

Resource Summary Report

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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](https://doi.org/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

Usage and Citation Metrics

We found 249 mentions in open access literature.

Listed below are recent publications. The full list is available at [kravitz2](#) .

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.

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.

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

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.

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.

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

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).

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.

Nemővi 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.

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.

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.

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.

Agyemang NB, et al. (2025) Synthetic, Computational, and Experimental Studies of a Class 3 Atropisomeric 1-Naphthyl Tropone. *The Journal of organic chemistry*, 90(32), 11501.

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.

Saito K, et al. (2025) Identification and design principles of far-red-absorbing chlorophyll in the light-harvesting complex. *The Journal of biological chemistry*, 301(6), 108518.

Kugawa M, et al. (2025) Structural insights into lipid chain-length selectivity and allosteric regulation of FFA2. *Nature communications*, 16(1), 2809.