

Code Number and Title:

LRI-ECO30: Mining data (bases) to expand the domain of applicability of chemical activity

Background

Society is facing a variety of challenges in environmental risk assessment (ERA): growing concerns about the effects of multiple stressors (both chemical and non-chemical); risks associated with exposure to complex mixtures; and demands to quantify local site-specific risks. At the same time, risk assessors are seeking to provide a more efficient framework on which to address these emerging problems and questions in a manner that reduces cost and the use of animals.

Recently there have been a number of studies that have aimed at demonstrating that chemicals that interact with biological systems through relatively weak and reversible hydrophobic interactions to cause non-specific baseline toxicity, or 'narcosis', are associated with a narrow range of internal body concentrations (2-8 mmol/kg) and chemical activities (0.1 to 0.001), [1, 2].

This observation has the potential to dramatically improve how we might do risk assessment for chemicals identified as baseline toxicants. Whereby, the risk assessment can be based on ensuring that the predicted environmental concentration is <1% of the solubility of the chemical. However, as highlighted within a recent ECETOC task force report, in which an extensive set of existing data provided a proof of concept for the relationship between chemical activity and toxicity for baseline toxicants, concerns were raised regarding the lack of high quality chronic aquatic toxicity data, and the data available for assessing the relationship of chemical activity with chemicals with other modes of action [3].

Scope and Objectives

The project's objectives are to evaluate a wide range of data and databases for the potential to expand the domain of applicability of chemical activity. In particular:

1. Expand the domain of applicability of chemical activity using existing data sets, including but not limited to other, i.e. non-baseline toxicity modes of action, other endpoints, *in vitro* data.
2. In the absence of high quality data, are there approaches/strategies for utilizing acute and chronic data of lesser quality.
3. Determine if MoA and chemical activities cluster in large *in vitro* data sets (e.g. USEPA ToxCast).

Deliverables

The final report shall contain an executive summary (2 pages max), a main part (max. 50 pages), a detailed bibliography illustrating data sources, the data and methods used to screen/classify data. It is expected that there will be recommendations on the implications of data gaps and on potential future experimentally-based projects. It is expected that

the findings will be developed into at least one peer reviewed publication, following poster/oral presentations at suitable scientific conferences.

Cost and Timing

Start in early 2015, duration 18-24 months
Budget in the order of €150,000

Partnering/Co-funding

Applicants should provide an indication of additional partners and funding opportunities that can be appropriately leveraged as part of their proposal. Partners can include, but are not limited to industry, government/regulatory organizations, research institutes, etc. Statements from potential partners should be included in the proposal package.

Fit with LRI objectives/Possible regulatory and policy impact involvements/Dissemination

Applicants should provide information on the fit of their proposal with LRI objectives and an indication on how and where they could play a role in the regulatory and policy areas. Dissemination plans should also be laid down.

References

- [1] MacKay D & Arnot JA 2011 The application of fugacity and activity to simulating the environmental fate of organic contaminants. *J Chem Eng Data* 56 1348-1355.
- [2] MacKay D, Arnot JA, Wania F, Bailey RE. 2011. Chemical activity as an integrating concept in environmental assessment and management of contaminants. *Environ Assess Manag* 7(2):248-255.
- [3] Activity-Based Relationships for Aquatic Ecotoxicology Data: Use of the Activity Approach to Strengthen MoA Predictions ECETOC Technical Report 120. ISSN 2079-1526-120 (online). European Centre for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium.

DEADLINE FOR SUBMISSIONS: August 31, 2014

Please visit www.cefic-lri.org for general information about the LRI funding programme, guidelines for grant applications and links to application documents.

For further assistance do not hesitate to contact the LRI Secretariat by e-mail at lri@cefic.be or by phone on 0032 (0)2 676 7368.