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Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation

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Computational chemogenomics approaches have emerged as a means to predict modulations of biomolecules by ligands. We implemented a method for the prediction of the macromolecular targets of small molecules combining state-of-the-art approaches that compare physicochemical properties and pharmacophoric features of query molecules with known drugs. Investigating similarity from multiple vantage points has been shown to increase the prediction accuracy in a retrospective evaluation. The method has been applied in multiple projects to "de-orphan" molecules with unknown main target and investigate potential side-effects of drug candidates. In a first application, the method identified a molecular scaffold as a potentially privileged structure of druglike compounds for chemoresistant tumor therapy [1]. In a second project, the tool revealed the potential of up to 5% of known bioactive substances to have unrecognized epigenetic effects by modulating histone deacetylase (HDAC) activity – thereby stressing the importance of probing for epigenetic effects in long-term drug toxicity studies [2].

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