Computational predictive programs (expert systems) in toxicology

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„...certain reactive 6roups. For instance, Ashby and Paton (1993) hsted many toxic residues responsi- ble ir adverse activity. **CompuDrug** starkd Eom thi approach and encoded into its ES, caHed HazardExpert the behaviour of selected residues based on a report by..."

Abstract

The increasing number of pollutants in the environment raises the problem of the toxicological risk evaluation of these chemicals. Several so called expert systems (ES) have been claimed to be able to predict toxicity of certain chemical structures. Different approaches are currently used for these ES, based on explicit rules derived from the knowledge of human experts that compiled lists of toxic moieties — for instance in the case of programs called HazardExpert and DEREK — or relying on statistical approaches, as in the CASE and TOPKAT programs. Here we describe and compare these and other intelligent computer programs because of their utility in obtaining at least a first rough indication of the potential toxic activity of chemicals.

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Abbreviations: AI, artificial intelligence; CASE, Computer Automated Structure Evaluation (a research program); COM-PACT, Computer Optimized Molecular Parametric Analysis of Chemical Toxicity (a research program); DEREK, Deductive Estimation of Risk from Existing Knowledge (a commercial program); ES, expert systems; HazardExpert, a commercial program; MULTICASE, the improved version of CASE; NMR, nuclear magnetic resonance; NTP, National Toxicology Program (US); QSAR, quantitative structure-activity relationship; TOPKAT, Toxicity Prediction by Komputer Assisted Technology (a commercial program)

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