

## *CURRICULUM VITAE*

### **Kalju Kahn**

#### **Professional address:**

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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, 4<sup>th</sup> 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

**Previous employment:**

*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

*Postdoctoral Researcher*, Department of Chemistry and Biochemistry, University of California, Santa Barbara, 1998–2001

Quantum chemical studies of enzymatic reactions, correlated motions in catalysis

*Assistant Research Chemist*, Department of Chemistry and Biochemistry, University of California, Santa Barbara, 2001–2003

Molecular simulations to understand enzyme catalysis and biological recognition

Development of accurate force fields to describe conformations and binding

affinities of complex polyketides with putative neuroregenerative activity

**Current employment:**

*Lecturer*, Department of Chemistry and Biochemistry, University of California, Santa Barbara, 2001–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

*Researcher*, Department of Chemistry and Biochemistry, University of California, Santa Barbara, 2001–present

Development of focal point analysis methods in quantum chemistry

Computer-based drug design

**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

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

**Professional interests:**

Application of computer simulation methods in enzymology and drug design

Experiment design and optimization in biophysical and bioanalytical chemistry

## BIBLIOGRAPHY

### for Kalju Kahn

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- (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  $\text{NAD}^+$  by  $\text{PhCH}_2\text{OH}$  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.  $\alpha$ -Ketoamides and  $\alpha$ -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<sup>+</sup>: 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 S<sub>N</sub>2 displacements by CH<sub>3</sub>CO<sub>2</sub><sup>-</sup> in water and by Asp124-CO<sub>2</sub><sup>-</sup> 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.
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- (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.* **2006** (accepted).

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.