

Metabolómica para la biomonitorización de contaminantes en organismos acuáticos (BIOAQUOMA)

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thinkⁱⁿ azul

This study forms part of the ThinkInAzul programme and was supported by MCIN with funding from European Union NextGenerationEU (PRTR-C17.11) and by *Generalitat Valenciana*



Descripción del Grupo de Trabajo



Dyana Vitale



Vicente Andreu



Yolanda Picó

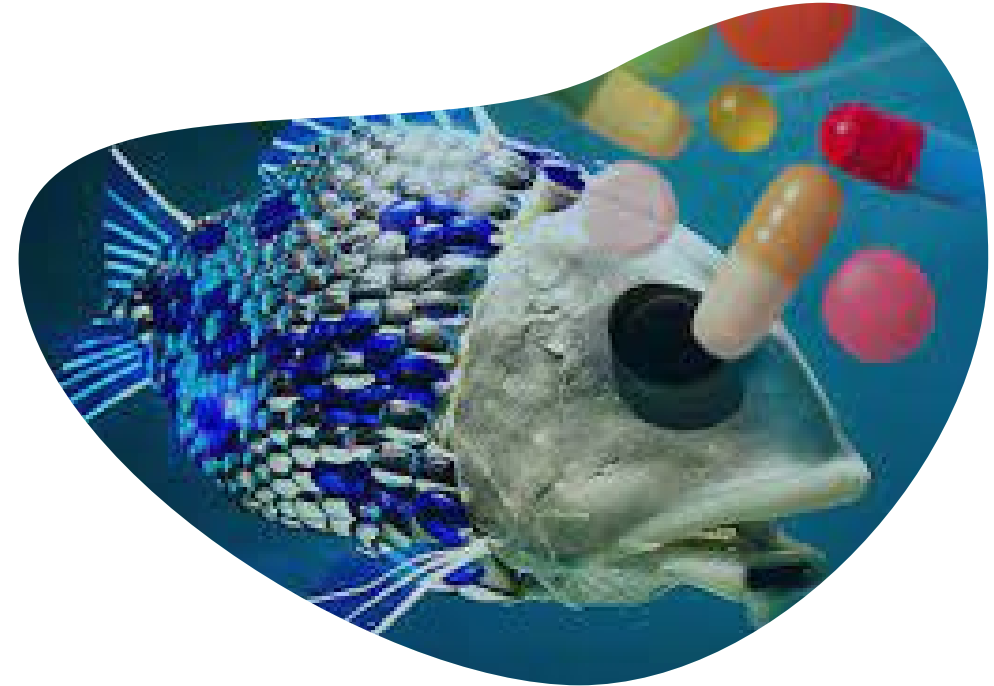


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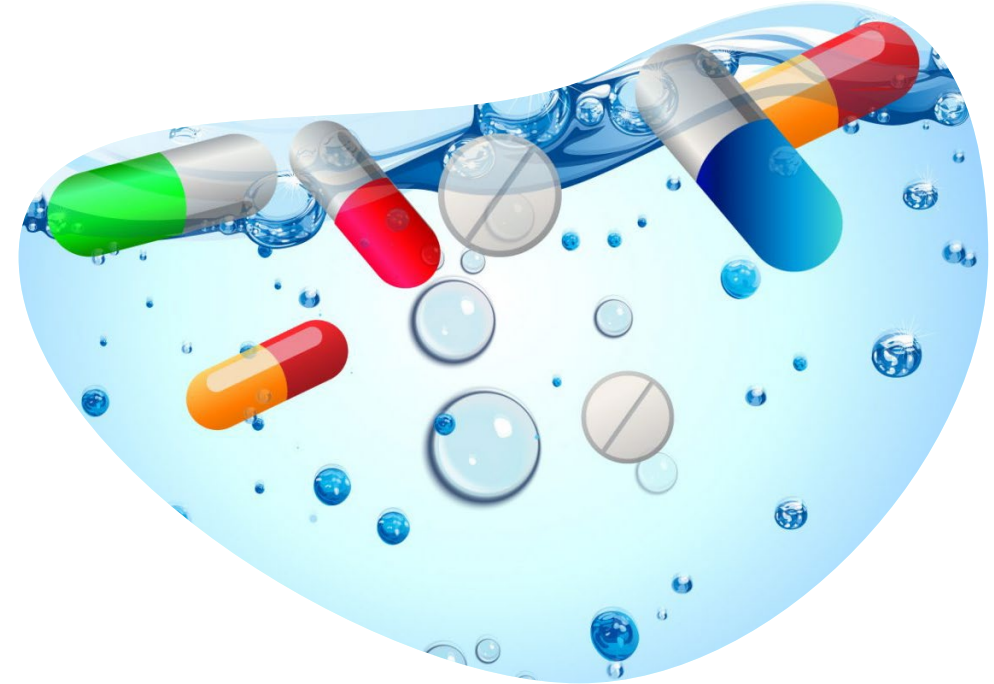
Objetivos

- Establecer mediante **métodos no dirigidos**, los contaminantes, metabolitos y compuestos endógenos en tejidos (músculo, hígado, mucus, etc.) y biofluidos (plasma)
- Descubrir los **perfiles metabolómicos e identificar los biomarcadores** alterados por la exposición de los peces a los contaminantes mediante estudios de bioacumulación en laboratorio y en el campo
- Evaluar críticamente la construcción de una **herramienta metabolómica** de alto rendimiento, que no sea lesiva para la biota acuática con los resultados anteriores, para establecer rápidamente el **exposoma** de los peces.



Tareas

- **Sistema de metabolómica** para identificar biomarcadores en peces → diferentes matrices (tejidos y fluidos biológicos)
- Métodos de análisis para **microplásticos** y **nanoplásticos**
- **Validación** del sistema de metabolómica para **ensayos en laboratorio con peces** → Dorada (*Sparus aurata*) y Lubina (*Dicentrarchus labrax*)
- **Métodos dirigidos** de metabolómica



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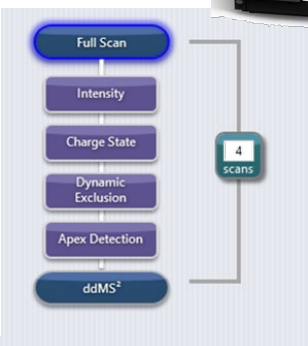
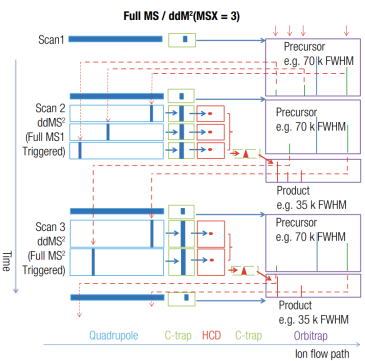
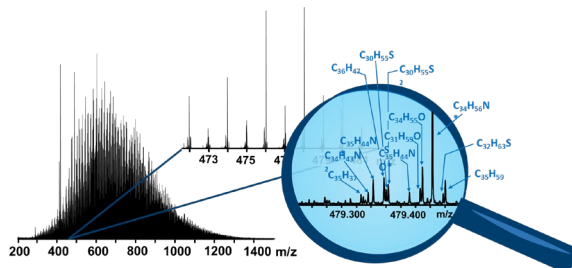
Resultados obtenidos hasta el momento

T.1. Sistema de metabolómica

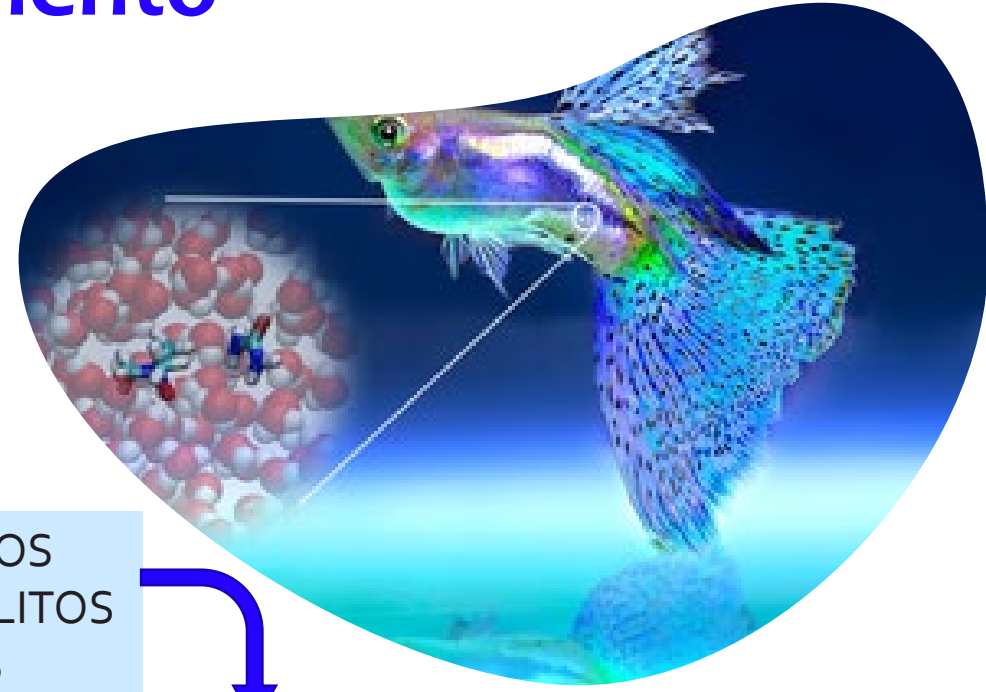
Métodos de extracción

Plasma – Metanol en frío (1:1 v/v)

Tejidos – Agua-methanol-dichlorometano (1:1:1 v/v) en frío



IDENTIFICADOS
260 METABOLITOS
ENDOGENOS



- Ejemplos:**
- | | | |
|--|--|--|
| <ul style="list-style-type: none"> Creatine Azelaic acid Δ^2-cis-Hexadecenoic acid Linoleic acid Δ^2-trans-Hexadecenoic acid 12,13-DHOME Mevalonic acid Oleic acid | <ul style="list-style-type: none"> Melatonin Epinefrine Progesterone Cortisol Cortisone Corticoesterone 5-HETE Phenylalanine Valine | <ul style="list-style-type: none"> Thriptophan Serotonine 1,2,4-Trihydroxybenzene 1-Methylhistidine 2,3,4-Trihydroxybutanoic acid 3-Methylhistidine 4-Deoxyglucose 4-Methyl-2-oxovaleric acid 4-oxo-proline |
|--|--|--|



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Chromatograms

MW: 341.07100 - File: SULTAN_PLANT_BI_BAGF_S2_dMS2pes.raw (F3) FTMS (+) MS1

Mass Spectrum

SULTAN_PLANT_BI_BAGF_S2_dMS2pes (F3) #6884, RT=9.166 min, MS1, FTMS (+)

F3 #6890, RT=9.176 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

F3 #6949, RT=9.244 min, MS1, FTMS (+)

F3 #6955, RT=9.255 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

F3 #6954, RT=9.252 min, MS1, FTMS (+)

F3 #6960, RT=9.257 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

F3 #6964, RT=9.307 min, MS1, FTMS (+)

F3 #6965, RT=9.318 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

F3 #6966, RT=9.316 min, MS1, FTMS (+)

F3 #6967, RT=9.327 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

RAWFILE(top): SULTAN_PLANT_BI_BAGF_S2_dMS2pes (F3) #9276, RT=12.420 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

REFERENCE(bottom): mzCloud library: Propiconazole, C15 H17 Cl2 N3 O2, MS2, FTMS, (HCD, 342.0771@20.3050)

SULTAN_PLANT_BI_BAGF_S2_dMS2pes (F3) #890, RT=9.176 min, MS2, FTMS (+), (HCD, DDA, 342.0783@18.3548, +1)

Tags	Checked	Name
<input type="radio"/>	<input type="checkbox"/>	Trinexapac-ethyl
<input type="radio"/>	<input type="checkbox"/>	Ethyl Paraben
<input type="radio"/>	<input type="checkbox"/>	3-Indoleacetic Acid
<input type="radio"/>	<input type="checkbox"/>	Atrazine-D5
<input checked="" type="radio"/>	<input checked="" type="checkbox"/>	Propiconazole
<input type="radio"/>	<input type="checkbox"/>	Piperonyl-butoxide
<input type="radio"/>	<input type="checkbox"/>	Dopamine
<input type="radio"/>	<input type="checkbox"/>	AZT
<input type="radio"/>	<input type="checkbox"/>	Methandienone
<input type="radio"/>	<input type="checkbox"/>	Dibutyl Phthalate
<input type="radio"/>	<input type="checkbox"/>	Fenoxycarb
<input type="radio"/>	<input type="checkbox"/>	11-nor-9-Carboxy-Delta-9-THC
<input type="radio"/>	<input type="checkbox"/>	(6E)-10-Heptyl-5,8,9-trihydroxy-3,4,5,8,9,10-hexahydro-

(Max.)	# C	394	0	0.558	0.517	0.909	0.909	0.987
8337825								
3732751		2		0.444	0.371	0.799	0.799	0.937
1349249		123		0.227	0.145	0.875	0.875	0.029
6322248		242		0.389	0.313	0.842	0.842	0.985
3296278		165		0.14	0.058	0.796	0.796	0.951
7331357		59		0.777	0.684	0.813	0.813	0.99
		1	3	0.978	0.89	0.819	0.819	0.985

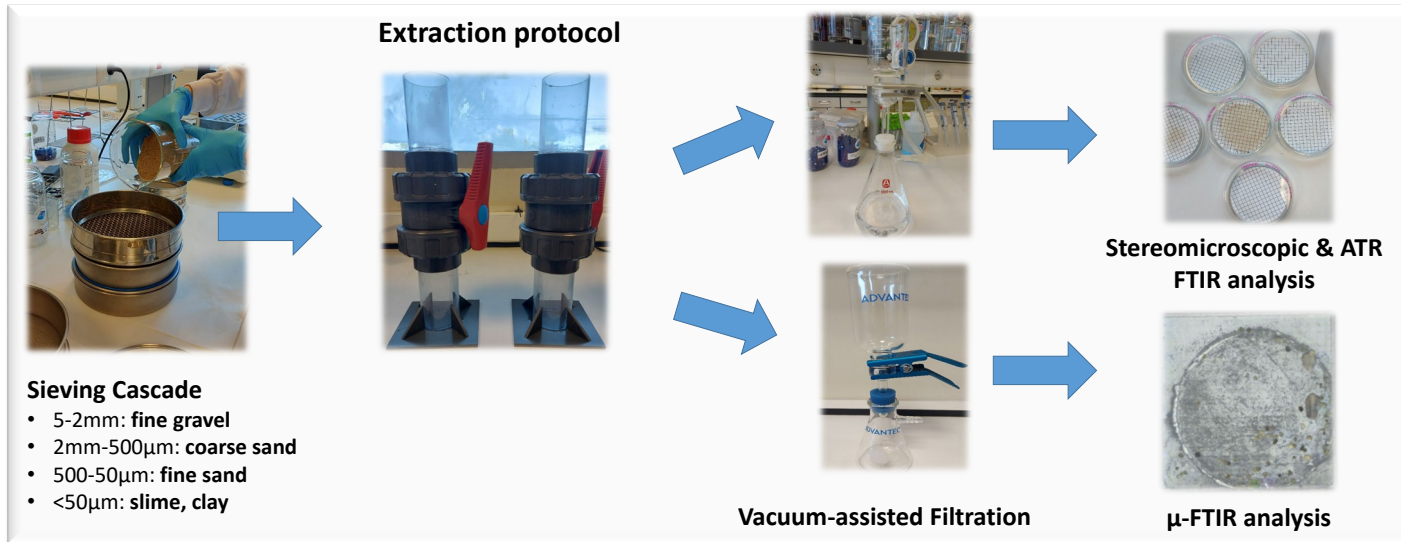
Show Related Tables



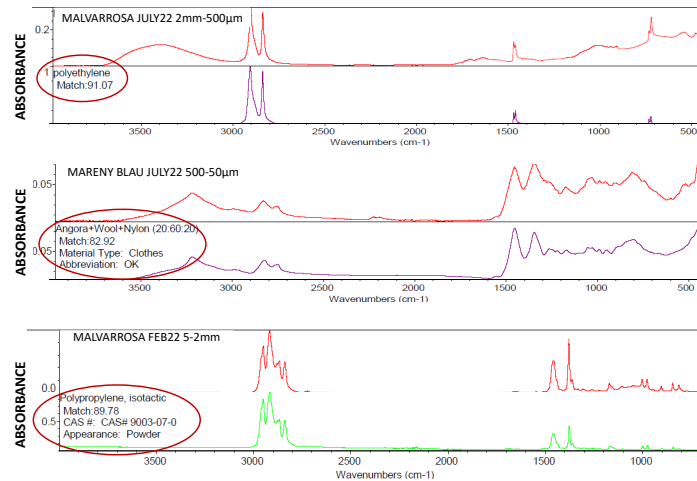
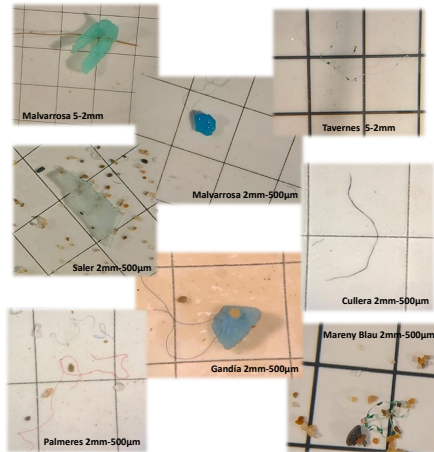
This study forms part of the ThinkInAzul programme and was supported by MCIN with funding from European Union NextGenerationEU (PRTR-C17.1a) and by Generalitat Valenciana



T.2. Analytical methods for MPs & NP



Stereomicroscopy
(Model EZ4, Leica AG,
Wetzlar, Germany)



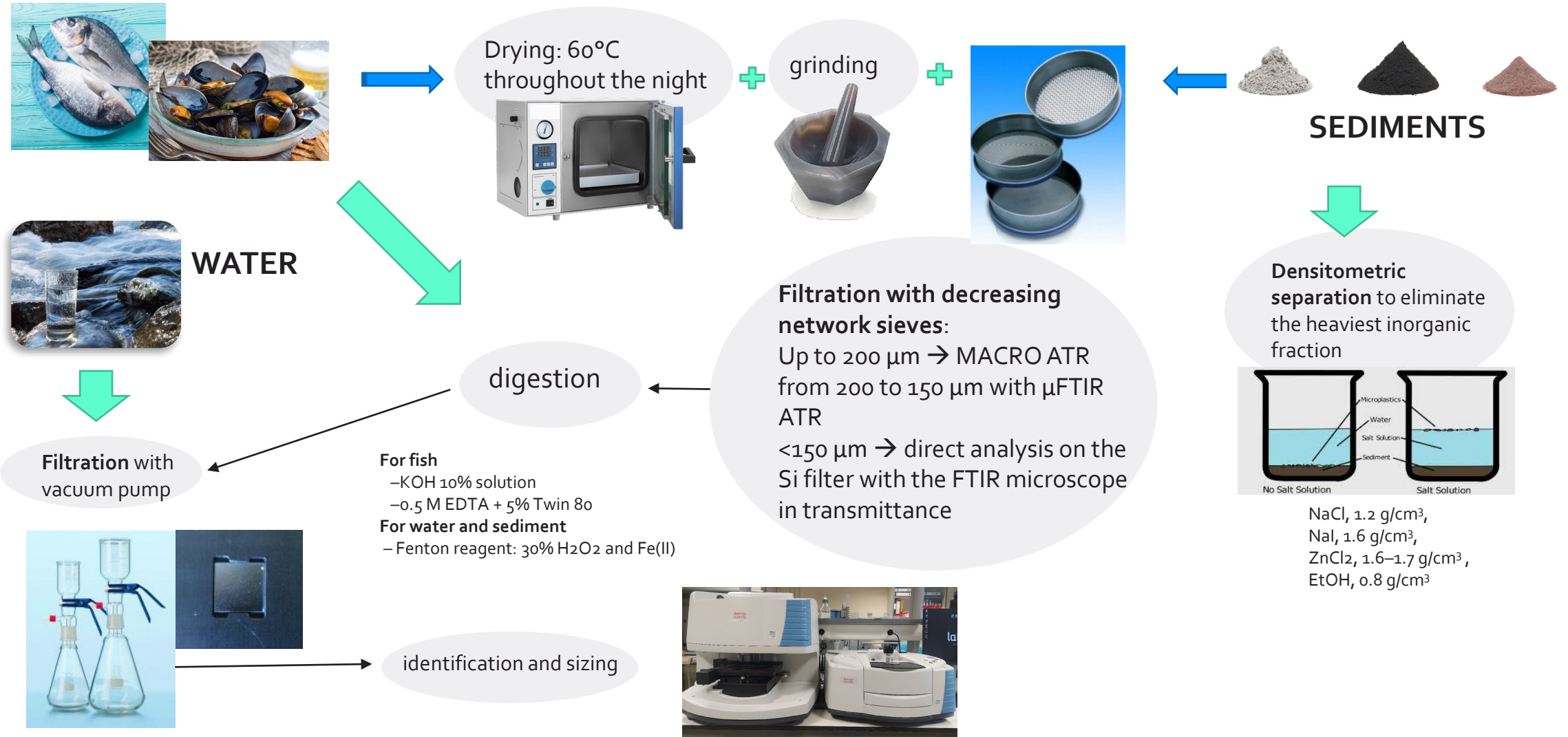
FTIR stereoscopy
(Nicolet iN10MX,
ThermoScientific,
Madison, USA)



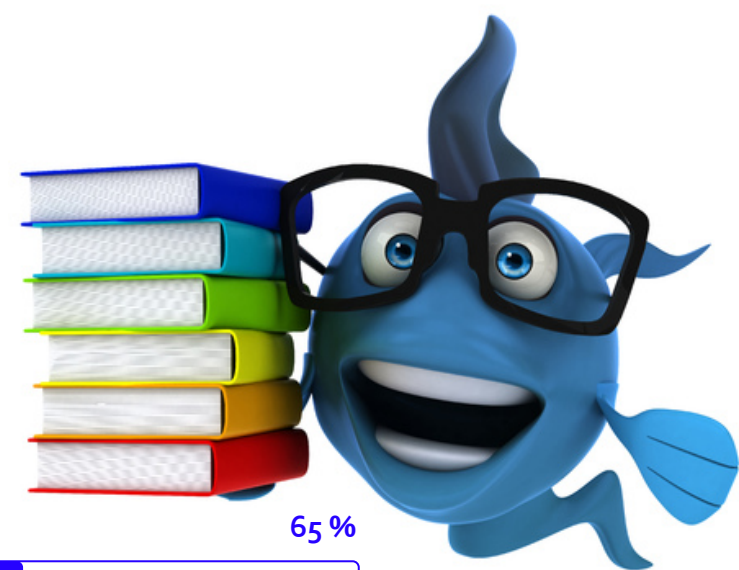
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Preparation of the sample for analysis in fish, sediments and water



Grado de consecución de las tareas



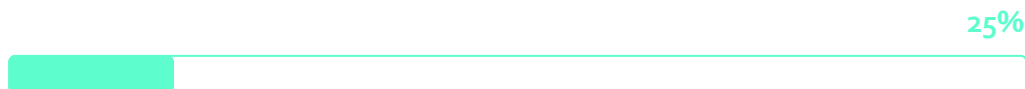
T. 1. Sistema de metabolómica non-target



T. 2. Métodos de análisis de MPs&NPs



T. 3. Validación metabólica con ensayos de laboratorio



T. 4. Métodos de metabolómica target



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Desviaciones del programa inicial



- **Determinación de nanoplasticos** – Pirolisis – Cromatografía de Gases Espectrometría de masas (Colaboraciones con grupos de investigación ajenos al Proyecto)

-University of Plymouth  UNIVERSITY OF PLYMOUTH

-Institut Català Recerca de l'Aigua 

- **Validación del método de metabolómica para metales** (Colaboración con la Universidad Católica de Valencia –Grupo Dr. José Tena)



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Hoja de ruta 6 próximos meses

- **T.1. Sistema de metabolómica:**
 - Sistema desarrollado para plasma (100 %)
 - Sistema desarrollado para tejidos (85-90 %)
- **T.2. Métodos para determinar MPs&NPs**
 - Método de análisis de microplásticos en líquidos biológicos y tejidos (100 %)
 - Método de análisis de nanoplásticos en líquidos biológicos y tejidos (85 %)
- **T.3. Validación del sistema de metabolómica mediante ensayos de laboratorio**
 - Ensayos de laboratorio aprobados por el comité de ética y realizados (100 %)
 - Análisis de muestras y evaluación de los resultados (30 %)
- **T.4. Método de metabolómica diana**



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We're thinking in azul

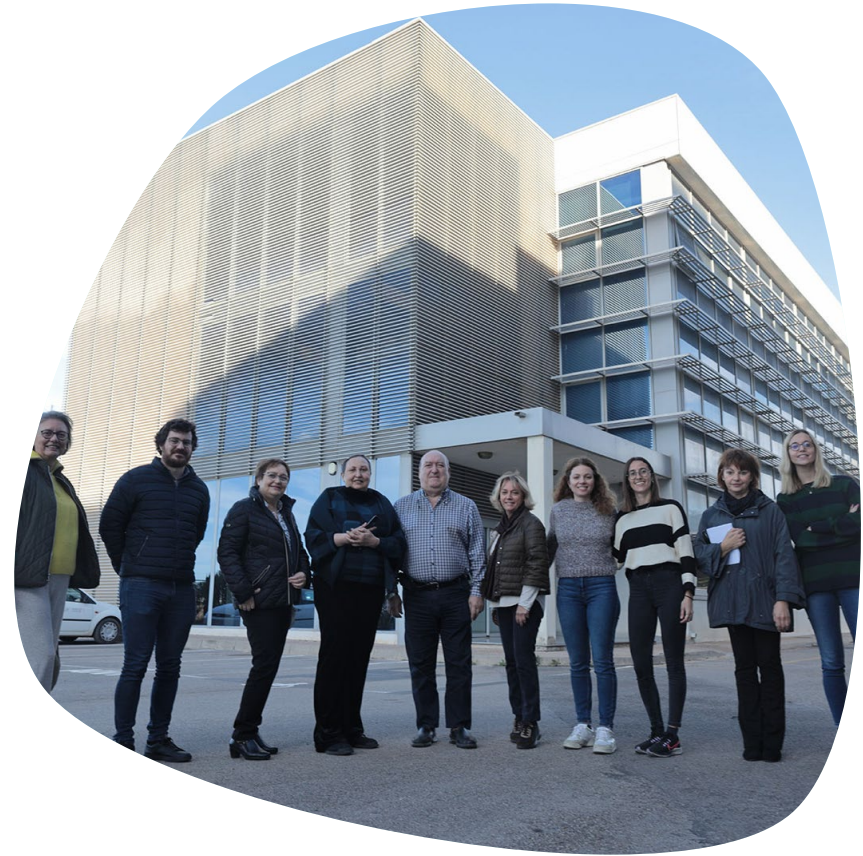
Thanks | Gràcies

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