

Assignment 6

The goal of this assignment is to analyze the 3D crystal structure of 3 G-protein coupled receptors (GPCRs). G-protein-coupled receptors (GPCRs) are the largest and most diverse group of membrane receptors in eukaryotes. These cell surface receptors act like an inbox for messages in the form of light energy, peptides, lipids, sugars, and proteins. Such messages inform cells about the presence or absence of life-sustaining light or nutrients in their environment, or they convey information sent by other cells.

Recent advances in creating and solving protein crystal structures on transmembrane proteins has resulted in the solving of a large number of GPCR structures. In this assignment, we will focus on three structures: 2RH1, the β 2-adrenergic receptor bound to the antagonist carazolol (a beta blocker used to treat heart arrhythmias), 4LD0, the β 2-adrenergic receptor bound to the agonist adrenaline (its natural ligand). We have uploaded modified versions of these two pdb files onto canvas called B2R_Inactive.pdb (carazolol inactivates the receptor) and B2R_Active.pdb (adrenaline activates the receptor). In each of these pdbs, the ligand has been renamed LIG to help you identify it.

Comparison of these two structures will allow us to understand how the protein changes when it is activated by adrenaline.

I have uploaded a template file that will guide you in writing the code for this assignment. For this assignment you **MUST** follow the suggestions in the template.

For many, this will be the most difficult assignment of the semester. It is imperative you start early and get help as early as possible if you need it. **We will not respond to last minute emails for help with this assignment.**