Hong Guo

List of Publications by Year
in descending order

68 papers	2,108 citations	331670 21 h-index	243625 44 g-index
73 all docs	73 docs citations	73 times ranked	2383 citing authors

#	Article	IF	Citations
1	The pineapple genome and the evolution of CAM photosynthesis. Nature Genetics, 2015, 47, 1435-1442.	21.4	472
2	Ab initio studies of hydrogen bonding of N-methylacetamide: structure, cooperativity, and internal rotational barriers. The Journal of Physical Chemistry, 1992, 96, 7273-7287.	2.9	185
3	The KalanchoÃ« genome provides insights into convergent evolution and building blocks of crassulacean acid metabolism. Nature Communications, 2017, 8, 1899.	12.8	159
4	Many-Body Effects in Systems of Peptide Hydrogen-Bonded Networks and Their Contributions to Ligand Binding:Â A Comparison of the Performances of DFT and Polarizable Molecular Mechanics. Journal of Physical Chemistry B, 2000, 104, 9746-9754.	2.6	93
5	Mechanism of histone methylation catalyzed by protein lysine methyltransferase SET7/9 and origin of product specificity. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 8797-8802.	7.1	91
6	Ab initio studies of polyenes. I. 1,3â€butadiene. Journal of Chemical Physics, 1991, 94, 3679-3699.	3.0	89
7	Ab initio force field for the planar vibrations of benzene. Journal of Chemical Physics, 1988, 89, 4235-4245.	3.0	62
8	An (E,E)â€Î±â€farnesene synthase gene of soybean has a role in defence against nematodes and is involved in synthesizing insectâ€induced volatiles. Plant Biotechnology Journal, 2017, 15, 510-519.	8.3	61
9	A 5-Enolpyruvylshikimate 3-Phosphate Synthase Functions as a Transcriptional Repressor in Populus. Plant Cell, 2018, 30, 1645-1660.	6.6	56
10	Combining ab initio and density functional theories with semiempirical methods. Journal of Chemical Physics, 2002, 117, 5617-5631.	3.0	55
11	Catalytic Mechanism of Cellulose Degradation by a Cellobiohydrolase, CelS. PLoS ONE, 2010, 5, e12947.	2.5	39
12	Origin of Tight Binding of a Near-Perfect Transition-State Analogue by Cytidine Deaminase:Â Implications for Enzyme Catalysis. Journal of the American Chemical Society, 2005, 127, 3191-3197.	13.7	38
13	Basis set and polarization function effects on optimized geometries and harmonic frequencies at the secondâ€order Mo/llerâ€“Plesset perturbation level. Journal of Chemical Physics, 1989, 91, 1719-1733.	3.0	37
14	Understanding the Role of Active-Site Residues in Chorismate Mutase Catalysis from Molecular-Dynamics Simulations. Angewandte Chemie - International Edition, 2003, 42, 1508-1511.	13.8	35
15	Stabilization and Destabilization of the Cî^'HÂ·Â·Â·OC Hydrogen Bonds Involving Proline Residues in Helices. Journal of Physical Chemistry B, 2004, 108, 18065-18072.	2.6	29
16	The Importance of Dynamics in Substrate-Assisted Catalysis and Specificity. Journal of the American Chemical Society, 2006, 128, 5994-5995.	13.7	29
17	A General Acidâ^'Base Mechanism for the Stabilization of a Tetrahedral Adduct in a Serineâ^'Carboxyl Peptidase:Â A Computational Study. Journal of the American Chemical Society, 2005, 127, 15662-15663.	13.7	28
18	The QM/MM Molecular Dynamics and Free Energy Simulations of the Acylation Reaction Catalyzed by the Serine-Carboxyl Peptidase Kumamolisin-Asâ€. Biochemistry, 2007, 46, 3784-3792.	2.5	25

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19	Understanding Product Specificity of Protein Lysine Methyltransferases from QM/MM Molecular Dynamics and Free Energy Simulations: The Effects of Mutation on SET7/9 beyond the Tyr/Phe Switch. Journal of Chemical Information and Modeling, 2012, 52, 449-456.	5.4	24
20	Energy Triplets for Writing Epigenetic Marks: Insights from QM/MM Freeâ€Energy Simulations of Protein Lysine Methyltransferases. Chemistry - A European Journal, 2009, 15, 12596-12599.	3.3	22
21	Understanding Energetic Origins of Product Specificity of SET8 from QM/MM Free Energy Simulations: What Causes the Stop of Methyl Addition during Histone Lysine Methylation?. Journal of Chemical Theory and Computation, 2010, 6, 1380-1389.	5.3	22
22	Overexpression of a Domain of Unknown Function 266-containing protein results in high cellulose content, reduced recalcitrance, and enhanced plant growth in the bioenergy crop Populus. Biotechnology for Biofuels, 2017, 10, 74.	6.2	22
23	Catalytic Role of Proton Transfers in the Formation of a Tetrahedral Adduct in a Serine Carboxyl Peptidase. Biochemistry, 2006, 45, 9129-9137.	2.5	21
24	Lysine Possesses the Optimal Chain Length for Histone Lysine Methyltransferase Catalysis. Scientific Reports, 2017, 7, 16148.	3.3	21
25	Understanding the Mechanism of Deacylation Reaction Catalyzed by the Serine Carboxyl Peptidase Kumamolisin-As: Insights from QM/MM Free Energy Simulations. Journal of Physical Chemistry B, 2010, 114, 10594-10600.	2.6	20
26	Biochemical characterization of microbial type terpene synthases in two closely related species of hornworts, Anthoceros punctatus and Anthoceros agrestis. Phytochemistry, 2018, 149, 116-122.	2.9	20
27	Substrate-Assisted Catalysis in the Reaction Catalyzed by Salicylic Acid Binding Protein 2 (SABP2), a Potential Mechanism of Substrate Discrimination for Some Promiscuous Enzymes. Biochemistry, 2015, 54, 5366-5375.	2.5	19
28	The nucleophilic amino group of lysine is central for histone lysine methyltransferase catalysis. Communications Chemistry, 2019, 2, .	4.5	19
29	QM/MM MD and Free Energy Simulations of G9a-Like Protein (GLP) and Its Mutants: Understanding the Factors that Determine the Product Specificity. PLoS ONE, 2012, 7, e37674.	2.5	18
30	VvMJE1 of the grapevine (Vitis vinifera) VvMES methylesterase family encodes for methyl jasmonate esterase and has a role in stress response. Plant Physiology and Biochemistry, 2016, 102, 125-132.	5.8	17
31	Biochemical characterization in Norway spruce (Picea abies) of SABATH methyltransferases that methylate phytohormones. Phytochemistry, 2018, 149, 146-154.	2.9	17
32	Stabilization of a Transition-State Analogue at the Active Site of Yeast Cytosine Deaminase:â€‰ Importance of Proton Transfers. Journal of Physical Chemistry B, 2007, 111, 6501-6506.	2.6	16
33	QM/MM Investigation of Substrate and Product Specificities of Suv4-20h2: How Does This Enzyme Generate Dimethylated H4K20 from Monomethylated Substrate?. Journal of Chemical Theory and Computation, 2017, 13, 2977-2986.	5.3	16
34	Quantum Mechanical/Molecular Mechanical Study of Catalytic Mechanism and Role of Key Residues in Methylation Reactions Catalyzed by Dimethylxanthine Methyltransferase in Caffeine Biosynthesis. Journal of Chemical Information and Modeling, 2014, 54, 593-600.	5.4	15
35	Î³-Thialysine versus Lysine: An Insight into the Epigenetic Methylation of Histones. Bioconjugate Chemistry, 2019, 30, 1798-1804.	3.6	15
36	Importance of the main chain of lysine for histone lysine methyltransferase catalysis. Organic and Biomolecular Chemistry, 2019, 17, 5693-5697.	2.8	14

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37	A peptide-linkage deletion procedure for estimate of energetic contributions of individual peptide groups in a complex environment: Application to parallel I2-Sheets. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 12-20.	3.6	12
38	QM/MM Free Energy Simulations of Salicylic Acid Methyltransferase: Effects of Stabilization of TS-like Structures on Substrate Specificity. Journal of Physical Chemistry B, 2011, 115, 389-396.	2.6	12
39	Evolution and divergence in the coding and promoter regions of the Populus gene family encoding xyloglucan endotransglycosylase/hydrolases. Tree Genetics and Genomes, 2012, 8, 177-194.	1.6	12
40	QM/MM MD and free energy simulations of the methylation reactions catalyzed by protein arginine methyltransferase PRMT3. Canadian Journal of Chemistry, 2013, 91, 605-612.	1.1	12
41	Understanding the Catalytic Mechanism of Xanthosine Methyltransferase in Caffeine Biosynthesis from QM/MM Molecular Dynamics and Free Energy Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1755-1761.	5.4	12
42	Clarification of the Mechanism of Acylation Reaction and Origin of Substrate Specificity of the Serine-Carboxyl Peptidase Sedolisin through QM/MM Free Energy Simulations. Journal of Physical Chemistry B, 2011, 115, 2470-2476.	2.6	11
43	Computational Study of Symmetric Methylation on Histone Arginine Catalyzed by Protein Arginine Methyltransferase PRMT5 through QM/MM MD and Free Energy Simulations. Molecules, 2015, 20, 10032-10046.	3.8	11
44	Catalytic mechanism and origin of high activity of cellulase TmCel12A at high temperature: a quantum mechanical/molecular mechanical study. Cellulose, 2014, 21, 937-949.	4.9	9
45	QM/MM free energy simulations of the reaction catalysed by (4S)-limonene synthase involving linalyl diphosphate (LPP) substrate. Molecular Simulation, 2018, 44, 1158-1167.	2.0	9
46	Lysine Ethylation by Histone Lysine Methyltransferases. ChemBioChem, 2020, 21, 392-400.	2.6	9
47	Structure and Dynamics of the Reactive State for the Histidine Methylation Process and Catalytic Mechanism of SETD3: Insights from Quantum Mechanics/Molecular Mechanics Investigation. ACS Catalysis, 2020, 10, 13314-13322.	11.2	9
48	Examining sterically demanding lysine analogs for histone lysine methyltransferase catalysis. Scientific Reports, 2020, 10, 3671.	3.3	9
49	Understanding the Autocatalytic Process of Proâ€kumamolisin Activation from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical (QM/MM) Freeâ€Energy Simulations. Chemistry - A European Journal, 2013, 19, 10849-10852.	3.3	7
50	Biosynthesis of methyl (E)-cinnamate in the liverwort Conocephalum salebrosum and evolution of cinnamic acid methyltransferase. Phytochemistry, 2019, 164, 50-59.	2.9	7
51	Title is missing!. Angewandte Chemie, 2003, 115, 1546-1549.	2.0	5
52	QM/MM and free-energy simulations of deacylation reaction catalysed by sedolisin, a serine-carboxyl peptidase. Molecular Simulation, 2013, 39, 206-213.	2.0	5
53	Sesquiterpene biosynthesis in a leafy liverwort Radula lindenbergiana Gottsche ex C. Hartm. Phytochemistry, 2021, 190, 112847.	2.9	5
54	Structural basis for the action of xyloglucan endotransglycosylases/hydrolases: Insights from homology modeling. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 133-139.	3.6	4

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55	PPCM: Combing Multiple Classifiers to Improve Protein-Protein Interaction Prediction. International Journal of Genomics, 2015, 2015, 1-7.	1.6	4
56	Histidine methyltransferase <scp>SETD3</scp> methylates structurally diverse histidine mimics in actin. Protein Science, 2022, 31, e4305.	7.6	4
57	QM/MM Analysis of Cellulase Active Sites and Actions of the Enzymes on Substrates. ACS Symposium Series, 2010, , 135-154.	0.5	3
58	Classification of Complete Proteomes of Different Organisms and Protein Sets Based on Their Protein Distributions in Terms of Some Key Attributes of Proteins. International Journal of Genomics, 2018, 2018, 1-12.	1.6	3
59	QM/MM MD and Free Energy Simulation Study of Methyl Transfer Processes Catalyzed by PKMTs and PRMTs. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 309-318.	3.6	2
60	Theoretical study of interaction of heteroaromatic compounds with a cluster model of kaolinite tetrahedral surface. International Journal of Quantum Chemistry, 2017, 117, e25352.	2.0	2
61	Catalytic Mechanism of the Ubiquitin-Like NEDD8 Transfer in RING E3-E2âˆ¼NEDD8-Target Complex from QM/MM Free Energy Simulations. Journal of Chemical Information and Modeling, 2018, 58, 422-429.	5.4	2
62	A Suggestion of Converting Protein Intrinsic Disorder to Structural Entropy Using Shannonâ€™s Information Theory. Entropy, 2019, 21, 591.	2.2	2
63	Catalytic Mechanism and Product Specificity of Protein Arginine Methyltransferase PRMT7: A Study from QM/MM Molecular Dynamics and Free Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5301-5312.	5.3	2
64	Computational Study of Methionine Methylation Process Catalyzed by SETD3. Interdisciplinary Sciences, Computational Life Sciences, 2022, 14, 929-936.	3.6	2
65	Understanding Enzyme Catalysis Mechanism Using QM/MM Simulation Methods. ACS Symposium Series, 2020, , 121-137.	0.5	1
66	Chorismate-Mutase-Catalyzed Claisen Rearrangement. , 0, , 1-23.		0
67	QM/MM MD and free energy simulation study of methyl transfer processes catalyzed by PKMTs and PRMTs. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 309.	3.6	0
68	Unraveling the Origins of Changing Product Specificity Properties of Arginine Methyltransferase PRMT7 by the E181D and E181D/Q329A Mutations through QM/MM MD and Free-Energy Simulations. Journal of Chemical Theory and Computation, 2022, 18, 2631-2641.	5.3	0