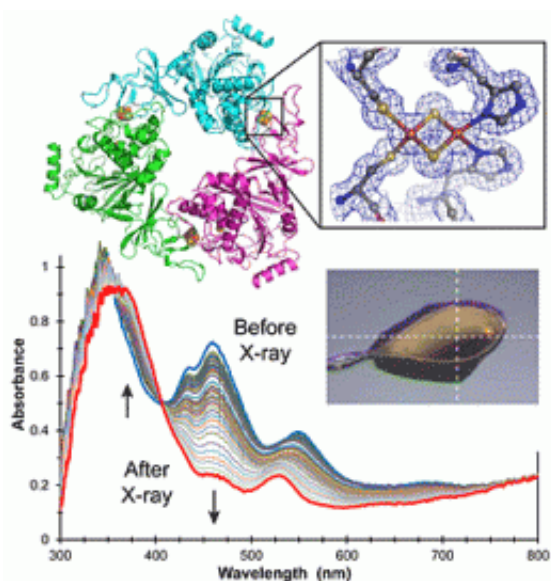


Combining crystallography and visible spectroscopy to understand enzymes

June 29 2012



The research team focused on the stachydrine demethylase from *Sinorhizobium meliloti* 1021. The applications of electronic absorption and resonance Raman spectroscopies, in conjunction with x-ray diffraction, all derive from the same $\sim 25 \mu\text{m}^2$ region of the crystal (intersection of the cross hairs). The x-ray beam alters the visible spectrum of the crystal with each exposure required to determine the crystal structure of the trimeric enzyme and the Fe-S cluster within each subunit.

Structure and function are intimately linked, but do not necessarily predict the other. For example, x-ray crystallography provides 3D atomic structural information about biological macromolecules but does not

define important details about metal ions.

However, the oxidation state of metal ions at an enzyme's active site has a critical effect on enzyme behavior. Thus, an enzyme's catalytic function derives from the electronic structure of those atoms influencing or directly participating in the reaction, information not revealed by the scattering methods used in x-ray [crystallography](#).

A new technology has been developed that simultaneously carries out crystallography and UV-visible and Raman spectroscopy to determine the atomic structure of the entire protein, and electronic and vibrational structures of the [metal ions](#) or cofactors within. The combined instrumentation has been used to study the process of demethylation of an organic substrate molecule by an enzyme whose active site includes an iron-sulfur cluster.

The researchers used spectroscopy to follow the change in the [oxidation state](#) of the cluster during the crystallography data collection, and to formulate a mechanism for the overall enzyme reaction mechanism. The results provide insight into a new demethylation reaction, an important class of phenomena that control cellular behavior.

The technology was developed by scientists at the Protein Crystallography Research Resource at the National Synchrotron Light Source at Brookhaven National Laboratory. The new study was led by Allen M. Orville of Brookhaven and Pinghua Liu and Karen N. Allen of Boston University, and is published in the *Journal of the American Chemical Society*.

Provided by Brookhaven National Laboratory

Citation: Combining crystallography and visible spectroscopy to understand enzymes (2012, June

29) retrieved 8 April 2024 from

<https://phys.org/news/2012-06-combining-crystallography-visible-spectroscopy-enzymes.html>

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