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Measurement report: Per- and polyfluoroalkyl substances (PFAS) in particulate matter (PM_{10}) from activated sludge aeration

Jishnu Pandamkulangara Kizhakkethil et al.

Correspondence to: Ivan Kourtchev (ivan.kourtchev@coventry.ac.uk, i.kourtchev@cantab.net)

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Table S1 Per- and polyfluoroalkyl substances (PFAS) in the EPA 533 PAR mix (Wellington laboratories Inc, Canada).

PFAS analyte	**Abbreviation**	**CAS RN**
Perfluorobutanoic acid	PFBA	375-22-4
Perfluoropentanoic acid	PFPeA	2706-90-3
Perfluorohexanoic acid	PFHxA	307-24-4
Perfluoroheptanoic acid	PFHpA	375-85-9
Perflurooctanoic acid	PFOA	335-67-1
Perfluorononanoic acid	PFNA	375-95-1
Perfluorodecanoic acid	PFDA	335-76-2
Perfluoroundecanoic acid	PFUDA	2058-94-8
Perfluorododecanoic acid	PFDoA	307-55-1
Hexafluoropropylene oxide dimer acid	HFPO-DA	13252-13-6
Perfluoro-3-methoxypropanoic acid	PFMPA	377-73-1
Perfluoro-4-methoxybutanoic acid	PFMBA	863090-89-5
Perfluoro-3,6-dioxaheptanoic acid	3,6-OPFHpA	151772-58-6
Perfluorobuatne sulfonic acid	L-PFBS	375-73-5
Perfluoropentane sulfonic acid	L-PFPeS	2706-91-4
Perfluorohexane sulfonic acid	PFHxS	355-46-4
Perfluoroheptane sulfonic Acid	L-PFHpS	375-92-8
Perfluorooctane sulfonic Acid	PFOS	1763-23-1
4:2 fluorotelomer sulfonate	4:2FTS	27619-93-8
6:2 fluorotelomer sulfonate	6:2FTS	27619-94-9
8:2 fluorotelomer sulfonate	8:2FTS	27619-96-1
Sodium dodecafluoro-3H-4,8-dioxanonanoate	NaDONA	2250081-67-3
Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid)	9Cl-PF3ONS	756426-58-1
11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid	11Cl-PF3OudS	763051-92-9
Perfluoro (2-ethoxyethane)sulfonic acid	PFEESA	113507-82-7

Table S2 16 ^{13}C labelled PFAS in the EPA 533 ES isotope dilution standard mix (Wellington laboratories Inc, Canada).

^{13}C labelled PFAS	**Abbreviation**
Perfluorobutanoic acid, $^{13}C_4$	MPFBA
Perfluorobutane sulfonic acid, $^{13}C_3$	M3PFBS
Perfluoropentanoic acid, $^{13}C_5$	M5PFPeA
4:2 fluorotelomer sulfonate, $^{13}C_2$	M2-4:2FTS
Perfluorohexanoic acid, $^{13}C_5$	M5PFHxA
Perfluoroheptanoic acid, $^{13}C_4$	M4PFHpA
Perfluorohexane sulfonic acid, $^{13}C_3$	M3PFHxS
Perflurooctanoic acid, $^{13}C_8$	M8PFOA
6:2 fluorotelomer sulfonate, $^{13}C_2$	M2-6:2FTS
Perfluorononanoic acid, $^{13}C_9$	M9PFNA
Perfluorooctane sulfonic acid, $^{13}C_8$	M8PFOS
Perfluorodecanoic acid, $^{13}C_6$	M6PFDA
8:2 fluorotelomer sulfonate, $^{13}C_2$	M2-8:2-FTS
Perfluoroundecanoic acid, $^{13}C_7$	M7PFUdA
Hexafluoropropylene oxide, $^{13}C_3$	M3HFPO-DA
Perfluorododecanoic acid, $^{13}C_2$	MPFDoA

Table S3 Concentrations of PFAS (pg m^{-3}) in the PM_{10} samples (blank corrected) collected above the activated sludge (AS) tank in October 2023.

PM_{10} PFAS concentrations (pg m^{-3}) - October 2023										
PFAS	**2 October 2023**		**3 October 2023**		**4 October 2023**		**5 October 2023**		**Median (pg m^{-3})**	**Mean (pg m^{-3})**
	Day	**Night**	**Day**	**Night**	**Day**	**Night**	**Day**	**Night**		
PFBA	CSB	CSB	CSB	13.78±0.71	19.60±0.77	10.38±0.80	14.53±0.64	15.24±0.83	12.08	9.19
PFBS	<LOD	0.24±0.01	0.34±0.03	0.35±0.02	0.34±0.03	0.33±0.02	0.43±0.04	0.55±0.01	0.34	0.32
PFHpA	<LOD	<LOD	<LOD	0.31±0.04	<LOD	0.28±0.05	<LOD	0.39±0.04	0.00	0.12
PFHxS	<LOD	<LOD	<LOD	0.15±0.01	<LOD	0.152±0.003	<LOD	0.18±0.01	0.00	0.06
PFOA	1.17±0.04	2.12±0.16	8.06±0.36	2.74±0.09	0.87±0.17	1.08±0.05	3.96±0.32	0.97±0.12	1.65	2.62
PFNA	0.95±0.11	1.32±0.01	<LOD	0.18±0.02	<LOD	0.25±0.03	<LOD	0.17±0.01	0.18	0.36
PFOS	12.48±0.51	17.35±0.15	0.72±0.03	0.81±0.02	0.44±0.07	1.79±0.07	0.71±0.03	1.14±0.04	0.98	4.43
PFDA	2.64±0.49	3.74±0.14	<LOD	0.24±0.02	<LOD	0.41±0.01	<LOD	0.29±0.02	0.26	0.91
∑PFAS									15.49	18.01

The reported standard deviation (SD) of the concentrations is from three replicate injections.

CSB - close to system blanks

LOD - Limit of detection

Other targeted PFAS amenable to the method but not listed in the table were either below the method's LOD or not detected in any of the collected samples.

Table S4 Concentrations of PFAS (pg m^{-3}) in the PM_{10} samples (blank corrected) collected above the AS tank in March 2024.

PM_{10} PFAS concentrations (pg m^{-3}) - March 2024										
PFAS	**4 March 2024**		**5 March 2024**		**6 March 2024**		**7 March 2024**		**Median (pg m^{-3})**	**Mean (pg m^{-3})**
	Day	**Night**	**Day**	**Night**	**Day**	**Night**	**Day**	**Night**		
PFBA	CSB	8.04±0.38	CSB	6.54±0.64	CSB	7.13±0.15	CSB	8.75±0.86	3.27	3.81
PFBS	ND	0.149±0.005	0.03±0.01	0.20±0.01	ND	0.21±0.01	ND	0.17±0.02	0.09	0.09
PFHpA	<LOD	0.22±0.02	<LOD	0.23±0.02	<LOD	0.26±0.03	<LOD	<LOD	0.00	0.09
PFHxS	<LOD	0.19±0.02	<LOD	0.20±0.02	<LOD	0.20±0.01	<LOD	0.12±0.01	0.06	0.09
PFOA	<LOD	1.62±0.13	<LOD	1.70±0.01	<LOD	1.21±0.07	<LOD	0.51±0.02	0.26	0.63
PFNA	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0	0
PFOS	<LOD	0.56±0.04	0.58±0.04	0.66±0.05	0.76±0.02	0.56±0.02	0.61±0.03	0.312±0.001	0.57	0.51
PFDA	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0	0
∑PFAS									4.25	5.22

The reported SD of the concentrations is from three replicate injections.

CSB - close to system blanks

ND - Not detected

LOD - Limit of detection

Other targeted PFAS amenable to the method but not listed in the table were either below the method's LOD or not detected in any of the collected samples.

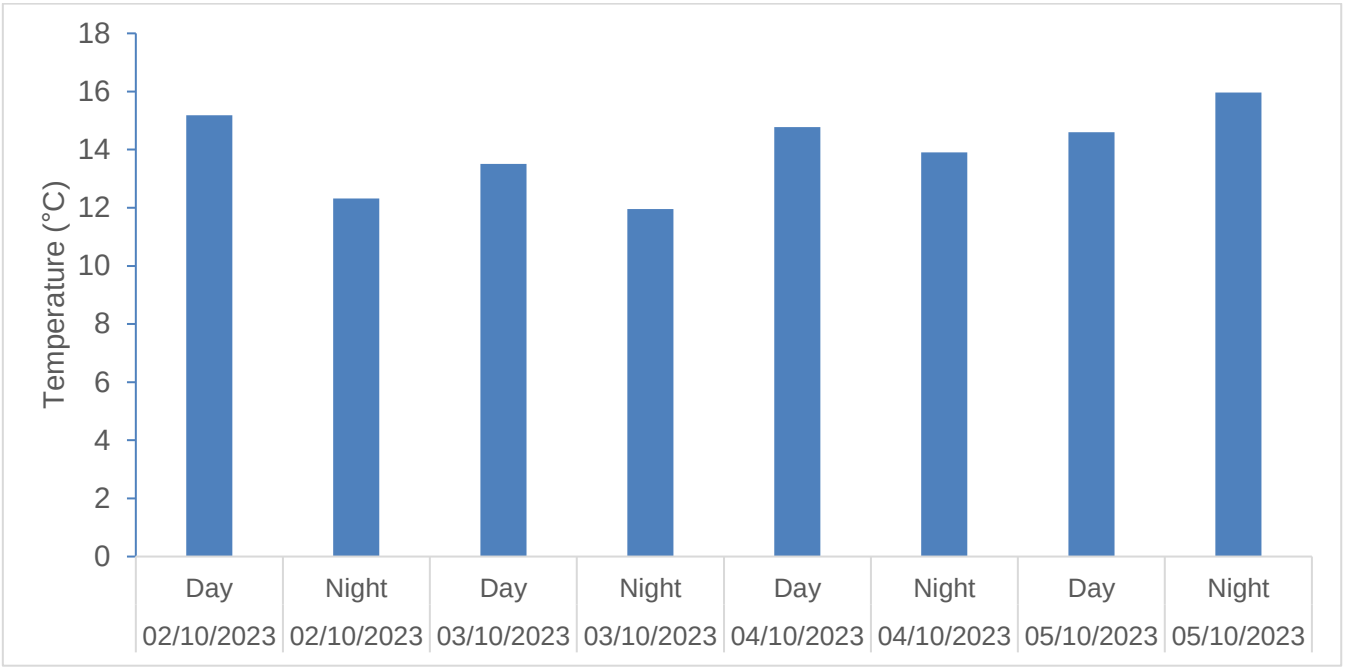

Figure S1 Average temperature (°C) during the sampling periods in October 2023. The data was obtained from ERA5-Land reanalysis data set. (https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land?tab=overview)

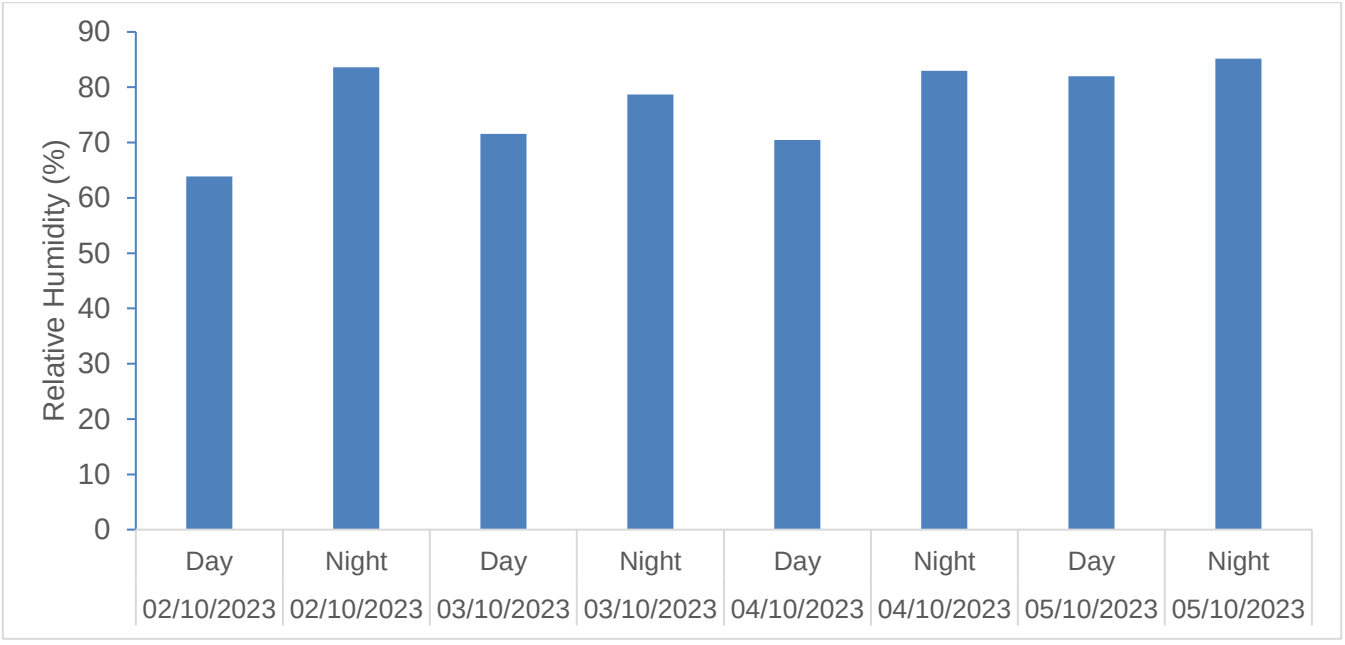

Figure S2 Average relative humidity (%) during the sampling periods in October 2023. The data was obtained from ERA5-Land reanalysis data set. (https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land?tab=overview)

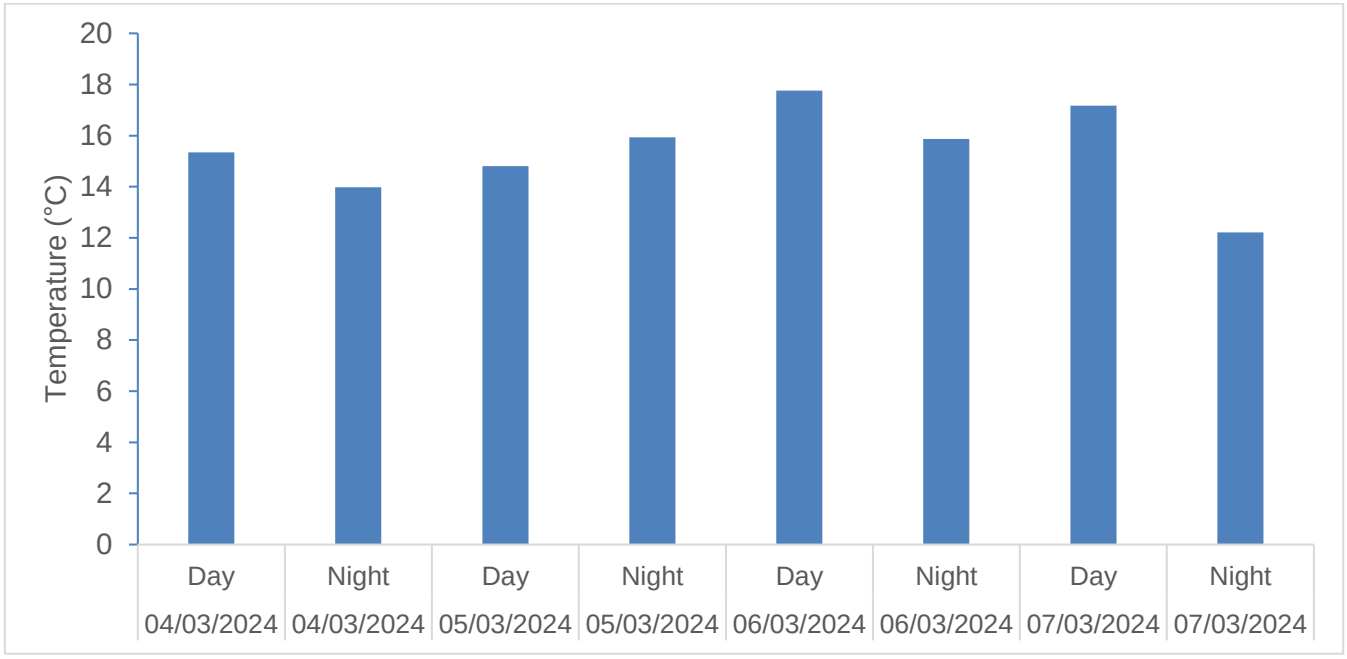

Figure S3 Average temperature (°C) during the sampling periods in March 2024. The data was obtained from ERA5-Land reanalysis data set. (https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land?tab=overview)

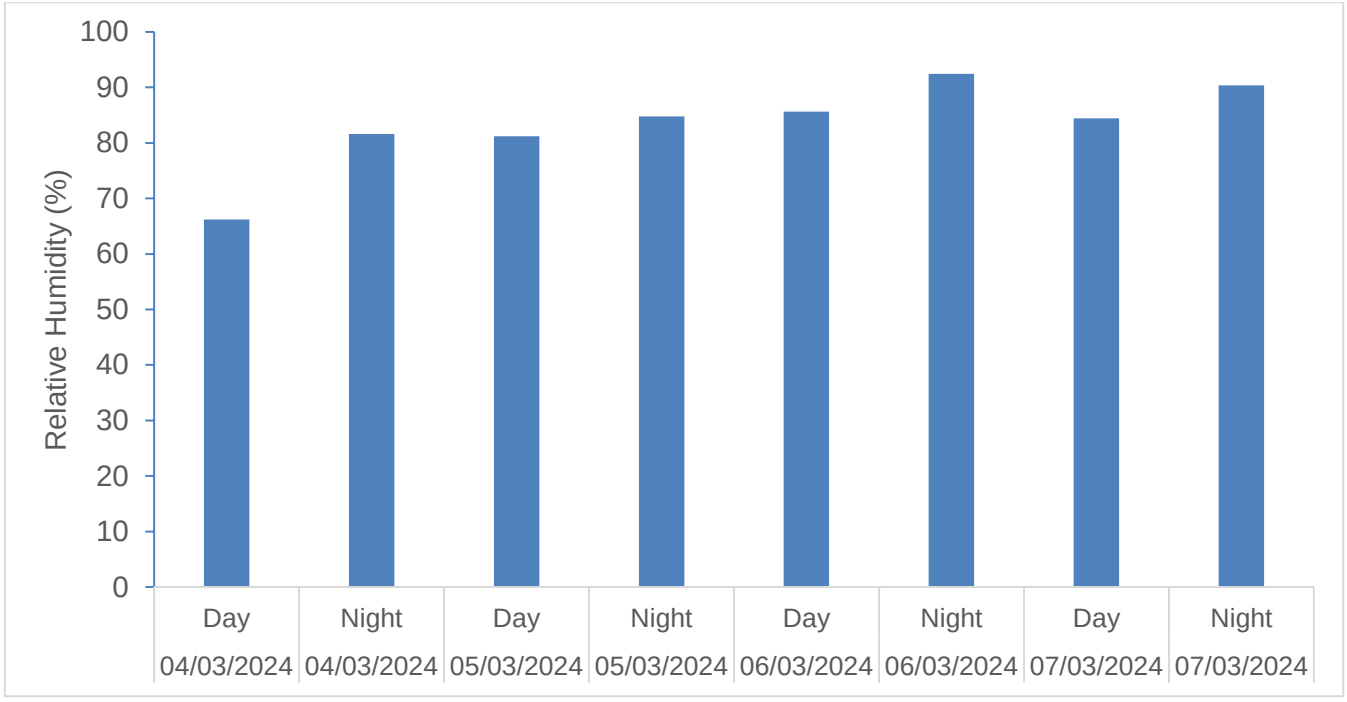

Figure S4 Average relative humidity (%) during the sampling periods in March 2024. The data was obtained from ERA5-Land reanalysis data set. (https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land?tab=overview)

Table S5 LOD and LOQ values for the PFAS.

PFAS	LOD (pg mL^{-1})	LOQ (pg mL^{-1})
PFBA	1.47	4.46
PFPeA	0.44	1.34
PFBS	0.21	0.65
4:2 FTS	0.27	0.81
PFHxA	0.37	1.13
PFPeS	0.21	0.63
PFHpA	0.42	1.27
PFHxS	0.26	0.79
PFOA	0.33	0.99
PFHpS	0.34	1.02
PFNA	0.22	0.66
PFOS	0.23	0.71
8:2 FTS	0.58	1.76
PFDA	0.38	1.14
PFUdA	0.38	1.15

Table S6 Blank concentrations of PFAS in October 2023. FB - filter blank, FLDB- field blank, ND - not detected, LOD - limit of detection.

Blank type	Largest concentration detected in the blanks (pg mL^{-1})							
	PFBA	PFBS	PFHpA	PFHxS	PFOA	PFNA	PFOS	PFDA
Baked filters (BF)	2.47	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Baked filters placed in MiniVol® air sampler and collecting air above the AS tank at 10 L min^{-1} for 2 min (FLDB)	2.75	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
System blanks (zero volume)	4.90	ND	<LOD	ND	<LOD	ND	ND	ND

The system blank values ('zero volume' injections) were estimated based on the analyte's chromatographic response without internal standard.

Table S7 Blank concentrations of PFAS in March 2024. FB- filter blank, FLDB- field blank, ND- not detected, LOD- limit of detection.

Blank type	Largest concentration detected in the blanks (pg mL^{-1})							
	PFBA	PFBS	PFHpA	PFHxS	PFOA	PFNA	PFOS	PFDA
Baked filters (BF)	<LOD	0.28	<LOD	ND	1.11	<LOD	<LOD	<LOD
Baked filters placed in MiniVol® air sampler and collecting air above the AS tank at 10 L min^{-1} for 2 min (FLDB)	<LOD	<LOD	<LOD	ND	<LOD	<LOD	<LOD	<LOD
System blanks (zero volume)	3.70	ND	<LOD	ND	<LOD	ND	ND	ND

The system blank values ('zero volume' injections) were estimated based on the analyte's chromatographic response without internal standard.

Table S8 Extraction efficiencies of the PFAS. The SD reported is between three replicate experiments. The data is published elsewhere (Kourtchev et al., 2022)

PFAS	Recovery (%)					
	1st Extraction	**SD**	**2nd Extraction**	**SD**	**3rd Extraction**	**SD**
PFBA	99.45	4.7	15.91	2.39	12.62	0.73
PFPeA	109.21	8.69	ND	0	ND	0
PFBS	103.21	0.75	3.29	0.16	ND	0
4:2 FTS	102.13	5.72	1.87	0.15	ND	0
PFHxA	107.11	5.84	10.49	0.93	6.3	0.76
PFPeS	105.40	1.46	3.28	0.52	ND	0
PFHpA	104.45	6.76	5.80	0.59	2.12	0.36
PFHxS	104.79	2.58	ND	0	ND	0
6:2 FTS	102.27	2.75	3.41	0.31	ND	0
PFOA	104.17	3.05	ND	0	ND	0
PFNA	104.16	3.73	0.91	1.58	ND	0
PFOS	106.96	4.06	3.80	0.33	ND	0
8:2 FTS	100.69	5.05	ND	0	ND	0
PFDA	104.44	7.56	ND	0	ND	0
PFUdA	103.99	4.50	16.35	4.37	ND	0
PFHpS	92.86	4.30	3.19	0.47	0	0

ND - Not detected

References

Kourtchev, I., Hellebust, S., Heffernan, E., Wenger, J., Towers, S., Diapouli, E., and Eleftheriadis, K.: A new on-line SPE LC-HRMS method for the analysis of Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS) in $PM_{2.5}$ and its application for screening atmospheric particulates from Dublin and Enniscorthy, Ireland, Sci. Total Environ., 835, 155496, https://doi.org/10.1016/j.scitotenv.2022.155496, 2022.