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ANALYTICAL REPORT

JWH-081 (C₂₅H₂₅NO₂)

(1-pentyl-3-(4-methoxy-1-naphthoyl)indole)

Remark – other active cpd. detected: none

Sample ID:	1488-16
Sample description:	liquid - clear
Sample type:	RM-reference material
Comments ¹ :	LGC Lot#12549, I-SEE - purchasing
Date of entry:	1/20/2016

Substance identified-structure ² (base form)	
Systematic name:	(1-pentyl-3-(4-methoxy-1-naphthoyl)indole)
Other names:	((4-Methoxynaphthalen-1-yl)(1-pentylindol-3-yl)methanone)
Formula (per base form)	C ₂₅ H ₂₅ NO ₂
M _w (g/mol)	371,47
Salt form:	base
StdInChIKey	UBMPKJKGUQDHRM-UHFFFAOYSA-N
Compound Class	Cannabinoids
Other active cpd. detected	none
Add.info (purity..)	1 mg in 1 mL acetonitrile

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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): 17,23 BP(1): 371; BP(2): 214,BP(3) :314,
FTIR-ATR		
GC-IR (condensed phase)		

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 °C.

Chromatographic separation

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 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 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) amu.

FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm-1

GC-method:

Injection volume 1 ml and split mode (1:5) .

Injector temperature: 280 °C.

Chromatographic separation

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 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

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 phase): IR scan range 4000 to 700, resolution 4cm-1

FIGURES OF SPECTRA

MS (EI)

Abundance

