Computer systems for the prediction of toxicity: an update

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„…QSAR Prediction DEREK MultiCASE TOPKAT HazardExpert TOXSYS COMPACT OncoLogic 1 Introduction...systems such as DEREK, OncoLogic and HazardExpert use rules about generalized relationships...be added or edited by the user. HazardExpert, produced by CompuDrug..."

Abstract

In order to survive in the current economic climate, the pharmaceutical, agrochemical and personal product companies are required to produce large numbers of new, effective products whilst significantly reducing development time and costs. With the advent of combinatorial chemistry and high-throughput screening (HTS), the numbers of new candidate structures coming out of the discovery cycle has increased significantly. This has created a demand for faster screening of the toxicological properties of these candidates. Not surprisingly, computer methods for toxicity prediction offer an attractive solution to this problem because of their ability to screen large numbers of structures even before synthesis has occurred. In this paper the major, commercially available computer software systems for toxicity prediction are discussed together with their main strengths and limitations.

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