Resource Summary Report

Generated by RRID on Aug 11, 2026

Jaguar

RRID:SCR_014895
Type: Tool

Proper Citation

Jaguar (RRID:SCR_014895)

Resource Information

URL: https://www.schrodinger.com/Jaguar

Proper Citation: Jaguar (RRID:SCR_014895)

Description: Ab initio molecular modeling software program that computes an array of molecular properties such as multipole moments, polarizabilities, and electrostatic potential. It can also map reaction coordinates between reactants, products, and transition states.

Resource Type: software application, software resource

Defining Citation: DOI:10.1002/qua.24481

Keywords: ab initio, molecular modeling, chemical properties, array

Availability: Commercial

Resource Name: Jaguar

Resource ID: SCR_014895

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260810T040612+0000

Ratings and Alerts

No rating or validation information has been found for Jaguar.

No alerts have been found for Jaguar.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 249 mentions in open access literature.

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

Wu R, et al. (2026) Structural and biochemical insight into allosteric regulation of the human 2-aminoadipic semialdehyde synthase, a bifunctional enzyme involved in lysine catabolism. Research square.

Siegbahn PEM, et al. (2026) The Intricate Mechanism of Nitric Oxide Synthase. Journal of computational chemistry, 47(17), e70448.

Ayaz M, et al. (2026) Exploring the anti-diabetic potential of bis-Schiff bases of ibuprofen: insights into the in vitro, molecular docking and density functional theory analyses. RSC advances, 16(12), 11005.

Wang Y, et al. (2026) Differentiating interfacial water structures via alkali metal cation promotor for H2O2 electrosynthesis in acid. Nature communications, 17(1).

Wallach J, et al. (2026) Bioisostere-Driven Discovery of SePP: A Selenium-Containing Polypharmacological Agent Relevant to Fragile X Syndrome. Journal of medicinal chemistry, 69(4), 4020.

Mirzahosseini A, et al. (2026) Phase-Specific Parameter Estimation in Chiral HPLC Using 1-Site, 2-Site Stochastic Models, and Unified Equation Approach. Analytical chemistry, 98(18), 13925.

Ahmad S, et al. (2026) Multitarget docking and molecular enumeration reveal DdpMPyPEPhU as a potent modulator of cell cycle, glucocorticoid, and estrogen signalling in breast cancer. PloS one, 21(3), e0344028.

Shah D, et al. (2026) Exploring imidazo[1,2-a]pyridine hybrids in cancer therapy: ADMET profiling, molecular docking, MD simulations and DFT calculations. Scientific reports, 16(1).

Madruga E, et al. (2026) Brain Permeable SGK1 Inhibitors: A Promising Therapeutic Strategy for Neurodegenerative Diseases. Journal of medicinal chemistry, 69(6), 6790.

Chirila CB, et al. (2026) Harnessing machine learning models to repurpose drugs targeting HIV-1 integrase, protease, and reverse transcriptase. Scientific reports, 16(1).

Gautrelet C, et al. (2026) Multiaxial vibration dataset obtained on a triaxial electrodynamic shaker rig using multiple control strategies. Data in brief, 67, 113008.

Shaheen K, et al. (2025) In vivo anti-inflammatory evaluation of oxadiazole derivatives bearing flurbiprofen moiety using experimental and computational approaches. Scientific reports, 15(1), 29144.

Bejcek LP, et al. (2025) Deconstruction of Desacetamidocolchicine's B Ring Reveals a Class 3 Atropisomeric AC Ring with Tubulin Binding Properties. The Journal of organic chemistry, 90(22), 7246.

R M, et al. (2025) Design, synthesis and evaluation of benzodioxole and bromofuran tethered 1,2,4-triazole hybrids as potential anti breast cancer agents with computational insights. Scientific reports, 15(1), 25680.

Agyemang NB, et al. (2025) Synthetic, Computational, and Experimental Studies of a Class 3 Atropisomeric ?-Naphthyl Tropone. The Journal of organic chemistry, 90(32), 11501.

Nem?ovi?ová I, et al. (2025) Small glycomimetic antagonists of the cytomegalovirus glycoprotein UL141 prevent binding to TRAIL death receptor. The Journal of biological chemistry, 301(5), 108490.

Mostafa EM, et al. (2025) Comparative study of the chemical profile, cytotoxic activity, and molecular docking of Serenoa repens extract and a pharmaceutical product. Scientific reports, 15(1), 34338.

Toth AR, et al. (2025) Novel Sigma-1 receptor agonist alleviates renal ischemic injury by targeting apoptotic and inflammatory pathways. Scientific reports, 15(1), 39762.

Noji T, et al. (2025) How the Electron-Transfer Cascade is Maintained in Chlorophyll-d Containing Photosystem I. Biochemistry, 64(1), 203.

Vemula D, et al. (2025) Proteome-wide identification of druggable targets and inhibitors for multidrug-resistant Pseudomonas aeruginosa using an integrative subtractive proteomics and virtual screening approach. Heliyon, 11(4), e42584.