GPCRDB: GPCR Data, Diagrams and Tools

www.gpcr.org/7TM

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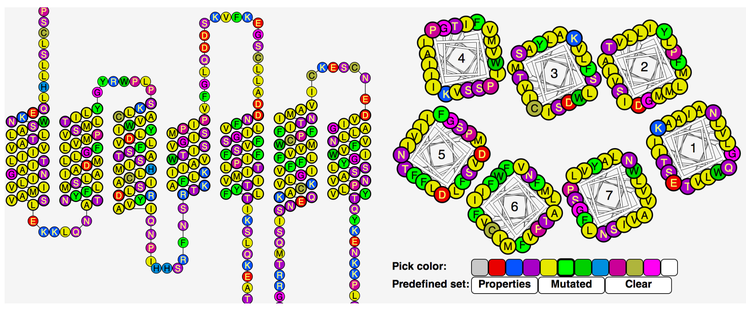
GPCRDB has served the GPCR community for 20 years and has ~1000 users every month. [1]

Receptor Diagrams

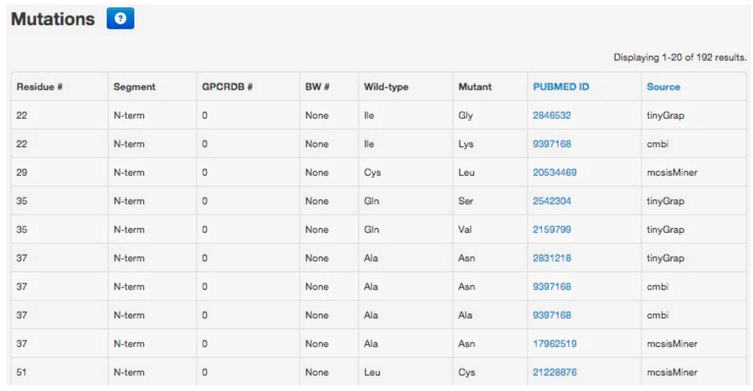
Snake plot -Side view

Helix Box -Top view



- Custom coloring
- Download for publication

Mutagenesis Data



Mutations

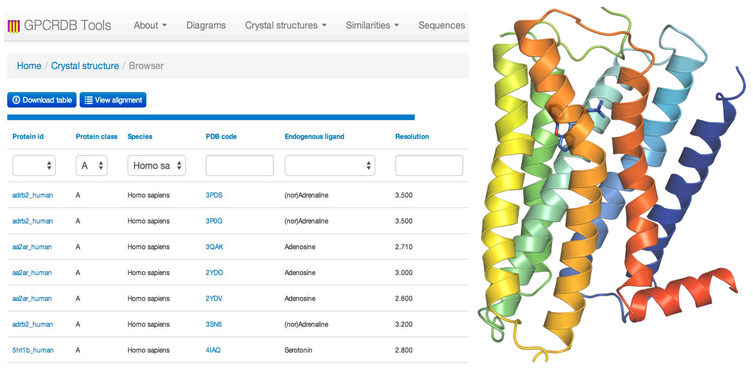
Displaying 1-20 of 192 results.

Residue #	Segment	GPCRDB #	BW #	Wild-type	Mutant	PUBMED ID	Source
22	N-term	0	None	Ile	Gly	2846532	tinyGrap
22	N-term	0	None	Ile	Lys	9397168	cmbi
29	N-term	0	None	Cys	Leu	20534469	mcsisMiner
35	N-term	0	None	Gln	Ser	2542304	tinyGrap
35	N-term	0	None	Gln	Val	2159799	tinyGrap
37	N-term	0	None	Ala	Asn	2831218	tinyGrap
37	N-term	0	None	Ala	Asn	9397168	cmbi
37	N-term	0	None	Ala	Ala	9397168	cmbi
37	N-term	0	None	Ala	Asn	17962519	mcsisMiner
51	N-term	0	None	Leu	Cys	21228876	mcsisMiner

- The largest collection of GPCR mutants

Crystal Structures

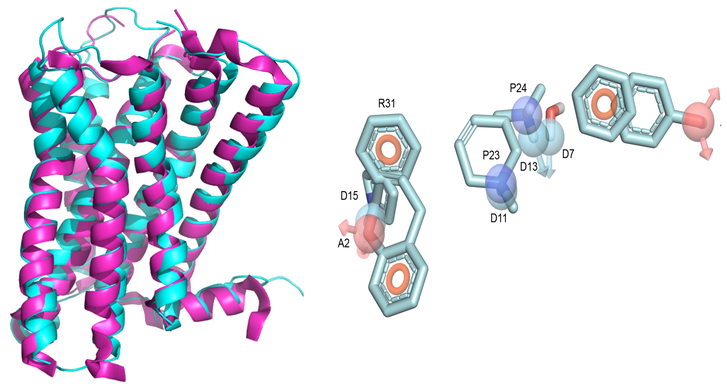
Browser with annotated PDB structures



Modeling

Homology Models -active and inactive

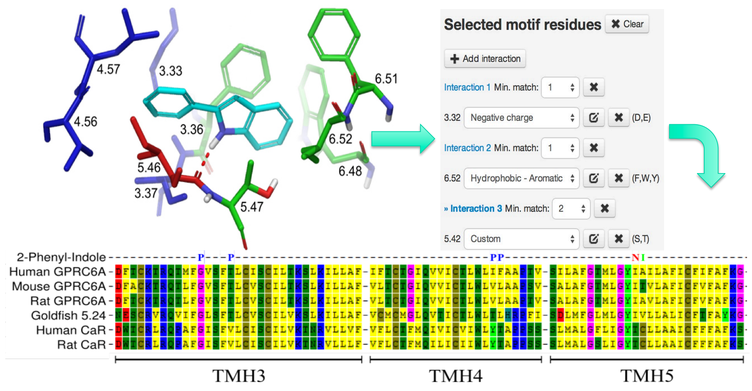
Pharmacophores [2] -crystal structure fragments



- Homology modeling template selection
- GPCR position-specific rotamer libraries
- Links to external modeling servers

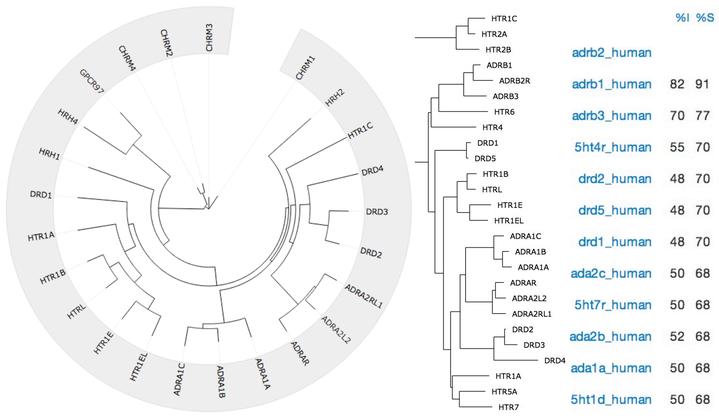
Site / Target Profiling

Sequence Motif Matching



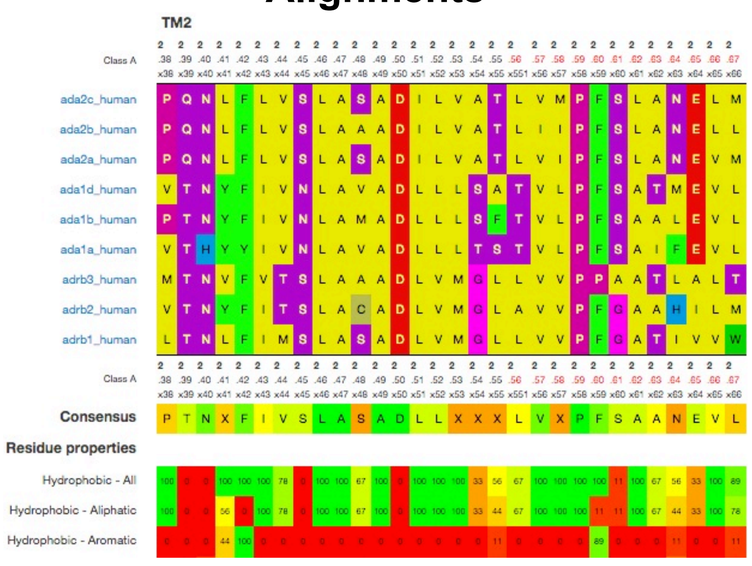
- Match binding sites to predict drug off-targets
- Match conserved structural features
- Match dimerisation sites

Similarities / Relationships



- Phylogenetic trees
- Sequence % similarities / identities
- Sequence similarity matrix

Alignments

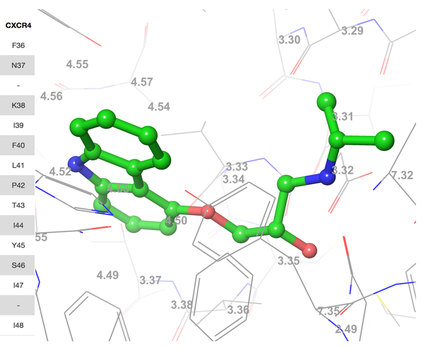


- Crystal structure-based
- Gaps for helix bulges and constrictions
- Residue conservation statistics

Generic Residue Numbers [3]

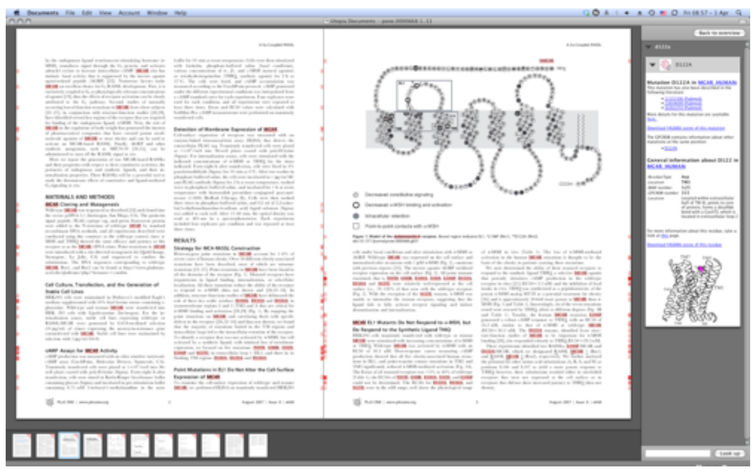
Lookup Tables **Structure Numbering**

GPCRDB	Class Spec.	HTR2B	ADRB1	ADRB2	HRH1	ADORA2A	P2RY12	EDG1	CXCR4
1x30	1.29-30	G51	Q56	V31	P25	M4	K22	N43	F36
1x31	1.30-31	N52	W57	W32	Q26	G5	I23	S44	N37
1x311	1.31	-	-	-	-	-	T24	-	-
1x32	1.31-32	K53	T58	V33	L27	S6	Q25	I45	K38
1x33	1.32-33	L54	A59	V34	M28	S7	V26	K46	I39
1x34	1.33-34	H55	G60	G35	P29	V8	L27	L47	F40
1x35	1.34-35	W56	M61	M36	L30	Y9	F28	T48	L41
1x36	1.35-36	A57	G62	G37	V31	I10	P29	S49	P42
1x37	1.36-37	A58	L63	I38	V32	T11	L30	V50	T43
1x38	1.37-38	L59	L64	V39	V33	V12	L31	V51	I44
1x39	1.38-39	L60	M65	M40	L34	E13	Y32	F52	Y45
1x40	1.39-40	I61	A66	S41	S35	L14	T33	I53	S46
1x41	1.40-41	L62	L67	L42	T36	A15	V34	L54	I47
1x411	1.41	M63	-	-	-	-	-	-	-
1x42	1.42	V64	I68	I43	I37	I16	L35	I55	I48



- Assign generic residue numbers
- Include new structure-based GPCRDB numbers
- Alignments are gapped according to helix bulges and constrictions

PDF Reader



- Enhances articles with information from GPRDB
- Recognizes terms and links to database entries
- Renumbers residues into generic numbering
- Finds similar info in related articles

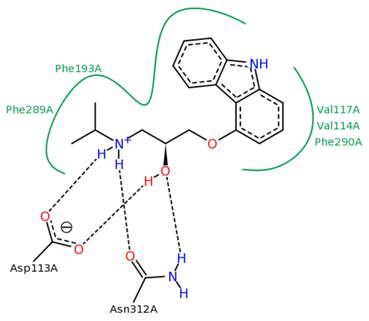
Coming Features

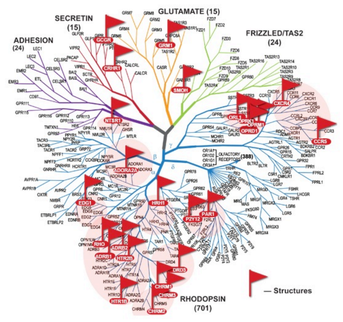
Mutants
- Submit your mutagenesis data
- Mutant design tool

Crystal Structures
- Statistics for crystallized receptors
- Superposition on substructures

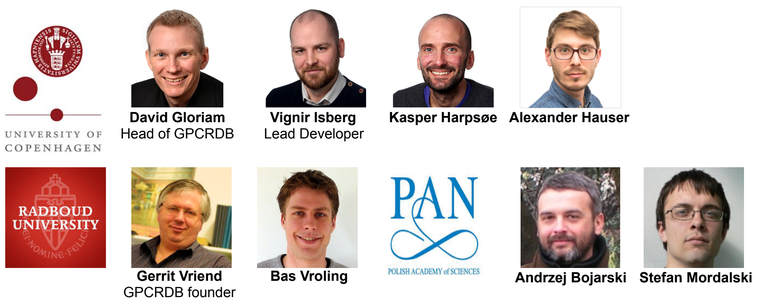
Modeling
- Chimeric templates for homology modeling
- All-against-all off-target prediction heat-map

Ligand Interactions
- From crystal structures
- Interaction plots





Developers



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LUNDBECKFONDEN

References

[1] Isberg V, Vroling B, van der Kant R, Li K, Vriend G, Gloriam DE GPCRDB: an information system for G protein-coupled receptors *Nucleic Acids Res*, 42 (2014) D422-425.

[2] Fidom K, Isberg V, Hauser A, Mordalski S, Lehto T, Bojarski AJ, Gloriam DE A New Crystal Structure Fragment-Based Pharmacophore Method for G Protein-Coupled Receptors, *In Review in Methods*

[3] Isberg V, de Graaf C, Bortolato A, Cherezov V, Katritch V, Marshall F, Mordalski S, Pin JP, Stevens RC, Vriend G, Gloriam DE Generic GPCR Residue Numbers - Aligning Topology Map Minding The Gaps, *Submitted*