visGReMLIN: An interactive strategy to visualize common substructures in protein-ligand interaction

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Interactions between proteins and ligands play an important role in biological processes of living systems. The comprehension of protein-ligand molecular recognition is an important step to ligand prediction, target identification and drug design, among others. Currently, we have a visual interactive interface to explore protein-ligand interactions and their conserved substructures for a set of similar proteins, which we named visGReMLIN, that allows to visualize protein-ligand interaction patterns computed by GReMLIN (**GR**aph **M**ining strategy to infer protein-**L**igand **IN**teraction patterns). This tool shows patterns in protein-ligand interaction for two test datasets: (i) CDK2 which comprehends 73 entries from Protein Data Bank (PDB) with identical sequences coupled with different ligands. CDK2 has an important role in cell cycle regulation; (ii) Ricin, 29 PDB entries, which share sequence identity greater than or equal 50% with ricin template 2AAI chain A. Ricin is a notorious protein that acts as a potent toxin. GReMLIN uses a strategy based on frequent subgraph mining, that is able to perceive structural arrangements relevant for protein-ligand interaction. In this abstract, we propose a generic version of visGREMLIN, in a way that it will enable biologists, biochemists and anyone who has interest in protein-ligand interactions to search and visualize patterns in compound structures from their own dataset of interest or from structures directly downloaded from PDB. With the PDB entries in hands, we will execute all steps from GreMLIN strategy to compute protein-ligand interaction patterns. Meanwhile, we give users a job number, to return to our website and explore the results when they are ready, as patterns computation can take some minutes.

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