Hiroshi Ishikita

List of Publications by Year
in descending order

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108 papers	3,500 citations	159358 30 h-index	168136 53 g-index
113 all docs	113 docs citations	113 times ranked	2626 citing authors

#	Article	IF	Citations
1	Î±-Helices direct excitation energy flow in the Fennaâ€“Matthewsâ€“Olson protein. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 16862-16867.	3.3	183
2	Energetics of a Possible Proton Exit Pathway for Water Oxidation in Photosystem II. Biochemistry, 2006, 45, 2063-2071.	1.2	167
3	Proton transfer reactions and hydrogen-bond networks in protein environments. Journal of the Royal Society Interface, 2014, 11, 20130518.	1.5	151
4	Mechanism of proton-coupled quinone reduction in Photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 954-959.	3.3	125
5	Short Hydrogen Bond between Redox-Active Tyrosine Y_Z and D1-His190 in the Photosystem II Crystal Structure. Biochemistry, 2011, 50, 9836-9844.	1.2	117
6	Energetics of proton release on the first oxidation step in the water-oxidizing enzyme. Nature Communications, 2015, 6, 8488.	5.8	111
7	How photosynthetic reaction centers control oxidation power in chlorophyll pairs P680, P700, and P870. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9855-9860.	3.3	104
8	Redox Potential of Quinones in Both Electron Transfer Branches of Photosystem I. Journal of Biological Chemistry, 2003, 278, 52002-52011.	1.6	103
9	Control of Quinone Redox Potentials in Photosystem II:Â Electron Transfer and Photoprotection. Journal of the American Chemical Society, 2005, 127, 14714-14720.	6.6	93
10	Distribution of the Cationic State over the Chlorophyll Pair of the Photosystem II Reaction Center. Journal of the American Chemical Society, 2011, 133, 14379-14388.	6.6	85
11	Redox Potentials of Chlorophylls in the Photosystem II Reaction Centerâ€. Biochemistry, 2005, 44, 4118-4124.	1.2	80
12	Theoretical studies of proton-coupled electron transfer: Models and concepts relevant to bioenergetics. Coordination Chemistry Reviews, 2008, 252, 384-394.	9.5	80
13	O2 evolution and recovery of the water-oxidizing enzyme. Nature Communications, 2018, 9, 1247.	5.8	68
14	Mechanism of tyrosine D oxidation in Photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7690-7695.	3.3	67
15	p<i>K</i>_a of a Proton-Conducting Water Chain in Photosystem II. Journal of Physical Chemistry Letters, 2016, 7, 1925-1932.	2.1	66
16	Origins of Water Molecules in the Photosystem II Crystal Structure. Biochemistry, 2017, 56, 3049-3057.	1.2	63
17	Function of Redox-Active Tyrosine in Photosystem II. Biophysical Journal, 2006, 90, 3886-3896.	0.2	58
18	Buffer-Assisted Proton-Coupled Electron Transfer in a Model Rheniumâˆ’Tyrosine Complex. Journal of the American Chemical Society, 2007, 129, 11146-11152.	6.6	58

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19	Variation of Ser-L223 Hydrogen Bonding with the QB Redox State in Reaction Centers from Rhodobacter sphaeroides. Journal of the American Chemical Society, 2004, 126, 8059-8064.	6.6	55
20	Redox Potential of Quinones in Photosynthetic Reaction Centers fromRhodobacter sphaeroides:â€‰ Dependence on Protonation of Glu-L212 and Asp-L213. Biochemistry, 2003, 42, 3882-3892.	1.2	54
21	Energetics of short hydrogen bonds in photoactive yellow protein. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 167-172.	3.3	54
22	Protein Conformational Gating of Enzymatic Activity in Xanthine Oxidoreductase. Journal of the American Chemical Society, 2012, 134, 999-1009.	6.6	49
23	Influence of the Ca2+ ion on the Mn4Ca conformation and the H-bond network arrangement in Photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 159-166.	0.5	46
24	Acquirement of water-splitting ability and alteration of the charge-separation mechanism in photosynthetic reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16373-16382.	3.3	46
25	Protonation States of Ammonia/Ammonium in the Hydrophobic Pore of Ammonia Transporter Protein AmtB. Journal of the American Chemical Society, 2007, 129, 1210-1215.	6.6	41
26	Electron transfer pathways in a multiheme cytochrome MtrF. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2916-2921.	3.3	41
27	Energetic insights into two electron transfer pathways in light-driven energy-converting enzymes. Chemical Science, 2018, 9, 4083-4092.	3.7	36
28	Structural basis for high selectivity of a rice silicon channel Lsi1. Nature Communications, 2021, 12, 6236.	5.8	34
29	Redox potentials of ubiquinone, menaquinone, phylloquinone, and plastoquinone in aqueous solution. Photosynthesis Research, 2017, 134, 193-200.	1.6	33
30	Predicting Drugâ€Resistant Mutations of HIV Protease. Angewandte Chemie - International Edition, 2008, 47, 697-700.	7.2	32
31	Mechanism of Radical Formation in the H-Bond Network of D1-Asn298 in Photosystem II. Biochemistry, 2018, 57, 4997-5004.	1.2	32
32	Redox Potential of the Oxygen-Evolving Complex in the Electron Transfer Cascade of Photosystem II. Journal of Physical Chemistry Letters, 2020, 11, 249-255.	2.1	32
33	Proton transfer pathway from the oxygen-evolving complex in photosystem II substantiated by extensive mutagenesis. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148329.	0.5	32
34	Oxidation of the Non-Heme Iron Complex in Photosystem II. Biochemistry, 2005, 44, 14772-14783.	1.2	31
35	H Atom Positions and Nuclear Magnetic Resonance Chemical Shifts of Short H Bonds in Photoactive Yellow Protein. Biochemistry, 2012, 51, 1171-1177.	1.2	31
36	Function of two Î²-carotenes near the D1 and D2 proteins in photosystem II dimers. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 79-87.	0.5	30

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37	Absorption-energy calculations of chlorophyll a and b with an explicit solvent model. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 358, 422-431.	2.0	30
38	Rigidly hydrogen-bonded water molecules facilitate proton transfer in photosystem II. Physical Chemistry Chemical Physics, 2020, 22, 15831-15841.	1.3	29
39	Contributions of the Protein Environment to the Midpoint Potentials of the A₁ Phylloquinones and the F_X Ironâˆ’Sulfur Cluster in Photosystem I. Biochemistry, 2007, 46, 10804-10816.	1.2	28
40	Origin of the p<i>K</i>_a shift of the catalytic lysine in acetoacetate decarboxylase. FEBS Letters, 2010, 584, 3464-3468.	1.3	27
41	Electrostatic Influence of PsaC Protein Binding to the PsaA/PsaB Heterodimer in Photosystem I. Biophysical Journal, 2006, 90, 1081-1089.	0.2	26
42	Quenching of Singlet Oxygen by Carotenoids via Ultrafast Superexchange Dynamics. Journal of Physical Chemistry A, 2020, 124, 5081-5088.	1.1	26
43	The origin of unidirectional charge separation in photosynthetic reaction centers: nonadiabatic quantum dynamics of exciton and charge in pigmentâ€“protein complexes. Chemical Science, 2021, 12, 8131-8140.	3.7	26
44	Redox potential of cytochrome c550 in the cyanobacterium Thermosynechococcus elongates. FEBS Letters, 2005, 579, 3190-3194.	1.3	25
45	Influence of the Protein Environment on the Redox Potentials of Flavodoxins from Clostridium beijerinckii. Journal of Biological Chemistry, 2007, 282, 25240-25246.	1.6	25
46	Formation of an unusually short hydrogen bond in photoactive yellow protein. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 387-394.	0.5	25
47	Structurally conserved channels in cyanobacterial and plant photosystem II. Photosynthesis Research, 2017, 133, 75-85.	1.6	25
48	Energetics of Proton Transfer Pathways in Reaction Centers from Rhodobacter sphaeroides. Journal of Biological Chemistry, 2005, 280, 12446-12450.	1.6	24
49	Dependence of the chlorophyll wavelength on the orientation of a charged group: Why does the accessory chlorophyll have a low site energy in photosystem II?. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 402, 112799.	2.0	24
50	Redox Potentials of Chlorophylls and Î²-Carotene in the Antenna Complexes of Photosystem II. Journal of the American Chemical Society, 2005, 127, 1963-1968.	6.6	23
51	Deformation of Chlorin Rings in the Photosystem II Crystal Structure. Biochemistry, 2012, 51, 4290-4299.	1.2	23
52	Structural Factors That Alter the Redox Potential of Quinones in Cyanobacterial and Plant Photosystem I. Biochemistry, 2017, 56, 3019-3028.	1.2	23
53	Induced conformational changes upon Cd2+ binding at photosynthetic reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16215-16220.	3.3	22
54	Light-induced Hydrogen Bonding Pattern and Driving Force of Electron Transfer in AppA BLUF Domain Photoreceptor. Journal of Biological Chemistry, 2008, 283, 30618-30623.	1.6	22

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55	The Existence of an Isolated Hydronium Ion in the Interior of Proteins. Angewandte Chemie - International Edition, 2017, 56, 9151-9154.	7.2	22
56	Energetics of Ionized Water Molecules in the H-Bond Network near the Ca²⁺ and Cl^{â€“} Binding Sites in Photosystem II. Biochemistry, 2020, 59, 3216-3224.	1.2	22
57	Cationic State of Accessory Chlorophyll and Electron Transfer through Pheophytin to Plastoquinone in Photosystem II. Angewandte Chemie - International Edition, 2006, 45, 1964-1965.	7.2	21
58	Factors That Differentiate the H-bond Strengths of Water Near the Schiff Bases in Bacteriorhodopsin and Anabaena Sensory Rhodopsin*. Journal of Biological Chemistry, 2012, 287, 34009-34018.	1.6	21
59	Tuning electron transfer by ester-group of chlorophylls in bacterial photosynthetic reaction center. FEBS Letters, 2005, 579, 712-716.	1.3	20
60	How Does the Q_B Site Influence Propagate to the Q_A Site in Photosystem II?. Biochemistry, 2011, 50, 5436-5442.	1.2	20
61	Insights into the Protein Functions and Absorption Wavelengths of Microbial Rhodopsins. Journal of Physical Chemistry B, 2020, 124, 11819-11826.	1.2	19
62	Mechanism of the formation of proton transfer pathways in photosynthetic reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	19
63	Rubredoxin Function: Redox Behavior from Electrostatics. Journal of Chemical Theory and Computation, 2011, 7, 742-752.	2.3	18
64	pKa of the ligand water molecules in the oxygen-evolving Mn4CaO5 cluster in photosystem II. Communications Chemistry, 2020, 3, .	2.0	18
65	pK a of ubiquinone, menaquinone, phylloquinone, plastoquinone, and rhodoquinone in aqueous solution. Photosynthesis Research, 2017, 133, 297-304.	1.6	17
66	Green-Sensitive, Long-Lived, Step-Functional Anion Channelrhodopsin-2 Variant as a High-Potential Neural Silencing Tool. Journal of Physical Chemistry Letters, 2020, 11, 6214-6218.	2.1	17
67	Role of redox-inactive metals in controlling the redox potential of heterometallic manganeseâ€“oxido clusters. Photosynthesis Research, 2021, 148, 153-159.	1.6	17
68	Redox potentials along the redox-active low-barrier H-bonds in electron transfer pathways. Physical Chemistry Chemical Physics, 2020, 22, 25467-25473.	1.3	17
69	Nature of Asymmetric Electron Transfer in the Symmetric Pathways of Photosystem I. Journal of Physical Chemistry B, 2021, 125, 2879-2885.	1.2	16
70	Electrostatic role of the non-heme iron complex in bacterial photosynthetic reaction center. FEBS Letters, 2006, 580, 4567-4570.	1.3	15
71	Cationic State Distribution over the P700 Chlorophyll Pair in Photosystem I. Biophysical Journal, 2011, 101, 2018-2025.	0.2	15
72	Identification of intermediate conformations in the photocycle of the light-driven sodium-pumping rhodopsin KR2. Journal of Biological Chemistry, 2021, 296, 100459.	1.6	15

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73	Vectorial Proton Transport Mechanism of RxR, a Phylogenetically Distinct and Thermally Stable Microbial Rhodopsin. Scientific Reports, 2020, 10, 282.	1.6	14
74	Mechanism of absorption wavelength shifts in anion channelrhodopsin-1 mutants. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148349.	0.5	13
75	Requirement of Chloride for the Downhill Electron Transfer Pathway from the Water-Splitting Center in Natural Photosynthesis. Journal of Physical Chemistry B, 2022, 126, 123-131.	1.2	13
76	A Single Amino Acid Mutation Converts (R)-5-Diphosphomevalonate Decarboxylase into a Kinase. Journal of Biological Chemistry, 2017, 292, 2457-2469.	1.6	11
77	Proton-Binding Sites of Acid-Sensing Ion Channel 1. PLoS ONE, 2011, 6, e16920.	1.1	10
78	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. Physical Chemistry Chemical Physics, 2017, 19, 17985-17997.	1.3	10
79	The Nature of the Short Oxygenâ€“Oxygen Distance in the Mn₄CaO₆ Complex of Photosystem II Crystals. Journal of Physical Chemistry Letters, 2020, 11, 10262-10268.	2.1	10
80	Structure-guided design enables development of a hyperpolarized molecular probe for the detection of aminopeptidase N activity in vivo. Science Advances, 2022, 8, eabj2667.	4.7	10
81	Correlation between Câ•O Stretching Vibrational Frequency and p<i>K</i>_a Shift of Carboxylic Acids. Journal of Physical Chemistry B, 2022, 126, 4999-5006.	1.2	10
82	Energetics of the Proton Transfer Pathway for Tyrosine D in Photosystem II. Australian Journal of Chemistry, 2016, 69, 991.	0.5	9
83	Mutational analysis of the conserved carboxylates of anion channelrhodopsin-2 (ACR2) expressed in <i>Escherichia coli</i> and their roles in anion transport. Biophysics and Physicobiology, 2018, 15, 179-188.	0.5	9
84	Redox potential of the non-heme iron complex in bacterial photosynthetic reaction center. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 1300-1309.	0.5	8
85	Redox Potential Difference between Desulfovibrio vulgaris and Clostridium beijerinckii Flavodoxins. Biochemistry, 2008, 47, 4394-4402.	1.2	8
86	Influence of the Axial Ligand on the Cationic Properties of the Chlorophyll Pair in Photosystem II from Thermosynechococcus vulcanus. Biophysical Journal, 2012, 102, 2634-2640.	0.2	8
87	Selective Removal of B800 Bacteriochlorophyll <i>a</i> from Light-Harvesting Complex 2 of the Purple Photosynthetic Bacterium <i>Phaeospirillum molischianum</i>. Biochemistry, 2018, 57, 3075-3083.	1.2	8
88	Mechanism of protonation of the over-reduced Mn4CaO5 cluster in photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 148059.	0.5	8
89	Modulation of the protein environment in the hydrophilic pore of the ammonia transporter protein AmtB upon GlnK protein binding. FEBS Letters, 2007, 581, 4293-4297.	1.3	7
90	Absorption wavelength along chromophore low-barrier hydrogen bonds. IScience, 2022, 25, 104247.	1.9	7

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91	Long-Range Exciton Diffusion via Singlet Revival Mechanism. Journal of Physical Chemistry Letters, 2019, 10, 7623-7628.	2.1	6
92	Proton transfer pathway in anion channelrhodopsin-1. ELife, 2021, 10, .	2.8	6
93	Two Distinct Oxygen-Radical Conformations in the X-ray Free Electron Laser Structures of Photosystem II. Journal of Physical Chemistry Letters, 2021, 12, 4032-4037.	2.1	5
94	Release of Electrons and Protons from Substrate Water Molecules at the Oxygen-Evolving Complex in Photosystem II. Journal of the Physical Society of Japan, 2022, 91, .	0.7	5
95	Tyrosine Deprotonation and Associated Hydrogen Bond Rearrangements in a Photosynthetic Reaction Center. PLoS ONE, 2011, 6, e26808.	1.1	4
96	Electron Acceptorâ€"Donor Iron Sites in the Ironâ€"Sulfur Cluster of Photosynthetic Electron-Transfer Pathways. Journal of Physical Chemistry Letters, 2021, 12, 7431-7438.	2.1	4
97	Long-Range Electron Tunneling from the Primary to Secondary Quinones in Photosystem II Enhanced by Hydrogen Bonds with a Nonheme Fe Complex. Journal of Physical Chemistry B, 2021, 125, 13460-13466.	1.2	4
98	Mechanism of Mixed-Valence Fe^{2.5+}Â·Â·Â·Fe^{2.5+} Formation in Fe₄S₄ Clusters in the Ferredoxin Binding Motif. Journal of Physical Chemistry B, 2022, 126, 3059-3066.	1.2	4
99	Cationic state distribution over the chlorophyll d-containing PD1/PD2 pair in photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 1191-1195.	0.5	3
100	Reply to Breuer et al.: Molecular dynamics simulations do not provide functionally relevant values of redox potential in MtrF. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10029-E10030.	3.3	3
101	Protein Environment that Facilitates Proton Transfer and Electron Transfer in Photosystem II. , 2019, , 191-208.		3
102	The Existence of an Isolated Hydronium Ion in the Interior of Proteins. Angewandte Chemie, 2017, 129, 9279-9282.	1.6	2
103	Redox Potentials of Quinones in Aqueous Solution: Relevance to Redox Potentials in Protein Environments. , 2020, , 115-120.		2
104	Computational Analysis of the Light-induced Electron Transfer Reactions in Photosynthetic Reaction Centers. Seibutsu Butsuri, 2010, 50, 286-289.	0.0	1
105	Exploring the Retinal Binding Cavity of Archaerhodopsin-3 by Replacing the Retinal Chromophore With a Dimethyl Phenylated Derivative. Frontiers in Molecular Biosciences, 2021, 8, 794948.	1.6	1
106	Release of a Proton and Formation of a Low-Barrier Hydrogen Bond between Tyrosine D and D2-His189 in Photosystem II. ACS Physical Chemistry Au, 0, , .	1.9	1
107	Electron Transfer Pathways in a Multiheme Cytochrome MtrF. Seibutsu Butsuri, 2017, 57, 151-152.	0.0	0
108	The Influence of Aspartate 575PsaBon the Midpoint Potentials of Phylloquinones A1A/A1Band the Fx Iron-Sulfur Cluster in Photosystem I. , 2008, , 101-104.		0