Resource Summary Report

Generated by RRID on Aug 15, 2026

xTB

RRID:SCR_026929
Type: Tool

Proper Citation

xTB (RRID:SCR_026929)

Resource Information

URL: https://github.com/grimme-lab/xtb

Proper Citation: xTB (RRID:SCR_026929)

Description: Software semiempirical extended tight-binding program package. Provides userfriendly interface for performing geometry optimizations, vibrational frequency calculations, and Molecular Dynamics simulations.

Synonyms: , eXtended TB (xTB), eXtended TB, extended Tight Binding

Resource Type: software toolkit, source code, software resource

Defining Citation: DOI:10.1002/wcms.1493

Keywords: performing geometry optimizations, vibrational frequency calculations, Molecular Dynamics simulations,

Availability: Free, Available for download, Freely available

Resource Name: xTB

Resource ID: SCR_026929

Alternate URLs: https://xtb-docs.readthedocs.io/en/latest/

License: LGPL v3

Record Creation Time: 20250513T055331+0000

Record Last Update: 20260815T183253+0000

Ratings and Alerts

No rating or validation information has been found for xTB.

No alerts have been found for xTB.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 4 mentions in open access literature.

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

Rojas WY, et al. (2025) Galaxy QCxMS for straightforward semi-empirical quantum mechanical EI-MS prediction. GigaByte (Hong Kong, China), 2025, gigabyte160.

Amin SA, et al. (2025) First 4D-QSAR Study of Human Kynurenine 3 Monooxygenase (hKMO) Inhibitors: Integrating Chemical Space Networks and an Explainable Artificial Intelligence Platform for Neurodegenerative Disease Drug Discovery. ACS omega, 10(35), 39751.

Boz E, et al. (2021) Accurate Receptor-Ligand Binding Free Energies from Fast QM Conformational Chemical Space Sampling. International journal of molecular sciences, 22(6).

Wilbraham L, et al. (2020) Mapping the optoelectronic property space of small aromatic molecules. Communications chemistry, 3(1), 14.