

Aquatic toxicity integrated testing and assessment strategies (ITS) for difficult substances: case study with thiochemicals

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Supplementary Information

Graphical presentation of trends in acute aquatic toxicities of mercaptopropionates and mercaptans based on the carbon chain length (# C) as a proxy for molecular size and hydrophobicity, log Kow and MW.

The trends are similar but for some of the descriptors with lower r^2 . Predictive applications of these trends requires that similarity in MoA, chemical structures and behaviour in aquatic media are adequately considered in terms of water solubility and stability of source and target compounds.

Table S1. Trends in acute aquatic toxicities of mercaptopropionates based on the carbon chain length (# C) as a proxy for molecular size and hydrophobicity, log Kow and MW.

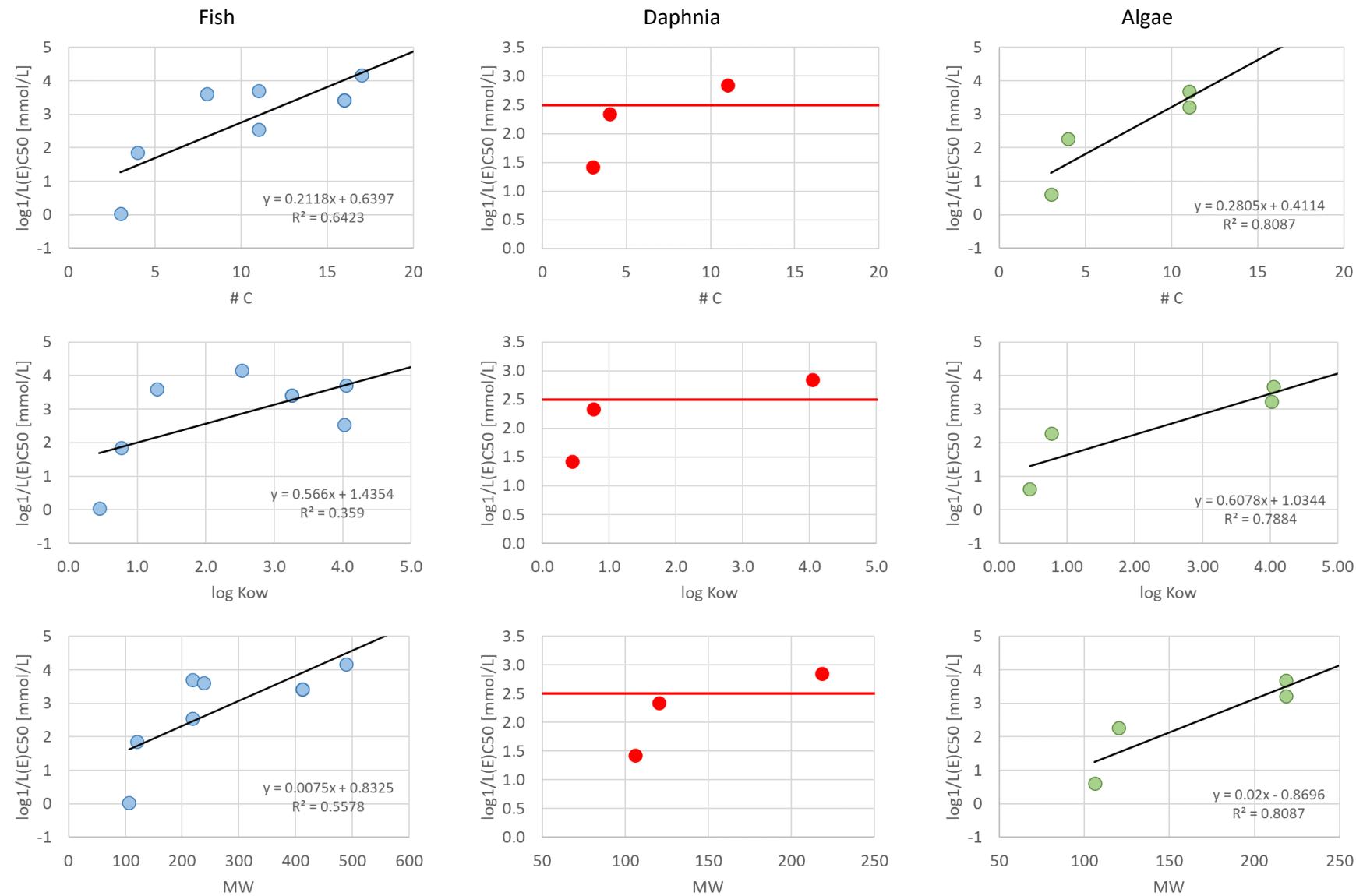


Table S2. Trends in acute aquatic toxicities of mercaptans based on the carbon chain length (# C) as a proxy for molecular size and hydrophobicity, log Kow and MW.

