



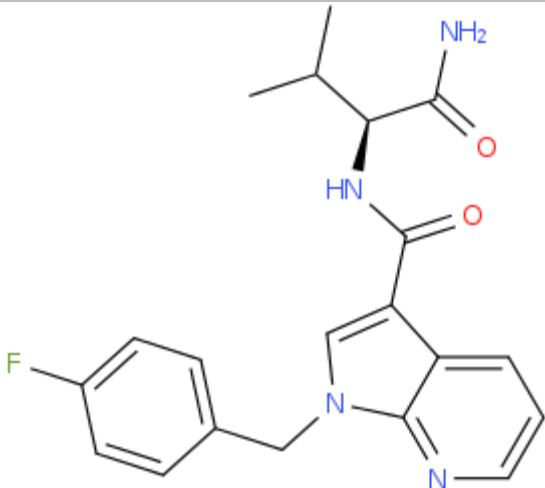
ANALYTICAL REPORT

AB-7-FUBAICA (C₂₀H₂₁FN₄O₂)

(2S)-2-({1-[(4-fluorophenyl)methyl]-1H-pyrrolo[2,3-b]pyridin-3-yl}formamido)-3-methylbutanamide

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

Sample ID:	1895-17
Sample description:	powder - white
Sample type:	RM-reference material
Comments:	CAY Lot#0513450-3,
Date of entry (DD/MM/YYYY):	07/12/2017

Substance identified-structure ¹ (base form)	
Systematic name:	(2S)-2-({1-[(4-fluorophenyl)methyl]-1H-pyrrolo[2,3-b]pyridin-3-yl}formamido)-3-methylbutanamide
Other names:	(S)-N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-pyrrolo[2,3-b]pyridine-3-carboxamide
Formula (per base form)	C ₂₀ H ₂₁ FN ₄ O ₂
M _w (g/mol)	368,41
Salt form:	base
StdInChIKey (per base form)	AIZFETCNFVMZGT-KRWDZBQOSA-N
Other active cpd. detected	none
Add.info (purity..)	100 %

¹ 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): 14,37 BP(1): 109; BP(2): 253,BP(3) :254,
FTIR-ATR		direct measurement
GC-IR (condensed phase)		always as base form
HPLC-TOF		exact monoisotopic mass: 368,1649 Δ ppm (difference from calculated): -1,05

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 μ m. 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^{-1} ; resolution 4 cm^{-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 °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.

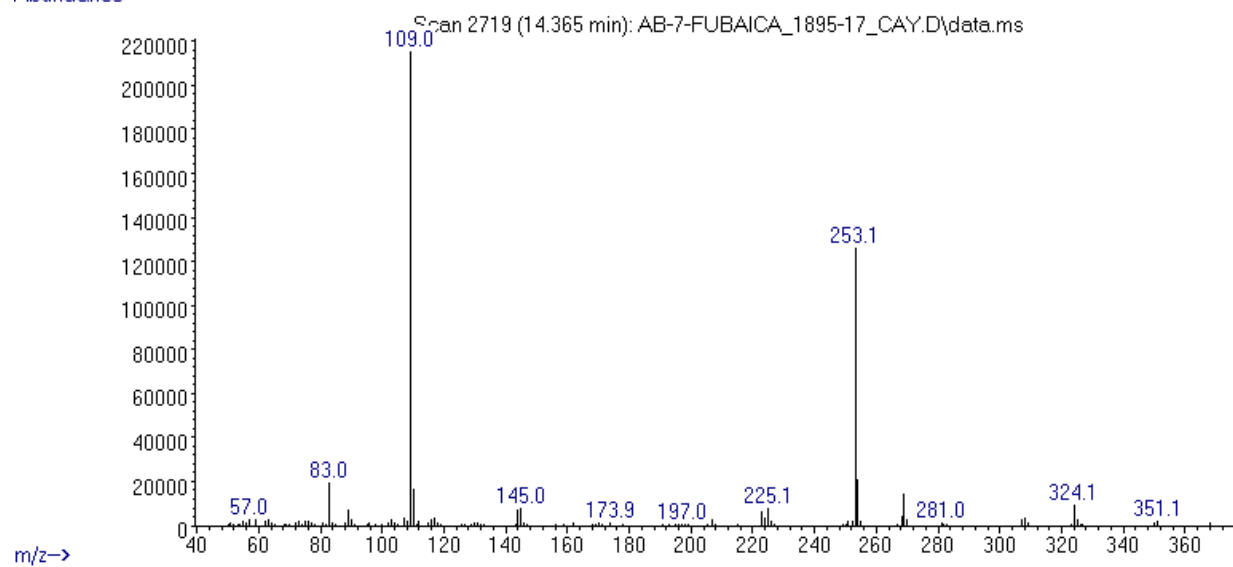
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1} .

4. HPLC-TOF for exact monoisotopic mass and empirical formula control

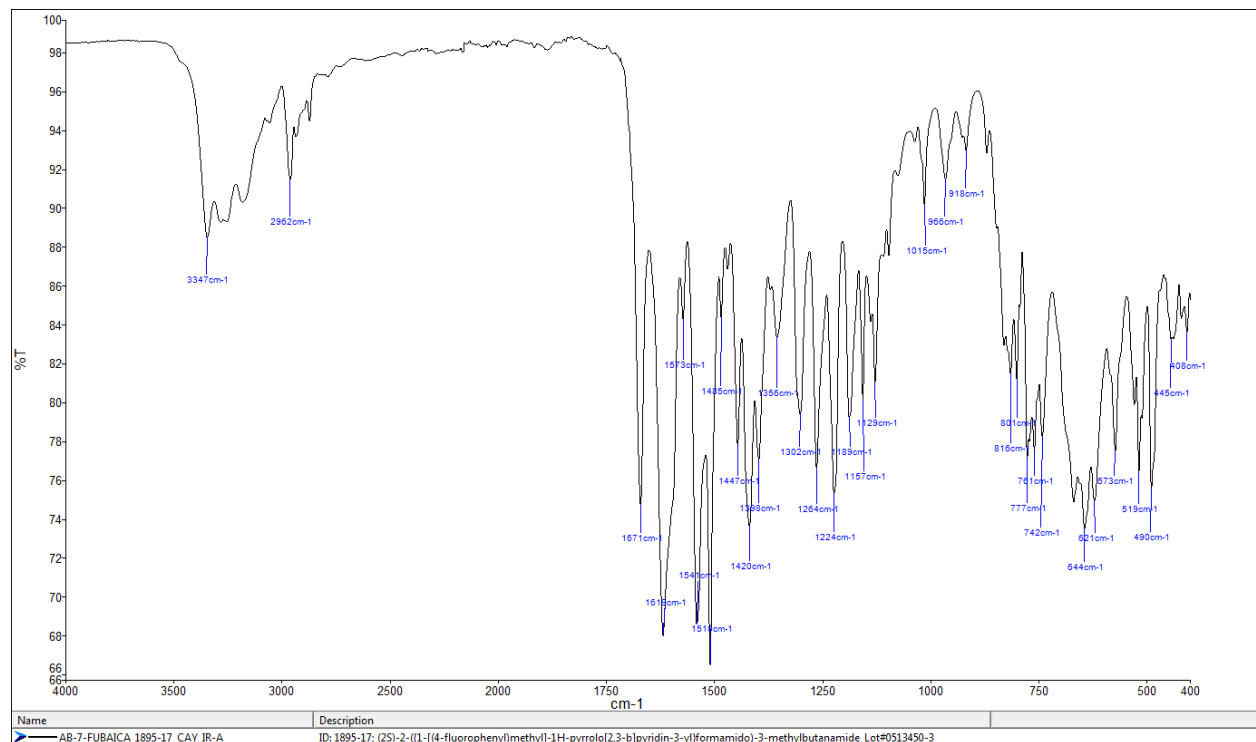
ANALYTICAL RESULTS

MS (EI)

Abundance



FTIR-ATR - sample as received



IR (condensed phase – after chromatographic separation)

