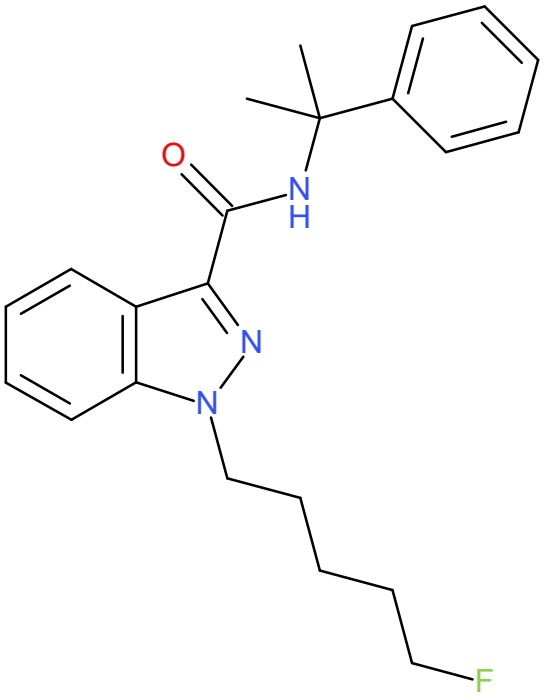
5F-Cumyl-PINACA



1-(5-fluoropentyl)-N-(1-methyl-1-phenylethyl)-1H-indazole-3-carboxamide

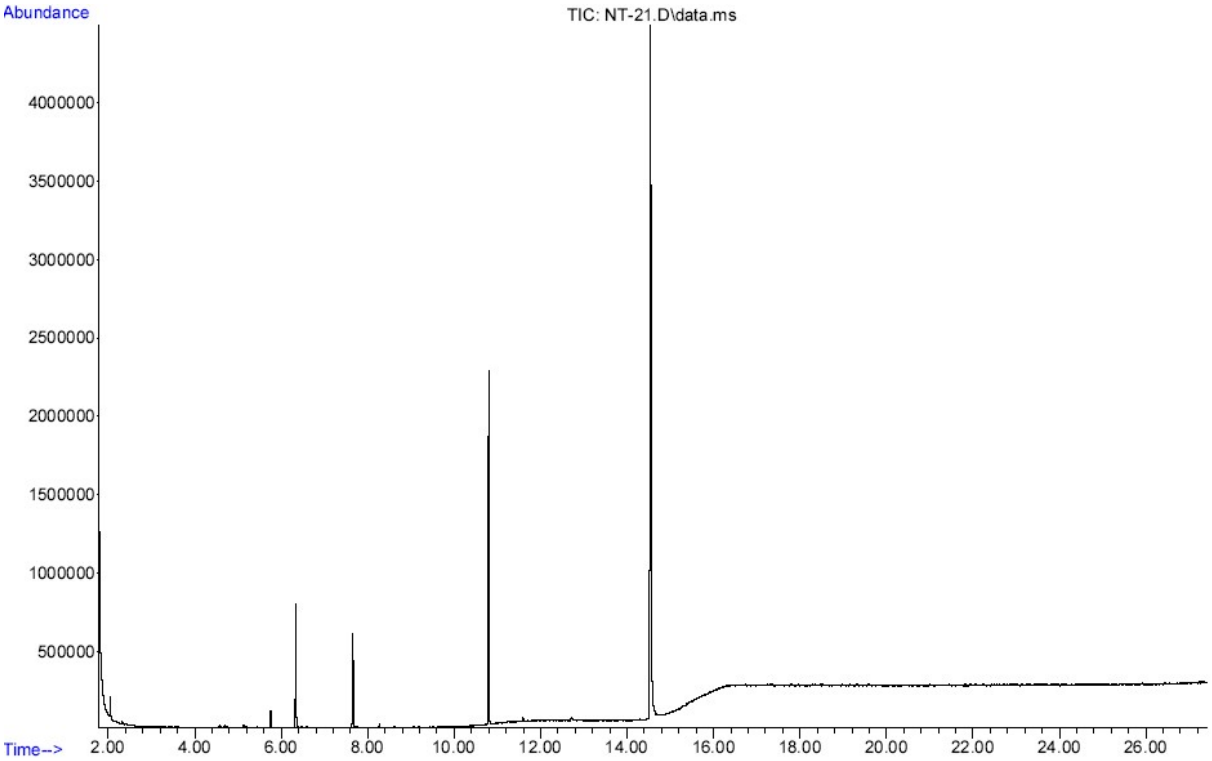
Formula: $C_{22}H_{26}FN_3O$
Formula weight: 367,47
Chemical Abstracts No.: 1400742-16-6
Smiles code: O=C(NC(C)(C)C1=CC=CC=C1)C2=NN(CCCCCF)C3=C2C=CC=C3
InChi key: XSHGVIPHMOTDCS-UHFFFAOYSA-N
Other names: 5F-Cumyl-PINACA, Cumyl-5F-PINACA

The components of the seized e-cigarette liquid were separated by column chromatography. The active component was analyzed by GC-MS and NMR methods.

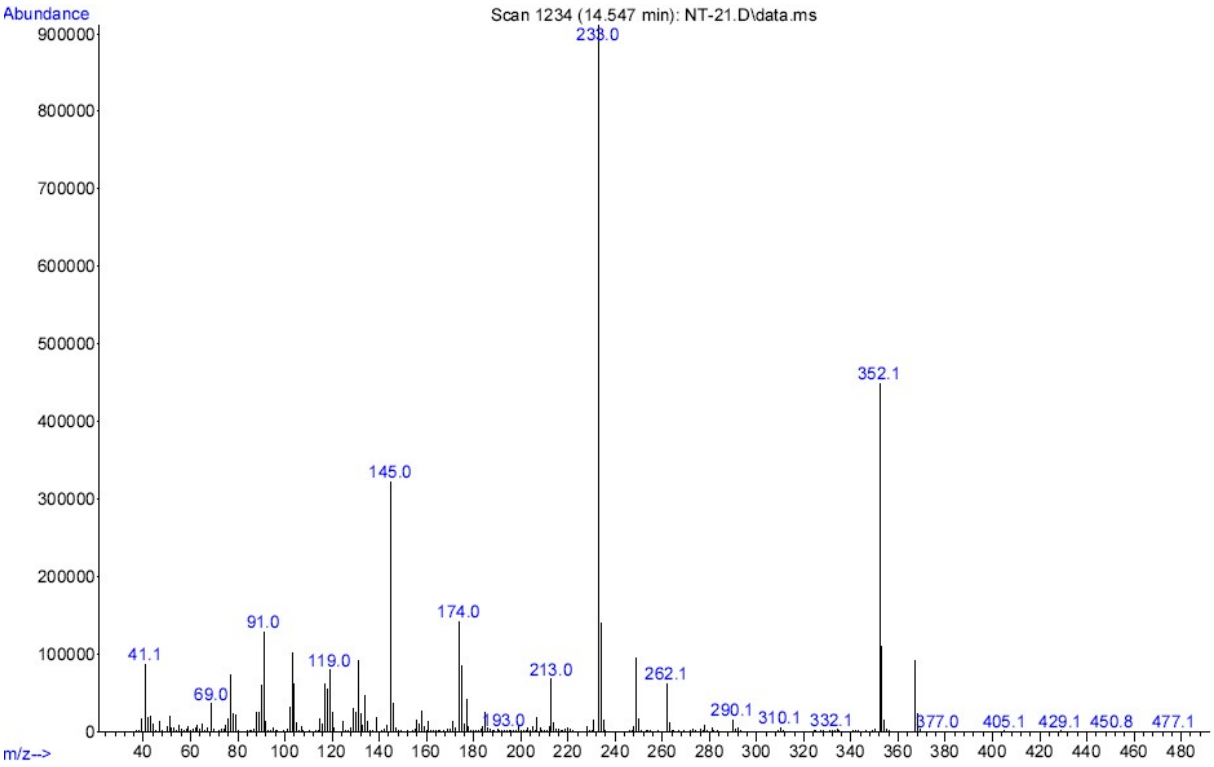
GC-MS

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 14.55 min retention time



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

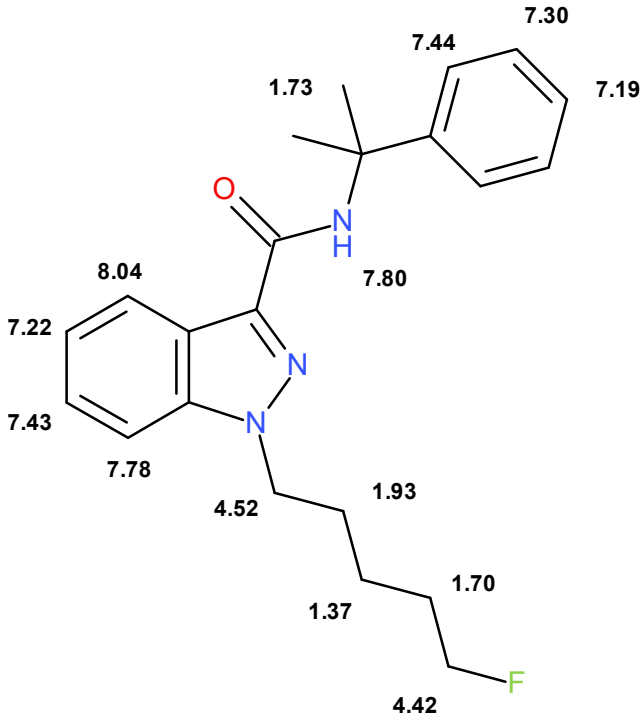
NMR

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.

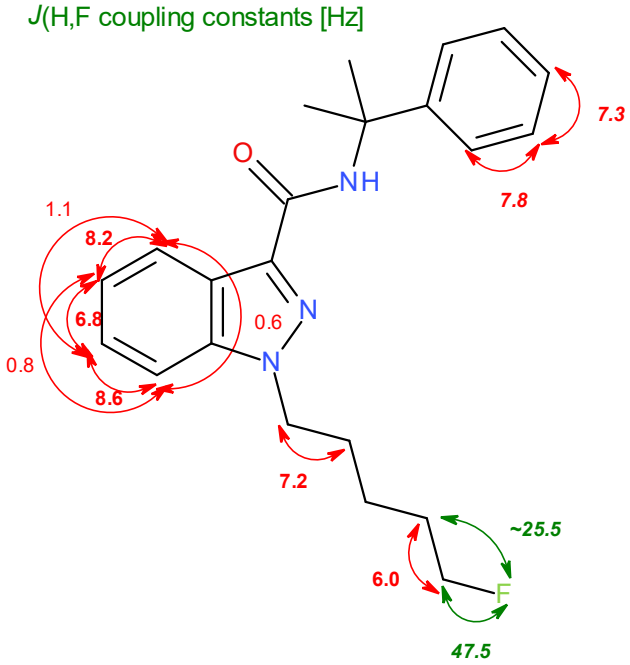
5F-Cumyl-PINACA
1-(5-fluoropentyl)-N-(1-methyl-1-phenylethyl)-1H-indazole-3-carboxamide
CC(C)(NC(=O)c1nn(CCCCCF)c2ccccc12)c3ccccc3
XSHGVIPHMOTDCS-UHFFFAOYSA-N

^{1}H-NMR chemical shifts δ [ppm]

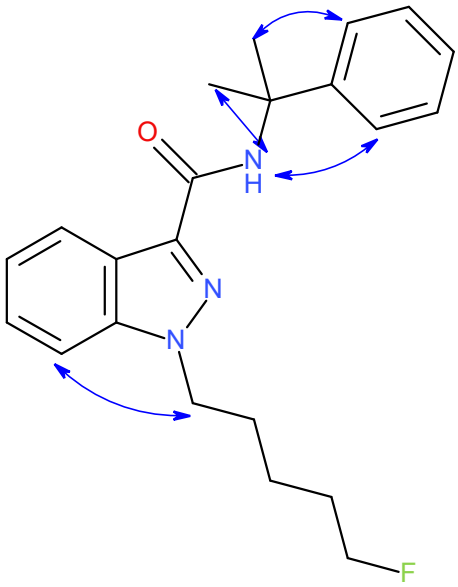
CAS No.: 1400742-16-6
Formula Weight: 367,45974
Exact Mass: 367,205990682
Molecular Formula: $C_{22}H_{26}FN_3O$



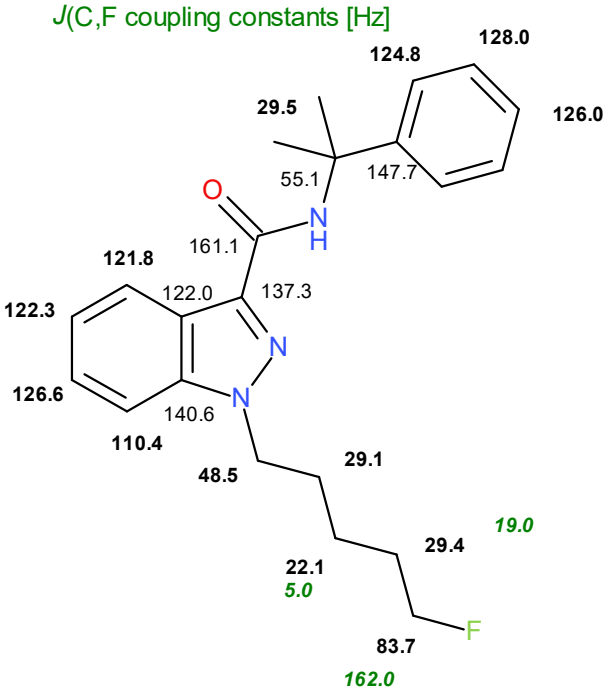
J(H,H coupling constants [Hz]
J(H,F coupling constants [Hz]



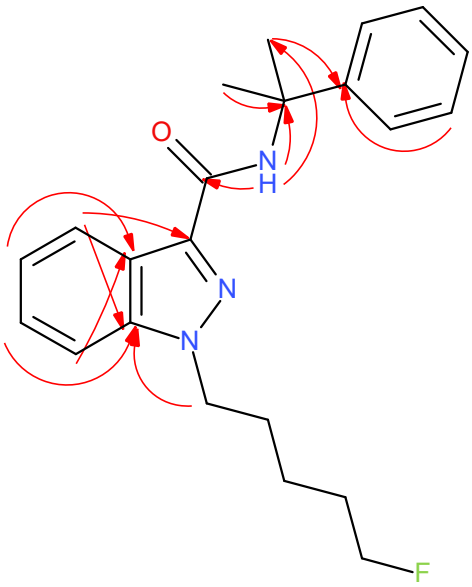
H-H steric proximities detected by zqs-NOESY measurement



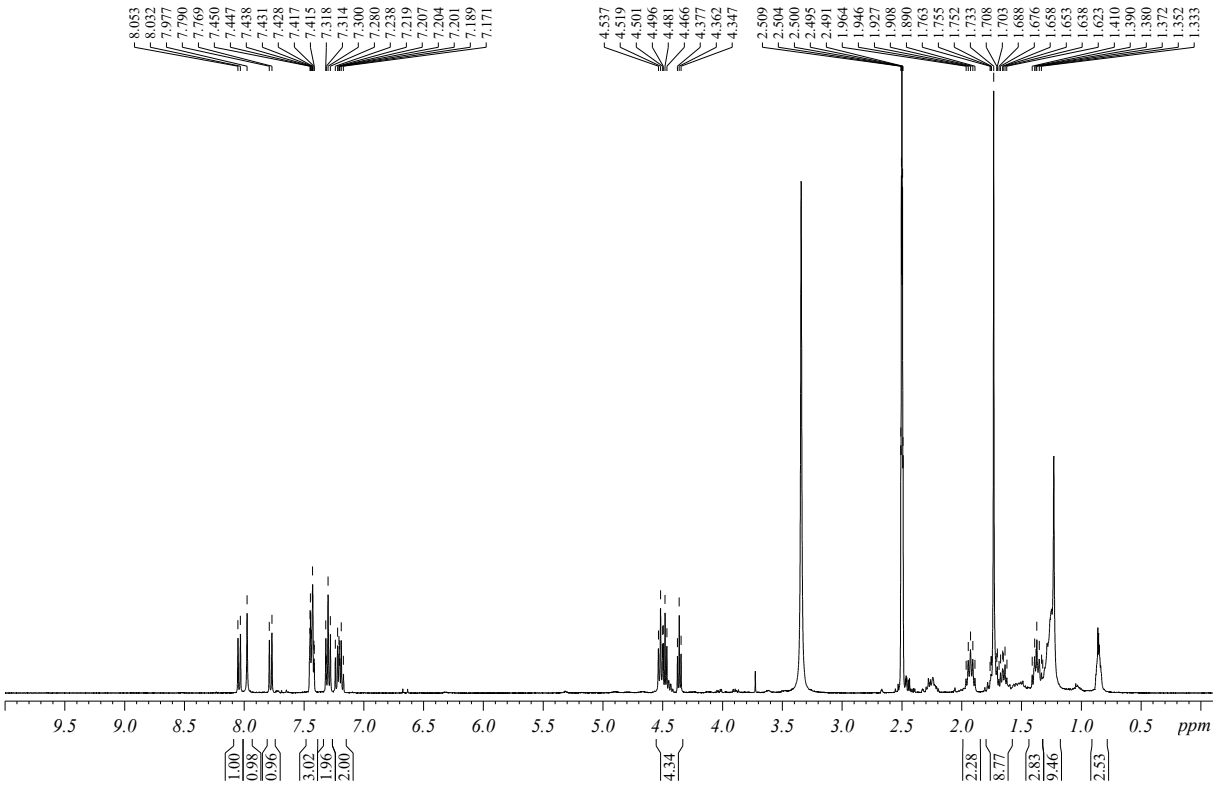
^{13}C-NMR chemical shifts δ [ppm]
J(C,F coupling constants [Hz]



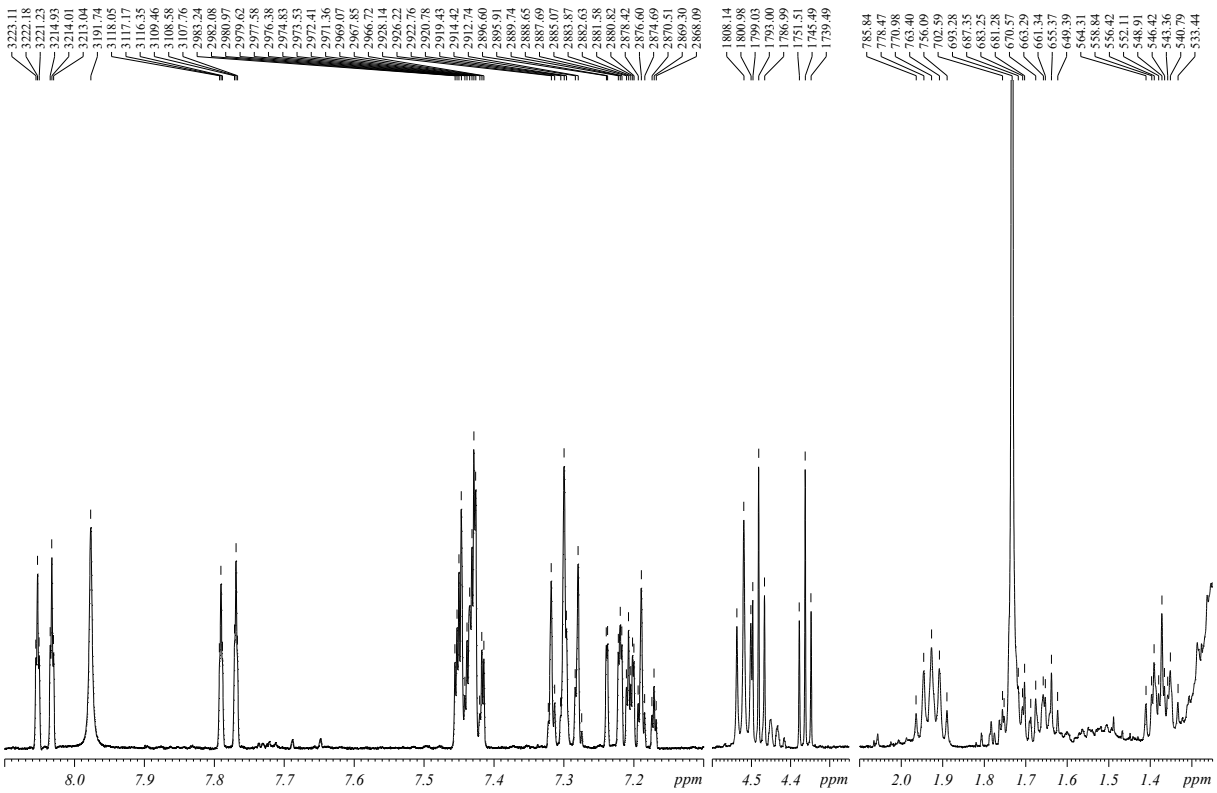
Characterictic heteronuclear long-range coupling detected by HMBC method H → C



^{1}H NMR spectrum (overview)

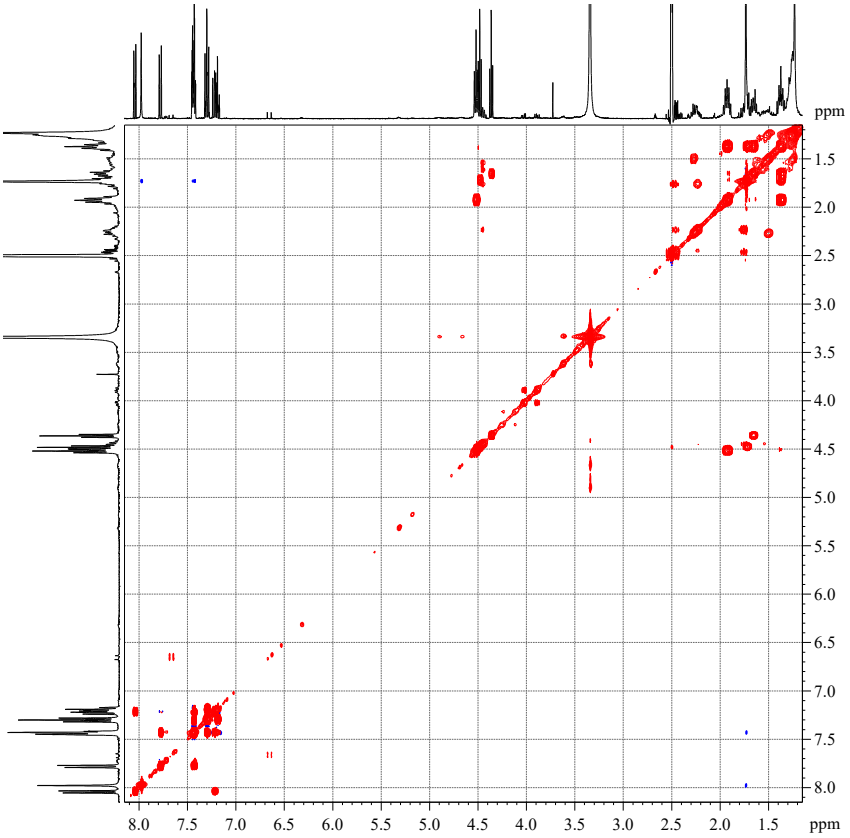


^{1}H NMR spectrum (characteristic sections)

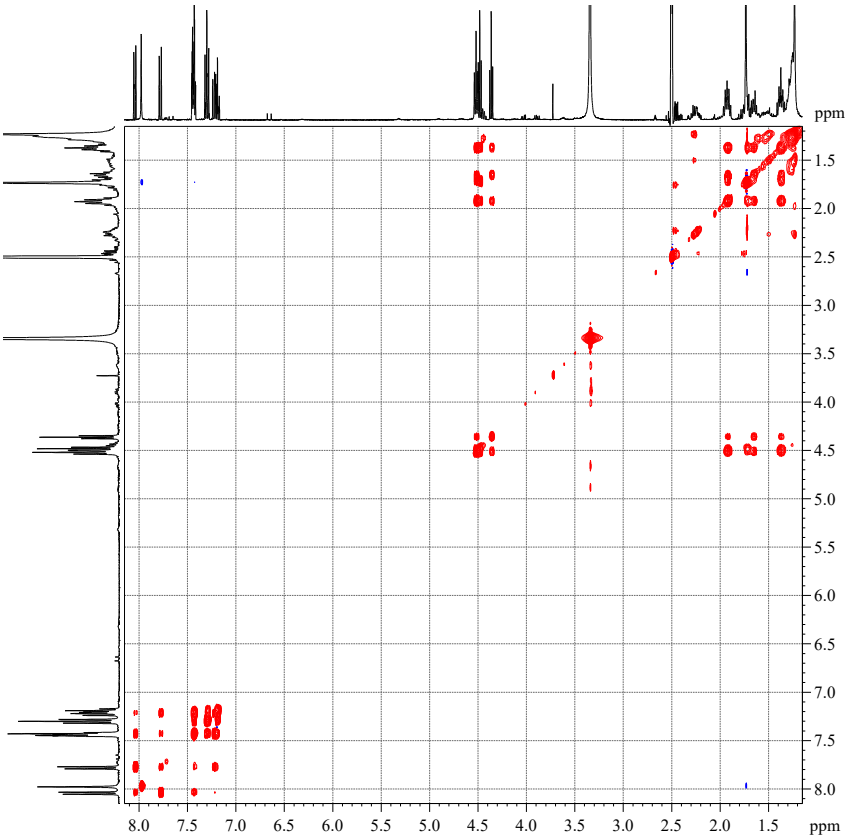


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-clip-COSY

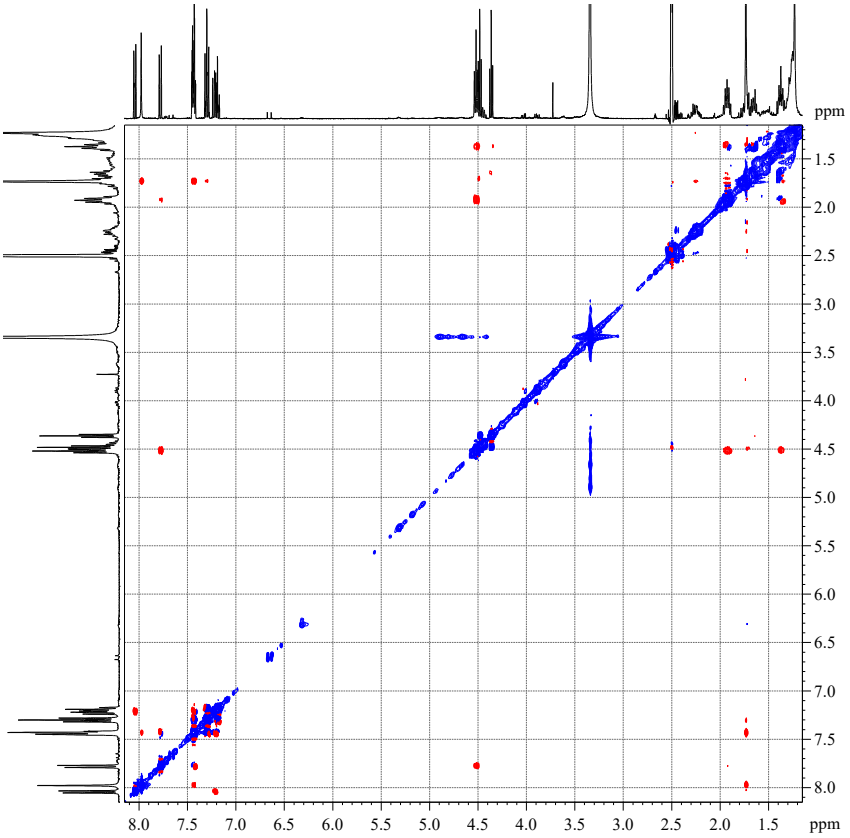


zqs-TOCSY

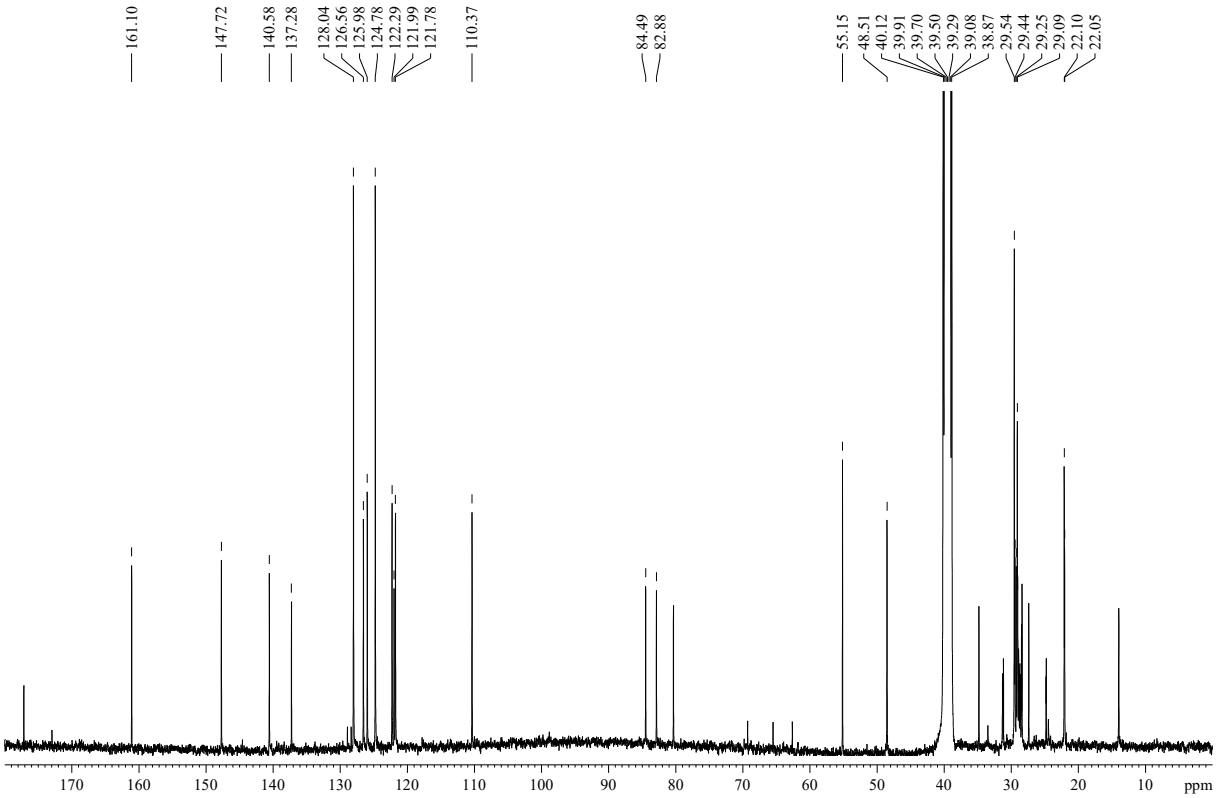


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-easy-ROESY

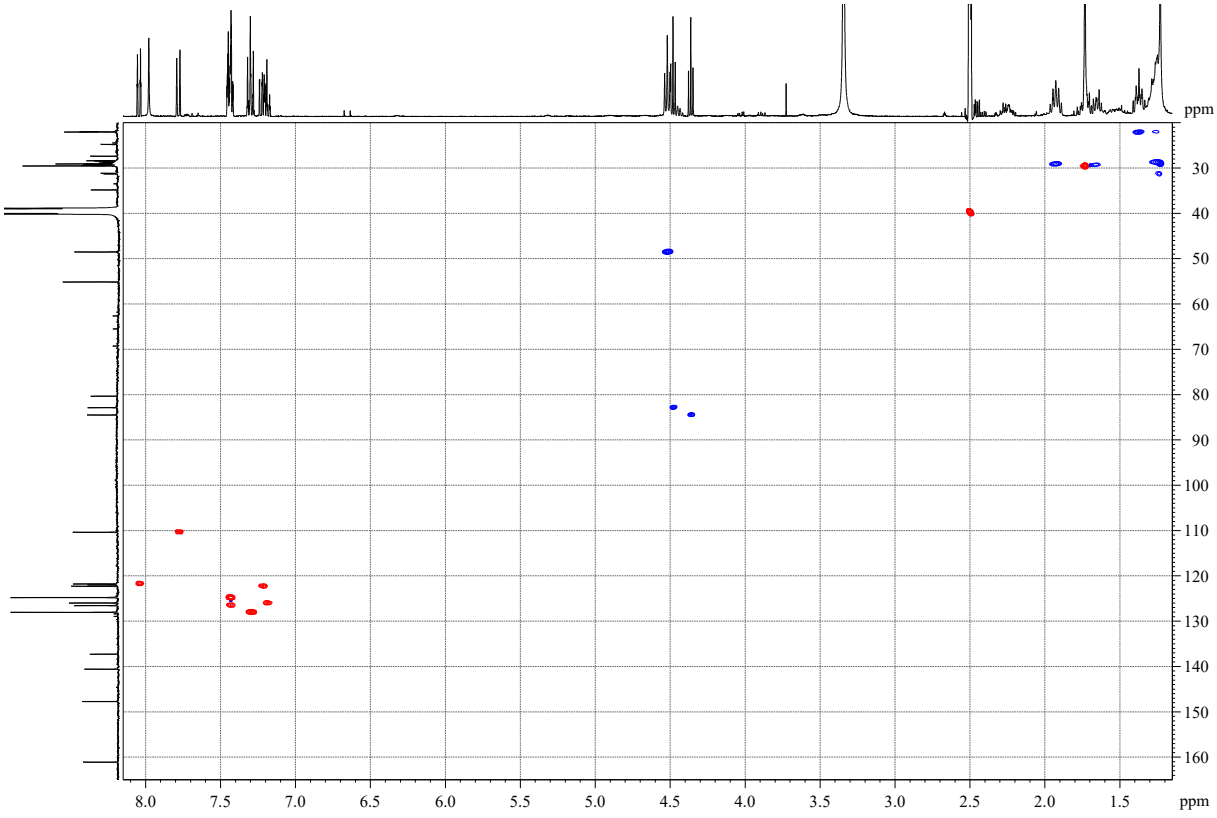


^{13}C NMR

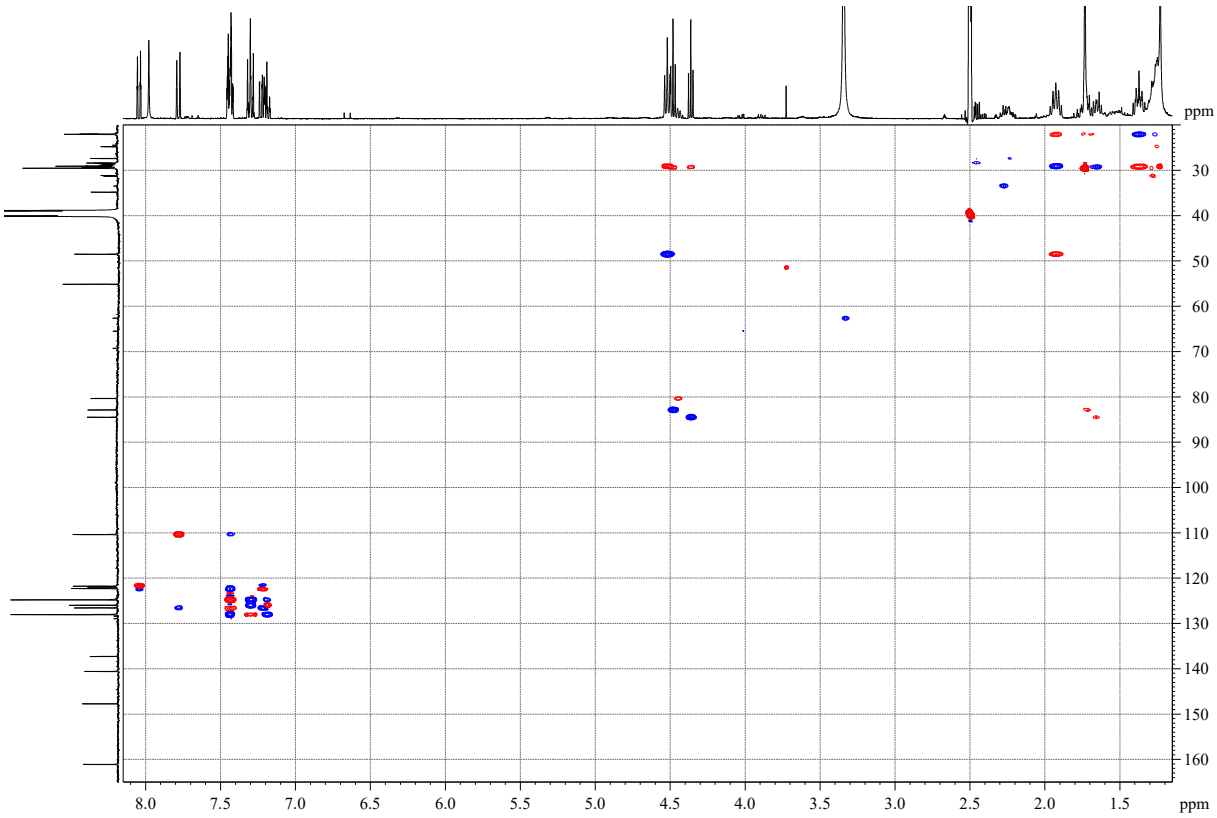


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC

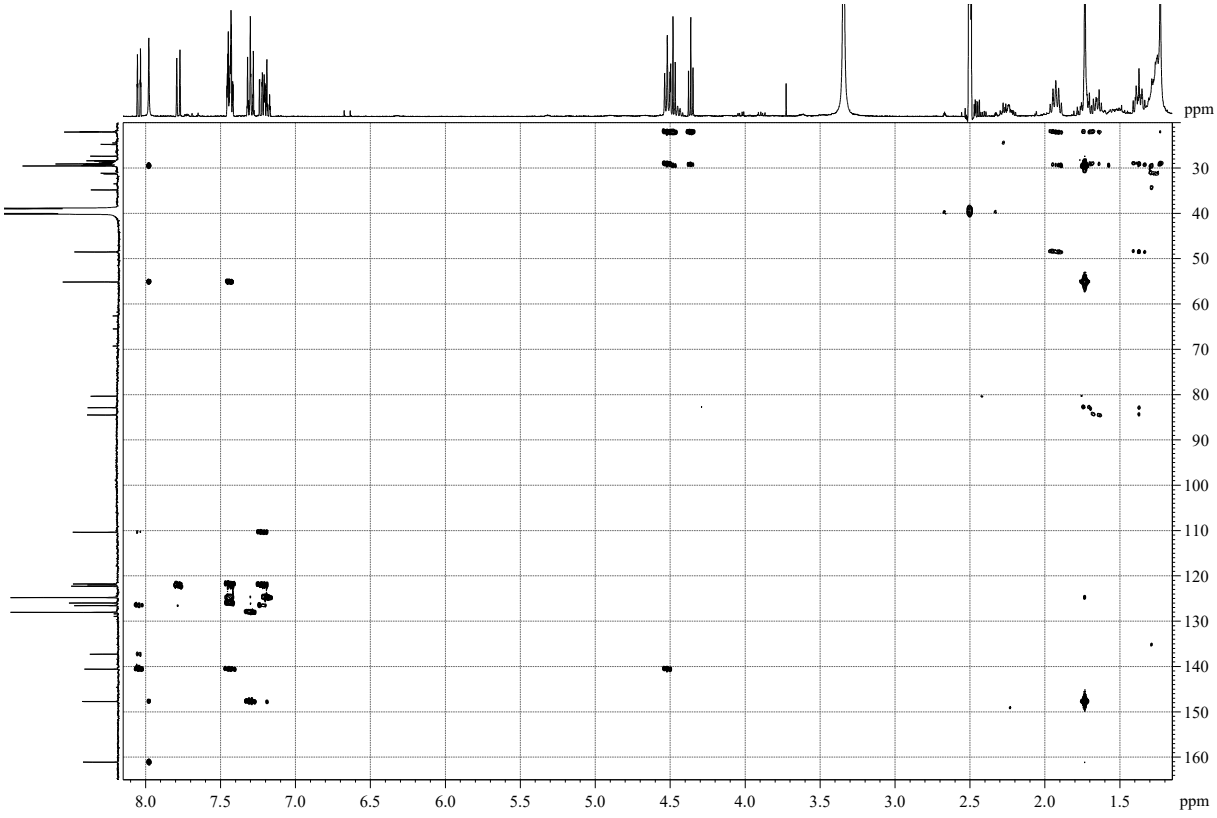


double edited-HSQC-zqs-clip-COSY

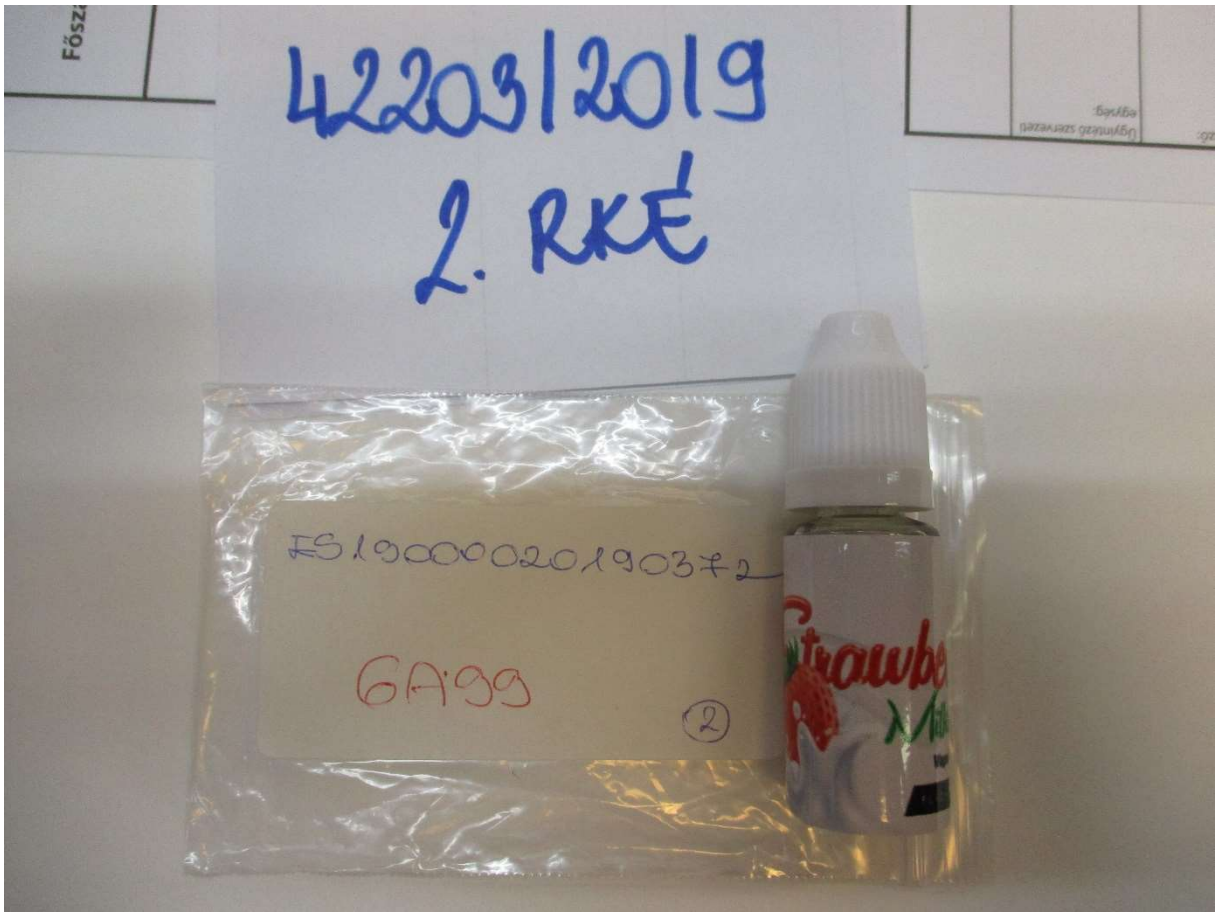


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

HMBC



Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6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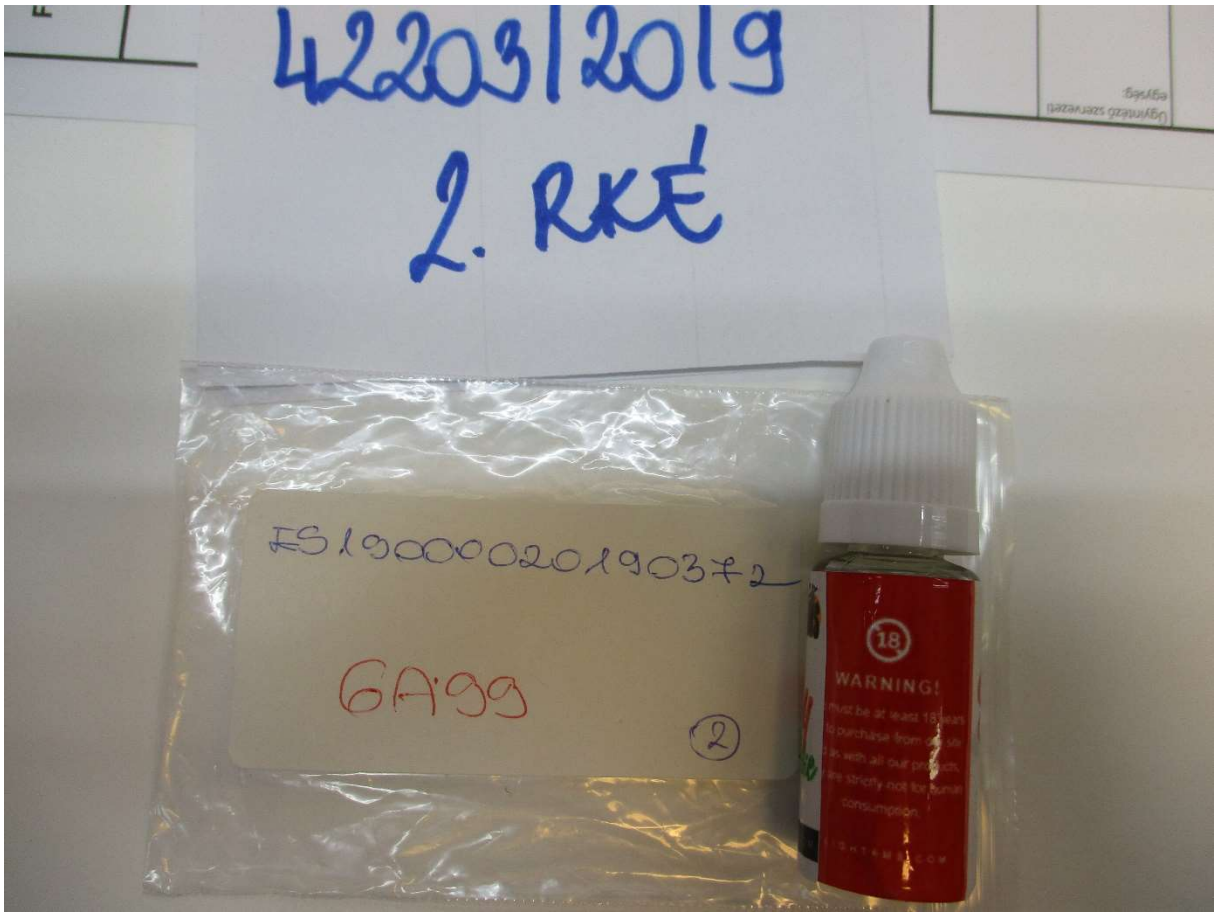
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18
WARNING!