MO092 Suspect and non-targeted strategies to investigate in vitro and in vivo biotransformation products of emerging environmental contaminants: the benzotriazoles and benzothiazoles C. Baduel, CNRS IGE UMR 5001, Univ. Grenoble / The Institute for Geosciences and Environmental research; F. Lai, Swedish University of Agricultural Sciences / Department of Aquatic Sciences and Assessment; A. Van Nuijs, A. Covaci, University of Antwerp / Toxicological Center.
Benzotriazoles (BTRs) and benzothiazoles (BTHs) derivatives are high production volume chemicals involved in a wide range of applications and consumer products. The widespread use of BTRs and BTHs and their occurrence in a wide range of environmental media (drinking water, indoor and outdoor air, indoor dust, textiles, etc.) as well as human urine samples across different countries suggest that the population is exposed continuously to these chemicals worldwide. However, while human exposure has been observed, exposure assessment to these chemicals is very limited and it is only based on the analysis of parent compounds in human specimens. The objective of this study was to investigate the *in vitro* human Phase I and Phase II biotransformation of six emerging contaminants (3 BTRs and 3 BTHs) through cytochrome P450 (CYP), uridine glucuronic acid transferase (UGT), and sulfotransferase (SULT). Highly used and ubiquitous BTRs and BTHs were selected as substrates in this present study. Moreover, they were considered as model compounds to predict potential biotransformation products of other BTRs and BTHs derivatives. Generated biotransformation products in the samples were investigated using liquid chromatography coupled to quadrupole-time-of-flight mass spectrometry (LC-QTOF-MS), followed by their identification and structural elucidation based on a workflow combining suspect and non-target strategies. Most of the proposed biotransformation products were identified and structurally elucidated for the first time and possible metabolic transformation pathways were presented for the studied compounds. The identified biotransformation products were then targeted for analysis in human urine samples. Our findings provide important insights for the selection of biomarkers in future biomonitoring studies and emphasize the importance to investigate the biotransformation products in order to assess overall exposure to xenobiotics.