Resource Summary Report

Generated by Kravitz on Sep 19, 2026

OpenEye

RRID:SCR_014880
Type: Tool

Proper Citation

OpenEye (RRID:SCR_014880)

Resource Information

URL: https://www.eyesopen.com/

Proper Citation: OpenEye (RRID:SCR_014880)

Description: Commercial organization which provides molecular modelling and cheminformatics software to the pharmaceutical industry.

Synonyms: OpenEye Scientific

Resource Type: resource

Keywords: commercial organization, pharmaceutical industry, molecular modelling, cheminformatics, durg discovery

Availability: Researchers may contribute to this organization

Resource Name: OpenEye

Resource ID: SCR_014880

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260919T195303+0000

Ratings and Alerts

No rating or validation information has been found for OpenEye.

No alerts have been found for OpenEye.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 426 mentions in open access literature.

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

Riedel C, et al. (2026) Identification and characterization of inhibitors of the tuberculosis phosphatase PstP. The Journal of biological chemistry, 302(4), 111316.

Okawa N, et al. (2026) Machine Learning Prediction for Fe(II) Spin-Crossover Complex in the Same Spin State Using Geometrical and Topological Descriptors. Journal of chemical information and modeling, 66(8), 4620.

Pushkaran AC, et al. (2026) Ensemble molecular dynamics for predicting binding energies of DNA intercalators. RSC advances, 16(15), 13696.

Silva-Mendonça S, et al. (2026) Structure- and Ligand-Based Discovery of Novel 3-Chymotrypsin-Like Protease Nonpeptidomimetic Hits. ChemMedChem, 21(7), e202501083.

Caldaruse AM, et al. (2026) Efficient Binding Affinity Estimation for Fragment-Based Compounds Using a Separated Topologies Approach. Journal of chemical information and modeling, 66(7), 4202.

Biswas B, et al. (2026) Cellular engagement of the SARS-CoV-2 macrodomain by GS-441524 and enhanced in vitro inhibition by its diphosphorylated metabolite. RSC chemical biology.

Raju B, et al. (2026) Exploration of Novel Chemical Spaces to Discover JAK1 Inhibitors: An Ensemble Docking-Guided Deep Learning Approach. ACS omega, 11(7), 11875.

Brezinova M, et al. (2026) Identification of potent high-affinity secondary nucleation inhibitors of A?42 aggregation from an ultra-large chemical library using deep docking. Molecular systems biology, 22(1), 69.

Williams HJ, et al. (2026) Query Matters: How Selection Strategies Influence Active Learning in Drug Discovery. Journal of chemical information and modeling, 66(6), 3288.

Cheng M, et al. (2026) The YAP-TEAD4 inhibitor M511-0965 suppresses triple-negative breast cancer progression by downregulating TGFB2. Translational oncology, 71, 102881.

Marín M, et al. (2026) Antimitotic Naphthalene Sulfonamides Are Potent Antitumor Agents Acting Differently from Colchicine. Pharmaceutics, 18(6).

Gkoutzivelaki A, et al. (2026) Design, Synthesis, Antiproliferative Potency and In Silico Studies of Novel Alkynyl Quinazolines as Potential EGFR Inhibitors. International journal of molecular sciences, 27(4).

Modric M, et al. (2026) A novel approach to combat Pseudomonas aeruginosa: repurposing pharmaceuticals for inhibition of phospholipase A. Microbiology spectrum, 14(3), e0130425.

Mottin M, et al. (2026) Enhanced Antiviral Activity of Novel Umifenovir Derivatives against SARS-CoV-2: Insights from an International Collaborative Study. ACS omega, 11(15), 23109.

Amorim AMB, et al. (2026) ViralBindPredict: empowering viral protein-ligand binding sites through deep learning and protein sequence-derived insights. GigaScience, 15.

Docken SS, et al. (2026) A hERG Blocker Facilitates K+ Channel Current by Agonizing Pore Opening while Blocking. bioRxiv : the preprint server for biology.

Zubatyuk R, et al. (2025) AQuaRef: machine learning accelerated quantum refinement of protein structures. Nature communications, 16(1), 9224.

Ricos MG, et al. (2025) Identification of New KCNT1-Epilepsy Drugs by In Silico, Cell, and Drosophila Modeling. Annals of neurology, 98(6), 1261.

Correy GJ, et al. (2025) Exploration of structure-activity relationships for the SARS-CoV-2 macrodomain from shape-based fragment linking and active learning. Science advances, 11(22), eads7187.

Osato M, et al. (2025) Evaluating the Functional Importance of Conformer-Dependent Atomic Partial Charge Assignment. Journal of computational chemistry, 46(13), e70112.