

# Robert J. Doerksen

209 Graduate House, University of Mississippi, University, MS, 38677-1848  
Phone: 1-662-915-7052; <http://www.robertjdoerksen.com>; E-mail: [rjd@olemiss.edu](mailto:rjd@olemiss.edu)

## EMPLOYMENT

### PRIMARY APPOINTMENTS

UNIVERSITY OF MISSISSIPPI, GRADUATE SCHOOL Associate Dean	OXFORD, MS 12/2017-present
UNIVERSITY OF MISSISSIPPI, DEPARTMENT OF BIOMOLECULAR SCIENCES Professor	OXFORD, MS 7/2019-present
UNIVERSITY OF MISSISSIPPI, DEPARTMENT OF BIOMOLECULAR SCIENCES Associate Professor	OXFORD, MS 4/2014-6/2019
UNIVERSITY OF MISSISSIPPI, DEPARTMENT OF MEDICINAL CHEMISTRY Associate Professor	OXFORD, MS 7/2010-4/2014
UNIVERSITY OF MISSISSIPPI, DEPARTMENT OF MEDICINAL CHEMISTRY Assistant Professor	OXFORD, MS 8/2004-6/2010
UNIVERSITY OF PENNSYLVANIA, DEPARTMENT OF CHEMISTRY Postdoctoral fellow with Prof. Michael L. Klein	PHILADELPHIA, PA 4/2001-7/2004
UNIVERSITY OF CALIFORNIA, BERKELEY, DEPARTMENT OF CHEMISTRY Postdoctoral fellow with Prof. Martin Head-Gordon	BERKELEY, CA 4/1999-3/2001
UNIVERSITY OF NEW BRUNSWICK, DEPARTMENT OF CHEMISTRY Postdoctoral fellow with Prof. Ajit J. Thakkar	FREDERICTON, NB, CANADA 10/1998-3/1999

### SECONDARY APPOINTMENTS

UNIVERSITY OF MISSISSIPPI, RESEARCH INST. OF PHARMACEUTICAL SCIENCES Research Professor	OXFORD, MS 7/2019-present
UNIVERSITY OF MISSISSIPPI, RESEARCH INST. OF PHARMACEUTICAL SCIENCES Research Associate Professor	OXFORD, MS 7/2010-6/2019
NATIONAL PINGTUNG UNIVERSITY OF SCIENCE TECHNOLOGY DEPARTMENT OF BIOLOGICAL SCIENCE & TECHNOLOGY Joint Appointment Associate Professor	NEIPU, PINGTUNG, TAIWAN 2/2014-6/2014
NATIONAL PINGTUNG UNIVERSITY OF SCIENCE TECHNOLOGY DEPARTMENT OF FOOD SCIENCE Visiting Associate Professor Joint Appointment Associate Professor	NEIPU, PINGTUNG, TAIWAN 12/2013-6/2014 2/2014-6/2014
UNIVERSITY OF MISSISSIPPI, RESEARCH INST. OF PHARMACEUTICAL SCIENCES Research Assistant Professor	OXFORD, MS 8/2004-6/2010

## EDUCATION

Ph.D., UNIVERSITY OF NEW BRUNSWICK, DEPARTMENT OF CHEMISTRY Thesis: "Geometries, polarizabilities and aromaticity of ring molecules" Supervisor: Prof. Ajit J. Thakkar	FREDERICTON, NB, CANADA 9/1993-9/1998
--	--

B.Sc., UNIVERSITY OF NEW BRUNSWICK, DEPARTMENTS OF PHYSICS AND MATHEMATICS 9/1982-4/1986  
 Double First Class Honours, Thesis: "An apparatus for zero-field NMR"  
 Supervisor: Prof. Reinhold Kaiser

## HIGHLIGHTED AWARDS

- University of Mississippi School of Pharmacy Distinguished Teaching Scholar 2017
- School of Pharmacy Faculty Service Award 2015-2016
- School of Pharmacy Faculty Instructional Innovation Award 2011-2012
- School of Pharmacy Faculty Service Award 2010-2011
- Junior Investigator, NIH Centers of Biomedical Research Excellence (COBRE) Centers of Research Excellence-Natural Products Neuroscience 2009-2015
- Phi Lambda Sigma, Pharmacy Leadership Society Elected in 2009
- Rho Chi, Academic Honors Society in Pharmacy Elected in 2009
- Who's Who in America 2008, 2009
- American Association of Colleges of Pharmacy New Investigator Award 2007-2008
- Searle Award Nominee, University of Mississippi 2005
- Fellow of University of Mississippi's Faculty Research Program 2004-2005
- Top 5 in the 'Science' category for the ComputerWorld 21st Century Achievement Award 2003
  - Supercomputer computations by RJ Doerksen in the antimicrobial polymer project (supported by National Institutes of Health) were chosen as the Case Study in the Pittsburgh Supercomputer Center's nomination for their new Lemieux Terascale Computer
- Natural Sciences and Engineering Research Council (NSERC) of Canada Postgraduate Scholarship 1995-1997
- Best Physical or Theoretical Student, UNB Chemistry Department 1996, 1997, 1998

## EDITORIAL ADVISORY BOARDS

*AIMS Biophysics*, Editorial Board, 2018-Present

*Pharmaceutical Sciences*, Editorial Board, 2017-Present

*Perspectives in Medicinal Chemistry*, Honorary Editorial Board, 2006-2019

## JOURNAL ARTICLES (85)

(# of Google Scholar citations listed for those articles which contribute to my h-index of 26)

J Liu; P Pandey; X Wang; K Adams; X Qi; J Chen; H Sun; Q Hou; D Ferreira; RJ Doerksen; S Li; MT Hamann "Hepatoprotective tetrahydrobenzocyclooctabenzofuranone lignans from *Kadsura longipedunculata*," accepted to *Journal of Natural Products* (8/30/2019).

AW Keasling; P Pandey; RJ Doerksen; GR Pedrino; EA Costa; LC da Cunha; JK Zjawiony; JO Fajemiroye "Salvindolin elicits opioid system-mediated antinociceptive and antidepressant-like activities," *Journal of Psychopharmacology* **33**, 865-881 (2019). doi: 10.1177/0269881119849821

ND Chaurasiya; J Zhao; P Pandey; RJ Doerksen; I Muhammad; BL Tekwani "Selective inhibition of human monoamine oxidase B by acacetin 7-methyl ether isolated from *Turnera diffusa* (damiana)," *Molecules* **24**, 810 (2019). doi: 10.3390/molecules24040810 PMID: 30813423 Special memorial issue honoring Dr. Charles F. Hufford.

Y Zou; X Wang; J Sims; B Wang; P Pandey; CL Welsh; RP Stone; MA Avery; RJ Doerksen; D Ferreira; C Anklin; FA Valeriote; M Kelly; MT Hamann "Computationally-assisted discovery and assignment of a highly strained and PANC-1 selective alkaloid from Alaska's deep ocean," *Journal of the American Chemical Society* **141**, 4338-4344 (2019). doi: 10.1021/jacs.8b11403 PMID: 30758203

P Pandey; KK Roy; RJ Doerksen "Negative allosteric modulators of cannabinoid receptor 2: Protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist," accepted to *Journal of Biomolecular Structure and Dynamics* (12/27/2018). doi: 10.1080/07391102.2019.1567384 PMID: 30652534

P Pandey; KK Roy; H Liu; G Ma; SA Pettaway; WF Alsharif; RS Gadepalli; JM Rimoldi; CR McCurdy; SJ Cutler; RJ Doerksen "Structure-based identification of potent natural product chemotypes as cannabinoid receptor 1 inverse agonists," *Molecules* **23**, 2630 (2018). Invited. Special issue on "Hit Generation and Verification for Novel Lead Compounds." doi: 10.3390/molecules23102630 PMID: 30322136

LG Malak; MA Ibrahim; AM Moharram; P Pandey; B Tekwani; RJ Doerksen; D Ferreira; SA Ross "Antileishmanial carbasugars from *Geosmithia langdonii*," *Journal of Natural Products* **81**, 2222-2227 (2018). doi: 10.1021/acs.jnatprod.8b00473 PMID: 30298736

X Wang; J Liu; P Pandey; FR Fronczek; RJ Doerksen; J Chen; X Qi; P Zhang; D Ferreira; FA Valeriote; H Sun; S Li; MT Hamann "Computationally assisted assignment of the kadsuraols, a class of chemopreventive agents for the control of liver cancer," *Organic Letters* **20**, 5559-5563 (2018). doi: 10.1021/acs.orglett.8b02207 PMID: 30192555

P Pandey; ND Chaurasiya; BL Tekwani; RJ Doerksen "Interactions of endocannabinoid virodhamine and related eicosanoids with human monoamine oxidase-A and -B," *Biochemical Pharmacology*, **155**, 82-91 (2018). doi: 10.1016/j.bcp.2018.06.024 PMID: 29958841

MF Sowaileh; AE Salyer; KK Roy; JP John; JR Woods; RJ Doerksen; GH Hockerman; DA Colby "Agonists of the  $\gamma$ -aminobutyric acid type B (GABA<sub>B</sub>) receptor derived from  $\beta$ -hydroxy and  $\beta$ -amino difluoromethyl ketones," *Bioorganic and Medicinal Chemistry Letters*, **28**, 2697-2700 (2018). doi: 10.1016/j.bmcl.2018.04.003 PMID: 29657102

J Liu; P Pandey; X Wang; X Qi; J Chen; H Sun; P Zhang; Y Ding; D Ferreira; RJ Doerksen; MT Hamann; S Li "Hepatoprotective dibenzocyclooctadiene and tetrahydrobenzocyclooctabenzofuranone lignans from *Kadsura longipedunculata*," *Journal of Natural Products* **81**, 846-857 (2018). doi: 10.1021/acs.jnatprod.7b00934 PMID: 29595972

GC Brandão; FCR Missias; LM Arantes; LF Soares; KK Roy; RJ Doerksen; A Braga de Oliveira; GR Pereira "Antimalarial naphthoquinones. Synthesis via click chemistry, in vitro activity, docking to PfDHODH and SAR of lapachol-based compounds," *European Journal of Medicinal Chemistry*, **145**, 191-205 (2018). doi: 10.1016/j.ejmech.2017.12.051 PMID: 29324340

J Pressly; SM Mustafa; AH Abidi; S Alghamdi; P Pandey; KK Roy; RJ Doerksen; BM Moore; F Park "Selective cannabinoid 2 receptor stimulation reduces tubular epithelial cell damage following renal ischemia-reperfusion injury," *Journal of Pharmacology and Experimental Therapeutics*, **364**, 287-299 (2018). doi: 10.1124/jpet.117.245522 PMID: 29187590 PMCID: PMC5774215

X Wang; J Liu; P Pandey; J Chen; FR Fronczek; S Parnham; X Qi; RJ Doerksen; D Ferreira; H Sun; S Li; MT Hamann "Assignment of the absolute configuration of hepatoprotective highly oxygenated triterpenoids using X-ray, ECD, NMR J-based configurational analysis and HSQC overlay experiments," *BBA (Biochimica et Biophysica Acta) General Subjects*, **1861**, 3089-3095 (2017). doi: 10.1016/j.bbagen.2017.09.001 PMID: 28919469

J Oh; H Liu; HB Park; D Ferreira; G-S Jeong; MT Hamann; RJ Doerksen; MK Na "In silico investigation of lavandulyl flavonoids for the development of potent FAS-inhibitory prototypes," *BBA (Biochimica et Biophysica Acta) General Subjects*, **1861**, 3180-3188 (2017). doi: 10.1016/j.bbagen.2016.08.001 PMID: 27531709

Y Ding; H Liu; BL Tekwani; NPD Nanayakkara; IA Khan; LA Walker; RJ Doerksen "Methemoglobinemia hemotoxicity of some antimalarial 8-aminoquinoline analogues and their hydroxylated derivatives: Density functional theory computation of ionization potentials," *Chemical Research in Toxicology*, **29**, 1132-1141 (2016). doi: 10.1021/acs.chemrestox.6b00063 PMID: 27223244

NN Mohammed; P Pandey; KM Elokely; HL Liu; RJ Doerksen; MA Repka "Clotrimazole-cyclodextrin

based approach for the management and treatment of Candidiasis. A formulation and chemistry based evaluation," *Pharmaceutical Development and Technology*, **21**, 619-629 (2016). doi: 10.3109/10837450.2015.1041041 PMID: 25923135

AD Priyanto; RJ Doerksen; C-I Chang; W-C Sung; SB Widjanarko; J Kusnadi; Y-C Lin; T-C Wang; J-L Hsu "Screening, discovery, and characterization of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins," *Journal of Proteomics*, **128**, 424-435 (2015). doi: 10.1016/j.jprot.2015.08.018 PMID: 26344130

AD Priyanto; RJ Doerksen; C-I Chang; W-C Sung; SB Widjanarko; J Kusnadi; Y-C Lin; T-C Wang; J-L Hsu "Data in support of optimized production of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins," *Data in Brief*, **5**, 403-407 (2015). doi:10.1016/j.dib.2015.09.038 PMID: 26958600

J Bae; LE McNamara; MA Nael; F Mahdi; RJ Doerksen; GL Bidwell III; NI Hammer; S Jo "Nitroreductase-triggered activation of a novel caged fluorescent probe obtained from methylene blue," *Chemical Communications*, **51**, 12787-12790 (2015). doi: 10.1039/C5CC03824C Cited >40 times. PMID: 26165999

KM Brown; KK Roy; GH Hockerman; RJ Doerksen; DA Colby "Activation of the  $\gamma$ -aminobutyric acid type B (GABA<sub>B</sub>) receptor by agonists and positive allosteric modulators," *Journal of Medicinal Chemistry*, **58**, 6336-6347 (2015). (Miniperspective) doi: 10.1021/jm5018913 Cited >25 times.

CC Chen; M-L Wu; C-T Ho; RJ Doerksen; T-C Huang "Apoptotic induction by andrographolide in HL-60 cells via Ras/ERK/NF- $\kappa$ B and Ras/Akt/NF- $\kappa$ B signaling dependent down-regulation of glyoxalase 1 and HMG-CoA reductase," *Journal of Functional Foods*, **14**, 226-235 (2015). doi: 10.1016/j.jff.2015.01.048

P-S Su; RJ Doerksen; S-H Chen; W-C Sung; RDS Rawendra; C-R Chen; J-W Li; Aisha; T-C Huang; C-I Chang; M-H Liao; J-L Hsu "Screening and profiling stilbene-type natural products with angiotensin-converting enzyme inhibitory activity from *Ampelopsis brevipedunculata* var. *hancei* (Planch.) Rehder," *Journal of Pharmaceutical and Biomedical Analysis*, **108**, 70-77 (2015). doi:10.1016/j.jpba.2015.01.053

H Liu; Y Ding; LA Walker; RJ Doerksen "Computational study on the effect of exocyclic substituents on the ionization potential of primaquine: Insights into the design of primaquine-based antimalarial drugs with less methemoglobin generation," *Chemical Research in Toxicology*, **28**, 169-174 (2015). doi: 10.1021/tx500230t PMID: 25222923

A Chatterjee; SJ Cutler; RJ Doerksen; IA Khan; JS Williamson "Discovery of novel thienoquinolone derivatives as selective and ATP non-competitive CDK5/p25 inhibitors by structure-based virtual screening," *Bioorganic & Medicinal Chemistry*, **22**, 6409-6421 (2014). doi: 10.1016/j.bmc.2014.09.043

G Fu; P. Sivaprakasam; OR Dale; SP Manly; SJ Cutler; RJ Doerksen "Pharmacophore modeling, ensemble docking, virtual screening, and biological evaluation on glycogen synthase kinase-3 $\beta$ ," *Molecular Informatics*, **33**, 610-626 (2014). doi: 10.1002/minf.201400044

G Fu; S Liu; X Nan; OR Dale; Z Zhao; Y Chen; DE Wilkins; SP Manly; SJ Cutler; RJ Doerksen "Quantitative structure-activity relationship analysis and a combined ligand-based/structure-based virtual screening study for glycogen synthase kinase-3," *Molecular Informatics*, **33**, 627-640 (2014). doi: 10.1002/minf.201400045

Y Ding; H Liu; NPD Nanayakkara; IA Khan; BL Tekwani; LA Walker; RJ Doerksen "Hydroxylated derivatives of NPC1161: Theoretical insights into their potential toxicity and the feasibility and regioselectivity of their formation," *Journal of Physical Chemistry A*, **118**, 5501-5507 (2014). doi: 10.1021/jp502612t

H Liu; RY Patel; RJ Doerksen "Structure of the cannabinoid receptor 1: Homology modeling of the

inactive state and enrichment study based on CB1 antagonist docking," *MedChemComm*, **5**, 1297-1302 (2014). doi: 10.1039/C4MD00121D **Inside cover article**.

MM Ghoneim; KM Elokely; AA El-Hela; AEI Mohammad; M Jacob; M Radwan; RJ Doerksen; SJ Cutler; SA Ross "Asphodosides A-E, anti-MRSA metabolites from *Asphodelus microcarpus*," *Phytochemistry*, **105**, 79-84 (2014). doi: 10.1016/j.phytochem.2014.06.011

MM Ghoneim, KM Elokely; AA El-Hela; AEI Mohammad; M Jacob; SJ Cutler; RJ Doerksen; SA Ross "Isolation and characterization of new secondary metabolites from *Asphodelus microcarpus*," *Medicinal Chemistry Research*, **23**, 3510-3515 (2014). doi: 10.1007/s00044-014-0928-x PMID: 25034614 PMCID: PMC4883109

J Bae; MA Nael; L Jiang; PT Hwang; F Mahdi; H-W Jun; WM Elshamy; Y-D Zhou; SN Murthy; RJ Doerksen; S Jo "Quinone propionic acid-based redox-triggered polymer nanoparticles for drug delivery: Computational analysis and in vitro evaluation," *Journal of Applied Polymer Science*, **131** (2014). doi: 10.1002/app.40461

H Liu; BL Tekwani; NPD Nanayakkara; LA Walker; RJ Doerksen "Methemoglobin generation by 8-aminoquinolines: Effect of substitution at 5-position of primaquine," *Chemical Research in Toxicology*, **26**, 1801-1809 (2013). doi: 10.1021/tx400067a

MAM Ibrahim; M Na; J Oh; RF Schinazi; TR McBrayer; T Whitaker; RJ Doerksen; DJ Newman; LG Zachos; MT Hamann "The significance of endangered and threatened plant natural products in the control of human disease," *Proceedings of the National Academy of Sciences of the United States of America*, **110**, 16832-16837 (2013). doi:10.1073/pnas.1311528110 **Featured article in University of Washington's Conservation Magazine and "Featured article recommended for teaching" in "F1000Prime"**. Cited >30 times.

Z Zhao; G Fu; S Liu; KM Elokely; RJ Doerksen; Y Chen; DE Wilkins "Drug activity prediction using multiple-instance learning via joint instance and feature selection," *BMC Bioinformatics*, **14** (Suppl 14), S16 (12 pp) (2013). (**2013 MCBIOS Proceedings**).

IH Hwang; J Oh; A Kochanowska-Karamyan; RJ Doerksen; M Na; MT Hamann "A novel natural phenyl alkene with cytotoxic activity," *Tetrahedron Letters*, **54**, 3872-3876 (2013). doi: 10.1016/j.tetlet.2013.05.032

H Liu; Y Ding; LA Walker; RJ Doerksen "Effect of antimalarial drug primaquine and its derivatives on the ionization potential of hemoglobin: A QM/MM study," *MedChemComm*, **4**, 1145-1147 (2013). doi: 10.1039/C3MD00045A **Cover article, August 2013**.

KM Elokely; RJ Doerksen "Docking challenge: Protein sampling and molecular docking performance," *Journal of Chemical Information & Modeling*, **53**, 1934-1945 (2013). doi: 10.1021/ci400040d PMID: 23530568 PMCID: PMC3755091 **Featured on the cover of Issue 11, November 2013**. Cited >85 times.

J Oh; JJ Bowling; Y Zou; AG Chittiboyina; RJ Doerksen; D Ferreira; TD Leininger; MT Hamann "Configurational assignments of conformationally restricted bis-monoterpene hydroquinones: Utility in exploration of endangered plants," *Biochemica et Biophysica Acta (BBA) - General Subjects*, **1830**, 4229-4234 (2013). doi: 10.1016/j.bbagen.2013.04.029; PMID: 23628705

MA Albadry; KM Elokely; B Wang; JJ Bowling; MF Abdelwahab; MH Hossein; RJ Doerksen; MT Hamann "Computationally assisted assignment of Kahalalide Y configuration using an NMR-constrained conformational search," *Journal of Natural Products*, **76**, 178-185 (2013). doi: 10.1021/np3006088; PMID: 23363083

A Shayanfar; S Ghasemi; S Soltani; K Asadpour-Zeynali; RJ Doerksen; A Jouyban "Quantitative structure-activity relationships of imidazole-containing farnesyltransferase inhibitors using different

- chemometric methods," *Medicinal Chemistry*, **9**, 434-448 (2013). doi: 10.2174/1573406411309030014
- G Fu; X Nan; H Liu; RY Patel; PR Daga; Y Chen; DE Wilkins; RJ Doerksen "Implementation of multiple-instance learning in drug activity prediction," *BMC Bioinformatics*, **13**, (Suppl 15) S3 (2012). doi:10.1186/1471-2105-13-S15-S3; PMID: 23046442 (**2012 MCBIOS Proceedings**). Cited >25 times.
- G Fu; H Liu; RJ Doerksen "Molecular modeling to provide insight into the substrate binding and catalytic mechanism of human biliverdin-IX $\alpha$  reductase," *Journal of Physical Chemistry B*, **116**, 9580-9594 (2012). doi: 10.1021/jp301456j; PMID: 22823425
- S Liu; RY Patel; PR Daga; H Liu; G Fu; RJ Doerksen; Y Chen; D Wilkins "Combined rule extraction and feature elimination in supervised classification," *IEEE Transactions on Nanobioscience*, **11**, 228-236 (2012). doi: 10.1109/TNB.2012.2213264; PMID: 22987128
- LK Brents; F Medina-Bolivar; KA Seely; V Nair; SM Bratton; A Gallus-Zawada; L Ćopó; RY Patel; H Liu; RJ Doerksen; PL Prather; A Radominska-Pandya "Natural prenylated resveratrol analogs arachidin-1 and -3 demonstrate improved glucuronidation profiles and have affinity for cannabinoid receptors," *Xenobiotica*, **42**, 139-156 (2012). doi: 10.3109/00498254.2011.609570 PMID: 21970716 PMCID: PMC3608422 Cited 30 times.
- H Liu; LA Walker; RJ Doerksen "DFT study on the radical anions formed by primaquine and its derivatives," *Chemical Research in Toxicology*, **24**, 1476-1485 (2011). doi: 10.1021/tx200094v; PMID: 21699254
- H Liu; A Dasmahapatra; RJ Doerksen "Computational study on the conformations of gambogic acid," *Chemical Physics Letters*, **511**, 405-412 (2011). doi: 10.1016/j.cplett.2011.06.035; PMID: 22991483
- X Nan; G Fu; Z Zhao; S Liu; RY Patel; H Liu; PR Daga; RJ Doerksen; X Dang; Y Chen; D Wilkins "Leveraging domain information to restructure biological prediction," *BMC Bioinformatics*, **12**, S22 (15 pp.) (2011) (2011 MCBIOS Proceedings). doi:10.1186/1471-2105-12-S10-S22; PMID: 22166097
- H Liu; LA Walker; NPD Nanayakkara; RJ Doerksen "Methemoglobinemia caused by 8-aminoquinoline drugs: DFT calculations suggest an analogy to H<sub>4</sub>B's role in nitric oxide synthase," *Journal of the American Chemical Society*, **133**, 1172-1175 (2011). doi: 10.1021/ja107472c; PMID: 21244096
- G Fu; RJ Doerksen; P Xu "Ab initio calculations of optical rotations and <sup>1</sup>H chemical shifts allow absolute configuration assignment of sulfinyl dilactones," *Journal of Molecular Structure*, **987**, 166-173 (2011). doi: 10.1016/j.molstruc.2010.11.076
- S Liu; RY Patel; PR Daga; H Liu; G Fu; RJ Doerksen; Y Chen; D Wilkins "Multi-class joint rule extraction and feature selection for biological data," In *Proceedings of the IEEE International Conference Bioinformatics & Biomedicine (BIBM 2011)*, pp. 476-481, Atlanta, GA, 11/12-15/2011. doi: 10.1109/BIBM.2011.82
- RY Patel; RJ Doerksen "Protein kinases-inhibitor database: analysis of structure variability and protein-inhibitor interactions within the P-loop," *Journal of Proteome Research*, **9**, 4433-4442 (2010). doi: 10.1021/pr100662s; PMID: 20681595 Cited 38 times.
- FE Dayan; PR Daga; SO Duke; RM Lee; PJ Tranel; RJ Doerksen "Biochemical and structural consequences of a glycine deletion in the  $\alpha$ -8 helix of protoporphyrinogen oxidase," *BBA - Proteins and Proteomics*, **1804**, 1548-1556 (2010). doi: 10.1016/j.bbapap.2010.04.004 Cited 42 times.
- R Mohammed; J Peng; M Kelly; M Yousaf; E Winn; S Odde; Z Bie; A Xie; RJ Doerksen; MT Hamann "Polyketide-peroxides from a species of Jamaican plakortis (Porifera: Demospongiae)," *Australian Journal of Chemistry*, **63**, 1-9 (2010). Special Issue. doi: 10.1071/CH09665
- PR Daga; J Duan; RJ Doerksen "Computational model of hepatitis B virus DNA polymerase: Molecular

dynamics and docking to understand resistant mutations," *Protein Science*, **19**, 796-807 (2010). doi: 10.1002/pro.359; PMID: 20162615 Cited 25 times.

H Liu; CR McCurdy; RJ Doerksen "Computational study on the conformations of mitragynine and mitragynaline," *Journal of Molecular Structure: Theochem*, **945**, 57-63 (2010). doi: 10.1016/j.theochem.2010.01.011; PMID: 21293786

J Peng; S Kudrimoti; S Prasanna; S Odde; RJ Doerksen; HK Pennaka; Y-M Choo; KV Rao; BL Tekwani; V Madgula; SI Khan; B Wang; AMS Mayer; MR Jacob; LC Tu; J Gertsch; MT Hamann "Structure activity relationship and mechanism of action studies of manzamine analogues for the control of neuroinflammation and cerebral infections," *Journal of Medicinal Chemistry*, **53**, 61-76 (2010). doi: 10.1021/jm900672t; PMID: 20017491 Cited >60 times.

PR Daga; RY Patel; RJ Doerksen "Template-based protein modeling: Recent methodological advances," *Current Topics in Medicinal Chemistry*, **10**, 84-94 (2010). PRD and RYP were joint first authors. (Invited review.) doi: 10.2174/156802610790232314 PMID: 19929829 Cited 42 times.

S Kudrimoti; SA Ahmed; PR Daga; AE Wahba; SI Khalifa; RJ Doerksen; MT Hamann "Semisynthetic latrunculin B analogs: Studies of actin docking support a proposed mechanism for latrunculin bioactivity," *Bioorganic & Medicinal Chemistry*, **17**, 7517-7522 (2009). doi:10.1016/j.bmc.2009.09.012; PMID: 19800245

P Sivaprakasam; PN Tosso; RJ Doerksen "Structure-activity relationship and comparative docking studies for cycloguanil analogs as PfDHFR-TS inhibitors," *Journal of Chemical Information & Modeling*, **49**, 1787-1796 (2009). doi: 10.1021/ci9000663; PMID: 19588935 Cited 25 times.

A Xie; S Odde; P Sivaprakasam; RJ Doerksen "Imidazole-containing farnesyltransferase inhibitors: 3D quantitative structure-activity relationship and molecular docking studies," *Journal of Computer-Aided Molecular Design*, **23**, 431-448 (2009). doi: 10.1007/s10822-009-9278-z; PMID: 19479325

A Xie; SR Clark; S Prasanna; RJ Doerksen "3D quantitative structure-farnesyltransferase inhibition analysis for some diaminobenzophenones," *Journal of Enzyme Inhibition & Medicinal Chemistry*, **24**, 1220-1228 (2009). doi: 10.3109/14756360902781389; PMID: 19912055

S Prasanna; RJ Doerksen "Topological polar surface area: A useful descriptor in 2D-QSAR," *Current Medicinal Chemistry*, **16**, 21-41 (2009). doi: 10.2174/092986709787002817 PMID: 19149561 Cited >75 times.

S Prasanna; PR Daga; A Xie; RJ Doerksen "Glycogen synthase kinase-3 inhibition by 3-anilino-4-phenylmaleimides: Insights from 3D-QSAR and docking," *Journal of Computer-Aided Molecular Design*, **23**, 113-127 (2009). doi: 10.1007/s10822-008-9244-1 PMID: 18839067

MA Ibrahim; AG Shilabin; S Prasanna; M Jacob; SI Khan; RJ Doerksen; MT Hamann "2-N-Methyl modifications and SAR studies of manzamine A," *Bioorganic & Medicinal Chemistry*, **16**, 6702-6706 (2008). PMID: 18595720 Cited 29 times.

PR Daga; RJ Doerksen "Stereo-electronic properties of spiroquinazolinones in differential PDE7 inhibitory activity," *Journal of Computational Chemistry*, **29**, 1945-1954 (2008). doi: 10.1002/jcc.20960 PMID: 18366018

SA Ahmed; S Odde; PR Daga; JJ Bowling; MK Mesbah; DT Youssef; SI Khalifa; RJ Doerksen; MT Hamann "Latrunculin with a highly oxidized thiazolidinone ring: Structure assignment and actin docking," *Organic Letters*, **9**, 4773-4776 (2007). doi: 10.1021/ol7020675 Cited 28 times.

P Sivaprakasam; A Xie; RJ Doerksen "Probing the physicochemical and structural requirements for glycogen synthase kinase-3 $\alpha$  inhibition: 2D-QSAR for 3-anilino-4-phenylmaleimides," *Bioorganic & Medicinal Chemistry*, **14**, 8210-8218 (2006). doi: 10.1016/j.bmc.2006.09.021; PMID: 17010615 Cited 46

times.

A Xie; P Sivaprakasam; RJ Doerksen "3D-QSAR analysis of antimalarial farnesyltransferase inhibitors based on a 2, 5-diaminobenzophenone scaffold," *Bioorganic & Medicinal Chemistry*, **14**, 7311-7323 (2006). doi: 10.1016/j.bmc.2006.06.041; PMID: 16837204 Cited 40 times.

Y Shao; LF Molnar; Y Jung; J Kussmann; C Ochsenfeld; ST Brown; ATB Gilbert; LV Slipchenko; SV Levchenko; DP O'Neill; RA DiStasio; RC Lochan; T Wang; GJO Beran; NA Besley; JM Herbert; CY Lin; T Van Voorhis; SH Chien; A Sodt; RP Steele; VA Rassolov; PE Maslen; PP Korambath; RD Adamson; B Austin; J Baker; EFC Byrd; H Dachsel; RJ Doerksen; A Dreuw; BD Dunietz; AD Dutoi; TR Furlani; SR Gwaltney; A Heyden; S Hirata; CP Hsu; G Kedziora; RZ Khalliulin; P Klunzinger; AM Lee; MS Lee; W Liang; I Lotan; N Nair; B Peters; EI Proynov; PA Pieniazek; YM Rhee; J Ritchie; E Rosta; CD Sherrill; AC Simmonett; JE Subotnik; HL Woodcock; W Zhang; AT Bell; AK Chakraborty; DM Chipman; FJ Keil; A Warshel; WJ Hehre; HF Schaefer; J Kong; AI Krylov; PMW Gill; M Head-Gordon "Advances in methods and algorithms in a modern quantum chemistry program package," *Physical Chemistry Chemical Physics*, **8**, 3172-3191 (2006). doi: 10.1039/B517914A **Cited >2440 times. Invited article.**

H Tang; RJ Doerksen; TV Jones; ML Klein; GN Tew "Biomimetic facially amphiphilic antibacterial oligomers with conformationally stiff backbones," *Chemistry & Biology*, **13**, 427-435 (2006). doi: 10.1016/j.chembiol.2006.02.007 Cited >75 times.

H Tang; RJ Doerksen; GN Tew "Synthesis of urea oligomers and their antibacterial activity," *Chemical Communications*, 1537-1539 (2005). doi: 10.1039/B413679A Cited >65 times.

RJ Doerksen; B Chen; D Liu; GN Tew; WF DeGrado; ML Klein "Controlling the conformation of arylamides: Computational studies of intramolecular hydrogen bonds between amides and ethers or thioethers," *Chemistry: A European Journal*, **10**, 5008 (2004). doi: 10.1002/chem.200400176 Cited 37 times.

D Liu; S Choi; B Chen; RJ Doerksen; DJ Clements; JD Winkler; ML Klein; WF DeGrado "Nontoxic membrane-active antimicrobial arylamide oligomers," *Angewandte Chemie International Edition*, **44**, 1158 (2004). doi: 10.1002/anie.200352791 **Cited >220 times. Cover article, February 20, 2004.**

RJ Doerksen; VJ Steeves; AJ Thakkar "Are polarizabilities useful as aromaticity indices? Tests on azines, azoles, oxazoles and thiazoles," Special issue on polarizabilities. *Journal of Computational Methods in Science and Engineering*, **3**, 427-438 (2004). Also appears in **Computational Aspects of Electric Polarizability Calculations: Atoms, Molecules and Clusters**, G Maroulis (Editor) IOS Press, Amsterdam (2004). ISBN: 158603495

RJ Doerksen; B Chen; J Yuan; JD Winkler; ML Klein "Novel conformationally-constrained  $\beta$ -peptides characterized by  $^1\text{H}$  NMR chemical shifts," *Chemical Communications*, 2534 (2003). doi: 10.1039/B309584C PMID: 14594267 Cited 26 times.

RJ Doerksen; B Chen; ML Klein "Intramolecular hydrogen bonds: Ab initio Car-Parrinello simulations of arylamide torsions," *Chemical Physics Letters*, **380**, 150 (2003). doi: 10.1016/j.cplett.2003.08.112

GN Tew; D Liu; B Chen; RJ Doerksen; J Kaplan; PJ Carroll; ML Klein; WF DeGrado "De novo design of biomimetic antimicrobial polymers," *Proceedings of the National Academy of Sciences of the United States of America*, **99**, 5110 (2002). **Featured in Chemical & Engineering News**, **80**, No. 23, 36-38 (June 10, 2002). Also, **featured in** the year-end Chemistry Highlights 2002 of *Chemical & Engineering News*, **80**, No. 50, 47 (December 16, 2002). doi: 10.1073/pnas.082046199 **Cited >450 times.**

RJ Doerksen; AJ Thakkar "Bond orders in heteroaromatic rings," *International Journal of Quantum Chemistry*, **90**, 534 (2002). doi: 10.1002/qua.998

RJ Doerksen; AJ Thakkar "Quadrupole and octopole moments of heteroaromatic rings," *Journal of Physical Chemistry A*, **103**, 10009 (1999). doi: 10.1021/jp992524v Cited >60 times.



RJ Doerksen; AJ Thakkar "Structures, vibrational frequencies and polarizabilities of diazaborinines, triazadiborinines, azaboroles, and oxazaboroles," *Journal of Physical Chemistry A*, **103**, 2141 (1999). doi: 10.1021/jp984256r Cited 39 times.

RJ Doerksen; AJ Thakkar; T Koga; M Hayashi "Geometries and multipole moments of  $\text{AlH}_4^-$ ,  $\text{SiH}_4$ ,  $\text{PH}_3$ ,  $\text{H}_2\text{S}$  and  $\text{HCl}$ ," *Theochem*, **488**, 217 (1999). doi:10.1016/S0166-1280(99)00020-2

RJ Doerksen; AJ Thakkar "Azaborinines: Structures, vibrational frequencies and polarizabilities," *Journal of Physical Chemistry A*, **102**, 4679 (1998). doi: 10.1021/jp980778v Cited 23 times.

RJ Doerksen; AJ Thakkar "Polarizabilities of heteroaromatic molecules: Azines revisited," *International Journal of Quantum Chemistry*, **60**, 421 (1996). doi: 10.1002/(SICI)1097-461X(1996)60:7<1633::AID-QUA45>3.0.CO;2-# Cited 26 times.

N El-Bakali Kassimi; RJ Doerksen; AJ Thakkar "Polarizabilities of oxazoles: *ab initio* calculations and simple models," *Journal of Physical Chemistry*, **100**, 8752 (1996). doi: 10.1021/jp953425u Cited 36 times.

N El-Bakali Kassimi; RJ Doerksen; AJ Thakkar "Polarizabilities of aromatic five-membered rings: Azoles," *Journal of Physical Chemistry*, **99**, 12790 (1995). doi: 10.1021/j100034a017 Cited 56 times.

## EDITORIALS

JD Wren; RJ Doerksen; IT Toby; B Nanduri; R Homayouni; P Manda; S Thakkar "Proceedings of the 2018 MidSouth Computational Biology and Bioinformatics Society (MCBIOS) conference," *BMC Bioinformatics* **20 (Suppl 2)**, 95 (2019). doi: 10.1186/s12859-019-2618-7

P Pandey; RJ Doerksen "New drugs from natural products around the world," *Pharmaceutical Sciences*, **22**, 215-216 (2016) doi: 10.15171/PS.2016.34 (Invited)

## PUBLISHED CONFERENCE ABSTRACTS

C Spencer; P Pandey; RJ Doerksen; M Godfrey. "A study of an active-state CB1 receptor model and JWH synthetic cannabinoids." *Proceedings of the American Academy of Forensic Sciences*, 70th Annual Scientific Meeting, Seattle, WA. 2018. K31.

C Spencer; KL Pettus; P Pandey; RJ Doerksen; M Godfrey "Study of an active-state CB1 receptor model and synthetic cannabinoid interactions." *Proceedings of the American Academy of Forensic Sciences*, 69th Annual Scientific Meeting, New Orleans, LA. 2017. K4.

MA Nael; RJ Doerksen "Identification of natural products as inhibitors of the protein kinase RNA-like endoplasmic reticulum kinase to manage Alzheimer's disease." *Planta Medica*, **80**, PF-10 (2014). doi: 10.1055/s-0034-1382588

P Pandey; KK Roy; H Liu; KM Elokely; S Pettaway; SJ Cutler; RJ Doerksen "Search for cannabinoid receptor 1 antagonists using structure-based virtual screening: identification of natural product hits." *Planta Medica*, **80**, PF-11 (2014). doi: 10.1055/s-0034-1382589

MM Ghoneim; KM Elokely; AA El-Hela; AEI Mohammad; SJ Cutler; RJ Doerksen; SA Ross "Computationally assisted assignment of highly strained isochromene nucleus." *Planta Medica*, **80**, PN-1 (2014). doi: 10.1055/s-0034-1382683

L Walker; P Fasinu; B Avula; N Chaurasiya; I Khan; M ElSohly; Y Wang; R Doerksen; Y Ding; H Liu; G Reichard; V Melendez; B Pybus; S Marcsisin; J Sousa; X Jin; R Rockford; J McChesney; B Herath; D Nanayakkara; B Tekwani "The metabolism of 8-aminoquinolines in relation to their efficacy and safety." 17th World Congress of Basic and Clinical Pharmacology (WCP2014), Cape Town, South Africa, July 2014. *Basic & Clinical Pharmacology & Toxicology*, **115**, 234 (2014).

J Oh; JJ Bowling; Y Zou; AG Chittiboyina; RJ Doerksen; D Ferreira; TD Leininger; MT Hamann "Configurational Assignments of Conformationally Restricted Bis-Monoterpene Hydroquinones: Utility in Exploration of Endangered Plants." *Planta Medica*, **79**, PN52 (2013). doi: 10.1055/s-0033-1348733

Y Ding; H Liu; RJ Doerksen; NPD Nanayakkara; BL Tekwani; IA Khan; L Walker "Hydroxylation Derivatives of Some 8-Aminoquinoline Compounds: Theoretical Insights into Their Toxicity, Feasibility, and Regioselectivity." *Planta Medica*, **78**, P-25 (2012). doi: 10.1055/s-0032-1307533

PR Daga; S Odde; MT Hamann; RJ Doerksen "Free energy calculations on the binding of natural latrunculins and semi-synthetic derivatives to G-actin," *Planta Medica* **75**, (P-52) 431-432 (2009). doi: 10.1055/s-2009-1216490

JJ Bowling; PR Daga; S Odde; SA Ahmed; MK Mesbah; DT Youssef; S Kudrimoti; S Khalifa; RJ Doerksen; MT Hamann "Actin-binding comparisons of the marine natural product latrunculin B with natural and semisynthetic latrunculin B analogs," *Planta Medica* **74**, (P-62) 341-342 (2008). doi: 10.1055/s-2008-1075258

AE Wahba; J Peng; P Sivaprakasam; S Odde; RJ Doerksen; MT Hamann "Regio-controlled nitration of manzamine A as intermediates for producing manzamine analogues with better docking scores with GSK-3 beta," *Planta Medica* **74**, (P-42) 335 (2008). doi: 10.1055/s-2008-1075238

P Sivaprakasam; M Hamann; RJ Doerksen "Blind docking of manzamines into glycogen synthase kinase-3 beta," *Planta Medica* **74**, (P-41) 335 (2008). doi: 10.1055/s-2008-1075237

RJ Doerksen; B Chen; D Liu; WF DeGrado; ML Klein "Designed intramolecular hydrogen bonds stabilizing antimicrobial amphiphilic polymers," *Polymer Preprints* **44**, 598 (2003).

## PATENT

RJ Doerksen; B Chen; WF DeGrado; ML Klein "Methods, systems, and computer program products for computational analysis and design of amphiphilic polymers." U.S. Patent Publication No. US 7590517 B2 published on 9/15/2009 (filed on May 28, 2003). Licensed by biotech start-up company, *Polymedix* (polymedix.com).

## COMPUTER PROGRAM AUTHORIZING

### *Author:*

WORKS: ab initio molecular dynamics

LENANG: molecular geometry manipulation

QUAD: quadrupole moment tensor manipulation

AROMIN: geometric indices of aromaticity

### *Co-author:*

Q-CHEM 3.0, a commercial quantum chemistry program, Y Shao, L Fusti-Molnar, Y Jung, J Kussmann, C Ochsenfeld, ST Brown, et al., Q-Chem, Inc., Inc.: Pittsburgh, PA; 2007. Cited >45 times.

ALFA1: uncoupled Hartree-Fock polarizability

POL201: finite-field polarizability fitting

## CURRENT RESEARCH FUNDING

NIH. R21. "Target-based chemotherapeutics development against Mycobacterium tuberculosis." Robert J. Doerksen, Co-I (PI: Dr. Sudeshna Roy, Division of Medicinal Chemistry). 7/1/2019-6/30/2021.

National Science Foundation. XSEDE (Extreme Science and Engineering Discovery Environment) Startup request. "Extended all-atom molecular dynamics simulations to shed light on the characteristic features from inactive- to active-state transition of the human CB2 receptor, energetically preferred binding pose recognition, and agonist-induced conformational changes during receptor activation." MCB190035. 4/15/2019-4/14/2020. Robert J. Doerksen, Co-Investigator (Pankaj Pandey, PI).

National Science Foundation. XSEDE (Extreme Science and Engineering Discovery Environment)

Startup request. "Computational modeling and dynamics studies of negative allosteric modulators within the orthosteric ligand-bound complexes of the human cannabinoid 1 (CB1) receptor." MCB190033. 4/3/2019-4/2/2020. Robert J. Doerksen, Principal Investigator.

National Institutes of Health. R15. "Computer-aided Design and In vitro Testing of Novel Cannabinoid Receptor Modulators." 5/1/2016-4/30/2019. Robert J. Doerksen, Principal Investigator. 1R15GM119061-01 No cost extension to 4/30/2020.

National Science Foundation. Research Experience for Undergraduates (REU). "Ole Miss Physical Chemistry Summer Research Program REU." Second Competitive Renewal. CHE-1757888. Robert J. Doerksen, Senior Personnel. (PI: Dr. Nathan Hammer, U. Mississippi.) 9/1/2018-8/31/2021.

## PAST RESEARCH FUNDING

MAD-ID (Make a Difference-Infectious Disease) Antimicrobial Stewardship Research Grant "Strategies to Optimize *Clostridium difficile* Classification and Treatment." 7/1/2017-6/30/2018. Doerksen, Co-PI. (PI: Jamie Wagner, Dept. of Pharmacy Practice). No cost extension to 8/15/2019.

National Institutes of Health. National Institute of General Medical Sciences Award Number P30GM122733. (PI: Dr. Soumyajit Majumdar) Center of Biomedical Research Excellence – Natural Products Neuroscience (COBRE-NPN) Voucher Program Award, "Computer-aided discovery of CB1 antagonists void of adverse neuropsychiatric effects." Robert J. Doerksen, Principal Investigator. 3/5/2019-5/31/2019.

National Science Foundation. Research Experience for Undergraduates (REU). "Ole Miss Physical Chemistry Summer Research Program REU." CHE-1460568. (Renewal) 9/1/2015-8/31/2018. Robert J. Doerksen, Senior Personnel. (PI: Dr. Nathan Hammer, Department of Chemistry, University of Mississippi.) Doerksen research group had one summer student each summer.

National Science Foundation. "MRI: A GPU Cluster for Computational Science in Mississippi." Award CHE-1338056. 9/15/2013-8/31/2016. Robert J. Doerksen, Co-Investigator. (PI: Dr. Greg Tschumper, University of Mississippi.) No cost extension to 8/31/2017.

University of Mississippi's National Institutes of Health (NIH) National Center for Research Resources (NCRR) Center of Research Excellence in Natural Products Neuroscience (CORE-NPN) Phase II. "CORE-NPN: Rational Design of Novel Natural Product-Derived Cannabinoid Ligands." P20GM104932. 9/1/2016-8/31/2017. Robert J. Doerksen, Chemistry Core Participant (PI: Dr. Soumyajit Majumdar, University of Mississippi.)

National Science Foundation. Mississippi EPSCoR Program. Targeted Seed Grant. NSF EPS 0903787. "Combined Computational Chemistry and Computational Biology Modeling for Understanding Protein-Protein and Protein-Ligand Interactions." 8/16/2015-8/15/2016. Robert J. Doerksen, Principal Investigator.

National Science Foundation. Mississippi EPSCoR Program "Modeling and Simulation of Complex Systems." NSF EPS 0903787 and NSF EPS 1006883. 8/2009-8/2016. Robert J. Doerksen, Co-Investigator. (PI: Dr. Sandra Harpole, Mississippi State University.) Year 7: 9/1/2015-8/31/2016.

University of Mississippi's National Institutes of Health (NIH) National Center for Research Resources (NCRR) Center of Research Excellence in Natural Products Neuroscience (CORE-NPN) Phase II. "CORE-NPN: Rational Design of Novel Natural Product-Derived Cannabinoid Ligands." P20GM104932. 9/1/2015-8/31/2016. Robert J. Doerksen, Chemistry Core Participant (PI: Dr. Stephen J. Cutler, University of Mississippi.)

Extreme Science and Engineering Discovery Environment (XSEDE) grant of supercomputer time, MCB140248 "Computational insights into the characteristic features of the active state 3D structure of the human CB2 receptor, mode of agonist recognition and agonist-induced conformational changes during receptor activation." Robert J. Doerksen, Co-Investigator. (PI: Dr. Kuldeep K. Roy, postdoctoral

fellow) 9/2014-11/2015.

University of Mississippi's National Institutes of Health (NIH) National Center for Research Resources (NCRR) Center of Research Excellence in Natural Products Neuroscience (CORE-NPN) Phase II. "CORE-NPN: Rational Design of Novel Natural Product-Derived Cannabinoid Ligands." P20GM104932. Robert J. Doerksen, Junior Investigator. (PI: Dr. Stephen J. Cutler, University of Mississippi.) 7/1/2012-8/31/2015.

National Science Foundation. Research Experience for Undergraduates (REU). "Ole Miss Physical Chemistry Summer Research Program REU." CHE-1156713. Robert J. Doerksen, Senior Personnel. (PI: Dr. Nathan Hammer, Department of Chemistry, University of Mississippi.) 9/1/2012-8/31/2015.

USAID (American Council on Education/US Agency for International Development). "Africa-U.S. Network of Centers of Excellence in Water & Environmental Science & Technology." AEG-A-00-05-00007. Robert J. Doerksen, Co-Investigator. (PI: Dr. Nosa Egiebor, University of Mississippi.) 8/1/2014-6/30/2015.

National Institutes of Health. "New Drugs for Opportunistic Infectious Diseases." NIAID, 2R0AI27094-20A1, PI: Alice M. Clark; Co-PI: Ameeta K. Agarwal. 7/2009-6/2014. Doerksen group received funding from this grant from 9/2013-12/2013.

National Science Foundation. Mississippi EPSCoR Program. Year 4 Seed Grant. "Computational modeling-aided design, synthesis and optimization of redox-sensitive polymer nanoparticles with optimal colloid-forming and DT-diaphorase-substrate properties." Robert J. Doerksen, Co-Investigator. (PI: Dr. Seongbong Jo, University of Mississippi.) 9/1/2012-8/31/2013.

Department of Defense USAMRMC. "Development of Safer Antimalarial and Antileishmanial Drugs for US Troops and Travelers." Robert J. Doerksen, Investigator. (PI: Dr. Larry Walker, University of Mississippi.) 9/2009-12/2012.

National Science Foundation. Mississippi EPSCoR Program. Year 3 Seed Grant. "Computational modeling-aided design, synthesis and evaluation of redox-sensitive polymer nanoparticles for cancer targeted drug delivery." Robert J. Doerksen, Co-Investigator. (PI: Dr. Seongbong Jo, University of Mississippi.) 9/1/2011-8/31/2012.

University of Mississippi's National Institutes of Health (NIH) National Center for Research Resources (NCRR) Center of Research Excellence in Natural Products Neuroscience (CORE-NPN) Junior Investigator Program. "CORE-NPN: Rational Design of Novel Natural Product-Derived Cannabinoid Ligands." Robert J. Doerksen, Principal Investigator. (PI: Dr. Stephen J. Cutler, University of Mississippi.) 7/1/2009-6/30/2011.

National Science Foundation. Mississippi EPSCoR Program. Targeted Seed Grant. "Combined Computational Chemistry and Computational Biology Modeling for Understanding Protein-Protein and Protein-Ligand Interactions." 1/1/2011-12/31/2011. Robert J. Doerksen, Principal Investigator.

National Science Foundation. Mississippi EPSCoR Program. Bridge Funding (between programs). "Innovations through Computational Sciences." EPS-0556308. Robert J. Doerksen, Investigator. (Dr. Sandra Harpole, PI, Mississippi State University.) 8/2009-10/31/2009.

American Association of Colleges of Pharmacy 2007-2008 New Investigators Program for Pharmacy Faculty. "Rational computer-aided drug design for glycogen synthase kinase-3 inhibition." Robert J. Doerksen (Principal Investigator). 12/15/2007-6/31/2008.

University of Mississippi's National Institutes of Health (NIH) National Center for Research Resources (NCRR) Center of Research Excellence in Natural Products Neuroscience (CORE-NPN) Small Grants Program. "Computational studies on manzamine inhibition of GSK-3beta and CDK5 for treatment of neuroinflammation." Robert J. Doerksen (PI). 7/1/2007-6/30/2009.

Centers for Disease Control and Prevention (CDC) National Center for Zoonotic, Vector-Borne, and Enteric Diseases (NCZVED). "Development and Testing of New Antimalarial Drugs." Robert J. Doerksen, Investigator. (Dr. Mitchell Avery, PI, University of Mississippi.) 8/1/2004-7/31/2009.

Centers for Disease Control and Prevention (CDC) National Center for Zoonotic, Vector-Borne, and Enteric Diseases (NCZVED). "Rational Design of Novel Drugs for the Treatment of Emerging Infectious Diseases." Robert J. Doerksen, Investigator. (Dr. Mitchell Avery, PI, University of Mississippi.) 9/15/2005-9/14/2006; 9/30/2006-9/29/2007.

National Science Foundation. Mississippi EPSCoR Program. "Innovations through Computational Sciences." EPS-0556308. Robert J. Doerksen, Investigator. (Dr. Sandra Harpole, PI, Mississippi State University). 5/1/2006-4/30/2009.

National Science Foundation. Mississippi EPSCoR Program. "Innovations through Computational Sciences." EPS-0556308. Robert J. Doerksen, Investigator. (Dr. Sandra Harpole, PI, Mississippi State University). Education & Outreach funding from 5/2008-8/2009 (administered at U. Mississippi by Dr. Peter Sukanek from Dept. of Chemical Engineering) provided support for several key personnel in the Doerksen research group. 5/1/2006-4/30/2009.

National Science Foundation - Division of Graduate Education (DGE), Integrative Graduate Education and Research Traineeship (IGERT); DGE 0333136. "Entrepreneurial Research and Education at the Interface of Polymers and Medicinal Chemistry." Robert J. Doerksen, Investigator. (Dr. Lon J. Mathias, PI). Cost-shared (no direct funds). 8/1/2004-9/31/2008.

University of Mississippi Ole Miss Partners Program Grant. "Uninterruptible Power Supplies for Continuous, Safe Operation of Research Computers." Robert J. Doerksen (PI). 12/2006-6/2007.

University of Mississippi Ole Miss Associates - Partners Program Grant. "Network-accessible computer storage device for computationally-intensive medicinal chemistry research." Robert J. Doerksen (PI). 1/2006-6/30/2006.

University of Mississippi Office of Research and Sponsored Programs. "Major Computer Purchase Assistance." Robert J. Doerksen (PI). 1/3/2006-6/30/2006.

University of Mississippi Faculty Research Program. "Ab initio Car-Parrinello QM/MM molecular dynamics study of the active site and catalytic functioning of biliverdin reductase." Robert J. Doerksen (PI). 1/1/2005-1/1/2006.

University of Mississippi Ole Miss Partners Program Grant. "Compiler for New Linux Computer Cluster." Robert J. Doerksen (PI). 11/2004-11/2005.

Travel Support. Funds received from a variety of sources. Selected examples:

For Robert J. Doerksen and group members to attend the 15th Conference on Current Trends in Computational Chemistry, Jackson, MS, 11/3-4/2006: Department of Medicinal Chemistry, University of Mississippi.

For Robert J. Doerksen to attend the 229th American Chemical Society National Meeting, San Diego, CA; support from: Michael Klein 65th Birthday Symposium, \$1250; School of Pharmacy, University of Mississippi, \$750; Office of Research and Sponsored Programs, University of Mississippi, \$750. 3/13-17/2005

For Robert J. Doerksen to attend the 13th Conference on Current Trends in Computational Chemistry, Jackson, MS: Office of Research and Sponsored Programs, University of Mississippi. 11/11-13/2004

## INVITED RESEARCH SEMINARS

RJ Doerksen "Beyond marijuana: Computational medicinal chemistry approaches targeting the

cannabinoid receptors." School of Pharmacy, Concordia University of Wisconsin, Mequon, WI, Sep 27, 2019.

RJ Doerksen "Discovering drugs at University of Mississippi: Calculations and experiments on the structure and properties of complex natural products." Department of Physical Sciences, School of Arts and Sciences, Concordia University of Wisconsin, Mequon, WI, Sep 27, 2019.

RJ Doerksen "Discovering drugs from nature: Accurate calculations and experiments to help determine the structure and properties of complex, flexible natural products." Drug Discovery and Development Colloquium 2019 (DDDC 2019), Little Rock, AR, Jun 13-15, 2019. Featured Speaker.

RJ Doerksen "Applying computational medicinal chemistry for discovery of cannabinoid receptor ligands." Department of Pharmaceutical Sciences, University of Arkansas for Medical Science, Little Rock, AR, Apr 19, 2019.

RJ Doerksen "Introduction to the University of Mississippi (UM) Graduate School and UM food science research: Nutrition, dietary supplements, and natural products as sources of drugs for human health." Department of Food Science, National Pingtung University of Science and Technology, Neipu, Taiwan, Jan 3, 2019.

RJ Doerksen "Flexible natural product molecules: Accurate calculations to help determine their structure and properties." Department of Biological Science and Technology, National Pingtung University of Science and Technology, Neipu, Taiwan, Jan 3, 2019.

RJ Doerksen "Challenges in the search for cannabinoid receptor ligands as CNS drugs." Symposium on "New and Emerging Therapeutic Targets for CNS Drug Discovery" at the 74th American Chemical Society Southwest Regional Meeting, Little Rock, AR, Nov 7-10, 2018.

RJ Doerksen "Laws of physics applied to molecules: Accurate electronic structure calculations and molecular dynamics simulations" Department of Physics, University of Mississippi, Sep 4, 2018.

RJ Doerksen "Cannabinoid receptor ligands: Search for new drugs to help human health." Drug Discovery and Development Colloquium 2018 (DDDC 2018), Lexington, KY, Jun 21-23, 2018. Featured Speaker.

RJ Doerksen "Docking of small molecules to the cannabinoid receptors: Finding value from big chemical datasets." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) 15<sup>th</sup> Annual Meeting in Starkville, MS, Mar 29-31, 2018. Session Featured Speaker.

RJ Doerksen "Computational medicinal chemistry: Connections to food science." Department of Food Science and Biotechnology, National Chung Hsing University, Taichung, Taiwan, Jul 4, 2017.

RJ Doerksen "Molecular docking: Striving for quantitative accuracy in addition to qualitative accuracy." Department of Chemistry, National Cheng Kung University, Tainan, Taiwan, Jun 21, 2017.

RJ Doerksen "Computational methods applicable to food chemistry: Molecular properties calculations and chemoinformatics." Department of Food Science, National Pingtung University of Science and Technology, Neipu, Taiwan, Jun 16, 2017.

RJ Doerksen "Molecular docking: A method to aid discovery of the mechanism of action for natural products." Department of Food Science, National Pingtung University of Science and Technology, Neipu, Taiwan, Jun 16, 2017.

RJ Doerksen "Search for cannabinoid receptor 1 antagonists as anti-obesity medicines." Department of Food Science, National Pingtung University of Science and Technology, Neipu, Taiwan, Jun 16, 2017.

RJ Doerksen "Computational chemistry and computational biology approaches to discovery of novel

cannabinoid receptor modulators.” Department of Biological Science and Technology, National Pingtung University of Science and Technology, Neipu, Taiwan, Jun 15, 2017.

RJ Doerksen “Computational medicinal chemistry approaches to discovery of novel cannabinoid receptor ligands.” Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS, Feb 3, 2017.

RJ Doerksen “Chemoinformatics and molecular dynamics approaches to discovery of novel cannabinoid receptor ligands.” Department of Chemical Engineering, University of Mississippi, Oct 19, 2016.

RJ Doerksen “Molecular docking: Striving for qualitative and quantitative accuracy.” Department of Chemistry, University of the Sciences, Philadelphia, PA, Mar 21, 2016.

RJ Doerksen “Computational medicinal chemistry: Striving towards qualitative and quantitative molecular docking.” Department of BioMolecular Sciences Seminar, University of Mississippi, Oct 13, 2015.

RJ Doerksen "Chemoinformatics approaches to discovery of drugs targeted to the cannabinoid receptors." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Little Rock, AR in Mar 6-7, 2015.

RJ Doerksen "Computational approaches to cannabinoid receptor drug hit discovery." 26th Canadian Symposium on Theoretical and Computational Chemistry, Montreal, Canada, Jul 6-11, 2014.

RJ Doerksen “Computational approaches to bioactive natural products: Conformation, configuration assignment, and drug hit discovery.” National Chung Hsing University, Department of Food Science and Biotechnology, Taichung, Taiwan, Friday, May 9, 2014.

RJ Doerksen “Computational approaches to find cannabinoid receptor modulators which can function as anti-obesity medicines.” Chung Shan Medical University, Department of Nutrition, Taichung, Taiwan, Friday, May 9, 2014.

RJ Doerksen “Computational approaches to bioactive marine natural products: Conformation, configuration assignment, and drug hit discovery.” National Kaohsiung Marine University, Department of Seafood Science, Kaohsiung, Taiwan, Wednesday, Apr 30, 2014.

RJ Doerksen “Computational approaches to marine natural products: Conformation, configuration assignment, and drug hit discovery.” National Museum of Marine Biology and Aquarium, Checheng, Pingtung, Taiwan, Monday, Apr 7, 2014.

RJ Doerksen “Computational approaches to bioactive natural products: Search for drugs that act on the cannabinoid receptors.” Tunghai University, Food Science Department, Taichung, Taiwan, Friday, Mar 14, 2014.

RJ Doerksen “Computational approaches to bioactive natural products: Search for cannabinoid-active anti-obesity medicines.” Hungkuang University, Department of Food Science and Technology, Taichung, Taiwan, Presented as part of “International Research Conference on Discovery and Applications of Bioactive Natural Products.” Friday, Mar 7, 2014.

RJ Doerksen “Computational approaches to bioactive natural products.” Department of Biological Science and Technology, National Pingtung University of Science and Technology, Neipu, Taiwan, Dec 27, 2013.

RJ Doerksen “Cannabinoid receptor modulator design: Ligand-based and protein structure-based approaches.” Department of Chemistry, Georgia State University, Atlanta, GA, Nov 8, 2013.

RJ Doerksen "Rational design of glycogen synthase kinase-3 inhibitors for the control of neuroinflammation and cerebral infections." The University of Mississippi Medical Center, Department of Neurobiology & Anatomical Sciences, Department of Psychiatry and Human Behavior and the Center for Psychiatric Neuroscience Seminar Series, Oct 29, 2013.

RJ Doerksen "Targeting glycogen synthase kinase-3 using a computational approach." School of Pharmacy Central Nervous System Brown Bag Lunch, Aug 15, 2013.

RJ Doerksen "Designer drugs through computational methods." The World Malaria Day: The Multidirectional Discovery Approach to Fight against Malaria. University of Mississippi, University, MS, Apr 24, 2013.

RJ Doerksen "Rational approaches to discovery of novel glycogen synthase kinase-3 inhibitors." SWRM 2012 Southwest Regional American Chemical Society (ACS) Meeting "Chemical and Structural Biology: New Frontiers in Therapeutic Development" Symposium, Baton Rouge, LA, Nov 4-7, 2012.

DA Kevin; S Prasanna; OR Dale; SP Manly; SJ Cutler; **RJ Doerksen** "Plant-derived human GSK-3beta inhibitors." 3rd Annual Conference American Council for Medicinally Active Plants (ACMAP), Jonesboro, AR, May 2012.

**P Prather**; A Radominska-Pandya; F Medina-Bolivar; RJ Doerksen "Natural prenylated and synthetic resveratrol analogs as novel ligands for cannabinoid receptors." 3rd Annual Conference American Council for Medicinally Active Plants (ACMAP), Jonesboro, AR, May 2012.

RJ Doerksen "Using computation and simulation to study complex nanoscale processes: Protein kinases and related topics." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 11, 2012.

RJ Doerksen "Modeling protein ligand interactions and protein domain interactions with the combined force of compbio and compchem." Mississippi NSF EPSCoR Research Meeting, Oxford, MS, Sep 20, 2011.

RJ Doerksen "Combined computational chemistry and computational biology modeling for understanding protein-protein and protein-ligand interactions." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 15, 2011.

H Liu; RJ Doerksen "Using computational approaches to understand the methemoglobinemia caused by 8-aminoquinolines." Department of Defense USAMRMC Research Project Annual Meeting. "Development of Safer Antimalarial and Antileishmanial Drugs for US Troops and Travelers." Oxford, MS, Mar 18, 2011.

RJ Doerksen "Computational approaches to aid natural product discovery and development." Department of Pharmacognosy, University of Mississippi, University, MS, Feb 22, 2011.

RJ Doerksen "Computational studies on protein kinase-inhibitor interactions." 2010 EPSCoR Research Fall Forum, University of Mississippi Medical Center, Jackson, MS, Sep 20, 2010.

RJ Doerksen "Quantum mechanical calculations on protein chemistry: Applications to hemoglobin and biliverdin reductase." Academia Sinica, Institute of Chemistry, Taipei, Taiwan, Jun 21, 2010.

RJ Doerksen "Computational studies on protein kinase-inhibitor interactions." Department of Chemistry, National Dong Hwa University, Hualien, Taiwan, Jun 18, 2010.

RJ Doerksen "Computational studies on protein kinase-inhibitor interactions." Academia Sinica, Institute of Atomic and Molecular Sciences, Taipei, Taiwan, Jun 8, 2010.

RJ Doerksen; H Liu; NPD Nanayakkara; LA Walker "DFT study on the methemoglobinemia caused by 8-aminoquinoline drugs." Department of Defense USAMRMC Research Project Annual Meeting.



"Development of Safer Antimalarial and Antileishmanial Drugs for US Troops and Travelers." Apr 23, 2010.

RJ Doerksen "Computational studies for rational design of GSK-3 and CDK5 inhibitors." 2nd Annual Meeting of the Mississippi Biophysical Consortium (MBC 2009), Mississippi State University, Starkville, MS, May 2009.

RJ Doerksen "Rational computer-aided drug design for glycogen synthase kinase-3 inhibition." American Association of Colleges of Pharmacy Annual Meeting, Chemistry Section, Chicago, IL, Jul 2008.

RJ Doerksen "Computational medicinal chemistry approaches for understanding protein-ligand interactions." National Changhua Education University, Department of Chemistry, Changhua, Taiwan, Jun 23, 2008.

RJ Doerksen "Novel peptidomimetic antimicrobial oligomers: Insights from computational modeling." National Taiwan University, School of Pharmacy, Taipei, Taiwan, Jan 19, 2006.

RJ Doerksen "Computational studies towards controlling the conformation of oligomers: Innovative functional backbones." Academia Sinica, Institute of Chemistry, Taipei, Taiwan, Jan 18, 2006.

RJ Doerksen "Novel internally hydrogen bonded peptidomimetic antimicrobials: Insights from computational modeling." Mississippi State University, Department of Chemistry, Starkville, MS, Oct 21, 2005.

RJ Doerksen "Controlling the conformation of novel arylamide and other nontoxic antimicrobial oligomers." University of Mississippi, Department of Chemistry and Biochemistry, University, MS, Oct 7, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." University of Montreal, Department of Chemistry, Montreal, QB, Canada, Mar 2, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." University of Missouri, St. Louis, Department of Chemistry and Biochemistry, St. Louis, MO, Feb 16, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." Yeshiva University, Albert Einstein College of Medicine, Department of Physiology and Biophysics, Bronx, NY, Jan 29, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." University of Mississippi, School of Pharmacy, Department of Medicinal Chemistry, University, MS, Jan 26, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." Illinois Institute of Technology, Department of Biological, Chemical, and Physical Sciences, Chicago, IL, Jan 21, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." University of Cincinnati, Department of Chemistry, Cincinnati, OH, Jan 13, 2004.

RJ Doerksen "A composite computational approach for design of nontoxic antimicrobial oligomers." Virginia Commonwealth University, Department of Chemistry, Richmond, VA, Dec 15, 2003.

RJ Doerksen "Computational modeling of antimicrobials." Colgate-Palmolive, Piscataway, NJ, Nov 20, 2003.

RJ Doerksen "Accurate density-functional theory torsional potentials for de novo amphiphilic antimicrobial peptide design." Taiwan National Health Research Institutes, Division of Biotechnology and Pharmaceutical Research, Taipei, Taiwan, Mar 21, 2002.

RJ Doerksen "Theoretical insight into the reaction of  $C + C_2H_2$  from ab initio molecular dynamics trajectories and transition state structures." Sandia National Laboratory, Livermore, CA, Jan 2001.

RJ Doerksen "Theoretical insight into the reaction of  $C(^3P) + C_2H_2$ ." University of Arizona, Department of Chemistry, Tucson, AZ, Jan 2001.

RJ Doerksen "Theoretical insight into the reaction of  $C(^3P_j)$  with acetylene." National Changhua Education University, Department of Chemistry, Changhua, Taiwan, Feb 2000.

## CONFERENCE TALKS

AO Aderibigbe; P Pandey; RJ Doerksen "Computer-aided design of peripherally-restricted antagonists of the cannabinoid receptor 1." 46<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2019.

AO Aderibigbe; P Pandey; RJ Doerksen "Use of chemoinformatics and molecular docking in the design of peripherally-restricted CB1 antagonists." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting, Birmingham, AL, Mar 2019.

P Pandey; KK Roy; RJ Doerksen "Identification of selective cannabinoid receptor 1 inverse agonists using protein structure-based virtual screening." Drug Discovery and Development Colloquium 2018 (DDDC 2018), Lexington, KY, Jun 21-23, 2018.

AO Aderibigbe; P Pandey; RJ Doerksen "Hybrid virtual screening for peripherally-restricted cannabinoid receptor 1 (CB1) antagonists and inverse agonists." 45<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, College Station, TX, May 2018.

AO Aderibigbe; P Pandey; RJ Doerksen "Sifting through big data: The search for peripherally-restricted CB1 receptor antagonists and inverse agonists." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Starkville, MS, Mar 29-31, 2018. AyoOluwa won an MCBIOS-JMP Young Scientist Excellence Award (Students: 2<sup>nd</sup> Place).

P Pandey; KK Roy; H Liu; RJ Doerksen "Protein structure-based virtual screening: Identification of potent natural product-chemotypes as cannabinoid receptor 1 inverse agonists." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Starkville, MS, Mar 29-31, 2018. Pankaj won an MCBIOS-JMP Young Scientist Excellence Award (Postdoctoral Fellows: Honorable Mention).

AO Aderibigbe; P Pandey; RJ Doerksen "Exploring the structural features of peripherally-restricted CB1 receptor antagonists and inverse agonists." 255<sup>th</sup> American Chemical Society National Meeting, Division of Computers in Chemistry, New Orleans LA, Mar 2018.

P Pandey; KK Roy; **RJ Doerksen** "Structural insights into conformation and dynamics of the cannabinoid CB2 receptor through an extended MD simulation of CP55,940–CB2 complex." 253<sup>rd</sup> American Chemical Society National Meeting, Division of Computers in Chemistry, San Francisco CA, Apr 2017.

P Pandey; KK Roy; RJ Doerksen "Exploring the allosteric inhibitory binding sites for known negative allosteric modulators within the cannabinoid CB2 receptor." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting, Memphis TN, Mar 2016. **Pankaj won First Place Postdoctoral Oral Presentation.**

N Nguyen; KK Roy; RJ Doerksen "Protein structure-based virtual screening for the discovery of novel CB2 receptor agonists." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual

Meeting, Memphis TN, Mar 2016.

P Pandey; KK Roy; **RJ Doerksen** "Cannabis-derived compounds as cannabinoid receptor modulators: Systematic analysis using molecular docking and binding free-energy studies." 25th Annual International Cannabinoid Research Society Symposium on the Cannabinoids, Wolfville, NS, Canada, Jun 29-Jul 2, 2015.

P Pandey; KK Roy; RJ Doerksen "Identification and characterization of allosteric site(s) for CB2 negative allosteric modulators (NAMS)." 42<sup>nd</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 17, 2015.

KK Roy; RJ Doerksen "Investigation of protein targets for antimalarial compounds/drugs with unknown mechanism of action (MOA): Computational approaches." 3rd University of Mississippi Malaria Symposium. Oxford, MS, Apr 2015.

P Pandey; KK Roy; RJ Doerksen "Identification and characterization of allosteric site(s) for dihydrogambogic acid (DHGA) and trans- $\beta$ -caryophyllene (TBC) as cannabinoid CB2 allosteric modulators." 249th American Chemical Society National Meeting, Division of Computers in Chemistry, Denver, CO, Mar 22-26, 2015.

SE Slater; G. Fu; MA Nael; MA Avery; RJ Doerksen "Structure-based lead optimization of a novel glycogen synthase kinase 3 beta (GSK-3 $\beta$ ) inhibitor." 248th American Chemical Society National Meeting, Division of Computers in Chemistry, San Francisco, CA, Aug 10-14, 2014.

SE Slater; J Kollar; KK Roy; KM Elokely; C-H Lu; S Krishna; RJ Doerksen; MA Avery "Finding a more feasible mechanism of action for artemisinin." 41<sup>st</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 18, 2014.

P Pandey; KK Roy; H Liu; KM Elokely; S Pettaway; SJ Cutler; RJ Doerksen "Identification of cannabinoid CB1 ligands through structure-based virtual screening." 41<sup>st</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 18, 2014.

AE Wahba; P Sivaprakasam; RJ Doerksen; MT Hamann "Modification and replacement of the  $\beta$ -carboline moiety to optimize antimalarial efficacy and toxicity of manzamine alkaloids." 2<sup>nd</sup> Annual University of Mississippi Malaria Symposium 2014, Oxford, MS, Apr 24, 2014.

P Pandey; KK Roy; RY Patel; RJ Doerksen "Utilizing the ensemble docking method for ranking and selection of representative cannabinoid receptor type 2 (CB2) models." 2013 Southeast Regional NIH IDeA Meeting, Little Rock, AR, Nov 2013. **P Pandey won Best Graduate Student Central Nervous System Oral Presentation award.**

MA Nael; RAS Gordji; J Bae; S Jo; RJ Doerksen "Prediction of paclitaxel loading into polymeric nano-systems for drug delivery." 16th Mid-South Annual Engineering and Science Conference (MAESC 2013), University of Mississippi, Oct 2013.

RAS Gordji; M Nael; J Bae; S Jo; RJ Doerksen "Computational design of nanoparticles based on calculations of the optimal properties for drug delivery." 16th Mid-South Annual Engineering and Science Conference (MAESC 2013), University of Mississippi, Oct 2013.

J Bae; MA Nael; F Mahdi; Y-D Zhou; RJ Doerksen; S Jo "Optimization of redox-triggered polymer nanoparticles for drug delivery via computational approaches." 16th Mid-South Annual Engineering and Science Conference (MAESC 2013), University of Mississippi, Oct 2013.

MN Nael; J Bae; S Jo; RJ Doerksen "Study of a redox sensitive polymer for drug delivery." 40th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Little Rock, AR, May 2013.

KM Elokely; **P Pandey**, MB Jekabsons; RJ Doerksen "Computational modeling: Structural insights into

Bax binding to the voltage dependent anion channel 1 (VDAC1)." 40th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Little Rock, AR, May 2013. **P. Pandey won the Nobles-Sam Award for best oral presentation by a University of Mississippi Department of Medicinal Chemistry student.**

KM Elokely; RJ Doerksen "Computational workflow for Human African trypanosomiasis phosphodiesterase inhibitor identification." 245<sup>th</sup> American Chemical Society (ACS) National Meeting & Exposition, New Orleans, LA, Apr 2013. **Received Teach-Discover-Treat KNIME Award.**

Z Zhao; G Fu; S Liu; KM Elokely; RJ Doerksen; Y Chen; DE Wilkins "Drug activity prediction using Multiple Instance Learning via joint instance and feature selection." 10th Annual MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Meeting, Columbia, MO, Apr 2013.

A Chatterjee; RJ Doerksen; SJ Cutler; IA Khan; A Dasmahapatra; JS Williamson "Virtual screening, synthesis and biological evaluation of novel CDK-5 inhibitors to target Alzheimer's disease." 39th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2012.

KM Elokely; G Fu; RJ Doerksen "CDK2/GSK-3 $\beta$  selectivity study." 39th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2012.

G Fu; X Nan; H Liu; RY Patel; PR Daga; K Elokely; Y Chen; D Wilkins; RJ Doerksen "Multiple-instance learning (MIL): A framework to identify bioactive conformations." 9th Annual MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Meeting, Oxford, MS, Feb 2012.

S Liu; RY Patel; PR Daga; H Liu; G Fu; RJ Doerksen; Y Chen; D Wilkins "Multi-class joint rule extraction and feature selection for biological data." IEEE International Conference Bioinformatics & Biomedicine (BIBM 2011), Atlanta, GA, Nov 2011.

H Liu; RY Patel; DA Kevin; RJ Doerksen "Classification models for cannabinoid receptor-2 antagonists." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

G Fu; P Sivaprakasam; OR Dale; SP Manly; SJ Cutler; RJ Doerksen "Pharmacophore modeling, ensemble docking and virtual screening studies on glycogen synthase kinase-3 $\beta$ ." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

G Fu; S Liu; X Nan; Z Zhao; Y Chen; DE Wilkins; RJ Doerksen "Implementation of machine-learning algorithms for identification and development of novel GSK-3 $\beta$  inhibitors." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

H Liu; LA Walker; RJ Doerksen "Computational approaches to understand the methemoglobinemia caused by 8-aminoquinolines." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

H Liu; RJ Doerksen; LA Walker "DFT study on the radical anions formed by 8-aminoquinoline drugs." 94th Canadian Chemistry Conference and Exhibition (CSC2011), Montreal, Canada, Jun 2011.

H Liu; LA Walker; RJ Doerksen "The effect of a substituent at the 5-position on the methemoglobinemia caused by primaquine analogs." 4th Annual Mississippi Biophysical Consortium 2011 Annual Meeting, Oxford, MS, Jun 2011.

G Fu; S Liu; X Nan; Z Zhao; Y Chen; D Wilkins; RJ Doerksen "Hierarchical quantitative structure-activity relationship analysis and virtual screening studies on glycogen synthase kinase-3 $\beta$ ," 38th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Houston, TX, May 2011. **G. Fu won the Nobles-Sam Award for best oral presentation by a University of Mississippi Department of Medicinal Chemistry student.**

H Liu; LA Walker; RJ Doerksen "Computational study on the mechanism of methemoglobinemia caused by primaquine and its derivatives." 2011 Southeast Theoretical Chemistry Association (SETCA) Annual Meeting, Starkville, MS, May 2011.

X Nan; G Fu; Z Zhao; S Liu; RY Patel; H Liu; PR Daga; RJ Doerksen; X Dang; Y Chen; D Wilkins "Leveraging domain information to restructure biological prediction." 8th Annual MidSouth Computational Biology and Bioinformatics Society Meeting, College Station, TX, Apr 2011. X Nan received a travel award from the conference.

G Fu; Y Chen; DE Wilkins; RJ Doerksen "Implementation of machine-learning algorithms for identification and development of novel GSK-3 $\beta$  inhibitors." Mississippi NSF EPSCoR Student Retreat, Jackson, MS, Nov 2010.

H Liu; LA Walker; NPD Nanayakkara; RJ Doerksen "Methemoglobinemia caused by 8-aminoquinoline drugs: DFT calculations suggest an analogy to H<sub>4</sub>B's role in nitric oxide synthase." 240th ACS National Meeting & Exposition, Boston, MA, Division of Computers in Chemistry, Aug 2010.

G Fu; P Sivaprakasam; OR Dale; SP Manly; SJ Cutler; RJ Doerksen "Pharmacophore modeling, ensemble docking, and virtual screening studies on glycogen synthase kinase-3 $\beta$ ." 37th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2010.

AE Wahba; P Sivaprakasam; RJ Doerksen; AMS Mayer; MT Hamann "Replacement of the  $\beta$ -carboline moiety in manzamine alkaloids: Opening the door for generating manzamine-like analogs with lower or no toxicity." 37th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2010.

PR Daga; RJ Doerksen "Hepatitis B virus DNA polymerase inhibition: Computational insight into resistance development." 36th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2009.

S Prasanna; PR Daga; A Xie; RJ Doerksen "Protein modeling and virtual screening to discover novel GSK-3 inhibitors." 237th ACS National Meeting & Exposition, Salt Lake City, UT, Division of Computers in Chemistry, Mar 2009.

PR Daga; RJ Doerksen "Hepatitis B virus DNA polymerase inhibition: Computational insight into resistance development." 237th ACS National Meeting & Exposition, Salt Lake City, UT, Division of Computers in Chemistry, Mar 2009.

RJ Doerksen; P Sivaprakasam "Topological polar surface area: A useful descriptor in 2D-QSAR." 236th ACS National Meeting & Exposition, Philadelphia, PA, Division of Chemical Information, Aug 2008.

PR Daga; RJ Doerksen "Binding of spiroquinazolinones to phosphodiesterase-7: Insights from Molecular Electrostatic Potential." 35th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Little Rock, AK, May 2008. **PR Daga won the Nobles-Sam Award for best oral presentation by a University of Mississippi Department of Medicinal Chemistry student.**

AE Wahba; J Peng; P Sivaprakasam; S Odde; RJ Doerksen; MT Hamann "Regio-controlled nitration of manzamine A as intermediates for producing manzamine analogues with better docking scores with GSK-3 $\beta$ ." 235th ACS National Meeting & Exposition, New Orleans, LA, Division of Medicinal Chemistry, Apr 2008.

P Sivaprakasam; S Odde; A Xie; RJ Doerksen "Genetic algorithm-guided QSPR model for drug absorption." PharmForum 2007, American Association of Pharmaceutical Scientists 6<sup>th</sup> Annual Southern Regional Discussion Group, Memphis, TN, May 2007.

P Sivaprakasam; S Odde; A Xie; RJ Doerksen "First pharmacophore model and novel qsar models for antimalarial farnesyltransferase inhibitors." 34th Annual MALTO Medicinal Chemistry-Pharmacognosy

Meeting, Monroe, LA, May 2007. **P. Sivaprakasam won the Nobles-Sam Award for best oral presentation by a University of Mississippi Department of Medicinal Chemistry student.**

RJ Doerksen; S Odde; A Xie; R Mohamed; R Stanikunite; Z. Bie; MT Hamann; SA Ross "Absolute configuration of bioactive flexible natural products from DFT optical rotations based on Monte Carlo conformational search and ab initio geometries." Division of Physical Chemistry, 233rd American Chemical Society National Meeting, Chicago, IL, Mar 2007.

P Sivaprakasam; A Xie; RJ Doerksen "Pharmacophore model for antimalarial farnesyltransferase inhibition." 2007 Annual Meeting of the Mississippi Academy of Sciences in Starkville, MS, Feb 2007. **P Sivaprakasam won an award for best graduate student oral presentation in the Health Sciences division of the meeting for this talk.**

RJ Doerksen "Computational approaches to antimalarial drug targets." Antimalarial Consortium Meeting, Oxford, MS, Oct 2006.

S. R. Clark, A. Xie and R. J. Doerksen "3D-QSAR analysis of inhibitors of farnesyltransferase." 2006 Summer Research Institute for Undergraduates Research Symposium, University of Mississippi, University, MS, Jul 2006.

P. N. Tosso, P. Sivaprakasam and R. J. Doerksen "2D and 3D-QSAR analysis of Plasmodium falciparum dihydrofolate reductase inhibitors." 2006 Summer Research Institute for Undergraduates Research Symposium, University of Mississippi, University, MS, Jul 2006.

RJ Doerksen; B Chen; D Liu; WF DeGrado; ML Klein "Joint computational-experimental approach to effective and selective antimicrobial oligomers." Division of Computers in Chemistry: Interplay between computer modeling and experiments on complex biological systems, 227th American Chemical Society National Meeting, Anaheim, CA, Mar 2004.

RJ Doerksen; B Chen; J Yuan; JD Winkler; ML Klein "Novel conformationally-constrained 8-helical  $\beta$ -peptides." Division of Organic Chemistry: Proteins, Peptides, Amino Acids, and Nucleotides, 227th American Chemical Society National Meeting, Anaheim, CA, Mar 2004.

RJ Doerksen; B Chen; D Liu; WF DeGrado; ML Klein "Designed intramolecular hydrogen bonds stabilizing antimicrobial amphiphilic polymers." Polymer Division: Polymer Design Using Non-covalent Methods, 225th American Chemical Society (ACS) National Meeting, New Orleans, LA, Mar 2003.

RJ Doerksen; B Chen; WF DeGrado; ML Klein "Accurate energetics for in-plane vs out-of-plane phenol, thiophenol, anisole, and thioanisole." Division of Computers in Chemistry General Contributions: Quantum Chemistry, 225th ACS National Meeting, New Orleans, LA, Mar 2003.

D Liu; J Yuan; B Chen; RJ Doerksen; Sungwok Choi, ML Klein; JD Winkler; WF DeGrado "De novo design and synthesis of antimicrobial oligo-amino acid-salicylamide." Division of Medicinal Chemistry: General Oral Session, 225th ACS National Meeting, New Orleans, LA, Mar 2003.

B Chen; RJ Doerksen; ML Klein "Computational design of biomimetic materials." Applying Computational Chemistry and Molecular Simulations: Functionalities Session, American Institute of Chemical Engineers Annual Meeting, Indianapolis, IN, Nov 2002.

B Chen; RJ Doerksen; ML Klein "Computational design of biomimetic materials." Division of Computers in Chemistry General Session, 224th ACS National Meeting, Boston, MA, Aug 2002.

RJ Doerksen; N El-Bakali Kassimi; VJ Steeves; AJ Thakkar "Bond orders and polarizabilities as measures of aromaticity: Azines, azoles, oxazoles, and thiazoles." Conference on Chemical Bonding: State of the art in conceptual quantum chemistry, La Colle-sur-Loup, France, Jun 2000.

RJ Doerksen; N El-Bakali Kassimi; VJ Steeves; AJ Thakkar "Quantitative aromaticity scales derived

from accurate polarizabilities and bond orders.” 13<sup>th</sup> Annual Symposium on Chemical Physics, University of Waterloo, Waterloo, ON, Canada, Oct 1997.

RJ Doerksen; AJ Thakkar “Confrontation between theory and experiment for properties of aromatic molecules.” 12<sup>th</sup> Annual Symposium on Chemical Physics, University of Waterloo, Waterloo, ON, Canada, Nov 1996.

## OTHER TALKS

RJ Doerksen “Donald R. Cole Award for Excellence in Promoting Inclusiveness in Graduate Education.” Flash Talk at Council of Graduate Schools 2019 Summer Workshop and New Deans Institute, San Diego, CA, Jul 2019.

RJ Doerksen “Computational Medicinal Chemistry: Applications to Neuroscience.” 1st University of Mississippi Neuroscience Research Showcase, Apr. 2015.

RJ Doerksen “179 Seconds of Computational Medicinal Chemistry.” University of Mississippi Research Day, Apr. 2015.

RJ Doerksen “Computational approaches for discovery of novel cannabinoid receptor modulators.” Department of Medicinal Chemistry Seminar Series, University of Mississippi, University, MS, Nov 2013.

RJ Doerksen “Ligand-based and protein-structure based approaches to new cannabinoid receptor modulators.” Institute for Computational Molecular Science, Department of Chemistry, Temple University, Philadelphia, PA, Aug 2013.

RJ Doerksen “Project 4: Rational design and testing of novel cannabinoid ligands.” NIH COBRE CORE-NPN Annual Meeting, University of Mississippi, University, MS, May 2013.

**V Gadepalli**; P Pandey; I Muhammad; RJ Doerksen “Docking of Leonotis leonurus and Leonurus cardiaca derived compounds to cannabinoid receptors.” 2013 UM COBRE Summer Undergraduate Research Fellows Reports, Jul 2013.

## CONFERENCE POSTER DISCUSSIONS

S Chatterjee; P Pandey; RJ Doerksen; TDH Bugg; CL Stallings; S Roy “Structure-based virtual screening approach to identify novel MraY inhibitors for tuberculosis chemotherapy.” 46<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2019.

P Pandey; B Avula; IA Khan; S Khan; VJ Navarro; RJ Doerksen; AG Chittiboyina “Potential modulation by EGCG and its metabolites of human NAD[P]H-quinone oxidoreductase 1 (NQO1) – A systematic computational study.” 19<sup>th</sup> Annual Oxford International Conference on the Science of Botanicals, Oxford, MS, Apr 2019.

RJ Doerksen; P Pandey; S Chatterjee; C Stallings; S Roy “Hybrid virtual screening approach for the identification of novel MraY inhibitors for tuberculosis chemotherapy.” MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting, Birmingham, AL, Mar 2019.

AO Aderibigbe; P Pandey; RJ Doerksen “Computer-aided design of peripherally-restricted antagonists of the cannabinoid CB1 receptor.” 9<sup>th</sup> University of Mississippi Graduate Student Council Research Symposium, Mar 2019.

AO Aderibigbe; P Pandey; RJ Doerksen “Computer-aided design of peripherally-restricted antagonists of the cannabinoid CB1 receptor.” 5<sup>th</sup> University of Mississippi Neuroscience Research Showcase, Mar 2019.

AO Aderibigbe; P Pandey; RJ Doerksen “Computational design of peripherally-restricted cannabinoid (CB1) receptor 1 blockers.” Drug Discovery and Development Colloquium 2018 (DDDC 2018),

Lexington, KY, Jun 21-23, 2018.

Z UI Haq; P Pandey; RJ Doerksen "Comparison of experimental and theoretical crystal structure of CB1: A molecular dynamics perspective." Drug Discovery and Development Colloquium 2018 (DDDC 2018), Lexington, KY, Jun 21-23, 2018.

P Pandey; KK Roy; RJ Doerksen "Identification of potent natural product chemotypes as cannabinoid receptor 1 inverse agonists using protein structure-based virtual screening." 45<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, College Station, TX, May 2018. Pankaj won the Dr. Ronald F. Borne Memorial Postdoctoral Poster Award.

Z UI Haq; P Pandey; RJ Doerksen "Dynamics of active site residues: Comparison of experimental and theoretical crystal structure of CB1." 45<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, College Station, TX, May 2018.

P Pandey; KK Roy; RJ Doerksen "Negative allosteric modulators of the cannabinoid receptor 2: Protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist." 255<sup>th</sup> American Chemical Society National Meeting, Division of Computers in Chemistry, New Orleans, LA, Mar 2018.

P Pandey; AO Aderibigbe; KK Roy; **RJ Doerksen** "Active-state cannabinoid 1 (CB1) receptor: Protein modeling and comparison to recently published X-ray structures of the inactive-state and active-state CB1 receptors." 255<sup>th</sup> American Chemical Society National Meeting, Division of Medicinal Chemistry, New Orleans, LA, Mar 2018.

C Spencer; P Pandey; RJ Doerksen; M Godfrey. "A study of an active-state CB1 receptor model and JWH synthetic cannabinoids." American Academy of Forensic Sciences 70<sup>th</sup> Annual Scientific Meeting, Seattle, WA, Feb 2018.

P Pandey; AO Aderibigbe; KK Roy; RJ Doerksen "Homology modeling of the active-state cannabinoid 1 (CB1) receptor: Quality assessment model validation and comparison to recently published X-ray structures of the inactive-state and active-state CB1 receptors." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2017.

P Pandey; ND Chaurasiya; BL Tekwani; RJ Doerksen "Mechanism of action and inhibition kinetics of the endocannabinoid virodhamine and other eicosanoids on human monoamine oxidase (MAO) -A and -B." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2017.

AO Aderibigbe; P Pandey; RJ Doerksen "Structural features of peripherally acting CB1 receptor antagonists." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2017.

P Pandey; KK Roy; AO Aderibigbe; RJ Doerksen "Homology modeling of the active state cannabinoid 1 (CB1) receptor: Quality assessment, model validation and comparison to recently published x-ray structures of the inactive state CB1 receptor." 44<sup>th</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2017.

P Pandey; ND Chaurasiya; BL Tekwani; RJ Doerksen "Mechanism of action and inhibition kinetics of the endocannabinoid virodhamine and other eicosanoids on human monoamine oxidase (MAO) -A and -B." 17<sup>th</sup> Annual Oxford International Conference on the Science of Botanicals, Oxford, MS, Apr 2017.

C Spencer; KL Pettus; P Pandey; RJ Doerksen; M Godfrey "Study of an active-state CB1 receptor model and synthetic cannabinoid interactions." American Academy of Forensic Sciences 69<sup>th</sup> Annual Scientific Meeting, New Orleans, LA, Feb 13-18, 2017.

C Popescu; VK Shankar; P Pandey; ZG Cuny; A Vo; RJ Doerksen; SN Murthy "Indomethacin:  $\beta$ -Cyclodextrin complexation and characterization." American Association of Pharmaceutical Scientists,



Denver, CO, Nov 2016. Abstract No. 35W1000.

C Popescu; VK Shankar; P Pandey; ZG Cuny; A Vo; RJ Doerksen; SN Murthy "Piroxicam solubility enhancement by native and modified  $\beta$ -cyclodextrins." American Association of Pharmaceutical Scientists, Denver, CO, Nov 2016. Abstract No. 01T0400.

VK Shankar; P Pandey; ZG Cuny; RJ Doerksen; SN Murthy "Preparation and characterization of Captisol® enabled silymarin constituents: A phase solubility and molecular modeling approach." American Association of Pharmaceutical Scientists, Denver, CO, Nov 2016. Abstract No. 20R1130.

C Popescu; VK Shankar; P Pandey; ZG Cuny; A Vo; RJ Doerksen; SN Murthy "Inclusion complex of valsartan with cyclodextrin derivatives." American Association of Pharmaceutical Scientists, Denver, CO, Nov 2016. Abstract No. 02R1130.

Y Ding; H Liu; PB Fasinu; NPD Nanayakkara; IA Khan; BL Tekwani; LA Walker; RJ Doerksen "Hydroxylated metabolites of primaquine by cytochrome P450 2D6: Theoretical investigations of enantiomeric regioselectivity by density functional theory, docking, MM/GBSA and molecular dynamics simulations." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2016.

MA Nael; RJ Doerksen "Design of new inhibitors of the cyclin dependant kinase 5 (CDK5) for Alzheimer's disease." MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting, Memphis TN, Mar 2016.

MA Nael; RJ Doerksen "Optimization of RNA-like endoplasmic reticulum kinase (PERK) inhibitors: Thermodynamic calculations of the active site." Mississippi NSF EPSCoR Annual Research Day @ The Capitol, Jackson MS, Feb 2016.

MA Nael; RJ Doerksen "Virtual screening of new inhibitors of the protein kinase RNA-like endoplasmic reticulum kinase (PERK)." 2015 American Association of Pharmaceutical Scientist (AAPS) Annual Meeting and Exposition, Orlando FL (Oct 2015). **Manal received the 2015 AAPS Graduate Student Research Award in Drug Discovery and Development Interface, including \$1250.**

MA Nael; RJ Doerksen "Insights into optimal design of protein kinase inhibitors: Role of waters in the binding site." 24<sup>th</sup> National NSF (National Science Foundation) EPSCoR Conference, Portsmouth, NH, Oct 2015.

KK Roy; P Pandey; RJ Doerksen "Cannabinoid receptor modeling and molecular dynamics simulations." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2, 2015.

MA Nael; RJ Doerksen "Design of multiple-kinase inhibitors to manage Alzheimer's disease." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2, 2015.

P Pandey; KK Roy; RJ Doerksen "Search of potential allosteric site(s) in the cannabinoid CB2 receptor for the discovery of novel CB2 allosteric modulators." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2, 2015.

RJ Doerksen, KK Roy, MA Nael, P Pandey "Computational medicinal chemistry capabilities and accomplishments." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2, 2015.

J Bae; LE McNamara; MA Nael; F Mahdi; RJD; GL Bidwell; NI Hammer; S Jo "Nitroreductase-triggered activation of a novel caged fluorescent probe obtained from methylene blue." University of Mississippi School of Pharmacy Annual Poster Session, Oxford, MS, Oct 2, 2015.

EA Peralta; E Ferreira; M Nael; RJ Doerksen "Docking studies of manzamine A and manzamine 8-OH

in the Mycobacterium tuberculosis shikimate kinase.” Universidad La Salle Pharmacobiology Chemistry Program Poster Day, Mexico City, Mexico, Sep 2015.

MA Nael; RJ Doerksen “Design of new inhibitors of the protein kinase RNA-like endoplasmic reticulum kinase (PERK).” Drug Discovery and Development Colloquium 2015, Oxford, MS, Jun 2015.

MA Nael; RJ Doerksen “Binding of bryostatin 1 to the C1B domain of protein kinase C epsilon (PKC- $\epsilon$ ).” 8th Annual Mississippi Biophysical Consortium 2015 Annual Meeting, Oxford, MS, Jun 2015.

V Gadepalli; P Pandey; KK Roy; SA Ross; I Muhammad; RJ Doerksen “Docking studies on leonotis leonurus and leonurus cardiac derived compounds for their potential activity at CB1 and CB2.” University of Mississippi Medical Center Annual Neuroscience Research Day, May 2015.

KK Roy; P Pandey; RJ Doerksen “Utilizing multiple GPCR templates for modeling of cannabinoid CB1 and CB2 receptors in their active states.” University of Mississippi Medical Center Annual Neuroscience Research Day, May 2015.

MA Nael; RJ Doerksen “Targeting protein kinase C epsilon (PKC- $\epsilon$ ) to manage Alzheimer’s disease.” 42<sup>nd</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2015.

V Gadepalli; MA Nael; RJ Doerksen “3D analysis and selective targeting of ERK2/caspase-9 interaction for the development of probes to suppress caspase-9 activation.” 42<sup>nd</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2015.

P Pandey; KK Roy; H Liu; KM Elokely; S Pettaway; SJ Cutler; RJ Doerksen “Protein structure-based virtual screening: Identification of natural product-derived hits as cannabinoid receptor 1 modulators.” 1st University of Mississippi Neuroscience Research Showcase, Apr 2015. **Pankaj won 2<sup>nd</sup> prize in the general science category.**

P Pandey; KK Roy; RJ Doerksen “Protein structure-based virtual screening led to identification of novel natural product-derived hits as cannabinoid receptor 1 modulators.” 249th American Chemical Society National Meeting, Division of Computers in Chemistry, Denver, CO, Mar 2015. **Pankaj Pandey won a \$1,150 Chemical Computing Group Research Excellence Award in Medicinal Chemistry and a copy of CCG's MOE (Molecular Operating Environment) software with a one-year license.**

KK Roy; P Pandey; RJ Doerksen “Structural insights into the mechanism of activation of the human cannabinoid type 2 (CB2) receptor: Molecular dynamics study of an agonist-bound state.” 249th American Chemical Society National Meeting, Division of Computers in Chemistry, Denver, CO, Mar 2015.

SE Slater; KK Roy; J Kollar; MA Nael; KM Elokely; RJ Doerksen; MA Avery “Determining alternative artemisinin binding sites in PfSERCA.” MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Little Rock, AR, Mar 2015. **Shuneize Slater won First Place Graduate Student Biological Bioinformatics Poster Presentation.**

MA Nael; SE Slater; RJ Doerksen “Analysis of water molecules in the active site of the protein kinase RNA-like Endoplasmic Reticulum Kinase (PERK): Insights for lead optimization.” Southeastern Regional Meeting of the American Chemical Society (SERMACS) 2014, Nashville, TN, Nov 2014.

P Pandey; KK Roy; RJ Doerksen “Identification and characterization of allosteric site(s) for known CB2 allosteric modulators.” University of Mississippi School of Pharmacy Research Day, Nov 2014.

P Pandey; KK Roy; H Liu; KM Elokely; S Pettaway; SJ Cutler; RJ Doerksen “Novel natural product-derived hits as cannabinoid receptor modulators identified through protein structure-based virtual screening.” University of Mississippi School of Pharmacy Research Day, Nov 2014.

KK Roy; DA Colby; RJ Doerksen “Molecular insights into the orthosteric and allosteric modulation of the

$\gamma$ -aminobutyric acid type B (GABAB) receptor." University of Mississippi School of Pharmacy Research Day, Nov 2014.

KK Roy; AK Agarwal; AM Clark; RJ Doerksen "Computational insights into the protein-ligand interactions of a new antifungal natural product that inhibits the yeast heat shock protein 90 (Hsp90) chaperone." University of Mississippi School of Pharmacy Research Day, Nov 2014.

J Bae; MA Nael; L Jiang, PT Hwang, F Mahdi; HW Jun; WM Elshamy; YD Zhou; SN Murthy; RJ Doerksen; S Jo "Quinone propionic acid-based redox-sensitive polymer nanoparticles for controlled drug delivery." American Association of Pharmaceutical Scientist (AAPS) Annual Meeting and Exposition, San Diego, CA, Oct 2014.

SE Slater; J Kollar; KK Roy; C-H Lu; S Krishna; RJ Doerksen; MA Avery "Ferrous ion/PfATP6 dual requirement for antimalarial activity: Making strides towards understanding the MOA of artemisinin." 248<sup>th</sup> American Chemical Society National Meeting, San Francisco, CA, Division of Medicinal Chemistry, Aug 2014.

MA Nael; RJ Doerksen "Identification of natural products as inhibitors of the protein kinase RNA-like endoplasmic reticulum kinase to manage Alzheimer's disease." American Society of Pharmacognosy 2014 Annual Meeting, Oxford, MS, Aug 2014.

P Pandey; KK Roy; H Liu; KM Elokely; S Pettaway; SJ Cutler; RJ Doerksen "Search for cannabinoid receptor 1 antagonists using structure-based virtual screening: identification of natural product hits." American Society of Pharmacognosy 2014 Annual Meeting, Oxford, MS, Aug 2014.

MM Ghoneim; KM Elokely; AA El-Hela; AI Mohammad; RJ Doerksen; SJ Cutler; SA Ross "Computationally assisted assignment of highly strained isochromene nucleus." American Society of Pharmacognosy 2014 Annual Meeting, Oxford, MS, Aug 2014.

KK Roy; P Pandey; RJ Doerksen "Computational modeling and simulation of the human cannabinoid CB2 receptor." NIH, NIGMS Fifth Biennial National IDeA Symposium of Biomedical Research Excellence (NISBRE), Washington, DC, Jun 2014.

V Gadepalli; P Pandey; KK Roy; SA Ross; I Muhammad; RJ Doerksen "Docking studies on Leonotis leonurus and Leonurus cardiaca derived compounds for their potential activity at CB1 and CB2." 41<sup>st</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2014.

MA Nael; RJ Doerksen "Targeting protein kinase RNA-like endoplasmic reticulum kinase to manage Alzheimer's disease." 41<sup>st</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2014.

S Slater; G. Fu; M Nael; MA Avery; RJ Doerksen "Identification of novel phthalimide inhibitors of GSK-3B: A computational study." 41<sup>st</sup> Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2014.

Y Ding; H Liu; NPD Nanayakkara; IA Khan; BL Tekwani; LA Walker; RJ Doerksen "Some 8-aminoquinoline analogues and their derivatives: Theoretical evaluation of their potential hemotoxicity as antimalarial candidates." 2<sup>nd</sup> Annual University of Mississippi Malaria Symposium 2014, Oxford, MS, Apr 2014.

Y Ding; H Liu; NPD Nanayakkara; IA Khan; BL Tekwani; LA Walker; RJ Doerksen "Hydroxylated derivatives of 8-aminoquinolines: Theoretical Insights into feasibility of formation, regioselectivity, and potential toxicity." 2<sup>nd</sup> Annual University of Mississippi Malaria Symposium 2014, Oxford, MS, Apr 2014.

J Kollar; SE Slater; KK Roy; RJ Doerksen; MA Avery "Possible mechanism of action of artemisinins: SERCA hypothesis expanded." 2<sup>nd</sup> Annual University of Mississippi Malaria Symposium 2014, Oxford, MS, Apr 2014.

SE Slater; J Kollar; KK Roy; RJ Doerksen; MA Avery "The artemisinin argument: Basis for questioning the accepted mechanism." 2<sup>nd</sup> Annual University of Mississippi Malaria Symposium 2014, Oxford, MS, Apr 2014. **Shuneize Slater won 2<sup>nd</sup> place.**

S Slater; G Fu; MA Nael; MA Avery; RJ Doerksen "Development of novel phthalimide inhibitors of glycogen synthase kinase-3 beta (GSK-3 $\beta$ )." University of Mississippi Graduate Student Council Research Forum Poster Competition, Oxford, MS, Apr 2014. **Shuneize Slater won 2<sup>nd</sup> place.**

MA Nael; J Bae; RAS Gordji; S Jo; RJ Doerksen "Prediction of hydrophobic drug loading into polymeric micelles for drug delivery." Mississippi National Science Foundation (NSF) EPSCoR Annual Meeting, Starkville, MS, Mar 2014.

V Gadepalli; RJ Doerksen "3D analysis and selective targeting of ERK2/caspase-9 interaction for the development of probes to suppress caspase-9 activation." Mississippi National Science Foundation (NSF) EPSCoR Annual Meeting, Starkville, MS, Mar 2014.

LE Jobe; KM Elokely; RJ Doerksen "Computational analysis of water...2-aminopyrimidine hydrogen bonding interactions with protein kinase GSK-3 $\beta$ ." 247<sup>th</sup> American Chemical Society National Meeting, CHED: Division of Chemical Education, Dallas, TX, Mar 2014.

RJ Doerksen; AW Boler; KM Elokely; V Gadepalli; H Liu; HM Matalgah; MC Ott; P Pandey; RY Patel; KK Roy; M Yadav "Cannabinoid receptor 1 models for protein structure based drug design of antagonists." 2013 Southeast Regional NIH IDeA Meeting, Little Rock, AR, Nov 2013.

V Gadepalli; P Pandey; KK Roy; I Muhammad; RJ Doerksen "Docking studies on *Leonotis leonurus* and *Leonuris cardiaca* derived compounds for their potential activity at human cannabinoid receptor type 1 (CB1)." 2013 Southeast Regional NIH IDeA Meeting, Little Rock, AR, Nov 2013.

KK Roy; P Pandey; RJ Doerksen "Uncovering the characteristic features of active state three-dimensional (3D) structure of the human cannabinoid type 2 receptor." 2013 Southeast Regional NIH IDeA Meeting, Little Rock, AR, Nov 2013.

P Pandey; NN Mohammed; Z Rahman; MA Repka; RJ Doerksen "Modeling studies on inclusion complex of clotrimazole in 2-hydroxypropyl [beta] cyclodextrin." 2013 American Association of Pharmaceutical Scientists Annual Meeting and Exposition, San Antonio, TX, Nov 2013.

RJ Doerksen; KM Elokely; **LE Jobe** "Computational analysis of water...2-aminopyrimidine hydrogen bonding interactions with protein kinase GSK-3 beta." Southeast Regional Meeting of the American Chemical Society (SERMACS) 2013, Atlanta, GA, Nov 2013.

V Gadepalli; P Pandey; KK Roy; I Muhammad; RJ Doerksen "Docking studies on *Leonotis leonurus* and *Leonuris cardiaca* derived compounds for their potential activity at CB1." 17th Annual University of Mississippi School of Pharmacy National Center for Natural Products Research Poster Day, Nov 2013.

J Bae; MA Nael; F Mahdi; Y Zhou; RJ Doerksen; S Jo "Redox-responsive polymeric nanoparticles for cytotoxic drug delivery via computational approaches." 17th Annual University of Mississippi School of Pharmacy National Center for Natural Products Research Poster Day, Nov 2013.

J Oh; W Zou; MA Ibrahim; AG Chittiboyina; RJ Doerksen; D Ferreira; M Na; MT Hamann "Investigation on endangered plant species for the alleviation of human diseases." 17th Annual University of Mississippi School of Pharmacy National Center for Natural Products Research Poster Day, Nov 2013. **J Oh won 2nd Prize.**

V Gadepalli; P Pandey; KK Roy; I Muhammad; RJ Doerksen "Docking studies on *Leonotis leonurus* and *Leonuris cardiaca* derived compounds for their potential activity at CB1." University of Mississippi School of Pharmacy Rho Chi Poster Day, Oct 2013. **Veena Gadepalli won First Place.**

A Chatterjee; SJ Cutler; RJ Doerksen; IA Khan; JS Williamson "Identification of novel, selective CDK5/p25 inhibitor: Structure based virtual screening, synthesis and SAR studies." 246<sup>th</sup> American Chemical Society National Meeting & Exposition, Indianapolis, IN, Sep 2013.

KM Elokely; RJ Doerksen "Shape constraints to identify new CB1 antagonist hits." Gordon Research Conference: "Cannabinoid Function in the CNS: Cannabinoids in Synapses, Circuits and the Human Brain." Waterville Valley, NH, Aug 2013.

P Pandey; KK Roy; RY Patel; RJ Doerksen "Ensemble docking approach toward the identification of representative cannabinoid 2 (CB2) receptor conformations for structure-based virtual screening." Gordon Research Conference: "Cannabinoid Function in the CNS: Cannabinoids in Synapses, Circuits and the Human Brain." Waterville Valley, NH, Aug 2013.

KM Elokely; RJ Doerksen "Preparation and validation of 3D models for the CB1 receptor." Gordon Research Seminar: "Cannabinoid Function in the CNS: Endocannabinoids in Neurophysiology and Neuropathology." Waterville Valley, NH, Aug 2013.

P Pandey; KK Roy; RY Patel; RJ Doerksen "Ensemble docking approach toward the identification of representative cannabinoid 2 (CB2) receptor conformations for structure-based virtual screening." Gordon Research Seminar: "Cannabinoid Function in the CNS: Endocannabinoids in Neurophysiology and Neuropathology." Waterville Valley, NH, Aug 2013.

J Oh; JJ Bowling; Y Zou; AG Chittiboyina; RJ Doerksen; D Ferreira; TD Leininger; MT Hamann "Configurational assignments of conformationally restricted bis-monoterpene hydroquinones: Utility in exploration of endangered plants." American Society of Pharmacognosy 2013 Annual Meeting, St. Louis, MO, Jul 2013.

H Liu; RY Patel; **RJ Doerksen** "Structure of the cannabinoid receptor 1: Homology modeling and enrichment study based on CB1 antagonist docking." 23rd Annual International Cannabinoid Research Society Symposium on the Cannabinoids, Vancouver, BC, Canada, Jun 2013.

V Gadepalli; RJ Doerksen "Targeting interactions of ERK2 and caspase-9 to suppress caspase-9 activation." 40th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Little Rock, AR, May 2013.

KM Elokely; **P Pandey**; MB Jekabsons; RJ Doerksen "Insights into interactions of voltage dependent anion channel 1 (VDAC1) and Bax." Mississippi NSF EPSCoR Annual Meeting, Hattiesburg, MS, Apr 2013.

MN Nael; J Bae; S Jo; RJ Doerksen "Prediction of paclitaxel loading into amphiphilic block copolymers comprised of polyethylene glycol and redox-sensitive polyester with pendant trimethyl-locked quinone propionate." Mississippi NSF EPSCoR Annual Meeting, Hattiesburg, MS, Apr 2013.

J Bae; MA Nael; F Mahdi; Y-D Zhou; RJ Doerksen; S Jo "Optimization of trimethyl-lock quinone propionic acid-based redox-sensitive polymer nanoparticles for drug delivery application." Mississippi NSF EPSCoR Annual Meeting, Hattiesburg, MS, Apr 2013.

KM Elokely; G Fu; RJ Doerksen "Structural assessment for active and selective kinase inhibitors: GSK-3 $\beta$  and CDK2 case studies." 245th American Chemical Society National Meeting & Exposition, New Orleans, LA, Apr 2013.

MN Nael; J Bae; S Jo; RJ Doerksen "Modeling of trimethyl-locked quinone based polymers for drug delivery." SOP/NCNPR Annual Research Day, University of Mississippi, MS, Nov 2012.

KM Elokely; **P Pandey**; MB Jekabsons; RJ Doerksen "Insights into interactions of voltage dependent anion channel 1 (VDAC1) and Bax." SOP/NCNPR Annual Research Day, University of Mississippi, MS,

Nov 2012.

J Bae; MA Nael; RJ Doerksen; S Jo "Trimethyl-locked benzoquinone based polymeric nanoparticles for targeted drug delivery." American Association of Pharmaceutical Scientist (AAPS) Annual Meeting and Exposition, Chicago, IL, Oct 2012.

MA Albadry; KM Elokely; B Wang; JJ Bowling; MF Abdelwahab; MH Hossein; RJ Doerksen; MT Hamann "Computationally assisted assignment of kahalalide Y Configuration using an NMR-constrained conformational search." 38th Northeast Regional Meeting of the American Chemical Society, Rochester, NY, NERM-145, Sep 2012.

H Liu; RY Patel; **RJ Doerksen** "Structure of the cannabinoid receptor 1: Homology modeling and enrichment study." NIH, NIGMS Fourth Biennial National IDeA Symposium of Biomedical Research Excellence (NISBRE), Washington, DC, Jun 25-27, 2012.

J Bae; MA Nael; JM Anderson; RJ Doerksen; H-W Jun; S Jo "Novel redox-sensitive polymeric nanoparticles for targeted delivery of anti-cancer agents." 5th Annual Mississippi Biophysical Consortium Annual Meeting, Hattiesburg, MS, Jun 21-22, 2012.

J Oh; JJ Bowling; Y Zou; MR Jacob; AG Chittiboyina; RJ Doerksen; TD Leininger MT Hamann "New hydroquinone melissifolanes from *Lindera melissifolia* (Lauraceae)." 3rd Annual Conference American Council for Medicinally Active Plants (ACMAP), Jonesboro, AR, May 2012.

KM Elokely; RJ Doerksen "Understanding the structure of CDK2." 39th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2012.

P Pandey; K Elokely; MB Jekabsons; RJ Doerksen "Prediction of binding modes for the interaction of voltage dependent anion channel 1 (VDAC1) and Bax." 39th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2012.

KM Elokely; RJ Doerksen "Protein-ligand docking challenge: Is making the protein flexible worth it?" Symposium on Biomolecular Structure, Dynamics and Function, Memphis, TN, Apr 2012.

P Pandey; K Elokely; MB Jekabsons; RJ Doerksen "Insights into interactions of voltage dependent anion channel 1 (VDAC1) and Bax." University of Mississippi Graduate Student Council Poster Competition, Oxford, MS, Apr 2012.

G Fu; X Nan; RY Patel; PR Daga; H Liu; KM Elokely; Y Chen; D Wilkins; RJ Doerksen "Multiple-instance learning (MIL): A framework to identify bioactive conformations." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 2012.

J Bae; MA Nael; RJ Doerksen; S Jo "Redox-sensitive polymeric nanoparticles for targeted cancer drug delivery." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 2012.

KM Elokely; G Fu; RJ Doerksen "Comparative selectivity study of GSK-3 $\beta$  vs CDK2 inhibitors." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 2012.

MA Nael; J Bae; S Jo; RJ Doerksen "Modeling of trimethyl-locked quinone based polymers for drug delivery." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 2012.

P Pandey; K Elokely; MB Jekabsons; RJ Doerksen "Insights into interactions of voltage dependent anion channel 1 (VDAC1) and Bax." Mississippi NSF EPSCoR Annual Meeting, Oxford, MS, Apr 2012.

Y Ding; H Liu; RJ Doerksen; BL Tekwani; IA Khan; LA Walker "Hydroxylation derivatives of some 8-aminoquinoline compounds: Theoretical insights into their toxicity, feasibility, and regioselectivity." 12<sup>th</sup> Annual Oxford International Conference on the Science of Botanicals, Oxford, MS, Apr 2012.

G Fu; X Nan; RY Patel; PR Daga; H Liu; KM Elokely; Y Chen; DE Wilkins; RJ Doerksen "Multiple-instance learning (MIL): A framework to identify bioactive conformations." 243rd American Chemical Society National Meeting & Exposition, San Diego, CA, Mar 2012.

Z Zhao; G Fu; X Nan; S Liu; RJ Doerksen; Y Chen; D Wilkins "Co-training in classifying scientific data." 9th Annual MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Meeting, Oxford, MS, Feb 2012.

G Fu; H Liu; RJ Doerksen "Substrate binding mode and catalytic mechanism studies on human biliverdin IX $\alpha$  reductase." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

H Liu; RY Patel; DA Kevin; RJ Doerksen "Classification models for cannabinoid receptor-2 antagonists." 242nd American Chemical Society (ACS) National Meeting & Exposition, Denver, CO, USA, Aug-Sep 2011.

G Fu; H Liu; RJ Doerksen "Substrate binding mode and catalytic mechanism studies on human biliverdin IX $\alpha$  reductase." 4th Annual Mississippi Biophysical Consortium 2011 Annual Meeting, Oxford, MS, Jun 2011.

KM Elokely; RJ Doerksen "Systematic analysis of cyclin dependent kinase 2 (CDK2)." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 2011.

G Fu; S Liu; X Nan; Z Zhao; Y Chen; DE Wilkins; RJ Doerksen "Implementation of machine-learning algorithms for identification and development of novel GSK-3 $\beta$  inhibitors." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 2011.

X Nan; G Fu; Z Zhao; S Liu; RY Patel; H Liu; PR Daga; RJ Doerksen; X Dang; Y Chen; D Wilkins "Leveraging domain information to restructure biological prediction." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 2011.

S Liu; RY Patel; PR Daga; H Liu; G Fu; Y Chen; D Wilkins; RJ Doerksen "Joint rule extraction and feature selection for multi-class biological data." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 2011.

S Liu; Z Huang; N Wang; RJ Doerksen; Y Chen; D Wilkins "Improving glycan classification with TF/IDF weighting scheme." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Apr 2011.

G Fu; S Liu; X Nan; Y Chen; DE Wilkins; RJ Doerksen "Implementation of machine-learning algorithms for identification and development of novel GSK-3 $\beta$  inhibitors." University of Mississippi Graduate Student Council Poster Symposium & Research Day, Apr 2011. **Gang Fu won the award for best Pharmaceutical Sciences presentation.**

S Liu; Y Chen; D Wilkins; RJ Doerksen "Joint rule extraction and feature selection for multi-class biological data." 8th Annual MidSouth Computational Biology and Bioinformatics Society Meeting, College Station, TX, Apr 2011.

S Liu; Z Huang; N Wang; RJ Doerksen; Y Chen; D Wilkins "Improving glycan classification with TF/IDF weighting scheme." 8th Annual MidSouth Computational Biology and Bioinformatics Society Meeting, College Station, TX, Apr 2011.

DA Kevin; RY Patel; RJ Doerksen "Virtual screening evaluation of the MarinLit natural products database for cannabinoid receptor 2 (CB2) agonist-like features." 241st ACS National Meeting & Exposition, Anaheim, CA, Division of Computers in Chemistry, Mar 2011.

LDN Craine; RJ Doerksen; G Fu "Evaluation and comparison of 3D-QSAR CoMSIA/CoMFA models for CDK1, CDK5, and GSK-3 $\beta$  inhibition by paullones." 2010 Annual Biomedical Research Conference for

Minority Students (ABRCMS), Charlotte, NC, Nov 2010.

RJ Doerksen; RY Patel; PR Daga "Predictive models of activity and selectivity for CB1 antagonists and CB2 agonists." 2010 International Cannabinoid Research Society, Lund, Sweden, Jul 2010.

H Liu; LA Walker; NPD Nanayakkara; RJ Doerksen "Computational study on the methemoglobinemia caused by 8-aminoquinoline drugs." 37th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2010.

RY Patel; RJ Doerksen "Homology model based enrichment study of CB2 receptor agonists." 37th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Oxford, MS, May 2010.

G Fu; H Liu, PR Daga; RY Patel; RJ Doerksen "Molecular modeling provides insight into the catalytic mechanism of biliverdin reductase." Mississippi NSF EPSCoR Annual Meeting, Jackson, MS, Apr 2010.

PR Daga; F Dayan; SO Duke; RM Lee; PJ Tranel; RJ Doerksen "Computational approaches elucidate how a glycine deletion enables plant protoporphyrinogen oxidase to resist herbicides." Division of Agrochemicals, 238th ACS National Meeting, Washington, DC, Aug 2009.

P Sivaprakasam; PN Tosso; RJ Doerksen "Structure-activity relationship and comparative docking studies for cycloguanil analogs as PfDHFR-TS inhibitors." American Association of Colleges of Pharmacy, Boston, MA, Jul 2009.

OR Dale; A Eslinger; S Prasanna; AE Wahba; MT Hamann; RJ Doerksen; SJ Cutler; SP Manly "Development of the invitrogen Z'-Lyte™ kinase assay kit to screen natural products for GSK-3beta inhibition." 50th Anniversary Meeting of the American Society of Pharmacognosy, Honolulu, HI, Jun-Jul 2009.

PR Daga; RJ Doerksen "Hepatitis B virus DNA polymerase inhibition: Computational insight into resistance development." 36th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2009.

R Patel; RJ Doerksen "Affinity and selectivity of indirubin analogs for GSK-3β and CDK5: A molecular dynamics simulation study." 36th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2009.

G Fu; PR Daga; H Liu; RY Patel; RJ Doerksen "Molecular modeling provides insight to catalytic mechanism of biliverdin reductase." 36th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Memphis, TN, May 2009.

PR Daga; S Odde; MT Hamann; RJ Doerksen "Free energy calculations on the binding of natural latrunculins and semi-synthetic derivatives to G-actin." Mississippi NSF EPSCoR Annual State Meeting, Starkville, MS, Apr 2009.

RY Patel; RJ Doerksen "Affinity and selectivity of indirubin analogs for GSK-3β and CDK5: A molecular dynamics simulation study." Mississippi NSF EPSCoR Annual State Meeting, Starkville, MS, Apr 2009.

G Fu; PR Daga; RY Patel; RJ Doerksen "Binding free energy calculations for biliverdin-IXα reductase." Mississippi NSF EPSCoR Annual State Meeting, Starkville, MS, Apr 2009.

PR Daga; S Odde; MT Hamann; RJ Doerksen "Free energy calculations on the binding of natural latrunculins and semi-synthetic derivatives to G-actin." 9th Annual Oxford International Conference on the Science of Botanicals, Oxford, MS, Apr 2009.

PR Daga; S Odde; MT Hamann; RJ Doerksen "Free energy calculations on the binding of natural latrunculins and semi-synthetic derivatives to G-actin." NIH CoBRE CORE-NPN, External Advisory Board Meeting, University of Mississippi, MS, Mar 23-25, 2009.



PR Daga; S Odde; MT Hamann; RJ Doerksen "Molecular dynamics and free energy calculations explain decreased inhibition of G-actin by oxalatrunculin B and semisynthetic analogs of latrunculin B." 237th ACS National Meeting & Exposition, Salt Lake City, UT, Division of Computers in Chemistry, Mar 2009.

P Sivaprakasam; RJ Doerksen "Discovery of novel leads for antimalarial, antimicrobial and antileishmanial activities using ligand and structure based virtual screening." American Association of Pharmaceutical Scientists Annual Meeting, Atlanta, GA, Nov 2008.

PR Daga; S Prasanna; J Peng; A Place; MT Hamann; RJ Doerksen "Computational efforts to predict absolute configuration and protein-ligand interactions of marine natural products." Gordon Research Conference on Oceans & Human Health, Tilton NH, Jun-Jul 2008.

PR Daga; RJ Doerksen "Homology modeling, docking and molecular dynamics simulation of hepatitis B virus DNA polymerase." 35th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Little Rock, AK, May 2008.

P Sivaprakasam; MT Hamann; RJ Doerksen "Computational binding site analysis of GSK-3 $\beta$  for manzamine A: Docking, molecular dynamics, MM/PBSA binding free energy and alanine scanning studies." Mississippi NSF EPSCoR Annual State Meeting, Starkville, MS, Apr 2008.

PR Daga; RJ Doerksen "Homology modeling and molecular dynamics simulation of hepatitis B virus DNA polymerase: Validation using molecular docking." Mississippi NSF EPSCoR Annual State Meeting, Starkville, MS, Apr 2008.

P Sivaprakasam; MT Hamann; RJ Doerksen "Blind docking of manzamines into glycogen synthase kinase-3 $\beta$ ." 7th Annual Oxford International Conference on the Science of Botanicals & American Society of Pharmacognosy 4th Interim Meeting, University, MS, Apr 2008.

AE Wahba; J Peng; P Sivaprakasam; S Odde; RJ Doerksen; MT Hamann "Regio-controlled nitration of manzamine a as intermediates for producing manzamine analogues with better docking scores with GSK-3." 7th Annual Oxford International Conference on the Science of Botanicals & American Society of Pharmacognosy 4th Interim Meeting, University, MS, Apr 2008.

JJ Bowling; PR Daga; S Odde; SA Ahmed; MK Mesbah; DT Youssef; S. Kudrimoti; SI Khalifa; RJ Doerksen; MT Hamann "Actin-binding comparisons of the marine natural product latrunculin B with natural and semi-synthetic latrunculin B analogs." 7th Annual Oxford International Conference on the Science of Botanicals & American Society of Pharmacognosy 4th Interim Meeting, University, MS, Apr 2008.

PR Daga; JR Rimoldi; RJ Doerksen "Homology modeling of CYP2B6 and insights into mechanism-based inactivation of phenyl diaziridines." Sigma Xi Undergraduate/Graduate Student Poster Symposium, University of Mississippi, University, MS, Apr 2008.

P Sivaprakasam; MT Hamann; RJ Doerksen "Computational binding site analysis of GSK-3 $\beta$  for manzamine A: Docking, molecular dynamics, MM/PBSA binding free energy and alanine scanning studies." Sigma Xi Undergraduate/Graduate Student Poster Symposium, University of Mississippi, University, MS, Apr 2008.

PR Daga; RJ Doerksen "Homology modeling and molecular dynamics simulation of hepatitis B virus DNA polymerase: Validation using molecular docking." Division of Medicinal Chemistry: Poster Session, 235th American Chemical Society (ACS) National Meeting, New Orleans, LA, Apr 2008.

JJ Bowling; SA Ahmed; PR Daga; S Odde; MK Mesbah; DT Youssef; S. Kudrimoti; SI Khalifa; RJ Doerksen; MT Hamann "Actin-binding studies of new natural product oxalatrunculin B, latrunculin B, and two semi-synthetic analogs of the latrunculin class." Division of Biological Chemistry: Poster

Session, 235th American Chemical Society (ACS) National Meeting, New Orleans, LA, Apr 2008.

S Prasanna; PR Daga; S Clark; PN Tosso; A Xie; S Odde; JR Duan; RJ Doerksen "Computational investigations of protein-ligand interactions." Mississippi NSF EPSCoR First Annual Legislative Day, Jackson, MS, Mar 2008.

P Sivaprakasam; MT Hamann; RJ Doerksen "Computational binding site analysis of GSK-3 $\beta$  for manzamine A: Docking, molecular dynamics, MM/PBSA binding free energy and alanine scanning studies." NIH CoBRE CORE-NPN, External Advisory Board Meeting, University of Mississippi, MS, Mar 2008.

J Peng; A Place; W Yoshida; C Anklin; PR Daga; RJ Doerksen; MT Hamann "A structure for a 50 year old toxin from *Karlodinium* sp. A product of improvements in cryodual NMR techniques." Marine Natural Products Gordon Conference, Ventura, CA, Feb 2008.

S Prasanna; PR Daga; S Clark; PN Tosso; A Xie; S Odde; JR Duan; RJ Doerksen "Computational investigations of protein-ligand interactions." 2007 National EPSCoR Meeting, Hawaii, Nov 2007.

PR Daga; S Prasanna; A Xie; G Fu; S Odde; RJ Doerksen "Computational medicinal chemistry using MCSR." SC07 (Supercomputer Conference), (Poster presented by Mr. Jason Hale of Mississippi Center for Supercomputing Research.) Reno, NV, Nov 2007.

P Sivaprakasam; MT Hamann; RJ Doerksen "Manzamine A interaction with CDK5: Docking, molecular dynamics simulations and binding free energy calculations." 16th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2007.

PR Daga; JR Rimoldi; RJ Doerksen "Homology modeling of CYP2B6 and insights into mechanism-based inactivation of phenyl diaziridines." 16th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2007.

P Sivaprakasam; RJ Doerksen "Active site analysis of wild type PfDHFR-TS using docking and molecular dynamics." Mississippi Center for Supercomputing Research (MCSR) Research Symposium, University, MS, Sep 2007.

P Sivaprakasam; PN Tosso; RJ Doerksen "Computational insights into PfDHFR-TS: Application of 2D, 3D-QSAR and docking studies to cycloguanil derivatives." 34th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting, Monroe, LA, May 2007. **P. Sivaprakasam won the Lemke Award for best poster presentation.**

P Sivaprakasam; PR Daga; A Xie; RJ Doerksen "Targeting glycogen synthase kinase-3: A promising Alzheimer's disease target." NIH CoBRE CORE-NPN, External Advisory Board Meeting, University of Mississippi, MS, Apr 2007.

P Sivaprakasam; PR Daga; A Xie; RJ Doerksen "3D-QSAR and docking studies on 3-anilino-4-phenylmaleimides for glycogen synthase kinase-3 inhibition." Division of Medicinal Chemistry, 233rd American Chemical Society National Meeting, Chicago, IL, Mar 2007.

S Odde; P Sivaprakasam; RJ Doerksen "Docking and 3D-QSAR analysis of HCV NS5B RNA-dependent RNA polymerase inhibitors based on a common benzothiadiazine scaffold." Division of Medicinal Chemistry, 233rd American Chemical Society National Meeting, Chicago, IL, Mar 2007.

A Xie; S Odde; P Sivaprakasam; RJ Doerksen "Imidazole-containing farnesyltransferase inhibitors: 3D quantitative structure-activity relationship and molecular docking studies." Division of Medicinal Chemistry, 233rd American Chemical Society National Meeting, Chicago, IL, Mar 2007.

P Sivaprakasam; A Xie; PN Tosso; RJ Doerksen "Genetic function approximation insights into Plasmodium falciparum dihydrofolate reductase and farnesyltransferase inhibition." Division of

Computers in Chemistry, 233rd American Chemical Society National Meeting, Chicago, IL, Mar 2007.

PR Daga; RJ Doerksen "Is the acidity of the N1 proton in spiroquinazolinones important for PDE7 inhibitory activity?" Sigma Xi Undergraduate/Graduate Student Poster Symposium, University of Mississippi, University, MS, Mar 2007.

SR Clark; A Xie; RJ Doerksen "3D-QSAR analysis of farnesyltransferase inhibition for antimalarial diaminobenzophenones." 2007 Annual Meeting of the Mississippi Academy of Sciences in Starkville, MS, Feb 2007.

P Sivaprakasam; PR Daga; J Duan; S Odde; A Xie; RJ Doerksen "Innovations through computational science: Computational analysis of enzyme active sites." Mississippi NSF EPSCoR Annual Meeting, Starkville, MS, Feb 2007.

SR Clark; A Xie; RJ Doerksen "3D-QSAR analysis of farnesyltransferase inhibition for antimalarial diaminobenzophenones." Annual Biomedical Research Conference for Minority Students, Anaheim, CA, Nov 2006.

PR Daga; RJ Doerksen "Is the acidity of the N1 proton in spiroquinazolinones important for PDE7 inhibitory activity?" 15th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2006.

A Xie; SR Clark; RJ Doerksen "3D quantitative structure-farnesyltransferase inhibition analysis for some diaminobenzophenones." 15th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2006.

P Sivaprakasam; A Xie; RJ Doerksen "DFT studies on structurally diverse farnesyltransferase inhibitors: Multivariate analysis of correlation between physicochemical properties and antimalarial activity." 15th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2006.

A Xie; P Sivaprakasam; SR Clark; S Odde; RJ Doerksen "Computational approaches to antimalarial drug targets: Non-thiol farnesyltransferase inhibitors." Antimalarial Consortium Meeting, Oxford, MS, Oct 2006.

P Sivaprakasam; A Xie; PR Daga; PN Tosso; RJ Doerksen "Computational approaches to antimalarial drug targets: Glycogen synthase kinase-3 and dihydrofolate reductase." Antimalarial Consortium Meeting, Oxford, MS, Oct 2006.

SR Clark; A Xie; RJ Doerksen "3D-QSAR analysis of inhibitors of farnesyltransferase." Oral presentation. 2006 Summer Research Institute for Undergraduates Research Symposium, University of Mississippi, University, MS, Jul 2006.

PN Tosso; P Sivaprakasam; RJ Doerksen "2D and 3D-QSAR analysis of Plasmodium falciparum dihydrofolate reductase inhibitors." Oral presentation. 2006 Summer Research Institute for Undergraduates Research Symposium, University of Mississippi, University, MS, Jul 2006.

P Sivaprakasam; PR Daga; A Xie; RJ Doerksen "Physico-chemical and structural requirements among 3-anilino-4-arylmaleimides for GSK-3 inhibitory activity enhancement through 2D and 3D quantitative structure activity relationships (QSARs)." 2006 Sigma Xi Student Research Symposium Poster Competition, University of Mississippi, University, MS, Apr 2006.

AH Xie; P Sivaprakasam; RJ Doerksen "CoMFA studies of antimalarial compounds based on 2, 5-diaminobenzophenone scaffold." 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2005.

P Sivaprakasam; PR Daga; AH Xie; RJ Doerksen "Probing the physico-chemical and structural requirements among 3-anilino-4-arylmaleimides for GSK-3 $\alpha$  inhibitory activity enhancement through 2D

and 3D QSAR investigations.” 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, Nov 2005.

RJ Doerksen “Computational approach to the role of hydrogen bonds in controlling the conformation of antimicrobial oligomers.” Division of Physical Chemistry: Poster Session and Sci-Mix Poster Session, 229th American Chemical Society National Meeting, San Diego, CA, Mar 2005.

RJ Doerksen; B Chen; D Liu; WF DeGrado; ML Klein “Conformational analysis of the ring-N torsion of de novo antimicrobial arylamide polymers.” 14<sup>th</sup> Biennial Philadelphia Organic Chemists Club' Day, Philadelphia, PA, May 2003.

D Liu; B Chen; RJ Doerksen; ML Klein; WF DeGrado “De novo design and synthesis of nonhemolytic biomimetic antimicrobial polymers.” Division of Medicinal Chemistry: Poster Session, 225<sup>th</sup> American Chemical Society (ACS) National Meeting, New Orleans, LA, Mar 2003.

RJ Doerksen; ML Klein “Accurate torsions and conformations around amide bonds.” 14<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Ottawa, ON, Canada, Aug 2001.

RJ Doerksen; RI Kaiser; YT Lee; M Head-Gordon “Theoretical studies on the crossed beam reaction of C(<sup>3</sup>P<sub>j</sub>) with acetylene.” 16<sup>th</sup> Annual Symposium on Chemical Physics, University of Waterloo, Waterloo, ON, Canada, Nov 2000.

RJ Doerksen; M Head-Gordon; RI Kaiser; YT Lee “Trajectories on the potential energy surface of C(<sup>3</sup>P<sub>j</sub>) reacting with acetylene.” Division of Physical Chemistry, 219<sup>th</sup> ACS National Meeting, San Francisco, CA, Mar 2000.

RJ Doerksen; M Head-Gordon; RI Kaiser; YT Lee “Theoretical insight into the reaction of C(<sup>3</sup>P<sub>j</sub>) with acetylene: transition state structures of triplet C<sub>3</sub>H<sub>2</sub>, effects of deuteration, and dynamics of the reaction.” Pitzer Memorial Symposium on Theoretical Chemistry, Berkeley, CA, Jan 2000.

RJ Doerksen; AJ Thakkar “Novel heteroaromatic boron-nitrogen monocycles: geometries and stabilities.” Division of Physical Chemistry, 216<sup>th</sup> ACS National Meeting, Boston, MA, Aug 1998.

RJ Doerksen; AJ Thakkar “Electron-correlated polarizabilities of 87 five- and six-membered-ring azaboracycles.” 13<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Vancouver, BC, Canada, Aug 1998.

RJ Doerksen; AJ Thakkar “Additive models of polarizability for heteroaromatic ring molecules.” 36<sup>th</sup> Sanibel Symposium, St. Augustine, FL, Feb 1996.

RJ Doerksen; N El-Bakali Kassimi; AJ Thakkar “Ab initio computations and additive models for the polarizabilities of aromatic five-membered rings: azoles.” 12<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Fredericton, NB, Canada, Aug 1995.

N El-Bakali Kassimi; RJ Doerksen; AJ Thakkar “Oxazoles: ab initio structures, polarizabilities, and additive models.” 12<sup>th</sup> Canadian Symposium on Theoretical Chemistry, Fredericton, NB, Canada, Aug 1995.

RJ Doerksen; AJ Thakkar “Uncoupled Hartree-Fock calculations of polarizabilities of heteroaromatic molecules: azines and azoles.” Chemcon 94, Fredericton, NB, Canada, Jul 1994.

## RESEARCH GROUP MEMBERS

### Current:

Postdoctoral fellows:

Dr. Pankaj Pandey (7/2019-present); partial support (mainly working for NCNPR)

PhD students:

AyoOluwa Aderibigbe (8/2016-present)

## Visiting MS student:

Chiu-Wen Li (8-12/2019), National Pingtung University of Science & Technology,  
Department of Food Science, MS student

**Alumni:**

## PhD students:

Dr. Manal Nael (1/2012-5/2016) "Targeting protein kinases to manage or prevent Alzheimer's disease"  
Dr. Pankaj Pandey (8/2010-12/2015) "Protein-ligand interaction studies and Identification of new drug-like hits as cannabinoid receptor modulators"  
Dr. Shuneize Slater (12/2011-8/2015) "The discovery of novel inhibitors of plasmodium falciparum atpase-6 obtained from a mechanistic study of artemisinin"  
Dr. Khaled M. Elokely (1/2009-11/2013)  
Dr. Gang Fu (7/2007-5/2012)  
Dr. Pankaj Daga (8/2005-5/2010)  
Dr. Prasanna Sivaprakasam (12/2004-4/2009)  
Mohammed Baradwan (9/2009-8/2010) (left the program to assist family)

## Postdoctoral fellows:

Dr. Pankaj Pandey (2/2016-4/2019)  
Dr. Zaheer UI Haq (4/2018-8/2018)  
Dr. Kuldeep K. Roy (6/2013-4/2016)  
Dr. Mukesh Yadav (7/2013-10/2013)  
Dr. Haining Liu (3/2009-8/2012)  
Dr. Ronal Patel (7/2008-6/2010)  
Dr. Aihua Xie (1/2005-1/2009)  
Dr. Jinsong Duan (11/2005-4/2007)  
Dr. Srinivas Odde (3/2006-6/2007)

## PharmD student:

Emily Lewis (6/2016-8/2016)  
G. D. (Nick) Walker (6/2016-8/2016)  
Dr. Veena Gadepalli (6/2011-8/2011; 9/2012-6/2016)

## Visiting MS student:

Wei Chen Zhang (8-12/2018), National Pingtung University of Science & Technology,  
Department of Food Science, MS student  
Ming-Yi Cheng (1-6/2016), graduated 7/2016 from National Pingtung University of Science & Technology, Department of Food Science, International MS

## Undergraduate students:

Anthony Sumlin [Junior, Arkansas St. U] (5/2019-8/2019)  
E. Ross Hodges [Freshman, U. Mississippi] (3/2018-8/2018)  
Rachel Boone [Junior, U. Mississippi] (5/2018-8/2018)  
Colin Welsh [Junior, Rhodes College, Memphis, TN] (5/2018-8/2018)  
Genevieve Haltingen-Verville [Junior, U. Mississippi] (5/2017-8/2017)  
Kamesha Adams [Sophomore, LeMoyné-Owen College, Memphis, TN] (5/2017-8/2017)  
Rachel Kroeger [Sophomore, U. Mississippi] (5/2017-8/2017)  
Jennifer Gross [Senior, U. Mississippi] (6/2017-8/2017)  
Mukesh Ghimire [Sophomore, U. Mississippi] (5/2017-7/2017)  
Zachary Cuny [Junior, Mississippi State U] (5/2016-8/2016), NSF REU Student;  
Commenced PhD in Chemistry, University of Alabama Birmingham (Fall 2017)  
Ngoc Nguyen [Senior, U. Mississippi] (6/2015-5/2016), NIH Predoctoral Fellow, Commenced PhD in Chemistry, University of Utah (Fall 2016)  
A. Caleb Ezell [Junior, U. Mississippi] (5/2014-8/2015), NIH Predoctoral Fellow  
Ennia Ferreira [Junior, Western Institute of Technology and Higher Education (ITESO), Guadalajara, Mexico] (7/2015-8/2015)  
Estefanía Aburto [Senior, Universidad La Salle, Mexico City, Mexico] (7/2015-8/2015)  
Valerie Huang [Freshman, U. Southern California] (5/2015-8/2015), NSF REU Student  
Cameron Lee [Freshman, Samford U.] (5/2015-8/2015), NSF REU Student  
Completed REU program at Ohio State U in 2016; enrolled in Pharm.D. program at

Sanford U in Fall 2016

Ashlee J. Colbert [Sophomore, Florida A&M] (5/2014-8/2014), NSF REU student  
Current: Graduate student at Purdue University, Department of Biomedical Engineering

Michael C. Santana [Sophomore, Universidad Metropolitana Recinto de Cupey, Sistema Universitario Ana G. Méndez, San Juan, Puerto Rico] (5/2014-8/2014), NSF REU student

Trent M. Todd [Junior, U. Mississippi] (5/2014-8/2014), NIH Predoctoral Fellow [MS Georgetown U]

Dion Kevin [Senior/Professional Pharmacy, U. Mississippi] (7/2009-5/2014) [BSPS]

Haneen M. Matalgah [Freshman, U. Mississippi] (6/2013-1/2014)

Austin W. Boler [Freshman, U. Mississippi] (6/2013-5/2014)

Madeline C. Ott [Freshman, U. Mississippi] (6/2013-8/2013) [Pharm.D. student]

Roya Gordji [Freshman, U. Mississippi] (6/2013-8/2013) [MD student at UMMC]

Lance Ezell [Junior, U. Mississippi] (6/2013-8/2013) [Entered PhD program in Pharmaceutical Sciences]

Laura Beth Jobe [Junior, Erskine College] (5/2013-7/2013), NSF REU student

Present: M.D. student at University of South Carolina School of Medicine, Greenville, SC

Caleb Swain [Junior, Georgia Southern U.] (5/2013-7/2013), NSF REU student

Present: M.D. student at Mercer University School of Medicine, Atlanta, GA

LaVar Craine [Junior, Rust College] (6/2010-8/2010) [Works for Monsanto in Memphis TN]

Atreyi Dasmahapatra [Senior, St. Xavier's College, Calcutta, India] (6/2010-7/2010) [PhD program at University of Texas, Arlington, in Chemistry & Biochemistry]

Justin Deloach [Junior, Rust College] (6/2009-7/2009)

Kitae Myoung [Junior, U. Mississippi] (5/2007-7/2009) [Received MS in Computer Science from Georgia Tech; working in industry]

Sidney Govan [Sophomore, Rust College] (6/2008-8/2008)

David Borzik [Freshman, U. Mississippi] (5/2008-7/2008) [Graduated from UMMC MD program; resident at Johns Hopkins University]

Karthik Maddhi [Junior, Vellore Inst. Tech.] (5/2008-8/2008) [PhD]

Ronald Kim [Senior, U. Mississippi] (1/2008-5/2008) [Pharm.D.]

Robin Finnamore [Senior, U. Mississippi] (1/2007-5/2007) [High School teacher, MS]

Steven Bie [Freshman, U. of Toronto] (5/2006-8/2006) [After B.A., currently Associate Director at Goldenwise Capital Management, Toronto, Canada]

Perrer Tosso [Junior, Norfolk State U.] (6/2006-7/2006) [Received PhD from Georgetown Medical Center]

Shawna Clark [Junior, Tougaloo College] (6/2006-7/2006) [Now a dentist in Memphis, TN]

Instructors:

Charles T. Rich, Rust College (6/2008-8/2008; 6/2009-8/2009)

## AWARDS WON BY RESEARCH GROUP MEMBERS

AyoOluwa Aderibigbe

- MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Starkville, MS, Mar 29-31, 2018. AyoOluwa won an MCBIOS-JMP Young Scientist Excellence Award (Students: 2nd Place).
- 2018 Nobles-Sam Graduate Research Award from the Division of Medicinal Chemistry, University of Mississippi, bestowed on the student with the best podium presentation at the annual MALTO meeting (May 2018)
- Honor Society Memberships: Phi Kappa Phi (2018), Rho Chi (2018)

Dr. Pankaj Pandey

- Travel award by University of Chicago for attending workshop on NSF- Multiscale Theory and Simulation, Chicago, IL, Jun 2012
- 2013 Nobles-Sam Graduate Research Award from the Department of Medicinal Chemistry, University of Mississippi, bestowed on the student with the best podium presentation at the annual MALTO meeting (May 2013)
- NIH Predoctoral Fellow 2013 "Virtual Screening of the ZINC Natural Products Database for

Rational Discovery of Anti-Alzheimer's Disease Agents" sponsored by the Center of Research Excellence in Natural Products Neuroscience (CORE-NPN), The University of Mississippi (Oct 2013)

- Best Graduate Student Central Nervous System Oral Presentation at the 2013 Southeast Regional IDeA Meeting, Little Rock, AR (Nov 2013)
- Who's Who for The University of Mississippi 2013-2014
- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2014-2015)
- \$1,150 Chemical Computing Group Research Excellence Award in Medicinal Chemistry Student Travel Award Stipend for the 2015 Spring American Chemical Society National Meeting (Mar 2015)
- 2014/2015 ACS Graduate Research Award from the Olemiss Local Section and the Department of Chemistry and Biochemistry (Apr 2015)
- 2<sup>nd</sup> place in the Applied Neuroscience poster section of the Neuroscience Research Showcase, The University of Mississippi (Apr 2015)
- 2015 Nobles-Sam Graduate Research Award from the Division of Medicinal Chemistry, University of Mississippi, bestowed on the student with the best podium presentation at the annual MALTO meeting (May 2015)
- Graduate School Dissertation Fellowship (Fall 2015)
- First Place at the MCBIOS XII (Midsouth Computational Biology & Bioinformatics Society), Postdoctoral Oral Presentation, Memphis, TN (Mar 2016)
- MCBIOS-JMP Young Scientist Excellence Award (Postdoctoral Fellows: Honorable Mention) at the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Starkville MS, Mar 2018
- Ronald F. Borne Outstanding Postdoctoral Poster Presentation Award at the 45th Annual MALTO Meeting, College Station TX, May 2018
- Honor Society Memberships: Phi Kappa Phi (2012), Rho Chi (2012)

#### Dr. Shuneize Slater

- NIH Predoctoral Fellow, Center for Biomedical Research Excellence (COBRE) in Natural Products Neuroscience (2011)
- Second Place Winner in the Graduate School Forum Annual Poster Session (Apr 2014)
- Second Place Winner in the Annual Malaria Day Poster Session (Apr 2014)
- First Place at the MCBIOS XII (Midsouth Computational Biology & Bioinformatics Society), Poster Presentation in Biological Bioinformatics, Little Rock, AR (Mar 2015)
- Graduate School Dissertation Fellowship (Spring 2015)
- Honor Society Membership: Phi Kappa Phi (2010), Rho Chi (2014)

#### Dr. Manal Nael

- Thomas L. Lemke Outstanding Poster Presentation Award for best poster, Forty-First Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting in-Miniature, Memphis, TN, May 2014.
- Selected to represent MS NSF EPSCoR Comp Chem in the 2015 National NSF EPSCoR meeting, Portsmouth NH (Nov 2015)
- Graduate Student Council (GSC) Research Award (2015-2016)
- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2015-2016)
- Graduate School Dissertation Fellowship (Spring 2016)
- Honor Society Membership: Phi Kappa Phi (2013), Rho Chi (2014), Golden Key (2015), Gamma Beta Phi (2015)

#### Dr. Veena Gadepalli (Pharm.D. student, 2011-2016)

- 1st place poster presentation, Rho Chi Research Day, University of Mississippi School of Pharmacy, 9/2013
- University of Mississippi Luckyday Scholar (8/2008-5/2012)
- UM Department of Medicinal Chemistry Distinguished Citation for Outstanding Contributions

to the Research Mission of Medicinal Chemistry, 2012-2013

- UM Department of BioMolecular Sciences Distinguished Citation for Outstanding Contributions to the Research Mission of the Department, 2013-2014; 2014-2015; 2015-2016
- Honor Society Membership: Gamma Beta Phi (4/2009-5/2012); Alpha Lambda Delta (4/2009-5/2012); National Society of Collegiate Scholars (8/2008-5/2012); Delta Phi Alpha (National German Honor Society) (2/2010-5/2012)

Dion Kevin (Pharm.D. student, 2009-2013)

- UM University of Mississippi School of Pharmacy Student Research Fellowship 2011-2012
- UM Department of Medicinal Chemistry Distinguished Citation for Outstanding Contributions to the Research Mission of Medicinal Chemistry, 2009-2010, 2010-2011, 2011-2012

Dr. Khaled Elokely

- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2012-2013)
- Teach-Discover-Treat KNIME Award to attend American Chemical Society 245th Meeting, K. M. Elokely, R. J. Doerksen, "Structure-based drug design for trypanosomal PDEB1", Apr 2013
- Honor Society Membership: Rho Chi (2011)

Dr. Gang Fu (8/2007–5/2012)

- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2011-2012)
- 2011 Nobles-Sam Graduate Research Award from the Department of Medicinal Chemistry, University of Mississippi, bestowed on the student with the best podium presentation at the annual MALTO meeting (May 2011)
- 2011 Graduate Student Research Award presented by the Ole Miss Local Section of the American Chemical Society (April 2011)
- Graduate School Council Annual Research Day Prize for Best Research in Pharmaceutical Sciences, The University of Mississippi (April 11, 2011)
- Graduate School Council research grant by The University of Mississippi (2010-2011)
- NIH Predoctoral Fellow 2008 "Virtual Screening of the ZINC Natural Products Database for Rational Discovery of Anti-Alzheimer's Disease Agents" sponsored by the Center of Research Excellence in Natural Products Neuroscience (CORE-NPN), The University of Mississippi (October 2009)
- Honor Society Membership: Rho Chi (2010)

Dr. Pankaj Daga (8/2005–5/2010)

- Travel award by NRBSC/Pittsburgh Supercomputer Center, Pittsburgh, PA for attending the workshop "Methods and Applications of Hybrid QM/MM Simulations to Biomolecular systems" (Sep 2007)
- Nobles-Sam Graduate Student Research Award for best graduate student oral presentation by a University of Mississippi, Department of Medicinal Chemistry PhD student at the 2008 MALTO Medicinal Chemistry / Pharmacognosy Meeting, Little Rock, AR (May 2008)
- Travel award by Office of Research and Sponsored Programs, The University of Mississippi, for attending the "Gordon Research Conference: Oceans and Human Health" (June 2008)
- NIH Predoctoral Fellow 2008 "Novel Approaches Towards Neurodegenerative Diseases: Design of Semi-Synthetic Latrunculin B Analogs" sponsored by the Center of Research Excellence in Natural Products Neuroscience (CORE-NPN), The University of Mississippi (Oct 2008)
- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2008-2009)
- Graduate School Council research grant by The University of Mississippi (2008-2009)
- Certificate for Honorable Mention, Graduate Student Poster Competition at 8th Annual Oxford International Conference on the Science of Botanicals, Oxford MS (Apr 2009)



- ACS Graduate Student Travel Grant, by American Chemical Society, AGRO division, for presenting the poster at 238th ACS National Meeting, Washington, DC (Aug 2009)
- NIH Predoctoral Fellow 2009 “Predictive Statistical Models for CB2 Receptor agonists Using Machine Learning Methods and Their Use in Drug Design” sponsored by the Center of Research Excellence in Natural Products Neuroscience (CORE-NPN), The University of Mississippi (Oct 2009)
- Honor Society Membership: Phi Kappa Phi (2006), Rho Chi (2008)

Dr. Prasanna Sivaprakasam (12/2004–4/2009)

- UM Graduate Student Achievement Award (1 of only 2 for University of Mississippi, School of Pharmacy) (2007-2008)
- The American Society of Pharmacognosy (ASP) 2008 Student Poster Award for poster presentation at 7th International Conference on Science and Botanicals-4th Interim ASP meeting held from April 30th - May 3rd 2008 at the University of Mississippi
- 2007 Natural Products Neuroscience Fellow, The Center of Research Excellence in Natural Products Neuroscience (CORE-NPN), The University of Mississippi
- First place graduate student oral presentation in the Health Sciences division, 2007 Annual Meeting of the Mississippi Academy of Sciences, Starkville, MS, February 21-23
- Thomas L. Lemke Outstanding Poster Presentation Award for best poster, Thirty-Fourth Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting in-Miniature, Monroe, LA, May 20-22, 2007.
- Selected as only student to represent the state of Mississippi to present a poster at the NSF EPSCoR National Meeting, November 2007, Hawaii.
- Graduate Research Award/Nobles-Sam Award, for the best MALTO presentation by a University of Mississippi Department of Medicinal Chemistry Graduate Student at the annual MALTO conference (May 2007) for the year 2006-2007
- Poster award at the 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, November 2005.
- Honor Society Membership: Rho Chi (2008)

## TEACHING

As a member of the Advisory Board for the University of Mississippi Center for Excellence in Teaching and Learning, I wrote an article entitled “Bonus! Encouraging student attendance of department seminars” for the February 2014 newsletter eMantle.

### Courses:

For the following if the number of lectures is not noted then I was the instructor of record and taught for the whole semester (~14 weeks); if the number of lectures is noted then I was not the instructor of record unless also noted.

Fall 2004

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design (3 credit hour graduate course)

MEDC 503. Medicinal Chemistry Research Methodology (3 credit hour graduate course), 1 lecture

Spring 2005

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design (3 credit hour graduate course)

Fall 2005

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design

MEDC 503. Medicinal Chemistry Research Methodology, 1 lecture

MEDC 541. Problems in Medicinal Chemistry: Advanced Computational Methods for Medicinal Chemistry (3 credit hour graduate course)

MEDC 543. Seminar on Current Medicinal Chemistry Topics (1 credit hour graduate course)

MEDC 643. Seminar on Current Pharmaceutical Topics (1 credit hour graduate course)

Spring 2006

MEDC 544. Seminar on Current Medicinal Chemistry Topics

MEDC 644. Seminar on Current Pharmaceutical Topics

Fall 2006

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 4 lectures

MEDC 501. Advanced Medicinal Chemistry I, 4 lectures

MEDC 543. Seminar on Current Medicinal Chemistry Topics

MEDC 643. Seminar on Current Pharmaceutical Topics

Spring 2007

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design

MEDC 544. Seminar on Current Medicinal Chemistry Topics

MEDC 644. Seminar on Current Pharmaceutical Topics

MEDC 417. Medicinal Chemistry of Therapeutic Agents II, 3 lectures

MEDC 502. Advanced Medicinal Chemistry II, 3 lectures

Fall 2007

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 11 lectures

MEDC 501. Advanced Medicinal Chemistry I, 11 lectures

Spring 2008

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design

MEDC 417. Medicinal Chemistry of Therapeutic Agents II, 4 lectures. Instructor of Record

MEDC 502. Advanced Medicinal Chemistry II, 4 lectures. Instructor of Record

Fall 2008

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 11 lectures

MEDC 501. Advanced Medicinal Chemistry I, 11 lectures

MEDC 503. Medicinal Chemistry Research Methodology, 1 lecture

Spring 2009

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design

MEDC 417. Medicinal Chemistry of Therapeutic Agents II, 3 lectures. Instructor of Record

MEDC 502. Advanced Medicinal Chemistry II, 3 lectures. Instructor of Record

Fall 2009

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 23 lectures

MEDC 501. Advanced Medicinal Chemistry I, 23 lectures

Fall 2010

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 26 lectures

MEDC 501. Advanced Medicinal Chemistry I, 26 lectures

Spring 2011

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design.

Fall 2011

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 24 lectures. Instructor of Record

MEDC 501. Advanced Medicinal Chemistry I, 24 lectures. Instructor of Record

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design

Fall 2012

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 24 lectures. Instructor of Record

MEDC 543. Seminar on Current Medicinal Chemistry Topics

MEDC 643. Seminar on Current Pharmaceutical Topics

Spring 2013

MEDC 612. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design

Fall 2013

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, 21 lectures

MEDC 501. Advanced Medicinal Chemistry I, 21 lectures

MEDC 611. Drug Action and Design I. Introduction to Computer-Aided Ligand Design

MEDC 543. Seminar on Current Medicinal Chemistry Topics

MEDC 643. Seminar on Current Pharmaceutical Topics

Fall 2014

MEDC 416. Medicinal Chemistry of Therapeutic Agents I. (whole course)

Spring 2015

MEDC 712. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design

CHEM 351. Individual Research. (1 undergraduate student enrolled.) Instructor of Record: Prof. C. Hussey

Fall 2015

MEDC 416. Medicinal Chemistry of Therapeutic Agents I, ~33 lectures. Instructor of record

MEDC 501. Advanced Medicinal Chemistry I, ~33 lectures. Instructor of record

CHEM 351. Individual Research. (1 undergraduate student enrolled.) Instructor of Record: Prof. C. Hussey

Spring 2016

MEDC 711. Drug Action and Design I. Introduction to Computer-Aided Ligand Design.

CHEM 351. Individual Research. (1 undergraduate student enrolled.) Instructor of Record: Prof. C. Hussey

BISC 533. Advanced Neuroscience. (1 lecture) Instructor of Record: Prof. Lainy Day

BISC 579 / SCI 582. Bioinformatics (4 hours, lectures/lab) Instructor of Record: Profs. Erik Hom, Dawn Wilkins, and Yixin Chen

Fall 2016

MEDC 319. Computer-Aided Structure Based Drug Design (CADD): Database Screening and de novo Design of Potential Drug Molecules. (professional pharmacy elective course). (2 credit hours)

MEDC 416. Medicinal Chemistry of Therapeutic Agents I. (whole course).

MEDC 501. Advanced Medicinal Chemistry I. (whole course).

MEDC 541. Special Topics in Medicinal Chemistry. Computer-Aided Structure Based Drug Design (CADD): Database Screening and de novo Design of Potential Drug Molecules.

Spring 2017

MEDC 712. Drug Action and Design II. Quantitative Structure-Activity Relationships in Drug Design.

Fall 2017

MEDC 319. Computer-Aided Structure Based Drug Design (CADD): Database Screening and de novo Design of Potential Drug Molecules. (professional pharmacy elective course). (2 credit hours)

MEDC 416. Medicinal Chemistry of Therapeutic Agents I. (whole course).

MEDC 501. Advanced Medicinal Chemistry I. (whole course).

### Theses and Dissertations

- \* Ibrahim Almarabi, Pharmacognosy (Ikhlas A. Khan, supervisor), MS thesis in progress
- \* Kimberley Poland, Chemistry & Biochemistry (Steven R. Davis, supervisor), PhD dissertation in progress
- \* Amna Adam, Medicinal Chemistry (David A. Colby, supervisor), PhD dissertation in progress
- \* AyoOluwa Aberibigbe, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation in progress
- \* Alexandra Baumann, Chemistry & Biochemistry (Gregory S. Tschumper, supervisor), PhD dissertation in progress
- \* Caroline Spencer, Chemistry & Biochemistry (Murrell Godfrey, supervisor), PhD completed, 2019.

- \* Abidah Parveen, Pharmacognosy (Ikhlas A. Khan, supervisor), PhD dissertation completed, 2019.
- \* Manal Alhusban, Pharmacognosy (Ikhlas A. Khan, supervisor), PhD dissertation completed, 2019.
- \* Katelyn Dreux, Chemistry & Biochemistry (Gregory S. Tschumper, supervisor), PhD dissertation completed, 2019.
- \* Sarah Johnson, Chemistry & Biochemistry (Gregory S. Tschumper, supervisor), PhD dissertation completed, 2019.
- \* Thomas Ellington, Chemistry & Biochemistry (Gregory S. Tschumper, supervisor), PhD dissertation completed, 2018.
- \* Michael Cunningham, Medicinal Chemistry (John M. Rimoldi, supervisor), PhD dissertation completed, 2018.
- \* Vedanjali Gogineni, Medicinal Chemistry (John M. Rimoldi, supervisor), PhD dissertation completed, 2017.
- \* Harshul Batra, Pharmacology (Tracy Brooks, supervisor), PhD dissertation completed, 2017.
- \* Lianyi Fan, Chemistry & Biochemistry (Susan D. Pedigo, supervisor), MS thesis completed, 2016.
- \* Kyoshin J. Choo, Computer & Information Science (Byunghyun Jang, supervisor), PhD dissertation completed, 2016.
- \* Manal Nael, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2016.
- \* J. Coleman Howard, Chemistry (Gregory S. Tschumper, supervisor), PhD dissertation completed, 2015.
- \* Pankaj Pandey, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2015.
- \* Shuneize Slater, Medicinal Chemistry (Robert J. Doerksen and Mitchell A. Avery, co-supervisors), PhD dissertation completed, 2015.
- \* Bei Cao, Chemistry & Biochemistry (T. Keith Hollis, supervisor), PhD dissertation not completed.
- \* Eric Van Dornshuld, Chemistry & Biochemistry (Gregory S. Tschumper, supervisor), PhD dissertation completed, 2014.
- \* Sheng Liu, Computer & Information Science (Yixin Chen, supervisor), PhD dissertation completed, 2014.
- \* Khaled Elokely, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2013.
- \* David Watson, Medicinal Chemistry (Christopher R. McCurdy, supervisor), PhD dissertation completed, 2013.
- \* Arindam Chatterjee, Medicinal Chemistry (Stephen J. Cutler and John S. Williamson, co-supervisors), PhD dissertation completed, 2013.
- \* Shana Stoddard, Chemistry & Biochemistry (Randy M. Wadkins, supervisor), PhD dissertation completed, 2013.
- \* Gang Fu, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2012.
- \* Ahmed Idris, Medicinal Chemistry (John S. Williamson, supervisor), MS thesis completed, 2012.
- \* Falgun Shah, Medicinal Chemistry (Mitchell A. Avery, supervisor), PhD dissertation completed, 2011.
- \* Mohamed Helal, Medicinal Chemistry (Mitchell A. Avery, supervisor), PhD dissertation completed, 2010.
- \* Pankaj R. Daga, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2010.
- \* Tammy Nolan, Medicinal Chemistry (Christopher R. McCurdy, supervisor), PhD dissertation completed, 2010.
- \* Sivaprakasam Prasanna, Medicinal Chemistry (Robert J. Doerksen, supervisor), PhD dissertation completed, 2009.
- \* S. Anand, Medicinal Chemistry (John M. Rimoldi, supervisor), PhD dissertation completed, 2008.
- \* Neha Vyas Philip, Medicinal Chemistry (Christopher R. McCurdy, supervisor), PhD dissertation completed, 2007.
- \* Nakul Telang, Medicinal Chemistry (Mitchell A. Avery, supervisor), PhD dissertation completed, 2007.
- \* Ashok Philip, Medicinal Chemistry (Christopher R. McCurdy, supervisor), PhD dissertation completed, 2006.
- \* Cassia Mizuno, Medicinal Chemistry (Mitchell A. Avery, supervisor), PhD dissertation completed, 2006.

#### Honors Theses

- \* Kalee Sigworth (Nathan Hammer, supervisor; Robert J. Doerksen second reader), "Raman spectroscopy of THC and CBD", thesis in progress, 9/2019-present.
- \* Marissa Teske (Murrell Godfrey, supervisor; Robert J. Doerksen second reader), "Fentanyl and derivatives and their interactions with the opioid receptors", thesis completed, 2019.
- \* Reba Chamblee (Murrell Godfrey, supervisor; Robert J. Doerksen second reader), "Kratom alkaloids and their interactions with the opioid receptors", thesis completed, 2019.
- \* Carly Rock (Greg Tschumper, supervisor; Robert J. Doerksen third reader), "Fentanyl and derivatives and their interactions with the opioid receptors", thesis completed, 2019.
- \* Carolyn Rader (Greg Tschumper, supervisor; Robert J. Doerksen third reader), "Benchmark structures and harmonic vibrational frequencies for hydrated halide ions:  $X^-(H_2O)_n$ ,  $X = F, Cl, Br$  and  $I$  (where  $n = 1 - 4$ )", thesis completed, 2019.
- \* Lyncyn L. R. Reliquias (Murrell Godfrey and Robert J. Doerksen, co-supervisors) "A study of the hydrophobic interactions between twenty-three CB1 selective JWH compounds with an active-state CB1 receptor model to

discover key structural features of the JWH compounds and key protein residues of the CB1 receptor”, thesis completed, 2017.

\* Kelsey Pettus (Murrell Godfrey and Robert J. Doerksen, co-supervisors), thesis completed, 2016.

### ORP (Original Research Proposal) Committees

\* Santu Singha (Asok Dasmahapatra, supervisor), 2016.

### Invited Teaching Presentations

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jun 2019.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jul 2018.

\* RJ Doerksen “Docking of small molecules to proteins: A method for rational drug discovery.” STEMS-REU Summer Program, University, MS, Jul 2018.

\* RJ Doerksen “Computational medicinal chemistry.” 4<sup>th</sup> Virtual Winter School of Computational Chemistry, 1/31-2/2/2018.

\* RJ Doerksen “Rational drug design.” STEMS-REU Summer Program, University, MS, Jul 2017.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jul 2017.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jun 2016.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jul 2015.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jul 2014.

\* RJ Doerksen “An introduction to computational medicinal chemistry.” Mississippi PChem/REU Summer Program, University, MS, Jun 2013.

\* RJ Doerksen “Computational medicinal chemistry approaches for understanding protein-ligand interactions.” Rust College, Holly Springs, MS, Mar 4, 2009.

\* RJ Doerksen “Computational medicinal chemistry approaches for understanding protein-ligand interactions.” Rust College, Holly Springs, MS, Oct 22, 2008.

\* RJ Doerksen “Teaching computational medicinal chemistry using modern MCSR supercomputers.” Mississippi Center for Supercomputing Research (MCSR) Research Symposium, University, MS, Sep 6-7, 2007.

### Leader of Conference Roundtable Discussions

\* RJ Doerksen “Pharmacy school admission criteria: What approach do you take?” as part of the morning Roundtable Discussions, American Association of Colleges of Pharmacy Annual Meeting, National Harbor, MD, Jul 2015.

\* RJ Doerksen “Motivating pharmacy students to attend, learn from and enjoy pharmaceutical science research seminars” as part of the morning Roundtable Discussions, American Association of Colleges of Pharmacy Annual Meeting, San Antonio, TX, Jul 2011.

\* RJ Doerksen “Molecular modeling assignments to aid professional pharmacy students' learning acquisition” as part of the morning Roundtable Discussions, American Association of Colleges of Pharmacy Annual Meeting, Seattle, WA, Jul 2010.

\* RJ Doerksen “School/College of pharmacy personal computer requirements for professional pharmacy students: necessary and/or advisable in 2009?” as part of the morning Roundtable Discussions, American Association of Colleges of Pharmacy Annual Meeting, Boston, MA, Jul 2009.

## SERVICE

### University-Wide Service

- Graduate Council, a University Standing Committee, Facilitator and Ex officio member  
12/2017-Present
- Search Committee for Dean of the Graduate School  
2-10/2018
- Reviewer for Graduate Student Council Grant Proposals  
4/2017

- Faculty Senate 5/2009-8/2013; 3/2015-8/2016
  - Faculty Senate Executive Committee 9/2015-8/2016
  - Faculty Senate Faculty Governance of Academic Policy Committee 8/2011-7/2012; 8/2015-8/2016
    - Chair 9/2015-8/2016
    - Faculty Senate General Academic Affairs Committee 8/2012-8/2013
    - Faculty Senate Academic Support Affairs Committee 8/2009-7/2011
- Instructional Technology Committee, a University Standing Committee 2007-2010; 2011-2012; 2015-8/2016
- Member, Faculty for Undergraduate Neuroscience Minor 3/2015-Present
- Judge for 3MT (3-Minute Thesis) Competition for UM Graduate Students 10/2015
- Advisory Board for the Center of Excellence in Teaching and Learning 8/2012-7/2015
- Undergraduate Council, a University Standing Committee 8/2012-7/2015
- Search Committee for Senior International Officer and Executive Director of the Office of Global Engagement, University of Mississippi 9/2013-2/2014
- Artist Series Committee, a University Standing Committee 2012-2013
- Dual and Second Degree Policy Task Force 11/2012-3/2013
- Library Council, a University Standing Committee 2011-2013

### School of Pharmacy Service

- American Association of Colleges of Pharmacy (AACP) Delegate for UM School of Pharmacy (2017-2018)
- American Association of Colleges of Pharmacy (AACP) Alternate Delegate for UM School of Pharmacy (2016-2017)
- Graduate Program Coordinator, Division of Medicinal Chemistry (1/2017-11/2017)
- Faculty Council (2015-2017); vice-chair (1-8/2017); chair (8-11/2017)
- Scholastic Standards (2007-2017); vice-chair (2007-2013;7-11/2017); chair (2013-6/2017)
- Division of Medicinal Chemistry Faculty Search Committee (2017); hired Prof. Sudeshna Roy
- Division of Pharmacognosy Faculty Search Committee (2016-2017); chair; hired Prof. Vitor Pomin
- Honors, Awards, and Commencement Committee (2004-2005; 2011-2016)
- Division of Medicinal Chemistry Faculty Search Committee (2015-2016); hired Prof. Hoang V. Le
- SOP Conduct Council Investigation (re. potential violation of Student Honor Code) (Dec 2015)
- SOP Conduct Council Review (re. violation of Student Honor Code) (Apr 2015)
- Information, Resources and Computing Committee (2005-2014); vice-chair (2006-2007); chair (2007-2009)
- School of Pharmacy Strategic Planning: Students Subcommittee for ACPE (Accreditation Council for Pharmacy Education) Self-Study conducted to prepare for reaccreditation (2006-2007; 2010-2012)
- School of Pharmacy Associate Dean of Academic Affairs Search Committee (2013); hired Prof. David Gregory
- Department of Medicinal Chemistry Faculty Search Committee (2012-2013); hired Prof. David A. Colby
- Department of Medicinal Chemistry Chair Search Committee (2005-2006); hired Prof. Stephen J. Cutler
- Facilities Subcommittee (ACPE Accreditation) (2004-2006)
- Instructional Technology and Computing Committee (2004-2005)

### Service to Students

- Faculty advisor to a Pharmacy student association, Christian Pharmacists Fellowship International, U. Mississippi chapter, founded Fall 2005 (2005-Present)
- Faculty advisor to a Pharmacy student association, American Association of Pharmaceutical Scientists, U. Mississippi student chapter (2010-2016)
- APhA Auction Participant (Feb 2015, Feb 2016, Mar 2017)
- Taste Contest Judge, SOP Relay for Life, 2<sup>nd</sup> Annual Taste of Relay (Mar 2016)

### Local/Regional Service to Profession

- MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Board of Directors (Mar 2018-Present)
- Conference of Southern Graduate Schools (CSGS) Faculty Awards Committee (May 2018-Present)
- Conference of Southern Graduate Schools (CSGS) Membership Committee (Feb 2018-Present)
- For the Drug Discovery and Development Colloquium 2019 (DDDC 2019), Little Rock, AR, Jun 2019.
  - Dr. Doerksen was a judge in the poster competition for graduate students
  - Dr. Doerksen was a judge in the podium presentation competition for graduate students
  - Dr. Doerksen was a panel member in the career panel for graduate students
- For the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting, Birmingham, AL in Mar 2019.
  - Dr. Doerksen was a session chair
  - Dr. Doerksen was a judge in the poster competition for graduate students
- For the Drug Discovery and Development Colloquium 2018 (DDDC 2018), Lexington, KY, Jun 2018, Dr. Doerksen was a judge in the poster competition for graduate students.
- For the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Starkville, MS in March 29-31, 2018.
  - Dr. Doerksen was a session chair
  - Dr. Doerksen was a judge in the poster competition for graduate students
- For the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Memphis, TN in March 3-5, 2016.
  - Dr. Doerksen was a judge in the oral presentation competition for graduate students
  - Dr. Doerksen was a judge in the poster competition for graduate students
- For the MidSouth Computational Biology and Bioinformatics Society (MCBIOS) Annual Meeting in Little Rock, AR in March 6-7, 2015.
  - Dr. Doerksen co-chaired an oral session
  - Dr. Doerksen was a judge in the oral presentation competition for undergraduate students
  - Dr. Doerksen was a judge in the poster competition for graduate students
- For the 2013 Southeast Regional National Institutes of Health (NIH) IDeA (Institutional Development Award) Meeting (Nov. 15-17) in Arkansas
  - Dr. Doerksen hosted a Breakfast Topic Table on Chemoinformatics
  - Dr. Doerksen co-chaired an oral session on the Central Nervous System
  - Dr. Doerksen was a judge in the oral presentation competition for undergraduate students
  - Dr. Doerksen was a judge in the poster competition for graduate students
- Ad-hoc Reviewer for NSF MS EPSCoR Seed Grant (Apr 2014)
- Internal Review for NSF Major Research Infrastructure Award competition, University of Mississippi (Dec 2014)
- Mississippi State Science & Engineering Fair Judge, Apr 2016, Oxford, MS
- Mississippi Region VII Science & Engineering Fair Judge, Feb 2016, Oxford, MS (high school)
- Mississippi Region VII Science & Engineering Fair Best of Fair Judge, Mar 2015, Oxford, MS (high school)
- Mississippi Region VII Science & Engineering Fair Judge, Apr 2015, Oxford, MS (elementary)
- Mississippi Region VII Science & Engineering Fair Best of Fair Judge, Mar 2013, Oxford, MS (high school)
- Mississippi Region VII Science & Engineering Fair Judge, Mar 2013, Oxford, MS (elementary)
- Steering Committee member for Mississippi NSF EPSCoR (12/2010-4/2012)
- Mississippi Region VII Science & Engineering Fair Judge, Mar 2011, Oxford, MS (high school)
- Mississippi Region VII Science & Engineering Fair Judge, Mar 2011, Oxford, MS (elementary)
- Mississippi Region VII Science & Engineering Fair Judge, Mar 2010, Oxford, MS (high school)
- Mississippi Region VII Science & Engineering Fair Judge, Mar 2010, Oxford, MS (elementary)
- Internal reviewer for Seed Grants for Mississippi NSF EPSCoR program, Jackson, MS, Dec 2009
- Mississippi State Science & Engineering Fair Judge, Spring 2008, Oxford, MS

## National/International Service to Profession

### Grant Review

#### *NIH Grant Review*

- Program Evaluation of NIH Peer Review Processes: The Role of Anonymization (Apr-Jul 2018)
- NIH ZRG1 BCMB-G (10) B Drug Discovery & Development SBIR/STTR Review Panel (Mar 2017)

- NIH MSFD (Macromolecular Structure and Function D) Study Section (Feb 2016)
- NIH Small Business: Biological Chemistry, Biophysics and Drug Discovery SBIR/STTR study section ZRG1 IMST-G (10) B (Jun 2015)
- NIH Small Business: Biological Chemistry, Biophysics and Drug Discovery SBIR/STTR study section ZRG1 IMST-G (10) B (Nov 2014)
- NIH National Cancer Institute (NCI) Special Emphasis Panel/Scientific Review Group 2012/01 ZCA1 SRLB-V (J1) R meeting (Nov 2011)

#### *DoD Grant Review*

- Department of Defense Congressionally Directed Medical Research Programs (CDMRP) peer review panel of the 2018 Peer Reviewed Medical Research Program (PRMRP), Reston VA (Nov, 2018)
- Department of Defense Medical Research and Material Command (MRMC) Medical Infectious Diseases Research Program (MIDRP) (Jan 2018)
- Department of Defense Congressionally Directed Medical Research Programs (CDMRP) Pre-Application peer review panel of the 2017 Peer Reviewed Medical Research Program (PRMRP) for Investigator Initiated Research Awards (IIRA) and Technology/Therapeutic Development Awards (TTDA) (Jul-Aug 2017)

#### *Other Grant Review*

- Wellcome Trust / DBT India Alliance (partnership between The Wellcome Trust, UK, and the Government of India) Early Career Fellowship Application (Mar 2018)
- AACP NIP (New Investigator Program) Review (Sep 2015)
- Ad-hoc Reviewer for ACS Petroleum Research Fund (2013-2014; 2014-2015)
- External reviewer for Louisiana Board of Regents' Pilot Funding for New Research (Pfund) program (12/2011)
- Ad-hoc Reviewer for National Science Foundation (2010)
- External reviewer for City University of New York Research Award (2009)
- Discovery Grant Application Referee for Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery Grant (2005)

#### *Peer Review of Publications*

- Journal Article Referee for **64 journals**, including: *Proceedings of the National Academy of Sciences of the United States of America*, *Journal of Medicinal Chemistry*, *Nature Protocols*, *Chemical Reviews*, *Protein Journal*, *Cancer*, *Journal of Biological Chemistry*, *Organic Letters*, *Journal of Organic Chemistry*, *Marine Drugs*, *Acta Pharmacologica Sinica*, *Journal of Computational Chemistry*, *Accounts of Chemical Research*, *Current Pharmaceutical Design*, *Journal of Functional Foods*, *Evidence-Based Complementary and Alternative Medicine*, *Expert Opinion on Drug Discovery*, *Biochemistry*, *Biochemical Pharmacology*, *Journal of Molecular Biology*, *Journal of Chemical Information & Modeling*, *Current Topics in Medicinal Chemistry*, *European Journal of Medicinal Chemistry*, *Bioorganic & Medicinal Chemistry*, *Bioorganic & Medicinal Chemistry Letters*, *Journal of Physical Chemistry*, *Journal of Pharmacy and Pharmacology*, *Journal of Natural Products*, *Natural Product Research*, *Chemical Physics Letters*, *Molecules*, *Structural Chemistry*, *Journal of Molecular Structure: THEOCHEM*, *Journal of Molecular Structure*, *Letters in Drug Design*, *Journal of Biomolecular Structure & Dynamics*, *International Journal of Molecular Sciences*, *Journal of Enzyme Inhibition & Medicinal Chemistry*, *Computational and Theoretical Chemistry*, *Theoretical Chemistry Accounts*, *Journal of Computational Chemistry*, *Journal of Theoretical and Computational Chemistry*, *Drug Discovery Today*, *SAR QSAR Environmental Research*, *Medicinal Chemistry Research*, *Perspectives in Medicinal Chemistry*, *Future Medicinal Chemistry*, *Pharmaceutical Research*, *Canadian Journal of Chemistry*, *Journal of Saudi Chemical Society*, *Biologia*, *PLOS Computational Biology*, *Computational Biology and Chemistry*, *Molecular Informatics*, *Journal of Molecular Graphics & Modeling*, *Currents in Pharmacy Teaching and Learning*, *Combinatorial Chemistry & High Throughput Screening*, *International Journal of Biological Macromolecules*, *Kuwait Journal of Science*, *Computers in Biology and Medicine*, *Scientific Reports*, *Tetrahedron*, *RSC Advances* and *Organometallics* (**185 manuscripts reviewed**, 286 review opportunities declined, 2006-2019)

#### *Other Review*

- Guest Associate Editor, Proceedings of MCBIOS 2018, *BMC Bioinformatics* (2018)
- Guest Editor, "Allosteric Modulators" *Molecules* (2017 Impact Factor 3.1), submission deadline Jan 2020



- Member of two Master's and three PhD Thesis examining committees for students for National Pingtung University of Science and Technology, Department of Food Science (Jun 2017)
- AACP 2017 National Meeting Poster Peer Review (Biological Sciences Section) (Mar 2017)
- External (foreign) examiner for PhD Dissertation from National Institute of Pharmaceutical Education & Research (NIPER), Nagar, Punjab, India by S. Abbat entitled 'Pharmacoinformatics Analysis of PfDHFR Substrate and Inhibitors' (2016-2017)
- National Cheng Kung University External Reviewer for new faculty applicants (Mar 2017)
- Member of several Master's Thesis examining committees for MS students of National Pingtung University of Science and Technology, Department of Food Science and Department of Biological Science and Technology (Jun 2014)
- External (foreign) examiner for a PhD Dissertation in Pharmacy from Birla Institute of Technology, Mesra (Ranchi, India) (2013)
- Reviewed a medicinal chemistry textbook proposal for John Wiley & Sons, Inc., 2010
- External (foreign) examiner for a PhD Dissertation in Pharmacy from Birla Institute of Technology, Mesra (Ranchi, India) by J. Venkatesan entitled 'Design, synthesis and pharmacological screening of mycobactin analogues' (2010)
- External (foreign) examiner for PhD Dissertation from National Institute of Pharmaceutical Education & Research (NIPER), Nagar, Punjab, India (2008)
- External (foreign) examiner for a PhD Dissertation in Pharmacy from Birla Institute of Technology, Ranchi, India for S. Vadivalen entitled 'Computer-aided design, synthesis and receptor binding studies for the discovery of potential PPAR ligands' (2008)

#### *Other Service*

- American Association of Colleges of Pharmacy Teachers of Chemistry Section Programming Committee (8/2018-7/2019)
- American Association of Colleges of Pharmacy Council of Sections Task Force for National Meeting Student Poster Competition Program (8/2017-Present; Co-Chair 7/2018-Present)
- American Association of Colleges of Pharmacy National Meeting Mentor (Jul 2015)
- Co-organizer of "Understanding molecular properties and interactions: A symposium in honour of Ajit Thakkar's 60th birthday" for the 94th Canadian Chemistry Conference and Exhibition (CSC2011), Montreal, Canada (Jun 2011)
- Intel International Science & Engineering Fair Grand Judge, Los Angeles, CA (May 2011)
- Session Chair, "Quantum chemistry. The quantum and physical worlds meet." 237th ACS National Meeting, Division of Computers in Chemistry, Salt Lake City, UT (Mar 2009)
- Session Chair, "Molecular Mechanics. General Oral Session." 236th ACS National Meeting, Division of Computers in Chemistry, Philadelphia, PA (Aug 2008)
- Co-organizer of Michael Klein 65th Birthday Symposium, 229th ACS National Meeting, Division of Computers in Chemistry, San Diego, CA (Mar 2005)
- Consultant for Medacorp and Round Table Group

## **MEMBERSHIPS**

- Council of Graduate Schools
- Council of Southern Graduate Schools
- American Chemical Society, Divisions of:
  - Medicinal Chemistry
  - Physical Chemistry
  - Computers in Chemistry
  - Chemical Information
- American Association of Colleges of Pharmacy
- American Association of Pharmaceutical Sciences (2010-2016)
- Mississippi Biophysical Consortium
- Rho Chi
- Phi Lambda Sigma
- Round Table Group
- University of Mississippi Big Data Research Constellation (2017-2019)