Victor Guallar

List of Publications by Year in descending order

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163 papers	6,939 citations	57631 44 h-index	76769 74 g-index
168 all docs	168 docs citations	168 times ranked	8202 citing authors

#	Article	IF	Citations
1	Small molecule interactions with the SARS-CoV-2 main protease: In silico all-atom microsecond MD simulations, PELE Monte Carlo simulations, and determination of in vitro activity inhibition. Journal of Molecular Graphics and Modelling, 2022, 110, 108050.	1.3	5
2	Investigation of small molecule inhibitors of the SARS-CoV-2 papain-like protease by all-atom microsecond modelling, PELE Monte Carlo simulations, and in vitro activity inhibition. Chemical Physics Letters, 2022, 788, 139294.	1.2	10
3	Clinical course impacts early kinetics,magnitude, and amplitude of SARS-CoV-2 neutralizing antibodies beyond 1 year after infection. Cell Reports Medicine, 2022, 3, 100523.	3.3	18
4	Heterogeneous Infectivity and Pathogenesis of SARS-CoV-2 Variants Beta, Delta and Omicron in Transgenic K18-hACE2 and Wildtype Mice. Frontiers in Microbiology, 2022, 13, .	1.5	39
5	Metagenomic Mining for Esterases in the Microbial Community of Los Rueldos Acid Mine Drainage Formation. Frontiers in Microbiology, 2022, 13, .	1.5	4
6	UEP: an open-source and fast classifier for predicting the impact of mutations in proteinâ€“protein complexes. Bioinformatics, 2021, 37, 334-341.	1.8	5
7	SARS-CoV-2 infection elicits a rapid neutralizing antibody response that correlates with disease severity. Scientific Reports, 2021, 11, 2608.	1.6	86
8	Comprehensive Insights into the Production of Long Chain Aliphatic Aldehydes Using a Copper-Radical Alcohol Oxidase as Biocatalyst. ACS Sustainable Chemistry and Engineering, 2021, 9, 4411-4421.	3.2	28
9	Identification of Plitidepsin as Potent Inhibitor of SARS-CoV-2-Induced Cytopathic Effect After a Drug Repurposing Screen. Frontiers in Pharmacology, 2021, 12, 646676.	1.6	40
10	Computationally Driven Rational Design of Substrate Promiscuity on Serine Ester Hydrolases. ACS Catalysis, 2021, 11, 3590-3601.	5.5	17
11	Stable neutralizing antibody levels 6Âmonths after mild and severe COVID-19 episodes. Med, 2021, 2, 313-320.e4.	2.2	77
12	Previous SARS-CoV-2 Infection Increases B.1.1.7 Cross-Neutralization by Vaccinated Individuals. Viruses, 2021, 13, 1135.	1.5	17
13	Structural-Based Modeling in Protein Engineering. A Must Do. Journal of Physical Chemistry B, 2021, 125, 6491-6500.	1.2	11
14	NetCleave: an open-source algorithm for predicting C-terminal antigen processing for MHC-I and MHC-II. Scientific Reports, 2021, 11, 13126.	1.6	7
15	Mapping Potential Determinants of Peroxidative Activity in an Evolved Fungal Peroxygenase from Agrocybe aegerita. Frontiers in Bioengineering and Biotechnology, 2021, 9, 741282.	2.0	6
16	Embelin potentiates venetoclax-induced apoptosis in acute myeloid leukemia cells. Toxicology in Vitro, 2021, 76, 105207.	1.1	2
17	Protection against reinfection with D614- or G614-SARS-CoV-2 isolates in golden Syrian hamster. Emerging Microbes and Infections, 2021, 10, 797-809.	3.0	42
18	Structural basis for substrate specificity of heteromeric transporters of neutral amino acids. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11

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19	SARS-CoV-2 interaction with Siglec-1 mediates trans-infection by dendritic cells. Cellular and Molecular Immunology, 2021, 18, 2676-2678.	4.8	36
20	Enhancing thermostability by modifying flexible surface loops in an evolved highâ€redox potential laccase. AICHE Journal, 2020, 66, e16747.	1.8	18
21	Sequential oxidation of 5-hydroxymethylfurfural to furan-2,5-dicarboxylic acid by an evolved aryl-alcohol oxidase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140293.	1.1	35
22	Genetically engineered proteins with two active sites for enhanced biocatalysis and synergistic chemo- and biocatalysis. Nature Catalysis, 2020, 3, 319-328.	16.1	90
23	aquaPELE: A Monte Carlo-Based Algorithm to Sample the Effects of Buried Water Molecules in Proteins. Journal of Chemical Theory and Computation, 2020, 16, 7655-7670.	2.3	8
24	Known Evolutionary Paths Are Accessible to Engineered ÃŸ-Lactamases Having Altered Protein Motions at the Timescale of Catalytic Turnover. Frontiers in Molecular Biosciences, 2020, 7, 599298.	1.6	3
25	Fatty-Acid Oxygenation by Fungal Peroxygenases: From Computational Simulations to Preparative Regio- and Stereoselective Epoxidation. ACS Catalysis, 2020, 10, 13584-13595.	5.5	25
26	Survivin modulation in the antimelanoma activity of prodiginines. European Journal of Pharmacology, 2020, 888, 173465.	1.7	13
27	Detection of SARS-CoV-2 in a cat owned by a COVID-19â˜affected patient in Spain. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24790-24793.	3.3	154
28	Predicting Antibody Neutralization Efficacy in Hypermutated Epitopes Using Monte Carlo Simulations. Polymers, 2020, 12, 2392.	2.0	0
29	Combining Monte Carlo and Molecular Dynamics Simulations for Enhanced Binding Free Energy Estimation through Markov State Models. Journal of Chemical Information and Modeling, 2020, 60, 5529-5539.	2.5	7
30	Mapping enzyme-substrate interactions: its potential to study the mechanism of enzymes. Advances in Protein Chemistry and Structural Biology, 2020, 122, 1-31.	1.0	11
31	FragPELE: Dynamic Ligand Growing within a Binding Site. A Novel Tool for Hit-To-Lead Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1728-1736.	2.5	14
32	Monte Carlo simulations using PELE to identify a proteinâ€“protein inhibitor binding site and pose. RSC Advances, 2020, 10, 7058-7064.	1.7	7
33	Efficiency of Siteâ€Specific Clicked Laccaseâ€“Carbon Nanotubes Biocathodes towards O₂ Reduction. Chemistry - A European Journal, 2020, 26, 4798-4804.	1.7	24
34	Engineering of a fungal laccase to develop a robust, versatile and highly-expressed biocatalyst for sustainable chemistry. Green Chemistry, 2019, 21, 5374-5385.	4.6	36
35	Structural and biochemical insights into an engineered high-redox potential laccase overproduced in Aspergillus. International Journal of Biological Macromolecules, 2019, 141, 855-867.	3.6	17
36	PELE-MSM: A Monte Carlo Based Protocol for the Estimation of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2019, 15, 6243-6253.	2.3	14

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37	Switching the substrate preference of fungal aryl-alcohol oxidase: towards stereoselective oxidation of secondary benzyl alcohols. Catalysis Science and Technology, 2019, 9, 833-841.	2.1	17
38	Modulating Fatty Acid Epoxidation vs Hydroxylation in a Fungal Peroxygenase. ACS Catalysis, 2019, 9, 6234-6242.	5.5	54
39	Structureâ€Guided Evolution of Aryl Alcohol Oxidase from Pleurotus eryngii for the Selective Oxidation of Secondary Benzyl Alcohols. Advanced Synthesis and Catalysis, 2019, 361, 2514.	2.1	27
40	Increasing Redox Potential, Redox Mediator Activity, and Stability in a Fungal Laccase by Computer-Guided Mutagenesis and Directed Evolution. ACS Catalysis, 2019, 9, 4561-4572.	5.5	96
41	Selective synthesis of 4-hydroxyisophorone and 4-ketoisophorone by fungal peroxygenases. Catalysis Science and Technology, 2019, 9, 1398-1405.	2.1	26
42	Atomistic simulations shed new light on the activation mechanisms of RORÎ³ and classify it as Type III nuclear hormone receptor regarding ligand-binding paths. Scientific Reports, 2019, 9, 17249.	1.6	9
43	Selective Synthesis of the Human Drug Metabolite 5â€²-Hydroxypropranolol by an Evolved Self-Sufficient Peroxygenase. ACS Catalysis, 2018, 8, 4789-4799.	5.5	70
44	Computational structureâ€based drug design: Predicting target flexibility. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1367.	6.2	13
45	Rational Engineering of Multiple Active Sites in an Ester Hydrolase. Biochemistry, 2018, 57, 2245-2255.	1.2	57
46	Determinants and Prediction of Esterase Substrate Promiscuity Patterns. ACS Chemical Biology, 2018, 13, 225-234.	1.6	106
47	Kauniolide synthase is a P450 with unusual hydroxylation and cyclization-elimination activity. Nature Communications, 2018, 9, 4657.	5.8	24
48	Automated Design of Efficient and Functionally Diverse Enzyme Repertoires. Molecular Cell, 2018, 72, 178-186.e5.	4.5	165
49	Multiple implications of an active site phenylalanine in the catalysis of aryl-alcohol oxidase. Scientific Reports, 2018, 8, 8121.	1.6	15
50	Description of a Non-Canonical Mn(II)-Oxidation Site in Peroxidases. ACS Catalysis, 2018, 8, 8386-8395.	5.5	21
51	Pushing the Limits of Computational Structure-Based Drug Design with a Cryo-EM Structure: The Ca²⁺ Channel Î±2Î´-1 Subunit as a Test Case. Journal of Chemical Information and Modeling, 2018, 58, 1707-1715.	2.5	19
52	Probing the Surface of a Laccase for Clues towards the Design of Chemoâ€Enzymatic Catalysts. ChemPlusChem, 2017, 82, 607-614.	1.3	14
53	Molecular Modeling in Enzyme Design, Toward In Silico Guided Directed Evolution. , 2017, , 257-284.		5
54	Simulating Substrate Recognition and Oxidation in Laccases: From Description to Design. Journal of Chemical Theory and Computation, 2017, 13, 1462-1467.	2.3	25

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55	Mapping the Long-Range Electron Transfer Route in Ligninolytic Peroxidases. Journal of Physical Chemistry B, 2017, 121, 3946-3954.	1.2	28
56	Oxidoreductases on their way to industrial biotransformations. Biotechnology Advances, 2017, 35, 815-831.	6.0	205
57	Exploring Binding Mechanisms in Nuclear Hormone Receptors by Monte Carlo and X-ray-derived Motions. Biophysical Journal, 2017, 112, 1147-1156.	0.2	22
58	Repurposing designed mutants: a valuable strategy for computer-aided laccase engineering â€“ the case of POXA1b. Catalysis Science and Technology, 2017, 7, 515-523.	2.1	17
59	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-Î² Fibrils. Journal of Physical Chemistry B, 2017, 121, 8926-8934.	1.2	34
60	Adaptive simulations, towards interactive protein-ligand modeling. Scientific Reports, 2017, 7, 8466.	1.6	58
61	Inhibition of Human Enhancer of Zeste Homolog 2 with Tambjamine Analogs. Journal of Chemical Information and Modeling, 2017, 57, 2089-2098.	2.5	5
62	Interactive GPU-based generation of solvent-excluded surfaces. Visual Computer, 2017, 33, 869-881.	2.5	10
63	Physics-Based Visual Characterization of Molecular Interaction Forces. IEEE Transactions on Visualization and Computer Graphics, 2017, 23, 731-740.	2.9	14
64	The ins and outs of vanillyl alcohol oxidase: Identification of ligand migration paths. PLoS Computational Biology, 2017, 13, e1005787.	1.5	23
65	Enhancing backbone sampling in Monte Carlo simulations using internal coordinates normal mode analysis. Bioorganic and Medicinal Chemistry, 2016, 24, 4855-4866.	1.4	1
66	Computer-Aided Laccase Engineering: Toward Biological Oxidation of Arylamines. ACS Catalysis, 2016, 6, 5415-5423.	5.5	54
67	Ecoupling server: A tool to compute and analyze electronic couplings. Journal of Computational Chemistry, 2016, 37, 1740-1745.	1.5	11
68	Synthesis of 1â€Naphthol by a Natural Peroxygenase Engineered by Directed Evolution. ChemBioChem, 2016, 17, 341-349.	1.3	83
69	Unveiling the basis of alkaline stability of an evolved versatile peroxidase. Biochemical Journal, 2016, 473, 1917-1928.	1.7	13
70	Asymmetric sulfoxidation by engineering the heme pocket of a dye-decolorizing peroxidase. Catalysis Science and Technology, 2016, 6, 6277-6285.	2.1	17
71	Computational Prediction of HIV-1 Resistance to Protease Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 915-923.	2.5	19
72	Combined Use of Oligopeptides, Fragment Libraries, and Natural Compounds: A Comprehensive Approach To Sample the Druggability of Vascular Endothelial Growth Factor. ChemMedChem, 2016, 11, 928-939.	1.6	10

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73	The unravelling of the complex pattern of tyrosinase inhibition. Scientific Reports, 2016, 6, 34993.	1.6	109
74	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
75	Activeâ€Siteâ€Directed Inhibitors of Prolyl Oligopeptidase Abolish Its Conformational Dynamics. ChemBioChem, 2016, 17, 913-917.	1.3	14
76	Re-designing the substrate binding pocket of laccase for enhanced oxidation of sinapic acid. Catalysis Science and Technology, 2016, 6, 3900-3910.	2.1	56
77	Molecular determinants for selective C₂₅-hydroxylation of vitamins D₂and D₃by fungal peroxygenases. Catalysis Science and Technology, 2016, 6, 288-295.	2.1	29
78	Rational Enzyme Engineering Through Biophysical and Biochemical Modeling. ACS Catalysis, 2016, 6, 1624-1629.	5.5	48
79	Real-Time Molecular Visualization Supporting Diffuse Interreflections and Ambient Occlusion. IEEE Transactions on Visualization and Computer Graphics, 2016, 22, 718-727.	2.9	12
80	High quality illustrative effects for molecular rendering. Computers and Graphics, 2016, 54, 113-120.	1.4	6
81	Porphyrin Binding to Gun4 Protein, Facilitated by a Flexible Loop, Controls Metabolite Flow through the Chlorophyll Biosynthetic Pathway. Journal of Biological Chemistry, 2015, 290, 28477-28488.	1.6	28
82	Aromatic stacking interactions govern catalysis in arylâ€alcohol oxidase. FEBS Journal, 2015, 282, 3091-3106.	2.2	22
83	Improving the Oxidative Stability of a High Redox Potential Fungal Peroxidase by Rational Design. PLoS ONE, 2015, 10, e0124750.	1.1	34
84	Steroid Hydroxylation by Basidiomycete Peroxygenases: a Combined Experimental and Computational Study. Applied and Environmental Microbiology, 2015, 81, 4130-4142.	1.4	36
85	Unveiling Prolyl Oligopeptidase Ligand Migration by Comprehensive Computational Techniques. Biophysical Journal, 2015, 108, 116-125.	0.2	20
86	Atomic Picture of Ligand Migration in Toluene 4-Monooxygenase. Journal of Physical Chemistry B, 2015, 119, 671-678.	1.2	8
87	Catalytic surface radical in dye-decolorizing peroxidase: a computational, spectroscopic and site-directed mutagenesis study. Biochemical Journal, 2015, 466, 253-262.	1.7	84
88	Basidiomycete DyPs: Genomic diversity, structuralâ€“functional aspects, reaction mechanism and environmental significance. Archives of Biochemistry and Biophysics, 2015, 574, 66-74.	1.4	71
89	Insights into Laccase Engineering from Molecular Simulations: Toward a Binding-Focused Strategy. Journal of Physical Chemistry Letters, 2015, 6, 1447-1453.	2.1	55
90	Direct Measurement of the Nanomechanical Stability of a Redox Protein Active Site and Its Dependence upon Metal Binding. Journal of Physical Chemistry B, 2015, 119, 12050-12058.	1.2	16

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91	New Monte Carlo Based Technique To Study DNAâ€“Ligand Interactions. Journal of Chemical Theory and Computation, 2015, 11, 5598-5605.	2.3	7
92	A theoretical multiscale treatment of proteinâ€“protein electron transfer: The ferredoxin/ferredoxin-NADP+ reductase and flavodoxin/ferredoxin-NADP+ reductase systems. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1530-1538.	0.5	10
93	Ligand Binding Mechanism in Steroid Receptors: From Conserved Plasticity to Differential Evolutionary Constraints. Structure, 2015, 23, 2280-2290.	1.6	96
94	Conformational Response to Ligand Binding in Phosphomannomutase2. Journal of Biological Chemistry, 2014, 289, 34900-34910.	1.6	34
95	Correlated Inter-Domain Motions in Adenylate Kinase. PLoS Computational Biology, 2014, 10, e1003721.	1.5	19
96	An Alternative Mechanism for the Methylation of Phosphoethanolamine Catalyzed by Plasmodium falciparum Phosphoethanolamine Methyltransferase*. Journal of Biological Chemistry, 2014, 289, 33815-33825.	1.6	12
97	Structural implications of the C-terminal tail in the catalytic and stability properties of manganese peroxidases from ligninolytic fungi. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 3253-3265.	2.5	33
98	Monte Carlo Free Ligand Diffusion with Markov State Model Analysis and Absolute Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2014, 10, 282-288.	2.3	37
99	pyProCT: Automated Cluster Analysis for Structural Bioinformatics. Journal of Chemical Theory and Computation, 2014, 10, 3236-3243.	2.3	7
100	Differential Control of Heme Reactivity in Alpha and Beta Subunits of Hemoglobin: A Combined Raman Spectroscopic and Computational Study. Journal of the American Chemical Society, 2014, 136, 10325-10339.	6.6	34
101	Atomic Level Rendering of DNA-Drug Encounter. Biophysical Journal, 2014, 106, 421-429.	0.2	9
102	Electron transfer in proteins: theory, applications and future perspectives. Physical Chemistry Chemical Physics, 2013, 15, 15271.	1.3	28
103	Single vs. multiple ligand pathways in globins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1739-1743.	1.1	6
104	Direct Observation of Single DNA Structural Alterations at Low Forces with Surface-Enhanced Raman Scattering. Biophysical Journal, 2013, 104, 156-162.	0.2	15
105	pyRMSD: a Python package for efficient pairwise RMSD matrix calculation and handling. Bioinformatics, 2013, 29, 2363-2364.	1.8	14
106	Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1957-1967.	1.1	6
107	In-silico Assessment of Protein-Protein Electron Transfer. A Case Study: Cytochrome c Peroxidase â€“ Cytochrome c. PLoS Computational Biology, 2013, 9, e1002990.	1.5	23
108	Formation of a tyrosine adduct involved in lignin degradation by Trametopsis cervina lignin peroxidase: a novel peroxidase activation mechanism. Biochemical Journal, 2013, 452, 575-584.	1.7	25

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109	PELE web server: atomistic study of biomolecular systems at your fingertips. Nucleic Acids Research, 2013, 41, W322-W328.	6.5	69
110	Tryptogalinin Is a Tick Kunitz Serine Protease Inhibitor with a Unique Intrinsic Disorder. PLoS ONE, 2013, 8, e62562.	1.1	32
111	Molecular Interactions of Prodiginines with the BH3 Domain of Anti-Apoptotic Bcl-2 Family Members. PLoS ONE, 2013, 8, e57562.	1.1	45
112	Role of Active Site Histidines in the Two Half-Reactions of the Aryl-Alcohol Oxidase Catalytic Cycle. Biochemistry, 2012, 51, 6595-6608.	1.2	51
113	Two Tyrosyl Radicals Stabilize High Oxidation States in Cytochrome c Oxidase for Efficient Energy Conservation and Proton Translocation. Journal of the American Chemical Society, 2012, 134, 4753-4761.	6.6	36
114	Exploration of Protein Conformational Change with PELE and Meta-Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 959-965.	2.3	36
115	An Atomistic View on Human Hemoglobin Carbon Monoxide Migration Processes. Biophysical Journal, 2012, 102, 887-896.	0.2	43
116	Hâ€bond network optimization in proteinâ€“protein complexes: Are allâ€atom force field scores enough?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 818-824.	1.5	12
117	Identification of dual mTORC1 and mTORC2 inhibitors in melanoma cells: Prodigiosin vs. obatoclax. Biochemical Pharmacology, 2012, 83, 489-496.	2.0	70
118	Stereoselective Hydride Transfer by Arylâ€Alcohol Oxidase, a Member of the GMC Superfamily. ChemBioChem, 2012, 13, 427-435.	1.3	48
119	Regulation of Electron and Proton Transfer by the Protein Matrix of CytochromecOxidase. Journal of Physical Chemistry B, 2011, 115, 3648-3655.	1.2	20
120	Modulating O2 Reactivity in a Fungal Flavoenzyme. Journal of Biological Chemistry, 2011, 286, 41105-41114.	1.6	46
121	Substrate diffusion and oxidation in GMC oxidoreductases: an experimental and computational study on fungal aryl-alcohol oxidase. Biochemical Journal, 2011, 436, 341-350.	1.7	62
122	Electron transfer pathways in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 1305-1313.	0.5	34
123	Mixed quantum mechanics and molecular mechanics methods: Looking inside proteins. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 315-322.	6.2	30
124	A New View of the Bacterial Cytosol Environment. PLoS Computational Biology, 2011, 7, e1002066.	1.5	39
125	Exploring hierarchical refinement techniques for induced fit docking with protein and ligand flexibility. Journal of Computational Chemistry, 2010, 31, 1224-1235.	1.5	50
126	QM/MM methods: Looking inside heme proteins biochemisty. Biophysical Chemistry, 2010, 149, 1-11.	1.5	37

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127	Temperature Effects on Donorâ^'Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2010, 6, 3241-3248.	2.3	7
128	Vibrational Resonances and CuB Displacement Controlled by Proton Motion in Cytochrome c Oxidase. Journal of Physical Chemistry B, 2010, 114, 1136-1143.	1.2	9
129	Ligand Migration in the Truncated Hemoglobin-II from Mycobacterium tuberculosis. Journal of Biological Chemistry, 2009, 284, 3106-3116.	1.6	52
130	Role of TolC in Klebsiella oxytoca resistance to antibiotics. Journal of Antimicrobial Chemotherapy, 2009, 63, 668-674.	1.3	31
131	Solvent Effects on Donorâ^'Acceptor Couplings in Peptides. A Combined QM and MD Study. Journal of Chemical Theory and Computation, 2009, 5, 3312-3320.	2.3	14
132	Raman Study of Mechanically Induced Oxygenation State Transition of Red Blood Cells Using Optical Tweezers. Biophysical Journal, 2009, 96, 209-216.	0.2	102
133	Peroxide-Dependent Formation of a Covalent Link between Trp51 and the Heme in Cytochrome c Peroxidase. Biochemistry, 2009, 48, 3593-3599.	1.2	18
134	Monitoring of mechanically induced transitions in biology using Raman tweezers. Biophysical Journal, 2009, 96, 311a.	0.2	0
135	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. Methods in Enzymology, 2008, 437, 477-498.	0.4	26
136	Mapping protein electron transfer pathways with QM/MM methods. Journal of the Royal Society Interface, 2008, 5, 233-239.	1.5	34
137	Electron Transfer in the P450cam/PDX Complex. The QM/MM e-Pathway. Journal of Physical Chemistry A, 2008, 112, 12989-12994.	1.1	27
138	Mechanism of Product Release in NO Detoxification from Mycobacterium tuberculosis Truncated Hemoglobin N. Journal of the American Chemical Society, 2008, 130, 1688-1693.	6.6	35
139	Heme Electron Transfer in Peroxidases: The Propionate e-Pathway. Journal of Physical Chemistry B, 2008, 112, 13460-13464.	1.2	32
140	Mechanism of thermal decomposition of carbamoyl phosphate and its stabilization by aspartate and ornithine transcarbamoylases. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16918-16923.	3.3	25
141	Modeling of Ligation-Induced Helix/Loop Displacements in Myoglobin:Â Toward an Understanding of Hemoglobin Allostery. Journal of the American Chemical Society, 2006, 128, 5427-5435.	6.6	40
142	The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450camCatalysis:Â A QM/MM Study. Journal of the American Chemical Society, 2006, 128, 3924-3925.	6.6	105
143	Hydrogen Bonding Pathways in Human Dihydroorotate Dehydrogenase. Journal of Physical Chemistry B, 2006, 110, 19704-19710.	1.2	7
144	The role of the heme propionates in heme biochemistry. Journal of Inorganic Biochemistry, 2006, 100, 755-760.	1.5	57

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145	Importance of accurate charges in molecular docking: Quantum mechanical/molecular mechanical (QM/MM) approach. Journal of Computational Chemistry, 2005, 26, 915-931.	1.5	365
146	A binding mechanism in protein-nucleotide interactions: Implication for U1A RNA binding. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3954-3959.	3.3	35
147	Molecular Dynamics Simulations of Salicylate Effects on the Micro- and Mesoscopic Properties of a Dipalmitoylphosphatidylcholine Bilayer. Biochemistry, 2005, 44, 13425-13438.	1.2	44
148	PELE:Â Protein Energy Landscape Exploration. A Novel Monte Carlo Based Technique. Journal of Chemical Theory and Computation, 2005, 1, 1304-1311.	2.3	190
149	AB INITIO QUANTUM CHEMICAL AND MIXED QUANTUM MECHANICS/MOLECULAR MECHANICS (QM/MM) METHODS FOR STUDYING ENZYMATIC CATALYSIS. Annual Review of Physical Chemistry, 2005, 56, 389-427.	4.8	493
150	Cytochrome P450CAM Enzymatic Catalysis Cycle:Â A Quantum Mechanics/Molecular Mechanics Study. Journal of the American Chemical Society, 2004, 126, 8501-8508.	6.6	130
151	Computational Modeling of the Catalytic Reaction in Triosephosphate Isomerase. Journal of Molecular Biology, 2004, 337, 227-239.	2.0	78
152	Peripheral heme substituents control the hydrogen-atom abstraction chemistry in cytochromes P450. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 6998-7002.	3.3	143
153	A New Semiempirical Approach to Study Ground and Excited States of Metal Complexes in Biological Systemsâ€. Journal of Physical Chemistry B, 2002, 106, 8038-8046.	1.2	13
154	Proton-Transfer Dynamics in the Activation of Cytochrome P450eryF. Journal of the American Chemical Society, 2002, 124, 1430-1437.	6.6	40
155	Dynamics of Alkane Hydroxylation at the Non-Heme Diiron Center in Methane Monooxygenase. Journal of the American Chemical Society, 2002, 124, 3377-3384.	6.6	85
156	Quantum chemical studies of methane monooxygenase: comparision with P450. Current Opinion in Chemical Biology, 2002, 6, 236-242.	2.8	45
157	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2â€²-hydroxyphenyl)â€“oxazole. Journal of Chemical Physics, 2000, 113, 9510-9522.	1.2	59
158	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers. Journal of Chemical Physics, 1999, 110, 9922-9936.	1.2	138
159	DNA Mutations Induced by Proton and Charge Transfer in the Low-Lying Excited Singlet Electronic States of the DNA Base Pairs:Â A Theoretical Insight. Journal of Physical Chemistry A, 1999, 103, 6251-6256.	1.1	104
160	Proton-Transfer Reaction in Isolated and Water-Complexed 8-Hydroxyimidazo[1,2-a]Pyridine in the S0 and S1 Electronic States. A Theoretical Study. Journal of Physical Chemistry A, 1999, 103, 5301-5306.	1.1	11
161	On the localization of the electronic excitation in supramolecules built up by equivalent units linked by hydrogen bonds. Chemical Physics, 1998, 228, 1-7.	0.9	4
162	H-Atom Transfer and Rotational Processes in the Ground and First Singlet Excited Electronic States of 2-(2â€˜-Hydroxyphenyl)oxazole Derivatives:Â Experimental and Theoretical Studiesâ€. The Journal of Physical Chemistry, 1996, 100, 19789-19794.	2.9	86

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163	Theoretical study of molecular dynamics in model base pairs. Chemical Physics Letters, 1996, 256, 370-376.	1.2	90