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From protein expression data to molecular dynamic simulation: Analysis of GRIP1 PDZ6 domain in AD

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Protein-protein interaction domain, PDZ (Postsynaptic density-95/Discs large/Zona occludens-1) plays a critical role in efficient synaptic transmission in brain. Dysfunction of synaptic transmission is thought to be the underlying basis of many neuropsychiatric and neurodegenerative disorders including Alzheimer's disease (AD). Glutamate receptor interacting protein 1 (GRIP1) family proteins contain six to seven PDZ domains which help in protein-protein interaction. GRIP1 interacts with the ionotropic glutamate receptors of the AMPA type which in turn are involved in the pathophysiology of several neurodegenerative processes including Alzheimer's, Parkinson's and Huntington's diseases. In this study we have used the protein expression data of AD patients obtained from liquid chromatography-tandem mass spectrometry (LC-MS/MS) experimental procedure. The differentially expressed proteins were then considered for construction of protein-protein interaction network (PPIN). GRIP1 was found to be differentially expressed in the protein expression data. Interestingly, it was also identified as one of the topologically significant proteins in the PPIN. Till date very few studies have analyzed the detailed structural basis of PDZ mediated protein interaction of GRIP1. In order to gain better understanding of structural and dynamic basis of these interactions we employed molecular dynamic simulations. The analysis of MD simulations shows considerable conformational flexibilities of the PDZ domain of GRIP1 which may require for its multimerization. Our study may provide detailed information about structural basis of PDZ mediated protein interaction of GRIP1 which may lead to novel therapeutic approaches in AD.

Biography

Paulami Chatterjee has completed her Post graduation in Biochemistry from Calcutta University. She is currently a Senior Research Fellow pursuing her PhD under the guidance of Dr. Debjani Roy at Biophysics Department, Bose Institute, Kolkata. She has so far published 2 papers in reputed journals and has presented her work in 1 national and 2 international conference.

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