# Resource Summary Report

Generated by NIF on Aug 5, 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:** 20260801T190509+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 380 mentions in open access literature.

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


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.

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

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

Ghattas M, et al. (2025) A Self-Consistent Approach to Rotamer and Protonation State Assignments (RAPA): Moving Beyond Single Protein Configurations. Journal of chemical information and modeling, 65(14), 7639.

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

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.

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.

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.

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

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

Errington D, et al. (2025) Assessing interaction recovery of predicted protein-ligand poses. Journal of cheminformatics, 17(1), 76.

Treeby J, et al. (2025) Guanine is an inhibitor of c-jun terminal kinases. Scientific reports, 15(1), 29374.

Jeon H, et al. (2025) STELLA provides a drug design framework enabling extensive fragment-level chemical space exploration and balanced multi-parameter optimization. Scientific reports, 15(1), 28135.

Zuanon M, et al. (2025) Identification of New Human P2X7 Antagonists Using Ligand- and Structure-Based Virtual Screening. Journal of chemical information and modeling, 65(13), 7143.

Jayashankar V, et al. (2025) Sphingosine simultaneously inhibits nuclear import and activates PP2A by binding importins and PPP2R1A. The EMBO journal, 44(16), 4473.

Singh S, et al. (2025) Prospective evaluation of structure-based simulations reveal their ability to predict the impact of kinase mutations on inhibitor binding. bioRxiv : the preprint server for biology.

Matias-Barrios VM, et al. (2025) Developing novel Lin28 inhibitors by computer aided drug design. Cell death discovery, 11(1), 5.

Guerrero-Rodríguez SL, et al. (2025) Identification of New CD36 Antagonists by Structure-Based Virtual Screening. Chemical biology & drug design, 106(5), e70205.

Hamakawa Y, et al. (2025) Understanding Conformation Importance in Data-Driven Property Prediction Models. Journal of chemical information and modeling, 65(7), 3388.

Osteen JD, et al. (2025) Pharmacology and Mechanism of Action of Suzetrigine, a Potent and Selective NaV1.8 Pain Signal Inhibitor for the Treatment of Moderate to Severe Pain. Pain and therapy, 14(2), 655.