

Computational Modelling of Copper Complexes Relevant to Alzheimer Disease

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Abstract. Metal cations, such as Cu^{2+} , have been shown to induce amyloid aggregation and formation of reactive oxygen species. Elucidation of the structural features of Cu^{2+} -Ab is thus, essential to understand their role in the aggregation of Ab, formation of reactive oxygen species and to rationally design new chelators with potential therapeutic applications. Present contribution reviews some of our computational studies in this field. First, computational strategies used to determine three dimensional structures for Cu^{2+} -Ab and the redox properties of these complexes will be presented^{1,2}. Second, we will summarize our studies on Cu^{2+} chelators³ and finally our recent advances on markers to identify Ab(1-40) fibrils⁴.

Keywords. Alzheimer disease, b-amyloid, metal chelation, Standard Reduction Potential, DFT, homology modelling, virtual screening.

References.

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