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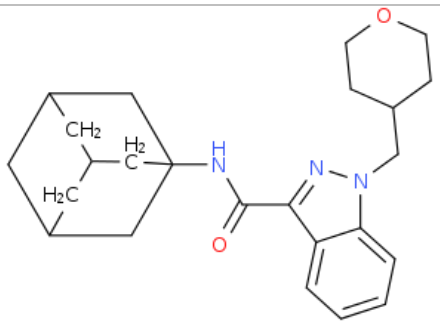
ANALYTICAL REPORT

ATHPINACA isomer 1 (C24H31N3O2)

N-(adamantan-1-yl)-1-[(oxan-4-yl)methyl]-1H-indazole-3-carboxamide

Remark – other active cpd. detected: none

Sample ID:	1807-17
Sample description:	powder - white
Sample type:	RM-reference material
Comments[1]:	CAY Lot#0492127-2; RESPONSE -purchasing
Date of entry:	4/10/2017

Substance identified-structure[2] (base form)	
Systematic name:	N-(adamantan-1-yl)-1-[(oxan-4-yl)methyl]-1H-indazole-3-carboxamide
Other names:	AD-THPINACA; Adamantyl-THPINACA; 1-[(tetrahydro-2H-pyran-4-yl)methyl]-N-tricyclo[3.3.1.13,7]dec-1-yl-1H-indazole-3-carboxamide; N-(1-adamantyl)-1-(tetrahydropyran-4-ylmethyl)indazole-3-carboxamide
Formula (per base form)	C24H31N3O2
M_w (g/mol)	393,53
Salt form:	base
StdInChIKey (per base form)	WFDRVDUEMGJILX-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	98%

[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)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 17,56 BP(1): 135; BP(2): 243,BP(3) :145,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form

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 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.

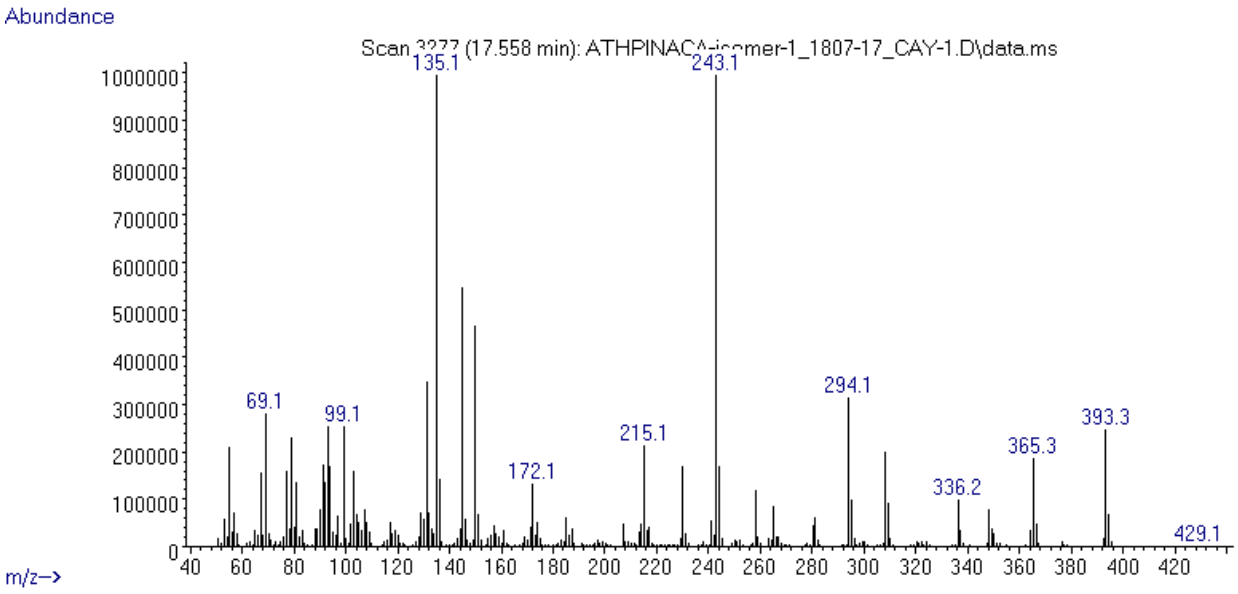
2. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm^{-1}; resolution 4cm^{-1}

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}.

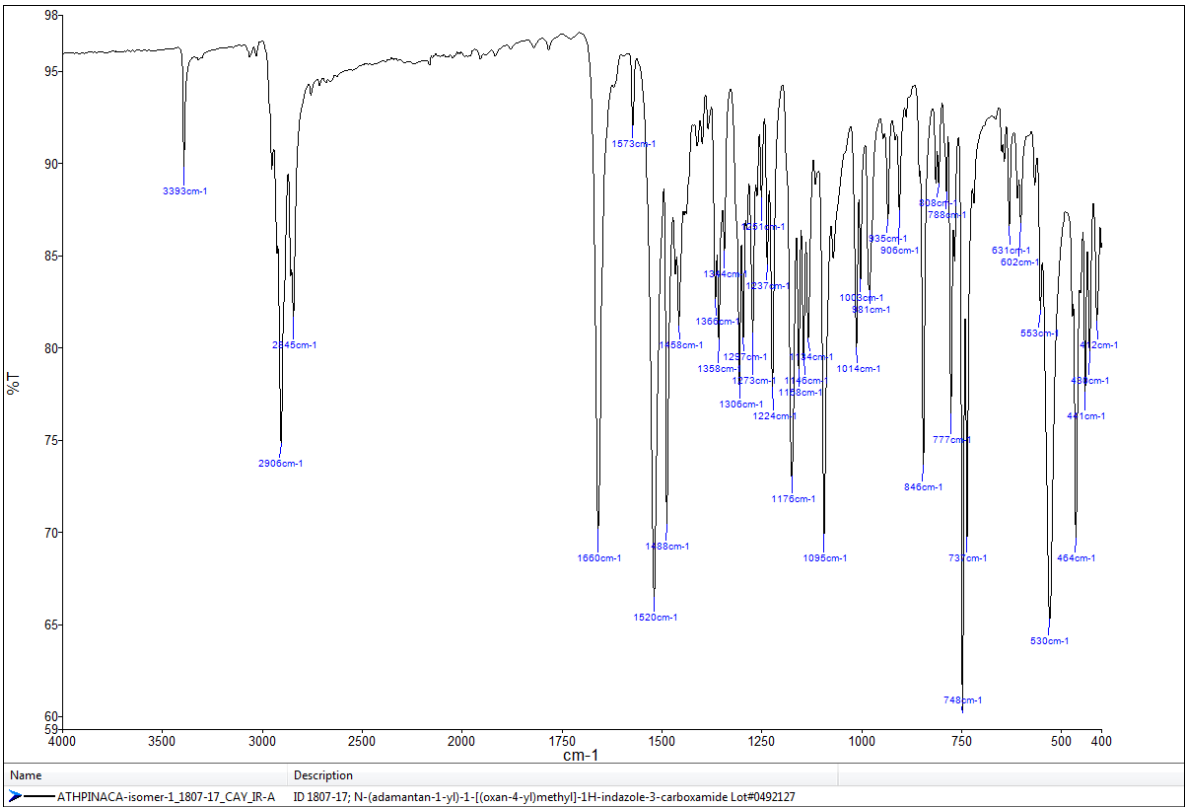
4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

ANALYTICAL RESULTS

MS (EI)



FTIR-ATR - sample as received



IR (condensed phase – after chromatographic separation)