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TODAY'S HEADLINES

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MOLECULAR IMPRINTING

BUILDING A BETTER BINDING SITE

Dendrimers built around template molecule offer shape selectivity

REBECCA RAWLS

Chemists at the University of Illinois, Urbana-Champaign, have a new twist on an old idea. For 50 years or more, chemists have been making polymers in the presence of a template in order to produce a cavity in the polymer that exactly matches the shape of the template. When the template is a single molecule, the resulting cavity can then be used to separate enantiomers, remove pollutants, and catalyze reactions.

But the approach has its problems. It's hard to completely remove the template, the imprinted polymer is insoluble, and the polymer contains many imprinted cavities, of which only some are really good matches for the template molecule.

To overcome these problems, chemistry professors Steven C. Zimmerman and Kenneth S. Suslick and their colleagues have made molecular imprints at the center of dendrimers [*Nature,* **418,** 399 (2002)].

The work represents a "merging of two areas of macromolecular chemistry: dendrimers and molecularly imprinted polymers," explains Andrew D. Hamilton, chemistry professor at Yale University, in a commentary accompanying publication of the work. The resulting family of easily prepared compounds shows "recognition properties that bear comparison to those of antibodies," Hamilton writes.

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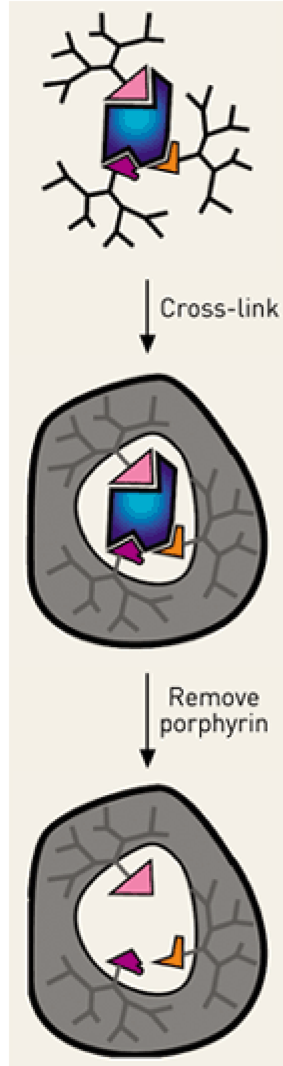
Dendrimers are large, roughly spherical macromolecules built from smaller precursors through repeated branching reactions around a single central molecule. The Illinois chemists construct their dendrimers around a central porphyrin ring. The ring is held at the center of the growing dendrimer by eight ester linkages that can later be cleaved to produce a porphyrin-sized cavity at the center of the dendrimer. The dendrimer is constructed so that its outer surface is covered with alkene groups, which can be cross-linked to one another using a Grubbs olefin metathesis catalyst. The result is a large, stable, but soluble macromolecule that contains a single binding site at its center.



IN A BIND **Dendrimer grown around target porphyrin (blue), when cross-linked, forms shape-specific cavity that selectively binds new porphryins.**

That single binding site is a key advantage over classic polymer imprinting, Zimmerman explains. "Our idea was, let's try and imprint a single binding site within a single polymer," he says. "We may not be any better than the polymer imprinting people at doing it, but at least we will have the opportunity to separate good binding sites from bad ones."

Cambridge University chemistry professor Jeremy K. M. Sanders calls the work "a very elegant approach to molecular recognition." Using alkene metathesis to cross-link the dendrimer into its final form is "a master stroke," Sanders says, because the reversible nature of this reaction means that the final product is the thermodynamically stable one.

Zimmerman characterizes the binding selectivity of the newly prepared dendrimers as "okay, but not great." While the researchers have established that the concept is workable, improving the binding is the next challenge. "I think we have our work cut out for us," Zimmerman says.

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