



ANALYTICAL REPORT

AB-FUBINACA (C₂₀H₂₁FN₄O₂)

2-({1-[(4-fluorophenyl)methyl]-1H-indazol-3-yl}formamido)-3-methylbutanamide

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

Sample ID:	1477-16
Sample description:	liquid - clear
Sample type:	RM-reference material
Comments ¹ :	Cayman Lot#0469561-1; I-SEE project RM and report I-SEE - purchasing
Date of entry:	5/12/2016

Substance identified- structure ² (base form)	
Systematic name:	2-({1-[(4-fluorophenyl)methyl]-1H-indazol-3-yl}formamido)-3-methylbutanamide
Other names:	N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide
Formula (per base form)	C ₂₀ H ₂₁ FN ₄ O ₂
M _w (g/mol)	368.41
Salt form:	base
StdInChIKey	AKOOIMKXADOPDA-UHFFFAOYSA-N
Compound Class	Cannabinoids
Other active cpd. detected	none
Add.info (purity..)	1 mg/ml in MeOH

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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): 13.34 BP(1): 109; BP(2): 253, BP(3) :324,
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 thickness 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, then 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 quadrupole 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 thickness 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, then 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 quadrupole 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)



