

Abstract Submitted
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**Investigation of copper(II) binding to the protein precursor of
Non-Amyloid-Beta Component of Alzheimer Disease Amyloid Plaque**

FRANCIS ROSE, MIROSLAV HODAK, JERRY BERNHOLC, N.C. State University — The Non-Amyloid-Beta Component Precursor (NACP) is a natively unfolded synaptic protein that is implicated in Alzheimers and Parkinsons diseases. Its aggregation into fibrillar structures is accelerated by the binding of copper(II). Experimental studies suggest that the dominant copper binding site is located at the histidine residue in NACP. Based on this evidence we assembled a model fragment of the binding site and used DFT to analyze the conformational details of the most probable binding motifs. We investigated the overall conformational effects with classical MD by constraining the copper binding site to the most energetically favorable geometry obtained from the DFT calculations. These results are compared and contrasted with those of the unbound NACP.

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