Computational analysis of the dominions CAH and FNIII of the Fosfacan DSD-1-PG and their union with the Tenascin R (TN-R) protein

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The cerebral injury are public health problems, they represent the first cause of incapacity and death between young people in all the world; this illness leads to a disabling process and functional loss in the long term, the implementation of new investigation lines such as the bioinformatics turn out to be a potential tool for the study and subsequent improvement of the medicaments, with which the neuronal deaths can be reduced and preserve the motor functions in persons that have suffered some type of cerebral injuries.

The biological responses of an organism after a lesion in the CNS correspond to demyelination and inflammation processes of the injured tissue, with the subsequent appearance of astrocytes, oligodendrocytes and microglial cells, which meet as a support, repairment and regeneration functions of the nervous tissue, what contributes to minimize the damage and neuronal death. Within this process, in the involved axons a glial scar is formed.

Inside the micro environment of the glial scar, subsequently there is an accumulation of cells and proteins, many of these with important functions such as migration, cellular regeneration, demyelination, axonal growth and cellular proliferation. Of the most expressed proteins in the glial scar are the proteoglycans, which are transmembrane proteins with inhibitory functions or of axonal growth, this depending of external stimulus and of unions with the proteins of the extracellular matrix.

Inside the family of the proteoglycans, we find the Fosfacan; this protein has been mentioned as a fundamental component of the SNC and has been reported as a highly expressed protein after a cerebral injury. The Fosfacan DSD-1-PG has plenty theoric evidence of its unions. To explain this computational model was used created by homology throughout a Schrödinger program of the extracellular region of the DSD-1-PG, which comprehends the dominions Fibronectin type III (FnIII) and Carbonic anhydrase (CAH).

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The prediction of a tridimensional model and the computational simulation of the Fosfacan DSD-1-PG is important to understand some processes that occur at the glial scar and that involve the regeneration, besides this model allowed to study the molecular recognition, just as its place of union to the extracellular protein Tenascin R, which has been reported as a modulator of axonal growth in different stages of the development, besides being highly present in cerebral lesions.

It was found that the union of the proteins DSD-1-PG and Tenascin R is a dependent union of calcium atoms; this interaction took place between the dominions FNIII for the protein DSD-1-PG and the dominion GDF for the Tenascin R in calcium dependent regions. This result can assume that inside the proteoglycans, the fosfakan and the agrecan are the only known proteoglycans until now that combine to other extracellular proteins throughout atoms, independently of the proteic binds that they posses.