Chun Wu

Assistant Professor
Chemistry & Biochemistry/Molecular & Cellular Biosciences

wuc@rowan.edu
http://users.rowan.edu/~wuc/

Education:
BS (Chemistry), Xiamen University
MS (Analytical Chemistry), Xiamen University
MS (Computer Science), University of Delaware
PhD (Chemistry), University of Delaware

Research Expertise:
Computer-aided Drug Design | Molecular Dynamics Simulation | Molecular Modeling

The long-term goal of my research program is to gain mechanic insights into the structure, dynamics and function of pharmacologically important biomolecules. The insights enable rational drug design using a hierarchical virtual screening protocol including docking, molecular dynamics simulation, and free energy perturbation methods. My current research aims to: 1) develop novel cancer drugs that target DNA/RNA-quadruples, transporter (ABCB1) and kinase (MLK); 2) develop novel analgesic and anti-drug-addiction agents that target G-protein coupled receptors (GPCR) (Dopamine, TAAR1, Opioid) membrane receptors; 3) develop novel anti-virus drugs against herpes virus entry (gD); 4) develop diabetes drug that simultaneously targets inflammation (PPAR).

Honors and Awards:
2010, Travel Award, the IBBI (Isolated Biomolecules and Biomolecular Interactions) conference, Berlin, Germany
2004, Named to the Dean's list in recognition of Scholastic Excellence, University of Delaware
1999, Excellent Thesis, Xiamen University

Member of:
American Chemical Society (www.acs.org)

Recent Publications:

Readmond C, Wu C (2017) Investigating detailed interactions between novel PAR1 antagonist F16357 and the receptor using docking and molecular dynamic simulations. J Mol Graphics Model 77:205-217.

Mulholland K, Siddiquei F, Wu C (2017) Binding Modes and Pathway of RHPS4 to Human Telomeric G-quadruplex and Duplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent. PCCP 19:18685-18694.

Sader S, Cai J, Muller A, Wu C (2017) Can human allergy drug fexofenadine, an antagonist of histamine (H1) receptor, be used to treat dog and cat? Homology modeling, docking and molecular dynamic Simulation of three H1 receptors in complex with fexofenadine. J Mol Graph Model 75:106-116.

Sader S, Wu C (2017) Computational analysis of Amsacrine resistance in human Topoisomerase II alpha mutants (R487K and E571K) using homology modeling and all-atom molecular dynamics simulation in explicit solvent, J Mol Graph Model 72:209-219.