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Mining public-source databases for structure-activity relationships

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Modeling off-target effects has become a highly important and relevant component of the computational chemistry toolset. The presentation will describe a new contribution that seeks to allow the extraction of 3D-structure-activity relationships from public information starting from a chemical structure. Several public source databases such as PubChem [1] offering structure as well as activity information for a number of targets have been examined for their value in extracting useful structure-activity relationships (SARs). A Topomer search [2] of public-source databases using the structures of a set of 255 marketed drugs [3] as queries yielded sets of shape- and pharmacophore similar hits. SAR-tables were constructed by collecting hits around each query structure and for a particular reported activity. A new method: quantitative series enrichment analysis (QSEA) [4] was applied to these SAR-tables to capture trends and to transform these trends into 3D-QSAR models. Overall more than 400 SAR-tables with Topomer CoMFA models were found by extracting trends from the PubChem and ChemBank [5] database. The resulting models were able to highlight the structural details of certain off-target effects of marketed drugs even in those cases where the traditional structural similarity would conclude that no off-target effect would exist. This demonstrates the usefulness of the approach in modeling off-target effects.

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