Group : Laboratory of Organic Chemistry

Project : **Functionalized pillararenes for PFAS absorption**

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Keywords. Functionalized pillar[5]arenes, PFAS absorption, host-guest chemistry, water treatment.

Introduction. Per- and polyfluoroalkyl substances (PFAS) are a group of man-made chemicals with water and lipid repellent properties.[1] These make them useful in non-stick coatings, firefighting foams, food packaging, clothing, and cosmetics.[2] Their extreme stability leads to accumulation in biological ecosystems and humans. The most common types of PFAS are perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS). Even though they are generally present at relatively low concentrations (in the order of ng/L), their toxicity causes cancers, immune disorders, and birth defects in humans.[3] Therefore, it is critical that PFAS are removed from the environment. State-of-the-art techniques for PFAS absorption involve granular activated carbon, anion resins, membranes, MOFs, and COFs. However, these techniques are either non-specific for PFAS, non-scalable, or expensive. Non-specificity for PFAS is detrimental, because it results in competition with natural organic matter, that is present in much higher concentrations, in real-life applications.[4] Therefore, new PFAS absorption technologies should be highly specific for PFAS.

Goal. Recently, our group discovered that hydroquinone-based macrocycles, called pillararenes,[5] can be used to absorb PFAS.[6] Ammonium-functionalized pillararenes demonstrated unprecedented 1:10 stoichiometry, high binding constants and robust performance.[6] However, the PFAS-binding mechanism is poorly understood. We aim for better understanding of this newfound technology to ultimately apply it for large-scale PFAS cleanup. This project is in collaboration with Wetsus, the Netherlands institute for water treatment technology.

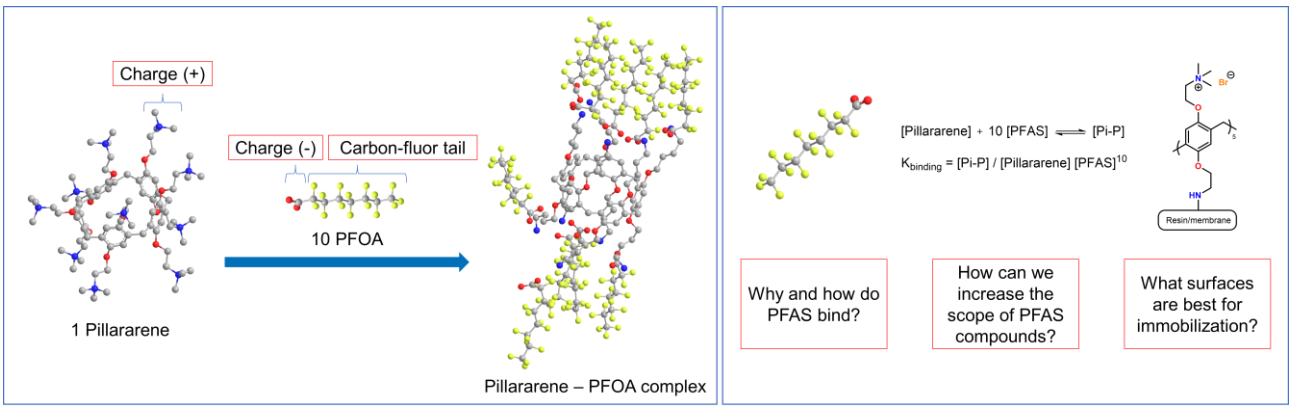

Figure 1. Left) One ammonium(+)-functionalized pillararene is able to bind 10 PFOA(-) molecules, leading to a pillararene-PFOA complex with stoichiometry of 1:10. Right) The main research questions for this project.

Topics to be studied. This project will investigate the underlying mechanisms of pillararene-PFAS binding. New insights will be applied to further improve binding constants. Additionally, this project attempts to broaden the scope of PFAS compounds that can be absorbed by functionalized pillararenes. This project works in parallel to the project of Rick Nooijen, who works on surface immobilization, regeneration of immobilized P5 materials and scaling up.

Techniques to be used. Organic synthesis; monitoring reactions by TLC and NMR; column chromatography; characterization of products with NMR, MS; ITC titrations to characterize binding.

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