

Abstract Submitted
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**Examining the Self Assembly of the Villin Headpiece Protein:
A Combined Experimental and Molecular Dynamics Study¹** BRIAN ANDREWS, KAHONG LONG, BRIGITA URBANC, Drexel Univ — The Villin Headpiece subdomain (VHP36) is a protein that is well studied experimentally and computationally such that its monomeric native structure and ability to self-assemble are well characterized. In this study, we present experimental evidence that VHP36 proteins in solution form a limited number of dimers while the large majority remain monomeric independent of concentration. We then use our in-house coarse-grain Discrete Molecular Dynamics (DMD) package DMD4B-HYDRA which combines discrete potential functionals with a four-bead protein model to observe VHP36 assembly in simulation. Dimers produced from the DMD simulations are converted from the four-bead model to an all-atom structure and their stability is analyzed via all-atom MD simulations in two frequently used MD force fields. Additional simulations of two unfolded VHP36 monomers are also simulated in the same MD force fields to observe the dimerization process in more detail. The purpose of this work is to assess and compare the ability of the MD force fields to capture the dimerization process and search for an explanation regarding the absence of larger order oligomers.

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