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Prediction of molecular targets responsible for adhesions (Lu/BCAM- α4β1) in sickle cell disease: Combined quantum mechanics and molecular mechanics study

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Sickle Cell Disease (SCD) is an inherited hemolytic anemia that substitution change valine to glutamic acid at 6th position of the β-globulin chain cause clinical manifestation, in addition to hemolysis and anemia. Simplified schemes of the main interaction involved in the abnormal adhesion of the sickle red blood cell to the endothelium, locally, endothelium damages expose sub-endothelial structure that also participate to the adhesion process. Some adhesion proteins are activated by extracellular stimuli. It is the case of the Basal Cell Adhesion Molecule (Lutherian blood group) (Lu/BCAM) that expresses its adhesion properties when phosphorylated via the protein kinase A-dependent (PKA) pathway downstream β2 adrenergic receptor. The first molecule partners identified as actors of the abnormal interaction on RBCs were the α4β1 integrin. RBCsthe main actor of this abnormal adhesion process are a population of young RBCs referred to as "stress reticulocytes". Although molecule basis of SCD Sickle cell disease via well characterized, underlying Vaso-occlusive painful crisis (VOC) has not been fully elucidated.Developing country like India Chhattisgarh region has that prevalence 10% population carries Sickle Cell Disease (SCD) gene and constitutes a large socio-economic burden on the economy of the state. Bioinformatics-based approach will give a new dimension in solving the (VOC) problem in sickle cell diseases.

Biography

Amiy Dutt Chaturvedi completed his MSc in Bioinformatics from SMU Univ., Gantok in the year 2006. Later He pursued for PhD (Biotechnology) from Pt R.S.U & SOS Biotechnology, Raipur and completed it in the year 2012. He worked as an Assistant Professor from 2006–2014 at SSMV, Bhilai Chhattisgarh, India. From 2013 till present date, he is working as a Scientist-II, Pt.JNM Medical College, Raipur, India.

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