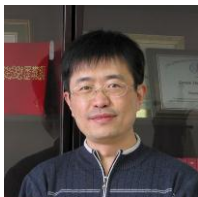


Ren-Xiao WANG

Professor, PhD

Macau Institute for Applied Research in Medicine and Health, State Key Laboratory for
Quality Research in Chinese Medicines
Macau University of Science and Technology



Prof. Renxiao Wang received both his B.S. degree (1994) and Ph.D. degree (1999) from Peking University. He did his postdoctoral research at the University of California Los Angeles (1999-2000) and Georgetown University (2000-2001). He worked for University of Michigan Medical School as a Research Investigator (2001-2005). Then he joined the faculty of Shanghai Institute of Organic Chemistry in 2005 as a “100-Talents Program” principal investigator. In 2013, he started to be a joint professor of Macau Institute for Applied Research in Medicine and Health at Macau University of Science and Technology.

Prof. Wang's research is across the field of drug design, chemical biology and biological physical chemistry. In particular, his interests focus on understanding how small organic molecules regulate their biological targets through molecular modeling approaches. Prof. Wang has published over 80 peer-reviewed papers in SCI journals with total citation over 3500 times and a H-index of 28. Prof. Wang has received a number of awards in recent years, including the prestigious Corwin Hansch Award by the Chemoinformatics & QSAR Society (2012), Biological & Chemical Research Excellency Award by WuxiPharma Inc. (2010), SCOPUS Young Researcher Momentum Award by Pfizer & Elsevier (2010), and Sevier Young Scientist Award by Chinese Pharmaceutical Association (2009). His research is financially supported by the National Natural Science Foundation of China, Chinese

Ministry of Sciences and Technology, Chinese Academy of Sciences as well as some international pharmaceutical companies.

Education:

July,1994, B. Sc. (Peking University, Beijing, China)

July 1999, Ph. D. (Peking University, Beijing, China)

Professional Chronology:

Aug.,1999- Jul., 2000 Postdoctoral fellow, Department of Chemistry and Biochemistry, University of California, Los Angeles, California, U.S.A

Aug.,2000-Aug.,2001 Postdoctoral fellow, Lombardi Cancer Center, Georgetown University, Washington D.C., U.S.A.

Sep.,2001-Jul.,2005 Research investigator, Department of Internal Medicine, University of Michigan Medical School, U.S.A.

Aug.,2005-present Professor, State Key Laboratory of Bioorganic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, P. R. China

Jul. 2013-present Professor, Macau Institute for Applied Research in Medicine and Health, Macau University of Science and Technology, Macau

Research Fields:

- 1) Molecular-targeted drug design
- 2) Chemical biology
- 3) Biological physical chemistry

Professional Associations

- 1) Editorial board members of "*ChemMedChem*" (Wiley), "*Molecular Informatics*" (Wiley) & "*Perspectives in Drug Design and Discovery*"(Springer)

- 2) Member of the Chinese Chemical Society, the Chinese Pharmaceutical Association, and the American Chemical Society

Awards:

- 1) Corwin Hansch Award, Chemoinformatics & QSAR Society (2012)
- 2) Biological & Chemical Research Excellency Award, WuxiPharma Inc. (2010)
- 3) SCOPUS Young Researcher Momentum Award, Pfizer & Elsevier (2010)
- 4) Sevier Young Scientist Award, Chinese Pharmaceutical Association (2009)
- 5) Advisor of Asian Outstanding Graduate Thesis Award, Eli Lilly Inc. (2009)
- 6) Young Investigator Award, CapCURE Foundation, USA (2001)
- 7) National Excellent Doctoral Theses Award, Chinese Ministry of Education (2001)

Selected Publications:

- 1) Zhao, Z.; Zhang, Z.; Li, Y.; Zhou, M.; Li, X.; Yu, B.; **Wang, R.-X.***, "Probing the Key Interactions Between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modelling", *ChemMedChem*, **2013**, 8, DOI: 10.1002/cmdc.201300256.
- 2) Xu, Y.; Zhou, M.; Li, Y.; Li, C.; Zhang, Z.; Yu, B*; **Wang, R.-X.***, "Characterization of the Stereochemical Structures of 2H-thiazolo[3,2-a]-Pyrimidine Compounds and Their Binding Affinities to Anti-Apoptotic Bcl-2 Family Proteins", *ChemMedChem*, **2013**, 8, DOI: 10.1002/cmdc.201300159.
- 3) Zhou, M.; **Wang, R.-X.*** "Small-Molecule Regulators of Autophagy and Their Potential Therapeutic Applications", *ChemMedChem*, **2013**, 8, 694-707.
- 4) Shi, Z. M.; Li, Y.; Liu, Z. H.; Mi, J.; **Wang, R.-X.*** "Theoretical Analysis of Fas Ligand-Induced Apoptosis with an Ordinary Differential Equation Model", *Molecular Informatics*, **2012**, 13(11-12), 793-807.
- 5) Xu, H.; Huang, W.; He, Q.-L.; Zhao, Z.-X.; Zhang, F.; **Wang, R.-X.**; Kang, J.-W.; Tang, G.-L. "Self-Resistance to an Antitumor Antibiotic: A DNA Glycosylase Triggers the Base-Excision Repair System in Yatakemycin Biosynthesis", *Angew. Chem. Int. Ed.* **2012**, 51(42), 10532-10536.
- 6) Li, Y.; Zhao, Y.; **Wang, R.-X.*** "Automatic Tailoring and Transplanting: A Practical

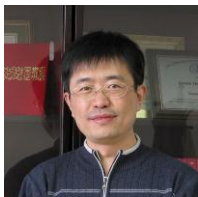
- Method that Makes Virtual Screening More Useful", *J. Chem. Inf. Model.*, **2011**, *51*, 1474–1491.
- 7) Zhou, B.; Li, X.; Li, Y.; Xu, Y.; Zhang, Z.; Zhou, M.; Zhang, X.; Liu, Z.; Zhou, J.; Cao, C.; Yu, B.*; **Wang, R.-X.*** "Discovery and Development of 2H-thiazolo[3,2-a]pyrimidine Derivatives as General Inhibitors of Bcl-2 Family Proteins", *ChemMedChem*, **2011**, *6*, 904–921.
 - 8) Lou, J.-P.; Liu, Z.; Li, Y.; Zhou, M.; Zhang, Z.-X., Zheng, S.; **Wang, R.-X.***; Li, J*. "Synthesis and anti-tumor activities of N'-benzylidene-2-(4-oxothieno[2,3-d]pyrimidin-3(4H)-yl) acetohydrazone derivatives", *Bioorgan. Med. Chem. Lett.* **2011**, *21*, 6662–6666.
 - 9) Li, Y.; Liu, Z.; **Wang, R.-X.***, "Test MM-PB/SA on True Conformational Ensembles of Protein-Ligand Complexes", *J. Chem. Inf. Model.* **2010**, *50*, 1682-1692.(cover story)
 - 10) Lin, F.; **Wang, R.-X.***, "Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc", *J. Chem. Theory Comput.* **2010**, *6*, 1852-1870.
 - 11) Cheng, T.; Liu, Z.; **Wang, R.-X.***, "A Knowledge-guided Strategy for Improving the Accuracy of Scoring Functions in Binding Affinity Prediction", *BMC Bioinformatics*, **2010**, *11*, 193-208.
 - 12) Li, X.; Li, Y.; Cheng, T.; Liu, Z.; **Wang, R.-X.***, "Evaluation of the Performance of Four Molecular Docking Programs on a Diverse Set of Protein-Ligand Complexes", *J. Comp. Chem.* **2010**, *31*, 2109-2125.
 - 13) Shi, H.; Zhou, B.; Li, W.; Shi, Z.; Yu, B.*; **Wang, R.-X.***, "Synthesis and Anti-tumor Activities of Methyl 2-O-Aryl-6-O-Aryl'-D-Glucopyranosides", *Bioorg. Med. Chem. Lett.*, **2010**, *20*, 2855-2858.
 - 14) Li, X.; Liu, Z.; Li, Y.; Li, J.; Li, J.; **Wang, R.-X.***, "A Statistical Survey on the Binding Constants of Covalently Bound Protein-Ligand Complexes", *Molecular Informatics*, **2010**, *29*, 87-96.
 - 15) Lin, F.; **Wang, R.-X.*** "Hemolytic Mechanism of Dioscin Proposed by Molecular Dynamics Simulations", *J. Mol. Model.* **2010**, *16*, 107-118.
 - 16) Cheng, T.; Li, X.; Li, Y.; Liu, Z.; **Wang, R.-X.*** "Comparative Assessment of Scoring Functions on a Diverse Test Set", *J. Chem. Inf. Model.* **2009**, *49*, 1079-1093.

- 17) Zhang, X.; Li, X.; **Wang, R.-X.*** “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)
- 18) Li, Y.; Zhou, B.; **Wang, R.-X.*** “Rational Design of Tamiflu Derivatives Targeting at the Open Conformation of Neuraminidase Subtype 1”, *J. Mol. Graph. Model.* **2009**, *28*, 203-219.
- 19) Lin, F.; **Wang, R.-X.*** “Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists”, *J. Mol. Model.* **2009**, *15*, 53-65.
- 20) Liu, Z. G.; Wang, G. T.; Li, Z. T.; **Wang, R.-X.*** “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.
- 21) Cheng, T.; Zhao, Y.; Li, X.; Lin, F.; Xu, Y.; Zhang, X.; Li, Y.; **Wang, R.-X.***; Lai, L. “Computation of Octanol-Water Partition Coefficients by Guiding an Additive Model with Knowledge”, *J. Chem. Inf. Model.* **2007**, *47*, 2140-2148.
- 22) Zhao, Y.; Cheng, T.; **Wang, R.-X.*** “Automatic Perception of Organic Molecules Based on Essential Structural Information”, *J. Chem. Inf. Model.* **2007**, *47*, 1379-1385.
- 23) **Wang, R.-X.***; 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.
- 24) Li, C.; Wang, G.; Yi, H.; Jiang, X.; Li, Z.*; **Wang, R.-X.*** “Diastereomeric Recognition of Chiral Foldamer Receptors for Chiral Glucoses”, *Org. Lett.* **2007**, *9*, 1797-1800.
- 25) Xu, Y.; **Wang, R.-X.*** “A Computational Analysis of the Binding Affinities of FKBP12 Inhibitors Using the MM-PB/SA Method”, *Proteins*, **2006**, *64*, 1058-1068.

王任小 特聘教授

澳門科技大學

澳門藥物與健康應用研究所，中藥質量研究國家重點實驗室



簡介: 王任小教授 1994 年畢業於北京大學化學學院，獲得理學學士學位。1999 年畢業於北京大學化學學院，獲得理學博士學位。1999 年 9 月至 2001 年 8 月先後在美國加利福尼亞州加州大學洛杉磯分校（University of California Los Angeles）化學系以及美國華盛頓喬治敦大學（Georgetown University）醫學中心做博士後研究。2001 年 9 月至 2005 年 7 月在美國密西根大學（University of Michigan）醫學院任助理研究員。2005 年入選中國科學院“百人計劃”，加入上海有機化學研究所任職至今。2013 年受聘為澳門科技大學特聘教授。

王任小教授課題組目前主要從事藥物分子設計以及化學生物學領域的研究。已在國際國內核心刊物上發表 SCI 索引論文 80 餘篇，引用總數 3500 餘次，H 指數為 27，並申請國家發明專利及軟件著作權 17 項。所取得的代表性成果創新性強，引用率高，在國際上也有一定的影響。近年來先後獲得國際 Chemoinformatics & QSAR society 頒發的 Corwin Hansch Award 以及藥明康德“生命化學研究獎”、中國藥學會“青年藥物化學家獎”等多項競爭性強的國內獎項，並受邀擔任 ChemMedChem 等國際刊物編委。近年來承擔和參與自然科學基金委、科技部以及上海市科委項目多項。

學歷:

- 1) 1994 年 7 月：北京大學化學學院，理學學士
- 2) 1999 年 7 月：北京大學化學學院，理學博士

工作經歷:

- 1) 1999 年 9 月至 2000 年 8 月：美國加州大學洛杉磯分校(University of California Los Angeles)，博士後
- 2) 2000 年 9 月至 2001 年 8 月：美國喬治敦大學(Georgetown University)，博士後
- 3) 2001 年 9 月至 2005 年 7 月：美國密西根大學(University of Michigan)，助理研究員
- 4) 2005 年 8 月至今：中國科學院上海有機化學研究所，生命有機化學國家重點實驗室，研究員
- 5) 2013 年 7 月至今：澳門科技大學，中藥質量控制國家重點實驗室，特聘教授

研究領域: 藥物分子設計，生物物理化學，化學生物學

專業會員:

- 1) 中國化學會會員，中國藥學會會員，中國化學會生物物理化學專業委員會委員，美國化學會會員
- 2) 國際刊物 *ChemMedChem* 編委，*Molecular Informatics* 顧問編委，*Perspectives in Drug Design and Discovery* 顧問編委

獲獎情況：

- 1) 國際化學信息學及定量構效關係研究學會 (Chemoinformatics & QSAR Society) "Cowin Hansch Award" (2012 年)
- 2) 藥明康德“生命化學研究獎”(2010 年)
- 3) SCOPUS“青年科學之星”(2010 年)
- 4) 中國藥學會-施維雅青年藥物化學家獎 (2009 年)
- 5) 明治乳業生命科學獎 (2009 年)

- 6) Eli Lilly 公司亞洲優秀畢業研究生導師獎 (2009 年)
- 7) 上海市科委“浦江人才”獎 (2006 年)
- 8) 中國科學院“百人計劃”擇優支持 (2006 年)
- 9) 美國 Cap CURE 癌症基金會 Young Investigator Award (2001 年)
- 10) 中國教育部“全國優秀博士學位論文”獎 (2001 年)

代表性研究論文：

- 1) Zhao, Z.; Zhang, Z.; Li, Y.; Zhou, M.; Li, X.; Yu, B.; **Wang, R.-X.***, "Probing the Key Interactions Between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modelling", *ChemMedChem*, **2013**, 8, DOI: 10.1002/cmdc.201300256.
- 2) Xu, Y.; Zhou, M.; Li, Y.; Li, C.; Zhang, Z.; Yu, B.*; **Wang, R.-X.***, "Characterization of the Stereochemical Structures of 2H-thiazolo[3,2-a]-Pyrimidine Compounds and Their Binding Affinities to Anti-Apoptotic Bcl-2 Family Proteins", *ChemMedChem*, **2013**, 8, DOI: 10.1002/cmdc.201300159.
- 3) Zhou, M.; **Wang, R.-X.*** "Small-Molecule Regulators of Autophagy and Their Potential Therapeutic Applications", *ChemMedChem*, **2013**, 8, 694-707.
- 4) Shi, Z. M.; Li, Y.; Liu, Z. H.; Mi, J.; **Wang, R.-X.*** "Theoretical Analysis of Fas Ligand-Induced Apoptosis with an Ordinary Differential Equation Model", *Molecular Informatics*, **2012**, 13(11-12), 793-807.
- 5) Xu, H.; Huang, W.; He, Q.-L.; Zhao, Z.-X.; Zhang, F.; **Wang, R.-X.**; Kang, J.-W.; Tang, G.-L. "Self-Resistance to an Antitumor Antibiotic: A DNA Glycosylase Triggers the Base-Excision Repair System in Yatakemycin Biosynthesis", *Angew. Chem. Int. Ed.* **2012**, 51(42), 10532-10536.
- 6) Li, Y.; Zhao, Y.; **Wang, R.-X.*** "Automatic Tailoring and Transplanting: A Practical Method that Makes Virtual Screening More Useful", *J. Chem. Inf. Model.*, **2011**, 51, 1474-1491.
- 7) Zhou, B.; Li, X.; Li, Y.; Xu, Y.; Zhang, Z.; Zhou, M.; Zhang, X.; Liu, Z.; Zhou, J.; Cao, C.; Yu, B.*; **Wang, R.-X.*** "Discovery and Development of 2H-thiazolo[3,2-a]pyrimidine Derivatives as General Inhibitors of Bcl-2 Family Proteins",

ChemMedChem, **2011**, *6*, 904–921.

- 8) Lou, J.-P.; Liu, Z.; Li, Y.; Zhou, M.; Zhang, Z.-X., Zheng, S.; **Wang, R.-X.***; Li, J*. "Synthesis and anti-tumor activities of N'-benzylidene-2-(4-oxothieno[2,3-d]pyrimidin-3(4H)-yl) acetohydrazone derivatives", *Bioorgan. Med. Chem. Lett.* **2011**, *21*, 6662–6666.
- 9) Li, Y.; Liu, Z.; **Wang, R.-X.***, "Test MM-PB/SA on True Conformational Ensembles of Protein-Ligand Complexes", *J. Chem. Inf. Model.* **2010**, *50*, 1682-1692.(cover story)
- 10) Lin, F.; **Wang, R.-X.***, "Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc", *J. Chem. Theory Comput.* **2010**, *6*, 1852-1870.
- 11) Cheng, T.; Liu, Z.; **Wang, R.-X.***, "A Knowledge-guided Strategy for Improving the Accuracy of Scoring Functions in Binding Affinity Prediction", *BMC Bioinformatics*, **2010**, *11*, 193-208.
- 12) Li, X.; Li, Y.; Cheng, T.; Liu, Z.; **Wang, R.-X.***, "Evaluation of the Performance of Four Molecular Docking Programs on a Diverse Set of Protein-Ligand Complexes", *J. Comp. Chem.* **2010**, *31*, 2109-2125.
- 13) Shi, H.; Zhou, B.; Li, W.; Shi, Z.; Yu, B.*; **Wang, R.-X.***, "Synthesis and Anti-tumor Activities of Methyl 2-O-Aryl-6-O-Aryl'-D-Glucopyranosides", *Bioorg. Med. Chem. Lett.*, **2010**, *20*, 2855-2858.
- 14) Li, X.; Liu, Z.; Li, Y.; Li, J.; Li, J.; **Wang, R.-X.***, "A Statistical Survey on the Binding Constants of Covalently Bound Protein-Ligand Complexes", *Molecular Informatics*, **2010**, *29*, 87-96.
- 15) Lin, F.; **Wang, R.-X.*** "Hemolytic Mechanism of Dioscin Proposed by Molecular Dynamics Simulations", *J. Mol. Model.* **2010**, *16*, 107-118.
- 16) Cheng, T.; Li, X.; Li, Y.; Liu, Z.; **Wang, R.-X.*** "Comparative Assessment of Scoring Functions on a Diverse Test Set", *J. Chem. Inf. Model.* **2009**, *49*, 1079-1093.
- 17) Zhang, X.; Li, X.; **Wang, R.-X.*** "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)
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203-219.

- 19) Lin, F.; **Wang, R.-X.*** “Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists”, *J. Mol. Model.* **2009**, *15*, 53-65.
- 20) Liu, Z. G.; Wang, G. T.; Li, Z. T.; **Wang, R.-X.*** “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.
- 21) Cheng, T.; Zhao, Y.; Li, X.; Lin, F.; Xu, Y.; Zhang, X.; Li, Y.; **Wang, R.-X.***; Lai, L. “Computation of Octanol-Water Partition Coefficients by Guiding an Additive Model with Knowledge”, *J. Chem. Inf. Model.* **2007**, *47*, 2140-2148.
- 22) Zhao, Y.; Cheng, T.; **Wang, R.-X.*** “Automatic Perception of Organic Molecules Based on Essential Structural Information”, *J. Chem. Inf. Model.* **2007**, *47*, 1379-1385.
- 23) **Wang, R.-X.***; 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.
- 24) Li, C.; Wang, G.; Yi, H.; Jiang, X.; Li, Z.*; **Wang, R.-X.*** “Diastereomeric Recognition of Chiral Foldamer Receptors for Chiral Glucoses”, *Org. Lett.* **2007**, *9*, 1797-1800.
- 25) Xu, Y.; **Wang, R.-X.*** “A Computational Analysis of the Binding Affinities of FKBP12 Inhibitors Using the MM-PB/SA Method”, *Proteins*, **2006**, *64*, 1058-1068.