In silico Design of Ligand Molecules Opening Blocked Aquaporins for Efficient Water Transport in Cystic Fibrosis Victims

Proceedings of the International Conference on Drug Discovery (ICDD) 2020

Joel Abraham
Sree Chitra Thirunal College of Engineering

Rohini Samadarsi
Assistant Professor, Dept. of BT & BCE, Sree Chitra Thirunal College of Engineering.
Email id: *rohinisasamadarsh@gmail.com*

Abstract

Aquaporins are transport proteins concerned with the transport of water in several parts of the body systems. They are found to be associated with and regulated by cystic fibrosis transmembrane conductance regulator (CFTR) proteins, which are chloride ion channels, in some regions of cells. Mutations in CFTR is found to be the primary cause of cystic fibrosis disease. One of the concerns with this disease is the absence of efficient water transport in tissue systems because of the non-regulation or block of water transport, by mutations in the CFTR gene and the formation of defective CFTR proteins. It can be found in the lungs, causing an absence of flushing of mucus and also in male sterility because of the lack of water in the male reproductive tract. In the present study the three-dimensional structures of aquaporin proteins were analyzed and ligands were developed by molecular modeling which could bind to blocked aquaporins to an open position for a short period of time.

Keywords: In silico, cystic fibrosis, aquaporin, lungs