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Quantification and visualization of structure-activity-relationships at multiple levels of detail

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The analysis of structure-activity relationships (SARs) plays an important role in medicinal chemistry and drug design [1]. SAR analysis attempts to establish relationships between chemical structure and biological activity of small molecules and is usually carried out for individual series of compounds active against a specific target. However, for the analysis of multiple SAR components that might exist in compound activity classes, systematic approaches are needed [2].

We have developed a framework for the quantification and visualization of SARs at multiple levels of detail. The SAR Index (SARI) provides a function to characterize activity landscapes defined by sets of active molecules in a quantitative manner [3]. Calculated from 2D similarity and compound potency, it distinguishes between three principal types of SARs that are essentially characterized by the way biological activity of small molecules responds to chemical modifications. Initially designed to capture global SAR characteristics, SARI scoring is extended to the analysis of local features within compound subsets including SAR contributions from individual compounds. Numerical analysis is complemented by graphical representations of similarity relationships and potency distributions within sets of active compounds.

Analysis of SAR graphs and global and local SARI scores facilitates the characterization of multiple SAR features both in qualitative and quantitative terms and aids in understanding how local SAR characteristics are related to each other. Furthermore, key compounds can be identified that have strong influence on global SAR features in a given set of active compounds.

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