

Impact of Macromolecular Crowding on the Structure and Function of *Escherichia coli* of Prolyl-tRNA Synthetase.

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Most computational and experimental studies to probe an enzyme-catalyzed reaction are typically performed in dilute solutions. However, enzymatic activities *in vivo* occur in a crowded environment composed of many macromolecules. The overall objective of this study is to investigate the role of macromolecular crowding on the structure and function of *Escherichia coli* prolyl-tRNA synthetase (ProRS). ProRS is a member of an important family of enzymes called aminoacyl tRNA synthetases (AARSs), which are essential for the biosynthesis of proteins in all living organisms. Combined molecular dynamics simulations and fluorescence spectroscopic studies have been employed to explore the impact of macromolecular crowding on structure and enzymatic functions. Upon completion of the study, we will be better able to assess if the macromolecular crowding impacts significantly in the structure-based drug design to inhibit the function of pathogenic prolyl-tRNA synthetases. Preliminary results of our computational and spectroscopic work will be presented.