LOYOLA UNIVERSITY CHICAGO

Synthesis of Tribenzo-1,4,7-triazacyclononene "N3-CTV" (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
Fine Chemicals
Qualitative/Quantitative ion analysis
Drug delivery vehicles & diagnostics
Materials science
Catalysis

Technology
Supramolecule scaffold and derivatives that can be solublized in water and tuned for host-guest specificity.

Key Features
- conformationally flexible 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 synthetic routes for parent compound and numerous derivatives

Stage of Development
- Basic synthesis route for key compound completed
- Substantial work on yield improvement
- Synthesic 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. 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, use as a transition-metal ligand, 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 (N3-CTV) 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 commonly-employed CTV (cyclotriveratrylene). The binding site or cavity, containing 3 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 popular supramolecular scaffold CTV (cyclotriveratrylene) is insoluble in water. Replacement of the three apical methylenes of CTV with nitrogen atoms significantly enhances water solubility aand also provides manifold functionalization possibilities. Additionn of substituents to its three benzene rings can be employed to fine tune binding characteristics, 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. Addition of apical 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 or by modulating pH. The current focus on binding appears to be nitrates, phosphates and other small anionic molecules with an environmental impact.

Opportunity

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

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Inventor

Dr. Daniel P. Becker received his Bachelor's degree in Chemistry from Kalamazoo College and his Ph.D. in Organic Chemistry from Indiana University, and he is presently a tenured member of the faculty as an Associate Professor of Chemistry at Loyola University in Chicago. His academic research encompasses both medicinal chemistry toward the design of novel enzyme inhibitors, and supramolecular chemistry in the construction of new supramolecular scaffolds for host-guest chemistry and analytical detection. Dr. Becker previously served as a Project Team Leader and Research Fellow in the Department of Medicinal Chemistry with Searle Pharmaceuticals and Pharmacia for seventeen years before moving to academia. He has authored over thirty publications in medicinal chemistry and synthetic organic methodology and has been awarded forty-seven U.S. patents for new pharmaceuticals in the areas of gastrointestinal diseases, cancer, arthritis and cardiovascular disease, and new synthetic organic methods.