INVITED PRESENTATION:
Molecular Diversity: Strategies and Concerns

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Abstract

Automation has produced the opportunity to test hundreds of thousands of compounds in a biological test. The challenge of the computational chemist is to select, from the 10^{180} possible drug-like molecules, those that are most attractive for screening, those that could form the basis of a medicinal chemistry program. Early work focused on selecting diverse compounds, leading to the question of how similar compounds must be in order for them to have similar biological activity. The issue, of course, is how to quantitate the similarity–which molecular descriptors and which similarity calculation provide the best result. More recent work has emphasized the consideration of physical properties to eliminate compounds, with the challenge of finding accurate and comprehensive methods to calculate these properties.