

Ernst-Walter Knapp

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3763945/publications.pdf>

Version: 2024-02-01

169
papers

7,668
citations

47006

47
h-index

62596

80
g-index

176
all docs

176
docs citations

176
times ranked

7095
citing authors

#	ARTICLE	IF	CITATIONS
1	Multivalency as a Chemical Organization and Action Principle. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10472-10498.	13.8	854
2	Protein dynamics. <i>Journal of Molecular Biology</i> , 1982, 161, 177-194.	4.2	357
3	Electrostatic models for computing protonation and redox equilibria in proteins. <i>European Biophysics Journal</i> , 1999, 28, 533-551.	2.2	250
4	Î±-Helices direct excitation energy flow in the Fennaâ€“Matthewsâ€“Olson protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 16862-16867.	7.1	183
5	Energetics of a Possible Proton Exit Pathway for Water Oxidation in Photosystem II. <i>Biochemistry</i> , 2006, 45, 2063-2071.	2.5	167
6	A consistent picture of protein dynamics.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1984, 81, 7088-7092.	7.1	162
7	Oxygen-Evolving Mn Cluster in Photosystem II: The Protonation Pattern and Oxidation State in the High-Resolution Crystal Structure. <i>Journal of the American Chemical Society</i> , 2012, 134, 7442-7449.	13.7	158
8	Analysis of optical spectra from single crystals of <i>Rhodospseudomonas viridis</i> reaction centers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1985, 82, 8463-8467.	7.1	145
9	Calculated pH-Dependent Population and Protonation of Carbon-Monoxo-Myoglobin Conformers. <i>Biophysical Journal</i> , 2001, 80, 1141-1150.	0.5	144
10	Recent advances in anionâ€“Î• interactions. <i>CrystEngComm</i> , 2011, 13, 3293.	2.6	144
11	Computational Simulation and Analysis of Dynamic Association between Plastocyanin and Cytochrome f. Consequences for the Electron-Transfer Reaction. <i>Journal of the American Chemical Society</i> , 1997, 119, 42-52.	13.7	129
12	Optimizing pK_A computation in proteins with pH adapted conformations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 1335-1348.	2.6	123
13	Metal Ligand Aromatic Cationâ€“Î• Interactions in Metalloproteins: Ligands Coordinated to Metal Interact with Aromatic Residues. <i>Chemistry - A European Journal</i> , 2000, 6, 3935-3942.	3.3	120
14	Electron Transfer between the Quinones in the Photosynthetic Reaction Center and Its Coupling to Conformational Changesâ€“. <i>Biochemistry</i> , 2000, 39, 10487-10496.	2.5	110
15	How to guarantee optimal stability for most representative structures in the protein data bank. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 79-96.	2.6	109
16	Energetics of Electron-Transfer and Protonation Reactions of the Quinones in the Photosynthetic Reaction Center of <i>Rhodospseudomonas viridis</i> â€“. <i>Biochemistry</i> , 1998, 37, 2488-2495.	2.5	104
17	How photosynthetic reaction centers control oxidation power in chlorophyll pairs P680, P700, and P870. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 9855-9860.	7.1	104
18	Redox Potential of Quinones in Both Electron Transfer Branches of Photosystem I. <i>Journal of Biological Chemistry</i> , 2003, 278, 52002-52011.	3.4	103

#	ARTICLE	IF	CITATIONS
19	Accurate pKa Determination for a Heterogeneous Group of Organic Molecules. ChemPhysChem, 2004, 5, 1513-1522.	2.1	103
20	The concentration dependence of the vibrational linewidth and shift in liquid binary mixtures: An analytical model. Journal of Chemical Physics, 1982, 76, 4730-4735.	3.0	97
21	The influence of protein dynamics on MÃ¶ssbauer spectra. Journal of Chemical Physics, 1983, 78, 4701-4711.	3.0	93
22	On the lineshapes of vibronically resolved molecular aggregate spectra. application to pseudoisocyanin (PIC). Chemical Physics Letters, 1984, 111, 481-486.	2.6	93
23	Structural fluctuations of myoglobin from normal-modes, MÃ¶ssbauer, Raman, and absorption spectroscopy. Biophysical Journal, 1996, 70, 2092-2099.	0.5	93
24	Control of Quinone Redox Potentials in Photosystem II:Â Electron Transfer and Photoprotection. Journal of the American Chemical Society, 2005, 127, 14714-14720.	13.7	93
25	Empirical Conversion of p <i>K</i> _a Values between Different Solvents and Interpretation of the Parameters: Application to Water, Acetonitrile, Dimethyl Sulfoxide, and Methanol. ACS Omega, 2018, 3, 1653-1662.	3.5	92
26	Magnetic field effect on the hyperfineâ€ induced electron spin motion in radicals undergoing diamagneticâ€ paramagnetic exchange. Journal of Chemical Physics, 1979, 71, 1878-1883.	3.0	80
27	Calculation of protonation patterns in proteins with structural relaxation and molecular ensembles - application to the photosynthetic reaction center. European Biophysics Journal, 1998, 27, 626-637.	2.2	80
28	Redox Potentials of Chlorophylls in the Photosystem II Reaction Centerâ€. Biochemistry, 2005, 44, 4118-4124.	2.5	80
29	Correlation of structural and spectroscopic properties of a photosynthetic reaction center. Chemical Physics Letters, 1985, 119, 1-4.	2.6	72
30	On the theory of homogeneous and inhomogeneous line broadening. An exactly solvable model. Journal of Chemical Physics, 1981, 74, 89-95.	3.0	68
31	Tuning Heme Redox Potentials in the Cytochrome c Subunit of Photosynthetic Reaction Centers. Journal of Biological Chemistry, 2003, 278, 51993-52001.	3.4	65
32	One-Electron Reduction Potential for Oxygen- and Sulfur-Centered Organic Radicals in Protic and Aprotic Solvents. Journal of the American Chemical Society, 2005, 127, 15730-15737.	13.7	62
33	Factors Determining the Orientation of Axially Coordinated Imidazoles in Heme Proteinsâ€. Biochemistry, 2001, 40, 7914-7928.	2.5	60
34	Protonation and Stability of the Globular Domain of Influenza Virus Hemagglutinin. Biophysical Journal, 2002, 82, 1050-1058.	0.5	60
35	Prediction using step-wise L1, L2 regularization and feature selection for small data sets with large number of features. BMC Bioinformatics, 2011, 12, 412.	2.6	60
36	Energetics of Radical Transfer in DNA Photolyase. Journal of the American Chemical Society, 2002, 124, 3775-3782.	13.7	59

#	ARTICLE	IF	CITATIONS
37	Quantum-mechanical treatment of collision-induced dissociation. <i>Journal of Chemical Physics</i> , 1977, 67, 4969-4975.	3.0	58
38	Function of Redox-Active Tyrosine in Photosystem II. <i>Biophysical Journal</i> , 2006, 90, 3886-3896.	0.5	58
39	Novel protein folds and their nonsequential structural analogs. <i>Protein Science</i> , 2008, 17, 1374-1382.	7.6	58
40	Variation of Ser-L223 Hydrogen Bonding with the QB Redox State in Reaction Centers from <i>Rhodobacter sphaeroides</i> . <i>Journal of the American Chemical Society</i> , 2004, 126, 8059-8064.	13.7	55
41	Vibrational energy relaxation of diatomic molecules isolated in rare-gas matrices: Role of orientational motions. <i>Journal of Chemical Physics</i> , 1978, 68, 4056-4065.	3.0	54
42	Redox Potential of Quinones in Photosynthetic Reaction Centers from <i>Rhodobacter sphaeroides</i> : Dependence on Protonation of Glu-L212 and Asp-L213. <i>Biochemistry</i> , 2003, 42, 3882-3892.	2.5	54
43	Proton conduction in linear hydrogen-bonded systems. <i>Chemical Physics</i> , 1980, 46, 215-229.	1.9	53
44	Comparison of the Physiologically Equivalent Proteins Cytochrome c6 and Plastocyanin on the Basis of Their Electrostatic Potentials. Tryptophan 63 in Cytochrome c6 May Be Isofunctional with Tyrosine 83 in Plastocyanin. <i>Biochemistry</i> , 1997, 36, 16187-16196.	2.5	53
45	Proton solvation in protic and aprotic solvents. <i>Journal of Computational Chemistry</i> , 2016, 37, 1082-1091.	3.3	53
46	A statistical mechanical method to optimize energy functions for protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000, 97, 3977-3981.	7.1	51
47	Artificial Cytochrome b: Computer Modeling and Evaluation of Redox Potentials. <i>Journal of the American Chemical Society</i> , 2001, 123, 6040-6053.	13.7	49
48	The Deacylation Step of Acetylcholinesterase: Computer Simulation Studies. <i>Journal of the American Chemical Society</i> , 2000, 122, 12254-12262.	13.7	48
49	Connectivity independent protein-structure alignment: a hierarchical approach. <i>BMC Bioinformatics</i> , 2006, 7, 510.	2.6	48
50	Statistical Thermodynamics of the Stability of Multivalent Ligand-Receptor Complexes. <i>Physical Review Letters</i> , 2008, 100, 178101.	7.8	48
51	Accurate redox potentials of mononuclear iron, manganese, and nickel model complexes*. <i>Journal of Computational Chemistry</i> , 2009, 30, 203-211.	3.3	47
52	Negative solubility coefficient of methylated cyclodextrins in water: A theoretical study. <i>Chemical Physics Letters</i> , 2001, 336, 504-510.	2.6	46
53	Polypeptide folding with off-lattice Monte Carlo dynamics: the method. <i>European Biophysics Journal</i> , 1996, 24, 387-403.	2.2	43
54	Protonation States of Ammonia/Ammonium in the Hydrophobic Pore of Ammonia Transporter Protein AmtB. <i>Journal of the American Chemical Society</i> , 2007, 129, 1210-1215.	13.7	41

#	ARTICLE	IF	CITATIONS
55	Vibrational line shapes in liquids. The role of resonant intermolecular coupling. <i>Journal of Chemical Physics</i> , 1984, 81, 643-652.	3.0	40
56	Structural alignment of ferredoxin and flavodoxin based on electrostatic potentials: Implications for their interactions with photosystem I and ferredoxin-NADP reductase. , 2000, 38, 301-309.		40
57	p <i>K_a</i> Values in Proteins Determined by Electrostatics Applied to Molecular Dynamics Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2827-2840.	5.3	38
58	Computational studies on imidazole heme conformations. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 343-354.	2.6	36
59	Electron transfer and protein dynamics. <i>Journal of Chemical Physics</i> , 1987, 87, 3880-3887.	3.0	34
60	Improved p <i>K_a</i> prediction: Combining empirical and semimicroscopic methods. <i>Journal of Computational Chemistry</i> , 2008, 29, 2575-2581.	3.3	33
61	Exploring classification strategies with the CoEPrA 2006 contest. <i>Bioinformatics</i> , 2010, 26, 603-609.	4.1	33
62	Exploring the Possible Role of Glu286 in C <i>c</i> O by Electrostatic Energy Computations Combined with Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12432-12441.	2.6	33
63	CONFORMATIONAL ENTROPY OF BIOMOLECULES: BEYOND THE QUASI-HARMONIC APPROXIMATION. , 2007, , .		32
64	Free Energy Computations on the Shift of the Special Pair Redox Potential:Â Mutants of the Reaction Center of <i>Rhodobacter sphaeroides</i> . <i>Journal of the American Chemical Society</i> , 1996, 118, 3743-3752.	13.7	31
65	A molecular docking study of estrogenically active compounds with 1,2-diarylethane and 1,2-diarylethene pharmacophores. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 6527-6537.	3.0	31
66	Oxidation of the Non-Heme Iron Complex in Photosystem II. <i>Biochemistry</i> , 2005, 44, 14772-14783.	2.5	31
67	Superimpose: a 3D structural superposition server. <i>Nucleic Acids Research</i> , 2008, 36, W47-W54.	14.5	31
68	Influence of Spacerâ€Receptor Interactions on the Stability of Bivalent Ligandâ€Receptor Complexes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2595-2604.	2.6	31
69	Function of two β^2 -carotenes near the D1 and D2 proteins in photosystem II dimers. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2007, 1767, 79-87.	1.0	30
70	Balanced and Bias-Corrected Computation of Conformational Entropy Differences for Molecular Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1235-1245.	5.3	30
71	Protein Secondary Structure Classification Revisited: Processing DSSP Information with PSSC. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2166-2179.	5.4	30
72	Exciton-phonon self-trapping: A continuous transition. <i>Chemical Physics Letters</i> , 1984, 106, 191-196.	2.6	28

#	ARTICLE	IF	CITATIONS
73	Contributions of the Protein Environment to the Midpoint Potentials of the A ₁ Phylloquinones and the F _X Iron-Sulfur Cluster in Photosystem I. <i>Biochemistry</i> , 2007, 46, 10804-10816.	2.5	28
74	Statistical Mechanics of the Stability of Multivalent Ligand-Receptor Complexes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5287-5304.	3.1	28
75	Computing p _K Values in Different Solvents by Electrostatic Transformation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3360-3369.	5.3	28
76	Close-coupling calculation of quantum-mechanical probabilities for collision-induced dissociation. <i>Chemical Physics Letters</i> , 1977, 49, 379-383.	2.6	26
77	Electrostatic Influence of PsaC Protein Binding to the PsaA/PsaB Heterodimer in Photosystem I. <i>Biophysical Journal</i> , 2006, 90, 1081-1089.	0.5	26
78	Computing p _K values of hexaaqua transition metal complexes. <i>Journal of Computational Chemistry</i> , 2015, 36, 69-78.	3.3	26
79	Redox potential of cytochrome c550 in the cyanobacterium <i>Thermosynechococcus elongates</i> . <i>FEBS Letters</i> , 2005, 579, 3190-3194.	2.8	25
80	DemQSAR: predicting human volume of distribution and clearance of drugs. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 1121-1133.	2.9	25
81	Multivalent Binding of Formin-binding Protein 21 (FBP21)-Tandem-WW Domains Fosters Protein Recognition in the Pre-spliceosome. <i>Journal of Biological Chemistry</i> , 2011, 286, 38478-38487.	3.4	25
82	The interdependence of small linewidth and frequency changes of a vibration in liquid mixtures of CDCl ₃ and CCl ₄ . <i>Journal of Chemical Physics</i> , 1984, 81, 3774-3778.	3.0	24
83	Protein dynamics with off-lattice Monte Carlo moves. <i>Physical Review E</i> , 1996, 53, 4221-4224.	2.1	24
84	Energetics of Proton Transfer Pathways in Reaction Centers from <i>Rhodobacter sphaeroides</i> . <i>Journal of Biological Chemistry</i> , 2005, 280, 12446-12450.	3.4	24
85	Stability and fluctuations of amide hydrogen bonds in a bacterial cytochrome c: a molecular dynamics study. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 26-40.	2.6	24
86	Can oxidation states and the protonation pattern of oxomanganese complexes be recognized from their structures?. <i>CrystEngComm</i> , 2011, 13, 6369.	2.6	24
87	Electrostatic p _K computations in proteins: Role of internal cavities. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3320-3332.	2.6	24
88	Lysine 362 in cytochrome c oxidase regulates opening of the K-channel via changes in p _K A and conformation. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2014, 1837, 1998-2003.	1.0	24
89	Folding Pathways of a Helix-Turn-Helix Model Protein. <i>Journal of Physical Chemistry B</i> , 1997, 101, 6734-6740.	2.6	23
90	Redox Potentials of Chlorophylls and β -Carotene in the Antenna Complexes of Photosystem II. <i>Journal of the American Chemical Society</i> , 2005, 127, 1963-1968.	13.7	23

#	ARTICLE	IF	CITATIONS
91	Diffusion of water molecules in crystalline β -cyclodextrin hydrates. <i>Journal of Molecular Graphics and Modelling</i> , 2000, 18, 143-152.	2.4	22
92	A Kunitz type protease inhibitor related protein is synthesized in <i>Drosophila</i> prepupal salivary glands and released into the moulting fluid during pupation. <i>Insect Biochemistry and Molecular Biology</i> , 2004, 34, 855-869.	2.7	22
93	Induced conformational changes upon Cd ²⁺ binding at photosynthetic reaction centers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 16215-16220.	7.1	22
94	Off-lattice Monte Carlo method with constraints: Long-time dynamics of a protein model without nonbonded interactions. <i>Journal of Computational Chemistry</i> , 1993, 14, 19-29.	3.3	21
95	Temperature dependent inelastic X-ray scattering of synchrotron radiation on myoglobin analyzed by the Mössbauer effect. <i>European Biophysics Journal</i> , 1996, 25, 43-46.	2.2	21
96	Cationic State of Accessory Chlorophyll and Electron Transfer through Pheophytin to Plastoquinone in Photosystem II. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1964-1965.	13.8	21
97	Protein Secondary Structure Prediction with SPARROW. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 545-556.	5.4	21
98	Unfolding of the cold shock protein studied with biased molecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 597-606.	2.6	20
99	Tuning electron transfer by ester-group of chlorophylls in bacterial photosynthetic reaction center. <i>FEBS Letters</i> , 2005, 579, 712-716.	2.8	20
100	Predicting protein complex geometries with a neural network. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1026-1039.	2.6	19
101	Proton Transfer in the K-Channel Analog of B-Type Cytochrome c Oxidase from <i>Thermus thermophilus</i> . <i>Biophysical Journal</i> , 2014, 107, 2177-2184.	0.5	19
102	C-H/O Interactions of Aromatic CH Donors within Proteins: A Crystallographic Study. <i>Crystal Growth and Design</i> , 2016, 16, 1948-1957.	3.0	19
103	Conformational entropy of biomolecules: beyond the quasi-harmonic approximation. <i>Genome Informatics</i> , 2007, 18, 192-205.	0.4	19
104	Exchange narrowing of correlated inhomogeneities. The dimer lineshape. <i>Chemical Physics Letters</i> , 1984, 103, 479-483.	2.6	18
105	Long time dynamics of a polymer with rigid body monomer units relating to a protein model: Comparison with the rouse model. <i>Journal of Computational Chemistry</i> , 1992, 13, 793-798.	3.3	18
106	Rubredoxin Function: Redox Behavior from Electrostatics. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 742-752.	5.3	18
107	PSII manganese cluster: Protonation of W2, O5, O4 and His337 in the S1 state explored by combined quantum chemical and electrostatic energy computations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2014, 1837, 1316-1321.	1.0	18
108	Energetics of the loop-to-helix transition leading to the coiled-coil structure of influenza virus hemagglutinin HA2 subunits. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 291-303.	2.6	17

#	ARTICLE	IF	CITATIONS
109	Understanding Rubredoxin Redox Potentials: Role of H-Bonds on Model Complexes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2898-2908.	5.3	17
110	Charge Transport in the ClC-type Chloride-Proton Anti-porter from <i>Escherichia coli</i> . <i>Journal of Biological Chemistry</i> , 2011, 286, 2976-2986.	3.4	17
111	The X-ray absorption spectroscopy Debye-Waller factors of an iron compound and of met-myoglobin as a function of temperature. <i>European Biophysics Journal</i> , 2001, 30, 393-403.	2.2	16
112	Symmetric Structures in the Universe of Protein Folds. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2147-2151.	5.4	16
113	mFES: A Robust Molecular Finite Element Solver for Electrostatic Energy Computations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5095-5112.	5.3	16
114	Merging Structural Information from X-ray Crystallography, Quantum Chemistry, and EXAFS Spectra: The Oxygen-Evolving Complex in PSII. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10899-10922.	2.6	16
115	Structural and Vibrational Characterization of the Chromophore Binding Site of Bacterial Phytochrome Agp1. <i>Photochemistry and Photobiology</i> , 2017, 93, 713-723.	2.5	16
116	Electrostatic role of the non-heme iron complex in bacterial photosynthetic reaction center. <i>FEBS Letters</i> , 2006, 580, 4567-4570.	2.8	15
117	Understanding Selectin Counter-Receptor Binding from Electrostatic Energy Computations and Experimental Binding Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16443-16454.	2.6	15
118	Protonation equilibria of transition metal complexes: From model systems toward the Mn-complex in photosystem II. <i>Coordination Chemistry Reviews</i> , 2017, 345, 16-30.	18.8	15
119	Redox induced protonation of heme propionates in cytochrome c oxidase: Insights from surface enhanced resonance Raman spectroscopy and QM/MM calculations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2017, 1858, 103-108.	1.0	15
120	Vibrational dephasing of diatomic molecules in liquids: role of anharmonicity of the diatom. <i>Chemical Physics Letters</i> , 1978, 58, 221-224.	2.6	14
121	An energy function for dynamics simulations of polypeptides in torsion angle space. <i>Journal of Chemical Physics</i> , 1998, 108, 8264-8276.	3.0	13
122	Driving Forces of Protein Association: The Dimer-Octamer Equilibrium in Arylsulfatase A. <i>Biophysical Journal</i> , 2002, 83, 3066-3078.	0.5	13
123	Circular permuted proteins in the universe of protein folds. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1618-1630.	2.6	13
124	Influence of Heterogeneity on the Ultrafast Photoisomerization Dynamics of Pfr in Cph1 Phytochrome. <i>Photochemistry and Photobiology</i> , 2017, 93, 703-712.	2.5	13
125	Understanding Properties of Cofactors in Proteins: Redox Potentials of Synthetic Cytochromes b. <i>ChemPhysChem</i> , 2010, 11, 1196-1206.	2.1	12
126	ProPairs: A Data Set for Protein-Protein Docking. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1495-1507.	5.4	12

#	ARTICLE	IF	CITATIONS
127	Relaxation in Self-Similar Hierarchical Spaces. <i>Physical Review Letters</i> , 1988, 60, 2386-2389.	7.8	11
128	A unified theory of electron transfer and internal conversion based on solitary electronic states. <i>Journal of Chemical Physics</i> , 1989, 90, 354-365.	3.0	11
129	Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6885-6893.	2.5	11
130	Optimized distance-dependent atom-pair-based potential DOOP for protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 881-890.	2.6	11
131	Analysis of the optical absorption spectra of diradical oligomers in diacetylene crystals. <i>Chemical Physics</i> , 1984, 84, 321-331.	1.9	10
132	Database of protein complexes with multivalent binding ability: Bival \hat{a} bind. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 744-751.	2.6	10
133	Combined NMR and computational study for azide binding to human manganese superoxide dismutase. <i>Solid State Nuclear Magnetic Resonance</i> , 2008, 34, 6-13.	2.3	9
134	Mechanical Rupture of Mono- and Bivalent Transition Metal Complexes in Experiment and Theory. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4333-4343.	3.1	9
135	Redox potential of the non-heme iron complex in bacterial photosynthetic reaction center. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2007, 1767, 1300-1309.	1.0	8
136	Merging Implicit with Explicit Solvent Simulations: Polyethylene Glycol. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1871-1883.	5.3	8
137	Geometry motivated alternative view on local protein backbone structures. <i>Protein Science</i> , 2013, 22, 1669-1674.	7.6	8
138	A complete decoupling of Faddeev-like equations for three arrangement systems; applications to H \hat{i} -H $\hat{2}$ collision. <i>Chemical Physics</i> , 1976, 15, 363-368.	1.9	7
139	Reprint of PSII Manganese Cluster: Protonation of W2, O5, O4 and His337 in the S1 state explored by combined quantum chemical and electrostatic energy computations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2014, 1837, 1389-1394.	1.0	7
140	Reply to \hat{a} Comment on: \hat{a} Cytochrome oxidation in bacterial photosynthesis \hat{a} . <i>Journal of Chemical Physics</i> , 1988, 89, 3394-3395.	3.0	6
141	GIS: a comprehensive source for protein structure similarities. <i>Nucleic Acids Research</i> , 2010, 38, W46-W52.	14.5	6
142	\hat{p} \hat{i} \hat{K} \hat{i} \hat{A} in proteins solving the \hat{P} oisson \hat{B} oltzmann equation with finite elements. <i>Journal of Computational Chemistry</i> , 2015, 36, 2147-2157.	3.3	6
143	Protonation-State-Dependent Communication in Cytochrome c Oxidase. <i>Biophysical Journal</i> , 2017, 113, 817-828.	0.5	6
144	The redox-coupled proton-channel opening in cytochrome \hat{i} \hat{c} oxidase. <i>Chemical Science</i> , 2020, 11, 3804-3811.	7.4	6

#	ARTICLE	IF	CITATIONS
145	Concentration dependence of the vibrational energy relaxation of O ₂ in liquid mixtures. <i>Chemical Physics</i> , 1981, 63, 203-208.	1.9	5
146	Equivalence of dynamics in ultrametric and hierarchical spaces. <i>Physical Review B</i> , 1988, 38, 2664-2668.	3.2	5
147	Diffusion of two different water models and thermal conductivity in a protein-water system. <i>International Journal of Quantum Chemistry</i> , 1996, 59, 271-279.	2.0	5
148	Beating Heart of Cytochrome <i>c</i> Oxidase: The Shared Proton of Heme <i>c</i> ₃ Propionates. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9668-9677.	2.6	5
149	Continuous-time random walks on a long-range hierarchical model. <i>Physical Review B</i> , 1988, 38, 6774-6778.	3.2	4
150	Quantification of Local Electric Field Changes at the Active Site of Cytochrome <i>c</i> Oxidase by Fourier Transform Infrared Spectroelectrochemical Titrations. <i>Frontiers in Chemistry</i> , 2021, 9, 669452.	3.6	4
151	Two-site-hopping time correlation functions. Application to radical pair recombination. <i>Chemical Physics Letters</i> , 1984, 110, 259-264.	2.6	3
152	Problems Evaluating Energetics of Electron Transfer from QA to QB: The Light-Exposed and Dark-Adapted Bacterial Reaction Center. <i>ACS Symposium Series</i> , 2004, , 71-92.	0.5	3
153	Structural alignment of ferredoxin and flavodoxin based on electrostatic potentials: Implications for their interactions with photosystem I and ferredoxin-NADP reductase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 38, 301-309.	2.6	3
154	Magnus approximation calculation of the energy-loss distribution of O ₂ ⁺ ions scattered from He. <i>Chemical Physics Letters</i> , 1976, 37, 485-487.	2.6	2
155	Dynamics on ultrametric spaces with random transfer rates. <i>Physical Review B</i> , 1989, 39, 4834-4837.	3.2	2
156	Mössbauer investigations on glass-forming organic liquids. <i>Hyperfine Interactions</i> , 1992, 70, 1125-1128.	0.5	2
157	Collinear reactive scattering of H on H ₂ in the magnus approximation. <i>Chemical Physics</i> , 1976, 18, 375-383.	1.9	1
158	Recombination of radicals in solution. A theoretical study on the influence of two- and many-site hopping on the microwave field effect. <i>Journal of Chemical Physics</i> , 1985, 83, 2913-2922.	3.0	1
159	Role of Ions on Structure and Stability of a Synthetic Gramicidin Ion Channel in Solution. A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10441-10448.	2.6	1
160	STRATEGIES OF NON-SEQUENTIAL PROTEIN STRUCTURE ALIGNMENTS. , 2010, , .		1
161	Models for Self-Avoiding Polymer Chains on the Tetrahedral Lattice. <i>Macromolecular Theory and Simulations</i> , 2014, 23, 452-463.	1.4	1
162	Chemically Realistic Tetrahedral Lattice Models for Polymer Chains: Application to Polyethylene Oxide. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2388-2400.	5.3	1

#	ARTICLE	IF	CITATIONS
163	Sampling geometries of protein-protein complexes. <i>Genome Informatics</i> , 2008, 20, 260-9.	0.4	1
164	Dynamics of hierarchical Brownian oscillators. <i>Physical Review B</i> , 1988, 38, 9474-9482.	3.2	0
165	Simulation of oligopeptide folding or how do residues talk. , 1999, , .		0
166	3P-271 Exploring the energetics of electron transfer events in photosynthetic reaction centers by electrostatic energy computations(The 46th Annual Meeting of the Biophysical Society of Japan). <i>Seibutsu Butsuri</i> , 2008, 48, S169.	0.1	0
167	Bound Ligand Conformer Revealed by Flexible Structure Alignment in Absence of Crystal Structures: Indirect Drug Design Probed for HIV-1 Protease Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 659-673.	5.3	0
168	EVALUATION OF SEQUENCE ALIGNMENTS OF DISTANTLY RELATED SEQUENCE PAIRS WITH RESPECT TO STRUCTURAL SIMILARITY. , 2007, , .		0
169	The Influence of Aspartate 575PsaBon the Midpoint Potentials of Phylloquinones A1A/A1Band the Fx Iron-Sulfur Cluster in Photosystem I. , 2008, , 101-104.		0