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LINKING ALGAL GROWTH INHIBITION TO CHEMICAL ACTIVITY

Stine N. Schmidt[1]*, James M. Amitage[2], Jon Arnot[2], Kresten Ole Kusk[1] and Philipp Mayer[1]

[1]Department of Environmental Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark and [2]ARC Arnot Research & Consulting Inc., Toronto, Canada. ***e-mail: stnsch@env.dtu.dk**

PART 1: Challenging the chemical activity range for baseline toxicity

Background

- Recently, high-quality data were published on the algal growth inhibition caused by 50 non-polar narcotic compounds, of which 39 were liquids with defined water solubility (Figure 1a, [1]).
- In the present study [2], the toxicity data for these liquids were applied to challenge the chemical activity range for baseline toxicity [3-6].
- Chemical activity (a, unitless) quantifies the energetic level of an organic compound relative to its pure liquid [0-1], and several studies have reported that baseline toxicity requires a chemical activity of at least 0.01-0.1 [e.g., 3-9].

Objectives

- To convert toxicity data for liquids to chemical activity.
- To challenge the proposed chemical activity range of 0.01-0.1 for baseline toxicity.
- To propose a framework for using the obtained findings.

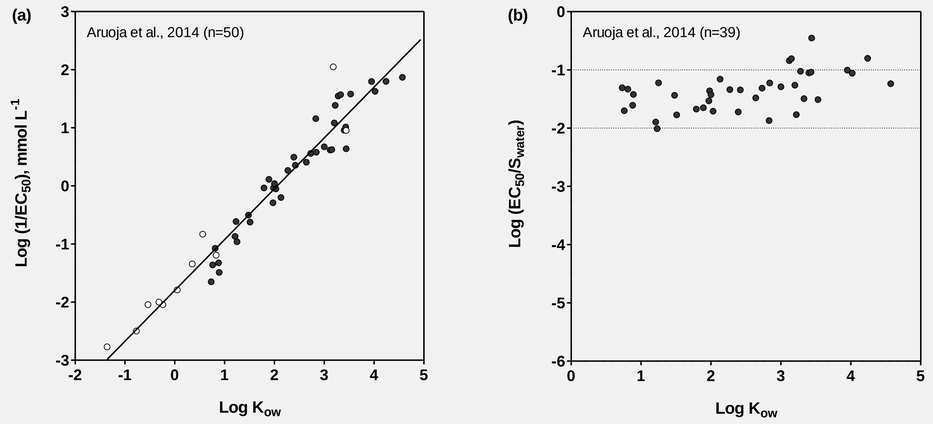

Figure 1. (a) Quantitative structure-activity relationship (QSAR) relating effective concentrations (EC_{50}) and octanol to water partition ratios (K_{ow}) for 50 non-polar narcotic compounds [1]. Water miscible and solid compounds (n=11) are indicated by light circles. (b) Ratios of EC_{50} (mg L^{-1}) and water solubility (S_{water}, mg L^{-1}) for the remaining 39 liquids plotted against K_{ow}.

Procedure

- Ratios of effective concentration (EC_{50}, mg L^{-1}) and water solubility (S_{water}, mg L^{-1}) were determined, which essentially equals the effective chemical activity (Ea_{50}).
- The EC_{50}/S_{water} ratios were plotted as a function of K_{ow} (Figure 1b, [2]).

Results

- Most EC_{50}/S_{water} ratios were within the expected chemical activity range of 0.01-0.1, and none were significantly below 0.01.
- These findings suggest EC_{50} values for baseline toxicity to be at or above 1% of liquid saturation, and EC_{50} values well below this limit would indicate excess toxicity.
- Methods for applying the chemical activity concept for ecological risk assessment and environmental quality guidelines for baseline (mixture) toxicity are being proposed [2] and refined in the CEFIC LRI-ECO30 project.

PART 2: Extending the utilisation of the chemical activity concept

Background

- As for the above data [1], aquatic toxicity data are most often expressed on a concentration basis (e.g., EC_{50} in mg L^{-1}).
- Whereas the data are useful within regulatory risk assessment, the actual EC_{50} values offer no direct information on whether the compounds exert baseline toxicity or excess toxicity.
- In the present study, algal growth inhibition data were plotted relative to a regression for the (sub-cooled) liquid solubility, which served as a visual reference for chemical activity of unity.
- The data came from three comprehensive and carefully conducted algal toxicity experiments [1, 10, 11].

Objectives

- To express aquatic toxicity data on a chemical activity basis.
- To identify and quantify excess toxicity and thereby compounds of concern.

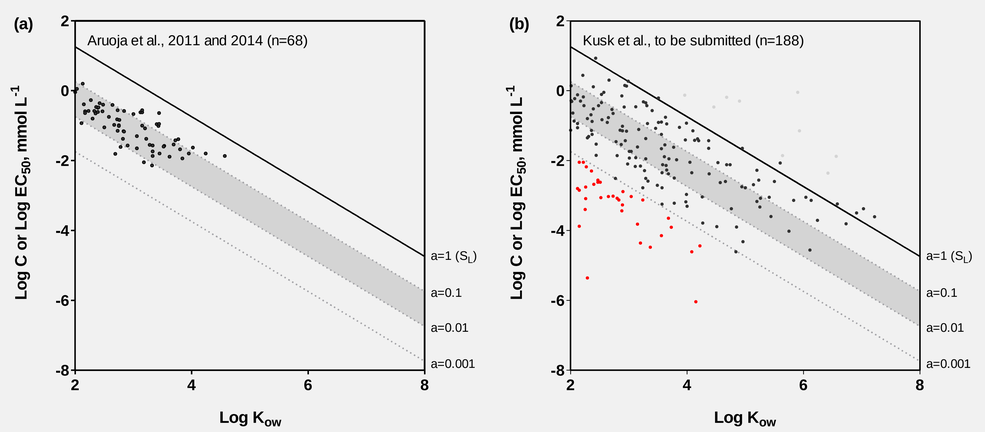

Figure 2. Regression of sub-cooled liquid solubility (S_L, mmol L^{-1}, a=1) as a function of K_{ow} [12] and lines representing the chemical activity levels of 0.1, 0.01 and 0.001. The shaded area is the chemical activity range 0.01 to 0.1 for the initiation of baseline toxicity. EC_{50} values (mmol L^{-1}) reported by (a) Aruoja and co-workers [1, 10] and (b) Kusk and co-workers [11] are plotted against their K_{ow}.

Procedure

- A regression of sub-cooled liquid solubility (S_L, mmol L^{-1}) [12] was plotted as a function of K_{ow}, representing a chemical activity of 1 (Figure 2).
- EC_{50} values (mmol L^{-1}) [1, 10, 11] were plotted against their K_{ow} in the same chart (Figure 2).

Preliminary Results

- The data analysis confirmed baseline toxicity for 68 compounds, which were characterised as polar and non-polar narcotic compounds by Aruoja and co-workers (Figure 2a).
- The data analysis of 188 compounds reported by Kusk and co-workers revealed 34 compounds exerting toxicity well below the limit of 1% of liquid saturation (a=0.01), and thereby indicating excess toxicity to algae (red circles, Figure 2b).
- In depth interpretation and further analyses on algal toxicity data, covering a wide range of solids and liquids, several expected modes of action and several algal species will be conducted.

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