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‘SUPERBOWL’ MOLECULE TO HELP DRUG DELIVERY

A new molecule shaped like a miniature football stadium that promises many applications, including precision drug delivery, has been developed by chemists at The Australian National University.

The molecule is capable of capturing and releasing drugs and chemicals, and has the potential for removing environmental toxins, catalysing chemical reactions and allowing new chemical purification.

Developed by synthetic chemist Dr Michael Sherburn and colleagues at the Research School of Chemistry, it belongs to a class of artificial bowl shaped molecules first developed more than a decade ago to mimic naturally occurring enzymes in the body.

The superbowl molecule has a unique shape: a rigid hollow sphere with the top chopped off. It is made through a chemical synthesis that unites five concave surfaces: four sides and a base. The open top allows ‘guests’ (such as drug molecules) to pass in and out.

“This is a very hot area at the moment and there is lot of great research being carried out around the world, particularly with assemblies of small bowl-like molecules,” Dr Sherburn said. “Our contribution is exciting and different because no one has made single molecule containers like this before.”

Its molecular structure is enormous by chemistry standards, containing 268 carbon atoms, 320 hydrogen atoms and 52 oxygen atoms. Nevertheless, the superbowl structure is only a few nanometres wide, thousands of times smaller than the width of a single human hair.

The researchers have shown that the hollow interior of the superbowl molecule can hold ‘guest’ molecules of up to 100 atoms — substantially larger than existing molecular containers and importantly, is big enough to encapsulate most common medicinal agents.

“Our compound is a much larger version of the original bowl molecules, hence the name ‘superbowl’. The original bowl molecules bind only the smallest ‘guests’ — one molecule of ethanol, for example. Our molecule has much greater capacity and selectivity than its predecessors and shows more promise for wider applications.

“The design allows us to do lots of new things, like changing the size and shape of the hole at the top of the molecule, which makes it easier or more difficult for, say a particular drug molecule, to pass in and out. This is ideal if you’re interested in modifying the rate of release of a particular guest.

“We’re particularly excited by the possibility of carrying out chemical reactions inside superbowl. The ability of one superbowl host to hold five guest molecules in precise locations in 3D space at the same time shows great promise for catalysis,” Dr Sherburn said.

The research team — group leader Dr Sherburn, PhD student Elizabeth Barrett, crystallographer Dr Alison Edwards and PhD student Jacob Irwin from the University of Sydney — published their results in the 29 December edition of the Journal of the American Chemical Society.

An animation and images of the superbowl molecule are available from the ANU Media Office.

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