

Ville R I Kaila

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

86
papers

2,906
citations

32
h-index

51
g-index

91
ext. papers

3,527
ext. citations

10.5
avg, IF

5.91
L-index

#	Paper	IF	Citations
86	Proton-coupled electron transfer in cytochrome oxidase. <i>Chemical Reviews</i> , 2010 , 110, 7062-81	68.1	414
85	New perspectives on proton pumping in cellular respiration. <i>Chemical Reviews</i> , 2015 , 115, 2196-221	68.1	175
84	Glutamic acid 242 is a valve in the proton pump of cytochrome c oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 6255-9	11.5	114
83	Redox-induced activation of the proton pump in the respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 11571-6	11.5	86
82	Long-range proton-coupled electron transfer in biological energy conversion: towards mechanistic understanding of respiratory complex I. <i>Journal of the Royal Society Interface</i> , 2018 , 15,	4.1	79
81	Redox-coupled substrate water reorganization in the active site of Photosystem II-The role of calcium in substrate water delivery. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016 , 1857, 740-8	4.6	79
80	Electrostatics, hydration, and proton transfer dynamics in the membrane domain of respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 6988-93	11.5	76
79	Symmetry-related proton transfer pathways in respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E6314-E6321	11.5	70
78	The identity of the transient proton loading site of the proton-pumping mechanism of cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2011 , 1807, 80-4	4.6	67
77	Conformational processing of oncogenic v-Src kinase by the molecular chaperone Hsp90. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E3189-98	11.5	62
76	Accessory NUMM (NDUFS6) subunit harbors a Zn-binding site and is essential for biogenesis of mitochondrial complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 5685-90	11.5	60
75	Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 12737-12742	11.5	58
74	Site-specific ubiquitylation and SUMOylation using genetic-code expansion and sortase. <i>Nature Chemical Biology</i> , 2019 , 15, 276-284	11.7	55
73	The low spin - high spin equilibrium in the S-state of the water oxidizing enzyme. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018 , 1859, 342-356	4.6	54
72	Redox-coupled quinone dynamics in the respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E8413-E8420	11.5	53
71	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 7043-7048	11.5	52
70	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. <i>Journal of Chemical Physics</i> , 2011 , 134, 214114	3.9	52

69	Mechanism and energetics by which glutamic acid 242 prevents leaks in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009 , 1787, 1205-14	4.6	46
68	Charge parameterization of the metal centers in cytochrome c oxidase. <i>Journal of Computational Chemistry</i> , 2008 , 29, 753-67	3.5	45
67	Energetics and dynamics of proton transfer reactions along short water wires. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 13207-15	3.6	43
66	Protein-Induced Color Shift of Carotenoids in β -Crustacyanin. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 11564-6	16.4	42
65	Terminal Electron-Proton Transfer Dynamics in the Quinone Reduction of Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16282-16288	16.4	41
64	The chemistry of the CuB site in cytochrome c oxidase and the importance of its unique His-Tyr bond. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009 , 1787, 221-33	4.6	41
63	Spectral tuning of rhodopsin and visual cone pigments. <i>Journal of the American Chemical Society</i> , 2014 , 136, 2723-6	16.4	40
62	To catalyze or not to catalyze: elucidation of the subtle differences between the hexameric capsules of pyrogallolarene and resorcinarene. <i>Chemical Science</i> , 2017 , 8, 1653-1657	9.4	39
61	The effect of protein environment on photoexcitation properties of retinal. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 2249-58	3.4	39
60	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2473-84	6.4	39
59	Redox-coupled proton pumping drives carbon concentration in the photosynthetic complex I. <i>Nature Communications</i> , 2020 , 11, 494	17.4	38
58	How cardiolipin modulates the dynamics of respiratory complex I. <i>Science Advances</i> , 2019 , 5, eaav1850	14.3	37
57	Electrostatic spectral tuning mechanism of the green fluorescent protein. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 4491-5	3.6	36
56	Dynamic Vesicles Formed By Dissipative Self-Assembly. <i>ChemSystemsChem</i> , 2020 , 2, e1900044	3.1	34
55	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 587-600	6.4	32
54	A combined quantum chemical and crystallographic study on the oxidized binuclear center of cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2011 , 1807, 769-78	4.6	30
53	Coupled-cluster studies of extensive green fluorescent protein models using the reduced virtual space approach. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 2933-45	3.4	28
52	A Protonated Water Cluster as a Transient Proton-Loading Site in Cytochrome c Oxidase. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 11940-4	16.4	27

51	Energetics of direct and water-mediated proton-coupled electron transfer. <i>Journal of the American Chemical Society</i> , 2011 , 133, 19040-3	16.4	27
50	Structure of inhibitor-bound mammalian complex I. <i>Nature Communications</i> , 2020 , 11, 5261	17.4	26
49	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2644-51	6.4	26
48	A switch point in the molecular chaperone Hsp90 responding to client interaction. <i>Nature Communications</i> , 2018 , 9, 1472	17.4	25
47	Contradictions in X-ray structures of intermediates in the photocycle of photoactive yellow protein. <i>Nature Chemistry</i> , 2014 , 6, 258-9	17.6	25
46	Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. <i>Nature Communications</i> , 2020 , 11, 1410	17.4	24
45	Architecture of bacterial respiratory chains. <i>Nature Reviews Microbiology</i> , 2021 , 19, 319-330	22.2	23
44	Prevention of leak in the proton pump of cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2008 , 1777, 890-2	4.6	21
43	Reciprocal Coupling in Chemically Fueled Assembly: A Reaction Cycle Regulates Self-Assembly and Vice Versa. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20837-20844	16.4	21
42	Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. <i>Nature Communications</i> , 2018 , 9, 1168	17.4	20
41	Linear energy relationships in ground state proton transfer and excited state proton-coupled electron transfer. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 2611-9	3.4	20
40	Interheme electron tunneling in cytochrome c oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 21470-5	11.5	20
39	Hsp90 dependence of a kinase is determined by its conformational landscape. <i>Scientific Reports</i> , 2017 , 7, 43996	4.9	19
38	Energetics and Dynamics of Proton-Coupled Electron Transfer in the NADH/FMN Site of Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2019 , 141, 5710-5719	16.4	19
37	Water-Gated Proton Transfer Dynamics in Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2020 , 142, 13718-13728	16.4	18
36	Tuning the Protein-Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. <i>Chemistry - A European Journal</i> , 2016 , 22, 8254-61	4.8	17
35	Dynamic water networks in cytochrome cbb3 oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2012 , 1817, 726-34	4.6	16
34	Aromatic pathways in conjugated rings connected by single bonds. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 848-857	2.1	16

33	The protease GtgE from Salmonella exclusively targets inactive Rab GTPases. <i>Nature Communications</i> , 2018 , 9, 44	17.4	15
32	Conversion of light-energy into molecular strain in the photocycle of the photoactive yellow protein. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2802-9	3.6	15
31	Structural snapshots of the minimal PKS system responsible for octaketide biosynthesis. <i>Nature Chemistry</i> , 2020 , 12, 755-763	17.6	14
30	Global collective motions in the mammalian and bacterial respiratory complex I. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018 , 1859, 326-332	4.6	14
29	Stabilization of the peroxy intermediate in the oxygen splitting reaction of cytochrome cbb(3). <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2011 , 1807, 813-8	4.6	14
28	Redox-coupled proton transfer in the active site of cytochrome cbb3. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2010 , 1797, 1512-20	4.6	13
27	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 6851-6858	3.6	12
26	Functional Water Wires Catalyze Long-Range Proton Pumping in the Mammalian Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2020 , 142, 21758-21766	16.4	12
25	A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. <i>Nature Communications</i> , 2020 , 11, 1219	17.4	12
24	How inter-subunit contacts in the membrane domain of complex I affect proton transfer energetics. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018 , 1859, 734-741	4.6	12
23	Dewetting transitions coupled to K-channel activation in cytochrome oxidase. <i>Chemical Science</i> , 2018 , 9, 6703-6710	9.4	11
22	Electric field modulated redox-driven protonation and hydration energetics in energy converting enzymes. <i>Chemical Communications</i> , 2019 , 55, 6078-6081	5.8	10
21	Molecular mechanism of polyketide shortening in anthraquinone biosynthesis of. <i>Chemical Science</i> , 2019 , 10, 6341-6349	9.4	9
20	Oxidative Unfolding of the Rubredoxin Domain and the Natively Disordered N-terminal Region Regulate the Catalytic Activity of Mycobacterium tuberculosis Protein Kinase G. <i>Journal of Biological Chemistry</i> , 2016 , 291, 27062-27072	5.4	8
19	Autophosphorylation activates c-Src kinase through global structural rearrangements. <i>Journal of Biological Chemistry</i> , 2019 , 294, 13186-13197	5.4	7
18	Protein-induzierte Farbverschiebung von Carotenoiden in β -Carotacyanin. <i>Angewandte Chemie</i> , 2015 , 127, 11726-11729	3.6	7
17	Molecular dynamics and structural models of the cyanobacterial NDH-1 complex. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2019 , 1860, 201-208	4.6	7
16	The central role of the metal ion for photoactivity: Zn- Ni-Mabiq. <i>Chemical Science</i> , 2021 , 12, 7521-7532	9.4	7

15	Deactivation blocks proton pathways in the mitochondrial complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	6
14	Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. <i>Journal of Hazardous Materials</i> , 2021 , 408, 124662	12.8	6
13	Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	6
12	Design of buried charged networks in artificial proteins. <i>Nature Communications</i> , 2021 , 12, 1895	17.4	5
11	C-H Oxidation by a Diiron Complex with Facially Opposing Active Sites. <i>ChemistrySelect</i> , 2018 , 3, 1602-1608		3
10	Quantum Chemical and QM/MM Models in Biochemistry. <i>Methods in Molecular Biology</i> , 2019 , 2022, 75-104		3
9	Molecular strain in the active/deactive-transition modulates domain coupling in respiratory complex I. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2021 , 1862, 148382	4.6	2
8	Dispersion forces drive water oxidation in molecular ruthenium catalysts.. <i>RSC Advances</i> , 2020 , 11, 425-437	3.7	2
7	Resolving Chemical Dynamics in Biological Energy Conversion: Long-Range Proton-Coupled Electron Transfer in Respiratory Complex I.. <i>Accounts of Chemical Research</i> , 2021 , 54, 4462-4473	24.3	2
6	Exploring the catalytic cascade of cembranoid biosynthesis by combination of genetic engineering and molecular simulations. <i>Computational and Structural Biotechnology Journal</i> , 2020 , 18, 1819-1829	6.8	1
5	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 486-490	16.4	1
4	Ion Binding and Selectivity of the Na/H Antiporter MjNhaP1 from Experiment and Simulation. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 336-344	3.4	1
3	Extended conformational states dominate the Hsp90 chaperone dynamics. <i>Journal of Biological Chemistry</i> , 2022 , 102101	5.4	1
2	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. <i>Angewandte Chemie</i> , 2018 , 130, 495-499	3.6	
1	Redox- and Light-Driven Hydration Dynamics in Biological Energy Transduction 2019 , 53-81		