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ESR distance measures show that Cu^{2+} coordinates to Histidine 114 in the EcoRI-DNA complex ZHONGYU YANG, University of Pittsburgh — Metal coordination of EcoRI is intimately connected to its function of cleaving viral DNA. In order to gain insight into this process pulsed ESR distance measurement methodology was extended to the case of copper-copper and copper-nitroxide in proteins. This talk will discuss the first results on $Cu^{2+}-Cu^{2+}$ and Cu^{2+} -nitroxide distances measured in proteins by pulsed ESR. A triangulation procedure that involved the measurement of several long range distances (2-4 nm) demonstrates that copper ions bind to histidines 114 in EcoRI. The combination of ESR distance measurement and molecular dynamics simulations show distinct differences in the coordination of Cu^{2+} versus the natural cofactor Mg^{2+} . This difference translates into the differences in roles of the metal ions - Mg^{2+} catalyzes cleavage while Cu^{2+} binding without cleavage of DNA.

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