

Resource Summary Report

Generated by [ASWG](#) on Aug 4, 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 resource, software application

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: 20260803T040722+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 5 mentions in open access literature.

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

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.