# Resource Summary Report

Generated by RRID on Apr 29, 2025

## SuperPred: Drug classification and target prediction

RRID:SCR_002691
Type: Tool

### Proper Citation

SuperPred: Drug classification and target prediction (RRID:SCR_002691)

### Resource Information

**URL:** http://bioinformatics.charite.de/superpred/

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**Description:** Publicly available web-server to predict medical indication areas based on properties and similarity of chemical compounds. The web-server translates a user-defined molecule into a structural fingerprint that is compared to about 6300 drugs, which are enriched by 7300 links to molecular targets of the drugs, derived through text mining followed by manual curation. Links to the affected pathways are provided. The similarity to the medical compounds is expressed by the Tanimoto coefficient that gives the structural similarity of two compounds. A similarity score higher than 0.85 results in correct ATC prediction for 81% of all cases. As the biological effect is well predictable, if the structural similarity is sufficient, the web-server allows prognoses about the medical indication area of novel compounds and to find new leads for known targets. The combination of physicochemical property and similarity searching provides the possibility to detect new biologically active compounds and novel targets for drug-like compounds. SuperPred can be applied for drug repositioning purposes, too. A further intention of SuperPred is to find side effects elicited by drugs caused through off-target hits.

**Abbreviations:** SuperPred

**Resource Type:** database, service resource, data or information resource, production service resource, data analysis service, analysis service resource

**Defining Citation:** PMID:18499712

**Keywords:** drug, drug class, drug target, addiction, anatomical therapeutic chemical, application area, biological activity, chemical, chemical classification, chemical property, classification, compound, molecular target, molecule, nervous system, pathway,

pharmacological property, physicochemical property, prediction, activity spectra, substance, structural similarity, structure, tanimoto coefficient, tanimoto score, target prediction, target-prediction server, therapeutic approach, therapeutic property, drug classification, target prediction, similarity score, target, bio.tools

**Funding:** SFB 449 ;
IRTG Berlin-Boston-Kyoto and Deutsche Krebshilfe. ;
DFG



**Resource Name:** SuperPred: Drug classification and target prediction

**Resource ID:** SCR_002691

**Alternate IDs:** biotools:superpred, nif-0000-00415

**Alternate URLs:** https://bio.tools/superpred

**Record Creation Time:** 20220129T080214+0000

**Record Last Update:** 20250429T054753+0000

## Ratings and Alerts

No rating or validation information has been found for SuperPred: Drug classification and target prediction.

No alerts have been found for SuperPred: Drug classification and target prediction.

## Data and Source Information

**Source:** SciCrunch Registry

## Usage and Citation Metrics

We have not found any literature mentions for this resource.