



Experiences of Predicting Acute Oral Toxicity in Industry

Richard Marchese Robinson, Surya Hari Lal, Sarah Whalley

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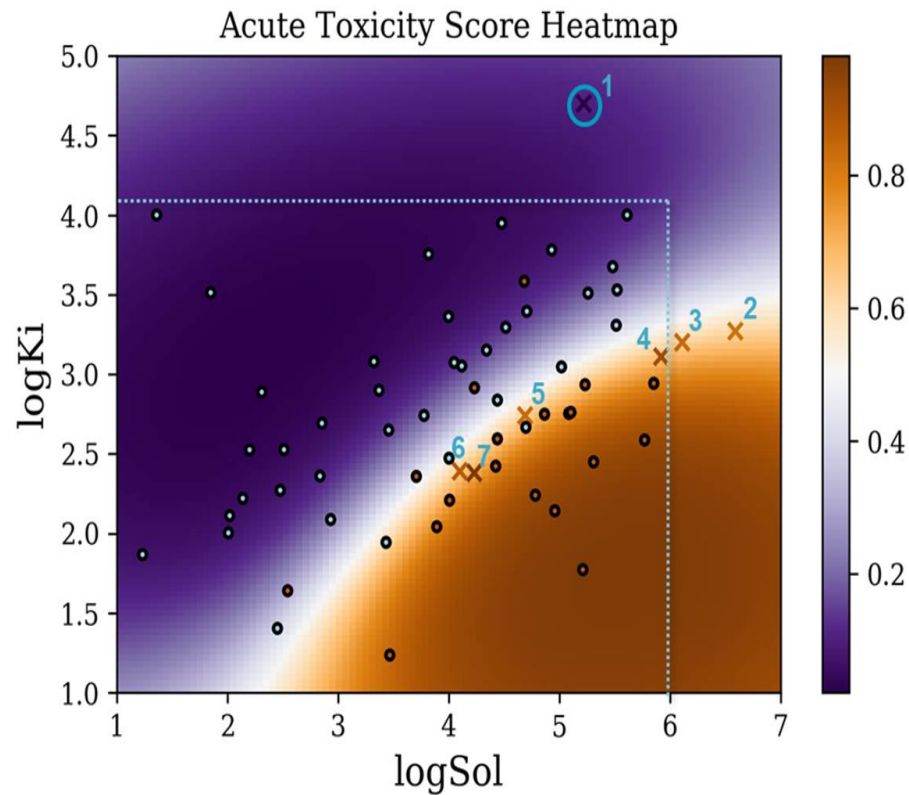
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Overview

- We want to predict the rodent oral acute toxicity – LD₅₀ or category based upon LD₅₀
- Ideally, make predictions directly from molecular structure using (Q)SARs
- Models could support screening, prioritisation, molecular design in early stage research
- Could they also support regulatory submissions, e.g., EPA 2035 target?
- A number of local models have been built and successfully deployed – but rely upon limited diversity in SAR and a known mode of toxicological action
- We are evaluating global models provided by external vendors and Open Source software, as well as exploring possibilities for building an in-house model

Examples

- Local model



- Leadscope predictions of GHS categories

