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Finding novel active scaffolds in GPCRs with 3D hydrophobic field-based screening

G protein-coupled receptors (GPCRs) represent an important type of proteins involved in transmembrane signaling heavily studied for the design of novel drugs. This family of receptors has been traditionally complex to crystallize due to their low expression and inherent instability. In this context, ligand-based techniques represent an interesting approach to find novel binders that can be used in drug discovery projects. We show the capabilities of PharmScreen1,2 in reporting novel hit scaffolds for a diverse set of GPCRs and in a real case study.