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Integrative structure of a histone chaperone-histone complex

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Histone chaperones play a crucial role in regulating the assembly and disassembly of chromatin. Our lab recently reported a novel chaperone binding mode in which histone chaperone APLF single-handedly assembled the histone complexes H2A-H2B and H3-H4 into the histone octamer. The chaperone domain of APLF consists of a short (~60 aa) intrinsically disordered, highly acidic domain (AD). As we could only solve the crystal structure of a peptide fragment of the AD bound to the histone octamer, we used an integrative structural biology approach to define the conformation of the rest of the AD. In this talk I will outline how the recent implementation of shape-based docking in the HADDOCK was used to integrate small angle xray and neutron scattering, cross-linking mass-spectrometry, NMR and the crystal structure to define the integrative structure of this challenging histone chaperone-histone complex.

Submitting to:

 Presenter:
 VAN INGEN, Hugo (Utrecht University)

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