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Refine restraints first-modeling next approach to improve trans-membrane protein modeling

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Gprotein-coupled receptors (GPCRs) are the top ranked drug targets in pharmaceutical industry because of their ability to induce wide variety of cellular responses. Therefore, structural information of such drug targets plays important role in accelerating drug discovery process. Results from GPCR DOCK competitions indicate that homology modeling of GPCRs based on low sequence identity is still a major challenge. To tackle this problem, we developed "refined restraints first-modeling next" approach that extracts unique distance restraints from multiple templates and incorporates them into homology modeling process. This method was applied to improve modeling of human beta 2 adrenergic receptor based on low sequence identity templates of bovine rhodopsin (1u19) and human protease-activated receptor 1 (3vw7). Results showed improvement over standard single-template and multiple-template methods in terms of generating low RMSD models. Our method is easy to implement and can be applied to all alpha helical trans-membrane proteins.

Biography

Rajan Chaudhari is a final year PhD student in the Department of Chemistry & Biochemistry with specialization in Computer-aided Drug Design at University of the Sciences in Philadelphia. He finished his Bachelors in Pharmacy from Pune University in 2007 and Masters in Bioinformatics from University of the Sciences in 2010. His research interests include improving homology modeling of membrane proteins and developing tools for accelerated drug design. He is a member of ACS and ISCB since 2011. He is also actively involved in organizing regional MACC meetings for computational chemists.

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