# Improving the prediction of in-sewer transformation of illicit drug biomarkers by identifying a new modelling framework

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# Improving the prediction of in-sewer transformation of illicit drug biomarkers by identifying a new modelling framework

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In the context of wastewater-based epidemiology, uncertainties associated with in-sewer transformation are often not considered. However, sewer systems are biological reactors in which the concentration of organic pollutants (primary pollutants, e.g. COD, and secondary pollutants, e.g. illicit drugs) is altered during transport. Although reduced stability of several drug biomarkers was shown in raw sewage and biofilm, evidence on the type of transformation (biotic or abiotic) and the effect of different redox conditions on transformation is currently insufficient. In this study, the biotransformation and abiotic transformation of 16 illicit drugs were assessed in wastewater and mineral water, respectively. The targeted illicit drugs were: cocaine and its metabolites benzoylecgonine, ecgonine methyl ester, and cocaethylene; heroin and its metabolites 6-monoacetylmorphine, morphine, and morphine-3-β-D-glucuronide; codeine and its metabolite norcodeine; methadone and its metabolite 2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP); mephedrone; and tetrahydrocannabinol (THC) and its metabolites 11-hydroxy-Δ9-THC (THCOH), and 11-nor-9-carboxy-Δ9-THC (THCCOOH). All the transformation studies were performed using batch experiments under both aerobic and anaerobic conditions, while concomitantly assessing the degradation of primary pollutants. Furthermore, sorption to suspended solids and to reactor walls was also considered and quantified. The transformation of primary pollutants and illicit drugs in wastewater was simulated using Wastewater Aerobic/anaerobic Transformations in Sewers model (WATS)[1] extended with the Activated Sludge Model for Xenobiotic trace chemicals (ASM-X)[2]. In addition, abiotic and biotic transformation pathways (based on available literature studies and statistical analysis) were considered for each drug biomarker. Our results suggest that ignoring the dynamics of biomass growth would result in significant overestimation (up to 385%) of aerobic biotransformation rate constants, whereas no significant difference was observed for anaerobic rate constants. Furthermore, abiotic transformation was found to be the main transformation mechanism for THC (aerobic conditions); mephedrone, methadone, cocaine, ecgonine methyl ester, cocaethylene, THCOH and THCCOOH (anaerobic conditions). By use of the proposed model the uncertainty of predicting illicit drug concentration at the excretion point can be reduced and hence the accuracy of back-calculation of illicit drug use in catchments can be improved.

[Wastewater-based epidemiology; drugs of abuse; in-sewer transformation; WATS; ASM-X]

**References**

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