

Abstract Submitted  
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**Thermodynamics and kinetics of apoazurin folding under macromolecular crowding effect and chemical interference**<sup>1</sup> FABIO ZEGARRA, MARGARET CHEUNG, University of Houston — Proteins fold in a cellular milieu crowded by different kinds of macromolecules. They exert volume exclusion impacting protein folding processes in vivo. Folding processes, however, has been studied by chemical denaturation under in vitro conditions. The impact of the two factors as an attempt to advance the understanding of folding mechanism in vivo is not understood. Here, we investigate the folding mechanisms of apoazurin affected by the macromolecular crowding and chemical interference by using coarse-grained molecular simulations. Crowding agents are modeled as hard-spheres and the chemical denaturation effects are implemented into an energy function of the side chain and backbone interactions. Protein folding stability, mechanism, and kinetics rates of apoazurin under chemical interference and macromolecular crowding conditions are being investigated.

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