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

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Introduction The IUPHAR/BPS Guide to PHARMACOLOGY (GtoPdb) (1), is an open-access, expert-curated, online database of human drug targets and their ligands (2). It provides succinct overviews, key references and recommended experimental ligands for 2,800 targets and related proteins organised into families. The database includes 9,100 ligand molecules, including approved drugs, investigational small molecules, endogenous or synthetic peptides, and antibodies.

Method The development of GtoPdb is overseen by NC-IUPHAR (3) 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 (4) medicinal chemistry dataset. Enhanced search facilities have been added, including a BLAST tool for sequence similarity searching, batch search allowing users to upload a set of target or ligand IDs, downloading of result sets in CSV format, and a pharmacology search tool to allow retrieval of data on ligands known to modulate sets of target protein/gene IDs. A disease list and disease summary pages are now provided, which combine data on curated targets and ligands associated to a particular disease. 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 (5). We now provide RDF files which users can download and view in a linked data browser, thereby allowing queries across the GtoPdb data in conjunction with other open linked data sources.

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.

References

(1) IUPHAR/BPS Guide to PHARMACOLOGY, http://www.guidetopharmacology.org/
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(5) IUPHAR Guide to IMMUNOPHARMACOLOGY, http://www.guidetoimmunopharmacology.org/