

Curriculum Vitae

Chenglong Li

Research Focus

Dr. Li's scholarly interests range from organic chemistry, biochemistry, medicinal chemistry 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, synthetic chemistry, X-ray protein crystallography, thermodynamic measurements, cellular techniques and *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) design and discovery of drugs targeting the IL-6/STAT3 inflammatory and oncogenic pathway for targeted therapy; 3) design and discovery of drugs targeting epigenetic histone arginine methylation enzymes, especially PRMT5; 4) design and discovery of drugs targeting specific nAChR and ASIC1 subtypes for drug addiction and neurodegenerative diseases; 5) design and discovery of "chemical chaperone" drugs targeting Δ F508 NBD1 misfolding intermediates for potential cystic fibrosis therapy.

- h-index: 34
- RG score: 42.08 (higher than 97.5% ResearchGate members)
- First-in-Class PRMT5-targeting epigenetic drug commercialization development licensing agreement signed with Prelude Therapeutics, Inc.
- NIH DDNS (Drug Discovery for the Nervous System) study section regular membership.

Contact Info

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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

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

Graduate Faculty Positions

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

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 biophysical chemistry, 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 or Adjunct 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
Guest Professorship	The University of Science and Technology of China (USTC)
Adjunct Professorship	Hong Kong Baptist University

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 pilot award, 2009.
Department of Defense Idea Grant Award, 2010.

Professional Service

a) Organizational duty

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

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

b) Grant reviewers

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

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-R²), 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 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
Proteins: Structure, Function, and Bioinformatics
Bioorganic & Medicinal Chemistry Letters
European Journal of Medicinal Chemistry
Medicinal Chemistry Communications
Cancer Research
Frontiers in Bioscience
BMC Genomics
Current Pharmaceutical Design
Chemical Biology & Drug Design
Current Chemical Genomics
Expert Opinion on Drug Discovery
Expert Opinion On Therapeutic Patents
Biochimie
Drug Discovery Today

Active Grants

a) as PI

“Small molecule *in vivo* probe development targeting the IL-6/STAT3 pathway for potential multiple sclerosis therapy”, PI: Chenglong Li, NIH/NINDS, 1R01NS088437-01A1, \$1,407,754, May 1, 2015 – April 30, 2018.

“A novel STAT3-selective inhibitor for medulloblastoma therapy”, mPI: Chenglong Li and Jiayuh Lin, NIH/NINDS, 1R01NS087213-01A1, \$1,660,665, July 1, 2015 – June 30, 2020.

“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, 2016.

b) as Co-I

“Studies of Childhood Sarcomas”, PI: Peter Houghton. Medicinal Chemistry and project 2: Chenglong Li. NIH/NCI (5P01CA165995-03). \$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, 1R21CA191751-01, \$426,688, Feb. 1, 2015 – Jan. 31, 2017.

“Role of HDAC6 in Platinum Resistance of Non-small Cell Lung Cancer”, PI: Xiaohong “Mary” Zhang, NIH/NCI (5R01CA164147-04), \$135,213.00, May 1, 2012 – April, 30, 2017.

“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.

“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.

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

“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.

Completed Grants

“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.

“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 Heterohexameric 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 – February 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.

Current Pending Grants

a) as PI

“Role and targeting of PRMT5 in prostate cancer”, mPI: Chenglong Li and Chang-Deng Hu, NIH/NCI, 1R01CA212403-01, \$ 2,780,638.00, Dec. 1, 2016 – Nov. 30, 2021.

b) as Co-I

“Mechanistic studies of the structure, function and inhibition of gamma-glutamyl transpeptidase: a novel therapeutic target”, PI: Marie Hannigan, NIH/NIGMS, \$591,360.00, Dec. 1, 2016 – Nov. 30, 2020.

Research Group/Lab Personnel (“Bold” marks current members)

a) Visiting Professors/Scientists

Yuepiao Cai, Ph.D., associate professor, 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., associate professor, department of pharmaceutical sciences, college of medicine, Xi’an Jiao-Tong University, Xi’an, China. 2/1/2010 – 7/31/2010. Working on lead discovery through virtual library screening, molecular dynamics simulation and binding free energy calculation.

Xiaojie Zhang, M. Sc., 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, M. Sc., 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.

b) Research Staff Scientists

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

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.

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. Now a postdoctoral scientist at NCI/NIH. She won the College of Pharmacy 2010-2011 Jane Chen Fellowship.

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 postdoc scientist at the University of Notre Dame. He won the College of Pharmacy 2009 Jack Beal Award.

Wenyong Yu, Ph.D. in Medicinal Chemistry. 4/1/2010 – 8/20/2013. Currently an Assistant 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.

e) Post-candidacy Ph.D. graduate students

Liguang Mao, M. Sc. in Medicinal Chemistry, 9/21/2011 – present, Currently in the graduate field of Medicinal Chemistry.

Guqin Shi, B.Sc. in Bioinformatics. 9/21/2011 – present, Currently in the graduate field of Medicinal Chemistry.

Wei Zhou, B. Sc. in Biochemistry. 2/28/2014 – present. Currently in the graduate field of Biochemistry (OSBP).

Linsen Li, B. Sc. in Chemistry. 8/21/2013 – present. Currently in the graduate field of Medicinal Chemistry.

Mohammad Ali Rezaei, M. Sc. in Biophysics. 5/1/2013 – present. Currently in the graduate field of Biophysics.

f) Pre-candidacy Ph.D. graduate students

Katherine Biggs, B. Sc. in Chemistry. 1/1/2013 – 12/31/2014. Obtained Pharm. D. and stopped to pursue PharmD/PhD dual degrees.

Nicolas Cockroft, B. Sc. in Chemistry. 8/21/2014 – present. Currently in the Chemistry-Biology Interface (CBI) Fellowship Program.

Xiaozhi Yang, M. Sc. in Medicinal Chemistry. 8/21/2014 – present. Currently in the 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.

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, 4th-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, 3rd-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.

Publications (Total: 107 peer-reviewed original research journal articles; independent work: 89 articles)

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

i) as Corresponding Author or Co-Corresponding Author

Tarighat, S. S., Santhanam, R., Frankhouser, D., Radomska, H. S., Lai, H., Anghelina, M., Wang, H., Huang, X., Alinari, L., Walker, A., Caligiuri, M. A., Croce, C. M., Li, L., Garzon, R., **Li, C.**, Baiocchi, R. A. and Marcucci, G. The dual epigenetic role of PRMT5 in acute myeloid leukemia: gene activation and repression via histone arginine methylation. ***Leukemia***, 2016, **30**, 789-799.

Alinari, L., Mahasenan, K. V., Yan, F., Karkhanis, V., Chung, J.-H., Smith, E. M., Quinion, C., Smith, P. L., Kim, L., Patton, J. T., Lapalombella, R., Yu, B., Wu, Y., Roy, S., De Leo, A., Pileri, S., Agostinelli, C., Bradner, J. E., Chen-Kiang, S., Elemento, O., Motiwala, T., Majumder, S., Byrd, J. C., Jacob, S., Sif, S, **Li, C.** and Baiocchi, R. A. Selective inhibition of protein arginine methyltransferase 5 blocks initiation and maintenance of B-cell transformation. ***Blood***, 2015, **125**, 2530-2543.

(impact factor: 9.775)

Li, H., Xiao, H., Lin, L., Jou, D., Kumari, V., Lin, J. and **Li, C.** Drug Design Targeting Protein–Protein Interactions (PPIs) Using Multiple Ligand Simultaneous Docking (MLSD) and Drug Repositioning: Discovery of Raloxifene and Bazedoxifene as Novel Inhibitors of IL-6/GP130 Interface. ***J. Med. Chem.***, 2014, **57**, 632-641. (Impact factor: 5.614)

Lai, H., Gallucci, J. C. and **Li, C.** N-[2-(9H-Carbazol-9-yl)ethyl]-4-(methylsulfonyl) aniline. ***Acta Cryst. E.***, 2014, **E70**, o332.

Lai, H., Gallucci, J. C. and **Li, C.** (E)-3-(9-Ethyl-9H-carbazol-3-yl)-1-(2-methoxyphenyl)prop-2-en-1-one. ***Acta Cryst. E.***, 2014, **E70**, o190.

Yu, W. and **Li, C.** Regioselective one-pot C-N coupling of substituted naphthoquinones: selective intramolecular ring fusion of sulfonamides. ***Tetrahedron***, 2014, **70**, 459-464.

(Impact factor: 2.803; 5-year IF: 2.899)

Chettiar, S. N., Cooley, J. V., Park, I.-H., Bhasin, D., Chakravarti, A., Li, P.-K., **Li, C.** and Jacob, N. K. Design, synthesis and biological studies of Survivin Dimerization Modulators that prolong mitotic cycle. ***Bioorg. Medicinal. Chem. Lett.***, 2013, **23**, 5429–5433.

Yu, W., Lin, J., Xiao, H. and **Li, C.** Discovery of Novel STAT3 Small Molecule Inhibitors via In Silico Site-Directed Fragment-Based Drug Design. ***J. Med. Chem.***, 2013, **56**, 4402-4412.

(Impact factor: 5.614; 5-year IF: 5.383)

Yu, W. and **Li, C.** 4-Nitro-phenyl N-(2-sulfamoylphen-yl)carbamate. ***Acta Cryst. E.***, 2013, **E69**, o355.

Mahasenan, K. V., **Li, C.** Novel inhibitor discovery through virtual screening against multiple protein conformations generated via ligand-directed modeling: a maternal embryonic leucine zipper kinase example. ***J. Chem. Info. & Modeling.***, 2012, **52**, 1345-1355.

(Impact Factor: 4.675; 5-year IF: 4.305)

Mahasenan, K. V., Pavlovicz, R. E., Henderson, B. J., Gonzalez-Cestari, T. F., Yi, B., McKay, D. B. and **Li, C.** Discovery of novel $\alpha 4\beta 2$ neuronal nicotinic receptor modulators through structure-based virtual screening. ***ACS Med. Chem. Lett.***, 2011, **2**, 855-860.

(Impact Factor: 3.355; 5-year IF: 3.355)

Pavlovicz, R. E., Henderson, B. J., Bonnell, A. B., Boyd, R. T., McKay, D. B. and Li, C. Identification of a negative allosteric site on human $\alpha 4\beta 2$ and $\alpha 3\beta 4$ neuronal nicotinic acetylcholine receptors. ***PLoS ONE***, 2011, **6**, e24949.

(Impact Factor: 4.092; 5-year IF: 4.537)

Li, H., Liu, A., Zhao, Z., Xu, Y., Lin, J., Jou, D. and Li, C. Fragment-based Drug Design and Drug Repositioning Using Multiple Ligand Simultaneous Docking (MLSD): Identifying Celecoxib and Template Compounds as Novel Inhibitors of Signal Transducer and Activator of Transcription 3 (STAT3). ***J. Med. Chem.***, 2011, **54**, 5592-5596.

(Impact Factor: 5.248; 5-year IF: 5.321)

Park, I.-H., and Li, C. Characterization of Molecular Recognition of STAT3 SH2 Domain Inhibitors through Molecular Simulation. ***J. Mol. Recog.***, 2011, **24**, 254-265.

(Impact Factor: 3.310; 5-year IF: 3.375)

Park, I.-H., and Li, C. Dynamic Ligand-Induced-Fit Simulation via Enhanced Conformational Samplings and Ensemble Dockings: A Survivin Example. ***J. Phys. Chem. B***, 2010, **114**, 5144-5153.

(Impact Factor: 3.696; 5-year IF: 4.061)

Li, H. and Li, C. Multiple Ligand Simultaneous Docking (MLSD): Orchestrated Dancing of Ligands in Binding Sites of Protein. ***J. Comp. Chem.***, 2010, **31**, 2014-2022.

(Impact Factor: 4.583; 5-year IF: 4.795)

Lin, L., Hutzen, B., Li, P.-K., Ball, S., Zuo, M., DeAngelis, S., Foust, E., Sobo, M., Friedman, L., Bhasin, D., Cen, L., Li, C. and Lin, J. A novel small molecule, LLL12 inhibits STAT3 phosphorylation and activities and exhibits potent growth suppressive activity in human cancer cells. ***Neoplasia***, 2010, **12**, 39-50.

(Impact Factor: 5.946; 5-year IF: 5.133)

Kumari, V., Farah, M. B., Langer, S. Z., Li, C. and Patil, P. N. Stereoselectivity of Norepinephrine Enantiomers at Pre- and Post-Junctional Adrenoceptors. ***Biogenic Amines: Pharmacological, Neurochemical and Molecular Aspects in the CNS(Book Chapter 12)***, Nova Science Publishers, published, December 2009.

(Impact Factor: N/A, book chapter)

Kumari, V. and Li, C. Comparative Docking Assessment of Glucokinase Interactions with Its Allosteric Activators. ***Current Chemical Genomics***, 2008, **2**, 76-89. (Invited contribution)

(Impact Factor: N/A)

ii) as Co-Author

Wu, X., Cao, Y., Xiao, W., Li, C. and Lin, J. Bazedoxifene as a Novel GP130 Inhibitor for Pancreatic Cancer Therapy. ***Mol. Cancer Ther.***, 2016, accepted.

Wu, X., Xiao, H., Wang, R., Liu, L., Li, C. and Lin, J. Persistent GP130/STAT3 Signaling Contributes to the Resistance of Doxorubicin, Cisplatin, and MEK Inhibitor in Human Rhabdomyosarcoma Cells. ***Curr. Cancer Drug Targets***, 2016, accepted.

Zhao, C., Wang, W., Yu, W., Jou, D., Wang, Y., Ma, H., Xiao, H., Qin, H., Zhang, C., Lu, J., Li, S., Li, C., Lin, J. and Lin, L. A Novel Small Molecule STAT3 Inhibitor, LY5, Inhibits Cell Viability, Colony Formation, and Migration of Colon and Liver Cancer Cells. ***Oncotarget***, 2016, **7**, 12917-12926.

Fu, W., Chen, L., Wang, Z., Zhao, C., Chen, G., Liu, X., Dai, Y., Cai, Y., Li, C., Zhou, J. and Liang, G. Determination of the binding mode for anti-inflammatory natural product xanthohumol with myeloid differentiation protein 2. ***Drug Design Dev. and Therapy***, 2016, **10**, 455-463.

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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.

Patents

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.

Li, P.-K., Li, C., Lin, J. Transcription factor inhibitors and related compositions, formulations and methods . PCT Int. Appl. (2011), WO 2011066263 A1 20110603. Language: English, Database: CAPLUS. STAT3 inhibitors, especially LLL12.

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Li, P.-K., Li, C., Lin, J., Fuchs, J. Curcumin analogs as dual JAK2/STAT3 inhibitors and methods of making and using the same . WO2010121007 (A1) 2010-10-21.

Baiocchi, R. A.; Li, C.; Lai, H.; Sif, S. Preparation of carbazole derivatives as inhibitors of prmt5. WO2014145214 (A2) 2014-09-18; WO2014145214 (A3) 2015-01-08.

Fuchs, J. R.; Li, C.; Li, P.-K.; Lin, J. Small molecule inhibitors of IL-6 and uses thereof. WO2013019690 (A1)

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Mohler, P.; Carnes, C.; Li, C.; Hund, T.; Li, P.-K. PP2A regulatory subunit modification in disease. US2014/0031291 A1, 2014-1-30.

Li, C.; Lin, J.; Wang, H. Compound XZH-5 inhibits constitutive and interleukin-6-induced STAT3 phosphorylation in human hepatocellular carcinoma cells. WO2012078982 (A2) 2012-06-14; WO2012078982 (A3) 2012-09-07.

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.

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/
- Science 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 oncogenic cycle involving Sp1/NF κ B/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>

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>

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)”.

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

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).

Wenyong 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 Targets, 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 β 2 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 γ S-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 $\alpha 4\beta 2$ and $\alpha 3\beta 4$ 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, Wenyong, 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.

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 chemoprevention 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.

Lin L, Zuo M, DeAngelis S, Li C, Li P-K, and Lin J. Target constitutive STAT3 pathway in Glioblastoma cells with a novel small molecular STAT3 inhibitor. The abstract was presented at the AACR Brain Tumor Meeting (San Diego, CA, Dec 13 – 15, 2009).

Ball S, Li C, Li P-K, and Lin J. Target constitutive STAT3 signaling in human medulablastoma cells with a novel small molecular STAT3 inhibitor. The abstract was presented at the AACR Brain Tumor Meeting (San Diego, CA, Dec 13 – 15, 2009).

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

Lin L., Hutzen B, Peng Z., Lin H., Li P-K., Li C., Wicha M., and Lin J. STAT3 is required for survival of human breast cancer stem cells. The abstract was presented at the AACR Annual Meeting (Washington DC, Apr 3 – 7, 2010) Received an AACR top-rated abstract award.

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.

Liu, A., Liu, Y., Xu, Z., Yu, W., Wang, H., Li, C. and Lin, J. A novel small molecule, XZH-5 inhibits constitutive and interleukin-6-induced STAT3 phosphorylation in human rhabdomyosarcoma cells. The 102nd AACR Annual Meeting, Orlando, Florida, April 6, 2011.

Demir, H., Ray-Chaudhury, A., Li, T., Li, C. and Nakano, I. Targeting therapy-resistant glioma cells with novel compounds that inhibit action of survivin. The 102nd AACR Annual Meeting, Orlando, Florida, April 5, 2011.

Lin, L., Li, P.-K., Fuchs, J., Li, C. and Lin, J. STAT3 is necessary for proliferation and survival in pancreatic cancer-initiating cells. The 102nd AACR Annual Meeting, Orlando, Florida, April 4, 2011.

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.

Jena, Nivedita; Hambira, Chido; Kumari, Vandana; Mok, May; Lin, Li; Li, Pui-Kai; Li, Jiayuh; Li, Chenglong; Fuchs, James R. Madindoline A as a lead for the development of new class of IL-6/GP130 homodimerization inhibitors. The 246th ACS National Meeting & Exposition, Indianapolis, IN, September 8-12, 2013.

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.

Collaborators

Dr. Candice Askwith, Neuroscience Program, The Ohio State University.

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

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

Dr. Chang-Deng Hu, Medicinal Chemistry and Molecular Pharmacology, Purdue University.

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

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

Dr. Hendrik Luesch, Department of Medicinal Chemistry, University of Florida, Gainesville, FL.

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

Dr. Mitch Phelps, Division of Pharmaceutics, College of Pharmacy, The Ohio State University.

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

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

Dr. David Wald, Divisions of Clinical and Experimental Pathology, Case Western Reserve University.

Dr. Yusu Wang, Computer Science and Engineering, The Ohio State University.

Dr. Karl Werbovetz, Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University.

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.

Faculty Hosted

Dr. Arthur Olson, 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, 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.

Graduate Committee Services

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)
Wenyong 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)

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)
Wenyong 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)

Teaching

I love teaching to undergraduate students and graduate 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 physical chemistry, computational chemistry, biochemistry/biophysics and molecular design.

Overall, my graduate teaching has been excellent. For undergraduate teaching, peer reviews are excellent. Curiously, student evaluation SEI dropped a little. I think that the main reasons are as follows.

1) The SEI is collected electronically, not in-class like before. The response rate is much lower for me, unlike in-class (close to 100%). I suspect that typically, the responding students are the ones who have lower grades and have complaints. 2) Most of our BSPS students aim for PharmD or other professional track, not for graduate research direction. My part of teaching is heavily physical chemistry/biophysics oriented. The students probably either have a bit weaker background or are not interested in these concepts and relatively abstract/quantitative relationships/models. However, I shall hold on certain standards as we are one of the top Colleges of Pharmacies in the country and I firmly believe that it'd be beneficial to them in the long run.

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, ADMET/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.

b) undergraduate level

Pharm 4100 “Biomedical 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.