BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Illinois/300 Knh
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UNRAVELING THE MOLECULAR MAGIC OF WITCHWEED

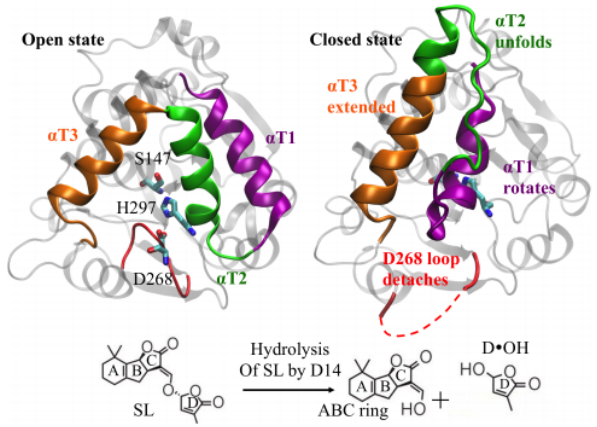

Fig. 1. Conformational change in the strigolactone receptor D14 leading to an open and closed state.

Research Challenge

Witchweed is a root parasite that is considered a serious agricultural pest affecting crops such as sorghum, maize (corn), rice, millet and cowpea, among other crops. Witchweed seeds remain in the soil for decades until favorable germination conditions are provided by a host plant. Globally, it leads to economic loss of $10 billion every year, and loss to livelihood of over 100 million farmers around the world. Currently, there is a need for a control technique to combat the outbreak of this menacing parasite.

Methods & Codes

The goal is to develop a molecular control strategy that inhibits growth of witchweed to avoid crop failure. To do this, there is the need to understand the activation process of the strigolactone receptors to which Witchweed is extremely susceptible to vs the host plants, therefore potentially stopping this pest. The project utilized Molecular Dynamics (MD) simulations that mimic and predict the time evolution of a system of atoms, assuming a given potential energy function.

Results & Impact

The simulations have revealed the flexible regions of the protein involved in the activation process. Also confirmed is the determination that the intermediate-bound protein has more potential activation pathways than the apo protein. The conclusion is that the witchweed protein has lower free energy for activation as compared to Arabidopsis (the host). This might explain the higher SL affinity in witchweed germination.

Why Blue Waters

Understanding the slow conformational transitions in proteins requires hundreds of microsecond-long simulations. Blue Waters provides the state-of-the-art computer architecture needed to perform such studies. This project employs large-scale adaptive sampling protocols, which can be efficiently performed on Blue Waters' GPU and CPU framework. This current work would not be possible without Blue Waters.