

# James W Gauld

## List of Publications by Year in descending order

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64  
papers

1,154  
citations

430874

18  
h-index

434195

31  
g-index

66  
all docs

66  
docs citations

66  
times ranked

1291  
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparative QM/MM study on the inhibition mechanism of $\hat{I}^2$ -Hydroxynorvaline to Threonyl-tRNA synthetase. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108224.	2.4	4
2	Molecular Dynamics Simulations of a Cytochrome P450 from <i>Tepidiphilus thermophilus</i> (P450-TT) Reveal How Its Substrate-Binding Channel Opens. <i>Molecules</i> , 2021, 26, 3614.	3.8	4
3	Simulated Breathing: Application of Molecular Dynamics Simulations to Pulmonary Lung Surfactant. <i>Symmetry</i> , 2021, 13, 1259.	2.2	6
4	Hydrolysis Mechanism of the Linkers by Matrix Metalloproteinase-9 Using QM/MM Calculations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5203-5211.	5.4	10
5	Antagonizing binding of cell cycle and apoptosis regulatory protein 1 (CARP-1) to the NEMO/IKK $\hat{I}^3$ protein enhances the anticancer effect of chemotherapy. <i>Journal of Biological Chemistry</i> , 2020, 295, 3532-3552.	3.4	4
6	Multiscale Computational Study on the Catalytic Mechanism of the Nonmetallo Amidase Maleamate Amidohydrolase (NicF). <i>Journal of Physical Chemistry A</i> , 2019, 123, 7710-7719.	2.5	1
7	Oligomerization of 3-substituted quinolines by catalytic activity of soybean peroxidase as a wastewater treatment. Product formation and computational studies. <i>Chemical Engineering Journal</i> , 2019, 364, 340-348.	12.7	15
8	The K <sub>2</sub> (9-ethylguanine) <sub>12</sub> <sup>2+</sup> quadruplex is more stable to unimolecular dissociation than the K(9-ethylguanine) <sub>8</sub> <sup>+</sup> quadruplex in the gas phase: a BIRD, energy resolved SORI-CID, IRMPD spectroscopic, and computational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15319-15326.	2.8	4
9	A H2AX-CARP-1 Interaction Regulates Apoptosis Signaling Following DNA Damage. <i>Cancers</i> , 2019, 11, 221.	3.7	10
10	Generation and Reactions of a Benzodehydrotropylium Ion-Co <sub>2</sub> (CO) <sub>6</sub> Complex. <i>ACS Omega</i> , 2019, 4, 18600-18608.	3.5	5
11	Evidence for an Allosteric S-Nitrosoglutathione Binding Site in S-Nitrosoglutathione Reductase (GSNOR). <i>Antioxidants</i> , 2019, 8, 545.	5.1	3
12	Unraveling the Critical Role Played by Ado76 <sup>2</sup> -OH in the Post-Transfer Editing by Archaeal Threonyl-tRNA Synthetase. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1092-1101.	2.6	10
13	An Assessment of Computational Methods for Calculating Accurate Structures and Energies of Bio-Relevant Polysulfur/Selenium-Containing Compounds. <i>Molecules</i> , 2018, 23, 3323.	3.8	9
14	A Pseudohypervalent Sulfur Intermediate as an Oxidative Protective Mechanism in the Archaea Peroxiredoxin Enzyme ApTPx. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6570-6579.	2.6	4
15	Roles of the Active Site Zn(II) and Residues in Substrate Discrimination by Threonyl-tRNA Synthetase: An MD and QM/MM Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6163-6174.	2.6	8
16	Computational insights into substrate binding and catalytic mechanism of the glutaminase domain of glucosamine-6-phosphate synthase (GlmS). <i>RSC Advances</i> , 2017, 7, 29626-29638.	3.6	5
17	Pretransfer Editing in Threonyl-tRNA Synthetase: Roles of Differential Solvent Accessibility and Intermediate Stabilization. <i>ACS Catalysis</i> , 2017, 7, 3102-3112.	11.2	8
18	A water-mediated and substrate-assisted aminoacylation mechanism in the discriminating aminoacyl-tRNA synthetase GlnRS and non-discriminating GluRS. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25598-25609.	2.8	12

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19	Enzymatic Post-Transfer Editing Mechanism of <i>E. coli</i> 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
20	Insights from molecular dynamics on substrate binding and effects of active site mutations in $\beta$ -pyrroline-5-carboxylate dehydrogenase. Canadian Journal of Chemistry, 2016, 94, 1151-1162.	1.1	3
21	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
22	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
23	Substrate-Assisted and Enzymatic Pretransfer Editing of Nonstandard Amino Acids by Methionyl-tRNA Synthetase. Biochemistry, 2015, 54, 5757-5765.	2.5	11
24	Glyceraldehyde 3-phosphate dehydrogenase (GAPDH) is inactivated by S-sulfuration in vitro. Free Radical Biology and Medicine, 2015, 89, 512-521.	2.9	97
25	Multi-Scale Computational Enzymology: Enhancing Our Understanding of Enzymatic Catalysis. International Journal of Molecular Sciences, 2014, 15, 401-422.	4.1	7
26	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
27	The catalytic formation of leukotriene C <sub>4</sub> : a critical step in inflammatory processes. Physical Chemistry Chemical Physics, 2014, 16, 16284.	2.8	3
28	A Multi-Scale Computational Study on the Mechanism of Streptococcus pneumoniae Nicotinamidase (SpNic). Molecules, 2014, 19, 15735-15753.	3.8	9
29	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
30	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
31	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
32	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
33	An assessment of pure, hybrid, meta, and hybrid-meta GGA density functional theory methods for open-shell systems: The case of the nonheme iron enzyme 8R-LOX. Journal of Computational Chemistry, 2013, 34, 141-148.	3.3	8
34	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
35	Applications of Potential Energy Surfaces in the Study of Enzymatic Reactions. Advances in Physical Chemistry, 2012, 2012, 1-15.	2.0	16
36	Model Iron-Oxo Species and the Oxidation of Imidazole: Insights into the Mechanism of OvoA and EgtB?. Inorganic Chemistry, 2012, 51, 13351-13356.	4.0	36

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37	Molecular Dynamics Investigation into Substrate Binding and Identity of the Catalytic Base in the Mechanism of Threonyl-tRNA Synthetase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5205-5212.	2.6	20
38	An Active Site Water Broadens Substrate Specificity in <i>S</i> -Ribosylhomocysteinase (LuxS): A Docking, MD, and QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8916-8929.	2.6	10
39	Reply to the "Comment on 'A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Study'" <i>Journal of Physical Chemistry B</i> , 2011, 115, 10776-10777.	2.6	1
40	A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9202-9212.	2.6	12
41	The $\beta$ -Amino Group of the Threonine Substrate as The General Base During tRNA Aminoacylation: A New Version of Substrate-Assisted Catalysis Predicted by Hybrid DFT. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13050-13060.	2.5	18
42	A QM/MM-Based Computational Investigation on the Catalytic Mechanism of Saccharopine Reductase. <i>Molecules</i> , 2011, 16, 8569-8589.	3.8	7
43	The first branching point in porphyrin biosynthesis: A systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogen III decarboxylase. <i>Journal of Computational Chemistry</i> , 2011, 32, 822-834.	3.3	17
44	Computational studies on Schiff-base formation: Implications for the catalytic mechanism of porphobilinogen synthase. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 479-489.	2.5	24
45	A DFT study on the catalytic mechanism of UDP-glucose dehydrogenase. <i>Canadian Journal of Chemistry</i> , 2010, 88, 804-814.	1.1	2
46	Protonation of guanine quartets and quartet stacks: insights from DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 278-287.	2.8	7
47	A DFT Study of Nucleobase Dealkylation by the DNA Repair Enzyme AlkB. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4887-4898.	2.6	64
48	DFT Investigation on the Mechanism of the Deacetylation Reaction Catalyzed by LpxC. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3462-3469.	2.6	26
49	A Density Functional Theory Investigation on the Mechanism of the Second Half-Reaction of Nitric Oxide Synthase. <i>Journal of the American Chemical Society</i> , 2008, 130, 3328-3334.	13.7	30
50	Substrate-assisted Catalysis in the Aminoacyl Transfer Mechanism of Histidyl-tRNA Synthetase: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16874-16882.	2.6	24
51	A Computational Study on the Interaction of the Nitric Oxide Ions NO <sup>+</sup> and NO <sup>-</sup> with the Side Groups of the Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1981-1989.	2.5	13
52	Second Half-Reaction of Nitric Oxide Synthase: Computational Insights into the Initial Step and Key Proposed Intermediate. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23706-23714.	2.6	28
53	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments. , 2004, , 565-580.		1
54	Quantum Chemical Calculations of the NHA Bound Nitric Oxide Synthase Active Site: O <sub>2</sub> Binding and Implications for the Catalytic Mechanism. <i>Journal of the American Chemical Society</i> , 2004, 126, 10267-10270.	13.7	18

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55	An Assessment of Theoretical Methods for the Calculation of Accurate Structures and SN Bond Dissociation Energies of S-Nitrosothiols (RSNOs). <i>Journal of Physical Chemistry A</i> , 2003, 107, 9946-9952.	2.5	57
56	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5155-5159.	2.5	188
57	Recent applications of density functional theory calculations to biomolecules. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 1-11.	1.4	47
58	Modeling the Action of an Antitumor Drug: A Density Functional Theory Study of the Mechanism of Tirapazamine. <i>Journal of the American Chemical Society</i> , 2001, 123, 7320-7325.	13.7	23
59	Hydrogen-Bond Mediated Catalysis: The Aminolysis of 6-Chloropyrimidine as Catalyzed by Derivatives of Uracil. <i>Journal of the American Chemical Society</i> , 2001, 123, 2047-2052.	13.7	8
60	Oxidative Degradation of Pyruvate Formate-Lyase. <i>Journal of the American Chemical Society</i> , 2000, 122, 2035-2040.	13.7	27
61	Catalysis Mediated by Hydrogen Bonding: A Computational Study of the Aminolysis of 6-Chloropyrimidine. <i>Journal of the American Chemical Society</i> , 2000, 122, 5384-5386.	13.7	8
62	Theoretical Studies of the Radiation Products of Hydroxyproline. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8583-8592.	2.5	20
63	A Density Functional Theory Study of the Radiation Products of Glycine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5080-5086.	2.5	36
64	Biocatalytic oligomerization of azoles; experimental and computational studies. <i>Environmental Science: Water Research and Technology</i> , 0, , .	2.4	1