CURRICULUM VITAE

(Updated December 2022)

Name: Junmei Wang, Ph.D.

Present Title: Associate professor

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EDUCATION AND TRAINING

1988-1992	Shandong Normal University, Jinan, China	BS in Chemistry
1992-1995	Graduate School of the University of Science and Technology of China, Beijing, China	MS in Physical Chemistry
1995-1998	Peking University, Beijing China	PhD in Computational Chemistry
2006-2007	Indiana University at Bloomington, IN	Certificate on Chemical Informatics and Bioinformatics

APPOINTMENTS AND POSITIONS

2017-Present	Associate Professor (tenure stream), Department of Pharmaceutical Sciences, School of Pharmacy, University of Pittsburgh, PA (Primary appointment)
2016-2017	Associate Professor (non-tenure stream) of Computational Chemistry and Biology, Green Center for Systems Biology, University of Texas Southwestern Medical Center, Dallas TX
2008-2016	Assistant Professor (non-tenure stream) of Computational Chemistry and Biology, Green Center for Systems Biology, University of Texas Southwestern Medical Center, Dallas TX
2008-2009	Adjunct Professor, School of Pharmacy, University of Pittsburgh, Pittsburgh, PA
2002-2007	Senior Scientist, Encysive Pharmaceuticals, Houston TX
2006-2007	Adjunct Professor, College of Pharmacy, University of Houston, Houston, TX

1998-2001	Postdoctoral Fellow, Department of Pharmaceutical Chemistry, University of California, San Francisco, CA
1995-1998	Graduate Research Assistant (Advisor: Dr Xiaojie Xu), Peking University, Beijing China

HONORS AND AWARDS

1992	Excellent Graduate graduates of Shandong Normal University, China
1992	Graduate School of the University of Science and Technology of China
1995	Research Scholarship, Peking University
1997	China Construction Bank “Excellent Graduate Student” award
1998	Award for Best Graduate Students, Peking University, Beijing, China
2006	Award for Best Employees in R&D, Encysive Pharmaceuticals, Houston, TX
2020	Graduate Faculty Member of The Year 2019, School of Pharmacy, University of Pittsburgh
2022	Certara/SimCYP 2022 Academic Award’s for “Most-Effective Teaching Application”
2024	Graduate Faculty Member of The Year 2023, School of Pharmacy, University of Pittsburgh

MEMBERSHIP IN PROFESSIONAL AND SCIENTIFIC SOCIETIES

2004-present	American Chemical Society
2004	Sigma Xi, the Scientific Research Society

TEACHING RESPONSIBLITIES

Graduate Courses

Institution	***Course***	***Role***	***Year***
UT Southwestern Medical Center	Computational & Systems Biology	Lecturer	2014-2017
University of Pittsburgh	Systems Pharmacology (Pharm 3068)	Lecturer & Course Coordinator	2018
University of Pittsburgh	Advanced Pharmacokinetics (Pharm 3002)	Lecturer	2018

University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2018
University of Pittsburgh	Pharmacometrics (Pharm 3069)	Lecturer & Course Coordinator	2019
University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2019
University of Pittsburgh	Systems Pharmacology (Pharm 3068)	Lecturer	2020
University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2020
University of Pittsburgh	Pharmacometrics (Pharm 3069)	Lecturer	2021
University of Pittsburgh	Advanced Pharmacokinetics (Pharm 3002)	Lecturer	2021
University of Pittsburgh	Applied Multivariate Statistical Analysis in Pharmaceutical Sciences (Pharm 3073)	Lecturer	2021
University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2021
University of Pittsburgh	Foundation in Pharmaceutical Sciences (Pharm 3071)	Lecturer	2022
University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2022
University of Pittsburgh	Systems Pharmacology (Pharm 3068)	Lecturer	2022
University of Pittsburgh	Foundation in Pharmaceutical Sciences (Pharm 3071)	Lecturer	2023
University of Pittsburgh	Pharmacometrics (Pharm 3069)	Lecturer	2023
University of Pittsburgh	Advanced Statistics (Pharm 3045)	Lecturer	2024
University of Pittsburgh	Foundation in Pharmaceutical Sciences (Pharm 3071)	Lecturer	2024

Professional Courses

Institution	***Course***	***Role***	***Year***
University of Pittsburgh	Principles of Drug Action (PDA) (Pharm 5118)	Lecturer	2021
University of Pittsburgh	Special Topics (Pharm 5851)	Instructor	2021
University of Pittsburgh	Principles of Drug Action (PDA) (Pharm 5118)	Instructor	2022
University of Pittsburgh	Principles of Drug Action (PDA) (Pharm	Instructor	2023

5118)

Education Program Development

2018	• Codeveloped Pharmacometrics and Systems Pharmacology (PSP), an MS/PhD graduate program to train the next-generation researchers who can conduct rational drug discovery and development via systems pharmacology and pharmacometrics methods.
2018	• Constructed and hosted a series of workshops to deliver knowledge of physiologically-based pharmacokinetics (PBPK) and train skills of applying SimCYP to conduct PBPK modeling and simulation

Graduate Course Development

2018	Systems Pharmacology (PHARM 3068)	• Codeveloped a core course for the PSP track which introduces knowledge and skills on conducting systems pharmacology analysis in rational drug discovery and drug development.
2018	Pharmacometrics (PHARM 3069)	• Codeveloped a core course for the PSP track which introduces knowledge and skills on performing pharmacokinetics and pharmacodynamics modeling and simulations.

Workshop Development

2018	SimCYP	• Constructed and hosted a series of workshops to deliver knowledge of physiologically-based pharmacokinetics (PBPK) and train skills of applying SimCYP to conduct PBPK modeling and simulation. These workshops adopted the “Teach me to teach you” style. Specially, I prepared the slides for students and students took turns to teach his/her fellow students after comprehending the slides.

MENTORING RESPONSIBLITIES (Not Provided)

SERVICE

A. Committees

- 2019, Member of the Outcome Faculty Search Committee, School of Pharmacy, University of Pittsburgh

- 2019-Present, Member of the GPCC Committee, School of Pharmacy, University of Pittsburgh

B. AMBER Support

As an AMBER developer, an important task is to provide service to AMBER users including answering questions and solving software-related problems. The service is provided via the AMBER mailing list (http://lists.ambermd.org/mailman/listinfo/amber) and individual emails.

C. Editor and Editorial Advisory Board

Journal	***Role***	***Starting Year***
Current Computer-Aided Drug Design	Member of Editorial Board	2011
Bioenergetics	Member of Editorial Board	2012
Biomedicine-Hub	Section Editor	2022
eDrug	Editor-In-Chief	2022
Antibiotics	Member of Editorial Board	2022
Journal of Alzheimer's Disease	Associate Editor	2023
Frontiers in Molecular Biosciences	Associate Editor	2023
NPJ Drug Discovery	Editorial Board Member	2024

D. Reviewer

Journal Review

Journals	***Number of Manuscripts Reviewed***	***Year***
ACS journals (JCIM, JCTC, JPC, JMC, Molecular Pharmaceutics, ACS Appl. Mater. Interfaces, J. Chem. Eng. Data, Environmental Science & Technology, JPC Letters, ACS Combinatorial Science, ACS Chemical Health & Safety, etc.)	114	2007-Present
Bioorganic & Medicinal Chemistry	1	2010
Combinatorial Chemistry & High Throughput Screening	1	2011
Bioorganic & Medicinal Chemistry	1	2011
Bioorganic & Medicinal Chemistry Letters	1	2011
Drug Discovery Today	1	2011
Proteins: Structure, Function, and Bioinformatics	1	2011
Letters in Drug Design & Discovery	1	2011
Current Computer-Aided Drug Design	1	2011
Current Computer-Aided Drug Design	2	2012
Journal of Molecular Graphics and Modeling	2	2012
Journal of Chemical Physics	1	2012

Journal of Computational Chemistry	3	2012
Journal of Cheminformatics	1	2012
Current Pharm Des	1	2012
Molecular BioSystems	1	2012
Molecular Pharmaceutics	1	2012
Current Pharmaceutical Design	1	2013
Journal of Biomolecular Structure and Dynamics	1	2013
Journal of Computational Chemistry	1	2013
Current Pharm Des	1	2013
AAPS	1	2014
Advanced Drug Delivery Reviews	1	2014
Computational Biology Chemistry	1	2014
Journal of Molecular Graphics and Modeling	2	2015
Molecular Biosystems	1	2016
Journal of Computational Chemistry	1	2016
Digestive Diseases and Sciences	1	2016
Drug Discovery Today	1	2016
Scientific Reports	2	2017
Journal of Computer-Aided Molecular Design	1	2017
Journal of Molecular Liquids	1	2018
Bioorganic & Medicinal Chemistry	1	2019
Physical Chemistry Chemical Physics	1	2019
Journal of Chemical Physics	1	2019
Journal of Computational Chemistry	1	2019
Cellular and Molecular Neurobiology	1	2019

Briefs in Bioinformatics	1	2019
Drug Discovery Today	1	2019
Current Computer-Aided Drug Design	1	2020
Dose Response	2	2020
Life Sciences	1	2020
Medicinal Chemistry	1	2020
Briefs in Bioinformatics	2	2020
Chemical Biology and Drug Design	1	2020
ChemMedChem	1	2020
Future Medicinal Chemistry	2	2020
Future Virology	2	2020
ChemistrySelect	2	2020
Drug Development Research	1	2020
Journal of Chemical Physics	1	2020
BMS Medicinal Chemistry	1	2020
Acta Pharmacologica Sinica	1	2020
Briefings in Bioinformatics	1	2020
Natural Communications	1	2020
Natural Machine Intelligence	1	2020
Coronaviruses	1	2020
Scientific Reports	1	2020
Chemical Science	1	2020
Journal of Chemical Physics	1	2020
RSC Advances	1	2020
Medicinal Chemistry	1	2020
ChemistrySelect	1	2020

iScience	1	2021
Briefings in Bioinformatics	3	2021
Advanced Drug Delivery Reviews	1	2022
Chemical Physics Letters	1	2022
Nucleic Acids Research	1	2022
Chemical Science	1	2022
Bioinformatics and Biology Insights	1	2022
New Journal of Chemistry	1	2022
Physical Chemistry Chemical Physics	5	2022
International Journal of Molecular Sciences	3	2022
Journal of Biomolecular Structure & Dynamics	2	2022
BMS Mini-Reviews in Medicinal Chemistry	1	2022
BMS Biomedicine Hub	3	2022
ChemBioChem	1	2022
Beni-Suef University Journal of Basic and Applied Science	1	2022
BMS Medicinal Chemistry	1	2022
iScience	2	2022
Molecular Genetics and Genomics	1	2022
Proteins: Structure, Function, and Bioinformatics	4	2022
Journal of Computational Chemistry	1	2022
Current Computer-Aided Drug Design	5	2022
Briefings in Bioinformatics	6	2022
International Journal of Molecular Sciences	3	2022
Neural Regeneration Research	1	2022
Communications Chemistry	1	2022

BMS Current Medicinal Chemistry	2	2022
Scientific Reports	2	2022
Expert Review of Clinical Pharmacology	1	2022
Computational & Structural Biotechnology Journal	1	2022
Molecules	1	2022
Vaccines	2	2022
ChemistrySelect	1	2022
Biomedicines	1	2022
Pharmaceuticals	2	2022
Frontiers in Medicine	2	2022
Journal of Alzheimer's Disease	1	2022
Journal of Molecular Liquids	1	2022
Annals of Translational Medicine	1	2022
Journal of Computational Biophysics and Chemistry	2	2022
Antibiotics	1	2022
Total	**259**	

Federal Grant Review

- Reviewer of Department of Energy (DOE), INCITE Biological Sciences I, September 2017
- Reviewer of NSF Study Section "Harnessing the Data Revolution (HDR): Institutes for Data-Intensive Research in Science and Engineering" [NSF 21-519], May 3-4, 2021
- Ad hoc reviewer for NIH study section "*Exploration of Antimicrobial Therapeutics and Resistance" (ZRG1)*, July 15-16, 2021
- Reviewer of an NSF Career Grant on September 1st, 2021.
- Ad hoc reviewer of the ZRG1 IMST-B (14) B study section: IMST-14: Small Business: Computational, Modeling, and Biodata Management, Nov 12th, 2021
- Ad hoc reviewer of ORAU-grant application, Oct. 31, 2022
- Ad hoc reviewer of the MCST-B(14) study section: MCST-14: Small Business: Computational, Modeling, and Biodata Management, March 15, 2023

- Mail reviewer for 2024 Transformative Research Award (TRA), April 2-3, 2024.
- Ad hoc reviewer of the Drug Discovery and Molecular Pharmacology B (DMPB) study section, June 27-28, 2024

Internal Grant Review

- Reviewer of Biomedical Modeling Pilot Awards, CTSI, University of Pittsburgh, July 2019
- Pharmacy Internal Grant Review, University of Pittsburgh, May 2021
- Pharmacy Internal Grant Review, University of Pittsburgh, September 2021
- Pharmacy Internal Grant Review, University of Pittsburgh, November 2021
- Pharmacy Internal Grant Review, University of Pittsburgh, January 2022
- Pharmacy Internal Grant Review, University of Pittsburgh, February 2022

Tenure/Promotion Review

- Dr. XXX, Promotion to tenured Associate Professor, Department of Pharmaceutical Sciences, University of North Texas Health Science Center, 2019
- Dr. XXX, Promotion to tenured Associate Professor, School of Pharmacy, University of Pittsburgh, 2019
- Dr. XXX, Promotion to Research Associate Professor, School of Pharmacy, University of Pittsburgh, 2020
- Dr. XXX, Promotion to Research Associate Professor, School of Pharmacy, University of Pittsburgh, 2020
- Dr. XXX, Professional performance quadrennial review, NIH, 2022.

Admission Review

- Graduate student interview, PSP track, Department of Pharmaceutical Sciences, 2017
- Admission interview, Sun Yat-Sen University Summer Internship Program, 2017
- Graduate student interview, Medicinal Chemistry track, Department of Pharmaceutical Sciences, 2017
- Graduate student interview, PSP track, Department of Pharmaceutical Sciences, 2018
- Graduate student interview, Medicinal Chemistry track, Department of Pharmaceutical Sciences, 2018
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2018

- Admission interview, Sun Yat-Sen University Summer Internship Program,2018
- Graduate student interview, PSP track, Department of Pharmaceutical Sciences, 2019
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2019
- Graduate student interview, PSP track, Department of Pharmaceutical Sciences, 2020
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2020
- Graduate student interview, PSP track, Department of Pharmaceutical Sciences, 2021
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2021
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2022
- Pharm.D. interview, School of Pharmacy, University of Pittsburgh, 2023

Other Review

- PharmD Portfolio review, 2019
- PharmD Portfolio review, 2020
- Member of the judge panel for the Grant Writing course (Pharm 3038), 2020
- PharmD Portfolio review, 2021
- Member of the judge panel for the Grant Writing course (Pharm 3038), 2021
- Member of the judger panel for 12th Annual Pharmaceutical Sciences Research Symposium (PSRS), 2021
- PharmD Portfolio review, 2022
- Member of the judge panel for the Grant Writing course (Pharm 3038), 2022
- Reviewer of ACS COMP Division Fellowship Awards, 2022
- PharmD Portfolio review, 2023
- Member of the judge panel for the Grant Writing course (Pharm 3038), 2023
- Reviewer of ACS COMP Division Fellowship Awards, 2023
- PharmD Portfolio review, 2024

E. Consultant

Served as a constant for XtalPI Inc., a company dedicated in drug solid state R&D and drug discovery

RESEARCH

A. Research Interests

I am a computational chemist and biophysicist with extensive experience in multiple areas of molecular simulations and computer-aided drug design. My research group is capable of developing and applying software tools to study the structures, dynamics, energetics, and functions of protein-ligand interactions. My research interests are driven by my desire to improve the success rate of rational drug design by developing highly accurate force field-based scoring functions, and to uncover the molecular mechanisms of biological events (such as amyloid protein oligomerization) through large- and multiscale molecular dynamics simulations.

Group Mission:
The mission of my group is to develop high-quality molecular mechanics force field models (MMFF), MMFF-based scoring functions, and software and web tools to enable accurate modeling of protein-ligand interactions. The successful pursuit of our mission will have a revolutionary impact on biomedical research and drug discovery & development. Together with the fast development of computer hardware especially on graphics processing unit (GPU), the era of true "Rational Drug Design" will come into being. I imagine medicinal chemists, even though having limited knowledge on molecular modeling, can routinely conduct high-level free energy calculations for their designed compounds prior to real synthesis via using our high-quality force field models/scoring functions and software/web tools.

Research Themes:
My research interests fall into nine themes.

THEME 1. Force Field Development
THEME 2. Force Field-Based Scoring Function Development
THEME 3. Structure-Based Drug Design Methodology Development
THEME 4. Application of Molecular Simulations in Molecular Property Calculations
THEME 5. Application of Molecular Simulations in Molecular Mechanism Studies
THEME 6. Drug Discovery Projects
THEME 7. Application of Machine Learning and Deep Learning in Drug Design
THEME 8. Software Tools and Web Tools Development
THEME 9. PBPK Modeling and Simulation

Instances of my success:

- Development of a set of general AMBER force fields (GAFF) which have been extensively utilized in structure-based drug design;
- Development of a set of GAFF-based descriptors and scoring functions to bridge the efficient yet less accurate molecular docking method and accurate yet less efficient free

energy-based methods;

- Development of a set of computational protocols and tools to enable us to study the kinetics of amyloid oligomerization via atomistic molecular dynamics simulations, and to screen inhibitors which can interfere with the pathogenic process related to Alzheimer's disease;
- Development of a hierarchical virtual screening strategy and successful application of the strategy in drug lead identification for many drug targets including HIV-1 RT and Eco-MscL;
- Development of a computational strategy to generate high-quality physiologically-based pharmacokinetic (PBPK) models for arbitrary drugs or drug candidates.

B. Publications

Peer Reviewed Articles

Summary of Peer Reviewed Articles

Peer-Reviewed Journal Name	2021 JCR Impact Factor (IF)	Number of Publications
Combinatorial Chemistry & High Throughput Screening	1.339	3
Current Computer-Aided Drug Design	1.606	1
Protein Engineering	1.65	1
Journal of Clinical Pharmacy and Therapeutics	1.668	1
Journal of Molecular Modeling	1.81	1
Journal of Mass Spectrometry	1.982	1
Acta Physico-Chimica Sinica	2.268	2
Journal of Physics-Condensed Matter	2.333	1
European Journal of Drug Metabolism and Pharmacokinetics	2.441	1
Journal of Molecular Graphics & Modelling	2.518	1
Drugs in R&D	2.594	1
Journal of Physical Chemistry A	2.781	1
JCO Clinical Cancer Informatics	2.95	1
Journal of Physical Chemistry B	2.991	12
Journal of the American Society for Mass Spectrometry	3.109	1
Biochemistry	3.162	1
Journal of Molecular Structure-Theochem	3.196	1
PLOS One	3.24	1
Chemistry and Physics of Lipids	3.329	1
Journal of Computational Chemistry	3.376	7
Journal of Biomolecular Structure & Dynamics	3.392	1
Journal of Chemical Physics	3.488	5
Chemometrics and Intelligent Laboratory Systems	3.491	3
Molecular Microbiology	3.501	1

ACS Omega	3.512	1
Biochemistry and Cell Biology	3.626	1
Physical Chemistry Chemical Physics	3.676	5
Journal of Computer-Aided Molecular Design	3.686	2
Langmuir	3.882	1
RNA	3.949	1
Biophysical Journal	4.033	2
Scientific Reports	4.379	1
Molecules	4.411	1
ACS Chemical Neuroscience	4.418	3
Journal of Alzheimer's Disease	4.472	1
PLOS Computational Biology	4.475	1
Expert Opinion on Drug Metabolism & Toxicology	4.481	1
Drug and Alcohol Dependence	4.492	2
Current Medicinal Chemistry	4.53	1
Antibiotics	4.64	2
Molecular Pharmaceutics	4.939	4
Journal of Personalized Medicine	4.945	1
Structure	5.006	1
Cellulose	5.044	1
FASEB Journal	5.191	1
Chemistry-a European Journal	5.236	1
Journal of Cheminformatics	5.514	5
International Journal of Molecular Sciences	5.923	1
Journal of Chemical Theory and Computation	6.006	8
Journal of Chemical Information and Modeling	6.162	23
Chinese Chemical Letters	6.779	3
Curr Opin Struct Biol	6.809	1
Journal of Medicinal Chemistry	7.446	4
PLOS Biology	8.029	1
eLife	8.14	1
Journal of Neuroinflammation	8.322	1
Proceedings of the National Academy of Sciences of the United States of America	11.202	4
Briefings in Bioinformatics	11.622	3
Science Advances	14.14	1
Journal of the American Chemical Society	15.419	2
Advanced Drug Delivery Reviews	15.47	2
Materials Today	26.94	1
Lancet Oncology	41.316	1
Cell	41.582	1
Nature	49.962	2
Chemical Reviews	60.622	1
Total: 65 journals		151

2021 JCF Impact Factor (IF)	< 4	4-10	10-20	>20
Number of Publications	61	72	12	6

Citations Report for Peer Reviewed Articles by Web of Knowledge

Total citations for the 151 articles: **29,491** according to Web of Knowledge accessed on March 14, 2022.

h-index: **54** according to Web of Knowledge (and h-index of 68 according to Google Scholar)

Total number of publications since joining PITT in 2017: **104**

Publication List (in Chronological Order)

Key #**:** Finished by students and fellows under my direction; ***:** Corresponding author

1. **Wang, J. M.**; Hu, Z. L.; Ye, X. Q., Conformational Analysis of Leu-enkephalin by Molecular Dynamics Method. *Acta Physico-Chimica Sinica* **1995,** *11* (8), 673-677.

2. **Wang, J. M.**; Zhao, Z. L.; Ye, X. Q., Parameterization Procedures in Molecular Mechanics Calculation. *Acta Physico-Chimica Sinica* **1995,** *11* (5), 424-428.

3. **Wang, J. M.**; Hou, T. J.; Li, Y. Y.; Xu, X. J., The QSAR research of pyrrolobenzothiazepinones and pyrrolobenzo-xazepinones - Novel and specific non-nucleoside HIV-1 reverse transcriptase inhibitors. *Chinese Chemical Letters* **1997,** *8* (10), 889-892.

4. Hou, T. J.; **Wang, J. M.**; Li, Y. Y.; Xu, X. J., Application of genetic algorithm to the QSAR research of pyrrolobenzothiazepinones and pyrrolobenzoxazepinones-novel and specific non-nucleoside HIV-1 reverse transcription inhibitors. *Chinese Chemical Letters* **1998,** *9* (7), 651-654.

5. **Wang, J. M.**; Zhang, H.; He, H. X.; Hou, T. J.; Liu, Z. F.; Xu, X. J., Theoretical studies on force titration of amino-group-terminated self-assembled monolayers. *Journal of Molecular Structure-Theochem* **1998,** *451* (3), 295-303.

6. Hou, T. J.; **Wang, J. M.**; Chen, L. R.; Xu, X. J., Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. *Protein Engineering* **1999,** *12* (8), 639-647.

7. Hou, T. J.; **Wang, J. M.**; Liao, N.; Xu, X. J., Applications of genetic algorithms on the structure-activity relationship analysis of some cinnamamides. *Journal of Chemical Information and Computer Sciences* **1999,** *39* (5), 775-781.

8. Hou, T. J.; **Wang, J. M.**; Xu, X. J., Applications of genetic algorithms on the structure-activity correlation study of a group of non-nucleoside HIV-1 inhibitors. *Chemometrics and Intelligent Laboratory Systems* **1999,** *45* (1-2), 303-310.

9. Hou, T. J.; **Wang, J. M.**; Xu, X. J., A comparison of three heuristic algorithms for molecular docking. *Chinese Chemical Letters* **1999,** *10* (7), 615-618.

10. **Wang, J. M.**; Hou, T. J.; Chen, L. R.; Xu, X. J., Automated docking of peptides and proteins by genetic algorithm. *Chemometrics and Intelligent Laboratory Systems* **1999,** *45* (1-2), 281-286.

11. **Wang, J. M.**; Hou, T. J.; Chen, L. R.; Xu, X. J., Conformational analysis of peptides using Monte Carlo simulations combined with the genetic algorithm. *Chemometrics and Intelligent Laboratory Systems* **1999,** *45* (1-2), 347-351.

12. **Wang, J. M.**; Cieplak, P.; Kollman, P. A., How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules? *Journal of Computational Chemistry* **2000,** *21* (12), 1049-1074.

13. **Wang, J. M.**; Kollman, P. A., Automatic parameterization of force field by systematic search and genetic algorithms. *Journal of Computational Chemistry* **2001,** *22* (12), 1219-1228.

14. **Wang, J. M.**; Morin, P.; Wang, W.; Kollman, P. A., Use of MM-PBSA in reproducing the binding free energies to HIV-1 RT of TIBO derivatives and predicting the binding mode to HIV-1 RT of efavirenz by docking and MM-PBSA. *Journal of the American Chemical Society* **2001,** *123* (22), 5221-5230.

15. **Wang, J. M**.; Wang, W.; Huo, S. H.; Lee, M.; Kollman, P. A., Solvation model based on weighted solvent accessible surface area. *Journal of Physical Chemistry B* **2001,** *105* (21), 5055-5067.

16. Wang, W.; Lim, W. A.; Jakalian, A.; Wang, J.; **Wang, J. M.**; Luo, R.; Bayly, C. T.; Kollman, P. A., An analysis of the interactions between the Sem-5 SH3 domain and its ligands using molecular dynamics, free energy calculations, and sequence analysis. *Journal of the American Chemical Society* **2001,** *123* (17), 3986-3994.

17. Huo, S. H.; **Wang, J. M.**; Cieplak, P.; Kollman, P. A.; Kuntz, I. D., Molecular dynamics and free energy analyses of cathepsin D-inhibitor interactions: Insight into structure-based ligand design. *Journal of Medicinal Chemistry* **2002,** *45* (7), 1412-1419.

18. Duan, Y.; Wu, C.; Chowdhury, S.; Lee, M. C.; Xiong, G. M.; Zhang, W.; Yang, R.; Cieplak, P.; Luo, R.; Lee, T.; Caldwell, J.; **Wang, J. M.**; Kollman, P., A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. *Journal of Computational Chemistry* **2003,** *24* (16), 1999-2012.

19. **Wang, J. M.**; Wolf, R. M.; Caldwell, J. W.; Kollman, P. A.; Case, D. A., Development and testing of a general amber force field. *Journal of Computational Chemistry* **2004,** *25* (9), 1157-1174.

20. Wu, C. D.; Decker, E. R.; Blok, N.; Bui, H.; You, T. J.; **Wang, J. M.**; Bourgoyne, A. R.; Knowles, V.; Berens, K. L.; Holland, G. W.; Brock, T. A.; Dixon, R. A. F., Discovery, modeling, and human pharmacokinetics of N-(2-acetyl-4,6-dimethylphenyl)-3-(3,4-

dimethylisoxazol-5-ylsulfamoyl)th iophene-2-carboxamide (TBC3711), a second generation, ETA selective, and orally bioavailable endothelin antagonist. *Journal of Medicinal Chemistry* **2004,** *47* (8), 1969-1986.

21. Shan, J. F.; Shi, D. L.; **Wang, J. M.**; Zheng, J., Identification of a specific inhibitor of the dishevelled PDZ domain. *Biochemistry* **2005,** *44* (47), 15495-15503.

22. Shan, J. F.; **Wang, J. M.**; Zheng, J., Identification of non-peptide inhibitor of the dishevelled PDZ domain. *Biophysical Journal* **2005,** *88* (1), 334A-334A.

23. **Wang, J. M.***; Kang, X. S.; Kuntz, I. D.; Kollman, P. A., Hierarchical database screenings for HIV-1 reverse transcriptase using a pharmacophore model, rigid docking, solvation docking, and MM-PB/SA. *Journal of Medicinal Chemistry* **2005,** *48* (7), 2432-2444.

24. Zhang, J. M.; **Wang, J. M.**; Brodbelt, J. S., Characterization of flavonoids by aluminum complexation and collisionally activated dissociation. *Journal of Mass Spectrometry* **2005,** *40* (3), 350-363.

25. Hou, T. J.; **Wang, J. M.**; Zhang, W.; Wang, W.; Xu, X., Recent advances in computational prediction of drug absorption and permeability in drug discovery. *Current Medicinal Chemistry* **2006,** *13* (22), 2653-2667.

26. **Wang, J. M.***; Hou, T. J.; Xu, X. J.*, Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. *Current Computer-Aided Drug Design* **2006,** *2* (3), 287-306.

27. **Wang, J. M.***; Krudy, G.; Xie, X. Q.; Wu, C. D.; Holland, G., Genetic algorithm-optimized QSPR models for bioavailability, protein binding, and urinary excretion. *Journal of Chemical Information and Modeling* **2006,** *46* (6), 2674-2683.

28. **Wang, J. M.***; Wang, W.; Kollman, P. A.; Case, D. A.*, Automatic atom type and bond type perception in molecular mechanical calculations. *Journal of Molecular Graphics & Modelling* **2006,** *25* (2), 247-260.

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Citation Report for book chapters

Total number of book chapters/software manuals: **18**

Total citations for book chapters/software manuals: **14,906** according to Google Scholar

Total citations for both peer-reviewed articles and book chapters: **56,812**

h-index: **65**

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Abstract at Meetings

Key *: Corresponding author; #: Students and fellows under my direction

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11. Man, V.; He, X. B.; **Wang, J. M.#**, Rational design of small molecules inhibiting amolyoid beta aggregation. *Abstracts of Papers of the American Chemical Society* **2019,** *257*.

12. Liu, S.; **Wang, J. M.#**, Molecular-Simulation-based Study on Action Mechanism of YIV-906(PHY906) as Adjuvant in Cancer Treatment, Quantitative Systems Pharmacology (QSP) Annual Meeting, July 20-21, 2019 Great Lakes Symposium, University at Buffalo.

13. Ji, B.; **Wang, J. M.#**, Pharmacokinetics Modeling and Molecular Modeling of Drug-Drug Interaction Between opioid and benzodiazepine, American Society for Clinical Pharmacology & Therapeutics (ASCPT)2019 Annual Meeting, March, **2019**, Washington, DC.

14. Ji, B.; **Wang, J. M.#**, A New Approach for In Silico Prediction of Oral Drug Concentration Profiles in Human for Drug Candidates Lack Experimental Pharmacokinetic Data, Quantitative Systems Pharmacology (QSP) Annual Meeting, Great Lakes Symposium, July 20-21, **2019,** University at Buffalo.

15. Ji, B.; **Wang, J. M.#**, Physiologically-based Pharmacokinetics Modeling of Drug-Drug Interaction between Oxycodone and Diazepam, Quantitative Systems Pharmacology (QSP) Annual Meeting, Great Lakes Symposium, July 20-21, **2019,** University at Buffalo.

16. **Wang, J. M.**, Development of the third generation of the general AMBER force field (GAFF3): Significantly improve the accuracy of free energy calculations. Abstracts of Papers of the American Chemical Society, **2021,** Spring Virtaul Meeting.

17. Ji, B.; **Wang, J. M.#**, Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. 12th Annual Pharmaceutical Sciences Research Symposium, March, **2021**.

18. Ji, B.; **Wang, J. M.#**, DRUGAN: A deep convolutional generative adversarial networks (DCGAN) model for druglike compound library construction. American Chemical Society National Meeting, March 21, **2022**.

19. Ji, B.; **Wang, J. M.#**, Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. American Chemical Society National Meeting, March 21, **2022**.

20. Sun, Y.; **Wang, J. M.#**, Accurate solvation free energy calculations using MM-PBSA methods, American Chemical Society National Meeting, March 21, **2022**.

21. Sun, Y.; **Wang, J. M.#**, Accurate solvation free energy calculations using MM-PBSA methods, American Chemical Society National Meeting, March 21, **2022**.

22. **Wang, J. M.#**; Cai, L.; Han, F. Predict infectability of SARS-CoV-2 spike mutations using a combination of evolution analysis, site-site correlation analysis and binding free energy analysis, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

23. Wang, L.; **Wang, J. M.#**, Rational design of lipid-based carriers for delivering small RNAs through MD simulations and free energy analysis, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

24. Niu, T.; Sun, Y.; **Wang, J. M.#**, Development and testing of endpoint solvation free energy models for binding free energy prediction, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

25. Ji, B.; Brock, M.; He, X.; Zhai, J.; **Wang, J. M.#**, Drugan: A deep convolutional generative adversarial networks (DCGAN),for durg-target-specific compound library construction, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

26. Man, V.; Gao, J.; He, X.; Ji, B.; Lin, D.; **Wang, J. M.#**, Inhibititor screening focusing on the oligomerization state of amyloid aggregation, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

27. Han, F.; Man, V.; **Wang, J. M.#**, Revealing open channel structures of Ec-MscL with multiple nonequilibrium molecular dynamics simulation methods, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

28. He, X.; Man, V.; **Wang, J. M.#**, Expansion of the ABCG2 charge model targeting solvation free energies, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

29. Hu, B.; Zhai, J.; He, X.; **Wang, J. M.#**, Toward predicting solubility of arbitrary solutes in arbitrary solvents: Prediction of density and refractive index using machine learning algorithms, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

30. Cai, L.; Ji, B.; Zhai, J.; **Wang, J. M.#**, Screening of potential flavonoid nutrients as inhibitors of SARS-CoV-2 3CL protease using machine learning trained classifiers and regression models, American Chemical Society National Meeting, March 21, 2022, March 26-30, **2023**.

Patent Invention

Wu, C.; Anderson, E.; Bui, H.; Gao, D.; Holland, G.; Kassir, J.; Li, W.; **Wang, J.**; Dupre, B. "Pyridine, pyrimidine, quinoline, quinazoline, and naphthalene urotensin-II receptor antagonists", WO/2004/078114.

C. Grant

ACTIVE

National Science Foundation/1955260, Wang, Junmei (PI) 07/01/20-06/30/23
Title: CDS&E: D3SC: Developing a molecular mechanics modeling platform (MMMP) for studying molecular interactions
Total Cost: $500,000 **Effort**: 8.3%
Goals: This proposal seeks to (1) develop and advance a set of computational tools to facilitate users from a broad range of disciplines to generate high quality molecular mechanics force field (MMFF) parameters; and (2) develop a set of MMFF-based models and software tools to facilitate study of molecular interactions with a focus on free energy calculation. The developed software and parameters will be released via the website https://clickff.org, and distributed through AMBER, a mainstream molecular simulation software package.
Role: PI

NIH/ R01GM147673 Wang, Junmei (PI) 09/24/2022-8/31/2026
Title: New generation of general AMBER force field for biomedical research
Total Cost: $1,252,000 **Effort:** 25%
Goals: We plan to (1) develop a new generation of general AMBER force field (GAFF3) for studying biomolecule-ligand interactions; (2) critically evaluate GAFF3 in protein-ligand and nucleic acid-ligand binding free energy predictions using a novel GPU-accelerated λ-dynamics based orthogonal space tempering (OST) algorithm; and (3) apply a variety of strategies to further

improve the performance of GAFF3 until it approaches the best performance an additive force field model can achieve.
Role: PI

NIH/R01 GM149705-01 Wang, Junmei (PI) 04/01/2023-3/31/2028
Title: AI-powered Biased Ligand Design
Total Cost: $1,252,000 **Effort:** 20%
Goals: Biased ligand design is an attractive approach for designing drugs that target a particular signaling pathway with high specificity and selectivity to minimize side effects, however, it is also a grand challenge due to lack of computational tools. Also, there is an urgent need to expand the druglike chemical space for promising drug targets which have plenty of potent ligands developed, but unfortunately, no approved drugs. We plan to apply artificial intelligence (AI) techniques to overcome the two challenges by developing interaction profile scoring function models to enable biased ligand design and Drug-GAN models to achieve de novo novel chemical structure design.
Role: PI

NIH/R01AG057555 Xie, Lei (PI) 06/01/2023-05/31/2028
Title: AI-Powered Quantitative Systems Pharmacology for AD Drug Repurposing
Total Award Amount: $464,315 (to PITT) **Effort:** 5%
Major Goals: The major goal of this proposal is to is to develop and experimentally validate innovative machine learning methods for predicting genome-wide protein-ligand interactions and ligand-induced functional activities for drug discovery targeting understudied proteins.
Role: PBPK expert

Eli Lilly/LRAP Wang, Junmei (PI) 07/01/2024-06/30/2026
Title: ABCG2 charge model-based platform for rational drug design
Total Award Amount: $250,513 (to PITT) **Effort:** 5%
Major Goals: The major goal of this proposal is to is to develop a platform to facilitate structure-based drug design. This ABCG2 charge model-based drug design platform, coined ADDP, seamlessly incorporate high-accurate electrostatic interaction calculation and machine learning/deep learning (ML/DL) to calculate protein-ligand binding free energy accurately and efficiently.
Role: PI

ACCESS/BIO220051 Wang, Junmei (PI) 6/1/2022-12/31/2022
Title: Discovery of structural and dynamic information of tau oligomerization process through molecular simulations of full-length tau proteins
Total GPU hours: 30,000
Goal: This proposal seeks to elucidate the oligomerization mechanism of full-length tau protein through multiscale molecular dynamics simulations
Role: PI

NIH/K25AG070277 Man, Viet (PI) 8/15/2021-7/31/2026
Title: Development of novel computational protocols to study amyloid oligomerization
Total Cost: $736,240 **Effort**: 0%
Goals: This career development grant provides support for research on amyloid oligomerization that is associated with neurodegenerative diseases.
Role: Primary Mentor

PENDING

NIH/R01LM014509-01 Wang, Junmei (PI) 09/01/2024 - 08/31/2028
Title: Development of a PBPK model repository for biomedical research
Total Cost: $1,590,000 **Effort**:10%
Goals: Physiologically based pharmacokinetic (PBPK) modeling plays an increasingly important role in drug development, therefore, global regulatory agencies including the FDA encourage inclusion of PBPK modeling in new drug applications, as PBPK models can be applied to study drug-drug interactions and design/optimize dosage regimens for special populations to achieve precision medicine. However, how to efficiently use those PBPK models can be challenging as they are disseminated in a variety of journals and many of them need further optimization. To overcome this challenge, we propose to build a public PBPK model repository to collect/optimize 200+ published PBPK models, develop 100+ new models, and then store the validated models in the SimCYP workspace format to guarantee model reproducibility, easy access, and retrieval.
Role: PI

NIH/R01000000-00 Wang, Junmei (PI) 02/01/2025 - 01/31/2030
Title: Discovery of Inhibitors for Tau Oligomerization
Total Cost: $1,590,000 **Effort**:20%
Goals: We plan to utilize large multiscale molecular simulations to elucidate the molecular mechanisms that govern pathological tau oligomerization in the earliest stage of tau aggregation, which will provide a structural basis for the subsequent drug screenings and de novo drug design. We will utilize an iterative process to develop 2-3 drug candidates which have optimal in vivo efficacy in reducing tauopathy and possess satisfactory DMPK and safety profiles for further preclinical development.
Role: PI

NIH/ R01CA281365 Xie, Lei (PI) 06/01/2023-05/31/2028
Title: Systems pharmacology-oriented humanized phenotype screening for precision drug discovery
Total Award Amount: $464,315 (to PITT) **Effort:** 5%
Major Goals: The goal of this project is to develop computational tools that can predict patient drug responses from cell line screens for anti-cancer drug discovery and personalized medicine

COMPLETED

NIH/NIGMS/1R01GM079383 Duan, Yong (PI) 09/28/2007-02/27/2014
Title: AMBER force field consortium: a coherent biomolecular simulation platform
Total Cost: $281,400 **Effort**:25%
Goals: The major goals of the project are to develop polarizable force fields for proteins, nucleic acids and organic molecules.
Role: co-PI of this MPI grant

NIH/NIGMS/5R01GM079383 Duan, Yong (PI) 03/26/2015-02/29/2020
Title: AMBER force field consortium: a coherent biomolecular simulation platform
Total Cost: $281,400 **Effort**:25%
Goals: The major goals of the project are to develop polarizable force fields for proteins, nucleic acids and organic molecules.
Role: co-PI of this MPI grant

NIH/NIGMS/ 5R21GM097617-02 Wang, Junmei (PI) 09/01/2011-08/31/2014
Title: Protein design using physical scoring functions integrated with site couplings
Total Cost: $396,875 **Effort**:35%
Goals: We intend to develop novel approaches to conquer the challenges in protein design. The new protein design strategies can facilitate us to engineer dynamical controls into a novel protein so that it can undertake a dynamic function. The novel approaches could be used to develop more effective biomedicine.
Role: PI

XtalPI/CGAFF Wang, Junmei 09/01/2019-08/31/2020
Title: Evaluation and reparameterization of GAFF2 for modeling crystal structures of drug molecules
Total Cost: $60,000 **Effort**:0%
Goals: We intend to develop a special version of GAFF2 force field for the prediction of crystal structures of drugs and drug candidates
Role: PI

NIH/ULITR001857/QUMP Wang, Junmei 02/01/2019-01/31/2020

Title: Quantitatively predict drug-drug interactions between oxycodone and other drugs by PBPK modeling and molecular modeling
Total Cost: $10,000 **Effort**:0%
Goals: We intend to predict drug-drug interactions between oxycodone and benzodiazepines and elucidate the underlying mechanisms through physiologically-based PK modeling and simulations as well as molecular modeling and simulations.
Role: PI for the QUMP grant

NIH/3R01MH113857 - 02W1 Price, Rebecca (PI) 12/01/18-06/30/22
Title: Improving precision of ketamine metabolite assays
Total Cost: $46,468 **Effort**: 7.0%
Goals: This project seeks to identify the neural and cognitive changes that accompany rapid relief from depressive symptoms following intravenous ketamine.
Role: Pharmacokinetics modeling expert

D. Seminars and Invited Lectureships

Invited Seminars/Talks

1. "GAFF and Antechamber Development", AMBER Developers' Annual Meeting, **2001**
2. "GAFF and Antechamber Development", AMBER Developers' Annual Meeting, **2002**
3. "GAFF and Antechamber Development", AMBER Developers' Annual Meeting, **2003**
4. "GAFF and Antechamber Development", AMBER Developers' Annual Meeting, **2004**
5. "GAFF and Antechamber Development", AMBER Developers' Annual Meeting, **2005**
6. "GAFF and Antechamber Development", AMBER/CHARMM Joint Meeting, **2006**

7. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2007**

8. “Computer-Aided Drug Design: My Understanding, Experience And Thinking.”, September **2007**, University of Texas Southwestern Medical Center, Dallas, TX

9. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2008**

10. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2009**

11. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2010**

12. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2011**

13. “Development And Test of AMBER Additive and Polarizable Force Fields.” June 16, **2011**, National Heart, Lung, and Blood Institute, Bethesda, MD.

14. “GAFF and Antechamber Development”, AMBER/CHARMM Joint Meeting, **2012**

15. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2013**

16. “Physical Scoring Function Development For Studying Protein Interaction“, April 21-22, **2013,** Zhejiang University, Hangzhou, China,

17. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2014**

18. Application of Molecular Dynamics (MD) Simulations in Biological Systems: Case Studies Dec. 15th, **2016**, Green Center for Systems Biology, University of Texas Southwestern Medical Center, Dallas, TX

19. “AMBER Force Field Development And Their Applications in Crystal Simulations”, Southern Methodist University, March 28, **2014**, Dallas, TX.

20. “Development And Test of Force Field-Based Scoring Functions in Ration Drug Design”, Soochow University, Feb. 25th, **2014***,* Suzhou, China.

21. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2015**

22. “Development of Molecular Mechanical Force Fields for Studying Biological Systems”, Feb. 15th, **2016**, Green Center for Systems Biology, University of Texas Southwestern Medical Center, Dallas, TX

23. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2016**

24. “Molecular Mechanical Force Field Development And Applications in Biomedical Research”, September., June 9th, **2016**, Green Center for Systems Biology, University of Texas Southwestern Medical Center, Dallas, TX

25. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2017**

26. “Physics-Based Scoring Function Development And Its Applications on Modeling Protein-Ligand Interactions”, CCGS, Department of Pharmaceutical Sciences, September. 22nd, **2017**.

27. “Applications of Molecular Dynamics Simulation And Free Energy Calculations in Studying Protein-Ligand Interactions”, Protein Structure & Dynamics, Science 2017, Oct. 20th, **2017**

28. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2018**

29. “Physics-Based Scoring Function Development And Its Applications on Modeling Protein-Ligand Interactions“, Pfizer Inc., June 25, **2018**, Boston, MA.

30. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2019**

31. “Improve the Binding Free Energy Calculations from Two Aspects: General Force Field and Practical Alchemical Free Energy Protocols. International conference of “Free energy calculations: entering the fourth decade of adventure in chemistry and biophysics”, June 16-21, **2019**, Santa Fe, NM. (Invited speaker and a session chair)

32. “GAFF and Antechamber Development”, AMBER Developers’ Annual Meeting, **2020**

33. “GAFF and Antechamber Development”, AMBER Developers’ Virtual Meeting, **2021**

34. “GAFF and GAFF-based scoring function development.” March 10, **2022**, National Heart, Lung, and Blood Institute, Bethesda, MD.

35. “GAFF and Antechamber Development”, AMBER Developers’ June 2-4, **2021** Tempa, FL.

36. “GAFF 2.2/2.3 Development”, AMBER Developers’ Meeting, on June 2-4, **2022**, Tempa

37. “Discovery of tau aggregation inhibitors by molecular simulation and experimental verification**”,** November 4, **2022,** Ohio State University**.**

38. “Discovery of small molecule inhibitors for amyloid oligomerization”, November 15, **2022**, University of Kansas.

39. “A Novel Strategy for Building PBPK Models for Arbitrary Molecules”, November 16, **2022**, Simcyp Scientific Webinar Series.

40. “A Novel Strategy for Building PBPK Models for Arbitrary Molecules” at the SimCYP Scientific Webinar Series on November 16, **2022**

41. “GAFF2 and GAFF3 Development” at Annual AMBER Developers’ Meeting, on March 1-4, **2023**, Tampa FL.

42. “Predict infectability of SARS-CoV-2 spike mutations using a combination of evolution analysis, site-site correlation analysis and binding free energy analysis” at ACS 2023 Spring National Meeting, on March 26-30, **2023**, Innianapolis, IN.

43. "Development of general-purpose molecular mechanics force fields (MMFF) and MMFF-based scoring functions for rational drug design", **2023**, NIH/NIH/NHLBI, Bethesta, MD.

44. "Accurate Free Energy Calculations Using Poisson-Boltzmann Surface Area (PBSA) Method" at "Free Energy Workshop", at the Novartis Institutes for BioMedical Research, May 10-12, **2023**, Cambridge, MA.

45. "GAFF2 and GAFF3 Development" at Annual AMBER Developers' Meeting, on Feb 28 to March 2nd, **2024**, Tampa FL.

46. "Development of the third generation of the general AMBER force field (GAFF3): Significantly improve the accuracy of free energy calculations" at ACS 2024 Spring National Meeting, on March 17th – March 21st in New Orleans.

International/National Conferences

47. "Antechamber: An accessory software package for molecular mechanical calculations.", *The #222nd American Chemical Society National Meeting,* **2001.**

48. "Development and test of a set of dipole interaction models.", The 236th *American Chemical Society National Meeting,* **2008.**

49. "Prediction of binding affinities with a Poisson-Boltzmann continuum solvent model", The 245th *American Chemical Society Conference,* **2013.**

50. "Prediction of Protein-Ligand Binding Using Continuum Models", 2nd International Conference on Bioinformatics and Computational Biology (ICBCB), April 21-22, **2013**, Beijing, China.

51. "Development and test of the second generation of the general AMBER force field.", The 247th *American Chemical Society National Meeting,* **2014.**

52. "Understanding the mechanisms of protein-ligand interactions through molecular dynamics simulations and free energy analysis", The 254th *American Chemical Society National Meeting,* **2017.**

53. "Development of the third generation of the general AMBER force field (GAFF3): Significantly improve the accuracy of free energy calculations", The *American Chemical Society National Meeting (Virtual),* **Spring 2021.**