

# CURRICULUM VITA

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## **Research Interests:**

- Enzymatic redox catalysis: Fundamental elements: electron transfer, proton transfer and coupling.
- Redox tuning: identification of hydrogen bonds, electrostatic and steric interactions by which proteins modulate properties of redox centers and thereby the nature of reactivity (1-e vs. 2-e, vs. bifurcation), non-heme Fe & flavins.
- NMR shielding tensors as reporters of flavin electronics, their relation to reactivity and their manipulation by the protein, via solid-state NMR in conjunction with high-level DFT calculations.
- Protein biophysics: coupling between protein dynamics and substrate (analog) binding.
- Dynamic nuclear polarization site-selective enhancements of NMR signals via radical states of bound cofactors.
- Enzyme-functionalized electrodes/membranes: remediation and enzymatic capture of chemical energy from waste products, and conversion into electrical energy.

## **Accomplishments:**

- Chemical and mechanistic explanation of the inactivity of metal-exchanged Mn-superoxide dismutase and Fe-superoxide dismutase (SODs). Demonstration that the two proteins exert  $\approx 0.5$  V different redox tuning on the bound metal ion, despite their superimposable structures.
- Redox tuning: designed mutations elevating FeSOD's reduction potential, by *over 600 mV* via a *single* second-sphere mutation, thus validating a general proposal for redox tuning via the energetics of proton transfer coupled to electron transfer and setting a record for rational redox tuning in an enzyme.
- Direct observation of pK proposed for the catalytic proton donor of reduced FeSOD, assignment of the pK to Tyr34.
- First observation of the  $^{15}\text{N}$  solid-state spectrum of a flavin, obtaining the *740 ppm wide* signal for N5.
- First dynamic nuclear polarization-enhanced NMR spectroscopy based on a stable natural endogenous radical.

## **Positions Held:**

**2012-present: Professor of Chemistry**

**2007-2008: Research Scientist (sabbatical)**, Massachusetts Institute of Technology, Department of Chemistry.

**1999-2012: Associate Professor**, University of Kentucky, Departments of Chemistry and Biochemistry.

**1998-1999: Associate Professor**, The Johns Hopkins University, Depts. of Chemistry and Biophysics.  
Left on good terms, in order to live with husband.

**1992-1998: Assistant Professor**, The Johns Hopkins University, Depts. of Chemistry and Biophysics.

**1990-1992: Postdoctoral Fellow**, Brandeis University, Dept. of Biochemistry, with Prof. A. G. Redfield.

Research: NMR spectroscopy: conformational changes in p21<sup>ras</sup> and thus regulation of cell proliferation.

**1989-1990: Postdoctoral**, Massachusetts Institute of Technology, Dept. Chemistry, with Prof. W. H. Orme-Johnson  
Research: Molecular biological and EPR spectroscopic study of assembly of the metal clusters of nitrogenase.

## **Education:**

**1982-1989: Ph.D. in (Biophysical) Chemistry**, Yale University, with Prof. G. W. Brudvig.

Thesis: "Assembly of the Catalytic Manganese Complex of Photosystem II." (An EPR and kinetic study.)

**1977-1982: B.Sc., Honours in Genetics and Minor in Physics**, University of Guelph, Canada, Sep. 1977-May 1982

Research: Fortran programming in statistical mechanics, cloning genes, solid state  $^2\text{H}$  NMR in membrane biophysics.

**Honours and Awards:**

President-elect, Division of Biological Chemistry, American Chemical Society.  
 Faculty Award for Distinguished Service and Engagement, April 2017 (College of Arts and Sciences, U. of Kentucky)  
 Chair: Southeast Enzyme Conference, 11 April 2015, Atlanta GA  
 Teacher Who Made A Difference, 2015 (University of Kentucky College of Education)  
 Plenary Speaker: Southeast Enzyme Conference, 20 April 2013, Atlanta GA  
 Teacher Who Made A Difference, 2012 (University of Kentucky College of Education)  
 Co-Chair, 2011 Gordon Research Conference on Enzymes, Coenzymes and Metabolic Pathways.  
 Chair, Midwest Enzyme Chemistry Conference, 2010.  
 Boston Marathon, 19 April 2010. Qualified for the Boston Marathon with 5 minutes to spare (Chicago, 11 Oct 2009).  
 Kate and Michael Barany Young Investigator Award, 2006, Biophysical Society.  
 Research Challenge Trust Fund professor, 1999, University of Kentucky.  
 Natural Sciences and Engineering Research Council of Canada Womens' Faculty Award, and Research Grant (1992).  
 Declined, to go to The Johns Hopkins University.  
 Life Sciences Research Foundation, Bristol-Myers Squibb Postdoctoral Fellow, 1991- 1992.  
 Natural Sciences and Engineering Research Council of Canada Postdoctoral Fellow, 1991.  
 Pfizer Fellowship, Yale University, 1982-1986.  
 Natural Sciences and Engineering Research Council of Canada Graduate Fellowship 1982  
 Winegard medal, University of Guelph, for best overall achievement as an undergraduate, 1982.  
 Natural Sciences and Engineering Research Council of Canada Undergraduate Research Scholarships, 1980, 1981, 1982.

**Current Grants:**

<b>1 Aug. 2014 - 31 July 2019</b>	<b>NSF KY EPSCoR #1355438</b>	<b>\$35,000/yr</b>	<b>Participant</b>
"Powering the Kentucky Bioeconomy for a Sustainable Future" (Rodney Andrews, P.I., total \$20M)			
<b>1 Aug. 2014 - 30 June. 2018</b>	<b>N. S. F. I/UCRC</b>	<b>\$10,000/yr</b>	<b>Participant</b>
"Nitroreductases a basis for breadth" as part of "Center for Pharmaceutical Development" (Munson and Bommarius, co P.I.s)			
<b>1 Aug. 2014 - 31 July 2018</b>	<b>D.O.E. DE-SC0012518</b>	<b>\$682,249 to UK</b>	<b>Co. I.</b>
"Biological Electron Transfer and Catalysis EFRC" Grant 11557967			

**Other Recent Submissions**

<b>Jan 2018 - Dec 2018</b>	<b>Alexander von Humboldt Foundation</b>	<b>\$60,000</b>	
Humboldt Research Award			
<b>1 Aug. 2017 - 31 July 2020</b>	<b>N.S.F. - MRI</b>	<b>\$381,259</b>	<b>P. I.</b>
"Acquisition of a 400 MHz automated NMR spectrometer for Chemical and Molecular Research" Pending			
<b>1 Jan. 2017 - 31 Dec. 2019</b>	<b>Arnold and Mabel Beckman Foundation</b>	<b>\$156,000</b>	<b>P.I.</b>
"2017 Beckman Scholars Program at the University of Kentucky" Declined			
<b>1 Jan. 2016- 31 Dec. 2018</b>	<b>Beckman Scholars Program</b>	<b>\$234,000 to U. K.</b>	<b>P. I.</b>
"2016 Beckman Scholars Program at the University of Kentucky" Declined			
<b>15 May 2015- 14 May 2016</b>	<b>NASA KY EPSCoR</b>	<b>\$40,000</b>	<b>P.I.</b>
"Possible participation of (deaza)flavins and pterins in primitive photobiochemistry and light-driven electron transfer."			
<b>1 July 2014-30 June 2018</b>	<b>N.I.H.</b>	<b>\$958,860</b>	<b>P. I.</b>
"Bases for the broad substrate repertoire of nitroreductase"			
<b>1 July 2014 - 30 June 2019</b>	<b>N.I.H.</b>	<b>\$1,880,000</b>	<b>Co. I.</b>
"Choline acetyltransferase in congenital motor disorders"			
<b>1 July 2013-30 June 2016</b>	<b>USDA-NIFA</b>	<b>\$500,000</b>	<b>Co. I.</b>
"Hydrogen Peroxide Generating Mechanisms in Hydrated Drink Mixes"			
<b>1 July 2013 - 30 June 2018</b>	<b>N.S.F. AISL</b>	<b>\$2,499,957</b>	<b>P.I.</b>
"Doing": Advancing Informal Stem Learning"			
<b>1 July 2013 - 30 June 2018</b>	<b>N.S.F. STEP</b>	<b>\$1,999,756</b>	<b>senior personnel</b>
"Systemic Teaching and Research Engagement in Applied Mathematical Sciences."			
<b>1 July 2013 - 30 June 2016</b>	<b>U. S. Department of Energy (BES)</b>	<b>\$500,000</b>	<b>(P.I.)</b>
"Tailoring the Reactivity of Flavins to Catch and Secure Electrons"			
<b>1 Jan. 13 – 31 Dec. 16</b>	<b>National Institutes of Health</b>	<b>\$812,144</b>	<b>(P.I.)</b>
"Managing the ping-pong problem, promiscuity and one-electron chemistry"			

**Past Grants:**

<b>15 Oct. 2010 - 14 Oct. 2013 N.S.F. MRI</b>	<b>\$150,276</b>	<b>(1 of 8 Co.Is)</b>
"Acquisition of a multifrequency phase modulated fluorimeter."		
<b>1 Feb. 2013 - 31 June 2014 University of Kentucky, Vice President for Research</b>	<b>\$20,000</b>	<b>(P.I.)</b>
"Dynamics and catalytic repertoire of two nitroreductases"		
<b>1 July 2009-30 June 2012: N.I.H. (1R01GM085302-01A1)</b>	<b>\$ 511,802</b>	<b>(P.I.)</b>
"Enzyme mis-metallation, consequences and opportunities."		
<b>1 April 2011 - 31 March 2012 USDA (AFRI award 2010-04130)</b>	<b>\$2,500</b>	<b>(P.I.)</b>
"The Midwest Enzyme Chemistry Conference, sharing recent advances in understanding and exploiting the chemistry of life."		
<b>1/Sep./06-31/Sep/10: Petroleum Research Foundation, 44321-AC4</b>	<b>\$80,000 Direct</b>	<b>(P.I.)</b>
"Solid-state NMR as a probe of flavin interactions, electronics and reactivity'."		
<b>1/Aug./08-31/July/10, U.S. Department of Agriculture, (2007-35107-18311)</b>	<b>\$286,000</b>	<b>(Co P.I.)</b>
"Inhibition of Fe(III) reduction by nitrate: Impact of anoxic chemical and biological Fe(II) oxidation."		
<b>May 2009-April 2010: Vice President for Research Support Grant</b>	<b>\$25,000</b>	<b>(P.I.)</b>
"Dynamic Nuclear Polarization Based on an Endogenous Radical"		
<b>1/Apr./06-31/Mar./09: N.S.F. -R.E.U. CHE-0552247</b>	<b>\$238,197</b>	<b>(Co-P.I.)</b>
"REU Site: Undergraduate Research for Appalachian Students at the Department of Chemistry, Univ. Kentucky"		
<b>1 Jan 2008, Vice President for Research Major Research Equipment Initiative</b>	<b>\$48,150</b>	<b>(P.I.)</b>
"Upgrade to the Electron Paramagnetic Resonance Spectrometer in CP26"		
<b>1/July/05-30/June/08, National Science Foundation MCB- 0019893001</b>	<b>\$300,000</b>	<b>(Co P.I.)</b>
"Sequence dependence of polyproline II helix formation"		
<b>1/Oct./03 – 30/Sep/06, N. I. H. R01 GM063921</b>	<b>\$150,000 Direct</b>	<b>(P. I.)</b>
"Understanding determinants of flavin enzyme activity"		
<b>1/July/03 – 30/June/06, N.S.F.</b>	<b>\$300,000 total,</b>	<b>(Co P.I.)</b>
"Chloroplast-localized N-terminal protein processing by peptide deformylase"		
<b>1/July/02 – 30/June/06, N.S.F. (0129599)</b>	<b>\$404,318 total</b>	<b>(P.I.)</b>
"How the superoxide dismutase protein specifies the reactivity of bound Fe"		
<b>2002 -2004, N. I. H.</b>	<b>\$461,310</b>	<b>(Co-P. I.)</b>
"Acquisition of a hybrid small/ macromolecule X-ray diffractometer system."		
<b>2002 - 2004, Kentucky Science Foundation</b>	<b>\$95,000 direct costs</b>	<b>(P.I.)</b>
"Engineering new catalytic activity into superoxide dismutase"		
<b>2002 - 2004, N. S. F.</b>	<b>\$2,300,000 total</b>	<b>(Co-P.I.)</b>
"Center for Structural Biology and Genetic Engineering: A Two-Campus Initiative for Research and Education"		
<b>2002 - 2003, N.C.S.A. 18,000 Service Units of supercomputer time on UK Superdome,</b>		<b>(P.I.)</b>
"Understanding Determinants of Flavin Enzyme Activity"		
<b>2002 Research Equipment Initiative</b>	<b>\$36,000</b>	<b>(P.I.)</b>
"Liquid He cryostat for EPR spectroscopy of biochemicals and materials"		
<b>1998 - 2002 N. I. H.</b>	<b>\$330,000 direct</b>	<b>(P.I.)</b>
"Proton Transfer Essential to Catalytic Activity in SOD"		
<b>1998 - 2000 Petroleum Research Foundation,</b>	<b>\$60,000,</b>	<b>(P.I.)</b>
"Identification of residues responsible for redox tuning and determination of the metal ion specificity of superoxide dismutase"		
<b>1998 - 2001: National Science Foundation,</b>	<b>\$330,000</b>	<b>(P.I.)</b>
"Understanding the basis for metal ion specificity in Fe- and Mn-superoxide dismutases"		
<b>1995 - 1997: National Science Foundation,</b>	<b>\$300,000</b>	<b>(P.I.)</b>
"Conformational Coupling and the Basis for Metal Ion Specificity in Superoxide Dismutase".		
<b>1993 - 1994: American Cancer Society:</b>	<b>\$15,000</b>	<b>(P.I.)</b>
"Nuclear Magnetic Resonance Studies of Superoxide Dismutase"		

**Postdoctoral Scholars Supervised**

Anush Karapetyan, James Maliekal, K. Padmakumar, Cungen Zhang, Rupam Sarma, Haijun (Diessel) Duan

**Ph. D. Dissertations Directed:**

- 1999 Ronald L. Koder, Jr.** The Johns Hopkins University,  
"A biochemical and biophysical investigation of *Enterobacter cloacae* nitroreductase."
- 1999 David L. Sorkin** The Johns Hopkins University,  
"Spectroscopic studies of ionization and anion binding events in the active sites of iron(II) and iron(III) superoxide dismutase."
- 1999 Carrie K. Vance** The Johns Hopkins University,  
"The metal ion specificity of the iron and manganese superoxide dismutases is explained by differences in the redox potentials and proton affinities between the native and metal ion substituted enzymes from *Escherichia coli*."
- 1999 Surekha Vathyam** The Johns Hopkins University,  
"Triple resonance assignments and comparison of the oxidized and reduced states of iron superoxide dismutase."
- 2001 Emine Yikilmaz** The Johns Hopkins University,  
"Redox tuning in *Escherichia coli* iron superoxide dismutase."
- 2002 Joseph Walsh** The Johns Hopkins University,  
"Theoretical and experimental investigations of flavin NMR shieldings, reduction potential tuning and hydrogen bonding."
- 2007 Peng Zhang** University of Kentucky  
"Nitroreductase: evidence for a fluxional low-temperature state and its possible role in enzyme activity"
- 2010 Dongtao Cui** University of Kentucky  
"<sup>15</sup>N Solid-State NMR Detection of Flavin Perturbation by H-bonding in Models and Enzyme Active Sites."
- 2014 Warintra Pitsawong** University of Kentucky  
"Bases for breadth: Insights into how the mechanism and dynamics of nitroreductase can explain this enzyme's broad substrate repertoire."
- 2017 Ting Wang** University of Kentucky  
"The Role of Gln146 in the Stability and Activity of Superoxide Dismutase."

**Masters Theses directed:**

- 2012 Xiaonan Mei** University of Kentucky  
"How a silent mutation suppresses the activity and iron incorporation in superoxide dismutase"
- 2014 Jianing Wang** University of Kentucky  
"The differences between iron and iron-substituted manganese superoxide dismutase with respect to hydrogen peroxide treatment"
- 2017 Madison J. Sloan** University of Kentucky  
"Biomimetic devices to drive a thermodynamically uphill reaction using light and to degrade industrial waste stream components"

**Undergraduates' Research Directed:**

Young Min Kang, Jonathan C. Lansing, Omolara Oyedele, David Duong, Amanda Hoetz (nee Lind), Magda Fuse, Dwight Willett, Natalie Meyer, Mallory Mueller, Nicole Scheff, Jack Challis, Yuriy Bronshteyn, Tessa Monday, Jennifer Watts, Kiran Haridas, Eleni Maroudas, Haibin Zheng, Anthony Johns, Haley Herrell, Tim Dodson, Karl Hempel, Annie Baker, Zachary Griffith

**High School Research Projects Directed:**

Shankar Miller-Murthy 2013-2015  
Bharath Chithrala 2013-2015  
Faizan Ahmed 2014-2015  
Ben Xie 2015-2017  
Julia Radhakrisnan 2016-

**Current Students and Associates**

Dr. Haijun Duan Postdoctoral Scholar

John Hoben Doctoral Student (Ph. D. candidate)  
Mason Daniel Graduate Student  
Nishya Mohamed Raseek Graduate Student

Andrew J. Bradley Graduate Student

Julia Radhakrishnan High School Student (P. L. Dunbar high school junior)

**Teaching:****At the University of Kentucky**

Biological Chemistry Laboratory, (CHE554 now CHE454) Experiments employing modern methods of molecular biology and biochemistry: PCR, ELISA, UV-vis, chromatography, transformation, protein overexpression, site-directed mutagenesis of green fluorescent protein, circular dichroism and fluorescence, Spring 2010, '11, '12, '13, '14. '16.

Biological Chemistry I (CHE550) Based on "Biochemistry" by Garrett and Grisham. Fall 2006, '08, '09.  
New in 2014 - revised to employ 'active learning' format based on "Lehninger's Principles of Biochemistry".  
Revised Fall 2015 to employ Sapling, REEF and Canvas on-line tools., 2016

Bio-Inorganic Chemistry, (CHE580-2 special topic) Fall 2008

Biological Chemistry Seminar (CHE776-5) Fall 2006, '08, '09, Spring 2010, '11, '12, Fall 2014.

Physical Chemistry Laboratory (CHE441G), No text (and different experiments) but comparable in level to the course by the same name at J.H.U. Spring 2000.

Homonuclear NMR (CHE555, "Practical NMR"). A *hands-on* course introducing common 1 and 2 dimensional NMR experiments. Based on my own instruction manual accompanied by Claridge's book "High-Resolution NMR Techniques in Organic Chemistry". Fall 2000, '01, Spring 2003, '04, '05, '06, '07. All new handouts and instruction sheets for VnmrJ, Fall 2010, 2012, spring 2015.

Molecular Biophysics (CHE559). How non-covalent and coupled interactions between molecules give rise to the properties of materials, molecular machines and the extraordinary complex behaviours of biological systems. Spring 2001, Fall 2003.

Communication in Chemistry (CHE572). Student presentations on literature and research, Spring & Fall 2002, Fall '04, '05.

Structural Biology (BCH604), 3 lectures on NMR spectroscopy of macromolecules, drawing on Cavanagh, Fairbrother, Palmer and Skelton's book "Protein NMR Spectroscopy" and current literature. Fall 2001, 02, 03, 04, 05, 06. Spring '09, '10, '11, '12, '13, '14.

Molecular Science for Citizens (CHE101). half of the course, based on Snyder's book "The Extraordinary Chemistry of Ordinary Things", with demonstrations using everyday materials. Fall 2002, '03, '04, '05.

Molecular Science for Citizens (CHE101). NEW: based on Suchocki's "Molecular Science for Citizens", Fall 2011.  
New again: UK core course re-reincarnation, Fall 2013.

**At the Johns Hopkins University**

Molecular Spectroscopy, Covered the bulk of Drago's Book, "Physical Methods for Chemists", with examples from the literature. Spring 1993, 1994, 1995.

Principles of Magnetic Resonance, Density matrix and product operator calculations to understand triple resonance, multidimensional NMR pulse sequences. Based on Farrar and Harriman's "Density Matrix Theory and its Applications in NMR Spectroscopy" and "Protein NMR Spectroscopy" by Cavanagh, Fairbrother, Palmer and Skelton. Fall 1992, 1993, 1994, 1995, 1996, Spring 1998.

Physical Chemistry, Based on Atkins' "Physical Chemistry". Chapters on the principles of quantum mechanics and spectroscopy. Spring 1996.

Physical Chemistry Lab, Experiments illustrating the principles of quantum mechanics and spectroscopy, many based on Shoemaker, Garland and Nibler's "Experiments in Physical Chemistry". Spring 1997, 1998, 1999.

Advanced Biochemistry, 3 lectures on redox catalysis, based on Walsh's "Enzymatic Reaction Mechanisms", and Lippard & Berg's "Principles of Bioinorganic Chemistry". Fall 1996, 1997.

Methods in Physical Biochemistry, 5 lectures on NMR spectroscopy at the level of Wüthrich's "NMR of Proteins and Nucleic Acids". Spring 1996, 1997, 1998, 1999.

Biophysical Chemistry, Half the course, on biochemical manifestations of thermodynamics such as ligand binding, linked equilibria and conformational transitions, based on van Holde, Johnson and Ho's book: "Principles of Physical Biochemistry". Spring 1999.

**Service:**

**International Organizing Committee:** 20th Symposium on Flavins and Flavoproteins, Gratz 2017-2020.

**President-Elect, Division of Biological Chemistry of the ACS:** To assume presidency in 2019.

**Advisory Board,** Living Arts and Sciences Center of Lexington KY 2016 - present.

**Department of Energy:** regular review panelist, 2016 - present

**Coordinator: Outreach in Chemistry:** 2011 - present

**Outdoor Education:** Lead series of bird-watching walks in local parks, 2016.

**Kentucky River Watershed Watch:** chemical and biological tests of water quality and stream health, 2014-16.

**Director of the NMR Spectroscopy Centre:** University of Kentucky: 2003-2017.

Oversaw 6 NMR spectrometers and one EPR spectrometer: Supervision of one staff person, trouble-shooting and instrument repairs, software updates, applications for instrumentation grants, user assistance and training, monthly skill sessions.

**College of Arts and Sciences,** Strategic Plan, outreach and community engagement

**College of Arts and Sciences Dean Review Committee,** Chair, 2014-2015.

**Academic Area Advisory Committee,** 2013-2015.

**American Soc. Biochem. Mol. Biol., Publications Committee.** 2013 - 2016.

**American Chemical Society - Division of Biological Chemistry Officer:** nominating committee 2012-2014.

**Committee on Undergraduate Education,** College of Arts and Sciences, University of Kentucky, 2012

**Co-Chair, Gordon Research Conference on Enzymes, Coenzymes and Metabolic Pathways** 2011.

**VPR's Periodic Review Committee for the Center for Applied Energy Research,** University of Kentucky 2011

**VPR's Center for Computational Sciences Futures Committee,** University of Kentucky 2011

**Program Chair Midwest Enzyme Chemistry Conference,** Northwestern University, 16 October 2010.

**Editorial Board, Journal of Biological Chemistry,** 2007-2012.

**National Institutes of Health study section,** member of Physical Biochemistry study section 1998; , Structure-Function study section 2005, Shared Instrumentation 2009; PSI:Biology 2010-2014.

**National Science Foundation MCB panel member** 2004; C.R.I.F. panel member on a regular basis; Life Sciences 2012.

**Advisory Panel,** NMR facility at Madison. 2002 – 2005.

**Section Editor,** Magnetic Resonance in Chemistry, 1999-2003.

**Referee** of manuscripts for *Biochemistry*, *Proceedings of the National Academy of Science*, *Biochimica Biophysica Acta*, *Journal of the American Chemical Society*, *Journal of Magnetic Resonance*, *The Journal of Molecular Biology*, *Inorganic chemistry*, *Analytical Biochemistry*, *European Journal of Biochemistry*, *Journal of Biomolecular NMR*, *Science*.

**Purchase of a 600 MHz four channel NMR spectrometer, two 400 MHz spectrometers** plus accessories, with Prof. M. Meier, University of Kentucky, 1999.

**Member:** American Chemical Society, American Association for the Advancement of Science, Biophysical Society, Society for Bioinorganic Chemistry, American Soc. Biochem. Mol. Biol.

**Curriculum Committee, School of Arts and Sciences,** The Johns Hopkins University, 1994- 1995.

**Deans Search Committee for the School of Arts and Sciences,** member, Johns Hopkins University, 1993-94, 1998-99.

**Member:** University Senate, and then University Board of Governors, University of Guelph.

**Park naturalist** for National Parks of Canada.

**Outreach** (recent)

**Chemistry Demonstrations** at local schools and the Lexington Living Arts and Sciences Center. Emphasis on experiments participants can repeat themselves with readily-available materials. Take-home message: fascinating chemistry is happening everywhere, all the time (not just in laboratories).

2009 two times: **Community Montessori School**: 'Atmospheric physics and weather',  
'Acids and bases, CO<sub>2</sub> emissions and acid rain'.

29 Sep. 2008: **Beaumont Middle School**: 'Physical properties vs. chemical properties'

4 March 2010: **Living Arts and Sciences Center**: 'Chemistry in the Kitchen' (65 in attendance)

17 March 2010: **Linlee Middle School**: 'Atmospheric physics and weather.'

23 Sep. 2010: **Winburn Middle School** 'Chemistry and light: chemoluminescence, fluorescence and phosphorescence'

30 Oct. 2010: **GEMS (Girls Enjoying Math and Sciences)**: 'Physical chemistry inherent in the making of fudge'.

17 March 2011: **Cassidy Art and Science Extravaganza**: 'Atmospheric physics of weather: the water cycle'

7 April 2011: **Discovery Night at the Living Arts and Science Center** (Lexington KY): "Glow in the Dark Chemistry"  
(135 in attendance)

11 April 2011: **Girl Scout troupe 813**: 'Physical chemistry of fudge making'.

10-19 May 2011: **Science Explore Club** (after-school science club in at-risk elementary schools) 5 demonstrations on the water cycle, states of matter, acids and bases in your home, and chromatography of plant pigments.

4 Nov. 2011: **Cassidy Art and Science Extravaganza**: 'States of Matter and the water cycle'

12 Nov. 2011: **GEMS (Girls Enjoying Math and Sciences)**: 'Physical chemistry inherent in the making of fudge'.

1 March 2012: **Discovery Night at the Living Arts and Science Center** (Lexington KY): "Glow in the Dark Chemistry"  
(210 in attendance).

2,4,6 April 2012: **Science in spring break at the Public Libraries**, 5 presentations, "Advanced Chemistry and Potions Class"

2 Nov. 2012: **Cassidy Art and Science Extravaganza**: 'States of Matter, mixtures and solutions'

10 Nov. 2012: **GEMS (Girls Enjoying Math and Sciences)**: 'Make-your-own spectroscope and emission spectra of atoms and molecules.

9 Feb. 2013: **Kentucky-American Water District Science Fair** (judge of high-school chemistry and biology projects).

12 March 2013: **What's New in Science "From Bits to Bonds"** lecture for Lexington teachers sponsored by the College of Arts and Sciences.

22 Feb. 2013: **Athens-Chilesburg Elementary Arts and Science Day** presenter: acids and bases.

18 April 2013: **Liberty Elementary School Science night**

9 May 2013: **Providence Montessori School** demonstrations on reactivity and states of matter

29 July 2013: Chemistry afternoon presented to the **middle school science camp** held at UK

25 October 2013: **National Chemistry Week Demonstration** evening (oversight of evening presented by our graduate students, 200 in attendance).

8 November 2013: **Cassidy Elementary Arts and Sciences Extravaganza**

16 November 2013: **GEMS (Girls Enjoying Math and Sciences)**: 'Make-your-own spectroscope and emission spectra of atoms and molecules. (60 in attendance)

27 Feb 2014: **Family night at Russell Cave Elementary School evening** with two SACS members (200 in attendance)

5 June 2014: **Discovery Night at the Living Arts and Science Center** (Lexington KY): "Chemistry in your garden" (35 in attendance).

9-11 June 2014: **Hope Hill "STEMulating Summer with UK" camp**. States of matter, wonderful water and plant pigments. (30 students exposed, three half-days, F. Ladipo coordinator).

28 June 2014, **Lexmark Youth Science Summit**: polymers we make, and polymers of which we are made. Two presentations to Lexington area high school students, ≈35 in each session.

21 August 2014: **FastTrack** program evening Chemistry demonstration presentation (50 in attendance).

24 October 2014: **National Chemistry Week Demonstration** evening (oversight of evening presented by our graduate students, 200 in attendance).

4 November 2014: **Discovery Night at the Living Arts and Science Center** (Lexington KY): "Plant pigments" (50 in attendance).

12 November 2014: **STEMcats chat**. "Enzymatic Catalysis for a better world" (100 in attendance)

15 January 2015: Winburn Middle School **Science Night**

8 March 2015: **Lexington Explorium** "color and light - how molecules capture, reflect and recreate light to create colour" as part of the Math, Arts and Science series.

23-25 July 2015: **Hope Hill School**: Organized a week-long chemistry program for girls from broken homes.

30 August 2015 : Boy Scout troupe "**make your own spectroscope** and observe the luminescent signatures of the elements"

23 October 2015 : **National Chemistry Week Demonstration** (200 in attendance)

30 October 2015 : '**Discovery Day** at Cassidy Elementary School with undergraduate presenter-trainee. (70 pupils)

5 November 2015: 'Glow in the dark Chemistry' **Discovery Night at the Living Arts and Science Center** (Lexington KY):  
(100 in attendance).

14 November 2015: "The Nose Knows" synthesis of some fragrant esters from some stinky organic acids. **GEMS (Girls Enjoying Math and Sciences)**. (≈ 75 in attendance).

19 November 2015: "polymer fun". **Science Night** at Meadowthorpe Elementary School (45 visitors).



- 11 April 2016: "Reaction Attraction" **Energy Fair** for 8 under-privileged schools hosted by Sayre School, Lexington KY (120 pupils)
- 22 April 2016: "**Science day**" at Russell Cave Elementary School (which serves a predominantly Hispanic community). (50 pupils)
- 14 October 2016: "**Reaction Attraction**" two productions of chemical reactions to the alumni and friends of the Chemistry Department on the occasion of its move to the new Jacobs Science Building. (50 and 15 people in attendance)
- 15 October 2016: "**Walk in the woods**, a (bio)chemical tour of reactions and compounds underpinning our native woodland ecosystem" (4 people - first time offering)
- 28 October 2016: "**Discovery day**" at Cassidy Elementary School, paper chromatography of plant pigments distinguishing polar from non-polar pigments. 60 grade-5 children, 6 teachers.
- 19 Jan. 2017: "**Science Night**" at Winburn Middle School, pigments and tie dye activity
- 11 Feb. 2017: Fayette County District **Science Fair** - Judge for High School Computer Science
- 4 March 2017: Fayette County Regional Science Fair - Judge

**Oral Presentations, Invited and at Meetings,** (Posters not listed but  $\approx 5$ /year, inc. recent invited lectures):

- "The Manganese and Calcium Dependence of Photoactivation in Photosystem II Membranes." Speaker, North Eastern Regional Photosynthesis Conference (1988).
- "Electron Transfer Events Involved in Assembly of the Catalytic Mn Complex of Photosystem II" Speaker, North Eastern Regional Photosynthesis Conference (1989).
- "Assembly of the Mn Complex of Photosystem II." **Invited Speaker**, 17<sup>th</sup> Annual Meeting of the American Society for Photobiology (1989).
- "The Conformational Switch of p21<sup>ras</sup>" Speaker, XV International Conference on Magnetic Resonance in Biological Systems, Jerusalem, (August 16-21, 1992).
- "<sup>15</sup>N-Edited NMR Studies of the Conformational Switch of Ras p<sup>21</sup>" Speaker, 24<sup>th</sup> Southeastern Magnetic Resonance Conference, Raleigh, N.C., (October 8-10, 1992).
- "NMR studies of proton donation in reduced superoxide dismutase: Tyr 34 can explain the pK of 8.5" Speaker, 213<sup>th</sup> A. C. S. National Meeting, (San Francisco April 13-17, 1997).
- "The Basis for Metal Ion Specificity in Fe- and Mn-superoxide Dismutase" **Invited Speaker**, Metals in Biology Gordon Research Conference, Ventura CA, (Jan. 18-22, 1998).
- "Direct observation of determinants of superoxide dismutase redox activity by NMR" Speaker, Keystone Meeting on frontiers of NMR in Molecular Biology VI, Breckenridge CO (Jan 9 - 15, 1999).
- "Mechanisms of redox tuning in Fe- and Mn-superoxide dismutases" **Invited Speaker**, International Congress on Bioinorganic Chemistry 99, Minneapolis MN (July 11-16 1999).
- "Redox tuning and metal ion specificity, SOD, a case in point" **Invited Speaker**, Central Regional Meeting of the ACS, Cincinnati OH (May 16-19 2000).
- "Elucidating the elements of redox catalysis in superoxide dismutase" **Invited Speaker**, Gordon Research Conference on Enzymes, Coenzymes and Metabolic Pathways, Meriden NH (July 16-21, 2001).
- "Enzymes of Eternal Youth" Distinguished Scholars Lecture, Research Challenge Trust Fund Series. **Invited Speaker**, W. T. Young Library, University of Kentucky (April 9, 2002).
- "Thermodynamic bases for the obligate two-electron, oxygen-insensitive reactivity of enteric nitroreductase.", **Invited Speaker**, American Chemical Society National Meeting, Boston MA (Aug 18-22, 2002).
- "Direct Observation of the Redox-Active Flavin Cofactor and Insights from NMR into How Proteins Control Flavin Reactivity." Speaker, International Congress for Magnetic Resonance in Biological Systems, Toronto, Canada (Aug. 25-30, 2002).
- "Redox Tuning over 600 mV in Superoxide Dismutase". **Invited Speaker**, National A.C.S. meeting, Anaheim CA (March 27-31. 2004).
- "Magnetic Resonance Studies of Substrate Analog Binding to Fe-Superoxide Dismutase, a 45 kDa Paramagnet-Containing Enzyme." **Invited Speaker**, 17<sup>th</sup> Waterloo NMR Summer School, Waterloo Canada (June 21-25, 2004).
- "Redox Tuning over 600 mV in Superoxide Dismutase" **Invited Speaker**, Biophysical and Bioinorganic Symposium, New Haven CT (June 26-27 2004).
- "Nitroreductase, Active Site Structure, Electronics and Dynamics", **Invited Speaker**, 15<sup>th</sup> International Symposium on Flavins and Flavoproteins, Shonan Village, Japan (April 17-22, 2005).
- "Enzyme Control over Redox Chemistry", **Invited Speaker**, 88<sup>th</sup> Canadian Chemistry Conference and Exhibition, Saskatoon, CA (May 28-June 1, 2005)
- "Does Tyr34 compensate for the different electronic configuration of Mn than Fe, in superoxide dismutase ?" Speaker, N.S.F. Workshop on Inorganic Chemistry, Landsdowne MD, July 2005
- "How proteins control electrons: Protons" **Invited Speaker**, 50<sup>th</sup> Biophysical Society Annual Meeting, Salt Lake City, Utah, Feb 18-22, 2006.
- "A plastic explosive-degrading enzyme" **Invited Speaker**, American Physical Society Meeting, Baltimore MD March 13-17, 2006.
- "The crucial importance of chemistry in the structure-function equation: manipulating H-bonding in Fe-superoxide dismutase" Speaker, American Chemical Society National Meeting, Atlanta GA March 26-30, 2006.

- "How proteins control electrons: Protons" **Invited Speaker**, 25th Summer Symposium in Molecular Biology, on Mechanism, Structure, and Assembly in Bioinorganic Chemistry. Penn State University, University Park, PA, June 7-10, 2006.
- "How proteins control electrons: Protons" **Invited Speaker**, 8<sup>th</sup> European Biological Inorganic Chemistry Conference, Aveiro Portugal 1– 6 July 2006.
- "How a protein modulates redox properties without significant structural change" **Invited Speaker**, Gordon Research Conference on Inorganic Chemistry, Salve Regina University, Newport, RI, July 15-20, 2007.
- "Redox tuning over 100s of mV via H-bonding and control of redox-coupled protons, in superoxide dismutase" **Invited Speaker**, A.C.S. National Meeting, special session on Catalysis, Boston MA, Aug 19-23, 2007.
- "Nitroreductase, a plastic explosive-degrading protein" **Invited Speaker**, 21<sup>st</sup> Annual Gibbs Conference on Biothermodynamics, Carbondale, IL, Sep 29- Oct. 2, 2007.
- "Redox tuning over almost 1 V with retention of structure" **Invited Speaker**, Central Regional Meeting of the A.C.S. , special session on Frontiers of Protein and Peptide Engineering, Columbus OH, June 10-14, 2008.
- "Nitroreductase, a plastic explosive-degrading protein" **Speaker**, Midwest Enzyme Chemistry Conference. Chicago IL 4 Oct. 2008.
- "How can one second-sphere mutation change the  $Fe^{III}/E_m$  by 660 mV ?" **Speaker**, Gordon Research Conference on Inorganic reaction mechanisms Galveston TX March 8-13, 2009.
- "Enzymes of eternal youth" **Invited Speaker**, Austin Peay State University, Clarksville, TN, 16 March 2009.
- "Solid-state NMR as a probe of flavin electronics and redox tuning produced by H-bonds." **Speaker**, Gordon Research Conference on Enzymes, Coenzymes and Metabolic Pathways, Waterville Valley NH, 5-10 July 2009.'
- "Redox tuning over almost 1 V with retention of structure" **Invited Speaker**, University of Wyoming, Laramie, WY, Nov. 13, 2009.
- "Nitroreductase: A Plastic Explosive Degrading Enzyme" **Invited Speaker**, DePauw University, Greencastle IN, Sep. 9, 2010.
- "Nitroreductase, a plastic explosive degrading enzyme." **Invited Speaker**, University of Tennessee as part of their "The Role of Intrinsic Disorder and Dynamics in Protein Function." series, Knoxville TN, 7 April 2011
- "Nitroreductase undergoes a thermal transition that affects substrate binding" **Invited Speaker**, Stanford University, Stanford CA, 2 May 2011.
- "Nitroreductase undergoes a dynamic transition that affects substrate analog binding" **Invited Speaker**, 17<sup>th</sup> International Symposium on Flavins and Flavoproteins, Berkeley CA, July 24-29 2011.
- "Why every flavin is special: towards understanding how proteins tune the reactivity of flavins, via solid-state NMR", **Invited Speaker**, Ohio State University, Columbus OH, Sept. 29 2011.
- Nitroreductase: a plastic explosive degrading enzyme." **Invited speaker**, Kennesaw State University, Atlanta GA, 11 Oct. 2011.
- "<sup>1</sup>H dynamic nuclear polarization based on an endogenous radical" Rocky Mountain Conference on Analytical Chemistry, Copper Mountain, CO, 15-19 July 2012.
- "When more is different: Dynamic Nuclear Polarization based on an endogenous paramagnet; 15-fold enhancement of NMR intensities and potential as a new means of obtaining structural information and characterizing physiological status." **Invited Speaker**, C. A Townsend Symposium, The Johns Hopkins University, Baltimore MD, 10-12 Aug. 2012.
- "How proteins control electrons: protons." **Invited Speaker**, University of Illinois, Urbana-Champaign, 4 Sept. 2012
- "<sup>1</sup>H dynamic nuclear polarization based on an endogenous radical" Southeastern Regional Meeting of the American Chemical Society and 41<sup>st</sup> Southeastern Magnetic Resonance Conference, Raleigh, N.C. 14-17 Nov. 2012.
- "How do proteins control electrons ?" **Invited Speaker**, Biochemistry seminar, City College New York, 13 Feb. 2013.
- "Extreme Redox Tuning from the Dawn of Aerobic Metabolism" **Invited Speaker**, Chemistry departmental seminar, University of Iowa, Iowa City, 29 March 2013.
- "Why Bother ?: why does nature make 21 kDa of protein to catalyze a reaction effected by a single Fe ion and a water molecule ?" (**Invited**), **Keynote speaker**, Southeastern Enzyme Conference, Atlanta GA, 20 April 2013.
- "How do proteins control electrons ?" **Invited Speaker**, Chemistry seminar, University of Alberta, Edmonton CA, 21 Oct. 2013.
- "Superoxide dismutase: a model for the evolution of an enzyme that makes aerobic life possible" **Invited Speaker**, Biochemistry seminar, University of Calgary, CA, 23 Oct. 2013.

- "How proteins control electrons: Protons" **Invited Speaker**, Chemistry seminar, University of Alabama, Huntsville AL, 23 Jan. 2015.
- "One Man's Trash Is an Enzyme's Substrate: Mechanistic and Structural Features of a Promiscuous Enzyme" **Invited Speaker**, Gordon Research Conference on Enzymes, Coenzymes and Metabolic Pathways. 13 July 2015, Waterville Valley NH.
- "Flavins at the foundation of life" Midwest Enzyme Chemistry Conference, 12 Sept. 2015, Chicago IL. **Keynote Speaker**, <https://sites.google.com/site/midwestenzyme2015/Program>
- "How proteins control electrons: protons" **Invited Speaker**, Department of Chemistry, Mississippi State University, 25 September 2015
- "<sup>1</sup>H dynamic nuclear polarization based on an endogenous flavin radical" **Invited Speaker**, Southeast Magnetic Resonance Conference, 9-11 October 2015, Daytona Beach FL. <https://nationalmaglab.org/news-events/events/for-scientists/south-east-magnetic-resonance-conference>
- "Flavins are Single- Molecule Switches that Couple Electron Transfer, Proton Transfer, Conformational Gating and energy reallocation in support of versatile high-efficiency energy transduction." **Speaker** Department of Energy Energy Frontier Research Centers P.I. Meeting, 26, 27 October 2015, Washington DC.
- "How proteins control electrons: protons" **Invited Speaker**, Department of Chemistry, University of Washington University, 29 September 2016
- "How proteins control electrons: protons" **Invited Speaker**, Department of Chemistry, Georgetown College, 3 October 2016
- "When more is different: dynamic nuclear polarization based on a naturally-occurring endogenous paramagnet" **Invited Speaker**, First Gateway NMR meeting, 12 November, Louisville KY.
- "Ultrafast kinetic studies reveal effects of electron transfer and charge recombination on the lifetime of flavin semiquinone" **Speaker**, 19th International Symposium on Flavins and Flavoproteins July 2-6, 2017 / Groningen / The Netherlands
- "Mechanism-informed refinement reveals altered substrate binding mode for catalytically competent nitroreductase." **Speaker**, ACS National meeting, Aug 20-24, Washington DC.

**Refereed Publications:**(To use DOI links, go to <http://dx.doi.org/> then enter the doi provided for the paper of interest.)

- 1 J. C. De Paula, P. M. Li, **A.-F. Miller**, B. W. Wu and G. W. Brudvig (1986) "Effect of the 17- and 23-Kilodalton Polypeptides, Calcium and Chloride on Electron Transfer in Photosystem II." *Biochemistry* 25, 6487-6494. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1986/25/i21/pdf/bi00369a022.pdf>
- 2 **A.-F. Miller**, J. C. De Paula, and G. W. Brudvig (1987) "Formation of the S<sub>2</sub> state and Structure of the Mn Complex in Photosystem II Lacking the Extrinsic 33 Kilodalton Polypeptide." *Photosynth. Res.* 12, 205-218.
- 3 J. C. De Paula, W. F. Beck., **A.-F. Miller**, R. B. Wilson and G. W. Brudvig (1987) "Studies of the Manganese Site of Photosystem II by Electron Spin Resonance Spectroscopy." *J. Chem. Soc. Faraday Transactions* 83, 3635-3651.
- 4 L. K. Thompson, **A.-F. Miller**, J. C. De Paula and G. W. Brudvig (1988) "Electron Donation in Photosystem II." *Israel J. Chem.* 28, 121-128.
- 5 **A.-F. Miller** and G. W. Brudvig (1989) "Manganese and Calcium Requirements for Reconstitution of Oxygen-Evolution Activity in Manganese-Depleted Photosystem II Membranes." *Biochemistry* 28, 8181-8190. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1989/28/i20/pdf/bi00446a033.pdf>
- 6 L. K. Thompson, **A.-F. Miller**, C. A. Buser, J. C. De Paula and G. W. Brudvig (1989) "Characterization of the Multiple Forms of Cytochrome b<sub>559</sub> in Photosystem II." *Biochemistry* 28, 8048-8056. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1989/28/i20/pdf/bi00446a012.pdf>
- 7 **A.-F. Miller** and G. W. Brudvig (1990) "Electron Transfer Events Leading to Reconstitution of Oxygen-Evolution Activity in Manganese-Depleted Photosystem II Membranes." *Biochemistry* 29, 1385-1392. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1990/29/i06/pdf/bi00458a007.pdf>
- 8 **A.-F. Miller** and G. W. Brudvig (1991) "A Guide to EPR Spectroscopy of Photosystem II Membranes." *Reviews in Bioenergetics, Biochim. Biophys. Acta.* 1056, 1-18. doi:10.1016/S0005-2728(05)80067-2
- 9 **A.-F. Miller** and W. H. Orme-Johnson (1992) "The Dependence on Iron Availability of Allocation of Iron to Nitrogenase Components in *K. pneumoniae* and *E. coli*" *J. Biol. Chem.* 267, 9398-9408. <http://www.jbc.org/cgi/reprint/267/13/9398>
- 10 **A.-F. Miller**, M. Z. Papastavros and A. G. Redfield (1992) "NMR Studies of the Conformational Change in Human N-p21<sup>ras</sup> Produced by Replacement of Bound GDP with the GTP Analog GTPγS" *Biochemistry* 31, 10208-10216. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/1992/31/i42/pdf/bi00157a007.pdf>
- 11 **Miller, A.-F.**, C. J. Halkides and A. G. Redfield (1993) "An NMR Comparison of the Changes Produced by Different Guanosine 5'-Triphosphate Analogs in Wild-Type and Oncogenic Mutant p21<sup>ras</sup>" *Biochemistry* 32, 7367-7376. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1993/32/i29/pdf/bi00080a006.pdf>
- 12 C. Abeygunawardana, D. J. Weber, A. G. Gittis, D. N. Frick, J. Lin, **A.-F. Miller**, M. J. Bessman, and A. S. Mildvan (1995) "Solution Structure of the MutT Enzyme, a Nucleoside Triphosphate Pyrophosphohydrolase" *Biochemistry* 34, 14997-15005. <http://pubs.acs.org/cgi-bin/archive.cgi/bichaw/1995/34/i46/pdf/bi00046a006.pdf>
- 13 D. M. Noll, **A.-F. Miller** and P. S. Miller (1996) "Effect of Third Strand Orientation on Oligonucleotide Intramolecular Triplex Stability" *J. Am. Chem. Soc.* 118, 8979-8980. <http://pubs.acs.org/cgi-bin/article.cgi/jacsat/1996/118/i37/pdf/ja9618816.pdf>
- 14 **A.-F. Miller** and D. L. Sorkin (1997) "Superoxide Dismutases: A Molecular Perspective" *Comments on Molecular and Cellular Biophysics*, 9(1) 1 - 48.
- 15 C. K. Vance, Y. M. Kang and **A.-F. Miller** (1997) "Selective Labeling and Direct Observation by NMR of the Active Site Glutamine of Fe-Containing Superoxide Dismutase" *J. Biomol. NMR*, 9, 201-206. doi:10.1023/A:1018662421878
- 16 D. L. Sorkin and **A.-F. Miller** (1997) "Observation of a Long-Predicted Active Site pK in Fe-Superoxide Dismutase from *E. coli*" *Biochemistry*, 36(16) 4916-4924. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/1997/36/i16/pdf/bi963047z.pdf>. doi:10.1021/bi963047z
- 17 **A.-F. Miller**, L. A. Egan and C. A. Townsend (1997) "Measurement of the Degree of Coupled Isotopic Enrichment of Different Positions in an Antibiotic Peptide by NMR" *J. Magn. Reson.*, 125(1) 120-131. doi:10.1006/jmre.1997.1107

- 18 D. L. Sorkin, D. K. Duong and **A.-F. Miller** (1997) "Mutation of Tyrosine 34 to Phenylalanine Eliminates the Active Site pK of Reduced Fe-SOD" *Biochemistry* 36, 8202 - 8208. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/1997/36/i27/pdf/bi970533t.pdf>
- 19 C. K. Vance and **A.-F. Miller** (1998) "A Simple Proposal that Can Explain the Inactivity of Metal-Substituted Superoxide Dismutases" *J. Am. Chem. Soc.*, 120 (3), 461-467. <http://pubs.acs.org/cgi-bin/article.cgi/jacsat/1998/120/i03/pdf/ja972060j.pdf>
- 20 C. K. Vance and **A.-F. Miller** (1998) "Spectroscopic Comparisons of the pH Dependencies of Fe-Substituted-(Mn) Superoxide Dismutase and Fe-Superoxide Dismutase", *Biochemistry* 37(16), 5518-5527. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/1998/37/i16/pdf/bi972580r.pdf>
- 21 R. L. Koder, Jr. and **A.-F. Miller** (1998) "Overexpression, Isotopic Labeling and Spectral Characterization of *Enterobacter cloacae* Nitroreductase" *Protein Expression and Purification*. 13, 53-60. doi:10.1006/prev.1997.0866
- 22 R. L. Koder, Jr. and **A.-F. Miller** (1998) "Steady State Kinetic Mechanism, Stereospecificity, Substrate and Inhibitor Specificity of *Enterobacter cloacae* Nitroreductase" *Biochim. Biophys. Acta*, 1385, 395-405. <http://www.sciencedirect.com/science/article/pii/S0167483898001514> doi:10.1016/S0167-4838(98)00151-4
- 23 J. Lou, F. Moshiri, M. K. Johnson, M. E. Lafferty, D. L. Sorkin, **A.-F. Miller**, and R. J. Maier (1999) "Mutagenesis Studies of the Fe<sup>II</sup> Protein of *Azotobacter vinelandii*: Roles of Histidine and Lysine Residues in the Protection of Nitrogenase from Oxygen Damage.", *Biochemistry*, 38(17) 5563-5571. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/1999/38/i17/pdf/bi9827823.pdf>
- 24 K. A. Campbell, E. Yikilmaz, C. V. Grant, W. Gregor, **A.-F. Miller**, and R. D. Britt (1999) "Parallel Polarization EPR Characterization of the Mn(III) Center of Oxidized Manganese Superoxide Dismutase", *J. Am. Chem. Soc.*, 121(19) 4714-4715. <http://pubs.acs.org/cgi-bin/article.cgi/jacsat/1999/121/i19/pdf/ja9902219.pdf>
- 25 S. Vathyam, R. A. Byrd and **A.-F. Miller** (1999) "Assignment of the Backbone Resonances of Oxidized Fe-Superoxide Dismutase, a 42 kDa Paramagnet-Containing Enzyme", *J. Biomol. NMR*, 14 (3) 293-294. doi:10.1023/A:1008348716066
26. R. L. Koder, Jr., M. E. Rodgers and **A.-F. Miller** (1999) "Flavin Binding Thermodynamics in *Enterobacter cloacae* Nitroreductase," in *Flavins and Flavoproteins*, S. Ghisla, P. Kroneck, P. Macheroux and H. Sund, Eds., Agency for Scientific Publications, Berlin, pp. 45-48.
- 27 J. D. Walsh and **A.-F. Miller** (1999) "Theoretical Destabilization of the Flavin Semiquinone of *Enterobacter cloacae* Nitroreductase by a Hydrogen-Bonding-Bending Mechanism," in *Flavins and Flavoproteins*, S. Ghisla, P. Kroneck, P. Macheroux and H. Sund, Eds., Agency for Scientific Publications, Berlin, pp. 63-66.
- 28 D. L. Sorkin and **A.-F. Miller** (2000) "Amino Acid Specific Labelling and Active Site Studies of Iron(II)- and Fe(III)-Superoxide Dismutase from *Escherichia coli*" *J. Biomol. NMR* 17, 311-322. doi:10.1023/A:1008344210662
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- 30 A. L. Schwartz, E. Yikilmaz, C. K. Vance, S. Vathyam, R. L. Koder, Jr. and **A.-F. Miller** (2000) "Mutational and Spectroscopic Studies of the Significance of the Active Site Glutamine to Metal ion Specificity in Superoxide Dismutase", *J. Inorg. Biochem.*, 80, 247-256. doi:10.1016/S0162-0134(00)00086-6
- 31 H. Nivinskas, R. L. Koder, Jr., Ž. Anusevičius, J. Šarlauskas, **A.-F. Miller**, N. Čenas (2000) "Two-Electron Reduction of Nitroaromatic Compounds by *Enterobacter cloacae* NAD(P)H Nitroreductase: Description of Quantitative Structure-Activity Relationships" *Acta Biochim. Pol.* 47 (4) 941-949.
- 32 H. Nivinskas, R. L. Koder, Jr., Ž. Anusevičius, J. Šarlauskas, **A.-F. Miller** and N. Čenas (2001) "Quantitative Structure-Activity Relationships in Two-Electron Reduction of Nitroaromatic Compounds by *Enterobacter cloacae* NAD(P)H:Nitroreductase" *Arch. Biochem. Biophys.* 385 (1), 170-178. doi:10.1006/abbi.2000.2127
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- 34 **A.-F. Miller** (2001) "Fe Superoxide Dismutase" in *Handbook of Metalloproteins*, Wieghardt, K., Huber, R., Poulos, T. L. and Messerschmidt, A, Eds., Wiley and Sons. pp. 668-682.
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- 36 C. K. Vance and **A.-F. Miller** (2001) "Novel Insights into the Basis for *E. coli* SOD's Metal Ion Specificity, from Mn-Substituted Fe-SOD and its Very High  $E_m$ ", *Biochemistry* 40, 13079-13087. <http://pubs.acs.org/cgi-bin/article.cgi/bichaw/2001/40/i43/pdf/bi0113317.pdf> doi:10.1021/bi0113317
- 37 J. Xie, E. Yikilmaz, **A.-F. Miller** and T. C. Brunold (2002) "Second-Sphere Contributions to Substrate-Analogue Binding in Iron(III) Superoxide Dismutase" *J. Am. Chem. Soc.* 124(14) 3769-3774. <http://pubs.acs.org/cgi-bin/article.cgi/jacsat/2002/124/i14/pdf/ja016254h.pdf>
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