

**SCIENCE NEWS FLASH:
New ECETOC report addresses environmental
exposure assessment of ionisable organic compounds**

Brussels, January 2014

When predicting the concentration of an ionisable chemical in the environment (an important step in risk assessment), it should be realised that the compound may have different key properties (acidity, partitioning and sorption) depending on pH, ionic strength, etc. While focusing on ionisable organic chemicals, particularly pharmaceutical ingredients and agrochemicals, this report explains the difficulties in applying current international standard methods (OECD test guidelines). Only hydrolysis and biodegradation can be measured as usual. Alternatively, if no measurement exists, the key data can be obtained mathematically, based on structural similarity. This works better for ionisable acids than for bases. Computerised 'chemical space' models can show the chemical's distribution into the environment (partitioning) at different acidities (pH values).

The report makes specific recommendations to take ionisability into account when measuring or estimating the acidity, sorption and partitioning. This should lead to more accurate prediction of environmental (wastewater effluent) concentrations and proper categorisation of ionisable chemicals before they are designated accumulative in environmental organisms or persistent in the environment.

The document is published as ECETOC Technical Report 123: *Environmental Exposure Assessment of Ionisable Organic Compounds*. The Summary and free PDF of the report are available at <http://bit.ly/ecetoc-tr123>



ECETOC is Europe's leading industry association for developing and promoting top-quality science in human and environmental risk assessment of chemicals.