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Synthesis of Tribenzo-1,4,7-triazacyclononene (Cyclophane family) and Derivatives as Supramolecular Scaffolds

A toolbox of supramolecular derivatives useful for high selectivity in host-guest recognition properties of anions in solution.

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Field

Qualitative/Quantitative ion analysis
Drug delivery vehicles &
diagnostics
Materials science
Catalysis

Technology

Supramolecule derivatives that can be solubilized in water and tuned for host-guest specificity.

Key Features

- Stereo selective/conformational binding site
- Binding site modified by peripheral substituents
- Soluble in aqueous and non aqueous solvents
- Attachment to solid support/resin systems

Key Benefits

- Patent contains broad coverage for synthesis routes for parent compound and numerous derivatives

Stage of Development

- Basic synthesis route for key compound completed
- Preliminary work on yield improvement
- Synthesis work on derivatives limited
- Functionality data for compounds needs development

Status

Seeking licensing partner

Patent Status

Provisional Status

Supramolecular compounds

Supramolecular chemistry finds commercial application over a wide range of analytical methodologies, materials science and medical diagnostics end uses. This results from their principle characteristic of being able to form non-covalent molecular complexes with a variety of ionic and non-ionic moieties in aqueous and non-aqueous solution via chelation. A particular supramolecule is selected for its unique functionality and targeted capacity for guest-host recognition, binding stability and working environment. General applications include, but are not limited to, qualitative and quantitative analysis of metal and non-metallic ions in solution, encapsulation of drugs, environmental analysis, catalysis, magnetic resonance and medical diagnostic imaging.

Synthesis of Tribenzo-1,4,7-triazacyclononene and derivatives

The inventors have developed a new, patented, synthetic route to the key compound designated as N3-CTV. Yields of the parent compound and its derivatives will need further improvement. They have synthesized some derivatives with enhanced water solubility over the parent. The binding site or cavity, containing 3 secondary nitrogens in a 9-membered ring, can produce pH-dependent binding and conformational properties which can be important in modulating its binding properties. The derivative compounds lend themselves to attachment to solid substrates/resins via alkylation, ester or amide formation.

N3-CTV supramolecule and its derivatives provide enhanced functionality as a family of compounds

The parent compound N3-CTV is insoluble in water. By substitution with polar substituents on its benzene rings it can be made water-soluble thereby greatly broadening its potential applications. This may also include biomedical applications such as drug delivery. These properties are not routinely found in the class of materials recognized as supramolecules. Further, derivatives of N3-CTV can allow one to produce host-binding sites/cavities that are tailored to specific guest ions or substrate size or polarity. This flexibility, derived from a parent material, is quite rare among this class of materials. Reactive ring substituents can allow for covalent binding to solid support systems and resins, and could potentially be applied to ion-specific sensors, electrodes and chromatographic columns thereby enhancing its application to various analytical methodologies.

Substrate specificity

N3-CTV and its derivatives may provide a toolbox of supramolecules to allow fine-tuning of selective host-binding characteristics either by the addition of electron-withdrawing or electron-donating groups. pH can also modulate the binding characteristics of the molecular cavity. The current focus on binding appears to be nitrates, phosphates and other small anionic molecules with an environment impact.

Opportunity

Loyola University Chicago is looking for commercial licensing partners for this patent.