G Matthias Ullmann

List of Publications by Year
in descending order

113 papers	4,506 citations	101384 36 h-index	114278 63 g-index
115 all docs	115 docs citations	115 times ranked	5225 citing authors

#	Article	IF	Citations
1	Anaerobic Microbial Degradation of Hydrocarbons: From Enzymatic Reactions to the Environment. Journal of Molecular Microbiology and Biotechnology, 2016, 26, 5-28.	1.0	615
2	Electrostatic models for computing protonation and redox equilibria in proteins. European Biophysics Journal, 1999, 28, 533-551.	1.2	250
3	A Novel View of pH Titration in Biomoleculesâ€. Biochemistry, 2001, 40, 3413-3419.	1.2	183
4	Structure of the non-redox-active tungsten/[4Fe:4S] enzyme acetylene hydratase. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 3073-3077.	3.3	135
5	pH Modulates the Quinone Position in the Photosynthetic Reaction Center from Rhodobacter sphaeroides in the Neutral and Charge Separated States. Journal of Molecular Biology, 2007, 371, 396-409.	2.0	132
6	Computational Simulation and Analysis of Dynamic Association between Plastocyanin and Cytochrome f. Consequences for the Electron-Transfer Reaction. Journal of the American Chemical Society, 1997, 119, 42-52.	6.6	129
7	Differential Effects of Cholesterol, Ergosterol and Lanosterol on a Dipalmitoyl Phosphatidylcholine Membrane:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 1786-1801.	1.2	129
8	Visualization of the Encounter Ensemble of the Transient Electron Transfer Complex of Cytochrome c and Cytochrome c Peroxidase. Journal of the American Chemical Society, 2010, 132, 241-247.	6.6	122
9	Density functional calculation of pK a values and redox potentials in the bovine Rieske iron-sulfur protein. Journal of Biological Inorganic Chemistry, 2002, 7, 632-639.	1.1	117
10	Electron Transfer between the Quinones in the Photosynthetic Reaction Center and Its Coupling to Conformational Changesâ€. Biochemistry, 2000, 39, 10487-10496.	1.2	110
11	Relations between Protonation Constants and Titration Curves in Polyprotic Acids:â€‰ A Critical View. Journal of Physical Chemistry B, 2003, 107, 1263-1271.	1.2	105
12	Energetics of Electron-Transfer and Protonation Reactions of the Quinones in the Photosynthetic Reaction Center ofRhodopseudomonas viridisâ€. Biochemistry, 1998, 37, 2488-2495.	1.2	104
13	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. Angewandte Chemie - International Edition, 2007, 46, 530-536.	7.2	95
14	McVol - A program for calculating protein volumes and identifying cavities by a Monte Carlo algorithm. Journal of Molecular Modeling, 2010, 16, 419-429.	0.8	95
15	The Î± Helix Dipole: Screened Out?. Structure, 2005, 13, 849-855.	1.6	89
16	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.	1.2	80
17	New Regioselectivity in the Cleavage of Histidine-Containing Peptides by Palladium(II) Complexes Studied by Kinetic Experiments and Molecular Dynamics Simulations. Journal of the American Chemical Society, 1999, 121, 3127-3135.	6.6	77
18	DNA-Induced Dimerization of Poly(ADP-ribose) Polymerase-1 Triggers Its Activationâ€. Biochemistry, 2005, 44, 14670-14681.	1.2	69

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19	Electron-Tunneling Paths in Various Electrostatic Complexes between Cytochrome c and Plastocyanin. Anisotropy of the Copper-Ligand Interactions and Dependence of the Iron-Copper Electronic Coupling on the Metalloprotein Orientation. Journal of the American Chemical Society, 1995, 117, 4766-4774.	6.6	66
20	pH-Dependent pK_a Values in Proteinsâ€”A Theoretical Analysis of Protonation Energies with Practical Consequences for Enzymatic Reactions. Journal of Physical Chemistry B, 2010, 114, 1994-2003.	1.2	60
21	Structural Basis for a Kolbe-Type Decarboxylation Catalyzed by a Glycyl Radical Enzyme. Journal of the American Chemical Society, 2011, 133, 14666-14674.	6.6	56
22	The Coupling of Protonation and Reduction in Proteins with Multiple Redox Centers:â€‰ Theory, Computational Method, and Application to Cytochrome c3. Journal of Physical Chemistry B, 2000, 104, 6293-6301.	1.2	54
23	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. Biochemistry, 1997, 36, 16187-16196.	1.2	53
24	Spectroscopic, Kinetic, and Mechanistic Study of a New Mode of Coordination of Indole Derivatives to Platinum(II) and Palladium(II) Ions in Complexes. Inorganic Chemistry, 2000, 39, 5004-5013.	1.9	50
25	Shifting the Equilibrium between the Encounter State and the Specific Form of a Protein Complex by Interfacial Point Mutations. Journal of the American Chemical Society, 2010, 132, 11487-11495.	6.6	48
26	Negatively Charged Residues and Hydrogen Bonds Tune the Ligand Histidine pKaValues of Rieske Ironâ^'Sulfur Proteinsâ€. Biochemistry, 2004, 43, 12383-12389.	1.2	46
27	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. Journal of Physical Chemistry A, 2004, 108, 3545-3555.	1.1	45
28	A molecular mechanics force field for biologically important sterols. Journal of Computational Chemistry, 2005, 26, 1383-1399.	1.5	45
29	Formation and characterization of an all-ferrous Rieske cluster and stabilization of the [2Fe-2S]0 core by protonation. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 10913-10918.	3.3	44
30	Redox-linked protonation state changes in cytochrome bc1 identified by Poissonâ€“Boltzmann electrostatics calculations. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 204-221.	0.5	42
31	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
32	Poly(ADP-ribose) Polymerase-1 Dimerizes at a 5â€˜ Recessed DNA Endin Vitro:Â A Fluorescence Studyâ€. Biochemistry, 2003, 42, 12409-12417.	1.2	40
33	GMCT : A Monte Carlo simulation package for macromolecular receptors. Journal of Computational Chemistry, 2012, 33, 887-900.	1.5	39
34	The Influence of a Transmembrane pH Gradient on Protonation Probabilities of Bacteriorhodopsin: The Structural Basis of the Back-Pressure Effect. Journal of Molecular Biology, 2004, 339, 571-589.	2.0	38
35	Theoretical investigation of the behavior of titratable groups in proteins. Photochemical and Photobiological Sciences, 2006, 5, 588.	1.6	38
36	Understanding the energetics of helical peptide orientation in membranes. Proteins: Structure, Function and Bioinformatics, 2005, 58, 913-922.	1.5	37

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37	Effects of Single and Double Mutations in Plastocyanin on the Rate Constant and Activation Parameters for the Rearrangement Gating the Electron-Transfer Reaction between the Triplet State of Zinc Cytochrome c and Cupriplastocyanin. Biochemistry, 1998, 37, 9557-9569.	1.2	36
38	Electrostatic potential at the retinal of three archaeal rhodopsins: Implications for their different absorption spectra. Proteins: Structure, Function and Bioinformatics, 2005, 61, 953-965.	1.5	35
39	Role of Hydrophobic Interactions in the Encounter Complex Formation of the Plastocyanin and Cytochrome f Complex Revealed by Paramagnetic NMR Spectroscopy. Journal of the American Chemical Society, 2013, 135, 7681-7692.	6.6	35
40	Glycerol Dehydratation by the B₁₂-Independent Enzyme May Not Involve the Migration of a Hydroxyl Group: A Computational Study. Journal of Physical Chemistry B, 2012, 116, 7076-7087.	1.2	33
41	The Electronically Excited States of LH2 Complexes from Rhodopseudomonas acidophila Strain 10050 Studied by Time-Resolved Spectroscopy and Dynamic Monte Carlo Simulations. II. Homo-Arrays Of LH2 Complexes Reconstituted Into Phospholipid Model Membranes. Journal of Physical Chemistry B, 2011, 115, 8821-8831.	1.2	31
42	Catalytic Mechanism of the Glycyl Radical Enzyme 4-Hydroxyphenylacetate Decarboxylase from Continuum Electrostatic and QC/MM Calculations. Journal of the American Chemical Society, 2013, 135, 14574-14585.	6.6	31
43	The Position of QB in the Photosynthetic Reaction Center Depends on pH: A Theoretical Analysis of the Proton Uptake upon QB Reduction. Biophysical Journal, 2003, 84, 2090-2098.	0.2	30
44	Structure and Function of the Unusual Tungsten Enzymes Acetylene Hydratase and Class II Benzoyl-Coenzyme A Reductase. Journal of Molecular Microbiology and Biotechnology, 2016, 26, 119-137.	1.0	29
45	Partitioning of amino-acid analogues in a five-slab membrane model. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 2234-2243.	1.4	26
46	Simulating the Proton Transfer in Gramicidin A by a Sequential Dynamical Monte Carlo Method. Journal of Physical Chemistry B, 2008, 112, 13401-13410.	1.2	26
47	The Electronically Excited States of LH2 Complexes from Rhodopseudomonas acidophila Strain 10050 Studied by Time-Resolved Spectroscopy and Dynamic Monte Carlo Simulations. I. Isolated, Non-Interacting LH2 Complexes. Journal of Physical Chemistry B, 2011, 115, 8813-8820.	1.2	26
48	pKa values and redox potentials of proteins. What do they mean?. Biological Chemistry, 2013, 394, 611-619.	1.2	26
49	Decomposing Complex Cooperative Ligand Binding into Simple Components:Â Connections between Microscopic and Macroscopic Models. Journal of Physical Chemistry B, 2004, 108, 11157-11169.	1.2	25
50	Experimental and DFT Studies:Â Novel Structural Modifications Greatly Enhance the Solvent Sensitivity of Live Cell Imaging Dyes. Journal of Physical Chemistry A, 2007, 111, 10849-10860.	1.1	25
51	Effects of pH on Protein Association:Â Modification of the Proton-Linkage Model and Experimental Verification of the Modified Model in the Case of Cytochromecand Plastocyanin. Journal of the American Chemical Society, 2001, 123, 10789-10798.	6.6	24
52	Influence of the Membrane Potential on the Protonation of Bacteriorhodopsin:Â Insights from Electrostatic Calculations into the Regulation of Proton Pumping. Journal of the American Chemical Society, 2006, 128, 12129-12139.	6.6	24
53	Thermodynamics of Transport Through the Ammonium Transporter Amt-1 Investigated with Free Energy Calculations. Journal of Physical Chemistry B, 2012, 116, 9690-9703.	1.2	24
54	Cysteine as a Modulator Residue in the Active Site of Xenobiotic Reductase A: A Structural, Thermodynamic and Kinetic Study. Journal of Molecular Biology, 2010, 398, 66-82.	2.0	23

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55	The dynamic complex of cytochrome c6 and cytochrome f studied with paramagnetic NMR spectroscopy. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1305-1315.	0.5	23
56	Investigating the mechanisms of photosynthetic proteins using continuum electrostatics. Photosynthesis Research, 2008, 97, 33-53.	1.6	22
57	Mechanistic Insights into Ferredoxinâ€“NADP(H) Reductase Catalysis Involving the Conserved Glutamate in the Active Site. Journal of Molecular Biology, 2010, 397, 814-825.	2.0	22
58	Simulation of the Electron Transfer between the Tetraheme Subunit and the Special Pair of the Photosynthetic Reaction Center Using a Microstate Description. Journal of Physical Chemistry B, 2007, 111, 2957-2968.	1.2	20
59	Breaking Benzene Aromaticityâ€”Computational Insights into the Mechanism of the Tungsten-Containing Benzoyl-CoA Reductase. Journal of the American Chemical Society, 2017, 139, 14488-14500.	6.6	19
60	Continuum electrostatic investigations of charge transfer processes in biological molecules using a microstate description. Faraday Discussions, 2011, 148, 173-193.	1.6	18
61	Structure and Function of 4-Hydroxyphenylacetate Decarboxylase and Its Cognate Activating Enzyme. Journal of Molecular Microbiology and Biotechnology, 2016, 26, 76-91.	1.0	18
62	Proton-Transfer Pathways in Photosynthetic Reaction Centers Analyzed by Profile Hidden Markov Models and Network Calculations. Journal of Molecular Biology, 2009, 388, 631-643.	2.0	17
63	Kinetic Characterization of Xenobiotic Reductase A from Pseudomonas putida 86. Biochemistry, 2009, 48, 11412-11420.	1.2	16
64	Electrostatic effects on the kinetics of photoinduced electron-transfer reactions of the triplet state of zinc cytochrome c with wild-type and mutant forms of Pseudomonas aeruginosa azurin. Journal of Biological Inorganic Chemistry, 1999, 4, 111-121.	1.1	15
65	Packing Density of the Erythropoietin Receptor Transmembrane Domain Correlates with Amplification of Biological Responses. Biochemistry, 2008, 47, 11771-11782.	1.2	15
66	Coupling of Protonation, Reduction, and Conformational Change in azurin from Pseudomonas aeruginosa Investigated with Free Energy Measures of Cooperativity. Journal of Physical Chemistry B, 2011, 115, 10346-10359.	1.2	15
67	Comparing the Rates and the Activation Parameters for the Forward Reaction between the Triplet State of Zinc Cytochrome c and Cupriplastocyanin and the Back Reaction between the Zinc Cytochrome c Cation Radical and Cuproplastocyanin. Biochemistry, 1999, 38, 1589-1597.	1.2	14
68	ATP Binding Enables Broad Antibiotic Selectivity of Aminoglycoside Phosphotransferase(3â€²)-IIIa: An Elastic Network Analysis. Journal of Molecular Biology, 2011, 409, 450-465.	2.0	14
69	Molecular dynamics simulation of HIV-1 fusion domain-membrane complexes: Insight into the N-terminal gp41 fusion mechanism. Biophysical Chemistry, 2012, 170, 9-16.	1.5	14
70	Loss of Electrostatic Interactions Causes Increase of Dynamics within the Plastocyaninâ€“Cytochrome f Complex. Biochemistry, 2013, 52, 6615-6626.	1.2	14
71	Low potential enzymatic hydride transfer via highly cooperative and inversely functionalized flavin cofactors. Nature Communications, 2019, 10, 2074.	5.8	14
72	An extended dead-end elimination algorithm to determine gap-free lists of low energy states. Journal of Computational Chemistry, 2007, 28, 2325-2335.	1.5	13

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73	Profile Hidden Markov Models for Analyzing Similarities and Dissimilarities in the Bacterial Reaction Center and Photosystem II. Biochemistry, 2009, 48, 1230-1243.	1.2	13
74	Efficient Encounter Complex Formation and Electron Transfer to Cytochromeâ€…c Peroxidase with an Additional, Distant Electrostatic Binding Site. Angewandte Chemie - International Edition, 2020, 59, 23239-23243.	7.2	13
75	Mechanisms and Specificity of Phenazine Biosynthesis Protein PhzF. Scientific Reports, 2017, 7, 6272.	1.6	12
76	Assessing density functional theory in real-time and real-space as a tool for studying bacteriochlorophylls and the light-harvesting complex 2. Journal of Chemical Physics, 2019, 151, 134114.	1.2	12
77	pHâ€dependent molecular dynamics of vesicular stomatitis virus glycoprotein G. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2601-2613.	1.5	10
78	A mathematical view on the decoupled sites representation. Journal of Mathematical Biology, 2013, 66, 477-503.	0.8	10
79	An Ensemble of Rapidly Interconverting Orientations in Electrostatic Proteinâ€“Peptide Complexes Characterized by NMR Spectroscopy. ChemBioChem, 2014, 15, 556-566.	1.3	10
80	PyCPR â€“ a python-based implementation of the Conjugate Peak Refinement (CPR) algorithm for finding transition state structures. Journal of Molecular Modeling, 2016, 22, 242.	0.8	10
81	Effect of HPr phosphorylation on structure, dynamics, and interactions in the course of transcriptional control. Journal of Molecular Modeling, 2007, 13, 431-444.	0.8	9
82	Continuum Electrostatic Analysis of Proteins. , 2014, , 135-163.		9
83	Serine and Cysteine Peptidases: So Similar, Yet Different. How the Active-Site Electrostatics Facilitates Different Reaction Mechanisms. Journal of Physical Chemistry B, 2022, 126, 4035-4048.	1.2	9
84	Effects of Histidine Protonation and Phosphorylation on Histidine-Containing Phosphocarrier Protein Structure, Dynamics, and Physicochemical Properties. Biochemistry, 2007, 46, 12314-12326.	1.2	8
85	Simultaneous true, gated, and coupled electron-transfer reactions and energetics of protein rearrangement. Journal of Inorganic Biochemistry, 2012, 106, 143-150.	1.5	7
86	CoMoDo: Identifying Dynamic Protein Domains Based on Covariances of Motion. Journal of Chemical Theory and Computation, 2015, 11, 2841-2854.	2.3	7
87	MCMapâ€”A Computational Tool for Mapping Energy Landscapes of Transient Proteinâ€“Protein Interactions. ACS Omega, 2018, 3, 6465-6475.	1.6	7
88	The Charge Distribution on a Protein Surface Determines Whether Productive or Futile Encounter Complexes Are Formed. Biochemistry, 2021, 60, 747-755.	1.2	7
89	Internal hydration of protein cavities: studies on BPTI. Physical Chemistry Chemical Physics, 2004, 6, 1906-1911.	1.3	6
90	A Generalized Free Energy Perturbation Theory Accounting for End States with Differing Configuration Space Volume. Journal of Physical Chemistry B, 2011, 115, 507-521.	1.2	6

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91	pH and Potential Transients of the bc₁ Complex Co-Reconstituted in Proteo-Lipobeads with the Reaction Center from Rb. sphaeroides. Journal of Physical Chemistry B, 2017, 121, 143-152.	1.2	6
92	Chemical properties of key metabolites determine the global distribution of lichens. Ecology Letters, 2022, 25, 416-426.	3.0	6
93	On the interaction of different types of ligands binding to the same molecule Part II: systems with n to 2 and n to 3 binding sites. Journal of Mathematical Chemistry, 2013, 51, 696-714.	0.7	5
94	The Open, the Closed, and the Empty: Time-Resolved Fluorescence Spectroscopy and Computational Analysis of RC-LH1 Complexes from Rhodopseudomonas palustris. Journal of Physical Chemistry B, 2015, 119, 1362-1373.	1.2	5
95	Computational Biochemistryâ€"Enzyme Mechanisms Explored. Advances in Protein Chemistry and Structural Biology, 2017, 109, 77-112.	1.0	5
96	On the interaction of two different types of ligands binding to the same molecule part I: basics and the transfer of the decoupled sites representation to systems with n and one binding sites. Journal of Mathematical Chemistry, 2013, 51, 672-695.	0.7	4
97	Aiding a Better Understanding of Molybdopterin: Syntheses, Structures, and pKa Value Determinations of Varied Pterin-Derived Organic Scaffolds Including Oxygen, Sulfur and Phosphorus Bearing Substituents. Journal of Molecular Structure, 2021, 1230, 129867.	1.8	4
98	Charge Transfer Properties of Photosynthetic and Respiratory Proteinsâ€â€his work was partially written at the Freie UniversitÃt Berlin, Department of Biology, Chemistry, and Pharmacy, Institute of Chemistry, Takustr. 6,14195 Berlin (Germany) and The Scripps Research Institute, Department of Molecular Biology, 10550 N. Torrey Pines Rd., TPC-15, La Jolla, CA 92037 USA.. , 2001, , 525-584.		3
99	Structural alignment of ferredoxin and flavodoxin based on electrostatic potentials: Implications for their interactions with photosystem I and ferredoxin-NADP reductase. , 2000, 38, 301.		3
100	Structural and Biophysical Analysis of the Phytochelatin-Synthase-Like Enzyme from Nostoc sp. Shows That Its Protease Activity is Sensitive to the Redox State of the Substrate. ACS Chemical Biology, 2022, 17, 883-897.	1.6	3
101	Distinguishing two groups of flavin reductases by analyzing the protonation state of an active site carboxylic acid. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2076-2085.	1.5	2
102	Theoretical Analysis of Electron Transfer in Proteins: From Simple Proteins to Complex Machineries. Advances in Photosynthesis and Respiration, 2016, , 99-127.	1.0	2
103	Chemical Evidence for the Dawn of Life on Earth. Australian Journal of Chemistry, 2011, 64, 16.	0.5	1
104	Corrigendum to: Chemical Evidence for the Dawn of Life on Earth. Australian Journal of Chemistry, 2011, 64, 228.	0.5	1
105	Continuum Electrostatic Calculation on Bovine Rhodopsin: Protonation and the Effect of the Membrane Potential. Photochemistry and Photobiology, 2017, 93, 1388-1398.	1.3	1
106	Efficient Encounter Complex Formation and Electron Transfer to Cytochromeâ€… c Peroxidase with an Additional, Distant Electrostatic Binding Site. Angewandte Chemie, 2020, 132, 23439-23443.	1.6	1
107	Role of electrostatic and hydrophobic interactions in the encounter complex formation of plastocyanin and cytochrome f. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, e120-e121.	0.5	0
108	Enhancing the population of the encounter complex affects protein complex formation efficiency. FEBS Journal, 2022, 289, 535-548.	2.2	0

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109	Conformational Transitions in Proteins and Membranes. , 2004, , 485-502.		0
110	Kinetic Simulations of the C-Subunit of the Bacterial Reaction Center. , 2008, , 553-557.		0
111	The Role of AspL213 for Stabilizing Semiquinone Binding to the Photosynthetic Reaction Center. , 2008, , 127-131.		0
112	Chemoselective Attachment of the Water-Soluble Dark Quencher Hydrodabcyl to Amino Groups in Peptides and Preservation of Its Spectroscopic Properties over a Wide pH Range. ACS Omega, 2021, 6, 32896-32903.	1.6	0
113	15 Methods based on continuum electrostatics and their application to flavoproteins â€“ a review. , 2013, , 335-360.		0