SYRACUSE UNIVERSITY

- Blood-brain barrier
- Bacterial membranes
- Nanocarrier design
- Drug-delivery
- Computational modeling

SHIKHA NANGIA

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Dr. Nangia is an expert in computational multiscale modeling of biophysical and biochemical systems. Broadly, her research is in the areas molecular and structural characterization of membrane protein, bacterial membranes, nanomedicine, and drug-delivery. A critical focus is on understanding the blood-brain barrier tight junction self-assembly using advanced computational techniques. Another component of her research focuses on designing novel nanocarriers of anticancer drug and protein delivery. More recently, her research effort has been on developing simulation parameter sets for bacterial membranes aimed to develop strategies to fight persistent bacterial infections.

Recent Research Projects:

Molecular architecture of the blood-brain barrier

The focus of this project is to provide new molecular-level strategies to deliver drug molecules to the brain, and characterize the thermodynamics and transport kinetics of the blood-brain barrier. The focus will be to elucidate the molecular structure of the tight junction using a combination of molecular docking, analysis tools, and molecular dynamics.

Designing drug-delivery nanocarriers

In this collaborative project, we focus on effective treatment of brain tumors, which remains a formidable task despite advances in radiation, surgery, and chemotherapeutic strategies. A major impediment in the success of chemotherapeutics in brain tumor treatment is their inability of crossing the blood-brain barrier. A class of extraordinarily potent protein toxins have emerged that are promising in killing cancer cells when administered systemically or locally during surgical removal of brain tumors. We employ synergistic computational and experimental approaches to engineer nanocarriers that encapsulate cytotoxic proteins and deliver them to malignant cancer cells in the brain.

Recent Awards:

2016 College Technology Educator of the Year, Technical Alliance of Central New York
2016 ACS OpenEye Outstanding Junior Faculty Award
2015 Nappi Research Competition Award
2015 NSF CAREER award
2015 Faculty Excellence Award, College of Engineering and Computer Science, Syracuse University

Recent Scholarship:

1. Molecular architecture of the blood-brain barrier tight junction proteins–A synergistic computational and in vitro approach, F. J. Irudayanathan, J. P. Trasatti, P. Karande, and **S. Nangia,** *Journal of Physical Chemistry B,* **120,** 77–88 (2016). http://dx.doi.org/10.1021/acs.jpcb.5b09977
2. Combinatorial approaches to evaluate nanodiamonds uptake and induced cellular fate, R. Eldawud, M. Reitzig, J. Opitz, Y. Rojanasakul, W. Jiang, **S. Nangia,** and C. Dinu, *Nanotechnology,* **27,** 085107 (2016). http://dx.doi.org/10.1088/0957-4484/27/8/085107
3. Simulating gram-negative bacterial outer membrane: A coarse grain model, H. Ma, F. J. Irudayanathan, W. Jiang, and **S. Nangia,** *Journal of Physical Chemistry B,* **119,** 14668–14682 (2015). Featured on the cover. http://dx.doi.org/10.1021/acs.jpcb.5b07122
4. Signaling factor interactions with polysaccharide aggregates of bacterial biofilms, S. C. DeSalvo, Y. Liu, G. Choudhary, D. Ren, **S. Nangia,** and R. Sureshkumar, *Langmuir,* **31** 1958-1966 (2015). http://dx.doi.org/10.1021/la504721b
5. Multiscale approach to investigate self-assembly of telodendrimer based nanocarriers for anticancer drug-delivery, W. Jiang, J. Luo, and **S. Nangia,** *Langmuir,* **31** 4270-4280 (2015). http://dx.doi.org/10.1021/la503949b
6. Optical signature of formation of protein corona in the firefly luciferase-CdSe quantum dot complex, J.M. Elward, F.J. Irudayanathan, **S. Nangia,** and A. Chakraborty, *Journal of Chemical Theory and Computation,* **10,** 5534-5524 (2014). *Featured on the cover.* http://dx.doi.org/10.1021/ct500681m

SUADVANCE

Syracuse University is driven by its vision, Scholarship in Action—a commitment to forging bold, imaginative, reciprocal, and sustained engagements with partners from all sectors of the economy: public, private, and non-profit. These profiles have been developed to facilitate cross-sector connections and are supported by the SU ADVANCE project with funding from the National Science Foundation under NSF Grant No. HRD-1008643.