The G protein-coupled receptor database, GPCRdb

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G protein-coupled receptors (GPCRs) are the most abundant mediators of both human signalling processes and therapeutic effects. The GPCR database, GPCRdb comprises reference data, online analysis tools and interactive visualisation (www.gpcrdb.org) (1).

New GPCRdb sections that will be presented:

1. Drugs: drug statistics, target mapping and browsing of drugs, targets, indications, clinical progression. Based on our analysis of the new trends for GPCR drugs, targets and indications covering FDA-approved drugs and agents in clinical trials (2).
2. Signal Proteins: facilitates investigation of GPCR-G protein coupling profiles, interfaces and in vitro mutations; and was added as part of a landmark study on GPCR-G protein selectivity (3).
3. Genetic variation: features variation statistics, browsing and an Estimated economic burden caused by genetic variation; and was added as part of a comprehensive report on pharmacogenomics of GPCR drug targets (4).
4. GPCRome-wide homology models: models of unprecedented quality are provided for inactive, intermediate and active states - except for classes C and F that only have inactive templates (1).
5. Ligand database with biological activities and commercial availability for 150,000 GPCR ligands from ChEMBL (1).
6. Crystallisation construct design tool based on all available GPCR structures (5)
7. Sequence signatures tool to elucidate functional determinants in evolutionary and functionally related receptors.
8. Residue contact networks data and tools to elucidate e.g. determinants of specific receptor conformational and activity states.
9. Biased agonist database. Preliminary results will be shared for a forthcoming resource of ligands with a proposed signal pathway-bias annotated from publications and patents.

References

- 1 Pandey-Szekeres, G. et al. GPCRdb in 2018: adding GPCR structure models and ligands. *Nucleic Acids Res*, 2017
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- 3 Flock, T. et al. Selectivity determinants of GPCR-G-protein binding. *Nature*, 2017
- 4 Hauser, A. S. et al. Pharmacogenomics of GPCR Drug Targets. *Cell* 2017
- 5 Munk, C. et al. GPCR crystallisation constructs and conditions - In-depth analysis and public resource. *Manuscript*.