ENVIRONMENTAL METABOLOMICS AS A POWERFULL TOOL TO ASSESS PHARMACEUTICAL POLLUTION

Katie O'Rourke[1], Beatrice Engelmann[2], Christina Virgiliou[34], Georgios Theodoridis[4], Eleni Gika[5], Rolf Altenburger[6], Ulrike E. Rolle-Kampczyk[2], Konstantinos Grintzalis[1]

[1]School of Biotechnology, Dublin City University, Republic of Ireland
[2]Laboratory of Pesticide Science, Agricultural University of Athens, Iera Odos 75, 118 55 Athens, Greece
[3]Department of Biology, University of Patras, Greece
[4]Department of Plant Science, McGill University, Macdonald Campus, Ste-Anne-de-Bellevue, Quebec H9X 3V9, Canada
[5]School of Nursing, Psychotherapy, and Community Health, Dublin City University, Republic of Ireland

Pharmaceuticals have been recognised as emerging contaminants of concern, with several pathways of entry to the environment. Pharmaceuticals eventuate into freshwater systems where they pose sub-lethal effects to aquatic organisms. Exacerbated by their increased consumption and poor removal rates from wastewater treatment plants, pharmaceutical compounds have been classified as pseudo-persistent in the aquatic environment and their monitoring is imperative.
The implementation of novel methods to water monitoring such as effect-based methods provide insight to the underlying mechanisms of toxicity of chemicals via adverse outcome pathways. Using the sentinel species *Daphnia magna*, and integrating holistic techniques such as metabolomics and biochemical markers, the molecular responses to individual pharmaceuticals or complex mixtures was explored in the wider concept of daphnids acting as the "canary in the coal mine" within the aquatic environment.
In this study we investigated the acute, chronic and transgenerational effects of frequently detected classes of pharmaceuticals including antibiotics, NSAIDs, anti-convulsants, anti-diabetics, lipid regulators and oestrogens, on the crustacean *Daphnia magna*. Exposure to these pharmaceuticals at sub-lethal concentrations, validated by toxicity tests and phenotypic endpoints, revealed significant changes in the polar metabolic profile and enzyme activities of daphnids. Metabolomic analysis provided significant changes in key metabolic pathways and revealed mechanistic insight of pharmaceuticals to non target species. Using these molecular signatures, we are able to detect pollution hotspots and timely predict pollution before reaching irreversible levels.