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Application of Interaction Patterns to Discriminate Ligand Preference to Target/Antitarget Protein.

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SIFts (Structural Interaction Fingerprints) are precise and rapid tool for binding site description. In this research, SIFt describing physical ligand-protein interactions consists of 9-bit fragments providing information with residues and type of interaction (hydrophobic, aromatic, charge, polar, sidechain, backbone). A collection of such fingerprints is then merged into an averaged string showing frequencies of occurrence of each interaction.
In this project, interaction patterns are generated for active (Ki < 10 nM) and inactive (Ki > 1000 nM) ligands docked into our target (5-HT6R) and antitarget (H1R) receptor structure.
Having those interaction profiles, we compare them with SIFt fingerprints produced for our test set. Basing on complementarity between those two we can select compounds with high affinity to our target and low affinity to antitarget.

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