Quantitative Structure-Based Modeling Applied to Characterization and Prediction of Chemical Toxicity[*1], [*2]

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„...**CompuDrug** Ltd, Budapest 45 Brown S. J. Raja A. A. Lewis D. F. V. Altern. Lab. Anim. 22 1994 482 500 46 **MetabolExpert**, 1989, **CompuDrug** Ltd, Budapest 47 Klopman G. Dimayuga M. Talafous J. J. Chem. Inf. Comput. Sci. 34 1994 1320 1325 48 Talafous..."

Abstract

Quantitative modeling methods, relating aspects of chemical structure to biological activity, have long been applied to the prediction and characterization of chemical toxicity. The early linear free-energy approaches of Hansch and Free Wilson provided a fundamental scientific framework for the quantitative correlation of chemical structure with biological activity and spurred many developments in the field of quantitative structure–activity relationships (QSARs). In addition to modeling of chemical toxicity, these methods have been extensively applied to modeling of medicinal properties of chemicals. However, there are important differences in the nature and objectives of these two applications, which have led to the evolution of different modeling approaches (namely, the need for treating sets of noncongeneric toxic compounds). In this paper are discussed those approaches to chemical toxicity that have taken a more "personalized" configuration and have undergone implementation into software programs able to perform the various steps of the assessment of the hazard posed by the chemicals. These models focus both on a variety of toxicological endpoints and on key elements of toxicity mechanisms, such as metabolism.

Methods
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