



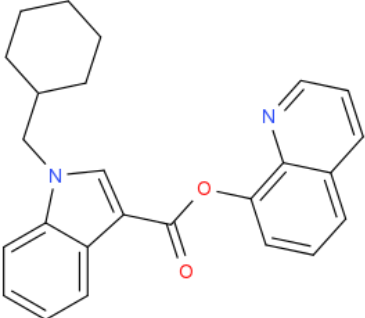
ANALYTICAL REPORT¹

BB-22 (C25H24N2O2)

quinolin-8-yl 1-(cyclohexylmethyl)-1H-indole-3-carboxylate

Remark – other NPS detected: **none**

Sample ID:	1299-15
Sample description:	powder - off white
Sample type:	test purchase /RESPONSE -purchasing
Date of sample receipt (M/D/Y):	10/1/2015
Date of entry (M/D/Y) into NFL database:	12/14/2015
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ² (base form)	
Systematic name	quinolin-8-yl 1-(cyclohexylmethyl)-1H-indole-3-carboxylate
Other names	QUCHIC
Formula (per base form)	C25H24N2O2
M _w (g/mol)	384,47
Salt form	base
StdInChIKey	RHYGTJXOHOGQGI-UHFFFAOYSA-N
Compound Class	Cannabinoids
Other NPS detected	none
Add.info (purity..)	pure by GC-MS, HPLC-TOF

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)

Instrumental methods (if applied) in NFL

1. 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: on 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 quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

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

4. 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 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

5. IC (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30°C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

Supporting information

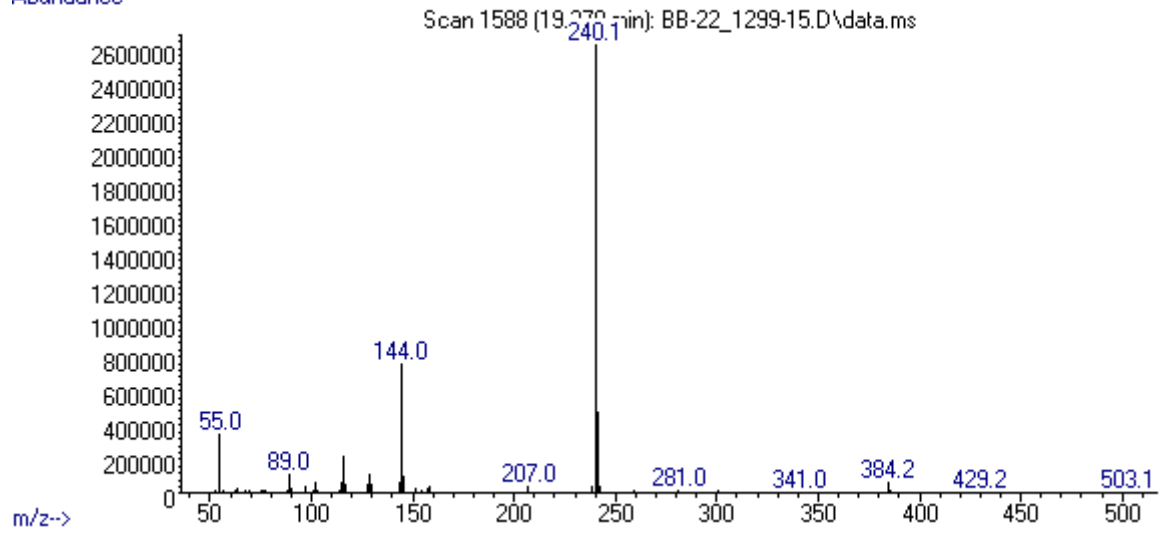
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 19,38 BP(1): 240; BP(2): 144,BP(3) :241,
HPLC-TOF	+	Exact mass (theoretical): 384,1838; measured value Δppm:0,42; formula:C ₂₅ H ₂₄ N ₂ O ₂
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	-	
NMR (in FKKT)	-	
validation		identification based on published data
other		

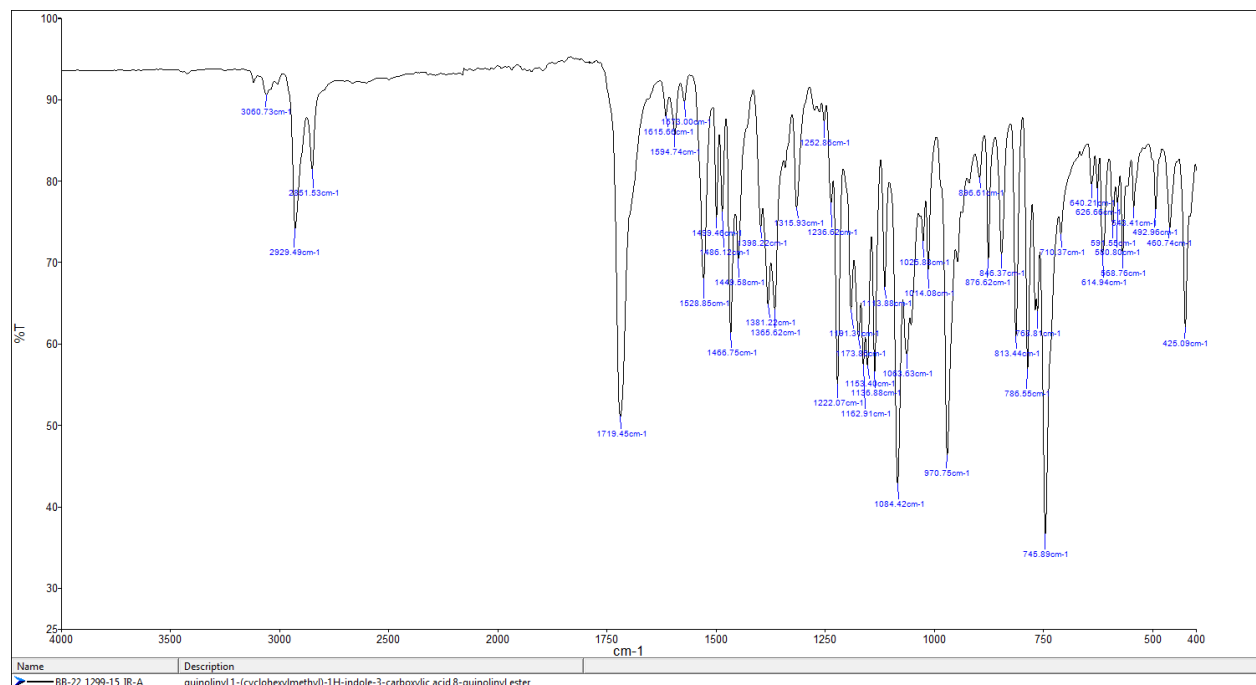
ANALYTICAL RESULTS

MS (EI)

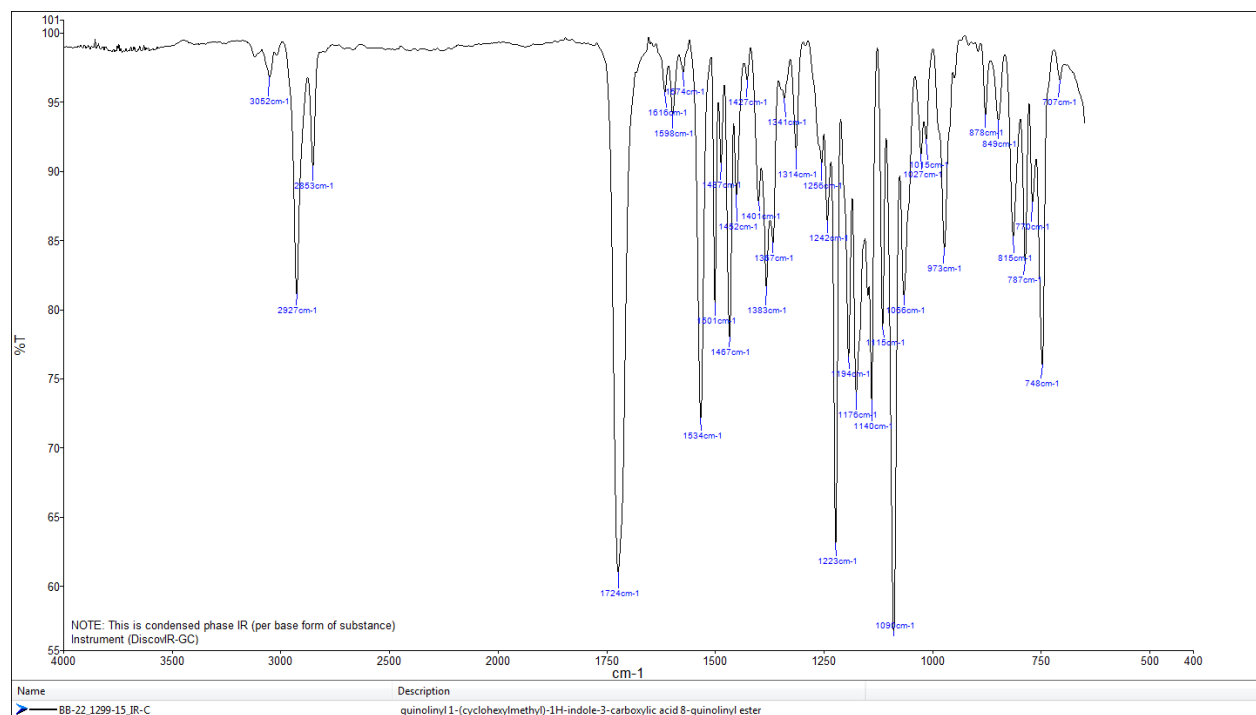
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

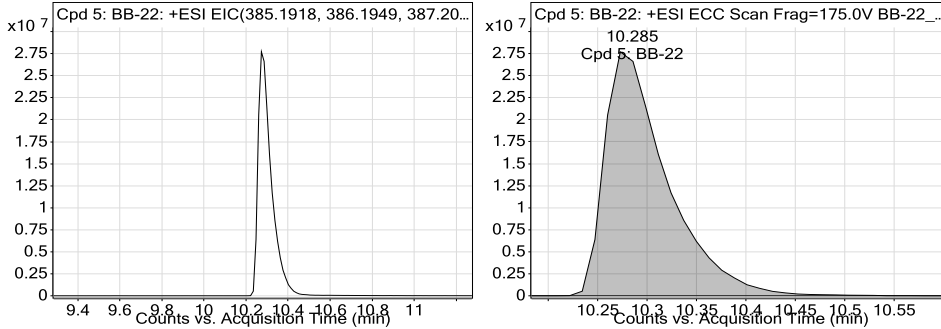
Data File	BB-22_1299-15_TOF.d	Sample Name	BB-22
Sample Type	Sample	Position	P1-B4
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-28052015-XDB-C18-ESI-poz.m	Acquired Time	10/23/2015 12:05:05 PM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	extract in MeOH		

Compound Table

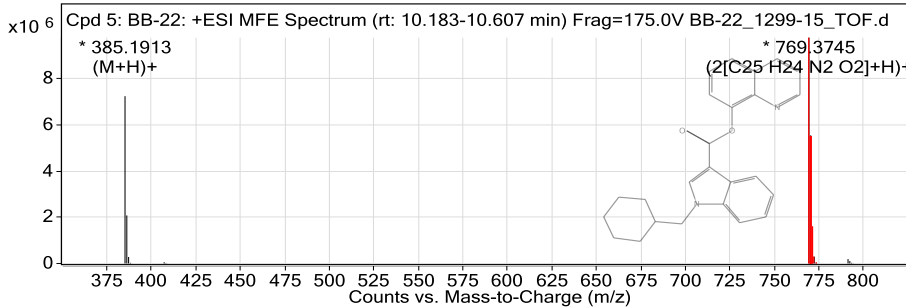
Label	Compound Name	Obs. RT	Obs. Mass
Cpd 5: BB-22	BB-22	10.285	384.1836

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
BB-22	769.3745	10.285	384.1836	10.3	C25 H24 N2 O2	384.1838	0.42

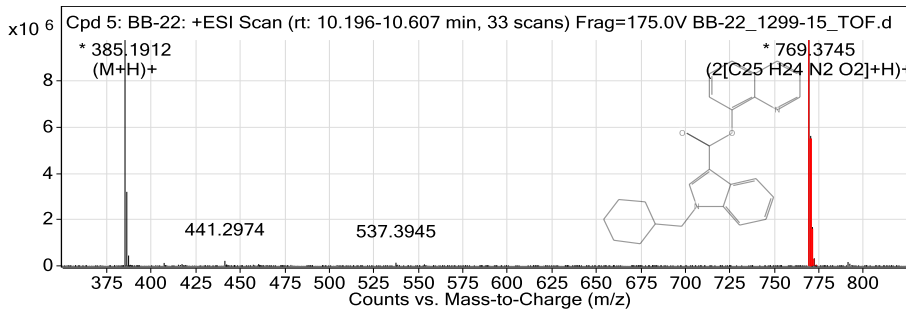
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
385.1913	1	7238041.5		(M+H)+
386.1947	1	2078874.75		(M+H)+
387.198	1	280155.73		(M+H)+
407.1732	1	54123.1		(M+Na)+
769.3745	1	9770139	C25 H24 N2 O2	(2M+H)+
770.3781	1	5544357.72	C25 H24 N2 O2	(2M+H)+
771.3815	1	1577416.79	C25 H24 N2 O2	(2M+H)+
772.3849	1	294370.05	C25 H24 N2 O2	(2M+H)+
791.3571	1	191078.36		(2M+Na)+
792.36	1	103575.7		(2M+Na)+

--- End Of Report ---