Two-way clustering method for QSAR modeling of diverse set of chemicals

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Toxicologists use a large number of tests to assess potential toxicity of chemicals to human and ecological health, a thorough analysis of one chemical requiring $2 to 4 million and a few years of time. One important toxicological property of chemicals is mutagenicity. Both drugs and environmental pollutants can be mutagenic. Gene mutilation related diseases have a major impact on human health. Some mutations may lead to increased susceptibility to some forms of heart disease, diabetes, or cancer. Laboratory bioassays used to assess the mutagenic potential of chemicals because the accumulation of mutations is prerequisite to tumor development. Therefore, testing a large number of chemical mutagens, both drug candidates in the discovery pipeline and environmental pollutants, can be expensive in terms of economic resources, testing facilities, and time.

An alternative approach is the use of computational toxicology tolls which use computed properties of the mutagens to predict their mutagenic potential using mathematical models. During the past five decades or so, mathematical chemistry has developed many new molecular descriptors. At the same time the power of computer has progress steadily following Moore's law. Currently we are witnessing an upsurge of research fueled by two important factors: a) Novel applications of mathematics to chemical and biological systems and ii) Availability of software which allows hypothesis driven as well as discovery oriented research within a reasonable time frame. This trend of research has led to numerous useful applications to scientifically, socially, technologically, and economically important areas such as drug

discovery, protection of human as well as ecological health.

The articles by Basak, Majumdar, and Grunwald developed in silico models for the estimation of potential mutagenicity of chemicals from their structure without the input of any other experimental data. Such models can also be used to prioritize laboratory testing based on estimated values.

More information: Subhabrata Majumdar et al. Adapting Interrelated Two-Way Clustering Method for Quantitative Structure-Activity Relationship (QSAR) Modeling of Mutagenicity/Non- Mutagenicity of a Diverse Set of Chemicals, *Current Computer Aided-Drug Design* (2013). DOI: 10.2174/15734099113096660045

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