World Academy of Science, Engineering and Technology
International Journal of
Vol:8, No:, 2014

On the Homology Modeling, Structural Function Relationship and Binding Site Prediction of Human Alsin Protein

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Abstract : Amyotrophic lateral sclerosis (ALS), also known as “Lou Gehrig’s disease”. It is a neurodegenerative disease associated with degeneration of motor neurons in the cerebral cortex, brain stem, and spinal cord characterized by distal muscle weakness, atrophy, normal sensation, pyramidal signs and progressive muscular paralysis reflecting. ALS2 is a juvenile autosomal recessive disorder, slowly progressive, that maps to chromosome 2q33 and is associated with mutations in the alsin gene, a putative GTPase regulator. In this paper we have done homology modeling of alsin2 protein using multiple templates (3KCI_A, 4LIM_A, 402W_A, 4D9S_A, and 4DNV_A) designed using the Prime program in Schrödinger software. Further modeled structure is used to identify effective binding sites on the basis of structural and physical properties using sitemap program in Schrödinger software, structural and function analysis is done by using Prosite and ExPASy server that gives insight into conserved domains and motifs that can be used for protein classification. This paper summarizes the structural, functional and binding site property of alsin2 protein. These binding sites can be potential drug target sites and can be used for docking studies.

Keywords : ALS, binding site, homology modeling, neuronal degeneration