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个人简介

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一．学习工作经历

1、学历背景：

1992年至1997年：北京大学化学学士

1997年至2002年：北京大学理学博士

2、工作经历：

2002年至2004年：北京大学化学系，博士后

2004年至2008年：美国加州大学圣地亚哥分校，博士后和项目研究员

2009年至2012年：苏州大学功能纳米与软物质研究院/药学院，特聘教授、博士生导师

2013年3月至今：浙江大学药学院，求是特聘教授、博士生导师。

二．研究方向

主要研究方向包括：(1). 基于靶标结构的虚拟筛选方法研究；(2). ADMET和类药性预测方法研究；(3). 重要靶点的药物分子设计和筛选；(4). 基于多尺度分子模拟的靶标-配体识别作用机制研究。

三．主要研究成果

(1). 学术成果简介

长期从事计算机辅助药物分子设计方法学和应用研究，主要研究成果包括：(1). 对MM/GB(PB)SA自由能预测方法中的核心理论问题进行了系统研究，发展了多种基于靶点结构的高精度及高效的虚拟筛选方法并成功用于重要靶点的药物分子设计；(2). 发展了一系列基于分子结构的ADMET性质和类药性预测新方法、新模型和新程序，并被国际大型分子模拟软件系统（如AMBER和MOE）、知名制药公司和国内外同行广泛采用；(3). 通过模拟和实验的结合成功发现多个重要靶标（ROCK1、MIF、ALK、A2A AR）的活性抑制剂分子。

在*PNAS*、*Adv Drug Delivery Rev*、*WIRES Comput Mol Sci*、*J Med Chem*、*Oncotarget*、*Mol Pharmaceutics*、*Mol Cell Proteomics*、*Drug Discov Today*、*J Chem Theory Comput*、*J Proteome Res*、*Mol Cancer Ther*、*PLoS Comput Biol*、*J Chem Inf Model*、*Bioinformatics*、*J Cheminformatics*、*J Mol Biol*、*PCCP*、*Antiviral Res*、*J Phys Chem B*、*J Comput Chem*等SCI收录期刊上发表论文280余篇，他引超过5600次，H因子为40。自计算机辅助药物分子设计和化学信息学领域最具影响力的专业性期刊J Chem Inf Model创刊50余年以来，在该期刊上发表论文数排名全世界第16位(共37篇)，华人第1位。获软件著作权和授权专利18项。

(2). 近期代表性论文.

1.Hui Liu, Fu Chen, Huiyong Sun, Dan Li, Tingjun Hou*, Improving the efficiency of non-equilibrium sampling in the aqueous environment via implicit-solvent simulations, *Journal of Chemical Theory and Computation*, 2017, 13, 1827-1836.

2.Shuangquan Wang, Huiyong Sun, Hui Liu, Dan Li, Youyong Li, Tingjun Hou*, ADMET evaluation in drug discovery. 16. Predicting hERG blockers by combining multiple pharmacophores and machine learning approaches, *Molecular Pharmaceutics*, 2016, 13, 2855-2866.

3.Hui Liu, Dan Li, Youyong Li, Tingjun Hou*, Atomistic molecular dynamics simulations of ATP-binding cassette transporters, *WIREs Computational Molecular Science*, 2016, 6, 255-265. (Inside Cover)

4.Fu Chen, Hui Liu, Huiyong Sun, Peichen Pan, Youyong Li, Dan Li, Tingjun Hou*, Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict protein-protein binding free energies and re-rank binding poses generated by protein-protein docking, *Physical Chemistry Chemical Physics*, 2016, 18, 22129-22139.

5.Mojie Duan, Na Liu, Wenfang Zhou, Dan Li, Minghui Yang*, Tingjun Hou*, Structural diversity of ligand-binding androgen receptors revealed by microsecond long molecular dynamics simulations and enhanced sampling, *Journal of Chemical Theory and Computation*, 2016, 12, 4611-4619.

6.Tailong Lei, Dan Li, Youyong Li, Huiyong Sun, Tingjun Hou*, ADMET Evaluation in Drug Discovery. 15. Accurate Prediction of Rat Oral Acute Toxicity Using Relevance Vector Machine and Consensus Modeling, *Journal of Cheminformatics*, 2016, 8, 1.

7.Huiyong Sun, Pengcheng Chen, Dan Li, Youyong Li, Tingjun Hou*, Directly-binding rather than induced-fit dominated binding affinity difference in (S) and (R)-crizotinib bound MTH1, *Journal of Chemical Theory and Computation*, 2016, 12, 851-860.

8.Huiyong Sun, Peichen Pan, Sheng Tian, Lei Xu, Xiaotian Kong, Youyong Li, Dan Li, Tingjun Hou*, Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery, *Scientific Reports*, 2016, 6, 24817.

9.Zhe Wang, Huiyong Sun, Xiaojun Yao, Dan Li, Lei Xu, Youyong Li, Sheng Tian, Tingjun Hou*, Comprehensive evaluation of ten docking programs on a diverse set of protein-ligand complexes: prediction accuracy of sampling power and scoring power, *Physical Chemistry Chemical Physics*, 2016, 18, 12964-12975.

10.Hui Liu, Tingjun Hou*, CaFE: a tool for binding affinity prediction using end-point free energy methods, *Bioinformatics*, 2016, 32, 2216-2218.

11.Sheng Tian, Junmei Wang, Youyong Li, Dan Li, Lei Xu, Tingjun Hou*, The application of in silico drug-likeness predictions in pharmaceutical research, *Advanced Drug Delivery Reviews*, 2015, 86, 2-10.

12.Mingyun Shen, Sheng Tian, Peichen Pan, Huiyong Sun, Dan Li, Youyong Li, Hefeng Zhou, Chuwen Li, Simon Ming-Yuen Lee*, Tingjun Hou*, Discovery of Novel ROCK1 Inhibitors via Integrated Virtual Screening Strategy and Bioassays, *Scientific Reports*, 2015, 5, 16749.

13.Jingyu Zhu, Man Wang, Yu Yang, Kunkun Han, Juan Tang, Lei Xu, Zubing Zhang, Guodong Chen, Jie Li, Chunhua Qiao,Tingjun Hou*, Xinliang Mao*, *Oncotarget*, 2015, 5, 3836-3848.

14.Huiyong Sun, Tingjun Hou*, Hongyu Zhang*, Finding Chemical Drugs for Genetic Diseases, *Drug Discovery Today*, 2015, 19, 1836-1840. (**feature article**)

15.Sheng Tian, Huiyong Sun, Peichen Pan, Dan Li, Xuechu Zhen*, Youyong Li*, Tingjun Hou*, Assessing ensemble docking-based virtual screening strategy for kinase targets by considering protein flexibility, *Journal of Chemical Information and Modeling*, 2014, 54, 2664-2679.(扩展**ESI**高引论文)

16.Lei Xu, Yu Zhang, Longtai Zheng, Chunhua Qiao, Youyong Li, Dan Li, Xuechu Zhen*, Tingjun Hou*, Discoveryof novel inhibitors targeting macrophage migration inhibitory factor via structure-based virtual screeningand bioassays, *Journal of Medicinal Chemistry*, 2014, 57, 3737-3745. (扩展**ESI**高引论文)

17.Huiyong Sun, Youyong Li, Mingyun Shen, Sheng Tian, Lei Xu, Peichen Pan, Yan Guan, Tingjun Hou*, Assessing the Performance of MM/PBSA and MM/GBSA Methods. 5. Improved Docking Performance by Using High Solute Dielectric Constant MM/GBSA and MM/PBSA Rescoring, *Physical Chemistry Chemical Physics*, 2014, 16, 22035-22045.(扩展**ESI**高引论文)

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(3). 课题

1.国家自然科学基金面上项目，新型ROCK抑制剂的设计和优化以及对脑出血治疗效果的研究，2018~2021，负责

2.国家重点研发计划，蛋白-蛋白相互作用及其网络的理论计算新方法与应用，2016~2021，骨干。

3.国家重点研发计划，生物医药服务社区建设，2016~2021，骨干。

4.国家自然科学基金面上项目，基于蛋白结构的成药性预测新方法研究，2016~2019，负责

5.973重大研究计划，纳米界面生物分子作用机制的基础研究及其在前列腺癌早期检测中的应用，2012~2016，骨干。

6.高等学校博士学科点专项科研基金，药物分子代谢和毒性的预测研究，2013~2015，负责。

7.江苏省高校青蓝工程科技创新团队，肿瘤纳米技术，2012~2014，负责

8.国家自然科学基金面上项目，蛋白质结构域介导的蛋白-蛋白相互作用网络的研究，2012~2015，负责

9.国家自然科学基金面上项目，基于hERG钾离子通道的药物分子心脏毒性的预测, 2009~2012，负责

(4). 著作

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2.罗旭, 化学统计学, 科学出版社, 2002 , 编委(第16章)

3.JunmeiWang, Tingjun Hou, Chapter 5 Recent Advances on *in silico* ADME Modeling, *Annual Reports in Computational Chemistry*, Elsevier, Volume 5, 2009, 101-127.

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5.MolecularConceptor courseware, Synergix Ltd. 2008. (Contributing the chapter: introduction to chemoinformatics).

(5). 授权专利和软件著作权

1.侯廷军等，*PharmacoKinetic Knowledge*Base软件著作权，2011SR076293

2.侯廷军等，分子键型自动生成软件Fixbond软件著作权，2012SR110379

3.侯廷军等，基于分子表面的构象熵计算软件SASCEC软件著作权，2012SR110382

4.侯廷军等，两点式自由能计算软件CaFE软件著作权，2016SR283150

5.侯廷军等，蛋白溶剂化能计算软件SolvationSAS软件著作权，2016SR283147

6.侯廷军等，面向CADD程序开发的基础库软件MORT软件著作权，2016SR283105

7.侯廷军等，分子模拟初始模型构建软件EMDY软件著作权，2017SR082307

8.侯廷军等，基于加权能量项的蛋白-蛋白打分软件NSFBWET软件著作权，2017SR088785

9.侯廷军，余慧东，沈明云，潘培辰，李有勇，周顺晔，3-[4-(磺酰)苯]脲类化合物及其在制备抗肿瘤药物中的应用，专利号：ZL201110263951.4，授权公告号：102327275B，授权公告日：2013.03.20

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13.侯廷军，余慧东，沈明云，潘培辰，李有勇，周顺烨，4,7-二氢四唑[1,5-a]嘧啶衍生物及其在制备抗肿瘤药物中的应用，专利号：ZL201110263953.3，授权公告号：102432612B，授权公告日：2015.07.08

14.侯廷军，沈明云，余慧东，潘培辰，李有勇，周顺晔，4-(2-甲基-1-哌啶基)-3-硝基苯甲酰胺在制备抗癌药物中的应用，专利号：ZL201410080657.3，授权公告号：103860556B，授权公告日：2015.06.17

15.崔孙良，张岩，侯廷军，反式邻羟基二苯乙烯衍生物及其制备方法和应用，专利号：201410432114.3，授权公告号：104193596B，授权公告日：2016.04.27

16.毛新良，侯廷军，朱景宇，乔春华，一种化合物及其制备与用途，专利号：201410191824.1，授权公告号：103951640B，授权公告日：2016.03.02

17.侯廷军，余慧东，沈明云，潘培辰，一种化合物在制备治疗乳腺癌药物中的应用，专利号：201310248134.0，授权公告号：103316002B，授权公告日：2015.04.15

四．社会兼职

中国化学会计算(机)化学专业委员会副主任委员

学术期刊编委：*Journal of Cheminformatics*、*Current Pharmaceutical Design* 、*Mini-Reviews in Medicinal Chemistry*、*Theoretical Biology & Medical Modelling*、*Current Computer-aided Drug Design*、*Medicinal Chemistry*、*Computational and Mathematical Methods in Medicine*、*Journal of Pharmaceutics*

学术期刊顾问编委：*Journal of Chemical Information and Modeling*、*Chemical Biology & Drug Design*

特刊客座编辑：*Advanced Drug Delivery Reviews*、*Current Drug Targets*、*Evidence-Based Complementary and Alternative Medicine*、*Combinatorial Chemistry & High Throughput Screening* 客座编辑

五．重要奖项和荣誉

1.2016年，英国皇家化学会“Top 1%高被引中国作者”

2.2015年，浙江省药学会医药科技一等奖（个人奖）

3.2014年，药明康德生命化学研究奖（学者奖）

4.2014年，全国高等学校科学研究优秀成果二等奖（排名第2），获奖项目：ADMET成药性评价关键技术和模型研究

5.2012年，第四届寻找青年科学之星（铜奖）

6.2008年，全国高等学校科学研究优秀成果二等奖（排名第2），获奖项目：药用天然产物高通量筛选及快速分离新途径