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Methodology in QSAR

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Quantitative structure-activity relationships (QSARs) are mathematical models that attempt to relate the structure derived feature of a compound to its biological or physicochemical activity. QSAR works on assumption that structurally similar compounds have similar activities. Therefore these models have predictive and diagnostic abilities. They can be used to predict the biological activity (e.g., IC_{50}) or class(e.g., inhibitor versus non inhibitors) of compounds before the actual biological testing. Quantitative structure-activity relationships (QSARs) attempt to correlate chemical structure with activity using statistical approaches. The QSAR models are useful for various purposes including the prediction of activities of untested chemicals. Quantitative structure-activity relationships and other related approaches have attracted broad scientific interest, particularly in the pharmaceutical industry for drug discovery and in toxicology and environmental science for risk assessment. An assortment of new QSAR methods have been developed during the past decade, most of them focused on drug discovery.

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