Hiroshi Ishikita

List of Publications by Year
in descending order

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	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
2	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
3	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
4	Absorption wavelength along chromophore low-barrier hydrogen bonds. IScience, 2022, 25, 104247.	1.9	7
5	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
6	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
7	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
8	Mechanism of absorption wavelength shifts in anion channelrhodopsin-1 mutants. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148349.	0.5	13
9	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
10	Nature of Asymmetric Electron Transfer in the Symmetric Pathways of Photosystem I. Journal of Physical Chemistry B, 2021, 125, 2879-2885.	1.2	16
11	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
12	Role of redox-inactive metals in controlling the redox potential of heterometallic manganeseâ€"oxido clusters. Photosynthesis Research, 2021, 148, 153-159.	1.6	17
13	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
14	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
15	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
16	Structural basis for high selectivity of a rice silicon channel Lsi1. Nature Communications, 2021, 12, 6236.	5.8	34
17	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
18	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

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19	Proton transfer pathway in anion channelrhodopsin-1. ELife, 2021, 10, .	2.8	6
20	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
21	pKa of the ligand water molecules in the oxygen-evolving Mn4CaO5 cluster in photosystem II. Communications Chemistry, 2020, 3, .	2.0	18
22	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
23	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
24	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
25	Insights into the Protein Functions and Absorption Wavelengths of Microbial Rhodopsins. Journal of Physical Chemistry B, 2020, 124, 11819-11826.	1.2	19
26	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
27	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
28	Rigidly hydrogen-bonded water molecules facilitate proton transfer in photosystem II. Physical Chemistry Chemical Physics, 2020, 22, 15831-15841.	1.3	29
29	Quenching of Singlet Oxygen by Carotenoids via Ultrafast Superexchange Dynamics. Journal of Physical Chemistry A, 2020, 124, 5081-5088.	1.1	26
30	Vectorial Proton Transport Mechanism of RxR, a Phylogenetically Distinct and Thermally Stable Microbial Rhodopsin. Scientific Reports, 2020, 10, 282.	1.6	14
31	Redox Potentials of Quinones in Aqueous Solution: Relevance to Redox Potentials in Protein Environments. , 2020, , 115-120.		2
32	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
33	Mechanism of protonation of the over-reduced Mn4CaO5 cluster in photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 148059.	0.5	8
34	Long-Range Exciton Diffusion via Singlet Revival Mechanism. Journal of Physical Chemistry Letters, 2019, 10, 7623-7628.	2.1	6
35	Protein Environment that Facilitates Proton Transfer and Electron Transfer in Photosystem II. , 2019, , 191-208.		3
36	O2 evolution and recovery of the water-oxidizing enzyme. Nature Communications, 2018, 9, 1247.	5.8	68

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37	Energetic insights into two electron transfer pathways in light-driven energy-converting enzymes. Chemical Science, 2018, 9, 4083-4092.	3.7	36
38	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
39	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
40	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
41	Mechanism of Radical Formation in the H-Bond Network of D1-Asn298 in Photosystem II. Biochemistry, 2018, 57, 4997-5004.	1.2	32
42	Structurally conserved channels in cyanobacterial and plant photosystem II. Photosynthesis Research, 2017, 133, 75-85.	1.6	25
43	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
44	A Single Amino Acid Mutation Converts (R)-5-Diphosphomevalonate Decarboxylase into a Kinase. Journal of Biological Chemistry, 2017, 292, 2457-2469.	1.6	11
45	pK a of ubiquinone, menaquinone, phylloquinone, plastoquinone, and rhodoquinone in aqueous solution. Photosynthesis Research, 2017, 133, 297-304.	1.6	17
46	Origins of Water Molecules in the Photosystem II Crystal Structure. Biochemistry, 2017, 56, 3049-3057.	1.2	63
47	The Existence of an Isolated Hydronium Ion in the Interior of Proteins. Angewandte Chemie - International Edition, 2017, 56, 9151-9154.	7.2	22
48	Structural Factors That Alter the Redox Potential of Quinones in Cyanobacterial and Plant Photosystem I. Biochemistry, 2017, 56, 3019-3028.	1.2	23
49	The Existence of an Isolated Hydronium Ion in the Interior of Proteins. Angewandte Chemie, 2017, 129, 9279-9282.	1.6	2
50	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
51	Redox potentials of ubiquinone, menaquinone, phylloquinone, and plastoquinone in aqueous solution. Photosynthesis Research, 2017, 134, 193-200.	1.6	33
52	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
53	Electron Transfer Pathways in a Multiheme Cytochrome MtrF. Seibutsu Butsuri, 2017, 57, 151-152.	0.0	0
54	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

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55	Energetics of the Proton Transfer Pathway for Tyrosine D in Photosystem II. Australian Journal of Chemistry, 2016, 69, 991.	0.5	9
56	Energetics of proton release on the first oxidation step in the water-oxidizing enzyme. Nature Communications, 2015, 6, 8488.	5.8	111
57	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
58	Proton transfer reactions and hydrogen-bond networks in protein environments. Journal of the Royal Society Interface, 2014, 11, 20130518.	1.5	151
59	Formation of an unusually short hydrogen bond in photoactive yellow protein. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 387-394.	0.5	25
60	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
61	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
62	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
63	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
64	Protein Conformational Gating of Enzymatic Activity in Xanthine Oxidoreductase. Journal of the American Chemical Society, 2012, 134, 999-1009.	6.6	49
65	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
66	Deformation of Chlorin Rings in the Photosystem II Crystal Structure. Biochemistry, 2012, 51, 4290-4299.	1.2	23
67	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
68	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
69	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
70	Rubredoxin Function: Redox Behavior from Electrostatics. Journal of Chemical Theory and Computation, 2011, 7, 742-752.	2.3	18
71	Cationic State Distribution over the P700 Chlorophyll Pair in Photosystem I. Biophysical Journal, 2011, 101, 2018-2025.	0.2	15
72	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

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73	How Does the Q_B Site Influence Propagate to the Q_A Site in Photosystem II?. Biochemistry, 2011, 50, 5436-5442.	1.2	20
74	Proton-Binding Sites of Acid-Sensing Ion Channel 1. PLoS ONE, 2011, 6, e16920.	1.1	10
75	Tyrosine Deprotonation and Associated Hydrogen Bond Rearrangements in a Photosynthetic Reaction Center. PLoS ONE, 2011, 6, e26808.	1.1	4
76	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
77	Computational Analysis of the Light-induced Electron Transfer Reactions in Photosynthetic Reaction Centers. Seibutsu Butsuri, 2010, 50, 286-289.	0.0	1
78	Theoretical studies of proton-coupled electron transfer: Models and concepts relevant to bioenergetics. Coordination Chemistry Reviews, 2008, 252, 384-394.	9.5	80
79	Predicting Drugâ€Resistant Mutations of HIV Protease. Angewandte Chemie - International Edition, 2008, 47, 697-700.	7.2	32
80	Redox Potential Difference between Desulfovibrio vulgaris and Clostridium beijerinckii Flavodoxins. Biochemistry, 2008, 47, 4394-4402.	1.2	8
81	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
82	The Influence of Aspartate 575PsaBon the Midpoint Potentials of Phylloquinones A1A/A1Band the Fx Iron-Sulfur Cluster in Photosystem I. , 2008, , 101-104.		0
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	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

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91	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
92	Electrostatic Influence of PsaC Protein Binding to the PsaA/PsaB Heterodimer in Photosystem I. Biophysical Journal, 2006, 90, 1081-1089.	0.2	26
93	Function of Redox-Active Tyrosine in Photosystem II. Biophysical Journal, 2006, 90, 3886-3896.	0.2	58
94	Energetics of a Possible Proton Exit Pathway for Water Oxidation in Photosystem II. Biochemistry, 2006, 45, 2063-2071.	1.2	167
95	Electrostatic role of the non-heme iron complex in bacterial photosynthetic reaction center. FEBS Letters, 2006, 580, 4567-4570.	1.3	15
96	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
97	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
98	Energetics of Proton Transfer Pathways in Reaction Centers from Rhodobacter sphaeroides. Journal of Biological Chemistry, 2005, 280, 12446-12450.	1.6	24
99	Redox Potentials of Chlorophylls in the Photosystem II Reaction Centerâ€. Biochemistry, 2005, 44, 4118-4124.	1.2	80
100	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
101	Oxidation of the Non-Heme Iron Complex in Photosystem II. Biochemistry, 2005, 44, 14772-14783.	1.2	31
102	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
103	Tuning electron transfer by ester-group of chlorophylls in bacterial photosynthetic reaction center. FEBS Letters, 2005, 579, 712-716.	1.3	20
104	Redox potential of cytochrome c550 in the cyanobacterium Thermosynechococcus elongates. FEBS Letters, 2005, 579, 3190-3194.	1.3	25
105	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
106	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
107	Redox Potential of Quinones in Both Electron Transfer Branches of Photosystem I. Journal of Biological Chemistry, 2003, 278, 52002-52011.	1.6	103
108	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