

## Curriculum Vitae of Prof. Ville R. I. Kaila, PhD



## PERSONAL INFORMATION

Full name: Ville Rolf Ilmari, KAILA  
 Date of birth: Dec 6, 1983 (age 39)  
 Civil status: Married, two children (3 and 9 years)  
 ORCID: 0000-0003-4464-6324  
 Web page: [villekaila.com](http://villekaila.com)  
 Nationality: Finnish

## EDUCATION

2007 – 2009 **Ph.D.** in Biochemistry, University of Helsinki, Finland. Grade: *excellent* (April/2009).  
*Supervisor:* Prof. Mårten Wikström, MD, PhD  
 2003 – 2007 **M.Sc.** in Biochemistry, University of Helsinki, Finland. Minors in Physical Chemistry,  
 Physics and Theoretical Physics.  
 1994 – 2004 Sibelius Academy, Finland. Training for a solo violin career.

## CURRENT POSITION

2019 – present **Full Professor of Biochemistry** (former Chair of Prof. Gunnar von Heijne)  
 Department of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden.

## PREVIOUS POSITIONS

2018 – 2019 **Professor (W3)**, tenured, Computational Biocatalysis, Department of Chemistry, Technical  
 University of Munich (TUM), Germany. Mentoring of TUM-PhD students until end of 2021.  
 2013 – 2018 **Tenure-track Professor (W2 to W3)** of Computational Biocatalysis, Department of  
 Chemistry, Technical University of Munich (TUM), Germany.  
 2018 **Visiting Professor program**, TUM-Imperial College London, UK. Collaboration with Prof.  
 A.W. Rutherford Lab.  
 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:* Prof. Dr. Gerhard Hummer (molecular biophysics)  
 2010 **Short-term post-doctoral researcher**, University of Helsinki, Finland.  
*Mentor:* Prof. Dr. Dage Sundholm (theoretical chemistry)  
 2006 – 2010 **Temporary Lecturer**, Department of Biology and Department of Chemistry, University of  
 Helsinki, Finland (physical chemistry, general chemistry).  
 2005 – 2009 **Researcher**, Helsinki Bioenergetics Group, University of Helsinki, Finland.  
*Mentor:* Prof. Dr. Mårten Wikström  
 2008 **Visiting scholar** in the research group of Prof. Dr. Peter Taylor, University of Warwick, UK.  
 2004 – 2005 **Research assistant** in NMR-laboratory and Helsinki Bioenergetics Group, University of  
 Helsinki, Finland.

HONOURS, FELLOWSHIPS, AND AWARDS (Total: *ca.* 7 Mio EUR during last 5 years)

2022 **Svedberg Prize in Biochemistry.**  
 2021 **Tage Erlander Prize** in Natural Sciences and Technology.  
 2021 – 2025 **Visiting Professorship** (Mercator Program, SFB1078), Freie Universität Berlin, Germany.  
 2020 – 2025 **Wallenberg Academy Fellow** (15 Mio SEK).  
 2020 **Recognition award** from Sven and Ebba-Christina Hagberg Foundation.  
 2020 Research Grant from Swedish Research Council (Vetenskapsrådet, 4.9 Mio SEK) and  
 Swedish Cancer Foundation (Cancerfonden, 3.1 Mio SEK).  
 2019 **Collaborative Wallenberg foundation project** (38 Mio SEK, Team: Högbom-Ädelroth-  
 Brzezinski-Kaila, "*The obligate respiratory supercomplex - augmented biological energy  
 conversion*").  
 2019 **Recognition award:** Ruth & Nils-Erik Stenbäck's foundation.  
 2018 **Recognition award:** Hans Fischer Memorial Award.  
 2018 **Excellence in teaching nomination, TU Munich.**

## KAILA

- 2018 – 2019 **Research funding** from Center of Integrated Protein Science Munich, 35 000 EUR.  
2016 – 2021 **European Research Council (ERC)**, Starting Grant, 1.5 Mio EUR.  
2015 **The Grand Prize** from Oskar Öflund's foundation, 15 000 EUR.  
2015 – Multiple **research grants** from German Research Foundation (DFG), Total 1.3 Mio EUR including Collaborative Research Grant (SFB1035), "*Emergence of Life*", and individual research projects.  
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 Erkkö Foundation: "Mechanisms of Biomimetic Water Splitting", 89 000 EUR.  
2010 – 2012 **Long-Term Postdoctoral Fellow**, European Molecular Biology Organization (EMBO).  
2010 **Recognition award**, Ruth & Nils-Erik Stenbäck's foundation, Finnish Science Foundation.  
2009 **The Alftan's prize** of the Finnish Chemical Society for best doctoral thesis of 2009.  
2007 – 2009 **Ph.D. fellowship** from Helsinki Graduate School of Biotechnology and Molecular Biology.  
2006 **Research Award**, Finnish Cultural Foundation for research in Computational Biochemistry.

## SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2013 – present Mentored **4** staff-scientist, **7** postdocs (3 now at PI/senior scientist positions), **14** PhD students (7 completed; 7 in progress), **>20** MSc/BSc/research-theses at TU Munich and Stockholm University. **Current team (2022)**: 3 staff scientists; 5 postdocs; 7 PhD students, 1 student.

## TEACHING ACTIVITIES (*selected*)

Developed and lectured *ca.* 20 courses at BSc, MSc, PhD level during 2013-present. See web page for further details. Nominated for excellence in teaching award at TU Munich 2018.

## ORGANISATION OF SCIENTIFIC MEETINGS (*selected*)

- 2022 Co-organizer of Psi-K (2021/2022) conference (C6 panel)  
2021 Co-organizer of German Physical Society (DPG) Spring Meeting 2021, Biophysics section.  
2017 Winter School of Theoretical Chemistry / Finland. *ca.* 100 Participants.

## INSTITUTIONAL RESPONSIBILITIES (*selected*)

- 2021 – Faculty and Recruitment board in Natural Sciences, Stockholm University.

## REVIEWING ACTIVITIES (*selected*)

- 2018 – Editorial Board Member, Journal of the Royal Society Interfaces, UK  
2014 – Ad-hoc reviewer for several journals including, *e.g.*, Angew Chemie, eLife, JACS, J Phys Chem Lett, NSMB, Nature Comms, Nature, Nature Chem, Science, PNAS.  
2013 – present Grant Reviewer for DFG, AvH, DAAD, ISF, NWO, ERC (Synergy and Advance Grants)  
2013 – present Served in > 40 PhD committees as examiner/opponent/chair

## MEMBERSHIPS OF SCIENTIFIC SOCIETIES (*selected*)

- 2020 – Elected Foreign Member of the Finnish Academy of Sciences and Letters

## MAJOR COLLABORATIONS

Prof. Judy **Hirst**, FRS, University Cambridge, Mitochondrial Biology Unit; Prof. Bill **Rutherford**, FRS, Imperial College London; Prof. Michael **Groll**/Prof. Michael **Sattler**/Prof. Johannes **Buchner**, TU Munich; Dr. Jan **Schuller**; Marburg University; Prof. Martin **Högbom**/Prof. Peter **Brzezinski**/Prof. Gunnar **von Heijne**, Stockholm University. Freie Universität Berlin (FUB), **SFB1078** Visiting Professor Program, 2021 – 2025.

## CAREER BREAKS

- 4/2009 – 4/2010 Compulsory military service (Finland), 12 months

## PUBLICATION SUMMARY AND INVITED TALKS

**> 100 peer-reviewed articles** (see selected publications), 4523 citations in total, *h*-index 40 (Google scholar), including multiple publications in *e.g.* PNAS (14), Nature Chemistry (2), Nature Comm (9), Nature Chem Biol (1), Science Adv (1), Angew Chemie (4), Chem Rev (2), Chem Science (2), and JACS (10); **> 60** invited/plenary talks during last five years.

**Selected publications***(See full publication list below)*

1. Röpke M, Riepl D, Di Luca A, Saura P, Mühlbauer M, Jussupow A, Gamiz-Hernandez AP, **Kaila VRI\*** (2021) Deactivation blocks proton pathways in the mitochondrial complex I. **PNAS** 118:e2019498118. • *Integration of molecular simulations, QM/MM, cryoEM data, bioinformatic analysis reveal a gating region that modulate complex I activity.*
2. Allgöwer FA, Gamiz- Hernandez AP, **Kaila VRI\*** (2022) Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II **JACS** 144: 7171-7180. • *Multiscale simulations of complex redox-driven proton transfer reactions in Photosystem II, showing that the enzyme utilizes electric field effects to control the water-splitting catalysis.*
3. Baumgart M, Röpke M, Mühlbauer M, Asami S, Mader S, Fredriksson K, Groll M, Gamiz-Hernandez AP, **Kaila VRI\*** (2021) Design of buried ion-pairs in artificial proteins. **Nature Comms** 12: 1895, 1–10 • *Our breakthrough work on artificial protein design integrated with computational, biochemical, biophysical and structural techniques to derive physical into function and stability of buried ion-pairs.*
4. Bridges HR, Fedor JG, Blaza JN, Di Luca A, Jussupow A, Jarman OD, Wright J, Agip ANA, Gamiz-Hernandez AP, Roessler MM, **Kaila VRI\***, Hirst J (2020) Structure of inhibitor-bound mammalian complex I, **Nature Comms**, 5261: 11, 1–11. • *Integration of cryoEM, computational, and functional studies to explore substrate binding in the mammalian complex I.*
5. 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. • *Our breakthrough work on describing the CO<sub>2</sub>-concentrating photosynthetic complex I.*
6. Mühlbauer ME, Saura P, Nuber F, Di Luca A, Friedrich T, **Kaila VRI\*** (2020) Water-gated proton transfer dynamics in respiratory complex I. **JACS** 142, 13718-13728. • *Mechanism of redox-driven proton pumping elucidating a link-between protein hydration, proton transfer, ion-pair dynamics, and validated with functional studies.*
7. 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 Comms** 11, 11410; 1-12. • *Enzyme engineering and modulating active site catalytic properties by combination of multiscale simulations, biophysical, biochemical, and functional studies.*
8. Jussupow A, Di Luca A, **Kaila VRI\*** (2019) How cardiolipin modulates the activity of complex I. **Science Adv** 5, eaav1850. • *The role of protein-lipid interactions in the function of membrane proteins and derivation of cardiolipin-binding sites in complex I.*
9. 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. • *The first prediction of a second Q-binding site in complex I that we validated based on free energy simulations. Experimental validation of this site is provided in Publication 4 (see above).*
10. Di Luca A, Gamiz-Hernandez AP, **Kaila VRI\*** (2017) Symmetry related proton transfer pathways in respiratory Complex I. **PNAS** 114, E6314-E6321. • *First prediction of proton wires in complex I.*

**PUBLICATIONS of Prof. Ville R. I. Kaila (updated Dec 2022)**N=109 incl. 5 in review; 4523 citations, *h*-index 40 (Google scholar)

\* corresponding author

**109.** Jussupow A, **Kaila VRI\*** (2022) Effective Molecular Dynamics from Neural-Network Based Structure Prediction Models (in review)

**108.** Kim H, Patricia Saura P, Pöverlein M.C.

Ana P. Gamiz-Hernandez A. P., Kaila V.R.I. (2022). Quinone Catalysis Modulates Proton Transfer Reactions in the Membrane-Domain of Respiratory Complex I (in review)

**107.** Saura P, Riepl D, Frey DM, Wikström M, Kaila VRI\* (2022). Electric Fields Control Water-Gated Proton Transfer in Cytochrome *c* Oxidase. **Proc. Natl. Acad. Sci. USA** 119(38):e2207761119.

**106.** John J, Aurelius O, Srinivas V, Saura P, Kim IS, Bhowmick A, Simon PS, Dasgupta M, Pham C, Gul S, Sutherlin KD, Aller P, Butryn A, Orville AM, Cheah MH, Owada S, Tono K, Fuller FD, Batyuk A, Brewster AS, Sauter NK, Yachandra VK, Yano J, **Kaila VRI**, Kern J, Lebrette H, Högbom M. (2022) Redox-controlled reorganization and flavin strain within the ribonucleotide reductase R2b-NrdI complex monitored by serial femtosecond crystallography. **eLife** 11: e79226.

**105.** Allgöwer F, Gamiz-Hernandez AP, Rutherford AW, **Kaila VRI\*** (2022). Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II. **J Am Chem Soc** 144: 7171-7180.

**104.** Fantuzzi A, Allgöwer F, Baker H, McGuire G, Kii Teh W, Gamiz-Hernandez AP, **Kaila VRI\***, Rutherford AW (2022) Bicarbonate-controlled reduction of oxygen by the Q<sub>A</sub> semiquinone in Photosystem II. **Proc Natl Acad Sci USA** 119(6):e2116063119.

**103.** Mühlbauer ME, Gamiz-Hernandez AP, **Kaila, VRI\*** (2021) Functional dynamics of an ancient membrane-bound hydrogenase. **J Am Chem Soc** 143: 20873-20883.

**102.** **Kaila VRI\*** (2021). Resolving Chemical Dynamics in Biological Energy Conversion: Long-range Proton-Coupled Electron Transfer in Respiratory Complex I. **Acc Chem Res** 54: 4462-4473.

**101.** Di Trani J, Moe A, Riepl D, Saura P, **Kaila VRI**, Brzezinski P, Rubinstein JL (2022). Structural basis of mammalian Complex IV inhibition by steroids. **Proc Natl Acad Sci USA** 119:e2205228119.

**100.** Katsyv A, Kumar A, Saura P, Pöverlein M.C., Freiber SA, Stripp S, Jain S, Gamiz-Hernandez AP, **Kaila VRI\***, Müller V, Schuller JM Molecular basis of a novel electron bifurcation mechanism in the HydABC complex. **JACS** (in review).

**99.** Jussupow A, Lopez A, Baumgart M, Mader S, Sattler M, **Kaila VRI\*** (2022) Extended conformational states dominate the Hsp90 chaperone dynamics. **J Biol Chem** 298(7):102101.

**98.** Melse O, Cho WY, Wu T, Antes I, **Kaila VRI\***, Sieber V, EnzymeMatch: Identification of Enzymes Capable of Catalyzing Target Reactions using Interaction Pattern Matching. (in review).

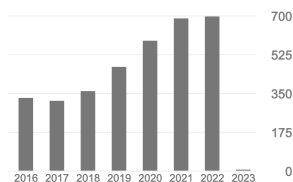
**97.** Melse O, Antes I, **Kaila VRI**, Zacharias, M. (2022) Benchmarking Biomolecular Force Field-based Zn<sup>2+</sup> Models for Mono- and Bimetallic Ligand Binding Sites. **J Comput Chem** (in press) doi: 10.1002/jcc.27052.

**96.** Auman D, Ecker F, Mader SL, Dorst KM, Bräuer A, Widmalm G, Groll M, **Kaila VRI\***. Peroxy intermediate drives carbon bond activation in the dioxygenase AsqJ. **J Am Chem Soc.** 144(34):15622-15632.

**95.** Röpke M, Riepl D, Di Luca A, Saura P, Mühlbauer M, Jussupow A, Gamiz-Hernandez AP, **Kaila VRI\*** (2021) Deactivation blocks proton pathways in the mitochondrial complex I. **Proc Natl Acad Sci USA** 118(29):e2019498118.

Cited by [VIEW ALL](#)

	All	Since 2018
Citations	4523	2819
h-index	40	31
i10-index	78	68



94. Baumgart M, Röpke M, Mühlbauer ME, Asami S, Mader S, Fredriksson K, Groll M, Gamiz-Hernandez AP, **Kaila VRI\*** (2021) Design of Buried Charged Networks in Artificial Proteins. **Nature Communications** 12: 1895.
93. Bridges HR, Fedor JG, Blaza JN, Di Luca A, Jussupow A, Jarman OD, Wright J, Agip ANA, Gamiz-Hernandez AP, Roessler MM, **Kaila VRI\***, Hirst J (2020) Structure of inhibitor-bound mammalian complex I, **Nature Communications** 5261: 11, 1–11.
92. **Kaila VRI\***, Wikström M (2021) Architecture of Bacterial Respiratory Chains. **Nature Rev Microbiol** 19: 319-330.
91. Johansson MP, Niederegger L, Rauhalahhti M, Hess CR, **Kaila VRI\*** (2021) Dispersion-Forces Drive Water Oxidation in Molecular Ruthenium Catalysts. **RSC Advances** 11: 425-432.
90. Lauenstein R, Mader S, Derondeau H, Block M, Römer A, Jandl C, Riedle E, **Kaila VRI**, Hauer J, Thyryhaug E, Hess CR (2021). The central role of the metal ion in photocatalysis: Zn- vs. Ni-Mabiq. **Chem Sci** 12(21): 7521-7532.
89. Di Luca A, **Kaila VRI\*** (2021) Molecular strain in the active/deactive-transition modulates domain coupling in respiratory complex I. **Biochim Biophys Acta Bioenerg** 1862(5):148382.
88. Röpke M, Saura P, Riepl D, Pöverlein M, **Kaila VRI\*** (2020) Functional water-wires catalyze long-range proton pumping in the mammalian respiratory complex I. **J Am Chem Soc** 142:21758-21766.
87. Kriebisch BAK, Jussupow A, Bergmann AM, Kohler F, Dietz H, **Kaila VRI**, Boekhoven J (2020) Reciprocal Coupling in Chemically Fueled Assembly: A Reaction Cycle Regulates Self-Assembly and Vice Versa. **J Am Chem Soc** 142(49): 20837-20844.
86. Mühlbauer ME, Saura P, Nuber F, Di Luca A, Friedrich T, **Kaila VRI\*** (2020) Water-gated proton transfer dynamics in respiratory complex I. **J Am Chem Soc** 142: 13718-13728.
85. 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.
84. 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 Comms** 11: 11410: 1-12.
83. Rehn A, Lawatscheck J, Mader SL, Luo Q, Blank B, Richter K, **Kaila VRI**, Buchner, J (2020) A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. **Nature Comms** 11: 1219; 1-14.
82. Bräuer A, Zhou Q, Grammbitter GLC, Schmalhofer M, **Kaila VRI**, Bode HB, Groll M (2020) Structural Snapshots of the Minimal PKS System Responsible for Octaketide Biosynthesis. **Nature Chemistry** 12(8):755-763.
81. Wild R, Di Luca A, Bisha I, **Kaila VRI\*** (2021) Ligand-dependent structural dynamics drives conformational switching in the human serotonin transporter (in review).
80. Farinelli G, Di Luca A, **Kaila VRI**, MacLachlan MJ, Tiraferri A (2020), Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. **J. Hazard Mater.** 408: 124662
79. Wanzke C, Jussupow A, Kohler F, Dietz H, **Kaila VRI**, Boekhoven J (2020) Dynamic vesicles formed by dissipative self-assembly, **ChemSystemsChem** 2: e1900044.

77. 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.
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<sup>+</sup>/H<sup>+</sup> Antiporter MjNhaP1. **J. Phys Chem B** 124: 336-344.
74. **Kaila VRI\*** (2019) Molekularen Mechanismen der biologischen Energieumwandlung. **Nachr Chem** 67.
73. 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.
72. Jussupow A, Di Luca A, **Kaila VRI\*** (2019) How cardiolipin modulates the activity of complex I. **Science Adv** 5: eaav1850.
71. Schrepfer P, Ugur I, Klumpe S., Metterlein M, Loll B, **Kaila VRI\***, Brück T (2020) Exploring the catalytic cascade of cembranoid biosynthesis by combination of genetic engineering and molecular simulations. **Comput Struct Biotechnol J** 18:1819-1829.
70. 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.
69. **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*.
68. 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.
67. 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.
66. 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.
65. 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.
64. 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.
63. Saura P, **Kaila VRI\*** (2018) Structure and dynamics of the cyanobacterial NDH-1 complex. **Biochim Biophys Acta - Bioenerg** 1860:201-208.
62. 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.
61. 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.
60. Supekar S, **Kaila VRI\*** (2018) Dewetting transitions coupled to K-channel activation in cytochrome *c* oxidase. **Chem Science** 9: 6703-6710.
59. 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 - Bioenerg** 1859: 734-741.

58. 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.
57. Saura P, Röpke M, Gamiz-Hernandez AP, Kaila VRI\* (2019) Quantum Chemical and QM/MM Models in Biochemistry. **Methods in Mol Biol** 2022:75-104.
56. Lindsay S, Mader SL, Kaila VRI\*, Hess CR (2018) C-H Oxidation by a Diiron Complex with Facially Opposing Active Sites. **ChemistrySelect** 3(5).
55. 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 - Bioenerg** 1859: 342-356.
54. Di Luca, Kaila VRI\* (2018) Global Collective Motions in the Mammalian and Bacterial Respiratory Complex I. **Biochim Biophys Acta - Bioenerg** 1859: 326-332.
53. 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.
52. 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.
51. 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.
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.

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