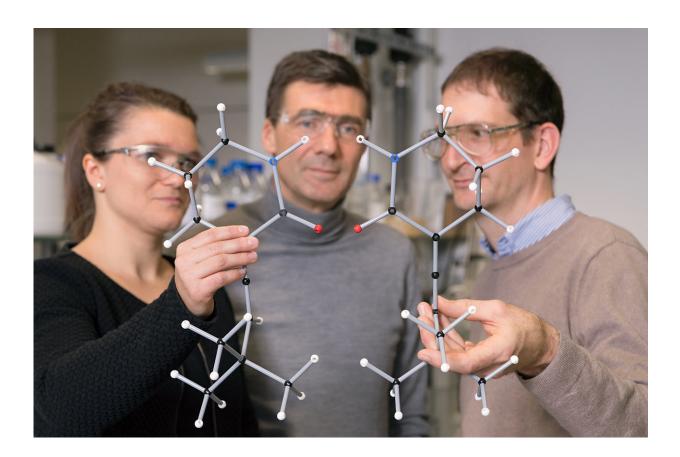


Photochemical deracemization of chiral compounds achieved

December 19 2018



Enantiomeric molecules resemble each other like right and left hands. While both variants normally arise in chemical reactions, frequently only one of them is effectual in biology and medicine. Hitherto, completely converting this mixture into the desired enantiomer was deemed impossible. Deploying a photochemical method, a team from the Technical University of Munich (TUM) has now achieved this feat. The image shows first authors Alena Hoelzl-Hobmeier and Andreas Bauer as well as Prof. Thorsten Bach (center) with the two enantiomers of one of the allenes studied. Credit: Uli Benz / TUM



Enantiomeric molecules resemble each other like right and left hands. Both variants normally arise in chemical reactions. But frequently, only one of the two forms is effective in biology and medicine. Completely converting this mixture into the desired enantiomer has been deemed impossible. However, via a photochemical method, a team from the Technical University of Munich (TUM) has now achieved this feat.

Producing <u>active ingredients</u> with very specific properties—antibacterial characteristics, for example—is not always so easy. The reason: Many of these <u>organic compounds</u> are chiral. They have two mirror-image forms, so-called enantiomers.

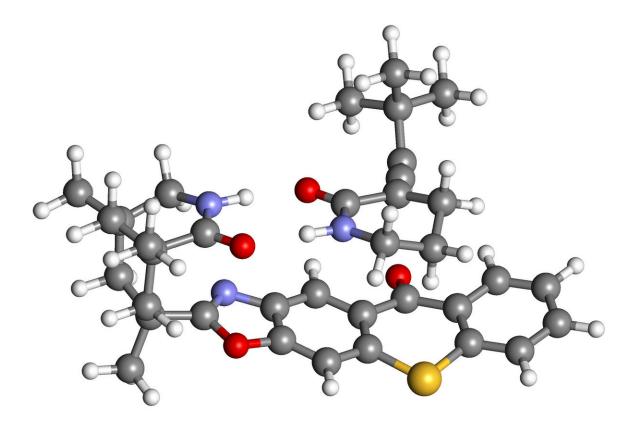
This small difference can be consequential because the two enantiomers can have different properties. While one has a healing effect, the other might be ineffective or even cause unwanted side effects.

Saving time, energy and resources

"For a long time, researchers around the world have been seeking ways to selectively synthesize only the desired <u>enantiomer</u> from a racemate," explains Prof. Thorsten Bach, Chair of Organic Chemistry at the Technical University of Munich. However, this has been very difficult, since <u>chemical reactions</u> usually produce both molecule variants.

Together with his team, the researcher has now developed a method with which the desired enantiomer can be obtained from a racemate, the mixture of both enantiomers, in high concentrations of up to 97 percent.





The allenic group of the unwanted enantiomer is much closer to the thioxanthone sensitizer and is therefore converted to the desired form. Credit: S. M. Huber and A. Bauer / TUM

Rather than painstakingly extracting the unwanted mirror-molecules from the mixture, the researchers use a photochemical reaction to transform them into the desired end product. "That saves time, energy and resources because all the <u>molecules</u> are used and you do not need to throw away half of them," explains Bach.

A catalyst for the "right" compounds



The secret of the transformation is a special photochemical catalyst. Originally, the thioxanthone sensitizer was developed for [2 + 2] photocycloadditions. The dye is itself chiral and therefore specifically converts only one of the enantiomers to the other. In the span of a few minutes, the equilibrium shifts in favor of the desired molecule. The undesirable mirror images disappear.

The chemists have successfully tested their new method on various molecular mixtures from the allene structural class. "We could thus demonstrate that selective and efficient catalysis to prepare enantiopure compounds from racemates is fundamentally possible," said Bach.

More information: Alena Hölzl-Hobmeier et al, Catalytic deracemization of chiral allenes by sensitized excitation with visible light, *Nature* (2018). DOI: 10.1038/s41586-018-0755-1

Provided by Technical University Munich

Citation: Photochemical deracemization of chiral compounds achieved (2018, December 19) retrieved 20 April 2024 from <u>https://phys.org/news/2018-12-photochemical-deracemization-chiral-compounds.html</u>

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