Abstract Submitted
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Insights on the Structural Details of Endonuclease EcoRI-DNA Complexes by Electron Spin Resonance JESSICA SARVER, University of Pittsburgh — Pulsed electron spin resonance (ESR) was used to probe the binding specificity of EcoRI, a restriction endonuclease. Using site-directed spin labeling, a nitroxide side chain was incorporated into the protein, enabling the use of ESR to study structural details of EcoRI. Distance measurements were performed on EcoRI mutants when bound to varying sequences of DNA using the Double Electron-Electron Resonance experiment. These distances demonstrated that the average structure in the arm regions of EcoRI, thought to play a major role in binding specificity, is the same when the protein binds to different sequences of DNA. Also, it was determined that the arms exhibit higher flexibility when bound to sequences other than the specific sequence due to the larger distance distributions acquired from these spin labeled complexes. Molecular dynamics (MD) simulations were performed on the spin-label-modified specific EcoRI-DNA crystal structure to model the average nitroxide orientation. The distance distributions from MD were found to be narrower than experiment, indicating the need for a more rigorous sampling of the nitroxide conformers in silico.

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