

Resource Summary Report

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PyRx

RRID:SCR_018548

Type: Tool

Proper Citation

PyRx (RRID:SCR_018548)

Resource Information

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

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

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: 20260808T190119+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 [PRECISE-TBI](#) .

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.

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).

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.

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).

Ataya F, et al. (2026) Identification of polyphenols as novel neuropilin-1 cendR pocket inhibitors to block SARS-CoV-2 entry and enhance variant resistance. *PloS one*, 21(3), e0345051.

de Araujo Monteiro AA, et al. (2026) Protective role of lycopene against salinity-induced oxidative stress in *Medicago sativa* L. seedlings. *Scientific reports*, 16(1).

Adeboye OM, et al. (2026) *Acanthospermum hispidum* and Its Metabolite Stigmasterol Modulates Anti-Inflammatory Antagonism of COX-1 and TGF- β 1. *Chemistry & biodiversity*, 23(1), e01647.

Ali MA, et al. (2026) Exploring potential phytochemicals from black cumin as drug molecules against SARS-CoV-2 infections through bioinformatics analysis. *PloS one*, 21(3), e0337970.

Bharati D, et al. (2026) Unraveling the Antioxidant, Antihyperlipidemic, and Antidiabetic Potential of *Jatropha integerrima* in Streptozotocin-Induced Diabetic Rats. *Life (Basel, Switzerland)*, 16(2).

Moetlediwa MT, et al. (2026) Identification of Enhanced Cyclooxygenase-2 (COX-2) Inhibitors Beyond Curcumin Through Virtual Screening to Target Inflammation-Related Metabolic Complications. *International journal of molecular sciences*, 27(4).

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).

Akter S, et al. (2026) Immunoinformatics approach to engineer a multi-epitope vaccine against SdrG in skin commensal *Staphylococcus epidermidis*. *PloS one*, 21(3), e0327534.