

Scientists solve structure of a mysterious protein found in cyanobacteria

EMSL's suite of NMR spectrometers now used to hunt for the protein's biological function

Scientists from the Pacific Northwest National Laboratory and Brookhaven National Laboratory have determined the crystal structure for the 78-residue protein *cce_0567* from the cyanobacteria *Cyanothece sp. PCC 51142*. Studies suggest that the protein may play a role in nitrogen fixation and/or the circadian control of nitrogen fixation. Nitrogen fixation is the rate-limiting step in the growth of cyanobacteria. Understanding the proteins involved in nitrogen fixation could help unlock the mysteries of how to efficiently turn this ubiquitous algae into a carbon-neutral fuel.

Using state-of-the-art resources at the Department of Energy's EMSL, the nuclear magnetic resonance chemical shift assignments for *cce_0567* were made using EMSL's 500-, 600-, 750-, and 800-MHz NMR spectrometers. The ^1H - ^{15}N HSQC spectrum is a "fingerprint" for the protein's conformation.

The assignment of the ^1H - ^{15}N HSQC spectrum is an important step in probing the biological function of *cce_0567*. Perturbations to these chemical shifts occur when other molecules are added to the solution. The perturbations are indicative of substrate binding. Following such chemical shifts allows researchers to identify protein-substrate interactions and then map them on to specific locations on the protein's surface using the structure determined by crystallographic methods.

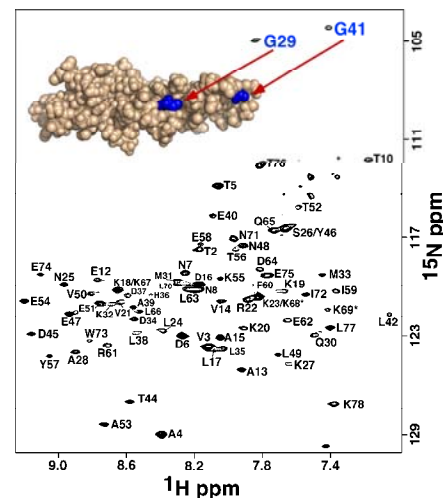
Scientific impact: Understanding the structure of *cce_0567* and other cyanobacteria proteins paves the way for further scientific inquiry, including biochemical experiments, into ubiquitous blue-green algae. This research is another example of EMSL's efforts to uncover biological functions from molecular and chemical data.

Social impact: This research is part of a broader endeavor to harness bacteria to efficiently produce hydrogen, a potential clean-burning alternative fuel.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

Citation: Buchko GW, and HJ Sofia. 2008. "Backbone ^1H , ^{13}C , and ^{15}N NMR Assignments for the *Cyanothece 51142* Protein *cce_0567*: A Protein Associated with Nitrogen Fixation in the DUF683 Family." *Biomolecular NMR Assignments* 2(1):25-28.

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The assigned ^1H - ^{15}N HSQC spectrum for *cce_0567* with the crystal structure of the protein (3CSX) is shown near the top. Understanding the function of this protein may help scientists use blue-green algae for producing energy and sequestering carbon.