News from the Outer Rim of Chemical Space

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Combinatorial descriptions of large chemical collections offer new roads for early phase drug discovery. Utilizing knowledge about robust reactions with large sets of available reactants spans chemical fragment spaces with tens of billions of small molecules. The readily available compounds such as from Enamine REAL enables one to do fast and cost-effective experimental testing. This frees one the restrictions of physical compound libraries. Due to their sheer size, fragment spaces require a different mind set in cheminformatics. Instead of solving problems for individual molecules or molecule pairs as it is traditionally done, the problem must be understood and solved in its entirety by understanding chemical fragment spaces as a single input entity. This talk will give an overview of techniques addressing the whole gamut of fragment space analyses, from design to search and analytics. For the key problem of searching chemical spaces, we address the full spectrum of searching, i.e. similarity, substructure and pattern matching as well as three-dimensional queries.

Bibliography :

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