Toxicity Database, QSAR and Read-Across

TOX NAVIGATION

Software for toxicology
Software for cheminformatics
Support and consultancy
Training

sales and support in the UK and Ireland for software from MN-AM

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MN-AM

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Toxicity Database, QSAR and Read-Across

TRAINING COURSE

Understanding QSARs and read-across and their applications in regulatory toxicology

London, 23-25 June 2020

Understanding QSARs and read-across and their applications in regulatory toxicology

With regulators encouraging the reduction of *in vivo* tests according to the principles of the 3Rs this 3 days course will provide an understanding of methods for *in silico* toxicology with an emphasis on appropriate use in regulatory toxicology.

23-25 June 2020

Program

Day 1: Understanding and using QSARs
Day 2: Understanding and applying read-across
Day 3: Hands-on (optional)

London, Interact, 138 Southwark Bridge Road, SE1 0DG

Day 1 + Day 2 £ 800 + VAT	3 Days £ 1,200 + VAT

Who should attend

- √ Scientists involved in chemical risk assessment and product development:
- √ toxicologists
- √ eco-toxicologists
- √ chemists
- √ cheminformaticians
- √ regulatory scientists
- √ risk assessors

Tutors

Prof Mark Cronin
Dr Judith Madden
Dr Elena Fioravanzo

Book your place
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Objectives of the course

- √ Review the current scientific basis and application of read-across and QSAR in toxicology
- √ Interpret the meaning of in silico predictions
- √ Describe the methods that will increase the probability of acceptance of predictions for regulatory use
- √ Use hands-on activities on selected case studies to put theory into practice.

Understanding and using QSARs

QSAR for the prediction of toxicity will be illustrated, focussing on:

- √ The description of freely available and commercial QSAR software for regulatory toxicology.
- √ The selection of QSAR models best suited for regulatory toxicology (OECD principles).
- √ The correct interpretation of predictions and description of the associated uncertainty.
- √ Combination of predictions to reduce uncertainty.
- √ Checking the applicability domain of models and analysis of nearest neighbours.
- √ Increasing the successful use of predicted values in regulatory toxi-

Understanding and applying read-across

The application of read-across for toxicity prediction will be described, focussing on:

- √ The read-across concept and its application using different methods and approaches.
- √ How to find suitable analogues.
- √ The creation and justification of a read-across hypothesis evaluating similarities and differences in chemical structures.
- √ The role of New Approach Methodology (NAM) data in supporting a read-across.
- √ The definition and evaluation of uncertainties for read-across.

Hands-on

- √ QSAR software for regulatory tocicology: **ToxTree, ToxGPS, ACD/Name, ACD/Percepta, ChemSpider, OChem**
- √ Finding data for source and target: **COSMOS DB, OECD Toolbox**
- √ Software to Support Read-Across: **OECD Toolbox and ToxGPS**