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Abstract in Englisch

A growing amount of open data in the area of life sciences has prompted the question of how useful these data are for drug discovery. In this work, one of the "hottest" therapeutic targets for pain research, the Transient Receptor Potential Vanilloid type 1 (TRPV1), was used to exploit the data available for it in the public domain with various computational methods. ChEMBLdb data retrieved for TRPV1 were heterogeneous with respect to descriptions of chemical and pharmacological information, which required manual comparison prior to in silico modeling.

From the applied ligand-based methods, pharmacophore modeling and subsequent virtual screening led to the discovery of two new antagonists of TRPV1. Furthermore, the structure-based methods were employed for evaluation of probable binding modes of two known classes of TRPV1 antagonists. Using a sequential workflow, including homology modeling, molecular docking, analysis of protein-ligand interactions and common scaffold clustering, the binding mode hypotheses for these antagonists were developed. Altogether, this work demonstrates the contribution of open data to successfully design novel bioactive molecules, using computational chemistry techniques.

The approach discussed in this thesis would particularly benefit the research on biological targets lacking structural information.