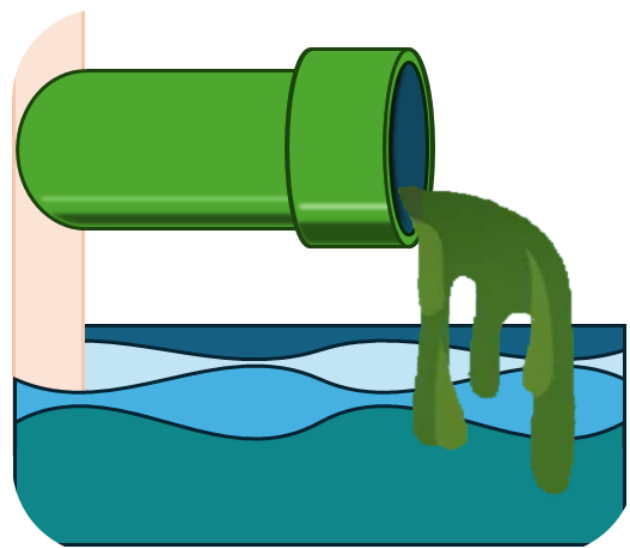


Removal of Organic Pollutants from Water using Supramolecular Containers

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Introduction



Pollution of British Wastewater¹

- Serious pollution incidents increased 60% in 2025.
- Environmental Agency targets have been missed since 2016.
- The yearly cost of water pollution is estimated to be up to £1.3 billion.

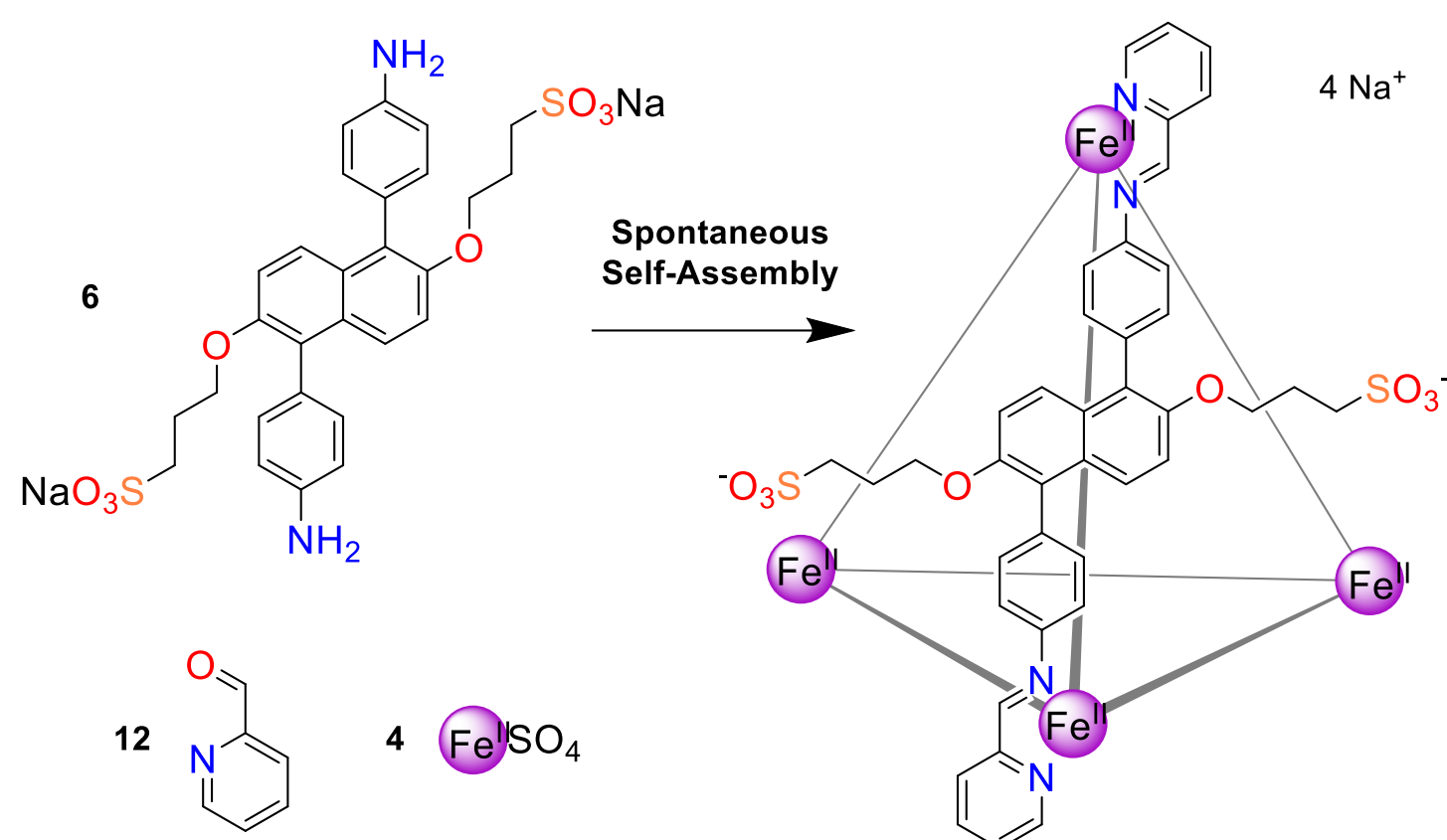
The Challenge²

- Urban, agricultural and industrial pollution are all waste streams of concern that have their own challenges.
- Standard physical and chemical separations are not feasible for every pollutant, each with unique, complex characteristics.
- Small organic chemicals remain a major issue and are time-consuming and costly to remove.

Our Approach - Sulfonate-functionalised Containers

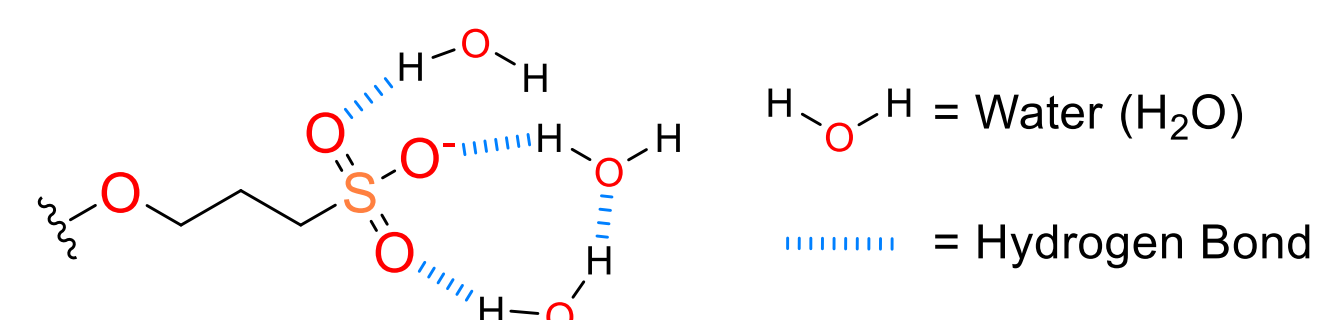
Synthesis of Containers³

Tetrahedral container molecules spontaneously assemble via heating and stirring of starting materials.



Fe₄L₆ tetrahedra are three-dimensional objects made of four iron ions connected by six organic ligands.

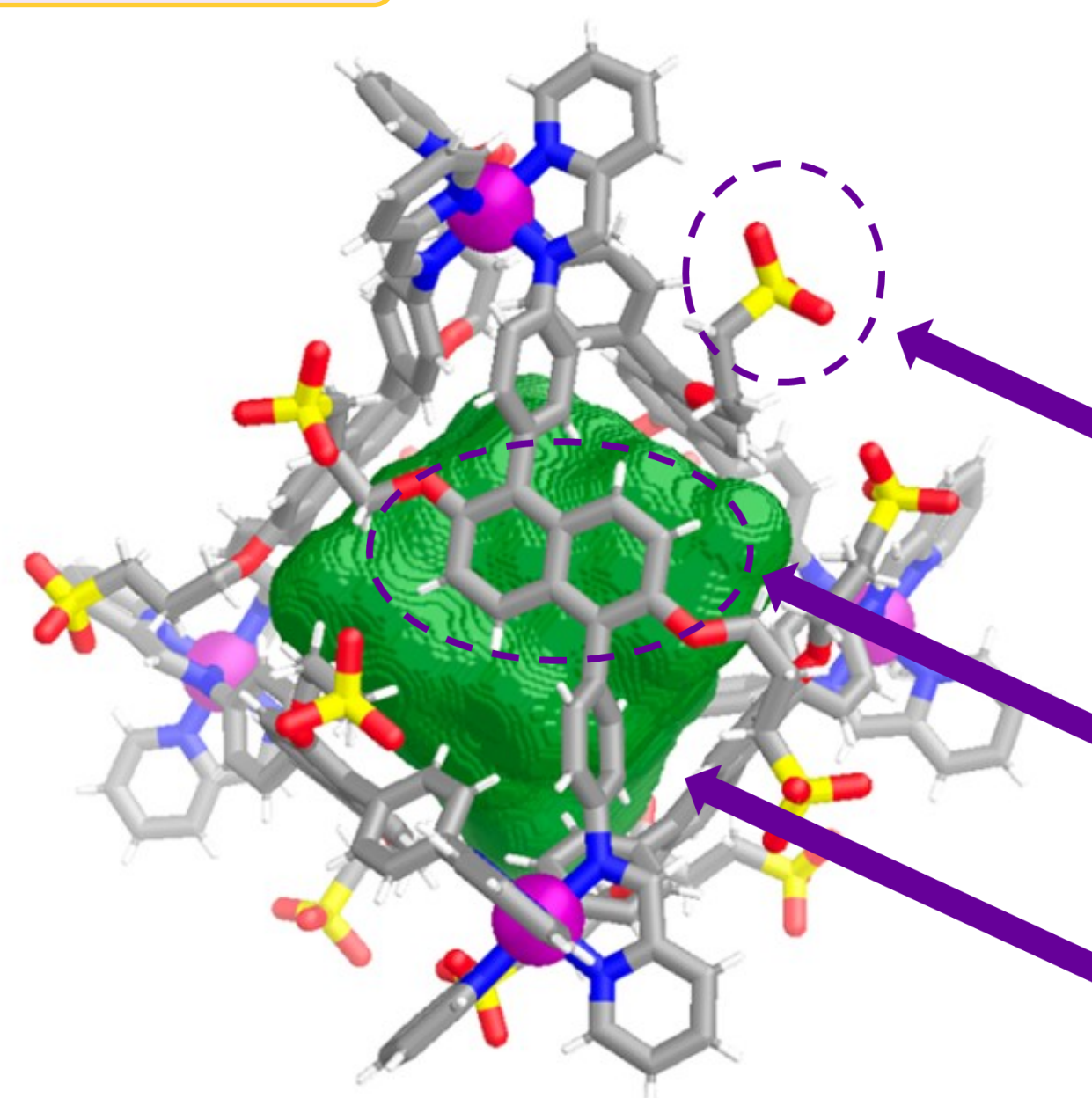
Functional Features



Sulfonate side chains form hydrogen bonds with water, stabilising the containers in solution.

Aromatic spacers create a zone for strong interactions with pollutants.

The large internal cavity (green mesh) can be used to remove a wide range of guest molecules from bulk water, forming Host-Guest Complexes in which pollutants can be isolated and stored.

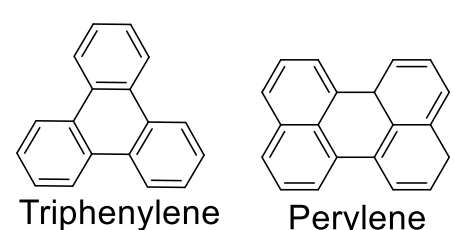
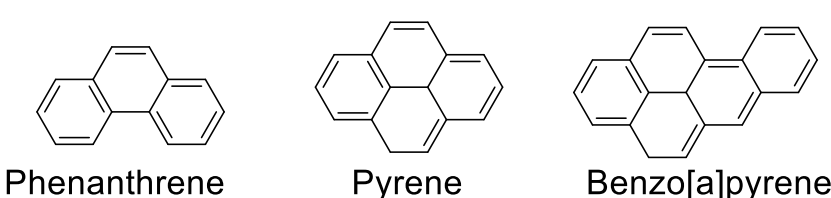


Model of the container and calculated internal cavity (green mesh) derived from single crystal X-ray data.

Our Findings - Pollutant Encapsulation via Host-Guest Complexes

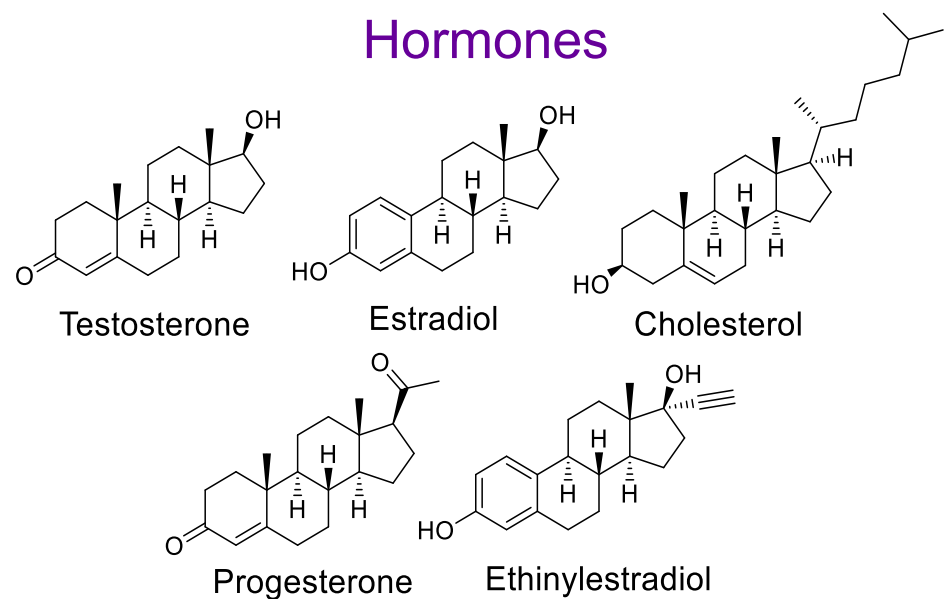
1. Isolatable Pollutants

Polycyclic Aromatic Hydrocarbons



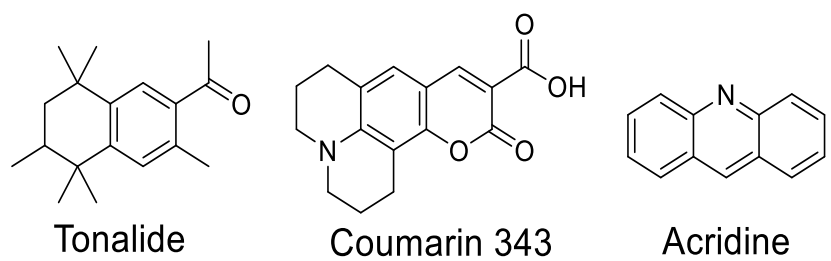
Known carcinogens and mutagens.

Hormones



Disruptive to biodiversity of aquatic ecosystems.

Scents and Dyes

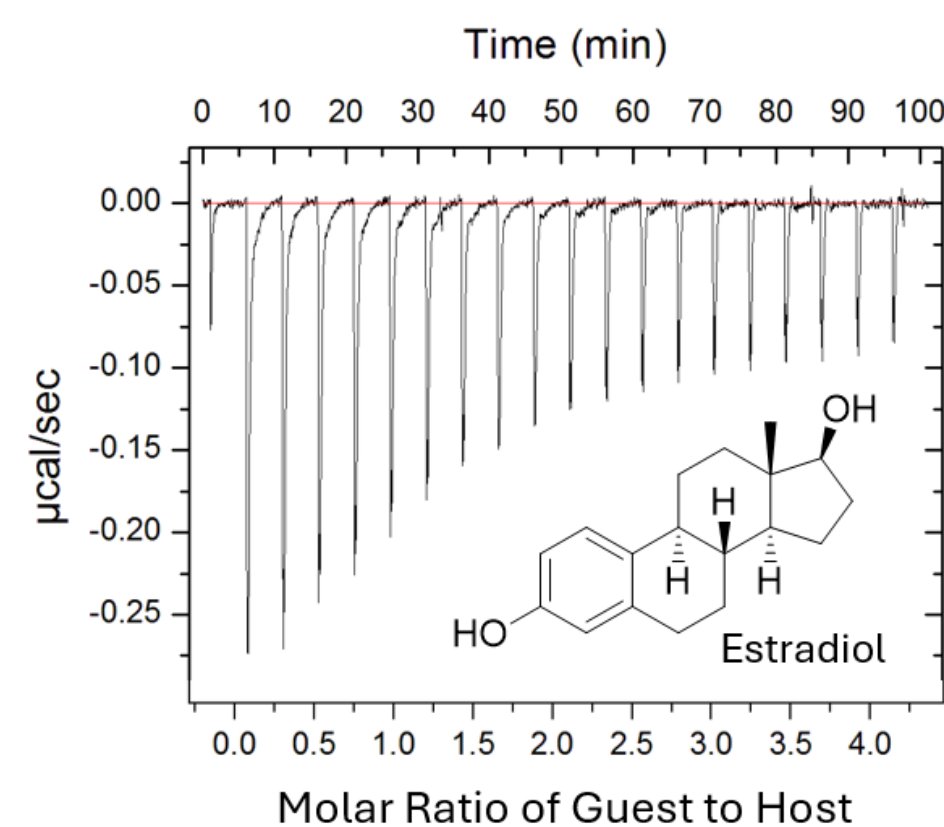


Used in industry but cause health concerns when improperly disposed of.

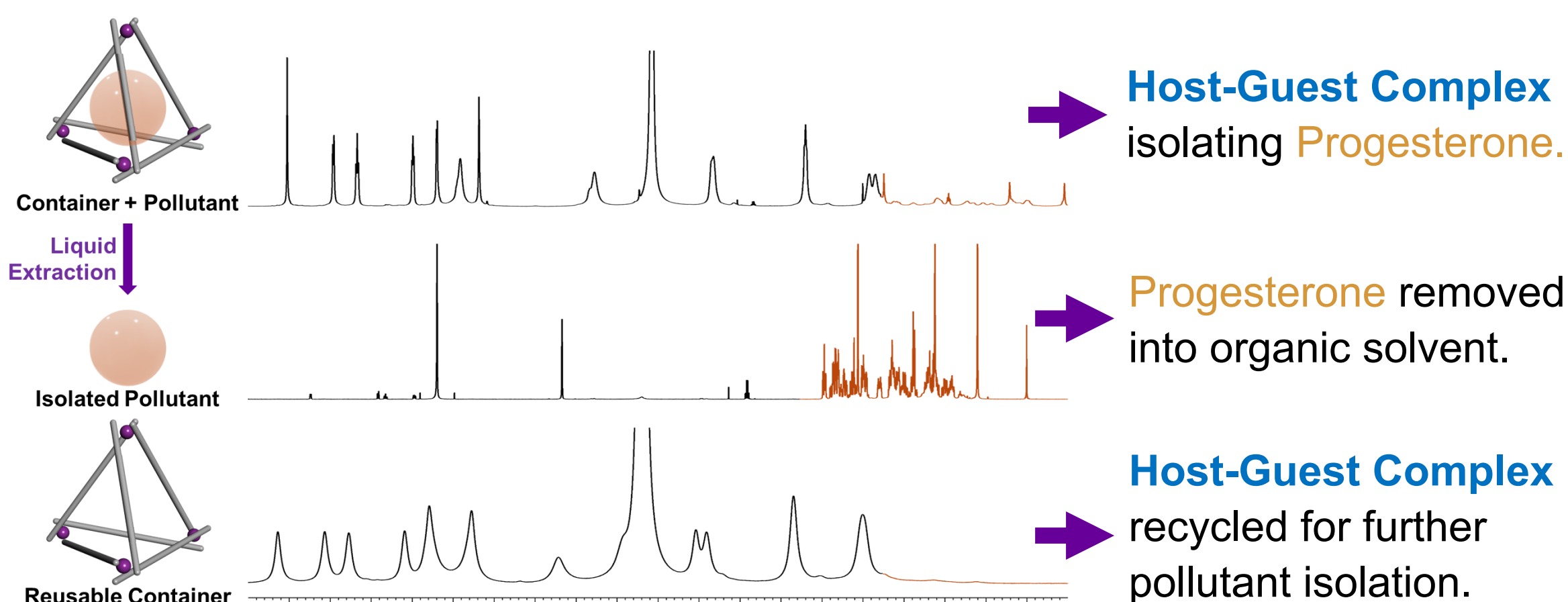
2. Binding Strength and Selectivity

Guest	Binding Strength - K_a (M ⁻¹)
Ethinylestradiol	$2.8 \times 10^5 (\pm 1.0 \times 10^5)$
Testosterone	$2.8 \times 10^5 (\pm 8.3 \times 10^5)$
Progesterone	$2.5 \times 10^5 (\pm 2.1 \times 10^4)$
Estradiol	$1.2 \times 10^5 (\pm 6.5 \times 10^3)$
Tonalide	$1.4 \times 10^4 (\pm 2.9 \times 10^3)$

Isothermal Titration Calorimetry measures heat released during Host-Guest Complex formation. Binding strength can be compared between each pollutant to assess specificity.



3. Recycling of Container Molecules

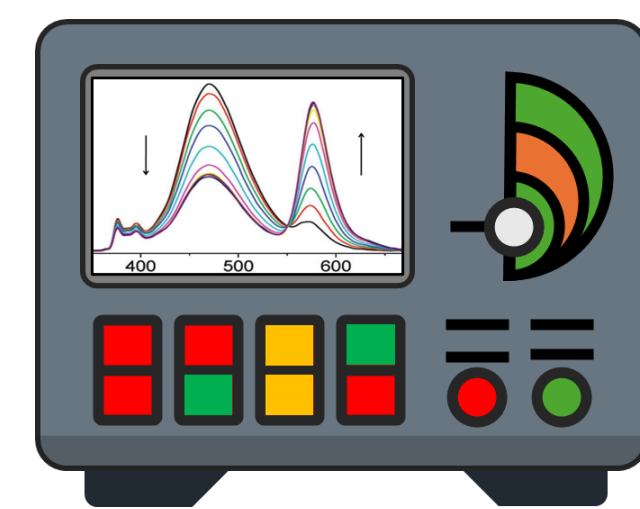


NMR spectra of an aqueous Host-Guest Complex, the isolation of Progesterone and subsequent regeneration of the container.

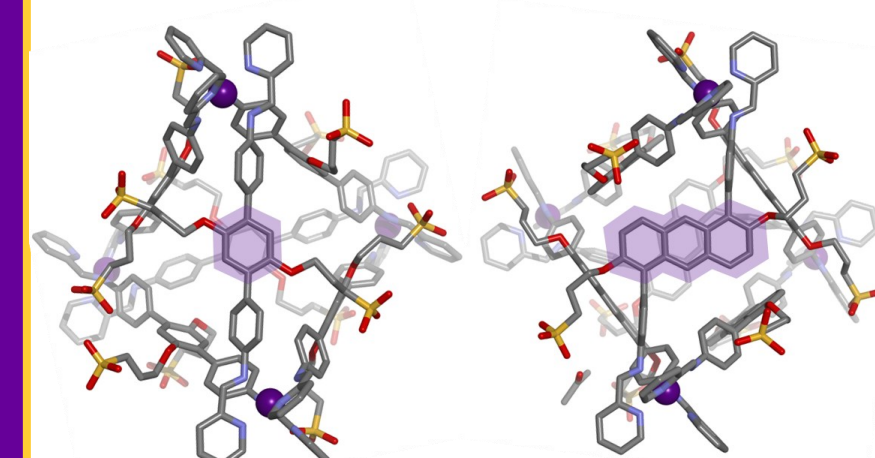
Applications



Prediction of suitable targets using computational analysis.



Optical spectroscopy detects pollutants at low concentrations.



Ongoing research into varied sizes for selective encapsulation.

Host-Guest Complexes enable analysis, isolation, and removal of pollutants from aquatic environments.

References

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3. J. D. Wright, E. O. Pyzer-Knapp, George F. S. Whitehead and I. A. Riddell, *Cell. Rep. Phys. Sci.*, 2025, **6**, 2,102404

Acknowledgements



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