Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Conformational Analysis on structural perturbations of the zinc finger NEMO[1] RYAN GODWIN, FREDDIE SALSBURY, Wake Forest Univ, SALSBURY GROUP TEAM — The NEMO (NF-kB Essential Modulator) Zinc Finger protein (2jvx) is a functional Ubiquitin-binding domain, and plays a role in signaling pathways for immune/inflammatory responses, apoptosis, and oncogenesis [*Cordier et al., 2008*]. Characterized by 3 cysteines and 1 histidine residue at the active site, the biologically occurring, bound zinc configuration is a stable structural motif. Perturbations of the zinc binding residues suggest conformational changes in the 423-atom protein characterized via analysis of all-atom molecular dynamics simulations. Structural perturbations include simulations with and without a zinc ion and with and without de-protonated cysteines, resulting in four distinct configurations. Simulations of various time scales show consistent results, yet the longest, GPU driven, microsecond runs show more drastic structural and dynamic fluctuations when compared to shorter duration time-scales. The last cysteine residue (26 of 28) and the helix on which it resides exhibit a secondary, locally unfolded conformation in addition to its normal bound conformation. Combined analytics elucidate how the presence of zinc and/or protonated cysteines impact the dynamics and energetic fluctuations of NEMO.

[1]Comprehensive Cancer Center of Wake Forest University Computational Biosciences shared resource supported by NCI CCSG P30CA012197

Ryan Godwin
Wake Forest Univ

Date submitted: 14 Nov 2013 Electronic form version 1.4