

Mission of Dr. Junmei Wang's Lab

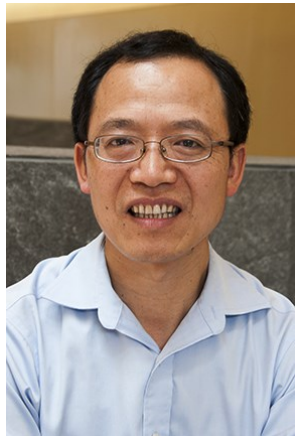


Mission: To develop a set of molecular mechanics force field (FF) models to accurately model the structures, dynamics, energetics and functions of biomolecular systems, specifically focused on:

1. Molecular interactions between proteins, nucleic acids, and small molecules.
2. Physical scoring functions for virtual screenings
3. Molecular mechanisms of biological processes, such as oligomerization/aggregation, and protein folding
4. Generative chemistry with cutting-edge deep learning algorithms

Impact: The successful pursuit of the above mission will bring revolutionary impact on biomedical research and drug discovery & development. With the continually increased computer power and significantly improved FF models, molecular modeling & simulation will become an indispensable tool in the above research fields.

Vision: The era of real “Rational Drug Design” will come into being. Medicinal chemists will routinely do computational prediction prior real synthesis

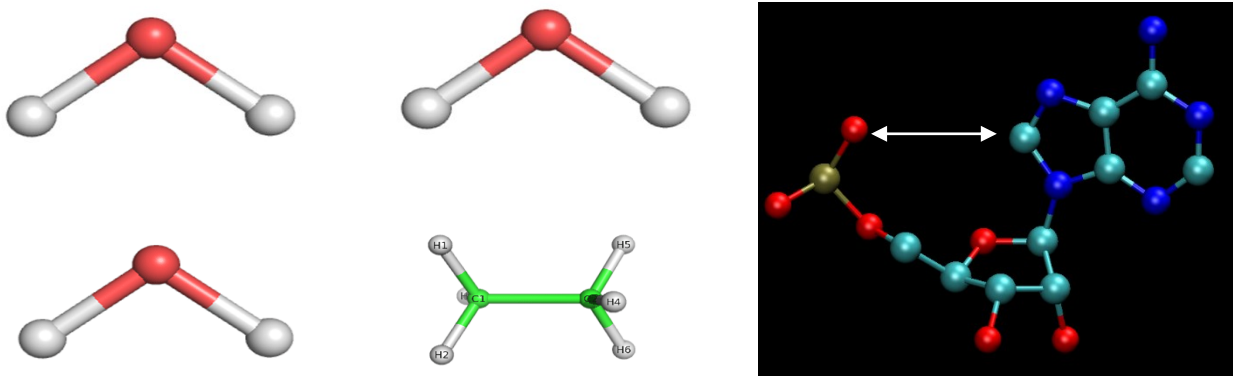


Dr. Junmei Wang,
Principal Investigator



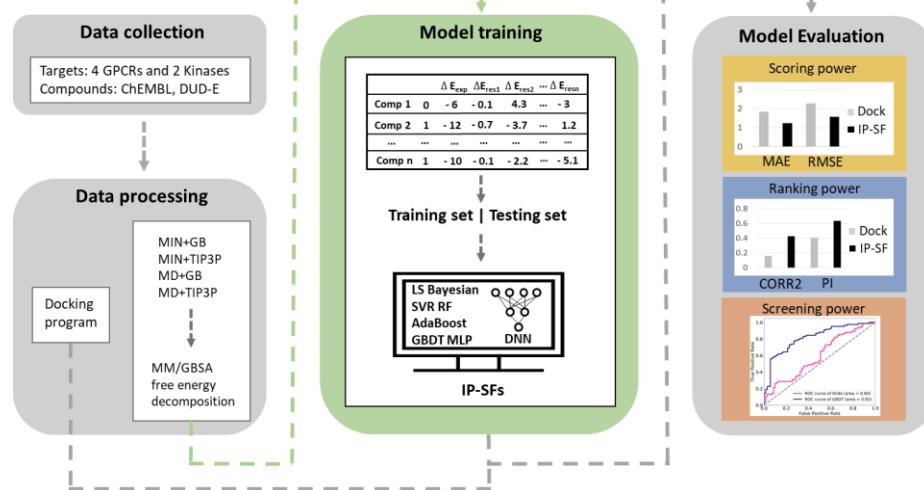
Research Focuses in Wang Lab

1. Molecular Mechanics Force Fields & Scoring Functions

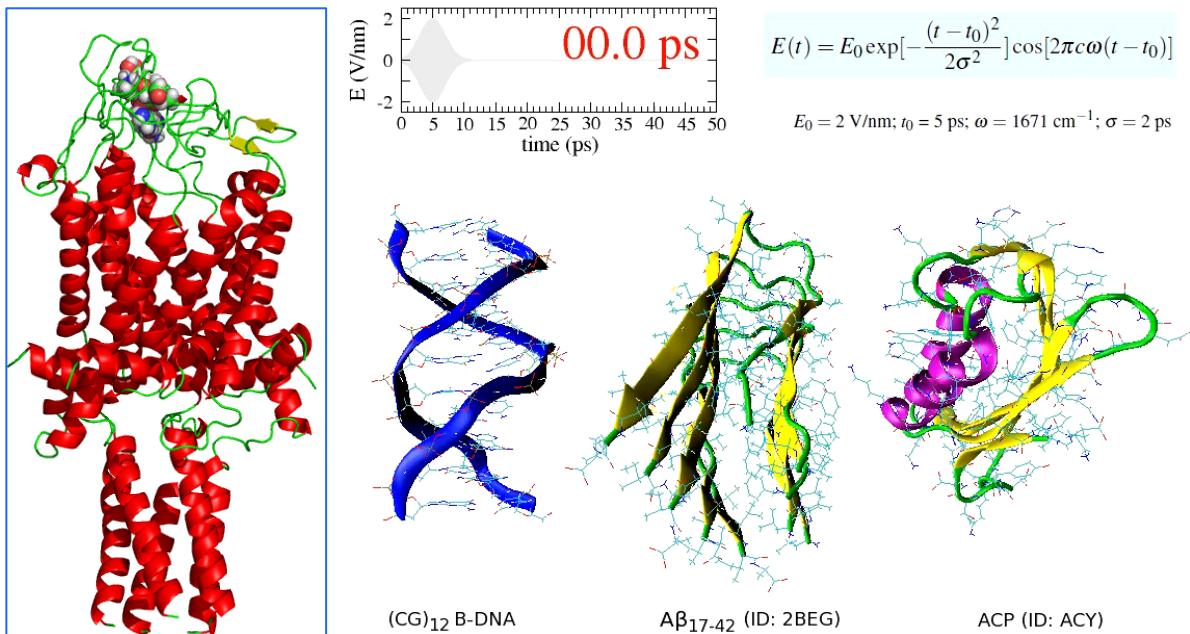


Non-bonded interaction

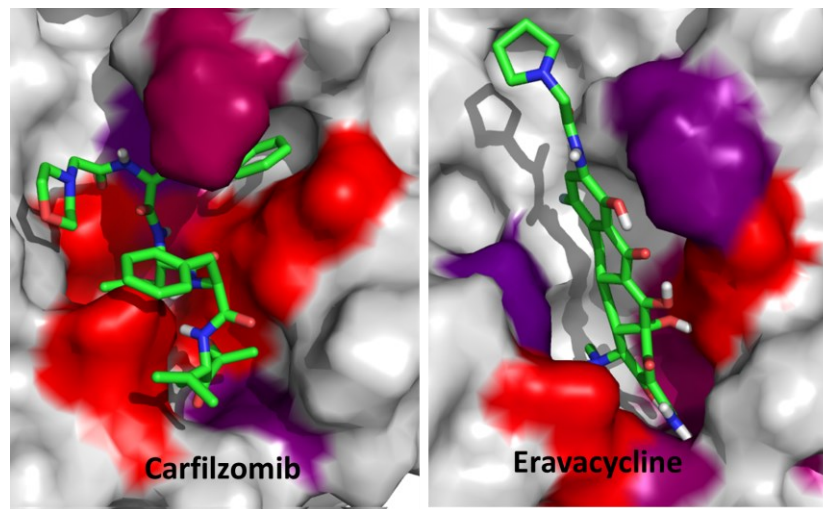
2. Machine Learning & Deeping Learning



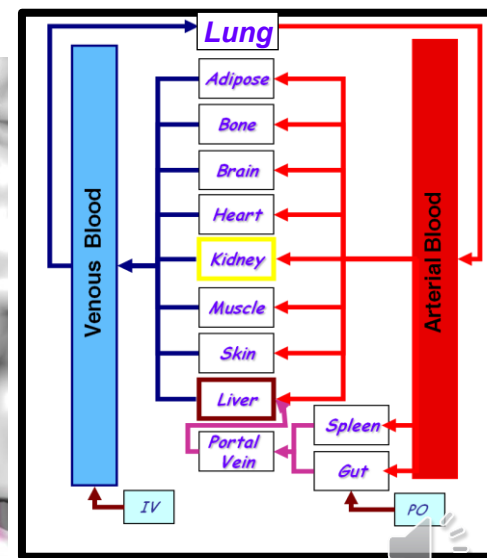
3. Molecular Mechanisms by MD Simulations



4. Computer-Aided Drug Design



5. PK/PD Modeling & Simulations



Group Information & Key Web Sites

▪ Current Members

1. Junmei Wang, PhD, PI, Associate Professor
2. Viet Man, PhD, Instructor
3. Xibing He, PhD, Research Scientist
4. Beihong Ji, PSP PhD student
5. Jingchen Zhai, PSP PhD student
6. Lianjin Cai, PSP MS student
7. Luxuan Wang, PSP MS student
8. Fengyan Han, PSP MS student
9. Taoyu Niu, PSP MS student

▪ Group Homepages

1. <https://clickff.org>
2. <https://clickff.org/wanglab>
3. <https://Mulan.pharmacy.pitt.edu>
4. <https://www.pharmacy.pitt.edu/directory/profile.php?profile=1639>



▪ Google Scholars

1. [Junmei Wang - Google Scholar](#)
2. [Xibing He - Google Scholar](#)
3. [Viet Man - Google Scholar](#)
4. [Beihong Ji - Google Scholar](#)

