Biophysical Society 61st Meeting, Feb. 11-15, 2017, New Orleans, Louisiana

How a Plant Resists Drought

Understanding of a key biochemical reaction could help future farmers protect plants from drought.

EMBARGOED for release until 2:45 p.m. Eastern Time on Tuesday, February 14, 2017

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WASHINGTON, D.C., February 14, 2017 -- Climate change will bring worsening droughts that threaten crops. One potential way to protect crops is by spraying them with a compound that induces the plants to become more drought resistant. Now, by identifying the key molecular mechanism that enables a plant to minimize water loss, researchers may be one step closer to that goal.

Faced with dry conditions, plants can mount a natural defense. They produce a hormone, called abscisic acid, or ABA, that binds to a protein, called a PYL receptor, triggering a chain of reactions that eventually closes the plant's pores on its leaves. "There is no or little water loss from the plants," explained Saurabh Shukla, a graduate student at the University of Illinois. "They conserve water resources and they survive for longer periods of time."

The key is the ABA hormone. Because of its moderate stability and molecular complexity, ABA can't be directly sprayed in fields. But, Shukla said, "If we can understand how the hormone works, we can design some molecule that can be sprayed and does the same job for us." If researchers can find a molecule that not only works the same way as the ABA hormone, but also is cheap, stable and environmentally friendly, then farmers can use it to make their crops become drought-resistant.

But the details for how ABA works have been elusive. Experimental techniques such as X-ray diffraction can take snapshots of the hormone before and after binding to the PYL receptor, but they can't catch the two in the act. So Shukla and his colleagues turned to supercomputers.

Using molecular dynamic simulations, the researchers have, for the first time, revealed the molecular details for how ABA binds with the PYL receptor. The simulations show, frame by frame, how and where the hormone binds with the protein and causes it to change shape, which allows it to activate the next protein in the sequence that eventually enables the plant to close its pores.

"You know exactly what is happening at the microscopic scale," Shukla said. "It's like a movie."

And the movie ends the way it should. The final frames of the hormone bound with the receptor precisely match the X-ray diffraction predicted crystal structures, confirming the accuracy of the simulations. The team will present its work during the 61st Meeting of the Biophysical Society held Feb. 11-15, 2017 in New Orleans.

The researchers simulated only two specific types of PYL receptors, found in a small, flowering plant called *A. thaliana*. Still, Shukla said, their results are widely applicable because the structure of PYL receptors is very similar across all species. For PYL receptors whose crystal structures are known, their binding pocket -- the part of the protein that binds to ABA -- is the same. The structure surrounding the pocket is also similar. Such similarities mean the same binding mechanism probably takes place in all plants.

While researchers may still want to confirm this mechanism in other plants, such as rice -- whose PYL receptor structure is known -- the hunt for an ABA mimic can now begin, Shukla said. Researchers will have to conduct rigorous computational and genetic studies to identify such a compound. The goal is to find a compound that can work on all species without resorting to genetic engineering. But it will likely be at least a decade before any product will be on the market, Shukla said.

Session 184.02 - Posters: Protein Small Molecule Interactions, 1721-Pos/B32, "Machine learning guided ligand-protein simulation approach elucidates the binding mechanism of abscisic acid," is authored by Saurabh Shukla, Moeen Meigooni, Chuankai Zhao and Diwakar Shukla. It will be at 1:45-3:45 p.m. Central Time on Tuesday, Feb 14, 2017 in Hall B-2 & C of the Ernest N. Morial Convention Center.

ABSTRACT: http://www.abstractsonline.com/pp8/#!/4279/presentation/2879

MORE MEETING INFORMATION

ABOUT THE MEETING

Each year, the Biophysical Society Annual Meeting brings together more than 6,000 researchers working in the multidisciplinary fields representing biophysics. With more than 3,600 poster presentations, over 200 exhibits, and more than 20 symposia, the BPS Annual Meeting is the largest meeting of biophysicists in the world. Despite its size, the meeting retains its small-meeting flavor through its subgroup symposia, platform sessions, social activities and committee programs. The 61st Annual Meeting will be held at Ernest N. Morial Convention Center in New Orleans, Louisiana.

PRESS REGISTRATION

The Biophysical Society invites professional journalists, freelance science writers and public information officers to attend its Annual Meeting free of charge. For press registration, contact Ellen Weiss at EWeiss@biophysics.org or the Media Line at the American Institute of Physics at media@aip.org or 301-209-3090.

NEWS RELEASES

Embargoed press releases describing in detail some of the breakthroughs to be discussed at the meeting are available on Newswise and Alpha Galileo or by contacting the Media Line at the American Institute of Physics at media@aip.org or 301-209-3090.

QUICK LINKS

Main Meeting Page: http://www.biophysics.org/2017meeting/Home/tabid/6672/Default.aspx
Symposia:
http://www.biophysics.org/2017meeting/Program/ScientificSessions/Symposia/tabid/6756/Default.aspx
Desktop planner: http://www.abstractsonline.com/pp8/#!/4279

ABOUT THE SOCIETY

The Biophysical Society, founded in 1958, is a professional, scientific Society established to encourage development and dissemination of knowledge in biophysics. The Society promotes growth in this expanding field through its annual meeting, monthly journal, and committee and outreach activities. Its 9,000 members are located throughout the U.S. and the world, where they teach and conduct research in colleges, universities, laboratories, government agencies, and industry. For more information on the Society, or the 2017 Annual Meeting, visit http://www.biophysics.org.

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