Visualising structural biology data of Class B1 GPCRs in 3D animations

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Class B1 peptide hormone GPCRs have a broad range of regulatory metabolic effects and are therefore important drug targets. Different steps of receptor activation through conformational and compositional changes, which are highly dynamic processes, are necessary to fine-tune downstream signalling. Recent advances in cryo-electron microscopy (cryo-EM) have enabled structure determination of the VPAC receptor family (PAC1 and VPAC receptors), which enhances our understanding of the molecular mechanisms of agonist binding and specificity.

We utilise data from a variety of (structural) biology methods (e.g., cryo-electron microscopy, molecular dynamics simulations, mass spectrometry, receptor pharmacology, etc.) and integrate these data to determine key features for receptor activation and agonist selectivity. To tell engaging stories about these complex biological processes, we load our data into Blender, an open-source 3D computer graphics software, to develop realistic and biologically relevant 3D animations. The illustrative images and movies, based on our experimental data, can tell visual stories about how these molecules work to both inform experts as well as appeal to broader audiences.

Four frames of a 3D animation to visualise molecular dynamics of the receptor in complex with ligand and G protein. The intracellular G protein and extracellular receptor domains are highly dynamic.

Receptor without ligand   Receptor with high affinity ligand   Receptor with high affinity ligand and G protein