Structure of desloratadine, a second–generation tricyclic antihistamine.

Drug **Repurposing**

We aimed to find off-targets and cases of drug repurposing for desloratadine , a second-generation tricyclic H1 inverse agonist used to treat allergies. Known off-targets include metabolic enzymes (P450 mono-oxygenases CYP3A4 or CYP2D6) and various subtypes of muscarinic acetylcholine receptors. In our approach a selection of experimentally determined receptor structures was used and cavity matching against the complete Protein Data Bank was performed. Notably, in the the final selection of high-ranked hits, known targets such as the previously described metabolic enzymes were found, along with less known off-targets such as serotonin receptors.

A list of new potential candidates that might bind desloratadine or its metabolites has been compiled based on the matching score from Catalophore™ analyses. To validate our approach, molecular docking of desloratadine has been performed.
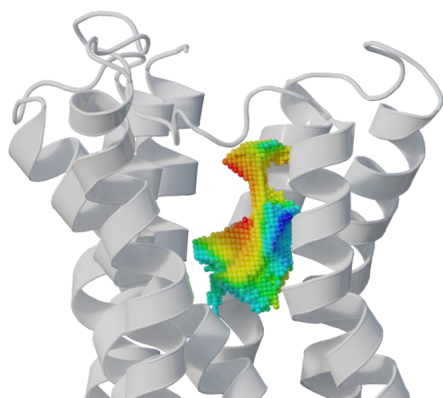
Point cloud depicting binding cavity found in a cavity matching against our dataset of 1 million cavities.
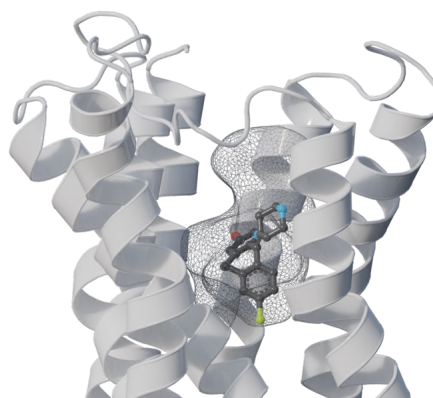
Result from docking with deslo–ratadine. Volume of point cloud is shown as mesh.

Unpublished Results