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Insights on copper coordination and reactivity of endonuclease EcoRI by ESR spectroscopy and modeling MING JI — The cleavage of DNA by restriction endonuclease EcoRI is catalyzed by metal ions such as Mg^{2+}. However, Cu^{2+} does not catalyze the cleavage of DNA by EcoRI. In order to understand the functional difference between Cu^{2+} and Mg^{2+}, coordination of Cu^{2+} in the EcoRI–DNA complex was clarified by ESR and MD simulation. There are two Cu^{2+} components in the specific EcoRI-DNA complex. Each component has one N atom from histidine imidazole and one oxygen atom from the phosphate backbone of DNA coordinate to Cu^{2+} based on the ESR experimental results. MD simulation further confirmed that the Nδ atom of His114 imidazole and one oxygen atom from the phosphate backbone of DNA coordinate to Cu^{2+}. Difference in the coordination of Cu^{2+} and Mg^{2+} explains their different functional behaviors.

Ming Ji

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