

[P13] Screening for small molecule ligands to a peptide binding GPCR

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At present, the members of the G protein-coupled receptor (GPCR) family are one of the main targets of the drugs on the market. For example treatment of pain, allergies, hypertension and asthma are mediated by targeting GPCRs. There is a wide variety of native ligands binding to GPCRs, including small organic molecules, peptides, proteins, lipids and nucleotides. Only few drugs on the market target peptide binding GPCRs, whereas GPCRs naturally binding a small molecule are more frequent drug targets.

The aim of my work is to find small molecule binders to a certain peptide binding GPCRs, among which some would have properties that lead to receptor activation. Small molecule library was virtually screened by a pharmacophore model, based on a weak agonist molecule and the native peptide. Several pharmacophoric point combinations were tested and the best performing set was used for screening. The chemical diversity collection by Institute of Molecular Medicine Finland was used as a source of small molecules for screening. A set of molecules was selected from the results to be tested *in vitro*.