

CURRICULUM VITAE

Kalju Kahn

Professional address:

Dr. Kalju Kahn
Department of Chemistry and Biochemistry
University of California, Santa Barbara
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Education:

B.S. Chemistry, Cum Laude (GPA 4.0), University of Tartu, Estonia, 1992

With specialty in biochemistry

Undergraduate thesis: "Differential conductometric studies of DNA–polylysine complexes in aqueous solutions". Thesis advisor Prof. Mati Karelson

M.S. Chemistry, University of Tartu, Estonia, 1994

Thesis "Poly-(N-ethyl-4-vinylpyridine): synthesis and complexes with DNA".

Thesis advisor: Prof. Mati Karelson

Fellowship at University of Joensuu, Finland. Studies in protein crystallography and molecular modeling.

Ph.D. Biochemistry, University of Missouri–Columbia, 1998

Dissertation: "Kinetic and mechanistic characterization of the urate oxidase reaction". Dissertation advisor: Prof. Peter A. Tipton

Honors:

Undergraduate research award in life sciences, University of Tartu, Estonia, 1992

Nordic Council of Ministers Scholarship at University of Joensuu, Finland, 1994

Phi Lambda Upsilon, Honorary Chemical Society, 1995

Sigma Xi, The Scientific Research Society, 1998

Research Poster Presentation Award, 4th Annual Spring Symposium on Enzymology, Iowa State University, 1998

Albert G. Hogan Dissertation Award—Best of Year, University of Missouri, 1999

"Teacher of the year" award by students in the Department of Chemistry and Biochemistry, UC Santa Barbara, 2005

Administrative duties:

Academic Senate, Committee on International Education, 2008-present

University Committee on International Education, 2009-present

Previous employment (International):

Scientific Advisor and Translator, the 26th International Chemistry Olympiad, 1994

Mentor in biochemistry for high school students

Member of the International Jury for the 26th International Chemistry Olympiad

Previous employment at the Department of Chemistry and Biochemistry, University of California Santa Barbara:

Postdoctoral Researcher, 1998–2001

Quantum chemical studies of enzymatic reactions, correlated motions in catalysis

Assistant Research Chemist, 2001–2003

Molecular simulations to understand enzyme catalysis and biological recognition

Temporary Lecturer and Researcher, 2001–2006

Curriculum development and teaching in biochemistry and related fields

Lecturer with Potential Security of Employment, 2006–2008

Curriculum development and teaching in biochemistry and related fields

Current employment:

Lecturer with Security of Employment, Department of Chemistry and Biochemistry,
University of California, Santa Barbara, 2008–present

Designing and teaching biochemistry laboratory courses: introductory biochemistry laboratory, laboratory techniques in biochemistry, biophysical and bioanalytical laboratory, molecular biology and protein purification graduate laboratory

Teaching organic chemistry, biochemistry, chemical kinetics, computational chemistry, and drug design lecture courses

Grants awarded:

Grant from the Christopher Reeve Paralysis Foundation for computational design of putative neuroregenerative drugs. P. I.: Prof. Thomas C. Bruice, 2000–2001

Computer time grants from the National Center for Supercomputing Applications (NCSA) and National Partnership for Advanced Computational Infrastructure (NPACI). P. I.: Dr. Kalju Kahn, 2000–2003, and 2006–2008.

Instructional Improvement Grants, UCSB, P.I.: Dr. Kalju Kahn, 2002–2003, 2003–2004, 2004–2005, 2006–2007, and 2008–2009.

Professional interests:

Application of theoretical chemistry methods to prediction of molecular properties

Experiment design and optimization in biophysical and bioanalytical chemistry

BIBLIOGRAPHY

for Kalju Kahn

- (1) Kahn, K.; Tipton, P. A. Kinetic mechanism and cofactor content of soybean root nodule urate oxidase. *Biochemistry* **1997**, *36*, 4731–4738.
- (2) Kahn, K.; Serfozo, P.; Tipton, P. A. Identification of the true product of the urate oxidase reaction. *J. Am. Chem. Soc.* **1997**, *119*, 5435–5442.
- (3) Kahn, K.; Tipton, P. A. Spectroscopic characterization of intermediates in the urate oxidase reaction. *Biochemistry* **1998**, *37*, 11651–11659.
- (4) Kahn, K. Theoretical study of intermediates in the urate oxidase reaction. *Bioorg. Chem.* **1999**, *27*, 351–362.
- (5) Sarma, A. D.; Serfozo, P.; Kahn, K.; Tipton, P. A. Identification and purification of hydroxyisourate hydroxylase, a novel ureide-metabolizing enzyme. *J. Biol. Chem.* **1999**, *274*, 33863–33865.
- (6) Luo, J.; Kahn, K.; Bruice, T. C. The linear dependence of $\log(k_{\text{cat}}/K_{\text{M}})$ for reduction of NAD^+ by PhCH_2OH on the distance between reactants when catalyzed by horse liver alcohol dehydrogenase and 203 single point mutants. *Bioorg. Chem.* **1999**, *27*, 289–296.
- (7) Kahn, K.; Tipton, P. A. Kinetics and mechanism of allantoin racemization. *Bioorg. Chem.* **2000**, *28*, 62–72.
- (8) Kahn, K.; Bruice, T. C. Transition state and ground state structures and their interaction with the active site residues in catechol *O*-methyltransferase. *J. Am. Chem. Soc.* **2000**, *122*, 46–51.
- (9) Kahn, K.; Bruice, T. C. α -Ketoamides and α -ketocarboxyls: Conformational analysis and development of all-atom OPLS force field. *Bioorg. Med. Chem.* **2000**, *8*, 1881–1891.
- (10) Lau, E. Y.; Kahn, K.; Bash, P. A.; Bruice, T. C. The importance of reactant positioning in enzyme catalysis: A hybrid quantum mechanics/molecular mechanics study of a haloalkane dehydrogenase. *Proc. Natl. Acad. Sci. USA* **2000**, *97*, 9937–9942.
- (11) Bruice, T. C.; Kahn, K. Computational enzymology. *Curr. Opin. Chem. Biol.* **2000**, *4*, 540–544.

- (12) Kahn, K.; Bruice, T. C. Diphtheria toxin catalyzed hydrolysis of NAD^+ : Molecular dynamics study of enzyme bound substrate, transition state, and inhibitor. *J. Am. Chem. Soc.* **2001**, *123*, 11960–11969.
- (13) Kahn, K.; Bruice, T. C. Parameterization of OPLS-AA force field for the conformational analysis of macrocyclic polyketides. *J. Comput. Chem.* **2002**, *23*, 977–996.
- (14) Mazumder, D.; Kahn, K.; Bruice, T. C. Computer simulations of trypanosomal nucleoside hydrolase: Determination of the protonation state of the bound transition-state analogue. *J. Am. Chem. Soc.* **2002**, *124*, 8825–8833.
- (15) Reddy, S. Y.; Kahn, K.; Zheng, Y.-J.; Bruice, T. C. Protein engineering of nitrile hydratase activity of papain: Molecular dynamics study of a mutant and wild-type enzyme. *J. Am. Chem. Soc.* **2002**, *124*, 12979–12990.
- (16) Hur, S.; Kahn, K.; Bruice, T. C. Comparison of formation of reactive conformers for the $\text{S}_{\text{N}}2$ displacements by CH_3CO_2^- in water and by Asp124- CO_2^- in a haloalkane dehalogenase. *Proc. Natl. Acad. Sci. USA* **2003**, *100*, 2215–2219.
- (17) Mazumder, D.; Kahn, K.; Bruice, T. C. Computational study of ketosteroid isomerase: Insights from molecular dynamics simulation of enzyme bound substrate and intermediate. *J. Am. Chem. Soc.* **2003**, *125*, 7553–7561.
- (18) Kahn, K.; Bruice, T. C. Comparison of reaction energetics and leaving group interactions during the enzyme-catalyzed and uncatalyzed displacement of chloride from haloalkanes. *J. Phys. Chem. B* **2003**, *107*, 6876–6885.
- (19) Kahn, K.; Bruice, T. C. Systematic convergence of energies with respect to basis set and treatment of electron correlation: focal point conformational analysis of methanol. *Theor. Chem. Acc.* **2004**, *111*, 18–24.
- (20) Mazumder-Shivakumar, D.; Kahn, K.; Bruice, T. C. Computational study of the ground state of thermophilic indole glycerol phosphate synthase: structural alterations at the active site with temperature. *J. Am. Chem. Soc.* **2004**, *126*, 5936–5937.
- (21) Kahn, K.; Bruice, T. C. Focal point conformational analysis of ethanol, propanol, and isopropanol. *ChemPhysChem.* **2005**, *6*, 487–495.
- (22) Kahn, K.; Granovsky, A. A.; Noga, J. Convergence of third order correlation energy in atoms and molecules. *J. Comput. Chem.* **2007**, *28*, 547–554.

- (23) Kahn, K.; Kahn, I. Improved efficiency of focal point conformational analysis with truncated correlation consistent basis sets. *J. Comput. Chem.* **2008**, *29*, 900–911.
- (24) Kahn, K.; Kirtman, B.; Noga, J.; Ten-no, S. Anharmonic vibrational analysis of water with traditional and explicitly correlated coupled cluster methods. *J. Chem. Phys.* **2010**, *133*, 074106.
- (25) Kahn, K.; Plaxco, K. W. Principles of Biomolecular Recognition in *“Recognition Receptors in Biosensors.”* M. Zourob (ed.), Springer, New York, **2010**.

Presentations in local, national, and international conferences including Midwest Enzyme Chemistry Conference, Gordon Conference, ACS National Meeting, and Sanibel Symposium.

Co-author of two booklets of original problems in the field of chemistry: “Study Materials for the Chemistry Olympiads”. Published by Tartu University Press, Tartu, 1994 and 1995.

Author of a PowerPoint slide-set with over 700 slides for the “Lehninger Principles of Biochemistry”, a leading biochemistry textbook (W. H. Freeman & Co), 2008.