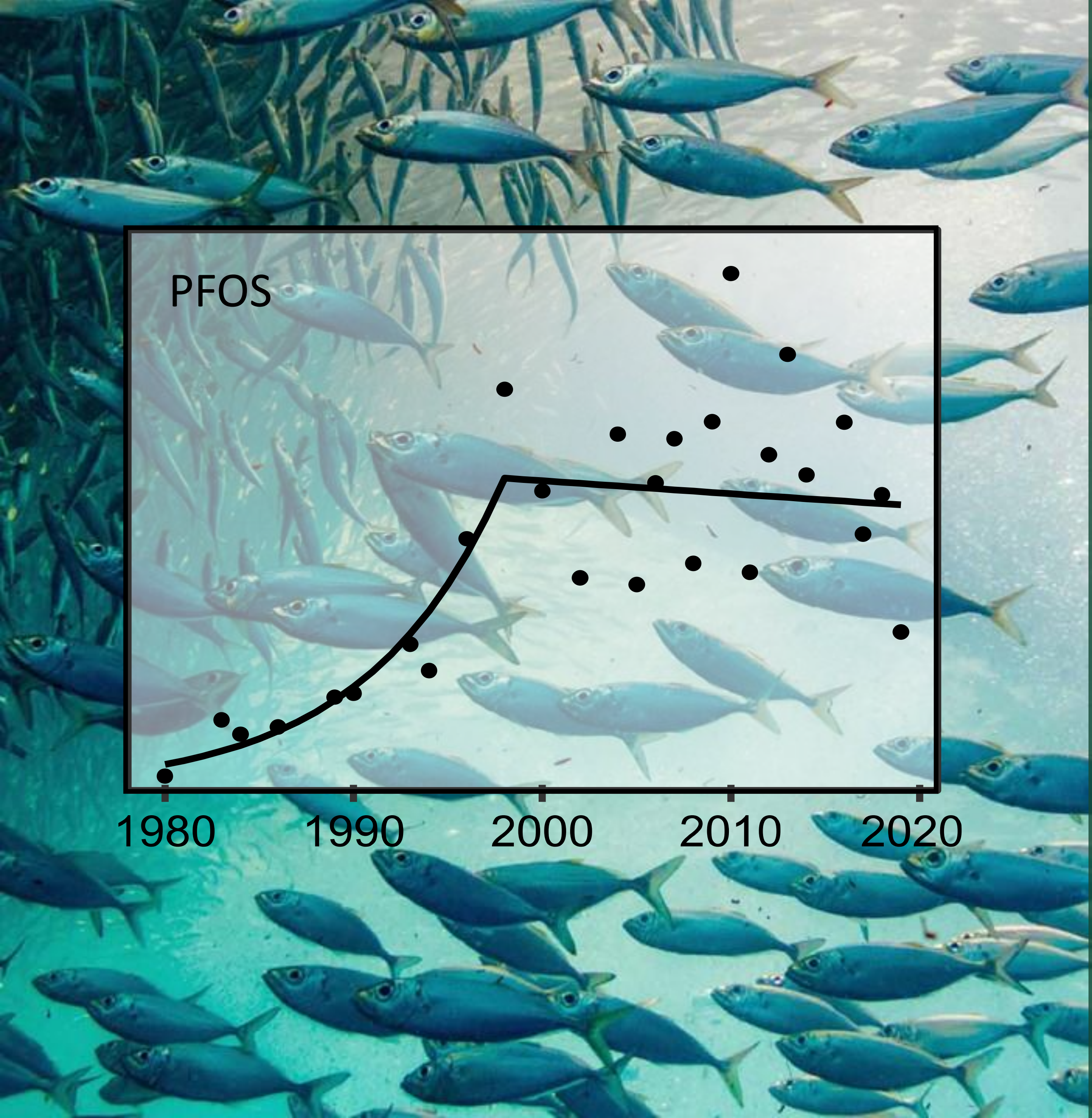

Outlook on PFAS in marine biota – spatiotemporal trends

Anne L. Soerensen

Global PFAS Modeling Initiative

HTAP, 7/5 2025

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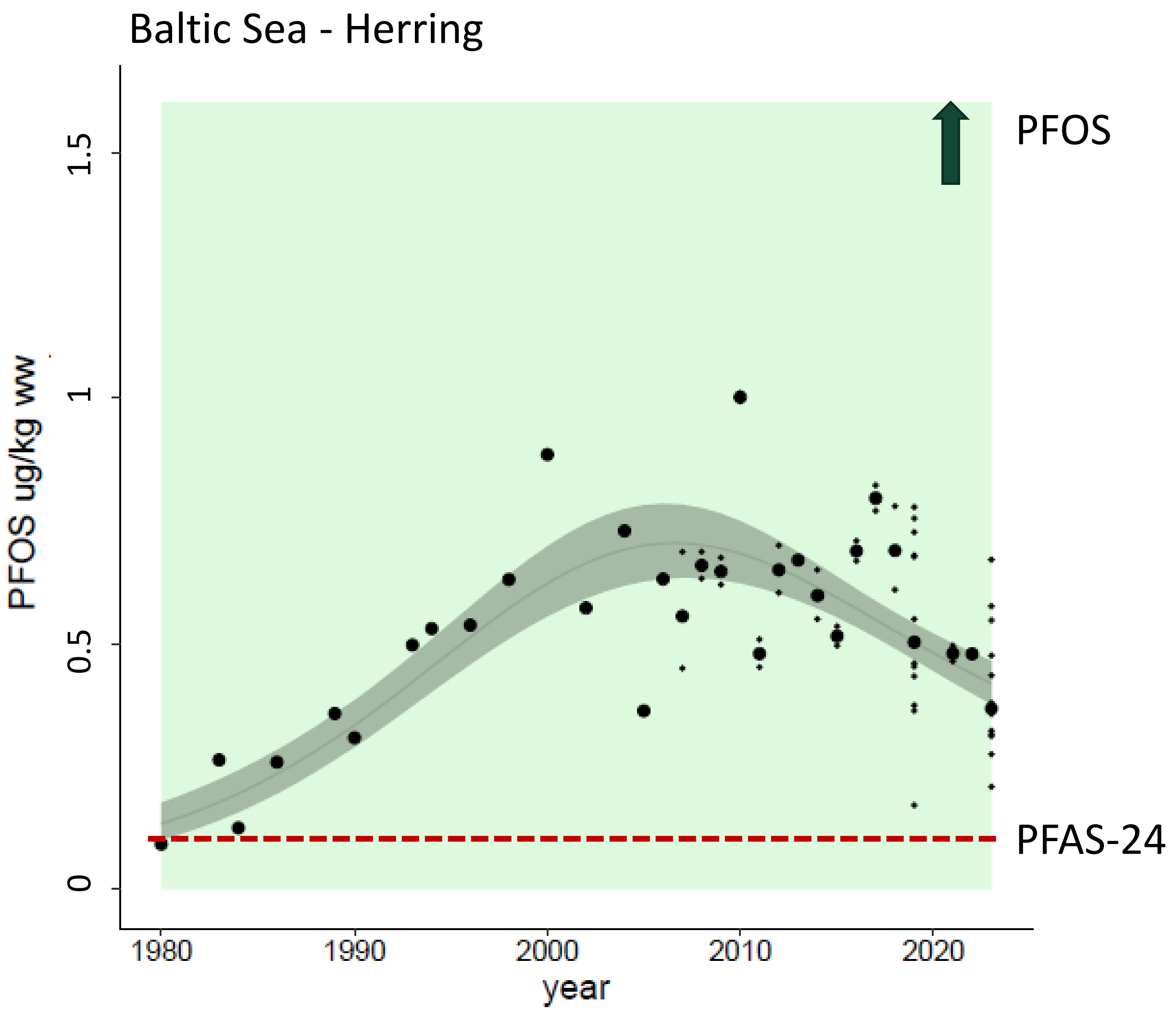
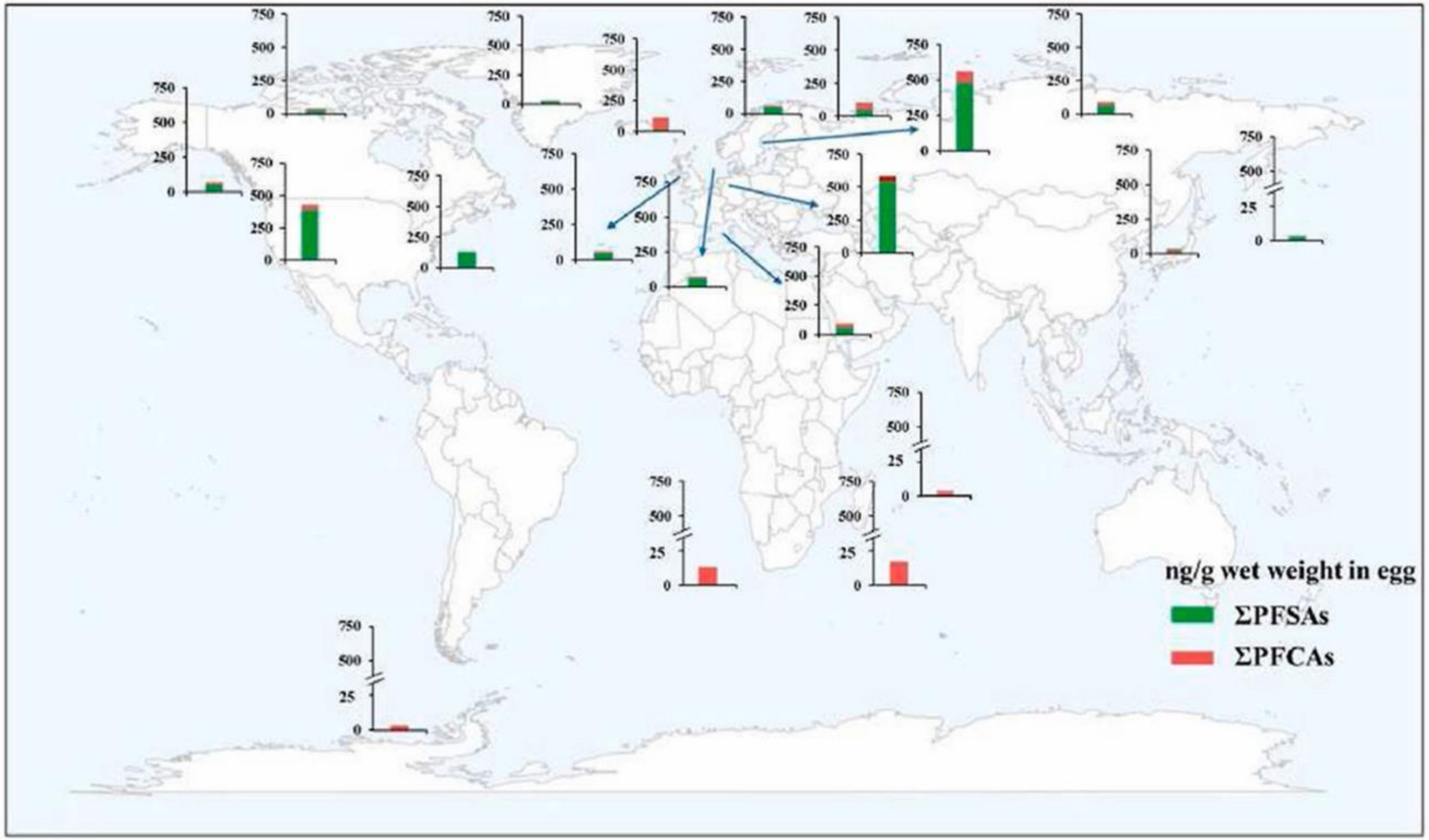
End goal...
predict the effect on humans and the environment

Human health EQS (EU target level)	
PFOS	9.1 ug/kg ww muscle
Proposed PFAS-24	0.077 ug/kg ww muscle

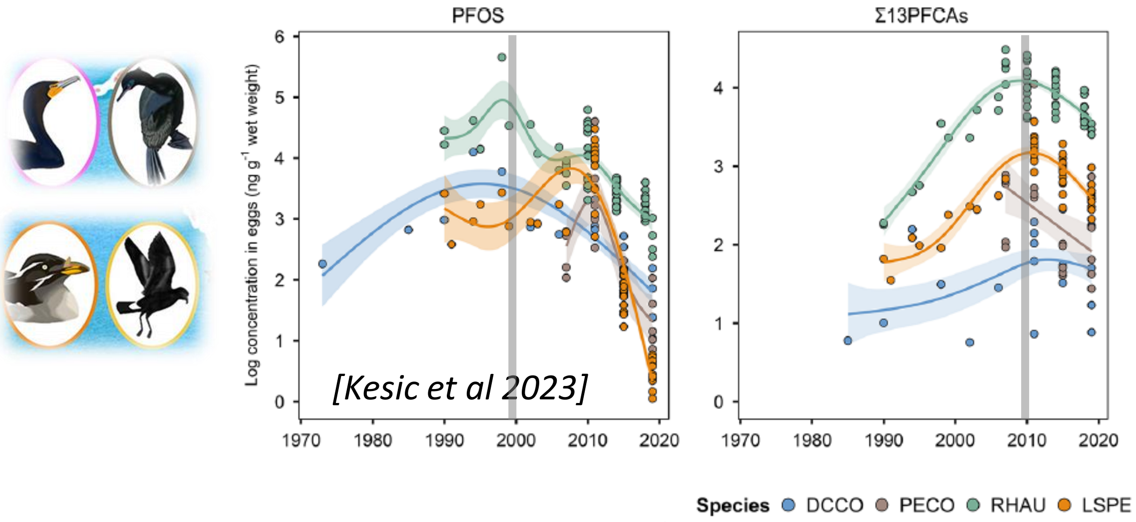


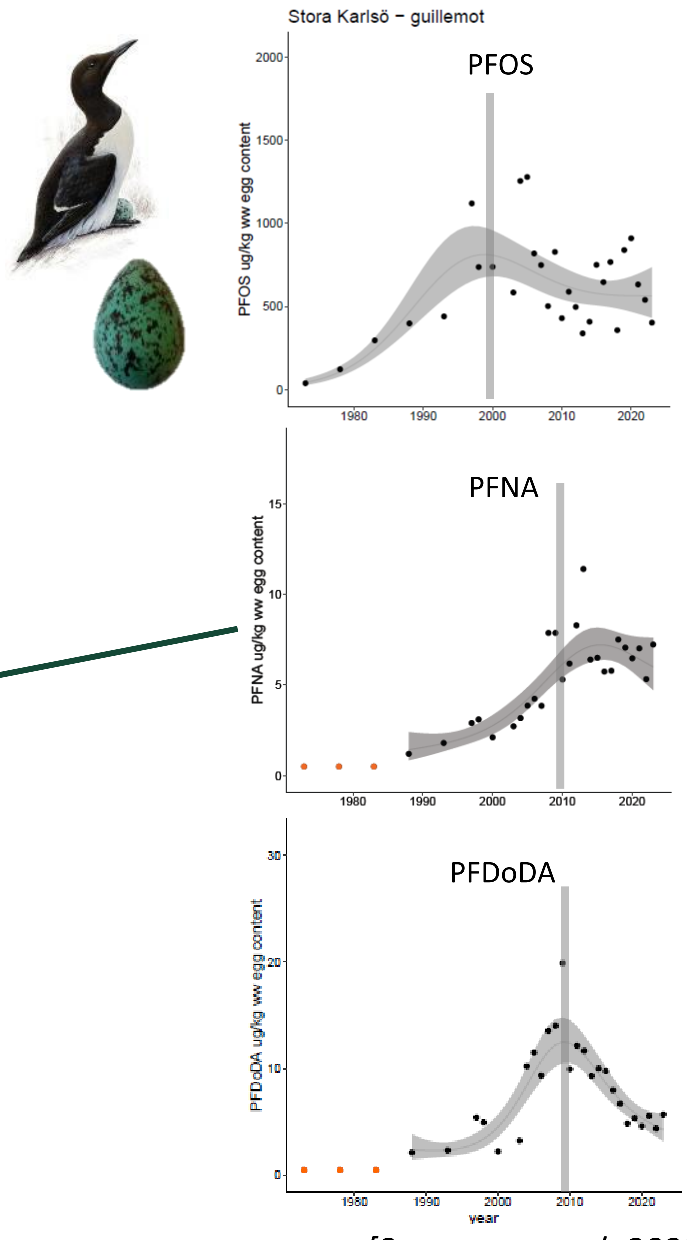
Sea bird (egg) PFAS concentrations



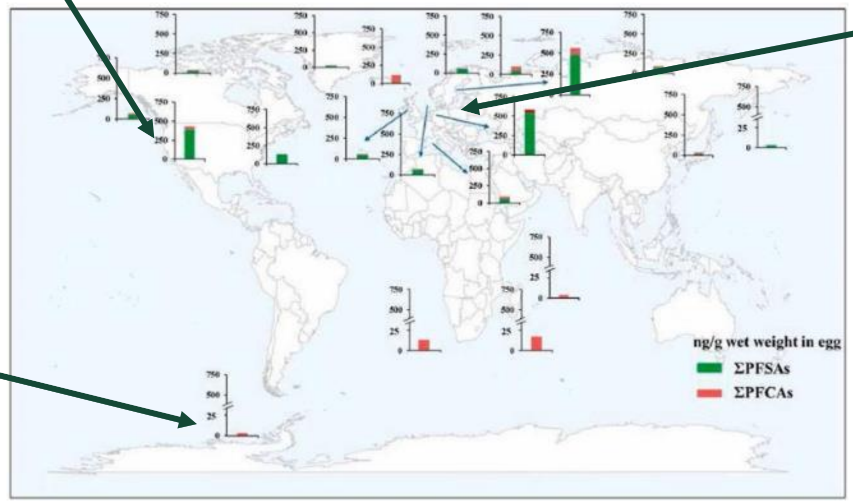
[Sun et al. 2023]

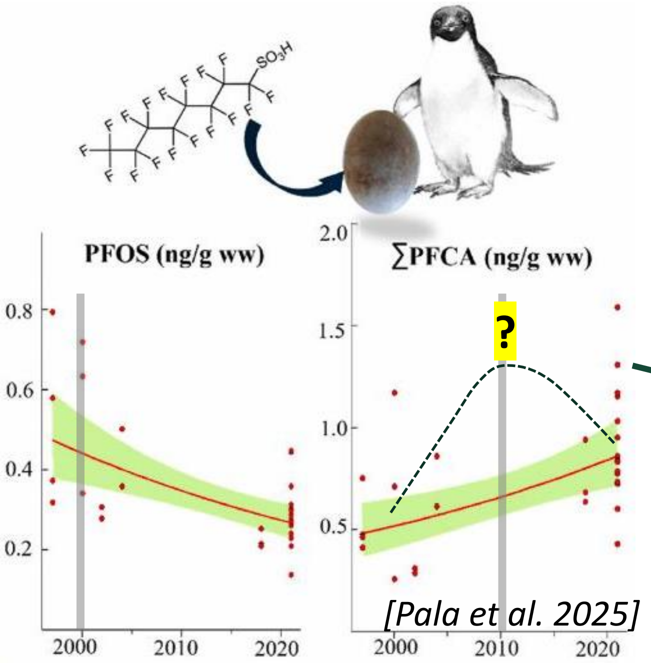
Global spatiotemporal trends





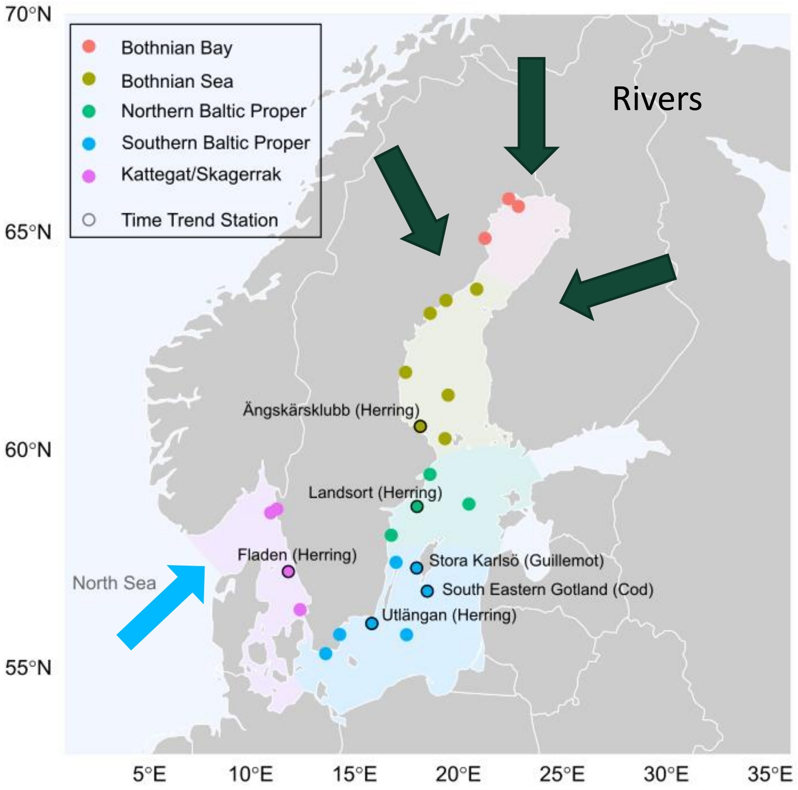
Sea bird (egg) PFAS concentrations

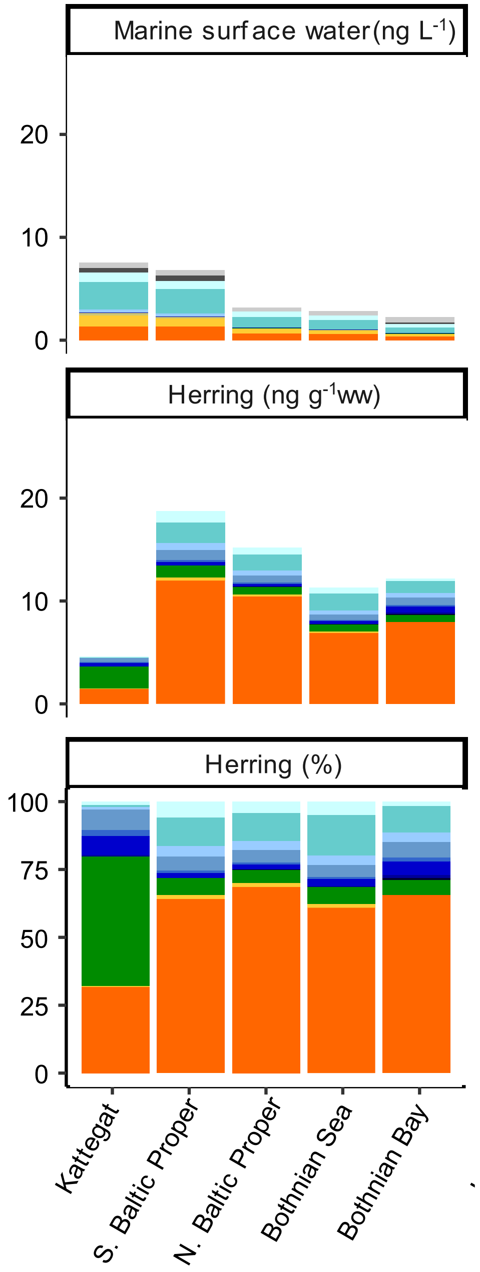


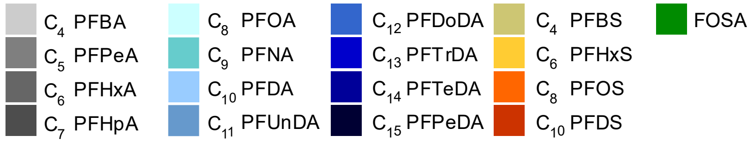


Regional spatiotemporal trends – the Baltic Sea

Coastal-marine







[Soerensen et al. 2024]

- PFOS highest bioconcentration
- PFAS in biota follow PFAS in water

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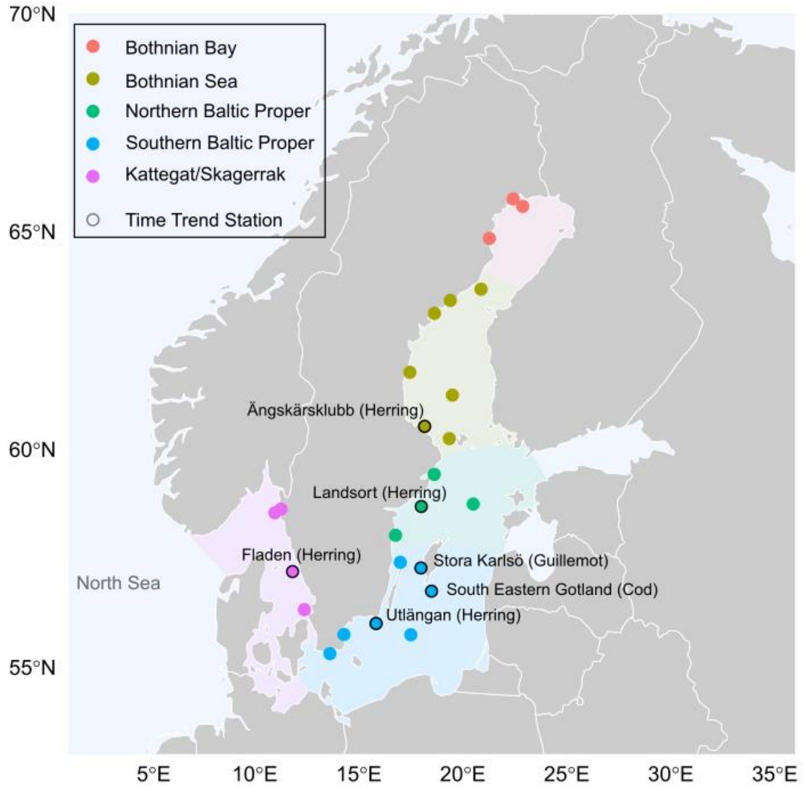
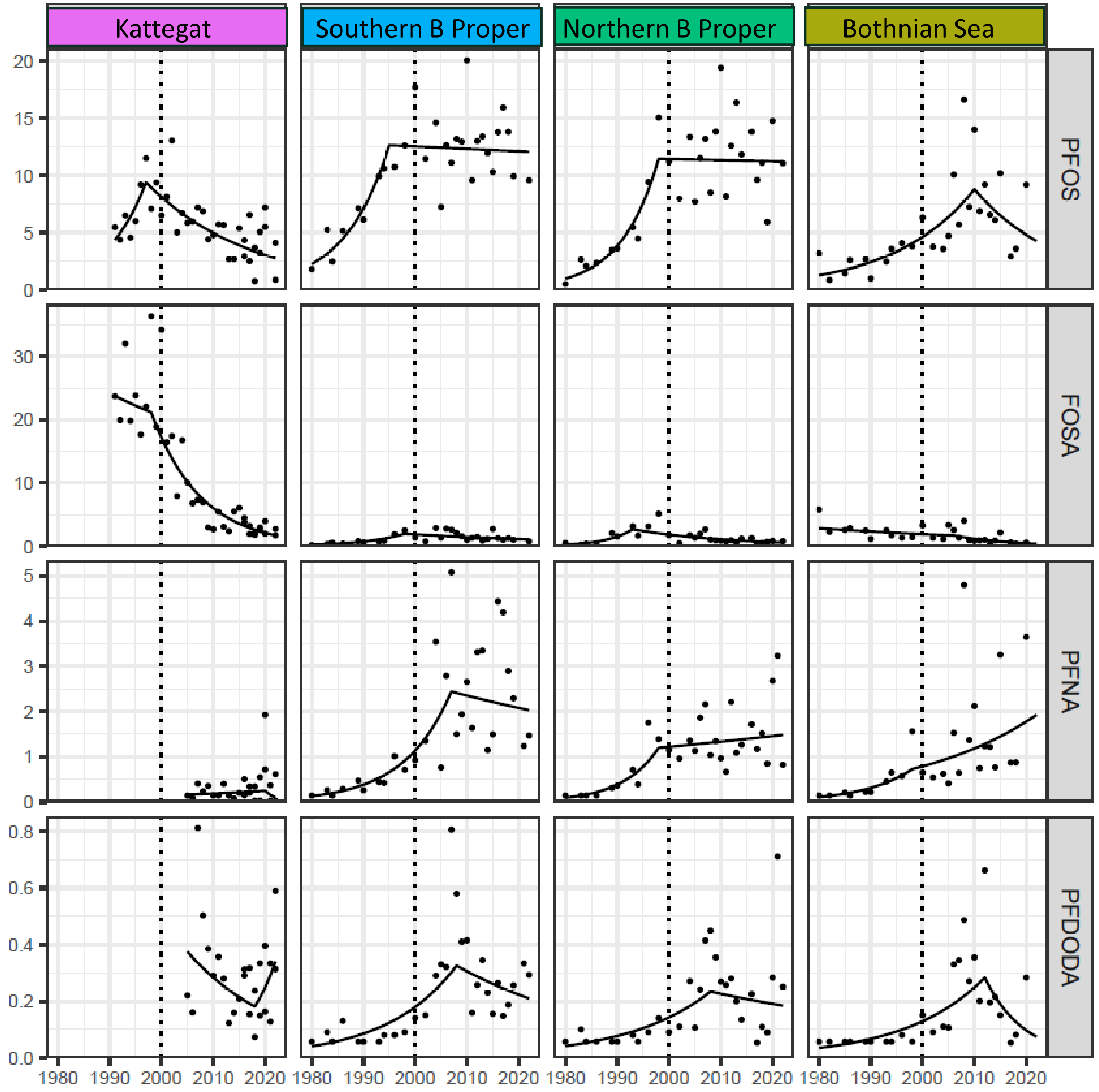
Regional spatiotemporal trends – the Baltic Sea

Coastal-marine



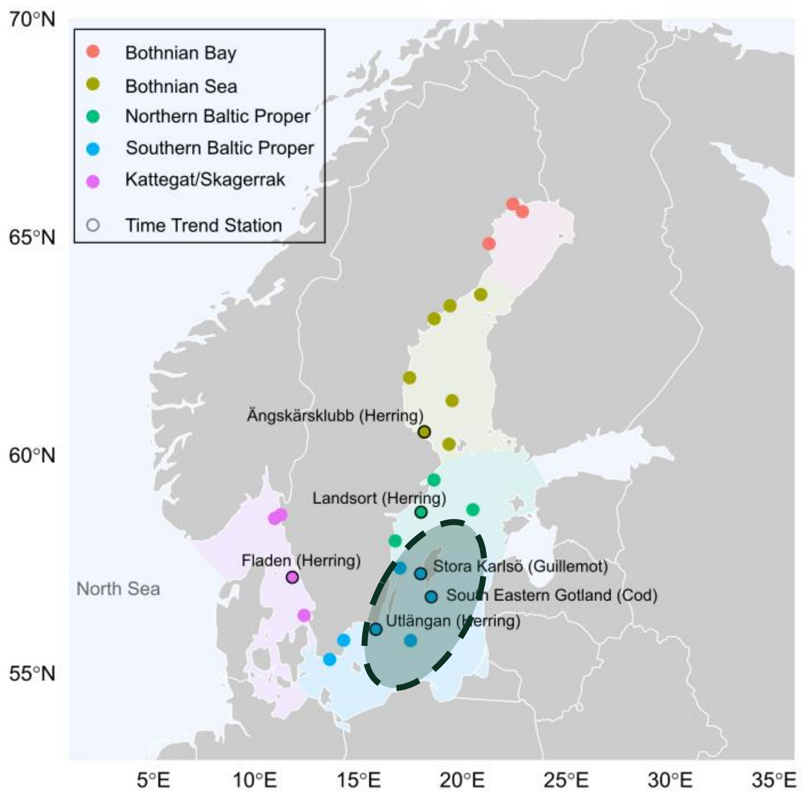


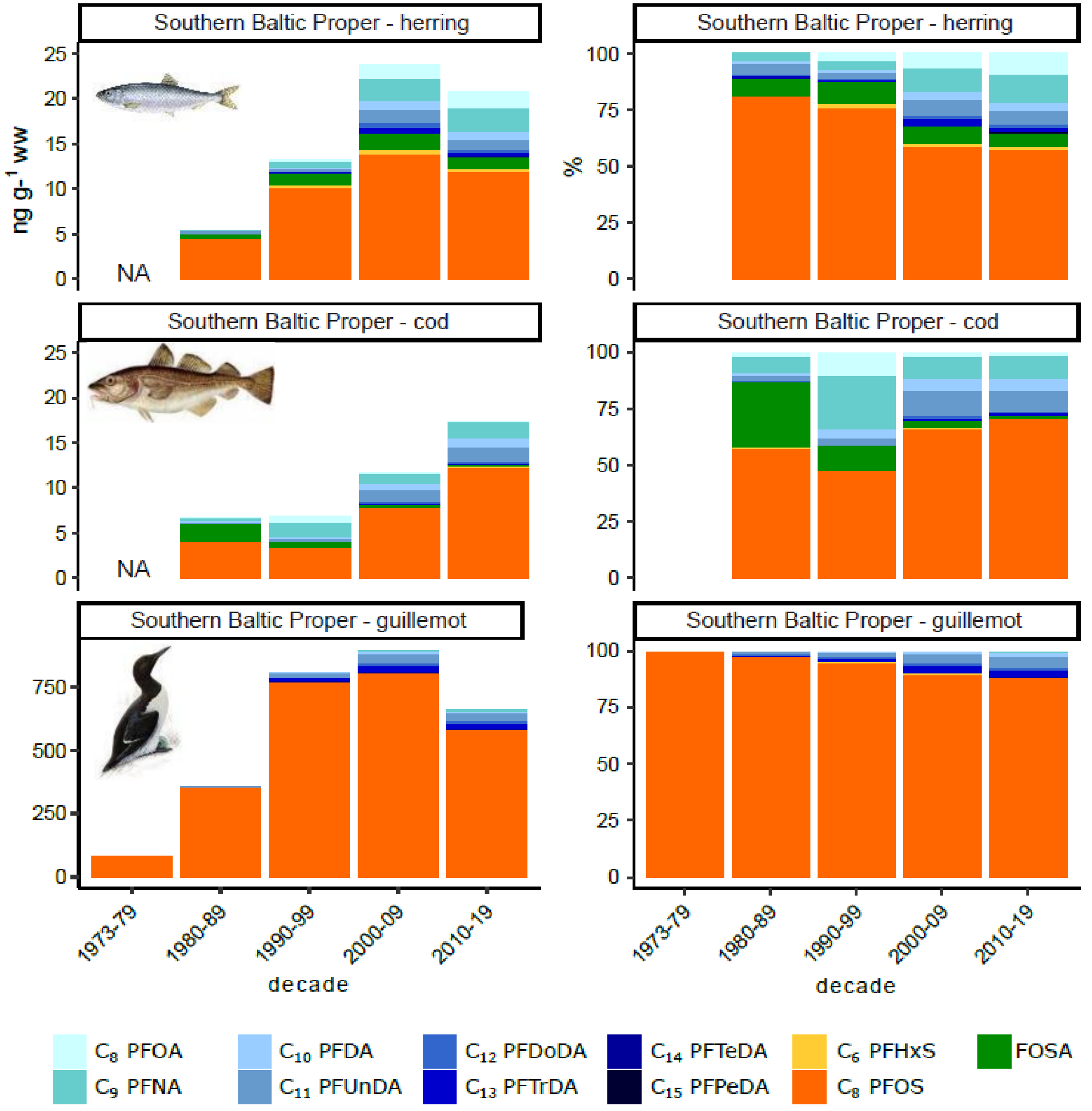
- Different responses in nearby regions
- Chain length dependence of PFCA response

Regional spatiotemporal trends – the Baltic Sea

Soerensen et al. 2024

Coastal-marine



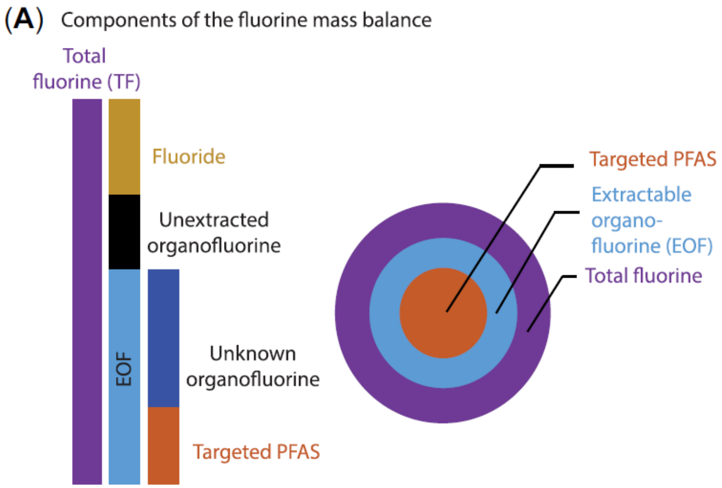


- PFOS highest biomagnification
- Increasing importance of PFCAs
- Species in same area show different trends

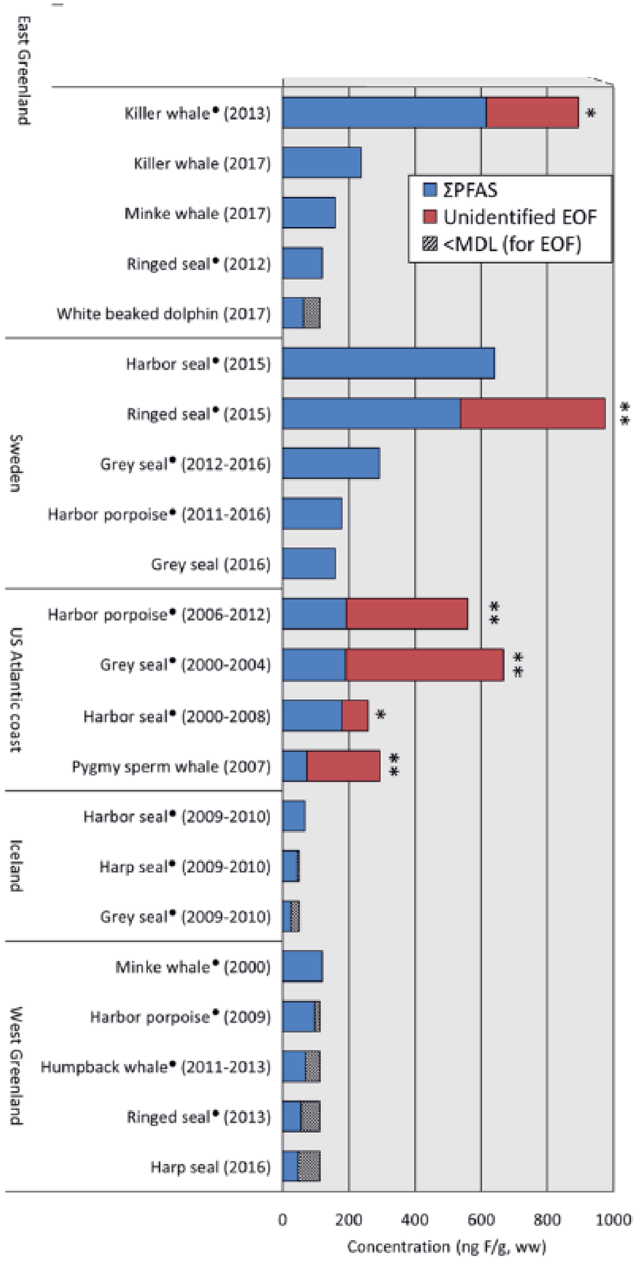
Novel PFAS - Fluorine mass balance & suspect screening

Extractable Organic Fluorine (EOF)

- PFAS exposure underestimated?
- EOF accounted for by ∑PFAS in target analysis differ widely



[De Silva et al, 2020]



[Spaan et al, 2020]

Novel PFAS - Fluorine mass balance & suspect screening

Additional PFAS detected in the Baltic region

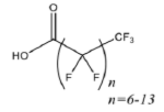
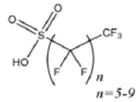
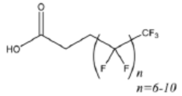
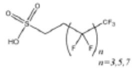
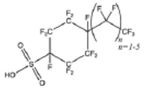
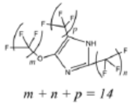
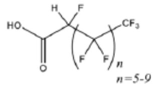
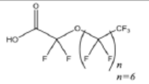
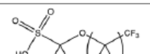
Table 13. PFAS homologues that have been found in various biota or in surface water or sediment in the Greater Baltic Sea. Bold text indicate that the PFAS homologues are part of the draft PFAS EQS dossier.

Class	Detected	Biota	Reference
PFSA and PFCA precursors	**PFBA**	**Surface water** **Sediment**	**[*Joerss et al.*, 2019; *Nguyen et al.*, 2017]**
	PFPeA	**Surface water**	**[*Joerss et al.*, 2019]**
	PFPeS	**Bird egg: guillemot**	**[*Kärrman et al.*, 2019]**
	PFHpS	**Fish liver: herring** **Marine mammal liver: grey seal, harbor seal, harbor porpoise** **Bird egg: eider, white-tailed sea eagle, guillemot**	**[*De Wit et al.*, 2020; *Kärrman et al.*, 2019; *Kratzer et al.*, 2011]**
	DiPAPs	Sediment Zooplankton	[*Gebbink et al.*, 2016; *Kärrman et al.*, 2022]
	diSAmPAP	Sediment	[*Kärrman et al.*, 2022]
FTSA	4:2 FTSA	Sediment* Fish liver: herring	[*Kärrman et al.*, 2022; *Kärrman et al.*, 2019]
	6:2 FTSA	Fish liver: herring, cod	[*Kärrman et al.*, 2019; *Schultes et al.*, 2019]
FTCA	7:3 FTCA	Sediment* Fish liver: herring Marine mammal liver: harbor porpoise	[*Kärrman et al.*, 2019]
FTUCA	FTUCA	Sediment*	[*Kärrman et al.*, 2022]
PFPiA	6:6 PFPiAs	Sediment	[*Joerss et al.*, 2019]
	6:8 PFPiAs	Sediment	[*Joerss et al.*, 2019]
Novel PFAS	PFECHS	Surface water Fish liver: herring, cod, flounder Marine mammal liver: grey seal, harbor seal, harbor porpoise Bird egg: eider, white-tailed sea eagle, guillemot	[*De Wit et al.*, 2020; *Joerss et al.*, 2019; *Kärrman et al.*, 2019; *Vainio*, 2022]
	HFPO-DA (Gen X)	**Surface water**	**[*Joerss et al.*, 2019]**
	11-Cl-PF	Bird egg: guillemot	[*De Wit et al.*, 2020]

* indicates that the presence has only been given at the level of class, not the specific homologue.

[Soerensen and Faxneld, 2023]

Suspect screening of white-tailed sea eagle eggs: 43 substances not included in targeted analysis

Class	General structure	ID	Target	$[M-H]^-$	*m/z*	Δ*ppm*	Verified fragments	RT (min)	CL	BP	GB	LP
PFCAs		PFOA (n=6)	x	$[C_8F_{15}O_2]^-$	412.9669	1.14	168.99 $[C_3F_7]^-$	3.24	1			
		PFNA (n=7)	x	$[C_9F_{17}O_2]^-$	462.9637	1.02	168.99 $[C_3F_7]^-$, 218.99 $[C_4F_9]^-$	3.65	1			
		PFDA (n=8)	x	$[C_{10}F_{19}O_2]^-$	512.9603	0.51	168.99 $[C_3F_7]^-$	4.03	1			
		PFUnDA (n=9)	x	$[C_{11}F_{21}O_2]^-$	562.9573	0.82	168.99 $[C_3F_7]^-$, 118.99 $[C_2F_5]^-$	4.38	1			
		PFDoDA (n=10)	x	$[C_{12}F_{23}O_2]^-$	612.9548	1.88	168.99 $[C_3F_7]^-$, 118.99 $[C_2F_5]^-$	4.72	1			
		PFTrDA (n=11)	x	$[C_{13}F_{25}O_2]^-$	662.9517	1.87	168.99 $[C_3F_7]^-$, 118.99 $[C_2F_5]^-$	5.05	1			
		PFTeDA (n=12)	x	$[C_{14}F_{27}O_2]^-$	712.9485	1.74	168.99 $[C_3F_7]^-$	5.36	1			
		PFPeDA (n=13)	x	$[C_{15}F_{29}O_2]^-$	762.9467	3.45	168.99 $[C_3F_7]^-$	5.64	1			
PFSAs		PFHxS (n=5)	x	$[C_6F_{13}SO_3]^-$	398.9371	1.25	No MS^2 triggered	3.27	1			
		PFHpS (n=6)		$[C_7F_{15}SO_3]^-$	448.9340	1.31	79.96 $[SO_3]^-$, 98.96 $[FSO_3]^-$	3.71	1			
		PFOS (n=7)	x	$[C_8F_{17}SO_3]^-$	498.9300	0.44	79.96 $[SO_3]^-$,	4.10	1			
		PFNS (n=8)		$[C_9F_{19}SO_3]^-$	548.9277	1.24	N/F	4.47	2b			
		PFDS (n=9)	x	$[C_{10}F_{21}SO_3]^-$	598.9249	1.79	N/F	4.80	1			
n:3 FTCAs		7:3 FTCA (n=6)		$[C_{10}F_{15}O_2H_4]^-$	440.9980	0.61	316.98 $[C_9F_{11}]^-$, 266.99 $[C_8F_9]^-$	4.20	1			
		8:3 FTCA (n=7)		$[C_{11}F_{17}O_2H_4]^-$	490.9952	1.36	366.98 $[C_{10}F_{13}]^-$, 316.98 $[C_9F_{11}]^-$, 62.99 $[CO_2F]^-$	4.70	2a			
		9:3 FTCA (n=8)		$[C_{12}F_{19}O_2H_4]^-$	540.9900	2.48	416.98 $[C_{11}F_{15}]^-$, 366.98 $[C_{10}F_{13}]^-$	5.15	2a			
		10:3 FTCA (n=9)		$[C_{13}F_{21}O_2H_4]^-$	590.9896	2.47	No MS^2 triggered	5.58	2b			
		11:3 FTCA (n=10)		$[C_{14}F_{23}O_2H_4]^-$	640.9861	1.79	No MS^2 triggered	5.99	2b			
n:2 FTSAs		6:2 FTSA (n=3)		$[C_8F_{13}SO_3H_4]^-$	426.9681	0.47	No MS^2 triggered	3.08	1			
		8:2 FTSA (n=5)		$[C_{10}F_{17}SO_3H_4]^-$	526.9618	0.53	No MS^2 triggered	3.87	1			
		10:2 FTSA (n=7)		$[C_{12}F_{21}SO_3H_4]^-$	626.9567	2.50	No MS^2 triggered	4.57	1			
FASAs		FBSA (n=3)		$[C_4HF_9NO_2S]^-$	297.9592	0.74	No MS^2 triggered	3.32	2b			
		FPeSA (n=4)		$[C_5HF_{11}NO_2S]^-$	347.9560	0.63	No MS^2 triggered	3.99	2b			
		FHxSA (n=5)		$[C_6HF_{13}NO_2S]^-$	397.9530	1.03	No MS^2 triggered	4.52	2b			
		FOSA (n=7)	x	$[C_8HF_{17}NO_2S]^-$	497.9469	1.41	No MS^2 triggered	5.44	1			
Cyclic/ unsaturated PFSAs		**d/C PFSA (PFECHS, n=1)**		$[C_8F_{15}SO_3]^-$	460.9341	1.50	380.98 $[C_8F_{15}]^-$, 98.96 $[FSO_3]^-$	3.65	1			
		d/C PFSA (n=2)		$[C_9F_{17}SO_3]^-$	510.9306	0.74	No MS^2 triggered	4.02	2b			
		d/C PFSA (n=3)		$[C_{10}F_{19}SO_3]^-$	560.9278	1.39	No MS^2 triggered	4.38	2b			
		d/C PFSA (n=4)		$[C_{11}F_{21}SO_3]^-$	610.9250	1.92	No MS^2 triggered	4.66	2b			
		d/C PFSA (n=5)		$[C_{12}F_{23}SO_3]^-$	660.9221	2.21	No MS^2 triggered	4.88	2b			
Perfluorinated N-heterocycle		PFNhcs (*m+n+p*=14)		$[C_{17}F_{31}N_2O]^-$	836.9537	1.90	217.97 $[C_5F_6N_2O]^-$	5.48	3			
H-PFCAs		H-PFOA (n=5)		$[C_8F_{14}HO_2]^-$	394.9765	2.78	No MS^2 triggered	2.72	4			
		H-PFNA (n=6)		$[C_9F_{16}HO_2]^-$	444.9731	2.31	No MS^2 triggered	3.14				
		H-PFDA (n=7)		$[C_{10}F_{18}HO_2]^-$	494.9702	2.44	No MS^2 triggered	3.52				
		H-PFUnDA (n=8)		$[C_{11}F_{20}HO_2]^-$	544.9669	2.39	No MS^2 triggered	3.85				
		H-PFDoDA (n=9)		$[C_{12}F_{22}HO_2]^-$	594.9637	1.51	No MS^2 triggered	4.20				
H-PFSAs		**H-PFOS (n=6)**		$[C_8HF_{16}SO_3]^-$	480.9400	1.84	No MS^2 triggered	3.89	4			
		H-PFDS (n=8)		$[C_{10}HF_{20}SO_3]^-$	580.9340	2.19	No MS^2 triggered	4.09				
Ether PFCAs		PFECA (n=9)		$[C_9F_{17}O_3]^-$	478.9589	1.57	No MS2 triggered	3.68	4			
Ether PFSAs		PFESA (n=4)		$[C_6F_{13}SO_4]^-$	414.9321	1.40	No MS^2		4			
		PFESA (n=5)		$[C_7F_{15}SO_4]^-$	464.9286	0.58	No MS^2					
		PFESA (n=6)		$[C_8F_{17}SO_4]^-$	514.9252	0.14	No MS^2 triggered	4.25				

[Haque et al, 2023]

Conclusions

- Legacy PFAS are beginning to decline in marine biota but we do not have a global spatiotemporal picture of trends
- There is a shift from PFSAs to PFCAs
- We are missing PFAS in biota with current targeted analysis – this will become more important in the future

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