**PUBLICATIONS**

[Suarez E, Lettieri S, Zwier, Meetthew C, et al. (2014) Simultaneous Computation of Dynamical and Equilibrium Information using a Weighted Ensemble of Trajectories](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=171&SID=4Ay8bd7L6Ps7fvTyMsp&page=1&doc=1). BIOPHYSICAL jOURNAL Volume: 106   Issue: 2   Supplement: 1   Pages: 406A-406A   [JIF= 3.832]

Spiriti JM, Zuckerman DM (2014). [A New Strategy for Coarse-Grained Protein Simulations: Smoothed Energy Tables](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=171&SID=4Ay8bd7L6Ps7fvTyMsp&page=1&doc=2). BIOPHYSICAL JOURNAL Volume: 106   Issue: 2   Supplement: 1   Pages: 412A-412A. [JIF=3.832]

Subramanian SR, Palli R, Zuckerman DM (2014) [Mixed-Resolution Monte Carlo: A Tool for Sampling Proteins and Ligands](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=171&SID=4Ay8bd7L6Ps7fvTyMsp&page=1&doc=3). BIOPHYSICAL JOURNAL Volume: 106   Issue: 2   Supplement: 1   Pages: 412A-412A. [JIF=3.832]

Palli R., Subramanian SR, Zuckerman DM. (2014). [Mixed-Resolution Monte Carlo: Application to Flexible Docking of the Estrogen Receptor](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=171&SID=4Ay8bd7L6Ps7fvTyMsp&page=1&doc=4). BIOPHYSICAL JOURNAL Volume: 106   Issue: 2   Supplement: 1   Pages: 475A-475A. [JIF=3.832]

**Active projects:**

Complementary methods for equilibrium sampling of biomolecules

High Performance Computing for Multiscale Modeling of Biological Systems

Dissecting the molecular mechanisms of stress-response proteins in cancer

**Proposals:**

High-performance weighted ensemble software for simulation of complex bio-events