

✧ 个人信息:

性别: 男

年龄: 30

最高学历: 博士

出生地: 广东佛山

政治面貌: 党员

语言: 国语/粤语/英语

✧ 联系方式:

E-mail: zhaozxcpu@hotmail.com

✧ 工作经历

- 2014.9-至今, 美国密歇根州立大学, 数学系(数学生物学方向), 博士后, 导师: Prof. Guowei Wei
- 2014.6-2014.9, 中国科学院上海有机化学研究所, 研究助理

✧ 教育经历

- 2008.9-2014.6, 理学博士(有机化学), 中国科学院上海有机化学研究所, 导师: 王任小研究员
- 2004.9-2008.7, 理学学士(药学), 中国药科大学

✧ 求职意向

- 分子模拟和计算生物/化学相关应用工作, 计算机辅助药物设计工作
- 生物信息学及数据分析相关工作; 软件开发等 IT 相关工作

✧ 个人技能

- 熟练掌握各种分子模拟技术, 如分子对接及虚拟筛选, 分子动力学模拟, 蛋白结构预测和优化, QSAR, 量化计算(反应过渡态计算, QM/MM)等。熟练使用 MOE、Schrodinger、Sybyl、Discovery Studio、Gaussian、Amber、Gold、Autodock、Pymol、VMD、Chimera 等软件。
- 熟练掌握多种编程语言(C++/Python/Shell/Fortran); 熟练使用和维护集群、Linux、Mac 等多系统; 掌握 Markdown、Html 等使用。
- 掌握数学和统计软件 Matlab 以及 R 的使用, 了解计算数学及应用。
- 熟练掌握有机化学知识及进行有机化学实验, 掌握核磁、质谱、红外、GC/LC 等分析手段。
- 掌握各种质谱仪器及其维护, 如 ESI-, MALDI-, APCI-, GC-及 MS/MS 等。精通各种质谱图谱的解释(ESI/MALDI/EI)。

项目经验

- 2015.6-至今: Poisson-Boltzmann 方法在蛋白等电点计算及残基突变亲和力变化的计算
- 2014.9-至今: 冷冻电镜数据的拓扑分析及结构拟合
- 2011.6-2014.6: 分子结构优化和全新设计程序 AutoT&T 的开发
- 2011.6-2014.6: 自吞噬相关靶点 Atg5 蛋白的先导化合物发现和设计
- 2013.6-2014.6: TSR 及 PYR 两种抗生素合成酶作用机制研究
- 2012.6-2013.6: 自组装超分子复合物结构模拟
- 2011.6-2012.6: DNA 糖基化酶 YtkR2 作用机制的研究
- 2009.6-2011.4: 微反应器串联质谱及敞开式质谱用于有机反应中间体研究和气相化学变化的研究
- 2007.9-2008.7: κ 阿片受体激动剂 MB-1c 类化合物制备方法的改进

◇ 奖项

- 2012-2013 以及 2013-2014 年度, 中科院三好学生
- 2013.10, 优秀墙报奖 (第十二届全国计算 (机) 化学学术会议)
- 2012.10, 优秀墙报奖 (第二届全国生物物理化学会议)
- 2012.6, 优秀墙报奖 (生命有机化学国家重点实验室 2012 年学术年会)
- 2004-2008, 中国药科大学数次奖学金及校三好学生

◇ 已发表及待发表论文:

1. **Zhixiong Zhao**[†], Zhengxi Zhang[†], Yan Li, Mi Zhou, Xun Li, Biao Yu, Renxiao Wang*. Probing the Key Interactions between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modeling. *ChemMedChem* **2013**, 8, 1270-1275. (Back Cover) [[Connect](#)]
2. **Zhixiong Zhao**, Haoyang Wang*, Yinlong Guo*. Study on Transient Intermediates in Fast Cyclopropenium-Activated Chlorination Reaction of Alcohols by ESI-MS. *J. Mass Spectrom.* **2011**, 46, 856-858. [[Connect](#)]
3. **Zhixiong Zhao**, Haoyang Wang*, Yinlong Guo*. Studies on CH₃CN-Assisted Decomposition of 1st Grubbs Catalyst by Electrospray Tandem Mass Spectrometry. *Rapid Commun. Mass Spectrom.* **2011**, 25, 3401-3410. [[Connect](#)]
4. **Zhixiong Zhao**, Haoyang Wang*, Yinlong Guo*. Studies of Heterogeneous/Homogeneous Ion-Molecule Reactions by Ambient Ionization Mass Spectrometry. *Curr. Org. Chem.* **2011**, 15, 3734-3749. [[Connect](#)]
5. **Zhixiong Zhao**, Haoyang Wang*, Chu Xu, Yinlong Guo*. Gas-phase Synthesis of Hydrodiphenylcyclopropenylium via Nonclassical Favorskii Rearrangement from Alkali-

- cationized α,α' -dibromodibenzyl Ketone. *Rapid Commun. Mass Spectrom.* **2010**, *24*, 2665-2672. [[Connect](#)]
6. **Zhixiong Zhao**, Shengjun Yao, Haoyang Wang*, Yinlong Guo*. Progress in ESI-MS Study for the Catalytic Asymmetric Reactions. *Chinese J. Org. Chem.* **2010**, *30*, 809-815. [[Connect](#)]
 7. Shoufeng Wang, Qingfei Zheng, Jianfeng Wang, **Zhixiong Zhao**, Qingye Li, Yunsong Yu, Renxiao Wang and Wen Liu*. Target-oriented design and biosynthesis of thioestrepton-derived thiopeptide antibiotics with improved pharmaceutical properties. *Org. Chem. Front.* **2015**, *2*, 106-109. (Cover)[[Connect](#)]
 8. Zhihai Liu, Yan Li, Li Han, Jie Li, Jie Liu, **Zhixiong Zhao**, Wei Nie, Yuchen Liu and Renxiao Wang*. PDB-wide Collection of Binding Data: Current Status of the PDBbind Database. *Bioinformatics*, **2015**, *31*, 405-412. [[Connect](#)]
 9. Yan Li, Zhihai Liu, Li Han, Jie Li, Jie Liu, **Zhixiong Zhao**, Chengke Li, Renxiao Wang*. Comparative Assessment of Scoring Functions on an Updated Benchmark: I. Compilation of the Test Set, *J. Chem. Inf. Model*, **2014**, *54*, 1700-1716. [[Connect](#)]
 10. Chunfang Wu, Zhiming Li, Xiaona Xu, **Zhixiong Zhao**, Xin Zhao, Renxiao Wang, ZhanTing Li*. Folding Induces Folding: The Assembly of Aromatic Amide and 1,2,3-Triazole Hybrid Helices. *Chem. Eur. J.* **2014**, *20*, 1418-1426. [[Connect](#)]
 11. Haoyang Wang*, **Zhixiong Zhao**, Yinlong Guo*. Chemical and Biochemical Applications of MALDI-TOF MS Based on Analyzing the Small Organic Compounds. *Top. Curr. Chem.* **2013**, *331*, 165-192. [[Connect](#)]
 12. Hui Xu[†], Wei Huang[†], Qingli He, **Zhixiong Zhao**, Feng Zhang, Renxiao Wang, Jingwu Kang, Gongli Tang*. Self-Resistance to an Antitumor Antibiotic: A DNA Glycosylase Triggers the Base-Excision Repair System in Yatakemycin Biosynthesis. *Angew. Chem. Int. Ed.* **2012**, *51*, 10532-10536. [[Connect](#)]
 13. Haoyang Wang*, Chu Xu, **Zhixiong Zhao**, Xiaoshuang He, Yinlong Guo*. Analysis of Low Molecular Weight Compounds by MALDI-FTICR-MS. *J. Chromatogr. B* **2011**, *879*, 1166–1179. [[Connect](#)]
 14. Chu Xu, Haoyang Wang, **Zhixiong Zhao**, Qinghong Tang, Yinlong Guo*, Long Lü. Studies of the Interesting Gas-Phase Rearrangement Reactions of 2-Pyrimidinyloxy-N-arylbenzylurea Promoted by Urea-Carbaminidic Acid Tautomerism by ESI-MS/MS and Theoretical Computation. *Chin. J. Chem.* **2010**, *28*, 1765-1772. [[Connect](#)]
 15. **Zhixiong Zhao**, Yuan Zhao, Yan Li, Zhihai Liu, Renxiao Wang*. Structure-Based Design by AutoT&T2: I. Efficient Process of Designed Ligand Structures. *In Preparation*.
 16. **Zhixiong Zhao**, Yuan Zhao, Yan Li, Zhihai Liu, Renxiao Wang*. Structure-Based Design by AutoT&T2: II. Pharmacophore- Directed De Novo Design. *In Preparation*.
 17. **Zhixiong Zhao**, Kelin Xia and Guowei Wei, Topological persistence between Cryo-EM data and fitting PDB structure. *In Preparation*.

18. Kelin Xia, **Zhixiong Zhao** and Guo-Wei Wei. Multiresolution topological persistence in biomolecular data, *J. Comp. Biol.* (2015)
19. Bao Wang, **Zhixiong Zhao** and Guowei Wei, Electrostatic solvation free energy based on Poisson-Boltzmann model and machine learning. *In Preparation.*
20. Xiaowei Sun, Chen Shi, Chengzhe Gao, **Zhixiong Zhao**, Renxiao Wang, Xiaolan Wen, Xiuhong Yang, Hongbin Sun*. Discovery of a Potent Octane-Carboxamide Based Renin Inhibitor Bearing a 4-(2-Hydroxyethyl)-1H-1,2,3-Triazole. *In preparation.*
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◇ 软件著作权:

21. AutoPhD 复合物药效团模型自动推导软件 V1.0, 正式登记号: 2014SR135134
22. AT&T-PG 药效团指导的药物分子结构设计软件 V1.0, 正式登记号: 2014SR135213
23. FWCluster 基于骨架的分子结构聚类软件 V1.0, 正式登记号: 2014SR135139
24. AT&T 先导化合物发现及结构优化软件 V2.0, 正式登记号: 2013SR160292
-

◇ 会议论文:

1. **Zhixiong Zhao**, Yuan Zhao, Yan Li, Zhihai Liu, Renxiao Wang*. Pharmacophore-Guided Automatic Tailoring and Transplanting for Lead Optimization. *The 12th National Symposium of Computational Chemistry*, Oct. 2013, Suzhou, Jiangsu province, China.
2. **Zhixiong Zhao**, Yuan Zhao, Yan Li, Zhihai Liu, Renxiao Wang*. Pharmacophore-Guided Automatic Tailoring and Transplanting for Lead Optimization. *The 8th National Conference on Chemical Biology*, Sep. 2013, Shanghai, China.
3. **Zhixiong Zhao**, Hui Xu, Yan Li, Gongli Tang*, Renxiao Wang*. Molecular Modeling Study on the Mechanism of DNA Glycosylase YtkR2 for the Self-Resistance to Antitumor Antibiotic. *The Second National Conference on Biophysical Chemistry*, Oct. 2012, Wuhan, Hubei province, China.
4. **Zhixiong Zhao**, Yan Li, Zhengxi Zhang, Mi Zhou, Renxiao Wang*. Virtual Screening of Small-Molecule Inhibitors Targeting the Protein-Protein Interactions Involving Autophagy-Related Protein Atg5. *The Second National Conference on Biophysical Chemistry*, Oct. 2012, Wuhan, Hubei province, China.