NAME Alvan C. Hengge
TITLE Professor

EDUCATION
B.S., University of Cincinnati, 1974
Ph.D., University of Cincinnati, 1982-1987
(Organic Chemistry, under R. Marshall Wilson)
Postdoctoral fellow, University of Wisconsin, 1987-1990
(Biochemistry, under W. W. Cleland)

ADDRESS Department of Chemistry and Biochemistry
Utah State University
Logan, UT 84322-0300
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WEB PAGE http://www.chem.usu.edu/~hengge/

RESEARCH INTERESTS

The goals of my laboratory's research lie in the areas of mechanistic organic chemistry and biochemistry. Specific areas focus on the molecular details of catalysis, especially of enzymatic reactions, involving phosphoryl transfer, sulfuryl transfer, and acyl transfer reactions. Of particular interest is the question of how mechanisms of enzymatic reactions compare with the analogous uncatalyzed reactions in solution.

PROFESSIONAL EXPERIENCE

Head, Department of Chemistry & Biochemistry, August 2009 - present
Professor of Chemistry, Utah State University, April 2004 - present
Associate Professor of Chemistry, Utah State University, 2000-2004
Assistant Professor of Chemistry, Utah State University, 1996-1999
Assistant Scientist, University of Wisconsin-Madison, Institute for Enzyme Research 1991-1996
NIH Postdoctoral Fellow, University of Wisconsin-Madison, Institute for Enzyme Research 1987-1990 (under W. W. Cleland)
Graduate Assistant, University of Cincinnati, 1983-1987
Chemistry and Physics Teacher, Cincinnati Public Schools, R.A. Taft High School, 1974-1982

PROFESSIONAL SOCIETY AFFILIATIONS

American Chemical Society (ACS):
Divisions of Organic Chemistry, Biological Chemistry, and Inorganic Chemistry
American Society for Biochemistry and Molecular Biology (ASBMB)
American Association for the Advancement of Science (AAAS)
Sigma Xi

HONORS

USU College of Science Undergraduate Research Mentor of the Year, 2008
USU College of Science Researcher of the Year, 2006
USU College of Science Teacher of the Year, 2005
NIH Postdoctoral Fellowship (GM 11942) 1987-1990
University of Cincinnati Research Council Summer Fellowship, 1985
Lowenstein-Schubert-Twitchell Fellowship, 1986
University of Cincinnati College of Engineering Scholastic Achievement Award, 1973
University of Cincinnati Honor Scholarship; 1971,1972

PROFESSIONAL ACTIVITIES

Scientific Reviewer for:

Biochemistry
Bioorganic and Medicinal Chemistry Letters
Biophysical Journal
Chemical Communications
Chemical Engineering Communications
Chemical Reviews
Geochimica et Cosmochimica Acta
Inorganic Chemistry
Industrial & Engineering Chemistry Research
The International Journal of Chemical Kinetics
Journal of the American Chemical Society
Journal of Biological Chemistry
Journal of Organic Chemistry
Journal of Physical Chemistry
Journal of Physical Organic Chemistry
Nucleic Acids Research
Protein Science
PLOS Biology
PNAS
Phytochemistry

Grant Reviewer for:

The National Science Foundation
The National Institutes of Health
American Chemical Society Petroleum Research Fund

Publicity Chair for the Joint ACS 59th Northwest and 18th Rocky Mountain Regional Meeting, June 6-9, 2004, at Utah State University, Logan, UT.

Organizer and Chair*,* Summer Chemistry and Biochemistry Department Internship program for high school students (2007-2011).

Project Leader for Chemistry, Northern Utah Science Teaching and Laboratory Initiative (a Utah Office of Education-funded project designed to enhance the effectiveness of high school science instruction). 2009-2011.

DEPARTMENTAL COMMITTEE ASSIGNMENTS

1996-1999	Safety Committee
1996-2006	Graduate Recruiting & Admission Committee (chair, 1999-2004, 2005-06)
1997	Visiting Speakers Committee
1998	Inorganic Faculty Search Committee (Lisa Berreau hired)
1998	Glassblower Search Committee (James Young hired)
1998-99	Chair, Organic Faculty Search Committee (Tom Chang hired)
1999	Departmental Secretary Search Committee (Beth Blaser hired)
1999	Department Head Search Committee (Steve Scheiner hired)
1999-2004	Graduate Studies Committee
2002	Chair, NMR/EPR Director Search Committee (Piotr Dobrowolski hired)
2002	Chair, Departmental Secretary Search (Maradean Holmes hired)
2002-2003	Hansen Professor of Biochemistry Search Committee (Joanie Hevel hired)
2002-present	NMR Users Committee (chair, 2003-2004)
2003-2006	Advisory committee
2007-2009	Graduate Studies Committee chair

UNIVERSITY-WIDE COMMITTEES

College of Science representative, Faculty Development, Diversity and Equity Committee, 2007-2010
Undergraduate Research Advisory Board, 2007 - 2009

TEACHING ASSIGNMENTS		EVALUATIONS	
		***Course** (course/dept.)	****Instructor** (course/dept.)
Chem 625 - Advanced Organic Chemistry	Fall 1996	4.7/4.7	5.3/4.8
Chem 733 - Special Topics in Organic Chemistry	Spring 1997	6.0/4.9	6.0/4.9
Chem 144 - Chemistry Laboratory	Spring 1997	4.0/4.9	4.6/4.9
Chem 625 - Advanced Organic Chemistry	Fall 1997	5.3/4.7	5.5/4.7
Chem 233 - Organic Chemistry III	Spring 1998	4.6/4.9	4.9/5.0
Chem 6300- Advanced Organic Chemistry	Fall 1998	5.2/4.3	5.6/4.3
Chem 2310-Organic Chemistry I	Spring 1999	4.8/4.6	5.0/4.5
Chem 6300-Advanced Organic Chemistry	Fall 1999	5.0/4.3	5.4/4.1
Chem 2310-Organic Chemistry I	Spring 2000	4.5/4.7	4.7/4.7
Chem 6300-Advanced Organic Chemistry	Fall 2000	5.8/4.5	5.8/4.6
Chem 2310-Organic Chemistry I	Spring 2001	4.8/4.6	4.9/4.6
Chem 6300-Advanced Organic Chemistry	Fall 2001	5.5/4.7	5.7/4.8
Chem 2310-Organic Chemistry I	Spring 2002	4.8/4.6	5.0/4.6
Chem 2310-Organic Chemistry I	Fall 2002	4.7/4.5	4.7/4.5
Chem 6300-Advanced Organic Chemistry	Spring 2003	5.7/4.8	5.7/4.8
Chem 2310-Organic Chemistry I	Fall 2003	5.0/4.5	5.2/4.6
Chem 2320-Organic Chemistry II	Spring 2004	4.9/4.9	5.0/5.0
Chem 6300-Advanced Organic Chemistry	Fall 2004	5.1/4.7	5.9/4.7
Chem 2330-Organic Chemistry Laboratory I	Fall 2004	lab - not evaluated	
Chem 2340-Organic Chemistry Laboratory II	Spring 2005	lab - not evaluated	
Chem 2310-Organic Chemistry I	Fall 2005	5.1/4.8	5.2/4.8
Chem 6300-Advanced Organic Chemistry	Spring 2006	5.3/4.8	5.5/4.9
Chem 6300-Advanced Organic Chemistry	Spring 2007	6.0/4.8	6.0/4.9
Chem 2310-Organic Chemistry I	Fall 2007	4.8/4.6	5.0/4.7
Chem 7330- Special Topics-Bioorganic Chemistry	Spring 2008	5.8/4.8	5.8/4.8
Chem 6300- Advanced Organic Chemistry	Fall 2008	5.7/4.8	5.7/4.8
Chem 2320-Organic Chemistry II	Spring 2009	4.4/4.7	4.4/4.6
Chem 6300- Advanced Organic Chemistry	Spring 2010	5.4/4.9	5.6/4.9
Chem 2320- Organic Chemistry II	Spring 2011	4.7/4.9	4.6/5.0
Chem 6300- Advanced Organic Chemistry	Fall 2011		

*Score for overall quality of course; first number is for my course, the second number is the semester average for the department. Range is from 0 – 6.
**Score for instructor effectiveness; first number is for my course, the second number is the semester average for the department. Range is from 0 – 6.

FUNDED RESEARCH GRANTS

Title	Source	Date	Amount (Direct + indirect)
NIH Postdoctoral Fellowship	NIH	1987-1990	
"Mechanisms of Acyl and Phosphoryl Transfer"	NIH R29/GM47297	5/1/1995 to 4/30/2000	$500,500
"Defining the Mechanisms of Uncatalyzed and Enzyme-Catalyzed Sulfuryl-Transfer Reactions"	USU New Faculty Research Grant	7/1/98 to 6/30/99	$25,000
"Investigations of Sulfate Ester Chemistry"	ACS PRF-AC	9/1/2000 to 8/31/2002	$60,000
"Mechanisms of Acyl, Phosphoryl and Sulfuryl Transfer"	NIH R01GM47297	5/1/2000 to 8/31/2004	$671,833
"US-Nigeria Cooperative Research: Transition States for Thiophosphoryl Transfer from Phosphinothioates and Related Compounds"	NSF INT-0217688	8/1/2002 to 7/31/2005	$30,000
"Mechanisms of Acyl, Phosphoryl and Sulfuryl Transfer"	NIH R01GM47297	9/1/2004 to 8/31/2009	$1,268,531
"Mechanisms of Phosphoryl Transfer"	NIH R01GM47297	9/1/2009 to 8/31/2012	$612,216
"New Antibacterial Approaches: Targeting the OspF Family of Virulence Factors"	USU Seed Program to Advance Research Collaboration (SPARC)	1/1/1010 to 12/31/2010	$34,943

PATENT

"Thiophosphonate Inhibitors of Phosphatase Enzymes and Metallophosphatases" Patent Number 6,943,267, issued September 13, 2005.

GRADUATE STUDENT THESIS/DISSERTATIONS MENTORED

Name	Degree	Status
Richard Hoff	Ph. D.	Degree awarded 1999; present position: Associate Professor, U. S. Military Academy, West Point

Dissertation title: "Investigation of the Cleavage of the Ester Bond in Phosphate Monoesters: Enzymatic and Solution Studies of Phosphoryl Transfer Reactions and Comparison with Sulfuryl Transfer Reactions."

Irina Catrina	Ph.D.	Degree awarded 2001; present position: Research Associate, Hunter College, Department of Biological Sciences

Dissertation title: "Phosphorothioates as Models for Studying Phosphoryl Transfer Reactions"

Piotr Grzyska	Ph.D.	Degree awarded 2003; present position: Research Assistant Professor, Michigan State University

Dissertation title: "Insights on Enzymatic and Uncatalyzed Phosphoryl Transfer"

Jamie Purcell	M.S.	Degree awarded 2005; presently a Ph.D. student at Emory University.

Thesis title: 1. "Thermodynamic Investigation of Phosphoryl and Thiophosphoryl Transfer. 2. Kinetic Isotope Effects on Zinc-Mediated Phosphotriester Hydrolysis."

Kerensa Sorensen-Stowell	Ph.D.	Degree awarded 2006; present position: Assistant Professor, Department of Chemistry, BYU-Idaho.

Dissertation title: Insights Into Solvation Effects on Phosphate, Phosphorothioate, and Sulfate Ester Hydrolysis Reactions.

Tim Humphry	Ph.D.	Degree awarded 2006; present position: Assistant Professor, Chemistry Department, Gonzaga University

Dissertation title: Investigations on the Effect of Metal Complexation Upon the Hydrolysis Reactions of Phosphate Esters

Robynn Cox	M.S.	Degree Awarded 2007

Thesis topic: A mechanistic study of purple acid phosphatases

Subashree Iyer	Ph.D.	Degree awarded 2007; present position: Research Scientist, Albany Molecular Research, Inc. Albany, NY.

Dissertation title: 1. Synthesis and evaluation of phosphonic acids as phosphatase inhibitors. 2. Transesterification thio effects and kinetic isotope effects of thio-substituted ribonucleoside models.

Alok Shenoy	M.S.	Degree Awarded 2011; present position: lab manager, Foster Agblevor, Dept. of Biological Engineering, USU.

Thesis topic: Mechanistic and Structural Investigations of the Phosphothreonine Lyase Class of Enzymes

Yuan Chu	Ph.D.	Degree awarded 2012; present position: Analytical Specialist, Great Salt Lake Minerals Company

Dissertation title: A Mechanistic Study of Catalytic Promiscuity in Protein Phosphatase I

Mark Haney	Ph.D.	Degree awarded 2013

Dissertation title: The Phosphoramidase Competency of Prototypical Phosphatase Catalytic Motifs.

Present Students:

Vyascheslov Kuznetsov, fifth year Ph. D student
Gwen Moise, second year student

POSTDOCTORAL RESEARCH FELLOWS

Dr. Przemyslaw Czyryca	October 1998-August 2003 (Present position: Fujitsu)
Dr. Krzysztof Swierczek	February 2001-April 2003 (Present position: SuperGen, Salt Lake City)
Dr. Eric Tanifum	April 2006 – February 2008 (Present position: Research fellow, Department of Pharmacology and Toxicology, University of Texas Medical Branch
Dr. Tiago Brandao	April 2007 – January 9, 2009 (Present position: Assistant Professor, Departamento de Química, Universidade Federal de Minas Gerais, Brazil

VISITING SCIENTISTS HOSTED

Dr. Ikenna Onyido, Department of Chemistry, Michael Okpara University of Agriculture Umuahia, Nigeria: Feb. – April, 2003; Sept. – Nov., 2004; Sept. – Dec., 2005.

UNDERGRADUATE RESEARCH STUDENTS MENTORED

Samantha Streicher	1997-1998
Paul Larsen	1998-1999 (2 papers)
Kelly Southwick-Small	1998-1999 (1 paper)
Sarah Fitch	1998-1999
Justin Golightly	1999 (1 paper)
David Cleverly	1999-2000
Stuart Gibby	2000-2002 (1 paper)
Jarod Younker	June 2001-August 2004 (3 papers, 3 poster presentations)
Jamie Purcell	June 2001-August 2004 (2 papers, 3 poster presentations)
Randy Christensen	January 2003-May 2003
Zahraa Al-Lawati	January 2004–August 2004
Darin Humphreys	January 2004–June 2005
Elise McKenna	May 2004-December 2004
Rebecca Mitchell	September 2004-January 2006, January 2008-2009 (1 paper)
Elizabeth Lund	May 2005-July 2007 (1 paper, 1 poster presentation)
Doug Holt	October 2005-December 2006
Sara Huefner	July 2007 – June 2009 (3 poster presentations)
Ryan Berry	January 2008 – June 2011 (2 poster presentations)
Rochelle Kellett	March 2008 – May 2010
Ben Brown	January 2010 – June 2011
Kelsey Klemm	January 2010 – August 2011 (2 poster presentations)
Emily Meacham	May 2011-May 2012 (1 poster presentation)
J. Tyler Gish	June 2011 – present (2 poster presentations)
Kyle Berg	January 2012 - present

RESEARCH-RELATED AWARDS WON BY UNDERGRADUATES

Jarod Younker:
URCO (Undergraduate Research and Creative Opportunities) award (2002)
Department Undergraduate Summer Research Award (2003)

Jamie Purcell
URCO (Undergraduate Research and Creative Opportunities) award (2003)
Department Undergraduate Summer Research Award (2002)

Darin Humphreys
Department Undergraduate Summer Research Award (2004)

Zahraa Al-Lawati
Department Undergraduate Summer Research Award (2004)

Rebecca Mitchell
URCO (Undergraduate Research and Creative Opportunities) award (2005)
Willard L. Eccles Undergraduate Research Fellowship (2005)

Elizabeth Lund
URCO (Undergraduate Research and Creative Opportunities) award (2006)
Willard L. Eccles Undergraduate Research Fellowship (2006)

College Science Scholar of the Year (2006-2007)
Department of Chemistry & Biochemistry Outstanding Graduating Senior (2007)

Douglas Holt
College of Science Undergraduate Minigrant (2006)

Sara Huefner
College of Science Undergraduate Minigrant (2008)
Best poster in the Life Sciences area, USU Student Showcase, April 2008
Dept. of Chemistry & Biochemistry Undergraduate Research Award, 2008
Center for Integrated BioSystems Undergraduate Student Research Award, 2008

Rochelle Kellett
College of Science Undergraduate Minigrant (2008)
Willard L. Eccles Undergraduate Research Fellowship (2009)
Maeser-Bauer Outstanding Graduating Senior in Biochemistry (2010)

Ryan Berry
Willard L. Eccles Undergraduate Research Fellowship (2008-2009)
College of Science Undergraduate Minigrant (2010)
Department of Chemistry & Biochemistry Undergraduate Research Award (2011)
Maeser-Bauer Outstanding Graduating Senior in Biochemistry (2011)

J. Tyler Gish
SURCO (Summer Undergraduate Research and Creative Opportunities) award (2012)
College of Science Minigrant (2013)

Kyle Berg
SURCO (Summer Undergraduate Research and Creative Opportunities) award (2013)

GRADUATE STUDENT SUPERVISORY COMMITTEES

Past Students

Name	Degree Sought	Status	Study Area (Advisor)
Ruihua Fang	Ph.D.	awarded 1998	Biochemistry (Ann Aust)
Mark Wathen	M.S.	awarded 2000	Organic Chemistry (Mike Wright)
Ryan Ball	M.S.	awarded 2000	Biochemistry (Ann Aust)
Travis Messenger	M.S.	awarded 2000	Organic Chemistry (Brad Davidson)
David Bienvenue	Ph.D.	awarded 2001	Biochemistry (Rick Holz)
Dan Clark	Ph.D.	awarded 2001	Biochemistry (Scott Ensign)
Yu Hui	M.S.	awarded 2002	Organic Chemistry (Vernon Parker)
Jonathan Krum	Ph.D.	awarded 2002	Biochemistry (Scott Ensign)
Geoffry Nadolski	Ph.D.	awarded 2002	Organic Chemistry (Brad Davidson)
Natasha Skoberla	M.S.	awarded 2003	Biochemistry (Steve Aust)
Russell Allred	Ph.D.	awarded 2003	Inorganic Chemistry (Lisa Berreau)
Bryan Elchert	M.S.	awarded 2003	Organic Chemistry (Tom Chang)
Magda Makowska-Grzyska	Ph.D.	awarded 2003	Inorganic Chemistry (Lisa Berreau)
Krzysztof Bzymek	Ph.D.	awarded 2003	Biochemistry (Rick Holz)
Aleksey Kuznetsov	Ph.D.	awarded 2003	Physical Chemistry (Alex Boldyrev)
Aleksander Baldys	Ph.D.	awarded 2004	Biochemistry (Rick Holz)
Matt Anderson	M.S.	awarded 2005	Organic Chemistry (Brad Davidson)
Shanghamitra Mitra	Ph.D.	awarded 2006	Biochemistry (Rick Holz)
Jinhua Wang	Ph.D.	awarded 2006	Organic Chemistry (Tom Chang)
Eric Tanifum	Ph.D.	awarded 2006	Organic Chemistry (Brad Davidson)
Laura Buelow	Ph.D.	awarded 2006	Biochemistry (Ann Aust/Joanie Hevel)
Gajendrasingh Ingle	M.S.	awarded 2007	Inorganic Chemistry (Lisa Berreau)
Jie Li	Ph.D.	awarded 2007	Organic Chemistry (Tom Chang)
Ian McAlexander	Ph.D.	awarded 2008	Organic Chemistry (Brad Davidson)
Bishnu Regmi	M.S.	awarded 2008	Biochemistry (Steve Aust)
Katarzyna Rudzka	Ph.D.	awarded 2008	Inorganic Chemistry (Lisa Berreau)
Whitney Wooderchak	Ph.D.	awarded 2008	Biochemistry (Joanie Hevel)
Yi Liang	M.S.	awarded 2008	Organic Chemistry (Tom Chang)
Christabel Tanifum	Ph.D.	awarded 2009	Organic Chemistry (Tom Chang)
James Danford	M.S.	awarded 2009	Inorganic Chemistry (Lisa Berreau)
Hanh Dinh	M.S.	awarded 2010	Analytical Chemistry (Bob Brown)
Jianjun Zhang	Ph.D.	awarded 2010	Organic Chemistry (Tom Chang)
Katarzyna Grubel	Ph.D.	awarded 2010	Inorganic Chemistry (Lisa Berreau)
Weifang Hao	Ph.D.	awarded 2011	Organic Chemistry (Vernon Parker)
Alina Sergeeva	Ph.D.	awarded 2012	Physical Chemistry (Alex Boldyrev)

Terri Alley	Ph.D.	left program	Physical Chemistry
Mitchell Berntson	Ph.D.	left program	Inorganic Chemistry
Vidhya Nagarajan	Ph.D.	left program	Biochemistry
Ben Philmus	Ph.D.	left program	Organic Chemistry
Lakshman Rajagopal	Ph.D.	left program	Biochemistry
Indranil Sen	Ph.D.	left program	Inorganic Chemistry

Current Students

Marina Fosso	Ph.D.	Organic Chemistry (Tom Chang)
Zhao Li	Ph.D.	Organic Chemistry (Vernon Parker)
Ryan Jackson	Ph.D.	Biochemistry (Sean Johnson)
Karamatullah Danyal	Ph.D.	Biochemistry (Lance Seefeldt)

Shangying Gui	Ph.D.	Biochemistry (Joanie Hevel)
Caleb Allpress	Ph.D.	Inorganic Chemistry (Lisa Berreau)
Jeremy Bakelar	Ph.D.	Bichemistry (Sean Johnson)
Anna Lytle	Ph.D.	Bichemistry (Sean Johnson)
	Ph.D.	Physical Chemistry (Alex Boldyrev)

INVITED TALKS:

1. "Insights from Heavy-Atom Isotope Effects on Sulfuryl and Phosphoryl Transfer Reactions," Gordon Research Conference on Isotopes in Biological and Chemical Sciences, Ventura, CA, January 1998.

2. "Insights from Heavy-Atom Isotope Effects on Phosphoryl and Thiophosphoryl Transfer Reactions," 26th Steenbock Symposium on Enzymatic Mechanisms, Madison, WI, May 28-31, 1998.

3. "Does Positive Charge at the Active Sites of Phosphatases Cause a Change in Mechanism?" Department of Molecular Pharmacology, Albert Einstein College of Medicine, Yeshiva University, Bronx, NY; October 26, 1999.

4. "Does Positive Charge at the Active Sites of Phosphatases Cause a Change in Mechanism?" Department of Chemistry, Washington State University, Pullman, WA; November 19, 1999

5. "Isotope Effects in Enzymatic Reactions of Phosphorothioates," 2001: An Isotope Odyssey, Zakopane, Poland, June 24-29, 2001

6. "Transition States for Phosphoryl Transfer Reactions of Phosphatases and Their Application to Inhibitor Design." Metals in Medicine Symposium, 222nd National Meeting of the ACS, Chicago, August 26-30, 2001.

7. "Are Phosphorothioates Valid Mechanistic Probes for Enzymatic Phosphoryl Transfer?" Physical Chemistry Division Symposium on Modern Aspects of Structure Function Correlations of Biomolecules: Phosphoryl and Nucleotidyl Transfer Reactions, 223^{d} National Meeting of the ACS, Orlando, April 7-11, 2002.

8. "Are Phosphorothioates Valid Mechanistic Probes for Enzymatic Phosphoryl Transfer?" Department of Chemistry, University of California-Davis, Davis, CA; April 25, 2002.

9. "Are Phosphorothioates Valid Mechanistic Probes for Enzymatic Phosphoryl Transfer?" Department of Chemistry, University of Utah, Salt Lake City, UT; May 21, 2002.

10. "Are Phosphorothioates Valid Mechanistic Probes for Enzymatic Phosphoryl Transfer?" Department of Biochemistry and Molecular Biology, Mayo Foundation, Rochester, MN; September 4, 2002.

11. "Are Phosphorothioates Valid Mechanistic Probes for Enzymatic Phosphoryl Transfer?" Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; February 3, 2003.

12. "Altered Hydrolysis Mechanisms for a Metal-Complexed Phosphate Monoester and Diester." International Isotope Effects Conference, Uppsala. Sweden, June 22-27, 2003.

13. "Recent Studies of Phosphoryl Transfer Mechanisms," McMaster University, Hamilton, Ontario, October 14, 2003.

14. "Recent Studies of Phosphoryl Transfer Mechanisms," Case Western University, Cleveland, Ohio, October 16, 2003.

15. “Recent Studies of Phosphoryl Transfer Mechanisms,” SUNY Buffalo, Buffalo, NY, October 17, 2003.

16. “The Effect of Metal Ions on Phosphoryl Transfer Reactions,” Isotopes 2005 Conference, June 27 – July 1, 2005, Bath, UK.

17. “The Effect of Metal Ions on Phosphoryl Transfer Reactions,” 8th Latin American Conference on Physical Organic Chemistry (CLAFQO8), Florianopolis, Brazil, October 9-14, 2005

18. “Mechanism of Phosphotriester Hydrolysis by Pyrazolylborate Zinc Hydroxide Complex,” Gordon Research Conference on Isotopes in Biological and Chemical Sciences, Ventura, CA, February 12-17, 2006

19. “Metals in Phosphoryl Transfer: From Model Systems to Purple Acid Phosphatases” ComBio meeting of the Australian Society for Biochemistry and Molecular Biology, in Brisbane, Australia, September 24-28, 2006

20. “Metals in Phosphoryl Transfer: From Model Systems to Purple Acid Phosphatases” Loyola University-Chicago, Department of Chemistry, November 30, 2006.

21. “Diesterase Activity and Substrate Binding in Purple Acid Phosphatases,” Isotopes 2007, Benicassim, Spain: May 27 – June 1, 2007.

22. "Protein Motions in Catalysis by Protein Tyrosine Phosphatases." Department of Chemistry at Queen's University, Kingston, ON, January 15, 2010.

23. "Protein Motions in Catalysis by Protein Tyrosine Phosphatases." Gordon Research Conference on Isotopes in Biological and Chemical Sciences, Galveston, TX, February 14-19, 2010.

24. "Protein Motions in Catalysis by Protein Tyrosine Phosphatases." Southern Illinois University-Edwardsville, October 5, 2010.

25. “Protein Motions and Catalytic Promiscuity in Phosphatases,” Nankai University, State Key Laboratory of Elemento-Organic Chemistry, Tianjin, China, September 21, 2011

26. “Protein Motions and Catalytic Promiscuity in Phosphatases,” Institute of Chemistry, Chinese Academy of Sciences, Beijing, China, September 23, 2011

27. “Protein Motions and Catalytic Promiscuity in Phosphatases,” Lanzhou University, State Key Laboratory of Applied Organic Chemistry, Lanzhou, China, September 27, 2011

28. “Effects of Protein Motions in Protein-Tyrosine Phosphatases on Catalysis and Inhibition by Vanadate,” Departamento de Química, Universidade Federal de Minas Gerais, Belo Horizonte, Brasil, October 18, 2012.

CONTRIBUTED PRESENTATIONS AT CONFERENCES as graduate student and postdoc *(oral and poster presentations; name of the presenter is underlined).*

1. A. C. Hengge and R.M. Wilson. "Oxidative Condensation Reactions Based Upon Triazolinedione Ylides," American Chemical Society 18th Central Regional Meeting, Bowling Green, Ohio, June 1-5, 1986.

2. A. C. Hengge and W. W. Cleland. "Secondary Oxygen-18 Isotope Effects on Phosphodiester Hydrolysis Reactions," Gordon Research Conference on Isotopes in the Physical and Life Sciences, January 22-26, 1990, Oxnard, CA.

3. A. C. Hengge and W. W. Cleland. "Determination of the Transition States for Phosphoryl Transfer and Hydrolysis Reactions," 23d Reaction Mechanisms Conference, June 10-14, 1990, University of Colorado-Boulder.

4. A. C. Hengge and W. W. Cleland. "Determination of the Transition States for Phosphoryl Transfer and Hydrolysis Reactions by Heavy Atom Isotope Effects," Gordon Conference on Enzymes, Coenzymes and Metabolic Pathways, July 2-6, 1990, Meriden, N.H.

5. A. C. Hengge and W. W. Cleland. "Solution and Enzymatic Phosphoryl Transfer Reactions of Phosphodiesters: Characterization of Transition States by Heavy Atom Isotope Effects," Twelfth Enzyme Mechanisms Conference, January 4-6, 1991, San Diego, CA.

6. A. C. Hengge. "Concertedness in Acyl Transfer Reactions of Esters," 24th Reaction Mechanisms Conference, June 5-11, 1992, University of Maine, Orono, Maine.

7. A. C. Hengge , R. A. Hess, A. E. Tobin, and W. W. Cleland. "Mechanistic Probes of Acyl and Phosphoryl Transfer Reactions Using Heavy Atom Isotope Effects," 13th Enzyme Mechanisms Conference, January 6-10, 1993, Key Largo, Florida.

8. J. Rawlings, A. C. Hengge, and W. W. Cleland. "Isotope Effects on the Hydrolysis of Cobalt (II)-Bound Phosphate Esters," American Society for Biochemistry and Molecular Biology Annual Meeting, May 21-25, 1994, Washington, D. C.

9. A. C. Hengge and Z.-Y. Zhang. "Kinetic Isotope Effects on Reactions of Tyrosine Phosphatases," ASBMB/DBC-ACS Joint Meeting, May 21-25, 1995, San Francisco, CA.

Conference poster presentations as independent investigator at USU. Presenter name is underlined. Graduate students are indicated with an asterisk, undergraduates by [#].

10. A. C. Hengge. "Phosphoryl Transfer Reactions of Protein Phosphatases," Gordon Research Conference on Isotopes in Biology and Chemistry, February 1996, Ventura, CA.

11. J. Rawlings and A. C. Hengge. "Co(III)-Cyclen Catalyzed Hydrolysis of *p*-Nitrophenyl Phosphate," American Chemical Society National Meeting, April 13-17, 1997, San Francisco, CA.

12. I. E. Catrina* and A. C. Hengge. "Thermodynamics, pH Behavior, and Effect of Metal Ions in Reactions of Phosphorothioates," American Chemical Society National Meeting, September 7-11, 1997, Las Vegas, Nevada.

13. R. H. Hoff* and A. C. Hengge. "Thermodynamics of Solvation Effects on Phosphoryl and Sulfuryl

Transfer Reactions," American Chemical Society National Meeting, September 7-11, 1997, Las Vegas, Nevada.

14. R. H. Hoff* and A. C. Hengge. "Entropy Effects in the Catalytic Efficiencies of Phosphatases," 27th Reaction Mechanisms Conference, June 28 - July 3, 1998, Pacific Grove, CA.

15. I. E. Catrina* and A. C. Hengge. "Solution and Enzymatic Reactions of Phosphorothioate Monoesters: Thermodynamics and Mechanisms," 27th Reaction Mechanisms Conference, June 28 - July 3, 1998, Pacific Grove, CA.

16. R. H. Hoff*, A. C. Hengge, Y.-F. Keng and Z.-Y. Zhang. "The Effect on the Function of the General acid Catalyst from Mutations of the Invariant Tryptophan and Arginine Residues in the Protein-Tyrosine Phosphatase from *Yersinia,*" 16th Enzyme Mechanisms Conference, January 6 - 10, 1999, Napa, CA

17. A. C. Hengge, R. H. Hoff*, P. Mertz, and F. Rusnak. "The Transition State of the Phosphoryl Transfer Reaction Catalyzed by the Lambda Ser/Thr Protein Phosphatase," 16th Enzyme Mechanisms Conference, January 6 - 10, 1999, Napa, CA.

18. J. Rawlings, A. C. Hengge and W. W. Cleland. "Co(III) and Zn(II) Catalyzed Hydrolysis of Phosphodiesters". 217th American Chemical Society National Meeting, March 21-25, 1999, Anaheim, CA.

19. F. Rusnak, R. H. Hoff*, P. Mertz and A. C. Hengge. "The Transition State of the Reaction Catalyzed by Bacteriophage λ Protein Phosphatase," International Conference on Biological Inorganic Chemistry, July 11-16, 1999, Minneapolis, Minnesota.

20. A. C. Hengge, R. H. Hoff*, Wu, L., Zhou, B. and Z.-Y. Zhang. "The Role of the Active Site Arginine in a Protein-Tyrosine Phosphatase. Does Positive Charge Cause a Change in Mechanism for Enzymatic Phosphoryl Transfer?" Gordon Conference on Enzymes, Coenzymes and Metabolic Pathways, July 11-16, 1999, Meriden, New Hampshire.

21. P. Mertz, R. H.Hoff*, F. Rusnak and A. C. Hengge. "A Model for the Catalytic Mechanism of the Metallophosphatases Calcineurin and λ Protein Phosphatase: Studies from Mutants Lacking an Active Site Histidine," Thirteenth Symposium of the Protein Society, July 24-28, 1999, Boston, MA.

22. P. Grzyska, P. Czyryca, R. Hoff*, K. Small[#], and A. C. Hengge. "Medium Effects in Phosphoryl Transfer Reactions: Information from Isotope Effects, Theoretical Studies, Kinetics, and Thermodynamics," Gordon Conference on Isotopes in Biological and Chemical Sciences, January 9-14, 2000, Ventura, CA

23. R. Hoff* and A. C. Hengge. "Does the Transition State for Sulfuryl Transfer Resemble That for Phosphoryl Transfer?," Gordon Conference on Isotopes in Biological and Chemical Sciences, January 9-14, 2000, Ventura, CA

24. P. Grzyska, P. Czyryca, J. Golightly[#], K. Small[#], P. Larsen[#], R. H. Hoff*, and A. C. Hengge. "Medium Effects on Phosphoryl Transfer Reactions and Their Possible Applicability to Enzymatic Phosphoryl Transfer," 222nd National Meeting of the ACS, August 26-30, 2001, Chicago, IL.

25. T. Humphry*, M. Forconi, A. C. Hengge, and N. H. Williams "Mechanism of Reaction of Phosphate Esters Coordinated to a Model of Dinuclear Metallophosphatases," 222nd National Meeting of the

ACS, August 26-30, 2001, Chicago, IL.

26. P. G. Czyryca and A. C. Hengge "A Novel Motif for the Design of Transition State Analogs for Phosphatases," 222nd National Meeting of the ACS, August 26-30, 2001, Chicago, IL.

27. P. G. Czyryca and A. C. Hengge "Kinetic Isotope Effect Studies of the Phosphoryl Transfer Reaction," Gordon Conference on Isotopes in Biological and Chemical Sciences , February 17-22, 2002, Ventura, CA

28. T. Humphry*, M. Forconi, N. H. Williams and A. C. Hengge "Mechanism of Reaction of Phosphate Esters Coordinated to a Model of Dinuclear Metallophosphatases," Gordon Conference on Isotopes in Biological and Chemical Sciences , February 17-22, 2002, Ventura, CA

29. J. Younker# and A.C. Hengge "Mechanistic Study of Aryl Aryl Sulfate Diesters" National Conference on Undergraduate Research, University of Utah, March 13-15, 2003.

30. P. G. Czyryca, J. Younker#, S. Iyer* and A. C. Hengge "Phosphonoethers: Analogs of the Phosphoryl Transfer Transition State," Structure-Based Drug Design 2003, Boston MA, April 28-29, 2003.

31. P. G. Czyryca and A. C. Hengge "HyperChem™ as a Programming Environment for De Novo Methodology" Structure-Based Drug Design 2003, Boston MA, April 28-29, 2003.

32. A. C. Hengge, T. Humphry*, M. Forconi, and N. H. Williams "Altered Hydrolysis Mechanisms for a Metal-Complexed Phosphate Monoester and Diester." International Isotope Effects Conference, Uppsala. Sweden, June 22-27, 2003.

33. I. Onyido, K. Swierczek, and A. C. Hengge "The Transition State for Thiophosporyl Transfer from Aryl Dimethylphosphinothioates to Oxygen Nucleophiles in Aqueous Solution" 39th IUPAC Congress and 86th Conference of The Canadian Society for Chemistry, Ottawa, Canada, August 10-15, 2003.

34. S.S. Iyer*, J. M. Younker, # P. G. Czyryca, A. C. Hengge. "Synthesis and evaluation of aryloxymethyl and aryloxyethyl phosphonates as inhibitors of phosphatases" 226th ACS National Meeting, September 7-11, 2003, New York, NY.

35. K. J. Swierczek, A. C. Hengge "Comparison of phosphonothioic acids with phosphonic acids as inhibitors of phosphatases," 226th ACS National Meeting, September 7-11, 2003, New York, NY.

36. J. Purcell# and A. C. Hengge "Mechanistic studies of phosphoryl and thiophosphoryl group transfer," 226th ACS National Meeting, September 7-11, 2003, New York, NY.

37. T. Humphry*, M. Forconi, N. H. Williams, A. C. Hengge "Alteration of the mechanisms of phosphate ester hydrolysis by complexation to a dinuclear metal center" 226th ACS National Meeting, September 7-11, 2003, New York, NY.

38. J. M. Younker# and A. C. Hengge "Mechanistic study of aryl aryl sulfate diesters" 226th ACS National Meeting, September 7-11, 2003, New York, NY.

39. J. M. Younker#, S.S. Iyer*, P. G. Czyryca, and A. C. Hengge "Aryloxymethano- and Aryloxyethano-Phosphonic Acids and Their Analogues as Motifs for Inhibition of Phosphatases."

Undergraduate Research Day at the State Capitol, Utah State Capitol, January 22, 2004.

40. J. Purcell[#] and A. C. Hengge "Mechanistic studies of phosphoryl and thiophosphoryl group transfer," Undergraduate Research Day at the State Capitol, Utah State Capitol, January 22, 2004.

41. K. Sorensen-Stowell* and A. C. Hengge "Use of ^{18}O Isotopic Shifts in ^{31}P NMR for Determination of P-O Bond Order of Various Phosphate Esters in Water," Gordon Conference on Isotopes in Biological and Chemical Sciences , February 15-20, 2004, Ventura, CA.

42. J. Purcell[#] and A. C. Hengge "Kinetic and Spectroscopic Investigations of Phosphate and Thiophosphate Esters" Joint 59th Northwest and 18th Rocky Mountain Regional Meeting of the American Chemical Society, June 6-9, 2004, Logan UT.

43. K. Sorensen-Stowell* and A. C. Hengge "Use of ^{18}O Isotopic Shifts in ^{31}P NMR for Determination of P-O Bond Order of Various Phosphate Esters in Water" Joint 59th Northwest and 18th Rocky Mountain Regional Meeting of the American Chemical Society, June 6-9, 2004, Logan UT.

44. J. M. Younker[#] and A. C. Hengge "Mechanistic Study of Aryl Aryl Sulfate Diesters" Joint 59th Northwest and 18th Rocky Mountain Regional Meeting of the American Chemical Society, June 6-9, 2004, Logan UT.

45. K. Sorensen-Stowell* and A. C. Hengge. "Use of ^{18}O isotope Shifts on ^{31}P NMR to Probe Potential Medium Effects on Phosphate Ester Bond Strengths." 229th ACS National Meeting, in San Diego, CA, March 13-17, 2005

46. A. C. Hengge, T. Humphry*, J. Morrow and J. Richards. "The Effect of Metal Ions on Phosphoryl Transfer Reactions," Isotopes 2005 Conference, June 27 – July 1, 2005, Bath, UK.

47. Robynn Cox* and Alvan C. Hengge. "Kinetic Isotope Effects on the Reactions of Purple Acid Phosphatases," Gordon Conference on Isotopes in Biological and Chemical Sciences, Ventura, CA, February 12-17, 2006

48. Subashree Iyer* and Alvan C. Hengge. "Effect of thio-substitution on the mechanisms of transesterification of ribonucleoside phosphodiester models" 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007.

49. Elizabeth A. Lund[#], Alvan C. Hengge, Nicholas H. Williams, Claire McWhirter, and Guoqiang Feng. "Mechanistic study of PP-1, a catalytically promiscuous enzyme," 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007.

50. N. Mitić, R. S. Cox*, M. Lanznaster, L. R. Gahan, A. Neves, A. C. Hengge, and G. Schenk**,** "The catalytic mechanism of purple acid phosphatases." *ICBIC 13*, Vienna, Austria, 2007.

51. Eric A. Tanifum, Alvan C. Hengge, Elizabeth A. Lund[#], Nicholas H. Williams, Guoqiang Feng, and Claire McWhirter. "Comparative mechanistic studies on the catalytically promiscuous serine/threonine protein phosphatase-1 (PP-1) and the dinuclear cobalt(III) complex $[Co_2(tacn)_2(OH)_3](ClO_4)_3$." 234th American Chemical Society National Meeting, Boston, MA, August 19-23, 2007.

52. Sara A. Huefner[#] and Alvan C. Hengge. "Mutations of critical amino acids in the human enzyme PTP1B." Research on Capitol Hill, Utah State Capitol, January 24, 2008.

53. Alvan C. Hengge, Tiago A. Brandao, Sara A. Huefner[#] and Sean J. Johnson "Differential Mutational Effects on Conformational Changes During Catalysis by Protein-Tyrosine Phosphatases." Gordon Conference on Isotopes in Biological and Chemical Sciences, Ventura, CA, February 17-22, 2008.

54. Sara A. Huefner[#], Tiago A. Brandão, Sean J. Johnson, and Alvan C. Hengge. "Protein-Tyrosine Phosphatases: Comparing the Effects of Mutation on Protein Conformation and Catalysis." Joint 63rd Northwest/21st Rocky Mountain American Chemical Society Conference, Park City, UT, June 15-18, 2008.

55. Sara A. Huefner[#], Tiago A. Brandão, Sean J. Johnson, and Alvan C. Hengge. "Protein-Tyrosine Phosphatases: Comparing the Effects of Mutation on Protein Conformation and Catalysis." 236th American Chemical Society National Meeting, Philadelphia, PA, Aug. 17-21 2008.

56. Ryan D. Berry[#], Sara A. Huefner[#], Tiago A. S. Brandão, and Alvan C. Hengge. "Analogous Mutations in Two PTP Enzymes Cause Differential Adverse Effects on Catalysis." Utah Conference on Undergraduate Research (UCUR), Westminster College, Salt Lake City, UT, February 20, 2009.

57. Vyacheslav I. Kuznetsov* and Alvan C. Hengge. "Kinetic studies of the dual-specificity phosphatase VHZ." Spring 2010 National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010. Division of Biological Chemistry, abstract #93.

58. Yuan Chu*, Nicholas H. Williams and Alvan C. Hengge. "Mechanistic study of phosphoryl transfer reactions catalyzed by protein phosphatase-1." Spring 2010 National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010. Division of Biological Chemistry, abstract #92.

59. Ryan D. Berry[#], Kelsey V. Klemm[#], and Alvan C. Hengge. "Elucidation of promiscuous catalytic activity of pseudomonas aeruginosa sulfatase." National Conference on Undergraduate Research, Ithaca, NY, March 31 – April 2, 2011.

60. Kelsey Klemm[#], J. Tyler Gish[#], Emily Measom[#], and Alvan C. Hengge. "Production of the Industrial Feedstock Chemical HMF From Algae." National Conference on Undergraduate Research, Ogden, UT, March 29 – 31, 2012.

61. Yuan Chu*, Nicholas H. Williams, and Alvan C. Hengge. "A simple Arg to Lys mutant of protein phosphatase 1 exhibits catalytic efficiencies toward monoanionic substrates superior to wild type." Annual Meeting of the American Society for Biochemistry and Molecular Biology, San Diego, CA, April 21-25, 2012.

62. Vyacheslav I. Kuznetsov*, Sean J. Johnson, and Alvan C. Hengge. "High resolution structure of the phosphatase VHZ explains unexpected substrate specificity, and suggests the presence of metavanadate at the active site." Annual Meeting of the American Society for Biochemistry and Molecular Biology, San Diego, CA, April 21-25, 2012.

63. Mark P. Haney* and Alvan C. Hengge. "The phosphoramidase competency of prototypical phosphatase motifs." Annual Meeting of the American Society for Biochemistry and Molecular Biology, San Diego, CA, April 21-25, 2012.

64. Sean S. Whittier, Alvan C. Hengge, and J. Patrick Loria. "Coupling of Loop Closure and Chemistry in Protein Tyrosine Phosphatases." 57th Annual meeting of the Biophysical Society, Philadelphia,

PA, February 2-6, 2013. Abstract published in the Biophysical Journal, **104**, *2*, Supplement 1, p 30a.

PEER-REVIEWED JOURNAL ARTICLES
The name(s) of corresponding author(s) are underlined.

1. R. M. Wilson and A. C. Hengge. "The Chemistry of an Azomethine Imine Derived From 2,3-Dimethylindole and *N*-Phenyl Triazolinedione: A New and Facile Condensation Method." *Tetrahedron Letters*. **1985**, *26*, 3673-3676.

2. R. M. Wilson and A. C. Hengge. "Nucleophilic Additions to Triazolinedione Ylides, Extremely Reactive Carbonyl Equivalents: A New Class of Condensation Reactions." *Journal of Organic Chemistry*, **1987,** *52*, 2699-2707.

3. R. M. Wilson, A. C. Hengge, A. Ataei, N. Chantarasiri. "Addition of 4- Phenyltriazolinedione to Carbonyl Compounds: The Formation of alpha-Urazolylcarbonyl Compounds." *J. Org. Chem.*, **1990,** *55*, 193-197.

4. R. M. Wilson, A. C. Hengge. "Synthesis and Chemistry of Acyltriazolinedione Ylides and Related Intermediates: New Methods for the Preparation of Di- and Tricarbonyl Compounds." *J. Org. Chem.*, **1990,** *55*, 197-202.

5. A. C. Hengge and W. W. Cleland. "Direct Measurement of Transition State Bond Cleavage in Hydrolysis of Phosphate Esters of *p*-Nitrophenol." *J. Am. Chem. Soc.* **1990,** *112*, 7421-7422.

6. A. C. Hengge and W. W. Cleland. "Mechanism of Phosphodiester Cleavage with β–Cyclodextrin.**"** *J. Org. Chem.* **1991,** *56*, 1972-1974.

7. A. C. Hengge and W. W. Cleland. "Phosphoryl Transfer Reactions of Phosphodiesters: Characterization of Transition States by Heavy Atom Isotope Effects." *J. Am. Chem. Soc.* **1991,** *113*, 5835-5841.

8. R. M. Wilson, A. C. Hengge, A. Ataei, D. M. Ho. "The Oxidative Alpha-Coupling of Carbonyl Compounds Via the Condensation of Acylated Triazolinedione (PTAD) Ylides With Enolates: A Facile Synthesis of Polyacylated Olefins," *J. Am. Chem. Soc.,* **1991,** *113*, 7240-7249.

9. A. C. Hengge. "Oxygen-18 Exchange in Nitrophenols: Significance for Labeling and Isotope Effect Experiments." *J. Am. Chem. Soc.***1991,** *113*, 2747-2748.

10 A. C. Hengge. "Can Acyl Transfer Occur by a Concerted Mechanism? Direct Evidence from Heavy Atom Isotope Effects." *J. Am. Chem. Soc.***1992,** *114*, 6575-6576.

11. A. C. Hengge, W.A. Edens, H. Elsing. "Transition-State Structures for Phosphoryl- Transfer Reactions of *p*-Nitrophenyl Phosphate." *J. Am. Chem. Soc.***1994,** *116*, 5045-5049.

12. A. C. Hengge, R.A. Hess. "Concerted or Stepwise Mechanisms for Acyl Transfer Reactions of *p*-Nitrophenyl Acetate? Transition State Structures from Isotope Effects." *J. Am. Chem. Soc.***1995,** *116*, 11256-11263.

13. A. C. Hengge, A.E. Tobin, W. W. Cleland. "Studies of Transition-State Structures in Phosphoryl Transfer Reactions of Phosphodiesters of *p*-Nitrophenol." *J. Am. Chem. Soc.* **1995,** *117*, 59159-5926.

14. A. C. Hengge, G.A. Sowa, L. Wu, Z.-Y. Zhang. "The Nature of the Transition State of the Protein-

Tyrosine Phosphatase-Catalyzed Reaction." *Biochemistry*, **1995,** *34*, 13982-13987. PMID: 7577995.

15. W. W. Cleland and A. C. Hengge. "Mechanisms of Phosphoryl and Acyl Transfer." *The FASEB Journal*, **1995,** *9*, 1585-1594. PMID: 8529838.

16. K. A. Deal, A. C. Hengge, J. N. Burstyn. "Characterization of Transition States in Dichloro (1,4,7-Triazacyclononane) Copper (II)-Catalyzed Activated Phosphate Diester Hydrolysis." *J. Am. Chem. Soc,* **1996,** *118*, 1713-1718.

.

17. A. C. Hengge, J. M. Denu, J. E. Dixon. "Transition-State Structures for the Native Dual-Specific Phosphatase VHR and D92N and S131A Mutants, Contributions to the Driving Force for Catalysis." *Biochemistry*, **1996,** *35*, 7084-7092. PMID: 8679534.

18. J. Rawlings, A. C. Hengge, and W. W. Cleland. "Heavy-Atom Isotope Effects on Reactions of Co(III)-Bound *p*-Nitrophenyl Phosphate: Nucleophilic Displacements of *p*-Nitrophenol and Dissociation of *p*-Nitrophenyl Phosphate." *J. Am. Chem. Soc.***1997,** *119,* 542-549.

19. G. A. Sowa, A.C. Hengge, and W. W. Cleland. "O-18 Isotope Effects Support a Concerted Mechanism for Ribonuclease A." *J. Am. Chem. Soc.***1997,** *119*. 2319-2320.

20. A. C. Hengge, Y. Zhao, L. Wu, Z.-Y. Zhang. "Examination of the Transition State of the Low-Molecular Mass Small Tyrosine Phosphatase 1. Comparisons with Other Protein Phosphatases." *Biochemistry*, **1997,** *36*, 7928-7936. PMID: 9201938.

21. R. A. Hess, A. C. Hengge, W. W. Cleland. "Kinetic Isotope Effects for Acyl Transfer from *p*-Nitrophenyl Acetate to Hydroxylamine Show a pH-Dependent Change in Mechanism." *J. Am. Chem. Soc* **1997,** *119*, 6980-6983.

22. A. C. Hengge and B. L. Martin. "Isotope Effect Studies on the Calcineurin Phosphoryl- Transfer Reaction: Transition State Structure and Effect of Calmodulin and Mn+2," *Biochemistry*, **1997,** *36*, 10185-10191. PMID: 9254616.

23. R. H. Hoff and A. C. Hengge. "A Facile High-Yield Synthesis and Purification of Tetrabutylammonium Tetrabutylborate." *J. Org. Chem.*, **1998,** *63*, 195. PMID: 11674064.

24. R. A. Hess, A. C. Hengge, and W. W. Cleland. "Isotope Effects on Enzyme-Catalyzed Acyl Transfer from *p*-Nitrophenyl Acetate: Concerted Mechanisms and Increased Hyperconjugation in the Transition State." *J. Am. Chem. Soc* **1998,** *120*, 2703-2709.

25. R. H. Hoff and A. C. Hengge. "Entropy and Enthalpy Contributions to Solvent Effects on Phosphate Monoester Solvolysis. The Importance of Entropy Effects in the Dissociative Transition State," *J. Org. Chem.*, **1998,** *63*, 6680-6688.

26. B. L. Martin, L. A. Jurado and A. C. Hengge "Comparison of the Reaction Progress of Calcineurin with Mn^{2+} and Mg^{2+}." *Biochemistry*, **1999,** *38*, 3386 –3392. PMID: 10079083.

27. I. E. Catrina and A. C. Hengge. "Comparisons of Phosphorothioate and Phosphate Monoester Transfer Reactions: Activation Parameters, Solvent Effects, and the Effect of Metal Ions." *J. Am. Chem. Soc.***1999,** *121*, 2156-2163.

28. R. H. Hoff, P. Mertz, F. Rusnak, and A. C. Hengge "The Transition State of the Phosphoryl Transfer Reaction Catalyzed by the Lambda Ser/Thr Protein Phosphatase." *J. Am. Chem. Soc.,* **1999,** *121***,** 6382-6390.

29. R. H. Hoff, L. Wu, B. Zhou, Z.-Y. Zhang, and A. C. Hengge. "Does Positive Charge at the Active Sites of Phosphatases Cause a Change in Mechanism? The Effect of the Conserved Arginine on the Transition State for Phosphoryl Transfer In the Protein-tyrosine Phosphatase from *Yersinia.*" *J. Am. Chem. Soc.***1999,** *121***,** 9514-9521.

30. R. H. Hoff, A. C. Hengge, L. Wu, Y.-F. Keng, and Z.-Y. Zhang. "Effects on General Acid Catalysis from Mutations of the Invariant Tryptophan and Arginine Residues in the Protein Tyrosine Phosphatase from *Yersinia*." *Biochemistry*, **2000**, *39*, 46 –54. PMID: 10625478.

31. K. M. Holtz, I. E. Catrina, A. C. Hengge, and E. R. Kantrowitz. "Mutation of Arg-166 of Alkaline Phosphatase Alters the Thio Effect but Not the Transition State for Phosphoryl Transfer. Implications for the Interpretation of Thio Effects in Reactions of Phosphatases." *Biochemistry*, **2000**, *39*, 9451-9458. PMID: 10924140.

32. A. C. Hengge, K. S. Bruzik, A. E. Tobin, W. W. Cleland, and M. D. Tsai. "Kinetic isotope effects and stereochemical studies on a ribonuclease model: Hydrolysis reactions of uridine 3 '-p-nitrophenyl phosphate." *Bioorg.Chem.* **2000,** 28 (3):119-133. PMID: 10915550.

33. M. A. Rishavy, A. C. Hengge, and W. W. Cleland . " Lanthanide Catalyzed Cyclization of Uridine 3'-p-Nitrophenyl Phosphate." *Bioorg.Chem.* **2000,** 28, (5), 283-292. PMID: 11133147.

34. J. D. Rigas, R. H. Hoff, A. E. Rice, A. C. Hengge, J. M. Denu. "Transition state analysis and requirement of Asp-262 general acid/base catalyst for full activation of dual-specificity phosphatase MKP3 by extracellular regulated kinase." *Biochemistry* **2001** 40, 4398-4406. PMID: 11284696.

35. P. G. Czyryca, A. C. Hengge. "The mechanism of the phosphoryl transfer catalyzed by Yersinia protein-tyrosine phosphatase: a computational and isotope effect study." *Biochim Biophys Acta* **2001**, *1547*, 245-53. PMID: 11410280.

36. A. C. Hengge "Isotope effects in the study of enzymatic phosphoryl transfer reactions." *FEBS Letters* **2001** *501*, 99-102. (invited review) PMID: 11470264.

37. R. H. Hoff, P. Larsen, and A. C. Hengge. "Isotope Effects and Medium Effects on Sulfuryl Transfer Reactions." *J. Am. Chem. Soc.,* **2001**, *123*, 9338-9344. PMID: 11562216.

38. A. C. Hengge "Isotope Effects In the Study of Phosphoryl and Sulfuryl Transfer Reactions." *Accounts of Chemical Research*, **2002**; 35(2); 105-112. PMID: 11851388.

39. P. K. Grzyska, P. G. Czyryca, J. Golightly, K. Small, P. Larsen, R. H. Hoff, and A. C. Hengge. "Generality of Solvation Effects on the Hydrolysis Rates of Phosphate Monoesters, and Their Possible Relevance to Enzymatic Catalysis." *J. Org. Chem.*, **2002**; 67(4); 1214-1220. PMID: 11846665.

40. D. F. McCain, I. E. Catrina, A. C. Hengge and Z.-Y. Zhang "The catalytic mechanism of Cdc25A phosphatase." *J. Biol. Chem*., **2002**, 277: 11190-11200. PMID: 11805096.

41. I. E. Catrina, P. G. Czyryca, and A. C. Hengge "Isotope effects on enzymatic and nonenzymatic reactions of phosphorothioates." *Nukleonika*, **2002**; 47 (Supplement 1); S17-S23.

42. T. Humphry, M. Forconi, N. H. Williams and A. C. Hengge "An Altered Mechanism of Hydrolysis for a Metal-Complexed Phosphate Diester." *J. Am. Chem. Soc.,* **2002**, *124*, 14860-14861. PMID: 12475323.

43. K. Swierczek, J. Peters and A. C. Hengge "A convenient synthesis of phosphonothioic acids." *Tetrahedron*, **2003**, *59/5,* 595 – 599.

44. J. Rawlings, W. W. Cleland and A. C. Hengge "Metal ion catalyzed hydrolysis of ethyl *p*-nitrophenyl phosphate." *Journal of Inorganic Biochemistry*, **2002**, *93*, (1-2), 61-65. PMID: 12538053.

45. I. E. Catrina and A. C. Hengge "Comparisons of Phosphorothioate with Phosphate Transfer Reactions for a Monoester, Diester and Triester: Isotope Effect Studies." *J. Am. Chem. Soc.,* **2003,** *125*, 7546-7552. PMID: 12812494.

46. K. Swierczek, A. S. Pandey, J. Peters and A. C. Hengge "A Comparison of Phosphonothioic Acids with Phosphonic Acids as Phosphatase Inhibitors." *J. Med. Chem.,* **2003**, *46*, 3703-3708. PMID: 12904075.

47. P. K. Grzyska, P. G. Czyryca, J. Purcell, and A. C. Hengge "Transition State Differences in Hydrolysis Reactions of Alkyl versus Aryl Phosphate Monoester Monoanions." *J. Am. Chem. Soc.,* **2003,** *125*, 13106-13111. PMID: 14570483.

48. S. G. Gibby, J. M. Younker, and A. C. Hengge "An Investigation of the Sulfuryl Transfer Step from Substrate to Enzyme by Aryl Sulfatases." *Journal of Physical Organic Chemistry,* **2004**, *17 (6-7),* 541-547; invited paper, special issue dedicated to William P. Jencks.

49. A. C. Hengge and Ross L. Stein "Role of Protein Conformational Mobility in Enzyme Catalysis - Acylation of α-Chymotrypsin by Specific Peptide Substrates", *Biochemistry.* **2004**; 43(3); 742-747. PMID: 14730979.

50. P. K. Grzyska, Y. Kim, M. D. Jackson, A. C. Hengge, and J. M. Denu, "Probing the Transition-State Structure of Dual-Specificity Protein Phosphatases Using a Physiological Substrate Mimic" *Biochemistry* **2004,** *43,* 8807-8814. PMID: 15236589.

51. D. F. McCain, P. K. Grzyska, L. Wu, A. C. Hengge, and Z.-Y. Zhang "Mechanistic Studies of Protein Tyrosine Phosphatases YopH and Cdc25A with *m*-Nitrobenzyl Phosphate" *Biochemistry* **2004,** *43,* 8256-8264. PMID: 15209522.

52. T. Humphry, M. Forconi, N. H. Williams and A. C. Hengge "Altered mechanisms of reactions of phosphate esters bridging a dinuclear metal center" *J. Am. Chem. Soc.,* **2004**, 126, 11864-11869. PMID: 15382921.

53. S. Iyer, J. M. Younker, P. G. Czyryca, and A. C. Hengge "A nonhydrolyzable analogue of phosphotyrosine, and related aryloxymethano- and aryloxyethano- phosphonic acids as motifs for inhibition of phosphatases" *Bioorganic & Medicinal Chemistry Letters*, **2004**, Vol 14/23 pp 5931-5935. PMID: 15501071.

54. J. M. Younker and A. C. Hengge "A Mechanistic Study of the Alkaline Hydrolysis of Diaryl Sulfate Diesters." *J. Org. Chem.* **2004**, 69(26) 9043-9048. PMID: 15609936.

55. A. C. Hengge and I. Onyido "Physical Organic Perspectives on Phospho Group Transfer from Phosphates and Phosphinates." *Curr. Org. Chem*. **2005**, *9*, 61-74.

56. I. Onyido, K. Swierczek, J. Purcell, and A. C. Hengge "A Concerted Mechanism for the Transfer of the Thiophosphinoyl Group from Aryl Dimethylphosphinothioate Esters to Oxyanionic Nucleophiles in Aqueous Solution." *J. Am. Chem. Soc.*, **2005**, 127(21); 7703-7711. PMID: 15913360.

57. K. Sorensen-Stowell and A. C. Hengge "Examination of P-OR Bridging Bond Orders in Phosphate Monoesters using ^{18}O Isotope Shifts in ^{31}P NMR." *J. Org. Chem.*, **2005**, 70 (12), 4805-4809. PMID: 15932321.

58. K. Sorensen-Stowell and A. C. Hengge "Probing Potential Medium Effects on Phosphate Ester Bonds Using ^{18}O Isotope Shifts on 31P NMR." *J. Org. Chem.*, **2005**, 70 (21): 8303-8308. PMID: 16209571.

59. J. Purcell and A. C. Hengge "The Thermodynamics of Phosphate versus Phosphorothioate Ester Hydrolysis." *J. Org. Chem.*, **2005**, 70 (21): 8437-8442. PMID: 16209589.

60. A. C. Hengge . "Mechanistic Studies on Enzyme-Catalyzed Phosphoryl Transfer." *Advances in Physical Organic Chemistry*, **2005**, 40: 49-108.

61. Y. Liu, B. A. Gregersen, A. C. Hengge and D. M. York. "Transesterification Thio Effects of Phosphate Diesters: Free Energy Barriers and Kinetic and Equilibrium Isotope Effects from Density-Functional Theory." *Biochemistry;***2006**; *45*(33); 10043-10053. PMID: 16906762.

62. K. Sorensen-Stowell and A. C. Hengge . "Thermodynamic Origin of the Increased Rate of Hydrolysis of Phosphate and Phosphorothioate Esters in DMSO/Water Mixtures." *J. Org. Chem.;* **2006**; *71*(19); 7180-7184. PMID: 16958510.

63. R. H. Hoff, P, G. Czyryca, M. Sun, T. S. Leyh, and A. C. Hengge. "The Transition State of the Sulfuryl Transfer Reaction of Estrogen Sulfotransferase." *Journal of Biological Chemistry,* **2006**, *281*, 30645-30649. PMID: 16899461.

64. W. W. Cleland and A. C. Hengge. **"**Enzymatic Mechanisms of Phosphate and Sulfate Transfer." *Chemical Reviews;* **2006**; *106*(8); 3252-3278. PMID: 16895327.

65. J. Rawlings, W. W. Cleland and A. C. Hengge. "Metal-Catalyzed Phosphodiester Cleavage: Secondary ^{18}O Isotope Effects as an Indicator of Mechanism." *J. Am. Chem. Soc.* **2006**; *128*(51); 17120-17125. PMID: 17177465.

66. Freeman M. Wong, Jianbo Wang, Alvan C. Hengge, and Weiming Wu "Mechanism of Rhodium-Catalyzed Carbene Formation from Diazo Compounds." *Org. Lett.;* **2007**; *9*(9); 1663-1665.

67. Irina Catrina, Patrick J. O'Brien, Jamie Purcell, Ivana Nikolic-Hughes, Jesse G. Zalatan, Alvan C. Hengge and Daniel Herschlag. "Probing the Origin of the Compromised Catalysis of *E. coli*

Alkaline Phosphatase in its Promiscuous Sulfatase Reaction." *J. Am. Chem. Soc.* **2007**; *129*(17); 5760-5765. PMID: 17411045.

68. R. S. Cox, G. Schenk, N. Mitic, L. Gahan and A. C. Hengge. "Diesterase Activity and Substrate Binding in Purple Acid Phosphatases." *J. Am. Chem. Soc*.; **2007**; *129* (31), 9550-9551. PMID: 17636903.

69. J. G. Zalatan, I. Catrina, R. Mitchell, P. K. Grzyska, P. J. O'Brien, D. Herschlag, and A. C, Hengge. "Kinetic Isotope Effects for Alkaline Phosphatase Reactions: Implications for the Role of Active-Site Metal Ions in Catalysis," *J. Am. Chem. Soc*. **2007**; *129* (31), 9789-9796. PMID: 17630738.

70. R. H. Hoff and A. C. Hengge. "The Use of Isotopes in the Study of Reactions of Acyl, Phosphoryl, and Sulfuryl Esters," Journal of Labelled Compounds and Radiopharmaceuticals, **2007;** *50*, 1026-1038.

71. Subashree Iyer and Alvan C. Hengge. "The Effects of Sulfur Substitution for the Nucleophile and Bridging Oxygen Atoms in Reactions of Hydroxyalkyl Phosphate Esters." *J. Org. Chem.*, **2008**; *73*(13), 4819-29. DOI: 10.1021/jo8002198. PMID: 18533704.

72. C. McWhirter, E. A. Lund, E. A. Tanifum, G. Feng, Q. L. Sheikh, A. C. Hengge, and N. H. Williams "Mechanistic Study of Protein Phosphatase-1 (PP1), A Catalytically Promiscuous Enzyme," *J. Am. Chem. Soc*. **2008**; *130*(41), 13673-13682. DOI: 10.1021/ja803612z. PMID: 18798625.

73. K. S. Hadler, E. A. Tanifum, S. H.-C. Yip, N. Mitić, L. W. Guddat, C. J. Jackson, L. R. Gahan, K. Nguyen, P. D. Carr, D. L. Ollis, A. C. Hengge, J. A. Larrabee, G. Schenk. "Substrate-Promoted Formation of a Catalytically Competent Binuclear Center and Regulation of Reactivity in a Glycerophosphodiesterase from Enterobacter aerogenes" *J. Am. Chem. Soc*. **2008**; *130 (41),* 14129-14138. DOI: 10.1021/ja803346w. PMID: 18831553.

74. Alvan C. Hengge. NMR Data do not Implicate a Phosphorane in the T4 Ligase Reaction. Proc. Natl. Acad. Sci. U S A. 2008 Nov 18;105(46):E84; author reply E85. doi: 10.1073/pnas.0806371105. PMID: 19004796.

75. T. Humphry, S. Iyer, O. Iranzo, J. R. Morrow, J. P. Richard, Piotr Paneth, and A. C. Hengge. "An Altered Transition State for the Reaction of an RNA Model Catalyzed by a Dinuclear Zinc(II) Catalyst" *J. Am. Chem. Soc*. **2008,** *130 (52),* 17858–17866**.** DOI: 10.1021/ja8059864. PMID: 19053445.

76. T. A. S. Brandão, H. Robinson, S. J. Johnson, and A. C. Hengge. "Impaired acid catalysis by mutation of a protein loop hinge residue in a YopH mutant revealed by crystal structures" *J. Am. Chem. Soc*. **2009,** *131 (2),* 778-786. DOI: 10.1021/ja807418b. PMID: 19140798.

77. Guoqiang Feng, Eric A. Tanifum, Harry Adams, Alvan C. Hengge and Nicholas H. Williams. "Mechanism and Transition State Structure of Aryl Methylphosphonate Esters Doubly Coordinated to a Dinuclear Cobalt(III) Center" *J. Am. Chem. Soc*. **2009,** *131 (35),* 12771-12779 . DOI: 10.1021/ja904134n. PMID: 19673521.

78. Gregory K. Smith, Zhihong Ke, Alvan C. Hengge, Dingguo Xu, Daiqian Xie and Hua Guo. "Active-Site Dynamics of SpvC Virulence Factor from *Salmonella typhimurium* and Density Functional Theory Study of Phosphothreonine Lyase Catalysis" *J. Phys. Chem. B*, **2009**, 113 (46),

15327–15333. DOI: 10.1021/jp9052677. PMID: 19715325.

79. Tiago A. S. Brandao, Alvan C. Hengge, and Sean J. Johnson. "Insights into the Reaction of Protein-tyrosine Phosphatase 1B: Crystal Structures for Transition State Analogs of Both Catalytic Steps." *J. Biol. Chem.* **2010**, *285 (21)*, 15874-15883. DOI: 10.1074/jbc.M109.066951. PMID: 20236928.

80. Natasa Mitic, Kieran S. Hadler, Lawrence R. Gahan, Alvan C. Hengge and Gerhard Schenk. "The Divalent Metal Ion in the Active Site of Uteroferrin Modulates Substrate Binding and Catalysis." *J. Am. Chem. Soc*. **2010**, 132 (*20*), pp 7049–7054. DOI: 10.1021/ja910583y. PMID: 20433174.

81. Gregory K. Smith, Zhihong Ke, Hua Guo, and Alvan C. Hengge. **"**Insights into the Phosphoryl Transfer Mechanism of Cyclin-Dependent Protein Kinases from ab Initio QM/MM Free-Energy Studies." *J. Phys. Chem. B*, **2011,** 115 (46), 13713-13722. PMID: 21999515.

82. Tiago A. S. Brandao, Alvan C. Hengge, and Sean J. Johnson. "The molecular details of WPD-loop movement differ in the protein-tyrosine phosphatases YopH and PTP1B." *Archives of Biochemistry and Biophysics* **2012**, 525, 53-59. DOI: 10.1016/j.abb.2012.06.002. PMID: 22698963.

83. Vyacheslav I. Kuznetsov, Anastassia N. Alexandrova, and Alvan C. Hengge. "Metavanadate at the Active Site of the Phosphatase VHZ." *J. Am. Chem. Soc.*, **2012**, *134* (35), 14298–14301. DOI: 10.1021/ja305579h. PMID: 22876963

84. Vyacheslav I. Kuznetsov, Alvan C. Hengge, and Sean J. Johnson. "New aspects of the phosphatase VHZ revealed by a high-resolution structure with vanadate and substrate screening." *Biochemistry*, **2012**, *51*, 9869-9879. DOI: 10.1021/bi300908y. PMID: 23145819

85. Alvan C. Hengge. "Chemistry and mechanism of phosphatases, diesterases and triesterases." Biochim. Biophys. Acta. **2013**, 1834(1):415-6. DOI: 10.1016/j.bbapap.2012.09.013. PMID: 23267546.

INVITED BOOK CHAPTERS AND RELATED MATERIALS:

1. "Transfer of the PO_3^{2-} Group," Alvan C. Hengge. In *Comprehensive Biological Catalysis: a Mechanistic Reference;* Sinnott, M., Ed., Academic Press, San Diego, CA, 1998; Chapter 14, Vol. 1, pp. 517-542.

2. "Insights from Heavy-Atom Isotope Effects on Phosphoryl and Thiophosphoryl Transfer Reactions," Alvan C. Hengge. In *Enzymatic Mechanisms*; Frey, P. A. and Northrop, D. B., Eds.; IOS Press, Amsterdam, The Netherlands, 1999; pp. 72-84.

3. "Phosphatases," Alvan C. Hengge. In *Encyclopedia of Catalysis*; Istvan Horvath, Editor In Chief; John Wiley & Sons, New Jersey, 2003; Volume 5, pp. 565-577.

4. "Kinases," Alvan C. Hengge. In *Encyclopedia of Catalysis*; Istvan Horvath, Editor In Chief; John Wiley & Sons, New Jersey, 2003; Volume 4, pp. 386-395.

5. "Phosphoryl Transfer Reactions," Alvan C. Hengge. In: *Encyclopedia of Life Sciences*. London: Nature Publishing Group. [doi: 10.1038/npg.els.0000608] http://www.els.net/

6. "Secondary Isotope Effects," Alvan C. Hengge. In *Isotope Effects in Chemistry and Biology*, Amnon Kohen and Hans-Heinrich Limbach, Editors. CRC Press, 2005. Chapter 39, pp. 955-974.

7. "Phosphoryl and Sulfuryl Transfer," Tiago A.S. Brandao and Alvan C. Hengge. In *Comprehensive Natural Products II: Chemistry and Biology*; Mander, L., Lui, H.-W., Eds.; Elsevier: Oxford, 2010; volume 8, pp.315–348

8. "Phosphatases," Yuan Chu and Alvan C. Hengge. In the *Encyclopedia of Catalysis, Second Edition*, John Wiley & Sons, New Jersey, 2011.

9. Guest Editor of special section entitled, "Chemistry and Mechanism of Phosphatases, Diesterases and Triesterases" in Biochimica et Biophysica Acta, Volume 1834, Issue 1, pages 415 – 478, January 2013.