Resource Summary Report

Generated by nidm-terms on Jul 30, 2026

MetabolExpert

RRID:SCR_014908
Type: Tool

Proper Citation

MetabolExpert (RRID:SCR_014908)

Resource Information

URL: http://www.compudrug.com/metabolexpert

Proper Citation: MetabolExpert (RRID:SCR_014908)

Description: Software tool for initial estimation of the structural formula of metabolites, which might be formed by a substance in humans, animals or in plants. MetabolExpert is also capable of predicting the most common metabolic pathways in animals, exporting results to SDF and RDF format and graphical highlighting that empasizes the essence of metabolic reactions that occurred.

Resource Type: software resource

Keywords: metabolites, metabolism, analysis, chemical, modeling, prediction

Availability: Commercial

Resource Name: MetabolExpert

Resource ID: SCR_014908

Record Creation Time: 20220129T080323+0000

Record Last Update: 20260725T190807+0000

Ratings and Alerts

No rating or validation information has been found for MetabolExpert.

No alerts have been found for MetabolExpert.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3 mentions in open access literature.

Listed below are recent publications. The full list is available at nidm-terms .

Furqan T, et al. (2020) Cannabis Constituents and Acetylcholinesterase Interaction: Molecular Docking, In Vitro Studies and Association with CNR1 rs806368 and ACHE rs17228602. Biomolecules, 10(5).

Kirchmair J, et al. (2012) Computational prediction of metabolism: sites, products, SAR, P450 enzyme dynamics, and mechanisms. Journal of chemical information and modeling, 52(3), 617.

Sun Y, et al. (2009) Oral bioavailability and brain penetration of (-)-stepholidine, a tetrahydroprotoberberine agonist at dopamine D(1) and antagonist at D(2) receptors, in rats. British journal of pharmacology, 158(5), 1302.