

Structural and dynamic characterization of copper(II) binding of the human prion protein outside the octarepeat region.

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Streszczenie

Human prion protein (hPrP) fragments encompassing the 91–120 region, namely hPrP92–100 (SP1), hPrP106–113 (SP2), hPrP91–120 (LP1), and hPrP91–114 (LP2), were considered for delineation of the Cu^{II}-binding site(s). NMR and EPR spectroscopy results obtained from LP1 or LP2 were compared with those obtained from SP1 and SP2. The coexistence of two binding sites, one centered at His96 and the other at His111, was evidenced and ratified by ESI mass spectrometry at low and high metal:peptide ratios. While room-temperature NMR spectroscopy data were consistent with the binding site centered on His111 being approximately fourfold stronger than that centered on His96, low-temperature EPR spectroscopy results yielded evidence for the opposite trend. This disagreement, which has also occurred in the literature, was clarified by temperature-dependent molecular dynamics runs that demonstrated Met112 approaching the metal at room temperature, a process that is expected to stabilize the His111-centered binding site through hydrophobic shielding of the metal coordination sphere.

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