New process improves catalytic rate of enzymes by 3,000 percent

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Light of specific wavelengths can be used to boost an enzyme's function by as much as 30 fold, potentially establishing a path to less expensive biofuels, detergents and a host of other products.

In a paper published in *The* Journal of Physical Chemistry *Letters,* a team led by Pratul Agarwal of the Department of Energy's Oak Ridge National Laboratory described a process that aims to improve upon nature – and it happens in the blink of an eye.

"When light enters the eye and hits the pigment known as rhodopsin, it causes a complex chemical reaction to occur, including a conformational change," Agarwal said. "This change is detected by the associated protein and through a rather involved chain of reactions is converted into an electrical signal for the brain."

With this as a model, Agarwal's team theorized that it should be possible to improve the catalytic efficiency of enzyme reactions by attaching chemical elements on the surface of an enzyme and manipulating them with the use of tuned light.

The researchers introduced a light-activated molecular switch across two regions of the enzyme Candida antarctica lipase B, or CALB – which breaks down fat molecules -- identified through modeling performed on DOE's Jaguar supercomputer.

"Using this approach, our preliminary work with CALB suggested that such a technique of introducing a compound that undergoes a light-inducible conformational change onto the surface of the protein could be used to manipulate enzyme reaction," Agarwal said.

While the researchers obtained final laboratory results at industry partner AthenaES, computational modeling allowed Agarwal to test thousands of combinations of enzyme sites, modification chemistry, different wavelengths of light, different temperatures and photo-activated switches. Simulations performed on Jaguar also allowed researchers to better understand how the enzyme's internal motions control the catalytic activity.

"This modeling was very important as it helped us identify regions of the enzyme that were modified by interactions with chemicals," said Agarwal, a member of ORNL's Computer Science and Mathematics Division. "Ultimately, the modeling helped us understand how the mechanical energy from the surface can eventually be transferred to the active site where it is used to conduct the chemical reaction."

Agarwal noted that enzymes are present in every organism and are widely used in industry as catalysts in the production of biofuels and countless other every day products. Researchers believe this finding could have immense potential for improving enzyme efficiency, especially as it relates to biofuels.

More information: "Engineering a Hyper-catalytic Enzyme by Photoactivated Conformation Modulation," dx.doi.org/10.1021/jz201675m

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