The polypharmacology browser for ligand based target prediction

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Target identification plays an important role in drug discovery. Its applications include the identification of biologically active molecules and promiscuous drugs, drug re-purposing, toxicity prediction, and understanding the molecular mechanism of action of bioactive compounds obtained from phenotypic screening.

Polypharmacology Browser (PPB) presented herein allows the target predictions for any given compound, by comparing the query to other small molecules with annotated targets information available in the ChEMBL database. Browser is unique in way that it performs the molecular comparison and target prediction simultaneously in ten different chemical spaces. We used PPB for the identification of off-targets of “CIS22a”, an inhibitor of the calcium channel TRPV6 recently developed in our group. “CIS22a” was found to be active against Dopamine receptor subtypes D2, D4, Alpha-1A adrenergic receptor (ADRA1A), and Serotonin receptor (5-HT1A).

PPB is freely accessible at www.gdb.unibe.ch.

[1] Keiser MJ, Roth BL, Armbruster BN, Ernsberger P, Irwin JJ, Shoichet BK (2007) Relating protein pharmacology by ligand chemistry. Nat Biotechnol 25(2):197–206.
[2] Awale M, Reymond JL (2017) The polypharmacology browser: a web-based multi-fingerprint target prediction tool using ChEMBL bioactivity data. J. Cheminform 9 **(**11)