

Curriculum Vitae of Prof. Dr. Ville R. I. Kaila

CONTACT AND PERSONAL INFORMATION

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Name: [Ville Rolf Ilmari Kaila](#)
Address (work): Department of Biochemistry and Biophysics
Stockholm University
Date of birth: December 6, 1983 (age 36)
Civil status: Married, two children (born 2013, 2019)
Country of citizenship: Finland
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EDUCATION

2007-2009 **Ph.D.** in Theoretical Biochemistry, University of Helsinki, Finland.
Ph.D. Thesis: "Theoretical Studies on Coupled Electron and Proton Transfer in Cytochrome *c* Oxidase". Grade: *excellent* (April/2009)
2003-2006 **M.Sc.** in Biochemistry, University of Helsinki, Finland.
Extended minors in Physical Chemistry, Physics and Theoretical Physics.
1994-2004 Sibelius Academy, Finland. Training for a solo violin career.

RESEARCH AND PROFESSIONAL EXPERIENCE

2019- **Full Professor and Chair** of Biochemistry, Department of Biochemistry and Biophysics, Stockholm University, Sweden.
2018-2019 **Professor (W3)** of Computational Biocatalysis, Department of Chemistry, Technical University Munich (TUM), Germany.
2013-2018 **Tenure-track Professor (W2 to W3)** of Computational Biocatalysis, Department of Chemistry, Technical University Munich (TUM), Germany.
2013 Offer for **Assistant Professor (W1)** at the Department of Chemistry and Biochemistry, Free University Berlin, Germany (declined).
2011 **Docent (Adjunct Professor)** of Physical Biochemistry, University of Helsinki.
2010-2013 **Post-doctoral researcher**, Laboratory of Chemical Physics (LCP), NIDDK, National Institutes of Health (NIH). Mentor: Gerhard Hummer
2010-2012 **Long-Term Postdoctoral Fellow**, European Molecular Biology Organization.
2010 **Short-term post-doctoral researcher**, University of Helsinki, Finland. Mentor: Prof. Dage Sundholm
2006-2010 **Temporary Lecturer**, Department of Biology and Department of Chemistry, University of Helsinki, Finland.
2005-2009 **Researcher**, Helsinki Bioenergetics Group, University of Helsinki, Finland. Mentor: Prof. Mårten Wikström
2008 **Visiting scholar** in the research group of Prof. Peter Taylor, University of Warwick, UK.
2005 **Research assistant** in NMR-laboratory, University of Helsinki, Finland.
2004 **Research assistant** in Helsinki Bioenergetics Group, University of Helsinki, Finland.

PUBLICATIONS SUMMARY AND INVITED TALKS

ca. **80 peer-reviewed articles** (see publications list below), 2886 citations in total, *h*-index 30 (Google scholar), including multiple publications in *e.g.* *PNAS* (11), *Nature Chemistry* (1), *Nature Comm* (5),

Nature Chem Biol (1), *Science Adv* (1), *Angew Chemie* (4), *Chem Rev* (2), *Chem Science* (2), and *JACS* (4); > 60 invited/plenary talks during 2014-present.

SUPERVISED RESEARCH

7 post-docs (3 now at PI/senior scientist positions), 11 PhD students (4 completed; 7 in progress), >20 research internships/BSc/MSc-theses. Lectured and developed *ca.* 20 courses at BSc, MSc, PhD level during 2013-present.

HONORS, AWARDS, AND GRANTS

2019	Wallenberg Academy Fellow
2019	Wallenberg foundation project (38 Mio SEK, Team: Högbom-Ädelroth-Brzezinski-Kaila, " <i>The obligate respiratory supercomplex – augmented biological energy conversion</i> ")
2019	Recognition award: Ruth & Nils-Erik Stenbäck's foundation.
2018	Recognition award: Hans Fischer Memorial Award
2018	Excellence in teaching nomination, TU Munich
2018	Research grant from German Research Foundation: Collaborative Research Grant (TRR235), " <i>Emergence of Life</i> " <i>ca.</i> 500 000 EUR
2018-2019	Research funding from Center of Integrated Protein Science Munich, 35,000 EUR
2016	European Research Council (ERC) , Starting Grant, "bioPCET", 1.5 Mio EUR for five years
2015	Recognition award: The Grand Prize ("Stora priset") from Oskar Öflunds foundation, 15 000 EUR
2016	Research grant from German Research Foundation (DFG): Collaborative Research Grant (SFB1035), 424 000 EUR
2015-2018	Research grant from DFG "Molecular Mechanism of Energy Conversion in Respiratory Complex I", 385 867 EUR
2015-2016	German Researcher exchange grant with Finland, "Computational Studies of Electronically Excited States of Biochromophores", 23 500 EUR
2014-2015	Research grant from Jane and Aatos Erkko Foundation: "Mechanisms of Biomimetic Water Splitting", 89 000 EUR
2010-2012	Long-Term Postdoctoral Fellow , European Molecular Biology Organization (EMBO).
2010	Recognition award from Ruth & Nils-Erik Stenbäck's foundation, the Finnish Science Foundation.
2009	The Alfthan's prize of the Finnish Chemical Society for best doctoral thesis of 2009 in Chemistry in Finland.
2007-2009	Ph.D. fellowship from Helsinki Graduate School of Biotechnology and Molecular Biology, University of Helsinki, Finland.
2006	Research Award from Finnish Cultural Foundation for research in Computational Biochemistry.

PROFESSIONAL EXPERIENCE

2014 - present	Served in >30 PhD committees as examiner/opponent/chair.
2018/4-present	Editorial board member of the <i>J. Royal Society of Interface</i> .
2017-2018	Second chairman of Munich Chemical Society (MChG).
2010-present	Reviewer for <i>Angew Chemie</i> , <i>BBA</i> , <i>Biochemistry</i> , <i>Biol Chem</i> , <i>Biophys J</i> , <i>ChemPhysChem</i> , <i>eLife</i> , <i>FEBS Lett</i> , <i>Int J Quant Chem</i> , <i>JACS</i> , <i>J Comput Chem</i> , <i>J Phys Chem</i> , <i>J Phys Chem Lett</i> , <i>NSMB</i> , <i>Nature</i> , <i>PCCP</i> , <i>PLOS journals</i> , <i>PNAS</i> , <i>Sci Rep</i> .
2014 -present	Grant reviewer for Humboldt Foundation, DAAD, DFG, ISF, NWO, Supercomputing Centers: Jülich, Irish, SuperMUC, Psi-K network.

10 Selected Publications of Prof. Ville R. I. Kaila

See full publications list below

1. Schuller JM, Saura P, Thiemann J, Schuller S, Gamiz-Hernandez AP, Kurisu G, Nowaczyk MM, **Kaila VRI** (2020) Redox-Coupled Proton Pumping Drives Carbon Concentration in the Photosynthetic Complex I, **Nature Comms** 11, 494: 1-7.
2. Jussupow A, Di Luca A, **Kaila VRI** (2019) How cardiolipin modulates the activity of complex I. **Science Adv** 5, eaav1850.
3. Warnau J, Sharma V, Gamiz-Hernandez AP, Di Luca A, Haapanen O, Vattulainen I, Wikström M, Hummer G, **Kaila VRI** (2018) Redox-Coupled Quinone Dynamics in the Respiratory Complex I. **PNAS** 115: E8413-E8420.
4. Mader SL, Bräuer A, Groll M, **Kaila VRI** (2018) Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. **Nature Comm** 9, 1168:1-8.
5. Gamiz-Hernandez AP, Jussupow A, Johansson MP, **Kaila VRI** (2017) Terminal Electron-Proton Transfer Dynamics coupled to Quinone reduction in Respiratory Complex I. **JACS** 139:16282-16288.
6. Suomivuori C-M, Gamiz-Hernandez AP, Sundholm D, **Kaila VRI** (2017) Energetics and dynamics of a light-driven sodium-pumping rhodopsin. **PNAS** 114:7043-7048. Cover issue.
7. Di Luca A, Gamiz-Hernandez AP, **Kaila VRI** (2017) Symmetry related proton transfer pathways in respiratory Complex I. **PNAS** 114:E6314-E6321.
8. Sharma V, Belevich G, Gamiz-Hernandez AP, Róg T, Vattulainen I, Wikström M, Hummer G, **Kaila VRI** (2015) Redox-Induced Activation of the Proton Pump in the Respiratory Complex I. **PNAS** 112:11571-11576.
9. **Kaila VRI**, Wikström M, Hummer G (2014) Electrostatics, Hydration, and Proton Transfer Dynamics in the Membrane Domain of Respiratory Complex I. **PNAS** 111:6988-6993.
10. **Kaila VRI**, Schotte F, Hyun S-C, Hummer G, Anfinrud PA (2014) Reconciling contradictions in time-resolved x-ray structures of early intermediates in the photocycle of photoactive yellow protein. **Nature Chem** 6:258-259.

Publications of Prof. Ville R. I. Kaila

N=82 incl. 5 in review; 2886 citations in total, *h*-index 30 (Google scholar)

* corresponding author contribution

82. Schuller JM, Saura P, Thiemann J, Schuller S, Gamiz-Hernandez AP, Kurisu G, Nowaczyk MM, **Kaila VRI*** (2020) Redox-Coupled Proton Pumping Drives Carbon Concentration in the Photosynthetic Complex I, **Nature Comms** 11, 494: 1-7.

81. Mader SL, Lopez A, Lawatscheck J, Luo Q, Rutz DA, Gamiz-Hernandez AP, Sattler M, Buchner J, **Kaila VRI*** (2020) Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. **Nature Comm** (accepted).

80. Wanzke C, Jussupow A, Kohler F, Dietz H, Kaila VRI, Boekhoven J (2019) Dynamic vesicles formed by dissipative self-assembly, **ChemSystemsChem** (in press) doi.org/10.1002/syst.201900044.

79. Johansson MP, Niederegger L; Rauhalampi M; Hess CR; Kaila VRI (2019) Dispersion-Driven Water Oxidation in Molecular Ruthenium Catalysts. (in review)

78. Shao Y, Mei Y, Sundholm D, **Kaila VRI*** (2020) Benchmarking the performance of time-dependent density functional theory methods on biochromophores. **J Chem Theor Comput** 16: 587-600

77. Lauenstein R; Mader S; Derondeau H; Block M; Römer A; Jandl C; Riedle E; Kaila VRI, Hauer J; Thyraug E; Hess CR (2019). The central role of the metal ion in photocatalysis: Zn- vs. Ni-Mabiq. (in review)

76. Bräuer A, Zhou Q, Grammbitter GLC, Schmalhofer M, **Kaila VRI**, Bode HB, Groll M (2019) Structural Snapshots of the Minimal PKS System Responsible for Octaketide Biosynthesis. (in review).

75. Warnau J, Wöhlert D, Okazaki K, Yildiz O, Gámiz-Hernández AP, **Kaila VRI***, Kühlbrandt W, Hummer G (2020) Ion Binding and Selectivity of the Na⁺/H⁺ Antiporter MjNhaP1. **J. Phys Chem B** 124: 336-344.

74. Saura P, **Kaila VRI*** (2019) Energetics and Dynamics of NADH-Driven Proton-Coupled Electron Transfer in Respiratory Complex I. **J Am Chem Soc** 41: 5710-5719.

73. Jussupow A, Di Luca A, **Kaila VRI*** (2019) How cardiolipin modulates the activity of complex I. **Science Adv** 5, eaav1850.

72. Suomivuori CM, Fliegl H, Starikov EB, Balaban TS, **Kaila VRI**, and Sundholm D (2019) Absorption Shifts of Diastereotopically Ligated Chlorophyll Dimers of Photosystem I. **Phys Chem Chem Phys** 21, 6851-6858.

71. **Kaila VRI*** (2019) Redox- and light-driven hydration dynamics (2019) in Oxygen Production and Reduction in Artificial and Natural Systems, *Eds. J. Barber, A. Ruban, P. Nixon*.

70. Jagtap PKA, Asami S, Sippel C, **Kaila VRI**, Hausch F, Sattler M (2019). Selective inhibitors of FKBP51 employ conformational selection of dynamic invisible states. *Angew Chemie Intl. Ed.* 58:9429-9433.
69. Saura P, Frey D, Gamiz-Hernandez AP, **Kaila VRI*** (2019) Electric Field Modulated Redox-Driven Protonation and Hydration Energetics in Energy Converting Enzymes. *Chem Comm* 55(43):6078-6081.
68. Zhou Q, Bräuer A, Adihou H, Schmalhofer M, Saura P, **Kaila VRI**, Groll M, Bode H (2019) Molecular mechanism of polyketide shortening in anthraquinone biosynthesis of *Photorhabdus luminescens*. *Chem Science* 10:6341-6349.
67. Boczek E, Luo Q, Dehling M, Röpke M, Mader S, Seidl A, **Kaila VRI***, Buchner J (2019) Auto-phosphorylation activates c-Src kinase through global structural rearrangements. *J Biol Chem* 294:13186-13197.
66. Rehn A, Lawatscheck J, Mader SL, Luo Q, Blank B, Richter K, **Kaila VRI**, Buchner, J. (2019) A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. *Nature Comm* (in review).
65. Fottner M, Brunner A-D, Bittl V, Horn-Ghetko D, Jussupow A, **Kaila VRI**, Bremm A, Lang K (2019) Site-specific ubiquitylation and SUMOylation using genetic code expansion and sortase-mediated transpeptidation. *Nature Chem Biol* 5:276-284.
64. Saura P, **Kaila VRI*** (2018) Structure and dynamics of the cyanobacterial NDH-1 complex. *Biochim Biophys Acta - Bioenergetics* 1860:201-208
63. Warnau J, Sharma V, Gamiz-Hernandez AP, Di Luca A, Haapanen O, Vattulainen I, Wikström M, Hummer G, **Kaila VRI*** (2018) Redox-Coupled Quinone Dynamics in the Respiratory Complex I. *Proc Natl Acad Sci USA* 115: E8413-E8420.
62. Mader SL, Bräuer A, Groll M, **Kaila VRI*** (2018) Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxxygenase AsqJ. *Nature Comm* 9, 1168: 1-8.
61. Supekar S, **Kaila VRI*** (2018) Dewetting transitions coupled to K-channel activation in cytochrome *c* oxidase. *Chem Science* 9: 6703-6710.
60. Di Luca A, Mühlbauer M, Saura P, **Kaila VRI*** (2018) How inter-subunit contacts in the membrane domain of complex I affect proton transfer energetics *Biochim Biophys Acta - Bioenergetics* 1859: 734-741.
59. **Kaila VRI*** (2018) Long-Range Proton-Coupled Electron Transfer in Biological Energy Conversion: Towards Mechanistic Understanding of Respiratory Complex I. *J. R. Soc. Interfaces* 15: 20170916.
58. Saura P, Röpke M, Gamiz-Hernandez AP, **Kaila VRI*** (2019) Quantum Chemical and QM/MM Models in Biochemistry. Biomolecular Simulations, *Methods in Mol Biol* 2022:75-104.

57. Lindsay S, Mader SL, **Kaila VRI***, Hess CR (2018) C-H Oxidation by a Diiron Complex with Facially Opposing Active Sites. **ChemistrySelect** 3(5). doi:10.1002/slct.201800192
56. Boussac A, Ugur I, Marion A, Sugiura M, **Kaila VRI**, Rutherford AW (2018) The low spin - high spin equilibrium in the S2-state of the water oxidizing enzyme. **Biochim Biophys Acta - Bioenergetics** 1859: 342-356.
55. Di Luca, **Kaila VRI*** (2018) Global Collective Motions in the Mammalian and Bacterial Respiratory Complex I. **Biochim Biophys Acta - Bioenergetics** 1859: 326-332.
54. Fedor J, Di Luca A, **Kaila VRI**, Hirst J (2017) Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. **Proc Natl Acad Sci USA** 114: 12737-12742.
53. Rutz DA, Luo Q, Freiburger L, Madl T, **Kaila VRI**, Sattler M, Buchner J (2018) A switch point in the molecular chaperone Hsp90 responding to client interaction. **Nature Comm** 9: 1472.
52. **Kaila VRI*** (2018) Multi-scale Molecular Simulations on Respiratory Complex I. in Chemical Biology No. 5, "Mechanisms of Primary Energy Transduction in Biology", *Ed.* Mårten Wikström, **The Royal Society of Chemistry** 2018 DOI:10.1039/9781788010405-00081
51. Schrepfer P, Ugur I, Klumpe S., Metterlein M, **Kaila VRI***, Brück T (2018) Deciphering and harmonizing catalytic events in cembranoid biosynthesis - a symphony of computational and synthetic biocatalysis. (in review)
50. Wachtel R, Bräuning B, Mader SL, Ecker F, **Kaila VRI**, Groll M, Itzen A (2018) The protease GtgE from Salmonella exclusively targets inactive Rab-proteins. **Nature Comm** 9: 44.
49. Gamiz-Hernandez AP, Jussupow A, Johansson MP, **Kaila VRI*** (2017) Terminal Electron-Proton Transfer Dynamics coupled to Quinone reduction in Respiratory Complex I. **J Am Chem Soc** 139: 16282-16288.
48. Suomivuori C-M, Gamiz-Hernandez AP, Sundholm D, **Kaila VRI*** (2017) Energetics and dynamics of a light-driven sodium-pumping rhodopsin. **Proc Natl Acad Sci USA** 114: 7043-7048. Cover issue.
47. Supekar S, Papageorgiou AC, Gemmecker G, Peltzer R, Johansson MP, Tripsianes K, Sattler M, **Kaila VRI*** (2018) Conformational Selection of Dimethylarginine Recognition by the SMN Tudor Domain. **Angew Chemie Intl Ed** 57: 486-490.
46. Di Luca A, Gamiz-Hernandez AP, **Kaila VRI*** (2017) Symmetry related proton transfer pathways in respiratory Complex I. **Proc Natl Acad Sci USA** 114: E6314-E6321.
45. Luo Q, Boczek EE, Buchner J, **Kaila VRI*** (2017) Conformational activation and Hsp90-dependence of c-Src and its oncogenic mutants. **Sci Rep** 7: 43996.

44. Suomivuori C-M, Winter N.O.C., Hättig C, Sundholm D, **Kaila VRI*** (2016) Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. **J Chem Theory Comput** 12: 2644-2651.
43. Wittwer M, Luo Q, **Kaila VRI**, Dames S (2016) Oxidative Unfolding of the Rubredoxin Domain and the Natively Disordered N-terminal Region Regulate the Catalytic Activity of M. tuberculosis Protein Kinase G. **J Mol Biol** 291: 27062-27072.
42. Gamiz-Hernandez AP, **Kaila VRI*** (2016) Conversion of light-energy into molecular strain in the photocycle of the photoactive yellow protein. **Phys Chem Chem Phys** 18: 2802-2809.
41. Zhang Q, Catti L, **Kaila VRI**, Tiefenbacher K (2016) To Catalyze or not to Catalyze: Elucidation of the Subtle Differences between the Hexameric Capsules of Pyrogallolarene and Resorcinarene. **Chem Sci** 8: 1653-1657.
40. Suomivuori CM, Lang L, Sundholm D, Gamiz-Hernandez AP, **Kaila VRI*** (2016) Tuning the protein-induced absorption shifts of retinal in engineered rhodopsin mimics. **Chem – Eur J**. 22: 8254-8861.
39. Supekar S, Gamiz-Hernandez AP, **Kaila VRI*** (2016) A Protonated Water Cluster as a Transient Proton Loading Site in Cytochrome c Oxidase. **Angew Chemie Intl Ed** 55: 11940-11944.
38. Ugur I, Rutherford AW, **Kaila VRI*** (2016) Redox-coupled substrate water reorganization in the active site of Photosystem II. **Biochim Biophys Acta – Bioenergetics** 1857: 740-748.
37. Sharma V, Belevich G, Gamiz-Hernandez AP, Róg T, Vattulainen I, Wikström M, Hummer G, **Kaila VRI*** (2015) Redox-Induced Activation of the Proton Pump in the Respiratory Complex I. **Proc Natl Acad Sci USA** 112:11571-11576.
36. Gamiz-Hernandez AP, Neycheva IA, Send R, Sundholm D, **Kaila VRI*** (2015) Protein-Induced Color Shift of Carotenoids in β -Crustacyanin. **Angew Chemie Intl Ed** 54:11564-11566.
35. Boczek EE, Reefschräger LG, Dehling M, Struller T, Häusler E, Seidl A, **Kaila VRI**, Buchner J (2015) Conformational processing of oncogenic v-Src kinase by Hsp90. **Proc Natl Acad Sci USA** 112: E3189-3198.
34. Kmita K, Wirth C, Warnau J, Guerrero-Castillo S, Hunte C, Hummer G, **Kaila VRI**, Zwicker K, Brandt U, Zickermann V. (2015) Accessory NUMM (NDUFS6) subunit harbors a Zn-binding site and is essential for biogenesis of mitochondrial complex I. **Proc Natl Acad Sci USA** 112: 5685-5690.
33. Wikström M, Sharma V, **Kaila VRI**, Hosler J, Hummer G (2015) New perspectives on proton pumping in cellular respiration. **Chem Rev** 115: 2196-2221.
32. Send R, Suomivuori CM, **Kaila VRI***, Sundholm D (2015) Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models using the Reduced Virtual Space Approach. **J Phys Chem B** 119: 2933-2945.

31. Gamiz-Hernandez AP, Magomedov A, Hummer G, **Kaila VRI*** (2014) Linear energy relationships in ground state proton transfer and excited state proton-coupled electron transfer **J Phys Chem B** 119: 2611-2619.
30. **Kaila VRI***, Wikström M, Hummer G (2014) Electrostatics, Hydration, and Proton Transfer Dynamics in the Membrane Domain of Respiratory Complex I. **Proc Natl Acad Sci USA** 111: 6988-6993.
29. **Kaila VRI**, Schotte F, Hyun S-C, Hummer G, Anfinrud PA (2014) Reconciling contradictions in time-resolved x-ray structures of early intermediates in the photocycle of photoactive yellow protein. **Nature Chem** 6: 258-259.
28. Zhou X, Sundholm D, Wesolowski A, **Kaila VRI*** (2014) Spectral Tuning of Rhodopsin and Visual Cone Pigments. **J Am Chem Soc** 136: 2723-2726.
27. **Kaila VRI***, Send R, Sundholm D (2013) Electrostatic Spectral Tuning Mechanism of the Green Fluorescent Protein. **Phys Chem Chem Phys** 15: 4491-4495.
26. Johansson MP, **Kaila VRI***, Sundholm D (2013) *Ab initio*, density functional theory, and semi-empirical calculations. **Methods in Mol Biol** 924: 3-27.
25. Schotte F, Hyun S-C, **Kaila VRI**, Kamikubo H, Dashdorja N, Henry E, Graber T, Henning R, Wulff M, Hummer G, Kataoka M, Anfinrud PA (2012) Picosecond Photobiology: Watching a Signaling Protein Function in Real Time via Time-resolved Laue Crystallography. **Proc Natl Acad Sci USA** 109: 19256-19261.
24. **Kaila VRI***, Send R, Sundholm D (2012) The effect of the protein environment on primary photoexcitation events of retinal. **J Phys Chem B** 116: 2249-2258.
23. Sharma V, Wikström M, **Kaila VRI*** (2012) Dynamic water networks in cytochrome *cbb3*. **Biochim Biophys Acta – Bioenergetics** 1817: 726-734.
22. **Kaila VRI***, Hummer G (2011) Energetics of direct and water-mediated proton-coupled electron transfer. **J Am Chem Soc** 133: 19040-19043.
21. **Kaila VRI***, Hummer G (2011) Energetics and dynamics of proton transfer reactions along short water wires. **Phys Chem Chem Phys** 13: 13207-13215.
20. Send R, **Kaila VRI**, Sundholm D (2011) Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. **J Chem Theory Comput** 7: 2473-2484.
19. Send R, **Kaila VRI**, Sundholm D (2011) Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. **J Chem Phys** 134: 214114.
18. Sharma V, Wikström M, **Kaila VRI*** (2011) Stabilization of the peroxy intermediate in the oxygen splitting reaction of cytochrome *cbb3*. **Biochim Biophys Acta – Bioenergetics** 1807: 813-818.

17. **Kaila VRI***, Oksanen E, Goldman A, Verkhovsky MI, Sundholm D, Wikström M (2011) A Combined Quantum Chemical and Crystallographic Study on the Oxidized Binuclear Center of Cytochrome *c* Oxidase. **Biochim Biophys Acta – Bioenergetics** 1807: 769-778.
16. Fliegl H, Lehtonen O, Sundholm D, **Kaila VRI*** (2011) Hydrogen-bond strengths by magnetically induced currents. **Phys Chem Chem Phys** 13: 434-437.
15. **Kaila VRI***, Sharma V, Wikström M (2011) The identity of the transient proton loading site of the proton-pumping mechanism of cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenergetics** 1807: 80-84.
14. Taubert S, **Kaila VRI**, Sundholm D (2011) Aromatic pathways in conjugated rings connected by single bonds. **Int J Quantum Chem** 111: 848-857.
13. **Kaila VRI**, Verkhovsky MI, Wikström M (2010) Proton-coupled electron transfer in cytochrome oxidase. **Chem Rev** 110: 7062-7081.
12. **Kaila VRI***, Johansson MP, Sundholm D, Wikström M (2010) Interheme electron tunneling in cytochrome *c* oxidase. **Proc Natl Acad Sci USA** 107: 21470-21475.
11. Sharma V, Wikström M, **Kaila VRI*** (2010) Redox-coupled proton transfer in the active site of cytochrome *cbb₃*. **Biochim Biophys Acta – Bioenergetics** 1797: 1512-1520.
10. **Kaila VRI***, Verkhovsky MI, Hummer G, Wikström M (2009) Mechanism and energetics by which glutamic acid 242 prevents leaks in cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenergetics** 1787: 1205-1214.
9. **Kaila VRI**, Johansson MP, Sundholm D, Laakkonen L, Wikström M (2009) The chemistry of the CuB site in cytochrome *c* oxidase and the importance of its unique His Tyr bond. **Biochim Biophys Acta – Bioenergetics** 1787: 221-233.
8. Sharma V, **Kaila VRI**, Annala A (2009) Protein folding as an evolutionary process. **Physica A** 388: 851-862.
7. **Kaila VRI**, Annala A (2008) Natural selection for least action. **Proc Roy Soc A** 464: 3055-3070.
6. **Kaila VRI**, Verkhovsky MI, Hummer G, Wikström M (2008) Prevention of leak in the proton pump of cytochrome *c* oxidase. **Biophys Biochim Acta – Bioenergetics** 1777: 890-892.
5. **Kaila VRI**, Verkhovsky MI, Hummer G, Wikström M (2008) Glutamic acid 242 is a valve in the proton pump of cytochrome *c* oxidase. **Proc Natl Acad Sci USA** 105: 6255-6259.
4. Johansson MP, **Kaila VRI**, Laakkonen L (2008) Charge parameterization of the metal centers in cytochrome *c* oxidase. **J Comput Chem** 29: 753-767.
3. Tuukkanen A^a, **Kaila VRI^a**, Laakkonen L, Hummer G, Wikström M (2008) Dynamics of the glutamic acid 242 side chain in cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenergetics** 1767: 1102-1106 (^ashared first authorship).

2. **Kaila VRI** (2009), “Theoretical Studies on Coupled Electron and Proton Transfer in Cytochrome Oxidase”. ISBN 978-952-10- 5263-7, ISSN 1795-7079, Yliopistopaino, Helsinki University Printing House. In electronic format: <https://oa.doria.fi/handle/10024/43396>

1. **Kaila VRI** (2006) “Beräkningskemiska studier av proton-translokeringsmekanismen i cytokrom *c* oxidas”, MSc thesis.