ChemProt-2.0: visual navigation in a disease chemical biology database - DTU Orbit (25/10/2018)

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.

General information
State: Published
Organisations: Center for Biological Sequence Analysis, Department of Systems Biology
Pages: D464-D469
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Nucleic Acids Research
Volume: 41
Issue number: D1
ISSN (Print): 0305-1048
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 10.84 SJR 9.025 SNIP 3.028
Web of Science (2017): Impact factor 11.561
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 9.28 SJR 7.883 SNIP 2.744
Web of Science (2016): Impact factor 10.162
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 9.48 SJR 7.358 SNIP 2.631
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.74 SJR 6.64 SNIP 2.552
Web of Science (2014): Impact factor 9.112
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 8.46 SJR 6.801 SNIP 2.284
Web of Science (2013): Impact factor 8.808
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Web of Science (2012): Impact factor 8.278
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2