



NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY

Vodovodna 95
1000 Ljubljana
SLOVENIJA

T: +386 (0)1 428 44 93

E: nfl@policija.si
www.policija.si

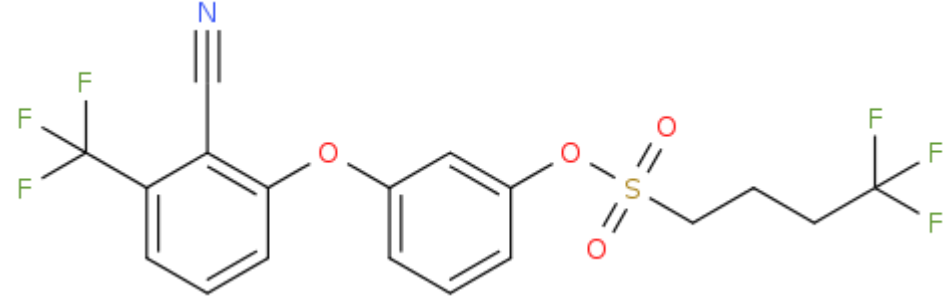
ANALYTICAL REPORT

BAY-59-3074 (C₁₈H₁₃F₆N₄O₄S)

3-[2-cyano-3-(trifluoromethyl)phenoxy]phenyl 4,4,4-trifluorobutane-1-sulfonate

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

Sample ID:	1804-17
Sample description:	powder - white
Sample type:	RM-reference material
Comments ¹ :	CAY Lot#0495371-1; RESPONSE -purchasing
Date of entry (DD/MM/YYYY):	14/04/2017

Substance identified-structure ² (base form)	
Systematic name:	3-[2-cyano-3-(trifluoromethyl)phenoxy]phenyl 4,4,4-trifluorobutane-1-sulfonate
Other names:	4,4,4-trifluoro-1-butanefulfonic acid, 3-[2-cyano-3-(trifluoromethyl)phenoxy]phenyl ester; BAY59-3074
Formula (per base form)	C ₁₈ H ₁₃ F ₆ N ₄ O ₄ S
M _w (g/mol)	453.36
Salt form:	base
StdInChIKey (per base form)	LWUSZIVDPJPVBW-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	98%

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)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 9.27 BP(1): 279; BP(2): 91,BP(3) :64,
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⁻¹; resolution 4cm⁻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.

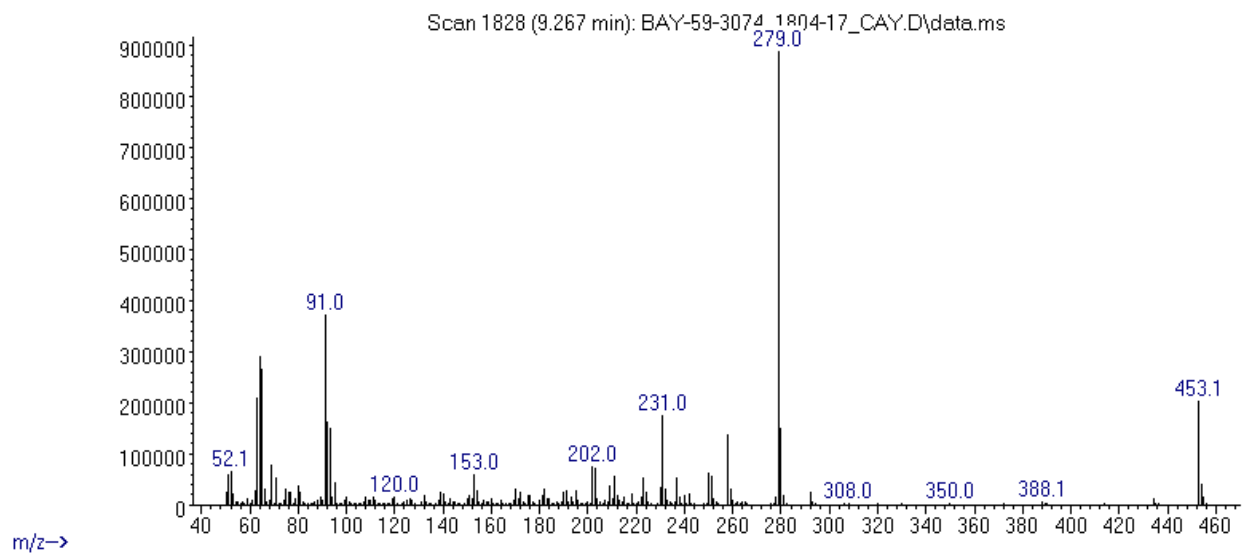
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

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

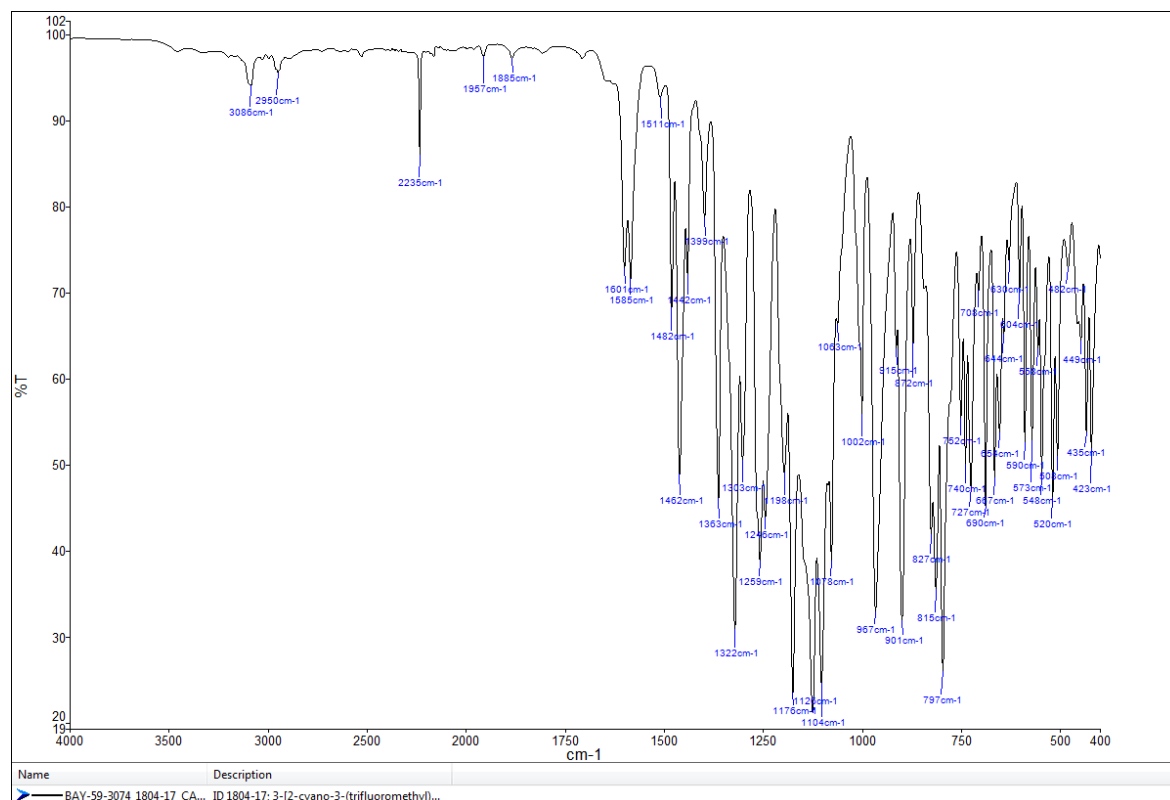
ANALYTICAL RESULTS

MS (EI)

Abundance



FTIR-ATR - sample as received



IR (condensed phase – after chromatographic separation)

