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Structural Integrity of Proteins under Applied Bias during Solid-State Nanopore Translocation[1] MOHAMMAD R. HASAN, RAJA RAHEEL KHANZADA, MOHAMMED A. I. MAHMOOD, ADNAN ASHFAQ, University of Texas at Arlington, SAMIR M. IQBAL, Nano-Bio Lab, Electrical Engineering, Bioengineering, University of Texas at Arlington — The translocation behavior of proteins through solid-state nanopores can be used as a new way to detect and identify proteins. The ionic current through a nanopore that flows under applied bias gets perturbed when a biomolecule traverses the Nanopore. It is important for a protein detection scheme to know of any changes in the three-dimensional structure of the molecule during the process. Here we report the data on structural integrity of protein during translocation through nanopore under different applied biases. Nanoscale Molecular Dynamic was used to establish a framework to study the changes in protein structures as these travelled across the nanopore. The analysis revealed the contributions of structural changes of protein to its ionic current signature. As a model, thrombin protein crystalline structure was imported and positioned inside a 6 nm diameter pore in a 6 nm thick silicon nitride membrane. The protein was solvated in 1 M KCl at 295 K and the system was equilibrated for 20 ns to attain its minimum energy state. The simulation was performed at different electric fields from 0 to 1 kCal/(mol.Å.e). RMSD, radial distribution function, movement of the center of mass and velocity of the protein were calculated. The results showed linear increments in the velocity and perturbations in ionic current profile with increasing electric potential.

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