Investigating a Novel Cyclodextrin Sorbent for Use Within an Integrative Passive Sampler for PFAS

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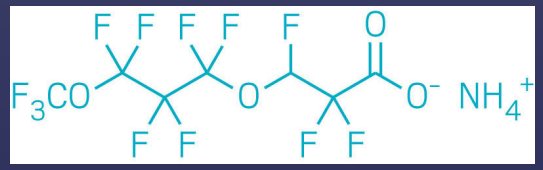
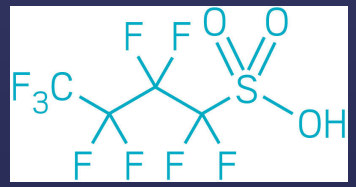
Slide 1

What Are All These Things?

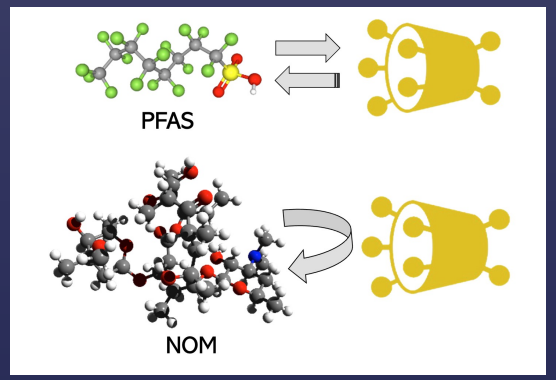
- PFAS[1,2,3]





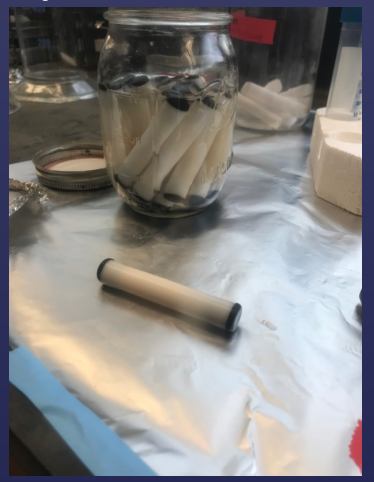
  - 4000+ man made compounds
  - Myriad of negative human health outcomes
  - Poorly regulated in US

- Dexsorb+[4,5,6,7,8]



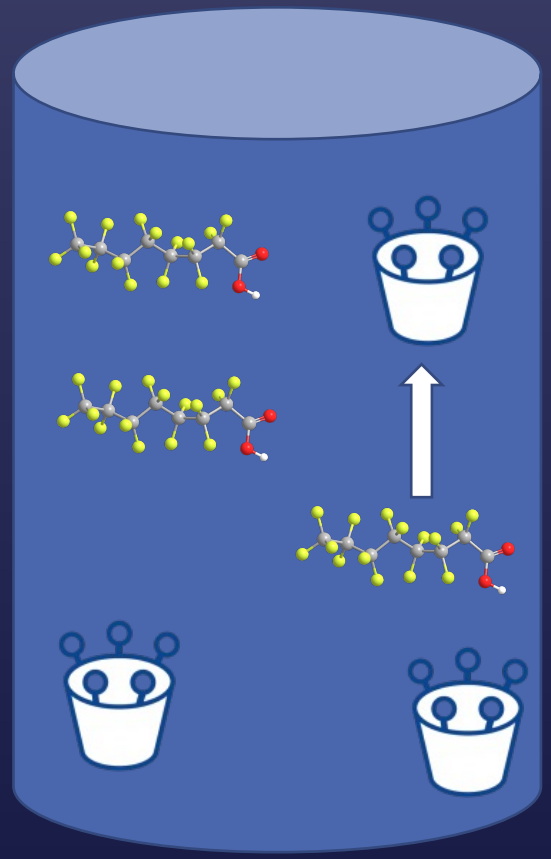
  - Affordable
  - Expand PFAS analysis
  - þeta-CDP with a positive surface charge

- Integrative Passive Samplers[9,10,11,12]



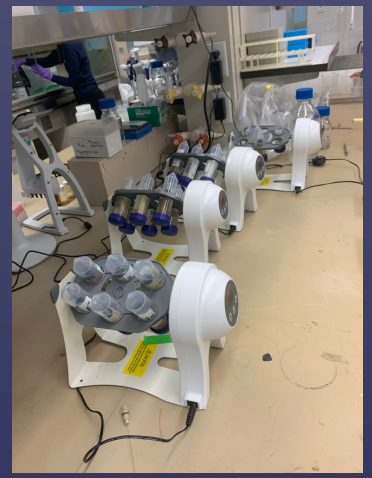
  - 7 cm long
  - Filled with sorbent (HLB or WAX)
  - Measure time weighted average

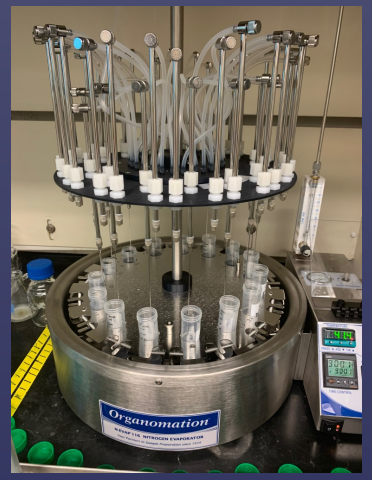
Can we use this in our passive sampler?



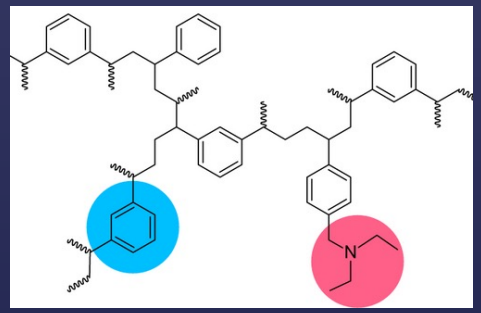
Methods and Process

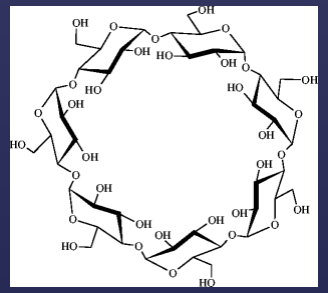
- Validate a method for extraction





- Quantify sorbent-water partitioning values (K_{sw})





- Deploy in contaminated waters

Step 1: Mass labeled surrogates recovered from Passive Sampler w/Dexsorb+

Tumble in ~20 mL
1% NaOH in LC
MeOH (v/v)

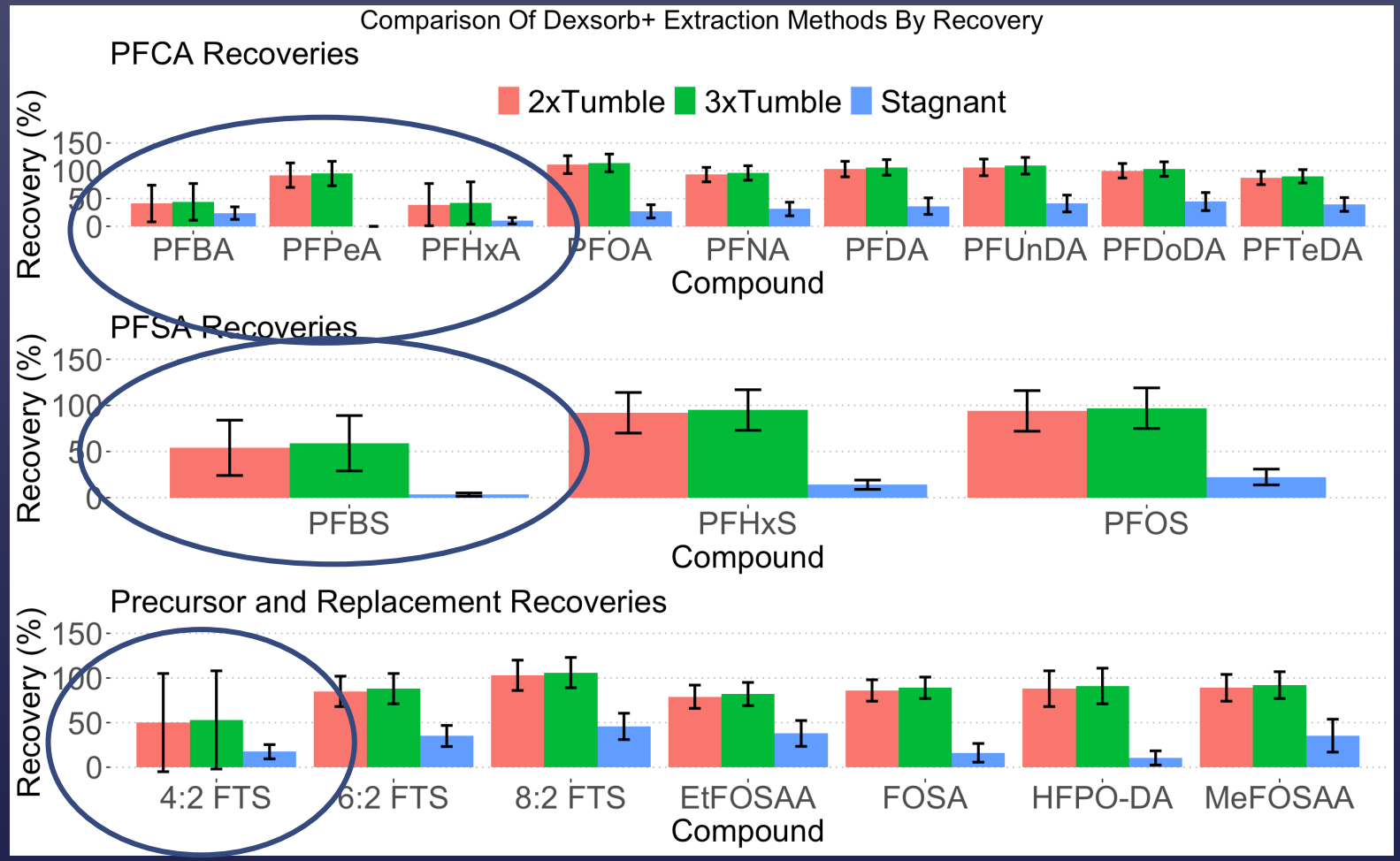
Collect

Tumble in ~20 mL
1% NaOH in LC
MeOH (v/v)

Collect

Concentrate at 40
C° under gentle
stream of N

Dilute with buffered
water and inject to LC-MS



Strong complexation with shorter chains, harder to break, may need correction factor[4]

Step 2: Batch experiments with environmental water

	DEX Log K_{sw}	WAX Log K_{sw}	HLB Log K_{sw}
PFBA	2.9	3.6	NR
PFPeA	3.4	3.7	NR
PFHxA	4.0	4.2	2.4
PFHpA	4.3	4.7	NR
PFOA	4.5	5.0	NR
PFNA	4.5	5.1	3.9
PFDA	4.7	5.1	4.9
PFPrS	4.0	4.1	3.2
PFBS	4.3	4.4	NR
PFPeS	4.7	4.9	3.0
PFHxS	4.9	5.3	3.7
PFHpS	4.9	5.4	4.2
PFOS	4.9	5.3	5.0
GenX	3.8	4.3	NR
FHxSA	4.5	5.0	5.2
8:2 FTS	4.6	5.1	4.9
4:2 FTS	4.1	4.2	NR
6:2 FTS	4.6	4.9	NR

- Units = dimensionless = g water / g sorbent
- Coefficient of variance (%) ranged from
  0.3-17 for DEX+
  1.5-13 for HLB
  1.1-14 for WAX

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Step 3: Deployments in Contaminated Surface Waters hit a snag…

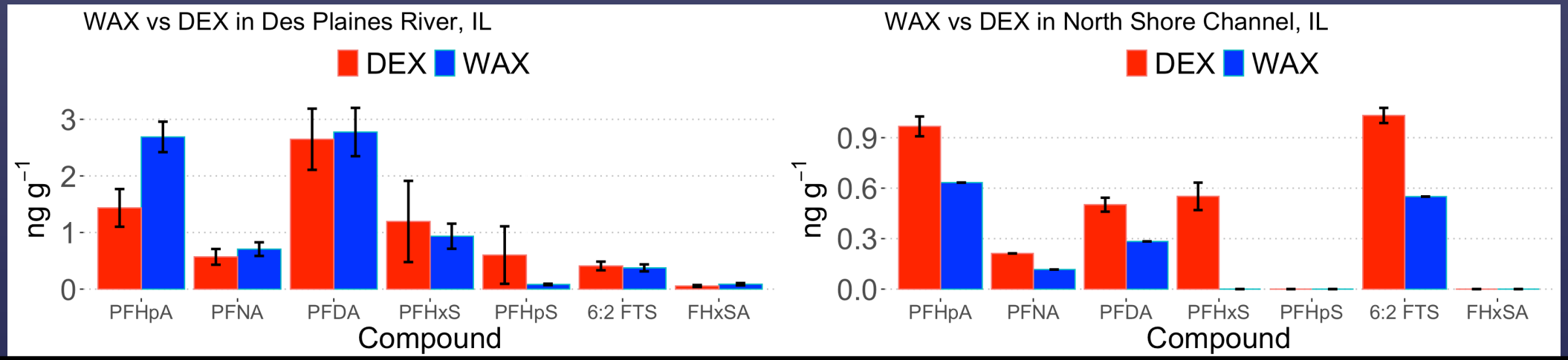
Unfortunately, the lab was contaminated with PFOA and PFOS from remediation efforts

Rendering much of the field deployed passive sampler data useless

Slide 8

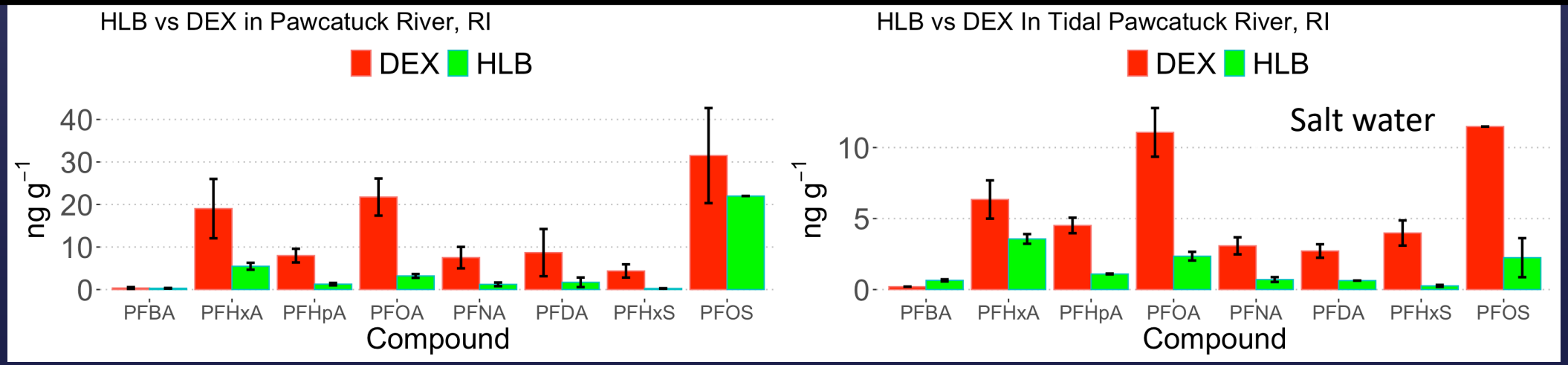
Step 3: There were some promising results to lead us forward….

CHICAGO



14 Days

Rhode Island



28 Days

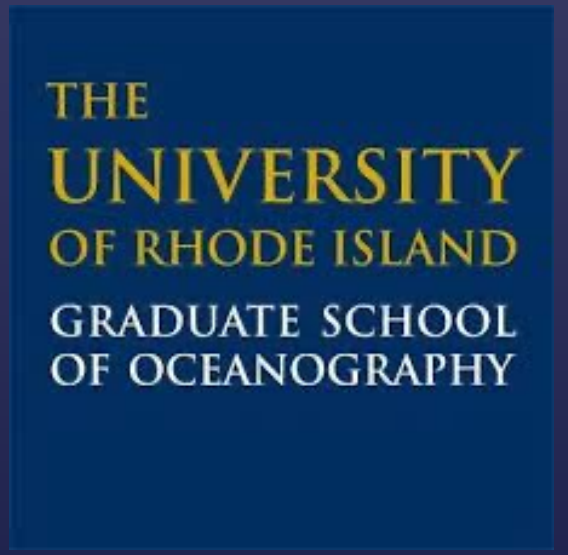
Dexsorb+ is suitable alternative to HLB/WAX sorbents for most PFAS compounds

1. Method of extraction results in good recovery of C5+ PFAS
2. K_{sw} may be lower than WAX, but shows more resistance to matrix than currently used HLB
3. Comparable uptake to WAX, better uptake than HLB, cheaper than both

Future Directions

- Explore alternative numerical models for sampler uptake
- Investigate how to improve recovery of short chain compounds

Acknowledgments



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References

- 1 Buck et al. 2011
- 2 Ojo et al. 2021
- 3 Cousins et al. 2020
- 4 Weiss-Errico et al. 2019
- 5 Wang et al. et al. 2020
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- 7 Xiao et al et al. 2017
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- 9 Fauvelle et al. 2017
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- 13 Urik & Vrana 2019
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