

SUPPORTING INFORMATION

Occurrence and fate of per/polyfluoroalkyl substances (PFASs) in residential wastewater treated with nitrogen-removing biofilters

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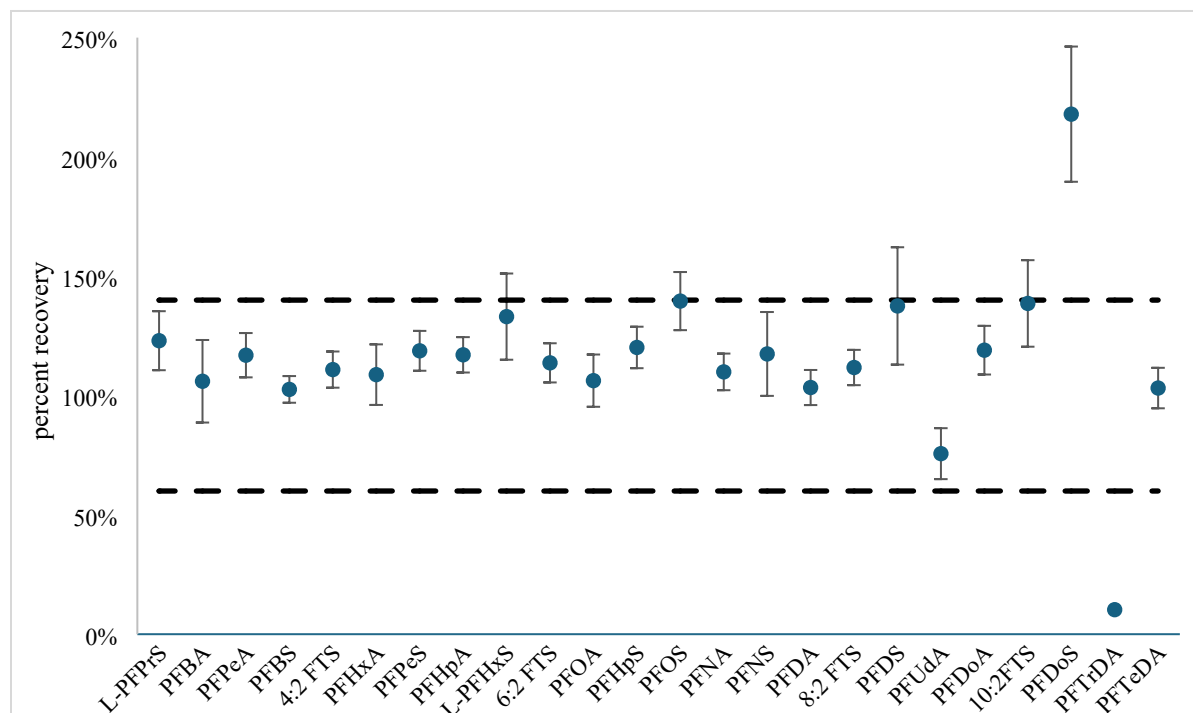


Figure S1: Average percent recoveries (\pm STDEV) for 24 PFASs in triplicate matrix spikes. Dashed lines represent $\pm 40\%$.

Text S1. Ion mobility data processing:

Raw IMS-QTOF files were demultiplexed using the PNNL Preprocessor (v4.1). A single field collision cross section (CCS) calibration was performed using MassHunter IM-MS Browser (v10.0) and reference mass correction was applied using MassHunter IM-MS Reprocessor (v10.00). Chromatographic features were extracted using Agilent Workstation MassHunter Mass Profiler software (v10.0.2). Minimum ion count was set to 600, and alignment tolerances were set to ± 0.10 minutes retention time (RT), $\pm 1.5\%$ drift time, and ± 10.0 ppm m/z . Detection frequency was filtered to require feature detection in $\geq 25\%$ of all samples. The raw peak list (feature table) including RT, m/z , CCS, and peak area for each extracted feature in each sample was loaded into FluoroMatch IM. The CCS library provided with FluoroMatch IM was used as the library file. Homologous series detection was set to search for CF_2 repeating units amongst the features. FluoroMatch IM screening parameters were set as follows: CCS window of $\pm 2\%$, mass window

of ± 0.01 Da, mass defect $-0.11 - 0.12$, polarity 'Neg'. Results were then examined in the output file and visualized in the Microsoft PowerBI Desktop application provided with FluoroMatch IM.

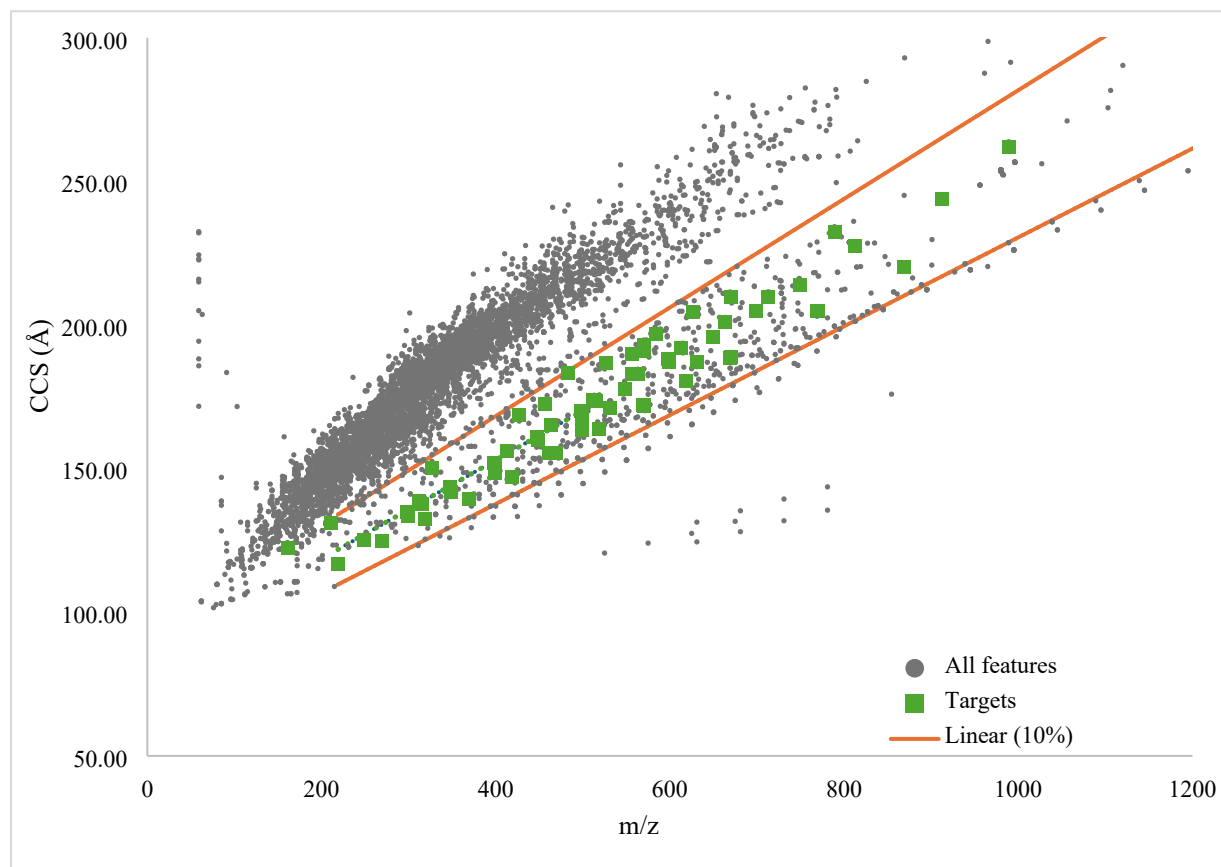


Figure S2: CCS vs m/z plot of in-house target PFASs. Dotted line is the linear fit for target compounds. The upper and lower solid lines represent the bounds of accepted CCS values for PFAS consideration

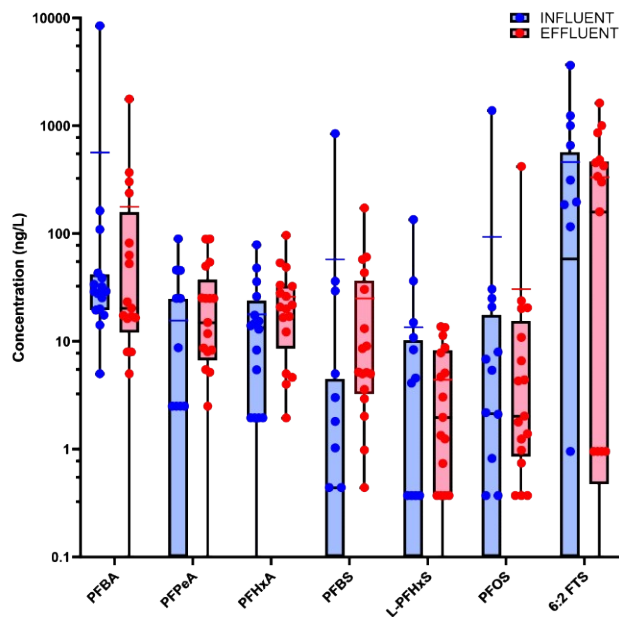


Figure S3: Concentrations of all grab samples for compounds with >50% detection frequency

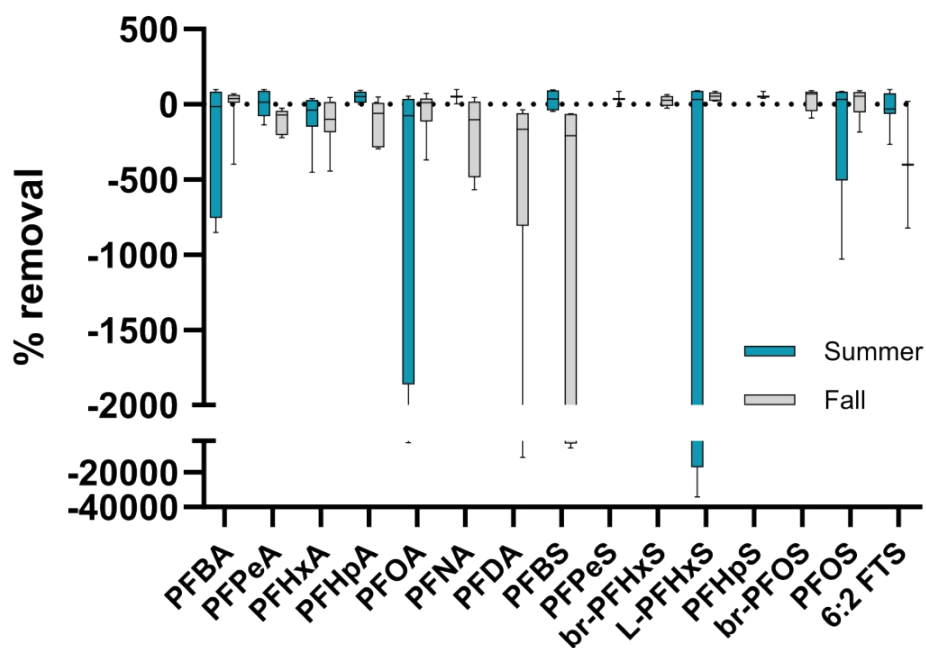


Figure S4: Percent removal of PFASs in grab samples at two time points. Raw, uncensored values.

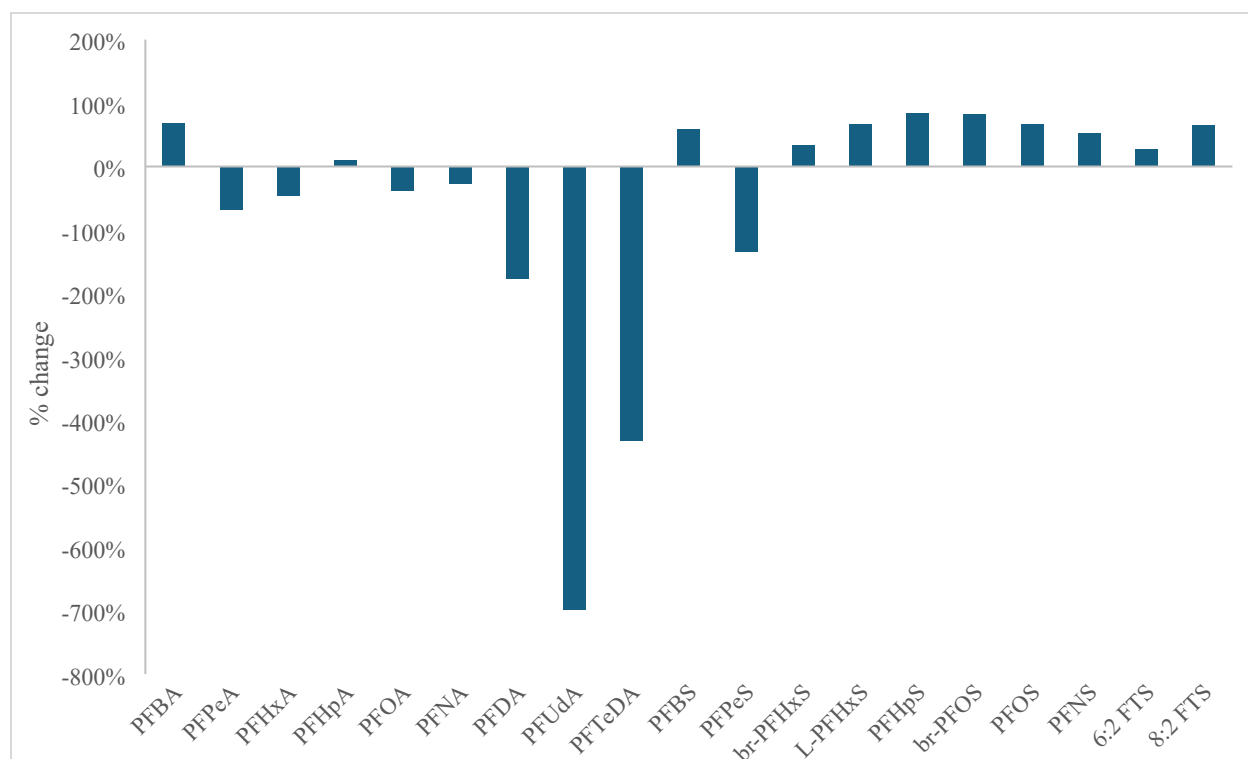


Figure S5: Average percent change of individual PFASs in multi-site grab samples based on average influent and effluent concentrations.