

Matt presented this poster at ISSX in October 2011.

Abstract:

Whether compounds are intended as drugs, cosmetics, agrochemicals or for other industrial application, it is essential to understand their potential to cause toxic effects. This can guide the prioritisation of compounds for further research or consideration of the most appropriate downstream experiments to confirm their safety. The ability to predict toxicities based on chemical structure alone would allow these factors to be considered prior to synthesis, allowing the safest options to be pursued and saving time and resources wasted on synthesis and testing of unsuitable compounds.

We will describe the automatic generation and validation of Quantitative Structure Activity Relationship (QSAR) models of key toxicity endpoints, based on data made available by the US Environmental Protection Agency (EPA) as part of its Toxicity Estimation Software Tool (T.E.S.T.) [1].

[1] [US Environmental Protection Agency](#)

[2] [Optibrium](#)

[3] O. Obrezanova et al. (2008) J. Comp.-Aided Mol. Desi. ,22, pp. 431-440

[4] M.D. Segall et al. (2009) Chem. & Biodiv. , 6 , pp. 2144-2151

[5] [Organisation for Economic Cooperation and Development](#)

A copy of this poster as available as a [PDF](#) .

Psychological research has demonstrated that reproducible biases affecting human decision-making, known as cognitive biases, threaten objectivity and balance in individual and team decision-making. Drug discovery leaders receive much conflicting advice on possible ways to improve productivity and restore the rate of successful drug launches; however with

Poster: Automatic Generation and Validation of QSAR Toxicity Models

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help to overcome these psychological barriers, better decision-making can enhance R&D performance [1].

We will discuss four of the common biases that have serious implications for decision-making in drug discovery (summarised below). We will suggest approaches for overcoming these, such as strategies adapted from evidence-based medicine and computational tools that seek to guide the decision-making process, encouraging objective consideration of all of the available information and explicit consideration of the impact of uncertainty in drug discovery.