HYBRID DISCOVERY WORKFLOW FOR ORGANIC MATERIALS AND SUPRAMOLECULAR SELF-ASSEMBLIES

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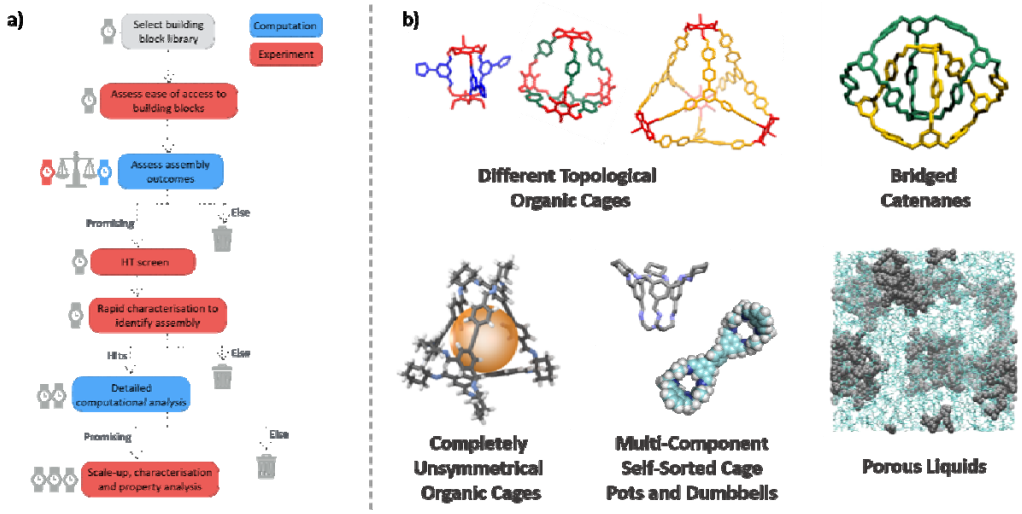
Supramolecular synthesis is a powerful tool for assembling complex organic molecules, such as macrocycles, cages, and catenanes. However, targeted design of such molecules can be challenging, especially as the systems become more elaborate. High-throughput automation can be used to screen a broad synthetic space, but when applied blindly, this approach is inefficient. We have developed a hybrid discovery workflow that fuses computational screening with robotic synthesis for discovering new organic cages – a class of self-assembled molecule that contain permanent intrinsic cavities accessible through windows, and by extension, other supramolecular assemblies [1]. By fusing our computational toolkit to predict the most likely topology and shape-persistence based on the precursors used, with a robust synthetic route which made translation onto an automated synthesis platform possible, the hybrid workflow led to the synthesis of 49 new cages, rapidly accelerating the discovery process. Furthermore, it led to the serendipitous discovery of a unique cage topology – covalently bridged cage catenanes, and has been applied in the discovery of a number of other organic materials and supramolecular assemblies, such as completely unsymmetrical cages [2], socially self-sorted pots and dumbbells, and porous liquids.



[1] R. L. Greenaway *et al.*, *Nature Communications*, **2018**, *9*, 2849.

[2] E. Berardo *et al.*, *Nanoscale*, **2018**, *10*, 22381.