The Similarity Principle (similar structures = similar activity) is at the heart of medicinal chemistry. A molecular descriptor is emerging as a general tool for the validation and interpretation of the similarity principle. The goal of a similarity search is to pick a novel chemotype fitting a given pharmacophore (that is, fit well the context of its expected extremes).

The average value of the activity dissimilarity score within the context of its expected extremes is a measure of the completeness of the similarity search. The average value of the activity dissimilarity score outside the context of its expected extremes is a measure of its consistency.

Two similarity scoring schemes – the Dice correlation coefficient scores (Σ) and respectively geometric (Ω) and respective geometric (γ) average scores (Ω) – are considered. The similarity score A(m,M) is related to the idea of the Neighborhood Behavior of descriptor space points (m) and (M).

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