Presence and distribution of pollutants of emerging concern in wild fish tissues using target and suspect analysis

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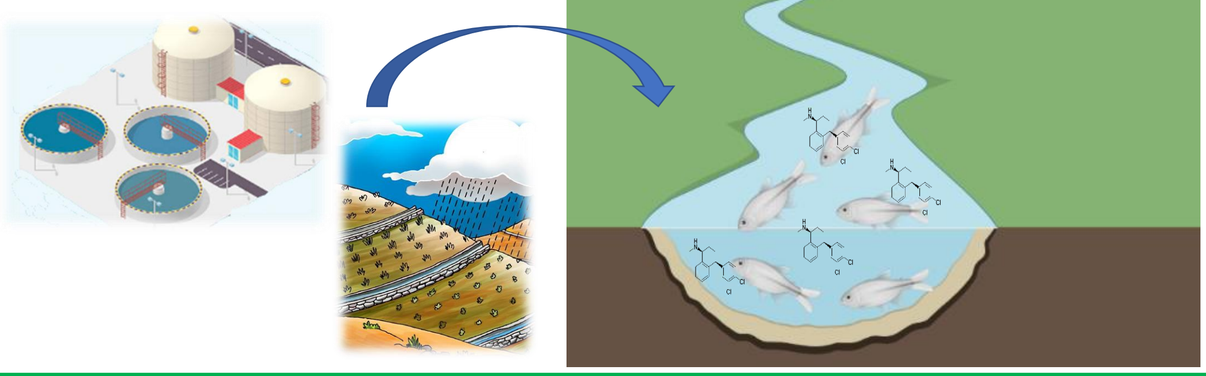
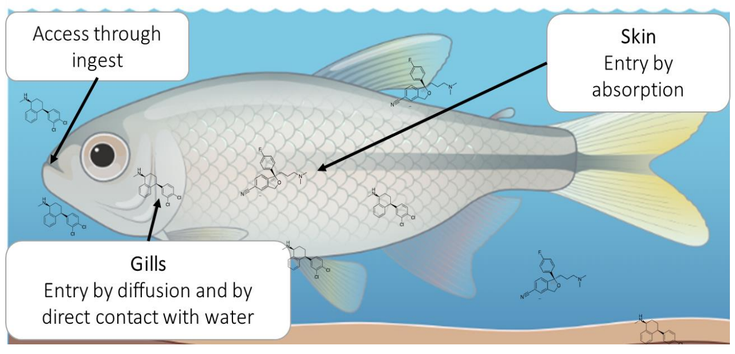
Introduction

Contaminants of emerging concern (CECs) are discharged into aquatic ecosystems through wastewater effluents, crop runoff water and other sources.



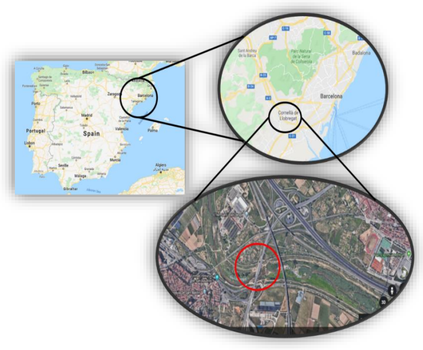


The pathways of entry of CECs into fish are ingestion of compounds accumulated in sediments, that is, depending on their diet, followed by absorption and diffusion through the gills or skin. Within the fish's body, various processes can take place, such as internal transport through the fish's fluids and the gastrointestinal tract, leading to their accumulation in fat and lipid tissue. Once the CECs are absorbed, it can reach the target organ through the bloodstream.

Objectives

- Distribution of 47 PhACs in wild fish from Llobregat river using a routine target method
- Using the capability of the SWATH mode, 1509 CECs were screened in fish samples to detect further compounds of interest

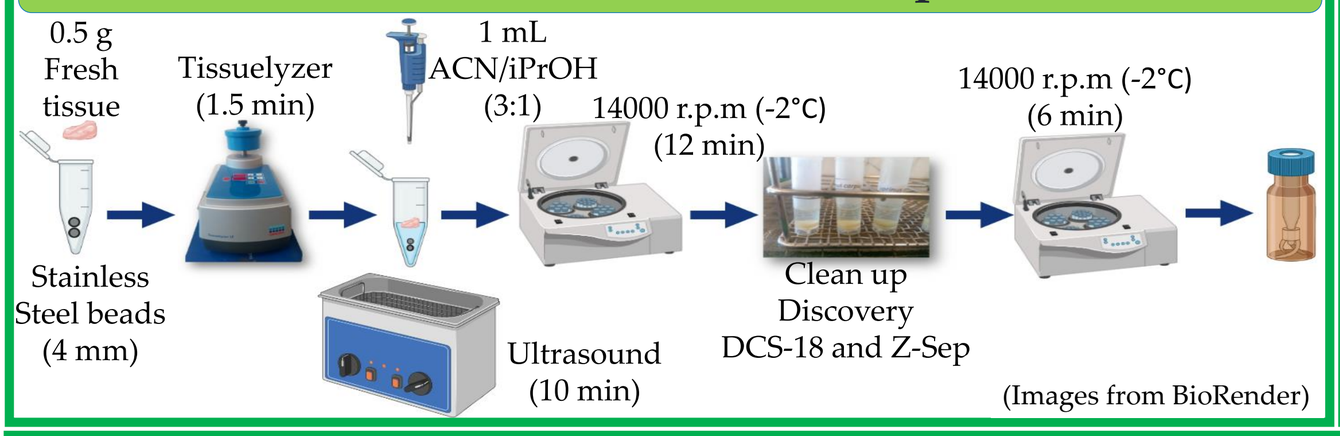
Sample collection



San Joan Despí (Catalonia, Spain).

Three individuals per species were captured: *Chelon ramada*, *Cyprinus Carpio*, *Anguilla anguilla*, and *Luciobarbus graellssi* and the tissues analyzed were brain, kidney, skin, liver, pancreas, heart, muscle, bile, and plasma.

Extraction method developed



(Images from BioRender)

LC-HR-MS/MS analysis

Q-TOF-MS system X500R (SCIEX).

Column: EVO C18 KINETEX.
Flow rate: 0.8 mL/min.
Ionization: ESI (+)
Acquisition mode: SWATH

Results and discussion

Compounds detected using our routine target method

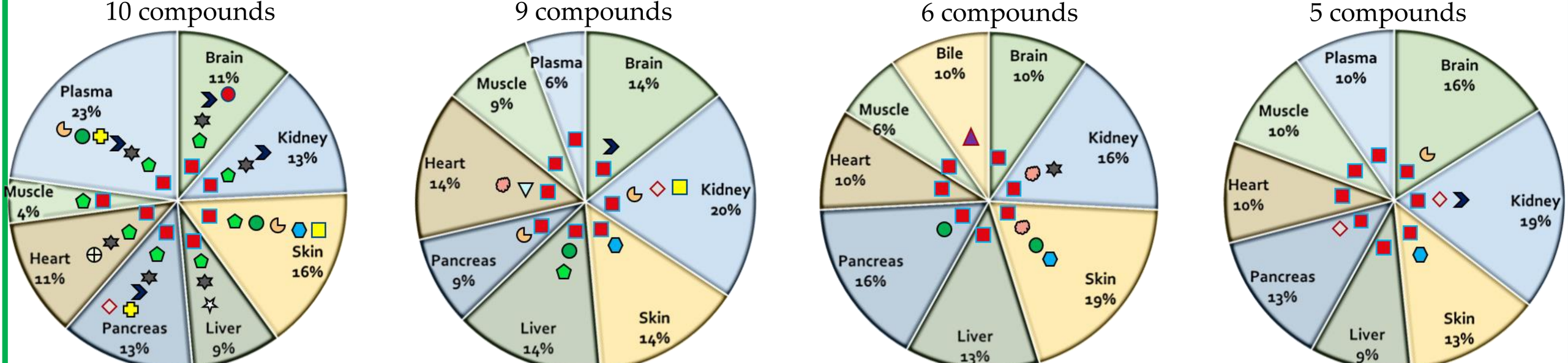
Acethaminophen, Acridone, Caffeine, Carbamazepine, Clarithromycin, Codeine, Diazepam, Diltiazem, Fluoxetine, Ketoprofen, Loratadine, Metoprolol, Sertraline, Sotalol, Trimethoprim, Venlafaxine

Chelon ramada
70 positive detections
10 compounds

Cyprinus carpio
35 positive detections
9 compounds

Anguilla anguilla
31 positive detections
6 compounds

Luciobarbus grellssi
31 positive detections
5 compounds



Distribution of the PhACs detected in each species. The percentages per tissue were calculated based on the positive detections obtained in the 3 individuals captured by species.

Compounds detected by suspect screening

Compound	RT	*Chelon ramada*									*Cyprunus Carpio*									*Anguilla anguilla*									*Luciobarbus graellsii*								
		Br	K	S	L	Pa	H	M	Bi	Pl	Br	K	S	L	Pa	H	M	Bi	Pl	Br	K	S	L	Pa	H	M	Bi	Pl	Br	K	S	L	Pa	H	M	Bi	Pl
Methylphenidate	0.1																																				
Amantadine	1.1																																				
o-desmethylvenlafaxine	1.7																																				
Tramadol	1.7																																				
Ondansetron	3.1																																				
Terazosin	3.3																																				
Bisoprolol	3.6																																				
Trazodone	4.0																																				
Clozapine	4.6																																				
Quetiapine	4.9																																				
Citalopram	5.1																																				
Desmethylcitalopram	5.1																																				
Tiamulin	6.5																																				
Telmisartan	7.5																																				
Terbutryn	8.3																																				
Triphenyl phosphate	8.5																																				
(2R,6S)-Fenpropimorph	8.6																																				

Detection frequency

1/3	
2/3	
3/3	
N.D	

Br	Brain
K	Kidney
S	Skin
L	Liver
Pa	Pancreas
H	Heart
M	Muscle
Bi	Bile
Pl	Plasma

Conclusions

- High detection frequency of antidepressant compounds, especially sertraline (■) in the routine target method.
- *Chelon ramada* was the species in which the highest number of compounds were detected.
- The majority of positive detections were presented in the pancreas and kidney, indicating that in these tissues there is a greater tendency to accumulate CECs.
- Priorization of amantadine, bisoprolol, and quetiapine to include them in our routine target method because they were the compounds that obtained the highest detection frequency in the suspect screening.
- Through the analysis by suspect screening, different classes of compounds were detected: triphenyl phosphate (flame retardant), terbutryn, and (2R, 6S) -Fenpropimorph (pesticides).

Future Work

Develop a method that facilitates the extraction of a greater number of compounds with different physicochemical properties an a wide polarity range.

Acknowledgements

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