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Macau Institute for Applied Research in Medicine and Health, State Key Laboratory for
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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.

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

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

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

1) Molecular-targeted drug design

2) Chemical biology

3) Biological physical chemistry

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
- 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)
- 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.
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- 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.
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 - 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.*** "AutomaÓ Mfn Pn of the mo C



1) 1994 7
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- 1) 1999 9 2000 8 (University of California Los Angeles)
- 2) 2000 9 2001 8 (Georgetown University)
- 3) 2001 9 2005 7 (University of Michigan)
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2) *ChemMedChem Molecular Informatics Perspectives in Drug Design and Discovery*

- 1) Chemoinformatics & QSAR Society "Cowin Hansch Award" 2012
- 2) " " " 2010
- 3) SCOPUS " " 2010
- 4) - 2009
- 5) 2009

- 6) Eli Lilly 2009
- 7) " " 2006
- 8) " " 2006
- 9) Cap CURE Young Investigator Award 2001
- 10) " " 2001

- 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.
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