BIOGRAPHICAL SKETCH

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NAME	POSITION TITLE
Yi Shang	Postdoctoral Research Associate
eRA COMMONS USER NAME (credential, e.g., agency login) NA	

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	MM/YY	FIELD OF STUDY
University of Science and Technology of China, China	B.S.	05/07	Biological Science
Stony Brook University, USA	Ph.D.	05/13	Molecular and Cellular Biology

A. Personal Statement

During my Ph.D studies, I carried out computer-aided drug design targeting aspartic proteases under the supervision of Professor Carlos Simmerling at Stony Brook University. First, I improved implicit solvent (AMBER GBOBC) simulations of small peptides as well as HIV-1 protease (HIVPR), by correcting the intrinsic radii parameters. Second, based on the improved implicit solvent model, I studied the active site gating mechanism in different HIV subtype proteases which explains corresponding experimental EPR spectrum and links to HIVPR drug resistance. Third, I performed free energy calculations and communication analysis on HIVPR bound to different inhibitors/substrate, in order to elucidate the impact of drug resistance mutations at different positions. At last, I extended the computational study of HIVPR to other non-HIV retroviral proteases, as well as bilobed aspartic proteases, many of which are important drug targets in human diseases. The comparative study involved sequence/structure comparison, evolutionary analysis, and MD simulations characterizing their active site gating and substrate recognition process.

I joined the Filizola lab to conduct research in computational biophysics of a notable subfamily of G protein-coupled receptors (GPCRs) involved in mechanisms of drug abuse.

B. Positions and Honors

Positions and Employment

2007-2008 Teaching Assistant, Molecular and Cellular Biology Graduate Program, Stony Brook University, NY, USA
2008-2013 Research Associate, Molecular and Cellular Biology Graduate Program, Stony Brook University, NY, USA
2013-present Postdoctoral Research Associate, Department of Structural and Chemical Biology, Mount Sinai School of Medicine, New York, NY, USA

Other Experience, Professional Memberships and Awards

2011 American Chemical Society, Chemical Computing Group (CCG) Research Excellence Award
2008-present American Chemical Society member

C. Selected Peer-Reviewed Papers

2. Shang, Y.; Simmerling, C., Molecular dynamics applied in drug discovery: the case of HIV-1 protease. Methods in Molecular Biology 2012, 819, 527-49.

1. Shang, Y.; Nguyen, H.; Wickstrom, L.; Okur, A.; Simmerling, C., Improving the description of salt bridge strength and geometry in a Generalized Born model. J Mol Graph Model 2011, 29 (5), 676-84.

D. Research Support

None