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UI researchers sculpt molecules

By GREG KLINE
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In the process of lost-wax metal casting, which sculptors have used for thousands of years, the sculpture is first rendered in wax and then covered in plaster.

The plaster gets heated in a kiln, and the wax melts out through a small hole, leaving a mold into which molten metal like bronze can be poured to cool in the shape of the wax sculpture.

University of Illinois chemistry professors Steve Zimmerman and Ken Suslick, who has done some bronze casting as a hobby, are doing something similar to create custom molecules that might be used for purposes ranging from medical diagnostics to detecting explosives in luggage.

"You can think about what Steve and I do as molecular sculpting," Suslick said recently.

The UI researchers are "sculpting" artificial molecules to perform a natural molecular recognition process chemists have been working to understand and mimic for decades.

In nature, molecules such as antibodies routinely recognize and attach to specific types of foreign molecules, called antigens, while ignoring the vast array of other substances in their orbit.

This molecular binding is a basic process of life, one that signals the body to gear up its infection-fighting defenses, for example, said Zimmerman and Suslick. Likewise, when the binding process goes wrong it can lead to problems such as diabetes, from the body's mistaken elimination of insulin-producing cells in the pancreas.

Almost all medical diagnostics rely on antibody-antigen binding, Zimmerman said. In blood tests, for instance, antibodies that bind with certain antigens are introduced into the sample. The binding process generates feedback that testers use to tell if a substance is present in the blood.

But the biologically created antibodies used in medical tests – they're often grown in lab animals like rabbits – have disadvantages, Zimmerman said. They are relatively expensive to produce and have a short shelf life.

Binding also could be used to detect molecules given off



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by chemical weapons, hidden explosives, or pollutants in water.

In one scenario, soldiers might wear tags designed to change colors in the presence of certain chemicals, Zimmerman said.

In part, that's why the UI research has drawn funding from both the Army and the National Institutes of Health.

But the trick is to be able to produce custom molecules that bind only to the substances being sought.

In the technique developed by Zimmerman, Suslick and colleagues, the researchers start with an antigen-type molecule to act as a template for their molecular mold, in the same way the wax sculpture functions in the metal-casting example.

They then use a larger molecule called a "dendrimer," which looks something like a tree sprouting many branches. Unlike a tree, dendrimers are flexible, and their arms can be wrapped around the molecular template to encase it.

After wrapping the template, the researchers fuse the dendrimer branches together using a chemical catalyst and chemically remove the template molecule inside.

The result is an imprint of the template on the inside of the dendrimer molecule, which now acts as an artificial antibody that will bind to any molecules with the same structure as the template's and to nothing else.

The UI researchers described the technique in this week's edition of the journal Nature. In addition to Zimmerman and Suslick, Ilya Zharov, a post-doctoral researcher at the UI's Beckman Institute, and former UI graduate students Neal Rakow and Michael Wendland worked on the study.

Zimmerman said the study proves the concept of being able to imprint a single molecule with another single molecule, the first time that's been done.

The next phase is to develop ways to do it more quickly and inexpensively in order to make the technique feasible for practical applications. The UI researchers also are working on better methods to capture and interpret the feedback from binding by the custom molecules.

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