Plenary-10

In silico predictions of 3D structures and binding sites for GPCR-ligand complexes

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G Protein Coupled Receptors (GPCRs) play a critical role in cell communications (dopamine, histamine, epinephrine, and serotonin) and in sensing the outside world (vision, smell, taste, and pain). Consequently they are potential targets for a large number of diseases. However multiple GPCRs may be affected by the same ligand (there are 14 human serotonin receptors) leading often to therapeutics with low selectivity and toxic side effects. Development of highly selective ligands has been hampered by a lack of x-ray crystal structures for most GPCRs.

We will first describe the recent progress in developing methods for predicting the 3D Structure of G Protein Coupled Receptors (GPCRs) and the binding sites for various agonists and antagonists then we will discuss the application of these methods to such systems as: CB1 cannabinoid receptor (target for obesity), CCR5 cytokine receptor (target for HIV inhibition), DP Prostaglandin receptors, GLP1 receptor (target for diabetes), TAS2R38 bitter taste receptor (target for GLP1 control in GI track).

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