吉林大学 生命科学学院
School of Life Sciences, Jilin University

教授

教授 (../../szdw/js.htm)

副教授 (../../szdw/fjs.htm)

讲师 (../../szdw/js1.htm)

实验技术人员 (../../szdw/syjsry.htm)

离退休人员 (../../szdw/ltxry.htm)

韩葳葳

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<tr><td>研究方向：</td><td colspan="2">酶结构与功能的关系 计算机辅助药物设计 计算结构生物学 机器学习</td></tr>
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2007.7-2009.9 分子酶学工程教育部重点实验室 讲师
1997.9-2002.7 装甲兵技术学院基础部数学室 教员</td></tr>
<tr><td>研究成果：</td><td colspan="2">1. Jingxuan Zhu,?Yishuo Lv,?XiaosongHan,?Dong Xu*, ?Weiwei Han*. Understanding the differences of the ligand binding/unbinding pathways between phosphorylated and non-phosphorylated ARH1 using molecular dynamics simulations. Sci Rep.?, 2017, 29;7(1):12439.
2. Qian Mengdan, Shan Yaming, Guan Shanshan, Zhang Hao, Han Weiwei*, Wang Song*. Structural Basis of Fullerene Derivatives as Novel Potent Inhibitors of Protein Tyrosine Phosphatase 1B: Insight into the Inhibitory Mechanism through Molecular Modeling Studies. J Chem Inf Model. ,2016, 56(10):2024-2034.
3. Weiwei Han#,?Jingxuan Zhu,?Song Wang,?Dong Xu. Understanding the Phosphorylation Mechanism by Using Quantum Chemical Calculations and Molecular Dynamics Simulations. J Phys Chem B.?,2017, 2121(15):3565-3573.
4. Jingxuan Zhu,?Yan Wang,?Xin Li,?Weiwei Han*, Li Zhao*. Understanding the interactions of different substrates with wild-type and mutant acylaminoacyl peptidase using molecular dynamics simulations. J Biomol</td></tr>
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Struct Dyn.?, 2017, 20:1-18.
5. Hanyong Jin, Jingxuan Zhu, Yang Dong, Weiwei Han*. Exploring the different ligand escape pathways in acylaminoacyl peptidase by random acceleration and steered molecular dynamics simulations. Rsc Advances,2016, 10987-10996.
6 Liyun Zou, Jingxuan Zhu, Yang Dong, Weiwei Han*, Yingjie Guo*, Hui Zhou *. Models for the binding channel of wild type and mutant transthyretin with glabridin. Rsc Advances, 2016,6.
7 Shanshan Guan, Li Zhao, Hanyong Jin, Ning Shan, Weiwei Han*, Song Wang*, Yaming Shan*. Binding modes of phosphotriesterase-like lactonase complexed with δ-nonanoic lactone and paraoxon using molecular dynamics simulations. J Biomol Struct Dyn. ,2016, 35: 273.
8 Hanyong Jin, Zhenhuan Zhou, Dongmei Wang, Shanshan Guan, Weiwei Han *. Molecular dynamics simulations of acylpeptide hydrolase bound WeiweMolecular Dynamics Simulations of Acylpeptide Hydrolase Bound to Chlorpyrifosmethyl Oxon and Dichlorvos. Int J Mol Sci., 2015, 16: 6217-6234.
9 Dongling Zhan, Shanshan Guan, Hanyong Jin, Weiwei Han *, Wang Song*. Stereoselectivity of phosphotriesterase with paraoxon derivatives: a computational study. J Biomol Struct Dyn.,?2016, 34(3):600-11.
10 Dongmei Wang,?Hanyong Jin,?Junling Wang,? Shanshan Guan, ?Zuoming Zhang?, Weiwei Han*. Exploration?of the?chlorpyrifos?escape?pathway?from?acylpeptide?hydrolases?using?steeredmolecular?dynamics?simulations. J Biomol Struct Dyn.?,2016, 34(4): 749-761.
11 Dongling Zhan, Aixi Bai, Lei Yu, Weiwei Han*, Feng Yan*. Characterization of the PH1704 protease from Pyrococcus horikoshii OT3 and the critical functions of Tyr120. Plos One., 2014,9, e103902.
12. Dongling Zhan, Dongmei Wang, Weihong Min*, Weiwei Han*. Exploring the molecular basis for selective binding of homoserine dehydrogenase from Mycobacterium leprae TN toward inhibitors: a virtual screening study. Int J Mol Sci.,2014, 15:1826-1841.
13. Dongling Zhan, Lei Yu, Hanyong Jin, Shanshan Guan, Weiwei Han *. Molecular modeling and MM-PBSA free energy analysis of endo-1,4-β-xylanase from Ruminococcus albus 8. Int J Mol Sci., 2014, 15: 17284-17303.
14. Han Weiwei#, Exploring the Molecular Basis for Selective Binding of Homoserine Dehydrogenase from Mycobacterium leprae TN toward Inhibitors: A Virtual Screening Study. Int. J. Mol. Sci. ,2014, 15: 1826-1841

15. Dongling Zhan, Zhenhuan Zhou, Shanshan Guan and Weiwei Han *. The effect of conformational variability of phosphotriesterase upon N-acyl-L-homoserine lactone and paraoxon binding: insights from molecular dynamics studie. Molecules, 2013, 18: 15501-15518.
16. Xun Sun, Mengdan Qian, Shanshan Guan, Yaming Shan, Ying Dong, Hao Zhang *, Song Wang *, Weiwei Han*. Investigation of an "alternate water supply system" in enzymatic hydrolysis in the processive endocellulase Cel7A from Rasamsonia emersonii by molecular dynamics simulation. Biopolymers, 2017, 107:46-61.
17. Dongmei Yan, Weiwei Han, Zehua Dong, Qihui Liu, Zheng Jin, Dong Chu, Yuan Tian, Jinpei Zhang, Dandan Song, Dunhuang Wang, Xun Zhu*. Homology modeling and docking studies of ENPP4: a BCG activated tumoricidal macrophage protein. Lipids Health Dis.,?2016 , 28:15-19.
18.Dongling Zhan, Weiwei Han*, Yan Feng*. Experimental and computational studies indicatethe mutation of Glu12 to increase the thermostability of oligomeric protease from Pyrococcus horikoshii. J Mol Model., 2011, 17:1241 - 1249.
19. Weiwei Han#, Ye Wang, Quan Luo, Yan Feng. Insights into a 3D homology model of arylesterase: the key residues upon protein-ligand docking and MM-PBSA calculations. J Chem Theory Comput Chem., 2011, 10: 165-177.
20. Weiwei Han#, Dongling Zhan, Quan Luo, Yihan Zhou, Yuan Yao, Zesheng Li, Yan Feng. The substrate specificity and the catalytic mechanism of N-carbamyl-D-amino acid amidohydrolase: a theoretical investigation. Chem Phys Lett., 2009, 472: 107-112.
21. Weiwei Han#, Ying Wang, Yihan Zhou, Yuan Yao, Zesheng Li *, Yan Feng*. Understanding structural/functional properties of amidase from rhodococcus erythropolis by computational approaches. J Mol Model., 2009,?15: 481-487.
22.Weiwei Han#, Dongling Zhan, Xi Zhao, Song Wang*.. Computational investigation on the ethylene-induced esterase from Citrus sinensis. Chem. Res in Chinese University.,2009, 26(1): 128-135.
23. Yuexi Wang, Ye Wang, Weiwei Han*, Yan Feng*. Improving the enzyme sensitivity of the organophosphorous compounds by combining experiment and theory methods. Chem. Res in Chinese University, 2012, 28(4): 707-711.
24. Weiwei Han#, Yihan Zhou, Quan Luo, Yuan Yao, Zesheng Li. On the 3D structure and catalytic mechanism study of AmiF formamidase of Helicobacter pylori. Polymer, 2007, 48: 3726-3731.
25.Weiwei Han#, Yihan Zhou, Yuan Yao, Zesheng Li*. The Three-dimensional

structure of Human aurora-C kinase predicted by homology modeling and docking study. Journal Molecular Struct. , 2007, 815: 87-93.
26. Weiwei Han#, Yihan Zhou, YuanYao, Zehheng Li*. Computational studies on bergaptol O-methyltransferase from Ammi majus L.: The substrate specificity. Polymer, 2006 , 47:7953-7961.
27. Weiwei Han#, Zesheng Li, Qingchuan Zheng, Chiachung Sun. Homology modeling and molecular dynamics studies on the tomato methyl jasmonate esterase. Polymer, 2006 , 47:1436-1442.
28. Weiwei Han#, Zesheng Li, Qingchuan Zheng, Chiachung Sun. Toward a blueprint for ?-Primeverosidase from tea leaves structure/function properties:Homology modeling study. J Chem Theory Comput Chem.,2006, 5:433-446.
29. Dongling Zhan, Nan Gao, Weiwei Han, Yan Feng. Quantum Chemistry Calculation of Thermophilic Protease PH1704 Allosteric Center and Mutant Dynamics. Chem. Res in Chinese University, 2014, 35(1) : 146-153.
30. Yuan Yao, Weiwei Han, Yihan Zhou, Zesheng Li*, Qiang Li, Xiaoyan Chen, Dafang Zhong*.The metabolism of CYP2C9 and CYP2C19 for gliclazide by homology modeling and docking study. Eur J Med Chem, 2009,44:854-861.
31. Quan Luo, Weiwei Han, Yihan Zhou, Yuan Yao, Zesheng Li*. The 3D Structure of the defense-related rice protein Pir7b predicted by homology modeling and ligand binding studies. J Mol Model., 2008, 14:559-569.
32. Yuan Yao, Weiwei Han, Yihan Zhou, Zesheng Li*, Qiang Li, Xiaoyan Chen, Dafang Zhong*.Catalytic Reaction Mechanism of Human Photoreceptor Retinol Dehydrogenase: A Theoretical Study. J Chem Theory Comput Chem., 2008 , 7: 565-578.
33. Yuan Yao, Weiwei Han, Yihan Zhou, Zesheng Li*. The 3D-Structure and Catalytic Reaction Mechanism of Human Photoreceptor Retinol Dehydrogenase. Polymer, 2007, 48: 2644-2648.
34. Yuan Yao, Weiwei Han, Yihan Zhou, Ze-sheng Li*. Molecular Docking Study of The Affinity of CYP2C9 and CYP2D6 for Imrecoxib. J Chem Theory Comput Chem., 2007, 6:514-548.
35. Chuan Xiao, Chao Sun , Weiwei Han, Feng Pan, Zhu Dan , Yu Li, Zhiguang Song, Yinghua Jin*. Synthesis of 6-(het) ary Xylocydine analogues and evaluating their inhibitory activities of CDK1 and CDK2 in vitro. Bloorgan Med Chem., 2011, 19: 7100－7110.
36. Quan Luo, Yuan Yao, Weiwei Han, Yihan?Zhou, Zesheng?Li*.? Homology modeling of a novel epoxide hydrolase (EH) from Aspergillus niger SQ-6:

structure-activity relationship in expoxides inhibiting EH activity. J Mol Model., 2009, 15:1125-1132.

项目：

1.吉林省科技发展极化项目 嗜热内脂酶：基于大分子反应通道的分子设计(3D517G951465)，2017. 1-2019.12

2.吉林省重大科技攻关项目 高效有机磷水解酶的制备及其在消除果蔬农药残留中的应用 (20140203025NY)，2014.1-2016.

3.973计划子课题 几类微生物代谢中的重要酶的结构与催化反应机理的理论研究(2012CB721003)，2012.1-2016.12

4.国家自然科学基金 嗜热寡聚蛋白酶别构调控机理的研究(31070638)，2011.1－2013.12

5.吉林省自然科学基金 磷酸三酯酶的分子改造(201015109)，2011.1-2013.12

6.吉林省教育厅“十二五”科学技术研究项目 碳纳米管和石墨烯诱导嗜热酶对有机磷化合物敏感性的研究，2015.1-2016.12