Est. 1993, ~4,000 users/month[1]

GPCRdb.org

The G protein-coupled receptor database GPCRdb[1,2]

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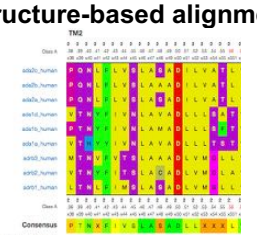
GPCR Cluster

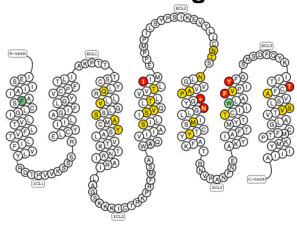
POPULAR

Structure-based alignments[3]



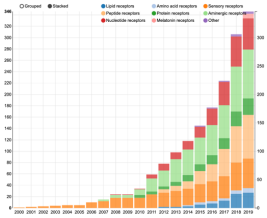
- Helix bulges/constriction gaps
- Residue conservation statistics
- Generic residue numbers[3]

Residue diagrams



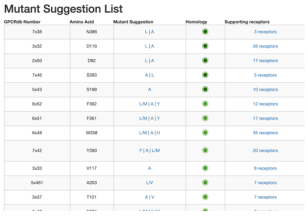
- Custom colouring
- Download for publication

Structures



- Structure browser
- Structure statistics

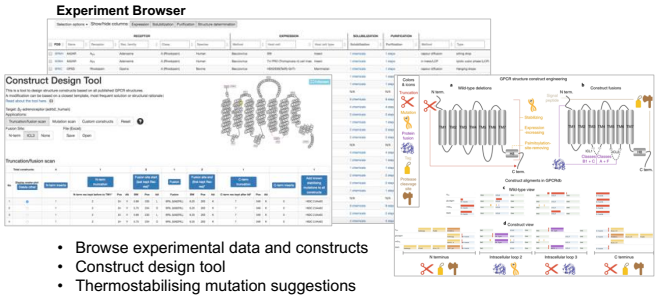
Binding site mutations[4]



- >30.000 mutagenesis data points
- Mutant design tool

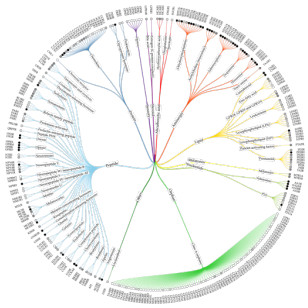
RECENTLY PUBLISHED

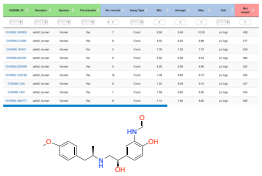
Structure determination resource[5]



- Browse experimental data and constructs
- Construct design tool
- Thermostabilising mutation suggestions

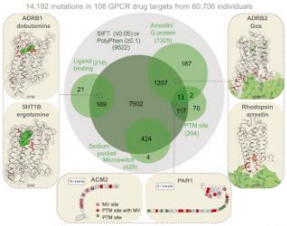
Ligand database[2]





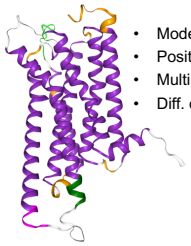
- Commercial availability
- GPCR ligand browser[1]
- GPCR ligand statistics
- >140K ligands from ChEMBL
- >280K experimental data points
- Ligand bioactivity profiles

Genetic variation[6]



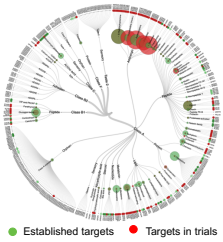
- Genetic variation in 60K humans
- Genetic variation statistics
- Receptor variant browser
- Estimated economic burden
- Post-translational modifications

Homology models[2]



- Models for whole GPCRome
- Position-specific rotamer libraries
- Multiple X-ray templates
- Diff. conformational states

Drugs[7]



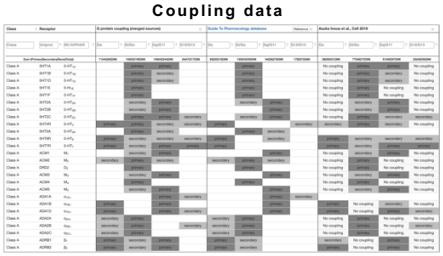
- GPCR drugs browser
- GPCR drugs statistics
- Primary/secondary targets
- Disease indications
- Clinical progression
- NHS prescription data[3]

NEW ONLINE

Signalling protein resource

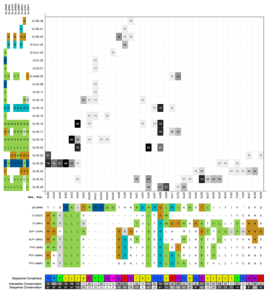
Find these resources under the *Signal Proteins* menu option on gpcrdb.org

Coupling data



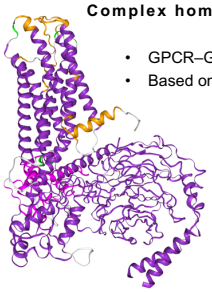
- Coupling data from Inoue et al., **2019**, and Guide to Pharmacology

Interaction matrix



- Complex structures analysing tool
- Align multiple interfaces to whole GPCR class

Complex homology models



- GPCR–G protein models
- Based on newest structures

Arrestin and G protein pages

- Find publication ready diagrams
- Overlay with other data sources (PTM, Variants etc)

IN DEVELOPMENT

Structure comparison resource[8]

- Intra-GPCR residue-residue interactions
- Residue angles and properties
- Compare interactions within or between sets of GPCR structures
- Identify unique and conserved interaction patterns
- Interactive visualization tools linked with a 3D protein viewer

References

1) Munk, C. et al. British Journal of Pharmacology, **2016**, 173(14), 2195-207
2) Pandy-Szekeres, G. et al. Nucleic Acids Res, **2018,** *46 (D1)*, D440-D446.
3) Isberg, V. et al. Trends Pharmacol Sci, **2015** 36(1), 22–31
4) Munk, C. et al. Current Opinion in Pharmacology, **2016**, 30, 51-58.
5) Munk, C. et al. Nat Methods, 2019, 16, 151–162.
6) Hauser, A. S. et al. Cell, 2018, 172 (1-2), 41-54 e19.
7) Hauser, A. S. et al. Nat Rev Drug Discov, 2017, 16 (12), 829-842.
8) Access given upon request

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