



Literature Review of PFAS Bioaccumulation Data

October 26, 2020

EPA-ECOS-ASTHO PFAS Science Call



Bioaccumulation: Background

- What is bioaccumulation?
 - Accumulation of a chemical in an organism
 - Occurs when uptake rates are faster than lost rates by excretion and biotransformation
- Bioaccumulation expressed using bioaccumulation factor (BAF)
- $BAF = \frac{\text{Concentration in organism}}{\text{Concentration in water}}$ $BAF > 1$
- PCBs: BAFs range from 10^5 to 10^8



Bioaccumulation: Background

- Why is chemical bioaccumulation important?
 - EPA's Ambient Water Quality Criteria (AWQC) for Protection of Human Health

Noncancer Effects²

$$AWQC = RfD \cdot RSC \cdot \left(\frac{BW}{DI + \sum_{i=2}^4 (FI_i \cdot BAF_i)} \right) \quad (\text{Equation 1-1})$$

2000 Methodology

DI = drinking water intake

FI = fish intake at trophic levels 2, 3 & 4

BAF = bioaccumulation factor at TLs 2, 3 & 4

BW = human body weight

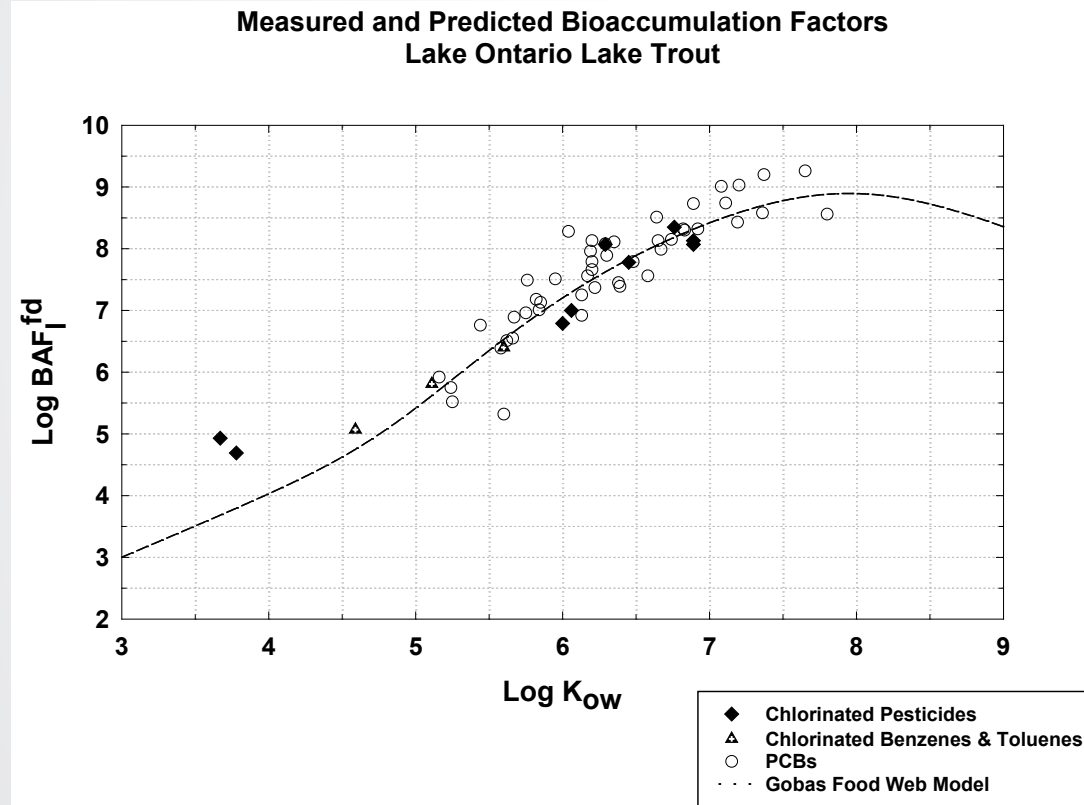
RfD = reference dose for noncancer effects

RSC = Relative source contribution factor

Equal exposures between DI and FI routes: $BAF \approx 5000$

$BAF > 5000$, dietary exposure primary uptake route

$BAF < 5000$, water exposure primary uptake route



- Models for legacy chemicals
 - PCBs, DDTs, PCDD/Fs ...
 - Uptake and excretion processes controlled by diffusional mass transport processes
 - Lipids major storage tissue
- **NOT applicable to PFAS**
 - Different processes
 - Renal transporters
 - Binding to cytosolic fatty acid binding proteins & to albumin
- Model development in its infancy
 - Decade or two to develop???



Needs & Path Forward

- OW
 - Actively developing ambient water quality criteria
 - Human health & aquatic life and aquatic dependent wildlife
 - PFOS and PFOA
- OLEM (Superfund)
 - Needs data for setting cleanup levels
- States & DOD actively developing their own criteria
 - Fish consumption advisories by states
- **Path Forwards:**
 - Use Empirical BAF data in criteria development



Path Forward

- Literature Review of Bioaccumulation
 - What do we know?
 - What are the gaps & limitations?
- Define and implement research to fill the gaps & limitations



Definitions

- Bioconcentration Factor (BCF)
- Laboratory experiment
 - Water only exposure

OECD 305, OPPTS 850.1730

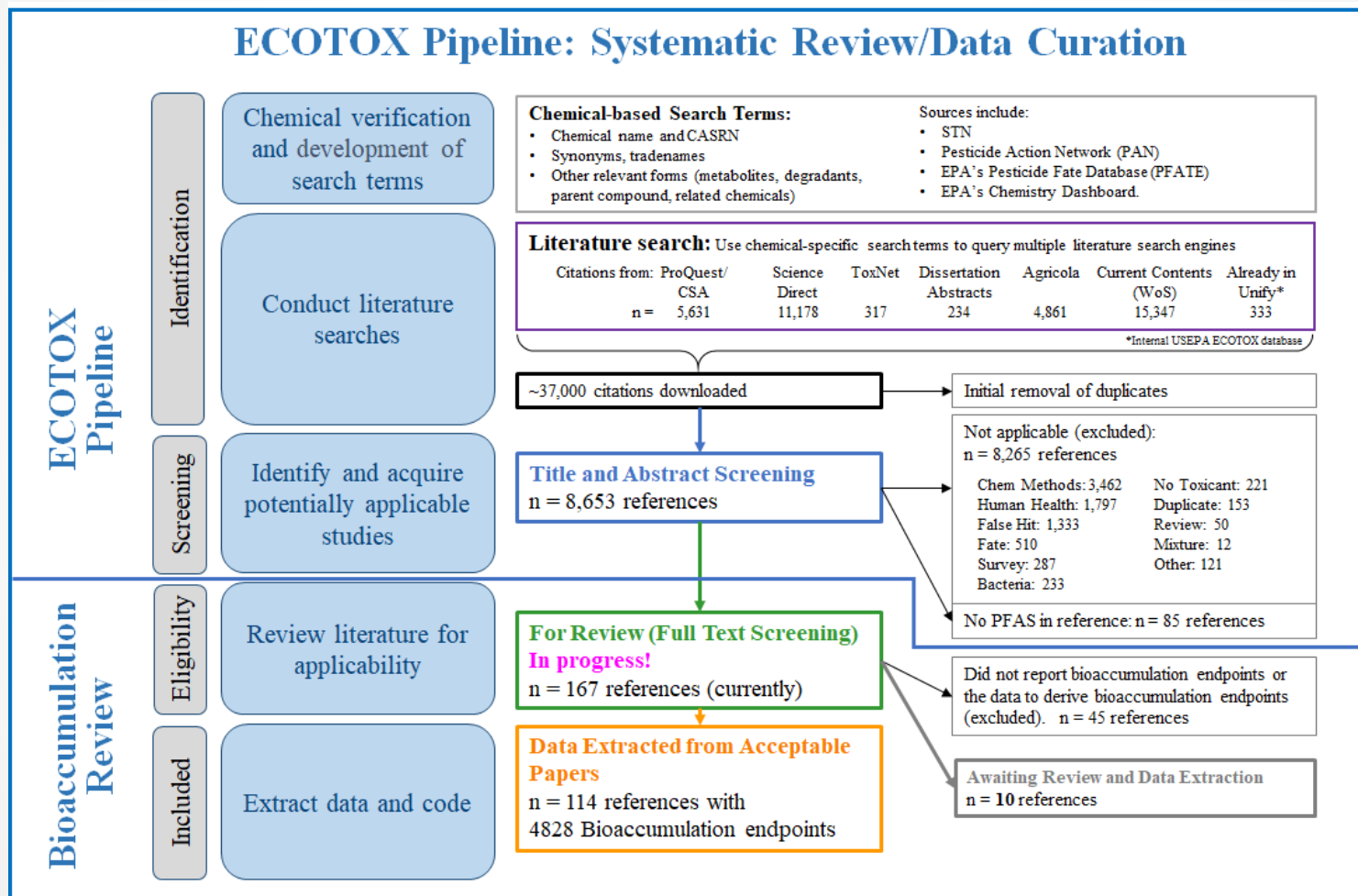
$$BCF = \frac{\textit{Concentration in biota}}{\textit{Concentration in water}}$$

- Bioaccumulation Factor (BAF)
 - Field measurement

$$BAF = \frac{\textit{Concentration in biota}}{\textit{Concentration in water}}$$



Search Strategy





Data Extraction Guidelines

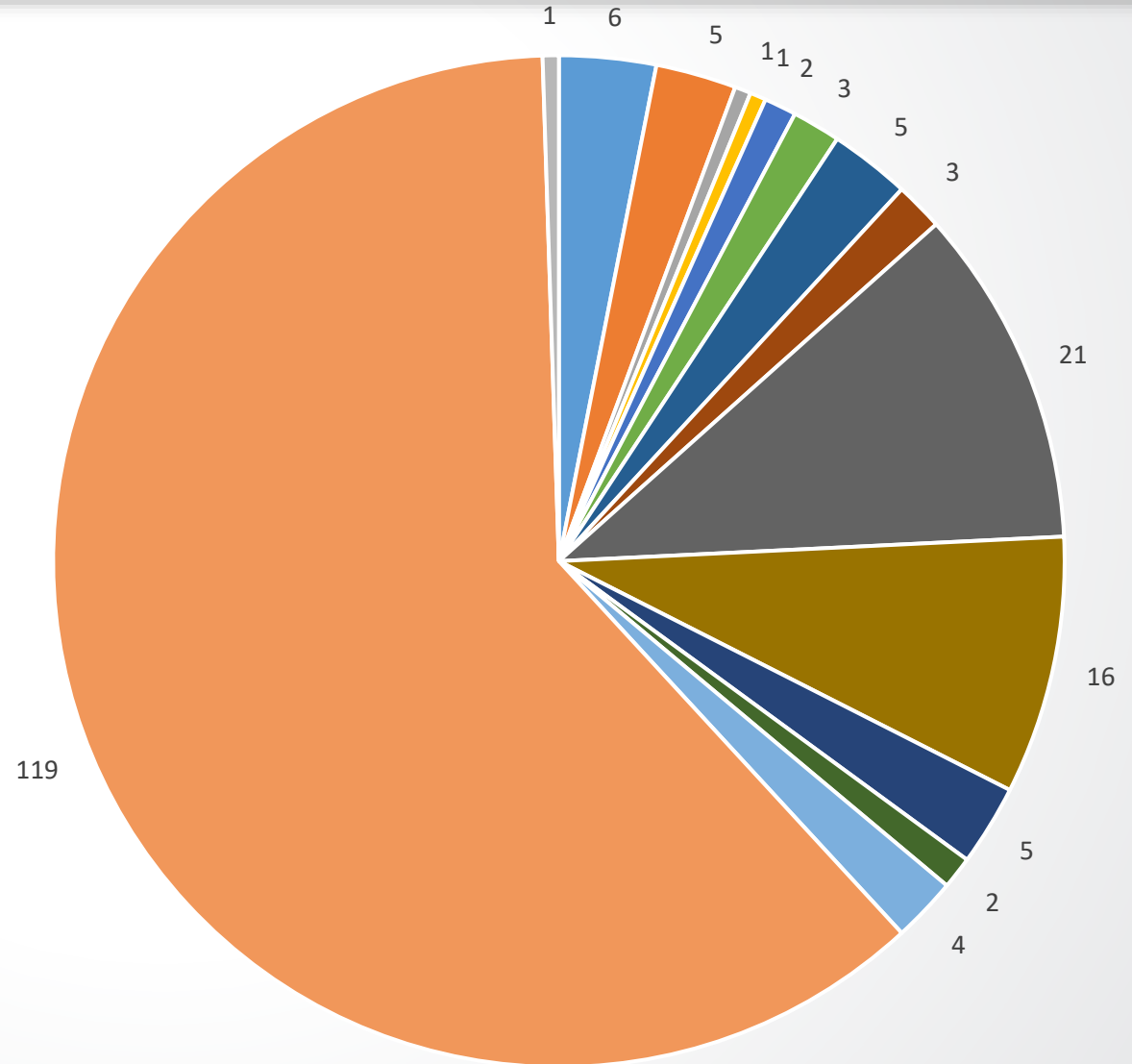
Data Extraction Guidelines

- Chemical & CASRN
- Exposure data
- Kinetic uptake and depuration rates & half-life
- Tissues: whole body, fillet, muscle, gills, brain, ...
- Species trophic level: Measured and Fishbase trophic level estimates
- Endpoints: BCF, BAF (lab & field), BSAF (lab & field), BMF (lab & field), & TMF
- Mixture or single chemical exposure
- Spatial and temporal coordination of biota, water and sediment data
- Number of samples for each matrix
- Do reported bioaccumulation endpoints align with reported data for biota, water and/or sediment?



What Species: Freshwater BCFs & BAFs

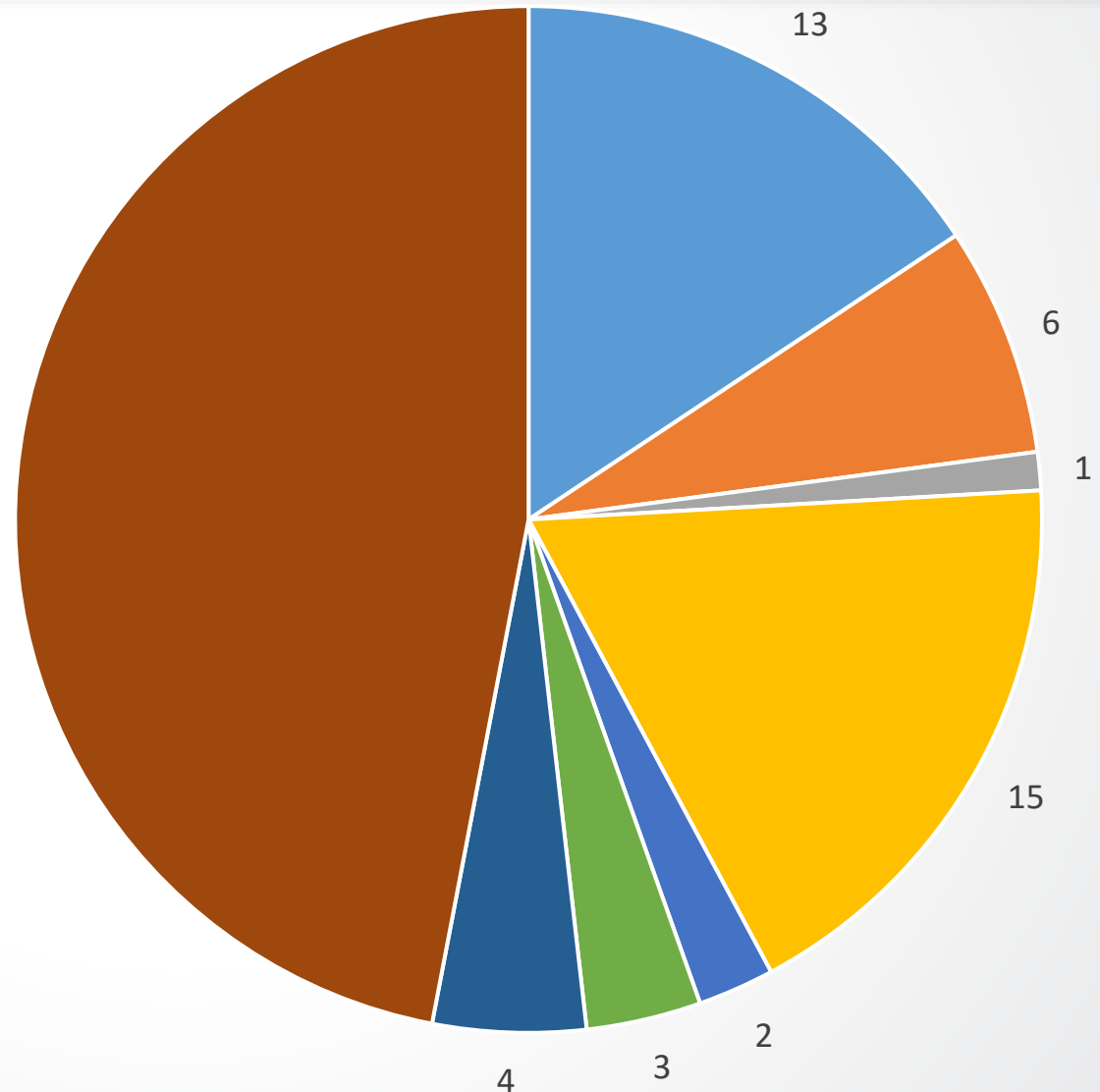
- Amphibia (frogs)
- Bivalvia (mussels)
- Branchiopoda (Daphnia)
- Chlorophyceae (algae)
- Florideophyceae (periphyton)
- Gastropoda (snails)
- Insecta (midges, mayfly)
- Liliopsida (macrophyte)
- Magnoliopsida (duckweed, lotus, hyacinth, hornwort)
- Malacostraca (shrimps, prawns, crabs, Gammarids, mysids)
- Plankton (Field net tows)
- Polypodiopsida (floating plants)
- Reptilia (turtles, alligators)
- Teleostei (fishes)
- Ulvophyceae (green algae)





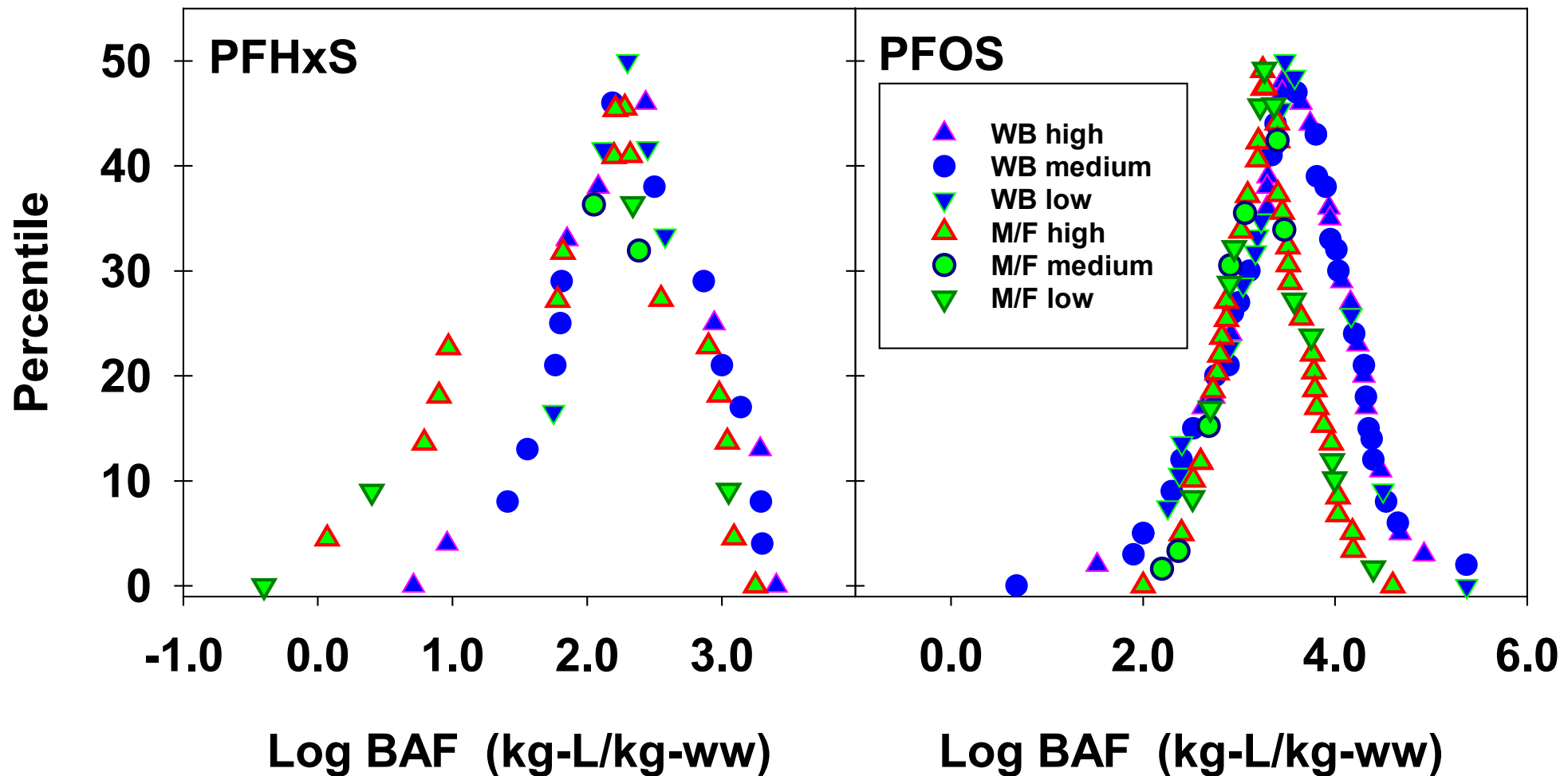
What Species: Marine/Brackish BCFs & BAFs

- Bivalvia (mussels)
- Gastropoda (snails)
- Holothuroidea (sea cucumber, starfish)
- Malacostraca (shrimps, prawns, crabs, Gammarids, mysids)
- Maxillopoda (Copepods)
- Plankton (Field net tows)
- Polychaeta (worms)
- Teleostei (fishes)



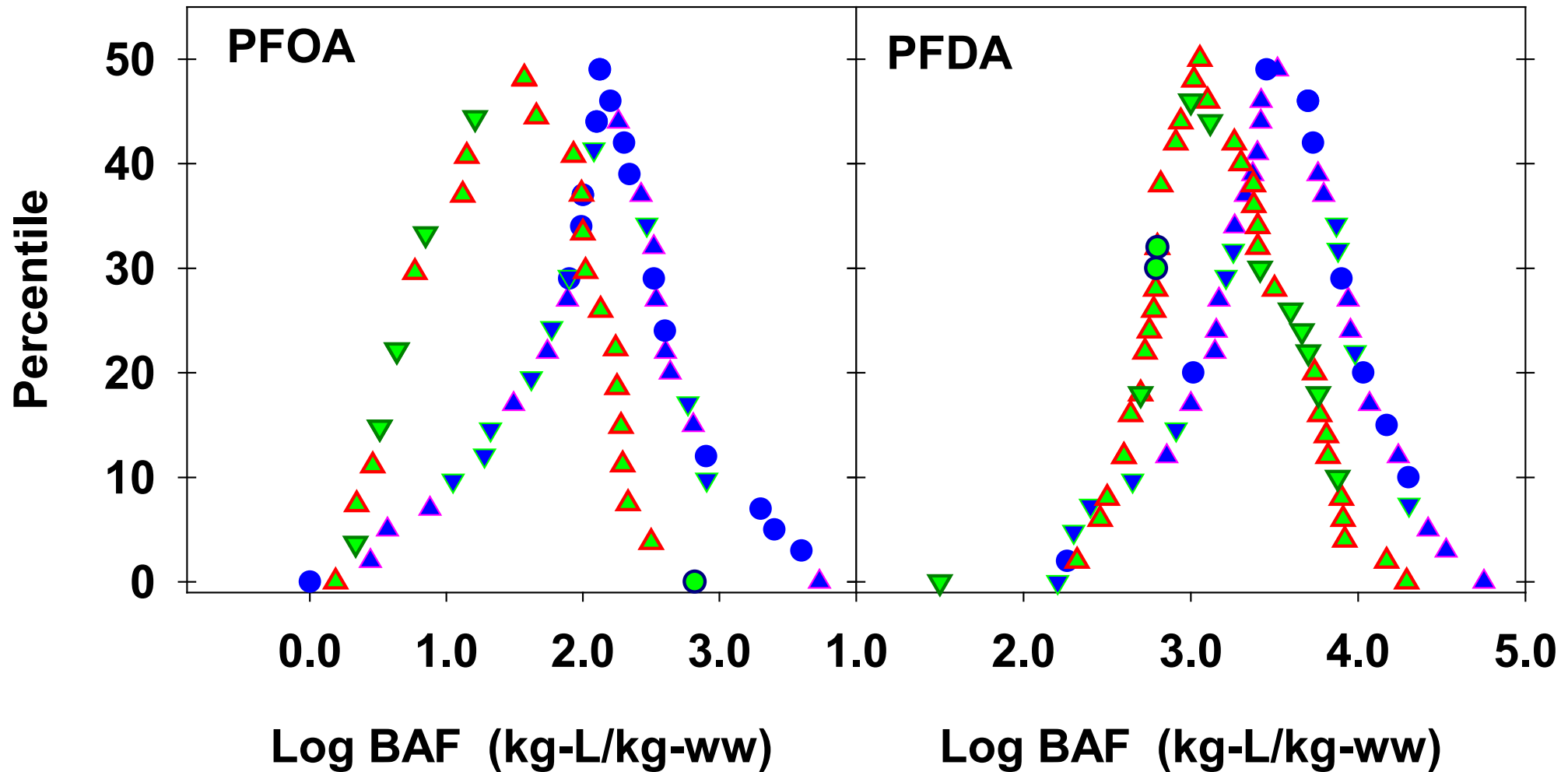


Comparison of BAFs: Whole Body vs Muscle/Fillet





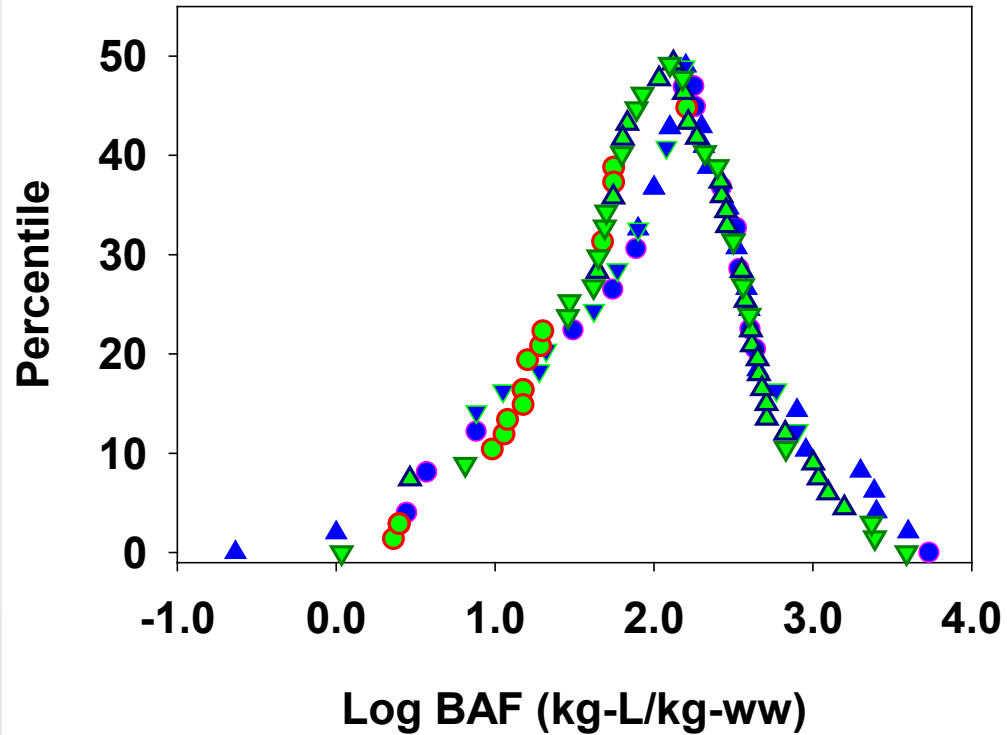
Comparison of BAFs: Whole Body vs Muscle/Fillet



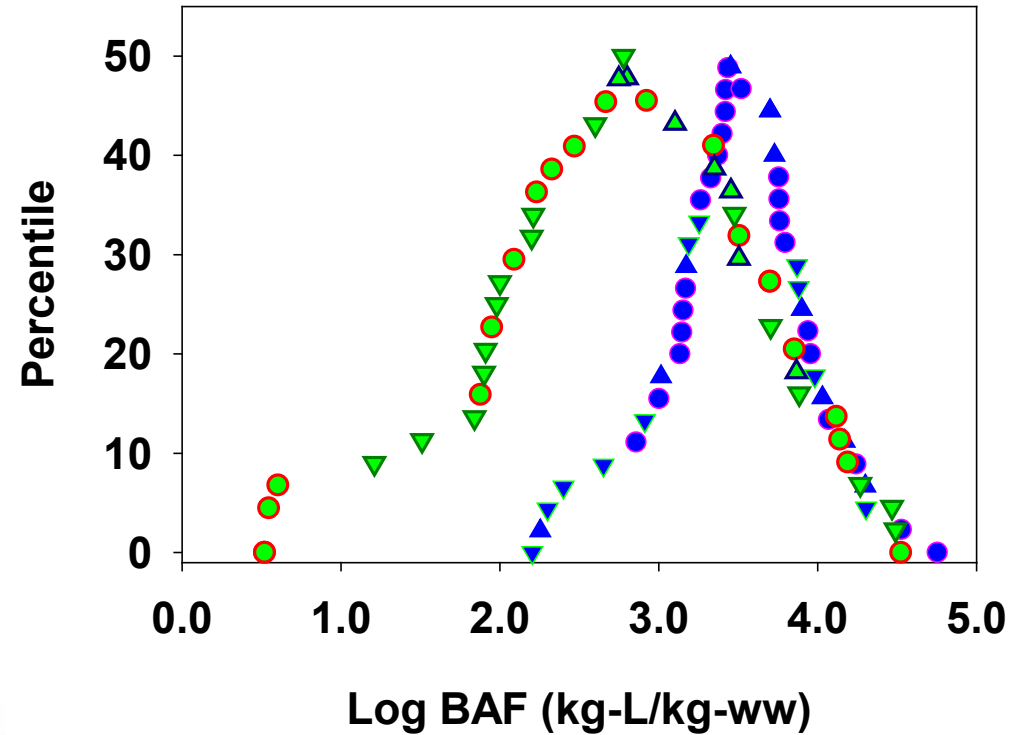


Comparison of Fish BAFs and Invertebrate BAFs

PFOA:
Fish Whole Body BAF
vs Invertebrate BAF



PFDA:
Fish Whole Body BAF
vs Invertebrate BAF





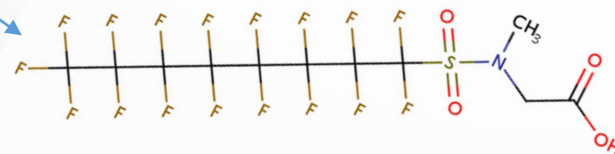
Fish: Carboxylic Acid BCFs & BAFs

	Log BCF Whole Body (L/kg) average ± sd (n)	Log BCF Muscle/Fillet (L/kg) average ± sd (n)	Log BAF Whole Body (L/kg) average ± sd (n)	Log BAF Muscle/Fillet (L/kg) average ± sd (n)
Carboxylic Acids - OECD Structure Category 102				
PFBA	1.18±0.08 (2)	-0.13±0.47 (4)	0.49±2.09 (3)	-0.78±0.11 (2)
PFPA		-0.83±0.22 (2)	2.31±2.89 (9)	
PFHxA	1.00±0.02 (2)	0.13±0.55 (4)	1.36±1.39 (16)	0.55±1.36 (9)
PFHpA		0.33±0.27 (2)	1.34±1.25 (12)	1.60±1.40 (9)
PFOA	1.45±0.83 (3)	1.20±0.76 (3)	2.04±0.93 (50)	1.28±0.84 (27)
PFNA	3.13±0.06 (2)	3.06±0.34 (2)	2.52±1.10 (46)	2.56±0.78 (25)
PFDA	3.88±0.13 (2)	3.51±0.76 (3)	3.49±0.59 (46)	3.15±0.60 (44)
PFUnDA	3.69±0.30 (4)	3.79±0.46 (3)	4.00±0.89 (24)	4.02±1.02 (27)
PFDoDA	4.08±0.18 (4)	4.16±0.46 (3)	4.57± --- (1)	4.79±0.45 (15)
PFTTrDA	4.34±0.46 (2)	4.51±0.85 (2)		4.59±0.16 (3)
PFTeDA	4.60±0.56 (4)	4.76±0.55 (3)		4.38± --- (1)
PFHxDA	3.68±0.01 (2)			
PFOcDA	2.57±0.09 (2)			



Fish: Sulfur based BCFs & BAFs

	Log BCF Whole Body (L/kg) average ± sd (n)	Log BCF Muscle/Fillet (L/kg) average ± sd (n)	Log BAF Whole Body (L/kg) average ± sd (n)	Log BAF Muscle/Fillet (L/kg) average ± sd (n)
Sulfonic Acids - OECD Structure Category 202				
PFBS	1.37±0.11 (2)	-0.09±0.32 (3)	1.83±1.24 (4)	1.09±1.05 (10)
PFH _x S	2.20±0.22 (3)	1.22±0.25 (3)	2.31±0.73 (31)	1.81±1.15 (17)
PFHpS				2.20± --- (1)
PFOS	3.30±0.43 (11)	3.18±0.22 (4)	3.30±1.11 (80)	3.27±0.61 (50)
PFDS	2.63± --- (1)		1.30± --- (1)	
PFECHS			2.79±0.19 (4)	
Sulfonamides - OECD Structure Category: 203.01				
PFOSA			3.43±0.51 (7)	2.59±0.67 (19)
Sulfonamidoacetic acids - OECD Structure Category: 203.05				
MePFOSAA			4.10±0.16 (2)	
EtPFOSAA			2.94±0.96 (3)	





Fish: Phosphorus based BCFs & BAFs

Log BCF Whole Body (L/kg)	Log BCF Muscle/Fillet (L/kg)	Log BAF Whole Body (L/kg)	Log BAF Muscle/Fillet (L/kg)
average ± sd (n)	average ± sd (n)	average ± sd (n)	average ± sd (n)

Perfluoroalkane sulfonyl amido ethanols, phosphate esters (SAmPAPs) - OECD Structure Category: 203.02

L-SAmPAP 1.42± --- (1)

Phosphonic acids - OECD Structure Category: 302

PFHxPA 1.47±0.36 (2) 1.44±0.14 (2)

PFOPA 1.92±0.13 (2) 1.75±0.12 (2)

PFDPA 2.21±0.13 (2) 1.87±0.04 (2)

Phosphinic acids - OECD Structure Category: 303

C6/C6 PFPiA 5.13±0.71 (2) 5.51±0.16 (2)

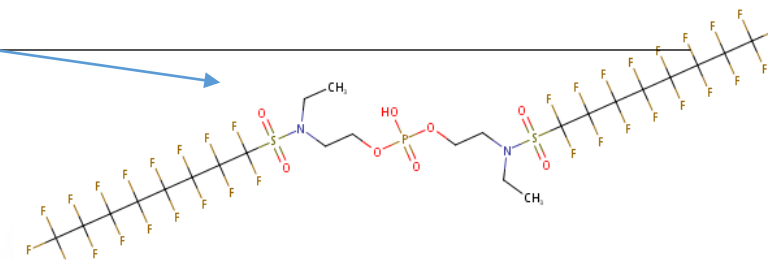
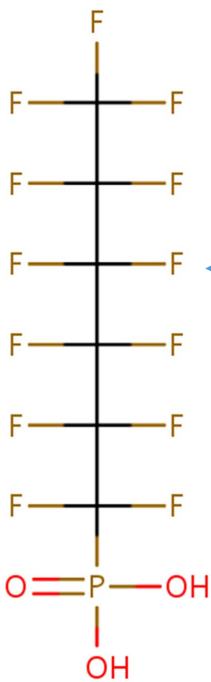
C6/C8 PFPiA 7.36±1.24 (2) 7.03±0.88 (2)

C8/C8 PFPiA 8.30±0.89 (2) 7.44±1.43 (2)

C6/C10 PFPiA 8.53±1.01 (2) 7.78±1.43 (2)


C8/C10 PFPiA 5.79±0.07 (2) 5.40± --- (1)

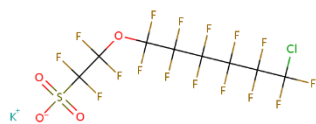
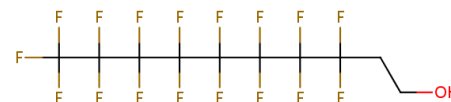
C6/C12 PFPiA 6.31±0.98 (2) 5.35±1.56 (2)



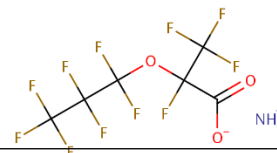


Fish: Alcohol and Ethers

	Log BCF Whole Body (L/kg)	Log BCF Muscle/Fillet (L/kg)	Log BAF Whole Body (L/kg)	Log BAF Muscle/Fillet (L/kg)
	average ± sd (n)	average ± sd (n)	average ± sd (n)	average ± sd (n)
n:2 fluorotelomer alcohol, phosphate esters (PAPs) - OECD Structure Category: 402.04				
6:2 diPAP			1.78± --- (1)	
Fluorotelomer alcohols - OECD Structure Category: 402.03				
8:2 FTOH	2.5±0.42 (2)			
Fluorotelomer sulfonate - OECD Structure Category: 402.07				
4:2 FTSA			4.14± --- (1)	1.49± --- (1)
6:2 FTSA	1.02±0.76 (2)			
8:2 FTSA			4.86±0.41 (2)	3.7±0.56 (4)
PFECAs, salts and esters - monoethers - OECD Structure Category: 502.01				
F-53B			4.24±0.11 (4)	3.87±0.04 (4)
6:2 Cl-PFESA				2.91± --- (1)
8:2 Cl-PFESA				4.69± --- (1)
HFPO-DA				0.61± --- (1)
PFECAs, salts and esters - diethers - OECD Structure Category: 502.02				
HFPO-TA				1.05± --- (1)



Gen-X





Observations and Gaps

- Observations:
 - Many species have measured bioaccumulation endpoints
 - Most measurements are for carbonyl and sulfonyl compounds:
 - Primarily PFCAs and PFSA's (OECD structure category 102 and 202)
 - Differences exist between BAFs based on whole body and muscle/fillet residues
 - Impacts on development of HH and Aquatic Life AWQC
- Gaps and Limitations
 - Limited data for alcohols, ethers, esters, and phosphorus PFASs
 - Effects of mixture exposures on accumulation
 - Fewer measurements for marine species
 - Should BAFs be similar between freshwater and marine species?
 - Plankton net tows
 - Usefulness a mixed blessing
 - Predictive models for assessing bioaccumulation in their infancy



Path Forward

- Data needs
 - Determinants of accumulation:
 - Albumin binding, Binding to cytosolic fatty acid proteins, Phospholipid binding, Renal clearance rates & Biotransformation rates
 - Field and laboratory (*in vivo*) data sets for model validation
 - “high throughput” *in vitro* tools
 - Causes of differences in accumulation across sites
- Can not test every chemical in the vast PFAS universe
 - Phasing out of existing chemicals
 - Replacement chemicals coming on-line
- My path
 - Submitted to Environ Toxicol Chem: Literature Review on BCFs and BAFs
 - In progress: Literature Review report on BMFs and BSAFs



- Questions

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