

## Development and Application of an analytical method using HRMS (Orbitrap) to estimate drug of abuse consumption through wastewater based epidemiology in post-pandemic Valencia (Spain)

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Wastewater-based epidemiology allows, among other estimations, to establish the consumption of drugs of abuse in any given population [1,2]. After two years of complete or partial quarantines and restrictions due to the Coronavirus (Covid-19) pandemic, calculating the concentrations of these substances excreted in wastewater permits the assessment of drug use trends and how they were affected during these last years. Thus, developing methods for the rapid screening and confirming of drugs of abuse and their metabolites in water samples can be considered a public health priority. Wastewater samples taken in four wastewater treatment plants of Valencia city, its metropolitan area and Sueca town during a whole week in 2021 and 2022. A method to quantify six illicit substances indicators using solid-phase extraction (SPE) and UHPLC-HRMS/MS (Orbitrap Exploris 120) was developed, validated and applied to the analysis of these water samples. As far as the HRMS/MS system is concerned, the correct tuning of instrumental parameters was crucial to achieve selectivity, sensitivity and reproducibility for the analytes. Different acquisition modes are available while using a Q-Orbitrap platform and the optimized protocol focused on targeted analysis. The best results were obtained by applying a full scan (FS) mode and then a target MS2 (ddMS2) mode after using a filter for dynamic exclusion. Amphetamine, benzoylecgonine, cocaine, methamphetamine and ecstasy were detected in positive mode, while 11-Nor-9-carboxi-delta-9-tetrahydrocannabinol, the main secondary metabolite of cannabis formed in the human body after consumption, was detected in negative mode. Intra- day precision (% RSD, n = 3) ranged from 0.03 to 18.7 %, while linearity (R<sup>2</sup>) values were higher than 0.9970 and the lowest method detection limit was 0.01 µg/ ml. Cannabis and cocaine estimated consumptions remain the highest in Valencia even after the pandemic, with calculated amounts up to 18 g/day/1000inh and 2.5 g/day/1000inh, respectively, in 2021, while in 2022 consumptions reached 26 g/day/1000inh for cannabis and 3 g/day/1000inh. It seems that the restrictions did affect the access to drugs of abuse analysed and their consumption tends to increase in wastewater samples in 2022, a year free from quarantines at national or city-wide level.

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### References

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- [2] Y. Picó, D. Barceló. TrAC- Trends Anal. Chem. 145 (2021) 116465

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