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Functionalized pillararenes for PFAS absorption from water

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Motivation

Per- and polyfluoroalkyl substances (PFAS) are a class of compounds that is known for their hydrophobicity and oleophobicity. These properties make them useful in many consumer products, such as non-stick coatings, firefighting foams, food packaging, etc. Their extremely high stability, however, causes them to accumulate in biological systems and humans. Despite low environmental concentrations (ng/L), they cause immune disorders, cancers, and birth defects in humans [1]. PFAS adsorption from the environment is key in preventing these toxic effects in the future. Granular activated carbon (GAC) is currently used in water treatment of PFAS-polluted waters, primarily since it is inexpensive. Several other techniques have been investigated, such as anion resins, membranes, and organic/metal frameworks. However, these are either non-specific, non-scalable, or expensive. Non-specificity of GAC and other techniques is detrimental, because it leads to competition with natural organic matter [2]. Thus, new, highly specific PFAS adsorbers are required.

Our group discovered that a type of macrocycle (called pillararenes) functionalized with positively charged groups binds PFOS and PFOA, the two most common PFAS compounds, strongly and specifically. A pillararene-PFAS complex (PiP) was formed with a unique 1:10 stoichiometry, and high breakthrough capacity of 90 mg/g for PFOS and 80 mg/g for PFOA. These findings confirmed their potential as PFAS adsorption technology [3].

Technological challenge

The innovative aspects of this research include:

- Pillararenes as a PFAS-adsorbing technology.
- Computational studies on the contribution of the fluorophilic effect in the mechanism of PiP formation.
- Synthesis of highly charged pillararenes, with the aim to improve stoichiometry and binding constant.
- Pillararene immobilization on different types of surfaces.

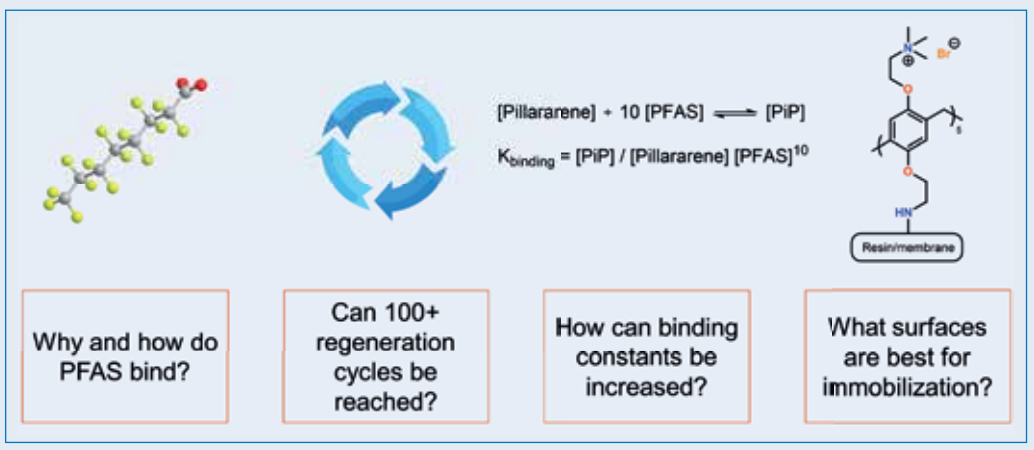

Figure 1. Main areas of focus: understanding the mechanism of PiP formation, improving the regeneration capabilities, increasing binding constants of PiP, and assessing what surfaces are best for immobilization..

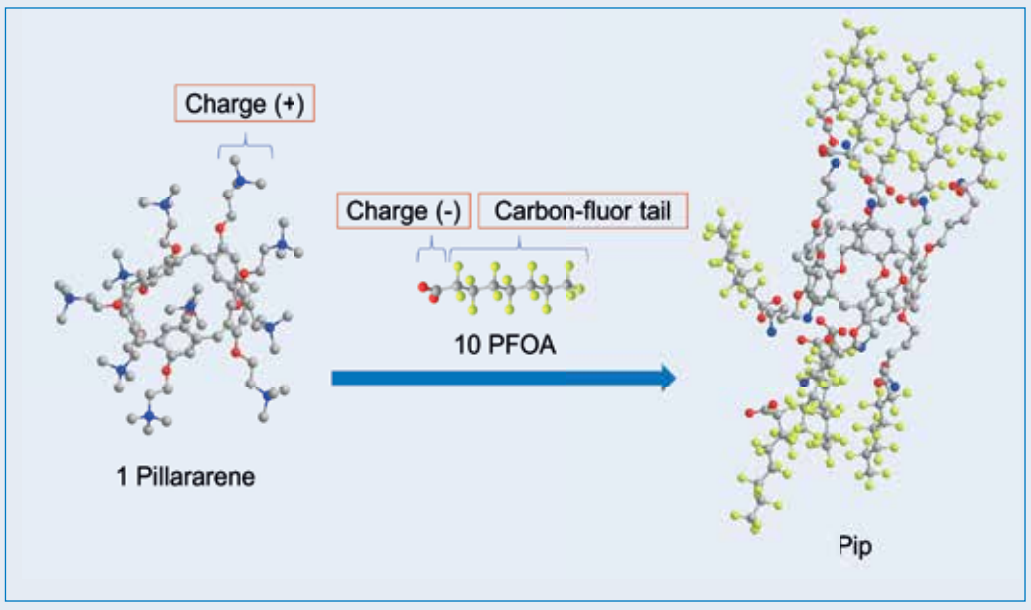

Figure 2.The formation of a PiP complex from 1 positively charged pillararene and 10 negatively charged PFOA.

Research goals

Thus far, the fundamentals of PiP formation are poorly understood. This understanding is paramount for the design of a next generation of PFAS-adsorbing pillararenes. Furthermore, the use of these pillararenes in larger-scale systems must be evaluated. This requires their immobilization on a surface. We have formulated the following objectives for our work:

- Computational study: 1) Study the PiP binding mechanisms.2) Investigate effects of different pillararene positively charged groups. 3) Review adsorption of different types of PFAS.
- Implement new knowledge on PiP formation in the design of a next generation of PFAS adsorbers.
- Surface modification: 1) Identify the optimal surface for pillararene immobilization. 2) Test pillararene immobilized surfaces on larger scales using real-life water samples.

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[2] K. Roest, T. ter Laak, H. Huiting, W. Siegers, N. Meekel, C. de Jong, M. de Jong, M. van Houten, T. Pancras, W. Plaisier, J. Dalmijn, Concawe Report no. 5/21 (2021).
[3] T. Gao, S. Huang, R. Nooijen, Y. Zhu, G. Kociok-Köhn, T. Stuerzer, G. Li, G. Salentijn, B. Chen, H. Bitter, F. M. Miloserdov, H. Zuilhof, ChemRxiv. (2023).