

Abstract Submitted
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Cu(II) coordination structure determinants of the fibrillization switch in Abeta peptides¹ JESSICA HERNANDEZ-GUZMAN, LI SUN, Emory University, Department of Physics, ANIL MEHTA, DAVID LYNN, Emory University, Department of Chemistry, KURT WARNCKE, Emory University, Department of Physics — Alzheimer’s Disease (AD) is associated with the aggregation and fibrillization of the beta-amyloid protein (Abeta). The coordination of Cu(II) by peptide histidine imidazole sidechains is proposed to play an important role in determining the fibrillization “switch” [1]. We have developed techniques of powder X-band electron spin echo envelope modulation (ESEEM) spectroscopy to determine the 3D molecular structure of the Cu(II)-histidine imidazole coordination in cryotrapped soluble and fibrillar forms of Abeta peptides, in order to gain insight into the factors that govern fibrillization. We use hybrid optimization-based OPTESIM [2] simulation of the double quantum harmonic feature to determine the mutual orientation of the imidazole rings in Cu(II)-bis-imidazole complexes and in Abeta(13-21) peptides. The Cu(II) coordination mode and assembly constraints in fibrils are revealed. [1] Dong , J., et al., *Proc. Natl. Acad. Sci.*, 2007, 104, 13313. [2] Sun, L., et al., *J. Magn. Reson.* 2009, 200, 21.

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