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In silico structure prediction and validation of homosapienβ-1 adrenergic receptor via threading based homology modelling and its docking studies

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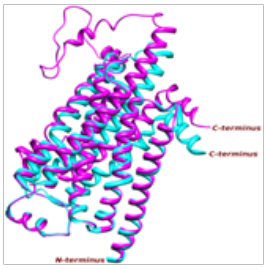

The use of rapidly generated *In silico* protein models provide a basis of structure-based drug design, analysis of protein function, interactions, and rational design of proteins with increased stability or novel functions. In addition, protein modelling is the only way to obtain structural information if experimental techniques fail. Many proteins like membrane embedded receptors are too large for NMR analysis and extremely difficult to be crystallized by X-ray diffraction. Hence homology modelling is the only way to predict the structure and function of these types of proteins. G-Protein coupled receptors which constitute the largest family of membrane receptors and mediate nearly 80% of signal transduction across cellular boundaries are challenging drug target due to their architecture and strong tendency of aggregation. Threading based homology modelling was applied to determine the structure and function of hsGPCRs. hsβADR1 is expressed primarily in cardiac tissue, where it regulates blood pressure and heart rate in responses to stress maintain blood pressure, autonomic control of heart, function myocardial hypertrophy , smooth muscle tone, heart failure or in other cardiovascular diseases, hormonal release and actions regulation of cell contraction and migration,carcinomas, asthma, mental disorder or inhibitory modulation of synaptic neurotransmission, regulation of carbohydrate and lipid metabolism, endocrinological disorder, inflammatory disorder, immunological disorder and sensory perceptions or cell growth and differentiation. This study will provide us clear understanding of GPCRs structure and its interactions with several agonists thus providing the remedial solutions of highly focuses cardiovascular and other diseases caused by malfunctioning of this protein.

Biography

Maria Saeed has completed M.Sc in Biochemistry in 2010 at the age of 22 years from Jinnah University for Women, Karachi, Pakistan. Currently, she is Research Officer at Computational Chemistry unit under the supervision of Dr. Zaheer Ul Haq Qasmi and Co-supervision with Dr. ReazUddin. She has participated in poster presentation in 13th international symposium on Natural Product Chemistry, 22nd-25th November 2012, International Center for Chemical and Biological Sciences (ICCBS) at the University of Karachi. She is working on multiple projects, wherein 2 are in publication process and two are in write up and running process.

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