Chemists successfully use light to regulate structural conversion of chiral molecules

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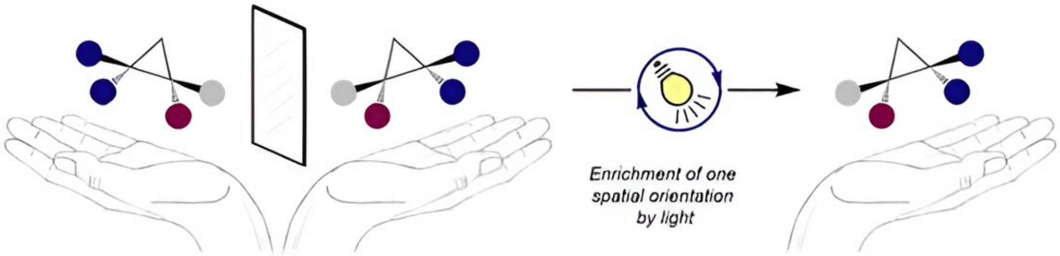

Just like our hands, certain organic molecules relate to each other like an image and its reflection—a phenomenon that chemists call "chirality" or "handedness." Credit: AG Gilmour

A team of chemists from the University of Münster have developed a novel concept in which a mixture of molecules that behave like mirror images is converted to a single form using light as external energy source. The conversion has applications in the preparation of drugs.

Just like our hands, certain organic molecules relate to each other like an image and its reflection—a phenomenon that chemists call "chirality," or "handedness." The two mirror images of the same molecule, namely both enantiomers, often possess different biological properties.

For drug discovery, for example, many times only one of the structures is relevant. However, chemical synthesis methods often create a 1:1 mixture of both forms. Therefore, the selective conversion of these mixtures into one selected form is of great importance.

A team of researchers from the Institute of Organic Chemistry and from the Center for Multiscale Theory and Computation at the University of Münster led by Prof. Ryan Gilmour and Prof. Johannes Neugebauer developed a novel concept in which this conversion is enabled by light as an external energy source. The study is now published in the journal *Nature*.

The researchers apply an aluminum complex that is activated by light as a catalyst to selectively convert a mixture of molecules that behave like mirror images to a single form. The reaction process was investigated experimentally and computationally. The detailed computer-based analyses contributed significantly to the understanding of the underlying processes.

The new paradigm impresses with its operational simplicity and broad applicability, as the aluminum complex used is a common catalyst for chemical reactions driven by heat. Translation to light-mediated processes is now envisaged to enable a plethora of new reactivities with great spatial control.

Achieving spatial control in light-mediated reactions is one of the main challenges in contemporary organic chemistry. To this end, usually two distinct catalysts are employed in one reaction: a photocatalyst, that initiates the reactivity, operates in concert with a second catalyst that controls the spatial arrangement of the molecules. Contrarily, the successful integration of both functions in a single catalyst structure was so far only achieved by incorporation of tailored recognition motifs in the catalyst and substrate structures.

In this work, the groups present a catalyst that regulates reactivity and selectivity simultaneously. It binds to simple ketones, a functional group that is prevalent in organic molecules, circumventing the need for tailored components. Furthermore, the catalyst is based on earth-abundant aluminum, which is cheaper that the transition metals that are commonly found in photocatalysts.

More information: Carina Onneken et al, Light-enabled deracemization of cyclopropanes by Al-salen photocatalysis, *Nature* (2023). DOI: 10.1038/s41586-023-06407-8

Provided by University of Münster

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