

Resource Summary Report

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Gamess

RRID:SCR_014896

Type: Tool

Proper Citation

Gamess (RRID:SCR_014896)

Resource Information

URL: <http://www.msg.chem.iastate.edu/gamess/>

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Description: Software program for ab initio molecular quantum chemistry. GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Capabilities include using nuclear gradients for automatic geometry optimization, modeling of solvent effects, computation of the energy hessian for prediction of vibrational frequencies, as well as computation of nuclear wavefunctions. The program can also compute variety of molecular properties, ranging from simple dipole moments to frequency dependent hyperpolarizabilities.

Synonyms: The General Atomic and Molecular Electronic Structure System

Resource Type: source code, software resource

Keywords: molecular quantum chemistry, molecular properties, computation, analysis, visualization

Resource Name: Gamess

Resource ID: SCR_014896

License URLs: http://www.msg.chem.iastate.edu/gamess/License_Agreement.html

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Ratings and Alerts

No rating or validation information has been found for Gamess.

No alerts have been found for Gamess.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 263 mentions in open access literature.

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

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.

Kumar A, et al. (2025) Molecular dynamics simulation and docking studies reveals inhibition of NF-kB signaling as a promising therapeutic drug target for reduction in cytokines storms. Scientific reports, 15(1), 15225.

Singh BG, et al. (2025) Experimental and Theoretical Studies on Reaction Kinetics, Mechanism, and Degradation of Quinoline-Based Herbicide with Hydroxyl Radical, Sulphate Radical Anion, and Hydrated Electron. Chemphyschem : a European journal of chemical physics and physical chemistry, 26(13), e202401135.

Paciotti R, et al. (2025) Unprecedented carbonic anhydrase inhibition mechanism: Targeting histidine 64 side chain through a halogen bond. Archiv der Pharmazie, 358(1), e2400776.

Azamat J, et al. (2025) The CH₄/CO₂ Gas Mixture Separation Using the Graphene, SiC, and BN Nanochannels: A Comprehensive Computational Approach. ACS omega, 10(30), 33295.

Randi PAS, et al. (2025) Stabilization Method as a Tool for Electronic State Spectroscopy. The journal of physical chemistry. A, 129(26), 5820.

Muñiz-Chicharro A, et al. (2025) A Multiscale Simulation Approach to Compute Protein-Ligand Association Rate Constants by Combining Brownian Dynamics and Molecular Dynamics. Journal of chemical information and modeling, 65(20), 11215.

Salvi E, et al. (2025) On the Role of Electronic Correlation and State-Specific Environment Polarization in Singlet-Triplet Gap Inversion. Journal of computational chemistry, 46(30), e70267.

Alrubia S, et al. (2025) Spectrophotometric and computational characterization of charge transfer complex of selumetinib with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone and its utilization in developing an innovative green and high throughput microwell assay for analysis of bulk form and pharmaceutical formulation. BMC chemistry, 19(1), 27.

Ghavi Z, et al. (2025) Molecular dynamics insights into non-covalent functionalization of boron nitride nanotubes for doxorubicin delivery. Scientific reports, 15(1), 30213.

Ibragimov S, et al. (2025) Isomers of Iron(III) Oxides and Cobalt(III) Oxides and Their Redox Properties: Quantum-Chemical Insights. *Molecules* (Basel, Switzerland), 30(21).

Lai R, et al. (2025) Mechanism of Ampicillin Hydrolysis by New Delhi Metallo- β -Lactamase 1: Insight From QM/MM MP2 Calculation. *Journal of computational chemistry*, 46(1), e27544.

Ali Q, et al. (2025) Assessment of the potential and application of Be₁₂O₁₂ nanocage for removal of ciprofloxacin from water employing density functional theory. *Scientific reports*, 15(1), 1020.

Ruiz-Gonzalez A, et al. (2025) Calcium Ion Sensors with Unrivalled Stability and Selectivity Using a Bilayer Approach with Ionically Imprinted Nanocomposites. *Nanomaterials* (Basel, Switzerland), 15(10).

Tsuneda T, et al. (2025) Bridging electron and nuclear motions in chemical reactions through electrostatic forces from reactive orbitals. *Communications chemistry*, 8(1), 158.

Serrano-Morrás Á, et al. (2025) The Quasi-Bound State as a Predictor of Relative Binding Free Energy. *Journal of chemical information and modeling*, 65(11), 5544.

Pompon D, et al. (2025) Geometry-encoded molecular dynamics enables deep learning insights into P450 regiospecificity control. *Scientific reports*, 15(1), 7512.

Gade P, et al. (2025) Different chemical scaffolds bind to L-phe site in *Mycobacterium tuberculosis* Phe-tRNA synthetase. *European journal of medicinal chemistry*, 287, 117335.

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.

Zandi P, et al. (2025) Detecting Cr⁶⁺ at $\sim$ 100 pM Concentration with Fluorescence Enhancement Signatures in a Novel Eco-Fluorophore: Matching WHO's 96 pM Recommended Standard for Drinking Water. *Advanced materials* (Deerfield Beach, Fla.), 37(29), e2504142.