

Resource Summary Report

Generated by [RRID](#) on Aug 16, 2026

Prediction of Activity Spectra for Substances

RRID:SCR_001971

Type: Tool

Proper Citation

Prediction of Activity Spectra for Substances (RRID:SCR_001971)

Resource Information

URL: <http://genexplain.com/pass>

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Description: PASS is a computer program which predicts the biological activity spectrum for a compound on the basis of its structural formula. The result of prediction is displayed for free. PASS Inet predicts 3678 pharmacological effects, mechanisms of action, mutagenicity, carcinogenicity, teratogenicity and embryotoxicity. PASS gives you hits in the following: - Finding most probable new leads with required activity spectra among the compounds from in-house and commercial data bases. - Revealing new effects and mechanisms of action for the old substances in corporate and private data bases. - Providing the basis for selection of the most prospective compounds for high throughput screening from the set of available samples. - Determining the assays that are more relevant for a particular compound. Sponsors: This work is supported by the Russian Foundation for Basic Research (Grant # 03-07-90282).

Synonyms: PASS

Resource Type: database, data processing software, data or information resource, data analysis software, software application, software resource

Keywords: element, embryotoxicity, activity, carcinogenicity, chemical, compound, mechanism, mutagenicity, pharmacological, spectrum, structural formula, teratogenicity

Availability: Restricted

Resource Name: Prediction of Activity Spectra for Substances

Resource ID: SCR_001971

Alternate IDs: nif-0000-10543

Old URLs: <http://195.178.207.233/PASS/>

Record Creation Time: 20220129T080210+0000

Record Last Update: 20260815T182205+0000

Ratings and Alerts

No rating or validation information has been found for Prediction of Activity Spectra for Substances.

No alerts have been found for Prediction of Activity Spectra for Substances.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 13 mentions in open access literature.

Listed below are recent publications. The full list is available at [RRID](#).

Islam Z, et al. (2026) Phytochemical Characterization and Neuropharmacological Assessment of Combretum indicum Methanolic Extract With Integrated Molecular Docking and Dynamics Simulation for Anxiety and Depression Therapy. Food science & nutrition, 14(5), e71918.

Tyurin VS, et al. (2026) Complexes of Zinc(II) Chloride with N-Vinyl-, N-Allyl- and N-Propargylimidazoles: Structural, Theoretical and Biological Studies. Pharmaceuticals (Basel, Switzerland), 19(6).

Hemdan A, et al. (2026) Assessment and Density Functional Theory of Bioactive Compounds of Curcuma longa L. Root Responsible for Its Cardio-Protective and Anti-Cancer Activities. Pharmaceuticals (Basel, Switzerland), 19(6).

Smirnova I, et al. (2026) Synthesis and Antitumor Potency of 2E,21E-bis-(2-Pyridinylidene)-hollongdione in NCI-60 Panel and Zebrafish Model. International journal of molecular sciences, 27(4).

Ebrahim Thaivalappil IA, et al. (2026) Structure-Based Identification of Allosteric Glucocerebrosidase Stabilizers from Xylia xylocarpa (Roxb.) Taub. for Parkinson's Disease Using LC-MS Profiling and Computational Analysis. Plants (Basel, Switzerland), 15(11).

Vijayan S, et al. (2025) The potential of Abrus precatorius leaves in arthritis alleviation computational approaches through IC-MS analysis. Future science OA, 11(1), 2483131.

Cinato M, et al. (2025) Transcriptome fingerprinting of aberrant fibroblast activation unlocks effective therapeutics to tackle cardiac fibrosis. Science advances, 11(33), eadx0968.

Daneman MR, et al. (2025) Cheminformatic identification of small molecules targeting acute myeloid leukemia. *bioRxiv : the preprint server for biology*.

Wahab S, et al. (2025) Exploring drug repurposing for PAK2 inhibition: a systematic virtual screening of FDA-approved drugs against cancer. *Discover oncology*, 16(1), 1747.

Wu F, et al. (2020) Computational Approaches in Preclinical Studies on Drug Discovery and Development. *Frontiers in chemistry*, 8, 726.

Lloyd K, et al. (2020) Using systems medicine to identify a therapeutic agent with potential for repurposing in inflammatory bowel disease. *Disease models & mechanisms*, 13(11).

Mehta AS, et al. (2015) Comparative sequence- and structure-inspired drug design for PilF protein of *Neisseria meningitidis*. *Human genomics*, 9(1), 5.

Corominas-Faja B, et al. (2014) Computer-aided discovery of biological activity spectra for anti-aging and anti-cancer olive oil oleuropeins. *Aging*, 6(9), 731.