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Category:Virtual instruments
Chemical shift perturbation-based de novo design of a generic GPCR-modulating scaffold. G protein-coupled receptors (GPCRs) are increasingly studied as drug targets, making them a wide-spread subfamily of protein targets. However, the low success rate of GPCR-targeting drugs and, even more so, the difficulties encountered in the GPCR-ligand design process make the identification of novel modulators a challenge. In this study, we have developed a GPCR-modulating scaffold by screening chemical shift perturbation data with the aim of taking advantage of the structural information present in these data. Starting from a library of structurally-related scaffolds, we have implemented a combinatorial design procedure which identifies the fragment best fitting the target conformation. The procedure was applied to a library of H-C-C-C-H-H scaffolds, composed of aromatic rings of three different sizes, such that the smallest aromatic ring would be able to occupy a cavity in GPCR ligand-binding sites. The results obtained indicate that the developed scaffolds, derived from a single fragment, are able to modulate GPCR activity with moderate potency (ca. 10 μ M). Their predicted conformation in the scaffold-GPCR complex compared to a ligand is excellent as confirmed by the docking. Furthermore, the scaffold-GPCR complex predicted in this work is compared to the available X-ray structures of ligand-bound complexes highlighting the best matching fragment that in this case is the smallest aromatic ring.

Vestibular coding strategies in the mormyrid fish Gym



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