

Resource Summary Report

Generated by [NIF](#) on Aug 27, 2026

Epik

RRID:SCR_016745

Type: Tool

Proper Citation

Epik (RRID:SCR_016745)

Resource Information

URL: <https://www.schrodinger.com/epik>

Proper Citation: Epik (RRID:SCR_016745)

Description: Software program for pKa prediction and protonation state generation for drug like molecules.

Resource Type: simulation software, software application, software resource

Defining Citation: [PMID:17899391](#)

Keywords: predict, pKa, value, chemical, structure, drug, profile, protonation, state, molecule, Schrodinger

Availability: Commercially available

Resource Name: Epik

Resource ID: SCR_016745

Record Creation Time: 20220129T080332+0000

Record Last Update: 20260821T194110+0000

Ratings and Alerts

No rating or validation information has been found for Epik.

No alerts have been found for Epik.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 6 mentions in open access literature.

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

Feher A, et al. (2026) A kinetic trap mechanism underlies hHv1 inhibition by NZ-58. The Journal of general physiology, 158(4).

Schneider C, et al. (2024) A Novel AMPK Inhibitor Sensitizes Pancreatic Cancer Cells to Ferroptosis Induction. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 11(31), e2307695.

Pedersen CN, et al. (2024) Cryo-EM structure of the dopamine transporter with a novel atypical non-competitive inhibitor bound to the orthosteric site. Journal of neurochemistry, 168(9), 2043.

Morales-Bayuelo A, et al. (2022) New findings on ligand series used as SARS-CoV-2 virus inhibitors within the frameworks of molecular docking, molecular quantum similarity and chemical reactivity indices. F1000Research, 11, 914.

Paradela LS, et al. (2021) Multiple unbiased approaches identify oxidosqualene cyclase as the molecular target of a promising anti-leishmanial. Cell chemical biology, 28(5), 711.

Borhade SR, et al. (2014) Inhibition of Insulin-Regulated Amino-peptidase (IRAP) by Arylsulfonamides. ChemistryOpen, 3(6), 256.