

# Effects of Common Drinking Water Cations on PFAS Removal Using Quaternary Ammonium Functionalized PolyHIPE Polymers

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## Abstract

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants widely detected in drinking water and associated with adverse human health effects. Quaternary ammonium functionalized high internal phase emulsion polymers (polyHIPEs) have emerged as promising PFAS sorbents due to combined electrostatic and hydrophobic interactions.

In this study, polyHIPE materials with 6 wt% and 12 wt% quaternary ammonium functionalization were evaluated for PFAS removal under environmentally relevant water chemistry conditions. A factorial design was used to assess the effects of common drinking water cations ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{Fe}^{2+}$ ) on adsorption performance, with analysis focused on preliminary 1-hour data.

Results indicate that polymer functionalization (% Quat) is the primary factor controlling removal for both PFPrA and PFBA.  $\text{Fe}^{2+}$  significantly enhanced PFPrA removal, while other cations showed no significant effects. These findings highlight the importance of polymer design in developing PFAS remediation materials effective under complex environmental conditions.

## Introduction

Per- and polyfluoroalkyl substances (PFAS) are a class of persistent environmental contaminants widely detected in drinking water systems and associated with adverse human health effects. Due to their chemical stability and resistance to degradation, PFAS accumulate in environmental and biological systems, making their removal a critical challenge. Current treatment methods, including reverse osmosis, ion exchange, and activated carbon, often show reduced efficiency under realistic water conditions where dissolved ions are present.

Polymer-based sorbents, particularly high internal phase emulsion polymers (polyHIPEs), offer a promising alternative due to their high surface area and tunable chemical functionality. Quaternary ammonium functionalization enhances PFAS adsorption through electrostatic and hydrophobic interactions. However, the influence of common drinking water cations on PFAS removal by these materials remains poorly understood.

## Materials and Methods

PolyHIPE materials containing 6 wt% and 12 wt% quaternary ammonium functionalization were synthesized using emulsion polymerization. A 16-condition factorial experimental design was constructed to evaluate the effects of five cations ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{Fe}^{2+}$ ) at low (0 ppm) and high (250 ppm) concentrations. PFAS adsorption experiments were conducted in 50 mL solutions, and samples were collected over time, with analysis focused on the 1-hour time point due to data availability. PFAS concentrations were quantified using LC-MS/MS (LC-QQQ), and statistical analyses were performed using Design-Expert software.

Std	Run	Factor 1 A:Na+	Factor 2 B:K+	Factor 3 C:Mg+2	Factor 4 D:Ca+2	Factor 5 E:Fe+2	Factor 6 F:Quat	Response 1 C R1
15	1	-1	1	1	1	-1	1	
1	2	-1	-1	-1	-1	-1	-1	
8	3	1	1	1	-1	1	-1	
13	4	-1	-1	1	1	1	-1	
7	5	-1	1	1	-1	-1	-1	
11	6	-1	1	-1	1	1	-1	
3	7	-1	1	-1	-1	1	1	
2	8	1	-1	-1	-1	1	-1	
6	9	1	-1	1	-1	-1	1	
4	10	1	1	-1	-1	-1	1	
9	11	-1	-1	-1	1	-1	1	
14	12	1	-1	1	1	-1	-1	
10	13	1	-1	-1	1	1	1	
16	14	1	1	1	1	1	1	
12	15	1	1	-1	1	-1	-1	
5	16	-1	-1	1	-1	1	1	

Figure M1. Experimental design matrix

## Results

Preliminary results at 1 hour indicate that polymer functionalization (% Quat) is the dominant factor controlling PFAS removal. For PFPrA, both % Quat and  $\text{Fe}^{2+}$  were identified as statistically significant factors, with higher levels of each resulting in increased removal efficiency. In contrast,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ , and  $\text{Ca}^{2+}$  did not significantly affect PFPrA adsorption.

For PFBA, % Quat was the only significant factor influencing removal, with no measurable impact from any of the tested cations. Half-normal plots and Pareto charts were used to identify factors that could be statistically important influences on PFAS adsorption while analysis of variance (ANOVA) was used to confirm whether the selected factors were statistically significant. Results for the ANOVA model using the selected factors demonstrated that the models using the selected factors reliably explain the observed trends.

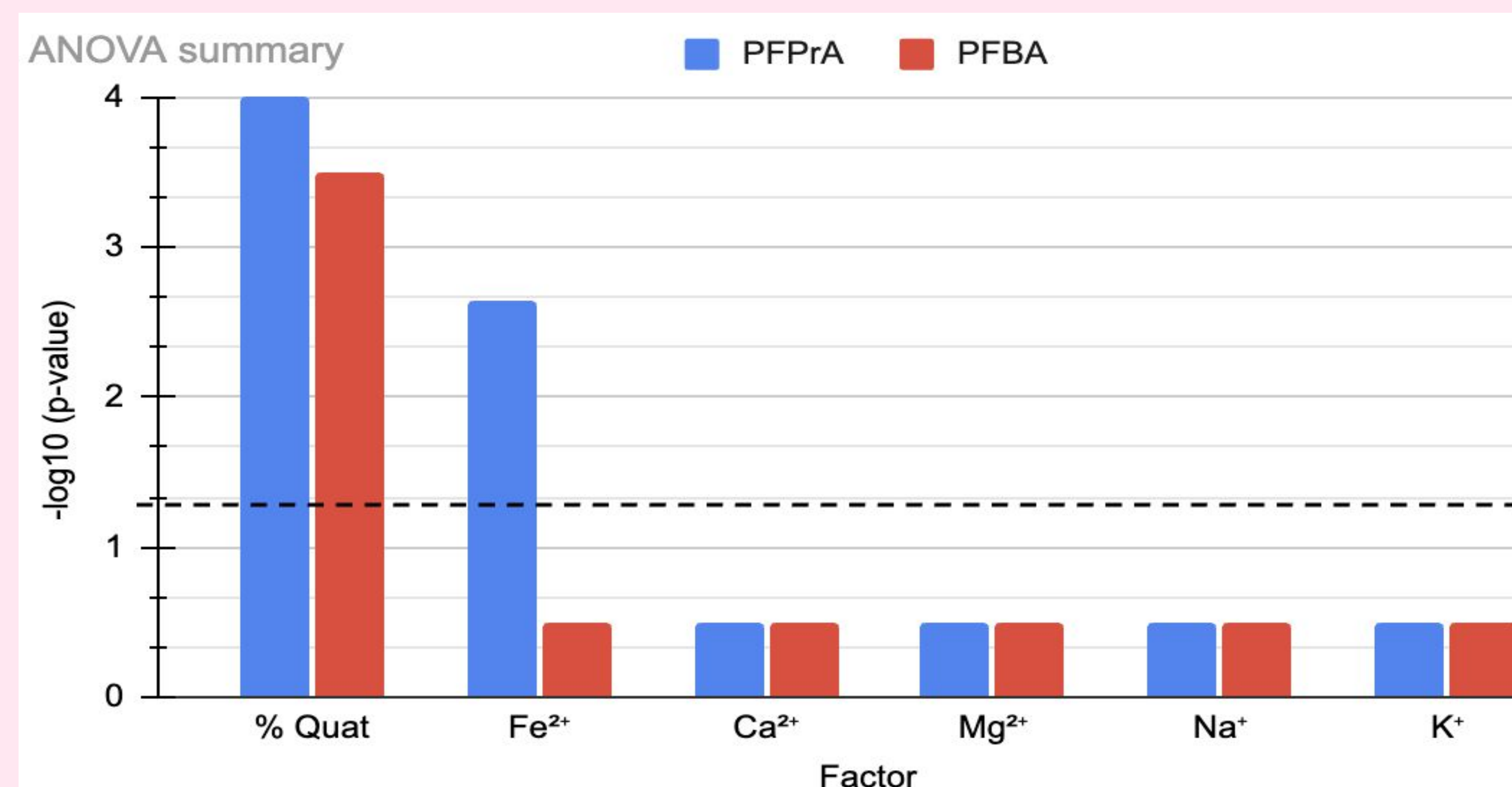


Figure R3. Summary of factor significance based on ANOVA analysis for PFPrA and PFBA at 1 hour. Bars represent  $-\log_{10}(\text{p-values})$ , with the dashed line indicating the significance threshold ( $p = 0.05$ ). Quaternary ammonium concentration (% Quat) is the dominant factor for both PFAS, while  $\text{Fe}^{2+}$  significantly affects PFPrA only.

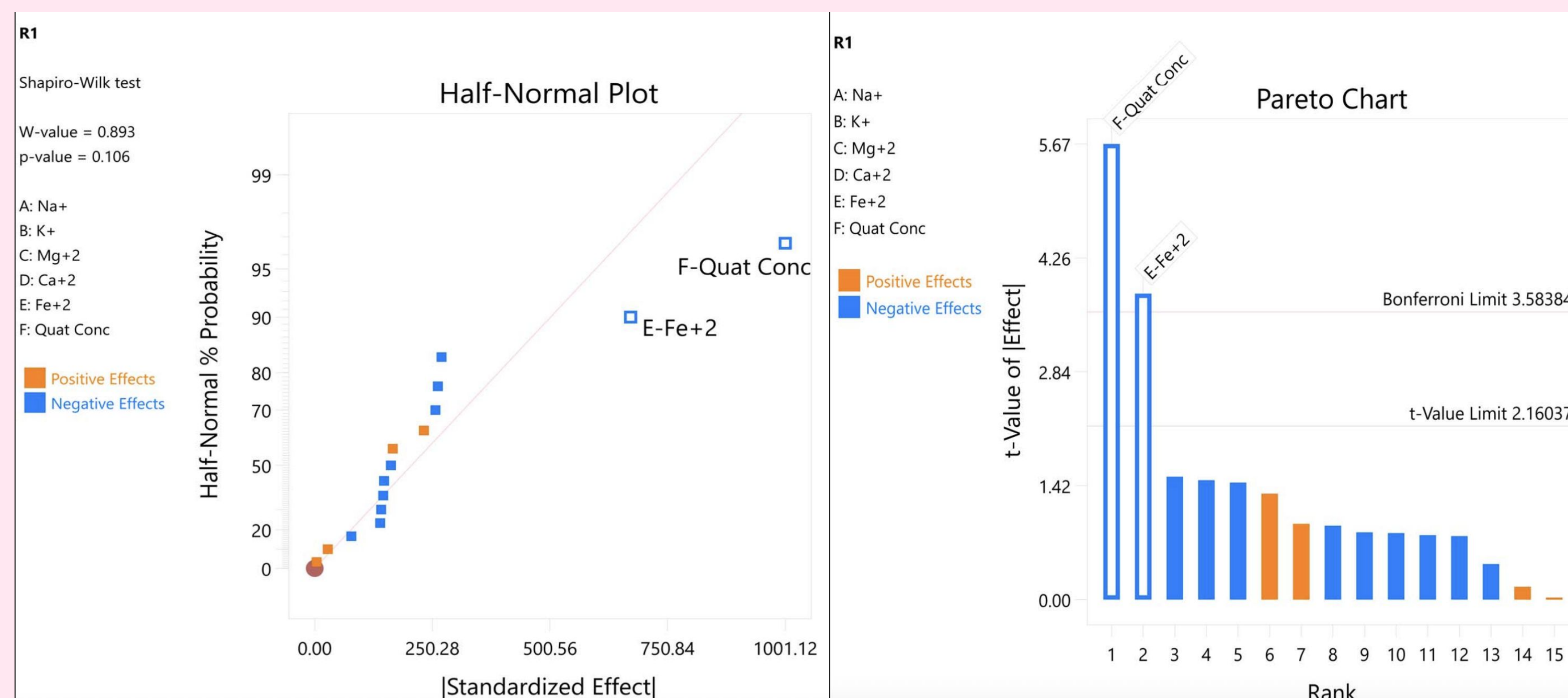


Figure R1. PFPrA half-normal + Pareto

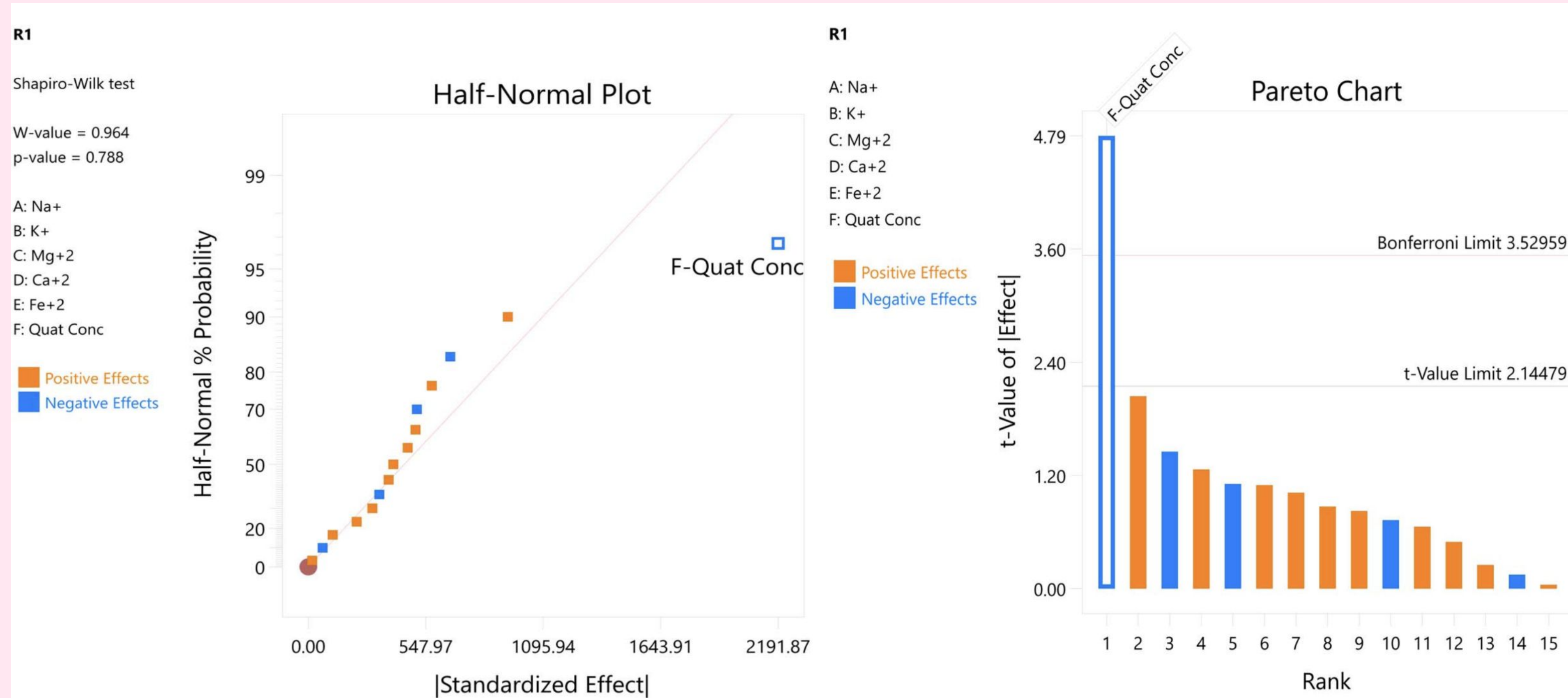


Figure R2. PFBA half-normal and Pareto

## SEM Results

Scanning electron microscopy revealed that both 6 wt% and 12 wt% polyHIPE materials exhibited similar porous, sponge-like morphologies with interconnected void structures. While average pore size did not differ significantly, the 12 wt% formulation displayed a higher frequency of smaller pores compared to the 6 wt% material. These observations suggest that increased quaternary ammonium content may influence pore distribution without significantly altering overall structure.

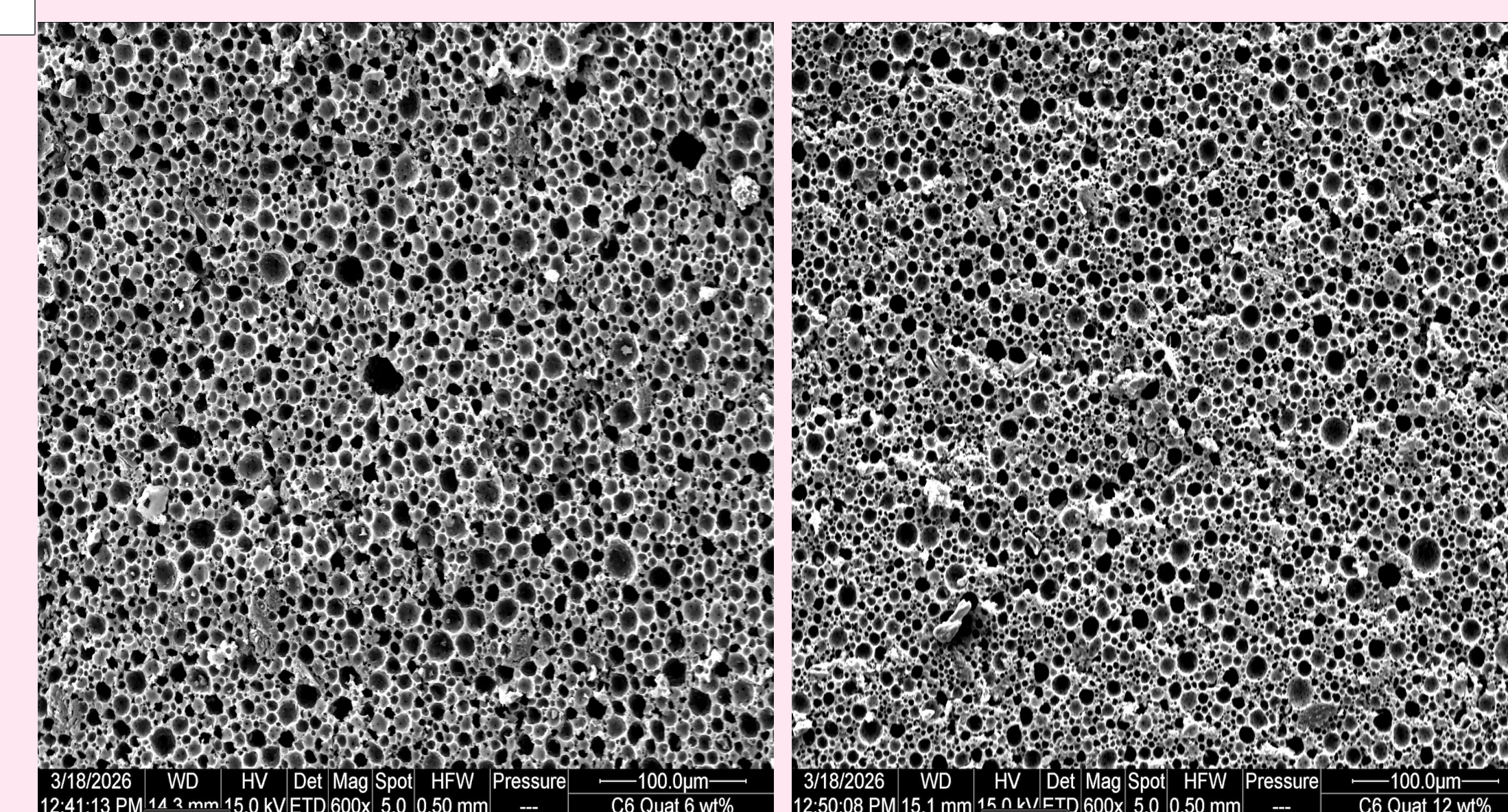


Figure R4: SEM images (6 wt% vs 12 wt%)

## Discussion

These findings indicate that PFAS removal is initially governed primarily by polymer functionalization rather than background water chemistry. The significant effect of % Quat supports the role of electrostatic interactions in PFAS adsorption, where increased functionalization enhances binding capacity. The observed influence of  $\text{Fe}^{2+}$  on PFPrA removal suggests that certain cations may facilitate adsorption through ion-specific interactions, potentially by altering solution chemistry or reducing electrostatic repulsion.

In contrast, the lack of cation effects for PFBA suggests that shorter-chain PFAS are less sensitive to environmental ionic conditions and more dependent on polymer properties. The minimal impact of  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ , and  $\text{Ca}^{2+}$  further indicates that most common drinking water cations do not significantly interfere with PFAS adsorption in this system.

**Conclusion:** PolyHIPE-based materials demonstrate effective PFAS removal under environmentally relevant conditions. Polymer functionalization (% Quat) was identified as the primary factor controlling adsorption, while most common drinking water cations had minimal impact.  $\text{Fe}^{2+}$  was the only cation observed to enhance PFAS removal for PFPrA. These results highlight the importance of polymer design in developing robust and effective PFAS remediation technologies.

## References

Tighe, M. et al., (2024). Pfas removal from water using quaternary amine functionalized porous polymers. *Chemical Engineering Journal*. <https://doi.org/10.2139/ssrn.4933692>

United States Environmental Protection Agency. (2026). *Ground water and drinking water*. <https://www.epa.gov/ground-water-and-drinking-water>

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