Electronic Supplementary Information for:

TITLE: Sorption and desorption of per- and polyfluoroalkyl substances (PFASs) on unmodified iron oxide and silica clay minerals

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Table S1. Details on suppliers, product numbers, solvents, and stock solution concentrations for all per- and polyfluoroalkyl substances (PFAS) and isotope-labelled internal standards (ILISs) used for this study. Supplier is Wellington Laboratories unless otherwise noted.

Product Name	Name	Acronym	Molecular Formula	Stock Concentration	Solvent[1]	Stock Solution
PFC-MXA	Perfluorobutanoic acid	PFBA	C4HF7O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluoropentanoic acid	PFPeA	C5HF9O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorohexanoic acid	PFHxA	C6HF11O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluoroheptanoic acid	PFHpA	C7HF13O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorooctanoic acid	PFOA	C8HF15O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorononanoic acid	PFNA	C9HF17O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorodecanoic acid	PFDA	C10H19O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluoroundecanoic acid	PFUnA	C11HF21O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorododecanoic acid	PFDoA	C12H23O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorotridecanoic acid	PFTrDA	C13HF25O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFC-MXA	Perfluorotetradecanoic acid	PFTA	C14HF27O2	2 mg L^{-1}	MeOH: (H2O < 1%)	PSS#1
PFS-MXA	Perfluorobutanesulfonic acid	PFBS	C4HF9O3S	2 mg L^{-1}	MeOH	PSS#1
PFS-MXA	Perfluorohexanesulfonic acid	PFHxS	C6HF13O3S	2 mg L^{-1}	MeOH	PSS#1

Product Name	Name	Acronym	Molecular Formula	Stock Concentration	Solvent[1]	Stock Solution
PFS-MXA	Perfluoroheptanesulfonic acid	PFHpS	C7HF15O3S	2 mg L^{-1}	MeOH	PSS#1
PFS-MXA	Perfluorooctanesulfonic acid	PFOS	C8HF17O3S	2 mg L^{-1}	MeOH	PSS#1
PFS-MXA	Perfluorodecanesulfonic acid	PFDS	C10HF21O3S	2 mg L^{-1}	MeOH	PSS#1
FTA-MXA	2-Perfluorohexyl ethanoic acid	6:2 FTCA	C8H3O2F13	2 mg L^{-1}	IPA: (H2O < 0.5%)	PSS#2
FTA-MXA	2-Perfluorooctyl ethanoic acid	8:2 FTCA	C10H3O2F17	2 mg L^{-1}	IPA: (H2O < 0.5%)	PSS#2
FTA-MXA	2-Perfluorodecyl ethanoic acid	10:2 FTCA	C12H3O2F21	2 mg L^{-1}	IPA: (H2O < 0.5%)	PSS#2
FPrPA	3-Perfluoropropyl propanoic acid	3:3 FTCA	C6H5F7O2	50 +/- 2.5 mg L^{-1}	Methanol	PSS#2
FPePA	3-Perfluoropentyl propanoic acid	5:3 FTCA	C8H5F11O2	50 +/- 2.5 mg L^{-1}	Methanol	PSS#2
FPePA	3-Perfluoroheptyl propanoic acid	7:3 FTCA	C10H5F15O2	50 +/- 2.5 mg L^{-1}	Methanol	PSS#2
FHUEA	2H-Perfluoro-2-octenoic acid	5:1:2 FTUCA	C8H2O2F12	50 +/- 2.5 mg L^{-1}	Anhydrous IPA	PSS#2
FOUEA	2H-Perfluoro-2-decenoic acid	7:1:2 FTUCA	C10H2O2F16	50 +/- 2.5 mg L^{-1}	Anhydrous IPA	PSS#2
FDUEA	2H-Perfluoro-2-dodecenoic acid	9:1:2 FTUCA	C12H2O2F20	50 +/- 2.5 mg L^{-1}	Anhydrous IPA	PSS#2
4:2 FTS	1H,1H,2H,2H-Perfluorohexanesulphonic acid	4:2 FTS	C6H5F9O3S	50 +/- 2.5 mg L^{-1}	MeOH	PSS#2
6:2 FTS[2]	1H,1H,2H,2H-Perfluorooctanesulphonic acid	6:2 FTS	C8H5F13O3S	1 g L^{-1}	MeOH	PSS#2
8:2 FTS	1H,1H,2H,2H-perfluorodecanesulfonic acid	8:2 FTS	C10H5F17O3S	50 +/- 2.5 mg L^{-1}	MeOH	PSS#2
Other	1H,1H,2H,2H-perfluorododecanesulfonic acid	10:2 FTS	C12H4F21SO3	50 +/- 2.5 mg L^{-1}	MeOH	PSS#2

Product Name	Name	Acronym	Molecular Formula	Stock Concentration	Solvent[1]	Stock Solution
FBSA	Perfluoro-1-butanesulfonamide	FBSA	C4H2F9NO2S	50 mg L^{-1}	IPA	PSS#2
FOSA	Perfluoro-1-octanesulfonamide	FOSA	C8H2F17NO2S	50 mg L^{-1}	MeOH: (H2O < 1%)	PSS#2
Other[3]	Perfluoro-N-(2- hydroxyethyl)-1butanesulfonamide	FBSE	C6H6F9NO3S	300 mg L^{-1}	IPA	PSS#2
TRC-N649510[3]	Perfluoro-N-(2- methoxyethyl)-1butanesulfonamide	MeFBSE	C7H8F9NO3S	300 mg L^{-1}	IPA	PSS#2
N-MeFOSAA	N-methylperfluoro-1octanesulfonamidoacetic acid	N-MeFOSAA	C11H6F17NO4S	50 +/- 2.5 mg L^{-1}	MeOH: (H2O < 1%)	PSS#2
N-EtFOSAA	N-ethylperfluoro-1octanesulfonamidoacetic acid	N-EtFOSAA	C12H8F17NO4S	50 +/- 2.5 mg L^{-1}	MeOH: (H2O < 1%)	PSS#2
5:3FTB	Undecafluorooctyl)dimethylammonio]acetate	5:3 FTB	C12H14F11NO2	50 +/- 2.5 mg L^{-1}	Methanol	PSS#2
5:1:2FTB	Dodecafluorooctyl)dimethylammonio]acetate	5:1:2 FTB	C12H13F12NO2	50 +/- 2.5 mg L^{-1}	Methanol	PSS#2
N-AmPr-FHxSA	(3-dimethylaminopropan-1-yl) perfluoro-1-hexane-sulfonamide	AmPr-FHxSA	C11H13F13N2O2S	50 +/- 2.5 mg L^{-1}	Methanol	PSS#3
N-TAmPFHxSA	[3-perfluoro-1-hexanesulfonamido) propan-1-yl]-N-trimethylammonium	TAmPr-FHxSA	C12H15F13N2O2S	50 +/- 2.5 mg L^{-1}	Methanol	PSS#3
N-CMAmP6:2FOSA	6:2 fluorotelomer sulfonamide alkylbetanine	6:2 FTAB	C15H19F13N2O4S	50 +/- 2.5 mg L^{-1}	Methanol	PSS#3
MPFAC-MXA	Sodium perfluoro-1hexane[$^{18}O_2$]sulfonate	$^{18}O_2$ - PFHxS	C6HF13[18]O2OS	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Sodium perfluoro-1-[1,2,3,4-$^{13}C_4$]octanesulfonate	$^{13}C_4$ - PFOS	[13]C4C4HF17O3S	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[$^{13}C_4$]butanoic acid	$^{13}C_4$ - PFBA	[13]C4HF7O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[1,2-$^{13}C_2$]hexanoic acid	$^{13}C_2$ - PFHxA	[13]C2C4HF11O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS

Product Name	Name	Acronym	Molecular Formula	Stock Concentration	Solvent[1]	Stock Solution
MPFAC-MXA	Perfluoro-n-[1,2,3,4-$^{13}C_4$]octanoic acid	$^{13}C_4$ - PFOA	[13]C4C4HF15O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[1,2,3,4,5-$^{13}C_5$]nonanoic acid	$^{13}C_5$ - PFNA	[13]C5C4HF17O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[1,2-$^{13}C_2$]decanoic acid	$^{13}C_2$ - PFDA	[13]C2C8HF19O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[1,2-$^{13}C_2$]undecanoic acid	$^{13}C_2$ - PFUnA	[13]C2C9HF21O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS
MPFAC-MXA	Perfluoro-n-[1,2-$^{13}C_2$]dodecanoic acid	$^{13}C_2$ - PFDoA	[13]C2C10HF23O2	2 mg L^{-1}	MeOH: (H2O < 1%)	ILIS

[1] H2O = water, MeOH = methanol, IPA = Isopropanol; [2] Supplier is Santa Cruz Biotech; [3] Supplier is Toronto Research Chemicals.

Table S2. A summary of all other chemicals and solvents used in this study.

Substance	CAS No.	Supplier	Purity
Methanol (OmniSolv®)	67-56-1	Sigma-Aldirch	LC-MS Grade
Water (OmniSolv®)	7732-18-5	Sigma-Aldirch	LC-MS Grade
Acetone	67-64-1	Sigma-Aldirch	HPLC Grade
Ammonium Acetate (for molecular biology)	631-61-8	Sigma-Aldirch	≥ 98%
Sodium Nitrate	7631-99-4	Fisher Scientific	> 99%
Magnesium Sulfate Heptahydrate (ACS)	10034-99-8	Alfa Aesar	98-102%
Barium Chloride Dihydrate	10326-27-9	Beantown Chemical	99%
Barium Hydroxide	12230-71-6	Fisher Scientific	≥ 98.0 %
Nitric Acid (Trace Metal Grade)	7697-37-2	Fisher Scientific	67-70%
Sodium Hydroxide	1310-73-2	VWR International	97%
Hydrochloric Acid (ACS Grade)	7647-01-0	VWR International	36.5-38%

Sorbent materials

Table S3. Details on the chemical composition and physical morphology of each of the four minerals.

Mineral	Type	Molecular Formula	Molecular Weight	CAS No.	BET SSA ($m^2\ g^{-1}$)	$d_{particle}$ (µm)	d_{pore} (average pore diameter (nm)	Pore volume ($mm^3\ g^{-1}$)	Source
Ferrihydrite	Iron-oxide	$Fe_{10}O_{14}(OH)_2 \cdot 3.8H_2O$	884.98	NA	360	10-38	3.3	220	Synthesized in lab
Goethite	Iron-oxide	$FeHO_2$	88.85	20344-49-4	10	10-38	35	26	Santa Cruz Biotechnology
Kaolinite	clay	$Al_2O_3 \cdot 2SiO_2 \cdot 2H_2O$	258.16	1318-74-7	6	10-38	47	16	Sigma-Aldrich
Montmorillonite	clay	$Al_2H_2O_{12}Si_4$	360.31	1318-93-0	264	10-38	4.6	370	Thermo Scientific

Batch experiments

Batch kinetic experiments

Stock solutions of each of the four minerals were prepared in 20 mL amber glass vials at concentrations of 5 g L^{-1} for ferrihydrite and 500 g L^{-1} for goethite, kaolinite, and montmorillonite, mixed for 30 minutes on a magnetic stirrer, ultra-sonicated for 10 minutes, and spiked at 0.5 mL into a 15 mL PP centrifuge tube containing 10 mL of 10 mmol $NaNO_3$. Final concentrations of each mineral in the experiments were 238 mg L^{-1} for ferrihydrite and 23.8 g L^{-1} for goethite, kaolinite, and montmorillonite. No pH adjustments were made in this experiment and pH levels were measured at the time of sampling to be approximately 4, 5, 6.3, and 8.3 for montmorillonite, ferrihydrite, kaolinite, and goethite, respectively. Next, 20 µL of one of the stock solutions (separate batch experiments were completed for PSS#1, PSS#2, and PSS#3) was spiked into each reactor tube to generate an initial concentration of 1 µg L^{-1} for each PFAS. The spiked reactor tubes were loaded onto a tube revolver (ThermoFisher Scientific), rotated at 40 rpm, and removed at time points of 1, 2, 3, 4, and 7 days. After removal, 8 mL of the experimental solution was transferred from the reactor tubes to a syringe and filtered into a new 15 mL PP centrifuge tube. Samples from batch experiments conducted with PSS#1 and PSS#2 were filtered with a 0.45 µm cellulose acetate filter (Restek) and samples from batch experiments conducted with PSS#3 were filtered with a 0.22 µm polyether sulfone filter (Restek). Previous studies have demonstrated adequate recoveries of the target PFASs in each of the respective stock solutions using these types of syringe filters.[1,2] Then, 8 mL of the filtrate was transferred to a 10 mL glass LC-MS vial (ThermoFisher Scientific) and spiked with 12 µL of the ILIS mixture (250 µg L^{-1}) to yield a target ILIS concentration (375 ng L^{-1}). We note that ILISs were not spiked in samples from experiments conducted with PSS#3 because no ILISs were available for the zwitterionic PFASs included in PSS#3. The samples were stored at 4 °C until analysis. Control samples were prepared following the same procedure without the addition of a mineral.

The percent sorption ($\% \, adsorption_{i,t}$) of each PFAS in each replicate sample was calculated by first using the following equation to calculate removal:

$$Rmvl_{i,t} = \frac{C_{control,i,t} - C_{sample,i,j,t}}{C_{control,i,t}} \qquad \text{Equation S1}$$

where *i* is any of the 40 PFASs; *j* is the number of triplicates and *j* = 1, 2, 3; *t* is the contact time at which the sample was taken and *t* = 1, 2, 3, 4, or 7 days; $C_{control,i,t}$ is the concentration of *i* in the control sample; and $C_{sample,i,j,t}$ is the concentration of *i* in replicate *j* taken at time *t*. Then, $\% \, adsorption_{i,t}$ of each PFAS was calculated as the arithmetic average of triplicates:

$$\% \, adsorption_{i,t} = \frac{Rmvl_{i,rep1} + Rmvl_{i,rep2} + Rmvl_{i,rep3}}{3} * 100 \qquad \text{Equation S2}$$

Error bars for $\% \, adsorption_{i,t}$ were calculated using the standard deviation of triplicates.

Batch isotherm experiments

Stock solutions of each of the four minerals were prepared in 20 mL amber glass vials at concentrations of 0.2, 1, and 5 g L^{-1} for ferrihydrite and 20, 100, and 500 g L^{-1} for goethite, kaolinite, and montmorillonite, mixed for 30 minutes on a magnetic stirrer, ultra-sonicated for 10 minutes, and spiked at 0.5 mL into a 15 mL PP centrifuge tube containing 10 mL of 10 mmol $NaNO_3$. Final concentrations of each mineral in the experiments were 10, 48, and 238 mg L^{-1} for ferrihydrite and 1.0, 4.8, and 23.8 g L^{-1} for goethite, kaolinite, and montmorillonite. Batch isotherm experiments were performed at pH levels of 4, 5, 6.3, and 8.3 to span the range of pH levels expected to be encountered in subsurface environments. The pH was adjusted using stock solutions of NaOH and HNO_3 to obtain the target pH level. After the initial pH was recorded, 20 µL of at least one of the PFAS stock solutions was spiked into each reactor tube to generate an initial concentration of 1 µg L^{-1} for each PFAS. For ferrihydrite, three separate batch experiments were completed using PSS#1, PSS#2, and PSS#3. For goethite, kaolinite, and montmorillonite, two separate batch experiments were completed using a combination of PSS#1 and PSS#2 or PSS#3. The spiked reactor tubes were loaded onto a tube revolver (ThermoFisher Scientific), rotated at 40 rpm, and removed at the equilibrium times predetermined by the kinetic batch experiments (two days for ferrihydrite, four days for goethite, seven days for kaolinite, and seven days for montmorillonite). During the equilibration period, the pH was measured at one or a few intermediate time points in side-by-side control experiments and at most one day prior to the prescribed equilibration time. In the case of pH drift, the pH was readjusted to the target pH level of the experiment using NaOH and HNO_3. After removal, 8 mL of the experimental solution was transferred from the reactor tubes to a syringe and filtered into a new 15 mL PP centrifuge tube. Samples from batch experiments conducted with PSS#1 and PSS#2 were filtered with a 0.45 µm cellulose acetate filter (Restek) and samples from batch experiments conducted with PSS#3 were filtered with a 0.22 µm polyether sulfone filter (Restek). Previous studies have demonstrated adequate recoveries of the target PFASs in each of the respective stock solutions using these types of syringe filters.[1,2] Then, 8 mL of the filtrate was transferred to a 10 mL glass LC-MS vial (ThermoFisher Scientific) and spiked with 12 µL of the ILIS mixture (250 µg L^{-1}) to yield a target ILIS concentration (375 ng L^{-1}). We note that ILISs were not spiked in samples from experiments conducted with PSS#3 because no ILISs were available for the zwitterionic PFASs included in PSS#3. The samples were stored at 4 °C until analysis by means of liquid chromatography coupled to mass spectrometry. Control samples were prepared following the same procedure without the addition of a mineral.

For all experiments, PFAS concentrations measured below the limit of quantification (LOQ) were conservatively estimated to be 1% of the control concentration to enable downstream calculations. Then, for batch experiments using PSS#1 and PSS#2, the equilibrium sorption capacity (ng g^{-1}) was calculated as:

$$q_{e_{u,j}} = \frac{C_{control,u} - C_{sample,u,j}}{C_M} \qquad \text{Equation S3}$$

where u is any of the 37 PFASs from PSS#1 and PSS#2; C_M is the mineral concentration and C_M= 10, 48, and 238 mg L^{-1} for ferrihydrite and 1.0, 4.8, and 23.8 g L^{-1} for goethite, kaolinite, and montmorillonite; and $C_{control}$ (ng L^{-1}) and C_{sample} (ng L^{-1}) represent the control and equilibrium PFAS concentrations. If calculated q_e values were negative (concentration measured in the sample was larger than the control) these negative values were replaced with the value of 1% of the control concentration, normalized by the mineral concentration to enable downstream calculations.

For experiments using PSS#3, controls were first averaged using the following equation:

$$\bar{C}_{control,z} = \frac{\sum_{c=1}^{n} C_{control,z,c}}{3} \qquad \text{Equation S4}$$

where z is any of the three zwitterions in PSS#3; C is the control associated with a batch experiment conducted at any one of the three concentrations and c = 10, 48, and 238 mg L^{-1} for ferrihydrite and 1.0, 4.8, and 23.8 g L^{-1} for goethite, kaolinite, and montmorillonite. Consequently, equilibrium sorption capacity (ng g^{-1}) for experiments using PSS#3 were calculated for each mineral as follows:

$$q_{e_{zj,M}} = \frac{\bar{C}_{control,z} - C_{sample,z,j}}{C_M} \qquad \text{Equation S5}$$

The distribution coefficient, K_d (L g^{-1}), was calculated using the following equation:

$$K_{d_{ij\ or\ zj}} = \frac{q_{\mathrm{e_{ij\ or\ zj}}}}{C_{sample,ij\ or\ zj}} \qquad \text{Equation S6}$$

where $q_{\mathrm{e_{ij\ or\ zj,M,pH}}}$ is the amount of sorbed PFAS at equilibrium to mineral *M*. We averaged the K_d values calculated from experiments of the smallest, middle, and largest mineral concentrations (nine K_d values) and we averaged K_d the values calculated from experiments of the middle and largest concentrations (six K_d values) and calculated the coefficient of variation for both sets of averages. The average K_d value that presented the lowest coefficient of variation was selected as the K_d value. This was done to ensure that the K_d value that we report is in the linear range of the otherwise nonlinear isotherm as previously described.[1,3] If the average K_d value across the smallest, middle, and largest concentration was equal to zero, we used the K_d value calculated from the average of the middle and largest concentrations. Error bars for log K_d values were determined using a previously described method for reporting uncertainty of log-transformed data.[4]

Batch desorption experiments

Batch desorption experiments were performed over three decanting cycles for all 40 PFASs and with all four minerals at a pH of 4. We selected this pH value because most PFASs exhibited the highest log K_d values for each of the four minerals at this pH value (data from the batch isotherm experiments) and we reasoned that desorption would be best quantified after the greatest extent of sorption. Stock solutions of each of the four minerals were prepared in 20 mL amber glass vials at concentrations of 1 g L^{-1} for ferrihydrite and 100 g L^{-1} for goethite, kaolinite, and montmorillonite, mixed for 30 minutes on a magnetic stirrer, ultra-sonicated for 10 minutes, and spiked at 0.5 mL into a 15 mL PP centrifuge tube containing 10 mL of 10 mmol $NaNO_3$. Final concentrations of each mineral in the experiments were 48 mg L^{-1} for ferrihydrite and 4.8 g L^{-1} for goethite, kaolinite, and montmorillonite. The pH was adjusted using stock solutions of NaOH and HNO_3 to obtain the target pH. After the initial pH was recorded, 20 µL of the PFAS stock solution was spiked into each reactor tube to generate an initial concentration each of 1 µg L^{-1}. For all four minerals, two separate batch experiments were completed using either a combination of PSS#1 and PSS#2 or PSS#3. The spiked reactor tubes were loaded onto a tube revolver (ThermoFisher Scientific) and rotated at 40 rpm and were removed at the equilibrium times predetermined by the kinetic batch experiments (two days for ferrihydrite, four days for goethite, seven days for kaolinite, and seven days for montmorillonite). During the equilibration period, the pH was measured at one or a few intermediate time points in side-by-side control experiments and at most one day prior to the prescribed equilibration time. In the case of pH drift, the pH was readjusted to the target pH level of the experiment using NaOH and HNO_3. After removal, the reactor tubes were centrifuged at 4,000 rpm for 20 minutes. For goethite only, the sample was filtered after being centrifuged (using the filters described for each PSS in the batch isotherm experiments) due to incomplete separation following centrifugation. Then, 8 mL of the supernatant (or filtrate for goethite) was transferred to a 10 mL glass LC-MS vial (ThermoFisher Scientific) and spiked with 12 µL of the ILIS mixture (250 µg L^{-1}) to yield a target ILIS concentration (375 ng L^{-1}). We note that ILISs were not spiked in samples from experiments conducted with PSS#3 because no ILISs were available for the zwitterionic PFASs included in PSS#3. Then, 8 mL of clean (PFAS-free) 10 mmol $NaNO_3$ was added back to the reactor tube and placed back on the tube revolver for desorption and re-equilibration. This process was repeated three times in total to assess desorption over three decanting cycles. All samples were stored at 4 °C until analysis by means of liquid chromatography coupled to mass spectrometry. Control samples were prepared following the same procedure without the addition of a mineral.

Two additional quality control criteria were needed to process the data from the batch desorption experiments prior to estimating the extent of desorption. First, we must observe some sorption of a PFAS to eventually estimate the extent of desorption. Therefore, we only considered PFASs for which $\%\ adsorption_{i,t}$ was at least 9%. Second, to account for potential PFAS losses on the reactor tubes, we only considered PFASs that exhibited the expected 80% reduction in PFAS concentration in the control reactors (this is the reduction expected when decanting 8 mL from a 10 mL reactor and replacing it with clean PFAS-free solution). For those PFASs that met these two criteria, the mass (m) of each PFAS remaining on the mineral after each desorption cycle was calculated using the following equation:

$$m_{i,d} = q_{\mathrm{e}_{\mathrm{j,i,d}}} * V * C_M \qquad \text{Equation S7}$$

where *i* is any of the 40 PFASs that pass the QC criteria, *j* is the number of triplicates and *j* = 1, 2, 3, *d* is the decanting cycle and *d* = 1, 2, 3, $q_{\mathrm{e}_{\mathrm{j,i,d}}}$ (ng g^{-1}) is the amount of PFAS sorbed at equilibrium, and *V* (L) is the volume of solution in the reactor tube. Percent desorption was then calculated using the following equation:

$$\%\, desorption_{i,d,j} = \left[\frac{m_{i,d,j} - m_{i,d+1,j}}{m_{i,d1,j}}\right] * 100 \qquad \text{Equation S8}$$

where *d+1* is the decanting cycle following the previous cycle (*d*), and *d1* is the first decanting cycle.

Analytical method

The HPLC-HRMS was operated with electrospray ionization in negative polarity mode for experiments spiked with PSS#1, in positive-negative polarity switching mode for experiments spiked with PSS#2 (or for experiments spiked with PSS#1 and PSS#2), and in positive polarity mode for experiments spiked with PSS#3. Analytical information for all PFASs and their ILISs is provided in **Table S4**. The mobile phase consisted of (A) 20 mM ammonium acetate in LC-MS grade water and (B) LC–MS grade methanol (100 %). Samples were injected at 5 mL volumes onto a Hypersil Gold dC18 12 µm 2.1 x 20 mm trap column (ThermoFisher Scientific) at room temperature (21- 22°C) via a loading pump delivering 1 mL min^{-1} of a mobile phase gradient at 99% A and eluted onto an Atlantis® dC18 5 µm 2.1 x 150 mm analytical column (Waters) at 25°C via an elution pump delivering 0.3 mL min^{-1} of a mobile phase gradient at 60% A. The mobile phase gradient program is described in **Table S5**. A matrix-matched calibration curve (n = 9) was prepared with concentrations ranging from 0 to 1000 ng L^{-1} and spiked with 12 µL of the ILIS mixture (250 µg L^{-1}). Quantification of PFASs was from the calibration curve using the PFAS product ion-to-ILIS peak area ratio responses by 1/x weighted linear least-squares regression. Calibration curves were run at the beginning of the analytical run. Instrument blanks (with no target PFASs or ILISs) were run before and after the calibration curve and each batch of triplicate samples. One quality control (QC) sample (with target PFASs and ILISs) was placed at the start of every analytical sequence, to ensure minimal contamination and adequate MS performance (QC tolerance set at ± 30%). Blanks containing LC-MS water were added after every three samples to prevent carryover. The limit of quantification (LOQ) for each PFAS was determined as the lowest point on the calibration curve with at least five MS scans and a PFAS product ion-to-ILIS peak area ratio that could be distinguished from the blank. PFAS spike controls were used to determine the PFAS recovery rate during analysis; recovery rate threshold was set at ± 50% for each PFAS to be considered as reliable data and a variable set of PFASs were considered as reliable data for each type of experiment after analysis.

Table S4. Analytical information of all PFASs and their assigned ILISs.

Name	Acronym	RT (min)	Polarity	Precursor Ion Mass (Da)	Product Ion Mass (Da)	ILIS [a]	pK_a [b]
Perfluorobutanoic acid	PFBA	9.2	neg	212.9786	168.9879	$^{13}C_4$ - PFBA	-0.21 to 0.37
Perfluoropentanoic acid	PFPeA	12.3	neg	262.9760	218.9863	$^{13}C_2$ - PFHxA	-0.80 to 0.40
Perfluorohexanoic acid	PFHxA	15.8	neg	312.9722	268.9829	$^{13}C_2$ - PFHxA	0.20 to 0.42
Perfluoroheptanoic acid	PFHpA	18.8	neg	362.9690	318.9794	$^{13}C_2$ - PFHxA	0.01 to 0.47
Perfluorooctanoic acid	PFOA	21.9	neg	412.9659	368.9767	$^{13}C_4$ - PFOA	0.34
Perfluorononanoic acid	PFNA	23.9	neg	462.9627	418.9737	^{13}C5 - PFNA	0.23 to 0.52
Perfluorodecanoic acid	PFDA	25.2	neg	512.9600	468.9703	$^{13}C_2$ - PFDA	0.40 to 0.52
Perfluoroundecanoic acid	PFUnA	26.7	neg	562.9563	518.9669	$^{13}C_2$ - PFUnA	0.52 to 0.54
Perfluorododecanoic acid	PFDoA	27.5	neg	612.9531	568.9635	$^{13}C_2$ - PFDoA	0.52 to 0.54
Perfluorotridecanoic acid	PFTrDA	28.7	neg	662.9499	618.9601	$^{13}C_2$ - PFDoA	0.52 to -0.54
Perfluorotetradecanoic acid	PFTA	29.6	neg	712.9467	668.9567	$^{13}C_2$ - PFDoA	0.52 to -0.54
Perfluorobutanesulfonic acid	PFBS	13.7	neg	298.9424	98.9543	$^{18}O_2$ - PFHxS	-3.57 to -1.61

Name	Acronym	RT (min)	Polarity	Precursor Ion Mass (Da)	Product Ion Mass (Da)	ILIS [a]	pK_a [b]
Perfluorohexanesulfonic acid	PFHxS	19.7	neg	398.9360	98.9543	$^{18}O_2$ - PFHxS	-3.34 to -1.64
Perfluoroheptanesulfonic acid	PFHpS	21.8	neg	448.9334	98.9543	$^{13}C_4$ - PFOS	-3.27 to -1.64
Perfluorooctanesulfonic acid	PFOS	23.7	neg	498.9296	98.9543	$^{13}C_4$ - PFOS	-3.27 to -1.64
Perfluorodecanesulfonic acid	PFDS	26.2	neg	598.9238	98.9543	$^{13}C_4$ - PFOS	-3.26 to -1.54
2-Perfluorohexyl ethanoic acid	6:2 FTCA	20.0	neg	376.9853	292.9833	$^{18}O_2$ - PFHxS	2.72 to 3.38
2-Perfluorooctyl ethanoic acid	8:2 FTCA	24.4	neg	476.9789	62.9875	^{13}C5 - PFNA	2.69 to 3.41
2-Perfluorodecyl ethanoic acid	10:2 FTCA	27.5	neg	576.9725	62.9873	$^{13}C_2$ - PFUnA	2.83 to 3.42
3-Perfluoropropyl propanoic acid	3:3 FTCA	13.8	neg	241.0105	116.9944	$^{13}C_4$ - PFOA	3.06 to 4.13
3-Perfluoropentyl propanoic acid	5:3 FTCA	19.8	neg	341.0041	216.9888	$^{13}C_2$ - PFHxA	3.54 to 4.18
3-Perfluoroheptyl propanoic acid	7:3 FTCA	23.6	neg	440.9977	316.9829	$^{13}C_2$ - PFHxA	3.36 to 4.22
2H-Perfluoro-2-octenoic acid	5:1:2 FTUCA	19.2	neg	356.9790	292.9832	$^{18}O_2$ - PFHxS	0.29 to 2.89
2H-Perfluoro-2-decenoic acid	7:1:2 FTUCA	24.2	neg	456.9727	392.9771	^{13}C5 - PFNA	0.45 to 2.73

Name	Acronym	RT (min)	Polarity	Precursor Ion Mass (Da)	Product Ion Mass (Da)	ILIS [a]	pK_a [b]
2H-Perfluoro-2-dodecenoic acid	9:1:2 FTUCA	26.7	neg	556.9663	492.9707	$^{13}C_2$ - PFUnA	0.57 to 2.75
1H,1H,2H,2H-Perfluorohexanesulphonic acid	4:2 FTS	16.5	neg	326.9743	80.9637	$^{13}C_2$ - PFHxA	0.93 to 1.25
1H,1H,2H,2H-Perfluorooctanesulphonic acid	6:2 FTS	21.5	neg	426.9679	80.9637	$^{13}C_4$ - PFOA	1.23 to 1.30
1H,1H,2H,2H-perfluorodecanesulfonic acid	8:2 FTS	24.7	neg	526.9615	80.9637	$^{13}C_2$ - PFDA	1.32 to 1.33
1H,1H,2H,2H-perfluorododecanesulfonic acid	10:2 FTS	27.6	neg	626.9551	80.9637	$^{13}C_2$ - PFDoA	1.32 to 1.48
Perfluoro-1-butanesulfonamide	FBSA	16.2	neg	297.9590	77.9638	$^{13}C_2$ - PFHxA	6.48 to 6.97
Perfluoro-1-octanesulfonamide	FOSA	26.5	neg	497.9462	77.9638	$^{13}C_2$ - PFUnA	6.78 to 7.01
Perfluoro-N-(2- hydroxyethyl)-1butanesulfonamide	FBSE	19.4	neg	341.9852	64.9689	$^{13}C_2$ - PFHxA	6.13 to 8.15
Perfluoro-N-(2- methoxyethyl)-1butanesulfonamide	MeFBSE	20.0	neg	356.0008	292.9833	$^{13}C_4$ - PFOA	6.17 to 14.1
N-methylperfluoro-1octanesulfonamidoacetic acid	N-MeFOSAA	26.2	neg	569.9673	82.9595	$^{13}C_2$ - PFUnA	-0.36 to 2.92
N-ethylperfluoro-1octanesulfonamidoacetic acid	N-EtFOSAA	26.4	neg	583.9830	168.9885	$^{13}C_2$ - PFUnA	0.57 to 2.93
Undecafluorooctyl)dimethylammonio]acetate	5:3 FTB	18.7	pos	414.0922	168.9885	No ILIS	1.76

Name	Acronym	RT (min)	Polarity	Precursor Ion Mass (Da)	Product Ion Mass (Da)	ILIS [a]	pK_a [b]
Dodecafluorooctyl)dimethylammonio]acetate	5:1:2 FTB	19.1	pos	432.0827	448.9334	No ILIS	1.73
(3-dimethylaminopropan-1-yl) perfluoro-1-hexane-sulfonamide	AmPr-FHxSA	28	pos	485.0563	85.0888	No ILIS	9.82
[3-perfluoro-1-hexanesulfonamido) propan-1-yl]-N-trimethylammonium	TAmPr-FHxSA	27	pos	499.0719	60.0815	No ILIS	5.86
6:2 fluorotelomer sulfonamide alkylbetanine	6:2 FTAB	22.9	pos	571.0931	58.0658	No ILIS	1.76 to 6.15
Sodium perfluoro-1hexane[$^{18}O_2$]sulfonate	$^{18}O_2$ - PFHxS	18.6	neg	402.9451	83.9643	NA	NA
Sodium perfluoro-1-[1,2,3,4-$^{13}C_4$]octanesulfonate	$^{13}C_4$ - PFOS	23	neg	502.9436	79.9558	NA	NA
Perfluoro-n-[$^{13}C_4$]butanoic acid	$^{13}C_4$ - PFBA	9.7	neg	216.9926	171.9984	NA	NA
Perfluoro-n-[1,2-$^{13}C_2$]hexanoic acid	$^{13}C_2$ - PFHxA	15.7	neg	314.9795	269.9864	NA	NA
Perfluoro-n-[1,2,3,4-$^{13}C_4$]octanoic acid	$^{13}C_4$ - PFOA	21.1	neg	416.9798	371.9862	NA	NA
Perfluoro-n-[1,2,3,4,5-$^{13}C_5$]nonanoic acid	$^{13}C_5$ - PFNA	23	neg	467.9800	422.9866	NA	NA
Perfluoro-n-[1,2-$^{13}C_2$]decanoic acid	$^{13}C_2$ - PFDA	24.7	neg	514.9667	469.9729	NA	NA
Perfluoro-n-[1,2-$^{13}C_2$]undecanoic acid	$^{13}C_2$ - PFUnA	26.3	neg	564.9636	519.9697	NA	NA

Name	Acronym	RT (min)	Polarity	Precursor Ion Mass (Da)	Product Ion Mass (Da)	ILIS [a]	pK$_a$ [b]
Perfluoro-n-[1,2-$^{13}C_2$]dodecanoic acid	$^{13}C_2$ - PFDoA	27.4	neg	614.9604	568.964	NA	NA

[a] ILISs were assigned to target analytes based on recommendations in previously established methods,[5] or based on better matches of retention time (RT), chain length, or head group [b] pK$_a$ values are estimated and were obtained from The CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard/).

Table S5. The mobile phase gradient program for LC-MS analysis.

Pump	**Retention Time (min)**	**Flow Rate (mL min^{-1})**	**Mobile Phase A (%)**[a]	**Mobile Phase B (%)**[b]
LPG	0.000	1.000	99	1
	5.100	1.000	99	1
	5.110	0.000	99	1
	37.200	0.000	99	1
	37.300	1.000	2	98
	41.300	1.000	2	98
	41.400	1.000	99	1
	42.100	1.000	99	1
HPG	0.000	0.300	60%	40%
	6.100	0.300	60%	40%
	6.1-30.1	0.300	decreasing rate 2.083 % min^{-1}	increasing rate 2.083 % min^{-1}
	30.100	0.300	10%	90%
	37.100	0.300	10%	90%
	37.110	0.300	60%	40%
	42.100	0.300	60%	40%

[a] Mobile Phase A consisted of 20 mM ammonium acetate in LC-MS grade water.

[b] Mobile Phase B consisted of LC–MS grade methanol (100 %).

Results and discussion

Quality Control for PFAS Data

All batch experiments were spiked with one or more of the three PFAS stock solutions (PSSs) that contained a total of 40 PFASs. However, the number of PFASs for which we report data for each type of batch experiment varies depending on our quality control (QC) criteria. For the batch kinetic experiments, we report data for any PFAS for which the concentrations in all control samples ($C_{control,i,t}$) is within ±50% of the expected spike concentration (1000 ng L^{-1}). For the batch isotherm experiments, we report data for any PFAS for which the average concentrations in all control samples across the three mineral concentrations ($C_{control,u,M,pH}$) is within ±55% of the expected spike concentration (1000 ng L^{-1}). An exception was made for the three zwitterions in PSS#3 (AmPr-FHxSA, TAmPr-FHxSA and 6:2 FTAB) for which we report data even when PFAS concentrations are outside ±55% QC threshold due to the lack of ILISs for those PFASs. For the batch desorption experiments, we report data for: any PFAS for which the concentrations in all control samples ($C_{control,i,t}$) are within ±50% of the expected spike concentration (1000 ng L^{-1}); for which $\%\ adsorption_{i,t}$ was at least 9% in the first cycle; and for which we observe the expected 80% (±10%) reduction in PFAS concentration in the control reactors across the three decanting cycles (this is the reduction expected when decanting 8 mL from a 10 mL reactor and replacing it with clean PFAS-free solution). One exception was made for 5:1:2 FTB for which we relaxed the range of the expected 80% reduction in PFAS concentration in the control from ±10% to ±15% to be able to report desorption behavior of at least one zwitterion across all four minerals.

Table S6. Summary of PFASs that pass our QC criteria for each type of batch experiment (X = pass).

Experiment	**Kinetics**				**Isotherm**																**Desorption**			
pH[1]	**5**	**8**	**6**	**4**	**4**	**5**	**6**	**8**	**4**	**5**	**6**	**8**	**4**	**5**	**6**	**8**	**4**	**5**	**6**	**8**	**4**	**4**	**4**	**4**
Mineral[2]	**F**	**G**	**K**	**M**	**F**	**F**	**F**	**F**	**G**	**G**	**G**	**G**	**K**	**K**	**K**	**K**	**M**	**M**	**M**	**M**	**F**	**G**	**K**	**M**
PFBA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X					
PFPeA					X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X
PFHxA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
PFHpA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			
PFOA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		
PFNA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			
PFDA	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X				
PFUnA	X	X	X	X		X	X	X		X	X						X		X	X				
PFDoA	X	X	X	X		X	X	X																
PFTrDA																								
PFTA																								
PFBS	X	X	X	X	X	X		X				X	X	X	X	X				X				
PFHxS	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			
PFHpS	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			
PFOS	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
PFDS	X		X																					
6:2 FTCA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X
8:2 FTCA	X	X	X	X		X	X	X		X	X	X		X	X	X	X	X	X	X				
10:2 FTCA	X						X							X										
3:3 FTCA				X	X	X	X	X				X	X	X				X	X	X		X		X
5:3 FTCA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X
7:3 FTCA		X	X	X		X	X	X		X	X	X		X	X	X	X	X	X	X				
5:1:2 FTUCA	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
7:1:2 FTUCA	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X				
9:1:2 FTUCA																								
4:2 FTS		X	X	X	X		X	X	X				X	X		X			X	X				
6:2 FTS	X	X	X	X	X	X	X	X					X	X		X		X		X	X			
8:2 FTS	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X				
10:2 FTS			X	X						X	X													
FBSA	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X			
FOSA																								
FBSE	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
MeFBSE	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X
N-MeFOSAA				X		X	X	X			X	X		X	X		X	X						
N-EtFOSAA						X	X	X			X													
5:3 FTB	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			X	X
5:1:2 FTB	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	
AmPr-FHxSA	X		X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X				
TAmPr-FHxSA	X		X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X				
6:2 FTAB	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
Total PFAS	29	27	31	32	27	33	32	34	23	27	29	26	26	31	27	27	27	28	28	29	11	7	5	7

[1] Actual pH levels were 4, 5, 6.3, and 8.3; [2] F = ferrihydrite, G = goethite, K = kaolinite, M = montmorillonite.

Mineral characterization

Table S7. Zeta-potential for each mineral at varying pH levels.

Mineral	**pH**	**zeta potential (mV)**	**standard deviation (mv)**
Ferrihydrite (238 mg L^{-1})	3.9	28.8	5.5
	4.2	23.7	4.7
	6.3	7.0	6.8
	8.3	-7.2	6.7
Goethite (4.8 g L^{-1})	3.9	14.9	4.9
	5.3	3.0	7.0
	6.2	-2.3	9.0
	8.7	-6.7	5.9
Kaolinite (4.8 g L^{-1})	4	-3.5	4.2
	5.2	-19.3	5.5
	6.2	-50.1	8.0
	8.2	-48.6	9.2
Montmorillonite (4.8 g L^{-1})	4.0	-17.9	6.6
	5	-21.3	7.6
	6.3	-29.6	9.0
	8.5	-30.4	5.6

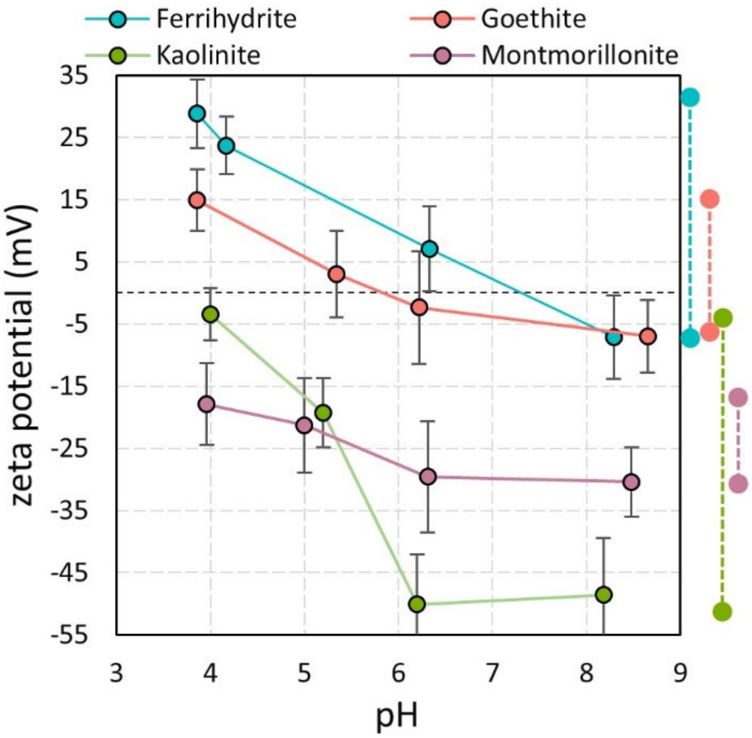

Figure S1. Zeta-potential (mV) as a function of pH (approx. 4 - 8.3) for ferrihydrite (blue), goethite (red), kaolinite (green), and montmorillonite (purple). The vertical dashed lines on the right represent the range of zeta-potential for each mineral. Error bars are the standard deviation of triplicate measurements.

Batch kinetic experiments

Table S8. Equilibrium sorption time for each PFAS on each mineral.

	Equilibrium sorption time [days]			
	Ferrihydrite	**Goethite**	**Montmorillonite**	**Kaolinite**
PFBA	2	2	2	4
PFHxA	2	3	2	2
PFHpA	2	3	2	2
PFOA	2	2	2	2
PFNA	2	2	2	2
PFDA	2	2	2	3
PFUnA	2	2	3	7
PFDoA	2	2	3	2
PFBS	2	2	2	2
PFHxS	2	2	2	2
PFHpS	2	2	2	2
PFOS	2	2	2	3
PFDS	2	NA	3	NA
6:2 FTCA	2	7	7	2
8:2 FTCA	2	4	2	4
10:2 FTCA	2	NA	NA	NA
3:3 FTCA	NA	NA	NA	2
5:3 FTCA	3	2	3	2
7:3 FTCA	NA	2	2	2
5:1:2 FTUCA	3	2	4	3
7:1:2 FTUCA	2	2	2	3
4:2 FTS	NA	2	7	3
6:2 FTS	2	7	4	3
8:2 FTS	2	2	7	2
10:2 FTS	NA	NA	2	2
FBSA	2	2	2	2
FBSE	3	2	2	2
MeFBSE	3	2	4	2
N-MeFOSAA	NA	NA	NA	3
5:3 FTB	3	2	2	2
5:1:2 FTB	2	2	3	2
AmPr-FHxSA	2	NA	2	4
TAmPr-FHxSA	2	NA	2	2
6:2 FTAB	3	2	2	2

Batch isotherm experiments

Table S9. log K_d values reported as average ± standard deviation for each PFAS on ferrihydrite.

log K_d values (units as L g^{-1} prior to log transformation) for each PFAS on ferrihydrite												
	pH 4			**pH 5**			**pH 6.3**			**pH 8.3**		
PFBA	-1.10	±	0.39	-0.60	±	0.42	-1.03	±	0.40	-0.97	±	0.38
PFPeA	0.40	±	0.60	-0.28	±	0.37	-0.96	±	0.36	-0.12	±	0.54
PFHxA	0.62	±	0.54	-0.08	±	0.28	-0.36	±	0.41	-0.92	±	0.34
PFHpA	0.53	±	0.51	0.38	±	0.19	-0.23	±	0.56	-0.32	±	0.41
PFOA	0.61	±	0.48	0.42	±	0.18	0.45	±	0.50	0.06	±	0.42
PFNA	1.37	±	0.37	0.92	±	0.13	-0.46	±	0.33	-0.02	±	0.42
PFDA	1.88	±	0.31	1.48	±	0.14	0.23	±	0.14	0.34	±	0.47
PFUnA	N/A	±	N/A	1.79	±	0.28	0.79	±	0.06	0.52	±	0.55
PFDoA	N/A	±	N/A	2.10	±	0.29	1.23	±	0.19	0.73	±	0.28
PFBS	-1.40	±	0.25	0.45	±	0.66	N/A	±	N/A	-1.07	±	0.36
PFHxS	0.72	±	0.63	0.01	±	0.33	-0.27	±	0.34	-0.28	±	0.41
PFHpS	1.11	±	0.51	0.38	±	0.28	0.10	±	0.54	0.58	±	0.60
PFOS	1.59	±	0.43	1.08	±	0.22	0.39	±	0.38	0.88	±	0.43
6:2 FTCA	0.85	±	0.30	0.65	±	0.26	-0.38	±	0.35	-1.08	±	0.45
8:2 FTCA	N/A	±	N/A	1.82	±	0.13	0.27	±	0.30	0.11	±	0.47
10:2 FTCA	N/A	±	N/A	N/A	±	N/A	1.21	±	0.59	N/A	±	0.67
3:3 FTCA	0.53	±	0.58	0.68	±	0.43	-0.98	±	0.39	0.10	±	0.65
5:3 FTCA	0.85	±	0.36	0.66	±	0.23	-0.24	±	0.38	-0.93	±	0.34
7:3 FTCA	N/A	±	N/A	2.10	±	0.11	0.74	±	0.24	0.40	±	0.47
5:1:2 FTUCA	0.49	±	0.50	-0.75	±	0.50	-0.94	±	0.36	-0.12	±	0.35
7:1:2 FTUCA	1.79	±	0.28	1.31	±	0.11	0.24	±	0.33	0.46	±	0.54
4:2 FTS	0.30	±	0.66	N/A	±	N/A	-0.23	±	0.69	0.02	±	0.64
6:2 FTS	0.45	±	0.47	0.69	±	0.34	-0.09	±	0.60	0.14	±	0.52
8:2 FTS	1.80	±	0.31	1.51	±	0.18	0.32	±	0.42	0.67	±	0.45
FBSA	0.52	±	0.59	0.27	±	0.66	N/A	±	N/A	-0.33	±	0.43
FBSE	0.05	±	0.61	0.32	±	0.66	-0.20	±	0.37	-0.17	±	0.42
MeFBSE	0.67	±	0.49	-0.20	±	0.53	-0.94	±	0.36	-0.24	±	0.46
N-MeFOSAA	N/A	±	N/A	2.66	±	0.11	1.07	±	0.15	0.65	±	0.49
N-EtFOSAA	N/A	±	N/A	2.47	±	0.10	1.10	±	0.19	0.77	±	0.47
5:3 FTB	0.03	±	0.52	-0.07	±	0.20	-1.01	±	0.35	-0.94	±	0.34
5:1:2 FTB	0.23	±	0.41	-0.46	±	0.27	-0.33	±	0.33	-0.53	±	0.33
AmPr-FHxSA	-1.19	±	0.32	0.89	±	0.61	1.54	±	0.59	-1.09	±	0.42
TAmPr-FHxSA	-0.37	±	0.42	-0.10	±	0.66	0.54	±	0.66	0.25	±	0.62
6:2 FTAB	0.43	±	0.25	0.71	±	0.36	0.53	±	0.28	-0.15	±	0.45

Table S10. log K_d values reported as average ± standard deviation for each PFAS on goethite.

log K_d values (units as L g^{-1} prior to log transformation) for each PFAS on goethite												
	pH 4			**pH 5**			**pH 6.3**			**pH 8.3**		
PFBA	-2.69	±	0.55	-2.92	±	0.67	-2.93	±	0.64	-2.50	±	0.55
PFPeA	-2.69	±	0.34	-2.26	±	0.47	-2.19	±	0.25	-1.90	±	0.39
PFHxA	-1.34	±	0.30	-1.27	±	0.30	-1.32	±	0.34	-2.59	±	0.14
PFHpA	-0.95	±	0.35	-1.19	±	0.25	-1.42	±	0.34	-1.93	±	0.67
PFOA	-0.46	±	0.31	-0.69	±	0.23	-0.96	±	0.29	-2.20	±	0.27
PFNA	-0.45	±	0.31	-0.55	±	0.26	-0.68	±	0.24	-1.50	±	0.36
PFDA	-0.13	±	0.28	-0.36	±	0.27	-0.51	±	0.32	N/A	±	N/A
PFUnA	N/A	±	N/A	-0.26	±	0.31	-0.29	±	0.32	N/A	±	N/A
PFBS	N/A	±	N/A	N/A	±	N/A	N/A	±	N/A	-1.27	±	0.44
PFHxS	-0.59	±	0.28	-0.81	±	0.26	-1.01	±	0.33	-2.11	±	0.39
PFHpS	-0.26	±	0.32	-0.57	±	0.25	-0.74	±	0.28	-1.56	±	0.37
PFOS	-0.43	±	0.35	-0.58	±	0.32	-0.57	±	0.31	-1.09	±	0.40
6:2 FTCA	-0.65	±	0.30	-0.73	±	0.21	-0.88	±	0.29	-1.36	±	0.32
8:2 FTCA	N/A	±	N/A	-0.24	±	0.28	-0.53	±	0.26	-0.50	±	0.32
3:3 FTCA	N/A	±	N/A	N/A	±	N/A	N/A	±	N/A	-0.72	±	0.26
5:3 FTCA	-0.36	±	0.32	-0.66	±	0.18	-1.16	±	0.29	-1.33	±	0.31
7:3 FTCA	N/A	±	N/A	0.24	±	0.25	-0.61	±	0.31	-1.46	±	0.67
5:1:2 FTUCA	-0.79	±	0.25	-1.05	±	0.21	-1.23	±	0.28	-1.44	±	0.33
7:1:2 FTUCA	N/A	±	N/A	-0.32	±	0.20	-0.55	±	0.28	-0.69	±	0.36
4:2 FTS	-2.74	±	0.55	N/A	±	N/A	N/A	±	N/A	N/A	±	N/A
8:2 FTS	-0.10	±	0.21	-0.61	±	0.16	-0.61	±	0.31	-0.31	±	0.37
10:2 FTS	N/A	±	N/A	-3.18	±	0.30	-3.09	±	0.81	N/A	±	N/A
FBSA	-1.55	±	0.36	-1.77	±	0.34	-1.95	±	0.57	-1.84	±	0.32
FBSE	-1.03	±	0.33	-1.10	±	0.26	-1.06	±	0.35	-1.68	±	0.40
MeFBSE	-0.64	±	0.23	-0.86	±	0.25	-1.08	±	0.31	-3.09	±	0.35
N-MeFOSAA	N/A	±	N/A	N/A	±	N/A	-0.46	±	0.41	-0.24	±	0.09
N-EtFOSAA	N/A	±	N/A	N/A	±	N/A	-0.08	±	0.33	N/A	±	N/A
5:3 FTB	-1.16	±	0.32	-0.95	±	0.23	-0.73	±	0.32	-0.63	±	0.27
5:1:2 FTB	-1.15	±	0.37	-0.91	±	0.18	-1.01	±	0.29	-0.84	±	0.24
AmPr-FHxSA	-0.21	±	0.16	-0.14	±	0.51	-0.77	±	0.17	-3.48	±	0.35
TAmPr-FHxSA	-0.36	±	0.20	-0.04	±	0.58	-0.46	±	0.15	-1.51	±	0.32
6:2 FTAB	-0.85	±	0.21	-0.71	±	0.13	-0.96	±	0.08	-0.85	±	0.09

Table S11. log K_d values reported as average ± standard deviation for each PFAS on montmorillonite.

log K_d values (units as L g^{-1} prior to log transformation) for each PFAS on montmorillonite												
	pH 4			**pH 5**			**pH 6.3**			**pH 8.3**		
PFBA	-2.79	±	0.18	-2.34	±	0.51	-1.68	±	0.50	N/A	±	0.48
PFPeA	-2.25	±	0.40	-2.65	±	0.18	-2.15	±	0.26	-1.20	±	0.39
PFHxA	-2.23	±	0.32	-1.63	±	0.36	-1.50	±	0.28	-1.52	±	0.39
PFHpA	-1.95	±	0.20	-1.45	±	0.44	-1.55	±	0.47	-2.19	±	0.56
PFOA	-2.04	±	0.45	-1.10	±	0.31	-1.03	±	0.37	-1.09	±	0.40
PFNA	-1.20	±	0.35	-0.97	±	0.32	-0.60	±	0.30	-0.88	±	0.56
PFDA	-0.68	±	0.35	-0.86	±	0.38	-0.53	±	0.22	-0.73	±	0.64
PFUnA	-0.13	±	0.38	N/A	±	N/A	-0.57	±	0.23	-0.94	±	0.46
PFBS	-2.91	±	0.35	N/A	±	N/A	N/A	±	N/A	-1.31	±	0.22
PFHxS	-0.73	±	0.32	-0.92	±	0.24	-0.87	±	0.26	-0.79	±	0.38
PFHpS	-0.07	±	0.32	-0.57	±	0.19	-0.45	±	0.20	-0.63	±	0.36
PFOS	0.71	±	0.37	-0.30	±	0.25	-0.23	±	0.15	-0.21	±	0.32
PFDS	0.40	±	0.47	-0.14	±	0.11	0.02	±	0.13	0.26	±	0.36
6:2 FTCA	0.15	±	0.29	-0.50	±	0.29	0.97	±	0.44	-0.10	±	0.67
8:2 FTCA	-0.67	±	0.18	-0.60	±	0.22	0.93	±	0.50	-0.09	±	0.65
3:3 FTCA	N/A	±	0.35	-0.25	±	0.40	-0.20	±	0.40	-0.22	±	0.40
5:3 FTCA	-0.92	±	0.10	-0.39	±	0.38	-0.71	±	0.43	-1.53	±	0.48
7:3 FTCA	0.35	±	0.15	-0.55	±	0.16	-0.60	±	0.42	-1.21	±	0.51
5:1:2 FTUCA	-1.77	±	0.08	-0.76	±	0.32	-0.50	±	0.42	-0.68	±	0.33
7:1:2 FTUCA	-1.32	±	0.29	-0.95	±	0.37	-0.35	±	0.30	-0.71	±	0.48
4:2 FTS	N/A	±	N/A	N/A	±	N/A	-1.11	±	0.47	-2.87	±	0.25
6:2 FTS	N/A	±	N/A	-2.43	±	0.41	N/A	±	N/A	-2.49	±	0.48
8:2 FTS	-0.50	±	0.32	-1.31	±	0.90	-1.10	±	0.46	-1.13	±	0.54
FBSA	-2.08	±	0.55	-1.26	±	0.45	-1.22	±	0.42	-1.27	±	0.41
FBSE	-1.68	±	0.16	-0.85	±	0.37	-0.76	±	0.38	-0.90	±	0.29
MeFBSE	-2.16	±	0.18	-1.86	±	0.41	-1.17	±	0.37	-1.58	±	0.35
N-MeFOSAA	-0.86	±	0.13	-0.60	±	0.42	N/A	±	N/A	N/A	±	0.44
5:3 FTB	0.94	±	0.24	0.20	±	0.12	-0.48	±	0.08	-0.65	±	0.10
5:1:2 FTB	0.91	±	0.35	0.01	±	0.29	-0.60	±	0.12	-0.85	±	0.15
AmPr-FHxSA	0.11	±	0.38	-0.16	±	0.15	-2.41	±	0.10	-0.69	±	0.38
TAmPr-FHxSA	0.26	±	0.43	1.01	±	0.39	0.75	±	0.41	0.78	±	0.19
6:2 FTAB	-0.34	±	0.41	1.01	±	0.27	0.72	±	0.14	0.55	±	0.27

Table S12. log K_d values reported as average ± standard deviation for each PFAS on kaolinite.

log K_d values (units as L g^{-1} prior to log transformation) for each PFAS on kaolinite												
	pH 4			**pH 5**			**pH 6.3**			**pH 8.3**		
PFBA	-2.26	±	0.46	-2.99	±	0.63	-1.68	±	0.56	-2.39	±	0.46
PFPeA	-2.07	±	0.32	-1.73	±	0.27	-2.01	±	0.32	-1.67	±	0.20
PFHxA	-2.20	±	0.27	-2.12	±	0.34	-2.39	±	0.43	-1.69	±	0.13
PFHpA	-1.71	±	0.41	-1.67	±	0.32	-2.57	±	0.46	-1.66	±	0.16
PFOA	-1.06	±	0.33	-0.96	±	0.23	-2.46	±	0.40	-1.77	±	0.52
PFNA	-0.71	±	0.33	-0.63	±	0.26	-1.75	±	0.27	-1.62	±	0.58
PFDA	-0.10	±	0.40	-0.19	±	0.55	-1.19	±	0.31	-1.63	±	0.73
PFBS	-2.10	±	0.44	-1.48	±	0.50	-2.72	±	0.36	-1.64	±	0.35
PFHxS	-1.02	±	0.38	-1.33	±	0.24	-1.51	±	0.32	-1.71	±	0.36
PFHpS	-0.81	±	0.30	-0.61	±	0.26	-0.73	±	0.31	-1.31	±	0.40
PFOS	-0.37	±	0.34	-0.64	±	0.28	-0.11	±	0.36	-1.30	±	0.52
6:2 FTCA	0.27	±	0.23	0.83	±	0.35	0.21	±	0.34	-1.37	±	0.33
8:2 FTCA	N/A	±	N/A	-0.36	±	0.34	-0.76	±	0.13	-1.32	±	0.20
10:2 FTCA	N/A	±	N/A	0.85	±	0.51	N/A	±	N/A	N/A	±	N/A
3:3 FTCA	N/A	±	N/A	-2.06	±	0.41	N/A	±	N/A	-1.24	±	0.75
5:3 FTCA	-1.40	±	0.28	-1.53	±	0.26	-2.09	±	0.37	-1.73	±	0.28
7:3 FTCA	N/A	±	N/A	-1.14	±	0.24	-1.87	±	0.94	-1.63	±	0.50
5:1:2 FTUCA	-1.42	±	0.33	-1.86	±	0.21	-2.55	±	0.18	-1.97	±	0.22
7:1:2 FTUCA	-1.21	±	0.13	-1.36	±	0.12	-2.65	±	0.31	-1.40	±	0.09
4:2 FTS	-2.09	±	0.57	-2.98	±	0.63	N/A	±	N/A	-1.37	±	0.95
6:2 FTS	-1.39	±	0.46	-1.29	±	0.63	N/A	±	N/A	-2.95	±	0.71
8:2 FTS	N/A	±	N/A	-1.08	±	0.38	-0.60	±	0.49	-1.91	±	0.24
FBSA	-2.93	±	0.32	-2.36	±	0.54	-1.91	±	0.28	-2.29	±	0.50
FBSE	-2.09	±	0.50	-2.34	±	0.39	-2.32	±	0.32	-2.26	±	0.56
MeFBSE	-2.26	±	0.29	-2.93	±	0.31	-2.07	±	0.42	-2.39	±	0.58
N-MeFOSAA	N/A	±	N/A	-0.85	±	0.17	-0.95	±	0.37	N/A	±	N/A
5:3 FTB	-1.00	±	0.37	-1.39	±	0.32	-3.04	±	0.32	-1.58	±	0.26
5:1:2 FTB	-0.79	±	0.52	-1.26	±	0.36	-3.04	±	0.34	-1.49	±	0.20
AmPr-FHxSA	-0.27	±	0.43	-1.30	±	0.51	-0.67	±	0.34	-0.45	±	0.00
TAmPr-FHxSA	-0.47	±	0.40	-0.50	±	0.31	-0.19	±	0.35	N/A	±	N/A
6:2 FTAB	-0.92	±	0.36	-1.24	±	0.56	-3.01	±	0.40	-0.97	±	0.72

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