OSV-45

Computational Exploration and Structural Modeling of Microbial Creatinase for Therapeutic Application in Humans

Ramya Keerthi Yennamsetti, Manisha Koyimadatha*, Mahalakshmi R

Department of Bioinformatics, Sathyabama Institute of Science and Technology, Chennai, India.

Creatine, a guanidino compound, is endogenously synthesized primarily in the liver and kidneys, playing a crucial role in cellular energy homeostasis, particularly in tissues with high energy demands such as muscle and the brain . This synthesis is a two-step enzymatic process involving arginine and glycine as precursors. Dysregulation in creatine metabolism, however, has been linked to various pathologies, underscoring the need for mechanisms to manage its levels. Specifically, elevated creatine levels have been associated with metabolic disorders and kidney dysfunction, highlighting the potential therapeutic utility of enzymes capable of creatine degradation .Creatinase (creatine amidinohydrolase), enzyme produced by microorganism *Pseudomonas putida*, catalyzes the hydrolysis of creatine into sarcosine and urea, offering a promising avenue for reducing excess creatine . Despite creatinase known efficacy in microbes, its potential in human therapeutic is largely unexplored, particularly in terms of computational modelling and structural adaptation. . This study addresses this gap by employing bioinformatics tools to identify, model, and computationally evaluate creatinase enzymes, with the ultimate goal of assessing their therapeutic potential in mitigating elevated creatine levels in humans. The absence of effective enzymatic therapies for direct creatine degradation in humans further underscores the critical need for this investigation.

Keywords: Bioinformatics, Creatine, Creatinase, Enzyme therapy, Therapeutic potential

***Correspondence:** Manisha Koyimadatha
manishamanu5198@gmail.com