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The role of His-50 of α-synuclein in binding Cu(II): pH dependence, speciation, thermodynamics and structure.

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Streszczenie

Copper interaction with alpha synuclein (αS) has been shown to accelerate aggregation and oligomerization of the protein. Three different αS copper binding domains have been proposed: (i) the N-terminal residues (1–9) that represent the minimal copper binding domain; (ii) the His-50 imidazole and (iii) the Asp and Glu residues within the acidic C-terminal domain. The copper coordination at the N-terminus has been extensively characterized and it is generally accepted that it provides the highest affinity site. The same does not hold for the role played by His-50 in copper binding. In this work Cu(II) coordination to peptide fragments encompassing residues 45–55 of αS has been exhaustively characterized, including systems containing the inherited mutations E46K and A53T, as model peptides of the His-50 site. Through potentiometric titrations all the speciation profiles have been determined and the stability constants have been used to estimate the dissociation constants of complexes corresponding to the binding modes at pH 6.5 and 7.5. Spectroscopic analyses allowed determination of (i) the copper coordination sphere, (ii) its geometry and (iii) the constraints wherefrom the 3D structural models of the copper complexes could be obtained.

Adres publiczny

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