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Renxiao Wang, Ph.D.

Research Interests

- Understand how small organic molecules regulate their biological targets through molecular modeling. Develop key computational methods for drug design and discovery.
- Discover novel small-molecule regulators of biological targets with pharmaceutical implication through a combination of molecular modeling, organic synthesis and biological experiments.

Professional Experience

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

2001–2005: Research investigator, Department of Internal Medicine, University of Michigan Medical School, U.S.A.

2000–2001: Postdoctoral fellow, *Lombardi Cancer Center, Georgetown University, Washington D.C., U.S.A.*

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

Education

1994-1999: Ph.D., *College of Chemistry, Peking University, Beijing, China*
- Majoring in computer-aided drug design and molecular modeling; Director: Prof. Youqi Tang, Academician Member of the Chinese Academy of Sciences

1989-1994: B.S., *College of Chemistry, Peking University, Beijing, China*
- Majoring in physical chemistry; Director: Prof. Luhua Lai

Honors and Awards

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

Professional Associations

- Editorial board members of "*ChemMedChem*" (Wiley), "*Molecular Informatics"* (Wiley) & "*Perspectives in Drug Design and Discovery"* (Springer)
- Member of the Chinese Chemical Society, the Chinese Pharmaceutical

Association, and the American Chemical Society

Selected Recent Publications

1. Zhao, Z.; Zhang, Z.; Li, Y.; Zhou, M.; Li, X.; Yu, B.; **Wang, R***, " Probing the Key Interactions Between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modelling", *ChemMedChem*, **2013**, *8*, *in press*.
2. Xu, Y.; Zhou, M.; Li, Y.; Li, C.; Zhang, Z.; Yu, B*; **Wang, R***, "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*, in press.
3. Zhou, M.; **Wang, R. X.*** "Small-Molecule Regulators of Autophagy and Their Potential Therapeutic Applications", *ChemMedChem*, **2013**, *8*, 694-707.
1. 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*, 793-807.
2. Li, Y.; Zhao, Y.; **Wang, R.*** "Automatic Tailoring and Transplanting: A Practical Method that Makes Virtual Screening More Useful", *J. Chem. Inf. Model.*, **2011**, *51*, 1474–1491.
3. Zhou, B.; Li, X.; Li, Y.; Xu, Y.; Zhang, Z.; Zhou, M; Zhang, X.; Liu, Z.; Zhou, J.; Cao, C.; Yu, B.;* **Wang, R.,*** "Discovery and Development of 2H-thiazolo[3,2-a]pyrimidine Derivatives as General Inhibitors of Bcl-2 Family Proteins", *ChemMedChem*, **2011,** *6*, 904–921.
4. Lou, J.-P.; Liu, Z.; Li, Y.; Zhou, M.; Zhang, Z.-X., Zheng, S.; **Wang, R***; 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.
5. Li, Y.; Liu, Z.; **Wang, R.***, "Test MM-PB/SA on True Conformational Ensembles of Protein-Ligand Complexes", *J. Chem. Inf. Model.* **2010,** *50,* 1682-1692.
6. Lin, F.; **Wang, R.*,** "Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc", *J. Chem. Theory Comput.* **2010***, 6,* 1852-1870.
7. Cheng, T.; Liu, Z.; **Wang, R.***, "A Knowledge-guided Strategy for Improving the Accuracy of Scoring Functions in Binding Affinity Prediction", *BMC Bioinformatics*, **2010**, *11*, 193-208.
8. 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.
9. 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.
10. Shi, H.; Zhou, B.; Li, W.; Shi, Z.; Yu, B.*; **Wang, R.***, "Synthesis and Anti-tumor Activities of Methyl 2-O-Aryl-6-O-Aryl'-D-Glucopyranosides", *Bioorg. Med. Chem. Lett.,* **2010**, *20*, 2855-2858.
11. 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.
12. 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.

13. 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.
14. 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.
15. 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.
16. Zhao, Y.; Cheng, T.; **Wang, R.*** “Automatic Perception of Organic Molecules Based on Essential Structural Information”, *J. Chem. Inf. Model.* **2007**, *47*, 1379-1385.
17. Xu, Y.; **Wang, R.*** “A Computational Analysis of the Binding Affinities of FKBP12 Inhibitors Using the MM-PB/SA Method”, *Proteins,* **2006**, *64*, 1058-1068.
18. **Wang, R.;** Fang, X.; Lu, Y.; Yang, C.-Y.; Wang, S. “The PDBbind Database: Methodologies and Updates”, *J. Med. Chem.* **2005**, *48*, 4111-4119.
19. Song, H.; **Wang, R.**; Wang, S; Lin, J. “A low-molecular-weight compound discovered through virtual database screening inhibits Stat3 function in breast cancer cells”, *Proc. Natl. Acad. Sci.* **2005**, *102*, 4700-4705.
20. **Wang R.;** Lu Y.; Fang X.; Wang S. “An Extensive Test of 14 Scoring Functions Using the PDBbind Refined Set of 800 Protein-Ligand Complexes”, *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 2114-2125.
21. **Wang, R.**; Fang, X.; Lu, Y.; Wang, S. “The PDBbind Database: Collection of Binding Affinities for Protein-Ligand Complexes with Known Three-Dimensional Structures”, *J. Med. Chem.* **2004**, *47*, 2977-2980.
22. **Wang, R.**; Lu, Y.; Wang, S. “Comparative Evaluation of Eleven Scoring Functions for Molecular Docking”, *J. Med. Chem.* **2003**, *46*, 2287-2303.
23. **Wang, R.**; Lai, L.; Wang, S. “Further development and validation of empirical scoring functions for structure-based binding affinity prediction”, *J. Comput.-Aided Mol. Des.* **2002**, *16*, 11-26.
24. **Wang, R.**; Wang, S. “How does consensus scoring work for virtual library screening? An idealized experiment”, *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 1422-1426.

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 and Georgetown University. He then worked for University of Michigan Medical School as a research investigator. In 2005, he joined the faculty of Shanghai Institute of Organic Chemistry as a principal investigator. His research interests focus on understanding how small organic molecules regulate their biological targets through molecular modeling approaches. In 2012, Prof. Wang received the Corwin Hansch Award by the Cheminformatics and QSAR Society in recognition of his contributions to the field of computer-aided drug design.