#### JOHN W. KELLER

#### **BIOGRAPHICAL SKETCH**

Dept of Chemistry & Biochemistry Email: jwkeller@alaska.edu
University of Alaska Fairbanks Tel: 907-888-7278

Fairbanks, AK 99775-6160 Profile: <a href="https://www.uaf.edu/chem/files/jkeller/">https://www.uaf.edu/chem/files/jkeller/</a>

# a. Professional Preparation

Undergraduate:The Ohio State UniversityChemistryB.S. 1968Graduate:University of Wisconsin-MadisonChemistryPh.D. 1976Post-Doctoral:University of Wisconsin-MadisonChemistry1976-79

## **b.** Appointments

2012-present	Professor of Chemistry Emeritus
2007-2010	Chair, Department of Chemistry and Biochemistry
1991-2012	Professor, University of Alaska Fairbanks
1986-1991	Associate Professor, University of Alaska Fairbanks
1979-1986	Assistant Professor, University of Alaska Fairbanks

# c. Selected Publications (graduate student; undergraduate student)

## (i) Five Relevant Publications

- J.W. Keller and A.L. Demmerly, "Investigating Crystal Violet Reactivity and Color with Quantum Theory and Interactive Webpages," *J. Chem. Educ.* 102, 2448–2453(2025). https://doi.org/10.1021/acs.jchemed.4c01544
- 2. J.W. Keller, T.I. Ayudhya, and N.N. Dingra, "Carbon monoxide formation from trimethylamine-boranecarboxylate: DFTstudies of S<sub>N</sub>i and chelotropic mechanisms", *RSC Advances*, **10**, 16038-16044 (2020). <a href="https://doi.org/10.1039/d0ra01572.e">https://doi.org/10.1039/d0ra01572.e</a>
- 3. J.W. Keller, <u>Bronwyn L. Harrod</u>, and <u>Sifat A. Chowdhury</u>, "Theoretical Study of Formic Acid-Sulfur Dioxide Dimers" *J. Phys. Chem. A* **114**, 13182-13188 (2010). <u>https://doi.org/10.1021/jp1076214</u>
- 4. J.W. Keller, "The Formic Acid-Trifluoroacetic Acid Bimolecule. Gas-Phase Infrared Spectrum and Computational Studies," *J. Phys. Chem. A* **108**, 4610-18 (2004). <a href="https://doi.org/10.1021/jp049883x">https://doi.org/10.1021/jp049883x</a>
- 5. J.W. Keller, "Lewis Acid Catalyzed Diels-Alder Reaction of Carvone with Isoprene. Using 2-Dimensional NMR and Molecular Modeling to Solve a Stereo- and Regiochemical Puzzle," *The Chemical Educator* **11**, 262-6 (2006). <a href="http://www.chemeducator.org/papers/0011004/1140262jk.pdf">http://www.chemeducator.org/papers/0011004/1140262jk.pdf</a>

## (ii) Five Significant Publications

- 1. J.W. Keller, "Sulfur Dioxide–Pyridine Dimer. FTIR and Theoretical Evidence for a Low-Symmetry Structure." *J. Phys. Chem. A* **119**, 10390-10398 (2015). https://doi.org/10.1021/acs.jpca.5b06122.
- E.J. Fogle, <u>See-Tarn Woon</u>, J.W. Keller, and M.D. Toney, "Role of Q52 in Catalysis of Decarboxylation and Transamination in Dialkylglycine Decarboxylase", *Biochemistry* 44, 16392-16404 (2005). <a href="https://doi.org/10.1021/bi051475b">https://doi.org/10.1021/bi051475b</a>
- 3. M.D. Toney, E. Hohenester, J.W. Keller, J.N. Jansonius, "Structural and Mechanistic Analysis of Two Crystal Structures of the Pyridoxal Phosphate-Dependent Dialkylglycine Decarboxylase", *J. Mol. Biol.* **245**, 151-79 (1995). https://doi.org/10.1006/jmbi.1994.0014
- 4. J.W. Keller, <u>K.B. Baurick, G.C. Rutt, M.V. O'Malley</u>, <u>N.B. Sonafranck, R.A. Reynolds, L.O.E. Ebbesson</u>, and <u>F.F. Vajdos</u>, "*Pseudomonas cepacia* 2,2-Dialkylglycine Decarboxylase. Cloning and Sequencing of Structural and Repressor Genes." *J. Biol. Chem.* **265**, 5531-5539 (1990). https://doi.org/10.1016/S0021-9258(19)39393-7

5. J.W. Keller and B. J. Hamilton, "Enzymatic Resolution of 2-Trifluoromethylalanine" *Tetrahedron Letters*, **27**,1249-1250 (1986). https://doi.org/10.1016/S0040-4039(00)84229-X

## d. Synergistic Activities

Poster at the Fall 2024 National Meeting of the American Chemical Society "Crystal violet quantum calculations for general chemistry students: Easing the load by combining interactive webpages with WebMO and Gaussian" https://doi.org/10.1021/scimeetings.5c10765

Poster at the Spring 2021 National Meeting of the American Chemical Society "Transition states for methyl transfer to a model quinonoid nucleophile", <a href="https://doi.org/10.1021/scimeetings.1c00198">https://doi.org/10.1021/scimeetings.1c00198</a>

System Administrator and consultant for UAF Computational Chemistry and WebMO site. 2009-present. <a href="https://antec12.cns.uaf.edu/~frank/cgi-bin/webmo/login.cgi">https://antec12.cns.uaf.edu/~frank/cgi-bin/webmo/login.cgi</a>

Recent invited seminar: University of Texas Permian Basin, Dept of Chemistry, "Theoretical Study of a Carbon Monoxide-Releasing Reaction", April 2022.

Organized and chaired session on "Computational Chemistry" at American Chemical Society's 2017 Northwest Regional Meeting, Anchorage, AK.

Published 40 YouTube videos on <u>chemistry seminars</u>, <u>general chemistry computational chem labs</u>, <u>organic chemistry</u>, and molecular graphics.

Panelist for NSF/DUE Course, Curriculum, and Laboratory Improvement program. 2002-2006.

PI on "Persistent Organic Pollutants in Alaska. New GC-MS Experiments and Experiences for College and Pre-College Students", National Science Foundation/ DUE. 2008-2010.

PI on "Enhancing Chemistry Curricula Through Molecular Modeling: A Multi-Campus Consortium Approach" NSF/DUE-CCLI. 2000-2004.

Consultation and collaboration on research and teaching applications of molecular modeling with students and professors across Alaska.

U.S. Patents "A Repressor Gene for Regulating Expression of Polypeptides and its Use in the Preparation of 2,2-Dialkylglycine Decarboxylase of Pseudomonas cepacia," 5,210,025. May 11,1993. Repressor Protein and Operon for Regulating Expression of Polypeptides and its Use In the Preparation of 2,2-Dialkylglycine Decarboxylase of Pseudomonas cepacia. 5,356,796. Oct. 18, 1994.

#### e. Collaborators and other affiliations:

### (i) Collaborators

Thep Ayudhya, Nin Dingra, University of Texas Permian Basin Thomas Green, University of Alaska Fairbanks Arianna Demmerly, University of Alaska Fairbanks

### (ii) Advisors

Graduate: (The late) Charles Heidelberger, UW-Madison, McArdle Laboratory for Cancer Research; (The late) Howard Whitlock, Department of Chemistry, University of Wisconsin-Madison Post-doctoral: Marion H. O'Leary, Univ. of Wisconsin-Madison, Cal State Sacramento (Emeritus).

#### (iii) Thesis Advisees (1998-2004)

See-Tarn Woon, Ph.D. 1998, University of Auckland, NZ

Honghong Sun, Ph.D., 2000 University of Pennsylvania Perelman School of Medicine, Philadelphia, PA Julie LaRocca-Brigham M.S. 2003, Molecular Profiling Institute, Phoenix, AZ Jeff Bickmeier, M.S., 2004, Arkea Bio, Arlington, MA