Curriculum Vitae

Chenglong Li
(January 2024)

Research Focus

Dr. Li's scholarly interests range from organic chemistry, biochemistry, medicinal chemistry, chemical biology to physical chemistry, computational chemistry, molecular biophysics and pharmacology. His research focuses on molecular recognition, with a strong application to structure-based computer-aided drug design. He combines molecular simulation, artificial intelligence, synthetic chemistry, X-ray protein crystallography, cryo-EM (electron microscopy), thermodynamic measurements, cellular techniques and (in collaboration) *in vivo* animal models to explore molecular interactions, especially protein-ligand interactions at molecular, cellular and organismal levels. His current working projects include both computational method development and drug design applications, for example: 1) pioneering development of a novel Multiple Ligand Simultaneous Docking (MLSD) strategy, with great potential for Fragment-Based Drug Design (FBDD); 2) development of AI-based deep learning models for molecular design (*Elion* platform); 3) design and discovery of drugs targeting the cytokine IL-6/STAT3 autoimmune, inflammatory and oncogenic pathway for targeted therapy; 4) design and discovery of drugs targeting epigenetic histone arginine methylation enzymes, especially PRMT5 with both active site and protein-protein interface inhibition; 5) design and discovery of drugs targeting specific nAChR and GPCR subtypes for drug addiction and neurodegenerative diseases; 6) design and discovery of "chemical chaperone" drugs targeting ΔF508 NBD1 misfolding intermediates for potential cystic fibrosis therapy; 7) design and discovery of drugs targeting the YAP/TEAD transcriptional machinery in the Hippo signaling pathway, etc.

- h-index (Google Scholar): 63

Contact and Personal Information

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Google: https://scholar.google.com/citations?user=cpPZNU0AAAAJ&hl=en&oi=ao
Date of Birth: April 24, 1965

Education

Ph.D. in Biophysics with minor in Organic Chemistry, Cornell University, Ithaca, New York, USA, 2000
M.Sc. in Physical Chemistry, Beijing University, Beijing, China, 1988
B.Sc. in Chemistry, Beijing University, Beijing, China, 1985

Current Position

Florida Preeminence Scholar and Nicholas Bodor Professorship in Drug Discovery, University of Florida, Gainesville, FL 32610, August 1, 2016 - present.

Associate Director, the Center for Natural Products, Drug Discovery and Development (CNPD3), College of Pharmacy, University of Florida, Gainesville, FL 32610, August 20, 2019 – present.

Director, the NIH/NIGMS Chemistry-Biology Interface T32 Predoctoral Training Program at the University of Florida, July 1, 2020 – present.

Investigator, UFHealth Cancer Center, August 1, 2016 – present.

Graduate Faculty Positions

Medicinal Chemistry	College of Pharmacy
Biophysics	College of Liberal Arts and Sciences
Biochemistry	College of Medicine

Adjunct Positions

Changjiang Scholar, Ministry of Education, China, July 2018 – June 2021
Visiting Professor, Xi'an Jiaotong University, Xi'an, China. May 1, 2018 – April 30, 2019
Adjunct Professor, The Ohio State University, Columbus, OH, August 1, 2016 – December 31, 2018
Adjunct Professor, Hong Kong Baptist University, Hong Kong. May 1, 2014 – April 30, 2017
Guest Professor, Wenzhou Medical University, Wenzhou, China. October 1, 2014 – September 30, 2017
Guest Professor, University of Science and Technology of China (USTC), Hefei, China. August 1, 2012 – July 31, 2017

Previous Positions

Full Professor with Tenure in Medicinal Chemistry, College of Pharmacy, The Ohio State University, Columbus, OH, June 2016 – July 2016.

Associate Professor with Tenure in Medicinal Chemistry, College of Pharmacy, The Ohio State University, Columbus, OH, 2011 – 2016.

Tenure-track Assistant Professor in Medicinal Chemistry, College of Pharmacy, the Ohio State University, Columbus, OH, 2005 – 2011.

Research Associate in computational chemistry, The Scripps Research Institute (TSRI), La Jolla, California, 2002-2005.

Postdoc in structural biology, the Burnham Institute, La Jolla, California, 2000-2002.

Research Associate in molecular biophysics, the Institute of Biophysics, Chinese Academy of Sciences, Beijing, China, 1988-1990.

Previous OSU Graduate Faculty Positions

Medicinal Chemistry	College of Pharmacy
Chemical Physics	College of Arts and Sciences
Biophysics	College of Arts and Sciences
Biochemistry	College of Arts and Sciences
Biomedical Engineering	College of Engineering

Other Previous OSU Research Positions

Translational Therapeutics	The Ohio State University Comprehensive Cancer Center (OSUCCC)
Disease-modifying Therapies	The Ohio State Neurological institute
Translational Data Analytics	The Ohio State University Data Analytics Collaborative
Chemistry-Biology Interface	The Ohio State University CBI Training Program
Molecular Biophysics	The Ohio State University Molecular Biophysics Training Program

Professional Organizations

American Chemical Society (ACS), 1991-
American Crystallographic Association (ACA), 1995-
American Association for Cancer Research (AACR), 2008-
Chinese-American Chemistry & Chemical Biology Professors Association, 2009-

Awards/Honors

Department of Defense Breast Cancer Postdoctoral Fellowship, 2001-2003.
NIH NCRR Postdoctoral Fellowship, 2003-2005.
Best poster award, OSUCCC annual meeting, 2008.
OSUCCC-ACS Institutional Research award, 2009.
Department of Defense Idea Grant Award, 2010.
Changjiang Chair Professor, 2017.

Professional Service

a) Organizational duty

Director, The Chemistry-Biology Interface Training Program at the University of Florida, funded by NIH/NIGMS, July 1, 2020 – present.

Co-Chair, UF Health Science Center (UFHSC) Diagnostics & Therapeutics AI Faculty Search Committee, January 1, 2021 – August 31, 2022.

Member, The University of Florida Task Force on AI Research. June 2020 – present.

Member, The UFHSC AI Advisory Committee, January 1, 2021 – present.

Associate Director, the Center for Natural Products, Drug Discovery and Development (CNPD3), College of Pharmacy, University of Florida, Gainesville, FL 32610, August 20, 2019 – present.

Member, The UF College of Pharmacy International Committee, August 16, 2020 – present.

Consultant, GLGroup, 2019 – present.

Member, NSF Center for Big Learning, 2018 – present.

Member, UF Computational Biophysics Faculty Search Committee, 2018-2019.

Graduate Coordinator, Department of Medicinal Chemistry, University of Florida, 2016 – 2019.

Member, the China Gateway Faculty Advisory Committee at The Ohio State University, 2015 – 2016.

Member and Data Collaborative Subcommittee Chair, the Provost-appointed University Data Analytics Faculty Advisory Committee, The Ohio State University, 2014 – 2016.

Member, the Ohio Supercomputer Center (OSC) Statewide Users Group (SUG) Executive Committee and Allocations Committee, 2009 – 2016.

Member, Choose Ohio First (COF) Bioinformatics Scholarship Program Committee, 2010 – 2016.

Faculty Advisor, Focus group on Structural and Computational Biology in the Biophysics Program, The Ohio State University, 2009 – 2014.

Chair, the Ohio Supercomputer Center (OSC) Statewide Users Group (SUG) Executive Committee, 2010 – 2011.

Vice Chair, the Ohio Supercomputer Center (OSC) Statewide Users Group (SUG) Executive Committee, 2009 – 2010.

Leader, the establishment of the Computational Medicinal Chemistry graduate track at the College of Pharmacy, The Ohio State University, 2009.

Chair, OSU College of Pharmacy Honors Committee, 2013 – 2015.

Chair, OSU College of Pharmacy Technology and Educational Resources Advisory Committee, 2010 – 2011.

Member, OSU College of Pharmacy Admissions and Financial Aid Committee, 2007 – 2010.

Member, The Ohio State Biochemical Program (OSBP) Admission Committee, 2007-2009.

b) Grant reviewers

NIH NCI Clinical and Translational Cancer Research grants review, Mar. 22, 2023.

NIH NIAID AViDD U19 center grants review, Feb. 9-17, 2022.

NIH CSR DDNS (Drug Discovery for the Nervous System) study section standing member, February 25, 2016 – June 30, 2020.

NIH NCI SEP Clinical and Translational R21 and Omnibus R03 Review, July 9, 2019.

UK MRC (Medical Research Council) grant review, December 2017.

NIH Special Emphasis Panel (SEP) 2017/05 ZHD1 DSR-L (50) 1 for U54 Contraception Centers Review, Apr. 6 - 7, 2017.

Polish Academy of Sciences Grants Review, March 2016.

NIH/NHLBI SBIR Grants Review, 2015.

The Cancer Commercialization reviews of health research grants, Oak Ridge Associated Universities, 2015.

NIH/NCI SEP Study Section Grants Review, 2014.

The Oklahoma Center of Biomedical Research Excellence in Structural Biology (OCSB), April, 2013.

NSF Review panel, BIO MCB, August, 2012.

Hong Kong RGC (Research Grants Council) Grants Review, 2011 – present.

Study section, ad hoc reviewer, NIH, Cellular and Molecular Biology of the Kidney (CMBK), February, 2010.

Special Emphasis Panel, center for scientific review, NIH, ZRG1, OTC-K RC1 ARRA Challenge grant mail reviews, 2009.

Grant proposal review on Academic Research Infrastructure Program: Recovery and Reinvestment (ARI-R^2), National Science Foundation (NSF), 2009.

Peer review, the Genesis Oncology Trust, New Zealand, 2009.

Peer review, Genome Canada, Canada, 2005-2006.

Grant computing resource units allocation reviews and allocations, regular member, Allocations Committee, the Ohio Supercomputer Center, State of Ohio, 2009 – 2016.

c) Journal reviewers

Journal of Medicinal Chemistry
Journal of Computational Chemistry
Journal of Physical Chemistry B
PLoS Computational Biology
Journal of the American Chemical Society
Journal of Chemical Information and Modeling
Journal of Chemical Theory and Computation
Journal of Computer-aided Molecular Design
Journal of Natural Products
Biochemistry
ACS Medicinal Chemistry Letters
ACS Chemical Biology
Molecular and Cellular Biochemistry
Molecular Informatics
Molecular Biosystems
Structure
Science
Advanced Science
Frontiers in Immunology
Scientific Reports
Proteins: Structure, Function, and Bioinformatics
Bioorganic & Medicinal Chemistry Letters
Bioorganic & Medicinal Chemistry
Molecular Cancer Therapeutics
European Journal of Medicinal Chemistry
Medicinal Chemistry Communications
Cancer Research
Cancers
Oncogene
Frontiers in Bioscience
BMC Genomics
Current Pharmaceutical Design
Chemical Biology & Drug Design
Current Medicinal Chemistry
Current Chemical Genomics
Expert Opinion on Drug Discovery
Expert Opinion On Therapeutic Patents
Biochimie
Drug Discovery Today
Frontiers in Pharmacology

d) Editorial duties

Editorial Board Member, Cells (ISSN 2073-4409; CODEN: CELLC6, MDPI. IF: 6.0)

Active Grants

a) as PI

"Chemistry-Biology Interface Training Program at the University of Florida", PI: Chenglong Li, NIH/NIGMS, 5T32GM136583-04, $800,510, July 1, 2020 – June 30, 2025.

"Developing YAP/TEAD inhibitors for novel NASH-associated hepatocellular carcinoma therapeutics", PI: Chenglong Li, DOD/CDMRP, W81XWH22PRCRP, $478,373, August 1, 2023 – July 31, 2025.

"Dual Inhibition of PARP and IL-6 as a Novel Therapeutic Approach for BRCA-Mutated Triple-Negative Breast Cancer", PI: Chenglong Li and Jiayuh Lin, DOD/CDMRP, BC230111, $1,139,152, September 15, 2023 – September 14, 2026.

b) as Co-I

"Integrative Multidisciplinary Discovery Platform to Unlock Marine Natural Products Therapeutic Opportunities", PI: Hendrik Luesch, NIH/MIGMS, 5RM1GM145426-02, $8,830,047, August 1, 2022 – July 31, 2027.

"Development of high-affinity and selective ligands as pharmacological tools to explore dopamine D4 receptor (D4R) subtype variants", PI: Comfort Boateng, NIH/NIDA, 1DP1DA058385-01, $2,235,000, April 1, 2023 – March 31, 2028.

"Mechanisms of Metal Ion Homeostasis of Oral Streptococci", PI: Jose Lemos, NIH/NIDCR, 1R01DE032555-01A1, $2,703,994, August 1, 2023 – July 31, 2028.

"Novel Targeted Anticancer Agents from Marine Cyanobacteria", PI: Hendrik Luesch, NIH/NCI, 5R01CA172310-10, $2,208,774, September 1, 2019 – August 31, 2024.

"Computationally designed IL-10 mutants for the treatment of inflammatory bowel diseases", PI: Sihong Song, DOD/CDMRP, W81XWH2210065, $305,000, Feb. 1, 2022 – Jan. 31, 2024.

Pending Grants

"Elion: an artificial intelligence-based computational platform for drug optimization", PI: Chenglong Li, NIH/NIGMS, $1,831,706, 1R01GM153863-01, April 1, 2024 – March 31, 2028.

"Regulation of enteric norovirus infection by host-derived and microbiota-transformed bile acids", PI: Stephanie Karst, NIH/NIAID, 2R01AI141478-06A1, $3,730,712, April 1, 2024 – March 31, 2029.

Completed Grants

"Role and targeting of PRMT5 in prostate cancer", mPI: Chenglong Li, Changdeng Hu and Jiaoti Huang, NIH/NCI, 5R01CA212403-05, $2,601,360, June 1, 2017 – May 31, 2023.

"QLCI-CG: Conceptualization of the Institute for Quantum Biology on Quantum Computers", PI: Beverly Sanders, NSF, 1936853, $149,999, August 14, 2019 – July 31, 2023.

"A Machine Learning Approach to Drug Hit Optimization", PI: Chenglong Li, UF Office of Research, $50,000, January 1, 2021 – June 30, 2022.

"Mechanistic studies of gamma-glutamyl transpeptidase inhibition: a novel approach to modulating serum levels of cysteine", PI: Marie Hanigan, NIH/NIGMS, 5R01GM125952-03, $325,224, Sep 1, 2018 – June 30, 2022.

"A novel STAT3-selective inhibitor for medulloblastoma therapy", mPI: Chenglong Li and Jiayuh Lin, NIH/NINDS, 5R01NS087213-05, $1,660,665, June 1, 2015 – May 31, 2021.

“Small molecule *in vivo* probe development targeting the IL-6/STAT3 pathway for potential multiple sclerosis therapy”, PI: Chenglong Li, NIH/NINDS, 5R01NS088437-04, $1,407,754, May 1, 2015 – April 30, 2019.

“Studies of Childhood Sarcomas”, PI: Peter Houghton. Medicinal Chemistry and project 2: Chenglong Li. NIH/NCI (5P01CA165995-05). $8,798,828. June 1, 2013 – May 31, 2018.

“Repositioning Bazedoxifene as a novel IL-6/GP130 inhibitor for sarcoma therapy”, PI: Jiayuh Lin, NIH/NCI, 1R21CA191751-03, $426,688, Feb. 1, 2015 – Nov. 30, 2017.

“Role of HDAC6 in Platinum Resistance of Non-small Cell Lung Cancer”, PI: Xiaohong “Mary” Zhang, NIH/NCI (5R01CA164147-05), $135,213.00, May 1, 2012 – August, 31, 2017.

“Development of novel therapeutics for neglected tropical disease leishmaniasis”, PI: Abhay Satoskar, DOD/CDMRP (PR130408), $994,937, September 30, 2014 – September 29, 2017.

“Targeting PRMT5 expression in diffuse large B cell and mantle cell lymphoma”, mPI: Robert Baiocchi and Chenglong Li. LLS (Leukemia & Lymphoma Society). $600,000. October 1, 2013 – September 30, 2017.

“Targeted delivery of microRNA-loaded microvesicles for cancer therapy”, PI: Thomas Schmittgen. NIH/NCATS. 5UH2TR000914-02, $1,500,000. August 1, 2013 – July 31, 2016.

“Novel therapeutic agents targeting Mps1/TTK in aggressive breast cancer”, PI: Robert Brueggemeier. OSU 2014 Pelotonia Idea Award. $100,000, July 1, 2014 – June 30, 2016.

“Targeted plan to discover lead compounds to selectively target PRMT5 in cancer”, mPI: Robert Baiocchi and Chenglong Li. OSU DDI (Drug Development Institute). $776,298. March 1, 2013 – June 30, 2016.

“Targeting PRMT5 as a Novel Radiosensitization Approach for Primary and Recurrent Prostate Cancer Treatment”, PI: Chang-Deng Hu, DOD/CDMRP (PC111190), $35,781.00, June 1, 2012 – May 31, 2016.

“Develop novel F508del modulators by targeting NBD1 conformation”, Pilot and Feasibility Program, PI: Eric Sorscher. NIH/NIDDK. 5P30DK072482-09, $231,000. May 1, 2013 – April 30, 2016.

“Novel Small Molecules Disabling the IL-6/IL-6R/GP130 Heterohexamer Complex”, PI: Chenglong Li. DOD/CDMRP (BC095473). $ 515,000. August 1, 2010 – October 31, 2013.

“Similarity-based indexing and integration of protein sequence and structure databases”, PI: Hakan Ferhatosmanoglu. NSF (0750891). $498,117. August 1, 2008 – July 31, 2012.

“Novel Lead Molecule Optimization Targeting Nicotinic Receptor Subtypes”, PI: Dennis McKay and Chenglong Li. NIH/NIDA (1R21DA029433-01). $457,500. September 30, 2009 – August 31, 2013.

“Development of novel compounds to inhibit PRMT5 enzyme in high grade astrocytomas”, PI: Robert Baiocchi and Chenglong Li. NIH/NINDS (1R21NS071346-01). $413,033. August 1, 2010 – July 31, 2013. (Score 17 and Percentile 1.0% at Feb. 2010 Study Section DMP: Drug Discovery and Molecular Pharmacology)

“Target Stat3 in Pancreatic Cancer Using Novel Small Molecule Inhibitors”, PI: Jiayuh Lin and Chenglong Li. NIH/NCI (5R21CA133652-02). $363,875. March 1, 2009 – February 28, 2012.

“SPORE - Experimental Therapeutics of Leukemia”, PI: John Byrd. NIH/NCI (1P50CA140158-01). $125,000 (Core D Medicinal Chemistry Co-I). August 17, 2009 – July 31, 2014.

“Novel STAT3 drug development for childhood osteosarcoma therapy using drug repositioning”, PI: Jiayuh Lin, Alex's Lemonade Stand Foundation for Childhood Cancer, $70,000, July 1, 2012 – June 30, 2014.

"Modulation of IL-6 signaling for MS therapy", PI: Yuhong Yang. National Multiple Sclerosis Society. PP2080. $44,000. January 1, 2014 – December 31, 2014.

"Development of novel STAT3 inhibitor in the treatment of psoriasis", PI: Henry Wong. OSU CCTS (center for clinical & translational science). $49,500, June 9, 2014 - June 8, 2015.

"Small Molecule Inhibitors of Stat3 Dimerization For Prostate Cancer", PI: Pui-Kai Li. DOD/CDMRP (PC073825). $518,538. September 1, 2008 – August 31, 2012.

"Development of Small Molecule Inhibitors of IL-6/GP130 for the Treatment of Prostate Cancer", PI: James Fuchs. DOD/CDMRP (PC094727) New Investigator, $337,500, September 1, 2009 – August 31, 2012.

"Evaluating the Anti-tumor Effects of Novel Curcumin Analogs in Melanoma", PI: Gregory Lesinski. NIH/NCI (1R21CA141434-01A1). $364,856. March 1, 2010 – Feburary 28, 2012.

"OSU Crystallography Facility: Acquisition of Crystallization Robot", PI: Michael Chan. NIH/NCRR (1S10RR027187-01). $111,200. January 6, 2009 – January 6, 2010.

"Dual inhibitors target JAK2/STAT3 for novel pancreatic cancer therapy", PI: Jiayuh Lin. AACR (2009-2011 AACR Pancreatic Pilot). $75,165. July 1, 2009 – June 30, 2011.

"Target Stat3 pathway in glioblastoma multiforme using novel small molecular inhibitors", PI: Jiayuh Lin. The James S. McDonnell Foundation. $100,000. September 1, 2007 – August 31, 2008.

"Targeting Stat3 pathway in pancreatic cancers using novel small molecular inhibitors", PI: Jiayuh Lin. National Foundation for Cancer Research. $50,000. September 1, 2007 – August 31, 2009.

"Molecular Targeting of Epstein Barr Virus (EBV) Kinases for Treatment of EBV-Related Malignancies", PI: Robert Baiocchi. OSUCCC seed grant. $30,000. January 1, 2007 – December 31, 2007.

Research Group/Lab Personnel ("**Bold**" marks current members)

a) Visiting Professors/Scientists

Yuepiao Cai, Ph.D., Professor and Vice Chair, department of pharmaceutical sciences, Wenzhou Medical University, Wenzhou, China. 2/16/2015 – 2/20/2016. Working on protein/drug modeling, computational design and free energy analysis.

Liqun Shen, Ph.D., Professor and Chair, department of chemistry and biochemistry, Guangxi University for Nationalities, Nanning, China. 1/16/2014 – 1/15/2015. Working on IL-6/STAT3 drug design and synthesis.

Yiping Li, Ph.D., Professor and Chair, department of pharmaceutical sciences, college of medicine, Xi'an Jiao-Tong University, Xi'an, China. 2/1/2010 – 7/31/2010; 12/19/2017 – 12/18/2018. Working on lead discovery through virtual library screening, molecular dynamics simulation and binding free energy calculation.

Xiaojie Zhang, Ph.D., graduate visiting scientist, department of biological sciences, Tsinghua University, Beijing, China. 8/8/2014 – 2/7/2015. Working on PRMT5 protein expression and purification.

Hongbo Li, Ph.D., graduate visiting scientist, department of pharmaceutical sciences, Tsinghua University, Beijing, China. 3/9/2015 – 12/31/2015. Working on drug design and synthesis for the IL-6/STAT3 pathway.

Mohammad Ali Rezaei, Visiting scholar, 6/1/2012 – 4/30/2013. Working on method development of fragment-based molecular design.

Lifang Yang, Ph.D., Professor, School of Chemistry and Chemical Engineering, Guangxi University for Nationalities. 12/19/2017 – 6/18/2018. Working on IL-6/STAT3 inhibitor compound synthesis and cellular evaluations.

Dejun Li, Ph.D., Associate Professor, Northeast Agricultural University. 1/1/2020- present. Working on IL-6/STAT3 inhibitor compound cellular evaluations.

Agrinaldo Jacinto do Nascimento, Ph.D., group leader, Integrated Reality Laboratory at Federal Institute of Education Science, and Technology of Brasília, Brazil. March 1, 2022 – Feb. 28, 2023. Working on YAP/TEAD structural complex simulations.

Tahira Noor, M.Sc., graduate visiting scientist, COMSATS University, Islamabad, Pakistan. Working on drug discovery targeting dihydropteroate synthetase (DHPS).

Clemens Alexander Wolf, graduate visiting scientist, Free University of Berlin, Germany. Working on drug metabolism mechanism and fragment-based design through molecular simulation.

b) Research Professors/Scientists

Gustavo Seabra, Ph.D., molecular design and simulation, AI-based design. 9/3/2019 – present.

Jinhua Song, Ph.D., Drug design and synthesis, and synthetic lab management. 7/27/2015 – 02/28/2019.

Yong Xu, Ph.D., Drug design and synthesis. 5/13/2013 – 2/21/2014.

c) Postdoctoral Research Associates

Ribai Yan, Ph.D. in Organic Chemistry, 1/1/2015 – 7/31/2015. Working on drug synthesis.

Min Wang, Ph.D. in Biochemistry. 8/1/2010 – 12/31/2011. Worked on protein structure and dynamics combining experimental and computational approaches.

Mohammad Ali Rezaei, Ph.D. in Biophysics. 8/1/2019 – present. Currently working on AI-based affinity model development.

Iram Hyder, M.D. in oncology. 1/1/2020 – present. Currently working on ovarian cancer biology.

Xiaozhi Yang, Ph.D. in Medicinal Chemistry. 8/21/2021 – present. Working on drug discovery targeting PRMT5.

d) Ph.D. graduate students graduated from my lab

In-Hee Park, Ph.D. in Chemical Physics. 4/1/2006 – 6/16/2010. After a postdoctoral study with joint appointment of the California Institute of Technology Materials and Process Simulation Center and the City of Hope Beckman Research Institute, she joined Novartis site at San Diego, California.

Vandana Kumari, Ph.D. in Pharmaceutical Sciences. 6/1/2006 – 8/20/2011. Then a postdoctoral scientist at NCI/NIH; now as Computational Scientist at NCI RAS Initiative. She won the College of Pharmacy 2010-2011 Jane Chen Fellowship. Currently Scientist at Leidos Biomedical Research, Inc./Frederick National Laboratory for Cancer Research.

Huameng Li, Ph.D. in Biophysics, 6/1/2007 – 12/31/2011. Now a senior IT staff at the State of Ohio Government.

Kiran Mahasenan, Ph.D. in Pharmaceutical Sciences. 1/1/2007 – 3/31/2012. Currently a research scientist at the University of Notre Dame. He won the College of Pharmacy 2009 Jack Beal Award.

Wenying Yu, Ph.D. in Medicinal Chemistry. 4/1/2010 – 8/20/2013. Currently a Full Professor of Medicinal Chemistry in the China Pharmaceutical University, Nanjing, China. She won the College of Pharmacy 2013 Jack Beal Award.

Somsundaram Chettiar, Ph.D. in Pharmaceutical Sciences, 9/1/2007 – 12/15/2013. Currently a postdoc at the Infectious Disease Research Institute (IDRI) at Seattle, Washington. He won 2013 COP Graduate Teaching Award.

Ryan Pavlovicz, Ph.D. in Biophysics, 8/1/2007 – 4/30/2014. Currently a postdoc in David Baker's Protein Design Institute at the University of Washington in Seattle. Ryan has won three prestigious graduate student awards: 1) the AFPE (American Foundation for Pharmaceutical Education) predoctoral graduate fellowship in pharmaceutical sciences, 2008-2011; 2) the NSF EAPSI (National Science Foundation East Asia and Pacific Summer Institute) fellowship for US graduate students, 2010; 3) the ACS Division of Medicinal Chemistry predoctoral fellowship for 2010-2011. Currently a Scientist at Cyrus Biotechnology Inc.

Liguang Mao, Ph.D. in Medicinal Chemistry, 9/21/2011 – 12/15/2017, Research on IL-6 small molecule inhibitors design, synthesis and evaluation.

Guqin Shi, Ph.D. in Medicinal Chemistry. 9/21/2011 – 12/15/2017, Currently Computational Chemist at WuXi AppTec. Worked on IL-6/GP130 modeling and small molecule design.

Mohammad Ali Rezaei, Ph.D.. in Biophysics. 9/1/2013 - 8/1/2019. Currently postdoc at Pfizer, Inc.

Wei Zhou, Ph.D. in Biochemistry. 2/28/2014 – 7/24/2020. Currently research scientist at Hansoh Bio.

Xiaozhi Yang, Ph.D. in Medicinal Chemistry. 8/21/2014 – 8/10/2021. Currently in the Li Lab as postdoc.

Daniel Schultz, B. Sc. in Mechanical Engineering and Chemistry. 8/21/2017 – 12/31/2022. Currently as postdoc at the Vanderbilt University.

e) Post-candidacy Ph.D. graduate students

Chen Zhou, B.Sc. and M.Sc. in Medicinal Chemistry, 8/21/2019 – present. Currently in the graduate field of Medicinal Chemistry.

Zhihang Shen, B. Sc. And M. Sc. In pharmacology, 10/1/2020 – present. Currently in the graduate field of Medicinal Chemistry.

f) Pre-candidacy Ph.D. graduate students

Peter Ramdhan, Pharm. D., 5/1/2023 – present. Currently in graduate field of Medicinal Chemistry.

Chi-Yuan Liu, B. Sc. and M. Sc. in Pharmacy. 8/16/2023 – present. Currently in graduate field of Medicinal Chemistry.

f) M.Sc. graduate students graduated from my lab

Heng Chiat Tai, 6/1/2007 – 8/31/2009. Non-thesis M.Sc. in Medicinal Chemistry.

Hongshan Lai, M. Sc. in Organic Chemistry, 9/20/2010 – 5/10/2014, Non-thesis M.Sc. in Medicinal Chemistry.

Benjamin Lewis, B. Sc. In Biochemistry, 8/16/2022 – present. Currently in the graduate field of Biochemistry.

g) Undergraduate Students

Michael Meyer, 3rd-year undergraduate student at MIT Bioengineering. 6/1/2009 – 8/15/2009. He won the College of Pharmacy 2009 Summer Undergraduate Fellowship and joined my lab to apply Bayesian analysis to protein-drug interactions. Currently a graduate student in Computational Biology at Cornell University.

Isaac Maison, 3rd -year undergraduate student at Morehouse College (Atlanta) Chemistry department. 6/20/2010 – 8/15/2010. He was learning molecular docking. He won the College of Pharmacy 2010 Summer Undergraduate Fellowship.

Kristyn Sturms, 3rd-year undergraduate student at the College of Pharmacy BSPS program. 4/1/2010 – 5/30/2012. She works on SH2 domain structural informatics project. She won the 2009 Choose Ohio First (COF) Bioinformatics Undergraduate Fellowship.

Olivia Sabik, 3rd-year undergraduate student at Kenyon College Chemistry program. 6/11/2012 – 8/19/2012. She works on PRMT5 project. She was selected as Kenyon-OSUCCC joint undergraduate training Fellow.

Charles Lin, 3rd-year BSPS student. 1/1/2013 – 4/21/2014. He works on ASIC1a drug design. He won the College of Pharmacy Undergraduate Research Scholarship for 2013 – 2014. He is a graduate student at UCSD.

Eileen Tran, 3rd-year Biochemistry and Mathematics student from University of North Carolina – Chapel Hill, 5/20/2013 – 8/15/2013. She works on SGT1 structural biology. She won the 2013 College of Pharmacy Summer Undergraduate Research Fellowship.

John Ziebro, 4rd-year undergraduate at OSU BSPS program, 1/1/2014 – 8/8/2014. He works on STAT3 drug synthesis. He won the 2014 College of Pharmacy Summer Undergraduate Research Fellowship.

Joshua Ong, 3nd-year undergraduate at OSU biological science program. 1/1/2014 – present. He works on PRMT5 inhibitor biological assays. He won the 2015 College of Arts and Sciences Undergraduate Research Award.

Justin Anderson, 3rd-year undergraduate at OSU BSPS program, 6/1/2014 - present. He works on IL-6 drug synthesis and cellular evaluation. He won the 2015 College of Pharmacy Summer Undergraduate Research Fellowship.

Kaitlyn Tenn, 3rd-year undergraduate majoring in Biochemistry from Florida State University. 5/26/2018 – 8/4/2018. She worked on IL-6 project. She won the 2018 College of Pharmacy Summer Undergraduate Research Fellowship.

Alyssa Mickle, 3rd-year undergraduate majoring in Biomedical Science and Mechanical Engineering from University of Central Florida. 5/25/2019 – 8/3/2019. She worked on IL-6 project. She won the 2018 College of Pharmacy Summer Undergraduate Research Fellowship.

Drew Gill, 3rd-year undergraduate majoring in computer science and biochemistry. He is working on kinase drug informatics.

Conner Booker, 3rd-year undergraduate majoring in chemistry. He is working on IL-6 compound synthesis.

Bari Weiner, 2nd-year undergraduate majoring on pre-med track. She is working on PRMT5 inhibitor compound synthesis.

h) Pharm. D. students

Peter Ramdhan, B.Sc., 1/1/2021 – 4/30/2023. Working on computational simulation for drug design.

Publications (Total: 171 peer-reviewed original research journal articles; independent work: 153 articles)

a) Independent Work (8/1/2005 – present)

i) as Corresponding Author or Co-Corresponding Author

Schultz, D. C., Pan, L., Wang, T., Booker, C., Hyder, I., Hanold, L., Rubin, G., Ding, Y., Lin, J. and **Li, C.** Carbohydrate-Small Molecule Hybrids as Lead Compounds Targeting IL-6 Signaling. ***Molecules***, 2023, 28, 677.

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b) Graduate and Postdoctoral work (before 8/1/2005)

Xu, L., Chong, Y., Hwang, I., D'Onofrio, A., Amore, K., Beardsley, G. P., **Li, C.**, Arthur J. Olson, A., Dale L. Boger, D. L. and Wilson, I. A. "Structure-based Design, Synthesis, Evaluation, and Crystal Structures of Transition State Analogue Inhibitors of Inosine Monophosphate Cyclohydrolase". ***J. Biol. Chem.,*** 2007, 282, 13033-13046.
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(**The collaborator Bruce *Beutler won the 2011 Nobel Prize in Physiology and Medicine***)

Wu, S.; Xie, P.; Welsh, K.; **Li, C**.; Ni, C.-Z.; Zhu, X.; Reed, J. C.; Satterthwait, A. C.; Bishop, G. A. and Ely, K. R. "LMP1 Protein from the Epstein-Barr Virus Is a Structural CD40 Decoy in B Lymphocytes for Binding to TRAF3". ***J. Biol. Chem.***, 2005, 280, 33620 - 33626.
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(IF: 5.328)

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(IF: 2.600)

Ma, C. and **Li, C.** Interaction between polyvinylpyrrolidone and sodium dodecyl sulfate at solid/liquid interface. ***J. Colloid and Interface Sci.***, 1989, 131, 485-92.
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Patents

Baiocchi, R. A., **Li, C.**, Li, P. K., Yan, F. Compositions and methods for cancer detection and treatment. WO 2011079236 (A1) 2011-06-30; US 9676749 (B2) 2017-06-13.

Li, C., Yu, W., Lin, J. Preparation of naphthalenesulfonamides, naphtho[1,8-cd]isothiazolones, and related compounds as STAT3 inhibitors and their use for treating cancer and other cell proliferation disorders. WO2014028909 (A1) 2014-02-20; US 20150232434 2015-8-20.

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Fuchs, J. R.; **Li, C**.; Li, P.-K.; Lin, J. Small molecule inhibitors of IL-6 and uses thereof. WO2013019690 (A1) 2013-02-07; US 20140315956 2014-10-23.

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Li, C. and Mao, L. Use of interleukin 6 inhibitors for treatment of cancer, autoimmune diseases and other inflammatory diseases. August 29, 2019, WO 2019165158 A1.

Yang, Y., **Li, C.** and Racke, M. Methods and compositions for inhibition of STAT3. April 4, 2019, WO 2019067696A1. May 25, 2020, PCT/US2018/053085.

Li, C., Yang, X. and Zhou, W. PRMT5 inhibitor compounds. October 8, 2020. WO 2020205660 A1.

Li, C. and Zhou, W. (UF Disclosure T18121) YAP-TEAD Inhibitors in The Hippo Signaling Pathway for Potential Cancer Therapeutics. March 16, 2020.

Li, C. and Hu, C.-D., (UF Disclosure T18505) Development and applications of a novel type of PRMT5 inhibitors targeting its interaction with pICln. May 10, 2021.

Li, C. and Mao, L., IL-6 inhibitors and methods of treatment, PCT/US2019/019069, Patent No. US 11,530,181 B2, December 20, 2022.

Li, C., Schultz, D. and Shen, Z. Multifaceted synthesis of pyrazole interleukin-6 inhibitors treating cancers, fibrosis, autoimmune, and inflammatory diseases. WO2022226133, October 27, 2022.

Yang, Y., **Li, C.** and Racke, M. Methods and compositions for inhibition of STAT3. US20230103257, March 30, 2023.

Software Release

The MLSD (Multiple Ligand Simultaneous Docking) code has been widely distributed around the world, usually upon request. It has been used for docking simulations, molecular design, mechanistic understanding, etc.

The deep-learning protein/ligand binding affinity server (DeepAtom) can be used for general public (under alpha version testing).

First-in-Class Cancer Drug Tech Licensing

PRMT5-targeting technology and Compound commercialization development licensing agreement has been signed with the Prelude Therapeutics, Inc. on May 20, 2016.

Media Attention

1) to MLSD simulation method development and application

- UPI (United Press International) science news: “Computer program may speed drug discovery” on April 19, 2010.
  http://www.upi.com/Science_News/2010/04/19/Computer-program-may-speed-drug-discovery/UPI-15241271700364/

- Sicence Daily news: “New Drug Design Technique Could Dramatically Speed Discovery Process” on April 15, 2010.
  http://www.sciencedaily.com/releases/2010/04/100413170707.htm

- The Ohio State University OnCampus faculty research news: “Drug design technique could speed discovery process” on May 5, 2010.
  http://oncampus.osu.edu/2010/05/drug-design-technique-could-speed-discovery-process/

2) to uncovering of a self-feeding ongogenic cycle involving Sp1/NFκB/HDAC/miR-29b regulatory molecular network in KIT-driven Acute Myeloid Leukemia (AML)

- Science Daily news: “’Vicious Cycle’ Offers New Acute Myeloid Leukemia Target” on April 21, 2010.
  http://www.sciencedaily.com/releases/2010/04/100413160905.htm

3) to a novel lead discovery through computational modeling to target prmt5 enzyme for potential epigenetic therapy to brain tumor

- The Ohio Supercomputer Center news release: “Biophysicist uses supercomputer to help fight brain tumors” on March 10, 2010.
  http://www.osc.edu/press/releases/2010/brainTumors.shtml

- OSUCCC Frontier story: “Drug Design In Silico” on Summer issue of 2012.
  http://cancer.osu.edu/about/publications/frontiers/archive/2012/07/19/drug-design-in-silico.aspx

- OSUCCC DDI story.

  https://cancer.osu.edu/news-and-media/news/drug-development-institute-collaborates-with-company-to-develop-epigentic-inhibitors-for-cancer

4) to a research project to simulate allosterics of nAChRs and to design allosteric-site-targeting molecules

- The Ohio State Supercomputer 2008 annual research report: “Finding treatments for neurological diseases” in December, 2008.
  http://www.osc.edu/research/report/biological_neuro.shtml

5) to a joint effort to engineer “designer” inhibitors based on natural compound curcumin, in collaboration with colleagues Drs. James Fuchs and Pui-Kai (Tom) Li

- Science Daily news: “Synthetic Molecules Could Add Spice to Fight against Cancer” on August 18, 2008.
  http://www.sciencedaily.com/releases/2008/08/080817223644.htm

6) to development of STAT3 and IL-6 inhibition drugs for targeted cancer therapy

- Science Daily news: **"**Common Anti-Inflammatory Coaxes Liver Cancer Cells to Commit Suicide" on May 16, 2011.
  http://www.sciencedaily.com/releases/2011/05/110516121545.htm
  http://oncampus.osu.edu/common-drug-makes-liver-cancer-cells-commit-suicide

- Science Daily news: "Blocking an Oncogene in Liver Cancer Could Be Potential Therapy Option" on October 13, 2010.
  http://www.sciencedaily.com/releases/2010/10/101012163303.htm

- Science Daily news: **"**Compounds Show Promise in Blocking STAT3 Signaling as Treatment for Osteosarcoma" on April 11, 2011.
  http://www.sciencedaily.com/releases/2011/04/110411152637.htm

- Science Daily news: "Biophysicist Targeting IL-6 to Halt Breast, Prostate Cancer" On April 25, 2011.
  http://www.sciencedaily.com/releases/2011/04/110419164213.htm

- Ohio Supercomputer Center research news: "Biophysicist Targeting IL-6 to Halt Breast, Prostate Cancer" on April 19, 2011.
  http://www.osc.edu/press/releases/2011/chenglongli.shtml

- Nature.com publication "SciBX: Science-Business eXchange" on novel STAT3 inhibitor LY5 on May 30, 2013.
  http://www.nature.com/scibx/journal/v6/n21/pdf/scibx.2013.516.pdf

- Nature.com publication "SciBX: Science-Business eXchange" on repositioning Raloxifene and Bazedoxifene as novel inhibitors of IL-6/GP130 interface on Feb. 13, 2014.
  http://www.nature.com/scibx/journal/v7/n6/full/scibx.2014.167.html

7) At the University of Florida

- UF College of Pharmacy receives training grant interfacing chemistry and biology.
  https://pharmacy.ufl.edu/2020/06/02/uf-college-of-pharmacy-receives-training-grant-interfacing-chemistry-and-biology/

- Celebrating Distinction in Pharmacy.
  https://pharmacy.ufl.edu/2016/11/03/celebrating-distinction-in-pharmacy-2/

Invited Talks

The echeminfo virtual conference on "Applications of Cheminformatics and Chemical Modeling to Drug Discovery" on November 8-19, 2004. Host: Dr. John Irwin (UCSF). Title: "Successful Virtual Screening for Human AICAR Transformylase Inhibitors against NCI Diversity set Using AutoDock".

Accelrys R & D center (San Diego) visit on June 27, 2005. Host: Dr. Lisa Yan. Title: "Virtual screening and free energy simulation: an example on AICAR transformylase".

Nationwide Children's Research Institute (Columbus) on November 28, 2005. Host: Dr. Jiayuh Lin and Dr. Stephen Qualman. Title: "Computer-aided drug design on cancer target STAT3".

ACS 38th Central Regional Meeting on May 22, 2007 at Covington, Kentucky. Host: Dr. William Seibel (University of Cincinnati). Title: "Novel inhibitors of DNA methyltransferase 1".

The Ohio State University Biomedical Engineering Lecture series on February 6, 2008. Host: Dr. Rita Alevriadou. Title: “Induced-fit simulation of survivin via combined replica-exchange molecular dynamics and virtual screening”.

2008 OCCBIO (Ohio Collaborative Conference on Bioinformatics) on June 2, 2008 at University of Toledo, Toledo, Ohio. Host: Dr. Michael Raymer (Wright State University). Title: “Biomolecular simulation and molecular design”.

The Ohio Supercomputer Center Guest Lecture series on September 11, 2008 at Columbus Ohio. Host: Dr. Russell Pitzer (Ohio State University). Title: “Induced-fit simulation of survivin via combined replica-exchange molecular dynamics and virtual screening”.

The Ohio State University Comprehensive Cancer Center Molecular Carcinogenesis and Chemoprevention Program seminar series on November 17, 2009. Host: Dr. Steven Clinton (Program Leader). Title: “Targeting IL-6/JAK2/STAT3 pathway using novel curcumin analogs”.

The Ohio State University Institute of Materials Research 2010 Symposium Session “Computational Materials Design – Are We There Yet?” on September 14, 2010. Host: Dr. Wolfgang Windl. Title: “Computational Drug Design”.

Einstein College of Medicine, New York City, March 22, 2011. Host: Dr. David Cowburn. Title: “Multiple Ligand Simultaneous Docking (MLSD) and its applications”.

Purdue University, April 14, 2011. Host: Dr. Changdeng Hu. Title: **“**Multiple Ligand Simultaneous Docking (MLSD)”.

The 42nd Central Regional Meeting of the American Chemical Society, Indianapolis, Indiana, June 9, 2011. Host: Dr. Samy Meroueh. Title: “Computational design of small molecule inhibitors disabling IL-6/IL-6R/GP130 functional hexamer for cancer therapy”.

The 2011 Era of Hope Breast Cancer Meeting, Orlando, Florida, August 5, 2011. Host: Dr. Angela Brodie. Title: “Novel IL-6 Inhibitors for Breast Cancer Therapy”.

Twelfth Annual Structure-based Drug Design Conference, Boston, June 6-8, 2012. Host: CHI and Bio-IT World, Title: “Drug Design and Repositioning Using Multiple Fragment Simultaneous Docking”.

Southern Illinois University College of Medicine, Springfield, IL, June 14-15, 2012. Host: Daotai Nie, Title: “Novel Small Molecule Inhibitors targeting the IL-6/STAT3 pathway”.

The 244th American Chemical Society National Meeting on August 21, 2012 in Philadelphia, Pennsylvania. Host: Jose L. Medina-Franco (Torrey Pines Institute for Molecular Studies). Title: “Drug design and repositioning using MLSD (multiple ligand simultaneous docking)”.

The 9th IUPAC international conference on biomolecular chemistry and Session Chair on “Molecular simulation and design”, Beijing, Aug. 25-29, 2012.

University of Science and Technology of China, Hefei, September, 25, 2012. Host: Haiyan Liu. Title: 1. “Multiple Ligand Simultaneous Docking (MLSD”; 2. “A Replica Exchange Molecular Dynamics (REMD) Simulation on Survivin”.

East China Normal University, Shanghai, September 27, 2012. Host: John Z. H. Zhang. Title: “Fragment-based Drug Design and Drug Repositioning Using Multiple Ligand Simultaneous Docking”.

National Lab on Structure of Matter at Microscale, Hefei, China, November 23, 2012. Host: Yi Luo. Title: “Unfolding Simulations of Di-domain Proteins: Crystallin and Survivin Examples”.

International Symposium on Laser and Computational Biophysics, Shanghai, June 15-17, 2014. Title: "Dissecting protein-ligand molecular recognition dynamics through Molecular simulation: survivin example and drug design implication".

ZING Conferences "Fragment-Based Drug Discovery", Punta Cana, Dominican Republic, July 19-22, 2014. Host: Steven Swann and Justin Bower. Title: "Fragment-based drug design and drug repositioning using multiple ligand simultaneous docking (MLSD): examples on targeting the IL-6/STAT3 pathway".

"Drug Discovery Chemistry" conference, San Diego, California, April 21-23, 2015. Host: Cambridge Health Institute. Title: "Discovery of a Potent and Specific Drug to Inhibit PRMT5 in Hematologic and Solid Tumors". (Not being able to attend due to schedule conflict)

The 11th SINO-US Chemistry Professors Conference, Suzhou, China, June 21-23, 2015. Host Suzhou University. Title: "Drug Discovery targeting IL-6/STAT3 Signaling Pathway".

University of Missouri at St. Louis, Department of Chemistry and Biochemistry, St. Louis, MO, Feb. 1-2, 2016. Host: Chung Wong. Title: "Drug Design Targeting the IL-6/STAT3 Signaling Axis".

Purdue University, Department of Medicinal Chemistry and Molecular Pharmacology, West Lafayette, IN, Mar. 1-2, 2016. Host: Mark Cushman. Title: "Drug Design Targeting the IL-6/STAT3 Signaling Axis".

BioOhio 2016, Columbus OH, June 16, 2016. Host: CAS (Chemical Abstract Service). Title: "Harnessing Big Data: Data Driven Insights in Health Care – A Novel Drug Hunting Strategy".

University of Maryland, Department of Biochemistry and Molecular Biology, Baltimore, MD. June 29, 2016. Host: Richard Eckert. Title: "Fragment-based drug design and drug repositioning using multiple ligand simultaneous docking (MLSD)".

"Drug Design Targeting PRMT5". Icahn School of Medicine at Mount Sinai. New York City. Apr 4, 2018 - Apr 6, 2018.

"A Data-Driven Deep-Learning Model to Evaluate Protein-Ligand Binding Affinity". Biophysical Society. Guangzhou, China. Jun 7, 2018 - Jun 10, 2018.

"The Role of Computational Biophysics in Drug Design". Department of Physics, University of Florida. Gainesville, Florida. Oct 11, 2018 - Oct 11, 2018.

"Drug Design Targeting the IL-6/STAT3 Signaling Pathway". College of Pharmacy and Pharmaceutical Sciences, Washington State University. Spokane, Washington. Mar 27, 2019 - Mar 27, 2019.

"Structure-based drug design towards small molecule interleukin-6 inhibitors". American Chemical Society. Orlando, Florida. Mar 31, 2019 - Apr 4, 2019.

"Revisiting STAT3 as a Drug Target". UFHealth Cancer Center. Gainesville, Florida. May 17, 2019 - May 17, 2019.

"Drug Design Targeting the IL-6/STAT3 Signaling Pathway". Host: Professor Lidia Moreira Lima, Symposium on Medicinal Chemistry and Molecular Pharmacology, Federal University of Rio de Janeiro, Brazil. December 1 – 4, 2019.

"Drug Design Targeting the IL-6/STAT3 Signaling Pathway". Host: Professor Hua Zhu, Guangxi University of Traditional Chinese Medicine. December 21-23, 2019.

"The Role of Computational Biophysics in Molecular Design". Host: Professor Hai Ping Cheng, UF Physics, Quantum Theory Project (QTP), March 11, 2020.

"Drug Design Targeting the IL6/STAT3 Signaling Pathway". Host: Jeffery Rudolf, UF Chemistry, Chemical Biology Division, Feb. 25, 2022.

Contributed Talks

The 236th American Chemical Society National Meeting on August 19, 2008 in Philadelphia, Pennsylvania. Host: Dr. Diane Joseph-McCarthy (Wyeth). Title: "Simulating molecular recognition through simultaneous multiple molecule docking".

The conference "Frontiers in Biological Sciences" on December 29, 2009 at San Diego, California. Host: Dr. Yishi Jin (UCSD) and Dr. Manyuan Long (University of Chicago). Title: "Molecular modeling of nAChRs".

The Ohio State University Mathematical Biosciences Institute (MBI) seminar series on April 22, 2010. Host: Dr. Dan Siegal-Gaskins. Title: "Multiple Ligand Simultaneous Docking (MLSD): Orchestrated Dancing of Ligands in Binding Sites of Protein".

Contributed Posters (not complete and updated**)**

a) by myself

Huameng Li and Chenglong Li, Multiple ligand simultaneous docking. Computer Aided Drug Design/Gordon Research Conferences, Tilton, NH, Jun 22, 2009. Chair: Prof. Brian K. Shoichet (UCSF); Vice Chair: Prof. Gerhard Klebe (Marburg).

Wenying Yu, Deepak Bhasin, Li Lin, Jiayuh Lin and Chenglong Li, Novel small molecule inhibitors targeting STAT3 oncoprotein for potential cancer therapy. The JAK-STAT Pathway: 20 Years from Discovery to Drugs, Natcher Conference Center, NIH campus, Bethesda, MD, Sep. 22-24, 2011. Organizers: John O'Shea (NIH/NIAMS), James Darnell (Rockefeller University), Richard Jove (City of Hope), David Levy (NYU), Warren Leonard (NIH/NHLBI), Lothar Hennighausen (NIH/ NIDDK).

Chenglong Li, Fragment-based drug design and drug repositioning using multiple ligand simultaneous docking (MLSD). Addressing the Challenges of Drug Discovery – Novel Tragets, New Chemical Space and Emerging Approaches/Keystone Symposia, Tahoe City, California, Mar. 21, 2012. Organizers: Dr. Stephen V. Frye (UNC-Chapel Hill), Dr. Michael Varney (Genentech), Prof. James A. Wells (UCSF).

Chenglong Li and Robert Baiocchi, Discovery of a first-in-class drug to inhibit PRMT5 in hematologic and solid tumors. Cancer Epigenetics/Keystone Symposia Conference, Santa Fe, NM, Feb. 4-9, 2014. Organizers: Sharon Y.R. Dent (MD Anderson Cancer Center), Jean-Pierre Issa (Temple University) and Peter A. Jones (Van Andel Institute).

Chenglong Li, Discovery of a potent and specific drug to inhibit PRMT5 in hematologic and solid tumors. Epigenetics and Cancer/ Keystone Symposia Conference, Keystone Resort, Keystone, CO, Jan. 25-30, 2015. Organizers: Tony Kouzarides (University of Cambridge) and Kristian Helin (University of Copenhagen).

Chenglong Li, Drug Design Targeting the IL-6/STAT3 Signaling Axis . Keystone Symposia: Cytokine JAK-STAT Signaling in Immunity and Disease, Steamboat Springs, Colorado, January 10-14, 2016.Organizers: Curt M. Horvath (Northwestern University), John J. O'Shea (National Institute of Arthritis and Musculoskeletal and Skin Diseases) and Stephanie S. Watowich (University of Texas MD Anderson Cancer Center).

b) by my students

In Hee Park and Chenglong Li, Novel ligand-induced survivin dimer conformation via Replica Exchange Molecular Dynamics (REMD) and receptor-based reverse Virtual Screening (VS). Biophysical Society annual meeting, Long Beach, California, Feb. 2-6. 2008.

In Hee Park and Chenglong Li. Novel ligand-induced Survivin dimer conformation via replica exchange molecular dynamics (REMD) and receptor-based reverse virtual screening (VS). The 235th ACS Spring national meeting; New Orleans, Louisiana. Apr. 6-10, 2008.

In Hee Park and Chenglong Li. Novel ligand-induced Survivin dimer conformation via replica exchange molecular dynamics (REMD) and receptor-based reverse virtual screening. ACS central regional meeting; June 6-10, 2008. Columbus, Ohio.

Katryna Cisek and Chenglong Li. Computational design of STAT3 inhibitors for targeted anti-cancer therapy. ACS central regional meeting; June 6-10, 2008. Columbus, Ohio.

Vandana Kumari and Chenglong Li. Molecular dynamics simulation of β2 adrenergic receptor. ACS central regional meeting; June 6-10, 2008. Columbus, Ohio.

Ryan Pavlovicz and Chenglong Li. Modeling nicotinic acetylcholine receptors for computational drug design. ACS central regional meeting; June 6-10, 2008. Columbus, Ohio.

Kiran V. Mahasenan and Chenglong Li. Comparative modeling of human protein arginine methyltransferase 5 (PRMT5) and substrate binding site characterization through molecular docking for target specific inhibitor design. ACS central regional meeting; June 6-10, 2008. Columbus, Ohio.

Park, In-Hee; Li, Chenglong. Simulation of age-related cataract causing monomeric two-domain misfolding pathway of γS-crystallin via enhanced sampling and 2D-potential of mean force (2D-PMF) mapping. 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010

Mahasenan, K. V., Yan, F., Li, Pui-Kai, Baiocchi, R., Li, C. Structure-based computational design of selective, small molecule PRMT5 inhibitors for experimental therapeutics of cancer: Protein modeling, virtual screening and lead validation. 13th Annual Meeting of the Translational Research Cancer Centers Consortium: Immune Suppression and The Tumor Microenvironment 2010, March 1-2, 2010, Columbus, Ohio.

Mahasenan, K. V., Yan, F., Li, Pui-Kai, Baiocchi, R., Li, C. Structure-based computational design of selective, small molecule PRMT5 inhibitors for experimental therapeutics of cancer: Protein modeling, virtual screening and lead validation. 12th OSUCCC-James Annual Scientific Meeting- Targeted Cancer Therapies: Discovery to Personalized Medicine, February 19, 2010, Columbus, Ohio.

Park, I.-H., Li, P.-K. and Li, C. Structure-based survivin dimerization inhibitor design: Transition from a putative computational simulation toward a practical drug design application. 13th Annual Meeting of the Translational Research Cancer Centers Consortium (TRC3) Immune Suppression and the Tumor Microenvironment, March 1-2, 2010, Columbus Ohio.

Kumari, V., Brachoni, C., Patel, T., Li, P.K., Li, C. Inhibition of Gp130 Homodimerization: An Approach towards Treatment of Prostate Cancer by Design of Selective IL-6 Inhibitors. 32nd National Medicinal Chemistry Symposium, June 6-9, 2010, Minneapolis, MN.

Li, Huameng and Li, Chenglong. Multiple land simultaneous docking (MLSD): Orchestrated dancing of ligands in binding sites of protein. The 240th ACS National Meeting, Boston, August 22-26, 2010.

Mahasenan, K., Yan, F., Baiocchi, R. and Li, C. Structure-based computational design of selective, small molecule PRMT5 inhibitors for experimental therapeutics of cancer: Protein modeling, virtual screening and lead validation, The 240th ACS National Meeting, Boston, August 22-26, 2010.

Mahasenan, Kiran V. and Li, Chenglong. Comparative modeling of maternal embryonic leucine zipper kinase inhibitor induced conformational ensembles: Improved structure-based virtual screen enrichment by incorporating protein flexibility. The 242nd ACS National Meeting & Exposition, Denver, CO, August 28-September 1, 2011.

Pavlovicz, Ryan, Henderson, Brandon, Bonnell, Andrew, Boyd, R. T., McKay, Dennis and Li, Chenglong. Identification of a novel negative allosteric site on human α4β2 and α3β4 nicotinic acetylcholine receptors. The 242nd ACS National Meeting & Exposition, Denver, CO, August 28-September 1, 2011.

Chettiar, Somsundaram N., Park, In-Hee, Cooley, James, Bhasin, Deepak, Li, Pui Kai, Chakravarti, Arnab, Naduparambil, Jacob and Li, Chenglong. Design, synthesis, and studies of novel survivin inhibitors. The 243rd ACS National Meeting & Exposition, San Diego, CA, March 25-29, 2012.

Yu, Wenying, Li, Jiayuh and Li, Chenglong. Discovery of novel STAT3 small molecule inhibitors via in silico site-directed fragment-based drug design. The 244th ACS National Meeting, Philadelphia, August 19-23, 2012.

Pavlovicz, Ryan and Li, Chenglong. Computational analysis of retinoic acid receptor antagonism using nonequilibrium molecular dynamics. Structural Analysis of Supramolecular Assemblies by Hybrid Methods/Keystone Symposia, Tahoe City, California, March 3-7, 2013.

Pavlovicz, Ryan and Li, Chenglong. Computational analysis of retinoic acid receptor antagonism using nonequilibrium molecular dynamics. Computational Chemistry/Gordon Research Conference, Mount Snow at West Dover, VT, July 20-25, 2014.

Mao, Liguang, Shi, Guqin and Li, Chenglong. Rational design, synthesis and evaluation of small molecule IL-6 /GP130 inhibitors as anticancer agents. MEDI-276. ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, 2016.

Shi, Guqin, Mao, Liguang and Li, Chenglong. Structure-based computer-aided IL-6/GP130 protein-protein interaction (PPI) inhibitor design. MEDI-370. ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, 2016.

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Shi, Guqin, Mao, Liguang, Kumari, Vandana and Li, Chenglong. Structure-based computer-aided IL-6/GP130 Protein-Protein Interaction (PPI) inhibitor design. MEDI-7. ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017.

c) by collaborators

Morris, Garrett M.; Huey, Ruth; Lindstrom, William; Li, Chenglong; Zhao, Yong; Hart, William E.; Belew, Richard; Sanner, Michel F.; Goodsell, David S.; Olson, Arthur J. Recent advances in AutoDock: Search, representation and scoring. 228th ACS National Meeting, Philadelphia, PA, August 22-26, 2004.

Hutzen B, Cen L, Friedman L, Sobo M, Ball S, Li P, Li C, Fuchs J, Bhasin D, Pandit B, Shibata H, Iwabuchi Y, Lin J. New curcumin analogues with enhanced growth suppressive activity in cancer cells. The 99th Annual Meeting of the American Association for Cancer Research; 2008 Apr 12-16; San Diego, CA.

Fuchs, James R.; Etter, Jonathan P.; Li, Pui-Kai; Abdelhamid, Dalia; Regan, Nicholas; Bhasin, Deepak; Pandit, Bulbul; Li, Chenglong; Cisek, Katryna; Lin, Jiayuh; Cen, Ling; Hutzen, Brian. Synthesis and antiproliferative activity of curcumin analogs. 236th ACS National Meeting, Philadelphia, PA. August 17-21, 2008.

Lin L., Hutzen B, Peng Z., Lin H., Li P-K., Li C., Wicha M., and Lin J. STAT3 as a novel therapeutic target in human breast cancer stem cells. The abstract was presented at The International society for biologic therapy of cancer annual meeting (Washington DC, Oct 29 – 31,2009).

Lin L., Hutzen B, Peng Z., Lin H., Li P-K., Li C., Wicha M., and Lin J. STAT3 as a novel therapeutic target in human breast cancer stem cells. The abstract was presented at the EORTC-NCI-AACR International Symposium on Molecular Targets and Cancer Therapeutics Annual Meeting (Boston, MA, Nov 16 – 19, 2009).

Zuo, M, Lin L. Li C, Li P-K, and Lin J. STAT3 as a checmoprevention target in liver cancer cells. The abstract was presented at the Eighth Annual AACR International Conference: Frontiers in Cancer Prevention Research (Houston, TX, Dec 6 – 9, 2009) Received an AACR travel award.

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Liu Y., Li C., Li P-K, Lin J. A small molecule, LLL12, inhibits IL-6 induced STAT3 phosphorylation and nuclear tanslocation. The abstract was presented at the AACR Annual Meeting (Washington DC, Apr 3 – 7, 2010) Received an AACR travel award.

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Fuchs, James R.; Schwartz, Eric B.; Abdelhamid, Dalia; Etter, Jonathan P.; Li, Chenglong; Li, Pui-Kai. Targeting the JAK/STAT pathway in cancer with curcumin derivatives. 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010.

Bhasin, D., Chettiar, S., Li, C., Lin, J. and Li, P.-K. Novel small molecule inhibitors of STAT3 in cancer, The 241st ACS National Meeting, Anaheim, California, March 27-31, 2011.

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Nicholas, C., Yan, F., Peters, S. B., Bill, M. A., Li, P.-K., Li, C., Fuchs, J. R., Baiocchi, R., Lesinski, G. B. The expression of PRMT5 methyltransferase mediates cell survival and metastatic phenotype in malignant melanoma. The 102nd AACR Annual Meeting, Orlando, Florida, April 2-6, 2011.

Fuchs, James R.; Jena, Nivedita; Kumari, Vandana; Mok, May; Li, Pui-Kai; Li, Chenglong. Disruption of IL-6 signaling in the IL-6/JAK/STAT pathway using small molecules. The 242nd ACS National Meeting & Exposition, Denver, CO, August 28-September 1, 2011.

Jena, Nivedita; Kumari, Vandana; Mok, May; Lin, Li; Li, Pui-Kai; Lin, Jiayuh; Li, Chenglong; Fuchs, James R. Small molecules targeting IL-6/GP130 homodimerization in the IL-6/JAK/STAT pathway. The 243rd ACS National Meeting & Exposition, San Diego, CA, March 25-March 29, 2012.

James V. Cooley, Somsundaram Chettiar, In-Hee Park, Deepak Bhasin, Arnab Chakravarti, Li Pui Kai, Chenglong Li, Naduparambil K. Jacob. Development of novel survivin inhibitors to target mitotic machinery in cancers. 2012 AACR Annual Meeting, Mar. 31 – Apr. 4, 2012. Chicago, IL.

Li Lin, Huameng Li, Minghao Xu, Zhenjiang Zhao, Veronica Olson, Yufang Xu, Chenglong Li, Jiayuh Lin. Novel drug discovery approach targeting STAT3 for breast cancer therapy using MLSD and drug repositioning. 2012

AACR Annual Meeting, Mar. 31 – Apr. 4, 2012. Chicago, IL.

Hemant K. Bid, Duane Oswald, Chenglong Li, Jiayuh Lin, Peter J. Houghton. Direct anti-angiogenic activity of a small molecular STAT3 inhibitor LLL12. 2012 AACR Annual Meeting, Mar. 31 – Apr. 4, 2012. Chicago, IL.

Woodard, John L.; Pan, Li; Chai, Heebyung; Mahasenan, Kiran; Li, Chenglong; Kinghorn, A. Douglas; Fuchs, James R. Flexible synthetic approach to the synthesis of the rocaglamide derivative silvestrol. The 244th ACS National Meeting & Exposition, Philadelphia, PA, August 19-23, 2012.

Fengting Yan, Kate Gordon, Kiran Mahasenan, Mark Lustberg, Lapo Alinari, Christian T. Earl, Balveen Kaur, Chenglong Li, Robert A. Baiocchi. Developing a first in class of drug to inhibit protein arginine methyltransferase 5 (PRMT5) enzyme dysregulation in glioblastoma multiforme. 2013 AACR Annual Meeting, Apr. 6-10, Washington DC.

Somayeh S. Tarighat, Kiran Mahasenan, Danilo Perrotti, Ramiro Garzon, Michael Caligiuri, Chenglong Li, William Blum, Guido Marcucci, Robert A. Baiocchi. Preclinical and pharmacological activities of protein arginine methyltransferase 5(PRMT5) enzyme inhibition in acute myeloid leukemia. 2013 AACR Annual Meeting, Apr. 6-10, Washington DC.

Hui Xiao, Wenying Yu, Veronica R. Olson, Chenglong Li, Peter Houghton, Jiayuh Lin. A novel small molecule, LY5, selectively inhibits STAT3 phosphorylation and activities and exhibits potent growth suppressive activity in cancer cells. 2013 AACR Annual Meeting, Apr. 6-10, Washington DC.

Schwartz, Eric B.; Etter, Jonathan; Abdelhamid, Dalia; Li, Chenglong; Li, Pui-Kai; Phelps, Mitch; He, Lei; Lesinski, Gregory B.; Lin, Jiayuh. Synthesis, optimization, and evaluation of dialkylated curcumin analogs as inhibitors of the JAK2/STAT3 pathway. The 246th ACS National Meeting & Exposition, Indianapolis, IN, September 8-12, 2013.

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Jennifer Yang, Kaitlin Keenan, Thomas Mace, Tanios Bekaii-Saab, James Fuchs, Eric Schwartz, Chenglong Li, Jiayuh Lin, Pui-Kai Li, Gregory Lesinski. STAT3 inhibitors elicit direct anti-tumor effects against human biliary cancer cell lines and limit release of immune suppressive cytokines in vitro. 2014 AACR Annual Meeting, Apr. 5-9, 2014, San Diego, CA.

Hui Xiao, Yang Bian, Chengguang Zhao, Li Lin, David Jou, Huameng Li, Chenglong Li, Jiayuh Lin. GP130 as a novel therapeutic target in il-6-dependent cancers. 2014 AACR Annual Meeting, Apr. 5-9, 2014, San Diego, CA.

Yuhong Yang, Chenglong Li, Patrick K Nuro-Gyina, Yue Liu, Wei Pei, Michelle Larson, Amy E. Lovett-Racke and Michael K. Racke. Modulating IL-6/STAT3 signaling pathway for Multiple Sclerosis therapy. The 2014 AAI (American Association of Immunologists) Annual Meeting, May 2-6, 2014, Pittsburgh, PA.

Liu, Liping; Park, In-Hee; Bakey, Michelle T.; Carver, Jessica R.; Kirby, Emily F.; Chettiar, Somsundaram; Regan, Nicholas; Bhasin, Deepak; Li, Pui-Kai; Sorscher, Eric J., Li, Chenglong, and Wang, Xiaodong R. INITIAL CHARACTERIZATION OF NBD1-TARGETING F508DEL CORRECTORS. The 29th Annual American Cystic Fibrosis Conference (NACFC), Oct. 9-11, 2014, Atlanta, GA.

Yonghua Ling, Xiaohua Zhu, Darlene Rozewski, Misty Bear, Jiayuh Lin, Chenglong Li, Pui-kai Li, Cheryl London, Mitch Phelps. Pharmacokinetic Evaluation of STAT3 Inhibitors LLL12 and LY5 in Mice. The 2014 AAPS Annual Meeting, Nov. 2-6, 2014, San Diego, CA.

Xiaojuan Wu, Hui Xiao, Chenglong Li, Jiayuh Lin. Persistent STAT3 signaling contributes to the resistance of anti-cancer drugs doxorubicin and cisplatin, and MEK inhibitor AZD6244 in human sarcoma cells. 2015 AACR Annual Meeting, Apr. 18-22, 2015. Philadelphia, PA.

Yina Wang, Chongqiang Zhao, Haiyan Ma, Huameng Li, Jiagao Lu, Chenglong Li, Jiayuh Lin, Li Lin. Inhibition of STAT3 signaling in human liver cancer cells using Evista. The 107th Annual Meeting of the American Association for Cancer Research; 2016 Apr 16-20; New Orleans, LA.
Da Silva, Lais; Song, Jinhua; Matthews, James; Jiang, Jinmai; Luesch, Hendrik; Li, Chenglong; Schmittgen, Thomas D. Inhibition of pancreatic acinar ductal metaplasia by a novel STAT3 inhibitor LLL12B. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019. MEDI-0304

Schultz, Daniel; Mao, Liguang; Shi, Guqin; Zhou, Wei; Huigens, Robert; Li, Chenglong. Structure-based drug design towards small molecule interleukin-6 inhibitors. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019. MEDI-0024

Yang, Xiaozhi; Zhou, Wei; Li, Chenglong. Discovery of SAM competitive and non-nucleoside derivative PRMT5 inhibitors with potent antitumor activity. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019. MEDI-0080

Zhou, Wei; Yang, Xiaozhi; Li, Chenglong. Biochemical study of human PRMT5 and its structure-based designer small molecule inhibitors for potential cancer therapeutics. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019. BIOL-0070

Rezaei, Mohammad; Li, Yanjun; Li, Xiaolin; Li, Chenglong. Improving the prediction of protein-ligand binding affinity using deep learning models. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019. COMP-0391

Zhou, Wei; Li, Yiping; Song, Jinhua; Li, Chenglong. Development of a fluorescence polarization assay for the identification and evaluation of inhibitors at the Ω-loop region of the YAP-TEAD protein-protein interface (PPI). 258th ACS National Meeting & Exposition, San Diego, CA, United States, August 25-29, 2019. BIOL-0195

Zhou, Wei; Yang, Xiaozhi; Yadav, Gaya P.; Jiang, Qiu-xing; Li, Chenglong. Structural and biochemical study of human PRMT5 and its peptide-competitive MTA-synergistic small molecule inhibitors for cancer therapeutics. 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020. MEDI-0268

Collaborators (past and present**)**

Dr. Robert Baiocchi, Division of Hematology, Internal Medicine, College of Medicine, The Ohio State University.

Dr. Comfort Boateng, Division of Pharmaceutical Sciences, High Point University.

Dr. Regine Bohacek, Boston *De Novo* Design, Boston, MA

Dr. Marie Hanigan, University of Oklahoma Health Sciences Center.

Dr. Chang-Deng Hu, Medicinal Chemistry and Molecular Pharmacology, Purdue University.
Dr. Robert Huigens III, Department of Medicinal Chemistry, University of Florida, Gainesville, FL.

Dr. Ralf Janknecht, Department of Cell Biology, College of Medicine, University of Oklahoma.

Dr. Joseph Kissil, Scripps Florida.

Dr. Jose Lemos, Center for Molecular Microbiology, University of Florida.

Dr. Yanjun Li, Department of Medicinal Chemistry, University of Florida.

Dr. Jiayuh Lin, Department of Biochemistry and Molecular Biology, University of Maryland, Baltimore, MD.

Dr. Hendrik Luesch, Debbie and Sylvia DeSantis Chair in Natural Products Drug Discovery and Development;

Professor and Chair of the Department of Medicinal Chemistry, University of Florida, Gainesville, FL.

Dr. Duane Mitchell, Center for Brain Tumor Therapy, University of Florida.

Dr. Arthur Olson, Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA.

Dr. Liya Pi, Department of Pathology and Laboratory Medicine, Tulane University School of Medicine.

Dr. Michael Racke, Department of Neurology, The Ohio State University.

Dr. Thomas Schmittgen, Chair of Pharmaceutics and The V. Ravi Chandran Professor of Pharmaceutical Sciences, University of Florida, Gainesville, FL.

Dr. Eric Sorscher, Hertz Professor, School of Medicine, Emory University, Atlanta, GA.

Dr. Gloria Su, Professor, Columbia University, NYC, NY.

Dr. John Z. H. Zhang, Department of Chemistry, New York University.

Dr. Xiaohong (Mary) Zhang, Department of Pathology and Cell Biology, College of Medicine, University of South Florida, Tampa, FL.

Dr. Zhe Jiang, Department of Computer & Information Science & Engineering, University of Florida.

Faculty Hosted

Dr. Arthur Olson, Anderson Chair, Department of Molecular Biology, The Scripps Research Institute. Visiting the Ohio State Biochemical Program (OSBP) on Feb. 19-21, 2007.

Dr. Weifan Zheng, BRITE Institute, North Carolina Central University. Visiting the College of Pharmacy on Nov. 13-15, 2007.

Dr. Regine Bohacek, Boston *De Novo* Design. Visiting the College of Pharmacy on Feb. 19-21, 2008.

Dr. Vern Schramm, Member of National Academy, Professor & Ruth Merns Chair in Biochemistry, Department of Biochemistry, Albert Einstein College of Medicine. Visiting the Ohio State Biochemical Program (OSBP) on March 2-4, 2009. Co-hosting with Dr. Dongping Zhong of Physics.

Dr. Ruth Nussinov, NIH/NCI and Tel Aviv. Visiting the Biophysics Program on Oct. 15, 2009.

Dr. Peter Houghton, Nationwide Children's Research Institute. Visiting the College of Pharmacy on Dec. 2, 2009.

Dr. Brian Shoichet, UCSF. Visiting the College of Pharmacy on Nov. 13, 2014 at the invitation of Dean Mann.

Dr. Shaomeng Wang, Warner-Lambert/Parke-Davis Professor in Medicine, Professor of Medicine, Pharmacology and Medicinal Chemistry, Co-Editors-in-Chief, Journal of Medicinal Chemistry, University of Michigan, March 6, 2019.

Dr. Haian Fu, Professor and Chair, Department of Pharmacology and Chemical Biology, Winship Partner in Research Endowed Chair, Emory University, Atlanta, GA. April 28, 2021.

Graduate Committee Services (not complete/updated)

a) final defense (Ph.D.)

Cen Ling (Biochemistry/OSBP, 2007)
Jason Fowler (Biochemistry/OSBP, 2009)
Janos Nadas (Organic Chemistry, 2009)
Justin Link (Biological Physics, 2009)
Erik Hill (Biochemistry/OSBP, 2010)
Joseph Huang (Medicinal Chemistry, 2010)
Ya-Ting Kao (Physical Chemistry, 2010)
Luyuan Zhang (Chemical Physics, 2010)
Yu Kay Law (Biophysics, 2010)
In Hee Park (Chemical Physics, 2010)
Justin Link (Biological Physics, 2011)
Yu-Yu Liu (Biochemistry/OSBP, 2011)
Ting-Fang He (Biochemistry/OSBP, 2011)
Tanping Li (Biophysics, 2011)
Nicholas Regan (Medicinal Chemistry, 2011)
Brandon Henderson (Pharmacology, 2011)
Deepak Bhasin (Medicinal Chemistry, 2011)
Veer Bhatt (Biophysics, 2011)
Vandana Kumari (Medicinal Chemistry, 2011)
Yihui Ma (Medicinal Chemistry, 2011)
Huameng Li (Biophysics, 2011)
Kiran V. Mahasenan (Medicinal Chemistry, 2012)
Hong Sun (Computer Science, 2012)
Jong-Kook Park (Pharmaceutics, 2012)
Chuan Tan (Biophysics, 2013)
Jonathan Etter (Medicinal Chemistry, 2013)
Wenying Yu (Medicinal Chemistry, 2013)
Somsundaram Chettiar (Medicinal Chemistry, 2013)
En-Chi (Andrew) Hsu (Medicinal Chemistry, 2014)
Ryan E. Pavlovicz (Biophysics, 2014)
Eric Schwartz (Medicinal Chemistry, 2015)
Bobo Shi (Biophysics, 2016)
Guangde Jiang (Medicinal Chemistry, 2019)
Xiao Liang (Medicinal Chemistry, 2019)
Mohammad Rezaei (Chemistry, 2019)
Julie Bray (Cancer Biology, 2020)
Peilan Zhang (Medicinal Chemistry, 2020)
Wei Zhou (Biochemistry, 2020)
Xiaozhi Yang (Medicinal Chemistry, 2021)
Kelton Schleyer (Medicinal Chemistry, 2021)
Yanjun Li (Computer Science, 2021)
Daniel Schultz (Medicinal Chemistry, 2022)
Jake Zhu (Chemistry, 2022)
Garret Rubin (Medicinal Chemistry, 2023)

b) candidacy exam

Cen Ling (Biochemistry, 2006)
Justin Link (Biological Physics, 2006)
Yu-Yu Liu (Biochemistry, 2006)
Jason Fowler (Biochemistry, 2007)
Jacqueline Lieblein (Biochemistry, 2007)
Rohit Tiwari (Medicinal Chemistry, 2007)
Ting-Fang He (Biochemistry, 2007)
Yu Kay Law (Biophysics, 2007)
Hong Sun (Computer Science, 2008)

In Hee Park (Chemical Physics, 2008)
Erik Hill (Biochemistry, 2008)
Janos Nadas (Organic Chemistry, 2008)
Brian Hutzen (Biochemistry, 2008)
Luyuan Zhang (Chemical Physics, 2008)
Chen Zang (Biological Physics, 2008)
Chuang Tan (Chemical Physics, 2008)
Tanping Li (Biophysics, 2008)
Ya-Ting Kao (Physical Chemistry, 2008)
Nicholas Regan (Medicinal Chemistry, 2008)
Brandon Henderson (Pharmacology, 2009)
Vandana Kumari (Medicinal Chemistry, 2009)
Joseph Huang (Medicinal Chemistry, 2009)
Sarah Ball (Biochemistry, 2009)
Yihui Ma (Medicinal Chemistry, 2009)

Thomas Haver (Biophysics, 2010)
Jonathan Etter (Medicinal Chemistry, 2010)
Deepak Bhasin (Medicinal Chemistry, 2010)
Jo Marie Bacusmo (Organic Chemistry, 2010)
David Mata (Organic Chemistry, 2010)
Huameng Li (Biophysics, 2010)
Kiran Mahasenan (Medicinal Chemistry, 2010)
Veer Bhatt (Biophysics, 2010)
Ryan Pavlovicz (Biophysics, 2011)
Wenying Yu (Medicinal Chemistry, 2012)
En-Chi (Andrew) Hsu (Medicinal Chemistry, 2012)
Hongshan Lai (Medicinal Chemistry, 2013)
Eric Schwartz (Medicinal Chemistry, 2013)
Bobo Shi (Biophysics, 2013)
Liguang Mao (Medicinal Chemistry, 2014)
Guqin Shi (Medicinal Chemistry, 2014)
Ahmed Abdelhameed (Medicinal Chemistry, 2014)
Janet Addae (Medicinal Chemistry, 2014)
Jack Tokarsky (Biophysics, 2015)
Wei Zhou (Biochemistry, 2015)
Kevin MaGarry (Biochemistry, 2015)
Linsen Li (Medicinal Chemistry, 2015)
Mohammad Ali Rezaei (Biophysics, 2016)
E. John Paul Tokarsky (Biophysics, 2016)
Xiao Luo (Pharmaceutics, 2016)
Julie Bray (Biomedical Sciences, 2017)
Guangde Jiang (Medicinal Chemistry, 2018)
Xiao Liang (Medicinal Chemistry, 2018)
Lais Da Silva (Pharmaceutics, 2018)
Peilan Zhang (Medicinal Chemistry, 2018)
Sutonuke Bhar (Cell Biology, 2018)
Xiaozhi Yang, (Medicinal Chemistry, 2019)
Manyun Chen (Medicinal Chemistry, 2020)
Yanjun Li (Computer Science, 2020)
Daniel Schultz (Medicinal Chemistry, 2020)
Garret Rubin (Medicinal Chemistry, 2020)
Chen Zhou (Medicinal Chemistry, 2022)
Jordan Stocks (Pharmaceutics, 2022)
Zhihang Shen (Medicinal Chemistry, 2023)
Yuzhao Zhang (Medicinal Chemistry, 2023)

Teaching

I love teaching to undergraduate, graduate and professional students. During my education, I was lucky to have many inspirational teachers, such as Professors Xuanshen Yan for inorganic chemistry, Gong-Du Zhou for structural chemistry and Zhaoxuan Zhu for nonlinear mechanics at Beijing University; Professors Benjamin Widom for statistical physics, Jon Clardy for crystallography and Gerry Feigenson for biochemistry at Cornell University. I have learned a lot from them and have been trying to apply the art of teaching to my students.

To me, teaching has to be a creative process in re-discovering knowledge and refining concepts and principles along the way. This makes learning as a lively "research" effort, and easier to grasp the most important/fundamental knowledge and skills, and bridges learning and research together.

I can teach medicinal chemistry, physical chemistry, computational chemistry, biochemistry/biophysics and molecular modeling and design.

Teaching courses:

a) graduate level

Pharm 8380 "Structure-based Computer-aided Molecular Design". I have been developing this biennial course since 2006. So far it has been taught in Spring Quarters of 2007 and 2009 and Spring Semester 2013. It covers topics like basic quantum chemistry, molecular mechanics, conformational sampling, molecular docking, virtual screening, fragment-based design, transition-state analog design, structure-based optimization, molecular dynamics at QM, MM and course-grained levels, free energy calculation, cheminformatics, library design, QSAR/QSPR, ADMT/Tox prediction.

Molbioc 7840 "Practical protein crystallography". I have been co-developing this biennial course with Dr. Charles Bell. So far it has been taught in summers of 2006 and 2008. Now Dr. Kotaro Nakanishi also teaches part of the course and we plan to resume it biennially. It covers basic diffraction physics, crystallography, phase problem, crystallization, instrumentation including synchrotron radiation, data collection and processing, molecular replacement, isomorphous replacement, anomalous diffraction phasing, density modification, model building and refinement, structural analysis and validation.

Pharm 7350 "Drug design and discovery". Offered each Spring. Four lectures on computer-aided design section covering molecular mechanics, molecular docking, structure-based optimization, QSAR.

Biochem 8990 "Advanced Topics in Biochemistry". Offered each year. One guest lecture on computational biochemistry each year.

PHA 6935 "Life Cycle of A Drug". Offered each year. One lecture on Structure-based Drug Design.

PHA 6936 "Drug Design II". Offered each Spring. Course coordinator. Five lectures on Computer-aided and AI-based Drug Design.

b) undergraduate level

Pharm 4100 "Biomedicinal Chemistry". Offered each Autumn. Fourteen lectures and four recitation sessions (40% for the total course). Topics cover protein structure, dynamics and function; enzyme mechanism, kinetics, regulation and inhibition; membrane transport; signaling transduction and drugs affecting signaling.

Pharm 4200 "Introduction to Medicinal Chemistry". Offered each Spring. Six lectures and two recitation sessions (20% for the total course). Topics cover molecular mechanics, molecular docking, molecular dynamics, QSAR and ADME/Tox modeling.

c) PharmD level

PHA5787C “Patient Care 5: Medicinal Chemistry of Diabetic Drugs”. Offered every Spring. Topics cover all types of drugs for diabetic therapy.

PHA5788C “Patient Care 6: Medicinal Chemistry of Non-Opioid Treatment Options: NSAIDS, Acetaminophen, Skeletal Muscle Relaxants, Common Adjuvant agents”. Offered every Autumn.