PO2-8-11 Poster session

# The IUPHAR/BPS Guide to PHARMACOLOGY database (GtoPdb) in 2018: new features and updates

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Background: The IUPHAR/BPS Guide to PHARMACOLOGY database (GtoPdb) is an open access, expert-curated, online database of human drug targets and their ligands. It provides succinct overviews, key references and recommended experimental ligands for 2,800 targets and related proteins organised into families. The database includes 9,000 ligand molecules, including approved drugs, investigational small molecules, endogenous and synthetic peptides, and antibodies.
Methods: The development of GtoPdb is overseen by NC-IUPHAR with data selected by its subcommittees and expert curators covering established drug targets as well as those of emerging interest for drug discovery. This update will provide details of recent developments to expand the data content and add new features to GtoPdb.
Results: We present a new visualisation tool to compare ligand affinity across species and explore additional targets that have been tested in the ChEMBL medicinal chemistry dataset. Enhanced search facilities have been added, including a BLAST tool for sequence similarity searching. A major recent effort has seen expansion in the area of immunopharmacology. Relevant targets and ligands have been added and linked to immunological cell types, processes and diseases. All this information has been gathered into a new portal aimed at immunologists wishing to search pharmacological data. The growing importance of 3D protein structures in pharmacology has been exploited in a tool called synPHARM, which was developed to help synthetic biologists find protein sequences that could be modulated using known tool compounds from GtoPdb, and holds useful data on 3D ligand-target binding. We present efforts to enhance interoperability of GtoPdb with other databases, which as an ELIXIR UK node resource, is increasingly important in bioinformatics. We developed web services and an RDF linked-data format providing computational access to the database, which allows other resources to easily subsume our content.
Conclusions: GtoPdb is a useful resource for scientists looking for expert-curated information on drug targets and recommended ligands, and we hope these new features will further enhance its utility, as well as ensure the data are as widely accessible as possible.