Dario A Estrin

List of Publications by Year
in descending order

200 papers	6,876 citations	57758 44 h-index	98798 67 g-index
203 all docs	203 docs citations	203 times ranked	6871 citing authors

#	Article	IF	Citations
1	When Galectins Recognize Glycans: From Biochemistry to Physiology and Back Again. Biochemistry, 2011, 50, 7842-7857.	2.5	238
2	Small Clusters of Water Molecules Using Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 8701-8711.	2.9	182
3	A Density Functional Study of Tautomerism of Uracil and Cytosine. The Journal of Physical Chemistry, 1994, 98, 5653-5660.	2.9	140
4	The Catalytic Mechanism of Peptidylglycine Î±-Hydroxylating Monooxygenase Investigated by Computer Simulation. Journal of the American Chemical Society, 2006, 128, 12817-12828.	13.7	137
5	Spectroscopy in Complex Environments from QMâ€“MM Simulations. Chemical Reviews, 2018, 118, 4071-4113.	47.7	136
6	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems:Â Application to Chorismate Mutase. Journal of Physical Chemistry B, 2003, 107, 13728-13736.	2.6	116
7	Aromaticâ€“Aromatic Interactions in Proteins: Beyond the Dimer. Journal of Chemical Information and Modeling, 2011, 51, 1623-1633.	5.4	115
8	Evidence for a ferryl intermediate in a heme-based dioxygenase. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 17371-17376.	7.1	113
9	Multiple-Steering QMâ˜MM Calculation of the Free Energy Profile in Chorismate Mutase. Journal of the American Chemical Society, 2005, 127, 6940-6941.	13.7	112
10	Theoretical Study of the Truncated Hemoglobin HbN:Â Exploring the Molecular Basis of the NO Detoxification Mechanism. Journal of the American Chemical Society, 2005, 127, 4433-4444.	13.7	111
11	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pKas: The Case of Nitrophorin 4. PLoS Computational Biology, 2012, 8, e1002761.	3.2	110
12	Discrimination of Nitroxyl and Nitric Oxide by Water-Soluble Mn(III) Porphyrins. Journal of the American Chemical Society, 2005, 127, 4680-4684.	13.7	109
13	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. Proteins: Structure, Function and Bioinformatics, 2006, 64, 457-464.	2.6	95
14	Heme Protein Oxygen Affinity Regulation Exerted by Proximal Effects. Journal of the American Chemical Society, 2006, 128, 12455-12461.	13.7	91
15	Dioxygen affinity in heme proteins investigated by computer simulation. Journal of Inorganic Biochemistry, 2006, 100, 761-770.	3.5	89
16	Fast Nitroxyl Trapping by Ferric Porphyrins. Journal of the American Chemical Society, 2003, 125, 15272-15273.	13.7	82
17	Naturally occurring fluorescence in frogs. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3672-3677.	7.1	81
18	Scavenging of NO by Melatonin. Journal of the American Chemical Society, 2000, 122, 10468-10469.	13.7	80

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19	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. Theoretical Chemistry Accounts, 2006, 116, 338-346.	1.4	79
20	Modeling heme proteins using atomistic simulations. Physical Chemistry Chemical Physics, 2006, 8, 5611-5628.	2.8	77
21	Solvent effects in density functional calculations of uracil and cytosine tautomerism. International Journal of Quantum Chemistry, 1995, 56, 615-625.	2.0	74
22	Structure and spin-state energetics of an iron porphyrin model: An assessment of theoretical methods. International Journal of Quantum Chemistry, 2002, 87, 158-166.	2.0	74
23	Reactions of Melatonin and Related Indoles with Free Radicals:Â A Computational Study. Journal of Medicinal Chemistry, 1998, 41, 3684-3689.	6.4	73
24	Complete Reaction Mechanism of Indoleamine 2,3-Dioxygenase as Revealed by QM/MM Simulations. Journal of Physical Chemistry B, 2012, 116, 1401-1413.	2.6	68
25	Catalysis of Peroxide Reduction by Fast Reacting Protein Thiols. Chemical Reviews, 2019, 119, 10829-10855.	47.7	68
26	Acidity and nucleophilic reactivity of glutathione persulfide. Journal of Biological Chemistry, 2020, 295, 15466-15481.	3.4	68
27	Molecular Basis for the Electric Field Modulation of Cytochrome c Structure and Function. Journal of the American Chemical Society, 2009, 131, 16248-16256.	13.7	66
28	Inhibitory effect of quercetin on matrix metalloproteinase 9 activity Molecular mechanism and structureâ€“activity relationship of the flavonoidâ€“enzyme interaction. European Journal of Pharmacology, 2010, 644, 138-145.	3.5	65
29	Nitric Oxide Interaction with Cytochromecâ€˜ and Its Relevance to Guanylate Cyclase. Why Does the Iron Histidine Bond Break?. Journal of the American Chemical Society, 2005, 127, 7721-7728.	13.7	64
30	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. Biochemistry, 2008, 47, 9793-9802.	2.5	62
31	Molecular Basis of the Mechanism of Thiol Oxidation by Hydrogen Peroxide in Aqueous Solution: Challenging the S_N2 Paradigm. Chemical Research in Toxicology, 2012, 25, 741-746.	3.3	61
32	Theoretical and Experimental Study of Medium Effects on the Structure and Spectroscopy of the [Fe(CN)5NO]2-Ion. Inorganic Chemistry, 1996, 35, 3897-3903.	4.0	59
33	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2009, 284, 14457-14468.	3.4	59
34	Exploring the molecular basis of heme coordination in human neuroglobin. Proteins: Structure, Function and Bioinformatics, 2008, 71, 695-705.	2.6	54
35	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. Journal of Biological Inorganic Chemistry, 2010, 15, 811-823.	2.6	53
36	Transnitrosation of Nitrosothiols:Â Characterization of an Elusive Intermediate. Journal of the American Chemical Society, 2005, 127, 486-487.	13.7	51

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37	Dynamical Characterization of the Heme NO Oxygen Binding (HNOX) Domain. Insight into Soluble Guanylate Cyclase Allosteric Transition. Biochemistry, 2008, 47, 9416-9427.	2.5	49
38	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. Journal of Physical Chemistry B, 2010, 114, 8536-8543.	2.6	49
39	A Surprisingly StableS-Nitrosothiol Complex. Journal of the American Chemical Society, 2006, 128, 2512-2513.	13.7	48
40	Exploring the molecular basis of human manganese superoxide dismutase inactivation mediated by tyrosine 34 nitration. Archives of Biochemistry and Biophysics, 2011, 507, 304-309.	3.0	48
41	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. Journal of Pineal Research, 2002, 33, 31-36.	7.4	47
42	Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O. Proteins: Structure, Function and Bioinformatics, 2008, 73, 372-379.	2.6	47
43	3-Nitrotyrosine and related derivatives in proteins: precursors, radical intermediates and impact in function. Essays in Biochemistry, 2020, 64, 111-133.	4.7	47
44	Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A quantum-classical simulation study. Journal of Chemical Physics, 2002, 117, 2718-2725.	3.0	46
45	Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Truncated Hemoglobin-N fromMycobacterium tuberculosis. Journal of the American Chemical Society, 2007, 129, 6782-6788.	13.7	46
46	Electronic energy shifts of a sodium atom in argon clusters by simulated annealing. Journal of Chemical Physics, 1990, 93, 7187-7200.	3.0	45
47	Copper-Transfer Mechanism from the Human Chaperone Atox1 to a Metal-Binding Domain of Wilson Disease Protein. Journal of Physical Chemistry B, 2010, 114, 3698-3706.	2.6	44
48	Structural basis of redox-dependent modulation of galectin-1 dynamics and function. Glycobiology, 2014, 24, 428-441.	2.5	44
49	AM1 Study of the Ground and Excited State Potential Energy Surfaces of Symmetric Carbocyanines. Journal of Physical Chemistry A, 1997, 101, 6998-7006.	2.5	43
50	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. Proteins: Structure, Function and Bioinformatics, 2009, 75, 885-894.	2.6	43
51	The extraordinary catalytic ability of peroxiredoxins: a combined experimental and QM/MM study on the fast thiol oxidation step. Chemical Communications, 2014, 50, 10070-10073.	4.1	43
52	Molecular Basis for the Substrate Stereoselectivity in Tryptophan Dioxygenase. Biochemistry, 2011, 50, 10910-10918.	2.5	42
53	Insights into the mechanism of the reaction between hydrogen sulfide and peroxynitrite. Free Radical Biology and Medicine, 2015, 80, 93-100.	2.9	41
54	Nitrosation of melatonin by nitric oxide: a computational study. Journal of Pineal Research, 2001, 31, 97-101.	7.4	40

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55	Theoretical insight into the hydroxylamine oxidoreductase mechanism. Journal of Inorganic Biochemistry, 2008, 102, 1523-1530.	3.5	40
56	NMR and molecular dynamics studies of the interaction of melatonin with calmodulin. Protein Science, 2008, 13, 2925-2938.	7.6	40
57	Tetrachlorocarbonyliridates: Water-Soluble Carbon Monoxide Releasing Molecules Rate-Modulated by the Sixth Ligand. Inorganic Chemistry, 2011, 50, 2334-2345.	4.0	40
58	Modulation of the NO trans effect in heme proteins: implications for the activation of soluble guanylate cyclase. Journal of Biological Inorganic Chemistry, 2003, 8, 595-600.	2.6	39
59	QMâ^'MM Study of Nitrite Reduction by Nitrite Reductase ofPseudomonas aeruginosa. Journal of Physical Chemistry B, 2004, 108, 18073-18080.	2.6	39
60	Comparing and combining implicit ligand sampling with multiple steered molecular dynamics to study ligand migration processes in heme proteins. Journal of Computational Chemistry, 2011, 32, 2219-2231.	3.3	39
61	Design, synthesis and biological evaluation of quinoxaline compounds as anti-HIV agents targeting reverse transcriptase enzyme. European Journal of Medicinal Chemistry, 2020, 188, 111987.	5.5	39
62	Bond or Cage Effect:â€‰ How Nitrophorins Transport and Release Nitric Oxide. Journal of the American Chemical Society, 2008, 130, 1611-1618.	13.7	38
63	Theoretical Investigation on the Electronic Structure of Pentacyano(L)ferrate(II) Complexes with NO+, NO, and NO-Ligands. Redox Interconversion, Protonation, and Cyanide-Releasing Reactions. Inorganic Chemistry, 2001, 40, 4127-4133.	4.0	37
64	pH-Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4. Journal of Physical Chemistry B, 2009, 113, 1192-1201.	2.6	37
65	Small ligandâ€“globin interactions: Reviewing lessons derived from computer simulation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1722-1738.	2.3	37
66	Unraveling the molecular basis for ligand binding in truncated hemoglobins: The trHbO Bacillus subtilis case. Proteins: Structure, Function and Bioinformatics, 2010, 78, 962-970.	2.6	36
67	Reactivity of Inorganic Sulfide Species toward a Heme Protein Model. Inorganic Chemistry, 2015, 54, 527-533.	4.0	36
68	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. PLoS Computational Biology, 2016, 12, e1004701.	3.2	36
69	Electric field effects on the reactivity of heme model systems. Chemical Physics Letters, 2007, 434, 121-126.	2.6	35
70	HNO trapping and assisted decomposition of nitroxyl donors by ferric hemes. Polyhedron, 2007, 26, 4673-4679.	2.2	35
71	Mechanism of Product Release in NO Detoxification from Mycobacterium tuberculosis Truncated Hemoglobin N. Journal of the American Chemical Society, 2008, 130, 1688-1693.	13.7	35
72	Substrate stereoâ€specificity in tryptophan dioxygenase and indoleamine 2,3â€dioxygenase. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2961-2972.	2.6	35

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73	Oxygen affinity controlled by dynamical distal conformations: The soybean leghemoglobin and the Paramecium caudatum hemoglobin cases. Proteins: Structure, Function and Bioinformatics, 2007, 68, 480-487.	2.6	33
74	Carbohydrate-Binding Proteins: Dissecting Ligand Structures through Solvent Environment Occupancy. Journal of Physical Chemistry B, 2009, 113, 8717-8724.	2.6	33
75	Characterization of the Galectin-1 Carbohydrate Recognition Domain in Terms of Solvent Occupancy. Journal of Physical Chemistry B, 2007, 111, 7360-7366.	2.6	31
76	Ligand Migration in Methanosarcina acetivorans Protoglobin: Effects of Ligand Binding and Dimeric Assembly. Journal of Physical Chemistry B, 2011, 115, 13771-13780.	2.6	31
77	Molecular basis of intramolecular electron transfer in proteins during radical-mediated oxidations: Computer simulation studies in model tyrosineâ€“cysteine peptides in solution. Archives of Biochemistry and Biophysics, 2012, 525, 82-91.	3.0	31
78	Protein dynamics and ligand migration interplay as studied by computer simulation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1054-1064.	2.3	30
79	Mechanism of cysteine oxidation by peroxynitrite: An integrated experimental and theoretical study. Archives of Biochemistry and Biophysics, 2013, 539, 81-86.	3.0	30
80	Fluoride as a Probe for H-Bonding Interactions in the Active Site of Heme Proteins: The Case of Thermobifida fusca Hemoglobin. Journal of the American Chemical Society, 2011, 133, 20970-20980.	13.7	29
81	Thiol redox biochemistry: insights from computer simulations. Biophysical Reviews, 2014, 6, 27-46.	3.2	29
82	Electronic spectra of indolyl radicals: a time-dependent DFT study. Chemical Physics Letters, 2002, 365, 15-21.	2.6	28
83	Mechanisms of NO Release by N1-Nitrosomelatonin:â€‰ Nucleophilic Attack versus Reducing Pathways. Journal of Organic Chemistry, 2005, 70, 5790-5798.	3.2	28
84	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. Journal of Biological Chemistry, 2013, 288, 6754-6762.	3.4	28
85	Access and Binding of H₂S to Hemeproteins: The Case of HbI of Lucina pectinata. Journal of Physical Chemistry B, 2016, 120, 9642-9653.	2.6	28
86	Biophysical Characterisation of Neuroglobin of the Icefish, a Natural Knockout for Hemoglobin and Myoglobin. Comparison with Human Neuroglobin. PLoS ONE, 2012, 7, e44508.	2.5	28
87	Concertedness and solvent effects in multiple proton transfer reactions: The formic acid dimer in solution. Journal of Chemical Physics, 2000, 112, 9498-9508.	3.0	27
88	Hydrogen Bonding and O2Affinity of Hemoglobins. Journal of the American Chemical Society, 2001, 123, 8436-8437.	13.7	27
89	The hemoglobins of the subâ€Antarctic fish Cottoperca gobio, a phyletically basal species â€“ oxygenâ€binding equilibria, kinetics and molecular dynamics. FEBS Journal, 2009, 276, 2266-2277.	4.7	27
90	Nitric Oxide Binding to Ferric Cytochrome P450:â€‰ A Computational Study. Inorganic Chemistry, 2000, 39, 2352-2359.	4.0	26

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91	Solvation and Structure of LiAlH4in Ethereal Solvents. Inorganic Chemistry, 2005, 44, 5286-5292.	4.0	26
92	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. Methods in Enzymology, 2008, 437, 477-498.	1.0	26
93	Structural Model for p75NTRâ€“TrkA Intracellular Domain Interaction: A Combined FRET and Bioinformatics Study. Journal of Molecular Biology, 2011, 414, 681-698.	4.2	26
94	Role of PheE15 Gate in Ligand Entry and Nitric Oxide Detoxification Function of Mycobacterium tuberculosis Truncated Hemoglobin N. PLoS ONE, 2012, 7, e49291.	2.5	26
95	Chemical Reactivity and Spectroscopy Explored From QM/MM Molecular Dynamics Simulations Using the LIO Code. Frontiers in Chemistry, 2018, 6, 70.	3.6	26
96	Electronic spectra of NaAr4and NaAr6: Isomerization and melting. Journal of Chemical Physics, 1992, 96, 7977-7991.	3.0	25
97	Structure, solvation, and bonding in pentacyano(L)ferrate(II) ions (L=aliphatic amine): a density functional study. Journal of Molecular Modeling, 2001, 7, 201-206.	1.8	25
98	Heme Pocket Structural Properties of a Bacterial Truncated Hemoglobin from Thermobifida fusca. Biochemistry, 2010, 49, 10394-10402.	2.5	25
99	Ligand Uptake Modulation by Internal Water Molecules and Hydrophobic Cavities in Hemoglobins. Journal of Physical Chemistry B, 2014, 118, 1234-1245.	2.6	25
100	Structure and Bonding in Pentacyano(L)ferrate(II) and Pentacyano(L)ruthenate(II) Complexes (L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6832-6837.	4.0	24
101	Coordination of peroxide to the CuM center of peptidylglycine Î±-hydroxylating monooxygenase (PHM): structural and computational study. Journal of Biological Inorganic Chemistry, 2013, 18, 223-232.	2.6	24
102	Structural flexibility of the heme cavity in the coldâ€adapted truncated hemoglobin from the Antarctic marine bacterium PseudoalteromonasÂhaloplanktis <scp>TAC</scp>125. FEBS Journal, 2015, 282, 2948-2965.	4.7	24
103	Environment effects on chemical reactivity of heme proteins. International Journal of Quantum Chemistry, 2002, 90, 1505-1514.	2.0	23
104	DFT study on the reactivity of iron porphyrins tuned by ring substitution. Journal of Inorganic Biochemistry, 2008, 102, 70-76.	3.5	23
105	A Unique Family of Stable and Water-Soluble S-Nitrosothiol Complexes. Inorganic Chemistry, 2008, 47, 4723-4733.	4.0	23
106	An Integrated Computational Analysis of the Structure, Dynamics, and Ligand Binding Interactions of the Human Galectin Network. Journal of Chemical Information and Modeling, 2011, 51, 1918-1930.	5.4	23
107	Role of the Distal Hydrogen-Bonding Network in Regulating Oxygen Affinity in the Truncated Hemoglobin III fromCampylobacter jejuni. Biochemistry, 2011, 50, 3946-3956.	2.5	23
108	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. Carbohydrate Research, 2011, 346, 939-948.	2.3	23

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109	Ligand Migration in the Apolar Tunnel of Cerebratulus lacteus Mini-Hemoglobin. Journal of Biological Chemistry, 2011, 286, 5347-5358.	3.4	23
110	Molecular Mechanism of Myoglobin Autoxidation: Insights from Computer Simulations. Journal of Physical Chemistry B, 2015, 119, 1802-1813.	2.6	23
111	PrxQ B from Mycobacterium tuberculosis is a monomeric, thioredoxin-dependent and highly efficient fatty acid hydroperoxide reductase. Free Radical Biology and Medicine, 2016, 101, 249-260.	2.9	23
112	Tertiary and quaternary structural basis of oxygen affinity in human hemoglobin as revealed by multiscale simulations. Scientific Reports, 2017, 7, 10926.	3.3	23
113	Stabilization of Aliphatic and Aromatic Diazonium Ions by Coordination:â€‰ An Experimental and Theoretical Study. Organometallics, 2000, 19, 3810-3817.	2.3	22
114	Exploring the Molecular Basis of Action of the Passive Antiglucocorticoid 21-Hydroxy-6,19-epoxyprogesterone. Journal of Medicinal Chemistry, 2008, 51, 1352-1360.	6.4	22
115	Interaction between Proteins and Ir Based CO Releasing Molecules: Mechanism of Adduct Formation and CO Release. Inorganic Chemistry, 2014, 53, 10456-10462.	4.0	22
116	Following Ligand Migration Pathways from Picoseconds to Milliseconds in Type II Truncated Hemoglobin from Thermobifida fusca. PLoS ONE, 2012, 7, e39884.	2.5	22
117	Two distinct heme distal site states define Cerebratulus lacteus mini-hemoglobin oxygen affinity. Proteins: Structure, Function and Bioinformatics, 2005, 62, 641-648.	2.6	21
118	The peculiar heme pocket of the 2/2 hemoglobin of cold-adapted Pseudoalteromonas haloplanktis TAC125. Journal of Biological Inorganic Chemistry, 2011, 16, 299-311.	2.6	21
119	H-bonding networks of the distal residues and water molecules in the active site of Thermobifida fusca hemoglobin. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1901-1909.	2.3	21
120	Coupling of tyrosine deprotonation and axial ligand exchange in nitrocytochrome c. Chemical Communications, 2014, 50, 2592-2594.	4.1	21
121	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. Biochemistry, 2016, 55, 2785-2793.	2.5	21
122	Kinetics, subcellular localization, and contribution to parasite virulence of a Trypanosoma cruzi hybrid type A heme peroxidase (Tc APx-CcP). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E1326-E1335.	7.1	21
123	Engineered chimeras reveal the structural basis of hexacoordination in globins: A case study of neuroglobin and myoglobin. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 169-177.	2.4	20
124	Thermal Stability of Globins: Implications of Flexibility and Heme Coordination Studied by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 441-452.	5.4	20
125	Hybrid Quantum Classical Molecular Dynamics Simulation of the Proton-Transfer Reaction of HO- with HBr in Aqueous Clusters. Journal of Physical Chemistry A, 1999, 103, 5105-5112.	2.5	19
126	Molecular structure effects on the kinetics of hydroxyl radical addition to azo dyes. Journal of Physical Organic Chemistry, 2002, 15, 287-292.	1.9	19

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127	Molecular Basis for the pH Dependent Structural Transition of Nitrophorin 4. Journal of Physical Chemistry B, 2009, 113, 2135-2142.	2.6	19
128	Mechanism of Sulfide Binding by Ferric Hemeproteins. Inorganic Chemistry, 2018, 57, 7591-7600.	4.0	19
129	Structural and Energetic Study of Cisplatin and Derivatives: Comparison of the Performance of Density Funtional Theory Implementations. Journal of Chemical Theory and Computation, 2008, 4, 740-750.	5.3	18
130	Linking the Structure and Thermal Stability of Î²-Galactoside-Binding Protein Galectin-1 to Ligand Binding and Dimerization Equilibria. Biochemistry, 2010, 49, 7652-7658.	2.5	18
131	Molecular Basis of Hydroperoxide Specificity in Peroxiredoxins: The Case of AhpE from Mycobacterium tuberculosis. Biochemistry, 2015, 54, 7237-7247.	2.5	18
132	Gating in plant plasma membrane aquaporins: the involvement of leucine in the formation of a pore constriction in the closed state. FEBS Journal, 2019, 286, 3473-3487.	4.7	18
133	Mapping the protein-binding sites for iridium(<scp>iii</scp>)-based CO-releasing molecules. Dalton Transactions, 2016, 45, 12206-12214.	3.3	18
134	Solvent Effects on Peroxynitrite Structure and Properties from QM/MM Simulations. Journal of Physical Chemistry A, 2005, 109, 9598-9604.	2.5	17
135	Lessons learned about steered molecular dynamics simulations and free energy calculations. Chemical Biology and Drug Design, 2019, 93, 1129-1138.	3.2	17
136	Proximal effects in the modulation of nitric oxide synthase reactivity: a QM-MM study. Journal of Biological Inorganic Chemistry, 2005, 10, 595-604.	2.6	16
137	Hemisuccinate of 21â€Hydroxyâ€6,19â€Epoxyprogesterone: A Tissueâ€Specific Modulator of the Glucocorticoid Receptor. ChemMedChem, 2008, 3, 1869-1877.	3.2	16
138	Impact of human galectin-1 binding to saccharide ligands on dimer dissociation kinetics and structure. Glycobiology, 2016, 26, 1317-1327.	2.5	16
139	Short-range and long-range solvent effects on charge-transfer-to-solvent transitions of Iâ¯ and K+Iâ¯ contact ion pair dissolved in supercritical ammonia. Journal of Chemical Physics, 2007, 126, 174504.	3.0	15
140	Mechanistic Insight into the Enzymatic Reduction of Truncated Hemoglobin N of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2014, 289, 21573-21583.	3.4	15
141	Interplay of the H-Bond Donorâ€“Acceptor Role of the Distal Residues in Hydroxyl Ligand Stabilization of Thermobifida fusca Truncated Hemoglobin. Biochemistry, 2014, 53, 8021-8030.	2.5	15
142	A quantitative model for oxygen uptake and release in a family of hemeproteins. Bioinformatics, 2016, 32, 1805-1813.	4.1	15
143	Role of Core Electrons in Quantum Dynamics Using TDDFT. Journal of Chemical Theory and Computation, 2017, 13, 77-85.	5.3	15
144	In Search of GABA_A Receptorâ€™s Neurosteroid Binding Sites. Journal of Medicinal Chemistry, 2019, 62, 5250-5260.	6.4	15

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145	Influence of Solvent Effects on the Basicity of Pentaammine(pyrazine)ruthenium(II) and Pentacyano(pyrazine)ruthenate(II) Ions:Â A Density Functional Study. Inorganic Chemistry, 1998, 37, 2033-2038.	4.0	14
146	N-Nitrosomelatonin. Acta Crystallographica Section C: Crystal Structure Communications, 2000, 56, 682-683.	0.4	14
147	Ab Initio Study of NMR15N Chemical Shift Differences Induced by Ca2+Binding to EF-Hand Proteinsâ€. Biochemistry, 2004, 43, 6554-6564.	2.5	14
148	QM-MM Investigation of the Reaction of Peroxynitrite with Carbon Dioxide in Water. Journal of Chemical Theory and Computation, 2007, 3, 1405-1411.	5.3	14
149	Electronic Perturbation in a Molecular Nanowire of [IrCl₅(NO)]^{â^'} Units. Chemistry - A European Journal, 2007, 13, 8428-8436.	3.3	14
150	Synthesis, Structure, and Reactivity of Aliphatic Primary Nitrosamines Stabilized by Coordination to [IrCl₅]^{2â^'}. Organometallics, 2008, 27, 1985-1995.	2.3	14
151	Protonation of histidine 55 affects the oxygen access to heme in the alpha chain of the hemoglobin from the Antarctic fish Trematomus bernacchii. IUBMB Life, 2011, 63, 175-182.	3.4	14
152	Tyrosine oxidation and nitration in transmembrane peptides is connected to lipid peroxidation. Archives of Biochemistry and Biophysics, 2017, 622, 9-25.	3.0	14
153	Structure and dynamics of Antarctic fish neuroglobin assessed by computer simulations. IUBMB Life, 2011, 63, 206-213.	3.4	13
154	Exploring the molecular basis of neurosteroid binding to the Î²3 homopentameric GABA A receptor. Journal of Steroid Biochemistry and Molecular Biology, 2015, 154, 159-167.	2.5	13
155	Application of the Hill determinant method to the vibrational motion of diatomic molecules. Journal of Chemical Physics, 1987, 87, 7059-7061.	3.0	12
156	Theoretical investigation of the mechanism of nitroxyl decomposition in aqueous solution. Journal of Inorganic Biochemistry, 2016, 162, 102-108.	3.5	12
157	Structure and function of crocodilian hemoglobins and allosteric regulation by chloride, ATP, and CO₂. American Journal of Physiology - Regulatory Integrative and Comparative Physiology, 2020, 318, R657-R667.	1.8	12
158	Generalized Hill determinant method. Physics Letters, Section A: General, Atomic and Solid State Physics, 1988, 130, 330-332.	2.1	11
159	Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules. F1000Research, 2015, 4, 22.	1.6	11
160	The Caenorhabditis elegans DAFâ€12 nuclear receptor: Structure, dynamics, and interaction with ligands. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1798-1809.	2.6	10
161	Quaternary structure effects on the hexacoordination equilibrium in rice hemoglobin rHb1: Insights from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2013, 81, 863-873.	2.6	10
162	The Nâ€terminal preâ€A region of MycobacteriumÂtuberculosis 2/2HbN promotes <scp>NO</scp>â€dioxygenase activity. FEBS Journal, 2016, 283, 305-322.	4.7	10

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