

2nd Bioinformatics Meeting
October 13 and 14, 2016, Universidad de Talca



SCIFORUM
BMEICB-02



Comparative study of molecular binding sites of nitrate and auxin in *Arabidopsis thaliana* NRT1.1 & NRT1.2 transporter.

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Abstract: Nitrogen is an essential macronutrient for plants and other living organisms. The main source of nitrogen for plants in agricultural soils is nitrate (NO_3^-). This ion is transported through specific nitrate transporters located in the plant cell plasma membrane. In addition to its role in metabolism, NO_3^- can also act as a signal to regulate many biological processes in plants. The Nitrate Transporter 1.1 (NRT1.1) protein is a dual-affinity transporter that has been shown to act as a nitrate sensor. Recent studies have shown that NRT1.1 can also transport the phytohormone auxin. Using molecular modelling techniques, we intend to determine the molecular binding sites of nitrate and auxin in the *Arabidopsis* NRT1.1 transporter. We aim to search for residues that differentiate the functionality of NRT1.1-nitrate and NRT1.1-auxin. To achieve our goal we performed molecular docking of auxin in the *Arabidopsis* NRT1.1 crystallographic structure and molecular dynamics simulations of NRT1.1-nitrate and NRT1.1-auxin complexes. Additionally, the same studies were performed over the nitrate transporter NRT1.2 with the aim to compare both transporters and begin to understand the transport mechanism of both nutrients.

Conflicts of Interest

The authors declare no conflict of interest.