

Development of a new using mathematical modeling to predict cocktail effects of Micro pollutants of diverse origins

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Abstract

Statement of the Problem: A wide variety of organic chemicals can be detected in waste and surface waters at very low concentrations (micrograms to Nano grams per litre). They are generally found in all matrices and also accumulate in wild-life organisms. These micro pollutants (MP) threaten ecosystems and human health as they exhibit potential harmful effects on non-target organisms. MP are predominantly aromatic compounds used as pesticides, pharmaceuticals or industrial chemicals that may act as endocrine disrupting compounds. The effect resulting from the interaction between chemicals is called cocktail effect but the impact of chemical mixtures is poorly documented and often limited to binary mixtures using MP of the same category. The purpose of this study is to propose a new methodology using mathematical modelling to easily determine cocktail effects within complex mixtures containing diverse categories of MP, whatever their mode of action. Six MP were selected: bisphenol A, diclofenac, tramadol, cyproconazole, diuron and terbutryn. A statistical design was used to reduce the number of in vitro experiments using MP mixtures. A response surface model was then applied to look for cocktail effects. **Findings:** Different mixtures were tested using MP at the concentration at which 10% or 25% of the maximal effect on human cytotoxicity was observed. A strong global cocktail effect between the micro pollutants was evidenced. This effect was further investigated by considering micro pollutant response surfaces taken in pairs. Hence, we showed that there was a neutralization effect between bisphenol A and tramadol. **Conclusion & Significance:** We present a study focusing on MP cocktail effects where a selection of micro pollutants was made to reflect the heterogeneity of water contamination. The proposed methodology was inspired by clinical methodologies developed to test the effect of drug combinations. Hopefully, new legislation dealing with priority cocktail monitoring will appear to reinforce micro pollutant monitoring policy.

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Biography

Hélène Duval is a lecturer at the University of South Brittany (UBS) in France and conducts her research activities at the IRDL laboratory (Institut de Recherche Dupuy de Lôme). She has her expertise in molecular and cellular approaches used to evaluate the deleterious effects of chemicals, including endocrine

disrupting compounds, on human cells. Recently, she collaborated with mathematicians in order to focus on cocktail effects associated with the presence of micro pollutant mixtures in the aquatic environment using mathematical modeling. She is also involved in the characterization of the human estrogen receptor and its splice variants in breast cancer.