Resource Summary Report

Generated by dkNET on Aug 30, 2026

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/

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

Description: THIS RESOURCE IS NO LONGER IN SERVICE. Documented on November 24,2025. 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: data access protocol, data or information resource, database, software resource, web service

Defining Citation: PMID:18499712, PMID:24878925

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

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IRTG Berlin-Boston-Kyoto and Deutsche Krebshilfe. ;
DFG

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

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: 20260829T182118+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 found 10 mentions in open access literature.

Listed below are recent publications. The full list is available at dkNET .

Amadea G, et al. (2026) Systems Biology and Atomistic Simulations Reveal Multi-Target Modulation of Alzheimer's Disease and Type 2 Diabetes by Caesalpinia sappan Bioactives. International journal of molecular sciences, 27(12).

Chulrik W, et al. (2026) In Silico Investigation Reveals IL-6 as a Key Target of Asiatic Acid in Osteoporosis: Insights from Network Pharmacology, Molecular Docking, and Molecular Dynamics Simulation. Medical sciences (Basel, Switzerland), 14(1).

Yuan J, et al. (2026) Integration of multi-omics and network toxicology reveals TLR4-mediated nephrotoxicity induced by arecoline. BMC pharmacology & toxicology, 27(1).

Ruankham W, et al. (2026) Unraveling Network Pharmacology-Based Therapeutics of Anthranilate Sulfonamides via Sirtuins/FOXO3a Cascade in Alzheimer's Disease. Journal

of neurochemistry, 170(2), e70377.

Guan X, et al. (2025) Peimine Alleviates DSS-Induced Colitis by Modulating Gut Microbiota and Attenuating Inflammation and Oxidative Stress. International journal of molecular sciences, 26(22).

Li S, et al. (2025) Elucidating the Mechanisms of Chrysanthemum Action on Atopic Dermatitis via Network Pharmacology and Machine Learning. International journal of molecular sciences, 26(23).

Qiu R, et al. (2025) Disclosure of Potential Therapeutic Targets in Plumbagin for Treating Osteosarcoma. Biomedical engineering and computational biology, 16, 11795972251405146.

Zhang T, et al. (2025) Exploring the Regulatory Mechanism of Total Alkaloids from Portulaca oleracea L. in UC Treatment Based on Network Pharmacology. International journal of molecular sciences, 26(14).

Yao L, et al. (2025) Exploring chamazulene as a novel therapeutic agent for breast cancer in silico and in vitro: apoptosis induction, cell cycle regulation, and antimetastatic effects. Frontiers in pharmacology, 16, 1680615.

Wei Z, et al. (2025) Anti-inflammatory effects of Lonicera macranthoides Hand.-Mazz based on Spectrum-effect relationship, network pharmacology and molecular docking technology. Scientific reports, 16(1), 3396.