Pyridinium Core Units for V-shaped Anthracene Dimers: Rapid Access to New Polyaromatic Amphiphiles

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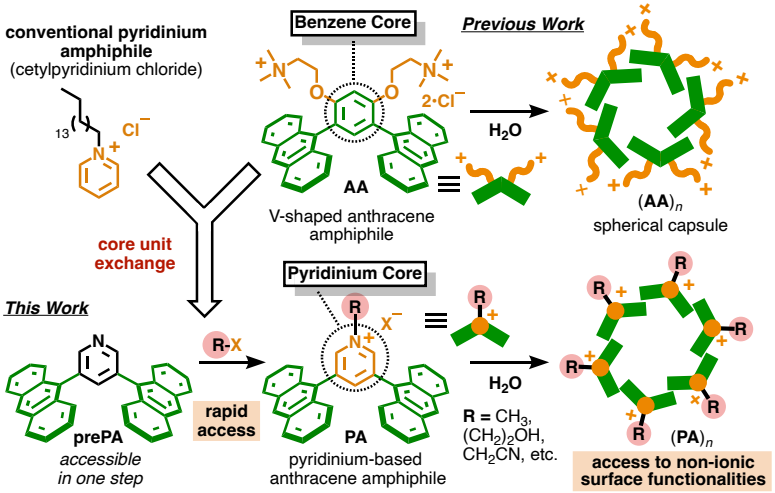
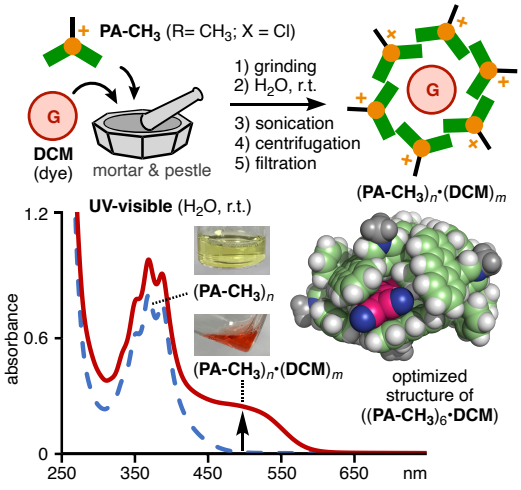
Rapid and facile access to functional building blocks is of fundamental importance for the field of supramolecular technology. Especially, building blocks that self-assemble into discrete capsular structures in water are highly desirable for advanced host-guest applications. Our group has established V-shaped amphiphile **AA** comprising an anthracene dimer with hydrophilic side-chains,[1] which self-assembles into a spherical capsule with wide-ranging host abilities in water.[2] Based on this design, here we report new V-shaped amphiphile **PA** featuring a pyridinium unit, which allows the rapid construction of spherical capsules with non-ionic surface groups and host functions.



N-Methylation of new building block **prePA** and subsequent ion-exchange yielded water-soluble **PA-CH$_3$** with chloride counterion in 3 facile synthetic steps. In water, **PA-CH$_3$** was shown to assemble into a discrete capsule of around 2 nm in size (0.5 mM based on **PA-CH$_3$**), in a manner similar to **AA**, as confirmed by DLS and DOSY analyses. The resultant capsule (**PA-CH$_3$**)$_n$ displayed good stability against heat. In addition, (**PA-CH$_3$**)$_n$ allowed the water-solubilization of hydrophobic dyes such as **DCM** and copper(II) phthalocyanine via a simple grinding protocol. Importantly, the present design enabled the construction of new polyaromatic capsules featuring a wide range of non-ionic surface functionalities in only 1 to 2 steps from **prePA**.



[1] K. Kondo, A. Suzuki, M. Akita, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2013**, *52*, 2308. [2] M. Yoshizawa, L. Catti, *Acc. Chem. Res.* **2019**, *52*, 2392.