

Dario A Estrin

List of Publications by Year in descending order

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200
papers

6,876
citations

66250

44
h-index

111975

67
g-index

203
all docs

203
docs citations

203
times ranked

7580
citing authors

#	ARTICLE	IF	CITATIONS
1	Mycobacterium tuberculosis DosS binds H ₂ S through its Fe ³⁺ heme iron to regulate the DosR dormancy regulon. <i>Redox Biology</i> , 2022, 52, 102316.	3.9	8
2	Profiling the Site of Protein CoAlation and Coenzyme A Stabilization Interactions. <i>Antioxidants</i> , 2022, 11, 1362.	2.2	6
3	Control of distal lysine coordination in a monomeric hemoglobin: A role for heme peripheral interactions. <i>Journal of Inorganic Biochemistry</i> , 2021, 219, 111437.	1.5	2
4	Distal lysine (de)coordination in the algal hemoglobin THB1: A combined computer simulation and experimental study. <i>Journal of Inorganic Biochemistry</i> , 2021, 220, 111455.	1.5	1
5	Reactivity of inorganic sulfide species towards a pentacoordinated heme model system. <i>Journal of Inorganic Biochemistry</i> , 2021, 220, 111459.	1.5	1
6	Multiscale Modeling of Thiol Overoxidation in Peroxiredoxins by Hydrogen Peroxide. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 843-853.	2.5	8
7	Design, synthesis and biological evaluation of quinoxaline compounds as anti-HIV agents targeting reverse transcriptase enzyme. <i>European Journal of Medicinal Chemistry</i> , 2020, 188, 111987.	2.6	39
8	Conformational Flexibility Drives Cold Adaptation in Pseudoalteromonas haloplanktis TAC125 Globins. <i>Antioxidants and Redox Signaling</i> , 2020, 32, 396-411.	2.5	6
9	Acidity and nucleophilic reactivity of glutathione persulfide. <i>Journal of Biological Chemistry</i> , 2020, 295, 15466-15481.	1.6	68
10	Electron transfer pathways from quantum dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 225102.	1.2	1
11	Substrate and Product-Assisted Catalysis: Molecular Aspects behind Structural Switches along Organic Hydroperoxide Resistance Protein Catalytic Cycle. <i>ACS Catalysis</i> , 2020, 10, 6587-6602.	5.5	4
12	Nucleotide-dependent dynamics of the Dengue NS3 helicase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2020, 1868, 140441.	1.1	7
13	Dioxygen Binding and Sensing Proteins. <i>Antioxidants and Redox Signaling</i> , 2020, 32, 1151-1154.	2.5	1
14	Structure and function of crocodilian hemoglobins and allosteric regulation by chloride, ATP, and CO ₂ . <i>American Journal of Physiology - Regulatory Integrative and Comparative Physiology</i> , 2020, 318, R657-R667.	0.9	12
15	In Silico Insight into the Reductive Nitrosylation of Ferric Hemeproteins. <i>Inorganic Chemistry</i> , 2020, 59, 3631-3641.	1.9	3
16	Reaction Path Analysis from Potential Energy Contributions Using Forces: An Accessible Estimator of Reaction Coordinate Adequacy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1618-1629.	2.3	3
17	3-Nitrotyrosine and related derivatives in proteins: precursors, radical intermediates and impact in function. <i>Essays in Biochemistry</i> , 2020, 64, 111-133.	2.1	47
18	Ligand Binding Rate Constants in Heme Proteins Using Markov State Models and Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2019, 20, 2451-2460.	1.0	1

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19	Catalysis of Peroxide Reduction by Fast Reacting Protein Thiols. <i>Chemical Reviews</i> , 2019, 119, 10829-10855.	23.0	68
20	Evaluation of quinoxaline compounds as ligands of a site adjacent to S2 (AS2) of cruzain. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2019, 29, 2197-2202.	1.0	8
21	Gating in plant plasma membrane aquaporins: the involvement of leucine in the formation of a pore constriction in the closed state. <i>FEBS Journal</i> , 2019, 286, 3473-3487.	2.2	18
22	Lessons learned about steered molecular dynamics simulations and free energy calculations. <i>Chemical Biology and Drug Design</i> , 2019, 93, 1129-1138.	1.5	17
23	In Search of GABA _A Receptor's Neurosteroid Binding Sites. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 5250-5260.	2.9	15
24	A computational investigation of the reactions of tyrosyl, tryptophanyl, and cysteinyl radicals with nitric oxide and molecular oxygen. <i>Free Radical Research</i> , 2019, 53, 18-25.	1.5	7
25	Thermal Stability of Globins: Implications of Flexibility and Heme Coordination Studied by Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 441-452.	2.5	20
26	Spectroscopy in Complex Environments from QM/MM Simulations. <i>Chemical Reviews</i> , 2018, 118, 4071-4113.	23.0	136
27	Understanding the molecular basis of the high oxygen affinity variant human hemoglobin Coimbra. <i>Archives of Biochemistry and Biophysics</i> , 2018, 637, 73-78.	1.4	7
28	Cold-Adaptation Signatures in the Ligand Rebinding Kinetics to the Truncated Hemoglobin of the Antarctic Bacterium <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11649-11661.	1.2	6
29	Mechanism of Sulfide Binding by Ferric Hemeproteins. <i>Inorganic Chemistry</i> , 2018, 57, 7591-7600.	1.9	19
30	Chemical Reactivity and Spectroscopy Explored From QM/MM Molecular Dynamics Simulations Using the LIO Code. <i>Frontiers in Chemistry</i> , 2018, 6, 70.	1.8	26
31	Kinetics, subcellular localization, and contribution to parasite virulence of a <i>Trypanosoma cruzi</i> hybrid type A heme peroxidase (<i>Tc</i> APx-CcP). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E1326-E1335.	3.3	21
32	Tyrosine oxidation and nitration in transmembrane peptides is connected to lipid peroxidation. <i>Archives of Biochemistry and Biophysics</i> , 2017, 622, 9-25.	1.4	14
33	Naturally occurring fluorescence in frogs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 3672-3677.	3.3	81
34	Tertiary and quaternary structural basis of oxygen affinity in human hemoglobin as revealed by multiscale simulations. <i>Scientific Reports</i> , 2017, 7, 10926.	1.6	23
35	Role of Core Electrons in Quantum Dynamics Using TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 77-85.	2.3	15
36	Structural Plasticity in Globins. <i>Advances in Protein Chemistry and Structural Biology</i> , 2016, 105, 59-80.	1.0	5

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37	The N-terminal pre-A region of <i>Mycobacterium tuberculosis</i> 2/HbN promotes NO -dioxygenase activity. <i>FEBS Journal</i> , 2016, 283, 305-322.	2.2	10
38	Impact of human galectin-1 binding to saccharide ligands on dimer dissociation kinetics and structure. <i>Glycobiology</i> , 2016, 26, 1317-1327.	1.3	16
39	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. <i>Biochemistry</i> , 2016, 55, 2785-2793.	1.2	21
40	Exploring the Catalytic Mechanism of Human Glutamine Synthetase by Computer Simulations. <i>Biochemistry</i> , 2016, 55, 5907-5916.	1.2	8
41	Experimental and Theoretical Study of the High-Temperature UV-Visible Spectra of Aqueous Hydroquinone and 1,4-Benzoquinone. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10547-10552.	1.2	4
42	Access and Binding of H_2S to Hemoproteins: The Case of Hbl of <i>Lucina pectinata</i> . <i>Journal of Physical Chemistry B</i> , 2016, 120, 9642-9653.	1.2	28
43	PrxQ B from <i>Mycobacterium tuberculosis</i> is a monomeric, thioredoxin-dependent and highly efficient fatty acid hydroperoxide reductase. <i>Free Radical Biology and Medicine</i> , 2016, 101, 249-260.	1.3	23
44	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3390-3397.	2.3	10
45	Theoretical investigation of the mechanism of nitroxyl decomposition in aqueous solution. <i>Journal of Inorganic Biochemistry</i> , 2016, 162, 102-108.	1.5	12
46	A quantitative model for oxygen uptake and release in a family of hemoproteins. <i>Bioinformatics</i> , 2016, 32, 1805-1813.	1.8	15
47	Mapping the protein-binding sites for iridium(III)-based CO-releasing molecules. <i>Dalton Transactions</i> , 2016, 45, 12206-12214.	1.6	18
48	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. <i>PLoS Computational Biology</i> , 2016, 12, e1004701.	1.5	36
49	Structural flexibility of the heme cavity in the cold-adapted truncated hemoglobin from the Antarctic marine bacterium <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>FEBS Journal</i> , 2015, 282, 2948-2965.	2.2	24
50	Insights into the mechanism of the reaction between hydrogen sulfide and peroxyxynitrite. <i>Free Radical Biology and Medicine</i> , 2015, 80, 93-100.	1.3	41
51	Molecular Mechanism of Myoglobin Autoxidation: Insights from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1802-1813.	1.2	23
52	Exploring the molecular basis of neurosteroid binding to the $\gamma^2\delta^3$ homopentameric GABA A receptor. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2015, 154, 159-167.	1.2	13
53	Destabilization of the torsioned conformation of a ligand side chain inverts the LXR γ activity. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2015, 1851, 1577-1586.	1.2	9
54	Molecular Basis of Hydroperoxide Specificity in Peroxiredoxins: The Case of AhpE from <i>Mycobacterium tuberculosis</i> . <i>Biochemistry</i> , 2015, 54, 7237-7247.	1.2	18

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55	Reactivity of Inorganic Sulfide Species toward a Heme Protein Model. <i>Inorganic Chemistry</i> , 2015, 54, 527-533.	1.9	36
56	Engineered chimeras reveal the structural basis of hexacoordination in globins: A case study of neuroglobin and myoglobin. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 169-177.	1.1	20
57	Ligand uptake in <i>Mycobacterium tuberculosis</i> truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , 2015, 4, 22.	0.8	8
58	Ligand uptake in <i>Mycobacterium tuberculosis</i> truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , 2015, 4, 22.	0.8	11
59	Mechanistic Insight into the Enzymatic Reduction of Truncated Hemoglobin N of <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2014, 289, 21573-21583.	1.6	15
60	Interplay of the H-Bond Donor–Acceptor Role of the Distal Residues in Hydroxyl Ligand Stabilization of <i>Thermobifida fusca</i> Truncated Hemoglobin. <i>Biochemistry</i> , 2014, 53, 8021-8030.	1.2	15
61	Thiol redox biochemistry: insights from computer simulations. <i>Biophysical Reviews</i> , 2014, 6, 27-46.	1.5	29
62	Molecular basis of thermal stability in truncated (2/2) hemoglobins. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2014, 1840, 2281-2288.	1.1	9
63	Structural basis of redox-dependent modulation of galectin-1 dynamics and function. <i>Glycobiology</i> , 2014, 24, 428-441.	1.3	44
64	Interaction between Proteins and Ir Based CO Releasing Molecules: Mechanism of Adduct Formation and CO Release. <i>Inorganic Chemistry</i> , 2014, 53, 10456-10462.	1.9	22
65	The extraordinary catalytic ability of peroxiredoxins: a combined experimental and QM/MM study on the fast thiol oxidation step. <i>Chemical Communications</i> , 2014, 50, 10070-10073.	2.2	43
66	Coupling of tyrosine deprotonation and axial ligand exchange in nitrocytochrome c. <i>Chemical Communications</i> , 2014, 50, 2592-2594.	2.2	21
67	Ligand Uptake Modulation by Internal Water Molecules and Hydrophobic Cavities in Hemoglobins. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1234-1245.	1.2	25
68	Coordination of peroxide to the CuM center of peptidylglycine β -hydroxylating monooxygenase (PHM): structural and computational study. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 223-232.	1.1	24
69	Molecular basis of the NO trans influence in quaternary T-state human hemoglobin: A computational study. <i>FEBS Letters</i> , 2013, 587, 2393-2398.	1.3	5
70	Mechanism of cysteine oxidation by peroxyxynitrite: An integrated experimental and theoretical study. <i>Archives of Biochemistry and Biophysics</i> , 2013, 539, 81-86.	1.4	30
71	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. <i>Journal of Biological Chemistry</i> , 2013, 288, 6754-6762.	1.6	28
72	H-bonding networks of the distal residues and water molecules in the active site of <i>Thermobifida fusca</i> hemoglobin. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1901-1909.	1.1	21

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73	Conformational States of 2-Methylpyrimidine Nucleosides in Single and Double Nucleic Acid Stranded Structures. <i>Journal of Physical Chemistry B</i> , 2013, 117, 57-69.	1.2	6
74	Small ligand-globin interactions: Reviewing lessons derived from computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1722-1738.	1.1	37
75	Quaternary structure effects on the hexacoordination equilibrium in rice hemoglobin rHb1: Insights from molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 863-873.	1.5	10
76	The key role of water in the dioxygenase function of <i>Escherichia coli</i> flavohemoglobin. <i>Journal of Inorganic Biochemistry</i> , 2013, 119, 75-84.	1.5	9
77	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pKas: The Case of Nitrophorin 4. <i>PLoS Computational Biology</i> , 2012, 8, e1002761.	1.5	110
78	Complete Reaction Mechanism of Indoleamine 2,3-Dioxygenase as Revealed by QM/MM Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1401-1413.	1.2	68
79	Molecular basis of intramolecular electron transfer in proteins during radical-mediated oxidations: Computer simulation studies in model tyrosine-cysteine peptides in solution. <i>Archives of Biochemistry and Biophysics</i> , 2012, 525, 82-91.	1.4	31
80	Role of PheE15 Gate in Ligand Entry and Nitric Oxide Detoxification Function of <i>Mycobacterium tuberculosis</i> Truncated Hemoglobin N. <i>PLoS ONE</i> , 2012, 7, e49291.	1.1	26
81	The <i>Caenorhabditis elegans</i> DAF-12 nuclear receptor: Structure, dynamics, and interaction with ligands. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1798-1809.	1.5	10
82	Molecular Basis of the Mechanism of Thiol Oxidation by Hydrogen Peroxide in Aqueous Solution: Challenging the S _N 2 Paradigm. <i>Chemical Research in Toxicology</i> , 2012, 25, 741-746.	1.7	61
83	Following Ligand Migration Pathways from Picoseconds to Milliseconds in Type II Truncated Hemoglobin from <i>Thermobifida fusca</i> . <i>PLoS ONE</i> , 2012, 7, e39884.	1.1	22
84	Biophysical Characterisation of Neuroglobin of the Icefish, a Natural Knockout for Hemoglobin and Myoglobin. Comparison with Human Neuroglobin. <i>PLoS ONE</i> , 2012, 7, e44508.	1.1	28
85	Tetrachlorocarbonyliridates: Water-Soluble Carbon Monoxide Releasing Molecules Rate-Modulated by the Sixth Ligand. <i>Inorganic Chemistry</i> , 2011, 50, 2334-2345.	1.9	40
86	Ligand Migration in <i>Methanosarcina acetivorans</i> Protoglobin: Effects of Ligand Binding and Dimeric Assembly. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13771-13780.	1.2	31
87	Fluoride as a Probe for H-Bonding Interactions in the Active Site of Heme Proteins: The Case of <i>Thermobifida fusca</i> Hemoglobin. <i>Journal of the American Chemical Society</i> , 2011, 133, 20970-20980.	6.6	29
88	When Galectins Recognize Glycans: From Biochemistry to Physiology and Back Again. <i>Biochemistry</i> , 2011, 50, 7842-7857.	1.2	238
89	An Integrated Computational Analysis of the Structure, Dynamics, and Ligand Binding Interactions of the Human Galectin Network. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1918-1930.	2.5	23
90	Role of the Distal Hydrogen-Bonding Network in Regulating Oxygen Affinity in the Truncated Hemoglobin III from <i>Campylobacter jejuni</i> . <i>Biochemistry</i> , 2011, 50, 3946-3956.	1.2	23

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91	Molecular Basis for the Substrate Stereoselectivity in Tryptophan Dioxygenase. <i>Biochemistry</i> , 2011, 50, 10910-10918.	1.2	42
92	Exploring the molecular basis of human manganese superoxide dismutase inactivation mediated by tyrosine 34 nitration. <i>Archives of Biochemistry and Biophysics</i> , 2011, 507, 304-309.	1.4	48
93	Structural Model for p75NTRâ€™TrkA Intracellular Domain Interaction: A Combined FRET and Bioinformatics Study. <i>Journal of Molecular Biology</i> , 2011, 414, 681-698.	2.0	26
94	Aromaticâ€™Aromatic Interactions in Proteins: Beyond the Dimer. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1623-1633.	2.5	115
95	The peculiar heme pocket of the 2/2 hemoglobin of cold-adapted <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 299-311.	1.1	21
96	Protonation of histidine 55 affects the oxygen access to heme in the alpha chain of the hemoglobin from the Antarctic fish <i>Trematomus bernacchii</i> . <i>IUBMB Life</i> , 2011, 63, 175-182.	1.5	14
97	Structure and dynamics of Antarctic fish neuroglobin assessed by computer simulations. <i>IUBMB Life</i> , 2011, 63, 206-213.	1.5	13
98	Comparing and combining implicit ligand sampling with multiple steered molecular dynamics to study ligand migration processes in heme proteins. <i>Journal of Computational Chemistry</i> , 2011, 32, 2219-2231.	1.5	39
99	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. <i>Carbohydrate Research</i> , 2011, 346, 939-948.	1.1	23
100	Protein dynamics and ligand migration interplay as studied by computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1054-1064.	1.1	30
101	Coordinated nitroxyl anion is produced and released as nitrous oxide by the decomposition of iridium-coordinated nitrosothiols. <i>Inorganica Chimica Acta</i> , 2011, 366, 85-90.	1.2	3
102	Ligand Migration in the Apolar Tunnel of <i>Cerebratulus lacteus</i> Mini-Hemoglobin. <i>Journal of Biological Chemistry</i> , 2011, 286, 5347-5358.	1.6	23
103	The first step of the dioxygenation reaction carried out by tryptophan dioxygenase and indoleamine 2,3-dioxygenase as revealed by quantum mechanical/molecular mechanical studies. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 811-823.	1.1	53
104	Inhibitory effect of quercetin on matrix metalloproteinase 9 activity Molecular mechanism and structureâ€™activity relationship of the flavonoidâ€™enzyme interaction. <i>European Journal of Pharmacology</i> , 2010, 644, 138-145.	1.7	65
105	Unraveling the molecular basis for ligand binding in truncated hemoglobins: The trHbO <i>Bacillus subtilis</i> case. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 962-970.	1.5	36
106	Substrate stereoâ€™specificity in tryptophan dioxygenase and indoleamine 2,3â€™dioxygenase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2961-2972.	1.5	35
107	Comparative Studies of Human Indoleamine 2,3-dioxygenase and Tryptophan Dioxygenase. , 2010, , .		1
108	High Protein Structural Flexibility Of A Truncated Hemoglobin From An Antarctic Cold-Adapted Bacterium. , 2010, , .		0

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109	Heme Pocket Structural Properties of a Bacterial Truncated Hemoglobin from <i>Thermobifida fusca</i> . <i>Biochemistry</i> , 2010, 49, 10394-10402.	1.2	25
110	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8536-8543.	1.2	49
111	Copper-Transfer Mechanism from the Human Chaperone Atox1 to a Metal-Binding Domain of Wilson Disease Protein. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3698-3706.	1.2	44
112	Linking the Structure and Thermal Stability of β -Galactoside-Binding Protein Galectin-1 to Ligand Binding and Dimerization Equilibria. <i>Biochemistry</i> , 2010, 49, 7652-7658.	1.2	18
113	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2009, 284, 14457-14468.	1.6	59
114	Evidence for a ferryl intermediate in a heme-based dioxygenase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 17371-17376.	3.3	113
115	Exploring the Nitric Oxide Detoxification Mechanism of <i>Mycobacterium tuberculosis</i> Truncated Haemoglobin N. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2009, , 33-47.	0.5	6
116	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 885-894.	1.5	43
117	The hemoglobins of the sub-Antarctic fish <i>Cottoperca gobio</i> , a phylogenetically basal species α oxygen-binding equilibria, kinetics and molecular dynamics. <i>FEBS Journal</i> , 2009, 276, 2266-2277.	2.2	27
118	Molecular Basis for the Electric Field Modulation of Cytochrome <i>c</i> Structure and Function. <i>Journal of the American Chemical Society</i> , 2009, 131, 16248-16256.	6.6	66
119	Molecular Basis for the pH Dependent Structural Transition of Nitrophorin 4. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2135-2142.	1.2	19
120	pH-Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1192-1201.	1.2	37
121	Carbohydrate-Binding Proteins: Dissecting Ligand Structures through Solvent Environment Occupancy. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8717-8724.	1.2	33
122	Exploring the molecular basis of heme coordination in human neuroglobin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 695-705.	1.5	54
123	Structural determinants of ligand migration in <i>Mycobacterium tuberculosis</i> truncated hemoglobin O. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 372-379.	1.5	47
124	Hemisuccinate of 21 α -Hydroxy-6,19 α -Epoxyprogesterone: A Tissue-Specific Modulator of the Glucocorticoid Receptor. <i>ChemMedChem</i> , 2008, 3, 1869-1877.	1.6	16
125	DFT study on the reactivity of iron porphyrins tuned by ring substitution. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 70-76.	1.5	23
126	Theoretical insight into the hydroxylamine oxidoreductase mechanism. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 1523-1530.	1.5	40

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127	QM-MM investigation of the reaction products between nitroxyl and O ₂ in aqueous solution. Chemical Physics Letters, 2008, 463, 112-116.	1.2	7
128	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. Methods in Enzymology, 2008, 437, 477-498.	0.4	26
129	NMR and molecular dynamics studies of the interaction of melatonin with calmodulin. Protein Science, 2008, 13, 2925-2938.	3.1	40
130	Bond or Cage Effect: How Nitrophorins Transport and Release Nitric Oxide. Journal of the American Chemical Society, 2008, 130, 1611-1618.	6.6	38
131	Structural and Energetic Study of Cisplatin and Derivatives: Comparison of the Performance of Density Functional Theory Implementations. Journal of Chemical Theory and Computation, 2008, 4, 740-750.	2.3	18
132	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. Biochemistry, 2008, 47, 9793-9802.	1.2	62
133	A Unique Family of Stable and Water-Soluble S-Nitrosothiol Complexes. Inorganic Chemistry, 2008, 47, 4723-4733.	1.9	23
134	Mechanism of Product Release in NO Detoxification from <i>Mycobacterium tuberculosis</i> Truncated Hemoglobin N. Journal of the American Chemical Society, 2008, 130, 1688-1693.	6.6	35
135	Dynamical Characterization of the Heme NO Oxygen Binding (HNOX) Domain. Insight into Soluble Guanylate Cyclase Allosteric Transition. Biochemistry, 2008, 47, 9416-9427.	1.2	49
136	Exploring the Molecular Basis of Action of the Passive Antiglucocorticoid 21-Hydroxy-6,19-epoxyprogesterone. Journal of Medicinal Chemistry, 2008, 51, 1352-1360.	2.9	22
137	Synthesis, Structure, and Reactivity of Aliphatic Primary Nitrosamines Stabilized by Coordination to [IrCl ₅] ²⁻ . Organometallics, 2008, 27, 1985-1995.	1.1	14
138	Short-range and long-range solvent effects on charge-transfer-to-solvent transitions of I ⁻ and K+I ⁻ contact ion pair dissolved in supercritical ammonia. Journal of Chemical Physics, 2007, 126, 174504.	1.2	15
139	QM-MM Investigation of the Reaction of Peroxynitrite with Carbon Dioxide in Water. Journal of Chemical Theory and Computation, 2007, 3, 1405-1411.	2.3	14
140	Characterization of the Galectin-1 Carbohydrate Recognition Domain in Terms of Solvent Occupancy. Journal of Physical Chemistry B, 2007, 111, 7360-7366.	1.2	31
141	Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Truncated Hemoglobin-N from <i>Mycobacterium tuberculosis</i> . Journal of the American Chemical Society, 2007, 129, 6782-6788.	6.6	46
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