LigTMap: Ligand and Structure-Based Target Identification and Activity Prediction for Small Molecular Compounds

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Motivation: Target prediction is a crucial step in modern drug discovery. However, existing experimental approaches to target prediction are time-consuming and costly. Results: The LigTMap server provides a fully automated workflow to identify targets from 17 target classes with >6000 proteins. It is a hybrid approach, combining ligand similarity search with docking and binding similarity analysis, to predict putative targets. In the validation experiment, LigTMap achieved a top-10 success rate of almost 70%, with an average precision rate of 0.34. The class-specific prediction method improved the success rate further with enhanced precision. In an independent benchmarking test, LigTMap showed good performance compared to the currently best target prediction servers. LigTMap provides straightaway the PDB of a predicted target and the optimal ligand binding mode, which could facilitate structure-based drug design and the repurposing of existing drugs.

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