

Coupling of HSP72 α -helix subdomains by the unexpected irreversible targeting of Lysine-56 over Cysteine-17; coevolution of covalent bonding

Aimen Aljoundi¹, Ahmed El Rashedy¹, Patrick Appiah-Kubi¹, and Mahmoud E.S Soliman^{1*}

¹Molecular Bio-computation and Drug Design Laboratory

School of Health Sciences, University of KwaZulu-Natal, Westville Campus, Durban 4001,
South Africa

*Corresponding Author: Mahmoud E.S. Soliman

Email: soliman@ukzn.ac.za

Telephone: +27 (0) 31 260 8048, Fax: +27 (0) 31 260 78

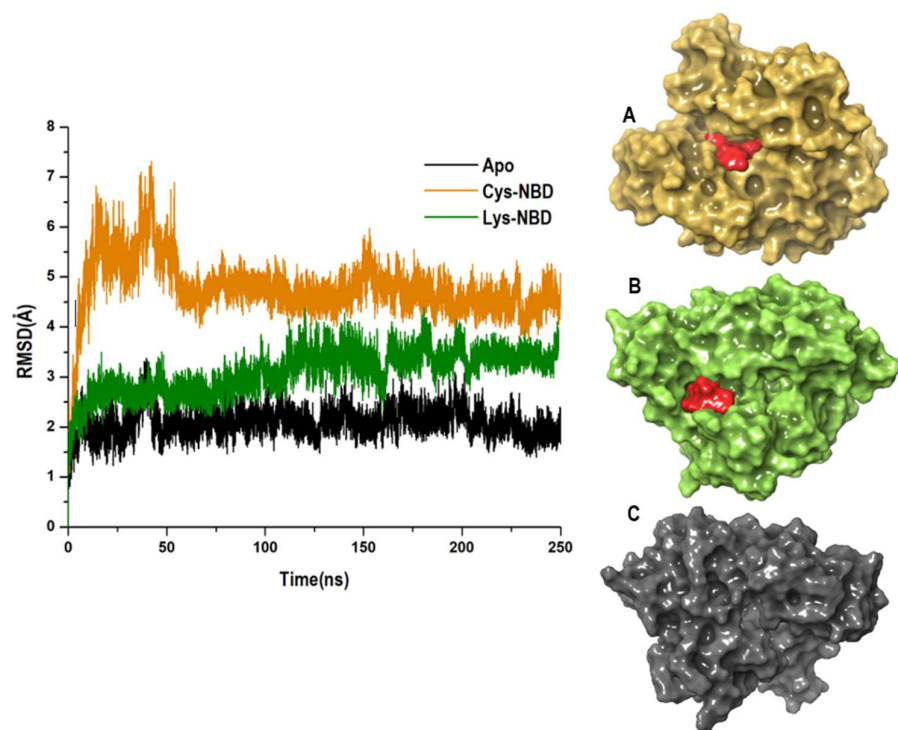


Figure S1. Comparative C- α RMSD plots showing the degree of stability and convergence of the studied systems over the 250ns MD simulation time; [A] Cysteine-NBD[B] Lysine-NBD [C] Apo.