UNIVERSITY of LIMERICK
OLLSCOIL LUIMNIGH

Chiral Identification and Separation

The Problem

Identification and separation of enantiomers has been a scientific and technological challenge since the dawn of stereochemistry when Pasteur discovered spontaneous resolution in 1848. This is particularly the case in drug discovery and natural products chemistry, where only trace amounts of novel compounds are initially available upon discovery.

Our Solution

Researchers at the University of Limerick (Ireland) and Nankai University (China) have just made a major breakthrough in terms of enantiomer identification and purification by creating a novel porous metal-organic material (MOM) that exhibits the following features:

- **Design from first principles.** The new chiral MOM (CMOM-3S) combines tight but adaptable binding sites and is a modular structure. CMOM-3S is therefore proprietary and prototypal for a large family of related materials because each of its components can be interchanged in modular fashion.
- **Extraordinary properties.** CMOM-3S synergistically combines two features that have not previously been brought together in the same material: the ability to serve a "crystalline sponge" for structural identification of trace amounts of compound (μg); tight binding chiral pores that exhibit enantioselectivity.
- **Immediate practical utility.** That CMOM-3S can serve as a crystalline sponge means that it can be used to identify molecular structure and chirality with precision on a lab x-ray diffractometer. The ability to function as an enantioselective crystalline sponge coupled with strong thermal and hydrolytic stability enables CMOM-3S to also serve as a chiral stationary phase for chromatographic separation of enantiomers.

Commercial Opportunity

HOW DOES CMOM-3S WORK? CMOM-3S enables the introduction of a new analytical method to identify and purify trace amounts of novel or existing chiral or achiral compounds in a manner that was hitherto beyond reach. This is accomplished in a parallel 2-step process:

CMOM-3S as chiral stationary phase (step 1): CMOM-3S is loaded onto the surface of a capillary column through a dynamic coating process. Even this crude column exhibits effective chiral separations of racemic compounds in a manner that is more efficient and more general than leading commercial chiral columns. Important features of CMOM-3S are the following:

- **Low cost:** The starting materials for the manufacture of CMOM-3S are commercially available and inexpensive. CMOM-3S is also facile to prepare through a one-step process that enables particle size to be controlled from nm to mm.
- **Durability:** The CMOM-3S coated column was evaluated after 10 months and 1000 injections with no loss of performance.
- **Versatility:** The efficiency of the CMOM-3S column is superior to that of commercial columns (figure below).

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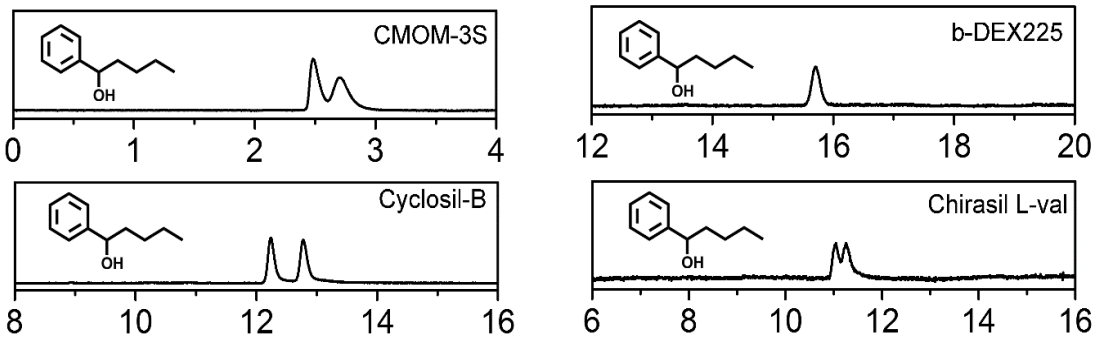
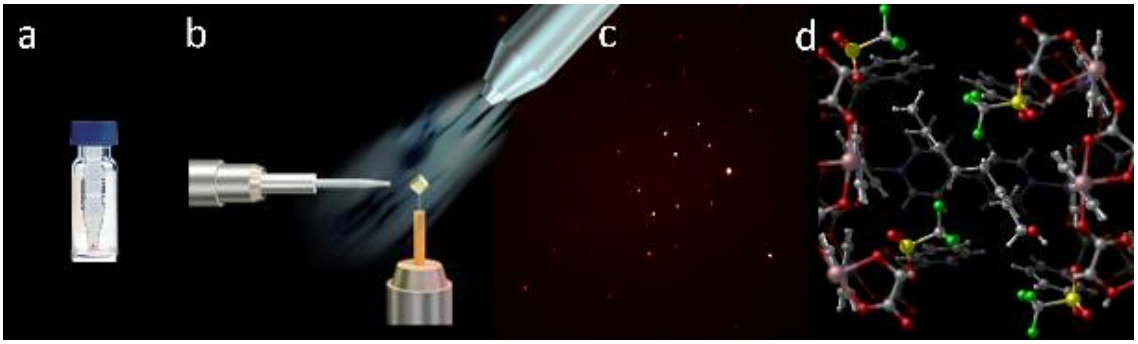


CMOM-3S as a crystalline sponge (step 2): enantiomer identification can be accomplished using a single crystal of CMOM-3S as follows: (a) a single crystal of CMOM-3S is placed in a microvial to which is added a solution of the target (e.g. 17 µg of the natural product geraniol as shown below); (b) After evaporation to dryness the crystal is mounted on a lab x-ray diffractometer; (c, d) the precise molecular structure of the target is thereby determined. The single crystal can be recycled and used again for a different target.



Intellectual Property

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