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Structure-based drug discovery for GPCRs: From receptors to ligands

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Abstract

G-Protein Coupled Receptors (GPCRs) have enormous physiological and biomedical importance, being the primary target of a large number of modern drugs. The availability of structural information on the binding site of the targeted GPCR plays a key role in rationalization, efficiency and cost-effectiveness of the drug discovery process. X-ray crystallography, a traditional source of structural information, is not currently feasible for every GPCR or GPCR-ligand complex. This situation significantly limits the ability of crystallography to impact the drug discovery process for GPCR targets in “real-time” and hence there is an urgent need for other practical alternatives. The goal of our research is the generation of GPCR 3D structures by applying integrated experimental-computational methods followed by their application in structure-based drug discovery. This research is done in collaboration with membrane protein molecular dynamics group lead by Dr. Philip Biggin from University of Oxford, UK and Structural-Biology group for membrane proteins lead by Prof. So Iwata from Imperial College London, UK. The research is supported by Royal Society UK and Evotec Ltd. The experimental validation of this research is provided mainly by Evotec within real drug discovery projects. The results of this research will be exemplified by MCH-1R, Orexin-1 and -2 Receptors, 5HT2c and/or other drug-discovery cases.

Biography

Dr. Alexander Heifetz is a Principal Scientist at Evotec (UK) Ltd**, a** drug discovery services company**.** He provides CADD expert support for drug discovery programs. He obtained his PhD from the Weizmann Institute of Science, Israel, in 2001 under supervision of former Israeli president and Foreign Member of the Royal Society Prof. Ephraim Katzir and Dr. Miriam Eisenstein. Dr. Heifetz has more than 12 years of experience in drug discovery industry (EPIX Pharmaceuticals and Evotec) and was involved in discovery of 3 clinical drug candidates for treatment of anxiety, major depressive disorder, pulmonary hypertension, and Alzheimer’s disease. He has more than 18 patents, patent applications and a wide range of publications in the area of medicinal chemistry and molecular modelling. Recently, he received the Royal Society Industry Award and established collaboration with academic group of Dr. Phillip Biggin from the University of Oxford, for development of methods for GPCR modelling.