

Resource Summary Report

Generated by [kravitz2](#) on Aug 8, 2026

Gaussian

RRID:SCR_014897

Type: Tool

Proper Citation

Gaussian (RRID:SCR_014897)

Resource Information

URL: <http://gaussian.com/>

Proper Citation: Gaussian (RRID:SCR_014897)

Description: Software program for electronic structure modeling that enables researchers to study and predict the properties of molecules and reactions under a wide range of conditions, especially those that are difficult or impossible to observe experimentally.

Resource Type: software resource, software application

Keywords: electronic structure modeling, simulation, visualization

Availability: Commercial

Resource Name: Gaussian

Resource ID: SCR_014897

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260808T042806+0000

Ratings and Alerts

No rating or validation information has been found for Gaussian.

No alerts have been found for Gaussian.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 642 mentions in open access literature.

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

Li J, et al. (2026) High-reactivity precursor C₂N₃H and its photo-induced stepwise growth toward 2D graphitic carbon nitride clusters. *iScience*, 29(3), 114933.

Li C, et al. (2026) Ultrahigh High-temperature Capacitive Energy Storage Via Proton Irradiation. *Advanced science* (Weinheim, Baden-Wurttemberg, Germany), 13(9), e22035.

Afzal M, et al. (2026) Integrated experimental and computational evaluation of Anagallis foemina derived terpenoids against carbapenem resistant *Acinetobacter baumannii*. *Scientific reports*, 16(1).

El-Maksoud SAA, et al. (2026) Effect of alkyl chain length on the corrosion inhibition performance of 2-thioxo-2,3-dihydroquinazolin-4(1H)-one derivatives for carbon steel in HCl solution. *Scientific reports*, 16(1).

Orji JN, et al. (2026) Synthesis, characterization, DFT and in silico anti-ulcer activities of novel sulphonamide derivatives. *Scientific reports*, 16(1).

Taspinar F, et al. (2026) Design, synthesis, and mechanistic evaluation of propargylated salicylaldehyde derivatives as dual apoptosis-autophagy modulator for pancreatic cancer. *Naunyn-Schmiedeberg's archives of pharmacology*, 399(8), 11785.

Schmidt-Dannert M, et al. (2026) Docking in the *Abies grandis* abietaenol synthase to investigate the mechanism underlying conifer resin acid diterpene synthase evolution. *The Biochemical journal*, 483(3), 365.

Abdel-Megid M, et al. (2026) Chemical reactivity of 2-methylchromone with some nitrogen-based nucleophiles: reactions, DFT analysis, anticancer activity and molecular docking studies. *RSC advances*, 16(7), 5814.

Braga E, et al. (2026) Zinc(II) Coordination Compounds on Acylhydrazones of 2-Tosylaminobenzaldehyde Basis as Promising Luminescent Agents. *International journal of molecular sciences*, 27(4).

Valdivieso Zárate LM, et al. (2026) Computational and Chemical Analysis of the Oxygen Atom Transfer Process of a Dioxo-Molybdenum Complex Incorporated into a Modified UiO-67 (Zr/Ti). *ACS organic & inorganic Au*, 6(3), 288.

Liu L, et al. (2026) Localization of the Au-Au bond strength in the triplet excited state of the [Au(CN)₂]⁻ oligomers revealed by ultrafast time-domain Raman spectroscopy. *Chemical science*, 17(5), 2676.

Sun F, et al. (2026) Rotational Detection of the Missing Conformers of 2-Chloropropionic Acid. *The journal of physical chemistry. A*, 130(4), 836.

Chen L, et al. (2026) Electric-field-driven CO₂ polarization and bioinspired proton blocking unlock CO₂ reduction in strong acid without metal cations. *Nature communications*, 17(1), 1734.

Badran AS, et al. (2026) Experimental, spectroscopic, thermodynamic, and DFT study of a novel cyanomethylchrome nopyridinecarbonitrile (CCPC). Scientific reports, 16(1).

Mozejko P, et al. (2026) On the Calculations of Electron Impact Ionization Cross-Sections for Selected Nucleosides and Deoxyribose Molecules. Molecules (Basel, Switzerland), 31(11).

Li Y, et al. (2026) Quadruple Bonding of Alkaline Earth Atoms in AeCLi₄ (Ae = Be - Ba) Complexes. Journal of computational chemistry, 47(18), e70449.

Chen X, et al. (2026) Reactivity of mammalian lipoxygenases (ALOX isoforms) with phospholipids, biomembranes and lipoproteins. Communications biology, 9(1).

Farinha AFM, et al. (2026) Quartz Crystal Microbalance Sensitivity Loss During Ionic Liquid Deposition: Insights into Film Structure and Morphology. Chemphyschem : a European journal of chemical physics and physical chemistry, 27(7), e70349.

Yoshine R, et al. (2026) Residue-resolved dynamically averaged interaction analysis of direct factor Xa inhibitors by MD-FMO combination calculations. Journal of computer-aided molecular design, 40(1).

Rewish NM, et al. (2026) Design, synthesis, and evaluation of novel triazole-based carbohydrazide derivatives with notable antioxidant activity: an integrated experimental and DFT study. BMC chemistry, 20(1).