个 人 简 历

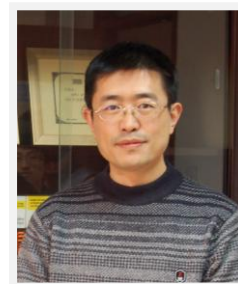## 王任小 博士

研究员，课题组长，博士生导师
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　　本人参加科研以来一直从事分子靶向药物设计方面的研究，尤其擅长发展分子靶向药物设计中的关键方法，工作具有很强的创新性和系统性，代表工作有 X-Score、XLOGP、AT&T 软件和 PDBbind 数据库。这些成果与国际上同类工作相比具有较高的水平，自公开发布以来在世界各地三十多个国家拥有超过 4700 名注册用户，其中许多来自国际著名的大学、研究所以及大型医药公司，形成了广泛的国际影响。除了在理论方法方面的建树之外，本人亦注重在实践中应用分子靶向药物设计，近年来领导课题组综合运用分子设计、化学合成以及生物学研究手段，针对重要生物靶标最终成功获得了多种活性化合物。本人已在 *J. Med. Chem., J. Chem. Inf. Model., J. Chem. Theor. Comput., Proc. Natl. Acad. Sci., J. Am. Chem. Soc.* 等国际国内核心刊物上发表学术论文超过 70 篇，截止至 2010 年 2 月底发表论文合计被引用达 2090 次，H 指数为 20。另外，近年来申请及拥有国家发明专利和计算机软件著作权合计 11 项。本课题组目前主要从事药物设计、计算生物学以及计算化学方面的研究工作，承担和参与多项自然科学基金委、科技部、中科院以及上海市科委项目。

主要研究方向

✧ 以分子模拟为手段研究生物大分子的结构和功能以及有机小分子与生物大分子的相互作用；研究和发展分子靶向药物设计中的关键理论和方法。

✧ 选择与重大疾病过程相关的生物大分子为靶标，综合运用分子模拟、化学合成以及生物学实验，发展可以有效调控生物靶标活性的有机小分子化合物。

教育背景及工作经历

✧ 2005 年 8 月至今：中国科学院上海有机化学研究所，"百人计划"研究员，课题组长，博士生导师

✧ 2001 年 9 月至 2005 年 7 月：美国密西根大学(University of Michigan)医学院，Research Investigator

✧ 2000 年 9 月至 2001 年 8 月：美国乔治敦大学(Georgetown University)癌症中心，博士后

✧ 1999 年 9 月至 2000 年 8 月：美国加州大学洛杉矶分校(University of California Los Angeles)化学系，博士后

✧ 1994 年 9 月至 1999 年 8 月：北京大学化学学院物理化学研究所，理学博士，导师：唐有祺院士。

✧ 1989 年 9 月至 1994 年 8 月：北京大学化学学院，理学学士，导师：来鲁华教授。

主要获奖情况

✧ 药明康德"生命化学研究奖"（2010 年）

✧ SCOPUS "青年科学之星"（2010 年）

✧ 中国药学会-施维雅青年药物化学家奖（2009 年）
✧ 明治乳业生命科学奖（2009 年）
✧ Eli Lilly 公司亚洲优秀毕业研究生导师奖（2009 年）
✧ 上海市科委"浦江人才"奖（2006 年）
✧ 中国科学院"百人计划"择优支持（2006 年）
✧ 美国 Cap CURE 癌症基金会 Young Investigator Award（2001 年）
✧ 中国教育部"全国优秀博士学位论文"奖（2001 年）

主要学术任职

✧ 国际刊物 *ChemMedChem, Molecular Informatics* 顾问编委
✧ 中国化学会及中国药学会高级会员

承担科研项目情况

✧ <u>作为项目负责人目前承担有</u>：自然科学基金委 "基于化学小分子探针的信号转导过程的研究" 重大研究计划培育项目（项目编号 90813006，2009-2011），自然科学基金委面上项目(项目编号 20772149，2008-2010)，自然科学基金委面上项目(项目编号 21072213，2010-2012)。
✧ <u>作为项目骨干目前参与的科研项目主要有</u>："重大新药创制" 科技重大专项关键技术类项目（项目编号 2009ZX09501-002，2009-2010），自然科学基金委创新群体（项目编号 20921091，2010-2012），中国科学院方向性项目（项目编号 KJCX2-YW-H08，2006-2010）。
✧ <u>近期已经结题的科研项目有</u>：中国科学院 "百人计划" 项目（2007-2009），自然科学基金委青年科学基金(项目编号 20502031，2006-2008)，上海市科委生物医药类重点项目（项目编号 074319113，2007-2010），上海市科委 "浦江人才" 计划(06PJ14115，2006-2008)，科技部 "863" 计划目标导向类专题项目（项目编号 2006AA02Z337，2006-2008）

发表论文清单

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2. Lin, F.; **Wang, R.*,** "Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc", *J. Chem. Theory Comput.* **2010***, 6,* 1852-1870.

3. Cheng, T.; Liu, Z.; **Wang, R.***, "A Knowledge-Based Strategy for Improving the Accuracy of Scoring Functions in Binding Affinity Prediction", *BMC Bioinformatics*, **2010**, *11*, 193-208.

4. Li, X.; Li, Y.; Cheng, T.; Liu, Z.; **Wang, R.***, "Evaluation of the Performance of Four Molecular Docking Programs on a Diverse Set of Protein-Ligand Complexes", *J. Comp. Chem.* **2010**, *31*, 2109-2125.

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6. Li, X.; Liu, Z.; Li, Y.; Li, J.; Li, J.; **Wang, R.***, "A Statistical Survey on the Binding Constants of Covalently Bound Protein-Ligand Complexes", *Mol. Informatics*, **2010**, *29*, 87-96.

7. Zheng, F.; Lin, F.; **Wang, R.**; Qing, F.-L. "Synthesis and conformational analysis of D-2-deoxy-2,2-difluoro-4-dihydro-4-thionucleosides", *Org. Biomol. Chem.*, **2010**, *8*, 163-170.

8. Lin, F.; **Wang, R.*** "Hemolytic Mechanism of Dioscin Proposed by Molecular Dynamics Simulations", *J. Mol. Model.* **2010**, 16, 107-118.

9. Cheng, T.; Li, X.; Li, Y.; Liu, Z.; **Wang, R.*** "Comparative Assessment of Scoring Functions on a Diverse Test Set", *J. Chem. Inf. Model.* **2009,** *49*, 1079-1093.

10. Zhang, X.; Li, X.; **Wang, R.*** "Interpretation of the Binding Affinities of PTP1B Inhibitors with the MM-GB/SA method and the X-Score Scoring Function", *J. Chem. Inf. Model.* **2009,** *49*, 1033-1048. (cover story)

11. Li, Y.; Zhou, B.; **Wang, R.*** "Rational Design of Tamiflu Derivatives Targeting at the Open Conformation of Neuraminidase Subtype 1", *J. Mol. Graph. Model.* **2009**, *28*, 203-219.

12. Li, X.; **Wang, R.*** "Automatic Identification of Antibodies in the Protein Data Bank", *Chinese Journal of Chemistry*, **2009**, *27*, 23-28.

13. Wang, K.; Wu, Y.-S.; Wang, G.-T.; **Wang, R.-X.**; Jiang, X.-K.; Fu, H.-B.; Li, Z.-T., "Hydrogen bonding-mediated foldamer-bridged zinc porphyrin-C60 dyads: ideal face-to-face orientation and tunable donor–acceptor interaction", *Tetrahedron*, **2009**, *65*, 7718–7729.

14. Zhu, Y.-Y.; Wang, G.-T.; **Wang, R.-X.**; Li, Z.-T. "Intramolecular Six-Membered and Three-Center C-H-O Hydrogen Bonding in 1,4-Diphenyl-1,2,3-Triazoles", *Cryst. Growth Des.,* **2009**, *9*, 4778–4783.

15. Liu, Z. G.; Wang, G. T.; Li, Z. T.; **Wang, R.*** "Geometrical Preferences of the Hydrogen Bonds on Protein-Ligand Binding Interface Derived from Statistical Surveys and Quantum Mechanics Calculations", *J. Chem. Theory Comput.* **2008,** *4,* 1959–1973.

16. Lin, F.; **Wang, R.*** "Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists", *J. Mol. Model*. **2008**, *15*, 53-65.

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19. Cheng, T.; Zhao, Y.; Li, X.; Lin, F.; Xu, Y.; Zhang, X.; Li, Y.; **Wang, R.***; Lai, L. "Computation of Octanol-Water Partition Coefficients by Guiding an Additive Model with Knowledge", *J. Chem. Inf. Model.* **2007**, *47*, 2140-2148.

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21. **Wang, R.***; Lin, F.; Xu, Y.; Cheng, T. "I-SOLV: A new surface-based empirical model for computing solvation free energies", *J. Mol. Graph. Model.* **2007**, *26*, 368-377.

22. Feng, D.-J.; Wang, G..-T.; Wu, J.; **Wang, R.-X.**; Li, Z.-T.* "Hydrogen bonding-driven elastic bis(zinc)porphyrin receptors for neutral and cationic electron-deficient guests with a sandwich-styled complexing pattern", *Tetrahedron Lett*. **2007**, *48*, 6181-6185.

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发表综述论文清单

1. Wang, Y.; Li, J.; **Wang, R.*** "Computational Approaches to Estimate Octanol-Water Partition Coefficient and Water Solubility of Organic Compounds", *Acta Phys.-Chim. Sinica* (物理化学学报)*,* **2010***,26,* 1742-1754

2. Li, Y.; **Wang, R.*** "Theoretical approaches to the prediction of the biological targets of small-molecular compounds based on chemogenomic information", *Chinese Bulletin of Life Sciences* (生命科学), **2009**, 21, 400-407.

近期发明专利申请清单

1. 王任小，马大为，李勋，孙威，周炳城，石志敏，张兴龙，朱翠侠，李雯雯，中科院上海有机化学研究所，"一种噻唑联吡唑酮类化合物及其作为 Bcl-2 家族蛋白拮抗剂的应用"，专利公开号：CN 101343268A

2. 王任小，俞飚，李勋，周炳城，石志敏，张兴龙，朱翠侠，李雯雯，中科院上海有机化学研究所，"一种噻唑并[3,2-a]嘧啶类化合物及其作为 Bcl-2 家族蛋白拮抗剂的应用"，专利公开号：CN 101348495A

3. 王任小，俞飚，史合方，李勋，周炳城，李嫣，石志敏，张兴龙，朱翠侠，李雯雯，中科院上海有机化学研究所，"2-芳基-6-芳基'-葡萄糖苷类化合物及其制备方法与应用"，专利公开号：CN 101348509A

4. 叶德泳，王任小，张亚，林赋，邓晓东，李勋，周璐，郑雪雁. 复旦大学药学院，"芳香胺类衍生物或其类似物及其应用"，中国专利申请号：200910194423.0。

近期计算机软件著作权申请清单

1. 中科院上海有机化学研究所，化学结构自动识别软件 I-interpret v1.0，登记号：2007SR15399.
2. 中科院上海有机化学研究所，脂水分配系数预测软件 XLOGP v3.0，登记号：2008SR05200.
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