Resource Summary Report

Generated by dkNET on Sep 22, 2026

PyRx

RRID:SCR_018548
Type: Tool

Proper Citation

PyRx (RRID:SCR_018548)

Resource Information

URL: https://pyrx.sourceforge.io/

Proper Citation: PyRx (RRID:SCR_018548)

Description: Open source virtual screening software for computational drug discovery with intuitive user interface. Runs on operating systems Linux, Windows, and Mac OS. Used to screen libraries of compounds against potential drug targets.

Resource Type: data processing software, simulation software, software application, software resource

Keywords: Virtual screening, computational drug discovery, drug, medicinal chemistry, target compound, compound screening, compound library, library screening

Availability: Restricted

Resource Name: PyRx

Resource ID: SCR_018548

Record Creation Time: 20220129T080340+0000

Record Last Update: 20260919T195353+0000

Ratings and Alerts

No rating or validation information has been found for PyRx.

No alerts have been found for PyRx.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 645 mentions in open access literature.

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

Ghasemi F, et al. (2026) Expansion, functional diversification, and gene fusion events in the Ato protein family. iScience, 29(7), 116467.

Arora M, et al. (2026) Integrated in silico and in vitro evaluation of Genistein and Apigenin as dual inhibitors of PARP1 and ESR1 in breast cancer. BMC pharmacology & toxicology, 27(1), 7.

Afroz M, et al. (2026) Abietic Acid Enhances the Sedative Activity of Diazepam: In vivo Approach along with Receptor Binding Affinity and Molecular Interaction with the GABAergic System. ChemistryOpen, 15(4), e202500397.

Putra WE, et al. (2026) Integrative computational approach to farnesyltransferase inhibition toward anti-liver cancer drug candidate from Syzygium cumini essential oils. Molecular biology research communications, 15(1), 49.

Khandakar MJ, et al. (2026) Integrated In Vitro, In Vivo, and In Silico Evaluation of Antioxidant, Anti-Inflammatory, Analgesic, and Anti-Arthritic Activities of Selected Marine Species. Bioengineering (Basel, Switzerland), 13(2).

Ren X, et al. (2026) Preparation and Identification of the Novel Umami Peptides from Sea Cucumber Viscera Hydrolysate. Foods (Basel, Switzerland), 15(4).

Rahaman HH, et al. (2026) In silico prediction, molecular docking and simulation of natural flavonoid apigenin and xanthoangelol E against human metapneumovirus. In silico pharmacology, 14(1), 40.

Tang G, et al. (2026) Bioinformatics and computational exploration of novel inhibitors targeting KRAS G12C mutant protein in lung adenocarcinoma. Discover oncology, 17(1).

Islam F, et al. (2026) Ameliorative Effects of Nypa fruticans Leaf Extract on Anxiety and Depression: Evidence From In Vivo and In Silico Studies. BioMed research international, 2026(1), e1243521.

Widiastuti D, et al. (2026) Antioxidant Activity, LC-MS/MS Identification and In Silico Analysis of the Ethanol Extract of Beneng Taro Leaves (Xanthosoma undipes K. Koch) Grown in Three Different Locations. Tropical life sciences research, 37(1), 31.

Abd El Salam HA, et al. (2026) New indole-linked 1,2,4-triazole derivatives as dual FAK inhibitors and apoptosis inducers targeting survival and migration in triple-negative breast cancer in-vitro. Scientific reports, 16(1).

Telli EE, et al. (2026) Optimization and Molecular Simulation of Gelatin-Free Marshmallow Formulation Using Gellan Gum and Aquafaba. Food science & nutrition, 14(5), e71898.

El-Halim MDA, et al. (2026) Biogenic selenium extract-mediated and total Convolvulus oxyphyllus extracts suppress IL6 and COX2 expression: insights from LC-MS metabolite

profiling and molecular docking. Scientific reports, 16(1).

Hoque N, et al. (2026) Investigating the Phytochemical Constituents, Anti-Inflammatory, and Neuropharmacological Activities of Podocarpus neriifolius Leaves Through FT-IR, GC-MS, Experimental Studies, Molecular Docking, and Molecular Dynamics Simulations. Pharmacology research & perspectives, 14(3), e70272.

Tayebi A, et al. (2026) Lipid-Lowering and Hepatoprotective Effects of Basil-Enriched Soybean Oil (BEO) in High-Fat-Diet-Fed Mice. Metabolites, 16(2).

Iftikhar N, et al. (2026) Polyphenol-rich Cucurbita formulation mitigates doxorubicin-induced cardiotoxicity in rats: biochemical, histological, and molecular docking insights. Scientific reports, 16(1).

Adedirin O, et al. (2026) Dual PTP1B/DPP4 Inhibitory Potential of Agathosma betulina, Cymbopogon citratus, and Artemisia afra: Structure-Based Modeling of Phytochemical Leads and Essential Oil Bioassays. Computational and structural biotechnology journal, 35(1), 0028.

Koparir A, et al. (2026) Clinical and genetic heterogeneity of syndromic hearing loss and its non-syndromic hearing loss mimics. Molecular medicine (Cambridge, Mass.), 32(1).

Khan MM, et al. (2026) In silico screening and molecular analyses identify apigenin from Scutellaria barbata as a potent AKT1 inhibitor in breast cancer. PloS one, 21(6), e0338874.

Rahman MM, et al. (2026) Unveiling the bactericidal effects of extracts and phytocompounds from Eichhornia crassipes (Mart.) Solms against methicillin-resistant Staphylococcus aureus (MRSA): An in vitro and in silico approach. PloS one, 21(6), e0349750.