Curriculum Vitae

KATHRYN A. THOMASSON

EDUCATIONAL BACKGROUND

Ph.D. Physical Chemistry May 1990
Iowa State University, Ames, IA
Ph.D. Thesis: Proline Side Chain Effects on Theoretical π-π^* Absorption and Circular Dichroic Spectra of Proline-containing Peptides
Advisor: Jon B. Applequist, (515)294-1157

B.A. Chemistry, Biology Minor May 1982
University of Virginia, Charlottesville, VA

PROFESSIONAL EXPERIENCE

Full Professor, July 2004; Associate Professor, Aug. 1999-2004; Assistant Professor: Chemistry, University of North Dakota, Grand Forks, ND, Aug. 1993 - July 1999.
Full Member of the Graduate Faculty, 1997
Associate Member of the Graduate Faculty, 1993

Dreyfus Postdoctoral Fellow Visiting Assistant Professor: Chemistry, Tennessee Technological University, Cookeville, TN, Aug. 1991 - 93.
Mentor: Scott H. Northrup, (931)-372-3421

Research Associate: Biosym Technologies Inc., San Diego, CA, 1990 - 91.

Graduate Research Assistant: Biochemistry & Biophysics, Iowa State University, Ames, IA, 1986-90.

Graduate Teaching Assistant: Chemistry, Iowa State University, Ames, IA, 1983-87; Molecular Cellular Developmental Biology, Iowa State University, Ames, IA, 1982-83.

Tutor: Iowa State University Tutoring Office, Ames, IA, 1985.

Laboratory Technician: Biochemistry, University of Virginia, Charlottesville, VA, 1982.

Grader: Mathematics, University of Virginia, Charlottesville, VA, 1981-82.

Ward Attendant: Woodworth Animal Hospital, Waynesboro, VA, 1980-81.

Lab Aide: Vivarium, University of Virginia Medical Center, Charlottesville, VA, 1978-80.

Substitute Latin Teacher: Western Albemarle High School, Crozet, VA, 1980.

TEACHING

A. Courses Taught at UND. Note: courses ≥ 500 denote graduate courses.

(i) Courses Taught After Promotion to Full Professor

Year	Term	Course No.	Title	Credits	Enrollment
2004	Fall	465	Physical Chemistry II	3	32
2005	Spring	466	Survey of Physical Chemistry	4	9
2005	Fall	465	Physical Chemistry II	3	22
2005	Fall	115L	Introductory Chemistry Laboratory	1	150
2006	Spring	466	Survey of Physical Chemistry	4	18
2006	Fall	465	Physical Chemistry II	3	21

(ii) Courses Taught After Promotion to Associate Professor

Year	Term	Course No.	Title	Credits	Enrollment
1999	Fall	464	Physical Chemistry I	3	28
1999	Fall	462	Physical Chemistry Laboratory	3	8
1999	Fall	467	Survey of Physical Chemistry Laboratory	2	3
2000	Spring	466	Survey of Physical Chemistry	4	8
2000	Fall	464	Physical Chemistry I	3	14
2000	Fall	462	Physical Chemistry Laboratory	3	11
2000	Fall	467	Survey of Physical Chemistry Laboratory	2	6
2001	Spring	466	Survey of Physical Chemistry	4	14
2001	Fall	462	Physical Chemistry Laboratory	3	5
2001	Fall	467	Survey of Physical Chemistry Laboratory	2	9
2002	Spring	466	Survey of Physical Chemistry	4	11
2002	Fall	465	Physical Chemistry II	3	18
2003	Spring	466	Survey of Physical Chemistry	4	16
2003	Fall	465	Physical Chemistry II	3	27
2004	Spring	466	Survey of Physical Chemistry	4	7

(iii) Courses Taught Prior to Promotion to Associate Professor

Year	Term	Course No.	Title	Credits	Enrollment
1993	Fall	151	Fundamental Concepts of Chemistry	3	57
1994	Spring	462	Physical Chemistry	2	12

			Laboratory		
1994	Fall	450	Physical Chemistry I	3	41
1994	Fall	539	Nonlinear Dynamics	1	3
1995	Spring	531	Chemical Dynamics	3	3
1995	Spring	462	Physical Chemistry Laboratory	2	13
1995	Fall	450	Physical Chemistry I	3	30
1995	Fall	509	Seminar	1	7
1996	Spring	462	Physical Chemistry Laboratory	2	10
1996	Spring	509	Seminar	1	2
1996	Fall	450	Physical Chemistry I	3	34
1997	Spring	107	Introduction to Organic and Biochemistry	4	107
1997	Spring	462	Physical Chemistry Laboratory	2	5
1997	Fall	450	Physical Chemistry I	3	38
1998	Spring	462	Physical Chemistry Laboratory	2	6
1998	Spring	107	Introduction to Organic and Biochemistry	4	95
1998	Fall	462	Physical Chemistry Laboratory	3	2
1999	Spring	107	Introduction to Organic and Biochemistry	4	101
1999	Spring	466	Survey of Physical Chemistry	4	4

B. Guest Lectured in the Following Courses

(i) Following Promotion to Associate Professor

(a) Graduate: Spring 2000, Chem 531: Chemical Dynamics
Spring 2002, Chem 531: Chemical Dynamics

(b) Undergrad: Spring 2003, Chem 464: Physical Chemistry I

(ii) Prior to Promotion to Associate Professor

(a) Graduate: Spring 1996, Biochem 530: Protein-Protein Interactions
Fall 1997, Chem 520: Advanced Organic Chemistry I

(b) Undergrad: Spring 1994-1999 Chem 388: Introduction to Research

C. Curriculum Development Activities:

(i) Physical Chemistry Laboratory:

(a) Following Promotion to Associate Professor

Developed a physical chemistry laboratory with an emphasis for the life sciences (1999-2000).

Developed a laboratory experiment in kinetics using a polarimeter (1999).

Developed a laboratory in enzyme kinetics (2000).

Developed a laboratory using semi-empirical quantum mechanics (2001).

(b) Prior to Promotion to Associate Professor

Developed a Raman laser experiment using a fluorimeter as a detector (1997).
Developed two experiments to teach statistics using absorption spectroscopy (1996).
Incorporated a greater variety of writing experiences in the Physical Chemistry lab (1995).
Developed an experiment in molecular modeling using INSIGHT/DISCOVER (1994).

(ii) Physical Chemistry Lecture:

(a) Following Promotion to Associate Professor

Created computational exercises for physical chemistry with emphasis for the life sciences (2003).

Created a computational recitation for solving kinetics problems with Mathematica (2002).

Created a computational recitation for solving quantum mechanical problems with Mathematica (1999-2000).

Developed a lecture physical chemistry course with an emphasis for the life sciences (1999-2000).

(b) Prior to Promotion to Associate Professor

Created a computational recitation for solving chemical thermodynamic problems with Mathematica (1996).

(iii) Other

(a) Following Promotion to Associate Professor

Ran a computational laboratory exercise for Chem 531 (Chemical Dynamics) 2000, 2002.

(b) Prior to Promotion to Associate Professor

Developed a computational laboratory exercise for Biochem 530 (Protein-Protein Interactions) 1996.

Developed a computational laboratory exercise for Chem 531 (Chemical Dynamics) 1997.

D. General Advisees (* after promotion to associate professor, †after promotion to full professor)

(i) Undergraduate:

Monica Francesconi	1994
Shawn Lee Jobe	1996
Nicholas Sheridan	1997
*Sarah Sundet	1999-03
*Erica Swanson	1999
*Christopher Dehen	2000-04
*Jessica Anderson	2000-01
*Todd Dupong	2002-04
*Stephanie Luithle	2002
*Shaine Lund	2003
*Shelia Nowatzki	2003
*Brieann Prommrehn	2003
*Jake Hager	2004-
†Sara Bush	2004-
†Lindsey Andrews	2004
†Christine Bentrup	2004
†Katy White Temple	2004-
†Kirsten M. Schneider	2005-
†Mitch S. Wahlsten	2005-
†Alex Thompson	2006-

(ii) Graduate:

Fan Yang	1997-99
*Felix Ngassa	1998-02
*Victor Waingeh	2001-2006
*Eric Njabon	2002-current
*Kristine Carlson	2002-current
*Neville Forlemu	2004-current

RESEARCH

A. Research Advised (* after promotion to associate professor, †after promotion to full professor)

(i) Postdoctoral Scholars (2)

Igor Ouporov (Ph.D. from Moscow State University, Moscow, Russia, 1982)
Jan. 1997- May 2000*

*†Stephen Lowe (Ph.D. from the University of Oregon, 1974)
Jan. 2000 - present

(ii) Graduate Students (6)

Fan Yang (B.S. Tsinghua University, Beijing, China, 1996) Jan. 1998-July 1999*, M.S. Thesis: "Brownian Dynamics of Nonspecific Protein-DNA Interactions".

*Felix Ngassa (B.S. University of Buea, Cameroon) Sept. 1998 - Dec. 2002
Ph.D. Thesis: "Synthetic and Computational Studies on Polycyclic Aromatic Hydrocarbon Derivatives, Nucleoside Analogs and Peptides".

*Victor Waingeh (B.S. University of Buea, Cameroon) Sept. 2001 - Ph.D. May 2006
Ph.D. Thesis: "Computer Simulations of Glyceraldehyde-3-Phosphate Dehydrogenase Interactions with Actin and Fructose-1,6-bisphosphate Aldolase, and Substrate Binding Dynamics"

*Kristine Carlson (B.S. U Minnesota - Morris) June 2002 - present
Ph.D. expected 2007

*Eric Njabon (B.S. University of Doula, Cameroon) Sept. 2002 - present
M.S. received 12/05. Ph.D. expected 2008
M.S. Thesis: "Brownian Dynamic Simulation of the Interaction Between Lactate Dehydrogenase (LDH) and G- or F-Actin"

*Neville Forlemu (B.S. University of Buea, Cameroon) Jan. 2004 - present
Ph.D. expected 2009

(iii) Visiting Scientists (3)

Ken Pierce (Ph.D. from UND, 1996 - now Assistant Professor of Chemistry at Dickinson State University) Summer 1997.

*Coretta Fernandes (MS from UND, 1997 - now Associate Professor of Chemistry at Lansing Community College, Lansing, MI) Summers 1999 & 2000.

*†Igor V. Ouporov, (Senior Research Scientist, Moscow State University) Summer 2002, Winter 2006, Winter 2007.

(iv) Undergraduate Students (26)

Name	School of Origin	Dates in Research
†Sara Bush	UND	Summer 2004-present
*Sarah Vollmer	UND	Fall 2001-2004
*Derek Atkinson	UND	2001-2002
*Karl Martin	UND	2001
*Lori Haagenson	UND	2000-2001
*Sarah Sundet	UND	Fall 2000
*Amanda Huber	UND	2000
*Megan Frykman	UND	Spring 2000
*Cathy Adrian	Bimidji State University	1999 (Summer)
Andrew Skalsky	UND	1998-9

Nathan Kadrmas	UND	1998 (Summer)
Tamara Baumgartner	UND	1995-7
Matthew Kuzel	UND	1996-97
Dagmara Motriuk	Casper College	1997 (Summer)
Michelle Humbert	UND	1994-6
Victoria Johnston	UND	1996 (Spring)
Jennifer Czlapinski	University of Wisconsin-Stevens Point	1996 (Summer)
Thea Kaldor	Mayville State University	1996 (Summer)
Cindy Bennedict	UND	1996
Rick Guo	University of Wisconsin-Eau Claire	1995 (Summer)
Glorianna Kie	New Mexico State University	1995 (Summer)
Karen McFarlane	UND	1994-5
Eric Nkabyo	University of Wisconsin-Whitewater	1994 (Summer)
Lisa Clark	UND	1994 (Summer)
Robert Warnock	Tennessee Technological University	1993
Kim Russell	Tennessee Technological University	1992

B. Theses & Dissertations Directed (* after promotion to associate professor, †after promotion to full professor)

Graduate Ph.D. Theses Directed (2)

*Felix Ngassa "Synthetic and Computational Studies on Polycyclic Aromatic Hydrocarbon Derivatives, Nucleoside Analogs and Peptides" December 2002.

‡Victor Waingeh "Computer Simulations of Glyceraldehyde-3-Phosphate Dehydrogenase Interactions with Actin and Fructose-1,6-bisphosphate Aldolase and Substrate Binding.

Graduate MS Theses Directed (2)

†Eric Njabon, "Brownian Dynamic Simulation of the Interaction between Lactate Dehydrogenase (LDH) And G- or F-Actin". December 2005.

†Fan Yang, "Brownian Dynamics of Nonspecific Protein-DNA Interactions". August 1999.

Undergraduate Senior Theses Directed (6):

*Sarah Vollmer, "Calculated Circular Dichroism of Cyclo(Gly-Pro-Pro)$_2$". May 2004.

*Derek Atkinson "Brownian Dynamics of Aldolase Mutants Interacting with F-Actin". May 2002.

*Amanda Huber "Predicting Circular Dichroism for the Flexible Peptide Cyclo(Gly-Pro-Gly)$_2$ Using a Variety of Methods to Determine Structure." January 2001.

*Lori Haagenson "Comparison of Calculation Methods and Conformations of Cyclo(L-proline)$_3$". May 2001.

Michelle Humbert "Prediction of Proton Uptake in the Complex Formation of Cytochrome c with Cytochrome b5" January 1996.

Karen McFarlane "Force Field Dependence of Boltzmann Weighting Factors on Predicted $\pi-\pi^*$ Circular Dichroic Spectra of Cyclo(Gly-Pro-Gly)2." May 1995.

C. Graduate Committee Service (* after promotion to associate professor, †after promotion to full professor)

(i) Chair

*Neville Forlemu (Ph.D. Physical Chemistry) 2004-present

*Kristine Carlson (Ph.D. Physical Chemistry) I am co-chair with Mark Hoffmann	2002-present
*Eric Njabon (Ph.D. Physical Chemistry)	2002-present
*Victor Waingeh (Ph.D. Physical Chemistry minor Biochemistry)	2001 - present
*Felix Ngassa (Ph.D. Organic and Physical Chemistry 12/02)	1998 - 2002
Fan Yang (M.S. Physical Chemistry, 8/99)	1998 - 1999*

(ii) Departmental Member

†Suhngwa Christian Jungong (Ph.D. Organic Chemistry)	2007-current
†Ganna Baglayeva (Ph.D. Physical Chemistry)	2007-current
†Daniel P. Theis (Ph.D. Physical Chemistry)	2006-current
†Rashel M. Mokambe (Ph.D. Physical Chemistry)	2006-current
†Carrie L. Amiot (Ph.D. Anaytical Chemistry)	2005-current
†Sheikh Mustakim (Ph.D. Physical Chemistry)	2005-current
†Divine Dugah (Ph.D. Inorganic Chemistry)	2005-current
†Kwame Shabass	2005
†Yvonne Bongfen (Ph.D. Physical Chemistry)	2004-current
*Walters Atmenkeng (M.S. Organic Chemistry)	2003-2006
*Larry Louisana	2003
*Rajeev Pandy (Ph.D. 12/03) Physical Chemistry	2003
*Hefeng Wang (M.S. 12/04) Physical Chemistry	2003-2004
*Ladislav Sallai (Ph.D. Organic Chemistry)	2003 - present
*Kristopher Keuseman (Ph.D. Organic Chemistry)	2002 - 2006
*Daniel McClintic	2000 - 2002
*Hina Baliyan (M.S. Analytical Chemistry)	2000 - 2003
*Eduard Tyapochkin (Ph.D. Physical Chemistry)	1999 - 2006
*Chris Dignan	1999
*Yen Dinh (M.S. Organic Chemistry, 12/01)	1999 - 2001
Michael Jager (M.S. Analytical Chemistry)	1998-9*
John Keeler	1998-9*
Jie Song (Ph.D. Physical Chemistry 8/02)	1998 - 2002*
Said Lubbad	1998
Bonnie Avery (Ph.D. Analytical Chemistry)	1994
Bill Brown (M.S. Physical Chemistry)	1996-7
Coretta Fernandes (M.S. Physical Chemistry)	1994-6
Chad Haraldson	1994
Sean Muller	1994
Ken Pierce (Ph.D. Physical Chemistry)	1994-6
Sherry Stein	1997-8
Stephanie Syverson (M.S. Analytical Chemistry)	1994
Jeff Vroman	1994
Ryan Winburn (M.S. Physical Chemistry)	1994-5
Naomi Winburn	1995

(iii) Outside Member

†Dagmar Hajkova (Ph. D. Biochemistry & Molecular Biology)	2005-present
†Maria Parnas (Ph.D. Biochemistry & Molecular Biology)	2005-2007
†Lata Balakrishnan (Ph.D. Biochemistry & Molecular Biology)	2004-2007
*Xuesong Chen (Ph.D. Pharmacology, Physiology & Therapeutics, 12/05)	2003-2005†
*Kelly Durick (Ph.D. Microbiology, 12/05)	2002-2005†
*Karl Wald (Ph.D. Biochemistry 5/02)	1999 - 2002
Karen Boeshans (Ph.D. Biochemistry 5/01)	1998 - 2001*

Mark Kapphahn (Ph.D. Biochemistry 8/97) 1994 -1997

SERVICE

(* after promotion to associate professor, †after promotion to full professor)

A. National

*†Serve on the National Council of Iota Sigma Pi, the National Honor Society for Women in Chemistry.

As Director of Student Awards. Elected 2005. My duties include:

- Manage three different national student awards including soliciting nominations, recruiting judging committees, and making the awards.
- Evaluate student applications for membership by national council action.
- Arrange for the printing of the membership and awards brochures for the organization.

As Coordinator for Members-at-Large. Elected in 1999-2005. My duties include:

- Maintaining membership database.
- Identifying potential new members.
- Fostering communications among the membership.
- Editing a quarterly newsletter.
- Assisted in planning the 2002 Triennial Convention & Centennial Celebration.
- Assisting in planning the 2005 Triennial Convention.
- Overseeing and awarding the annual National Education Re-Entry Award.

B. State

*†Co-Director with Stefan Balaz, Computational Chemistry and Biology Network (2002 -present).

- Recommend purchases of hardware and software.
- Educate biomedical researchers about molecular modeling software.
- Maintain the software and computer network locally.
- Teach periodic workshops about modeling for the state of North Dakota.
  - April 29, 2005 Introduction to InsightII/Discover, I was primary instructor.
  - Oct. 25, 2002 Introduction to InsightII/Discover, I was primary instructor.
  - Feb. 14, 2003 Introduction to Flexidoc, I was remote instructor for Stefan Balaz.
  - May 20-22, 2003 InsightII/Discover/Homology, I was primary instructor.
  - April 29, 2005 Introduction to InsightII/Discover, I was primary instructor.
  - May 17, 2006 Introduction to InsightII/Discover3, I advised instructor, Kristine Carlson.

*Served on the Board of Red River Valley Chapter of the American Chemical Society, 1999-2000. Duties included:

- Assisting in planning the Great Lakes Regional ACS Meeting in 2000.
- Joined discussions of maintaining the organization.

C. University

†Member, College of Arts and Sciences Tenure and Promotion Committee, 2007-2010

†Member, Search Committee for Genomics position in Biology, 2006-2007

†Member, Presidential ad hoc Committee for Promotions, 2005

†Member, UND Assistant Vice President for Research Search Committee, 2005

*Member, Internal Advisory Panel, UND NIH COBRE project, 2002-2004†.

*Member, Scholarly Activities Forum Committee, 2003.

*Member, Graduate Constitution Committee, 2002.

*Served on Tenure/Promotion Panel for PACW Discussion of Promotion and Tenure 9/14/99.

Member, Chemical Engineering Faculty Search Committee Member (Fall 1998)
Assisted Chem. Engineering identify candidates that overlap well with Chemistry and the Medical School.

*President, UND Chapter of Sigma Xi, June 1999- May 2000
- Ran monthly meetings of the chapter.
- Oversaw and awarded the Chapter's research award.

Vice President, UND Chapter of Sigma Xi, June 1998-May 1999
- Recruited speakers for the monthly meeting.

D. Department:
†Chair, Graduate Admissions Committee (2006-present).

†Member, Tenure, Reappointment, and Promotion Committee (2005-present).

*†Editor, Chemistry Alumni Newsletter (2003-present).

†Member, Chair Advisory Committee (2004-present).

*Analytical Chemistry Search Committee (2002-2004).

*†Chair, Chemistry Computer Committee (*1999-2005); member (1995-9, 2005-current).
*As chair:
- Called meeting to decide issues concerning the department's computer labs and computer uses.
- Wrote grants to obtain software from university funds
- Made policy for departmental computer labs.

As a member:
- I participate in the decision making.
- Recommend software,

*†Member, Graduate Program (2003-2004)
Assisted in rewriting graduate student policy manual. Assisted in changes to the graduate program.

*Chemical Education Search Committee (1999-2000).

Chair, Undergraduate Chemistry Curriculum Committee (1994-2000*, 2004-2005), member since 1993-present.
As a member
- I participated in recertification of the B.S. in Chemistry approved by the American Chemical Society (1993).

As chair, I:
- †Organized department undergraduate self-study (2005).
- †Worked with department chair to maintain ACS certification of the department BS program. (2004-2005)

- †Currently streamlining the last two years of the Chemistry programs (2004-present).
- Streamlined the first two years of the Chemistry programs including updating the Minor in Chemistry (1994-5).
- Developed standard guidelines for Chem 490 papers, the Senior Thesis (1996).
- Streamlined the second two years of the Chemistry programs (1996-7).
- Am developing a new curriculum in Chemistry with emphasis for the Health Sciences (1998).

Director, Chemistry Research Experience for Undergraduates (REU) Program (1997-2000*)

As co-PI on the NSF REU proposal:

- I ran the day to day business for the REU students during the summer.
- Organized weekly meetings, which included instruction on writing research papers and giving research presentations.
- Coordinated with other REU programs on campus for tours of local research centers and picnics.
- Was the primary contact person for all applicants during the school year and organizing the selection process.

Chair, Seminar Committee (1995-96), member (1993-4, 1999-2001*)

As chair:

- I organized student seminars, led grading, and held discussions with students about their seminars.

As a member:

- I assisted in determining the final grade for each student seminar.

Chair, Lectures Committee (1995-96). *Member (2003-2004)

As chair

- Organized and invited speakers for the Chemistry lectures program.

As a member.

- Aided in the selection of speakers.

Physical Chemistry Search Committee (1994-95).

Chemistry Graduate Admissions Committee (1993-7).

E. Recruiting

*Made contact with the University of Buea, Cameroon, Africa. Worked with a faculty member to identify potential graduate students.
*Assisted Graduate Recruiting officer in developing a letter for international applicants.
*Visited Concordia College, Moorhead, MN, 10/12/00.
Visited Mayville State University, Mayville, ND, 10/14/98.
Visited University of Minnesota, Morris, MN, 11/17/94.
Visited Mankato State University, Mankato, MN, 11/16/94.
Visited Moorhead State University, Moorhead, MN, 10/12/94.
Visited Winona State University, Winona, MN, 12/12/93.
Visited St. John's University, St. Joseph, MN, 12/13/93.
Visited St. Cloud State University, St. Cloud, MN, 12/14/93.

C. Community Service

*Assisted the Dakota Science Center in July 4th Celebration, July 4, 1999.
*Represented the Chemistry Department at the Girls State Career-Fair, June 1, 1999.
Represented the Chemistry Department at the UND Major Exploration Day, Oct. 21, 1998.

Represented the Chemistry Department at the UND Fall Open House, Sept. 27, 1998 and September 20, 1997.
Visited Broadus Wood Elementary, Earlysville, VA, to describe the Grand Forks flood, 5/2/97.
Assisted Brainy Bunch Science Club host Summerthing95, July 22, 1995.

PUBLICATIONS (70 total, 36 after promotion to associate professor, 15 after promotion to full professor)

(* after promotion to associate professor, ‡ after promotion to full professor)

A. Refereed (27 total, 12 after promotion to associate professor, 7 after promotion to full professor):

‡Mahesh K. Lakshman, John C. Keeler, Felix N. Ngassa, John H. Hilmer, Padmanava Pradhan, Barbara Zajc, Kathryn A. Thomasson. "Highly Diastereoselective Synthesis of Nucleoside Adducts From the Carcinogenic Benzo[*A*]Pyrene Diol Epoxide and a Computational Analysis." *J. Amer. Chem. Soc. 129* (**2007**) 68-76.

‡Neville Y. Forlemu, Victor F. Waingeh, Igor V. Ouporov, Stephen L. Lowe, Kathryn A. Thomasson. Theoretical Study of Interactions between Aldolase and F-actin: Insight into Different Species. *Biopolymers*, *85* (**2007**) 60-71. Figure 3 of this paper was featured on the cover of the journal.

‡Sugato Banerjee, Janel Evanson, Erik Harris, Stephen L. Lowe, Robert C. Speth, Kathryn A. Thomasson and James E. Porter. Correction: Identification of specific calcitonin-like receptor residues important for calcitonin gene-related peptide high affinity binding. *BMC Pharmacology, 6* (**2006**) 14.

‡V. F. Waingeh, C.D. Gustafson, E. I. Kozliak, S. L. Lowe, H. R. Knull, K. A. Thomasson. "Glycolytic Enzyme Interactions with Yeast and Skeletal Muscle F-actin." *Biophys. J. 90* (**2006**) 1371-1384.

‡K. L. Carlson, M. R. Hoffmann, K. A. Thomasson. "Geometric Optimization of Cyclo(L-Proline-L-Proline) and Prediction of its UV Circular Dichroic Spectrum." *J. Phys. Chem. A 110* (**2006**) 1925-1933.

‡Sugato Banerjee, Janel Evanson, Erik Harris, Stephen L. Lowe, Kathryn A. Thomasson, James E. Porter. Identification of Specific Calcitonin-like Receptor Residues Important for Calcitonin Gene-Related Peptide High Affinity Binding. *BMC Pharmacology, 6*:9 (**2006**) available online at http://www.biomedcentral.com/1471-2210/6/9.

‡K. L. Carlson, S. L. Lowe, M. R. Hoffmann, K. A. Thomasson. "Theoretical UV Circular Dichroism of Aliphatic Cyclic Dipeptides." *J. Phys. Chem. A*, *109* (**2005**) 5463-5470.

*V. Waingeh, S. Lowe, K. Thomasson. Brownian Dynamics of Interactions between Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants and F-actin. *Biopolymers*, *73*, 533-541 (**2004**).

*A. Hayen, M. A. Schmitt, F. Ngassa, K. A. Thomasson, S. H. Gellman. Foldamers with Heterogeneous Backbones: Two Helical Conformations from a Single Foldamer Backbone: Split Personality in Short α/β–Peptides. *Angewandte Chemie, 43,* 505-510 (**2004**).

*A. Huber, E. Nkabyo, R. Warnok, A. Skalsky, M. Kuzel, V. J. Gelling, T. B. Dillman, M. Ward, R. Guo, G. Kie-Adams, S. Vollmer, F. N. Ngassa, S. L. Lowe, I. V. Ouporov, K. A. Thomasson. "A Conformational Search and Calculation of the Circular Dichroic Spectrum of the

Flexible Peptide Cylco(Gly-Pro-Gly)$_2$ Using the Dipole Interaction Model". *J. Undergrad. Chem. Res.*, *4*, 145-161 (**2003**).

*S. Lowe, C. Adrian, I. Ouporov, V. Waingeh, K. Thomasson. "Brownian Dynamics Simulations of Glycolytic Enzyme Subsets with F-actin." *Biopolymers*, *70*, 456-470 (**2003**).

S. L. Lowe, K. S. Pierce, J. Czlapinski, G. Kie-Adams, Rajeev Pandey, M. R. Hoffmann, K. A. Thomasson· "Dipole Interaction Model Predicted π–π Circular Dichroism of Cyclo(L-Pro)3 Using Structures Created by Semi-empirical, Ab Initio, and Molecular Mechanics Methods." *J. Peptide Research*, *61*, 189-201 (**2003**).

*S. L. Lowe, D. M. Atkinson, V. Waingeh, K. A. Thomasson. "Brownian Dynamics of Interactions Between Aldolase Mutants and F-Actin." *J. Mol. Recognition*, *15*, 423-431 (**2002**).

*F. Yang, I. V. Ouporov, C. Fernandes, D. Motriuk, K. A. Thomasson. "Brownian Dynamics Simulating the Ionic Strength Dependence of the Nonspecific Association of 434 Cro Repressor Binding B-DNA." *J. Phys. Chem. 105*,12601-12608 (**2001**).

*I. Ouporov, H. Knull, A. Huber K. Thomasson. "Brownian Dynamics Simulations of Aldolase Binding GAPDH and the Possibility of Substrate Channeling." *Biophysical Journal, 18*, 2527-2535 (**2001**).
This article was cited (9/02) by the Rebecca Wade in the Faculty of Thousand as recommended reading for structural biology:

*I. Ouporov, H. Knull, S. L. Lowe, K. Thomasson. "Interactions of Glyceraldehyde-3-phosphate Dehydrogenase with G- and F-actin Predicted by Brownian Dynamics." *J. Molecular Recognition*, *14* (**2001**) 29-41.

*I. Ouporov, T. Kieth, H. Knull, K. Thomasson. "Computer Simulations of Glycolytic Enzyme Interactions with F-actin." *J. Biomolecular Structure and Dynamics 18* (**2000**) 311-323.

*I. Ourporov, H. R. Knull, K. A. Thomasson. "Brownian Dynamics Simulations of the Specific Interactions Between Rabbit Aldolase and G- or F-Actin." *Biophys. J.*, *76* (**1999**) 17-27.
This article was quoted in *Current Awareness in Biomedicine, Cytoskeleton*, March 1999.

S. Sun, J. Saltmarsh, S. Mallik, K. Thomasson. "Molecular Recognition of a Tris(Histidine) Ligand." *Chemical Communication*, *4* (**1998**) 519-520.

K. A. Thomasson, S. Merschman, M. Humbert, N. Kulevsky. "Applying Statistics in the Undergraduate Chemistry Laboratory: Experiments with Food Dyes." *Journal of Chemical Education*, *75* (**1998**) 231-233.

K. A. Thomasson, I. V. Ouporov, T. Baumgartner, J. Czlapinski, T. Kaldor, S. H. Northrup. "Free Energy of Nonspecific Binding of Cro Repressor Protein to DNA." *Journal of Physical Chemistry B*, *101* (**1997**) 9127-9136.

K. J. MacFarlane, M. M. Humbert, K. A. Thomasson. "Force Field Dependence of Boltzmann Weighting Factors on Predicted π–π^* Circular Dichroic Spectra of Cyclo(Gly-Pro-Gly)2." *International Journal of Peptide Protein Research*, *47* (**1996**) 447-459.

D. A. Fitzwater, K. A. Thomasson, R. J. Glinski. "A Modular Raman Spectroscopy System Using a Helium-Neon Laser That Is Also Suited For Emission Spectrophotometry Experiments." *Journal of Chemical Education*, *72* (**1995**) 187-189.

S. M. Andrew, K. A. Thomasson, S. H. Northrup. "Simulation of Electron Transfer Self-Exchange Kinetics of Cytochromes c and b_5", *Journal of the American Chemical Society*, *115*, (**1993**) 5516-5521.

S. H. Northrup, K. A. Thomasson, C. M. Miller, L. D. Eltis, P. D. Barker, A. G. Mauk. "Effects of Charged Amino Acid Mutations on the Bimolecular Kinetics of Reduction of Yeast iso-1-ferricytochrome c by Bovine ferrocytochrome b_5", *Biochemistry*, *32*, (**1993**) 6613-6623.

K. A. Thomasson, J. B. Applequist. "Effects of Proline Ring Conformation on Theoretical π-π^* Absorption and Circular Dichroic Spectra of Helical Poly(L-proline) Forms I and II". *Biopolymers*, *31* (**1991**) 529-535.

K. A. Thomasson, J. B. Applequist. "Bond Optimized Ring Closure for Proline: Comparison of Conformations and Semiempirical Energies with Small Molecule X-ray Structure". *Biopolymers*, *30* (**1990**) 437-450.

B. Abstracts (18 total, 6 after promotion to associate professor and 7 after promotion to full professor):

‡N. Y. Forlemu, Victor F. Waingeh, Eric N. Njabon, Kristine L. Carlson, Kathryn A. Thomasson. Brownian Dynamics Simulations of Enzyme-Enzyme Interactions and Ligand Transfer, accepted for presentation at the Biophysical Society Meeting, Long Beach CA, Feb. 2-6, 2008.

‡N. Y. Forlemu, E. N. Njabon, K. L. Carlson, V. F. Waingeh, K. A. Thomasson. Computer Simulation of the Ionic Strength Dependence of the Association of Glycolytic Enzymes to F-actin. *Biophysical Journal,* January **2007**, *Abstracts Issue*, 565a.

‡E. N. Njabon, V. F. Waingeh, K. L. Carlson, S. L. Lowe, K. A. Thomasson. "Brownian Dynamics Simulations of the Interaction between Lactate Dehydrogenase (LDH) Isoforms and F-actin. *Biophysical Journal,* January **2007**, *Abstracts Issue*, 565a.

‡V. F. Waingeh, K. A. Thomasson. "Computer Simulations of Enzyme/Enzyme Association in the Glycolytic Pathway." *Biophysical Journal*, January **2006**, *90* (1), 576a.

‡N. Y. Forlemu, V. F. Waingeh, S. L. Lowe, K. A. Thomasson. "Brownian Dynamics Simulations of Interactions between Fish Aldolase and G- or F-actin." *Biophysical Journal Supplement,* **2005**, *88*(1 part 2) 398a.

‡K. L. Carlson, S. L. Lowe, M. R. Hoffmann, K. A. Thomasson. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." *Biophysical Journal Supplement,* **2005**, *88*(1 part 2) 530a.

*V. F. Waingeh, K. A. Thomasson. "Computer Simulations of Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Interactions with Actin in Different Species." *Biophysical Journal Supplement,* **2004**, *86*(1 part 2) 266a.

*S. L. Lowe, C. Adrian, V. F. Waingeh, I. V. Ouporov, K. A. Thomasson. "Brownian Dynamics of Interactions Between F-actin and Dimers of Peptides of Rabbit Aldolase or GAPDH." *Biophysical Journal*, **2003**, 84(2) 257a.

*S. L. Lowe, D. M. Atkinson, K. A. Thomasson. "Brownian Dynamics of Interactions Between Mutants of Aldolase and F-actin." *Biophysical Journal*, **2002**, 82(1) 383a.

*K. A. Thomasson, S. L. Lowe, K. S. Pierce, J. Czlapinski, G. Kie. "Predicting the UV $\pi-\pi^*$ Circular Dichroism Spectrum of Cylco(L-Pro)$_3$. *Biophysical Journal,* **2001**, 80(1) 322a.

*I. V. Ouporov, H. R. Knull, K. A. Thomasson, "BD Simulations of Aldolase & GAPDH Binding and the Possibility of Substrate Channeling." *Biophysical Journal*, **2000**, 78(1) 292A.

*F. Yang, I. Ouporov, K. A. Thomasson. "Ionic Strength Dependence of the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA Predicted by Brownian Dynamics." *Biophysical Journal*, **1999**, *76*(2) A132.

I. Ouporov, K. A. Thomasson. "Modeling of Interactions Between Rabbit Aldolase and G- or F-Actin." *Biophysical Journal*, **1998**, *74*(2) A47.

K. A. Thomasson, T. Baumgartner, J. Czlapinski, T. Kaldor, S. H. Northrup. "Predicting the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA." *Biophysical Journal*, **1997**, *72*(2) A96.

T. Baumgartner, K. A. Thomasson. "Side Chain Effects on UV $\pi-\pi^*$ Circular Dichroic Spectra of Cation Complexes of Cyclo(Pro-Gly)3", *Biophysical Journal*, **1996**, *70*(2), A104.

K. A. Thomasson, S. H. Northrup, M. M. Humbert. "Simulated Proton Uptake in Complex Formation Between Cytochrome c and Cytochrome b5", *Biophysical Journal*, **1995**, *68*(2), A79.

K. A. Thomasson, S. H. Northrup. "Brownian Dynamics Simulation of Nonspecific Binding of Cro Repressor Protein to DNA", *Biophysical Journal*, **1994**, *66*(2) A187.

S. M. Andrew, K. A. Thomasson. "Simulation of Electron Transfer Self-Exchange in Cytochromes C and B5." *Biophysical Journal*, **1993**, *64*(2) A157.

S. H. Northrup, K. A. Thomasson. "Electrostatic Calculations of 2:1 Complexes of Cytochrome C and Cytochrome C Peroxidase". *Biophysical Journal*, **1992**, *61*(2), A2735.

C. Non-refereed (19 total, 15 after promotion to associate professor, 3 after promotion to full professor):

‡N. Y. Forlemu, V. F. Waingeh, S. L. Lowe, K. A. Thomasson. Brownian Dynamics Simulations of Interactions between Fish Aldolase and G- or F-Actin. *Proceedings of the North Dakota Academy of Sciences*, *59*, (**2005**) 40.

‡E. N. Njabon, S. L. Lowe, V. F. Waingeh, K. A. Thomasson. Computer Modeling of Electrostatic Interactions between LDH and Actin. *Proceedings of the North Dakota Academy of Sciences*, *59*, (**2005**) 48.

‡V. F. Waingeh, S. L. Lowe, E. I. Kozliak, C. D. Gustafson, H. R. Knull, K. A. Thomasson. Glycolytic Enzyme Interactions with F-Actin: Comparing Rabbit and Yeast. *Proceedings of the North Dakota Academy of Sciences*, *59*, (**2005**) 57.

*K. A. Thomasson. "What happens when your spouse is tenured and you still want to work as a chemist?" *Members-at-Large Newsletter of Iota Sigma Pi*, March **2004**.

*K. A. Thomasson. Book Review of *The Modem Nutritional Diseases - Heart Disease, Stroke, Type-2 Diabetes, Obesity, Cancer - and How to Prevent Them*, by Fred and Alice Ottoboni. *Members-at-Large Newsletter of Iota Sigma Pi*, Jan. **2003**.

*V. F. Waingeh, S. L. Lowe, and K. A. Thomasson. "Brownian Dynamics of Rabbit Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants Binding Rabbit F-actin." *Proceedings of the North Dakota Academy of Sciences*, *56* **(2002)** 50.

*K. A. Thomasson. "MAL Quilt Story" and "Members-at-Large Triennial Chapter Report". *Members-at-Large Newsletter of Iota Sigma Pi*, July **2002**.

*K. A. Thomasson. "ΙΣΠ Members-at-Large, Quilting for the Future of Interrupted Careers". *Members-at-Large Newsletter of Iota Sigma Pi*, March **2002**.

*K. A. Thomasson. "Question for Thought and Response Why Didn't We Receive Any MAL Scholarship Applicants This Year?" *Members-at-Large Newsletter of Iota Sigma Pi*, June **2001**.

*K. A. Thomasson. "Why are Women Faculty Still Underrepresented at Research Institutions?" *Members-at-Large Newsletter of Iota Sigma Pi*, March **2001**.

*K. A. Thomasson. "What do you do when you encounter someone in authority who is threatened by a strong, competent female and tries to make that person's work life unpleasant?" *Members-at-Large Newsletter of Iota Sigma Pi*, October **2001**.

*K. A. Thomasson. "My Interviewing Experience" *Members-at-Large Newsletter of Iota Sigma Pi*, March **2001**.

*K. A. Thomasson. "How far away are you from a local chapter?" *Members-at-Large Newsletter of Iota Sigma Pi*, Spring **2000**.

*S. L. Lowe, N. Kadrmas, T. Baumgartner, K. A. Thomasson. "Predicted Circular Dichroic Spectra of Cyclo(Pro-Gly)$_3$ by the Dipole Interaction Model Using Revised Parameters." *Proceedings of the North Dakota Academy of Science, 54* **(2000)** 37.

*K. A. Thomasson. "How to Nominate People for the Awards of Iota Sigma Pi." *Members-at-Large Newsletter of Iota Sigma Pi*, Winter **1999**.

*K. A. Thomasson. "Had any experience with premenopause? Might it be work related?" *Members-at-Large Newsletter of Iota Sigma Pi*, Winter **1999**.

*K. A. Thomasson. "News from the 1999 Triennial Convention." *Members-at-Large Newsletter of Iota Sigma Pi*, Fall **1999**.

*K. A. Thomasson. "Teaching statistical methods - Reply". *Journal of Chemical Education*, *76* (**1999**) 469. Concerns a discussion of the following article: K. A. Thomasson, S. Merschman, M. Humbert, N. Kulevsky. "Applying Statistics in the Undergraduate Chemistry Laboratory: Experiments with Food Dyes." *Journal of Chemical Education*, *75* (**1998**) 231-233.

K. A. Thomasson. "Physical Chemistry Education: A Comparison of American and Chinese Universities" *The Iotan*, May **1997**, No. 69, p. 2. *The Iotan* is the national newsletter for Iota Sigma Pi, the National Honor Society for Women in Chemistry.

D. Invited (refereed) (3 total, 3 after promotion to associate professor (*))

*****K. A. Thomasson. "Using Brownian Dynamics to Predict Interactions Between Large Biological Molecules." *Proceedings of the 91st Annual Meeting of the North Dakota Academy of Science, 53* **(1999)** 106-111.

*I. V. Ouporov, K. A. Thomasson, and Harvey R. Knull. "Brownian Dynamics Simulations of Rabbit Muscle Aldolase Binding Rabbit Muscle Actin, Actin Mutants and Yeast Actin." *Proceedings of the 91st Annual Meeting of the North Dakota Academy of Science, 53* **(1999)** 113.

*F. Yang, I. V. Ouporov, K. A. Thomasson. "Ionic Strength Dependence of the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA Predicted by Brownian Dynamics." *Proceedings of the 91st Annual Meeting of the North Dakota Academy of Science, 53* **(1999)** 112.

E. Invited (non-refereed) (2 total, both before promotion):

K. A. Thomasson. "Observing Culture in China: Part 1." *Members-at-Large Newsletter of Iota Sigma Pi*, Fall **1997**.

K. A. Thomasson. "Observing Culture in China: Part 2." *Members-at-Large Newsletter of Iota Sigma Pi*, Winter **1997**.

F. Manuscripts in Preparation (5 total)

Felix N. Ngassa, Eric M. Nkabyo, Kathryn A. Thomasson, and Samuel H. Gellman. Understanding The Interactions of β-Peptides with Each Other and with the Fos and Jun Units of the Human Leucine Zipper: A Computational Modeling Study.

Eric N. Njabon, Victor F. Waingeh, Kristine L. Carlson, Stephen L. Lowe, Kathryn A. Thomasson. Brownian Dynamics Simulations of the Interactions between Lactate Dehydrogenase (LDH) and G- or F-Actin. Part I: Muscle and Heart Homo-Isoforms.

Eric N. Njabon, Victor F. Waingeh, Neville Forlemu, Kristine Carlson, Steve L. Lowe, Kathryn A. Thomasson. Brownian Dynamics Simulations of the Interactions between Lactate Dehydrogenase (LDH) and G- or F-actin. Part II: Mixed Isoforms.

Neville Y. Forlemu, Eric N. Njabon, Kristine L. Carlson, Victor F. Waingeh, Kathryn A. Thomasson. Brownian Dynamics Simulating the Ionic Strength Dependence of the Association of Glycolytic Enzymes with F-actin.

S. Bush, S. Vollmer, K. L. Carlson, I. V. Ouporov, Kathryn A. Thomasson. Turn Structures of a Model Peptide System - Insights from Circular Dichroism.

PROFESSIONAL PRESENTATIONS (151 total, 71 since promotion to associate professor, 33 after promotion to full professor)

(† denotes principal authorship, underline denotes presenting author)
(* after promotion to associate professor, ‡ after promotion to full professor)

A. National/International (52 total, 22 since promotion to associate professor, 11 after promotion to full professor)

(i) Invited Participant (2 total, 1 since promotion to full professor)

K. A. Thomasson‡. "Brownian Dynamics Simulations of the Interactions between Lactate Dehydrogenase and G- or F-actin. Presented at the Gordon Conference on Macromolecular Organization and Cell Function, August 6-11, 2006, Mount Holyoke College, South Hadley, MA, USA.

K. A. Thomasson†. "Discussions of (1) Brownian Dynamics and (2) Physical Chemistry Education", as part of the Physical Chemistry People to People Delegation to the People's Republic of China (Beijing University, Tsinghua University, China Northern University, Fudan University, East China University of Science and Technology) June 7-20, 1996.

(ii) Invited Speaker (7 total, 3 since promotion to associate professor, 2 since promotion to full professor)

‡K. A. Thomasson†, S. H. Northrup. "Introducing MacroDox." Presented at the BDBDB: Biological Diffusion and Brownian Dynamics Brainstorm, March 26-29, 2007, Villa Bosch, Heidelberg, Germany.

‡K. A. Thomasson†. "Brownian Dynamics Simulations of Glycolytic Enzymes/Actin Interactions." Presented at the BDBDB: Biological Diffusion and Brownian Dynamics Brainstorm, March 26-29, 2007, Villa Bosch, Heidelberg, Germany.

*K. A. Thomasson†. "Computer Simulations of Glycolytic Enzyme/F-actin Interactions." Presented at the Gordon Conference on Macromolecular Organization and Cell Function, August 4-9, 2002, at Queens College/Oxford University in Oxford, UK.

*K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Chemistry and Biochemistry, Auburn University, Auburn, AL, January 31, 2000.

*K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Chemistry and Biochemistry, Worchester Polytechnic Institute, Worchester, MA, November 18, 1999.

K. A. Thomasson†. "Brownian Dynamics Simulations of the Specific Interactions Between Rabbit Aldolase and G- or F-Actin." Protein-Protein Interaction Conference, Grand Forks, ND, May 29, 1998.

K. A. Thomasson†. "My Accomplishments Within the Dreyfus Scholar/Fellow Program". Presented at the National American Chemical Society Dreyfus Symposium, San Diego, CA March 15, 1994.

(iii) Papers Presented (48 total, 18 since promotion to associate, 13 since promotion to full professor)

‡Eric N. Njabon, Neville Y. Forlemu, Kathryn A. Thomasson†. Brownian Dynamics Simulations of Glycolytic Enzymes Interacting with Tubulin. Presented at the National American Chemical Society Conference, Boston, MA, August 19-23, 2007.

‡Eric N. Njabon, Kristine L. Carlson and Kathryn A. Thomasson†. Brownian dynamics simulations of lactate dehydrogenase isoforms with F-actin. Presented at the National American Chemical Society Conference, Boston, MA, August 19-23, 2007.

‡Kristine L. Carlson, Sara J. Bush, Sarah Vollmer, and Kathryn A. Thomasson†. Turn structures of a model peptide system: Insights from circular dichroism. Presented at the National American Chemical Society Conference, Boston, MA, August 19-23, 2007.

‡N. Y. Forlemu, E. N. Njabon, K. L. Carlson, V. F. Waingeh, K. A. Thomasson†. Computer Simulation of the Ionic Strength Dependence of the Association of Glycolytic Enzymes to F-actin. Presented at the International Biophysical Society Meeting, Baltimore, MD, March 7 2007.

‡E. N. Njabon, K. L. Carlson, V. F. Waingeh, S. L. Lowe, K. A. Thomasson†. "Brownian Dynamics Simulations of the Interaction between Lactate Dehydrogenase (LDH) Isoforms and F-actin. Presented at the International Biophysical Society Meeting, Baltimore, MD, March 7 2007.

‡V. F. Waingeh, I. V. Ouporov, K. A. Thomasson†. Computer Simulations of Glycolytic Enzyme/Enzyme Association and Implications for Substrate Binding. Presented at the National American Chemical Society Meeting, Atlanta, GA, March 28, 2006.

‡Eric N. Njabon, Victor F. Waingeh, Steve L. Lowe, Kathryn A. Thomasson†. Brownian Dynamics Simulations of the Interactions between Lactate Dehydrogenase (LDH) and G- or F-Actin. Presented at the National American Chemical Society Meeting, Atlanta, GA, March 29, 2006.

‡V. F. Waingeh, I. V. Ouporov, K. A. Thomasson†. Computer Simulations of Enzyme/Enzyme Association in the Glycolytic Pathway. Presented at the 50th Annual Biophysical Society Meeting, Salt Lake City, UT, February 22, 2006.

‡K. L. Carlson, M. R. Hoffmann, K. A. Thomasson†. Structural Minimization & Theoretical UV Circular Dichroism of Cyclic Dipeptides. Presented at the 10th International Conference on Circular Dichroism, Sandestin Golf and Beach Resort, Destin, FL, August 21-25, 2005.

‡N. Forlemu, K. A. Thomasson†. "Brownian Dynamics Simulations of Interactions between Fish Aldolase and G- or F-actin." Presented at the National Biophysical Society Meeting, Long Beach, CA**,** February 15, 2005.

‡K. L. Carlson, S. L. Lowe, M. R. Hoffmann, K. A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD spectra." Presented at the National Biophysical Society Meeting, Long Beach, CA**,** February 15, 2005.

‡K. L. Carlson, M. R. Hoffmann, K. A. Thomasson†. "Ab initio studies of cyclo(L-proline-L-proline) and theoretical calculation of the UV-CD Spectrum." Presented at the 228th National American Chemical Society Meeting, Philadelphia, PA August 25, 2004.

‡K. A. Thomasson†, V. F. Waingeh, S. L. Lowe, E. I. Kozliak, C. D. Gustafson, K. H. Wald, K. A. Sukalski, H. R. Knull. "Glycolytic Enzyme Interactions with F-actin, a Comparison of Different Species." Presented at the Gordon Research Conference on Macromolecular Organization and Cell Function, Queen's College, Oxford, U.K. August 15-20, 2004.

*V. F. Waingeh, K. A. Thomasson†. "Computer Simulations of Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Interactions with Actin in Different Species." Presented at the 48th Annual Biophysical Society Meeting, Baltimore, MD, Feb. 16, 2004.

*S. L. Lowe, C. Adrian, V. F. Waingeh, I. V. Ouporov, K. A. Thomasson†. "Brownian Dynamics of Interactions Between F-actin and Dimers of Peptides of Rabbit Aldolase or GAPDH." Present at the 47th Annual Biophysical Society Meeting, San Antonio, TX, March 3, 2003.

*K. L. Carlson, M. R. Hoffmann, K. A. Thomasson† "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the 225th National Meeting of the American Chemical Society, New Orleans, March 26, 2003.

*V. F. Waingeh, S. L. Lowe, K. A. Thomasson.† "Brownian Dynamic Simulations of Glyceraldehyde-3-phopshate Dehydrogenase (GAPDH) Mutants Binding F-actin. Presented at the 225th National Meeting of the American Chemical Society, New Orleans, March 26, 2003. This poster won the student poster prize in Physical Chemistry.

*S. Vollmer, K. A. Thomasson.† "Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency Toward β-Turns, and the Calculated UV Circular Dichroism." Presented at the National Meeting of Sigma Xi, Galveston Island, TX, November 16, 2002.

*K. A. Thomasson†, B. Gordon, D. Iannotti. "ΙΣΠ Members-at-Large, Quilting for the Future of Interrupted Careers." Presented at the Triennial Convention and Centennial Celebration of Iota Sigma Pi, Berkeley, CA, June 12-15, 2002.

*S. L. Lowe, D. M. Atkinson, K. A. Thomasson†. "Brownian Dynamics of Interactions Between Mutants of Aldolase and F-actin." Presented at the Triennial Convention and Centennial Celebration of Iota Sigma Pi, Berkeley, CA, June 12-15, 2002.

*V. F. Waingeh, S. L. Lowe, K. A. Thomasson†. "Brownian Dynamics of Rabbit Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants Binding Rabbit F-Actin." Presented at the North Dakota Academy of Sciences, Grand Forks, ND, April 25, 2002.

*S. L. Lowe, D. M. Atkinson, K. A. Thomasson†. "Brownian Dynamics of Interactions Between Mutants of Aldolase and F-actin." Presented at the 46th Annual Meeting of the Biophysical Society, San Francisco, CA, February 23-27, 2002.

*S. L. Lowe, D. M. Atkinson, K. A. Thomasson†. "Brownian Dynamics of Interactions Between Mutants of Aldolase and F-actin." Presented at the 223 National Meeting of the American Chemical Society, Orlando, FL, April 7-11, 2002.

*F. N. Ngassa, M. A. Gelman, S. H. Gellman, K. A. Thomasson†. "Computer Simulations of Linkages Between α- and β-Peptide Helices." Presented at the 223 National Meeting of the American Chemical Society, Orlando, FL, April 7-11, 2002.

*D. J. Nelson†, S. Vercellotti, S. S. Marine, J. Clark, K. Louie, A. T. Sherren, P. Fish, K. A. Thomasson, C. Hermann, L. M. Ng, L. C. Brazdil, J. M. Buccigross, "Iota Sigma Pi: a century of fostering females in chemistry". Presented at the 223 National Meeting of the American Chemical Society, Orlando, FL, April 7-11, 2002.

*Felix N. Ngassa, Eric M. Nkabyo, Samuel H. Gellman, and Kathryn A. Thomasson†· "Computational Modeling Studies of the Interactions of β-Peptides with Each Other and with the Products of the Nuclear Oncogenes FOS and JUN". Presented at the 220th National American Chemical Society Meeting, Chicago, August 28, 2001.

K. A. Thomasson†, S. L. Lowe, K. S. Pierce, J. Czlapinski, G. Kie. "Predicting the UV π–π Circular Dichroism Spectrum of Cylco(L-Pro)$_3$. Presented at the 45th Annual Biophysical Society Meeting, Boston, MA, February 19, 2001.

*Coretta Fernandes, Fan Yang, Igor Ouporov, & Kathryn Thomasson†. "Dynamics of Nonspecific Interactions Between Cro Repressor Protein and B-DNA." Presented at the 219th National American Chemical Society Meeting, San Francisco, CA, March 26, 2000.

*I. V. Ouporov, H. R. Knull, K. A. Thomasson†, "BD Simulations of Aldolase & GAPDH Binding and the Possibility of Substrate Channeling." Presented at the 44th Annual Biophysical Society Meeting, New Orleans, February 15, 2000.

*I. V. Ouporov, K. A. Thomasson†, and Harvey R. Knull. "Brownian Dynamics Simulations of Rabbit Muscle Aldolase Binding Rabbit Muscule Actin, Actin Mutants and Yeast Actin." Presented at the National Triennial Convention of Iota Sigma Pi, Portland, OR, June 24th, 1999.

*F. Yang, I. Ouporov, K. A. Thomasson†. "Ionic Strength Dependence of the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA Predicted by Brownian Dynamics." Presented at the Biophysical Society Meeting, Baltimore, MD, Feb. 14, 1999.

I. Ouporov, K. A. Thomasson†. "Brownian Simulations of the Specific Interactions Between Rabbit Aldolase and G- or F-Actin." Protein-Protein Interaction Conference, Grand Forks, ND, May 29, 1998.

M. Humbert, I. Ouporov, T. Baumgartner, T. Kaldor, K. A. Thomasson†. "Simulated Proton Uptake In Complex Formation Between Cytochrome C And Cytochrome B5". Protein-Protein Interaction Conference, Grand Forks, ND, May 29, 1998.

F. Yang, D. Motriuk, I. Ouporov, K. A. Thomasson†. "Effect Of Ionic Strength On Brownian Dynamics Of Cro Repressor Protein With B-DNA." Protein-Protein Interaction Conference, Grand Forks, ND, May 29, 1998.

I. Ouporov, K. A. Thomasson†. "Modeling of Interactions Between Rabbit Aldolase and G- or F-Actin." Presented at the Biophysical Society Meeting, Kansas City, MO, February 23, 1998.

K. S. Pierce, K. A. Thomasson†. "Comparison of predicted circular dichroism of peptides using semi-empirical, ab initio, and molecular mechanics methods". Presented at the 215th American Chemical Society National Meeting, Dallas, TX, April 1, 1998.

D. Motriuk, K. A. Thomasson†. "Energetics of Nonspecific Binding of Cro repressor protein to DNA." Presented at the CUR Second Undergraduate Poster Session on Capitol Hill, Washington, DC, April 21, 1998.

K. A. Thomasson†, T. Baumgartner, J. Czlapinski, T. Kaldor, S. H. Northrup. "Predicting the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA." Presented at the Biophysical Society Meeting, New Orleans, LA, March 3, 1997.

T. Baumgartner, K. A. Thomasson†. "Side Chain Effects on UV $\pi-\pi^*$ Circular Dichroic Spectra of Cation Complexes of Cyclo(Pro-Gly)3". Presented at the Biophysical Society Meeting, Baltimore, MD, February 17, 1996.

K. A. Thomasson†, S. H. Northrup, M. M. Humbert. "Simulated Proton Uptake in Complex Formation Between Cytochrome c and Cytochrome b5". Presented at the Biophysical Society Meeting, San Francisco, CA, February 12, 1995.

K. J. MacFarlane, M. M. Humbert, K. A. Thomasson†. "Force Field Dependence of Boltzmann Weighting Factors on Predicted $\pi-\pi^*$ Circular dichroic Spectra of Cyclo(Gly-Pro-Gly)$_2$." Presented at the National American Chemical Society Meeting, Anaheim, CA, April 3, 1995.

K. A. Thomasson†, S. H. Northrup. "Brownian Dynamic Simulations of Nonspecific Binding of Cro Repressor Protein to DNA." Presented at the National American Chemical Society Dreyfus Symposium, San Diego, CA March 13, 1994.

R. P. Warnock, S. L. Syverson, K. A. Thomasson†, and K. Russell "Circular Dichroism of Multiple Conformations of Cyclo(Gly-Pro-Gly)$_2$ in Solution". Presented at the National American Chemical Society Undergraduate Research Symposium, San Diego, CA, March 14, 1994.

K. Russell, K. A. Thomasson†, S. H. Northrup "Theoretical Predictions of the $\pi-\pi^*$ Circular Dichroic Spectra of Cyclo(Gly-Pro-Gly)$_2$". Presented at the National Meeting of the American Chemical Society, Denver, Colorado, March 28 - April 2, 1993.

S. M. Andrew, K. A. Thomasson, S. H. Northrup†. "Simulations of Electron Transfer Self-Exchange in Cytochromes C and B5." Presented at the Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

S. H. Northrup†, K. A. Thomasson, S. M. Andrew. "Dynamical Simulation of Cytochrome Association and Electron Transfer." Presented at the National American Chemical Society Meeting, Denver, Colorado, March 28-April 2, 1992.

S. H. Northrup†, K. A. Thomasson. "Electrostatic Calculations of 2:1 Complexes of Cytochrome C and Cytochrome C Peroxidase". Presented at the Biophysical Society Meeting, Houston, TX, February 1992.

R. H. Lee†, K. A. Thomasson. "Automatic Determination of Structurally Conserved Regions in Proteins". Presented at the Lorne Protein Conference, Lorne, Victoria, Australia, February 9-13, 1992.

B. Regional (66 total, 37 since promotion to associate professor, 7 since promotion to full professor)

(i) Symposia Organized (1 since promotion to associate professor)

*Biomolecular Recognition Symposium, American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

(ii) Invited Speaker (18 total, 10 since promotion of associate professor, 1 after promotion to full professor)

‡K. A. Thomasson†. "Brownian Dynamics of Protein-Protein Interactions." Seminar for the Department of Physics, North Dakota State University, January 19, 2005.

*K. Carlson, M. Hoffmann, K. Thomasson†. "Calculations of Circular Dichroism for Cyclic Dipeptides." Seminar for the ND BRIN Statewide Research IVN Seminar Series, Feb. 23, 2004.

*S. Vollmer and K. A. Thomasson†. Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency Toward beta-Turns, and the

Calculated UV Circular Dichroism. Seminar for the ND BRIN Statewide Research IVN Seminar Series, Oct. 6, 2003.

*K. A. Thomasson†. "Computer Simulations for Predicting Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Physics, University of North Dakota, January 31, 2003.

*K. A. Thomasson†. "Computer Simulations for Predicting Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Physics, North Dakota State University, Oct. 2, 2002.

*K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Chemistry, North Dakota State University, June 7, 2002.

*K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Chemistry, Concordia College, Moorhead, MN, Oct. 12, 2000.

*K. A. Thomasson†. "Brownian dynamics simulation of the ionic strength dependence of the nonspecific association of Cro repressor binding B-DNA. For the Biomolecular Recognition Symposium at the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

*K. A. Thomasson†. "Computer Simulations of Protein-Protein and Protein-DNA Interactions." For the UND Chapter of Sigma Xi, January 19, 2000.

*K. A. Thomasson†. "Computer Modeling of protein/DNA interactions." For the USDA Human Nutrition Research Center, July 14, 1999, Grand Forks, ND.

*K. A. Thomasson.† "Using Brownian Dynamics to Predict Interactions Between Large Biological Molecules." For the Biosystems Modeling Symposium of the 91st Annual Meeting of the North Dakota Academy of Science, April 15, 1999, Grand Forks, ND.

K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for Mayville State University, 10/14/98.

K. A. Thomasson†. "Using Brownian Dynamics to Predict Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Biochemistry, NDSU, 9/11/98.

K. A. Thomasson†. "Free Energy Of Nonspecific Association of Cro Repressor Protein with B-DNA". Presented at the joint North Dakota/South Dakota EPSCoR conference, Brookings, South Dakota, Sept. 27, 1997.

K. A. Thomasson†. "Applications of Brownian Dynamic Simulations to Nonspecific Protein-Protein Binding and Protein-DNA Binding". Department of Chemistry, Mankato State University, 11/16/95.

K. A. Thomasson†. "Applications of Brownian Dynamic Simulations to Nonspecific Protein-Protein Binding and Protein-DNA Binding". Department of Chemistry, University of Minnesota at Morris, 11/17/95.

K. A. Thomasson†. "Applications of Brownian Dynamic Simulations to Nonspecific Protein-Protein Binding and Protein-DNA Binding". Department of Chemistry, Moorhead State University, 10/19/94.

K. A. Thomasson†. "Applications of Brownian Dynamic Simulations to Nonspecific Protein-Protein Binding and Protein-DNA Binding". Seminar for the Department of Chemistry, NDSU, 10/20/94.

(iii) Papers Presented (47 total, 26 since promotion to associate professor, 6 after promotion to full professor)

(a) Invited (10 total, 9 since promotion to associate, 1 since promotion to full)

‡Victor F. Waingeh, C. D. Gustafson, E. I. Kozliak, S. L. Lowe, H. R. Knull, K. A. Thomasson†. "Glycolytice Enzyme Interaction with Yeast and Skeletal Muscle F-actin. Presented at the Joint SD/ND EPSCoR Conference, 9/9/05, Brookings, South Dakota.

*Felix N. Ngassa, Michael A. Gelman, Samuel H. Gellman & Kathryn A. Thomasson†. "Computer Simulation of Linkers between α- and β-Peptide Helices." Presented at the ND EPSCoR Conference, University of North Dakota, Oct. 26, 2002.

*Victor F. Waingeh & Stephen L. Lowe & Kathryn A. Thomasson†. "Brownian Dynamics of Interactions between Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants and F-actin." Presented at the ND EPSCoR Conference, University of North Dakota, Oct. 26, 2002.

*Derek M. Atkinson, Stephen L. Lowe & Kathryn A. Thomasson†. "Brownian Dynamics of Aldolase Mutants Interacting with F-Actin." Presented at the 3rd Biennial Joint EPSCoR Conference, Brookings, SD, Oct. 2, 2001.

*Felix N. Ngassa, Eric M. Nkabyo, Samuel H. Gellman, and Kathryn A. Thomasson†· "Computational Modeling Studies of the Interactions of β-Peptides with Each Other and with the Products of the Nuclear Oncogenes FOS and JUN". Presented at the 3rd Biennial Joint EPSCoR Conference, Brookings, SD, Oct. 2, 2001.

*I. V. Ouporov, H. R. Knull, K. A. Thomasson†. "The Theoretical Studies of Channeling of Glyceraldehyde-3-phosphate Between Aldolase and Glyceraldehyde-3-Phosphate Dehydrogenase." For the 2nd Biennial Joint EPSCoR Conference, North Dakota State University, Fargo, ND, Sept. 10, 1999.

*Coretta Fernandes, Fan Yang, Igor Ouporov, & Kathryn Thomasson†. "Dynamics of Nonspecific Interactions Between Cro Repressor Protein and B-DNA." For the 2nd Biennial Joint EPSCoR Conference, North Dakota State University, Fargo, ND, Sept. 10, 1999.

*F. Ngassa, J. Keeler, M. Laksman, and K. Thomasson†, "Synthetic and Computational Studies in Polycyclic Aromatic Hydrocarbon Induced Chemical Carcinogensis." For the 2nd Biennial Joint EPSCoR Conference, North Dakota State University, Fargo, ND, Sept. 10, 1999.

*I. V. Ouporov, K. A. Thomasson†, and Harvey R. Knull. "Brownian Dynamics Simulations of Rabbit Muscle Aldolase Binding Rabbit Muscule Actin, Actin Mutants and Yeast Actin." For the Biosystems Modeling Symposium of the 91st Annual Meeting of the North Dakota Academy of Science, April 15, 1999, Grand Forks, ND.

*F. Yang, I. V. Ouporov, K. A. Thomasson†. "Ionic Strength Dependence of the Free Energy of Nonspecific Association of Cro Repressor Protein with B-DNA Predicted by Brownian Dynamics." For the Biosystems Modeling Symposium of the 91st Annual Meeting of the North Dakota Academy of Science, April 15, 1999, Grand Forks, ND.

(b) Contributed (37 total, 17 since promotion to associate, 5 since promotion to full)

‡ N. Y. Forlemu, E. N. Njabon, K. L. Carlson, V. F. Waingeh, K. A. Thomasson†. Computer Simulation of the Ionic Strength Dependence of the Association of Glycolytic Enzymes to F-actin. Presented at the Joint ND/SD EPSCoR Conference, 9/7/07, Fargo, ND.

‡S. J. Bush**,** K. L. Carlson, S. Vollmer, K. A. Thomasson†. It Fits! Molecular Shape By Circularly Polarized Light Absorbtion Patterns. 74 Annual Meeting of the Minnesota Academy of Sciences, Hamline University, St. Paul, MN, April 20, 2007.

‡Neville Y. Forlemu, Victor F. Waingeh, Stephen L. Lowe, Kathryn A. Thomasson†. Brownian Dynamics Simulations of Interactions between Fish Aldolase and G- or F-actin. Presented at the Joint SD/ND EPSCoR Conference, 9/9/05, Brookings, South Dakota.

‡Kristine L. Carlson, Mark R. Hoffmann, Kathryn A. Thomasson†. "Structural Minimization and Theoretical UV Circular Dichroism of Cyclic Dipeptides." Presented at the Joint SD/ND EPSCoR Conference, 9/9/05, Brookings, South Dakota.

‡N. Y. Forlemu, V. F. Waingeh, S. L. Lowe, K. A. Thomasson. Brownian Dynamics Simulations of Interactions between Fish Aldolase and G- or F-Actin. Presented at the North Dakota Academy of Science, 4/28/05, Grand Forks, ND.

‡E. N. Njabon, S. L. Lowe, V. F. Waingeh, K. A. Thomasson†. Computer Modeling of Electrostatic Interactions between LDH and Actin. Presented at the North Dakota Academy of Science, 4/28/05, Grand Forks, ND.

‡V. F. Waingeh, S. L. Lowe, E. I. Kozliak, C. D. Gustafson, H. R. Knull, K. A. Thomasson†. Glycolytic Enzyme Interactions with F-Actin: Comparing Rabbit and Yeast. Presented at the North Dakota Academy of Science, 4/28/05, Grand Forks, ND.

*Sarah Vollmer & Kathryn Thomasson†. "Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency Toward β-Turns, and the Calculated UV Circular Dichroism." Presented at the ND/SD Joint EPSCoR Conference, Ramada Plaza Suites, Fargo, ND, Sept. 5, 2003.

*Kristine Carlson, Mark R. Hoffmann†, Kathryn A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the ND/SD Joint EPSCoR Conference, Ramada Plaza Suites, Fargo, ND, Sept. 5, 2003.

*Victor F. Waingeh, Stephen L. Lowe, Kathryn A. Thomasson†. "Brownian Dynamics of Rabbit Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants Binding Rabbit F-Actin." Presented at the ND/SD Joint EPSCoR Conference, Ramada Plaza Suites, Fargo, ND, Sept. 5, 2003.

*Eric N. Njabon, Michael A. Gelman, Felix N. Ngassa, Samuel H. Gellman†, Kathryn A. Thomasson†. Computer Modeling of α- and β-Peptide Helices in Natural and Synthetic Polymers. Presented at the ND/SD Joint EPSCoR Conference, Ramada Plaza Suites, Fargo, ND, Sept. 5, 2003.

*Kristine Carlson, Mark R. Hoffmann†, Kathryn A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the 35th Midwest Theoretical Chemistry Conference, Ames, IA, sponsored by Iowa State University and IBM, June 12, 2003.

*Kristine Carlson, Mark R. Hoffmann†, Kathryn A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the ND EPSCoR Conference, University of North Dakota, Oct. 26, 2002.

*Sarah Vollmer & Kathryn Thomasson†. "Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency Toward β-Turns, and the Calculated UV Circular Dichroism." Presented at the ND EPSCoR Conference, University of North Dakota, Oct. 26, 2002.

*S. L. Lowe, C. Adrian, V. F. Waingeh, I. V. Ouporov, K. A. Thomasson†. "Brownian Dynamics of Interactions between F-Actin and Dimers or Peptides of Rabbit Aldolase or GAPDH." Presented at the ND EPSCoR Conference, University of North Dakota, Oct. 26, 2002.

*Victor F. Waingeh, Stephen L. Lowe, Kathryn A. Thomasson. "Brownian Dynamics of Rabbit Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants Binding Rabbit F-Actin." Presented at the ND Academy of Sciences, April 25, 2002.

*Derek M. Atkinson, Stephen L. Lowe & Kathryn A. Thomasson†. Brownian Dynamics of Aldolase Mutants Interacting with F-Actin." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 25, 2001.

*Felix Ngassa, John Keeler, Mahesh Laksman, K. A. Thomasson†. "Synthetic and computational studies in polycyclic aromatic hydrocarbon induced chemical carinogenesis." For the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 4, 2000.

*Amanda Huber, Andrew Skalsky, Matthew Kuzel, Eric Nkabyo, Kathryn A. Thomasson†. "Predicting the UV circular dichroism of a flexible peptide, cyclo(Gly-Pro-Gly)$_2$ using the dipole interaction model." For the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

*S. L. Lowe, K. S. Pierce, J. Czlapinski, G. Kie, K. A. Thomasson†. "Comparison of experimental and predicted circular dichroism spectra of cyclo(L-Pro)$_3$." For the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

*Coretta Fernandes, Fan Yang, Igor Ouporov, Kathryn Thomasson†. "Further dynamics of nonspecific interactions between Cro repressor protein and B-DNA" . For the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

*Igor V. Ouporov, Harvey R. Knull, Kathryn A. Thomasson†. "BD Simulations of aldolase and GAPDH and the possibility of substrate channeling." For the American Chemical Society, Great Lakes Regional Meeting, Fargo, ND, June 5, 2000.

*Cathy Adrian, Igor Ouporov & Kathryn Thomasson†. "Brownian Dynamics Simulations of Aldolase or Aldolase Subsets with F-Actin." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Grand Forks, North Dakota, July 28, 1999.

*Coretta Fernandes, Fan Yang, Igor Ouporov, & Kathryn Thomasson†. "Dynamics of Nonspecific Interactions Between Cro Repressor Protein and B-DNA." ." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Grand Forks, North Dakota, July 28, 1999.

N. Kadrmas, T. Baumgartner, K. A. Thomasson†. "Solution Conformations and Predicted Circular Dichroism of Cation Complexes of Cyclo(Pro-Gly)3." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, University of North Dakota, Grand Forks, North Dakota, July 31, 1998.

K. S. Pierce, K. A. Thomasson†. "Comparison of UV Circular Dichroism of Peptides Using Semi-empirical and Molecular Mechanics Methods." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 30, 1997.

I. V. Ouporov, K. A. Thomasson†. "Modeling of Interactions Between Rabbit Aldolase and G-actin." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 30, 1997.

D. Motriuk, K. A. Thomasson†. "Energetics of Nonspecific Binding of Cro Repressor Protein to DNA" Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 30, 1997.

M. F. Kuzel, K. A Thomasson†. "Predicting the UV Circular Dichroism of Cyclo(Gly-Pro-Gly)2." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 30, 1997.

T. Baumgartner, K. A. Thomasson†. "Theoretical UV $\pi-\pi^*$ Circular Dichroism of Cyclo(Pro-Gly)3". Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, University of North Dakota, Grand Forks, North Dakota, July 31, 1996.

J. Czlapinski, K. A. Thomasson†. "Predicting the UV Circular Dichroism of Cyclo(Pro)3". Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, University of North Dakota, Grand Forks, North Dakota, July 31, 1996.

T. Kaldor, K. A. Thomasson†. "Simulated Proton Uptake in Complex Formation Between Cytochrome c and Cytochrome b5". Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, University of North Dakota, Grand Forks, North Dakota, July 31, 1996.

R. Guo, K. A. Thomasson†. "Homology and Dynamic Modeling of Plastocyanin". Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 28, 1995.

G. Kie, K. A. Thomasson†. "Side Chain Preferences of Cyclo(Pro)3". Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 28, 1995.

T. Baumgartner, K. A. Thomasson†. "Side Chain Effects on $\pi-\pi^*$ Circular Dichroic Spectra of Magnesium Complexes of Cyclo(Pro-Gly)3." Presented at the North Dakota Science, Engineering, & Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 28, 1995.

M. Humbert, K. A. Thomasson†. "Simulated Proton Uptake in Complex Formation Between Cytochrome c and Cytochrome b5". Presented at the North Dakota Science, Engineering,

& Mathematics Undergraduate Poster Session, North Dakota State University, Fargo, North Dakota, July 28, 1995.

E. Nkabyo, K. A. Thomasson†. "A Thorough Conformational Search of Cyclo(Gly-Pro-Gly)$_2$". Presented at the Joint UND/NDSU Undergraduate Poster Session, University of North Dakota, Grand Forks, August 4, 1994.

K. A. Thomasson, J. B. Applequist†. "Proline Conformations by Bond Optimized Ring Closure; Comparison with Semiempirical Energies and X-ray Structures". Presented at the Joint Meeting of the Ames and Iowa Sections of the American Chemical Society, Grinnell College, Grinnell Iowa, April 29, 1989.

K. A. Thomasson, J. B. Applequist†. "A Theory of Side Chain Effects on π-π^* Circular Dichroism of Cyclo(Pro-Gly)$_3$". Presented at the Joint Meeting of the Ames and Iowa Sections of the American Chemical Society, Grinnell College, Grinnell Iowa, April 16, 1988.

C. Local (33 total, 12 since promotion to associate professor, 15 since promotion to full professor)

(i) Invited Speaker (10 total, 3 since promotion to associate professor, 1 since promotion to full professor)

‡K. A. Thomasson. "Protein-Protein Interactions: A Computational Approach." Seminar for the Department of Biology, University of North Dakota, November 3, 2006.

*K. A. Thomasson†. "Computer Simulations of Biomacromolecular Interactions." Seminar for the Department of Biochemistry, University of North Dakota, January 29, 2004.

*K. A. Thomasson†. "Computer Simulations for Predicting Protein-Protein and Protein-DNA Interactions." Seminar for the Department of Physics, University of North Dakota, Jan. 31, 2003.

*K. A. Thomasson†. "Computer Simulations of Protein-Protein Interactions and Protein-DNA Interactions." Sigma Xi Luncheon Series, Jan. 20, 2000.

K. A. Thomasson†. "Panel Discussion of Undergraduate Research: Opportunities for Students." UND Office of Instructional Development Lunch Box Series, Jan. 14, 1998.

K. A. Thomasson†. "Brownian Dynamic Simulations of Protein-DNA Interactions." Presented at the Biochemistry Cluster Meeting, UND Medical School, 10/4/96.

K. A. Thomasson†. "Simulated Proton Uptake in Complex Formation Between Cytochrome c and Cytochrome b$_5$." Presented at the Biochemistry Cluster Meeting, UND Medical School, 11/95.

K. A. Thomasson†. "Simulations of Interactions between Cytochrome c and Cytochrome b$_5$." Presented at the Biochemistry Cluster Meeting, UND Medical School, 10/94.

K. A. Thomasson†. "Simulation of Electron Transfer Self-Exchange Kinetics of Cytochromes c and b$_5$". Special Lecture for the department of Biochemistry and Molecular Biology, UND, 12/7/93.

K. A. Thomasson†. "Applications in Molecular Modeling." Seminar for the department of Chemical Engineering, UND, 10/93.

(ii) Contributed (23 total, 9 since promotion to associate professor, 14 since promotion to full professor)

‡N. Y. Forlemu, E. N. Njabon, K. L. Carlson, V. F. Waingeh, K. A. Thomasson†. Computer Simulation of the Ionic Strength Dependence of the Association of Glycolytic Enzymes to F-actin. Presented at the Scholarly Activities Forum, March 1, 2007.

‡E. N. Njabon, K. L. Carlson, V. F. Waingeh, S. L. Lowe, K. A. Thomasson†. "Brownian Dynamics Simulations of the Interaction between Lactate Dehydrogenase (LDH) Isoforms and F-actin. Presented at the Scholarly Activities Forum, March 1, 2007.

‡K. L. Carlson, S. J. Bush, S. Vollmer, K. A. Thomasson†. " It Fits! Molecular Shape by Circularly Polarized Light Absorbtion Patterns." Presented at the Scholarly Activities Forum, March 1, 2007.

‡Eric N. Njabon, Victor F. Waingeh, Steve L. Lowe, Kathryn A. Thomasson†. Brownian Dynamics Simulations of the Interactions between Lactate Dehydrogenase (LDH) and G- or F-Actin. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Kristine L. Carlson, Kathryn A. Thomasson†, Mark R. Hoffmann†. Insights from Circular Dichroism. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Victor F. Waingeh, Igor V. Ouporov, Kathryn A. Thomasson†. Computer Simulations of Glycolytic Enzyme-Enzyme Interaction and Substrate Binding. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Neville Y. Forlemu, Victor F. Waingeh, Igor V. Ouporov, Stephen L. Lowe, Kathryn A. Thomasson†. Theoretical Study of Interactions between Aldolase and F-actin: Insight into Different Species. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Sara Bush, Sarah Vollmer, Kristine L. Carlson, Kathryn A. Thomasson†. Turn Structures of a Model Peptide System - Insights from Circular Dichroism. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Stephen L. Lowe, Karl Wald, Eric Njabon, Sarh Vollmer, Harvey Knull, Kathy Sulalsky, Kathryn A. Thomasson†. Interactions of Enzyme/Green Fluorescent Protein Constructs with F-actin. Presented at the UND Scholarly Activities Forum, February 28 - March 2, 2006.

‡Sara Bush, Kristine L. Carlson and K. A. Thomasson†. "Cyclo(Gly-Pro-Pro)$_2$ Modeled Structure and Calculated Circular Dichroism." Presented at the UND Scholarly Activities Forum, February 22, 2005.

‡Victor. F. Waingeh, Stephen L. Lowe, Evguennii I. Kozliak, Carol D. Gustafson, Karl H. Wald, Katherine A. Sukalski, Harvey R. Knull and Kathryn A. Thomasson†. "Glycolytic Enzyme Interactions with F-actin, a Comparison of Different Species." Presented at the UND Scholarly Activities Forum, February 22, 2005.

‡Kristine L. Carlson, Mark R. Hoffmann and Kathryn A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the UND Scholarly Activities Forum, February 22, 2005.

‡Neville Y. Forlemu, Victor F. Waingeh, Stephen L. Lowe and Kathryn A. Thomasson†. "Brownian Dynamics Simulations of the Interactions between Aldolase and G- or F-actin." Presented at the UND Scholarly Activities Forum, February 22, 2005.

‡Eric N. Njabon and Kathryn A. Thomasson†. "Computer Modeling of Electrostatic Interactions of LDH and F-actin." Presented at the UND Scholarly Activities Forum, February 22, 2005.

*Eric N. Njabon, Victor F. Waingeh, Stephen L. Lowe, and Kathryn A. Thomasson†. "Computer Simulations of Electrostatic Interactions between Models of Lactate Dehydrogenase with G- and F-actin.' Presented at the UND Scholarly Activities Forum, March 4, 2004.

*Victor F. Waingeh and Kathryn A. Thomasson†. "Computer Simulations of Glyceradehyde-3-Phosphate (GAPDH) Interactions with Actin in Different Species." Presented at the UND Scholarly Activities Forum, March 4, 2004.

*Kristine L. Carlson, Mark R. Hoffmann, and Kathryn A. Thomasson†. "Geometric Optimization of Cyclo(L-Proline-L-Proline) and Prediction of its UV Circular Dichroic Spectrum." Presented at the UND Scholarly Activities Forum, March 4, 2004.

*Sarah Vollmer and Kathryn Thomasson†. Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency toward β–turns, and the Calculated UV Circular Dichroism. Presented at the UND REU Poster Session, August 6, 2003.

*Kristine Carlson, Mark R. Hoffmann†, Kathryn A. Thomasson†. "Modeling Cyclic Dipeptides and Calculations of Their UV CD Spectra." Presented at the UND Scholarly Activities Forum, Feb. 13, 2003.

*Sarah Vollmer & Kathryn Thomasson†. "Comparing Structures of Cyclo(Gly-Pro-Pro)$_2$ Minimized by Force Fields at Various Dielectrics, the Tendency Toward β-Turns, and the Calculated UV Circular Dichroism." Presented at the UND Scholarly Activities Forum, Feb. 13, 2003.

*S. L. Lowe, C. Adrian, V. F. Waingeh, I. V. Ouporov, K. A. Thomasson†. "Brownian Dynamics of Interactions between F-Actin and Dimers or Peptides of Rabbit Aldolase or GAPDH." Presented at the UND Scholarly Activities Forum, Feb. 13, 2003.

*Victor F. Waingeh, Stephen L. Lowe, Kathryn A. Thomasson. "Brownian Dynamics of Rabbit Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH) Mutants Binding Rabbit F-Actin." Presented at the UND Scholarly Activities Forum, Feb. 13, 2003.

*S. L. Lowe, D. M. Atkinson, K. A. Thomasson†. "Brownian Dynamics of Interactions Between Mutants of Aldolase and F-actin." Presented at the UND Scholarly Activities Forum, Feb. 12, 2002.

GRANTS

(* after promotion to associate professor; ‡ after promotion to full professor)

A. Funded (47 total: $19,539,777; 17 since promotion to associate: $6,059,591; 8 since promotion to full: $10,309,755)

(i) Single Investigator Grants (31: $473,888; 14 since promotion to associate professor: $41,270; 5 since promotion to full professor: $19,755)

(externally reviewed: (10 total: $452,322; 6 since promotion to associate professor: $307,717; 1 since promotion to full professor: $15,633)

*Brownian Dynamics Simulations of Actins with Aldolase. National Institutes of Health, General Medical Sciences, 7/03-6/06 ($140,200).

*Incorporation of Hydrophobic Forces Into Brownian Dynamics Computer Program MacroDox - NATO Visiting Expert, 5/27/02-6/60/02 ($3,300).

*Computational Studies of β-Peptides and Their Interactions with Each Other and with Leucine Zippers FOS and JUN. ND EPSCoR Doctoral Dissertation Assistantship for Felix Ngassa. 8/16/01-8/15/02 ($17,417) ND EPSCoR, 8/16/01-8/15/02.

*Undergraduate Involvement in Computational Bioinformatics. National Science Foundation - REU Supplement. 12/01-2/28/02, $2,500.

* Brownian Dynamics Simulations of Actin with Aldolase. National Institutes of Health, General Medical Sciences, 7/1/00 - 6/30/03, $141,300.

*Undergraduate Involvement in Computational Biochemistry. National Science Foundation - REU Supplement. 11/99-8/00, $3,000.

Brownian Dynamics Simulations of Actin with Aldolase ($107,972) National Institutes of Health - General Medical Sciences, 6/1/97-5/31/00.

Theoretical $\pi-\pi^*$ Absorption and Circular Dichroic Spectra of Peptides ($18,000) NSF, 8/94-6/96.

Protein Flexibility in Brownian Dynamic Simulations of Protein-Protein and Protein-DNA Interactions ($30,000) ND EPSCoR, 5/1/94-8/31/95.

(internally reviewed: 21 total: $21,566.22; 8 since promotion to associate professor: $10,553; 4 since promotion to full professor: $4,122.22)

‡Travel to the Biological Diffusion and Brownian Dynamics Brainstorm, Villa Bosh, Heidelberg, Germany. Senate Scholarly Activities Committee, $848, 3-24-07.

‡Brownian Dynamics of Glyceraldehyde-3-phosphate Dehydrogenase Interactions with Actin. ND EPSCoR Doctoral Dissertation Fellowship for Victor Waingeh. 8/16/04-8/15/06 ($15,633).

‡Senate Scholarly Activities Committee, Travel Award ($293.22) to travel to the Biophysical Society meeting in Salt Lake City, UT, 2/18-2/23/06.

‡Senate Scholarly Activities Committee, Travel Award ($426) to travel to the Biophysical Society meeting in Long Beach, CA, 1/28/05-7/15/05.

‡Science Bound Award for Sara Bush. Molecular Modeling of Cyclic Peptides. NDEPSCoR, $2,903.00, 7/13/04-5/15/05.

‡Travel Costs for the Gordon Conference titled Macromolecular Structure and Cell Function held in Oxford, England, 8/15/04-8/20/04 (ORPD $500).

*Travel Costs for the Biophysical Society meeting in San Antonio, TX, March 2003, from the Senate Scholarly Activities Committee ($471).

*Plane Ticket for the Gordon Conference titled Macromolecular Structure and Cell Function held in Oxford, England, 8/3/02-8/9/02, ORPD ($1181)

*Travel Costs for the national American Chemical Society Meeting in Orlando, FL April 2002 from Senate Scholarly Activity Committee ($435).

*Publication Costs from ORPD ($1,350) for I. Ouporov, H. Knull, A. Huber K. Thomasson. "Brownian Dynamics Simulations of Aldolase Binding GAPDH and the Possibility of Substrate Channeling." *Biophysical Journal* 4/24/01.

*Travel Costs to travel to the Biophysical Society meeting in Boston, MA from ORPD ($460) Feb. 2001.

*Cambridge Structural Database and SpartanPro Molecular Modeling Software ($771) OID Faculty Instructional Development Grant. 11/21/00.

*UND Summer Graduate Research Professorship ($5,400), 6/99-7/99.

*Faculty Research Committee Award ($485) for travel to the Biophysical Society Meeting in Baltimore, MD, 2/99.

Faculty Research Committee Award ($988) for publication costs, 11/98.

Faculty Research Committee Award ($420) for travel to the Biophysical Society Meeting in Kansas City, MO, 2/98.

Visit to the People's Republic of China as a Citizen Ambassador in the People to People Program ($1300: $300 from ND EPSCoR and $1,000 Instructional Development), 4/96.

Theoretical UV Circular Dichroic Spectra of Cyclo(Pro-Gly)$_3$ and Cyclo(Pro)$_3$ ($500) UND Faculty Research Committee, 10/18/95.

Undergraduate Involvement in Protein Flexibility in Brownian Dynamic Simulations of Protein-Protein Interactions ($1,000) ND EPSCoR, 10/95.

UND WAC Half-Day Workshop to coordinate the teaching of writing in the discipline of chemistry ($625) UND Writing Across the Curriculum, 3/95.

Supplemental Award for Molecular Modeling Software for use in protein and peptide dynamic simulations ($1500) ND EPSCoR, 12/1/93.

Instructional Development Award ($75) for the purchase of the program DIATOMIC for use in the Physical Chemistry Laboratory, 3/11/94.

Faculty Research Committee Award ($483) for travel to the national American Chemical Society Meeting in San Diego, CA 3/94.

(ii) Multiple Investigator Grants (16 total: $19,065,889; 3 since promotion to associate professor: $6,018,321; 3 since promotion to full professor: $10,290,000)

(participation as PI or co-PI: 6 total: $307,367; 2 since promotion to associate professor: 23,021; 2 since promotion to full professor $90,000)

‡Computational Approaches to Modeling the Mercury Interactions on Activated Carbons. DOE/EERC. 7/1/04 ($40,000). I am co-PI with PI, Mark Hoffmann.

‡ Computational Approaches to Modeling the Mercury Interactions on Activated Carbons. EPA. 7/1/04 ($50,000). I am co-PI with PI, Mark Hoffmann.

*Three-Dimensional Folding of Biologically Important Molecules. UND Seed Money. 6/1/02-11/30/03 ($22,250). I am PI with co-PI, Mark Hoffmann.

*Cambridge Structural Database and SpartanPro Molecular Modeling Software ($771) Faculty Instructional Development Committee 11/2000 (I was PI with Harmon Abrahamson).

Computer Operated Undergraduate Chemistry Instrumentation ($46,346) NSF 6/98 (I was co-PI with Irina Smoliakova).

Undergraduate Research in Chemistry: A Site Emphasizing Native American Participation ($148,000) NSF 3/97-8/30/99 (I was co-PI with David Pierce)

(participation as contributor: 10 total: $18,758,522; 1 since promotion to associate professor, 5,995,300; 1 since promotion to full professor, $10,200,000)

‡North Dakota Biomedical Research Infrastructure, NIH/INBRE (Shabb, PI), $4.2 million to the UND campus, 10/1/04-9/30/09. I contribute by coordinating the Computational Chemistry and Biology Network.

‡National Institutes of Health - INBRE "Building Biomedical Research in North Dakota", 10/01/01 - 9/30/04, ($6,000,000). John Shabb, (PI).

*National Institutes of Health - BRIN "Building Biomedical Research in North Dakota", 10/01/01 - 9/30/04, $5,995,300. John Shabb, (PI).

Purchase of Circular Dichroism Spectrometer for Research in Carcinogen-DNA Interactions ($79,218) NSF 3/15/99 (Harmon Abrahamson, PI).

Brownian Dynamics Simulations of F-Actin with Glycolytic Enzymes (approximately $50,000 to my program over three years) as part of a NSF vBNS hookup, 10/98 (Carl Fox, PI)

Acquisition of a 400 MHz NMR Spectrometer for Research and Education in Chemistry ($329,764) 7/98 (Irina Smoliakova, PI)

National Science Foundation, ARI Program (buildings), "Renovation of Abbott Hall, Chemistry Department", 1996-99, $1,771,000. R.J. Baltisberger (PI).

Supramolecular Protein Complexes: Roles in Cellular Regulation, Biochemistry Cluster ($1,474,000) NSF EPSCoR (Harvey Knull and John Shabb, PIs) ($86,000 to my program) 10/95-7/31/98.

National Science Foundation, ILI Program (instrumentation), "Curriculum Improvement in Undergraduate Chemistry Laboratories Using Rapid-Scanning Spectroscopic Techniques", 1995, $115,240. H. B. Abrahamson (PI) and N. F. Woolsey (co-PI).

National Science Foundation, Research Experiences for Undergraduates, "Undergraduate Research in Chemistry," 5/94-5/97, $132,000. David Pierce (PI).

B. Pending (1)

(i) Single Investigator (0)

(ii) Multiple Investigator (0)
(participation as PI or co-PI)
NATO: Investigation of Interaction Specificity and Possibility of Channelling between Neuron Specific Enolase and Brain Phosphoglycerate Mutase. 1/1-2008-1/30/2009, $13,987, Kathryn Thomasson, PI; Karen Nazaryan, co-PI.

(participation as contributor)

C. Declined (38 total: 11 since promotion to associate professor, 9 since promotion to full professor)

(i) Single Investigator Grants (31 total, 10 since promotion to associate professor, 4 since promotion to full professor)
(external: 27 total; 8 since promotion to associate professor; 4 since promotion to full professor)
‡Brownian Dynamics Simulations of Glycolytic Enzymes with Actin. NIH/NIGMS. PI: Kathryn Thomasson. 7/1/06-6/30/09. $209,400.

†Development of MacroDox & HARLEM Biomodeling Package. National Institutes of Health, National Center for Research Resources/DHHS ($1,604,799) 8/15/05-7/31/10.

‡The Apple Workgroup Cluster for Bioinformatics. Apple Computers, Inc. ($40,000 for a G5 cluster with bioinformatics software). 6/29/04-6/28/07.

†Development of MacroDox & HARLEM Biomodeling Package. National Institutes of Health, National Center for Research Resources/DHHS ($1,432,250) 12/1/04-11/30-09.

*Substrate Channeling in Glycolysis: Theory & Experiment. National Institutes of Health, General Medical Sciences, 1/1/04-12/31-07 ($134,592).

*Experiments of Substrate Channeling among the Glycolytic Enzymes and the Effect of the Presence of F-actin. National Institutes of Health, General Medical Sciences, ($140,200). Jenya Kozliak (PI).

*Substrate Channeling in Glycolysis: Theory & Experiment. National Institutes of Health, General Medical Sciences, 6/1/03-5/31-06 ($134,592).

*Enhancements to Docking Macromolecules with MacroDox. National Institutes of Health, General Medical Sciences, 11/02-10/05 ($115,773).

*Predicting Complexes of Glycolytic Enzymes & Substrate Channeling Chances. NSF, 1/01/03-12/31/05 ($559,837)

*National Institutes of Health - General Medical Sciences "Brownian Dynamics of Helical Structures." 6/01/02-5/31/06 ($953,775).

*National Science Foundation - REU Supplement "Undergraduate Involvement in Computational Biochemistry ($5000) declined 8/00.

*Brownian Dynamics Simulations of Glycolytic Enzymes ($569,759) NIH, declined 7/6/99.

Brownian Dynamics of Protein-DNA Interactions ($411,041) American Cancer Society 8/1/98.

Brownian Dynamics of Protein-DNA Interactions ($350,000) NIH, 3/30/98.

Theoretical UV Circular Dichroic Spectra of Peptides and Amides ($656,554) NSF, 1/1/98.

Brownian Dynamics Simulations of Actin with Aldolase ($30,000) ND EPSCoR, 2/24/97.

Brownian Dynamics Simulations of Actin with Aldolase ($75,000) American Chemical Society - Petroleum Research Fund Type AC, 2/15/97.

Predicting Electronic UV Circular Dichroism: Applications of the Dipole Interaction Model to Include a Greater Variety of Amino Acids ($50,000) Research Corporation, 5/96.

Prediction of Absorption and Circular Dichroic Spectra of Peptides ($50,000) ND EPSCoR 12/95.

Theoretical UV Absorption and Circular Dichroic Spectra of Conformationally Restricted Peptides ($477,949)NSF Career Development Plan, 10/95.

Dynamic Simulations of Diffusion Influenced Protein-Protein Association: Cytochrome c Binding to Plastocyanin or Monoclonal Antibody ($20,000) American Chemical Society - Petroleum Research Fund of the American Chemical Society, 6/95.

Protein Flexibility in Brownian Dynamic Simulations of Protein-Protein and Protein-DNA Interactions ($350,000) NIH First Program, 3/95.

Brownian and Molecular Dynamics of Cytochrome Proteins" ($20,000) American Chemical Society - Petroleum Research Fund Type G, 3/95.

Theoretical π–π^* Absorption and Circular Dichroic Spectra of Peptides ($400,000) NSF Career Development Plan, 10/94.

Theoretical Investigations of Structure-Function Relationships of Peptides and Proteins Using Brownian Dynamics and Optical Property Predictions ($20,000) American Chemical Society - Petroleum Research Fund, 3/94.

Brownian Dynamics of Protein-Protein Associations and Prediction of Optical Properties of Peptides ($25,000) Dreyfus Foundation, 6/93.

Optical and Binding Properties of Peptides and Proteins ($350,000) NIH, 3/93.

(internal: 5 total, 2 since promotion to associate professor, one since promotion to full professor)

‡Glycolytic Enzyme Interactions with F-actin and the Influence of These Interactions on Enzyme Catalysis. ND EPSCoR AURA Program. PI: Kathryn Thomasson. $7,400. 5/16/06-12/8/06.

*Physical Chemistry Laboratory, Why Do Students Burn Out? ($3,000) Bush Teaching Scholars, 2/01.

*Applying the Dipole Interaction Model to the Prediction of the Circular Dichroic Spectrum of the Flexible Peptide, Cyclo(Gly-Pro-Gly)$_2$. ($1,232) Senate Scholarly Activities Committee, 11/00.

Purchase of a Constant Temperature Water Bath to Teach Temperature Dependent Kinetics to Students in Physical Chemistry Laboratories. ($1,000) Instructional Development, 1/99.

The Effect of Ionic Strength on Brownian Dynamics Simulations of Cro Repressor Protein Interacting with DNA ($5,400) UND Summer Graduate Research Professorship, 1/98.

(ii) Multiple Investigator Grants (8 total; 2 since promotion to associate professor, 5 since promotion to full)

(participation as PI or co-PI)

‡Interactions of Glycolytic Enzymes with Cytoskeletal Structures in the Brain. NIH/NIGMS. PI: Kathryn Thomasson, co-PIs: Evguenii Kozliak and Barry Milavetz. $837,600, 1/1/2007-12-31-2009.

‡MRI: Acquisition of a High Performance Computer to Support Multi-Scale, Multi-Phenomena Modeling at the University Of North Dakota. NSF. PI: Mark Hoffmann, Co-PIs: Kathryn Thomasson, Juana Moreno, Leon Osborne, Richard Schultz. $992,324, 7/1/06-6/30/07.

‡Quantum & Classical Predictions of UV CD for Proteins, NIH/NIGMS, ($1,000,000). I am PI with Mark Hoffmann as co-PI (12-04).

‡Development of MacroDox & HARLEM Biomodeling Package. NIH/NIGMS. PI: Kathryn Thomasson. Co-PI: Igor Kurnikov, University of Pittsburgh. 11/04.

‡MRI: Acquisition of a High Performance Computer to Support Multi-scale, Multi-phenomena Modeling at the University of North Dakota. NSF/MRI. PI: Mark Hoffmann, co-PIs: Richard Schultz, Leon Osborne, Kathryn Thomasson. Contributors: Juana Moreno, Ronald Marsh. Requested $2,000,000. Declined June 2005.

‡Graduate Training and Research in Multi-scale, Multi-phenomena Modeling. NSF/IGERT. PI: Mark Hoffmann, co-PIs: Richard Schultz, Leon Osborne, Kathryn Thomasson. $2 Contributors: Juana Moreno, Ronald Marsh. Declined May 2005.

(participation as contributor)

‡Two-prong Approach: Carbonic Anhydrase Inhibitor Design. NIH/NIGMS. PIs: Sanku Mallik and D. K. Srivistava. Fall 2004.

*Environmental and Biological Fates of Combustion Generated Heavy Metals, DOE EPSCoR ($1,000,000). Mark Hoffmann (PI). Fall 2004.

Acquisition of a 500 MHz NMR Spectrometer for Research and Education in Chemistry ($389,984) National Science Foundation, MRI Program (instrumentation), S. Mallik and I. Smoliakova (PIs), 2/97.

PROFESSIONAL ASSOCIATIONS

(* after promotion to associate professor, ‡after promotion to full professor)

A. Memberships:

American Chemical Society:
Very active in local section and attend national meetings.

Biophysical Society:
Attend national meetings.

Iota Sigma Pi, National Honor Society for Women in Chemistry:
Very active on both the local and *‡national level including sitting on scholarship committees, writing articles for national newsletters, recruiting and nominating members, and serving as a local representative at national meetings.

Sigma Xi:
Active in local section.

Association for Women in Science:
Active locally. Occasional correspondence with other members nationally.

B. Offices Held:

‡National Director for Student Awards for Iota Sigma Pi, July 2005 - current.
*Members at Large Coordinator (worldwide) for Iota Sigma Pi, July 1999 - June 2005.
*President, UND Chapter of Sigma Xi, June 1999-2000
Vice President, UND Chapter of Sigma Xi, June 1998-May 1999
Faculty Liaison Officer, Members at Large Chapter, Iota Sigma Pi, 1997-current
Member at Large Officer in the Red River Valley ACS section, 1997-1999*
Members at Large Scholarship Committee Member, Iota Sigma Pi, 1992-current
Undergraduate Excellence Award Committee Member, Iota Sigma Pi, 1996
Gladys Emerson-Anderson Scholarship Committee Member, Iota Sigma Pi, 1995
Anna Louise Hoffman Award Committee Member, Iota Sigma Pi, 1994
President, Iota Sigma Pi, Aurum Chapter, 1985-1986
Treasurer, Iota Sigma Pi, Aurum Chapter, 1988-1989
Membership Chair, Iota Sigma Pi, Aurum Chapter, 1987-1988
Historian, Iota Sigma Pi, Aurum Chapter, 1984-1985

PROFESSIONAL EDUCATION

(* after promotion to associate professor, ‡after promotion to full professor)

‡Invited Participant, "A Short Course in Circular Dichroism Spectroscopy of Proteins & Nucleic Acids", Brookhaven National Laboratory, June 25-29, 2007.

*Participant, OID Discussion "Undergraduate Teaching Assistants - Good Pedagogy or Economic Necessity?" April 21, 2004.

*Participant, OID Discussion "Informing Practice: Getting Students to Value Research". Feb. 19, 2003.

*Participant in NCSA Workshop on Biomedical Applications of Molecular Dynamics on the TeraGrid. University of Illinois. Participated through the AccessGrid at North Dakota State University, April 17-19, 2002.

*Participant in the First Annual Institutional Development Award (IDeA), BRIN Bioinformatics Workshop, Los Alamos, NM March 8-9, 2002.

*Participant in the UND Grantwriting Workshop, Feb - May, 2001.
*Participant, WAC Discussion "Teaching with Writing Groups", Nov. 30, 2000.
*Participant, OID Discussion "Teaching with Technology" Nov. 14, 2000.
*Participant, OID Discussion "Reshaping Undergraduate Science Education" Nov. 9, 1999.
*Participant, WAC Discussion " Teaching with Writing - Getting Students to Take Writing Seriously" Oct 20, 1999.
*Participant, WAC Discussion "Grading Student Writing - Working with Rubrics" Sept. 23, 1999.
*Panel Member, "Promotion and Tenure Forum" Faculty Panel. Sept. 14, 1999.
*Participant, OID Discussion "Setting and Maintaining High Expectations for Our Students", Sept. 8, 1999.
Participant, NSF Fastlane Workshop, North Dakota State University, Sept. 27, 1998.
Regularly attend Writing Across the Curriculum Meetings, Fall 1994 - current.
Regularly attend Instructional Development meetings, Fall 1996 - current.
Panel Member, "Undergraduate Research: Opportunities for Students.", OID Discussion Series, 1/14/98.
Participant, Putting Your Syllabus on the World Wide Web, August 18 & 19, 1997.
Participant, Text and Academic Authors Workshop #1, Writing A Textbook, Oct. 24, 1997.
Participant in the Faculty Writing Seminar, September 1995 - May 1996.
Participant, Writing Across the Curriculum Half-Day Workshop in Chemistry, May 18, 1995.
Participant, "Filling in the Gaps: What You Always Wanted to Know About Teaching Over Delayed Video", August 28, 1995.
Participant Writing Across the Curriculum Workshop, May 1994.
Participant Alice T. Clark/UND Foundation Scholars Mentoring Program, 1993-4.

AWARDS

*1999	Elected to National Council of Iota Sigma Pi
*1999	(Department of Chemistry) University Award for Departmental Excellence in Research
1994	Elected Full Member of Sigma Xi, The Scientific Research Society
1992	Elected Associate Member of Sigma Xi, The Scientific Research Society
1991	Dreyfus Postdoctoral Fellow (one of 10 in the nation named to teach and do postdoctoral research at an undergraduate institution)
1990 & 93	Official Delegate to Triennial National Convention of Iota Sigma Pi, elected to represent membership
1988	Sigma Xi Grant-in-Aid for graduate research funding
1985	Graduate Teaching Assistant Award, Chemistry
1983	Elected Member Iota Sigma Pi, Honor Society for Women in Chemistry
1979	Earlysville Women's Club Scholarship (for college funding)
	Western Albemarle Library League Scholarship (for college funding)
1978	Ruth B. Huff Scholarship (for college funding)
	Greenwood Ruitan Scholarship (for college funding)
	Charlottesville Soroptomist Scholarship (for college funding)

OTHER

(*After promotion to associate professor. ‡After promotion to full professor.)

Paper Reviewer:
‡Reviewer for *Chemical Research in Toxicology,* 2006- ‡2

‡Reviewer for *Journal of Molecular Graphics and Modeling*, 2006 ‡1
‡Reviewer for *Chirality*, 2005 ‡1
‡Reviewer for *Biochimia et Biophysica Acta*, 2005 ‡1
‡Reviewer for *J. Biomolecular Structure and Dynamics,* 2005 ‡2
‡Reviewer for *Journal of Undergraduate Chemistry Research*, 2004 ‡1
‡Reviewer for *Biophysical Journal*, 2004 — 2006 ‡2
*Reviewer for *Journal of Biological Inorganic Chemistry*, 2002 *1
*Reviewer for *Current Opinions in Structural Biology*, 2001 *1
*Reviewer for *Biochemistry and Cell Biology*, 2001 *1
*Reviewer for *Biopolymers,* 2001 — *2
Reviewer for *Journal of Physical Chemistry*, 1995 — *8, ‡4
Reviewer for *Journal of Chemical Education*, 1998 — *2, ‡1

Grant Reviewer

‡Member, F04B Study Section, National Institutes of Health, Biological Chemistry & Macromolecular Biophysics, July 2007.
‡The BSF (United States-Israel Binational Science Foundation) 2007
‡Reviewer for NSF International Research Fellowship Program Winter 2005/2006
‡Reviewer for NIH Superfund, Summer and Fall 2005
‡Reviewer of grant proposal for the Research Corporation Cottrell College Science Awards, June 2005
‡Reviewer of grant proposal for the Welcome Trust Fund Fellowship. December 2004.
*Ad hoc member of the NIH BBCA study section. October 2003
‡*Ad hoc reviewer for NSF, Chemistry Division Spring 2000, Spring 2004, Fall 2006
*External Reviewer of NDSU Research Development Support Program - Fall 2000
*‡Reviewer of grant proposal for the American Chemical Society's Petroleum Research Fund, 1999, 2003, 2004, 2005
Reviewer for ND EPSCoR REU program, 1995.

External Reviewer for promotion of

‡Barbara Zjac, City University of New York, 2007
*Susan Marine, Miami University, 2003
*John Harwood, Tennessee Tech, 1996 and *2000
Robert Glinski, Tennessee Tech, 1997

‡*Madison's Who's Who*, 2005, 2006 Editions
‡*International Who's Who of Professionals*, 2005-2006 Edition
‡*Strathmore's Who's Who* 2002-2003 and 2003-2004, 2005-2006, 2007-2008 Editions
**Dictionary of International Biography*, Thirty-First Edition, 2004
**International Who's Who of Professional & Business Women*, 2000-2002
**International Who's Who of Professional Educators,* 2004-2005
**Marquis Who's Who in America*, 2002-2004, 2005-2006, 2007.
**Marquis Who's Who of American Women* 2002-2003, 2004-2005 Editions
**America's Registry of Outstanding Professionals* 2002-2003 Edition
**Marquis Who's Who in Science and Engineering* 2003-2004 Edition
‡**Empire Who's Who Executive and Professional Registry*, 2004, 2005-2006 Editions
**AcademicKeys Who's Who in Sciences Higher Education*, 2004 Edition