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Chemists develop new 'light switch' chloride binder

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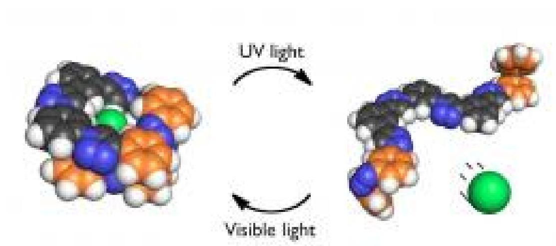

When azobenzene units (blue) at the ends of the receptor are struck with UV light, the receptor unfolds the helix and releases the chloride ion (green). Image by Amar Flood

Chemists at Indiana University Bloomington have designed a molecule that binds chloride ions -- but can be conveniently compelled to release the ions in the presence of ultraviolet light.

Reporting online in the Journal of the American Chemical Society today, IU Bloomington chemist Amar Flood and Ph.D. student Yuran Hua explain how they designed the molecule, how it works and, just as importantly, how they know it works.

"One of the things we like most about this system is that the mechanism is predictable -- and it functions in the way we propose," said Flood, who led the project.

Chloride is a relatively common element on Earth, ubiquitous in seawater and in the bodies of living organisms.

"We have two main goals with this research," Flood said. "The first is to design an effective and flexible system for the removal of toxic, negatively charged ions from the environment or industrial waste. The second goal is to develop scientific and even medical applications. If a molecule similar to ours could be made water soluble and non-toxic, it could, say, benefit people with cystic fibrosis, who have a problem with chloride ions accumulating outside of certain cells."

Many organic molecules exist that can bind positively charged ions, or cations, and this has much to do with the fact that it is easy to synthesize organic molecules with negatively charged parts. Synthesizing organic molecules that bind negatively charged ions, or anions, like chloride, presents special challenges.

The binding molecule or "foldamer" Flood and Hua designed is both a folding molecule and a (small) polymer, meaning the foldamer's constituent parts can be synthesized with relative ease. Under visible light of 436 nanometers (nm), the foldamer prefers a tight spiral structure that allows specially configured residues to interact with each other, which improves stability, and creates an attractive pocket for chloride. In the presence of ultraviolet light (365 nm), the foldamer absorbs energy and the tight spiral is destabilized, weakening the chloride binding pocket and freeing chloride to re-enter the solution.

The "light switch" properties of the foldamer could make it an invaluable tool to biochemists and molecular biologists who seek to adjust the availability of chloride in their experiments by simply turning a UV light emitter on or off.

The foldamer is not quite ready for that, however. It can only be dissolved at present in organic (fatty) solutions, whereas living systems operate mostly in water-based solutions.

"That's the direction we're headed," Flood said. "It actually wouldn't be that difficult to modify the molecule so that it is water soluble. But first we need to make sure it does all the things we want it to do."

In their *JACS* paper, Flood said he and Hua wanted to bring sythentic chemistry together with modern diagnostic approaches to demonstrate the efficacy of their foldamer.

"A lot of the ideas in our paper have been floating around for some time," Flood said. "The idea of a foldamer that binds anions, the idea of a foldamer that you can isomerize with light, the idea of receptor that can bind anions ... But none of the prior work uses conductivity to show that the chloride concentrations actually go up and down as intended. What's new is that we've put all these things together. We think we have something here that allows us to raise our heads to the great research that's preceded us."

Flood and Hua used an electrical conductivity test to show that when voltage is applied to the solution containing chloride ions and the binding molecule, electricity flows more freely in the presence of UV light, when the binder is relaxed and chloride is disassociated from it. That was proof, Flood said, that the foldamer was working as intended.

"My training is in building molecular machines," Flood said. "I create machines that do what we want them to do -- and to show what's possible in chemical and biological laboratory science."

The binding molecule Flood and Hua describe is an improvement on a previous binder developed by Flood and then-postdoctoral fellow Yongjun Li that was also an oligomer of sorts but did not fold. This previous iteration of the chloride binder was closed and donut-shaped, using space restrictions and strategically placed atoms to yield a binding pocket with a special affinity for chloride.

Provided by Indiana University

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