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DESIGN AND SYNTHESIS OF MOLECULAR BUILDING BLOCKS FOR MODULAR SUPRAMOLECULAR CAVITANDS

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Cavitands are macrocyclic molecules containing a permanent intramolecular cavity for non-covalent binding of guest molecules. The most commonly encountered types of cavitands are cyclodextrins and cyclic phenol-formaldehyde oligomers. Such compounds have many potential applications as synthetic enzymes[1], drug delivery systems[2], or filters for removing polyaromatic contaminants from aqueous systems[3]. However, existing cavitand designs suffer from high symmetry and poor capabilities of functionalization and cavity size modification, which severely limits their potential.

Our current research is based around a system that enables the modular synthesis of various different-sized cavitands from a small selection of molecular building blocks through cyclocondensation reactions. The system is centered around derivatives of bicyclic V-shaped compound **1**. Methods for the synthesis and resolution of enantiomerically pure **(+)-1**[4] and both enantiomers of the heterocyclic variant **(+)-2** and **(-)-2**[5] have been developed. Bifunctionalized symmetric synthons **5** and **6** for Friedlander and Fischer cyclocondensations have also been successfully synthesized and tested in the corresponding condensation reactions. However, synthesis of cavitands has been unsuccessful due to solubility problems and self-condensation side reactions emerging after functionalization with bulky solubilizing groups. Future plans include alternative routes of functionalization and synthesis of model cavitands.

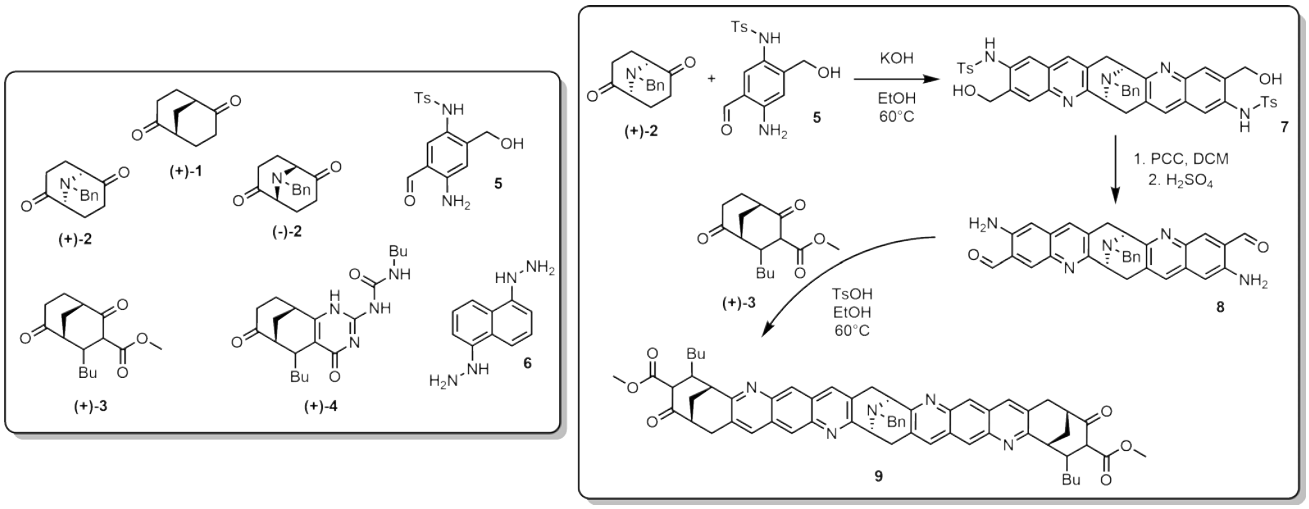

Fig. 1. Prepared molecular building blocks (left) and model cavitand synthesis (right).

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