PP-8

Application of Structural Interaction Fingerprints (SIFt) in Identification and Analysis of GPCR Binding-Sites.

Stefan Mordalski, Tomasz Kościółek, Andrzej J. Bojarski

Department of Medicinal Chemistry, Institute of Pharmacology, Polish Academy of Sciences, Smętna 12, 31-343 Kraków
e-mail: tomek.kosciolek@gmail.com

Since high-throughput computational analyzes has become vital aspect of receptor focused studies, as well as ligand research, tools aiding such tasks are strongly desirable. Yet, targets of unknown binding sites are even more challenging computational objectives. Thus, a mean of numerically analyzing docking data becomes extremely helpful while facing such difficulties.
Structural Interaction Fingerprints (SIFt) describe protein-ligand interactions in a simplified binary manner. SIFts employed in our modelling agenda form a nine-digit pattern for each amino-acid in the receptor. This binary pattern portrays interaction as follows:
any | backbone | side-chain | polar | hydrophobic | H-bond acceptor | H-bond donor | aromatic | charged.
Calculations focused on receptor or ligand population give information concerning an average position of ligand groups in each receptor or particular ligand among alternative receptor models.
Averaged, real number SIFt elegantly depicts overall preferences towards particular interactions, enabling construction of a compact scheme of crucial interactions which then facilitate design of a binding mode hypothesis and description of preferred ligand positions within the active site.
Knowledge about metabotropic glutamate receptors' allosteric binding sites (their structural features in particular) is still incomplete. Transmembrane helices boundaries, binding site composition and architecture have not been definitely determined since only indirect data is available. Processed SIFts data yield information about potential binding site, preferred binding mode and facilitate rapid exclusion of incoherent docking results, and so becoming a tool-of-choice for tackling such demanding targets as metabotropic glutamate receptors.

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