New Hierarchical Graph Representation of Pharmacophore Models Extracted from Molecular Dynamics Simulations

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In the past years, the concept and representation of chemical space played a central role in the medicinal chemistry field. [1] With the emergence of graph databases, various network-based representations are daily used to display chemical features and structural information. [2] Recently, a pharmacophore network has been developed to analyze and extract the structure activity relationship of small molecule databases. [3] In a previous work, we observed an important amount of pharmacophore related information that can be extracted from molecular dynamics simulations (MD) of protein and ligand complexes. [4]

The work presented in this presentation aims to display the relationships between these pharmacophore models under a hierarchical graph representation. This single view of an entire MD will help the user to detect the key pharmacophoric features of their model and simplify the overall understanding of the observed binding modes.

Hierarchical graph representation of the pharmacophore models extracted from a molecular dynamics simulation of the Cyclin-dependent Kinase 2 (PDB code: 1ke7).

Bibliography :

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