

SUPPORTING INFORMATION for

Uptake of Per- and Polyfluorinated Alkyl Substances by Dry Farmed Oats Following the Agricultural Application of Biosolids and Compost

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Figure S1. (a) Site A biosolids; (b) Site B biosolids; (c) Site C compost



Figure S2. (a) Recoveries of all surrogates in each matrix and extraction blank; (b) recoveries of surrogates used for internal calibration of analytes after removal of poorly recovered surrogates per matrix.

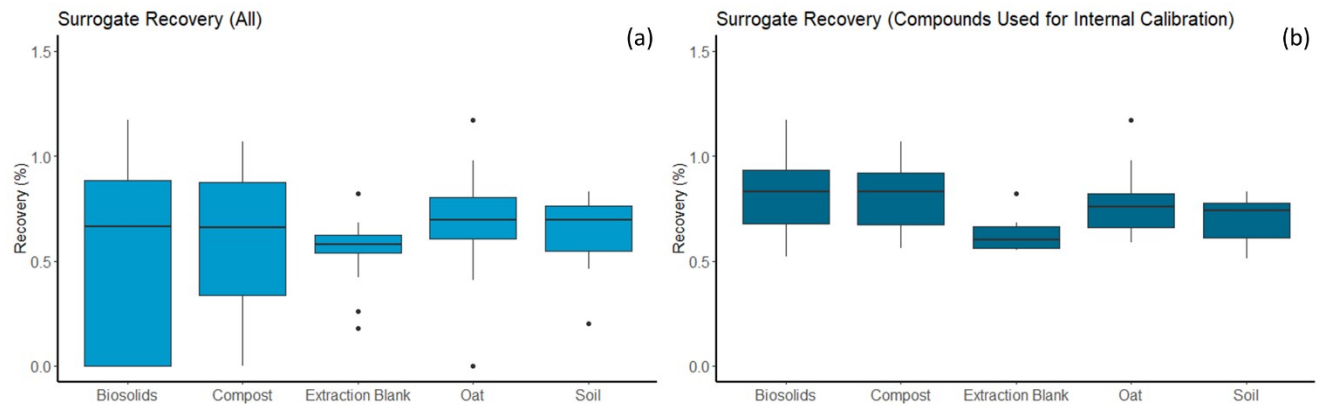


Figure S3. (a) Analyte recovery for all analytes per matrix (b) Analyte recovery after removing poorly recovered (<20%) analytes that were excluded from quantification.

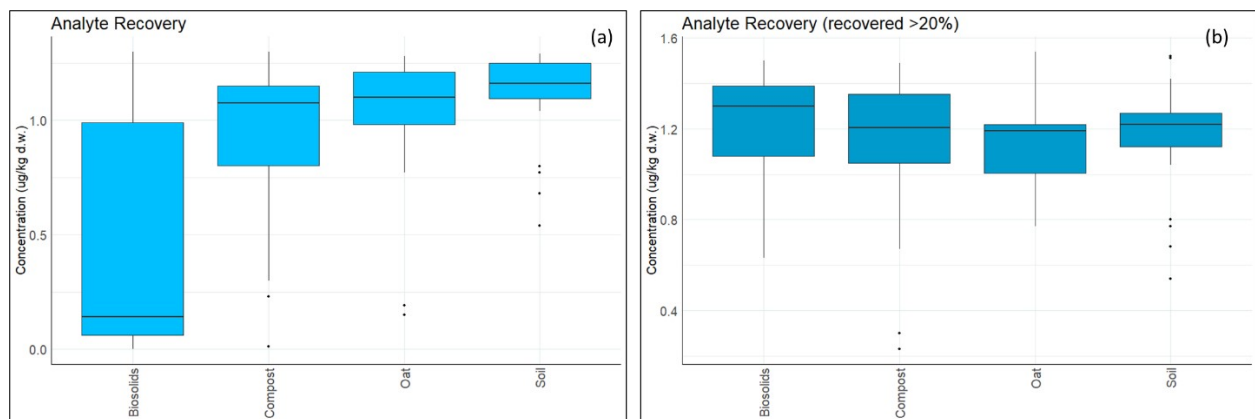


Figure S4. Physical characteristics of soil from three sites receiving five types of amendment. Site A: biosolids + lime application; Site B: biosolids + lime application; Site C1: USDA organic site, no amendment; Site C2: USDA organic site, compost application; Site C3: USDA organic site, compost and lime application.

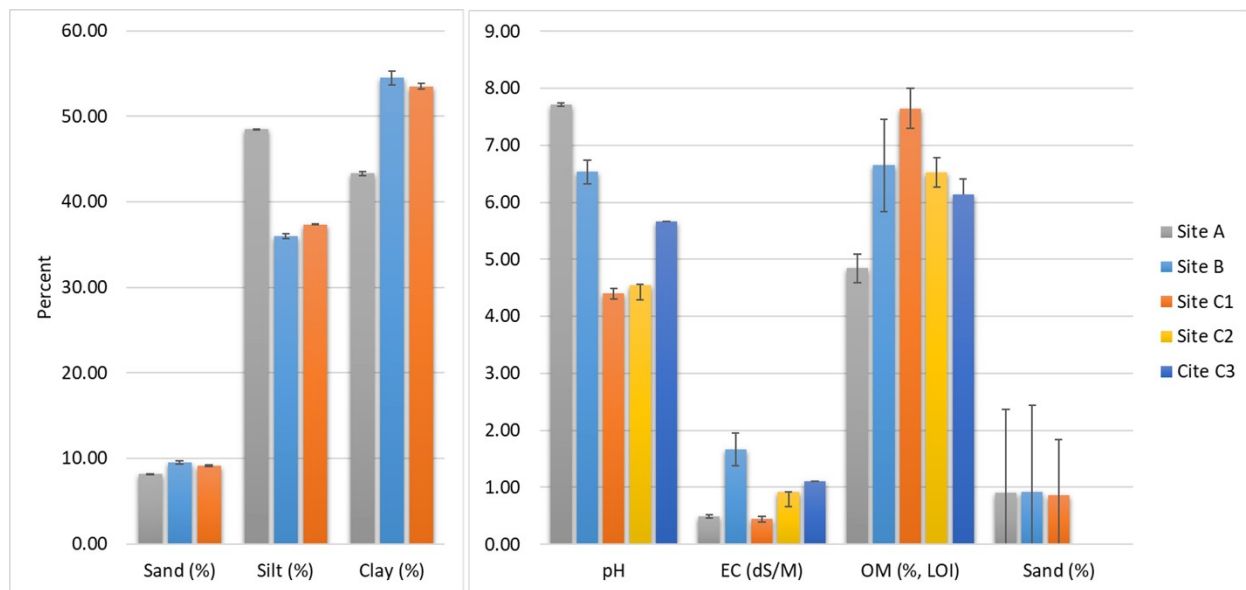


Table S1. Target analytes

Target Analyte	Abbreviation
1H,1H,2H,2H-perfluorohexane sulfonate	4:2 FTS
1H,1H,2H,2H-perfluoro-1-octanesulfonate	6:2 FTS
1H,1H,2H,2H-Perfluorodecane sulfonate	8:2 FTS
Perfluoro-1-butanesulfonate	PFBS
Perfluoro-1-pentanesulfonate	PFPeS
Perfluoro-1-hexanesulfonate	PFHxS
Perfluoro-1-heptanesulfonate	PFHpS
Perfluoro-1-octanesulfonate	PFOS
Perfluoro-1-nonanesulfonate	PFNS
Perfluoro-1-decane sulfonate	PFDS
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonate	9-Cl-PF3ONS
11-Chloroeicosafluoro-3-oxaundecane-1-sulfonate	11-Cl-PF3OudS
Perfluoro-n-butanoic acid	PFBA
Perfluoro-n-pentanoic acid	PFPeA
Perfluoro-n-hexanoic acid	PFHxA
Perfluoro-n-heptanoic acid	PFHpA
Perfluoro-n-octanoic acid	PFOA
Perfluoro-n-nonanoic acid	PFNA
Perfluoro-n-decanoic acid	PFDA
Perfluoro-n-undecanoic acid	PFUnA
Perfluoro-n-dodecanoic acid	PFDoA
Perfluoro-n-tridecanoic acid	PFTTrDA
Perfluoro-n-tetradecanoic acid	PFTeDA
bis(1H,1H,2H,2H-perfluorooctyl)phosphate	6:2 diPAP
Perfluorooctane sulfonamide	FOSA
N-methylperfluorooctanesulfonamidoacetic acid	MeFOSAA
N-ethylperfluorooctanesulfonamidoacetic acid	EtFOSAA
N-methylperfluoro-1-octanesulfonamide	N-MeFOSA-M
2-(N-methylperfluoro-1-octanesulfonamido)-ethanol	N-MeFOSE-M
2-(N-ethylperfluoro-1-octanesulfonamido)-ethanol	N-EtFOSE-M
N-ethylperfluoro-1-octanesulfonamide	N-EtFOSA-M
Tetrafluoro(heptafluoropropoxy)propanoic acid	HFPO-DA
Dodecafluoro-3H-4,8-dioxanonoate	NaDONA

Table S2. Isotopically labelled surrogate standards

Standard	Type
Sodium 1H,1H,2H,2H-[1,2-13C2]perfluorooctylphosphate	Surrogate
Perfluoro-n-[2,3,4-13C3]butanoic acid	Performance Standard
Perfluoro-n-[13C4]butanoic acid	Surrogate
Perfluoro-n-[13C5]pentanoic acid	Surrogate
Perfluoro-n-[1,2,3,4,6-13C5]hexanoic acid	Surrogate
Perfluoro-n-[1,2,3,4-13C4]heptanoic acid	Surrogate
Perfluoro-n-[1,2-13C2]octanoic acid	Performance Standard
Perfluoro-n-[13C8]octanoic acid	Surrogate
Perfluoro-n-[13C9]nonanoic acid	Surrogate
Perfluoro-n-[1,2-13C]decanoic acid	Performance Standard
Perfluoro-n-[1,2,3,4,5,6-13C6]decanoic acid	Surrogate
Perfluoro-n-[1,2,3,4,5,6,7-13C7]undecanoic acid	Surrogate
Perfluoro-n-[1,2-13C2]dodecanoic acid	Surrogate
Perfluoro-n-[1,2-13C2]tetradecanoic acid	Surrogate
2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-13C3-propanoic acid	Surrogate
Sodium perfluoro-1-[2,3,4-13C3]butanesulfonate	Surrogate
Sodium perfluoro-1-[1,2,3-13C3]hexanesulfonate	Surrogate
Sodium perfluoro-1-[1,2,3,4-13C4]octanesulfonate	Performance Standard
Sodium perfluoro-1-[13C8]octanesulfonate	Surrogate
Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2)	Surrogate
N-methyl-d3-perfluoro-1-octanesulfonamide	Surrogate
N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	Surrogate
2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	Surrogate

Table S3. Surrogate recoveries in matrix spikes. Reported recovery is the average of a matrix spike and matrix spike duplicate. Gray shaded cells denote recoveries $\leq 50\%$. For analytes that were matched with low recovery surrogates, external calibration curves were used to quantify analyte concentrations.

Surrogate analyte	Performance Standard	Oat	Compost	Soil	Biosolids	Extraction Blank
Perfluoro-n-[1,2,3,4,5,6,7-13C7]undecanoic acid	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	66%	0%	46%	0%	60%
Perfluoro-n-[1,2-13C2]tetradecanoic acid	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	76%	40%	78%	0%	82%
Perfluoro-n-[13C5]pentanoic acid	Perfluoro-n-[1,2-13C2]octanoic acid	89%	92%	79%	92%	42%
Perfluoro-1-[13C8]octanesulfonate	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	71%	69%	66%	70%	68%
Perfluoro-n-[13C8]octanoic acid	Perfluoro-n-[1,2-13C2]octanoic acid	66%	65%	64%	66%	56%
Perfluoro-n-[13C9]nonanoic acid	Perfluoro-n-[1,2-13C2]octanoic acid	77%	92%	73%	79%	55%
Perfluoro-1-{1,2,3-13C3}hexanesulfonate	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	61%	67%	60%	67%	66%
Perfluoro-n-[1,2,3,4,6-13C5]hexanoic acid	Perfluoro-n-[1,2-13C2]octanoic acid	98%	93%	83%	94%	50%
Perfluoro-n-[1,2,3,4-13C4]heptanoic acid	Perfluoro-n-[1,2-13C2]octanoic acid	82%	86%	75%	95%	55%
Perfluoro-n-[1,2-13C2]dodecanoic acid	Perfluoro-n-[1,2-13C]decanoic acid	80%	36%	82%	0%	67%
Perfluoro-n-[1,2,3,4,5,6-13C6]decanoic acid	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	59%	56%	54%	52%	60%
Perfluoro-1-[2,3,4-13C3]butanesulfonate	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	68%	80%	75%	87%	61%
N-methyl-d3-perfluoro-1-octanesulfonamide	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	41%	27%	55%	0%	60%
2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	0%	27%	51%	0%	56%
N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	Perfluoro-1-[1,2,3,4-13C4]octanesulfonate	45%	0%	20%	0%	18%
Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate	Perfluoro-n-[1,2-13C2]octanoic acid	117%	107%	76%	117%	26%

Table S4. Analyte recoveries in each matrix. Gray shaded boxes denote external calibration was performed due to poorly recovered surrogates in one or more matrix

Target Analyte	Surrogate Analyte (used for Internal Standardization)	Soil	Oat	Biosolids	Compost
4:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	104%	143%	150%	143%
6:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	127%	120%	131%	132%
8:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	77%	101%	70%	67%
PFBS	Perfluoro-1-[2,3,4-13C3]butanesulfonate	127%	121%	142%	137%
PFPeS	Perfluoro-1-{1,2,3-13C3}hexanesulfonate	116%	100%	127%	122%
PFHxS	Perfluoro-1-{1,2,3-13C3}hexanesulfonate	119%	114%	131%	127%
PFHpS	Perfluoro-1-[13C8]octanesulfonate	108%	91%	108%	105%
PFOS	Perfluoro-1-[13C8]octanesulfonate	129%	121%	143%	139%
PFNS	Perfluoro-1-[13C8]octanesulfonate	134%	110%	124%	140%
PFDS	Perfluoro-1-[13C8]octanesulfonate	133%	142%	6%	30%
9-Cl-PF3ONS	Perfluoro-1-[13C8]octanesulfonate	151%	124%	135%	149%
11-Cl-PF3ONS	Perfluoro-1-[13C8]octanesulfonate	152%	143%	81%	130%
PFBA*	Perfluoro-n-[13C4]butanoic acid	108%	121%	90%	110%
PFPeA	Perfluoro-n-[13C5]pentanoic acid	111%	104%	123%	115%
PFHxA	Perfluoro-n-[1,2,3,4,6-13C5]hexanoic acid	122%	112%	130%	135%
PFHpA	Perfluoro-n-[1,2,3,4-13C4]heptanoic acid	127%	124%	146%	139%
PFOA	Perfluoro-n-[13C8]octanoic acid	124%	122%	144%	136%
PFNA	Perfluoro-n-[13C9]nonanoic acid	123%	120%	139%	135%
PFDA	Perfluoro-n-[1,2,3,4,5,6-13C6]decanoic acid	128%	119%	136%	131%
PFUnA*	Perfluoro-n-[1,2,3,4,5,6,7-13C7]undecanoic acid	117%	154%	6%	23%
PFDoA*	Perfluoro-n-[1,2-13C2]dodecanoic acid	127%	122%	12%	133%
PFTTrDA*	Perfluoro-n-[1,2-13C2]tetradecanoic acid	131%	98%	6%	112%
PFTeDA*	Perfluoro-n-[1,2-13C2]tetradecanoic acid	125%	121%	7%	137%
6:2 diPAP*	N-methyl-d3-perfluoro-1-octanesulfonamide	68%	96%	0%	1%
FOSA*	N-methyl-d3-perfluoro-1-octanesulfonamide	80%	98%	10%	92%
MeFOSAA*	N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	142%	128%	63%	104%
EtFOSAA*	N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	112%	108%	12%	113%
N-MeFOSA-M*	N-methyl-d3-perfluoro-1-octanesulfonamide	112%	105%	2%	115%
N-MeFOSE-M	2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	125%	92%	4%	82%
N-EtFOSE-M*	2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	113%	19%	14%	119%
N-EtFOSA-M*	N-methyl-d3-perfluoro-1-octanesulfonamide (N-MeFOSA)	116%	15%	6%	105%
HFPO-DA	2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-13C3-propanoic acid (HFPO)	54%	77%	70%	75%
NaDONA	Sodium perfluoro-1-[13C8]octanesulfonate	113%	96%	127%	114%

Table S5. Method detection limits (LOD) and limits of quantification (LOQ) for the target PFAS analytes

Target Analyte	Surrogate Analyte (used for Internal Standardization)	LOD (µg/kg)	LOQ (µg/kg)
4:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	1.25	5.00
6:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	1.25	5.00
8:2 FTS	1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (6:2 FTS)	2.50	12.5
PFBS	Perfluoro-1-[2,3,4-13C3]butanesulfonate	1.25	5.00
PFPeS	Perfluoro-1-{1,2,3-13C3}hexanesulfonate	1.25	5.00
PFHxS	Perfluoro-1-{1,2,3-13C3}hexanesulfonate	1.25	5.00
PFHpS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
PFOS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
PFNS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
PFDS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
9-Cl-PF3ONS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
11-Cl-PF3ONS	Perfluoro-1-[13C8]octanesulfonate	1.25	5.00
PFBA*	Perfluoro-n-[13C4]butanoic acid	5.00	25
PFPeA	Perfluoro-n-[13C5]pentanoic acid	2.50	12.5
PFHxA	Perfluoro-n-[1,2,3,4,6-13C5]hexanoic acid	2.50	12.5
PFHpA	Perfluoro-n-[1,2,3,4-13C4]heptanoic acid	1.25	5.00
PFOA	Perfluoro-n-[13C8]octanoic acid	1.25	5.00
PFNA	Perfluoro-n-[13C9]nonanoic acid	2.50	12.5
PFDA	Perfluoro-n-[1,2,3,4,5,6-13C6]decanoic acid	2.50	12.5
PFUnA*	Perfluoro-n-[1,2,3,4,5,6,7-13C7]undecanoic acid	2.50	12.5
PFDoA*	Perfluoro-n-[1,2-13C2]dodecanoic acid	2.50	12.5
PFTeDA*	Perfluoro-n-[1,2-13C2]tetradecanoic acid	2.50	12.5
PFTeDA*	Perfluoro-n-[1,2-13C2]tetradecanoic acid	2.50	12.5
6:2 diPAP*	N-methyl-d3-perfluoro-1-octanesulfonamide	12.5	50
FOSA*	N-methyl-d3-perfluoro-1-octanesulfonamide	1.25	5.00
MeFOSAA*	N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	5.00	25
EtFOSAA*	N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	2.50	12.5
N-MeFOSA-M*	N-methyl-d3-perfluoro-1-octanesulfonamide	1.25	5.00
N-MeFOSE-M	2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	12.5	50
N-EtFOSE-M*	2-(N-ethyl-d5-perfluoro-1-octanesulfonamido)ethan-d4-ol	12.5	50
N-EtFOSA-M*	N-methyl-d3-perfluoro-1-octanesulfonamide (N-MeFOSA)	2.50	12.5
HFPO-DA	2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-13C3-propanoic acid (HFPO)	12.5	50
NaDONA	Sodium perfluoro-1-[13C8]octanesulfonate	2.50	12.5