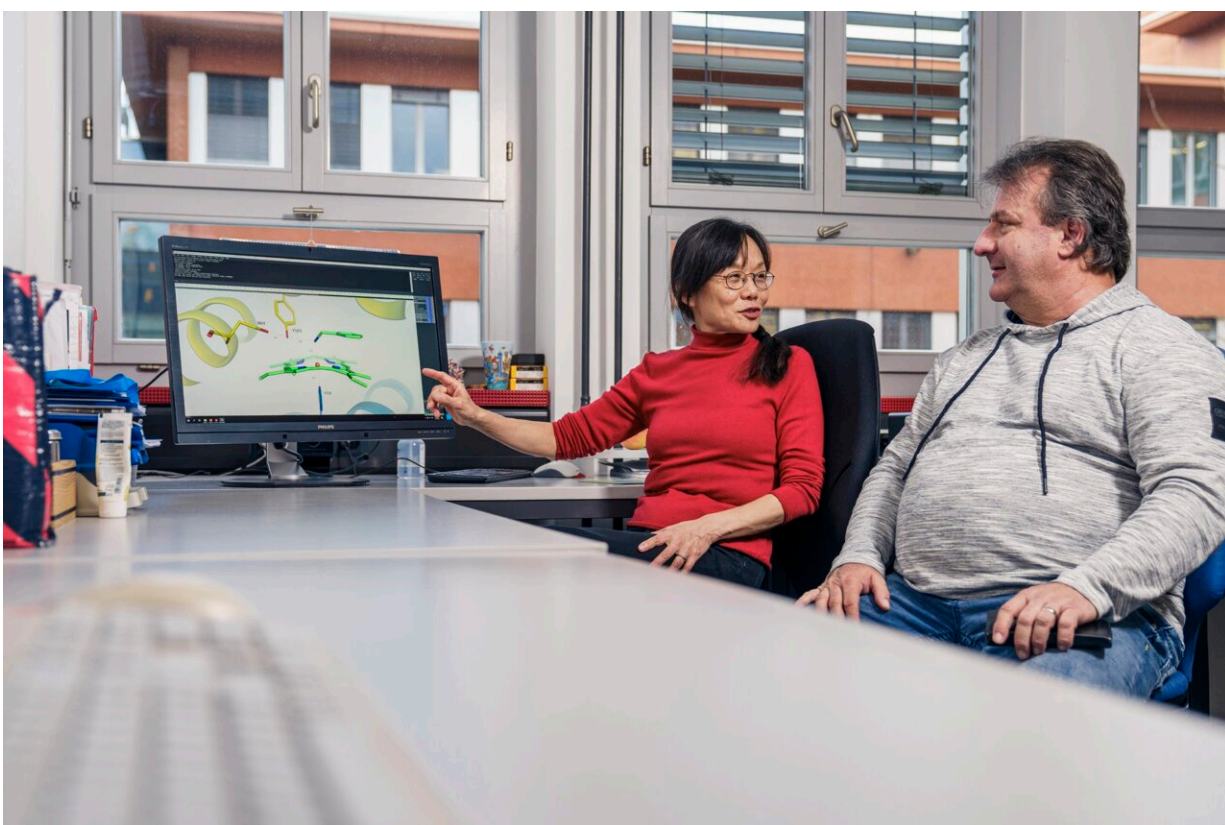


# Researchers precisely characterize styrene oxide isomerase, which could help yield 'green' chemicals and drug precursors

May 14 2024, by Brigitte Osterath

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Xiaodan Li and Richard Kammerer have characterized an enzyme for the first time that could become an important tool for the circular economy. The monitor shows a schematic representation of the key part of the active center of this enzyme. Credit: Paul Scherrer Institute/Markus Fischer

Researchers at the Paul Scherrer Institute PSI have—for the first time—precisely characterized the enzyme styrene oxide isomerase, which can be used to produce valuable chemicals and drug precursors in an environmentally friendly manner. The study appears in the journal *Nature Chemistry*.

Enzymes are powerful biomolecules that can be used to produce many substances at ambient conditions. They enable "green" chemistry, which reduces [environmental pollution](#) resulting from processes used in synthetic chemistry. One such tool from nature has now been characterized in detail by PSI researchers: the [enzyme styrene](#) oxide isomerase. It is the biological version of the Meinwald reaction, an important chemical reaction in [organic chemistry](#).

"The enzyme, discovered decades ago, is made by bacteria," says Richard Kammerer of PSI's Biomolecular Research Laboratory. His colleague Xiaodan Li adds, "But because the way it functions was not known, its practical application has been limited up to now." The two researchers and their team have elucidated the structure of the enzyme as well as the way it works.

## Simple mechanism for a complicated reaction

Microorganisms possess specific enzymes with which they can, for example, break down harmful substances and use them as nutrients. Styrene oxide isomerase is one of these. Together with two other enzymes, it enables certain environmental bacteria to grow on the hydrocarbon styrene.

The styrene oxide isomerase catalyzes a very specific step in the reaction: It splits a three-membered ring in the styrene oxide consisting of one oxygen and two carbon atoms, a so-called epoxide. Thereby the enzyme is highly specific and creates only one product. It is also capable

of converting a number of additional substances, producing important precursors for medical applications.

One particular advantage has to do with the fact that in many chemical reactions, both an image and a mirror image of a chemical compound are formed, which may have completely different biological effects. But this enzyme specifically creates only one of the two products. In chemistry this property is called stereospecificity—it is particularly important for the generation of precursor molecules for drugs.

"The enzyme is an impressive example of how nature makes [chemical reactions](#) possible in a simple and ingenious way," Li says.

In the course of their investigations, which they conducted in part at the Swiss Light Source SLS, the PSI researchers discovered the enzyme's secret: an iron-containing group in its interior, similar to the iron-containing pigment in our red blood cells. This heme group binds the epoxide ring, and that's how it makes the reaction so simple and efficient.

Other parts of the investigations were carried out by the group of Volodymyr Korkhov, also from the PSI Laboratory for Biomolecular Research and Associate Professor in the Department of Biology at ETH Zurich, using cryo-electron microscopy.

Li and Kammerer feel certain that the enzyme will prove extremely useful in the chemical and pharmaceutical industries. "It is so far the only bacterial enzyme known to catalyze the Meinwald reaction," Kammerer emphasizes. With the enzyme's help, industry could produce precursors for drugs and important chemicals under energy-saving and environmentally friendly conditions.

Li adds, "The enzyme could potentially be altered so that it can produce

a great many new substances."

In addition, the enzyme is very stable and thus is suitable for large-scale industrial applications.

"It will certainly become a new, important tool for the [circular economy](#) and [green chemistry](#)," the PSI researchers are convinced.

**More information:** Structural basis of the Meinwald rearrangement catalyzed by styrene oxide isomerase, *Nature Chemistry* (2024). [DOI: 10.1038/s41557-024-01523-y](#)

Provided by Paul Scherrer Institute

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