

Resource Summary Report

Generated by [dkNET](#) on Sep 18, 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, drug discovery

Availability: Researchers may contribute to this organization

Resource Name: OpenEye

Resource ID: SCR_014880

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260912T195822+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 [dkNET](#) .

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.

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

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

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

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.

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 β 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.

Han Y, et al. (2025) Molecular simulations reveal intricate coupling between agonist-bound β -adrenergic receptors and G protein. iScience, 28(2), 111741.

Luttens A, et al. (2025) Virtual fragment screening for DNA repair inhibitors in vast chemical space. Nature communications, 16(1), 1741.

Wang Y, et al. (2025) An AI-assisted fluorescence microscopic system for screening mitophagy inducers by simultaneous analysis of mitophagic intermediates. Nature communications, 16(1), 5179.

Harnying W, et al. (2025) Gas-phase Curtius and Wolff rearrangement reactions investigated by tandem-MS, IR ion spectroscopy and theory. Physical chemistry chemical physics : PCCP, 27(25), 13543.