

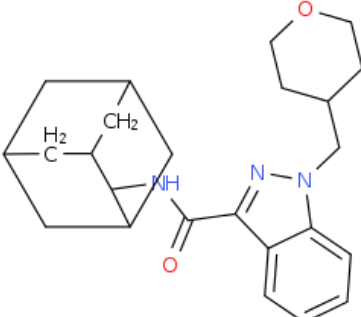
## ANALYTICAL REPORT

### ATHPINACA isomer 2 (C<sub>24</sub>H<sub>31</sub>N<sub>3</sub>O<sub>2</sub>)

#### N-(adamantan-2-yl)-1-[(oxan-4-yl)methyl]-1H-indazole-3-carboxamide

Remark – other active cpd. detected: **none**

Sample ID:	1808-17
Sample description:	powder - white
Sample type:	RM-reference material
Comments <sup>1</sup> :	CAY Lot#0491080-3; RESPONSE -purchasing
Date of entry:	4/10/2017

Substance identified-structure <sup>2</sup> (base form)	
Systematic name:	N-(adamantan-2-yl)-1-[(oxan-4-yl)methyl]-1H-indazole-3-carboxamide
Other names:	Adamantyl-THPINACA; AD-THPINACA;N-(2-Adamantyl)-1-(tetrahydro-2H-pyran-4-ylmethyl)-1H-indazole-3-carboxamide
Formula (per base form)	C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub>
M <sub>w</sub> (g/mol)	393,53
Salt form:	base
StdInChIKey (per base form)	XFZLBNDGZVRJNJ-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	98%

<sup>1</sup> 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.

<sup>2</sup> 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): 17,95 BP(1): 150; BP(2): 151,BP(3) :131,
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 °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. FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**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 °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.

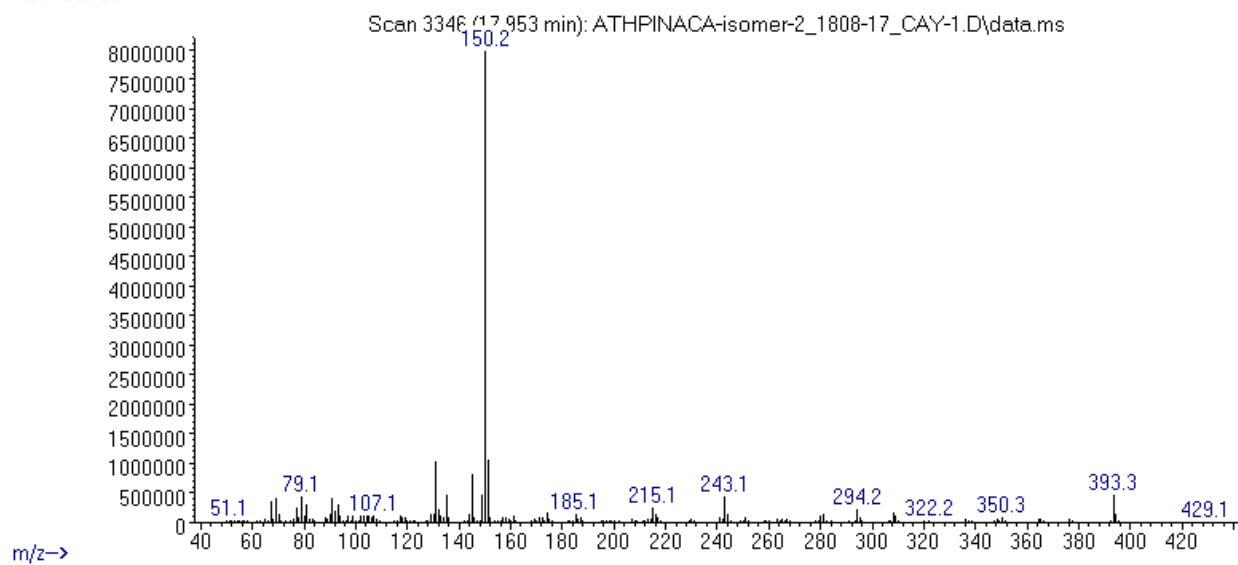
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm<sup>-1</sup>.

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

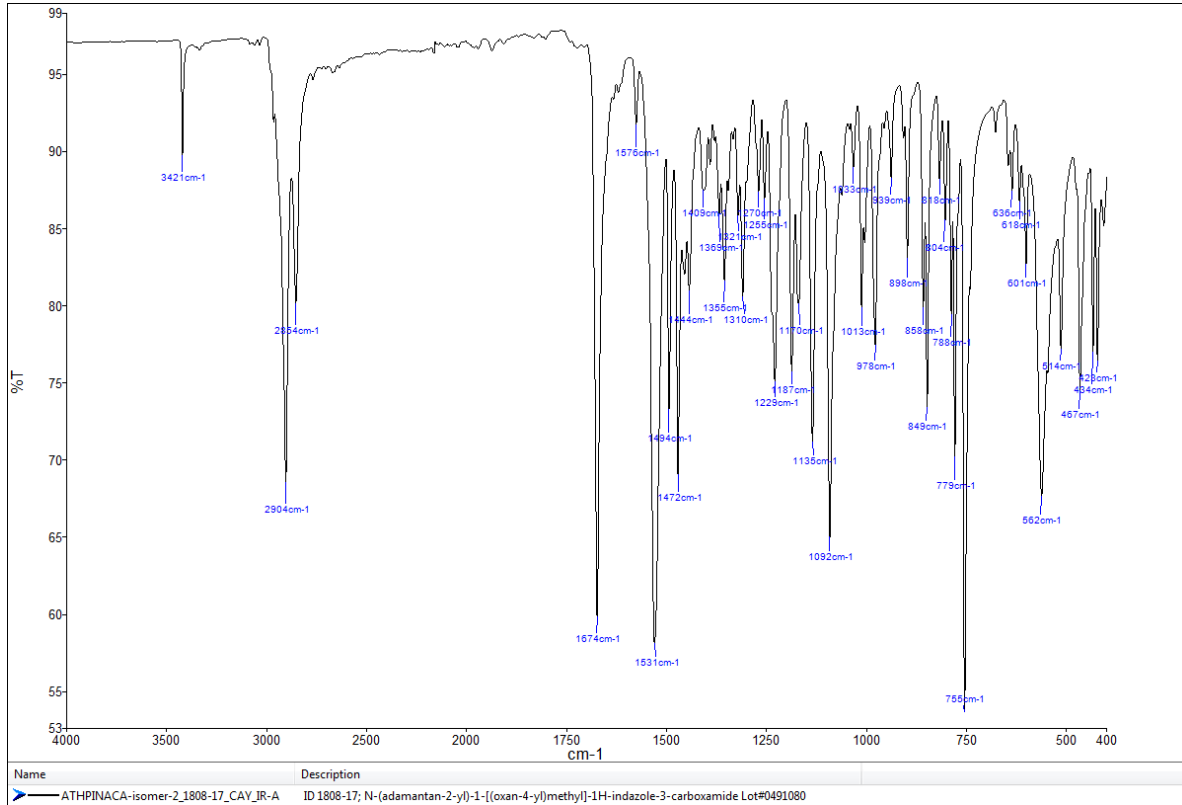
# ANALYTICAL RESULTS

MS (EI)

Abundance



FTIR-ATR - sample as received



IR (condensed phase – after chromatographic separation)

