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New tool accurately predicts toxic effects of chemical mixtures

A new tool that predicts the effects of complex mixtures in water has shown promising results. It correctly predicted the impacts of toxic mixtures on the model species *Daphnia magna,* or water fleas, in over 90 per cent of cases.

The most common approaches for predicting the toxicity of chemical mixtures are 'Concentration Addition' and 'Independent Action'. Both these methods focus on specific effects of the mixtures (e.g. on growth) and the results do not apply to other organisms, endpoints, points in time or chemicals.

The research was supported by the EU-funded NoMiracle[1] project. It compared predicted survival with observed survival of water fleas in water samples taken from the Delfland region of the Netherlands, an area with a high concentration of greenhouses. At the time of the research there was no sewage treatment in this region so it is contaminated with heavy metals, pesticides, nutrients and minerals.

The concentrations of over 90 chemical contaminants were measured and, by analysing the chemical composition, the study predicted whether the NECs were exceeded and what the effect on water flea survival was after one week of exposure. 37 datasets were analysed from 17 locations. In 17 of these datasets all water fleas died, but in the other 20 all water fleas survived. Other datasets were also examined which showed partial effects, i.e. some water fleas died, but large differences in mortality levels made it difficult to include these in the main analysis.

The researchers predicted the survival of water fleas using no effect concentrations (NEC) of detected chemical compounds in the water samples. NECs are the concentrations below which there are no effects on the water fleas. For the first time, NECs were also derived for mixtures. They distinguished the following groups on the basis of having similar NECs: poly-aromatic hydrocarbons (PAHs), organophosphorus insecticides, inhibiting acetyl-choline esterases and metals. All other compounds were assumed to have their own individual NECs. The study also considered the impacts of the acidity of water and the level of oxygen.

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In 19 out of the 20 cases, where all water fleas survived, the model correctly predicted survival. In 15 out of the 17 cases, where all water fleas died, the model correctly predicted death. In the samples where there was complete mortality the model could identify the contaminant, group of contaminants or conditions that was the cause of death, by checking which of the NECs were exceeded. These were mainly high pH, individual pesticides and low oxygen levels.

There was only one case where the observed mortality was caused by a mixture. This was from a mixture of organophosphorus pesticides. However, the researchers suggested that if partial or sub-lethal effects were evaluated then the role of mixtures could be more apparent.

1. NoMiracle was supported by the European Commission under the Sixth Framework Programme, under the theme 'Global Change and Ecosystems'. See: http://nomiracle.jrc.ec.europa.eu/default.aspx

Source: Baas, J., Willems, J., Jager, T. *et al.* (2009). Prediction of Daphnid Survival after *in Situ* Exposure to Complex Mixtures. *Environmental Science & Technology.* 43(15): 6064-6069.

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