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Designer protein enriched with large neutral amino acids: A new approach for treating phenylketonuria

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Phenylketonuria (PKU) is a genetically inherited disease caused by the defective phenylalanine hydroxylase (PAH) enzyme. In case of phenylketonuria, the body fails to convert phenylalanine (Phe) to tyrosine (Tyr), resulting in the elevated blood Phe level and consequent neurological damage. Of all therapies, large neutral amino acid (LNAA) supplementation has emerged as a promising approach for the dietary treatment of PKU. The LNAAs compete with Phe for the same L-type LNAA transporter (LAT1, SLC7A5) across the blood-brain barrier, decreasing brain Phe level. Thus, the aim of this study was to design an easily digestible protein enriched with LNAA (except Phe) in accordance with WHO/FAO/UNU specification by homology modeling using αs1 casein as template. The challenge was to maximize the LNAAs content (except Phe) in the protein model by finding a suitable scaffold (like α-helix) for homology modeling. Out of 63 different protein models designed, protein model-54 was selected for its compact 3D structure with only α-helices, high sequence similarity with template (60.4%) and good *in silico* digestibility. Different softwares like, SWISS-MODEL, EXPASY tool, PROFUNC, I-TASSER, RaptorX and SAVeS Server were used for the structure prediction and validation of the designed protein. The structures obtained from tertiary predicting software were visualized by discovery, UCSF chimera and Pymol tools. Based on these evaluations, the protein model-54 was found to be the best and reliable model. The presentation will review the strategies used for homology modeling, secondary structure and tertiary structure prediction and validation of the designed protein and discuss its nutritional significance for PKU treatment.

Biography

Prakruthi Appaiah has completed her MSc in Microbiology (2010) from University of Mysore and currently pursuing her PhD (Life Science) in CSIR-Central Food Technological Research Institute, Mysore, India. After her Post-graduation, she worked as Project Assistant (2011) in Lipid Science and Traditional Food Department, CSIR-CFTRI, Mysore, during which she has published three papers in reputed journals and won Best Oral Presentation Award in the National Conference on Functional Foods in Health & Well-being, Bangalore, India. She has presented a poster in 22nd Indian Convention of Food Scientists and Technologists (ICFOST-2012), organized by AFSTI at CSIR-CFTRI, Mysore, India.

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