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Relative Orientation of Imidazole Ligands in Cu(II) Model and Abeta peptides Complexes revealed by ESEEM Spectroscopy[1] JESSICA HERNANDEZ, LI SUN, KURT WARNCKE, Department of Physics, Emory University — 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 X-band electron spin echo envelope modulation (ESEEM) spectroscopy to determine the 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. Focusing on the ESEEM double quantum harmonic feature, we use our hybrid optimization-based OPTESIM simulation software [2] to determine the mutual orientation of the imidazole rings in Cu(II)–bis-imidazole complexes that include *cis*- versus *trans*- coordination. The technique has been applied to Abeta(13-21) peptide to reveal the Cu(II) coordination mode in fibrils. [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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