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Molecular Interactions Between Mismatch Repair Protein MutS and DNA from the Perspective of Colorectal Cancer.[1] SANJAY KARIMBANAMLAYIL BABU, KAVYA CHANDRIKA HEMMANUR, ISAAC MACWAN, PRABIR PATRA, University of Bridgeport — It is estimated that about 30% of the colorectal cancer (CRC) cases are hereditary and related to known syndromes, particularly Lynch Syndrome. This study aims to understand the molecular interactions between a mismatch repair protein, MutS and a mismatched DNA through a DNA-graphene-polypyrole (DGP) biosensor and molecular dynamics. Electrochemical impedance spectroscopy (EIS) analysis of the DGP biosensor confirms the adsorption of the DNA probe and its interactions with MutS. These results are supported by a set of all-atom molecular dynamics simulations using NAMD and CHARMM force fields. Within the first 200ns of the molecular interactions between MutS and mismatched DNA, we portray the conformational changes of the human MutS protein as it binds to the DNA. It is further found that within the first 50ns, the reactive site on the MutS protein (residues 1 to 124) start to favorably interact with the DNA for the onset of the scan cycle. This investigation additionally provides crucial insights into the interactive energetic events at the interface of MutS and the DNA through non-binding energies, thereby mapping out the events during scanning and locating the mismatch.

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