Constructing Networks of Pharmacologically Relevant Molecular Fragments Based on Target-Proteins

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As the amount of pharmacologically relevant biological and chemical information is constantly growing, more and more emphasis is put on the systematization of these informations into a unified system. Here we report a technique that groups and relates proteins based on the maximum common substructures (MCS) of their ligands. Over 55,000 ligands for 242 of drug target proteins formed the base of the study. The MCSes of all possible combination of the molecules were determined. Various statistical analyses were carried out to compare these characteristic substructures. Furthermore networks of the target proteins were created based on the existence of common MCS between their ligands. The potential application of the gathered informations for drug research will be discussed.

In order to help the interpretation of molecular networks, the molecular viewer software Marvinview were integrated to the biology-oriented network visualizer software Cytoscape.