First NMR Signal of a Copper Site in Azurin Obtained

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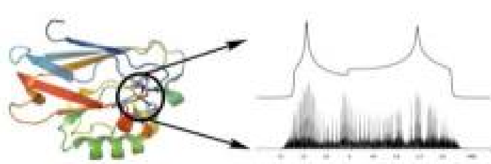

On the right is the reconstruction of the solid-state NMR lineshape of copper (I) in azurin, shown in the structure at left, with its corresponding simulation.

(PhysOrg.com) -- Metalloproteins, such as the copper-containing azurin, play a major role in catalyzing electron transfer in cellular reactions. Understanding how their structure relates to function can give rise to advances in biotechnology and medicine. To accurately characterize the nature of the bonding -- covalent vs. ionic vs. hybrid -- around azurin's metal center, a team of researchers from Pacific Northwest National Laboratory and the University of Nebraska at Lincoln obtained the first high-field nuclear magnetic resonance (NMR) signal of a copper site in a copper protein.

Using NMR to study copper-containing proteins is a technique previously ignored because copper's inherent NMR properties give rise to broad NMR lines that are difficult to detect. In this study, the researchers integrated 800-MHz NMR spectroscopy and the Chinook supercomputer, both housed at the Department of Energy's EMSL.

This combination of tools turned the properties of the copper ion into an advantage; the researchers gained an "exquisitely sensitive measure of the electron density around the nuclear site," revealing previously unknown details about the electronic structure and environment of azurin's copper center. Their results were published in the Journal of the American Chemical Society.

Developing the novel ability to use high-field NMR to characterize the electronic structure of metalloproteins containing metals such as the copper isotope ^{65}Cu provides a powerful new tool that advances the field of bioinorganic chemistry—the study of how living systems use nonliving elements to perform fundamental biological functions. The team's strategy broadens the arena of NMR samples and is applicable to any diamagnetic metalloprotein—those proteins that create a magnetic field in opposition to an externally applied magnetic field.

The advent of high magnetic fields and theoretical supercomputing capabilities allows opportunities for scientists to perform previously impossible experiments and validate the results with powerful calculations and models. The team used these advances to fill gaps in azurin's data pool. Data were then reproduced using theoretical calculations, confirming details of the electronic structure. In addition to yielding new information on azurin, this study helps demonstrate that high-field, low-temperature NMR, when combined with electronic structure theory, provides a detailed and precise probe of metal nuclei in metalloproteins.

Understanding metalloproteins at the molecular level provides researchers with the knowledge necessary to alter, support, inhibit, or direct these proteins' functions in support of human health, energy production, and environmental remediation.

More information: Lipton AS, RW Heck, WA de Jong, AR Gao, X

Wu, A Roehrich, GS Harbison, and PD Ellis. 2009. "Low Temperature 65Cu NMR Spectroscopy of the Cu+ Site in Azurin." *Journal of the American Chemical Society* 131(39):13992 - 13999. doi:10.1021/ja901308v

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