I-SEE
European Project
on New Psychoactive Substance

Co-funded by the Prevention of and Fight against Crime Programme of the European Union
JUST/2013/ISEC/DRUGS/AG/6426

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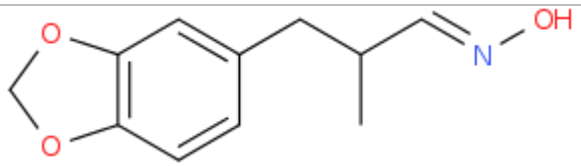
ANALYTICAL REPORT

MDA 2-aldoxime analog (C11H13NO3)

N-[3-(2H-1,3-benzodioxol-5-yl)-2-methylpropylidene]hydroxylamine

Remark – other active cpd. detected: two isomers

Sample ID:	1648-16
Sample description:	liquid - colourless
Sample type:	RM-reference material
Comments[1]:	Chiron Lot#16657; I-SEE project RM and report
Date of entry:	12/3/2016

Substance identified-structure[2] (base form)	
Systematic name:	N-[3-(2H-1,3-benzodioxol-5-yl)-2-methylpropylidene]hydroxylamine
Other names:	alpha-Methyl-1,3-benzodioxole-5-propanal oxime;
Formula (per base form)	C11H13NO3
M_w (g/mol)	207.23
Salt form:	base
StdInChIKey	ISLHQWBNLXYVQG-UHFFFAOYSA-N
Compound Class	Phenethylamines
Other active cpd. detected	two isomers
Add.info (purity..)	98.1 % declared; analyses in NFL revealed mixture of two isomers (this should be written on RM certificate but it is not)!

[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/6426). 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)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 5.36 (isomer 1); 5.46 (isomer 2 BP(1): 135; BP(2): 77,BP(3) :51,
FTIR-ATR	+	
GC-IR (condensed phase)	-	

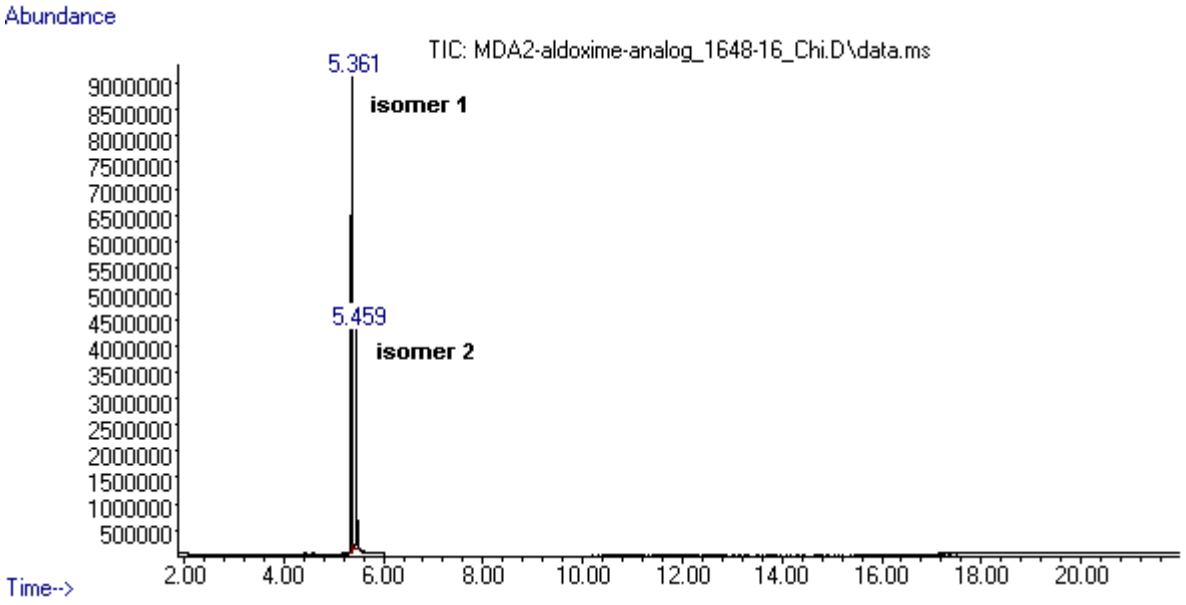
1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 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 6.1 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. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm^{-1}; resolution 4cm^{-1}

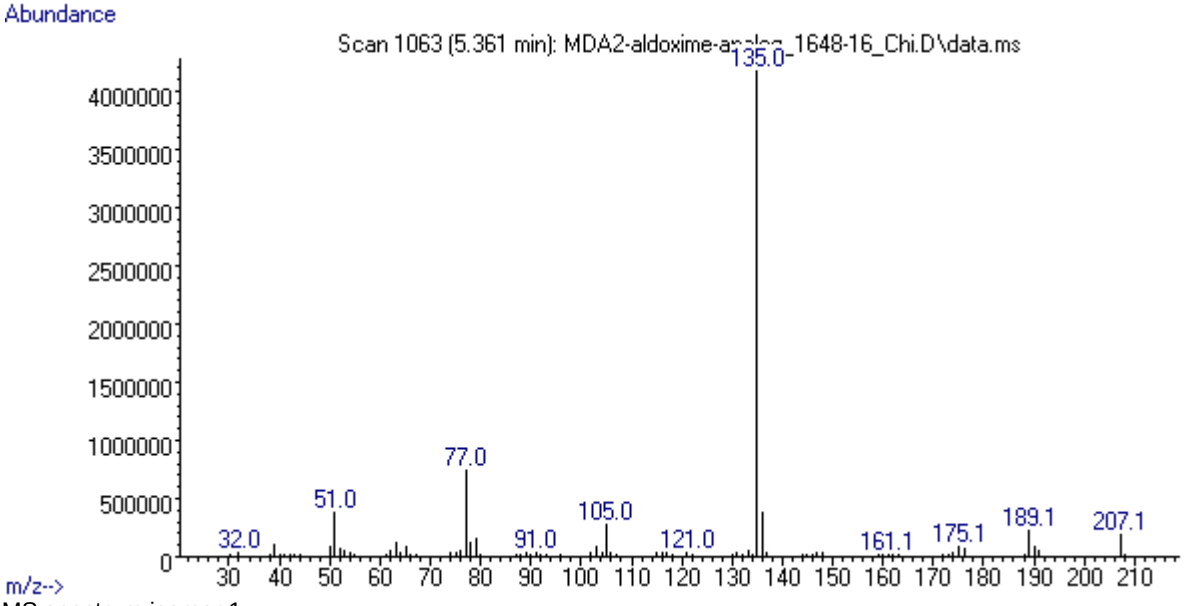
3. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).**
Split MS : IR = 1 : 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole 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 (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1} .

FIGURES OF SPECTRA

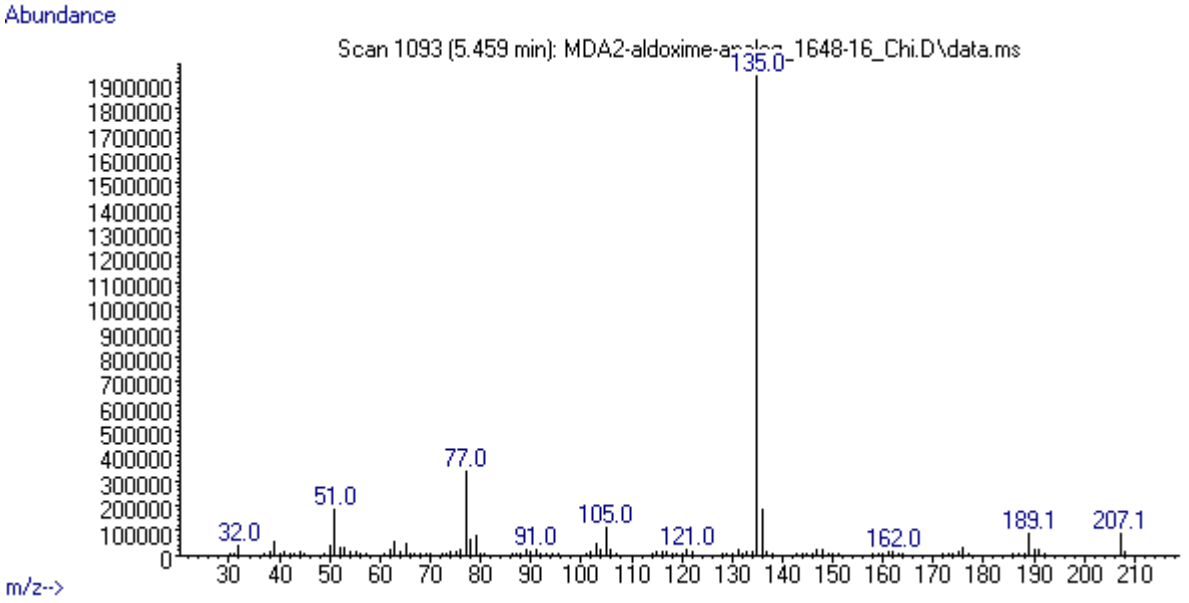
GC



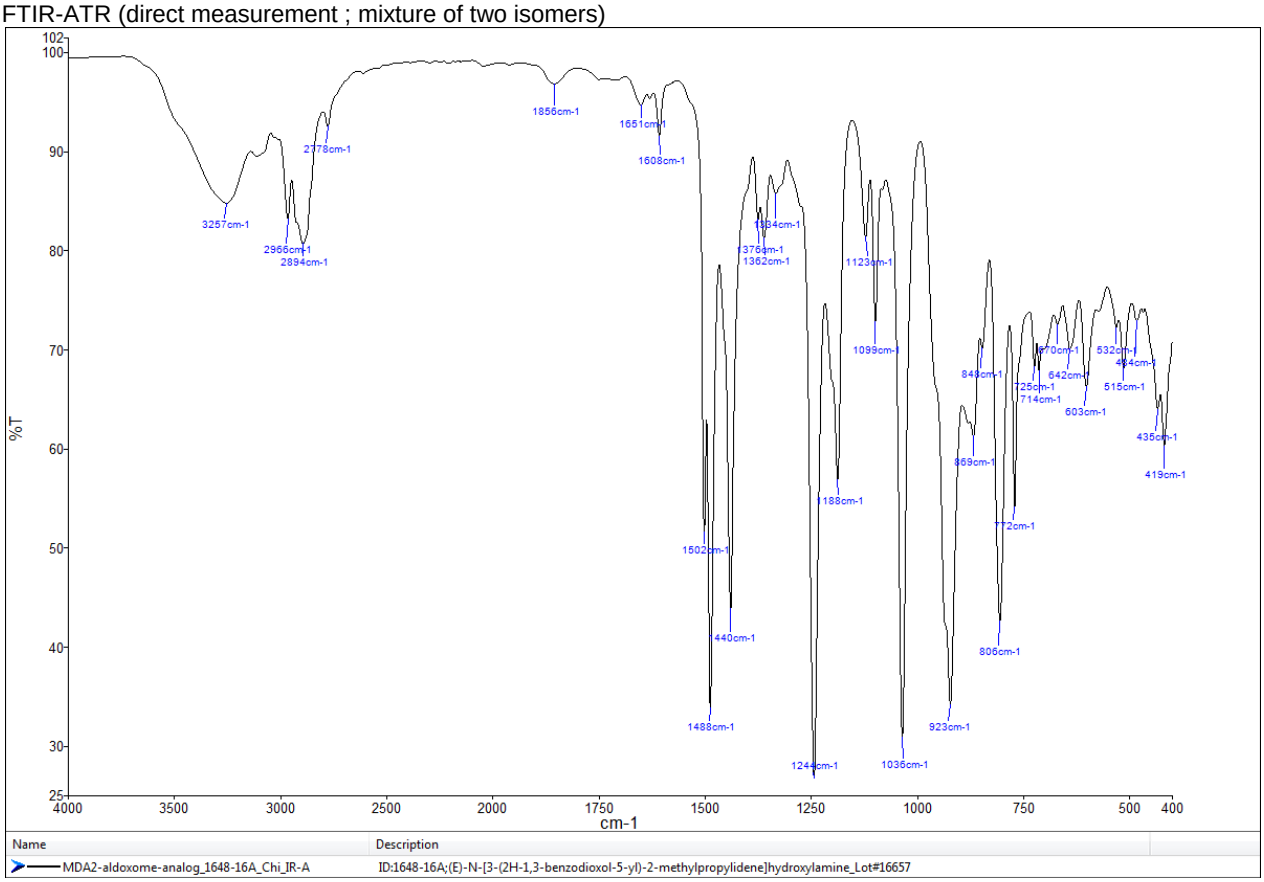
MS (EI)



MS spectrum isomer 1



FTIR-ATR (direct measurement ; mixture of two isomers)



TOF REPORT

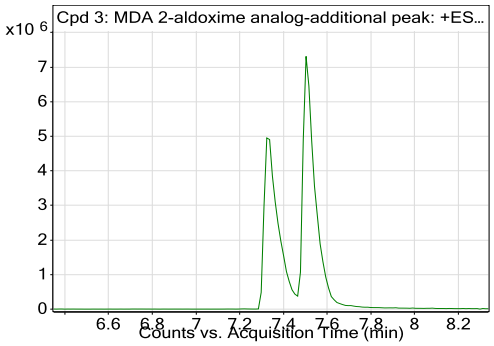
Data File	MDA 2-aldoxime analog_1648-16_TOF.d	**Sample Name**	ID_1648-16
Sample Type	Sample	**Position**	P1-C3
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-24_08_2016-XDB-C18-ESI-poz-soft.m	**Acquired Time**	8/29/2016 12:08:10 PM
IRM Calibration Status	Success	**DA Method**	Drugs_NFL.m
Comment	extract in MeOH		

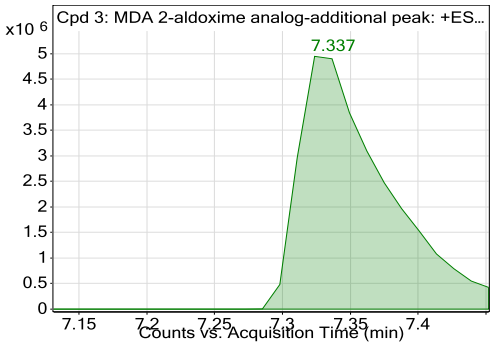
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 3: MDA 2-aldoxime analog-additional peak	MDA 2-aldoxime analog-additional peak	C11 H13 N O3	7.337	207.0895
Cpd 7: MDA 2-aldoxime analog	MDA 2-aldoxime analog	C11 H13 N O3	7.512	207.0899

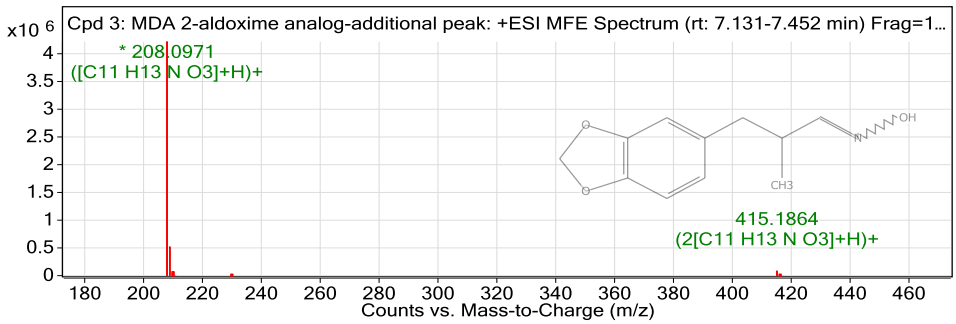
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
MDA 2-aldoxime analog-additional peak	208.0971	7.337	207.0895	7.34	C11 H13 N O3	207.0895	0.38

Compound Chromatograms

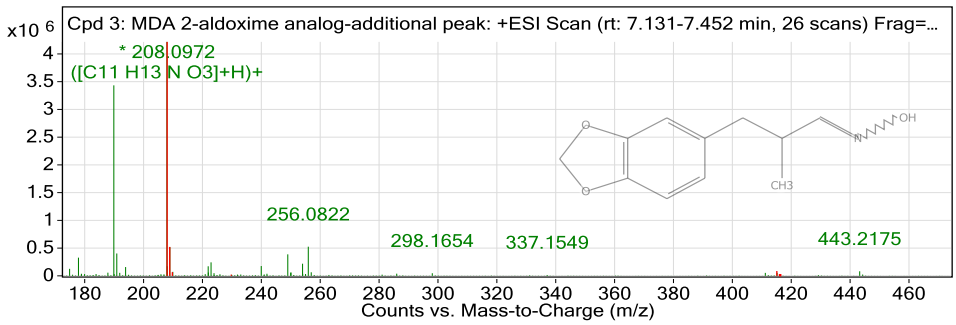




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

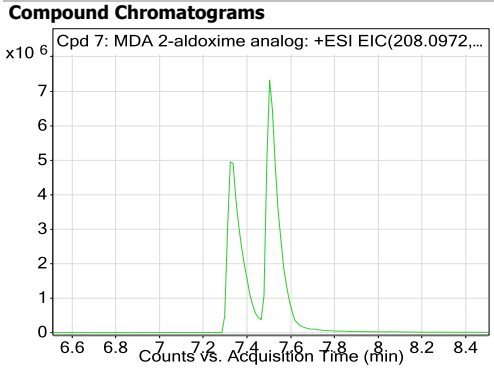
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
208.0971	1	4209918.5	C11 H13 N O3	(M+H)+
209.1008	1	515251.39	C11 H13 N O3	(M+H)+
210.1034	1	71758.3	C11 H13 N O3	(M+H)+
211.1032	1	7769.84	C11 H13 N O3	(M+H)+
230.079	1	24463.12	C11 H13 N O3	(M+Na)+
415.1864	1	74747.64	C11 H13 N O3	(2M+H)+
416.1893	1	18897.06	C11 H13 N O3	(2M+H)+
417.192	1	4482.97	C11 H13 N O3	(2M+H)+

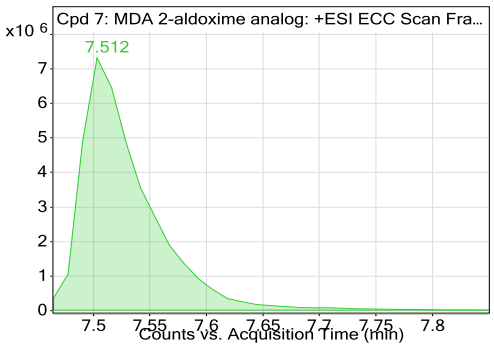
TOF REPORT

437.1725	1	1880.15		(2M+Na)+
439.1552	1	1123.29		(2M+Na)+

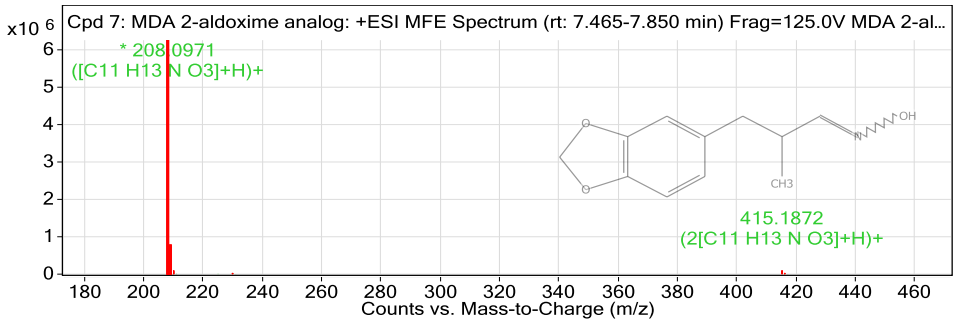
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
MDA 2-aldoxime analog	208.0971	7.512	207.0899	7.51	C11 H13 N O3	207.0895	-1.76

Compound Chromatograms

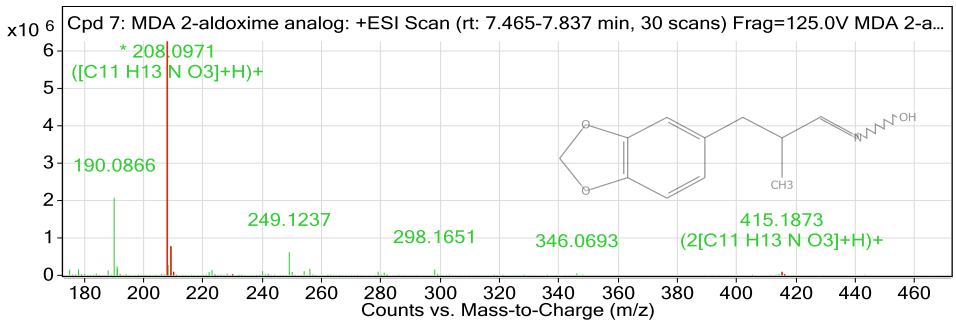




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
208.0971	1	6262099.5	C11 H13 N O3	(M+H)+
209.1008	1	781510.6	C11 H13 N O3	(M+H)+
210.1036	1	84457.53	C11 H13 N O3	(M+H)+
211.1065	1	9101.11	C11 H13 N O3	(M+H)+
225.1218	1	9001.38	C11 H13 N O3	(M+NH4)+
230.0788	1	21947.19	C11 H13 N O3	(M+Na)+
231.0923	1	3627.54	C11 H13 N O3	(M+Na)+
415.1872	1	88373.24	C11 H13 N O3	(2M+H)+
416.1899	1	21584.52	C11 H13 N O3	(2M+H)+
417.1933	1	4211.86	C11 H13 N O3	(2M+H)+

--- End Of Report ---