

Sunday 9th May 2004 Training Course “Building Better QSARs” 9.30am – 4.30pm

The Training Course is being held at Liverpool John Moores University. More details are available on the Workshop Web-Site. Please note that the Training Course is not included in the Workshop registration. The Training Course is free to students, and a nominal fee is payable by academics and non-academics.

Sunday 9th May 2004

Opening Session

Chairs: John Dearden and Mark Cronin

18:00-18:15 Opening of QSAR2004, Chairman's Introduction

18:15-19:00 Plenary talk by Gilman Veith
Benchmarking Progress in QSAR Research

19:00 Reception

Monday 10th May 2004

Session 1 9:00-10:35

Knowledge Discovery and Data Mining. This session is sponsored by KDNNet.org.

Chairs: Dan Neagu and Alex Tropsha

9:00-9:35 Plenary: Christoph Helma
Data Mining and Knowledge Discovery in Predictive Toxicology

9:35-9:55 Alka Kurup
CQSAR database and its utility

9:55-10:15 Marian Craciun
Applications of Artificial Intelligence Techniques in Predictive Toxicology: an Overview

10:15-10:35 Uko Maran
Large Scale Molecular Design and Engineering in Grid

10:35-10:55 Joanna Jaworska
Chemical similarity and grouping: is SAR different from QSAR?

Coffee Break 10:55-11:25

Session 2 11:25-12:40

Toxicogenomics / Molecular Mechanisms

Chairs: Subash Basak and Terry Schultz

11:25-12:00 Plenary: Bruno Sobrol

Data and Tool Interoperation in Life Sciences - The ToolBus Federation
12:00-12:20 Terry Schultz
Structure-Activity Relationships for PAH Induced Apoptosis
12:20-12:40 Subhash Basak
Prediction of toxicity of chemicals using chemodescriptors and biodescriptors

12:40-14:00 Lunch

Session 3 14:00-17:20

Predicting Environmental Toxicity

Chairs: Gerrit Schüüuurmann and Gil Veith

14:00-14:20 Jacques Chretien
Advances in SAR and QSAR modeling of ecotoxicity
14:20-14:40 Iglia Lessigiarska
QSAR investigation of a large data set for fish, algae and Daphnia toxicity
14:40-15:00 Klaus Kaiser
TerraQSAR programs for quantitative property and effect computations: PNN-based software for E2-RBA, FHM, logP, and RMIV estimation
15:00-15:20 Pat Schmieder
Integrating Toxicity Pathway-Specific In Vitro Testing with Advanced Chemical Selection Strategies for Environmental QSAR Development
15:20-15:40 Hristo Aladjov
Strategic Chemical Selection to Optimize QSAR Design for Large Inventories
15:40-16:00 Markus Lill
In silico prediction of receptor-mediated toxic phenomena
16:00-16:20 James Devillers
Prediction of Mammalian Toxicity of Pesticides from QSTR modelling

16:20-17:20 Coffee and Poster Session 1

Tuesday 11th May 2004

Session 4 9:00-10:35

Modelling Environmental Fate

Chairs: Alistair Boxall and Roger Breton

9:00-9:35 Plenary: Michael McLachan
Are Partitioning Properties Important in Determining Human Exposure?
9:35-9:55 Eric Clarke
The Application of Abraham Solvation Descriptors to the Prediction of Soil Sorption Parameters
9:55-10:15 William Doucette
Estimating the uptake of organic chemical by plants
10:15-10:35 Chris Sinclair
Predictive techniques, their use in the environmental risk assessment of pesticide transformation products

Coffee Break 10:35-11:05

Session 5 11:05-12:55

Regulatory Use of QSAR. This session is sponsored by CEFIC Long-Range Research Initiative.

Chairs: John Walker and Mike Comber

11:05-11:40 Plenary: Kees van Leeuwen

The Prospects for Using (Q)SARs in a Changing Political Environment – High Expectations and a Key Role for the Commission's Joint Research Centre

11:40-12:15 Plenary: Joanna Jaworska

Review of Methods to assess applicability domain

12:15-12:35 Jay Tunkel

Practical Considerations on the Use of Predictive Models for Regulatory Purposes

12:35-12:55 Robert Boethling

Using Biowin, Bayes and Batteries to Predict Ready Biodegradability

Lunch 12:55-14:00

Session 6 14:00-17:40

Validation of QSARs

Chairs: Kees van Leeuwen and Joanna Jaworska

14:00-14:35 Plenary: Andrew Worth

The role of the European Centre for the Validation of Alternative Methods (ECVAM) in the validation of (Q)SARs

14:35-15:10 Plenary: Etje Hulzebos

Validity and Validation of Expert (Q)SAR systems

15:10-15:30 Nina Jeliaskova

A review of methods for accuracy estimation and model selection

Coffee Break 15:30-16:00

16:00-16:20 Alexander Tropsha

Integrated Workflow for Predictive QSAR Modeling and Virtual Screening

16:20-16:40 Tatiana Netzeva

On the Purpose of Validation: Valid versus Validated QSARs

16:40-17:00 Chandrika Moudgal

Assessment of the Rat Chronic Lowest Observed Adverse Effect Level (LOAEL) Model in TOPKAT

17:00-17:20 Robert Clark

Trials and Tribulations of Building a Robust pKa Predictor

17:20-17:40 Paola Gramatica

Validated prediction of rate constants for the tropospheric degradation of heterogeneous chemicals by hydroxyl radical.

Wednesday 12th May 2004

Session 7 9:00-12:40

QSAR Methods: Statistical Analysis and Physicochemical Properties

Chairs: John Dearden and Ovanes Mekenyan

9:00-9:35 Plenary: Lowell Hall

Topological Approaches to QSAR of Properties of Interest for Human Health

9:35-10:10 Plenary: Gerrit Schüürmann

Quantum Chemical Characterisation of the Molecular Bioreactivity of Compounds

10:10-10:30 Assia Kovatcheva

The development of novel chirality sensitive descriptors and their application in QSAR modelling

Coffee Break 10:30-11:00

11:00-11:20 Lennart Eriksson

Three-block bi-focal PLS (3BIF-PLS) and its application in QSAR

11:20-11:40 Marjana Novic

Variables Selection with Genetic Algorithm in Non-linear Modelling of Structure - Affinity Correlation of Estrogen Receptor Binding

11:40-12:00 Taravat Ghafourian

Linear and Non-linear QSAR Methods in Prediction of Oestrogen Receptor Binding Affinities

12:00-12:20 Marjan Vracko

Self Organizing Maps (SOM) and Counter Propagation Neural Networks (CP NN) in Structure-Property Relationship Studies

12:20-12:40 Philip Howard

Estimating Octanol-Air Partition Coefficients with Octanol-Water Partition Coefficients and Henry's Law Constants

12:40-12:50 Presentation for QSAR2006

Lunch 12:50-14:00

Session 8 14:00-16:15

Prediction of Human Health Endpoints. This session is sponsored by Unilever's Safety and Environmental Assurance Centre (SEAC).

Chairs: Aldo Benigni and Andrew Worth

14:00-14:35 Plenary: Edwin Matthews

Risk Assessment of Health Effects of Xenobiotics in Humans

14:35-14:55 Yin-tak Woo

Mechanistic consideration in SAR/QSAR studies and development of a mechanism-based expert system for predicting carcinogenic potential of chemicals. Yin-tak Woo, U.S. Environmental Protection Agency, Washington, DC

14:55-15:15 Sabcho Dimitrov

Skin sensitization: modeling based on skin metabolism simulation and formation of protein conjugates

15:15-15:35 Michael Abraham

Effects of Volatile Organic Compounds on Humans

15:35-15:55 Kannan Krishnan

Quantitative structure-pharmacokinetic relationship modeling for inhaled volatile organic chemicals in humans

15:55-16:15 John Walker

Can QSARs identify emerging chemical contaminants that will threaten human health and the environment?

Coffee and Poster Session 16:15-17:15

**17:15-18:15 Workshop and Round-Table Discussion
on the Role of QSAR for Permeability Assessment**

**19:00 Banquet at the Liverpool Athenaeum Club – Formal
Dress Required**

Thursday 13th May 2004

Session 9 9:00-12:25

In silico ADMET

Chairs: Ed Matthews and Mark Cronin

9:00-9:35 Plenary: Ulf Norinder

In silico modelling of ADMET - a review of recent work and new applications

9:35-9:55 Na'ngono Manga

Structure-Based Methods for the Prediction of the Dominant P450 Enzyme in Human Drug Biotransformation; CYP3A, 2C9, 2D6

9:55-10:15 Ovanes Mekenyan

TIMES: Simulating toxic behaviour of chemicals resulting from their metabolic activation

10:15-10:35 Adam Ibrahim

The prediction of drug tissue-distribution in humans and rats

Coffee Break 10:35-11:05

11:05-11:25 Oleg Raevsky

Analysis of water solubility of volatile, liquid and solid chemicals and drugs on the basis of similarity and physicochemical descriptors.

11:25-11:45 Michael Bolger

A method for estimation of the composite solubility vs. pH profile

11:45-12:05 John S. Delaney

ESOL: Estimating Aqueous Solubility Directly from Molecular Structure

12:05-12:25 Aynur O. Aptula

Prediction of HERG K⁺ Blocking Potency: Application of structural knowledge

Close of Meeting: 12.25- 12.30

Disclaimer: This is a draft program and subject to change and alteration. The organisers will make every effort to keep alterations to a minimum.