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Boron Uptake in Salt Cedars via Aquaporins
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Background

Salt Cedar (Tamarix) is a dicot plant highly tolerant to the chemical boron. For most plants boron is an essential yet toxic metalloid. Plants have a hard time excluding it. The goal of the project is to identify a potential protein sequence (order of amino acids forming a protein) for an aquaporin that allows the transport of boron, moving through a pore. In addition to selecting the sequences, a 3D model of the protein has been constructed to see how boron is entering the cells through the channels of these proteins. A dynamic model is being made to examine the structure in a cell membrane.

Methods

In addition to selecting the sequences, a 3D model of the protein has been constructed to see how boron is entering the cells through the channels of these proteins. A dynamic model is being made to examine the structure in a cell membrane. We have assembled 3D models of these channel proteins using computer software programs that build models based on the sequences. The models are based on Pichia pastoris Aquaporin 1 structure (Pp.AQY1). The models of Arabidopsis thaliana (A.t.) and Cucumis sativus (C.s.) were then analyzed in a second program to determine the size of the protein’s channel. The known structure of Homo sapiens Aquaporin 1 (H.s.AQP1) was used to determine the validity of programs’ results. The diameter of the channel/pore is a critical value being calculated. Molecular dynamic simulations are being run on these models as well. (See flowchart for molecular dynamics steps.)

Results

The radius of the channel is a critical value; it determines whether or not boron fits through the protein channel. The results of the sequence C.s.N.I.P5.1 (closest sequenced relative found) did not show a large enough radius to allow the movement of boron through the protein in a static model. The nearly identical A.t.N.I.P5.1 has been shown to move boron, yet also does not show a large enough pore radius either. This raises the question of how dynamic the pore channel must be to allow boron to pass through. In the dynamic model the pore should have a larger size at times. The pore size will determine if boron will fit through the channel. We expect this channel to have a lower presence in the roots of this plant, thus limiting boron uptake.

Figures: Left: Salt cedars in the laboratory. Middle Top: Fine grain molecular dynamics system of C.s.N.I.P5.1 monomer using CHARMM-GUI Membrane Builder Module. Middle Bottom: Course grain molecular dynamics system of C.s.N.I.P5.1 monomer using CHARMM-GUI PACE CG Bilayer Builder Module. Top Right: All atom coarse grain model using CHARMM-GUI PACE CG to All-atom Converter Module.

Bibliography


Molecular Dynamics Design Steps using CHARMM-GUI
Select PDB model to use and define unit cell
Select system model to construct
Design bilayer with lipids and insert protein
Select energy minimization constraints and forcefields.
Equilibrade model and run simulation