

Synthetic molecules emulate enzyme behavior for the first time

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When chemists want to produce a lot of a substance -- such as a newly designed drug -- they often turn to catalysts, molecules that speed chemical reactions. Many jobs require highly specialized catalysts, and finding one in just the right shape to connect with certain molecules can be difficult. Natural catalysts, such as enzymes in the human body that help us digest food, get around this problem by shape-shifting to suit the task at hand.

Chemists have made little progress in getting synthetic molecules to mimic this shape shifting behavior -- until now.

Ohio State University chemists have created a synthetic catalyst that can fold its molecular structure into a specific shape for a specific job, similar to natural catalysts.

In laboratory tests, researchers were able to cause a synthetic catalyst -- an enzyme-like molecule that enables hydrogenation, a reaction used to transform fats in the food industry -- to fold itself into a specific shape, or into its mirror image.

The study appears in the June 25 issue of the *Journal of the American Chemical Society*.

Being able to quickly produce a catalyst of a particular shape would be a boon for the pharmaceutical and chemical industries, said Jonathan Parquette, professor of chemistry at Ohio State.

The nature of the fold in a molecule determines its shape and function, he explained. Natural catalysts reconfigure themselves over and over again in response to different chemical cues -- as enzymes do in the body, for example.

When scientists need a catalyst of a particular shape or function, they synthesize it through a process that involves a lot of trial and error.

"It's not uncommon to have to synthesize dozens of different catalysts before you get the shape you're looking for," Parquette said. "Probably the most important contribution this research makes is that it might give scientists a quick and easy way to get the catalyst that they want."

The catalyst in this study is just a prototype for all the other molecules that the chemists hope to make, said co-author and professor of chemistry T.V. RajanBabu.

"Eventually, we want to make catalysts for many other reactions using the fundamental principles we unearthed here," RajanBabu said.

For this study, Parquette, RajanBabu, and postdoctoral researcher Jianfeng Yu synthesized batches of a hydrogenation catalyst in the lab and coaxed the molecules to change shape.

The technique that the chemists developed amounts to nudging certain atoms on the periphery of the catalyst molecule in just the right way to initiate a change in shape. The change propagates to a key chemical bond in the middle of the molecule. That bond swings like a hinge, to initiate a twist in one particular direction that spreads throughout the rest of the molecule.

Parquette offered a concrete analogy for the effect.

"Think of the Radio City Rockettes dance line. The first Rockette kicks her leg in one direction, and the rest of them kick the same leg in the same direction -- all the way down the line. A change in shape that starts at one end of a molecule will propagate smoothly all the way to the other end."

In tests, the chemists caused the catalysts to twist one way or the other, either to form one chemical product or its mirror image. They confirmed the shape of the molecules at each step using techniques such as nuclear magnetic resonance spectroscopy.

That's what the Ohio State chemists find most exciting: the molecule does not maintain only one shape. Depending on its surroundings -- the chemical "nudges" that it receives on the outside -- it will adjust.

"For many chemical reactions to work, molecules must be able to fit a catalyst like a hand fits a glove," RajanBabu said. "Our synthetic molecules are special because they're flexible. It doesn't matter if the hand is a small hand or a big hand, the 'glove' will change its shape to fit it, as long as there is even a slight chemical preference for one of the hands. The 'flexible glove' will find a way to make a better fit, and so it will assist in specifically making one of the mirror image forms."

Despite decades of research, scientists aren't sure exactly how this kind of propagation works. It may have something to do with the polarity of different parts of the molecule, or the chemical environment around the edges of the molecule.

But Parquette says the new study demonstrates that propagation can be used to make synthetic catalysts change shape quickly and efficiently -- an idea that wasn't apparent before. The use of adaptable synthetic molecules may even speed the discovery of new catalysts.

Source: Ohio State University

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