Peng Tao, Ph.D.

Department of Chemistry
Center for Drug Design, Discovery, Delivery
Center for Scientific Computation
Southern Methodist University
Email: ptao@smu.edu

PO Box 750314
Dallas, TX 75275-0314
Phone: (214) 768-8802
Fax: (214) 768-4089

CAREER

2013 ~ Southern Methodist University, Dallas, TX
Assistant professor, Department of Chemistry

2010 ~ 2013 NHLBI/NIH, Rockville, MD
Research Fellow, advisor: Dr. Bernard R. Brooks

2007 ~ 2010 Wayne State University, Detroit, MI
Postdoctoral Research Fellow, advisor: Professor H. Bernhard Schlegel

EDUCATION

2007 The Ohio State University, Columbus, OH
Ph.D., Physical Chemistry, advisor: Professor Christopher M. Hadad

2001 Peking University, P. R. China
M.S., Physical Chemistry, advisor: Professor Luhua Lai

1998 Peking University, P. R. China
B.S., Chemistry (Honors), advisor: Professor Luhua Lai

AWARD

2017 Sam Taylor Fellowship ($1,000)

2015 Ralph E. Powe Junior Faculty Enhancement Award ($10,000)

2014 Sam Taylor Fellowship ($2,000)

EXTERNAL GRANTS

2017-2019 American Chemical Society (ACS) Petroleum Research Fund (PRF) Doctoral New Investigator (DNI) Grants (Total: $110,000)

2014 Computing allocation (400,000 System Units) awarded from Texas Advanced Computing Center

2013 Computing allocation (300,000 System Units) awarded from Texas Advanced Computing Center

INTERNAL GRANTS

2017 Just-in-Time Teaching and Technology Grants from Center for Teaching Excellence (Total: $900)

2016 Just-in-Time Teaching and Technology Grants from Center for Teaching Excellence (Total: $500)

2016-2017 Southern Methodist University, Dean's Research Council, Research Grant, (Total: $28,900)

2013 Internal grant from Center for Drug Design, Discovery, Delivery, SMU

PEER REVIEWED PUBLICATIONS

32. Wang, F.; Zhou, H.; Olademehin, O. P.; Kim, S. J.; Tao, P., Insights into Key Interactions between Vancomycin and Bacteria Cell Wall Structure. *ACS Omega* **2018**, *3*, 37−45 DOI: 10.1021/acsomega.7b01483.

31. Zhou, H.; Tao, P., Dynamics Sampling in Transition Pathway Space. *J. Chem. Theory Comput.* **2018**, *14*, 14−29 DOI: 10.1021/acs.jctc.7b00606.

30. Dong, Z.; Zhou, H.; Tao, P., Combining Protein Sequence, Structure and Dynamics: A Novel Approach for Functional Evolution Analysis of Pas Domain Superfamily. *Protein Sci.* **2017**, *27*: 421-430 DOI: 10.1002/pro.3329.

29. Zhou, H.; Zoltowski, B.; Tao, P.*; "Revealing Hidden Conformational Space of LOV Protein VIVID Through Rigid Residue Scan Simulations" *Sci. Rep.* **2017**, *7*: 46626. DOI:10.1038/srep46626

28. Tao, P.; Hackett, J. C.; Kim, J. Y.; Saffen, D.; Hayes, C. J.; Hadad, C. "Molecular Determinants of TRPC6 Channel Recognition by FKBP12" in Computational Chemistry Methodology in Structural Biology and Materials Sciences, ISBN 978-1-77188-568-3, Apple Academic Press, Inc., **2017**.

27. Kalescky, R.; Zhou, H.; Liu, J.; Tao, P.*; "Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery" *PLoS Comput. Biol.* **2016**, *12(4):* e1004893.

26. Chang, J.; Zhou, H.; Preobrazhenskaya, M.; Tao, P.;Kim, S. J. "The Carboxyl Terminus of Eremomycin Facilitates Binding to the Non-d-Ala-d-Ala Segment of the Peptidoglycan Pentapeptide Stem" *Biochemistry* **2016**, *55*, 3383–3391.

25. Kalescky, R.; Liu, J.; Tao, P.*; "Identifying Key Residues for Protein Allostery Through Rigid Residue Scan" *J. Phys. Chem. A.* **2015**, *119*, 1689-1700.

24. Cao, J.; Lopez, M.; Thacker, J. M.; Moon, J. Y.; Jiang, K.; Morris, S. N. S.; Bauer, J. H.; Tao, P.; Mason, R. P.; Lippert, A. R. "Chemiluminescent Probes for Imaging H2S in Living Animals" *Chem. Sci.* **2015**, *6*, 1979-1985.

23. Sodt, A. J.; Mei, Y.; Tao, P.; Steele, R. P.; Brooks, B. R; Shao, Y.; "Multiple Environment Single System Quantum Mechanical/molecular Mechanical (MESS-QM/MM) Calculations. I. Estimation of Polarization Energies.". *J. Phys. Chem. A.* **2015**, *119*, 1511-1523.

22. Tao, P.*; Sodt, A. J.; Shao, Y.; König, G.; Brooks, B. R; "Computing the free energy along a reaction coordinate using rigid body dynamics". *J. Chem. Theory Comput.* **2014**, *10*, 4198-4207.

21. Tao, P.; Larkin, J. D.; Brooks, B. R. "Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events" in Some Applications of Quantum Mechanics, ISBN 979-953-51-0059-1, InTech, **2012**.

20. Tao, P.; Hodošček, M.; Larkin, J. D; Shao, Y.; Brooks, B. R; "Comparison of Three Chain-of-States Methods: Nudged Elastic Band, Replica Path with Restraints or Constraints". *J. Chem. Theory Comput.* **2012**, *8*, 5035-5051.

19. Tao, P.; Wu, X.; Brooks, B. R; "Maintain Rigid Structures in Verlet Based Cartesian Molecular Dynamics Simulations". *J. Chem. Phys.* **2012**, *137*, 134110.

18. Tao, P.; Parquette, J. R; Hadad, C. M; "Right- and Left-Handed Helices, What is in between? Interconversion of Helical Structures of Alternating Pyridinedicarboxamide/m-(phenylazo)azobenzene Oligomers". *J. Chem. Theory Comput.* **2012**, *8*, 5137-5149.

17. Bao, X.; Tao, P.; Villamena, F. A.; Hadad, C. M; "Spin Trapping of Hydroperoxyl Radical by a Cyclic Nitrone Conjugated to β-Cyclodextrin: A Computational Study". *Theor. Chem. Acc.* **2012**, *131*, 1248-1257.

16. Zhang, S.; Qu, Z.; Tao, P.; Brooks, B. R; Shao, Y.; Chen, X.; Liu, C.; "Quantum Chemical Study of the Ground and Excited State Electronic Structures of Carbazole Oligomers with and without Triarylborane Substitutes", *J. Phys. Chem. C,* **2012**, *116*, 12434-12442.

15. Zhou, J.; Tao, P.; Fisher, J. F.; Shi, Q.; Mobashery, S.; Schlegel, H. B. "QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S) SB-3CT and its Oxirane Analogue", *J. Chem. Theory Comput.* **2010**, *6*, 3580-3587. (Selected as cover article)

14. Tao, P.; Gatti, D. L.; Schlegel, H. B. "Common Basis for the Mechanism of Metallo and Non-metallo KDO8P Synthases", *J. Inorg. Biochem.* **2010***, 104*, 1267-1275.

13. Psciuk, T. B.; Tao, P.; Schlegel, H. B. "Ab Initio Classical Trajectory Study of the Fragmentation of C3H4 Dications on the Singlet and Triplet Surfaces", *J. Phys. Chem. A* **2010**, *114, 7653*-7660.

12. Tao, P.; Schlegel, H. B. "A Toolkit to Assist ONIOM Calculations", *J. Comput. Chem.* **2010**, *31*, 2363-2369.

11. Sanan, T. T.; Muthukrishnan, S.; Beck, J. M.; Tao, P.; Hayes, C. J.; Otto, T. C.; Cerasoli, D. M.; Lenz, D. E.; Hadad, C. M. "Computational modeling of human paraoxonase 1: preparation of protein models, binding studies, and mechanistic insights", *J. Phys. Org. Chem.*, **2010***, 23,* 357-369.

10. Tao, P.; Fisher, J. F.; Shi, Q.; Mobashery, S.; Schlegel, H. B. "Matrix Metalloproteinase 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Deprotonation-Initialized Ring-Opening Reaction of Sulfoxide Analog of SB-3CT", *J. Phys. Chem. B*, **2010***, 114,* 1030-1037.

9. Tao, P.; Gatti, D. L.; Schlegel, H. B. "The energy landscape of 3-Deoxy- D-*manno*-octulosonate 8-Phosphate Synthase"*, Biochemistry,* **2009***, 48, 11706*-11714

8. Tao, P.; Fisher, J. F.; Shi, Q.; Vreven, T.; Mobashery, S.; Schlegel, H. B. "Matrix Metalloproteinase 2 (MMP2) Inhibition: Combined Quantum Mechanics and Molecular Mechanics Studies of the Inhibition Mechanism of (4-Phenoxyphenylsulfonyl) methylthiirane and Its Oxirane Analogue", *Biochemistry*, **2009***, 48,* 9839-9847

7. Tao, P.; Fisher, J. F.; Mobashery, S.; Schlegel, H. B. "DFT Studies of the Ring-Opening Mechanism of SB-3CT, a Potent Inhibitor of Matrix Metalloproteinase 2", *Org. Lett.*, **2009**, *11*, 2559-2562

6. Kona, F.; Tao, P.; Martin, P.; Xu, X.; Gatti, D. L.. "Electronic Structure of the Metal Center in the Cd^{2+}, Zn^{2+}, and Cu^{2+} Substituted Forms of KDO8P Synthase: Implications for Catalysis", *Biochemistry*, **2009**, *48*, 3610-3630 (Kona, K. and Tao, P. contributed equally to this work)

5. King, E. D.; Tao, P.; Sanan, T. T.; Hadad, C. M.; Parquette, J. R. "Photomodulated chiral induction in helical azobenzene oligomers**".** *Org. Lett.* **2008**, *10*, 1671-1674

4. Mendlik, M. T.; Tao, P.; Hadad, C. M.; Coleman, R. S.; Lowary, T. L. "Synthesis of L-Daunosamine and L-Ristosamine Glycosides via Photoinduced Aziridination. Conversion to Thioglycosides for Use in Glycosylation Reactions." *J. Org. Chem.* **2006**, *71*, 8059-8070

3. Tao, P.; Lai, L. "Protein Ligand Docking Based on Empirical Method for Binding Affinity Estimation" *J. Comput.-Aided Mol. Des.* **2001**, *15*, 429-446.

2. Tao, P.; Wang, R.; Lai, L. "Calculating Partition Coefficients of Peptides by the Addition Method" *J. Mol. Mod.* **1999**, *5*, 189-195.

1. Tao, P.; Wang, R.; Lai, L. "Calculation of Peptide's Partition Coefficients by Amino Acid Addition Method" *Wuli Huaxue Xuebao* **1999**, *15*, 449-453.

ORAL PRESENTATIONS

- Invited Presentation, "Probing protein allostery as dynamical process through systematic perturbation and machine learning" Southwest Regional ACS Meeting, Lubbock, TX, October 29-November 1, 2017
- Invited presentation, "Artificial Intelligence in Computational Chemistry: Hope or Hype?" IEEE MetroCon 2017 Conference, Arlington, TX, October 26, 2017
- Invited Seminar, Department of Chemistry and Chemical Biology, Indiana University – Purdue University Indianapolis, Indianapolis, IN, October 10, 2017
- Invited Seminar, Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, September 25, 2017
- Invited Seminar, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, September 22, 2017
- Invited presentation, "Application of machine learning methods in computer simulations of protein dynamics", American Mathematical Society, Sectional Meeting, University of North Texas, Denton, TX, September 9-10, 2017
- Invited Seminar, Department of Chemistry, University of Louisville, Louisville, KY, September 8, 2017
- Invited Seminar, Chemistry Department, University of Colorado Denver, Denver, CO, September 1, 2017
- Invited Seminar, The Laboratory of Computational Biology, National Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD, August 23, 2017
- Invited presentation, "Chain-of-states method based dynamical sampling", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- Oral presentation, "Computational investigation of cell nitroxyl (HNO) fluorescent probe", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- Invited Seminar, Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore, MD, August 18, 2017
- Invited Seminar, National Heart, Lung, and Blood Institute, National Institutes of Health, Rockville, MD, August 17, 2017
- Invited Seminar, Biotechnology High Performance Computing Software Applications Institute (BHSAI), Department of Defense, Frederick, MD, August 16, 2017
- Invited Seminar, Center for Cancer Research, National Cancer Institute, Frederick, MD, August 15, 2017
- Invited Seminar, Department of Pharmacology, Baylor College of Medicine, Houston, TX, August 1, 2017

- Invited presentation, "Enhanced Transition Pathway Dynamical Sampling Method", Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics Workshop Telluride Science Research Center (TSRC), Telluride, CO, July 11-15, 2017
- Invited presentation, "Surveying key residues for protein allostery using rigid residue scan method", 253rd ACS National Meeting, San Francisco, CA, April 2-6, 2017
- SMU BioMath Monthly Seminar Series, March 6th, 2017
- Invited Seminar, ACS DFW 4th Young Investigators Symposium, University of Texas Dallas, Dallas, TX, January 28, 2017
- Invited Seminar, Department of Chemistry, Southeastern Louisiana University, Hammond, LA, January 20, 2017
- Invited Seminar, Department of Chemistry, University of North Texas, Denton, TX, December 2, 2016
- "Protein allostery: What we can learn from nudging the protein structure systematically?" Invited Presentation, Southwest Regional ACS Meeting, Galveston, TX, November 12, 2016
- "Direct pathway dynamical sampling method", Invited Presentation, Southwest Regional ACS Meeting, Galveston, TX, November 12, 2016
- Invited Seminar, Department of Chemistry and Biochemistry, Baylor University, Waco, TX, November 18, 2016
- Invited Seminar, College of Chemistry, Peking University, P. R. China, July 26, 2016
- "Bolstering Antibiotics: How to Fight Superbugs and Conquer Drug Resistance" Invited Seminar at Inside SMU Forum of Founder's Day Event, April 16, 2016
- Invited Departmental Seminar, Department of Mathematics, SMU, April 7, 2016.
- Invited Departmental Seminar, Department of Chemistry, Wichita State University, March 9, 2016
- "Exploring enzymatic reaction pathways using QM/MM methods", Southwest Regional ACS Meeting, Memphis, TN, November 7, 2015
- "Application of rigid body dynamics in free energy simulation and protein allostery", Southwest Regional ACS Meeting, Fort Worth, TX, November 19-22, 2014
- "Computational Enzymology and Methodology", Chemistry Departmental Seminar, Texas Christian University, November 13, 2014
- "Free Energy Profile Along Reference Reaction Path Through Rigid Body Dynamics", 244th ACS National Meeting, Philadelphia, PA, United States, August 19-23, 2012
- "Replica Path Method and Rigid Body Dynamics in CHARMM", Telluride Science Research Center, Telluride, CO, United States, June 17-21, 2012
- "Computational Methods in Enzymatic Reaction Mechanism Study", 241st ACS National Meeting, Anaheim, CA, United States, March 27-31, 2011

- "Postdoctoral research: why and how", 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009
- "Folding of helical structures of alternating pyridinedicarboxamide/M-(phenylazo) azobeneze oligomers." Abstracts of Papers, 234th ACS National Meeting, Boston, MA, United States, August 19-23, 2007
- "Computational sof the N5-CAIR mutase mechanism in the purine biosynthesis pathway. Abstracts of Papers, 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006
- "Applying molecular dynamics to understand signal transduction: Recognition of TRPC6 by FKBP12." Abstracts of Papers, 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006
- "Computational Study of Epoxide Ring-Opening Reactions of 2,3-Anhydrosuars" 229th ACS National Meeting, San Diego, CA, March 13-17, 2005

POSTER PRESENTATIONS

- "Protein evolution analysis integrating different levels of structures and simulations", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- "Correlating individual amino acid residues with protein allostery through rigid residue scan", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- "Computational Study of Allostery of Protein VIVID, a PAS/LOV Domain in Circadian Clock System". Cancer Prevention and Research Institute of Texas (CPRIT) Innovations Conference at Austin, TX on November 9, 2015.
- "Computational Enzymology: Methodology Development and Application", 3rd DFW's New Young Investigators Symposium, University of Texas at Arlington, Arlington, Texas January 25, 2014
- "Computational Study of Epoxide Ring-Opening Reactions of 2,3-Anhydrosuars" 229th ACS National Meeting, San Diego, CA, March 13-17, 2005

COMMITTEE SERVICE

2013-present	Research Committee for Center for Scientific Computation, SMU
2015	Panelist of "Bridging the gap between theory and experiments in Nanomedicine", Southwest Regional ACS Meeting, Memphis, TN, November 7, 2015

AFFILIATIONS

2003-present	American Chemical Society
2007-2011	Member of Younger Chemists Committee charted by American Chemical Society
2010-2011	Chair of Communication Subcommittee of Younger Chemists Committee

PEER-REVIEW ACTIVITIES

Foundation for Frontier Research in Chemistry (FRC)
National Science Foundation, Panelist, Chemistry division,
Chemical Structure, Dynamics and Mechanisms Program
Chemical Theory, Models and Computational Methods program
Major Research Instrumentation Program
American Chemical Society Petroleum Research Fund
PLoS Computational Chemistry
European Journal of Medicinal Chemistry
International Journal of Quantum Chemistry
Journal of Biological Physics
Journal of Molecular Graphics and Modelling
Journal of Physical Chemistry B
Journal of Physical Chemistry C
Nanoscience
Molecular Simulation
Scientific Reports