PTI-3

N-([1-(5-Fluoropentyl)-1H-indol-3-yl]-1,3-thiazol-4-yl)methyl)-2-methoxy-N-methylethanamine

Formula: C\textsubscript{21}H\textsubscript{28}FN\textsubscript{3}OS
Formula weight: 389.53
Chemical Abstracts No.: n. a.
Smiles code: COCCN(C)Cc1csc(n1)c2cn(CCCCCF)c3cccc23
InChi key: LXQIIHJBHSFWQW-UHFFFAOYSA-N
Other names: PTI-3
The components of the seized e-cigarette liquid were separated by column chromatography. The active component was analyzed by GC-MS and NMR methods.

**GC-MS**

An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. Samples were subjected to electron ionization (EI) mode. GC-MS conditions: HP-5MS column was temperature programmed from 100 °C (which was held for 2 minutes) to 280 °C at 20 °C/min, 280°C was held for 3 minutes, then to 315 °C at 25 °C/min, the temperature was stated at 315 °C for 12 minutes. The carrier gas was helium. Tribenzyl-amine was applied as an internal standard (locked to 10.8 minutes). Data handling was carried out with GC/MSD ChemStation software.
GC-MS chromatogram

Mass spectrum at 16.30 min retention time

Agilent 6890N Network GC system set up with Agilent HP-5MS
NMR

The NMR spectra were recorded on a Bruker Avance Neo 400 NMR operating at 9.4 Tesla magnetic field, equipped with Prodigy BBO-H&F-D-05 Z-gradient probe. The spectra were recorded at 25°C in DMSO-d$_6$ solution. The spectrometer was controlled, and the data were processed using TopSpin 4.0 software package. Chemical shifts (δ) are given in parts per million unit, referenced to tetramethylsilane (δ$_{TMS}$ = 0.00 ppm). The determination of the structure was based on $^1$H, zqs-clip-COSY, zqs-easy-ROESY, as well as $^{13}$C, multiplicity edited HSQC, HMBC as well as double-edited HSQC-zqs-clip-COSY spectra.

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N-((1-(5-Fluoropentyl)-1H-indol-3-yl)-1,3-thiazol-4-yl) methyl-2-methoxy-N-methylethanamine

COCCN(C)Cc1csc(n1)c2cn(CCCCCF)c3cccccc23

LXQIIHJBHSFWQW-UHFFFAOYSA-N
$J_{\text{H,H coupling constants [Hz]}}$

$J_{\text{H,F coupling constants [Hz]}}$

H-H steric proximities detected by zqs-easy-ROESY measurement

$^{13}$C-NMR chemical shifts $\delta$ [ppm]

$J_{\text{C,F coupling constants [Hz]}}$

Characteristic heteronuclear long-range coupling detected by HMBC method
1H NMR spectrum (overview)

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d6
zqs-clip-COSY

zqs-easy-ROESY

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-\textsubscript{d}\textsubscript{6}
$^{13}$C NMR

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-$d_6$
**Hungarian Institute for Forensic Science**

**Analytical data for PTI-3**

**double edited-HSQC-zqs-clip-COSY**

**HMBC**

*Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d$_6$*