

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: software application, simulation software, software resource, 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: 20260728T043552+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 518 mentions in open access literature.

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

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.

Ali IJ, et al. (2026) Anti-Inflammatory, Antioxidant, Molecular Docking and Pharmacokinetics Properties of Cycloeucalenone Isolated From *Musa × paradisiaca* L. Fruit Peels. *Chemistry & biodiversity*, 23(1), e02342.

Buhlak S, et al. (2025) Design, Synthesis, and Computational Evaluation of 3,4-Dihydroquinolin-2(1H)-One Analogues as Potential VEGFR2 Inhibitors in Glioblastoma Multiforme. *Pharmaceuticals (Basel, Switzerland)*, 18(2).

Bhuia MS, et al. (2025) Anxiolytic Activity of Morellic Acid: Modulation of Diazepam's Anxiolytic Effects, Possibly Through GABAergic Interventions. *CNS neuroscience & therapeutics*, 31(2), e70276.

Ravindranath KJ, et al. (2025) Regulating the expression of matrix metalloproteinases to inhibit ovarian carcinoma using isoquinoline alkaloid from *Allium ascalonicum*. *Scientific reports*, 15(1), 9228.

Akwu NA, et al. (2025) Phytochemistry, Antibacterial and Antioxidant Activities of *Grewia lasiocarpa* E. Mey. Ex Harv. Fungal Endophytes: A Computational and Experimental Validation Study. *Chemistry & biodiversity*, 22(5), e202402908.

Abdallah HA, et al. (2025) A comparative study of the essential oil extracts of *Centaurea alexanderina* different parts: GC-MS analysis, antimicrobial, antioxidant, and anti-hyperglycemic activities. *BMC complementary medicine and therapies*, 25(1), 90.

Eyong ED, et al. (2025) In vitro and in silico pharmaco-nutritional assessments of some lesser-known Nigerian nuts: *Persea americana*, *Tetracarpidium conophorum*, and *Terminalia catappa*. *PloS one*, 20(4), e0319756.

Juzer T, et al. (2025) *Camellia sinensis* mediated silver nanoparticles: eco-friendly antimicrobial agent to control multidrug resistant Gram-positive *Staphylococcus aureus*. *Discover nano*, 20(1), 92.

Abo-El-Sooud K, et al. (2025) Combined in vivo and silico assessment of melatonin's protective effects on rifampicin-induced liver damage in rats. *Scientific reports*, 15(1), 31104.

Oloyede OI, et al. (2025) In Silico evaluation of phytoconstituents from *Carica Papaya* and its anti-hyperglycemic activities on high sucrose-induced oxidative stress in *Drosophila melanogaster*. *Scientific reports*, 15(1), 29834.

Pradeep S, et al. (2025) Exploring shared therapeutic targets for Alzheimer's disease and glioblastoma using network pharmacology and protein-protein interaction approach.

Frontiers in chemistry, 13, 1549186.

Naveed M, et al. (2025) Exploring the therapeutic potential of *Thymus vulgaris* ethanol extract: a computational screening for antimicrobial compounds against COVID-19 induced mucormycosis. *Scientific reports*, 15(1), 15906.

Aati HY, et al. (2025) Bioactivity Profiling of Chemically Characterized Extract of Saudi Jackfruit (*Artocarpus heterophyllus*) Using In Vitro and In Silico Approaches. *Scientifica*, 2025, 8015648.

Külahc? MB, et al. (2025) *Arenaria serpyllifolia* as a Natural Antiviral Agent: Phytochemical, Biological, and Molecular Approaches. *ChemistryOpen*, 14(11), e202500236.

Shanthappa PM, et al. (2025) Deciphering highly potent natural abscisic acid agonists for binding to pyrabactin resistance 1 receptor through computational approaches. *Scientific reports*, 15(1), 20999.

Azme E, et al. (2025) Computational identification of potential natural terpenoid inhibitors of MDM2 for breast cancer therapy: molecular docking, molecular dynamics simulation, and ADMET analysis. *Frontiers in chemistry*, 13, 1527008.

Kamau SW, et al. (2025) Antiproliferative activity of *Grewia villosa* ethyl acetate extract on cervical cancer HeLa cell line: Mechanistic insights through network pharmacology and functional assays approach. *PloS one*, 20(9), e0331649.

Hossain MR, et al. (2025) Green synthesis of silver nanoparticles from *Brownlowia tersa* leaf extract: multifaceted evaluation of antibacterial, antioxidant, cytotoxic, and anti-alzheimer potential. *PloS one*, 20(11), e0335524.

Xie J, et al. (2025) A blueprint of synergistic effect in *Crataegus pinnatifida* and obesity-related gut microbiota against obesity via systems biology concept. *PloS one*, 20(10), e0332038.