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Toxico-Cheminformatics:
Merging biological and chemical information domains in support of toxicity prediction.

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Major trends affecting public toxicity information resources have the potential to significantly alter the future of predictive toxicology. Chemical toxicity screening is undergoing shifts towards greater use of more fundamental information on gene/protein expression patterns and bioactivity profiles, the latter generated with high-throughput screening technologies. In addition, curated, systematically organized, and web-accessible toxicity and biological activity data in association with chemical structures are becoming more widely available. Merging of these biological and chemical informatics domains will fuel the next frontier of advancement for structure-activity relationship (SAR) and activity-activity relationship (AAR) prediction methods and data mining technologies. Biological profiling, in order to be most successful, should optimally employ chemical structure-space considerations and design criteria, essential for accurately assessing the biological and chemical applicability domain of any predictive models. Likewise, building of SAR models within more chemically diverse, yet mechanistically coherent areas of bioassay profile space, offers a means for extending the predictive reach of such technologies. Progress towards the goal of providing effective data linkages to support toxicity prediction models is illustrated by the DSSTox project and collaborations among the NIH Molecular Libraries Initiative, PubChem, Leadscope ToxML, the National Toxicology Program, and the EPA ToxCast initiative.