JamesÂ W Gauld

List of Publications by Year
in descending order

64	1,154	430874	434195
papers	citations	18 h-index	31 g-index

66	66	66	1291
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. Journal of Physical Chemistry A, 2002, 106, 5155-5159.	2.5	188
2	Glyceraldehyde 3-phosphate dehydrogenase (GAPDH) is inactivated by S-sulfuration in vitro. Free Radical Biology and Medicine, 2015, 89, 512-521.	2.9	97
3	A DFT Study of Nucleobase Dealkylation by the DNA Repair Enzyme AlkB. Journal of Physical Chemistry B, 2009, 113, 4887-4898.	2.6	64
4	An Assessment of Theoretical Methods for the Calculation of Accurate Structures and SN Bond Dissociation Energies of S-Nitrosothiols (RSNOs). Journal of Physical Chemistry A, 2003, 107, 9946-9952.	2.5	57
5	Recent applications of density functional theory calculations to biomolecules. Theoretical Chemistry Accounts, 2002, 108, 1-11.	1.4	47
6	A Density Functional Theory Study of the Radiation Products of Glycine. Journal of Physical Chemistry A, 2000, 104, 5080-5086.	2.5	36
7	Model Ironâ€“Oxo Species and the Oxidation of Imidazole: Insights into the Mechanism of OvoA and EgtB?. Inorganic Chemistry, 2012, 51, 13351-13356.	4.0	36
8	A Density Functional Theory Investigation on the Mechanism of the Second Half-Reaction of Nitric Oxide Synthase. Journal of the American Chemical Society, 2008, 130, 3328-3334.	13.7	30
9	Second Half-Reaction of Nitric Oxide Synthase:â€‰ Computational Insights into the Initial Step and Key Proposed Intermediate. Journal of Physical Chemistry B, 2005, 109, 23706-23714.	2.6	28
10	Oxidative Degradation of Pyruvate Formate-Lyase. Journal of the American Chemical Society, 2000, 122, 2035-2040.	13.7	27
11	DFT Investigation on the Mechanism of the Deacetylation Reaction Catalyzed by LpxC. Journal of Physical Chemistry B, 2008, 112, 3462-3469.	2.6	26
12	Substrate-assisted Catalysis in the Aminoacyl Transfer Mechanism of Histidylâ˜tRNA Synthetase: A Density Functional Theory Study. Journal of Physical Chemistry B, 2008, 112, 16874-16882.	2.6	24
13	Computational studies on Schiff-base formation: Implications for the catalytic mechanism of porphobilinogen synthase. Computational and Theoretical Chemistry, 2011, 963, 479-489.	2.5	24
14	Modeling the Action of an Antitumor Drug:Â A Density Functional Theory Study of the Mechanism of Tirapazamine. Journal of the American Chemical Society, 2001, 123, 7320-7325.	13.7	23
15	Insights into the Catalytic Mechanism of Coral Allene Oxide Synthase: A Dispersion Corrected Density Functional Theory Study. Journal of Physical Chemistry B, 2013, 117, 6701-6710.	2.6	21
16	Theoretical Studies of the Radiation Products of Hydroxyproline. Journal of Physical Chemistry A, 2000, 104, 8583-8592.	2.5	20
17	Molecular Dynamics Investigation into Substrate Binding and Identity of the Catalytic Base in the Mechanism of Threonyl-tRNA Synthetase. Journal of Physical Chemistry B, 2012, 116, 5205-5212.	2.6	20
18	Quantum Chemical Calculations of the NHA Bound Nitric Oxide Synthase Active Site:Â O2Binding and Implications for the Catalytic Mechanism. Journal of the American Chemical Society, 2004, 126, 10267-10270.	13.7	18

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19	The Î±-Amino Group of the Threonine Substrate as The General Base During tRNA Aminoacylation: A New Version of Substrate-Assisted Catalysis Predicted by Hybrid DFT. Journal of Physical Chemistry A, 2011, 115, 13050-13060.	2.5	18
20	The first branching point in porphyrin biosynthesis: A systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogenâ€III decarboxylase. Journal of Computational Chemistry, 2011, 32, 822-834.	3.3	17
21	Applications of Potential Energy Surfaces in the Study of Enzymatic Reactions. Advances in Physical Chemistry, 2012, 2012, 1-15.	2.0	16
22	Oligomerization of 3-substituted quinolines by catalytic activity of soybean peroxidase as a wastewater treatment. Product formation and computational studies. Chemical Engineering Journal, 2019, 364, 340-348.	12.7	15
23	A Computational Study on the Interaction of the Nitric Oxide Ions NO+ and NO- with the Side Groups of the Aromatic Amino Acids. Journal of Physical Chemistry A, 2007, 111, 1981-1989.	2.5	13
24	A Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) Study on Ornithine Cyclodeaminase (OCD): A Tale of Two Iminiums. International Journal of Molecular Sciences, 2012, 13, 12994-13011.	4.1	13
25	A Molecular Dynamics and Quantum Mechanics/Molecular Mechanics Study of the Catalytic Reductase Mechanism of Methionine Sulfoxide Reductase A: Formation and Reduction of a Sulfenic Acid. Biochemistry, 2013, 52, 1814-1827.	2.5	13
26	A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Study. Journal of Physical Chemistry B, 2011, 115, 9202-9212.	2.6	12
27	A water-mediated and substrate-assisted aminoacylation mechanism in the discriminating aminoacyl-tRNA synthetase GlnRS and non-discriminating GluRS. Physical Chemistry Chemical Physics, 2017, 19, 25598-25609.	2.8	12
28	Gaining insight into the chemistry of lipoxygenases: a computational investigation into the catalytic mechanism of (8R)-lipoxygenase. Journal of Biological Inorganic Chemistry, 2013, 18, 343-355.	2.6	11
29	A Molecular Dynamics Examination on Mutation-Induced Catalase Activity in Coral Allene Oxide Synthase. Journal of Physical Chemistry B, 2013, 117, 14635-14641.	2.6	11
30	Substrate-Assisted and Enzymatic Pretransfer Editing of Nonstandard Amino Acids by Methionyl-tRNA Synthetase. Biochemistry, 2015, 54, 5757-5765.	2.5	11
31	An Active Site Water Broadens Substrate Specificity in S-Ribosylhomocysteinase (LuxS): A Docking, MD, and QM/MM Study. Journal of Physical Chemistry B, 2012, 116, 8916-8929.	2.6	10
32	Formation of a Stable Iminol Intermediate in the Redox Regulation Mechanism of Protein Tyrosine Phosphatase 1B (PTP1B). ACS Catalysis, 2015, 5, 2195-2202.	11.2	10
33	Unraveling the Critical Role Played by _{Ado76}2â€²OH in the Post-Transfer Editing by Archaeal Threonyl-tRNA Synthetase. Journal of Physical Chemistry B, 2018, 122, 1092-1101.	2.6	10
34	A H2AXâ€“CARP-1 Interaction Regulates Apoptosis Signaling Following DNA Damage. Cancers, 2019, 11, 221.	3.7	10
35	Hydrolysis Mechanism of the Linkers by Matrix Metalloproteinase-9 Using QM/MM Calculations. Journal of Chemical Information and Modeling, 2021, 61, 5203-5211.	5.4	10
36	A Multi-Scale Computational Study on the Mechanism of Streptococcus pneumoniae Nicotinamidase (SpNic). Molecules, 2014, 19, 15735-15753.	3.8	9

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37	Enzymatic Post-Transfer Editing Mechanism of E. coli Threonyl-tRNA Synthetase (ThrRS): A Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) Investigation. ACS Catalysis, 2017, 7, 5180-5193.	11.2	9
38	An Assessment of Computational Methods for Calculating Accurate Structures and Energies of Bio-Relevant Polysulfur/Selenium-Containing Compounds. Molecules, 2018, 23, 3323.	3.8	9
39	Catalysis Mediated by Hydrogen Bonding:Â A Computational Study of the Aminolysis of 6-Chloropyrimidine. Journal of the American Chemical Society, 2000, 122, 5384-5386.	13.7	8
40	Hydrogen-Bond Mediated Catalysis:â€‰ The Aminolysis of 6-Chloropyrimidine as Catalyzed by Derivatives of Uracil. Journal of the American Chemical Society, 2001, 123, 2047-2052.	13.7	8
41	An assessment of pure, hybrid, meta, and hybridâ€meta GGA density functional theory methods for openâ€shell systems: The case of the nonheme iron enzyme 8Râ€“LOX. Journal of Computational Chemistry, 2013, 34, 141-148.	3.3	8
42	Roles of the Active Site Zn(II) and Residues in Substrate Discrimination by Threonyl-tRNA Synthetase: An MD and QM/MM Investigation. Journal of Physical Chemistry B, 2017, 121, 6163-6174.	2.6	8
43	Pretransfer Editing in Threonyl-tRNA Synthetase: Roles of Differential Solvent Accessibility and Intermediate Stabilization. ACS Catalysis, 2017, 7, 3102-3112.	11.2	8
44	Protonation of guanine quartets and quartet stacks: insights from DFT studies. Physical Chemistry Chemical Physics, 2009, 11, 278-287.	2.8	7
45	A QM/MMâ€“Based Computational Investigation on the Catalytic Mechanism of Saccharopine Reductase. Molecules, 2011, 16, 8569-8589.	3.8	7
46	Multi-Scale Computational Enzymology: Enhancing Our Understanding of Enzymatic Catalysis. International Journal of Molecular Sciences, 2014, 15, 401-422.	4.1	7
47	Computational investigations on the catalytic mechanism of maleate isomerase: the role of the active site cysteine residues. Physical Chemistry Chemical Physics, 2014, 16, 12462-12474.	2.8	6
48	Simulated Breathing: Application of Molecular Dynamics Simulations to Pulmonary Lung Surfactant. Symmetry, 2021, 13, 1259.	2.2	6
49	Computational insights into substrate binding and catalytic mechanism of the glutaminase domain of glucosamine-6-phosphate synthase (GlmS). RSC Advances, 2017, 7, 29626-29638.	3.6	5
50	Generation and Reactions of a Benzodehydrotropylium Ionâ€“Co₂(CO)₆ Complex. ACS Omega, 2019, 4, 18600-18608.	3.5	5
51	A Pseudohypervalent Sulfur Intermediate as an Oxidative Protective Mechanism in the Archaea Peroxiredoxin Enzyme ApTPx. Journal of Physical Chemistry B, 2017, 121, 6570-6579.	2.6	4
52	The K₂(9-ethylguanine)₁₂²⁺ quadruplex is more stable to unimolecular dissociation than the K(9-ethylguanine)₈⁺ quadruplex in the gas phase: a BIRD, energy resolved SORI-CID, IRMPD spectroscopic, and computational study. Physical Chemistry Chemical Physics, 2019, 21, 15319-15326.	2.8	4
53	Antagonizing binding of cell cycle and apoptosis regulatory protein 1 (CARP-1) to the NEMO/IKKÎ³ protein enhances the anticancer effect of chemotherapy. Journal of Biological Chemistry, 2020, 295, 3532-3552.	3.4	4
54	Molecular Dynamics Simulations of a Cytochrome P450 from Tepidiphilus thermophilus (P450-TT) Reveal How Its Substrate-Binding Channel Opens. Molecules, 2021, 26, 3614.	3.8	4

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55	Comparative QM/MM study on the inhibition mechanism of Î²-Hydroxynorvaline to Threonyl-tRNA synthetase. Journal of Molecular Graphics and Modelling, 2022, 115, 108224.	2.4	4
56	The catalytic formation of leukotriene C₄: a critical step in inflammatory processes. Physical Chemistry Chemical Physics, 2014, 16, 16284.	2.8	3
57	Insights from molecular dynamics on substrate binding and effects of active site mutations in Î”¹-pyrroline-5-carboxylate dehydrogenase. Canadian Journal of Chemistry, 2016, 94, 1151-1162.	1.1	3
58	Evidence for an Allosteric S-Nitrosoglutathione Binding Site in S-Nitrosoglutathione Reductase (GSNOR). Antioxidants, 2019, 8, 545.	5.1	3
59	A DFT study on the catalytic mechanism of UDP-glucose dehydrogenase. Canadian Journal of Chemistry, 2010, 88, 804-814.	1.1	2
60	The Importance of the MM Environment and the Selection of the QM Method in QM/MM Calculations. Advances in Protein Chemistry and Structural Biology, 2015, 100, 153-185.	2.3	2
61	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments. , 2004, , 565-580.		1
62	Reply to the â€œComment on 'A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Studyâ€™â€• Journal of Physical Chemistry B, 2011, 115, 10776-10777.	2.6	1
63	Multiscale Computational Study on the Catalytic Mechanism of the Nonmetallo Amidase Maleamate Amidohydrolase (NicF). Journal of Physical Chemistry A, 2019, 123, 7710-7719.	2.5	1
64	Biocatalytic oligomerization of azoles; experimental and computational studies. Environmental Science: Water Research and Technology, 0, , .	2.4	1