

Indrek Kalvet

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Education

- 2018 –** **University of Washington**, Seattle, USA
HFSP & HHMI Postdoctoral Fellow with Prof. David Baker
- 2013 – 2017** **RWTH Aachen University**, Aachen, Germany
Doctoral studies with Prof. Franziska Schoenebeck (*summa cum laude*)
- 2011 – 2013** **University of Tartu**, Tartu, Estonia
MSc in chemistry (*cum laude*)
- 2008 – 2011** **University of Tartu**, Tartu, Estonia
BSc in chemistry

Internships and Trainings

- 08/2016** **Kings College**, London, UK
Ab initio Molecular Dynamics (CP2K) summer school
- 06/2013 –** **TBD Biodiscovery**, Tartu, Estonia
08/2013 Internship in synthetic chemistry
- 10/2012 –** **Queen's University**, Kingston, Canada
01/2013 Visiting researcher with Prof. Victor Snieckus.
- 09/2011** **Aalto University**, Helsinki, Finland
Workshop in computational chemistry (Prof. Per-Ola Norrby)

Awards and Honors

- 2018** HFSP Cross-Disciplinary Postdoctoral Fellowship
- 2017** Estonian Student Research Contest, main prize
- 2017** Best flash talk award, 2nd prize (*ISySyCat 2017*)
- 2017** MS_CEC Young Researcher Award (*for superb scientific contributions in Germany*)
- 2017** Poster prize at the 9th New Year's Symposium (*Aachen, Germany*)
- 2016** DAAD Travel award (*For participating EuCheMS 2016 in Seville*)
- 2016** GDCh Travel award (*For participating ORCHEM 2016 in Weimar*)
- 2012** Rotalia Foundation scholarship
- 2012** ESF DoRa 7 Travel award (*For studies in Canada*)
- 2008** Finalist at the Estonian National Chemistry Olympiad

Publications

- [20] R. Krishna,[†] J. Wang,[†] W. Ahern,[†] P. Sturmfels, P. Venkatesh,[‡] I. Kalvet,[‡] G. R. Lee,[‡] F. S. Morey-Burrows, I. Anishchenko, I. R. Humphreys, R. McHugh, D. Vafeados, X. Li, G. A. Sutherland, A. Hitchcock, C. N. Hunter, A. Kang, E. Brackenbrough, A. K. Bera, M. Baek, F. DiMaio, D. Baker, “Generalized Biomolecular Modeling and Design with RoseTTAFold All-Atom” *Science* **2024**, *384*, eadl2528.
- [19] K. H. Sumida, R. Núñez-Franco, I. Kalvet, S. J. Pellock, B. I. M. Wicky, L. F. Milles, J. Dauparas, J. Wang, Y. Kipnis, N. Jameson, A. Kang, J. De La Cruz, B. Sankaran, A. K. Bera, G. Jiménez-Osés, D. Baker, “Improving protein expression, stability, and function with ProteinMPNN” *J. Am. Chem. Soc.* **2024**, *146*, 2054.
- [18] I. Kalvet,[†] M. Ortmayer,[†] J. Zhao,[†] R. Crawshaw, N. M. Ennist, C. W. Levy, A. Roy, A. P. Green, D. Baker, “Design of Heme Enzymes with a Tunable Substrate Binding Pocket Adjacent to an Open Metal Coordination Site” *J. Am. Chem. Soc.* **2023**, *145*, 14307.
- [17] I. Kalvet, K. Deckers, I. Funes-Ardoiz, G. Magnin, T. Sperger, M. Kremer, F. Schoenebeck, “Selective Ortho Functionalization of Adamantylarenes enabled by Dispersion and an Air-Stable Pd(I) Dimer” *Angew. Chem. Int. Ed.* **2020**, *59*, 7721.
- [16] M. Mendel, I. Kalvet, D. Hupperich, G. Magnin, F. Schoenebeck, “Site-Selective, Modular Diversification of Polyhalogenated Aryl Fluorosulfates (ArOSO₂F) Enabled by an Air-Stable Pd^I Dimer” *Angew. Chem. Int. Ed.* **2020**, *59*, 2115.
- [15] J. Ye, I. Kalvet, F. Schoenebeck, T. Rovis, “Direct α -alkylation of primary aliphatic amines enabled by CO₂ and electrostatics” *Nature Chem.* **2018**, *10*, 1037.
- [14] A. B. Dürr,[†] H. C. Fisher,[†] I. Kalvet, K. N. Truong, F. Schoenebeck, “Striking Divergence in Reactivity of a Dinuclear (NHC)Ni(I) Catalyst vs Ni(0) enables Chemoselective Trifluoromethylselenolation” *Angew. Chem. Int. Ed.* **2017**, *56*, 13431.
- [13] I. Kalvet, T. Sperger, T. Scattolin, G. Magnin, F. Schoenebeck, “Pd^(I) Dimer Enabled Extremely Rapid and Chemoselective Alkylation of Aryl Bromides over Triflates & Chlorides in Air” *Angew. Chem. Int. Ed.* **2017**, *56*, 7078.
- [12] I. Kalvet, Q. Guo, G. J. Tizzard, F. Schoenebeck, “When Weaker Can Be Tougher: On the Role of Oxidation State (I) in P- vs. N-Ligand Derived Ni-Catalyzed Trifluoromethylthiolation of Aryl halides” *ACS Catal.* **2017**, *7*, 2126.
- [11] I. Kalvet, G. Magnin, F. Schoenebeck, “Rapid Room Temperature Chemoselective C_{sp}²-C_{sp}² Coupling of Poly(pseudo)halogenated Arenes enabled by Pd(I) Catalysis in Air” *Angew. Chem. Int. Ed.* **2017**, *56*, 1581.
- [10] H. P. L. Gemoets, I. Kalvet, A. V. Nyuchev, N. Erdmann, V. Hessel, F. Schoenebeck, T. Noël, “Mild and selective base-free C–H arylation of heteroarenes: Experiment and computation” *Chem. Sci.* **2017**, *8*, 1046.
- [9] M. Lorentzen, I. Kalvet, F. Sauriol, T. Rantanen, K. B. Jørgensen, V. Snieckus, “Atropisomerism in Tertiary Biaryl 2-Amides: A Study of Ar-CO and Ar-Ar’ Rotational Barriers” *J. Org. Chem.* **2017**, *82*, 7300.
- [8] I. Kalvet, J. Tammiku-Taul, U. Mäeorg, K. Tamm, P. Burk, L. Sikk, “NMR and DFT Study of the Copper(I)-Catalyzed Cycloaddition Reaction: H/D Scrambling of Alkynes and Variable Reaction Order of the Catalyst” *ChemCatChem* **2016**, *8*, 1804.
- [7] X. Liu, C.-C. Hsiao, I. Kalvet, M. Leiendecker, L. Guo, F. Schoenebeck, M. Rueping, “Lewis Acid Assisted Nickel-Catalyzed Cross-Coupling of Aryl Methyl Ethers by C–O Bond-Cleaving Alkylation: Prevention of Undesired β -Hydride Elimination” *Angew. Chem. Int. Ed.* **2016**, *55*, 6093.

- [6] A. B. Dürr, G. Yin, I. Kalvet, F. Napoly, F. Schoenebeck, "Nickel-catalyzed Trifluoromethylthiolation of Csp²–O Bonds" *Chem. Sci.* **2016**, 7, 1076.
- [5] T. Sperger, I. A. Sanhueza, I. Kalvet, F. Schoenebeck, "Computational Studies of Synthetically Relevant Homogeneous Organometallic Catalysis Involving Ni, Pd, Ir, and Rh: An Overview of Commonly Employed DFT Methods and Mechanistic Insights" *Chem. Rev.* **2015**, 115, 9532.
- [4] G. Yin, I. Kalvet, F. Schoenebeck, "Trifluoromethylthiolation of Aryl Iodides and Bromides Enabled by a Bench-Stable and Easy-To-Recover Dinuclear Palladium(I) Catalyst" *Angew. Chem. Int. Ed.* **2015**, 54, 6809.
- [3] G. Yin, I. Kalvet, U. Englert, F. Schoenebeck, "Fundamental Studies and Development of Nickel-Catalyzed Trifluoromethylthiolation of Aryl Chlorides: Active Catalytic Species and Key Roles of Ligand and Traceless MeCN Additive Revealed" *J. Am. Chem. Soc.* **2015**, 137, 4164.
- [2] A. Kipper, I. Kalvet, L. Sikk, K. Kõiv, U. Mäeorg, P. Burk, K. Tamm, "Synthesis of Unprotected CH₂-Skipped Piperazine-Pyridine Alternating Cycles with Azide End-Group" *Heterocycles* **2015**, 90, 625.
- [1] I. Kalvet, K. J. Bonney, F. Schoenebeck, "Kinetic and Computational Studies on Pd(I) Dimer-Mediated Halogen Exchange of Aryl Iodides" *J. Org. Chem.* **2014**, 79, 12041.

Conference Presentations

Oral presentations:

ACS Spring, 2024, New Orleans, USA.

Enzyme Engineering XXVII, 2023, Singapore (virtual).

RosettaCON, 2022, Leavenworth, USA.

Estonian Student Research Award Ceremony, 2017, Tartu, Estonia.

2nd International Symposium on Synthesis and Catalysis, 2017, Evora, Portugal.

8th Münster Symposium on Cooperative Effects in Chemistry (MS_CEC), 2017, Münster, Germany.

Tallinn University of Technology, 2017, Tallinn, Estonia.

6th EuCheMS Chemistry Congress, 2016, Seville, Spain.

RSC Physical Organic Chemistry Postgraduate Meeting, 2016, Syngenta/Bracknell, UK.

8th New Year's Symposium, 2016, Aachen, Germany.

Poster presentations:

Enzyme Engineering XXV, 2019, Whistler, Canada.

RosettaCON, 2019, Leavenworth, USA.

19th HFSP Awardees meeting, 2019, Tsukuba, Japan.

WATOC, 2017, Munich, Germany.

European Symposium on Organic Chemistry, 2017, Cologne, Germany.

Computational Molecular Science (CMS), 2017, University of Warwick, UK.

9th New Year's Symposium, 2017, Aachen, Germany.

ORCHEM, 2016, Weimar, Germany.

7th Münster Symposium on Cooperative Effects in Chemistry, 2016, Münster, Germany.

OMCOS 18, 2015, Sitges, Spain.

13th European Symposium on Organic Reactivity, 2011, Tartu, Estonia.

Teaching and Mentoring Activities

- 2024 -** Jihun Jeung (graduate student, University of Washington)
- 2023 -** Seth Woodbury (graduate student, University of Washington)
- 2022** Jacob North (rotation student, University of Washington)
- 2021** Richard Muniz (rotation student, University of Washington)
- 2020 -** Anna Lauko (graduate student, University of Washington)
- 2020** Caroline Langley (rotation student, University of Washington)
- 2019-20** Susana Vasquez-Torres (graduate student, University of Washington)
- 2017** Leonard Reuter (master's student, RWTH Aachen University)
- 2017** Daniel Hupperich (master's student, RWTH Aachen University)
- 2017** Nils Kurig (master's student, RWTH Aachen University)
- 2017** Teaching assistant in a master's course "Metal mediated synthesis".
- 2015** Teaching assistant at an introductory laboratory course in organic synthesis (2 semesters).