




Panel Discussion

- **Challenges and opportunities in QSAR today**
 - What do we need to do to make (Q)SAR more widely accepted as an alternative to experimentation?
 - What are the most significant remaining challenges for (Q)SAR modellers and how should we address them?
 - Where are the new opportunities for *(people entering)* the (Q)SAR modelling field?
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Thank you

Toxicology Session (chair: Thierry Hanser, Lhasa Limited)

Improving predictions of Ames mutagenicity by correcting unbalanced training data

Jonathan Vessey, Lhasa Limited

Use of Read-Across in Filling Data Gap for Assessments

Nora Aptula, Unilever

Poster Flash presentations

Coffee Break / Posters

Identification of novel anti-convulsant drugs using a larval zebrafish model

Simon Hand, University of Sheffield

Towards an MIE atlas – Tools for toxicity prediction

Tim Allen, University of Cambridge

Metabolism Session (chair: Carol Marchant, Lhasa Limited)

Combining an expert system with machine learning to rank metabolites

Edward Rosser, Lhasa Limited

Drug Metabolism Prediction: Experiment and/or Computation?

Johannes Kirchmair, University of Hamburg

Coffee Break / Poster

Using QSAR for metabolic network completion and metabolic engineering

Jean-Loup Faulon, Manchester Institute of Biotechnology

