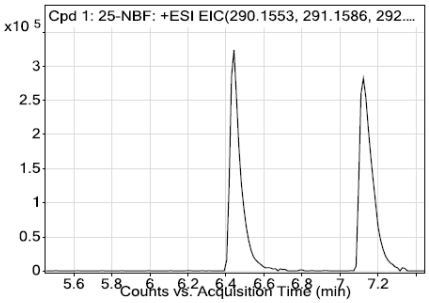
Data File	25I-NBF_1386-15_TOF.d	**Sample Name**	ID_1386-15
Sample Type	Sample	**Position**	P1-A6
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-17112015-XDB-C18-ESI-poz.m	**Acquired Time**	12/11/2015 11:40:13 AM
IRM Calibration Status	Success	**DA Method**	Drugs_NFL.m
Comment	extract in MeOH		

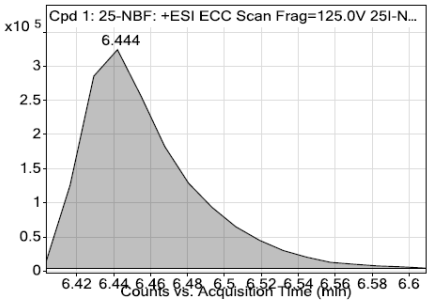
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 1: 25-NBF	25-NBF	C17 H20 F N O2	6.444	289.1483
Cpd 2: 25C-NBF	25C-NBF	C17 H19 Cl F N O2	6.853	323.1094
Cpd 3: 25I-NBF	25I-NBF	C17 H19 F I N O2	7.126	415.0444

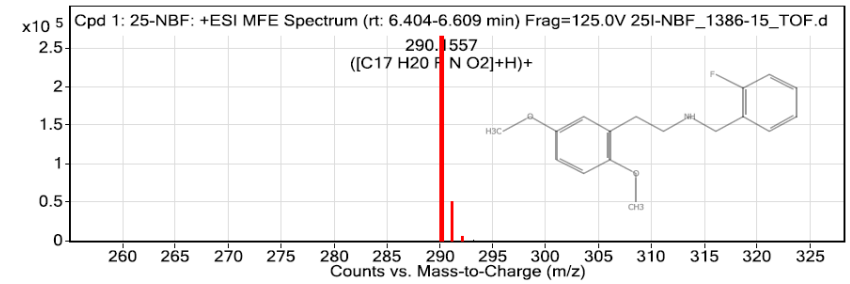
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
25-NBF	290.1557	6.444	289.1483	6.44	C17 H20 F N O2	289.1478	-1.8

Compound Chromatograms

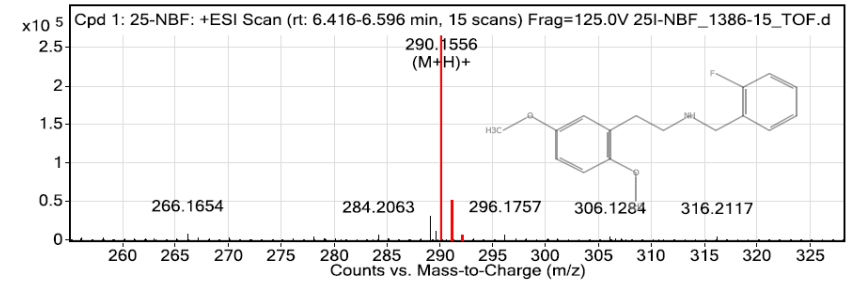




MFE MS Zoomed Spectrum



MS Zoomed Spectrum

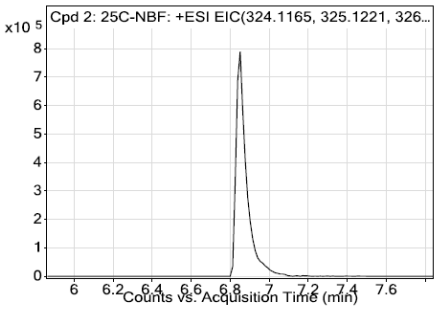


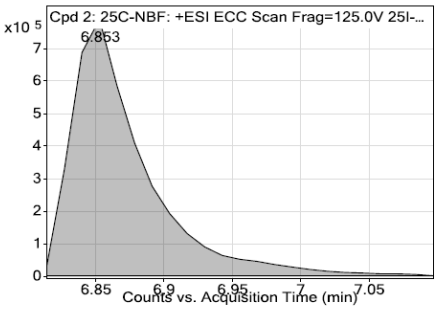
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
290.1557	1	265549.31	C17 H20 F N O2	(M+H)+
291.1583	1	50949.87	C17 H20 F N O2	(M+H)+
292.1617	1	5900.94	C17 H20 F N O2	(M+H)+
293.1636	1	518.21	C17 H20 F N O2	(M+H)+

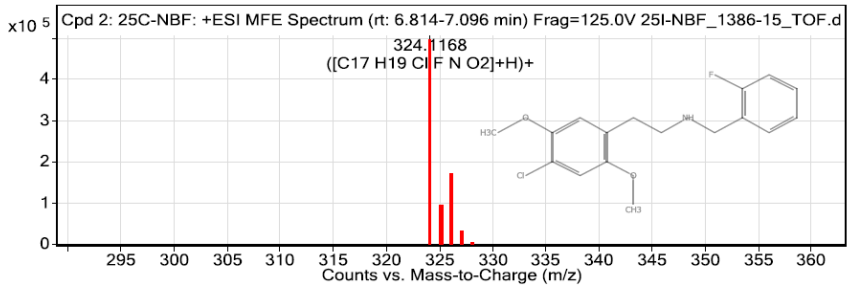
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
25C-NBF	324.1168	6.853	323.1094	6.84	C17 H19 Cl F N O2	323.1088	-1.7

Compound Chromatograms

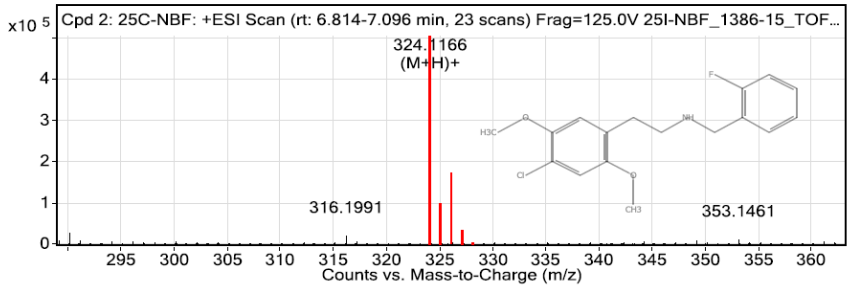




MFE MS Zoomed Spectrum



MS Zoomed Spectrum

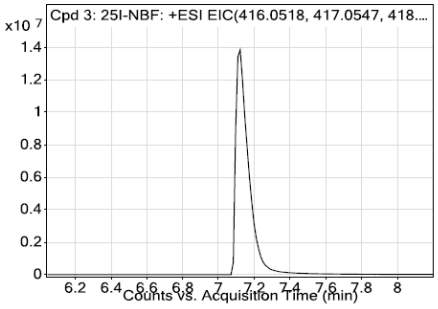


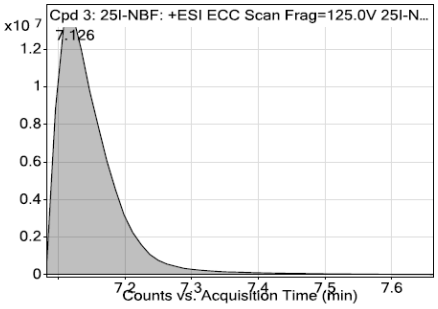
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
324.1168	1	505156.63	C17 H19 Cl F N O2	(M+H)+
325.1195	1	93316.27	C17 H19 Cl F N O2	(M+H)+
326.1141	1	162648.1	C17 H19 Cl F N O2	(M+H)+
327.1168	1	29718.43	C17 H19 Cl F N O2	(M+H)+
328.1203	1	3428.15	C17 H19 Cl F N O2	(M+H)+

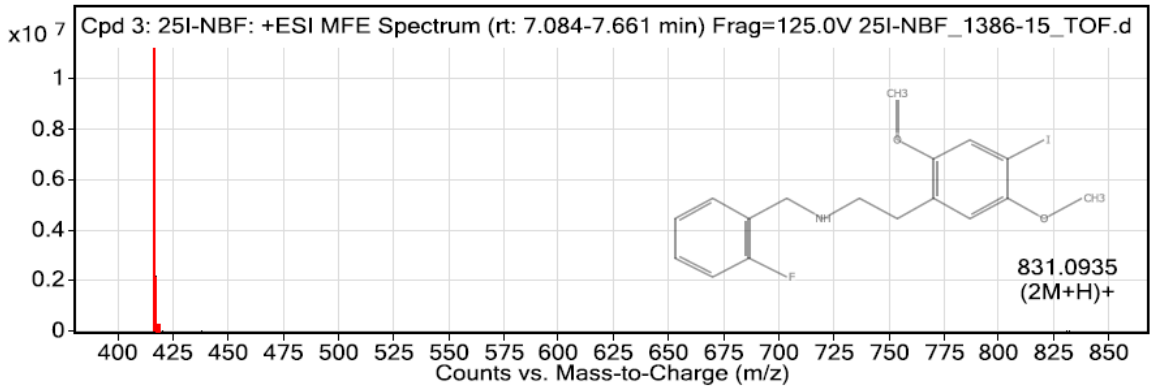
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
25I-NBF	416.0517	7.126	415.0444	7.11	C17 H19 F I N O2	415.0445	0.04

Compound Chromatograms

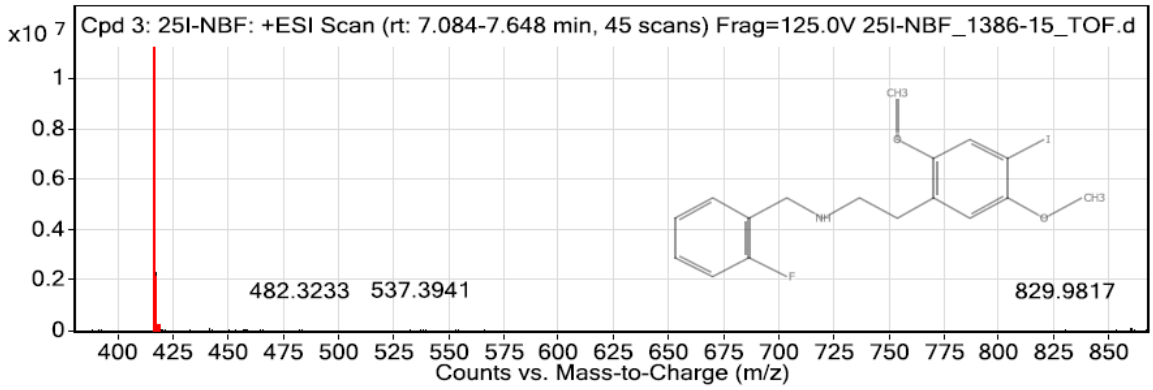




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
416.0517	1	11217121	C17 H19 F I N O2	(M+H)+
417.0552	1	2151217.03	C17 H19 F I N O2	(M+H)+
418.0582	1	221432.79	C17 H19 F I N O2	(M+H)+
419.0602	1	15627.18	C17 H19 F I N O2	(M+H)+
420.0627	1	494.56	C17 H19 F I N O2	(M+H)+
438.0338	1	2689.3	C17 H19 F I N O2	(M+Na)+
831.0935	1	4018.43		(2M+H)+
832.0996	1	1521.81		(2M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**25I-NBF_1386-15_IC**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Program:	**ANIONI**	*Operator:*	**kemija**
Inj. Date / Time:	**11-dec-2015 / 15:36**	*Run Time:*	**42,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1,00	8,92	**Chloride**	BMB	7,32	32,77	n.a.
		TOTAL:		7,32	32,77	0,00