Screening of new psychoactive substances in Swiss wastewaters by high-resolution mass spectrometry

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STSM purpose: Analyse wastewater samples collected in Switzerland via liquid chromatography coupled to high-resolution mass spectrometry (HR-MS). Provide stakeholders in Switzerland information about the possible use of new psychoactive substances in the country.

Description of the work carried out during the STSM:

During the eight weeks period, 46 wastewater samples (from the cities of Lausanne and Neuchâtel and from two major public events in the area) were analysed using a Waters Acquity UPLC system (Waters, Milford, MA, USA) coupled to a hybrid quadrupole-orthogonal acceleration time-of-flight mass spectrometer (Xevo G2 QTOF, Waters, Milford, MA, USA) available at the host institution. All samples were initially analysed using two different acquisition functions simultaneously (i.e., MS’ experiment): low collision energy (LE, at 4 eV) and high collision energy (HE, ramped from 10 to 40 eV). Acquisition was made in positive and negative mode. After collection, results were confronted to a database containing approximately 300 NPS (synthetic cannabinoids, cathinones, amphetamines, piperazines, tryptamines, lysergamines, cocaine, opioids and kratom derivatives).

The first step consisted in selecting candidate compounds (i.e., potentially present in the samples) using mainly the data acquired in LE and the exact mass of the molecular ion for all compounds contained in the database. The second step consisted in investigating the fragmentation pattern observed with the HE function for the candidates selected in the previous stage. The retained fragments were then compared to the molecular structure of the parent compound to verify if their occurrence followed a plausible fragmentation pattern. At this stage, 20 compounds were retained. These were mainly observed in samples from the city of Lausanne grasping during the period of an electronic music festival and during the weekends. The final step of the work consisted in conducting MS/MS experiments on the selected compounds. Four fragmentation energies were used (i.e., 10, 20, 30 and 40 eV) and the TOF was operated in full scan mode, so to obtain a large fragmentation pattern. Analogously to the previous step, candidates were retained if matches were found with the literature and/or if the observed fragments were plausible with regard to the molecular structure of the parent compound.

Description of the main results obtained:

After the various selection steps, 5 compounds (in one case structural isomers could not be discriminated) were retained in samples collected during the music festival:

- 5-IT, 6-IT and α-Methyltryptamine which are structural isomers. Six fragments, all corresponding to the literature, were observed. According to the literature and the observed fragmentation patterns (relative intensity), α-Methyltryptamine is the most likely of the three. 5-IT had been previously reported by Swiss authorities (seized at border control/post offices).
- 2-Methoxyamphetamine. Three fragments, all corresponding to the literature, were observed.
- 3,4-Methylenedioxypropylamphetamine (or 3,4-MDPA)
- O-Acetylpseudoephedrine
- Hu-210