CURRICULUM VITAE

Andrew David Mesecar, Ph.D.

Purdue University
Department of Biochemistry (Primary)
Department of Biological Sciences (Secondary)
Department of Chemistry (Courtesy)

214 South Martin Jischke Drive
West Lafayette, IN 47097-1971

Telephone: 765-494-1924; e-mail: amesecar@purdue.edu

EDUCATION

University of California Berkeley, CA.	**Post-Doctoral Fellow**	**1999**
University of Notre Dame Notre Dame, IN.	**Ph.D. Biochemistry**	**1995**
Purdue University West Lafayette, IN.	**B.S. Chemistry**	**1988**

POSITIONS AND EXPERIENCE

Purdue University, West Lafayette (August 2015 to present). Head, Department of Biochemistry.

Purdue University, West Lafayette (August 2010 to present) Walther Professor of Cancer Structural Biology. Departments of Biological Sciences (minor) and Chemistry (courtesy).

Purdue University, West Lafayette (August 2010 to present) Deputy Director, Purdue University Center for Cancer Research.

University of Illinois, Chicago (August 2009 to August 2010) Assistant Head, Department of Medicinal Chemistry and Pharmacognosy.

University of Illinois, Chicago (August 2008 to August 2010) Professor, Department of Medicinal Chemistry and Pharmacognosy, the Center for Pharmaceutical Biotechnology and the Institute for Tuberculosis Research.

University of Illinois, Chicago (August 2004 to August 2008) Associate Professor with Tenure, Department of Medicinal Chemistry and Pharmacognosy and the Center for Pharmaceutical Biotechnology.

University of Illinois, Chicago (January 1999 to August 2004) Assistant Professor, Department of Medicinal Chemistry and Pharmacognosy and the Center for Pharmaceutical Biotechnology.

University of California, Berkeley (1995 to 1999) Postdoctoral Research Fellow under *Professor Daniel E. Koshland Jr.*–Department of Molecular and Cell Biology. Research focused on mapping the structural changes that occur along the reaction trajectory of an enzyme-catalyzed reaction by using a combination of methods including cryogenic X-ray crystallography, Laue X-ray diffraction, site-directed mutagenesis, enzyme kinetics and chemical modification.

University of Notre Dame (1988 to 1994) Graduate Research Scientist under *Professor Thomas Nowak*–Department of Chemistry and Biochemistry. Dissertation Title: *"Kinetic Responses and Conformational Changes Required for Yeast Pyruvate Kinase Activation and Catalysis".* Research focused on constructing a kinetic and thermodynamic model for the allosteric regulation of yeast pyruvate kinase and identifying amino acid residues involved in catalysis and regulation.

Purdue University (1987 to 1988) Undergraduate Research Assistant under *Professor Robert F. Brush*–Department of Psychobiology and Endocrinology. Research focused on correlating rat adrenal gland size, weight and in-vitro corticosteroid output with rat behavioral responses, i.e. low or high tolerances to stress and pain.

Purdue University (1986 to 1988) Undergraduate Research Assistant under *Professor David Gorenstein*–Department of Chemistry. Research focused on the isolation and purification of the *lac* repressor head-piece for NMR structure determination.

FELLOWSHIPS, SCHOLARSHIPS AND AWARDS

- **(2014)** Purdue Cancer Research Award – Lafayette Lions Club
- (**2012-2014**) Purdue Bindley Biosciences Center - Research Scholar Award
- **(2010, 2015)** Purdue University Seed Award for research grants over $1M
- (**1999–2000)** American Association of Colleges of Pharmacy New Investigator Award
- (**1995–1998)** U.S. Department of Energy: Post-Doctoral Fellowship Center for Advanced Materials, Lawrence Berkeley National Laboratory
- (**1993–1994)** Reilly Graduate Fellowship: University of Notre Dame
- (**1989–1992)** U.S. Department of Education: Graduate Fellowship. GAANNP Scholarship Program
- (**1984)** U. S. Air Force ROTC Four-Year Scholarship

EDITORIAL BOARDS

- **(2006 to 2008)** Associate Editor, Crystallography Reviews

PROFESSIONAL NOMINATIONS AND SERVICE

- **(2011 to 2014)** Faculty of 1000
- **(2006 to 2008)** Defense Science Study Group. U.S. Department of Defense, DARPA and the Institute for Defense Analyses.
- **(2005 to 2008)** Executive Committee Chairman Macromolecular Diffractometer (MaNDi)-Instrument Development Team (IDT). Elected by an international group of my peers.
- **(2002 to present)** NIH Study Sections –Various

SCIENTIFIC ADVISORY BOARDS

- **(2003 to 2009)** Shamrock Structures, LLC. Woodridge, IL.

PROFESSIONAL COURSES TAUGHT

- (**2003-2004)** American Crystallographic Association Summer School in X-ray Crystallography

PROFESSIONAL COURSES ATTENDED

- **(1999)** Cold Spring Harbor Course in Macromolecular Crystallography

MEMBERSHIPS AND PROFESSIONAL AFFILIATIONS

American Chemical Society-Division of Biological Chemistry, AAAS, American Association for Cancer Research, Protein Society, American Crystallographic Association, American Society of Microbiology.

RESEARCH FUNDING (Current – see next page)

Agency	*Grant Title*	*Total Project Period*	*Total Award*	*Total Direct Costs*	*Total Indirect Costs*	*Current Project Period*	*Current Direct Costs*	*Current Indirect Costs*
Current Grants:								
Agency	***Title***	***Dates***	***Total***	***Direct***	***Indirect***	***Past Year***	***Direct***	***Indirect***
NIH/DHHS 1R01AI085089 (w/ Loyola)	Mechanisms of viral proteases in coronavirus replication and pathogenesis (Role: co-PI)	07/01/2015-6/30/2020	$1,602,986	$1,066,824	$536,162	07/01/2017-6/30/2018	$195,000	$90,000
Walther Cancer Institute	Purdue Cancer Center Recruitment of Cancer-Focused Structural Biologist	07/01/2010-06/30/2018	$2,147,208	$2,147,208	$0	07/01/2017-06/30/2018	$572,932	$0
Walther Cancer Institute	Request for Support to Recruit Deputy Director PUCCR	07/01/2010-06/30/2018	$225,000	$225,000	$0	07/01/2017-06/30/2018	$108,688	$0
NIH/DHHS	Indiana CTSI (Therapeutics)	05/01/2015-04/30/2020	$33,381	$25,559	$7823	05/01/2017-04/30/2018	$33,381	$25,559
Walther Cancer Institute	Medicinal Chemistry Support for Drug Development (w/T. Ratliff)	07/01/2012-10/31/2018	$484,054	$484,054	$0	07/01/2017 -10/31/2018	$338,499	$338,499
PU-EVPRP	New R01 Program w/Arun Ghosh	05/01/2016-12/31/2017	30,000	$28,281	$0	05/01/2016-12/31/2017	$15,980	$15,980

RESEARCH FUNDING

COMPLETED

1R01AI085089 (PI: Mesecar, Andrew and Co-PI Baker, Susan) 07/01/2010-6/30/2015
NIH/NIAID ~$185,000 (Direct /yr to Mesecar)
Proposal Title: Mechanisms of viral proteases in coronavirus replication and pathogenesis
The major objectives of this proposal were to study the structure of coronavirus papain-like proteases (PLPs) and to engineer the PLPs to attenuate the innate immune response of the host.

PC131237
Department of Defense 10/01/2014-9/30/2017
Role (Co-PI:Mesecar) PI: Tim Ratliff, Purdue ~$100K (direct/yr-Mesecar)
Prostate Cancer Research Program Idea Development Award
Project Title: Targeting Sulfotranferase (Sult2B1b) as a regulator of cholesterol metabolism in prostate cancer.
This proposal aims to identify and develop inhibitors of Sult2B1b as a potential treatment of prostate cancer.

NIH/DHHS (Probe Development Center – University of Kansas) 4/01/2014-5/31/2015
Role (PI: Mesecar – Compound Testing) $60,518 direct/yr - Mesecar
Project Title: SARS CoV inhibitors and imaging probes that target the papain-like protease.
The goals of this project were to test the compounds synthesized by the University of Kansas for their potency against the papain-like protease from SARS virus.

2 R01 AI026603-21A1 **(**NIH/NIAID) 7/01/2010 to 6/30/2015
Title: Polymerase Proteins in Coronavirus Replication ~$40K (direct/yr-Mesecar)
Role: Co-Investigator (PI: Mark Denison, Vanderbilt)
The major objectives are to characterize the biochemical, thermal, structure and dynamic properties temperature sensitive mutants of 3CL protease from MHV.

1U01AI077949 (Co-I: Mesecar, Andrew) 10/01/2009 to 08/31/2012
NIH/NIAID $296,160 direct/yr-Mesecar
Proposal Title: Novel antibiotic development for biodefense
PI: Mike Johnson, UIC
This multi-project, collaborative proposal aims to develop an advanced series of broad spectrum antibacterial lead compounds that are safe, efficacious, and orally bioavailable in established animal models.

5 P01 CA48112 (PI: Mesecar, Andrew: Project 3) 05/1/2005 to 4/31/2012
NIH/NCI $129,788 direct/yr-Mesecar
Proposal Title: Natural Inhibitors of Carcinogenesis
Project 4: *Structure-Function Studies of Chemoprevention Targets.*
The major objectives of this project are to determine the mechanisms and x-ray structures of novel chemopreventive protein targets.

5 P01 CA48112 (PI: Mesecar, Andrew: Project 3) 10/1/10 to 9/30/11
NIH/NCI (Competing Supplement) $61,818 direct/yr-Mesecar
Proposal Title: Natural Inhibitors of Carcinogenesis (Supplemental Proposal to Parent P01)
1 P01 AI060915 (PI: Mesecar, Andrew: Project 2) 05/15/2005 to 4/31/2010

NIH NIAID $169,036 direct/yr-Mesecar
Proposal Title: Development of Novel Protease Inhibitors as SARS therapeutics
Project 2: *Mechanistic and crystallographic studies of SARS proteases.*
This was a large program grant aimed at developing novel therapeutic compounds via structure-based approaches to treat SARS infections.

1U19 MH085193-01 (Co-Invest. Project 1: Mesecar, Andrew) 06/01/2009 to 3/30/12
NIH NIMHS NCDDG $75,000 direct/yr -Mesecar
(PI: Kozikowski, Alan)
Proposal Title: Design and Study of New Nicotine Analogs for Use in Depression
This is a multi-project, collaborative proposal. The Mesecar lab role is to determine X-ray structures of the nicotinic acid receptor in complex with designed inhibitors.

1 P01 AI060915 (PI: Mesecar, Andrew: Core B) 05/15/2005 to 4/31/2010
NIH NIAID $94,031 direct/yr-Mesecar
Proposal Title: Development of Novel Protease Inhibitors as SARS therapeutics
Core B: *Protein Expression and Purification.*
This was a large program grant aimed at developing novel therapeutic compounds via structure-based approaches to treat SARS infections. (1 year no cost extension)

1 U19 AI056575 (PI: Mesecar, A. D. Core B) 08/15/2003 to 1/31/2009
NIH/NIAID $145,665 (direct) per year
Novel Therapeutics for Bacillus anthracis
This was a large program grant aimed at developing novel therapeutic compounds via structure-based approaches to treat *Bacillus anthracis* infections. Core B is "Protein Expression and Purification."

R03MH084162 (Co-PI-Mesecar, Andrew) 9/30/2008 - 8/31/2009
NIH NIMH $15,923 direct/yr-Mesecar
Proposal Title: High Throughput Screening for Identifying Lead Compounds Against 3CLpro
Dr. Valerie Grum-Tokars, a research assistant professor in my lab, is serving as the PI.
This was a MLPCN probe-development project.

R03 CA128095 (Co-investigator-Mesecar, Andrew) 4/1/08 to 3/31/10
NIH NCI $50,000 direct/yr-Mesecar
Proposal Title: Investigating Nrf2 phosphorylation in the mechanism of cancer prevention agents
Dr. Aimee Eggler is the PI. She is a research assistant professor in my lab. (1 year no cost extension)

2R01 AI056351-06 (Co-Invest. Mesecar, Andrew) 06/01/09 to 5/31/10 5%
NIH/NIAID $49,370 direct/yr-Mesecar
Proposal Title: Susceptibility and protective immunity to noroviruses
This was a collaborative proposal with Ralph Baric at the University of North Carolina, Chapel Hill to look at the structural evolution of norovirus capsid (PI: Ralph Baric)
1R01CA138762-01 (Co-Investigator. Mesecar, Andrew) 05/01/09 to 4/30/12
$35,100 direct/yr-Mesecar
Proposal Title: Splicing factors as therapeutic targets for the treatment of ovarian cancer
This is an NIH roadmap initiative for novel HTS assay development projects. Our role is to help develop the assays and transition to a robotics platform

1 U19 AI056575 (PI: Mesecar, A. D. Core E) 08/15/2003 to 1/31/2009
NIH/NIAID $269,609 (direct) per year
Novel Therapeutics for Bacillus anthracis
This is a large program grant aimed at developing novel therapeutic compounds via structure-based approaches to treat *Bacillus anthracis* infections. Core E is "High Throughput Bioassays"

2 R41 GM072357 (PI: Mesecar, Andrew) 4/01/2006 to 3/31/2009
NIH/NIGMS $265,708 (Direct for two years)
Novel organophosphorous hydrolases for decontamination (Phase II Application)
This is a Phase II STTR proposal aimed at engineering and industrial scale production of an enzyme that degrades soman gas. Our industrial partner is Lybradyn, Inc.

0410100Z (PI: Mesecar, A. D.) 01/01/2003 to 12/31/2005
American Heart Association $49,000 total grant
Allosteric-site-targeted drug design for pyruvate kinase deficiency.
This is a pre-doctoral fellowship for my graduate student Sasi Kiran Chilukuri. The project involves computational-based discovery of compounds that can modulate the function of red blood cell pyruvate kinase.

5 P01 CA48112 (PI: Mesecar, Andrew) 09/20/2004 to 06/3/2005
NIH/NCI- Bridge Funding $36,613 (direct)
Natural Inhibitors of Carcinogenesis
O235416Z (PI: Mesecar, A. D.) 07/01/2002 to 6/30/2005
American Heart Association $247,500 total grant
The molecular basis for non-spherocytic hemolytic anemia caused by pyruvate kinase deficiency.

The project involves biochemical and structural characterization of point-mutations that cause pyruvate kinase deficiency.

1 R41 GM072357-01 (PI: Mesecar, A. D.) 08/15/2004 to 2/14/2004
NIH/NIGMS $97,082 (Total Direct)
Novel Organophosphorous Hydrolases for Decontamination
This is a Phase 1 STTR grant in collaboration with Lybradyn, Inc. The grant is to develop expression vectors for industrial scale production of our enzymes that degrade chemical warfare agents.

1 S10 RR017744-01 (PI: Mesecar, A. D.) 03/01/2003 to 02/31/2004 NIH/NCRR
$346,385 (Total Direct)
Macromolecular x-ray structure facility instrumentation.
This proposal is for the acquisition of a new x-ray detector system for protein crystallography and an update to our existing detector.

N000140210956 (PI: Mesecar, A. D.) 08/15/2002 to 08/14/2004
Office of Naval Research $200,000 (Total)
"Novel Organophosphorous Hydrolases for Homeland Defense"
This project involves structure-based engineering of organophosphorous hydrolases with enhanced activity towards chemical warfare agents and pesticides.

1 R03 CA92744-01 (PI: Mesecar, A. D.) 07/01/2001 to 06/30/2003
NIH/NCI $155,870 (Total)
A Molecular basis for phytoestrogen chemoprevention

The project involves the x-ray structure determination of phytoestrogen compounds, isolated from plant extracts such as hops and licorice, in complex with the estrogen receptors alpha and beta.

1 S10 RR-16848-01 (PI: Mesecar, A. D.) 04/01/2002 to 03/30/2003
NIH/NCRR $273,800 (Total Direct)
Small molecule x-ray diffraction instrumentation
The proposal is for the acquisition of small molecule x-ray instrumentation.

Type 1 Project (PI: Mesecar, A. D.) 06/01/2001 to 05/31/2002
UIC Campus Research Board $15,000 (Total Direct)
Structural Changes During Enzyme Catalysis
The project involves solving the x-ray structures of trapped enzyme intermediate complexes of the isocitrate dehydrogenase reaction and constructing a molecular movie from the data.

P50 AT00155 (PI: Farnsworth, N.) 08/31/2000 to 08/30/2001
UIC/NIH Center for Botanical Dietary Supplements Research $36,862 (Total)
A 3D-Structure based approach to characterization of natural products in dietary botanical extracts that exhibit estrogenic or anti-estrogenic activity
The project involves determination of estrogenic activity of phytoestrogen compounds isolated from soy and red clover plant extracts via x-ray crystallography.

Functional Foods for Health (PI: Mesecar, A. D.) 03/01/2001 to 03/31/2003
$20,000 (Total Direct)
Do green tea catechins act as phytoestrogens?
This project involves determining the dissociation constants for of a series of catechins with the estrogen receptors and then determining the x-ray structure of the tightest binding ligand.

Hans Vahlteich Foundation (PI: Mesecar, A.D.) 02/01/00 to 01/31/01
$40,000 (Total Direct)
"Structure and function studies of pyruvate kinase isozymes implicated in disease"

New Investigators Award (PI: Mesecar, A.D.) 12/1/1999 to 11/30/2000
American Association of Colleges of Pharmacy $10,000 total
A new paradigm for rational drug design: Allosteric-site based drug design as a potential therapy for treating pyruvate kinase associated diseases
The project involves making site-directed mutants to study the allosteric activation of pyrvuate kinase.

United States Department of Energy (PI: Mesecar, A.D.) 06/15/1999 to 03/31/2000
$76,850 total
"*Enzyme engineering for biodegradation of chlorinated organic pollutants"*
The project involves purification and crystallization of the enzyme pentachlorophenol hydroxylase.

Type 1 Project (PI: Mesecar, A.D.) 12/31/1998 to 12/30/1999
UIC Campus Research Board $15,000
"Molecular Basis for pyruvate kinase associated diseases"
The project involves making site-directed mutants to study the allosteric activation of pyrvuate kinase.

PUBLICATIONS

Google Scholar Statistics: Overall h-Index = 44, i10-index = 111, Citations = 7,076

My Graduate Students are highlighted in **Bold** with an **Asterisk ***

Graduate Students who got a publication from a rotation in my lab are indicated with **

2019

135. Vickman RE, Yang J, Lanman NA, Cresswell GM, Zheng F, Zhang C, Doerge RW, Crist SA, Mesecar AD, Hu CD, Ratliff TL. Cholesterol Sulfotransferase SULT2B1b Modulates Sensitivity to Death Receptor Ligand TNFα in Castration-Resistant Prostate Cancer. Mol Cancer Res. 2019 Mar 1.

134. Ghosh AK, Brindisi M, ***Yen YC**, ***Lendy EK**, Kovela S, Cárdenas EL, Reddy BS, Rao KV, Downs D, Huang X, Tang J, Mesecar AD. Highly Selective and Potent Human β-Secretase 2 (BACE2) Inhibitors against Type 2 Diabetes: Design, Synthesis, X-ray Structure and Structure Activity Relationship Studies. ChemMedChem. 2019 Mar 5;14(5):545-560. **(Featured on the Journal Cover)**

2018

133. Ghosh AK, Ghosh K, Brindisi M, ***Lendy EK**, ***Yen YC**, Kumaragurubaran N, Huang X, Tang J, Mesecar AD. Design, synthesis, X-ray studies, and biological evaluation of novel BACE1 inhibitors with bicyclic isoxazoline carboxamides as the P3 ligand. Bioorg Med Chem Lett. 2018 Aug 15;28(15):2605-2610.

2017

132. Abuhammad, A., R.A. Al-Aqtash, ***B.J.Anson,** A.D. Mesecar, and M.O. Taha, *Computational modeling of the bat HKU4 coronavirus 3CLpro inhibitors as a tool for the development of antivirals against the emerging Middle East respiratory syndrome (MERS) coronavirus.* J Mol Recognit, 2017. **30**(11).

131. ***Clasman, J.R.**, ***Y.M. Baez-Santos**, R.C. Mettelman, A. O'Brien, S.C. Baker, and A.D. Mesecar, *X-ray Structure and Enzymatic Activity Profile of a Core Papain-like Protease of MERS Coronavirus with utility for structure-based drug design.* Sci Rep, 2017. **7**: p. 40292.

130. Daczkowski, C.M., J.V. Dzimianski, ***J.R. Clasman**, O. Goodwin, A.D. Mesecar, and S.D. Pegan, *Structural Insights into the Interaction of Coronavirus Papain-Like Proteases and Interferon-Stimulated Gene Product 15 from Different Species.* J Mol Biol, 2017. **429**(11): p. 1661-1683.

129. Ghosh, A.K., M. Brindisi, ***Y.C. Yen**, E.L. Cardenas, J.R. Ella-Menye, N. Kumaragurubaran, X. Huang, J. Tang, and A.D. Mesecar, *Design, synthesis, and X-ray structural studies of BACE-1 inhibitors containing substituted 2-oxopiperazines as P1'-P2' ligands.* Bioorg Med Chem Lett, 2017. **27**(11): p. 2432-2438.

2016

128. ***Hjortland, N.M.** and A.D. Mesecar, *Steady-state kinetic studies reveal that the anti-cancer target Ubiquitin-Specific Protease 17 (USP17) is a highly efficient deubiquitinating enzyme.* Arch Biochem Biophys, **2016**. **612**: p. 35-45.

127. Ghosh, A.K., B.S. Reddy, ***Y.C. Yen**, E. Cardenas, K.V. Rao, D. Downs, X. Huang, J. Tang, and A.D. Mesecar, Design of Potent and Highly Selective Inhibitors for Human beta-Secretase 2 (Memapsin 1), a Target for Type 2 Diabetes. Chem Sci, **2016**. 7: p. 3117-3122.

126. St John, S.E., ***B.J. Anson**, and A.D. Mesecar, X-Ray Structure and Inhibition of 3C-like Protease from Porcine Epidemic Diarrhea Virus. Sci Rep, **2016**. 6: p. 25961.

125. Vickman, R.E., S.A. Crist, K. Kerian, L. Eberlin, R.G. Cooks, G.N. Burcham, K.K. Buhman, C.D. Hu, A.D. Mesecar, L. Cheng, and T.L. Ratliff, Cholesterol Sulfonation Enzyme, SULT2B1b, Modulates AR and Cell Growth Properties in Prostate Cancer. Mol Cancer Res, **2016**. 14(9): p. 776-86.

2015

124. ***Baez-Santos, Y.M.**, S.E. St John, and A.D. Mesecar, The SARS-coronavirus papain-like protease: structure, function and inhibition by designed antiviral compounds. Antiviral Res, **2015**. 115: p. 21-38. ***Highlighted Paper of the Month -January***

123. ***Chen, Y.,** S.N. Savinov, A.M. Mielech, T. Cao, S.C. Baker, and A.D. Mesecar, X-ray Structural and Functional Studies of the Three Tandemly Linked Domains of Non-structural Protein 3 (nsp3) from Murine Hepatitis Virus Reveal Conserved Functions. J Biol Chem, **2015**. 290(42): p. 25293-306.

122. Ghosh, A.K., M. Brindisi, ***Y.C. Yen**, X. Xu, X. Huang, T. Devasamudram, G. Bilcer, H. Lei, G. Koelsch, A.D. Mesecar, and J. Tang, Structure-based design, synthesis and biological evaluation of novel beta-secretase inhibitors containing a pyrazole or thiazole moiety as the P3 ligand. Bioorg Med Chem Lett, **2015**. 25(3): p. 668-72.

121. Jain, A.D., H. Potteti, B.G. Richardson, L. Kingsley, ***J.P. Luciano**, ***A.F. Ryuzoji**, H. Lee, A. Krunic, A.D. Mesecar, S.P. Reddy, and T.W. Moore, Probing the structural requirements of non-electrophilic naphthalene-based Nrf2 activators. Eur J Med Chem, **2015**. 103: p. 252-68.

120. Mielech, A.M., X. Deng, ***Y. Chen**, E. Kindler, D.L. Wheeler, A.D. Mesecar, V. Thiel, S. Perlman, and S.C. Baker, Murine coronavirus ubiquitin-like domain is important for papain-like protease stability and viral pathogenesis. J Virol, **2015**. 89(9): p. 4907-17.

119. St John, S.E., ****M.D. Therkelsen**, P.R. Nyalapatla, H.L. Osswald, A.K. Ghosh, and A.D. Mesecar, X-ray structure and inhibition of the feline infectious peritonitis virus 3C-like protease: Structural implications for drug design. Bioorg Med Chem Lett, **2015**. 25(22): p. 5072-7.

118. St John, S.E., ***S. Tomar**, S.R. Stauffer, and A.D. Mesecar, Targeting zoonotic viruses: Structure-based inhibition of the 3C-like protease from bat coronavirus HKU4--The likely reservoir host to the human coronavirus that causes Middle East Respiratory Syndrome (MERS). Bioorg Med Chem, **2015**. 23(17): p. 6036-48. ***Featured on the Cover***

117. ***Tomar, S.,** M.L. Johnston, S.E. St John, H.L. Osswald, P.R. Nyalapatla, L.N. Paul, A.K. Ghosh, M.R. Denison, and A.D. Mesecar, Ligand-induced Dimerization of Middle East

Respiratory Syndrome (MERS) Coronavirus nsp5 Protease (3CLpro): IMPLICATIONS FOR nsp5 REGULATION AND THE DEVELOPMENT OF ANTIVIRALS. J Biol Chem, **2015**. 290(32): p. 19403-22. ***Featured in August, 2015 Edition of ASBMB Today. Targeting the Achilles' heel of MERS virus: Molecules shut down activity of an essential viral replication enzyme. By Elizabeth Gardner.***

2014

116. Zhai, X., Go, M. K., O'Donoghue, A. C., Amyes, T. L., Pegan, S. D., Wang, Y., Loria, J. P., Mesecar, A. D. and Richard, J. P. (**2014**). "Enzyme architecture: the effect of replacement and deletion mutations of loop 6 on catalysis by triosephosphate isomerase." *Biochemistry* **53**(21): 3486-501.

115. ***Ratia, K.,** Kilianski, A., ***Baez-Santos**, Y. M., Baker, S. C. and Mesecar, A. D. (**2014**). "Structural Basis for the Ubiquitin-Linkage Specificity and deISGylating activity of SARS-CoV papain-like protease." *PLoS pathogens* **10**(5): e1004113.

114. Molland, K., ***Zhou, Q.** and Mesecar, A. D. (**2014**). "A 2.2 A resolution structure of the USP7 catalytic domain in a new space group elaborates upon structural rearrangements resulting from ubiquitin binding." *Acta crystallographica. Section F, Structural biology communications* **70**(Pt 3): 283-7.

113. Mielech, A. M., Kilianski, A., ***Baez-Santos, Y. M.,** Mesecar, A. D. and Baker, S. C. (**2014**). "MERS-CoV papain-like protease has deISGylating and deubiquitinating activities." *Virology* **450-451**: 64-70.

112. Mielech, A. M., ***Chen, Y.,** Mesecar, A. D. and Baker, S. C. (**2014**). "Nidovirus papain-like proteases: Multifunctional enzymes with protease, deubiquitinating and deISGylating activities." *Virus research* **194**: 184-90.

111. Lv, W., Banerjee, B., Molland, K. L., Seleem, M. N., Ghafoor, A., Hamed, M. I., Wan, B., Franzblau, S. G., Mesecar, A. D. and Cushman, M. (**2014**). "Synthesis of 3-(3-aryl-pyrrolidin-1-yl)-5-aryl-1,2,4-triazines that have antibacterial activity and also inhibit inorganic pyrophosphatase." *Bioorganic & medicinal chemistry* **22**(1): 406-18.

110. Deng, X., St. John, S. E., Osswald, H. L., O'Brien, A., Banach, B. S., Sleeman, K., Ghosh, A. K., Mesecar, A. D. and Baker, S. C. (**2014**). "Coronaviruses resistant to a 3C-like protease inhibitor are attenuated for replication and pathogenesis, revealing a low genetic barrier but high fitness cost of resistance." *Journal of virology* **88**(20): 11886-98.

109. Deng, X., Agnihothram, S., Mielech, A. M., Nichols, D. B., Wilson, M. W., St.John, S. E., Larsen, S. D., Mesecar, A. D., Lenschow, D. J., Baric, R. S. and Baker, S. C. (**2014**). "A chimeric virus-mouse model system for evaluating the function and inhibition of papain-like proteases of emerging coronaviruses." *Journal of virology* **88**(20): 11825-33.

108. ***Baez-Santos, Y. M.,** Mielech, A. M., Deng, X., Baker, S. and Mesecar, A. D. (**2014**). "Catalytic function and substrate specificity of the papain-like protease domain of nsp3 from the Middle East respiratory syndrome coronavirus." *Journal of virology* **88**(21): 12511-27.

107. ***Baez-Santos, Y. M.,** Barraza, S. J., Wilson, M. W., Agius, M. P., Mielech, A. M., ***Davis, N. M.**, Baker, S. C., Larsen, S. D. and Mesecar, A. D. (**2014**). "X-ray structural

and biological evaluation of a series of potent and highly selective inhibitors of human coronavirus papain-like proteases." *Journal of medicinal chemistry* **57**(6): 2393-412.

106. Agnihothram, S., Yount, B. L., Jr., Donaldson, E. F., Huynh, J., Menachery, V. D., Gralinski, L. E., Graham, R. L., Becker, M. M., ***Tomar, S.,** Scobey, T. D., Osswald, H. L., Whitmore, A., Gopal, R., Ghosh, A. K., Mesecar, A., Zambon, M., Heise, M., Denison, M. R. and Baric, R. S. (**2014**). "A mouse model for Betacoronavirus subgroup 2c using a bat coronavirus strain HKU5 variant." *mBio* **5**(2): e00047-14.

2013

105. Turlington, M., Chun, A., ***Tomar, S.,** Eggler, A., Grum-Tokars, V., Jacobs, J., Daniels, J. S., Dawson, E., Saldanha, A., Chase, P., ***Baez-Santos**, Y. M., Lindsley, C. W., Hodder, P., Mesecar, A. D. and Stauffer, S. R. (**2013**). "Discovery of N-(benzo[1,2,3]triazol-1-yl)-N-(benzyl)acetamido)phenyl) carboxamides as severe acute respiratory syndrome coronavirus (SARS-CoV) 3CLpro inhibitors: identification of ML300 and noncovalent nanomolar inhibitors with an induced-fit binding." *Bioorganic & medicinal chemistry letters* **23**(22): 6172-7.

104. Stobart, C. C., Sexton, N. R., Munjal, H., Lu, X., Molland, K. L., ***Tomar, S.,** Mesecar, A. D. and Denison, M. R. (**2013**). "Chimeric exchange of coronavirus nsp5 proteases (3CLpro) identifies common and divergent regulatory determinants of protease activity." *Journal of virology* **87**(23): 12611-8.

103. St John, S. E., ***Jensen, K. C.,** Kang, S., ***Chen, Y.,** ***Calamini, B.,** Mesecar, A. D. and Lipton, M. A. (**2013**). "Design, synthesis, biological and structural evaluation of functionalized resveratrol analogues as inhibitors of quinone reductase 2." *Bioorganic & medicinal chemistry* **21**(19): 6022-37.

102. Pegan, S. D., Rukseree, K., Capodagli, G. C., Baker, E. A., Krasnykh, O., Franzblau, S. G. and Mesecar, A. D. (**2013**). "Active site loop dynamics of a class IIa fructose 1,6-bisphosphate aldolase from Mycobacterium tuberculosis." *Biochemistry* **52**(5): 912-25.

101. Jacobs, J., Grum-Tokars, V., Zhou, Y., Turlington, M., Saldanha, S. A., Chase, P., Eggler, A., Dawson, E. S., ***Baez-Santos, Y. M.**, ***Tomar, S.**, Mielech, A. M., Baker, S. C., Lindsley, C. W., Hodder, P., Mesecar, A. and Stauffer, S. R. (**2013**). "Discovery, synthesis, and structure-based optimization of a series of N-(tert-butyl)-2-(N-arylamido)-2-(pyridin-3-yl) acetamides (ML188) as potent noncovalent small molecule inhibitors of the severe acute respiratory syndrome coronavirus (SARS-CoV) 3CL protease." *Journal of medicinal chemistry* **56**(2): 534-46.

2012

100. Hu, C., Nikolic, D., Eggler, A. L., Mesecar, A. D. and van Breemen, R. B. (**2012**). "Screening for natural chemoprevention agents that modify human Keap1." *Analytical biochemistry* **421**(1): 108-14.

99. Reddy, P. V., ***Jensen, K. C.,** Mesecar, A. D., Fanwick, P. E. and Cushman, M. (**2012**). "Design, synthesis, and biological evaluation of potent quinoline and pyrroloquinoline ammosamide analogues as inhibitors of quinone reductase 2." *Journal of medicinal chemistry* **55**(1): 367-77.

98. Volkova, M. S., ***Jensen, K. C.**, Lozinskaya, N. A., Sosonyuk, S. E., Proskurnina, M. V., Mesecar, A. D. and Zefirov, N. S. (**2012**). "Synthesis of novel capital EM, Cyrilliccapital TE, Cyrillic3 receptor ligands via an unusual Knoevenagel condensation." *Bioorganic & medicinal chemistry letters* **22**(24): 7578-81.

2011

97. Yang, J. H., Kondratyuk, T. P., ***Jermihov, K. C.,** Marler, L. E., Qiu, X., Choi, Y., Cao, H., Yu, R., ***Sturdy, M.**, Huang, R., Liu, Y., Wang, L. Q., Mesecar, A. D., van Breemen, R. B., Pezzuto, J. M., Fong, H. H., Chen, Y. G. and Zhang, H. J. (**2011**). "Bioactive compounds from the fern Lepisorus contortus." *Journal of natural products* **74**(2): 129-36.

96. ***Wubben, T.** and Mesecar, A. D. (**2011**). "Structure of Mycobacterium tuberculosis phosphopantetheine adenylyltransferase in complex with the feedback inhibitor CoA reveals only one active-site conformation." *Acta crystallographica. Section F, Structural biology and crystallization communications* **67**(Pt 5): 541-5.

95. Pegan, S. D., ***Sturdy, M.,** Ferry, G., Delagrange, P., Boutin, J. A. and Mesecar, A. D. (**2011**). "X-ray structural studies of quinone reductase 2 nanomolar range inhibitors." *Protein science : a publication of the Protein Society* **20**(7): 1182-95.

94. Park, S. K., Pegan, S. D., Mesecar, A. D., Jungbauer, L. M., LaDu, M. J. and Liebman, S. W. (**2011**). "Development and validation of a yeast high-throughput screen for inhibitors of Abeta(4)(2) oligomerization." *Disease models & mechanisms* **4**(6): 822-31.

93. Kozikowski, A. P., Gunosewoyo, H., Guo, S., Gaisina, I. N., Walter, R. L., Ketcherside, A., McClung, C. A., Mesecar, A. D. and Caldarone, B. (**2011**). "Identification of a glycogen synthase kinase-3beta inhibitor that attenuates hyperactivity in CLOCK mutant mice." *ChemMedChem* **6**(9): 1593-602.

92. Kondratyuk, T. P., Park, E. J., Marler, L. E., Ahn, S., Yuan, Y., Choi, Y., Yu, R., van Breemen, R. B., Sun, B., Hoshino, J., Cushman, M., ***Jermihov, K. C.,** Mesecar, A. D., Grubbs, C. J. and Pezzuto, J. M. (**2011**). "Resveratrol derivatives as promising chemopreventive agents with improved potency and selectivity." *Molecular nutrition & food research* **55**(8): 1249-65.

91. Hu, C., Eggler, A. L., Mesecar, A. D. and van Breemen, R. B. (**2011**). "Modification of keap1 cysteine residues by sulforaphane." *Chemical research in toxicology* **24**(4): 515-21.

90. Choi, Y., ***Jermihov, K.,** Nam, S. J., ***Sturdy, M.,** Maloney, K., Qiu, X., Chadwick, L. R., Main, M., Chen, S. N., Mesecar, A. D., Farnsworth, N. R., Pauli, G. F., Fenical, W., Pezzuto, J. M. and van Breemen, R. B. (**2011**). "Screening natural products for inhibitors of quinone reductase-2 using ultrafiltration LC-MS." *Analytical chemistry* **83**(3): 1048-52.

2010

89. Yang, J. H., Kondratyuk, T. P., Marler, L. E., Qiu, X., Choi, Y., Cao, H., Yu, R., ***Sturdy, M.,** Pegan, S., Liu, Y., Wang, L. Q., Mesecar, A. D., Van Breemen, R. B., Pezzuto, J. M., Fong, H. H., Chen, Y. G. and Zhang, H. J. (**2010**). "Isolation and evaluation of kaempferol glycosides from the fern Neocheiropteris palmatopedata." *Phytochemistry* **71**(5-6): 641-7.

88. ***Wubben, T. J.** and Mesecar, A. D. (**2010**). "Kinetic, thermodynamic, and structural insight into the mechanism of phosphopantetheine adenylyltransferase from Mycobacterium tuberculosis." *Journal of molecular biology* **404**(2): 202-19.

87. Sun, B., Hoshino, J., ***Jermihov, K.,** Marler, L., Pezzuto, J. M., Mesecar, A. D. and Cushman, M. (**2010**). "Design, synthesis, and biological evaluation of resveratrol analogues as aromatase and quinone reductase 2 inhibitors for chemoprevention of cancer." *Bioorganic & medicinal chemistry* **18**(14): 5352-66.

86. ***Small, E.,** Eggler, A. and Mesecar, A. D. (**2010**). "Development of an efficient E. coli expression and purification system for a catalytically active, human Cullin3-RINGBox1 protein complex and elucidation of its quaternary structure with Keap1." *Biochemical and biophysical research communications* **400**(4): 471-5.

85. Pegan, S. D., ***Tian, Y., *Sershon, V.** and Mesecar, A. D. (**2010**). "A universal, fully automated high throughput screening assay for pyrophosphate and phosphate release from enzymatic reactions." *Combinatorial chemistry & high throughput screening* **13**(1): 27-38. ***(Featured on Cover)***

84. Ghosh, A. K., Takayama, J., Rao, K. V., ***Ratia, K.,** Chaudhuri, R., Mulhearn, D. C., Lee, H., Nichols, D. B., Baliji, S., Baker, S. C., Johnson, M. E. and Mesecar, A. D. (**2010**). "Severe acute respiratory syndrome coronavirus papain-like novel protease inhibitors: design, synthesis, protein-ligand X-ray structure and biological evaluation." *Journal of medicinal chemistry* **53**(13): 4968-79.

83. Conda-Sheridan, M., Marler, L., Park, E. J., Kondratyuk, T. P., ***Jermihov, K.,** Mesecar, A. D., Pezzuto, J. M., Asolkar, R. N., Fenical, W. and Cushman, M. (**2010**). "Potential chemopreventive agents based on the structure of the lead compound 2-bromo-1-hydroxyphenazine, isolated from Streptomyces species, strain CNS284." *Journal of medicinal chemistry* **53**(24): 8688-99.

82. Clementz, M. A., Chen, Z., Banach, B. S., Wang, Y., Sun, L., ***Ratia, K., *Baez-Santos, Y. M.,** Wang, J., Takayama, J., Ghosh, A. K., Li, K., Mesecar, A. D. and Baker, S. C. (**2010**). "Deubiquitinating and interferon antagonism activities of coronavirus papain-like proteases." *Journal of virology* **84**(9): 4619-29.

81. ***Calamini, B., *Ratia, K.**, Malkowski, M. G., Cuendet, M., Pezzuto, J. M., Santarsiero, B. D. and Mesecar, A. D. (**2010**). "Pleiotropic mechanisms facilitated by resveratrol and its metabolites." *The Biochemical journal* **429**(2): 273-82.

80. Burks, E. A., Fleming, C. D., Mesecar, A. D., Whitman, C. P. and Pegan, S. D. (**2010**). "Kinetic and structural characterization of a heterohexamer 4-oxalocrotonate tautomerase from Chloroflexus aurantiacus J-10-fl: implications for functional and structural diversity in the tautomerase superfamily." *Biochemistry* **49**(24): 5016-27. ***(Featured on Cover)***

2009

79. Zhang, H., Rothwangl, K., Mesecar, A. D., Sabahi, A., Rong, L. and Fong, H. H. (**2009**). "Lamiridosins, hepatitis C virus entry inhibitors from Lamium album." *Journal of natural products* **72**(12): 2158-62.

78. ***Sershon, V. C.,** Santarsiero, B. D. and Mesecar, A. D. (**2009**). "Kinetic and X-ray structural evidence for negative cooperativity in substrate binding to nicotinate

mononucleotide adenylyltransferase (NMAT) from Bacillus anthracis." *Journal of molecular biology* **385**(3): 867-88.

77. Pegan, S. D., Rukseree, K., Franzblau, S. G. and Mesecar, A. D. (**2009**). "Structural basis for catalysis of a tetrameric class IIa fructose 1,6-bisphosphate aldolase from Mycobacterium tuberculosis." *Journal of molecular biology* **386**(4): 1038-53. (**Featured on Cover of JMB and Featured as Molecular of the Month, Rigaku MSC**).

76. Maiti, A., Reddy, P. V., ***Sturdy, M.,** Marler, L., Pegan, S. D., Mesecar, A. D., Pezzuto, J. M. and Cushman, M. (**2009**). "Synthesis of casimiroin and optimization of its quinone reductase 2 and aromatase inhibitory activities." *Journal of medicinal chemistry* **52**(7): 1873-84.

75. Kim, K. H., Gaisina, I., Gallier, F., Holzle, D., Blond, S. Y., Mesecar, A. and Kozikowski, A. P. (**2009**). "Use of molecular modeling, docking, and 3D-QSAR studies for the determination of the binding mode of benzofuran-3-yl-(indol-3-yl)maleimides as GSK-3beta inhibitors." *Journal of molecular modeling* **15**(12): 1463-79.

74. ***Hawwa, R., *Larsen, S. D., *Ratia, K.** and Mesecar, A. D. (**2009**). "Structure-based and random mutagenesis approaches increase the organophosphate-degrading activity of a phosphotriesterase homologue from Deinococcus radiodurans." *Journal of molecular biology* **393**(1): 36-57.

73. ***Hawwa, R.,** Aikens, J., Turner, R. J., Santarsiero, B. D. and Mesecar, A. D. (**2009**). "Structural basis for thermostability revealed through the identification and characterization of a highly thermostable phosphotriesterase-like lactonase from Geobacillus stearothermophilus." *Archives of biochemistry and biophysics* **488**(2): 109-20. ***(Featured on August 15th Cover)***

72. Guo, S., Tipparaju, S. K., Pegan, S. D., Wan, B., Mo, S., Orjala, J., Mesecar, A. D., Franzblau, S. G. and Kozikowski, A. P. (**2009**). "Natural product leads for drug discovery: isolation, synthesis and biological evaluation of 6-cyano-5-methoxyindolo[2,3-a]carbazole based ligands as antibacterial agents." *Bioorganic & medicinal chemistry* **17**(20): 7126-30.

71. Ghosh, A. K., Takayama, J., Aubin, Y., ***Ratia, K.,** Chaudhuri, R., ***Baez, Y.,** Sleeman, K., Coughlin, M., Nichols, D. B., Mulhearn, D. C., Prabhakar, B. S., Baker, S. C., Johnson, M. E. and Mesecar, A. D. (**2009**). "Structure-based design, synthesis, and biological evaluation of a series of novel and reversible inhibitors for the severe acute respiratory syndrome-coronavirus papain-like protease." *Journal of medicinal chemistry* **52**(16): 5228-40.

70. Frieman, M., ***Ratia, K.,** Johnston, R. E., Mesecar, A. D. and Baric, R. S. (**2009**). "Severe acute respiratory syndrome coronavirus papain-like protease ubiquitin-like domain and catalytic domain regulate antagonism of IRF3 and NF-kappaB signaling." *Journal of virology* **83**(13): 6689-705.

69. Eggler, A. L., ***Small, E.,** Hannink, M. and Mesecar, A. D. (**2009**). "Cul3-mediated Nrf2 ubiquitination and antioxidant response element (ARE) activation are dependent on the partial molar volume at position 151 of Keap1." *The Biochemical journal* **422**(1): 171-80.

68. Tipparaju, S. K., Mulhearn, D. C., ***Klein, G. M.,** Chen, Y., Tapadar, S., ****Bishop, M. H.**, Yang, S., Chen, J., Ghassemi, M., Santarsiero, B. D., Cook, J. L., Johlfs, M., Mesecar, A.

D., Johnson, M. E. and Kozikowski, A. P. (**2008**). "Design and synthesis of aryl ether inhibitors of the Bacillus anthracis enoyl-ACP reductase." *ChemMedChem* **3**(8): 1250-68.

2008

67. Tipparaju, S. K., Joyasawal, S., ****Forrester, S.,** Mulhearn, D. C., Pegan, S., Johnson, M. E., Mesecar, A. D. and Kozikowski, A. P. (**2008**). "Design and synthesis of 2-pyridones as novel inhibitors of the Bacillus anthracis enoyl-ACP reductase." *Bioorganic & medicinal chemistry letters* **18**(12): 3565-9.

66. ***Tian, Y.**, Suk, D. H., Cai, F., Crich, D. and Mesecar, A. D. (**2008**). "Bacillus anthracis o-succinylbenzoyl-CoA synthetase: reaction kinetics and a novel inhibitor mimicking its reaction intermediate." *Biochemistry* **47**(47): 12434-47.

65. ***Ratia, K.,** Pegan, S., Takayama, J., Sleeman, K., Coughlin, M., Baliji, S., Chaudhuri, R., Fu, W., Prabhakar, B. S., Johnson, M. E., Baker, S. C., Ghosh, A. K. and Mesecar, A. D. (**2008**). "A noncovalent class of papain-like protease/deubiquitinase inhibitors blocks SARS virus replication." *Proceedings of the National Academy of Sciences of the United States of America* **105**(42): 16119-24.

64. Pegan, S. D., Serrano, H., Whitman, C. P. and Mesecar, A. D. (**2008**). "Structural and mechanistic analysis of trans-3-chloroacrylic acid dehalogenase activity." *Acta crystallographica. Section D, Biological crystallography* **64**(Pt 12): 1277-82.

63. Mesecar, A. D. and ***Ratia, K.** (**2008**). "Viral destruction of cell surface receptors." *Proceedings of the National Academy of Sciences of the United States of America* **105**(26): 8807-8.

62. McAdams, K., Casper, E. S., Matthew Haas, R., Santarsiero, B. D., Eggler, A. L., Mesecar, A. and Halkides, C. J. (**2008**). "The structures of T87I phosphono-CheY and T87I/Y106W phosphono-CheY help to explain their binding affinities to the FliM and CheZ peptides." *Archives of biochemistry and biophysics* **479**(2): 105-13.

61. Holland, R., Hawkins, A. E., Eggler, A. L., Mesecar, A. D., Fabris, D. and Fishbein, J. C. (**2008**). "Prospective type 1 and type 2 disulfides of Keap1 protein." *Chemical research in toxicology* **21**(10): 2051-60.

60. Grum-Tokars, V., ***Ratia, K.,** Begaye, A., Baker, S. C. and Mesecar, A. D. (**2008**). "Evaluating the 3C-like protease activity of SARS-Coronavirus: recommendations for standardized assays for drug discovery." *Virus research* **133**(1): 63-73.

59. Ghosh, A. K., Gong, G., Grum-Tokars, V., Mulhearn, D. C., Baker, S. C., Coughlin, M., Prabhakar, B. S., Sleeman, K., Johnson, M. E. and Mesecar, A. D. (**2008**). "Design, synthesis and antiviral efficacy of a series of potent chloropyridyl ester-derived SARS-CoV 3CLpro inhibitors." *Bioorganic & medicinal chemistry letters* **18**(20): 5684-8.

58. Eggler, A. L., ****Gay, K. A.** and Mesecar, A. D. (**2008**). "Molecular mechanisms of natural products in chemoprevention: induction of cytoprotective enzymes by Nrf2." *Molecular nutrition & food research* **52 Suppl 1**: S84-94.

57. ***Calamini, B.,** Santarsiero, B. D., Boutin, J. A. and Mesecar, A. D. (**2008**). "Kinetic, thermodynamic and X-ray structural insights into the interaction of melatonin and analogues with quinone reductase 2." *The Biochemical journal* **413**(1): 81-91.

2007

56. ***May, M.,** Mehboob, S., Mulhearn, D. C., Wang, Z., Yu, H., Thatcher, G. R., Santarsiero, B. D., Johnson, M. E. and Mesecar, A. D. (**2007**). "Structural and functional analysis of two glutamate racemase isozymes from Bacillus anthracis and implications for inhibitor design." *Journal of molecular biology* **371**(5): 1219-37.

55. Luo, Y., Eggler, A. L., Liu, D., Liu, G., Mesecar, A. D. and van Breemen, R. B. (**2007**). "Sites of alkylation of human Keap1 by natural chemoprevention agents." *Journal of the American Society for Mass Spectrometry* **18**(12): 2226-32.

54. Ghosh, A. K., Xi, K., Johnson, M. E., Baker, S. C. and Mesecar, A. D. (**2007**). "Progress in Anti-SARS Coronavirus Chemistry, Biology and Chemotherapy." *Annual reports in medicinal chemistry* **41**: 183-196.

53. Ghosh, A. K., Xi, K., Grum-Tokars, V., Xu, X., ***Ratia, K.,** Fu, W., Houser, K. V., Baker, S. C., Johnson, M. E. and Mesecar, A. D. (**2007**). "Structure-based design, synthesis, and biological evaluation of peptidomimetic SARS-CoV 3CLpro inhibitors." *Bioorganic & medicinal chemistry letters* **17**(21): 5876-80.

52. Eggler, A. L., Luo, Y., van Breemen, R. B. and Mesecar, A. D. (**2007**). "Identification of the highly reactive cysteine 151 in the chemopreventive agent-sensor Keap1 protein is method-dependent." *Chemical research in toxicology* **20**(12): 1878-84.

51. Chen, Z., Wang, Y., ***Ratia, K.,** Mesecar, A. D., Wilkinson, K. D. and Baker, S. C. (**2007**). "Proteolytic processing and deubiquitinating activity of papain-like proteases of human coronavirus NL63." *Journal of virology* **81**(11): 6007-18.

2006

50. Zhang, H. J., Ma, C., Nguyen, V. H., Nguyen, M. C., Tan, G. T., Santarsiero, B. D., Mesecar, A. D., Soejarto, D. D., Pezzuto, J. M. and Fong, H. H. (**2006**). "Miliusanes, a class of cytotoxic agents from Miliusa sinensis." *Journal of medicinal chemistry* **49**(2): 693-708.

49. Su, B. N., Chai, H., Mi, Q., Riswan, S., Kardono, L. B., Afriastini, J. J., Santarsiero, B. D., Mesecar, A. D., Farnsworth, N. R., Cordell, G. A., Swanson, S. M. and Kinghorn, A. D. (**2006**). "Activity-guided isolation of cytotoxic constituents from the bark of Aglaia crassinervia collected in Indonesia." *Bioorganic & medicinal chemistry* **14**(4): 960-72.

48. ***Ratia, K.,** Saikatendu, K. S., Santarsiero, B. D., Barretto, N., Baker, S. C., Stevens, R. C. and Mesecar, A. D. (**2006**). "Severe acute respiratory syndrome coronavirus papain-like protease: structure of a viral deubiquitinating enzyme." *Proceedings of the National Academy of Sciences of the United States of America* **103**(15): 5717-22.

47. Mason, T. E., Abernathy, D., Anderson, I., Ankner, J., Egami, T., Ehlers, G., Ekkebus, A., Branroth, G., Hagen, M., Herwig, K., Hodges, J. P., Hoffman, C., Horak, C., Horton, L., Klose, F., Larese, J., Mesecar, A. D., Myles, D. A. A., Neuefeind, J., Ohl, M., Tulk, C., Wang, X.-L. and Zhao, J. (**2006**). "The spallation neutron source in Oak Ridge: A powerful tool for materials research." *Physica B: Condensed Matter* **385-386**: 955-960.

46. Liu, A., Pajkovic, N., Pang, Y., Zhu, D., ***Calamini, B.**, Mesecar, A. D. and van Breemen, R. B. (**2006**). "Absorption and subcellular localization of lycopene in human prostate cancer cells." *Molecular cancer therapeutics* **5**(11): 2879-85.

45. Homhual, S., Zhang, H. J., Bunyapraphatsara, N., Kondratyuk, T. P., Santarsiero, B. D., Mesecar, A. D., Herunsalee, A., Chaukul, W., Pezzuto, J. M. and Fong, H. H. (**2006**). "Bruguiesulfurol, a new sulfur compound from Bruguiera gymnorrhiza." *Planta medica* **72**(3): 255-60.

44. Deng, S., Chen, S. N., Lu, J., Wang, Z. J., Nikolic, D., van Breemen, R. B., Santarsiero, B. D., Mesecar, A., Fong, H. H., Farnsworth, N. R. and Pauli, G. F. (**2006**). "GABAergic phthalide dimers from Angelica sinensis (Oliv.) Diels." *Phytochemical analysis : PCA* **17**(6): 398-405.

43. Cuendet, M., Mesecar, A. D., DeWitt, D. L. and Pezzuto, J. M. (**2006**). "An ELISA method to measure inhibition of the COX enzymes." *Nature protocols* **1**(4): 1915-21.

42. Barretto, N., Jukneliene, D., ***Ratia, K**., Chen, Z., Mesecar, A. D. and Baker, S. C. (**2006**). "Deubiquitinating activity of the SARS-CoV papain-like protease." *Advances in experimental medicine and biology* **581**: 37-41.

2005

41. Barretto, N., Jukneliene, D., ***Ratia, K.,** Chen, Z., Mesecar, A. D. and Baker, S. C. (**2005**). "The papain-like protease of severe acute respiratory syndrome coronavirus has deubiquitinating activity." *Journal of virology* **79**(24): 15189-98.

40. Dietz, B. M., Kang, Y. H., Liu, G., Eggler, A. L., Yao, P., Chadwick, L. R., Pauli, G. F., Farnsworth, N. R., Mesecar, A. D., van Breemen, R. B. and Bolton, J. L. (**2005**). "Xanthohumol isolated from Humulus lupulus Inhibits menadione-induced DNA damage through induction of quinone reductase." *Chemical research in toxicology* **18**(8): 1296-305.

39. ***Dombrauckas, J. D.,** Santarsiero, B. D. and Mesecar, A. D. (**2005**). "Structural basis for tumor pyruvate kinase M2 allosteric regulation and catalysis." *Biochemistry* **44**(27): 9417-29.

38. Eggler, A. L., Liu, G., Pezzuto, J. M., van Breemen, R. B. and Mesecar, A. D. (**2005**). "Modifying specific cysteines of the electrophile-sensing human Keap1 protein is insufficient to disrupt binding to the Nrf2 domain Neh2." *Proceedings of the National Academy of Sciences of the United States of America* **102**(29): 10070-5.

37. Ghosh, A. K., Xi, K., ***Ratia, K.,** Santarsiero, B. D., Fu, W., Harcourt, B. H., Rota, P. A., Baker, S. C., Johnson, M. E. and Mesecar, A. D. (**2005**). "Design and synthesis of peptidomimetic severe acute respiratory syndrome chymotrypsin-like protease inhibitors." *Journal of medicinal chemistry* **48**(22): 6767-71.

36. Grimsley, J. K., ***Calamini, B.,** Wild, J. R. and Mesecar, A. D. (**2005**). "Structural and mutational studies of organophosphorus hydrolase reveal a cryptic and functional allosteric-binding site." *Archives of biochemistry and biophysics* **442**(2): 169-79.

35. Liu, G., Eggler, A. L., Dietz, B. M., Mesecar, A. D., Bolton, J. L., Pezzuto, J. M. and van Breemen, R. B. (**2005**). "Screening method for the discovery of potential cancer

chemoprevention agents based on mass spectrometric detection of alkylated Keap1." *Analytical chemistry* **77**(19): 6407-14.

34. Schultz, A. J., Thiyagarajan, P., Hodges, J. P., Rehm, C., Myles, D. A. A., Langan, P. and Mesecar, A. D. (**2005**). "Design of the next generation Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source." *Journal of Applied Crystallography* **38**: 964-974.

2004

33. Rumthao, S., Lee, O., Sheng, Q., Fu, W., Mulhearn, D. C., Crich, D., Mesecar, A. D. and Johnson, M. E. (**2004**). "Design, synthesis, and evaluation of oxyanion-hole selective inhibitor substituents for the S1 subsite of factor Xa." *Bioorganic & medicinal chemistry letters* **14**(20): 5165-70.

32. Nguyen, Q. C., Nguyen, V. H., Santarsiero, B. D., Mesecar, A. D., Nguyen, M. C., Soejarto, D. D., Pezzuto, J. M., Fong, H. H. and Tan, G. T. (**2004**). "New 3-O-acyl betulinic acids from Strychnos vanprukii Craib." *Journal of natural products* **67**(6): 994-8.

31. Li, Y., Yao, J., Chang, M., Nikolic, D., Yu, L., Yager, J. D., Mesecar, A. D., van Breemen, R. B. and Bolton, J. L. (**2004**). "Equine catechol estrogen 4-hydroxyequilenin is a more potent inhibitor of the variant form of catechol-O-methyltransferase." *Chemical research in toxicology* **17**(4): 512-20.

30. Hwang, B. Y., Su, B. N., Chai, H., Mi, Q., Kardono, L. B., Afriastini, J. J., Riswan, S., Santarsiero, B. D., Mesecar, A. D., Wild, R., Fairchild, C. R., Vite, G. D., Rose, W. C., Farnsworth, N. R., Cordell, G. A., Pezzuto, J. M., Swanson, S. M. and Kinghorn, A. D. (**2004**). "Silvestrol and episilvestrol, potential anticancer rocaglate derivatives from Aglaia silvestris." *The Journal of organic chemistry* **69**(10): 3350-8.

29. Graham, J. G., Zhang, H., Pendland, S. L., Santarsiero, B. D., Mesecar, A. D., Cabieses, F. and Farnsworth, N. R. (**2004**). "Antimycobacterial Naphthopyrones from Senna obliqua." *Journal of natural products* **67**(2): 225-7.

2003

28. Burdette, J. E., Liu, J., Chen, S. N., Fabricant, D. S., Piersen, C. E., Barker, E. L., Pezzuto, J. M., Mesecar, A., Van Breemen, R. B., Farnsworth, N. R. and Bolton, J. L. (**2003**). "Black cohosh acts as a mixed competitive ligand and partial agonist of the serotonin receptor." *Journal of agricultural and food chemistry* **51**(19): 5661-70.

27. Jang, D. S., Park, E. J., Hawthorne, M. E., Vigo, J. S., Graham, J. G., Cabieses, F., Santarsiero, B. D., Mesecar, A. D., Fong, H. H., Mehta, R. G., Pezzuto, J. M. and Kinghorn, A. D. (**2003**). "Potential cancer chemopreventive constituents of the seeds of Dipteryx odorata (tonka bean)." *Journal of natural products* **66**(5): 583-7.

26. Park, S., Hayes, B. L., Marankan, F., Mulhearn, D. C., Wanna, L., Mesecar, A. D., Santarsiero, B. D., Johnson, M. E. and Venton, D. L. (**2003**). "Regioselective covalent modification of hemoglobin in search of antisickling agents." *Journal of medicinal chemistry* **46**(6): 936-53.

25. Rao, K. V., Santarsiero, B. D., Mesecar, A. D., Schinazi, R. F., Tekwani, B. L. and Hamann, M. T. (**2003**). "New manzamine alkaloids with activity against infectious and

tropical parasitic diseases from an Indonesian sponge." *Journal of natural products* **66**(6): 823-8.

24. Su, B. N., Kang, Y. H., Pinos, R. E., Santarsiero, B. D., Mesecar, A. D., Soejarto, D. D., Fong, H. H., Pezzuto, J. M. and Kinghorn, A. D. (**2003**). "Isolation and absolute stereochemistry of coussaric acid, a new bioactive triterpenoid from the stems of Coussarea brevicaulis." *Phytochemistry* **64**(1): 293-302.

23. Su, B. N., Park, E. J., Nikolic, D., Santarsiero, B. D., Mesecar, A. D., Vigo, J. S., Graham, J. G., Cabieses, F., van Breemen, R. B., Fong, H. H., Farnsworth, N. R., Pezzuto, J. M. and Kinghorn, A. D. (**2003**). "Activity-guided isolation of novel norwithanolides from depreasubtriflora with potential cancer chemopreventive activity." *The Journal of organic chemistry* **68**(6): 2350-61.

22. Yao, J., Li, Y., Chang, M., Wu, H., Yang, X., Goodman, J. E., Liu, X., Liu, H., Mesecar, A. D., Van Breemen, R. B., Yager, J. D. and Bolton, J. L. (**2003**). "Catechol estrogen 4-hydroxyequilenin is a substrate and an inhibitor of catechol-O-methyltransferase." *Chemical research in toxicology* **16**(5): 668-75.

21. Zhang, H. J., Tan, G. T., Santarsiero, B. D., Mesecar, A. D., Hung, N. V., Cuong, N. M., Doel Soejarto, D., Pezzuto, J. M. and Fong, H. H. (**2003**). "New Sesquiterpenes from Litsea verticillata." *Journal of natural products* **66**(5): 609-15.

2002

20. Zhang, X., Gan, L., Pan, H., Guo, S., He, X., Olson, S. T., Mesecar, A., Adam, S. and Unterman, T. G. (**2002**). "Phosphorylation of serine 256 suppresses transactivation by FKHR (FOXO1) by multiple mechanisms. Direct and indirect effects on nuclear/cytoplasmic shuttling and DNA binding." *The Journal of biological chemistry* **277**(47): 45276-84.

19. Su, B. N., Park, E. J., Mbwambo, Z. H., Santarsiero, B. D., Mesecar, A. D., Fong, H. H., Pezzuto, J. M. and Kinghorn, A. D. (**2002**). "New chemical constituents of Euphorbia quinquecostata and absolute configuration assignment by a convenient Mosher ester procedure carried out in NMR tubes." *Journal of natural products* **65**(9): 1278-82.

18. Su, B. N., Misico, R., Park, E. J., Santarsiero, B. D., Mesecar, A. D., Fong, H. H. S., Pezzuto, J. M. and Kinghorn, A. D. (**2002**). "Isolation and characterization of bioactive principles of the leaves and stems of Physalis philadelphica (Tomatillos)." *Tetrahedron* **58**(17): 3453-3466.

17. Su, B. N., Chang, L. C., Park, E. J., Cuendet, M., Santarsiero, B. D., Mesecar, A. D., Mehta, R. G., Fong, H. H., Pezzuto, J. M. and Kinghorn, A. D. (**2002**). "Bioactive constituents of the seeds of Brucea javanica." *Planta medica* **68**(8): 730-3.

16. Li, S.-H., Zhang, H.-J., Qiu, S.-X., Niu, X.-M., Santarsiero, B. D., Mesecar, A. D., Fong, H. H. S., Farnsworth, N. R. and Sun, H.-D. (**2002**). "Vitexlactam A, a novel labdane diterpene lactam from the fruits of Vitex angnus-castus." *Tetrahedron Letters* **43**(29): 5131-5134.

15. Jang, D. S., Park, E. J., Hawthorne, M. E., Vigo, J. S., Graham, J. G., Cabieses, F., Santarsiero, B. D., Mesecar, A. D., Fong, H. H., Mehta, R. G., Pezzuto, J. M. and Kinghorn, A. D. (**2002**). "Constituents of Musa x paradisiaca cultivar with the potential to

induce the phase II enzyme, quinone reductase." *Journal of agricultural and food chemistry* **50**(22): 6330-4.

14. Cui, J., Marankan, F., Fu, W., Crich, D., Mesecar, A. and Johnson, M. E. (**2002**). "An oxyanion-hole selective serine protease inhibitor in complex with trypsin." *Bioorganic & medicinal chemistry* **10**(1): 41-6.

13. Chen, S. N., Li, W., Fabricant, D. S., Santarsiero, B. D., Mesecar, A., Fitzloff, J. F., Fong, H. H. and Farnsworth, N. R. (**2002**). "Isolation, structure elucidation, and absolute configuration of 26-deoxyactein from Cimicifuga racemosa and clarification of nomenclature associated with 27-deoxyactein." *Journal of natural products* **65**(4): 601-5.

2001

12. Velichutina, I. V., Hong, J. Y., Mesecar, A. D., Chernoff, Y. O. and Liebman, S. W. (**2001**). "Genetic interaction between yeast Saccharomyces cerevisiae release factors and the decoding region of 18 S rRNA." *Journal of molecular biology* **305**(4): 715-27.

2000

11. Bond, C. J., Jurica, M. S., Mesecar, A. and Stoddard, B. L. (**2000**). "Determinants of allosteric activation of yeast pyruvate kinase and identification of novel effectors using computational screening." *Biochemistry* **39**(50): 15333-43.

10. Freiberg, G., Mesecar, A. D., Huang, H., Hong, J. Y. and Liebman, S. W. (**2000**). "Characterization of novel rad6/ubc2 ubiquitin-conjugating enzyme mutants in yeast." *Current genetics* **37**(4): 221-33.

9. Mesecar, A. D. and Koshland, D. E., Jr. (**2000**). "Sites of binding and orientation in a four-location model for protein stereospecificity." *IUBMB life* **49**(5): 457-66.

8. Mesecar, A. D. and Koshland, D. E., Jr. (**2000**). "A new model for protein stereospecificity." *Nature* **403**(6770): 614-5.

1999

7. Bollenbach, T. J., Mesecar, A. D. and Nowak, T. (**1999**). "Role of lysine 240 in the mechanism of yeast pyruvate kinase catalysis." *Biochemistry* **38**(28): 9137-45.

6. Rombel, I., Peters-Wendisch, P., Mesecar, A., Thorgeirsson, T., Shin, Y. K. and Kustu, S. (**1999**). "MgATP binding and hydrolysis determinants of NtrC, a bacterial enhancer-binding protein." *Journal of bacteriology* **181**(15): 4628-38.

1998

5. Jurica, M. S., Mesecar, A., Heath, P. J., Shi, W., Nowak, T. and Stoddard, B. L. (**1998**). "The allosteric regulation of pyruvate kinase by fructose-1,6-bisphosphate." *Structure* **6**(2): 195-210.

4. Stoddard, B. L., Cohen, B. E., Brubaker, M., Mesecar, A. D. and Koshland, D. E., Jr. (**1998**). "Millisecond Laue structures of an enzyme-product complex using photocaged substrate analogs." *Nature structural biology* **5**(10): 891-7.

1997

3. Mesecar, A. D. and Nowak, T. (**1997**). "Metal-ion-mediated allosteric triggering of yeast pyruvate kinase. 2. A multidimensional thermodynamic linked-function analysis." *Biochemistry* **36**(22): 6803-13.

2. Mesecar, A. D. and Nowak, T. (**1997**). "Metal-ion-mediated allosteric triggering of yeast pyruvate kinase. 1. A multidimensional kinetic linked-function analysis." *Biochemistry* **36**(22): 6792-802.

1. Mesecar, A. D., Stoddard, B. L. and Koshland, D. E., Jr. (**1997**). "Orbital steering in the catalytic power of enzymes: small structural changes with large catalytic consequences." *Science* **277**(5323): 202-6.

UNIVERSITY, COLLEGE, DEPARTMENT AND CENTER SERVICE AND LEADERSHIP

PURDUE UNIVERSITY (2010 TO PRESENT)

PURDUE CAMPUS AND DISCOVERY PARK (PURDUE)

Purdue Center for Cancer Research (PCCR)

Deputy Director (August 2010 to present).
The PCCR is an NIH/NCI Funded Basic Sciences Cancer Center. As Deputy Director, I report directly to the PCCR Director (Tim Ratliff). I am responsible for the overall direction of the 7 PCCR Shared Resources, and am the direct supervisor for the Developmental Shared Resource (Computational and Medicinal Chemistry), the review of pilot proposals and allocation of funds, the coordination of shared resources and campus resources for a drug discovery pipeline for center members, industrial relations and administrative review and allocation of funds for graduate student fellowships and travel awards and undergraduate SROP awards etc. I work closely with the director in every aspect of the center operations which has annual expenditures exceeding $3M.

Bindley Biosciences Center

Director, Biomolecular Screening and Drug Discovery Core Facility (BSDDCF) (2013 to 2016). I provided scientific oversight of the core facility direction in coordination with our BSDDCF advisory board that is composed of faculty members from campus and BBC scientists. We changed the name of the facility from Integrated Screening Technologies in 2013 and we established the BSDDCF as an Indiana Core Facility in May, 2014.

Directors Advisory Board (2011 to 2015)
Facilities Advisory Board (2011 to 2015)
Space Advisory Committee (2011 to 2015)
Integrated Screening Technologies Advisory Board (2011-2013)

Purdue Institute for Drug Discovery (PIDD)

Internal Advisory Board (2016-present). This committee meets once per month to advise the director as to strategic vision, programmatic themes etc.
Website design team (2013 to 2014)-worked with a team of individuals from the Office of the Vice President of Research and the center director to collect and organize data and material for the design and launch of the current center website. The center was transformed into an institute in 2016,
Chemical Genomics Facility (2016-present). Scientific Advisory Board. The CGF replaced the Biomolecular Screening and Drug Discovery Core Facility in 2016. Prof. Zhong-Yin Zhang was recruited from IU Medical School to setup up a brand new facility with state-of-the-art resources.

Purdue Institute for Inflammation, Immunology & Infectious Disease (PI4D)

Internal Advisory Board (2016-present) This committee meets once per month to advise the director as to strategic vision, programmatic themes etc.

Purdue Select Agent Program

Faculty Point of Contact (2013 to 2015) I spearheaded an effort to obtain Select Agent Status at Purdue to study the coronavirus that causes SARS (SARS-CoV) in our BSL3 lab in Hockmeyer. This is the first time that Purdue was designated to work with a select agent on campus. It took considerable coordination between our Office of the Vice President for Research, Biological Safety Office, Police Department, Center for Disease Control and the Department of Justice.

Purdue Institutional Review Entity (IRE)

Committee Member(2016-Present). This committee was appointed by the Associate Vice President of Research to review all IBC protocols which present a Dual-Use Research of Concern. This committee meets once per year.

Indiana Clinical and Translational Sciences Institute (iCTSI)

Executive Committee member of the Experimental Therapeutics Program (2015-present). This committee meets once per month (telecom/Videocon) to review applications for funding, set programmatic goals, discuss proposals and advise iCTSI members on projects etc.

COLLEGE OF AGRICULTURE (PURDUE)

Strategic Governance Committee. (2015 to present). This committee has the charge of identifying college level IT needs to meet its strategic goals.

COLLEGE OF SCIENCE (PURDUE)

College of Science Faculty Council. (2013 to 2015). Elected by my peers to represent the Department of Biological Sciences on the council.

College of Science Undergraduate Curriculum and Academic Policy (UCAP) Committee (2013 to 2015). Elected to be the College of Science Faculty Council to be their UCAP committee representative. This is a separate position from the UCAP committee elected by the individual departments.

Dean's Leadership Council (September 2011 to September 2014). 3 year appointment. I was appointed by the Dean of the College of Science to serve as one of 3 faculty members on this council. The council was a working council that was divided into 3 different groups with different missions. We met twice per year for two days to go over our projects.

Member, Search Committee for Chaired Professorship's in Drug Discovery (March 2012 to 2014). I was appointed by the Dean of the College of Science to serve on this search committee that had the goal of hiring 2 senior faculty members in drug discovery. After much effort, we were unsuccessful. The search started since before I arrived in 2010 and is now underway with a new committee composition.

DEPARTMENT OF BIOLOGICAL SCIENCES (PURDUE)

Cryo-EM Facilities Oversight Committee (August 2016-present). This committee provides guidance and oversight for the cryo-EM facilty in Hockmeyer Hall of Structural Biology. This facility is mainly for high-resolution structural studies of viruses and proteins.

Chair, Structural Biology Search Committee (September 2014 – May 2015). I was appointed by the department head to lead a search committee to hire a senior level structural biology faculty member with an emphasis in cancer biology. The person in this position will hold the title of the Walther Professor of Cancer Structural Biology. I also co-wrote the proposal to the Walther Cancer Foundation with Tim Ratliff, Director of the Center for Cancer Research, that secured $750K to contribute to the start-up package of the successful candidate.

Chair, Structural Biology Search Committee (September, 2013-May, 2014). I was appointed by the department head to lead a search committee to hire a structural biologist. We successfully hired Nick Noinaj who joined the faculty in August, 2014.

Leading Faculty Scholar Search Committee (April 2011 to December 2011)
This program was been established by the provost is intended to bring substantial university resources to bear on the targeted recruitment of NAS level faculty. Our charge was to search, identify, and then help with the recruitment of a possible Leading Faculty Scholar. The program was dismantled after the arrival of the new president.

Primary Promotions Committee (2011-2015). I was a member of the primary promotions committee for Jason Lanman, Assistant Professor, Seema Matoo, Assistant Professor, and Nick Noinaj, Assistant Professor.

DEPARTMENT OF CHEMISTRY (PURDUE)

Search Committee, Biochemistry Division (September 2013 to May, 2014). I was a member on the search committee for a biochemistry position(s) at the assistant professor level. We were successful and hired Angeline Lyon and Matthew Tantama who both joined the faculty in August, 2014.

Primary Promotions Committees (2014-present). I am currently serving on the primary promotions committee for Angeline Lyon (assistant professor), Mingjie Dai (assistant professor) and Mark Lipton (associate professor)

DEPARTMENT OF BIOCHEMISTRY (PURDUE) –While in Biological Sciences

Faculty Mentor. (2014 -2015). I was formally an external department committee member for Jeremy Lohman, Assistant Professor. This was before I became the department head.

DEPARTMENT OF NUTRITION SCIENCE

Chair, Search Committee for the New Head of the Department of Nutrition Science (January 2016 – June 2016). I was asked by Dean Christine Ladisch to chair this committee to find a new head to replace Connie Weaver after her 25 years of service. We successfully hired Dr. Michele Foreman.

Faculty Search Committee -Nutrition Science (July 2017 – present). Member of the search committee to hire new faculty members (assistant to full professor).

UNIVERSITY OF ILLINOIS AT CHICAGO (1999-2010)

CAMPUS LEVEL LEADERSHIP AND ACTIVITIES

University of Illinois at Chicago, College of Medicine – Medical Scientist Training Program (MSTP) – Executive Committee (2007-2010). We wrote and were funded an NIH Training grant for our MSTP program at UIC. I was on the executive committee which had oversight on the program. I was fortunate to have two MD/Ph.D from this highly competitive program.

University of Illinois at Chicago, Summer Research Opportunities Program (SROP) (2006, 2007). Faculty mentor and advisor to 2 students during each of the summers.

***Search Committee for Proteomics Faculty* (2007-2008)** Appointed by the Vice Chancellor of Research.

***University of Illinois, Board of Governors for CARS* (2002 to 2010)**. Alternate member to the Board of Governors for Consortium for Advances Radiation Sources (CARS) at the Advanced Photon Source, Argonne National Laboratory. The University of Illinois at Chicago has become an institutional member of this Consortium.

***Faculty Advisory Committee*, UIC Center for Structural Biology (2000 to 2010).** My role is to provide advice to the Director on how to fulfill the missions of the Center in the areas of Teaching Initiatives, Research Initiatives, and Facilities Development.

Faculty Advisory and User Committee-Macromolecular Crystallography Facility (2000 to 2010). Committee member for Research Resources Center to oversee the operations and usage of x-ray diffraction instrumentation.

Faculty Advisory and User Committee-Small Molecule X-ray Diffraction Facility (2002 to 2010). Committee member for Research Resources Center to oversee the operations and usage of x-ray diffraction instrumentation.

***Search Committee* (2001)**. for a scientific coordinator between UIC and the Consortium for Advances Radiation Sources (CARS) at the Advanced Photon Source, Argonne National Laboratory.

COLLEGE OF PHARMACY (UIC)

Chair, Basic Sciences Faculty Search Committee (2009-2010). College of Pharmacy Rockford Expansion. Appointed by the Dean to chair the search committee to hire 4 basic sciences faculty to start in Fall of 2010 for our expansion to the University of Illinois at Chicago, at Rockford. I was able to lead the committee to the fulfillment of all 4 positions as a result of a highly coordinated effort of the committee members.

Executive Committee (2007 to 2009)
Elected Position. Two year service term.

American Council on Pharmaceutical Education (ACPE) Self-Study Committee **(April to October, 2007)** Appointed by the Dean. This committee works on professional certification for the PharmD program.

Search Committee **(2007)** for Head, Department of Pharmacy Practice
Appointed by the Dean.

Academic Standing Committee (2005 to 2007)
Elected Position. Two year service term.

Hahns Valteich Awards Committee (2006 & 2007)
Appointed by the Dean

Institute for Tuberculosis Awards Committee (2006)
Appointed by the Dean

Image and Public Relations Committee **(2003 to 2004).**
Chairperson. Appointed by Dean.

Student Faculty Relations Committee **(2001 to 2003).**
Elected Position. Two year service term.

Student Discipline Committee **(2003 to 2004).**
Elected Position. 1 year service term.

Search Committee **(2003 to 2005)** for Head, Department of Medicinal Chemistry and Pharmacognosy. Appointed by the Dean.

American Council on Pharmaceutical Education (ACPE) Self-Study Committee **(April to November, 2001).** Appointed by the Dean.

DEPARTMENTAL OF MEDICINAL CHEMISTRY AND PHARMACOGNOSY (UIC)

Assistant Head of Medicinal Chemistry and Pharmacognosy (2009-2010). Responsible for curriculum and teaching organization and assignments for the Pharm.D. professional program as well as the Medicinal Chemistry and Pharmacognosy graduate programs.

Department Faculty Advisory Committee (2003 to 2010). Department of Medicinal Chemistry and Pharmacognosy. Elected Position. (2 year terms) Major responsibilities included promotion and tenure, curriculum decisions, and providing advice to the department head.

Program Chair, Structural Biology Track, Medicinal Chemistry Graduate Program (2001-2009).

Department Technical Resources Committee (2005-2006). Department of Medicinal Chemistry and Pharmacognosy. Appointed by the Head.

Search Committee **(2003, 2004, 2005, 2006, 2007)** for Medicinal Chemistry and Pharmacognosy faculty positions. Appointed by the Head.

Department Webmaster-Supervisor (2001-2005). I supervised the design, construction and maintenance of the Department of Medicinal Chemistry and Pharmacognosy website.

Department Strategic Planning Committee (2005 - 2006). Department of Medicinal Chemistry and Pharmacognosy. Appointed by the Head.

Search Committee **(2001)** for NMR Spectroscopist position, Department of Medicinal Chemistry and Pharmacognosy. Appointed by the Head.

Comprehensive Exam Committee (June, 2000 and 2002)-Written Exam. Medicinal Chemistry Graduate Program. Member. Was responsible or creation and grading of a portion of the year 2000 Preliminary Written Exam.

Medicinal Chemistry Graduate Program Revision Committee (2000-2001). Member. Worked on a plan to revise the Medicinal Chemistry Graduate program. Program was implemented in Fall of 2002.

CENTER FOR PHARMACEUTICAL BIOTECHNOLOGY (UIC)

Center for Pharmaceutical Biotechnology-Faculty Search Committee (2005, 2006, 2007). Appointed by the Center Director.

Center for Pharmaceutical Biotechnology-Recruiting Committee Chair (August 2000 to 2001). Appointed by the Center Director.

Faculty Sponsor**, Undergraduate Student Research Outreach Program (2001).**

PROFESSIONAL SCIENTIFIC SERVICE

NATIONAL AND INTERNATIONAL SCIENTIFIC INFRASTRUCTURE

Chair, Executive Committee **(2003-2008) for the Instrument Development Team (IDT) for "MaNDi" a Macromolecular Neutron Diffractometer at the Spallation Neutron Source (SNS)**. Over a period of 5 years, I worked with other members of the MaNDi executive committee, the IDT and the international scientific community to build a case for the design and construction of a state-of-the-art macromolecular neutron diffractometer at SNS at Oakridge National Laboratory, Oakridge, TN. After about 2 years of work including presentations of our scientific case and scientific workshops, we were able to convince the SNS administration to allocate at the SNS for us to build a neutron beamline. After an additional 2 years of presentations and workshops, we were able to secure funding (~$12 million) from the DOE to build a world renowned, best-in-class neutron diffractometer for macromolecular neutron structures. In January of 2007, we hired a Beamline scientist to oversee the construction of MaNDi. The beamline is now built and fully operational, as of 2013, and is in the final commissioning phase.

Our original design and vision papers for MaNDi (I was the one who actually named the beamline) can be found in the following publications;

- Schultz, A. J., Thiyagarajan, P., Hodges, J. P., Rehm, C., Myles, D. A. A., Langan, P. and Mesecar, A. D. (**2005**). "Design of the next generation Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source." *Journal of Applied Crystallography* **38**: 964-974.

- Mason, T. E., Abernathy, D., Anderson, I., Ankner, J., Egami, T., Ehlers, G., Ekkebus, A., Branroth, G., Hagen, M., Herwig, K., Hodges, J. P., Hoffman, C., Horak, C., Horton, L., Klose, F., Larese, J., Mesecar, A. D., Myles, D. A. A., Neuefeind, J., Ohl, M., Tulk, C., Wang, X.-L. and Zhao, J. (**2006**). "The spallation neutron source in Oak Ridge: A powerful tool for materials research." *Physica B: Condensed Matter* **385-386**: 955-960.

Steering Committee-**(2002-2003)** An international committee of prominent scientists was formed to develop a plan to build a state-of-the-art Neutron Diffraction Facility at the Spallation Neutron Source (SNS) at Oakridge National Laboratory.

NIH Site-Visit Support Presentations for BioCARS, Advanced Photon Source (2001, 2006)
BioCARS is a National Resource that is funded by NCRR (NIH). BioCARS provides 3 state-of-the-art beamlines for monochromatic and polychromatic Laue x-ray diffraction experiments. BioCARS is located at the Advanced Photon Source, Argonne National Laboratory. These presentations were to highlight our (Mesecar lab) cutting-edge research being conducted at BioCARS beam lines.

Site-Visit Support Presentations for the Advanced Photon Source (2007). The Advanced Photon Source at Argonne National Laboratory is funded by the DOE. The APS is periodically reviewed by the DOE for scientific progress. This presentation is to highlight our (Mesecar lab) cutting-edge research being conducted at the various beam lines provided by the APS.

Support Presentation for BioCARS to the Advanced Photon Source (2007) BioCARS is periodically reviewed by the APS for their scientific progress. This presentation was to highlight our (Mesecar lab) cutting-edge research being conducted at the various beam lines provided by the BioCARS.

NATIONAL GRANT REVIEW PANELS (PURDUE)

National Science Foundation Chemistry of Life Processes: Enzymes and Metalloproteins 1-P141024 Study Section. Max Funk, SRO April 3rd, 2014

NIH Study Section - Special Emphasis Panel/Scientific Review Group 2014/01 ZAI1 AWA-M (J1) 1 meeting, scheduled for 01/07/2014-01/07/2014. Partnerships for Biodefense (R01) Annie Walker-Abbey SRO

NIH Study Section - Special Emphasis Panel/Scientific Review Group 2012/01 ZRG1 F04-A (20) L meeting, scheduled for 11/14/2011-11/15/2011. Ross Shonat, SRO Fellowship: Chemistry, Biochemistry, Biophysics, and Bioengineering

NIH Study section - Special Emphasis Panel/Scientific Review Group 2012/05 MSFE meeting, scheduled for 02/16/2012-02/17/2012. Macromolecular Structure and Function E Study Section. Nitsa Rosenzweig SRO

NIH Study Section February 3rd and 4th, 2011 Special Emphasis Panel/Scientific Review Group 2011/05 ZRG1 IDM-L (02) M meeting, scheduled for 03/03/2011-03/04/2011. Drug discovery/drug resistance. Joana Pyper, SRO

NIH/NCI Site Visit team – University of Colorado June 14th-16th, 2011 Site visit: Cancer Center Support Grant (P30) application for University of Colorado Comprehensive Cancer Center, University of Colorado, 2 P30 CA046934 [comprehensive cancer center/ competing renewal] PI: Dr. Dan Theodorescu Location: Aurora, CO Date/Time: Tuesday, June 14, 2011– Thursday, June 16, 2011

NIH Study Section. Special Emphasis Panel/Scientific Review Group 2010/05 ZRG1 BST-J (51) R meeting, scheduled for 01/28/2010-01/29/2010. IAR Reviewer Invitation for meeting 2010/05 ZRG1 BST-J (51) R - Roadmap HTS Assay Development. Sergei Ruvinov, SRO

NATIONAL GRANT REVIEW PANELS (UIC)

NIH Study Sections (2001 to present)
-NIH MSFE Study Section (2009 – ad hoc)
-National Center for Research Resources (NCRR) Study Section-(2003 to 2005, 2007,2009)
-NIH Special Emphasis Panels-various from 2003-2010
-Chemical Pathology Study Section (Ad hoc, 2001, 2002, 2003).
-National Center for Research Resources (NCRR) Study Section-2001 (Ad Hoc-Site Review).

Proposal Review Panel (2001-Present) Advanced Photon Source, Argonne National Laboratory. I continually review proposals for requests for synchrotron beamtime.

Proposal Reviewer (2003,2004)-Research Corporation, Genome Canada (Ad Hoc)

NATIONAL AND INTERNATIONAL PROFESSIONAL JOURNALS

Editorial Boards
Associate Editor, Crystallography Reviews (2006 to 2008)

Journal Reviewer (Ad Hoc)
Nature Structure and Molecular Biology, Proceedings from the National Academy of Sciences, EMBO Journal, Biochemistry, Journal of Biological Chemistry, PLoS Biology, PLoS Pathogens, Biochemistry, Journal of the American Chemical Society, Applied and Environmental Microbiology, Chemical Research in Toxicology, Combinatorial Chemistry and High Throughput Screening, Protein Science, Clinical Chemistry, Journal of Molecular Biology, Journal of Virology, Virus Research, Biochemical Journal, Acta Crystallographica Sections D and F and others.

NATIONAL, PROFESSIONAL SCIENTIFIC CONFERENCES ORGANIZED

Ubiquitination Processes and Their Role in Cancer Mini-Symposium. (April 19th, 2013). Purdue University, W. Lafayette, IN. Co-organized with Chitta Das, Department of Chemistry. Sponsored by the Purdue University centerof ro Cancer Research.

27th Midwest Enzyme Chemistry Conference (September, 2007)-Local Chairman & UIC site hos (With Drs Aimee Eggler and Valerie Grum-Tokars). September 29th, 2007. This meeting was held in the College of Pharmacy. See http://www.midwestenzyme.org/

Conference on New Frontiers in Neutron Macromolecular Crystallography (July 2005). July 12-13, 2005 at the Spallation Neutron Source**,** Oak Ridge National Laboratory, Oak Ridge, TN, USA. See http://www.sns.gov/workshops/mandi2005/. There were over 100 participants.

23rd Midwest Enzyme Chemistry Conference (October, 2003)-Local Chairman & UIC site host. October 4th, 2003. This meeting was held in the college of Pharmacy. There were approximately 200 registered participants and over 100 posters and presentations.

A Workshop for MaNDi: a Macromolecular Neutron Diffractometer at the Spallation Neutron Source (October, 2003).-Workshop Organizer. This workshop was held from October 2nd to 3rd, 2003 at the Intense Pulsed Neutron Source at Argonne National Laboratory.

***Session Chair, "*Time Resolved Diffraction in Chemistry & Biology Symposium" (July, 2003).** American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31.

Session Chair, "Macromolecular Motions and Dynamic Processes." (May, 2002). American Crystallographic Association, Annual Meeting, San Antonio, Texas. May 25th - 30th.

TEACHING AND MENTORING ACTIVITIES

PURDUE UNIVERSITY (2010 to present)

UNDERGRADUATE COURSE TEACHING AT PURDUE

BIOL 495 Biological and Structural Aspects of Drug Design and Action (Spring 2011 to present). This is a new 3 credit hour course that I created in Spring, 2011 during my first year at Purdue. I am teaching the entire course and give about 40 lectures. Over the past 4 years, the course has had enrollments between 11 and 24 students. In its 5th year (2015), it has 13 students enrolled. **This course has been reviewed by the departments, colleges and Purdue and is now a permanent course. Starting in 2017, the new numbers will be BCHM 536 and BIOL 536.**

Student Evaluations of BIOL 495
Spring 2011
24 students enrolled, **15** responded
Overall I would rate this instructor **4.6** /5.0
Overall I would rate this course **4.1** /5.0

Spring 2012
16 students enrolled, **6** responded
Overall I would rate this instructor **4.1** /5.0
Overall I would rate this course **4.0** /5.0

Spring 2013
11 students enrolled, **5** responded
Overall I would rate this instructor **4.9** /5.0
Overall I would rate this course **4.7** /5.0

Spring 2014
19 students enrolled, **7** responded
Overall I would rate this instructor **4.8** /5.0
Overall I would rate this course **4.4** /5.0

Spring 2015
10 students enrolled, responded **10**
Overall I would rate this instructor **4.** /5.0
Overall I would rate this course **4.** /5.0

Spring 2016
19 students enrolled, **17** responded
Overall I would rate this instructor **4.2** /5.0
Overall I would rate this course **4.1** /5.0

GRADUATE COURSE TEACHING AT PURDUE

BIOL 696 Enzymes as Drug Targets (Fall 2014)
12 students enrolled, 9 responded
Overall I would rate this instructor **4.4** /5.0
Overall I would rate this course **4.4** /5.0

BCHM 695 Macromolecules (Fall 2011-2013)
Gave 3 lectures on structure-based drug design each year and provided exam questions for lectures.

CHEM 696 Drug Design (Fall 2013-2014)
Gave guest lectures each year to students on drug design research ongoing in our lab.

GRADUATE STUDENTS (PURDUE)

1) **Katie (Jermihov) Jensen (2009 to 2012)**. Graduated with a Ph.D in the Biological Sciences graduate program in December, 2012. Dissertation Title: *"Crystallographic, Kinetic and Cellular Studies on Natural Product Inspired Inhibitors of Quinone Reductase 2".* She is currently a Patent Agent at the law firm of Mintz Levin in Boston, MA. She is also currently working on her law degree with a specialization in patent law.
2) **Sakshi Tomar (2011 to Dec 2015)**. Graduated with a Ph.D in the Biological Sciences graduate program in December, 2015. Dissertation Title: *"Understanding the Determinants for Substrate Specificity, Regulation of Enzymatic Activity and the Development of Broad-Spectrum Inhibitors of Coronavirus 3-Chymotrypsin-like Proteases".* She is currently a post-doc working in the lab of Prof. Melanie Ott at the Gladstone Institutes at the University of California, San Francisco.
3) **Yafang Chen (2011 to Dec. 2015)** Graduated with a PhD in the PULSe graduate program in May, 2016. Dissertation Title: *"Structural and Functional Studies of the Papain-like Protease 2 from Mouse Hepatitis Virus"*. She is currently in Seattle, WA working on an advanced degree in computer programming and bioinformatics.
4) **Nicole (Davis) Hjortland (2012 to 2016)** Graduated with a PhD student in the PULSe graduate program in December, 2016. Dissertation Title: "*Defining the Regulatory Determinants in Substrate Catalysis by Biochemical, Biophysical, and Kinetic Studies for the Development of Specific Small-Molecule Inhibitors of Ubiquitin Specific Protease 7 and 7".* She is currently a Medical Writer at ArticulateScience, a division of Nucleus Global, in Decatur, GA.
5) **Qing Zhou (2012 to 2017)** Graduated with a PhD student in the Biological Sciences graduate program in August, 2017. Dissertation Title: *"Towards the Identification of Human Sulfotransferase 2B1b (Sult2B1b) Inhibitors for the Treatment of Prostate Cancer".* She is currently a Senior Analyst for A. T. Kearney, which is a global management consulting firm, in Chicago, IL.
6) **Yu-Chen Yen (2013 to 2017)** Graduated with a PhD in the Biological Sciences graduate program in August, 2017. Dissertation Title: *"Structure-based Drug Design of Selective BACE1 and BACE2 Inhibitors for the Treatments of Alzheimer's Disease and Type II Diabetes".* She is currently a post-doc in the lab of Prof. John Tesmer at Purdue University.

7) **Aya Ryuzoji (2014 to 2016)** Graduated with a non-thesis MS degree in the Biological Sciences graduate program in December, 2016. She is currently a research scientist in protein production at Eli Lilly in Indianapolis, IN.
8) **Jozlyn Clasman (2015 to May, 2019) She** graduated with a PhD in the PULSe and Biological Sciences graduate program in May, 2019. Dissertation title: *"Investigating the Substrate Specificity of the Equivalent Papain-Like Protase 2 Domain of NSP3 Across Alpha- and Beta-Coronaviruses"*. She is conducting post-doctoral research with Prof. Karen Allen at Boston University.
9) **Julia Luciano (2011 to present/delay)**. PhD student in the Biological Sciences graduate program. She is currently on a leave of absence for family reasons.
10) **Brandon Anson (2015 to present)** PhD student in the PULSe and Biological Sciences graduate program.
11) **Corey Moore (2015 to present)** PhD student in the Biological Sciences graduate program.
12) **Emma Lendy (2017-present)** PhD student in the PULSe and Biochemistry graduate programs.
13) **Yamasingha Pathiranage Samadhi Kulathunga (2017-present)** PhD student in the Chemistry (Biochemistry Division) graduate program.
14) **Mackenzie Chapman (August 2018-present).** PhD student in the Biological Sciences graduate program.
15) **Noah Danielson (August 2018-present).** PhD student in the Biochemistry graduate program.
16) **Adam Hamdani (August 2018-present).** PhD student in the Biochemistry graduate program.

POST-DOCTORAL RESEARCH FELLOWS (PURDUE)

1) **Courtney Daczkowski (2018-present).**
2) **Kristina Kesely (2016-present).**
3) **Renata Everett (2015-2017).** She recently moved to Seattle with her partner and is searching for a faculty position.
4) **Sarah St. John (2013-2016)** She is currently a Technical Account Manager at Phenomenex, Chicago, IL.
5) **Yahira Baez (2012 -2014)** She is currently a Clinical Project Manager at Cook Research Inc. in W. Lafayette, IN
6) **Katie Molland (2011 - 2014)** Currently a Regulatory Affairs Scientist at Cook Biotech, Inc. in W. Lafayette, IN.
7) **Soma Mukhopadhyay (2011 to 2013).** Currently teaching at Ivy Tech in Lafayette, IN.

RESEARCH-TRACK PROFESSORS (PURDUE)

1) **Aimee Eggler, Ph.D. (August 2010 to July 2012)** Research Assistant Professor of Biological Sciences. Aimee was the first one in our department with this title. Currently an Assistant Professor (tenure-track) in the Biochemistry Program at Villanova University, Philadelphia, PA.

RESEARCH STAFF SUPERVISED (PURDUE)

1. **Antonella Pepe, Ph.D. (October 2013 to June 2018).** Senior Research Scientist. Center for Cancer Research. Leader of the Medicinal Chemistry component of the Computational and Medicinal Chemistry Shared Resource. She is now a Visiting Associate Professor amd Senior Research Scientist, Department of Chemistry at Stony Brook University, NY.
2. **Nicole Kinkner, B.S. (January 2015 to present).** Research Assistant and Lab Manager
3. **Nadia Attalah, Ph.D.** (**September 2015 to September, 2018.**) Research Scientist. Center for Cancer Research. Bionformatician. She was promoted to Research Assistant Professor in 2018 in the Department of Comparative Pathobiology. She is now also Director of Bioinformatics for the Purdue Center for Cancer Research.
4. **Laura Kingsley, Ph.D. (August 2014 to May 2015).** Research Associate. Center for Cancer Research. Leader of the Computational Chemistry component of the Computational and Medicinal Chemistry Shared Resource. She is currently a research scientist at the Genomics Institute of the Novartis Research Foundation
5. **Sergey Savinov, Ph.D.** (**January 2012-August 2014).** Senior Research Scientist. Center for Cancer Research. Leader of the Computational Chemistry component of the Computational and Medicinal Chemistry Shared Resource. He is currently an Extension Associate Professor at University of Massachusetts Amherst in the Department of Biochemistry and Molecular Biology.

ROTATION GRADUATE STUDENTS SUPERVISED (PURDUE)

Student Name	**Graduate Program**	**Rotation Year**
		2010/2011
*Julia Luciano	Biological Sciences	*Fall*
*Sakshi Tomar	Biological Sciences	*Fall*
Michael Barney	PULSe	*Spring*
*Yafang Chen	PULSe	*Spring*
		2011/2012
Ross VerHeul	PULSe	*Fall*
Qing Zhou	Biological Sciences	*Fall*
Erin Kischuk	PULSe	*Fall*
Karthik Padmanabhan	Biological Sciences	*Spring*
*Nicole (Davis) Hjortland	PULSe	*Spring*
Ampa Suksatu	Biological Sciences	*Spring*
		2012/2013
*Yu-Chen Yen	Biological Sciences	*Fall*
James Grant	PULSe	*Fall*
Xiangying Sun	Biological Sciences	*Spring*
Amar Parvate	Biological Sciences	*Spring*
Joselyn Cruz	PULSe	*Spring*
		2013/2014
Songyao Ma	PULSe	*Fall*

Patrick Backman	PULSe	*Fall*
Paola Montenegro	PULSe	*Fall*
*Aya Ryuzoji	Biological Sciences	*Fall*
Starupa Bhaduri	Biological Sciences	*Spring*
Erh-Ting Hsu	PULSe	*Spring*
Mike Dibiasio-White	PULSe	*Spring*
**Xin Wen	PULSe	*Spring*
Thu Cao	Biological Sciences	*Spring*
		2014/2015
*Jozlyn Clasman	PULSe	*Fall*
*Brandon Anson	PULSe	*Fall*
Aslihan Terzi	Biological Sciences	*Fall*
*Corey Moore	Biological Sciences	*Fall*
Jacob Milton	PULSe	*Fall*
Matt Therkelsen	PULSe	*Fall*
		2015/2016
Zach Beck	Biochemistry	*Fall*
Veronica Heintz	PULSe	*Fall*
Bethany Manning	Biochemistry	*Fall*
Chelsea Theisen	PULSe	*Fall*
Alan Yi-Hui Hsu	Biological Sciences	*Fall*
**Thays Carvalho	PULSe	*Spring*
		2016/2017
Matt Eckhart	PULSe	*Fall*
*Emma Lendy	PULSe	*Spring*
Sue Heidi Loperena-Medina	PULSe	*Spring*
		2017/2018
Melaku Garsamo	Biochemistry	*Fall*
Karthik Srinivasan	Biological Sciences	*Fall*
Sherlene Brown	Biochemistry	*Spring*
		2018/2019
Kedrick Milholland	Biochemistry	*Fall*
Adam Hadmani	Biochemistry	*Fall*
Sarah McGovern	Biochemistry	*Fall*
Matt Russon	Biochemistry	*Fall*
Noah Danielson	Biochemistry	*Spring*
Andrew Demarco	Biochemistry	*Spring*

PULSe = Purdue University Interdisciplinary Life Sciences Program
*Student ultimately joined my lab
**Student ultimately joined my lab but left the graduate program due to personal issues.

GRADUATE STUDENT COMMITTEES (PURDUE)

Katie Jensen (Jermihov) Preliminary Exam, November 3rd, 2011
Katie Jensen (Jermihov) Committee Meeting, May23, 2012
Katie Jensen (Jermihov), Dissertation Defense, October 18th, 2012
Yafang Chen – Committee Meeting, March 21st, 2012
Saskshi Tomar – Preliminary Exam, April 30th 2012
Caroline Botting, Committee meeting, October 4th, 2011
Caroline Botting, Committee meeting, October 2nd, 2012
Caroline Botting, MS Theses defense, October 20th, 2012
Chao Feng, Committee Meeting, October 3rd, 2012
Marie Marrow, Oral Preliminary Exam (OP) October 26th, 2012
Nicole Davis committee meeting March 22nd, 2013
Nicole Davis committee meeting March 13th, 2014
Mary Zhang committee meeting April 1st, 2013
Qing Zhou Preliminary exam April 18th, 2013
Ross Verhul Committee Meeting April 26th 2013
Chun Ligan preliminary exam May 6th, 2013
Biaobin Jiang, May 15th 2013
Mark Ridella defense July 26th, 2013
Yafang Chen – August 21st, 2013 committee meeting
Rosemary Morman Prelim exam –Oct 3rd, 2013
Mary Zheng Committee meeting – Oct 4th, 2013
Ampa Suksatu Preliminary Exam October 17th, 2013
Shashir Poudyal committee meeting March 31st, 2014
Qing Zhou committee meeting April 14th, 2014
Mary Zhang dissertation defense April 15th, 2014
Chao Feng dissertation committee meeting April 21st, 2014
Cinthia Sanchez dissertation defense, April 23rd, 2014
Biaobing Jiang committee meeting May 12th, 2014
Rosemary Morman committee meeting May 27th, 2014
Yu-Chen Yen preliminary exam May 27th, 2014
Sara Johnson OP prelim exam May 29th, 2014
Paola Montenegro (agreed to be on committee)
Sakshi Tomar Committee Meeting, September 9th 2014
Kaibo committee meeting September 22nd, 2014
Healther Osswald, OP Exam, October 1st, 2014
Prasanthy Nyalapatla OP Exam, Oct 3rd, 2014
Phillip R, Prelim Exam, Cynthia Stauffacher student PULSe, October 6th, 2014
Julia Luciano, Committee Meeting, November 3rd, 2014
Yafang Chen, Committee Meeting, November 7th, 2014
Amy Funk, OP preliminary Exam, November 14th, 2014 –Chem, Chris Hyrcyna's student
Wen Zhu, OP preliminary Exam, Nov. 18th, 2014 – Chem student, IUPUI
Need to add 2015 Graduate Student Activities
Boning Zhang Prelim Exam March 22nd, 2016
Gillian Barth Prelim May 16th, 2016
Xusi Han Prelim Exam May 18th, 2016
Jacqueline Williams, OP exam (Chemistry) Sept. 26th, 2016

Yu-Chen committee meeting May 25th, 2016
Shishir Poudyal committee meeting, June 16th, 2016
Qing Zhou committee meeting August 30th, 2016
Nicole Hjortland PhD defense, September 2nd, 2016
Ross Verheul committee meeting, September 13th, 2016
Need to add 2017 Graduate Student Activities

UNDERGRADUATE STUDENTS (PURDUE)

I am only listing these Purdue undergraduate students who worked in the lab for at least two years and stayed at least one summer in the lab under a fellowship or research grant support.

1. **Annalissa Kammeyer (2013-2015)** – Biological Sciences
2. **Lendsey Thicklin (2012-2014)** – Biological Sciences (also Purdue SROP student)
3. **Melanie Johnston (2012-2014)** – Chemistry (Biochemistry), Chemistry Department fellowship.
4. **Caitlin Specht (2012-2014)** – Biological Sciences and SURF fellowship
5. **Samantha Pazak (2013-2014)** – Biological Sciences
6. **Rebeccca Twedell (2011-2012)** – Biological Sciences

The students listed below are from other universities who I mentored over the summer via Summer Research Opportunities Program (SROP) grant or the Purdue HHMI Undergraduate–Statistics Quantitative Biology program.

1. **Sue Heidi Loperena-Medina (2014)** University of Puerto Rico, Aguadilla (SROP student). She is now in the PULSe program at Purdue.
2. **KaLeigh Hurley (2014)** – Franklin College- Purdue HHMI Undergraduate–Statistics Quantitative Biology
3. **Jancita Wilson (2013)** – Chiminade University (SROP student)
4. **Belessing Aroh (2012)** – University of Maryland Eastern Shore (SROP student)
5. **Tamuka Chikyausiku (2011)** –Claflin University (SROP student)

UNIVERSITY OF ILLINOIS AT CHICAGO (1999-2010)

GRADUATE STUDENTS (UIC)

17) **Qi Sheng (2000 to 2003)**. Graduated with a MS degree in the Pharmacognosy graduate program-Biotechnology Track. Currently a research specialist at UIC.

18) **Sasikiran Chilukuri (2000 to 2006)** Graduated from my lab with a Ph.D. in the Pharmacognosy graduate program-Biotechnology Track. Currently the Publications Excellence Lead, Vaccines R&D, GSK Pharmaceuticals India
19) **Melissa May (2001 to 2006**). Graduated with a Ph.D. in the Pharmacognosy graduate program-Biotechnology Track. She is currently Vice President of Strategic Planning at NetBio in Boston, MA.
20) **Jill (Dombrauckas) Collins (2001 to 2006)** Graduated with a Ph.D. in the Medicinal Chemistry graduate program. She is currently Head of Accounts, Science, Marketing and Advertising Health and Science brands for Audacity, Inc. in San Diego, CA.
21) **Barbara Calamini (2001 to 2007)** Graduated with a Ph.D. in the Medicinal Chemistry graduate program. Currently is currently the Group Leader of Cell Biology, Sanofi Pharmaceuticals, Paris, France.
22) **Sonia Larsen (2001 to 2008)** Graduated with a Ph.D. in the Pharmacognosy Graduate Program-Biotechnology Track. She did a post-doc at Lybradyn, Inc. and then decided to be a stay-at-home mom.
23) **Huidong Yu (2001 to 2007)** Graduated with a Ph.D. in the Pharmacognosy graduate program-Biotechnology Track. He is currently a scientist for Rongene Pharma in China.
24) **Patrick Miller (2002 to 2008)** Graduated with a Ph.D. in the Pharmacognosy Graduate Program-Biotechnology Track. He is currently a Senior Scientist for Celerion in Lincoln, Nebraska.
25) **Kiira Ratia (2003 to 2008)** Graduated with her Ph.D. in the Pharmacognosy graduate program-Biotechnology Track. She is currently a Research Assistant Professor at the University of Illinois at Chicago and she is also the Director of the High-throughput Screening Center.
26) **Gary Klein (2004 to 2007)** Graduated with a MS degree in the Medicinal Chemistry graduate program. He had to leave the Ph.D. program since he was an active duty officer in the US Army. He is currently a US Army, Major stationed at Fort Leavenworth, Kansas. He is attending the U.S. Army School of Advanced Military Studies.
27) **Yang Tian (2004 to 2008)** Graduated with a Ph.D. in the Pharmacognosy graduate program-Biotechnology Track. He is currently a Senior Research Scientist at Gilead Sciences, Inc. in South San Francisco, CA.
28) **Renda Hawwa (2004 to 2009).** Graduated with a Ph.D. in the Medicinal Chemistry graduate program, Feb 22nd. She is currently a Regulatory Affairs Associate at Fresenius Medical Care in Boston, MA.
29) **Valerie Sershon (2004 to 2009)** Graduated with a Ph.D. in the Medicinal Chemistry graduate program. She is currently a Senior Research Scientist (Enzymologist) at Kraft Foods Group in Northfield, IL.
30) **Evan Small (2007 to 2010)** Graduated with an MD/PhD in Biochemistry. He finished the PhD portion of his degree in my lab in 2010 and his MD in 2012. He is now a Doctor of Emergency Medicine and Toxicology at the Mayo Clinic in Rochester, MN.
31) **Megan Sturdy (2006 to 2010).** Graduated with a Ph.D in the Medicinal Chemistry graduate program. She was co-advised with Dr. Jimmy Orjala. She is currently completing her Doctor of Osteopathic Medicine degree at Western University (2015).
32) **Thomas Wubben (2008 to 2011).** Graduated with an MD/PhD in Biochemistry. He finished the PhD portion of his degree in my lab in 2011 and his MD in 2013. He is currently doing is residency in Ophthalmology at the University of Michigan.

33) **Yahira Baez-Santos (2007 to 2012)** Graduated with a Ph.D. in the Pharmacognosy graduate program-Biotechnology Track in December 2012. She is now a Clinical Project Manager at Cook Research, Inc. West Lafayette, IN.

POST-DOCTORAL RESEARCH FELLOWS MENTORED AT UIC

8) **Chris Fleming, Ph.D. (August 2007 to August 2009)** Currently a Research Scientist at Syngenta in Raleigh, NC.
9) **Aimee Eggler, Ph.D. (April, 2003 to April 2006)**. Currently an Assistant Professor (tenure track) at Villanova University, Philadelphia, PA.
10) **Scott Pegan, Ph.D. (September, 2006 to May, 2009).** Currently an Associate Professor (tenure track) at the University of Georgia, Athens.
11) **Magdalini Vamvouka, Ph.D. (January, 2001 to August, 2003)**. Currently an Adjunct Professor at the University of Detroit Mercy.
12) **Kiira Ratia, Ph.D. (December, 2008 to March, 2010).** Post-doctoral research associate and senior research specialist.

RESEARCH-TRACK PROFESSORS SUPERVISED AT UIC

1) **Bernard Santarsiero (August 2001 to December 2007)**. Research Professor. He is still a Research Professor in the Department of Medicinal Chemistry and Pharmacognosy at UIC and is the Associate Director for the U of I Biorepository.
2) **Valerie Grum-Tokars (August 2005 to August 2008; September 2009 to Aug 2010)** Research Assistant Professor. She is currently a Research Assistant Professor in Pharmacology and the Core Facility Operations Director at Northwestern University Feinberg School of Medicine, Chicago, IL.
3) **Aimee Eggler, Ph.D. (April 2006 to August 2010)** Research Assistant Professor. Currently an Assistant Professor (tenure track) in the Biochemistry Program at Villanova University, Philadelphia, PA.
4) **Scott Pegan, Ph.D**. **(May 2009 to September 2009).** Research Assistant Professor. Currently an Associate Professor (tenure track) at the University of Georgia, Athens. In the Department of Pharmaceutical & Biomedical Sciences.
5) **Kiira Ratia, Ph.D. (March 2010 to August 2010).** Research Assistant Professor. She is currently a Research Assistant Professor in the Department of Medicinal Chemistry and Pharmacognosy at the University of Illinois at Chicago.

GRADUATE COURSE TEACHNING AT UIC (My last year at UIC)

I taught the courses below for 11 years at UIC. The number of lectures for each course varied slightly each year, but the number of didactic course lectures I gave each year was approximately 50.

Spring 2010

PMPG 513	Structure of Biopolymers
MDCH 571	Organic Medicinal Chemistry II
MDCH 592	Research Techniques in Medicinal Chemistry
PMPG 599	Doctoral Research in Pharmacognosy
MDCH 599	Doctoral Research in Medicinal Chemistry
PMPG 522	Laboratory Techniques in Pharmaceutical Biotechnology 1

Fall 2009

PMPG 510	Research Techniques in Pharmacognosy
MDCH 599	Doctoral Research in Medicinal Chemistry
MDCH 561	Medicinal Chemistry
PMPG 599	Doctoral Research in Pharmacognosy
PMPG 523	Laboratory Techniques in Pharmaceutical Biotechnology II.
PMPG 507	Drug Discovery

PROFESSIONAL COURSES TAUGHT AT UIC

Fall 2009

BPS 385	Professional Development Seminar

Spring 2010

PHAR 408	PDAT Series-Required Course

INVITED SCIENTIFIC SEMINARS AND SYMPOSIA

1. Mesecar, A. D. (2019) "Taxonomically-Driven Inhibitor Development." NIAID Centers for Structural Genomics of Infectious Disease Annual Meeting. May 8th -10th. Chicago, IL.
2. Mesecar, A.D. (2019). "The Yin and Yang of Developing Selective and Broad-Spectrum Therapeutics: Lessons from Coronavirus Proteases." University of Notre Dame , Department of Chemistry and Biochemistry. April 18th (Invited Seminar)
3. Mesecar, A.D. (2019). "Discovery and Design of Selective Ubiquitin Specific Protease (USP) Inhibitors." Sanford Burnham Prebys Medical Discovery Institute in La Jolla, CA as part of their NCI Cancer Center seminar series. April 29th (Invited Seminar)
4. Mesecar, A. D. (2018) "Taxonomically-Driven Inhibitor Development." NIAID Centers for Structural Genomics of Infectious Disease Annual Meeting. (May 2nd -4th). Seattle, WA
5. Mesecar, A.D. (2017). "Ubiquitin Specific Proteases (USPs) as Emerging Therapeutic Targets" Department of Pharmaceutical & Biomedical Sciences, University of Georgia, Athens. September 26th-28th. (Invited Seminar)
6. Mesecar, A.D. (2017). "Discovery & Development of Coronavirus Protease Inhibitors as Potential Therapeutics". XIVth International Nidovirus Symposium. June 4th to 9th. Kansas City, MO. (Invited Talk)
7. Mesecar, A.D. (2016). "Selective (Yin) and Broad-Spectrum (Yang) Targeting of Coronavirus Proteases". Vanderbilt Institute of Chemical Biology. Vanderbilt University School of Medicine. Nashville, TN. September 6th -8th. (Invited Seminar)
8. Mesecar, A.D. (2016). "Proteases as antiviral drug targets: successes and challenges". 4th Antivirals Congress. Sitges, Spain. September 17th-22nd. (Invited Talk)
9. Mesecar, A.D. (2016). "Structural Biology at Purdue". Indiana Structural Biology Forum. Indianapolis, IN. March 2nd. (Invited Talk)
10. Mesecar, A.D. (2015). "Oxidative Stress and Chronic Disease". Bioactives and Health Symposium. Purdue University. August 28th. (Invited seminar).
11. Mesecar, A.D. (2015). "Purdue Moves: Investing in drug discovery". The 6th Joint Great Lakes/Central Regional Meeting of the American Chemical Society. Grand Rapids, MI. May 28th.
12. Mesecar, A.D. (2015). "Natural and dietary-derived chemopreventive agents that modulate Keap1 and NRF2". Department of Nutrition Science, Interdepartmental Nutrition Program Seminar. Purdue University. Jan. 23rd – Forthcoming
13. Mesecar, A.D. (2015). "Discovery and Design of Selective Ubiquitin Specific Protease (USP) Inhibitors". Department of Chemistry seminar series. Indiana University Purdue University Indianapolis. March 4th (Invited Seminar)
14. Mesecar, A.D. (2014). "Mechanistic and Structural Studies of Cancer Chemopreventive Targets. Department of Medicinal Chemistry and Pharmacognosy seminar series, University of Illinois at Chicago. Sept. 19th (Invited Seminar)

15. Mesecar, A.D. (2014). "Discovery and Design of Selective Ubiquitin Specific Protease (USP) Inhibitors". Center for Drug Discovery Dedication Symposium. Purdue University. Sept. 4th
16. Mesecar, A.D. (2014). "Coronaviruses-21st Century Threats". Given at the 'Science on Tap' seminar series, sponsored by the Lafayette Brewing Company, Lafayette, IN. Sept. 25th.
17. Mesecar, A.D. (2014). "Mechanistic and Structural Basis for Nrf2 ubiquitination by Keap1-Cul3-Rbx1". Seminar presented at Eli Lilly. Indianapolis, IN. Oct. 29th
18. Mesecar, A.D. (2014). "Dietary derived cancer preventive agents". Lecture given as part of an educational series entitled "Cancer Research at Purdue". Wabash Area Lifetime Learning Association (WALLA). Morton Center. West Lafayette, IN. Oct. 22nd
19. Mesecar, A.D. (2014). "Identifying Deubiquitinating Enzyme inhibitors via HTS". Laboratory Robotics Interest Group (LRIG), Midwest Chapter annual meeting. Indianapolis, IN. April 24th.
20. Molland, K. and Mesecar, A.D. (2013). "A 2.2 A structure of the USP7 catalytic domain in a new space group elaborates upon structural rearrangements reulting from ubiquitin binding". Katie Molland presented our seminar at the 33rd Midwest Enzyme Chemistry Conference. Loyola University, Chicago. Oct. 12th
21. Mesecar, A.D. (2013). "Structure-based Approach to Discovering DUB Inhibitors". Pre-Conference Workshop on Challenegs in Identifying Selective Inhibitors of DUBs & Ligases. Ubiquitin Drug Discovery & Diagnostics conference. Philadelphia, PA. July 22nd to 24th.
22. Molland, K. and Mesecar, A.D. (2013). "New Structures of the USP7 Catalytic Domain Elaborate upon Structural Plasticity Caused by Ubiquitin Binding". Katie Molland delivered our invited talk in the Ubiquitin, A New Fronteir in Cancer session of the Ubiquitin Drug Discovery & Diagnostics conference. Philadelphia, PA. July 22nd to 24th.
23. Baker, S. and Mesecar, A.D. (2013). "Development of antiviral compounds against MERS-CoV". MERS-CoV Research: Current Status and Future Priorities Meeting. National Institutes of Health. Bethesda, MD. June 23rd.
24. Mesecar, A.D. (2011). "Orientational requirements in enzyme catalyzed reactions". Enzyme Mini-Symposium to Celebrate the Career of Thomas Nowak. University of Notre Dame. November 4th-5th, South Bend, IN.
25. Mesecar, A.D. (2011). "Structure & Function of Coronavirus Papain-Like Proteases". Department of Microbiology and Immunology seminar series. Loyola University, Stritch School of Medicine. Oct. 20th.
26. Mesecar, A.D. (2011). "Structural & mechanistic studies of nutritional and natural product derived cancer chemopreventive agents". Purdue University Oncological Sciences Center Prevention & Control Program seminar. Purdue University. April 5th.
27. Mesecar, A.D. (2011). "Identification of non-covalent, antiviral DUB inhibitors that block human SARS and NL63 viruses. Invited oral presentation for the 241st American Chemical Society National Meeting, Anaheim, CA. Division of Medicinal Chemistry. Targeting the Ubiquitiliation System session. Abstract #151. March 28-31st th.
28. Mesecar, A.D. (2011). "Structural & Chemical Approaches to Understanding Mechanisms of Natural Cancer Preventive Agents". Department of Pharmaceutical Sciences and

Experimental Therapeutics seminar series on Medicinal and Natural Products Chemistry. University of Iowa. March 1st.

29. Mesecar, A.D. (2011). "SARS virus papain-like protease: A drug target with multiple functions". College of Science Colloquium Seminar. Illinois Institute of Technology, Chicago, IL.
30. Mesecar, A.D. (2011). "Biochemical and Structural Basis for Natural Product Induction of that Antioxidant Responsive Element". Department of Biochemistry seminar series. Purdue University. Feb. 22nd.
31. Mesecar, A.D. (2011). "Orientational requirements in enzyme catalyzed reactions". Marsico Visiting Scholars Named Lectureship Program. Department of Chemistry, University of Denver. January 11th.
32. Mesecar, A.D. (2011). "Chemical and structural basis for induction of cytoprotective enzymes involved in cancer prevention". Marsico Visiting Scholars Named Lectureship Program. Department of Chemistry, University of Denver. January 10th.
33. Mesecar, A.D. (2011). "Development of potent, non-covalent cysteine protease inhibitors that target viral deUbiquitination and deISGylation". GlaxoSmithKline Pharmaceuticals. Cancer Research-Protein Dynamics. Collegeville, PA. January 23rd.
34. Mesecar, A.D. (2009). "Targeting deubiquitinating enzymes (DUBS) with antiviral and anticancer agents: Lessons from the SARS virus papain-like protease". The Institute for Genomics & Systems Biology and Section of Hematology/Oncology. The University of Chicago. December 14th.
35. Mesecar, A.D. (2009). "Therapeutic targeting of the papain-like protease from SARS virus that multitasks as a viral deubiqitinating and deISGylating enzyme". University of California, San Diego. November 17th, 2009.
36. Mesecar, A.D. (2009). "Lead discovery and probe-development in smaller academic-based labs". Probe Discovery Conference, November 19-20, La Jolla, CA.
37. Mesecar, A.D. (2009). "A non-covalent class of papain-like protease/deubiquitinase inhibitors blocs SARS virus replication." Ubiquitin in Drug Discovery & Diagnostics Conference. October 12-14, Philadelphia, PA.
38. Mesecar, A.D. (2009). "The role of the Keap1-Nrf2-Cul3 system in cancer chemoprevention". UIC Cancer Center Seminar, University of Illinois at Chicago. September 10th.
39. Mesecar, A.D. (2009). "Natural product based cancer preventive agents: New targets and lead discovery". Department of Medicinal Chemistry. University of Michigan, Ann Arbor, MI. June 18th.
40. Mesecar, A.D. (2009). "Lead discovery and development of SARS virus cysteine-protease inhibitors-targeting a double-edged sword". Department of Medicinal Chemistry. University of Michigan, Ann Arbor, MI. March 12th.
41. Mesecar, A.D. (2009). "The use of light-based probes in academic lead discovery". Promega Corporation, Madison, WI. March 9th.

42. Mesecar, A.D. (2009). "Development of non-covalent inhibitors that target the papain-like cysteine protease from SARS virus: New horizons for targeting deubiquitinating enzymes." Department of Biochemistry Seminar Series. Emory University, Atlanta, GA. February 26th.
43. Mesecar, A.D. (2009). "Natural products and their pleiotropic interactions with molecular targets: towards the molecular basis for cancer chemoprevention". 3rd International Conference on Molecular Mechanism of Environmental Response to Food and Oxygen. February 9th to 12th. Sendai, Japan.
44. Mesecar, A.D. (2009). "Development of Non-Covalent Inhibitors that Target the Papain-Like Cysteine Protease from SARS Virus: New Horizons for Targeting Deubiquitinating Enzymes". University of Missouri, Kansas City. Department of Biochemistry Seminar Series. January 29th.
45. Mesecar, A.D. (2009)."Proteinase inhibitor design for SARS 3CLpro and PLpro. Conference on Respiratory Virus Pathogenesis, Aging, and Models of ARDS. University of North Carolina, Chapel Hill. January 12th-13th.
46. Mesecar, A.D. (2008). "Mapping Enzyme Reaction Coordinates by X-ray Crystallography". Workshop on Time-resolved Macromolecular Crystallography. Advanced Photon Source, Argonne National Laboratory. November 20-22, 2008
47. Mesecar, A.D. (2008). "Drug Discovery and Biotechnology in Academia". Department of Chemistry and Biochemistry. Indiana University, South Bend. November 10th.
48. Mesecar, A.D. (2008). "Therapeutic targeting of a protease from SARS virus that multitasks as a viral deubiqitinating and deISGylating enzyme". University of Maryland Baltimore County, Department of Chemistry Seminar Series. September 23rd.
49. Mesecar, A.D. (2008). "Therapeutic targeting of a protease from SARS virus that multitasks as a viral deubiqitinating and deISGylating enzyme". Purdue University, Department of Biological Sciences, Structural Biology Seminar. September 3rd.
50. Mesecar, A.D. (2008). "Deubiquitinating enzymes (DUBS) as therapeutic targets: From antiviral to anticancer agents" The University of Chicago, Institute for Genomics & Systems Biology and Department of Medicine Seminar Series. March 17th.
51. Mesecar, A. D. (2007) "The tale of two proteases:Therapeutic Development Against Coronavirus Infections" Department of Pharmacology Seminar. University of Pennsylvania, December 10th.
52. Mesecar, A. D. (2007) "The application of X-ray crystallography to medicinal chemistry and natural product lead discovery". University of Minnesota. Department of Medicinal Chemistry Seminar. December 17th.
53. Mesecar, A. D. (2007) "Using X-ray Structural Information in Drug Design". ***Keynote Lecture.*** The 3rd International Meeting on Medicinal and Pharmaceutical Chemistry. Antalya, Turkey, October 16 – 21.
54. Mesecar, A.D., Eggler, A. L., Calamini, B., van Breemen, R., Pezzuto, J.M. (2007) "Natural products and their pleiotropic interactons with molecular targets: Toward the molecular basis for cancer chemoprevention" 233rd ACS National Meeting in Chicago. (Paper ID: 1048367

Paper ID AGFD 27). Sunday, March 25th. Section on Natural Products, Diets and Cancer Prevention. (Invited Oral Presentation)

55. Mesecar, A. D. (2006)." Molecular odysseys in mapping enzyme reaction coordinates by x-ray crystallography" Workshop on Time-resolved and Laue X-ray Crystallography. Advanced Photon Source, Argonne National Laboratory. May 6th, 2006.

56. Mesecar, A. D. (2006)."Drug Discovery and Structural Biology in Biodefense" Northwestern University. Department of Biochemistry, Molecular Biology, and Cell Biology. Biophysics Seminar. May 1st, 2006.

57. Mesecar, A. D. (2006)."Drug Discovery in Biodefense: Our progress here at UIC. MD/PHD Seminar. College of Medicine, UIC October 4th, 2006

58. Mesecar, A. D. (2005) "Towards a molecular-level understanding of the cancer chemopreventive properties of dietary and other natural compounds", Department of Human Nutrition, University of Illinois at Chicago, November 17th, 2005.

59. Mesecar, A. D. (2005) Crystallographic Studies of Enzyme Reaction Coordinates: Molecular Odysseys in Four Dimensions". Department of Chemistry, Loyola University, October 27th, 2005.

60. Mesecar, A. D. (2005) "Time-resolved Laue x-ray diffraction studies at the Advanced Photon Source." 2nd Annual SER-CAT Symposium, St. Jude Children's Research Hospital, Memphis, TN. March 18th, 2005.

61. Mesecar, A. D. (2005) "The Potential Impact of Structural Genomics on Time-resolved X-ray and Time-of-Flight (Spallation) Neutron Diffraction". Biosciences Division Seminar, Argonne National Laboratory. March 3rd, 2005.

62. Mesecar, A. D. (2004). "Structural Motions During the Catalytic Cycles of Isocitrate Dehydrogenase and Phosphotriesterase Revealed by Monochromatic and Laue X-ray Crystallography". The 62nd Annual Pittsburgh Diffraction Conference, October 28th-30, Pittsburgh, PA.

63. Mesecar, A. D. (2004). "New horizons in protein crystallography: Time-resolved x-ray diffraction and time-of-flight (Spallation) neutron diffraction" The University of Kansas Structural Biology Center, Building Dedication and Symposium on Protein Structure and Function. University of Kansas. October 15-16, 2004.

64. Mesecar, A. D. (2004). "The role of protein dynamics in enzyme catalysis and inhibitor design for the SARS 3C proteinases". Stritch School of Medicine, Loyola University Chicago. September 16th, 2004.

65. Mesecar, A. D. (2004). "Protein crystallography in four dimensions: New horizons for dynamic structure-guided design". Molecular Pharmacology and Experimental Therapetuics Seminars. Division of Cardiovascular Diseases, Department of Medicine. Mayo Clinic. September 3rd, 2004.

66. Andrew Mesecar, Kiira Ratia, Bernard Santarsiero, Kai Xi, Dalia Jukneliene, Brian Harcourt, Paul Rota, Susan Baker, Arun Ghosh (2004). "Crystallographic and Kinetic Studies of Novel SARS-CoV 3CLpro Protease Inhibitors that Inhibit SARS-CoV and MHV-A59 Replication".

The 7th International Symposium on Positive-Strand RNA Viruses. San Francisco, CA. May 27-June 1. ***Plenary Lecture***.

67. Mesecar, A. D. (2004) "Molecular Movies of Enzyme Catalysis: Implications for Dynamic, Structure-Based Drug Design". Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN. May 3rd.

68. Mesecar, A. D. (2004) "Crystallographic Studies of Enzyme Reaction Coordinates: Molecular Odysseys in Four Dimensions". Department of Chemistry, University of Toledo. April 5th, 2004.

69. Mesecar, A. D. (2004) "A new organophosphorous hydrolase from *Deinococcus radiodurans*". NATO Army Armaments Group. Project Group 31 on "Non-Corrosive, Biotechnology-Based Decontaminants fro CBW Agents. Eighteenth Meeting held at the McGowan Institute for Regenerative Medicine, Pittsburgh, PA. March 30 -31.

70. Mesecar, A. D. (2003) "Settling Controversies in Enzyme Catalysis via Macromolecular Neutron Diffraction". Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, NM. Sixth User Group Meeting. October 19 - 21.

71. Mesecar, A. D. (2003) "Enzyme Catalyzed Reactions in Four Dimensions". The University of Iowa, Iowa City, IA. Department of Biochemistry. September 25th.

72. Mesecar, A.D. (2003) "Dynamic motions of enzymes revealed by static and time-resolved x-ray structures". The University of Minnesota, Minneapolis, MN. Department of Biochemistry, Molecular Biology and Biophysics (BMMB). October 8th.

73. Mesecar, A.D., Barry Stoddard, Bernie Santarsiero, Sonia Larsen, Kiira Ratia, Magdalini Vamvouka, Zhong Ren, Reinhard Pahl and Vukica Srajer. (2003) "Static and Time-Resolved Studies of Enzyme Reaction Coordinates: Molecular Odysseys in Four Dimensions". Time Resolved Diffraction in Chemistry & Biology Symposium. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31.

74. Mesecar, A.D. (2003) "Prospecting the biosphere for novel enzyme functions" Fred Hutchinson Cancer Research Center. Basic Sciences Division. Seattle, WA. Monday, May 19th, 2003.

75. Mesecar, A.D. (2002) "Dynamic motions of enzymes during catalysis revealed by time-resolved x-ray structures" University of Illinois at Chicago, Department of Biochemistry. Chicago, Illinois. Thursday, November 21st.

76. Mesecar, A.D. (2002) "Making molecular movies of enzyme reaction coordinates. This isn't Hollywood. XXII Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, September 28th.

77. Mesecar, A.D. (2002) "A new paradigm for rational drug design: Thinking out of the static, active site box". MediChem, Inc. Woodridge, Illinois. Thursday, March 7th.

78. Mesecar, A.D. (2001) Molecular Movies of Enzyme Action: This isn't Hollywood. Purdue University. West Lafayette, Indiana. Structural Biology Seminar Series. Department of Biology. Wednesday, November 14th.

79. Mesecar, A.D. (2001) Molecular Movies and Enzyme Reaction Coordinates. The 11th Users Meeting of the Advanced Photon Source, Argonne National Laboratory. Argonne, Illinois. Tuesday, October 9th.
80. Mesecar, A.D. (2001) Molecular Movies of Enzyme Action: This isn't Hollywood. Northern Illinois University. DeKalb, Illinois. Monday, September 10th. Graduate Colloquium Seminar.
81. Mesecar, A.D. (2001) "Making Molecular Movies of Enzyme Catalysis: This isn't Hollywood" BioCARS Workshop on Time-Resolved Crystallography. Monday, March 12th. Argonne National laboratory, Argonne, Illinois.
82. Mesecar, A.D. (2001) "The Experiment: Caging Strategies for Triggering Enzyme Reaction in the Crystalline State " BioCARS Workshop on Time-Resolved Crystallography. Tuesday, March 13th. Argonne National laboratory, Argonne, Illinois..
83. Mesecar, A.D. (2001) "Rational Drug Design: Past, Present and Future" Forty-Ninth Annual Honors Convocation. Thursday, February 22nd. College of Pharmacy, University of Illinois at Chicago. Chicago, Illinois. *Honors Address-Invited Speaker.*
84. Mesecar, A.D. (2001) "A New Paradigm for Rational Drug Design". Vahlteich Award Recipient Series. Friday, March 2nd. University of Illinois at Chicago. Chicago, Illinois.
85. Mesecar, A.D. (2000) "Molecular Movies of Enzymes in Action." Friday, November 17th. Medical College of Wisconsin.
86. Mesecar, A.D. (2000). "Creating a Molecular Movie of an Enzyme Catalyzed Reaction." Finch University of Health Sciences/The Chicago Medical School. Thursday, February 24th.
87. Mesecar, A.D. (1999). "Protein Conformational Changes: How small is Big Enough? University of Wisconsin, Madison." Friday, October 29th.
88. Mesecar, A.D. (1999). "Protein Conformational Changes: How small is Big Enough?" Illinois Institute of Technology, Chicago, Illinois. Monday, November 15th.
89. Mesecar, A.D. (1999). "Protein Conformational Changes: How small is Big Enough?" University of Notre Dame. June 10th and 11th.
90. Mesecar, A.D. (1996)"Revealing the Regulatory Role of the Divalent Metal of the Pyruvate Kinase Reaction by a Complete Thermodynamic Analysis of the Ligand Binding Parameters" (1995). University Federal do Rio de Janeiro, Brazil.
91. Mesecar, A. D. and Nowak, T. (1993) "Non-concerted Allosteric Behavior of Yeast Pyruvate Kinase." XIIIth Midwest Enzyme Chemistry Conference (1993).

CONFERENCE AND SYMPOSIA ABSTRACTS AND PRESENTATIONS (Also Student and Post-doc Presentations at Purdue)

1. Jozlyn Clasman, Yahira M. Baez-Santos, Robert C. Mettelman, Amornrat O'Brian, Susan C. Baker and Andrew D. Mesecar. Structure and kinetics of a core MERS papain-like protease

with utility for structure-based drug design. Abstract S2. O-08. XIVth International Nidovirus Symposium (2017). June 4th to 9th. Kansas City, MO. (Invited Talk for my graduate student Jozlyn Clasman)

2. Leticia Sofia Gonzalez, Brandon Anson and Andrew D. Mesecar (2017). "Effect of Allosteric Changes in MERS 3CL protease Enzymatic Activity and Dimerization". The FASEB Journal. Vol. 31 no.1 Supplement 601.7 Abstract from the Experimental Biology meeting, April 22-26, Chicago, IL.
3. Jozlyn R. Clasman, Yahira M. Baez-Santos, Robert C. Mettelman, Amornrat O'Brieen, Susan C. Baker and Andrew D. Mesecar (2016). "Crystal Structure and Kinetic Profile of a Core Papain-like Protease of MERS Coronavirus with Utility for Structure-based Drug Design". Poster #19. The 34th Midwest Enzyme Chemistry Conference. The University of Illinois at Chicago, October 1st. Chicago, IL.
4. Kristina R. Kelsey, Yafang Chen, Xufang Deng, Susan C. Baker and Andrew D. Mesecar (2016). "X-ray Structural and Functional Studies of Four Tandemly Linked Domains of Non-structural Protein 3 (nsp3) from Murine Hepatitis Virus (MHV) and their Involvement in Mediating Viral Escape from the Innate Immune Response". Poster #124 The 34th Midwest Enzyme Chemistry Conference. The University of Illinois at Chicago, October 1st. Chicago, IL.
5. Yu-Chen Yen, Annalissa Kammeyer, Katherine C. Jensen, Arun K. Ghosh and Andrew D. Mesecar (2016). "Development of an efficient structure-based drug discovery platform for BACE1 Inhibitors for the treatment of Alzheimer's Disease". The FASEB Journal. Vol. 30. No. 1. Supplement 607.9. The FASEB Journal. Vol. 30. No. 1. Supplement 612.14. Abstract from the Experimental Biology Meeting. April 2-6, San Diego, CA.
6. Qing Zhou and Andrew D. Mesecar. (2016) A Fluorescent, HTS-Adaptable Coupled-Enzyme Assay for Measurement of Human Cytosolic Sulfotransferase (SULT) 2B1b Activity and Identification of Small-Molecule Inhibitors. The FASEB Journal. Vol. 30. No. 1. Supplement 612.14. Abstract from the Experimental Biology Meeting. April 2-6, San Diego, CA.
7. Sarah E. St. John and Andrew D. Mesecar. (2016) Design, Synthesis, and Development of Broad Spectrum Coronaviral 3C-Like Protease Inhibitors to Target Emerging Human Pathogens: A Phylochemical Approach". The FASEB Journal. Vol. 30. No. 1. Supplement 842.14. Abstract from the Experimental Biology Meeting. April 2-6, San Diego, CA.
8. Nicole M. Hjortland, Antonella Pepe, Katrina Molland and Andrew D. Mesecar (2016). "Decoupling the Allosteric Activation of Ubiquitin Specific Protease 7 by Its Ubiquitin-like Domains for the Development of Small Molecule Inhibitors". The FASEB Journal. Vol. 30. No. 1. Supplement 835.6. Abstract from the Experimental Biology Meeting. April 2-6, San Diego, CA.
9. Midwest Enzyme Chemistry Conference (2016). University of Illinois at Chicago. Chicago, IL. October, 1st. (Multiple posters presented by lab members).
10. Defense Science Study Group – 30th Anniversary Conference (2016). Washington, DC. March 29th-31st. (Attended)
11. St. John, S.E. and Andrew Mesecar (2015). "Phylochemical approach for the development of broad spectrum coronavirual 3C-like protease inhibitors to target emerging human pathogens". The 6th Joint Great Lakes/Central Regional Meeting of the American Chemical Society. Grand Rapids, MI. May 28th. (Poster)

12. St. John, S.E. and Andrew Mesecar (2014). "Structural Insights into the Inhibition of the bat HKU4 3C-like protease." Presented at The 34th Midwest Enzyme Chemistry Conference, Chicago, IL. September (Poster)
13. Sakshi Tomar, Aimee Eggler, Valerie Grum-Tokars, Craig W. Lindsley, Shaun R. Stauffer, Anna Mielech, Susan Baker, Andrew Mesecar (2014). Discovery of potent, non-covalent inhibitors of SARS-CoV 3CLpro. Office of Interdisciplinary Graduate Programs, Purdue University, West Lafayette, IN. April 2nd. (poster)
14. Julia Luciano and Andrew D. Mesecar (2014) Single-Particle Electron Microscopy Analysis of Keap1 reveals a novel domain organization and conformational variability NRAMM Workshop on Advanced Topics in EM Structure Determination: Where do we go from here? November 9th -14th, 2014 – The Scripps Research Institute (poster)
15. Julia Luciano and Andrew D. Mesecar (2014) Single-Particle Electron Microscopy Analysis of Keap1 reveals a novel domain organization and conformational variability. Presented at the 34th Midwest Enzyme Chemistry Conference – September 27th, 2014 – Northwestern University, Evanston – IL (poster).
16. Qing Zhou and Andrew D. Mesecar (2014). A fluorescent, HTS-adaptable coupled-enzyme assay for activity measurement of human cytosolic sulfotransferase (SULT) 2B1b. Presented at the 34th Midwest Enzyme Chemistry Conference – September 27th, 2014 – Northwestern University, Evanston – IL (poster).
17. Sakshi Tomar (2014). Characterization of 3CL protease (3CLpro) from recently emerged MERS coronavirus. Infectious Disease Seminar series, Department of Biological Sciences, Purdue University, West Lafayette, IN. March 6th. (Talk)
18. Nicole Davis and Andrew D. Mesecar (2014). Targeted Inhibition of Ubiquitin Specific Proteases for Cancer Treatment. Purdue University Center for Cancer Research Scientific Retreat. West Lafayette, IN. November 12. (Poster)
19. Sakshi Tomar (2014). Ligand-induced dimerization of MERS coronavirus 3CL protease (3CLpro): implications for 3CLpro regulation and the development of antivirals. Graduate Student Research In Progress Seminar series, Department of Biological Sciences, Purdue University, West Lafayette, IN. November 6th. (Talk)
20. Sakshi Tomar (2014). Ligand-induced dimerization of MERS coronavirus 3CL protease (3CLpro): implications for 3CLpro regulation and the development of antivirals. Infectious Disease Seminar series, Department of Biological Sciences, Purdue University, West Lafayette, IN. November 6th. (Talk)
21. Molland, K. and Mesecar, A.D. (2014) "Structure, Function and Inhibition of Deubiquitinating Enzymes" . Structural Biology Seminar Series, March 26, 2014 Purdue University, West Lafayette, Indiana (Invited talk – K. Molland)
22. Katrina Molland, Qing Zhou, Andrew Mesecar. (2013)"A 2.2 Å structure of the USP7 catalytic domain in a new space group elaborates upon structural rearrangements resulting from ubiquitin binding" Walther Cancer Foundation Symposium. University of Notre Dame, South Bend, IN. October 5th (poster)
23. Julia Luciano and Andrew D. Mesecar (2013) Preliminary Single-Particle Electron Microscopy Analysis of Keap1 reveals a novel domain organization and conformational variability. Presented at the 33rd Midwest Enzyme Chemistry Conference – October 12th, 2013 – Loyola University, Chicago – IL (Poster)

24. Nicole Davis and Andrew D. Mesecar (2013). From E.coli to Baculovirus, the Expression and Purification of USP17. Purdue University Center for Cancer Research Scientific Retreat. West Lafayette, IN. November 6th. (Poster)
25. Julia Luciano and Andrew D. Mesecar (2013) Preliminary Single-Particle Electron Microscopy Analysis of Keap1 reveals a novel domain organization and conformational variability. Presented at the Walther Cancer Foundation Symposium – October 4th-5th, 2013 – University of Notre Dame – IN (poster)
26. Julia Luciano and Andrew D. Mesecar (2013) The Role of Keap1-Cul3-mediated Ubiquitination in Regulation of Nrf2 and Nf-κB Signaling. Presented at the Purdue Center for Cancer Research CIS Seminar – February 21st, 2013 – West Lafayette – IN (Invited talk – J. Luciano)
27. Nicole Davis and Andrew D. Mesecar (2013). From E.coli to Baculovirus, the Expression and Purification of USP17. Midwest Enzyme Chemistry Conference. Loyola University Chicago, IL. October 12th. (Poster)
28. Katrina Molland, Qing Zhou, Andrew Mesecar. (2013) "A 2.2 Å structure of the USP7 catalytic domain in a new space group elaborates upon structural rearrangements resulting from ubiquitin binding" 33rd Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 12th. (poster)
29. Katrina Molland, Qing Zhou, Andrew Mesecar. (2013) "A new 2.2 Å structure of the USP7 catalytic domain elaborates upon structural rearrangements that accompany ubiquitin binding" Ubiquitin Workshop and Conference, July 22-24, 2013 Philadelphia, Pennsylvania (invited talk - K. Molland and poster).
30. Nicole Davis and Andrew D. Mesecar (2013). From E.coli to Baculovirus, the Expression and Purification of USP17. Walther Cancer Foundation Symposium. Notre Dame , IN. October 5th. (poster)
31. Katrina Molland, Caitlin Specht, Andrew Mesecar. (2013) "A new tool to probe the cleavage preferences of coronaviral 3CL protease" Purdue University Disease and Pathogenesis Seminar Series, March 21, 2013 Purdue University, West Lafayette, IN (invited talk –K. Molland)
32. Sakshi Tomar, Aimee Eggler, Valerie Grum-Tokars, Craig W. Lindsley, Shaun R. Stauffer, Anna Mielech, Susan Baker, Andrew Mesecar (2013). Discovery of potent, non-covalent inhibitors of SARS-CoV 3CLpro. Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IN. October 12th. (poster)
33. St. John, S.E., Lipton, M. and Mesecar, A.D. (October 2013). "Design, Synthesis, & Evaluation of Resveratrol Analogues for the Inhibition of Quinone Reductase 2." Poster Presentation. Presented at The 33rd Midwest Enzyme Chemistry Conference. Chicago, IL.
34. Nicole Davis and Andrew D. Mesecar (2013). From E.coli to Baculovirus, the Expression and Purification of USP17. Ubiquitin Processes and Their Role in Cancer Mini-Symposium and Poster Session. West Lafayette, IN. April 19th. (poster)
35. Nicole Davis, Yahira Baez and Andrew D. Mesecar (2013). Protease Analysis of Inhibitor Interaction with Residue Q270. Purdue University Life Sciences Poster Session. West Lafayette, IN.
36. St. John, S.E.; Jensen, K., Mesecar, A.D. & Lipton, M. (March 2013). "Design, Synthesis, Biological Evaluation and X-Ray Structure Determination of Functionalized Resveratrol

Analogues as Inhibitors of Quinone Reductase 2." Poster Presentation. Presented at the Purdue Univeristy Obesity & Cancer Discovery Group. West Lafayette, IN.

37. Jensen, K. and Mesecar, A.D. (2013) Kinetic, crystallographic and biological studies on nanomolar ammosamide analogs as quinone reductase 2 inhibitors. Purdue Structural Biology Seminar Series, August 2013 (Invited Talk – K. Jensen)
38. Yu-Chen Yen, Jillian M. Jespersen, Michele Patterson, Tyler S. Crum, Daniel Garman, Nicholas Anzideo, Daniel K. Clark Jr., Craig N. Streu, and Andrew D. Mesecar (2013). Kinetic and X-ray Structural Analysis of Azo-stilbene Inhibitors of Quinone Reductase 2. 33th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 12th.
39. Jensen, K. and Mesecar, A.D. (2013) Structure-activity relationship of sub-micromolar quinone reductase 2 inhibitors in dietary foods identified via X-ray crystallography-assisted dereplication. Purdue Biophysics Symposium May 2013 (Invited Talk – K. Jensen)
40. Jensen, K. and Mesecar, A.D. (2012) Kinetic, crystallographic and biological evaluation of nanomolar ammosamide analogs as quinone reductase 2 inhibitors. Purdue Cancer Research Day Fall 2012 West Lafayette, IN (poster)
41. Jensen, K. and Mesecar, A.D.(2010) Natural fruit extracts produce potent inhibitors of human quinone reductase 2- a potential enzyme target for cancer chemopreventive compounds. Purdue Cancer Research Day, Fall 2010, Lafayette Indiana. (poster)
42. Sakshi Tomar (2012). Anticoronaviral drug discovery: An effort towards the development of broad spectrum Coronavirus 3CLpro Inhibitors. Infectious Disease Seminar series, Department of Biological Sciences, Purdue University, West Lafayette, IN. November 8th. (Talk)
43. Thomas Wubben, Scott D Pegan and Andrew D Mesecar (2009). Insight into the Enzymatic Mechanism of Phosphopantetheine Adenylyltransferase from *Mycobacterium tuberculosis*. 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)
44. Yahira M. Baez, Susan C. Baker, Andrew D. Mesecar (2009). Characterization of amino acids and structural motifs important for SARS PLpro substrate specificity**.** 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)
45. Megan Sturdy, Scott Pegan, Susana Gaudencio, Sang-Jip Nam, Katherine Maloney, Shunyan Mo, Jimmy Orjala, William Fenical, and Andrew D. Mesecar (2009). *CrystAssist*: a macromolecular, X-ray crystallographic deconvolution method to assist in the discovery of potent inhibitors of quinone reductase 2. 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)
46. Katherine Jermihov, Megan Sturdy, Scott Pegan, Andrew Mesecar (2009). Kinetic and X-Ray structural studies of fruit extracts reveal potent inhibitors of human quinone reductase 2 (QR2). 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)
47. Evan Small, Aimee Eggler and Andrew D. Mesecar (2009). Shining Light on Cancer Chemoprevention. 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)

48. Niciole Freedman, Benjamin E. Ramirez and Andrew D. Mesecar (2009). Enzymatic and NMR characterization of Shikimate kinase from *Mycobacterium tuberculosis*. 29th Midwest Enzyme Chemistry Conference, Loyola University, Chicago, IL. October 10th. (poster)
49. Megan Sturdy, Scott Pegan, Susana Gaudencio, Sang-Jip Nam, Katherine Maloney, Shunyan Mo, Jimmy Orjala, William Fenical, and Andrew D. Mesecar (2009). CRYSTASSIST. A macromolecular, X-ray crystallographic deconvolution method to assist in the discovery of potent inhibitors of quinone reductase 2. The 50th Anniversary Meeting of the American Society of Pharmacognosy. Honolulu, Hawaii. June 24th-July 2nd. (Poster P-228).
50. Yegao Chen, Jianhong Yang, Tamara P. Kondratyuk, Xi Qiu, Yongsoo Choi, Megan Sturdy, Scott Pegan, Ying Liu, Liqin Wang, Andrew D. Mesecar, Richard B. Van Breemen, John, M. Pezzuto, Harry H. S. Fong, and Hongjie Zhang (2009). New cancer chemopreventive kaempferol glycosides from *Neocheiropteris palmatopedata*. The 50th Anniversary Meeting of the American Society of Pharmacognosy. Honolulu, Hawaii. June 24th-July 2nd. (Poster P-535).
51. Scott D. Pegan, Kamolchanok Rukseree, Scott G. Franzblau and Andrew D. Mesecar (2008). "Structural characterization of tetrameric *Mycobacterium tuberculosis fructose* 1,6-bisphosphate aldolase-substrate binding and catalysis mechanism of a class IIa bacterial aldolase. 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
52. Elizabeth A. Burks, Christopher D. Fleming, Andrew D. Mesecar, Christian P. Whitman and Scott D. Pegan (2008). "Kinetic and structural characterization of a heterohexameric 4-oxalocrotonate tautomerase from *Chlorflexus autantiacus* J-10-fl:Implications for structural diversity in the tautomerase superfamily. 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
53. Kiira Ratia, S. Pegan, J. Takayama, K. Sleeman, M.Coughlin, R. Chaudhuri, W. Fu, M.E Johnson, S.C. Baker , A.K. Ghosh and A.D. Mesecar (2008). "The identification and characterization of a non-covalent inhibitor with antiviral activity that targets the papain-like protease from SARS virus". 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
54. Renda Hawwa, John Aikens, Robert Turner, Bernard Santarsiero and Andrew D. Mesecar (2009). "Kinetic and structural characterization of a new organophosphorous hydrolase with high thermostability and activity towards ogranophosphates and lactones. 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
55. Thomas Wubben, Scott D. Pegan, Glen Capodagli and Andrew D. Mesecar (2008). "Characterization and preliminary crystallization of phosphopantetheine adenylyltransferase from *Bacillus anthracis*. 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
56. Valerie Sershon, Bernard Santarsiero and Andrew D. Mesecar (2008). "Negative cooperativity in the nicotinate mononucleotide adenylyltransferase reaction and implications for pathway regulation in *Bacillus anthracis*. 28th Midwest Enzyme Chemistry Conference, University of Chicago, Chicago, IL. October 4th. (poster)
57. Katrina Sleeman, Melissa Coughlin, Kiira Ratia, Scott Pegan, Jun Takayama, Arun Ghosh, Bellur S. Prabhakar, Andrew D. Mesecar and Susan C. Baker. (2008). "Identification of

inhibitors of SARS-CoV papain-like protease with antiviral activity". Twenty-seventh Annual Meeting of the American Society for Virology, Ithica, New York, USA. July. (Invited Oral Presentation)

58. K. Sleeman, M. Coughlin, K. Ratia, A.D. Mesecar and S.C. Baker. (2008). "Screening of PLpro protease inhibitors as potential SARS-CoV antiviral compounds". CAVA (Chicago Area Virology Association) Symposium, Rush University Medical Center, Chicago, IL, USA. January. (Oral Presentation)
59. S.C. Baker, K.Ratia, N. Barretto, Z.Chen, K. Sleeman, M. Coughlin, B.S. Prabhakar, S..G. Devaraj, Nan Wang, Chien-Te K., Tseng, K., Li, A.K. Ghosh, M.E. Johnson and A.D. Mesecar "Developing proteinasae inhibitors to SARS-CoV". The XIth International Nidovirus Symposium, St. Catherine's College, Oxford, UK. June 2008. (Poster)
60. John M. Pezzuto, Ching J. Chang, Bruce A. Craig, Mark S. Cushman, William Fenical, Harry H.S. Fong, Andrew D. Mesecar, Richard C. Moon, Richard B. van Breemen. "Natural product cancer chemopreventive agents". Annual Meeting of the Phytochemical Society of North America June 25-30, 2008 Washington State University, Pullman, WA
61. Sipak Joyasawal, Suresh K. Tipparaju, Scott Pegan, Andrew D. Mesecar, and Alan P. Kozikowski (2008). "Synthesis and biological activity of A-33853 and its analogs".
62. 236th ACS National Meeting & Exposition August 17-21, 2008. Philadelphia, PA, USA. (poster).
63. Susan C. Baker, Kiira Ratia, Naina Barretto, Zhongbin Chen, Katrina Sleeman, Melissa Coughlin, Santhana G. Devaraj, Chien-Te K. Tseng, Kui Li, Arun K. Ghosh, Michael E. Johnson and Andrew D. Mesecar. (2007) "Developing protease inhibitors for Severe Acute Respiratory Syndrom (SARS). Focus Meeting on Viral Pathogenesis. Great Lakes Center of Excellence in Biodefense & Emerging Infectious Diseases. The University of Chicago. October 26, 2007. (Invited oral presentation by Susan Baker).
64. M.E. Johnson, S.C. Baker, A. Ghosh, A.D. Mesecar, Y. Baez, N. Barretto, R. Chaudhuri, Z. Chen, M. Coughlin, W. Fu, V. Grum-Tokars, S. Pegan, K. Ratia, B.D. Santarsiero, H. K. Sleeman, J. Takayama and X. Xi. (2007) "Development of 3CLpro and PLpro inhbitors as SARS therapeutics". SARS: Current progress, future directions. National Institutes of Health. October 1st and 2nd, NIH Campus, Bethesda, MD. (Oral presentation by Mike Johnson)
65. Yang Tian, Bernard D. Santarsiero and Andrew D. Mesecar (2007). "X-ray crystal structures of bacterial o-succinylbenzoyl-CoA (OSB-CoA) synthetase: insight into its reaction mechanism and inhibitor design". 27th Midwest Enzyme Chemistry Conference. University of Illinois at Chicago, College of Pharmacy. Saturday, September 29th. (Poster)
66. Yahira Baez, Kiira Ratia and Andrew D. Mesecar (2007). "Site-directed mutagenesis of the papain-like protease from SARS Coronavirus: Analysis of substrate specificity and stabilization". 27th Midwest Enzyme Chemistry Conference. University of Illinois at Chicago, College of Pharmacy. Saturday, September 29th. (Poster)
67. Kiira Ratia and Andrew D. Mesecar (2007). Kinetic comparison of two human coronavirus papain-like proteases with deubiquitinating activity". 27th Midwest Enzyme Chemistry Conference. University of Illinois at Chicago, College of Pharmacy. Saturday, September 29th. (Poster)

68. Hawwa, R., Santarsiero, BD and Mesecar. AD. (2007). "Structure, Function, and Directed Evolution of an Organophosphate and Homoserine Lactone Degrading Enzyme". 21st Symposium of the Protein Society. July 21-25, Boston, MA. (Poster Abstract 140, B81) (Poster)

69. Tian, Y, Santarsiero, BD and Mesecar, AD (2007). "X-Ray Crystal Structures of Bacterial o-Succinylbenzoyl-CoA Synthetase: Insight into Its Reaction Mechanism and Inhibitor Design". 21st Symposium of the Protein Society. July 21-25, Boston, MA. (Poster Abstract 206, B147)

70. Sershon, V., Santarsiero, BD and Mesecar, AD (2007). "Kinetic and Structural Evidence for Negative Cooperativity in Substrate Binding to Nicotinate Mononucleotide Adenylyltransferase from *Bacillus anthracis*". 21st Symposium of the Protein Society. July 21-25, Boston, MA. (Poster Abstract 287, B43).

71. S.C. Baker, Z. Chen, M. Coughlin, B.S. Prabhakar, V. Grum-Tokars, K. Ratia, A. D. Mesecar, M.E. Johnson, K. Xi and A. K. Ghosh (2007). "Developing protease inhibitors that block replication of coronaviruses". The 8th International Symposium on Postive-Strand RNA Viruses. (Invited oral presentation given by Susan Baker).

72. Kiira Ratia, Kumar S. Saikatendu, Bernard D. Santarsiero, Naina Barretto, Susan C. Baker, Raymond C. Stevens, and Andrew D. Mesecar. (2006) "Crystal structure of a deubiquitinating papain-like protease from SARS coronavirus". American Society for Virology Madison, WI. July 15th. (Invited Seminar: given by my student Kiira Ratia)

73. Patrick Miller, Andrew D. Mesecar (2006) "Characterization of the 1-Deoxy-D-Xylulose-5-Phosphate Reductoisomerase, DXR-2, from *Bacillus anthracis*". 26th Annual Midwest Enzyme Chemistry Conference. Northwestern University, Evanston, IL. September 30th. (Poster).

74. Aimee L. Eggler, Guowen Liu, John M. Pezzuto, Richard B. van Breemen, Andrew D. Mesecar (2005) "Alkylating specific cysteines of the human electrophile-sensing protein Keap1 does not disrupt the tight association with the Nrf2 domain Neh2" American Association for Caner Research (AACR) National Meeting in Anaheim, CA. April 16th-20th. (Poster)

75. Aimee L. Eggler, Guowen Liu, John M. Pezzuto, Richard B. van Breemen, Andrew D. Mesecar (2005)"Alkylating specific cysteines of the human electrophile-sensing protein Keap1 does not disrupt the tight association with the Nrf2 domain Neh2". 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)

76. Barbara Calamini**,** Bernie Santarsiero, Kiira Ratia and Andrew Mesecar. "The Molecular Basis for the Health Benefits of Resveratrol and Its Metabolites". 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)

77. Huidong Yu, Melissa May, Andrew Mesecar, Michael Johnson. "High-throughput screening bioassay against glutamate racemase from *Bacillus anthracis.* (2005) 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)

78. Yang Tian, Bernard D. Santarsiero and Andrew D. Mesecar. (2005) "Purification, characterization and crystallization of bacterial menaquinone biosynthetic enzymes". 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)

79. Renda L Hawwa, Sonia D Larsen, Bernie D Santarsiero and Andrew D Mesescar (2005)

"Improving catalytic activity of an organophosphate degrading enzyme via random and site-directed mutagenesis" 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)

80. Jill D. Dombrauckas and Andrew Mesecar. "Structural Analysis and Allosteric Regulation of Human Tumor PK." 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Invited Talk: J. Dombrauckas)
81. Melissa L. May, Bernard S. Santarsiero, Andrew D. Mesecar, and Michael E. Johnson.(2005) "Characterization of Two putative Glutamate Racemases from *Bacillus anthracis*" 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)
82. Patrick S. Miller and Andrew D. Mesecar. (2005) "Initial Studies On Targeting the First Steps of Isoprenoid Biosynthesis Via the DXP Pathway for Drug Discovery Against *Bacillus anthracis*." 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)
83. Valerie C. Sershon and Andrew Mesecar. (2005) **"**Characterization of Nicotinate Mononucleotide Adenyltransferase from *Bacillus anthracis*" 43rd Annual MIKI Meeting (Medicinal Chemistry) in Minneapolis, MN. June 3rd-5th. (Poster)
84. Aimee L. Eggler and Andrew D. Mesecar. (2005) "A new molecular mechanism model in cancer prevention:modifying specific cysteines of the human Keap1 protein is insufficient to disrupt binding to Neh2" 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Invited Talk: A. Eggler).
85. Barbara Calamini, Bernie Santarsiero, Kiira Ratia, and Andrew Mesecar (2005) "Structural Basis for Potent Inhibition of COX by Resveratrol-A Natural Product in Wine". 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
86. Jill D. Dombrauckas, Bernard D. Santarsiero, and Andrew D. Mesecar. (2005) "Targeting Allosteric Sites of Tumor Pyruvate Kinase M2 for Anti-Cancer Drug Leads." 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
87. Gary M. Klein, Bernard D. Santarsiero, and Andrew D. Mesecar. "Characterization of Enoyl Reductase (FabI) from Bacillus anthracis – an Antibacterial Drug Target," (2005) 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
88. Huidong Yu, Melissa May, Michael Johnson, Andrew Mesecar. (2005) "High-throughput screening to identify the inhibitors for glutamate racemase from *Bacillus anthracis*. 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
89. Sonia Larsen, Kiira Ratia, Bernard D. Santarsiero and Andrew D. Mesecar. (2005) **"**Macromolecular X-ray Crystallographic studies of a Phosphotriesterase capable of degrading soman" 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
90. Yang Tian, Bernard D. Santarsiero and Andrew D. Mesecar. (2005) "Purification, characterization and crystallization of *Bacillus anthracis* menaquinone biosynthetic enzymes".

25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)

91. Renda L Hawwa, Sonia D Larsen, Bernie D Santarsiero and Andrew D Mesescar (2005) "Engineering of an Organophosphate Degrading Enzyme via Random and Site-Directed Mutagenesis" 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
92. Kiira Ratia, Bernard Santarsiero, Diana Arsenieva, Evan Small, Kai Xi, Dalia Jukneliene, Brian Harcourt, Michael Johnson, Susan Baker, Arun Ghosh, and Andrew D. Mesecar. (2005) "Kinetic and Crystallographic Comparison of a Series of SARS 3CLpro AG7088-based Inhibitors. 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
93. Sasi K. Chilukuri and Andrew D. Mesecar. (2005) "Molecular Basis for Hereditary Non-Spherocytic Hemolytic Anemia: Prevalent Mutations in Human Erythrocyte Pyruvate Kinase" 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
94. Patrick S. Miller and Andrew D. Mesecar (2005) "Steps toward drug discovery against Bacillus anthracis by targeting enzymes in the DXP pathway for isoprenoid biosynthesis" 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
95. Valerie C. Sershon and Andrew Mesecar (2005). "Characterization of nicotinate mononucleotide adenyltransferase from *Bacillus anthracis*". 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
96. Melissa May, Bernard Santarsiero, Michael E. Johnson and Andrew D. Mesecar (2005) "Structure-function studies of glutamate racemases from *Bacillus anthracis*". 25th Annual Midwest Enzyme Chemistry Conference. Loyola University of Chicago, Chicago, IL. October 8th. (Poster)
97. Aimee L. Eggler, Yan Luo, Guowen Liu, John M. Pezzuto, Richard B. van Breemen, Andrew D. Mesecar (2005) "Modifying Cysteines of the Electrophile-sensing Human Keap1 Protein: Mapping locations and the Effect on binding to Nrf2" Fourth Annual American Association for Cancer Research (AACR) International Conference on Frontiers in Cancer Prevention Research, Baltimore, MD, USA. October 30th-November 2nd , 2005. (Poster)
98. Barbara Calamini**,** Bernie Santarsiero, Kiira Ratia and Andrew Mesecar. (2005) "The Molecular Basis for the Health Benefits of Resveratrol and Its Metabolites". Fourth Annual American Association for Cancer Research (AACR) International Conference on Frontiers in Cancer Prevention Research, Baltimore, MD, USA. October 30th-November 2nd. (Poster)
99. Barbara Calamini**,** Bernie Santarsiero, Kiira Ratia and Andrew Mesecar. (2005) "The Molecular Basis for the Health Benefits of Resveratrol and Its Metabolites". Fourth Annual American Association for Cancer Research (AACR) International Conference on Frontiers in Cancer Prevention Research, Baltimore, MD, USA. October 30th-November 2nd. (Invited Talk: B. Calamini)

100. Barbara Calamini, Bernie Santarsiero, Kiira Ratia, and Andrew Mesecar. (2005) "Structural Basis for Potent Inhibition of COX by Resveratrol-A Natural Product in Wine". XX Congress of the International Union of Crystallography, Florence, Italy, August 23rd -31st (Poster)

101. Jill D. Dombrauckas, Bernard D. Santarsiero, and Andrew D. Mesecar. (2005) "Structural Basis for Tumor Pyruvate Kinase M2 Allosteric Regulation and Catalysis." XX Congress of the International Union of Crystallography, Florence, Italy, August 23rd -31st (Poster)

102. Kiira Ratia, Bernard Santarsiero, Diana Arsenieva, Evan Small, Kai Xi, Dalia Jukneliene, Brian Harcourt, Michael Johnson, Susan Baker, Arun Ghosh, and Andrew Mesecar. (2005) "Kinetic and Crystallographic Analyses of SARS Coronavirus 3CLpro Inhibitors". XX Congress of the International Union of Crystallography, Florence, Italy, August 23rd -31st (Poster)

103. Sonia Larsen, Kiira Ratia, Bernard D. Santarsiero and Andrew D. Mesecar. "Structural Studies of a Novel Phosphotriesterase capable of degrading soman" XX Congress of the International Union of Crystallography, Florence, Italy, August 23rd -31st (Poster)

104. Pappannan Thiyagarajan, Art. J. Schultz, Christine. Rehm, Jason. P. Hodges, Dean.A. Myles, Paul. A. Langan, Andrew D. Mesecar (2005) "Design of a High Resolution Macromolecular Neutron Diffractometer (MaNDi) for Structural Biology Research at the SNS". XX Congress of the International Union of Crystallography, Florence, Italy, August 23rd -31st (Poster)

105. Arthur Schultz, P. Thiyagarajan, Christine Rehm, Jason Hodges, Dean Myles, Paul Langan, Andrew Mesecar. (2005) "A High Resolution Macromolecular Neutron Diffractometer (MaNDi) at the SNS". American Crystallographic Association (ACA) Annual Meeting, Orlando, Florida. May 28th – June 2nd. (Poster)

106. Paul Langan, P. Thiyagarajan, Art.J. Schultz, Christine Rehm, Jason P. Hodges, Dean A. Myles, Andrew D. Mesecar. (2005) "Opportunities for Fiber Diffraction With the Proposed Macromolecular Neutron Diffractometer MaNDi at the Spallation Neutron Source". American Crystallographic Association (ACA) Annual Meeting, Orlando, Florida. May 28th – June 2nd. (Invited Talk: P. Langan)

107. Bao-Ning Su, Heebyung Chai, Qiuwen Mi, Johar J. Afriastini, Soedarsono Riswan, Bernard D. Santarsiero, Andrew D. Mesecar, Norman R. Farnsworth, Geoffrey A. Cordell, Steven M. Swanson, and Douglas A. Kinghorn. (2005) "Activity-guided isolation of cytotoxic constituents from the bark of Aglaia crassinervia". 46th Annual Meeting of the American Society of Pharmacognosy at Oregon State University, Corvallis Oregon, July 23rd to 25th. (Poster)

108. Guowen Liu; Aimee Eggler; Birgit M. Dietz; Andrew D. Mesecar; Judy L. Bolton; Richard B. van Breemen. (2005) "A mechanism based high throughput screening mass spectrometry assay for identification of potential chemopreventive agents" 53rd American Society for Mass Spectrometery (ASMS) Conference. June 5th-9th, San Antonio, TX. (Poster)

109. Melissa May, Bernard Santarsiero, Michael Johnson, and Andrew D. Mesecar (2005) "Characterization of two putative glutamate racemases from *Bacillus anthracis*". The 3rd Annual American Society of Microbiology Biodefense Research Meeting. March 20th -23rd , Baltimore, Maryland.

110.Melissa May, Bernard Santarsiero, Andrew D. Mesecar and Michael E. Johnson (2005) "Characterization of two putative glutamate racemases from *Bacillus anthracis*". The Protein Society 19th Symposium. Boston, MA July 30th –August 3rd.

111.P. Thiyagarajan, Arthur Schultz, Christine Rehm, Jason Hodges, W.T. Lee, Andrew Mesecar (2004). "Design of a single crystal macromolecular neutron diffractometer at SNS." 2nd American Conference on Neutron Scattering, College Park, MD. June 6 to 10th.

*112.*Bang Yeon Hwang, Bao-Ning Su, Soyoung Kim, Heebyung Chai, Qiuwen Mi, Leonardus B. S. Kardono, Johar J. Afriastini, Soedarsono Riswan, Bernard D. Santarsiero, Andrew D. Mesecar, Robert Wild, Craig R. Fairchild, Gregory D. Vite, William C. Rose, Norman R. Farnsworth, Geoffrey A. Cordell, John M.Pezzuto, Steven M. Swanson, and A. Douglas Kinghorn. (2004) "Structure and stereochemistry of the rocaglate derivative, silvestrol, a constituent of *Aglaia silvestris* with antineoplastic activity". International Conference on Natural Products Research. July 31 – August 4th, Phoenix AZ.

*113.*Bao-Ning Su, Heebyung Chai, Qiuwen Mi, William P. Jones, Leonardus B. S. Kardono, Johar J. Afriastini, Soedarsono Riswan, Bernard D. Santarsiero, Andrew D. Mesecar, Norman R. Farnsworth, Geoffrey A. Cordell, Steven M. Swanson, and A. Douglas Kinghorn. (2004). "Activity-guided isolation of cytotoxic constituents from the bark of an Indonesian *Aglaia* species. International Conference on Natural Products Research. July 31 – August 4th, Phoenix AZ.

*114.*Christopher J Halkides, Andrew Mesecar, Eric S Casper, and Kenneth McAdams. (2004) The structures of T87I Phosphono-CheY and T87I/Y106W Phosphono-CheY and their binding affinities to the FliM and CheZ peptides. 56th Souteast Regional Meeting of the American Chemical Society, Research Triangle Park. November 11th, 2004.

*115.*A. J. Schultz, P. Thiyagarajan, C. Rehm, J. P. Hodges, W. T. Lee, A. D. Mesecar, D. A. Myles, P. A. Langan. (2004) "Design of a Single Crystal Macromolecular Neutron Diffractometer at the SNS.*"* American Crystallographic Association Annual Meeting. Chicago, IL. July 17-22, 2004

116.Kiira Ratia, Bernard Santarsiero, Kai Xi, Dalia Jukneliene, Brian Harcourt, Susan Baker, Arun Ghosh, and Andrew Mesecar. (2004) Kinetic and Crystallographic Analyses of SARS Coronavirus 3Clpro Inhibitors. 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9.

117.Kiira Ratia, Bernard Santarsiero, Kai Xi, Dalia Jukneliene, Brian Harcourt, Susan Baker, Arun Ghosh, and Andrew Mesecar (2004) "Crystallographic and Kinetic Studies of Novel SARS-CoV 3Clpro Protease Inhibitors that Inhibit SARS-CoV and MHV-A59 Replication" 42nd Annual MIKI Meeting (Medicinal Chemistry). The University of Iowa, Iowa City, Iowa. April 17. *Poster*

118.Sasi K. Chilukuri, Bernard D. Sanstersiero, Andrew D. Mesecar. (2004) "Functional Characterization of the Most Prevalent Mutations in Pyruvate Kinase associated with

Hemolytic Anemia" 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9.

119. Sasi K. Chilukuri, Bernard D. Sanstersiero, Andrew D. Mesecar. (2004) "Allosteric Regulation of prevalent PK mutations associated with Hemolytic Anemia." 42nd Annual MIKI Meeting (Medicinal Chemistry). The University of Iowa, Iowa City, Iowa. April 17. *Poster.*
120. Guowen Liu, Kiira Ratia, Andrew D. Mesecar and Richard van Breemen. (2004). "Screening for ligands binding to human retinoic acid receptor gamma ligand binding domain using pulsed ultrafiltration-MS-MS. 42nd Annual MIKI Meeting (Medicinal Chemistry). The University of Iowa, Iowa City, Iowa. April 17. *Poster.*

121. Calamini B., Santarsiero B., Eggler A., and Mesecar A. D. (2004) "The Molecular Basis for Cancer Chemoprevention and Longevity Promotion by Resveratrol and Its Human Metabolites". 42nd Annual MIKI Meeting, The University of Iowa, Iowa City, IA. April 17. *Poster*

122. Pajkovic N., Nikolic D., Calamini B., Sawant A., Mesecar A. D., van Breemen R.(2004) "Ultrafiltration LC-MS Screening of Natural Products for Ligands to the Androgen Receptor" 52nd American Society for Mass Spectrometry (ASMS) Conference, May 23rd-27th, Nashville, TN. *Poster*

123. Sonia Larsen, Kiira Ratia, Bernard D. Santarsiero and Andrew D. Mesecar. (2004) "Monochromatic and Polychromatic Laue X-ray Crystallographic Studies of a Novel Phosphotriesterase Capable of Hydrolyzing Soman Gas". 42nd Annual MIKI Meeting, The University of Iowa, Iowa City, IA. April 17. *Poster.*

124. Sonia Larsen, Kiira Ratia, Bernard D. Santarsiero and Andrew D. Mesecar (2004). "Structural Studies of a Novel Phosphotriesterase Capable of Degrading Soman Using Monochromatic and Polychromatic Laue X-ray Techniques" 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9.

125. Jill Dombrauckas, Bernard D. Santarsiero, Andrew D. Mesecar. (2004) "Structural Analysis of the Tumor-Specific Pyruvate Kinase for Structure-based Drug Design." 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9, 2004. Poster.

126. Jill Dombrauckas, Bernard D. Santarsiero, Andrew D. Mesecar. (2004) "Structure Determination of Tumor-Specific Pyruvate Kinase M2." 42nd Annual MIKI Meeting, The University of Iowa, Iowa City, IA. April 17, 2004. *Poster*

127. Patrick Miller and Andrew D. Mesecar. (2004) "Preliminary X-Ray Analysis of BphC1, an Extradiol Dioxygenase from *Sphingomonas* strain BN6". 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9, 2004. Poster.

128.Patrick Miller, Kiira Ratia, Andrew D. Mesecar. (2004) "Preliminary X-Ray Analysis of BphC1, an Extradiol Dioxygenase from *Sphingomonas* strain BN6" American Crystallographic Association Annual Meeting. Chicago, IL. July 17-22, 2004.

129.Melissa May, Bernard D. Santarsiero, Michael E. Johnson, Andrew D. Mesecar. (2004) "Characterization of Two Putative Glutamate Racemases from *Bacillus Anthracis*." 24th Annual Midwest Enzyme Chemistry Conference. University of Chicago, Chicago, IL. October 9, 2004. Poster.

130.Li, Yan; Yao, Jiaqin; Chang, Minsun; Yu, Linning; Yager, James D.; Mesecar, Andrew D.; van Breemen, Richard B.; Bolton, Judy. "Equine estrogen metabolite 4-hydroxyequilenin (4-OHEN) is a more potent inhibitor of the variant form of catechol O-methyltransferase (COMT)". Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), TOXI-071.

131.Chang, Minsun; Calamini, Barbara; Nikolic, Dejan; Ratia, Kiira; van Breemen, Richard B.; Mesecar, Andrew D.; Bolton, Judy L. "Differential modification of the ligand binding domains of human estrogen receptors alpha and beta by the equine estrogen metabolite, 4-hydroxyequilenin." Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), TOXI-060.

132.Sonia Larsen, Kiira Ratia, Bernard Santarsiero and Andrew Mesecar. (2003) "Monochromatic and Polychromatic Laue Studies of a Novel Phosphotriesterase that Degrades Soman Gas." Center for Pharmaceutical Biotechnology, Dept. of Medicinal Chemistry and Pharmacognosy, Univ. of Illinois at Chicago. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

133.Barbara Calamini*, Bernie Santarsiero*, Kiira Ratia*, Michael Malkowski[§], John Pezzuto[#], and Andrew Mesecar*. (2003) Structural Basis for Potent Inhibition of Cox-1 and Cox-2 by Resveratrol-A Natural Product in Wine.*Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, [§]Hauptman-Woodward Medical Research Institute, and [#]Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

134. Jill Dombrauckas, Bernard Sanstersiero, and Andrew D. Mesecar. (2003) "X-ray structure determination of tumor-specific pyruvate kinase type-M2 from humans". Department of Medicinal Chemistry, University of Illinois at Chicago; 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

135.Kiira Ratia and Andrew Mesecar. (2003) Directed Evolution of a Novel Phosphotriesterase Reveals Dynamic Contributions to Catalysis. Center for Pharmaceutical Biotechnology and the Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

136.Sasi K. Chilukuri, Bernard D. Santarsiero, and Andrew D. Mesecar. (2003) Structure of Pyruvate Kinase with a Novel Allosteric Activator Identified via Computational Docking. Center for Pharmaceutical Biotechnology, Dept. of Medicinal Chemistry and Pharmacognosy,

Univ. of Illinois at Chicago. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

137. Magdalini Vamvouka and Andrew Mesecar (2003) High Resolution Structures of THT-Dioxygenase Mutants: Insight into Extradiol Catalysis., The Center for Pharmaceutical Biotechnology and the Dept. of Medicinal Chemistry and Pharmacognosy, The Univ. of Illinois at Chicago. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

138. Bernard Santarsiero, Kiira Ratia, and Andrew D. Mesecar. (2003) A Comparison of Bromide Ion "Quick Soak" and Se-Met Derivatives for Structure Determination of a Novel Hydrolase. The Center for Pharmaceutical Biotechnology and the Dept. of Medicinal Chemistry and Pharmacognosy, The Univ. of Illinois at Chicago. 23rd Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, October 4th. *Poster.*

139. Sonia Larsen, Kiira Ratia, Bernard Santarsiero and Andrew Mesecar. (2003) Monochromatic and Polychromatic Laue Studies of a Novel Phosphotriesterase that Degrades Soman Gas. Center for Pharmaceutical Biotechnology, Dept. of Medicinal Chemistry and Pharmacognosy, Univ. of Illinois at Chicago. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Invited oral presentation.*

140. Barbara Calamini*, Bernie Santarsiero*, Kiira Ratia*, Michael Malkowski[§], John Pezzuto[#], and Andrew Mesecar*. (2003) Structural Basis for Potent Inhibition of Cox-1 and Cox-2 by Resveratrol-A Natural Product in Wine.*Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, [§]Hauptman-Woodward Medical Research Institute, and [#]Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

141. Jill Dombrauckas[1], Dagny L. Ulrich[2], Bernard Sanstersiero[1], Pat Loria[2], Andrew D. Mesecar[1]. (2003) DeNovo X-ray Structure Determination of the Bacterial Quorum-Sensing Phoshorelay Protein Lux U. [1]Department of Medicinal Chemistry, University of Illinois at Chicago; [2]Department of Chemistry, Yale University. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

142. Kiira Ratia and Andrew Mesecar. (2003) Directed Evolution of a Novel Phosphotriesterase Reveals Dynamic Contributions to Catalysis. Center for Pharmaceutical Biotechnology and the Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

143. Sasi K. Chilukuri, Bernard D. Santarsiero, and Andrew D. Mesecar. (2003) Structure of Pyruvate Kinase with a Novel Allosteric Activator Identified via Computational Docking. Center for Pharmaceutical Biotechnology, Dept. of Medicinal Chemistry and Pharmacognosy, Univ. of Illinois at Chicago. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

144. Magdalini Vamvouka and Andrew Mesecar (2003) High Resolution Structures of THT-Dioxygenase Mutants: Insight into Extradiol Catalysis., The Center for Pharmaceutical Biotechnology and the Dept. of Medicinal Chemistry and Pharmacognosy, The Univ. of Illinois at Chicago. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

145. Bernard Santarsiero, Kiira Ratia, and Andrew D. Mesecar. (2003) A Comparison of Bromide Ion "Quick Soak" and Se-Met Derivatives for Structure Determination of a Novel Hydrolase. The Center for Pharmaceutical Biotechnology and the Dept. of Medicinal Chemistry and Pharmacognosy, The Univ. of Illinois at Chicago. American Crystallographic Society Meeting. Covington, Kentucky, July 26 - 31. *Poster.*

146. Su, B-N, Kang, Y-H, Pinos, R. E., Santarsiero, B. D., Mesecar, A. D., Soejarto, D. D., Fong, H.H.S., Pezzuto, J. M., and Kinghorn, A. D. (2003). Isolation and absolute stereochemistry of coussaric acid, a new bioactive triterpenoid from the stems of *Coussarea brevicaulis*. 44th Annual Meeting of the American Society of Pharmacognosy "The Changing Face of Natural Products Chemistry". Chapel Hill, NC. July 12-16.

147. Calamini, B. and Mesecar, A.D. (2002). A structural basis for chemopreventive activity of resveratrol-a natural product of wine. XXII Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, September 28th. *Poster.*

148. Sheng, Q. Johnson, M. and Mesecar, A. D. (2002). Accelerating structure-based drug design of factor Xa inhibitors via engineered bovine trypsin. XXII Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, September 28th. *Poster.*

149. Vamvouka, M. and Mesecar, A. D. (2002). A proton shuttle mechanism for extradiol dioxygenases revealed by high resolution crystal structures and kinetic characterization of site-directed mutants. XXII Midwest Enzyme Chemistry Conference. Chicago, Illinois. Saturday, September 28th. *Poster.*

150. Grubjesic, S., Santersiero, B., Kosmeder II, J.W., Gigli, H., Moriarty, R.M., and Mesecar, A.D. Synthesis of caged catechol substrates for time resolved Laue x-ray studies of trihydroxytoluene dioxygenase. Abstracts of Papers, 224th National Meeting of the American Chemical Society, Boston, MA, August 18-22, 2002; MEDI 182.

151. Santarsiero, B.D., Mesecar, A.D., Su, B,-N., Fong H.H.S., Pezzuto, J.M., Kinghorn, A.D. (2002) "Using 10^9 molecules and a synchrotron to determine a crystal structure". American Crystallographic Association, Annual Meeting, San Antonio, Texas. May 25th - 30th. *Oral Paper Presentation.*

152. Su, B. N., Park, E.J., Vigo, J.S., Graham, J.G., Cabieses, F., Santarsiero, B., Mesecar, A.D., Fong, H. H. S., Farnsworth, N.R., Pezzuto, J. M., Kinghorn, A.D. (2002) "Activity-guided isolation and cancer chemopreventive potential of unusual 18-norwithanolides with a new type of carbon skeleton from *Solanum altissiumum*." 43rd Annual Meeting of the American Society of Pharmacognosy and 3rd Monroe Wall Symposium. July 27th-31st. New Brunswick, New Jersey. *Poster*

153. Su, B.N. Park, E.J., Mbwambo, Z. H., Santarsiero, B., Mesecar, A.D., Fong, H. H. S., Pezzuto, J. M., Kinghorn, A.D. (2002) "Chemical constituents of Euphorbia quinquecostata and absolute configuration assignment by a Mosher ester procedure conveniently carried out in a NMR tube. 43rd Annual Meeting of the American Society of Pharmacognosy and 3rd Monroe Wall Symposium. July 27th-31st. New Brunswick, New Jersey. *Poster*

154. Jang, D. S., Park, E. J., Hawthorn, M.E., Vigo, J. S., Graham, J.G., Cabieses, F., Santarsiero, B.D., Mesecar, A.D., Fong, H.H.S., Mehta, R.G., Pezzuto, J.M. and Kinghorn, A.D. (2002) "Constituents of Musa Sapientum (Banana) with the potential to induce the phase II enzyme,

quinoine reductase. 43rd Annual Meeting of the American Society of Pharmacognosy and 3rd Monroe Wall Symposium. July 27th-31st. New Brunswick, New Jersey. *Poster.*

155. Ratia, K., Falzarim, K., Santarsiero, B. D. and Mesecar, A.D. (2001) Kinetic and thermal characterization of pyruvate kinase mutants associated with hemolytic anemia. XXI Midwest Enzyme Chemistry Conference. *Poster.*

156. Gunter, H. and Mesecar, A.D. (2001) Evidnece for a CO_2 Binding pocket in isocitrate dehydrogenase. XXI Midwest Enzyme Chemistry Conference. *Poster.*

157. Santarsiero, B.D. and Mesecar, A.D. (2001) New insights into extradiol ring-cleaving mechanisms as revealed from the by the x-ray structures of trihydroxytoluene dioxygenase. The native structure at 1.20Å and the 4-Nitrocatechol complex at 1.20Å. XXI Midwest Enzyme Chemistry Conference. *Poster.*

158. Simonida Grubjesic, Bernard Santersiero, Jerry Kosmeder, Zhong Ren, Reinhard Pahl, and Andrew Mesecar. (2001) Trihydroxytoluene dioxygenase as a model system for time-resolved laue x-ray diffraction studies. XXI Midwest Enzyme Chemistry Conference. *Poster.*

159. Su, B-N, Chang, L.C., Park, E.J., Cuendet, M., Santarsiero, B.D., Mesecar, A.D., Mehta, R.G., Fong, H.H.S., Pezzuto, J.M. and Kinghorn, A.D. (2001) Bioactive constituents of the seeds of *Brucea javanica.* Amer. Chem. Soc. Natl. Meeting. Chicago. MEDI: Abst. #0134. *Poster.*

160. Santarsiero, B., Ren, Z. Pahl, R. and Mesecar, A.D. (2001) Monochromatic and Laue Structural Studies of Trihydroxytoluene Dioxygenase. BioCARS Workshop on Time-Resolved Crystallography. Argonne National laboratory. *Poster.*

161. Mesecar, A.D. (2001) A Molecular Movie of the isocitrate dehydrogenase reaction." BioCARS Workshop on Time-Resolved Crystallography. Argonne National laboratory. *Poster.*

162. Kloss, P. and Mesecar, A.D. (2000). Over-expression and purification of an FAD utilizing monooxygenase involved in bioremediation of dinitrotoluene (DNT). XXth Midwest Enzyme Chemistry Conference. *Poster.*

163. Binutu, O. and Mesecar, A.D. (2000). Crystallization and preliminary x-ray characterization of a ring cleaving dioxygenase involved in bioremediation of dinitrotoluene. XXth Midwest Enzyme Chemistry Conference. *Poster.*

164. Mesecar, A.D. and Koshland, D.E. (2000). A New Model for Protein Stereospecificity. 14th Symposium of the Protein Society, August 5 - 9, 2000, in San Diego, California. Abstract #00441, *Protein Science.*

165. Mesecar, A. D. and Daniel E. Koshland Jr. (1999). X-ray structural evidence for metal-ion dependent enantiomeric specificity of isocitrate dehydrogenase: "Four-Point Location" in enzymatic stereospecificity. XIXth Midwest Enzyme Chemistry Conference.

166. Barry L. Stoddard, Jill Bolduc, and Dave Dyer (The Fred Hutchinson Cancer Research Center) and Andrew Mesecar, Bruce Cohen, Mike Brubaker, and Daniel E. Koshland, Jr. (University of California, Berkeley) "Time-resolved Crystallographic Studies of Isocitrate Dehydrogenase: Using Intermediate Trapping, Photolytic Triggering, and Synchrotron Radiation". The Sixth International Conference on Biophysics and Synchrotron Radiation, August 4-8, 1998, Advanced Photon Source, Argonne National Laboratory, USA.

167. Mesecar, A. D., Stoddard, B. L. and Daniel E. Koshland, Jr. (1997) Small Conformational Changes of an Enzyme Under Catalytic Turnover: The Isocitrate Dehydrogenase Catalyzed Reaction.. 17th IUBMB/ASBMB Conference-San Francisco. FASEB Journal, v. 11, n.9, A2672.

168. Mesecar, A. D. Larry, J. P. and Nowak, T. (1995). The Function of Active Site Residues in Pyruvate Kinase. ASBMB/DBC-ACS Joint Meeting-San Francisco. FASEB Journal, v.9, n.6,: A1286. *Poster.*

169. Mesecar, A. D. and Nowak, T. (1994) The Role of Lysine-269 in the Pyruvate Kinase Reaction. XIVth Midwest Enzyme Chemistry Conference. *Poster.*

170. Mesecar, A.D. and Nowak, T. (1993) Non-Concerted Allosteric Interactions of phosphoenolpyruvate, fructose 1,6-diphosphate and Mn^{2+} with Pyruvate Kinase from *Saccharomyces cerevisiae.* ASBMB/DBC-ACS Joint Meeting-San Diego. FASEB Journal, v.7, n.7: A1102.

171. Mesecar, A. D. and Nowak, T. (1992) Allosteric Interactions of phosphoenolpyruvate and fructose 1,6-diphosphate with Mn^{2+} activated pyruvate kinase from *Saccharomyces cerevisiae.* XIIth Midwest Enzyme Chemistry Conference. *Poster*

172. Mesecar, A.D. and Nowak, T. Kinetic and Genetic Studies of Yeast Pyruvate Kinase. (1992) ASBMB/Biophysical Society Joint Meeting-Houston, Biophysical Journal, v.61, n.2 Part 2: A331.

173. Mesecar, A. D. and Nowak, T. (1991). Lysine-269 in the Pyruvate Kinase Reaction: pH Studies and Site-Directed Mutagenesis. XIth Midwest Enzyme Chemistry Conference. *Poster*.

174. Mesecar, A. D. and Nowak, T. (1990) pH Studies on Yeast Pyruvate Kinase: Mn^{2+} Activation and the Substrate Phosphoenolpyruvate. Xth Midwest Enzyme Chemistry Conference. *Poster*.

175. Mesecar, A. D. and Nowak, T. (1989) pH Effects on Mn^{2+} Activation of Yeast Pyruvate Kinase IXth Midwest Enzyme Chemistry Conference. *Poster*