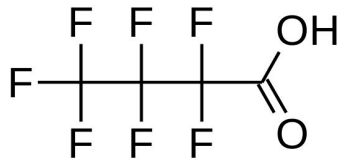
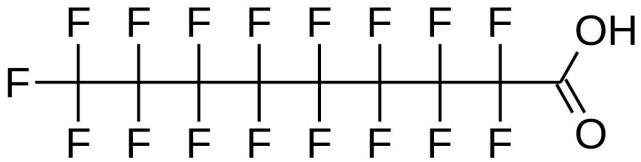
applied sciences

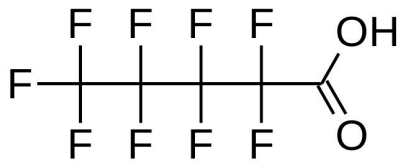
Supplementary Materials



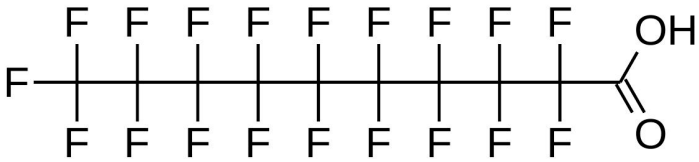
Perfluorobutanoic acid (PFBA)



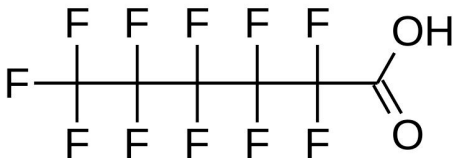
Perfluorononanoic acid (PFNA)



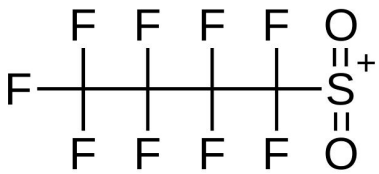
Perfluoropentanoic acid (PFPeA)



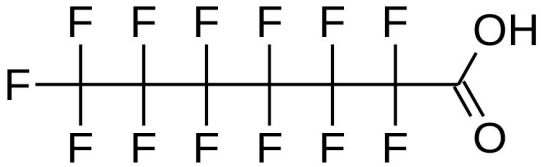
Perfluorodecanoic acid (PFDA)



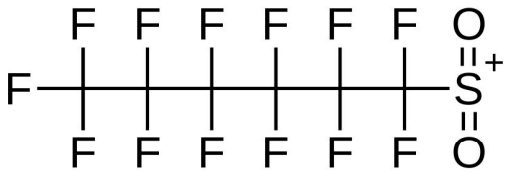
Perfluorohexanoic acid (PFHxA)



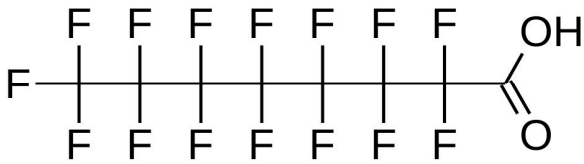
Perfluorobutane sulfonate (PFBS)



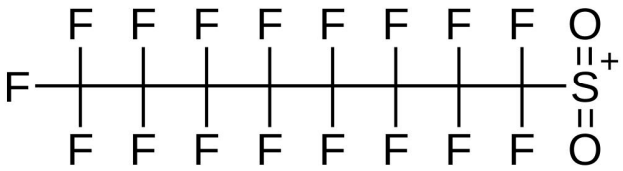
Perfluoroheptanoic acid (PFHpA)



Perfluorohexane sulfonate (PFHxS)



Perfluorooctanoic acid (PFOA)



Perfluorooctane sulfonate (PFOS)

Figure S1. The structures of the investigated analytes.

Table S1. Retention times and MRM ion pairs of analyzed PFAS.

PFAS Name	Acronym	Rt [min]	MRM ion pairs
Perfluorobutanoic acid	PFBA	0.71	217/172
Perfluoropentanoic acid	PFPeA	1.05	263/219
Perfluorohexanoic acid	PFHxA	1.19	313/269; 313/119
Perfluorobutane sulfonate	PFBS	1.30	299/80; 299/99
Perfluoroheptanoic acid	PFHpA	1.87	363/319; 363/169
Perfluorooctanoic acid	PFOA	2.28	413/369; 413/169
Perfluoro-n-[$^{13}C_8$] octanoic acid	L-PFOA	2.30	417/372; 417/172
Perfluorohexane sulfonate	PFHS	2.10	399/80; 399/99
Perfluorononanoic acid	PFNA	2.41	463/419; 463/219
Perfluorodecanoic acid	PFDA	2.83	513/469; 513/119
Perfluorooctane sulfonate	PFOS	2.88	499/80; 499/99
perfluoro-1-[$^{13}C_8$] octanesulfonate	L-PFOS	2.89	503/80

Abbreviations: Rt – retention time, MRM – Multiple Reaction Monitoring.

PFBA	Multiple Comparisons p values (2-tailed); PFBA (Spreadsheet4) Independent (grouping) variable: Product Kruskal-Wallis test: H (14, N= 89) =87.19836 p =.0000														
	wholemeal bread	boltona bread	wheat roll	graham roll	wheat noddle	durum-wheat noddle	white rice	brown rice	unroasted buckwheat groats	roasted buckwheat groats	millet groats	wheat bran	rye bran	rye flour	wheat flour
	R:27.500	R:27.500	R:27.500	R:27.500	R:65.200	R:70.200	R:27.500	R:27.500	R:57.000	R:27.500	R:27.500	R:86.000	R:82.200	R:77.000	R:66.400
wholemeal bread		1.000000	1.000000	1.000000	0.810476	0.267647	1.000000	1.000000	1.000000	1.000000	1.000000	0.003743	0.011642	0.049221	0.627801
boltona bread	1.000000		1.000000	1.000000	0.810476	0.267647	1.000000	1.000000	1.000000	1.000000	1.000000	0.003743	0.011642	0.049221	0.627801
wheat roll	1.000000	1.000000		1.000000	0.933816	0.319798	1.000000	1.000000	1.000000	1.000000	1.000000	0.005164	0.015452	0.062227	0.729393
graham roll	1.000000	1.000000	1.000000		1.000000	0.941844	1.000000	1.000000	1.000000	1.000000	1.000000	0.036058	0.085595	0.257334	1.000000
wheat noddle	0.810476	0.810476	0.933816	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
durum-wheat noddle	0.267647	0.267647	0.319798	0.941844	1.000000		0.941844	0.941844	1.000000	0.941844	0.941844	1.000000	1.000000	1.000000	1.000000
white rice	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844		1.000000	1.000000	1.000000	1.000000	0.036058	0.085595	0.257334	1.000000
brown rice	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000		1.000000	1.000000	1.000000	0.036058	0.085595	0.257334	1.000000
unroasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
roasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000		1.000000	0.036058	0.085595	0.257334	1.000000
millet groats	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000		0.036058	0.085595	0.257334	1.000000
wheat bran	0.003743	0.003743	0.005164	0.036058	1.000000	1.000000	0.036058	0.036058	1.000000	0.036058	0.036058		1.000000	1.000000	1.000000
rye bran	0.011642	0.011642	0.015452	0.085595	1.000000	1.000000	0.085595	0.085595	1.000000	0.085595	0.085595	1.000000		1.000000	1.000000
rye flour	0.049221	0.049221	0.062227	0.257334	1.000000	1.000000	0.257334	0.257334	1.000000	0.257334	0.257334	1.000000	1.000000		1.000000
wheat flour	0.627801	0.627801	0.729393	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	

PFPeA	Multiple Comparisons p values (2-tailed); PFPeA (Spreadsheet4) Independent (grouping) variable: Product Kruskal-Wallis test: H (14, N= 89) =87.85250 p =.0000														
	wholemeal bread	boltona bread	wheat roll	graham roll	wheat noddle	durum-wheat noddle	white rice	brown rice	unroasted buckwheat groats	roasted buckwheat groats	millet groats	wheat bran	rye bran	rye flour	wheat flour
	R:40.000	R:40.000	R:40.000	R:40.000	R:40.000	R:40.000	R:82.200	R:40.000	R:40.000	R:40.000	R:86.800	R:40.000	R:40.000	R:40.000	R:40.000
wholemeal bread		1.000000	1.000000	1.000000	1.000000	1.000000	0.300566	1.000000	1.000000	1.000000	0.098948	1.000000	1.000000	1.000000	1.000000
boltona bread	1.000000		1.000000	1.000000	1.000000	1.000000	0.300566	1.000000	1.000000	1.000000	0.098948	1.000000	1.000000	1.000000	1.000000
wheat roll	1.000000	1.000000		1.000000	1.000000	1.000000	0.357757	1.000000	1.000000	1.000000	0.122202	1.000000	1.000000	1.000000	1.000000
graham roll	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.439087	1.000000	1.000000	1.000000	1.000000
wheat noddle	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	0.439087	1.000000	1.000000	1.000000	1.000000
durum-wheat noddle	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	0.439087	1.000000	1.000000	1.000000	1.000000
white rice	0.300566	0.300566	0.357757	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
brown rice	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	0.439087	1.000000	1.000000	1.000000	1.000000
unroasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	0.439087	1.000000	1.000000	1.000000	1.000000
roasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		0.439087	1.000000	1.000000	1.000000	1.000000
millet groats	0.098948	0.098948	0.122202	0.439087	0.439087	0.439087	1.000000	0.439087	0.439087	0.439087		0.439087	0.439087	0.439087	0.439087
wheat bran	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.439087		1.000000	1.000000	1.000000
rye bran	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.439087	1.000000		1.000000	1.000000
rye flour	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.439087	1.000000	1.000000		1.000000
wheat flour	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.439087	1.000000	1.000000	1.000000	

PFHxA	Multiple Comparisons p values (2-tailed); PFHxA (Spreadsheet4) Independent (grouping) variable: Product Kruskal-Wallis test: H (14, N= 89) =80.86452 p =.0000														
	wholemeal bread	boltona bread	wheat roll	graham roll	wheat noddle	durum-wheat noddle	white rice	brown rice	unroasted buckwheat groats	roasted buckwheat groats	millet groats	wheat bran	rye bran	rye flour	wheat flour
	R:78.300	R:77.250	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500	R:35.500
wholemeal bread		1.000000	0.032716	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473	0.261473
boltona bread	1.000000		0.045824	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309	0.333309
wheat roll	0.032716	0.045824		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
graham roll	0.261473	0.333309	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
wheat noddle	0.261473	0.333309	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
durum-wheat noddle	0.261473	0.333309	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
white rice	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
brown rice	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
unroasted buckwheat groats	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
roasted buckwheat groats	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000
millet groats	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000
wheat bran	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000
rye bran	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000
rye flour	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000
wheat flour	0.261473	0.333309	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	

PFOA	Multiple Comparisons p values (2-tailed); PFOA (Spreadsheet4) Independent (grouping) variable: Product Kruskal-Wallis test: H (14, N= 89) =76.29295 p =.0000														
	wholemeal bread	boltona bread	wheat roll	graham roll	wheat noddle	durum-wheat noddle	white rice	brown rice	unroasted buckwheat groats	roasted buckwheat groats	millet groats	wheat bran	rye bran	rye flour	wheat flour
	R:81.300	R:60.400	R:65.000	R:65.400	R:23.300	R:71.400	R:41.600	R:42.500	R:16.000	R:41.800	R:34.600	R:16.000	R:16.000	R:16.000	R:16.000
wholemeal bread		1.000000	1.000000	1.000000	0.004363	1.000000	0.527569	0.641468	0.000414	0.551169	0.101473	0.000414	0.000414	0.000414	0.000414
boltona bread	1.000000		1.000000	1.000000	0.918595	1.000000	1.000000	1.000000	0.178858	1.000000	1.000000	0.178858	0.178858	0.178858	0.178858
wheat roll	1.000000	1.000000		1.000000	0.399775	1.000000	1.000000	1.000000	0.070687	1.000000	1.000000	0.070687	0.070687	0.070687	0.070687
graham roll	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	0.262596	1.000000	1.000000	0.262596	0.262596	0.262596	0.262596
wheat noddle	0.004363	0.918595	0.399775	1.000000		0.340561	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
durum-wheat noddle	1.000000	1.000000	1.000000	1.000000	0.340561		1.000000	1.000000	0.073274	1.000000	1.000000	0.073274	0.073274	0.073274	0.073274
white rice	0.527569	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
brown rice	0.641468	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
unroasted buckwheat groats	0.000414	0.178858	0.070687	0.262596	1.000000	0.073274	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
roasted buckwheat groats	0.551169	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000
millet groats	0.101473	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000
wheat bran	0.000414	0.178858	0.070687	0.262596	1.000000	0.073274	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000
rye bran	0.000414	0.178858	0.070687	0.262596	1.000000	0.073274	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000
rye flour	0.000414	0.178858	0.070687	0.262596	1.000000	0.073274	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000
wheat flour	0.000414	0.178858	0.070687	0.262596	1.000000	0.073274	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	

PFOS	Multiple Comparisons p values (2-tailed); PFOS (Spreadsheet4) Independent (grouping) variable: Product Kruskal-Wallis test: H (14, N= 89) =60.95383 p =.0000														
	wholemeal bread	boltona bread	wheat roll	graham roll	wheat noddle	durum-wheat noddle	white rice	brown rice	unroasted buckwheat groats	roasted buckwheat groats	millet groats	wheat bran	rye bran	rye flour	wheat flour
	R:38.500	R:38.500	R:38.500	R:38.500	R:55.300	R:74.900	R:81.200	R:38.500	R:38.500	R:38.500	R:58.300	R:38.500	R:38.500	R:38.500	R:38.500
wholemeal bread		1.000000	1.000000	1.000000	1.000000	1.000000	0.267647	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
boltona bread	1.000000		1.000000	1.000000	1.000000	1.000000	0.267647	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
wheat roll	1.000000	1.000000		1.000000	1.000000	1.000000	0.319798	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
graham roll	1.000000	1.000000	1.000000		1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
wheat noddle	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
durum-wheat noddle	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
white rice	0.267647	0.267647	0.319798	0.941844	1.000000	1.000000		0.941844	0.941844	0.941844	1.000000	0.941844	0.941844	0.941844	0.941844
brown rice	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
unroasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
roasted buckwheat groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000	1.000000
millet groats	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000	1.000000
wheat bran	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000	1.000000
rye bran	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000	1.000000
rye flour	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000		1.000000
wheat flour	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.941844	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	

Figure S2. The results of the Kruskal-Wallis H non-parametric test for detected variables (PFBA, PFPeA, PFHxA, PFOA, and PFOS).

Table S2. Clustering of samples using hierarchical sample clustering analysis.

Group/cluster	Sample name	No. of samples
1	boltona bread (1 pc), wheat roll (7 pcs), graham roll (4 pcs), wheat noodle (5 pcs), durum-wheat noodle (3 pcs), white rice (5 pcs), brown rice (5 pcs), unroasted buckwheat groats (5 pcs), roasted buckwheat groats (5 pcs), millet groats (5 pcs), wheat bran (5 pcs), rye bran (5 pcs), wheat flour (5 pcs), rye flour (5 pcs)	65
2	wholemeal bread (10 pcs), boltona bread (9 pcs), wheat roll (2 pcs), graham roll (1 pc), durum-wheat noodle (2 pcs)	24