Ville R I Kaila

List of Publications by Year
in descending order

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88 papers	4,007 citations	94269 37 h-index	133063 59 g-index
91 all docs	91 docs citations	91 times ranked	3954 citing authors

#	Article	IF	Citations
1	Proton-Coupled Electron Transfer in Cytochrome Oxidase. Chemical Reviews, 2010, 110, 7062-7081.	23.0	466
2	New Perspectives on Proton Pumping in Cellular Respiration. Chemical Reviews, 2015, 115, 2196-2221.	23.0	238
3	Glutamic acid 242 is a valve in the proton pump of cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6255-6259.	3.3	125
4	Redox-induced activation of the proton pump in the respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11571-11576.	3.3	122
5	Long-range proton-coupled electron transfer in biological energy conversion: towards mechanistic understanding of respiratory complex I. Journal of the Royal Society Interface, 2018, 15, 20170916.	1.5	114
6	Site-specific ubiquitylation and SUMOylation using genetic-code expansion and sortase. Nature Chemical Biology, 2019, 15, 276-284.	3.9	96
7	Electrostatics, hydration, and proton transfer dynamics in the membrane domain of respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6988-6993.	3.3	94
8	Redox-coupled substrate water reorganization in the active site of Photosystem IIâ€"The role of calcium in substrate water delivery. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 740-748.	0.5	94
9	Architecture of bacterial respiratory chains. Nature Reviews Microbiology, 2021, 19, 319-330.	13.6	92
10	Symmetry-related proton transfer pathways in respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6314-E6321.	3.3	91
11	Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12737-12742.	3.3	91
12	Redox-coupled quinone dynamics in the respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E8413-E8420.	3.3	84
13	The identity of the transient proton loading site of the proton-pumping mechanism of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 80-84.	0.5	81
14	The low spin - high spin equilibrium in the S2-state of the water oxidizing enzyme. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 342-356.	0.5	77
15	Conformational processing of oncogenic v-Src kinase by the molecular chaperone Hsp90. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3189-98.	3.3	73
16	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7043-7048.	3.3	73
17	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. Journal of Chemical Theory and Computation, 2020, 16, 587-600.	2.3	69
18	Structure of inhibitor-bound mammalian complex I. Nature Communications, 2020, 11, 5261.	5.8	68

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19	Accessory NUMM (NDUFS6) subunit harbors a Zn-binding site and is essential for biogenesis of mitochondrial complex I. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5685-5690.	3.3	64
20	Terminal Electronâ€“Proton Transfer Dynamics in the Quinone Reduction of Respiratory Complex I. Journal of the American Chemical Society, 2017, 139, 16282-16288.	6.6	62
21	Redox-coupled proton pumping drives carbon concentration in the photosynthetic complex I. Nature Communications, 2020, 11, 494.	5.8	62
22	Proteinâ€Induced Color Shift of Carotenoids in Î²â€Crustacyanin. Angewandte Chemie - International Edition, 2015, 54, 11564-11566.	7.2	57
23	How cardiolipin modulates the dynamics of respiratory complex I. Science Advances, 2019, 5, eaav1850.	4.7	56
24	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. Journal of Chemical Physics, 2011, 134, 214114.	1.2	55
25	Dynamic Vesicles Formed By Dissipative Selfâ€Assembly. ChemSystemsChem, 2020, 2, e1900044.	1.1	53
26	Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. Nature Communications, 2020, 11, 1410.	5.8	50
27	To catalyze or not to catalyze: elucidation of the subtle differences between the hexameric capsules of pyrogallolarene and resorcinarene. Chemical Science, 2017, 8, 1653-1657.	3.7	49
28	Charge parameterization of the metal centers in cytochrome c oxidase. Journal of Computational Chemistry, 2008, 29, 753-767.	1.5	48
29	The chemistry of the CuB site in cytochrome c oxidase and the importance of its unique Hisâ€“Tyr bond. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 221-233.	0.5	47
30	Mechanism and energetics by which glutamic acid 242 prevents leaks in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 1205-1214.	0.5	47
31	Electrostatic spectral tuning mechanism of the green fluorescent protein. Physical Chemistry Chemical Physics, 2013, 15, 4491.	1.3	47
32	Energetics and dynamics of proton transfer reactions along short water wires. Physical Chemistry Chemical Physics, 2011, 13, 13207.	1.3	44
33	The Effect of Protein Environment on Photoexcitation Properties of Retinal. Journal of Physical Chemistry B, 2012, 116, 2249-2258.	1.2	43
34	Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726.	6.6	43
35	Reciprocal Coupling in Chemically Fueled Assembly: A Reaction Cycle Regulates Self-Assembly and Vice Versa. Journal of the American Chemical Society, 2020, 142, 20837-20844.	6.6	42
36	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. Journal of Chemical Theory and Computation, 2011, 7, 2473-2484.	2.3	40

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37	A combined quantum chemical and crystallographic study on the oxidized binuclear center of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 769-778.	0.5	39
38	A Protonated Water Cluster as a Transient Protonâ€Loading Site in Cytochromeâ€…c Oxidase. Angewandte Chemie - International Edition, 2016, 55, 11940-11944.	7.2	36
39	Energetics and Dynamics of Proton-Coupled Electron Transfer in the NADH/FMN Site of Respiratory Complex I. Journal of the American Chemical Society, 2019, 141, 5710-5719.	6.6	36
40	Water-Gated Proton Transfer Dynamics in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 13718-13728.	6.6	36
41	Structural snapshots of the minimal PKS system responsible for octaketide biosynthesis. Nature Chemistry, 2020, 12, 755-763.	6.6	35
42	Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II. Journal of the American Chemical Society, 2022, 144, 7171-7180.	6.6	35
43	The protease GtgE from Salmonella exclusively targets inactive Rab GTPases. Nature Communications, 2018, 9, 44.	5.8	33
44	Energetics of Direct and Water-Mediated Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2011, 133, 19040-19043.	6.6	32
45	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2644-2651.	2.3	32
46	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. Journal of Physical Chemistry B, 2015, 119, 2933-2945.	1.2	30
47	A switch point in the molecular chaperone Hsp90 responding to client interaction. Nature Communications, 2018, 9, 1472.	5.8	30
48	Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. Nature Communications, 2018, 9, 1168.	5.8	30
49	Contradictions in X-ray structures of intermediates in the photocycle of photoactive yellow protein. Nature Chemistry, 2014, 6, 258-259.	6.6	28
50	Interheme electron tunneling in cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21470-21475.	3.3	26
51	Functional Water Wires Catalyze Long-Range Proton Pumping in the Mammalian Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 21758-21766.	6.6	25
52	A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. Nature Communications, 2020, 11, 1219.	5.8	24
53	Hsp90 dependence of a kinase is determined by its conformational landscape. Scientific Reports, 2017, 7, 43996.	1.6	23
54	Prevention of leak in the proton pump of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 890-892.	0.5	22

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55	Linear Energy Relationships in Ground State Proton Transfer and Excited State Proton-Coupled Electron Transfer. Journal of Physical Chemistry B, 2015, 119, 2611-2619.	1.2	21
56	Deactivation blocks proton pathways in the mitochondrial complex I. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	21
57	Resolving Chemical Dynamics in Biological Energy Conversion: Long-Range Proton-Coupled Electron Transfer in Respiratory Complex I. Accounts of Chemical Research, 2021, 54, 4462-4473.	7.6	21
58	Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. Journal of Hazardous Materials, 2021, 408, 124662.	6.5	20
59	Aromatic pathways in conjugated rings connected by single bonds. International Journal of Quantum Chemistry, 2011, 111, 848-857.	1.0	19
60	Autophosphorylation activates c-Src kinase through global structural rearrangements. Journal of Biological Chemistry, 2019, 294, 13186-13197.	1.6	18
61	Molecular mechanism of polyketide shortening in anthraquinone biosynthesis of Photorhabdus luminescens. Chemical Science, 2019, 10, 6341-6349.	3.7	18
62	Tuning the Proteinâ€Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. Chemistry - A European Journal, 2016, 22, 8254-8261.	1.7	17
63	Dynamic water networks in cytochrome cbb3 oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 726-734.	0.5	16
64	Global collective motions in the mammalian and bacterial respiratory complex I. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 326-332.	0.5	16
65	Dewetting transitions coupled to K-channel activation in cytochrome c oxidase. Chemical Science, 2018, 9, 6703-6710.	3.7	16
66	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	1.3	16
67	Stabilization of the peroxy intermediate in the oxygen splitting reaction of cytochrome cbb3. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 813-818.	0.5	15
68	Conversion of light-energy into molecular strain in the photocycle of the photoactive yellow protein. Physical Chemistry Chemical Physics, 2016, 18, 2802-2809.	1.3	15
69	Redox-coupled proton transfer in the active site of cytochrome cbb3. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 1512-1520.	0.5	14
70	Bicarbonate-controlled reduction of oxygen by the Q _A semiquinone in Photosystem II in membranes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	14
71	How inter-subunit contacts in the membrane domain of complex I affect proton transfer energetics. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 734-741.	0.5	13
72	Electric field modulated redox-driven protonation and hydration energetics in energy converting enzymes. Chemical Communications, 2019, 55, 6078-6081.	2.2	13

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73	Oxidative Unfolding of the Rubredoxin Domain and the Natively Disordered N-terminal Region Regulate the Catalytic Activity of Mycobacterium tuberculosis Protein Kinase G. Journal of Biological Chemistry, 2016, 291, 27062-27072.	1.6	12
74	The central role of the metal ion for photoactivity: Znâ€“ vs. Niâ€“Mabiq. Chemical Science, 2021, 12, 7521-7532.	3.7	11
75	Molecular dynamics and structural models of the cyanobacterial NDH-1 complex. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 201-208.	0.5	10
76	Functional Dynamics of an Ancient Membrane-Bound Hydrogenase. Journal of the American Chemical Society, 2021, , .	6.6	10
77	Ion Binding and Selectivity of the Na⁺/H⁺ Antiporter MjNhaP1 from Experiment and Simulation. Journal of Physical Chemistry B, 2020, 124, 336-344.	1.2	8
78	Design of buried charged networks in artificial proteins. Nature Communications, 2021, 12, 1895.	5.8	7
79	Molecular strain in the active/deactive-transition modulates domain coupling in respiratory complex I. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148382.	0.5	7
80	Câ€H Oxidation by a Diiron Complex with Facially Opposing Active Sites. ChemistrySelect, 2018, 3, 1602-1608.	0.7	4
81	Dispersion forces drive water oxidation in molecular ruthenium catalysts. RSC Advances, 2021, 11, 425-432.	1.7	4
82	Quantum Chemical and QM/MM Models in Biochemistry. Methods in Molecular Biology, 2019, 2022, 75-104.	0.4	3
83	Exploring the catalytic cascade of cembranoid biosynthesis by combination of genetic engineering and molecular simulations. Computational and Structural Biotechnology Journal, 2020, 18, 1819-1829.	1.9	3
84	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. Angewandte Chemie - International Edition, 2018, 57, 486-490.	7.2	2
85	Extended conformational states dominate the Hsp90 chaperone dynamics. Journal of Biological Chemistry, 2022, 298, 102101.	1.6	2
86	Chapter 4. Multi-scale Molecular Simulations on Respiratory Complex I. Chemical Biology, 0, , 81-103.	0.1	1
87	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. Angewandte Chemie, 2018, 130, 495-499.	1.6	0
88	Redox- and Light-Driven Hydration Dynamics in Biological Energy Transduction. , 2019, , 53-81.		0