

Table S9. Molecular characteristics and analytical performance of the target PFAS compounds

PFAS compounds	Molecular formula	LOD (ng/mL)	LOQ (ng/mL)	ULOQ (ng/mL)	R ²	Calibration (ng/mL)	Recovery (%)	Precision (RSD, %)
11Cl-PF3OUdS	C ₁₀ HClF ₂₀ O ₄ S	0.02	0.05	200.00	0.9986	20.0	106.44	3.22
9Cl-PF3ONS	C ₉ HClF ₁₈ O ₄ S	0.02	0.05	100.00	0.9989	20.0	98.70	5.62
PFBS	C ₄ HF ₉ O ₂ S	0.02	0.05	100.00	0.9992	20.0	96.59	5.71
PFHpS	C ₇ HF ₁₃ O ₂ S	0.02	0.05	200.00	0.9991	20.0	94.73	7.88
PFHxS	C ₈ HF ₁₅ O ₂ S	0.10	0.20	200.00	0.9993	20.0	91.36	14.13
PFOS	C ₈ HF ₁₇ O ₂ S	0.01	0.02	100.00	0.9999	20.0	99.64	3.08
PFPeS	C ₅ HF ₁₁ O ₂ S	0.01	0.02	100.00	0.9994	20.0	96.78	3.78
PFUnA	C ₁₁ HF ₂₁ O ₂	0.01	0.02	100.00	0.9998	20.0	112.22	6.53
PFDA	C ₁₀ HF ₁₉ O ₂	0.10	0.20	200.00	0.9982	20.0	105.12	4.81
PFBA	C ₄ HF ₇ O ₂	0.10	0.20	25.00	0.9963	20.0	99.99	2.97
PFDoA	C ₁₂ HF ₂₃ O ₂	0.01	0.02	25.00	0.9999	20.0	117.53	3.09
PFHpA	C ₇ HF ₁₃ O ₂	0.01	0.02	200.00	0.9991	20.0	98.67	3.91
PFNA	C ₉ HF ₁₇ O ₂	0.10	0.20	100.00	0.9979	20.0	100.10	6.76
PFOA	C ₈ HF ₁₅ O ₂	0.05	0.10	50.00	0.9983	20.0	102.32	2.82
PFPeA	C ₅ HF ₉ O ₂	0.39	0.78	200.00	0.9994	20.0	98.39	3.07
PFTeDA	C ₁₄ HF ₂₇ O ₂	0.39	0.78	200.00	0.9989	20.0	96.82	4.72
PFTTrDA	C ₁₅ HF ₂₉ O ₂	0.01	0.02	50.00	0.9999	20.0	116.20	3.90

Note: LOD, limit of detection; LOQ, limit of quantification; ULOQ, upper limit of quantification; R², coefficient of determination.