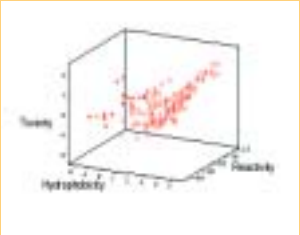
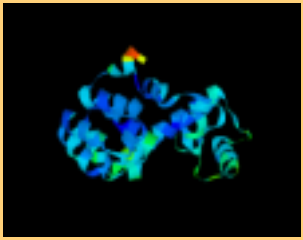
Predictive Toxicology

In Silico Modelling and Expert Systems

Thursday 27 February 2003





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PROGRAMME

09.00 Coffee and Registration

10.00 Chairmen's Introduction
Han van de Waterbeemd & Mark Cronin

Section 1 QSAR

10.10 **Has QSAR helped to predict toxic endpoints?**
Mark Cronin, Liverpool John Moores University, UK

10.45 **Quality and validation of QSARs for toxicity**
Joanna Jaworska, Procter and Gamble, Belgium

Section 2 Expert systems

11.20 **Using logic induction for toxicity prediction**
Ross King, University of Aberystwyth, UK

11.55 **Consensus model building**
Bobby Glen, Cambridge University, UK

12.30 Lunch, posters and exhibition open

Section 3 Learning from experiments

14.00 **Integrated structure-based toxicity prediction**
John Ashby, Syngenta Central Toxicology Laboratory, UK

14.35 **Importance of modelling metabolism in the prediction of toxicity**
Kevin Park and Dominic Williams, Liverpool University, UK

15.10 Tea

Section 4 Early toxicity studies in drug discovery

15.40 **High-throughput toxicity**
Mark Smith, GlaxoSmithKline, UK

16.15 **Industry experience with predictive toxicity tools**
Nigel Greene, Pfizer, UK

16.50 Closing remarks

17.00 Close

For the opportunity to participate in the poster display, please send a brief abstract of your poster by email to Alex Jennings at the SCI Conference Office **(alex.jennings@soci.org)**.

Predictive Toxicology - *in Silico* Modelling and Expert Systems

There is considerable impetus to reduce animal toxicity testing by the use of computer-aided techniques. This one-day meeting will examine the latest technology in the prediction of toxicity directly from chemical structure. The meeting will also refer particularly to human health effects.

The programme brings together a variety of speakers from industry (including pharmaceuticals and personal products) and academia. The main themes of the meeting will address topical issues in the use, development and validation of quantitative structure-activity relationships (QSAR) in predicting toxicity; the use of expert systems; and how these techniques are applied to screen and develop novel non-toxic molecules.

The meeting is highly relevant to researchers (both academic and industrial), technical support personnel, medics and regulators who are involved in the assessment of toxicity of pharmaceuticals, nutraceuticals, personal products and agrochemicals.

Scientific Organising Committee

Mark Cronin, Liverpool John Moores University

Han van de Waterbeemd, Pfizer

REGISTRATION FORM

Predictive Toxicology - *in Silico* Modelling and Expert Systems

27 February 2003,
SCI,14/15 Belgrave Square, London, UK

FEE: Includes refreshments as stated in the programme.

Non-members ..... £130 ❑ SCI members ..... £90 ❑

Non-member students .. £30 ❑ SCI students ..... £20 ❑

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