



## CURRICULUM VITAE

### Personal Information

Name: JingYuan Liu  
Work Address: 2443 Derek Dr. Carmel, Indiana  
Telephone: (317) 341-1100 (cell)  
E-mail: JingYuan.Liu@UToledo.Edu

### Education

|           |                                |                                                                                         |
|-----------|--------------------------------|-----------------------------------------------------------------------------------------|
| 1991-1995 | B.Sc. in Biochemistry          | Department of Biochemistry<br>Shandong University, China                                |
| 1995-1998 | M.Sc. in Molecular Genetics    | Institute of Genetics<br>Chinese Academy of Sciences, China                             |
| 1998-2004 | Ph.D. in Structure Biology     | Department of Biochemistry & Molecular Biology<br>Indiana University School of Medicine |
| 2006-2011 | Postdoc in Computation Biology | Department of Medical & Molecular Genetics<br>Indiana University School of Medicine     |

### Positions

|              |                                                                                                                                          |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------|
| 2012-present | Assistant Professor, Department of Pharmacology and Toxicology, Indiana University School of Medicine, Indianapolis, IN                  |
| 2012-present | Assistant Professor, Department of Computer and Information Science, Indiana University Purdue University Indianapolis, Indianapolis, IN |
| 2013-present | Member, Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN                     |

### Honors

|      |                                                                           |
|------|---------------------------------------------------------------------------|
| 1994 | Annual Outstanding Student Award, Shandong University                     |
| 2002 | Outstanding Departmental Poster Presentation Award, IU School of Medicine |
| 2004 | Travel award, 10th SCBA International Meeting                             |
| 2005 | Ralph W. and Grace M. Showalter Research Trust Young Investigator Award   |

### Teaching Activities

|           |                                                                                                                                                          |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
|           | CSCI590 Algorithms for Bioinformatics, 3 hours/week                                                                                                      |
| 2012-2014 | Graduate core course (14 lectures, 3 homework, 2 projects and 2 exams)<br>Number of students: Varies each year. About 15-25/Year.<br>Role: Sole lecturer |

### Student and Fellow Mentoring Activities

#### Master students

Abhinav Kuru (M.Sc., 2012)  
Divya Neelagiri (M.Sc., 2013)  
Hema Kasi (M.Sc., 2014)  
Vinit Shah (M.Sc., 2016)

#### Ph.D. Students

Valerie Fako (Ph.D., 2014)



JoAnne Babula (Ph.D. expected 2019)  
Catherine Rajendran (Ph.D. expected 2023)

**Postdoctoral fellow**

Ravi Yadav (2012-2013)  
Taolan Zhang (2018-present)

**Professional Services**

|              |                                                                                 |
|--------------|---------------------------------------------------------------------------------|
| 2012-present | Associate Editorial Board Member, Int. J. Biochem Mol Biol                      |
| 2013-present | Advisory Board Member, Current Cancer Drug Target                               |
| 2014-present | Editorial Board Member, Aperiato Journal of Computer Science and Biology        |
| 2015-present | Editorial Board Member, Journal of Bioinformatics and Comparative Genomics      |
| 2015-present | Reviewer, Physical Chemistry, Theoretical and Computational Chemistry           |
| 2015-present | Reviewer, Cellular and Molecular Life Sciences                                  |
| 2015-present | Reviewer, American Journal of Chemical Information and Modeling                 |
| 2017         | Grant Reviewer (Biostatistician), Indiana CTSI                                  |
| 2017         | Grant Reviewer (Biostatistician), Mesothelioma Panel, DoD-PRCRP                 |
| 2018         | Grant Reviewer (Biostatistician), Stomach cancer, DoD-PRCRP                     |
| 2018-2019    | Member, Biochemistry Department Computational Faculty Search & Screen Committee |

**Research Support**

**Active:**

- National Institute Of General Medical Sciences (R01 GM127656)  
Effective targeting survivin dimerization interface with small molecule inhibitors  
Total Costs: \$ 1,757,100 (Direct Costs: \$ 1,117,250); Dates: 2018-2024  
Role: PI
- DOD Breast Cancer Research Program (BC150290)  
Targeting FASN for breast cancer treatment by repositioning PPIs  
Total Costs: \$1,170,000 (Direct Cost: \$750,000); Dates: 2016-2019 (NCE)  
Role: Co-PI
- National Cancer Institute (R01 CA211904)  
Translational control in Wnt/ $\beta$ -catenin signaling and colon tumorigenesis  
Total Costs: \$1,793,515 (Direct Costs: \$1,130,025); Dates: 2017-2022  
Role: Co-I

**Pending**

- NIH/NCI  
A novel STAT3-targeting anti-cancer nanomedicine with dual function and targeted delivery  
Requested Direct Costs: \$2,200,000  
Role: Co-I

**Past**

- Start-Up Fund (Liu) 2012-2015  
The start-up fund is to help Dr. Liu establish her laboratory and independent research career in computational biology and drug discovery.
- IUPUI iM2CS-GEIRE  
Analysis of protein-protein interactions by identification and investigation of the dimerization

cores

Total Costs: \$15,000; Date: 2012-2013

Role: PI

- ACS Institutional Grant  
A novel approach targeting “undruggable” oncogenic protein dimers for drug discovery  
Total Costs: \$40,000; Dates: 2013-2014  
Role: PI
- Showalter Young Investigator Grant  
Characterization of Newly Synthesized Lead Analogs Targeting Survivin for Cancer Treatment  
Total Costs: \$60,000; Dates: 2015-2017  
Role: PI
- NIH/NCI (R41 CA19577)  
A Novel STAT3 Inhibitor Targeting its DNA-Binding Site for Drug Development  
Total Costs: \$225,000 (Direct Costs: \$204,000); Dates: 2016-2018 (NCE)  
Role: PI
- DOD Prostate Cancer Research Program (PC131242)  
Targeting survivin to overcome acquired taxol resistance in prostate cancer chemotherapy Total Costs: \$584,999 (Direct Cost: \$375,000); Dates: 2014-2018 (NCE)  
Role: Co-I

### Invited Presentations

- 2013 Department of Chemistry & Chemical Biology, Indiana University-Purdue University at Indianapolis, Indianapolis, IN
- 2014 Department of Chemistry and Biochemistry, Andrews University, Berrien Springs, MI
- 2015 The 15th SCBA International Symposium, Taipei, Taiwan
- 2015 EDT program, Indiana University, Cancer Center, Indianapolis, IN
- 2016 Bimolecular Science Institute, Florida International University, Miami, FL
- 2018 College of Pharmacy, Ohio State University, Columbus, OH

### Publications (\* corresponding author).

1. Timm, D.E.; **Liu, J.Y.**; Baker, L.J.; Harris, R.A. Crystal structure of thiamin pyrophosphokinase. *J Mol Biol* 310(1): 195-204; 2001.
2. **Liu, J.Y.**; Timm, D.E.; Harris, R.A.; Hurley, T.D. Studies in the structure and function of thiamin pyrophosphokinase. In: Patel MS, Jordan F, editors. Thiamine: Catalytic mechanism and role in normal and disease states. New York: Marcel Dekker. 2002.
3. **Liu, J.Y.**; Timm, D.E.; Hurley, T.D. Pyrithiamine as a substrate for thiamine pyrophosphokinase. *J Biol Chem* 281(10): 6601-6607; 2006
4. Li, Z.; **Liu, J.Y.**; Zhang, J.T. 14-3-3 $\sigma$ , the double-edged sword of human cancers. *Am. J. Transl. Res.* 1:312-324; 2009.
5. Liu, H.; **Liu, J.Y.**; Wu, X.; Zhang, J.T. Biochemistry, molecular biology, and pharmacology of fatty acid synthase, an emerging therapeutic target and diagnosis/prognosis marker. *Int. J. Biochem. Mol. Biol.* 1:69-89; 2010.
6. Neher, T.M.; Shuck, S.C.; **Liu, J.Y.**; Zhang, J.T.; Turchi, J.J. Identification of novel small molecule inhibitors of the XPA protein using *in silico* based screening. *ACS Chem. Biol.* 15:953-965; 2010.
7. **Liu, J.Y.**; Mooney, S. Characterization of Ligand Type of Estrogen Receptor by MD Simulation

- and mm-PBSA Free Energy Analysis. *Int J Biochem Mol Biol* 2(2):190-198; 2011.
8. **Liu, J.Y.**; Hurley, T.D. A new crystal form of mouse thiamin pyrophosphokinase. *Int J Biochem Mol Biol* 2:111-118; 2011.
9. **Liu, J.Y.**\*; Li, Z.; Li, H.; Zhang, J.T. A critical residue that promotes protein dimerization: a story of partially exposed Phe<sup>25</sup> in 14-3-3 $\sigma$ . *J. Chem. Inf. Model.* 51:2612-25; 2011.
10. Mo, W.; **Liu, J.Y.**; Zhang, J.T. Biochemistry and pharmacology of human ABCC1/MRP1 and its role in detoxification and in multidrug resistance of cancer chemotherapy. Recent Advances of Cancer Research and Therapy (ed X.Y. Liu; S. Pestka; Y. Shi). Elsevier pp371-404; 2012
11. Li, Z.; Peng, H.; Qin, L.; Qi, J.; Zuo, X.; **Liu, J.Y.\***; Zhang, J.T\*. Determinants of 14-3-3 $\sigma$  dimerization and function in drug resistance. *J Biol Chem.* 1;288(44):31447-57; 2013
12. Huang, W.; Dong, Z.; Wang, F.; Peng, H.; **Liu, J.Y.\***; and Zhang, J.T.\* A small molecule inhibitor targeting the “undruggable” DNA-binding site of human STAT3 inhibits cancer cell proliferation, migration, and invasion. *ACS Chem. Biol.* 9:1188–1196; 2014. (cover story)
13. Hu, G.; **Liu, J.Y.\***; and Wang, J.\* Insight into conformational change for 14-3-3 $\sigma$  protein by molecular dynamics simulation. *Int. J. Mol. Sci.* 15(2), 2794-2810; 2014.
14. Fako, V.E.; Zhang, J.T.; and **Liu, J.Y.\*** Mechanism of Orlistat Hydrolysis by the Thioesterase of Human Fatty Acid Synthase. *ACS Catal.*, 4, 3444–3453; 2014
15. Fako, V.E.; Pflug, B; **Liu, J.Y.\*** and Zhang, J.T.\* Repositioning Proton Pump Inhibitors as Anti-Cancer Drugs by Targeting the Thioesterase Domain of Human Fatty Acid Synthase. *J. Med. Chem.* 58 (2), 778–784, 2015 (cover story)
16. Babula, J.; **Liu, J.Y.\*** Integrate omics data and molecular dynamics simulation and energy calculation to understand specificity of 14-3-3 isoforms. *J Genet Genomics.* 42:531-547; 2015.
17. Wu, X.; Fako, V.E.; Dong, Z.; Serrano, M.A.; Zou, Y.; **Liu, J.Y.** and Zhang, J.T. FASN regulates cellular response to genotoxic treatments by increasing PARP-1 expression and DNA repair activity via NF-kappa B and SP1. *Proc. Natl. Acad. Sci. USA* 113:E6965–E6973; 2016.
18. Qi, J.; Dong, Z.; Liu, J.; Peery, R.C.; Zhang, S.; **Liu, J.Y.\*** and Zhang, J.T.\* Effective targeting of the survivin dimerization interface with a small molecule inhibitor. *Cancer Res.* 76:453-462; 2016 (cover and editor’s pick as the “must-read” article for the January 15<sup>th</sup> issue in 2016).
19. Huang, W; Dong, Z.; Wang, F.; Chen, Y.; Wang, C.; He, Y.; Hangoc, G.; Pollok, K.; Sandusky, G.; Fu, X.Y.; Broxmeyer, H.; Zhang, Z.Y.; Liu, J.Y.\* and **Zhang, J.T.\*** Small-molecule inhibitors targeting the DNA-binding domain of STAT3 suppress tumor growth, metastasis and STAT3 target gene expression in vivo. *Oncogene* 35:783-792; 2016.
20. Zhang, J.T.; **Liu, J.Y.** Drugging the “undruggable” DNA-binding domain of STAT3. *Oncotarget* 7:66324-66325; 2016.
21. Peery, R.; **Liu, J.Y.** and Zhang, J.T. Targeting survivin for therapeutic discovery: past, present, and future promises. *Drug Discovery Today* 22:1466-1477; 2017.
22. Peery R.C.; **Liu J.Y.** and Zhang J.T. Targeting survivin for therapeutic discovery: past, present, and future promises. *Drug discovery today* 2017; 22(10):1466-1477
23. Li, X.; Ma, X.; Li, L.; Sun, X.; **Liu, J.Y.\***; Zhu, W.\* and Zhang, J.T.\* Novel synthetic bisindolylmaleimide alkaloid analogue inhibits activation of STAT3 and induces apoptosis in human breast cancer cells. *Oncogene* 2018; 37(18):2469-2480
24. Beebe, J.D.; **Liu J.Y.** and Zhang J.T. Two decades of research in discovery of anticancer drugs targeting STAT3, how close are we? *Pharmacology & therapeutics* 2018; 191:74-91
25. Li, D.; Wang, C.J.; Danielson, J.; Zhang, E.H.; Miller, K; Li, L.; Jian-Ting Zhang and **Liu, J.Y.\*** PPI usage benefits breast cancer patient with increased overall survival and reduced recurrence by inhibiting DNA repair via inhibiting FASN (submitted).
26. Babula, J.; and **Liu, J.Y.\*** Significant different conformation and dynamics of HIV-1 protease when bound to Darunavir derivatives differentiated by single atom substitution (submitted).



27. Li, D.; Fang, S.; and **Liu, J.Y.\*** Principles and predictions of specific protein-protein interactions (manuscript in preparation).
28. Babula, J.; Yadav, R.P.; and **Liu, J.Y.\*** Distinct properties of conserved 14-3-3 human isoforms revealed by molecular dynamic simulation and SAXS (manuscript in preparation)
29. Babula, J.; Zhang, JT; and **Liu, J.Y.\*** Parallel vs anti-parallel conformation of nonphosphorylated STAT1 (manuscript in preparation)

#### **Patent**

1. Inhibitors Targeting the DNA-Binding Domain of Human STAT3 for Treatment of Metastatic Cancers (provisional patent application, 61/883,814 filed on July 27, 2013, PCT filed on September 24, 2014; **PCT/US2015/0094353**)  
**(US Patent # 9,382,204 issued on July 5, 2016).**
2. Survivin-targeting anti-tumor agents and uses thereof (provisional patent, 62/162 291, filed on May 15, 2015, PCT filed on May 14, 2016)
3. Combination drug therapy reduces PARP-1 related DNA repair and increase the efficacy of genotoxic agents. (provisional patent, 62/403,423, filed on October 10, 2016, PCT filed on October 10, 2017)