ChemProt-2.0: visual navigation in a disease chemical biology database

ChemProt-2.0 (http://www.cbs.dtu.dk/services/ChemProt-2.0) is a public available compilation of multiple chemical-protein annotation resources integrated with diseases and clinical outcomes information. The database has been updated to > 1.15 million compounds with 5.32 millions bioactivity measurements for 15 290 proteins. Each protein is linked to quality-scored human protein-protein interactions data based on more than half a million interactions, for studying diseases and biological outcomes (diseases, pathways and GO terms) through protein complexes. In ChemProt-2.0, therapeutic effects as well as adverse drug reactions have been integrated allowing for suggesting proteins associated to clinical outcomes. New chemical structure fingerprints were computed based on the similarity ensemble approach. Protein sequence similarity search was also integrated to evaluate the promiscuity of proteins, which can help in the prediction of off-target effects. Finally, the database was integrated into a visual interface that enables navigation of the pharmacological space for small molecules. Filtering options were included in order to facilitate and to guide dynamic search of specific queries.

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