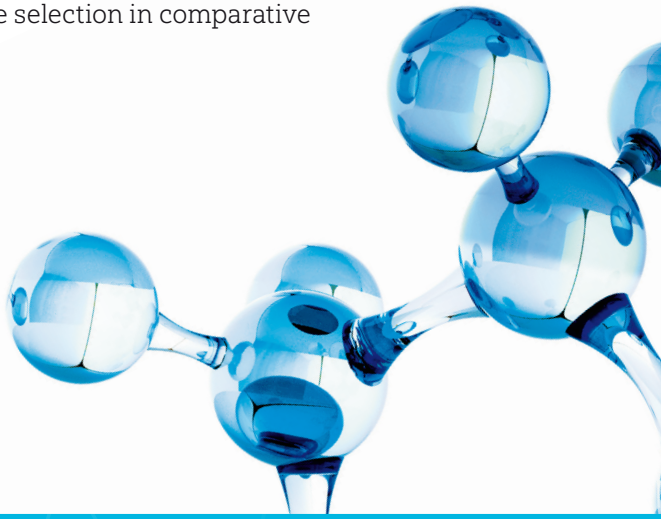
QSAR MODELLING

Predicting toxicity, identifying suitable analogues for read-across, and selecting lead candidates through combined use of public and commercial structure activity modelling tools

ToxMinds has substantial experience in applying QSAR modelling tools to support the safety evaluation and risk assessment of chemicals, food-contact materials, cosmetic ingredients or impurities present in pharmaceuticals. We routinely identify analogue substances and utilise a range of public and proprietary QSAR tools including Derek Nexus, Sarah Nexus and Meteor Nexus from Lhasa Ltd for structure activity and metabolism predictions.

Our **services** include:

- QSAR-based (eco)toxicological hazard profiling and/or metabolism prediction
- Quantitative prediction of physico-chemical and ecotoxicological properties
- Identification of analogues for read-across purposes
- SAR-based chemical and biological similarity assessments
- ECHA guideline-compliant read-across justification for (eco)toxicology endpoints and analogue-based derivation of safe exposure levels
- ICH guideline-compliant mutagenicity assessment of manufacturing impurities, extractables and leachables
- Identification of low toxicity molecules and lead candidate selection in comparative toxicity screens



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ToxMinds
THINKING AHEAD IN TOXICOLOGY