
BIOGRAPHICAL SKETCH

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NAME Yi Shang		POSITION TITLE Postdoctoral Research Associate	
eRA COMMONS USER NAME (credential, e.g., agency login) NA			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable.)</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	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