From dendrimers to macrocycles: exploring covalent templates in the synthesis of large aromatics

One of the most important tasks of chemistry is creating new and unique molecules and investigating how such compounds interact with the surrounding environment. A lions' share of the overwhelming diversity of novel chemical substances made every year are those based on carbon. They not only form the basic building blocks of life (proteins, sugars, enzymes etc.), but also create our modern civilization in the form of materials and related technologies. A lot of such compounds take the shape of circles built from smaller circular parts, and we call them macrocycles. The structural diversity and unique repertoire of methods used to synthesize aromatic macrocycles – cyclic, carbon-based chemical entities of nanometer scale (one millionth of a meter!), has made them one of the fastest developing fields of modern organic chemistry. Such architectures represent a vibrant and interesting conglomerate of structure-property relationships, ranging from nature-based, functional molecules (such as porphyrins, responsible for oxygen transport in our blood and photosynthesis in plants), through industrial reaction mediators (by changing the reaction speed, facilitating contact between reactive species), to enormous, human-made assemblies acting as models for molecular wires or chemical sensors.

A general challenge in constructing nanoscale, shape-persistent structures lies in harnessing the macrocyclization step, where we want to fuse the smaller building blocks together to form a loop. We also need to search for ways to drive the reactions toward a specific ring size and to compete with other processes – linear assembly being the main villain. One of the possible solutions is the use of templates: supporting structures, which act as an internal scaffolding (or mold, just like the ones needed for a cake of a certain shape). My project aims to create templates in the form of dendrimers – web-like, branching molecules, which can be expanded very fast using simple, iterative procedures into much larger assemblies. The dendrimers would act as tethers to bring various aromatic building blocks together in space, thus facilitating their coupling into cycles. This requires multiple testing of different designs, dendrimer lengths and configurations to maximize the target product outcome. Once made, the macrocycles would be put into a series of experiments to see how they interact with different kinds of light and magnetic fields, which would unambiguously prove their structure and lead the way to more advanced studies aimed at checking how they can be used as functional materials.