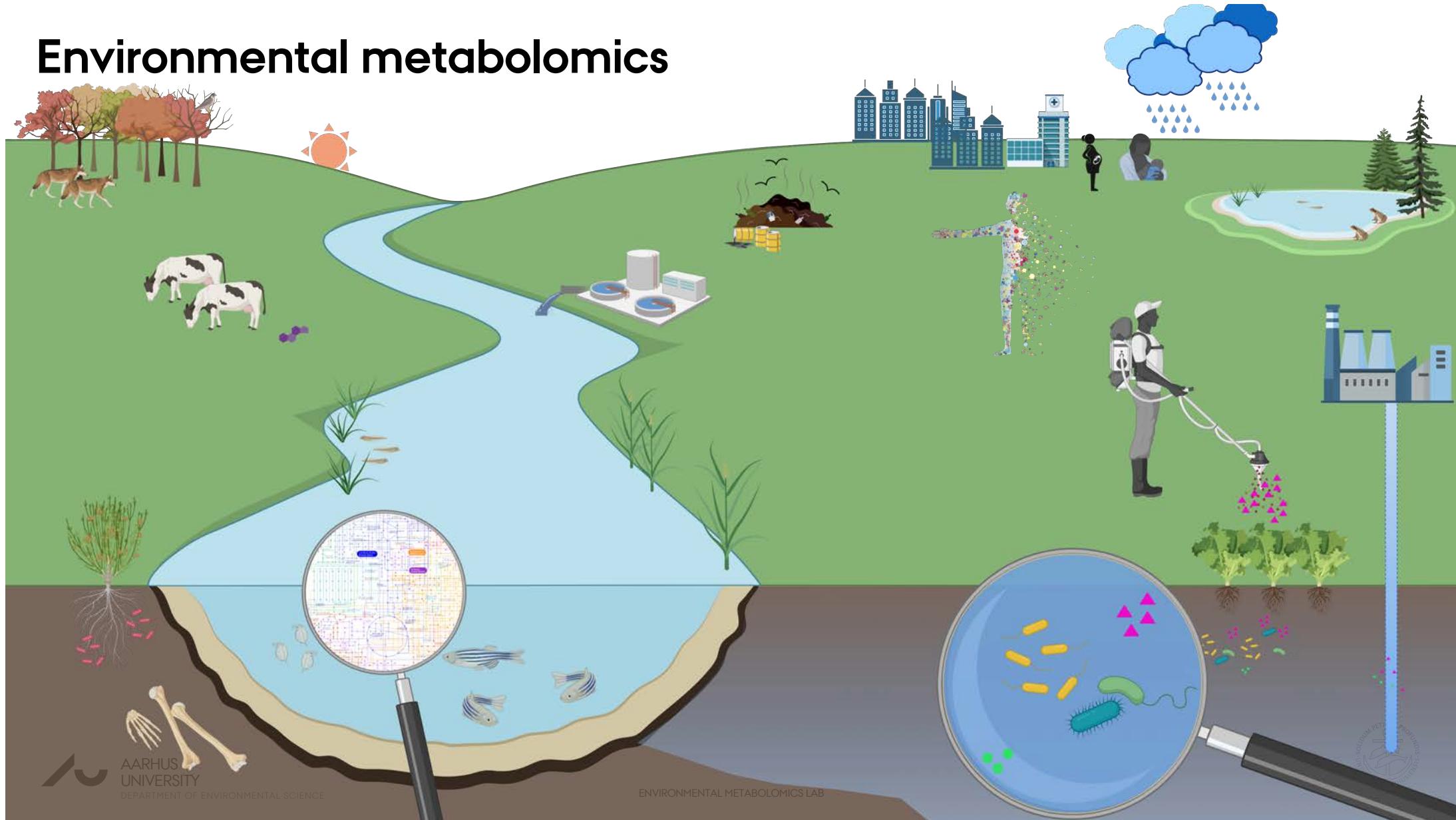


# Holistic non-targeted screening analysis: Cases and challenges

Martin Hansen, Emil Egede Frøkjær, Mulatu Y Nanusha, Petros Pousinis, Xiaomin Zhou, Thorsten KO Gravert, Marie Rønne Aggerbeck, Joseph D Martin, Robert B Young, Anna M Brun Hansen, Rikke Poulsen, Eva L Doting, Laura Halbach, Ate HJ Jaarsma, Kristina Dicová, Diego AB Sanchez, Amalie Ask and Alexandra Morton Hayward



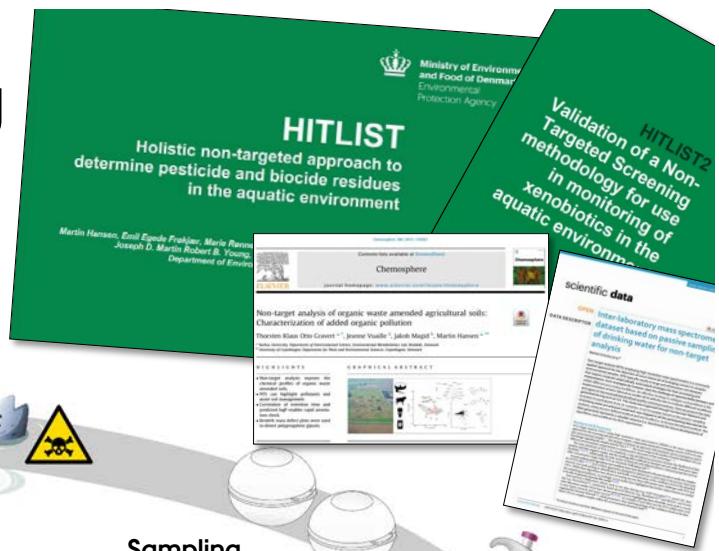
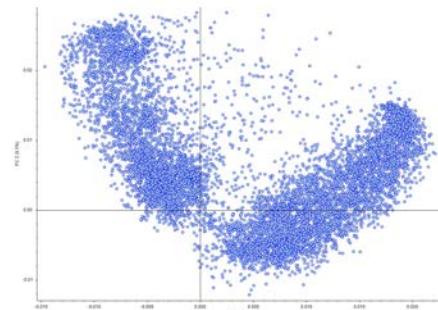
# Environmental metabolomics



# Holistic non-targeted and suspect screening



Non-targeted screening analysis



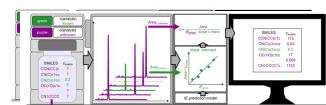
Retrospective analysis



Suspect list



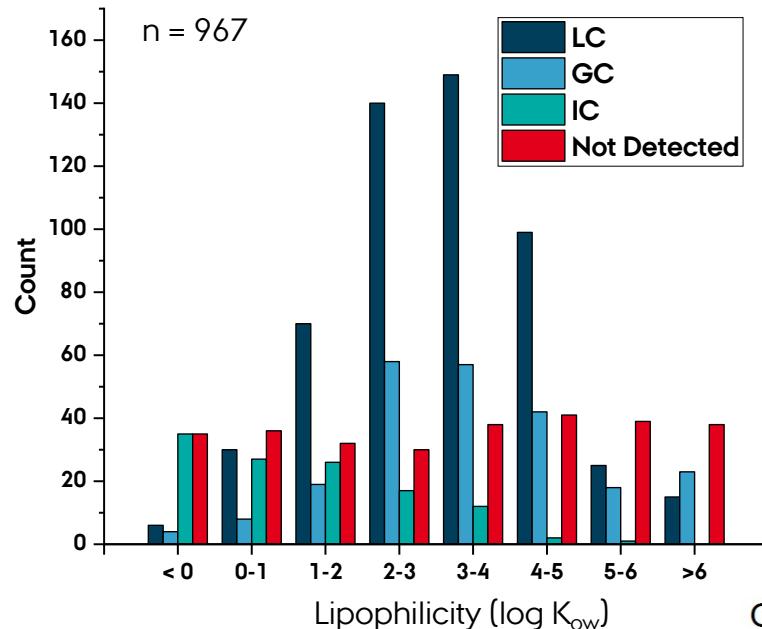
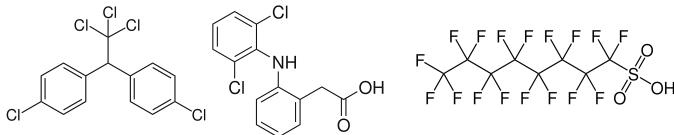
Semi quantitation



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# Validation: Mapping of chemical space

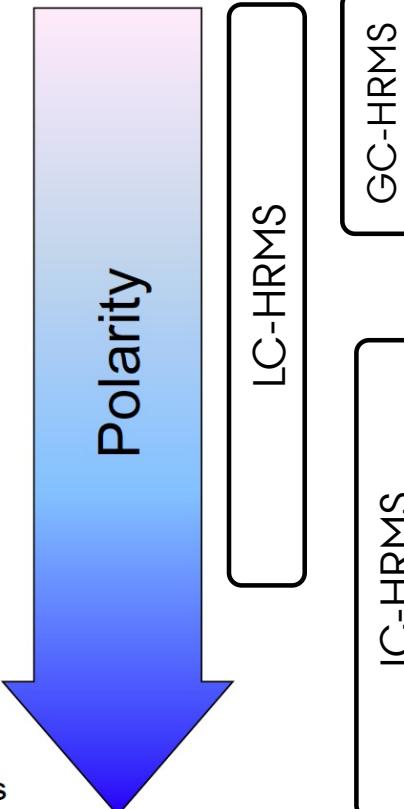
## Anthropogenic chemicals



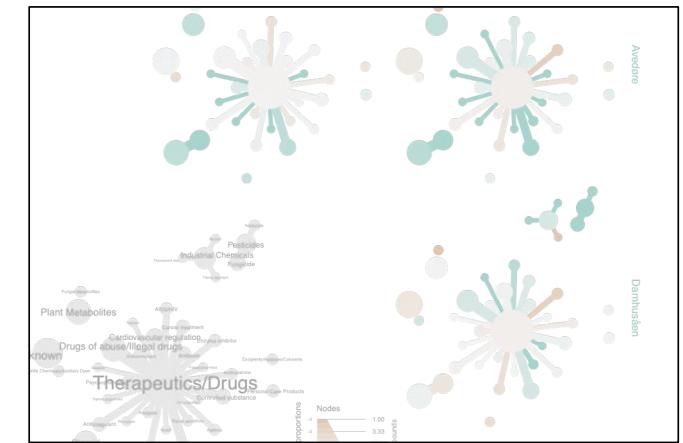
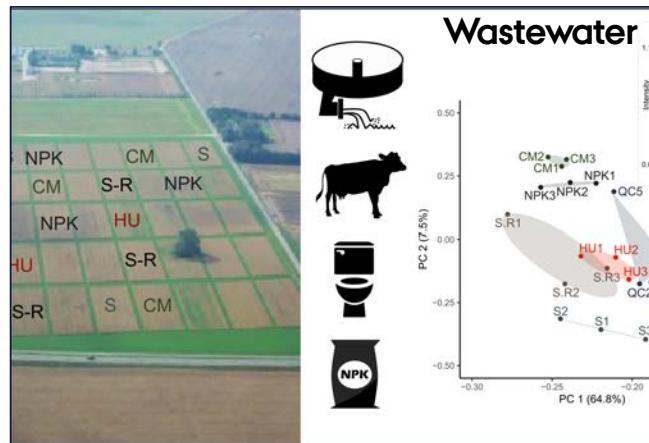
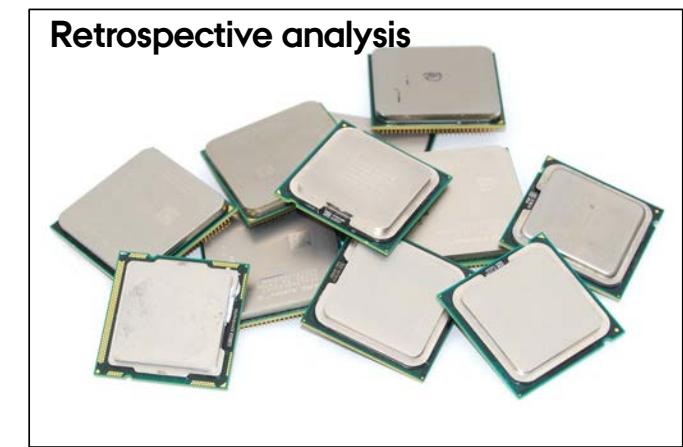
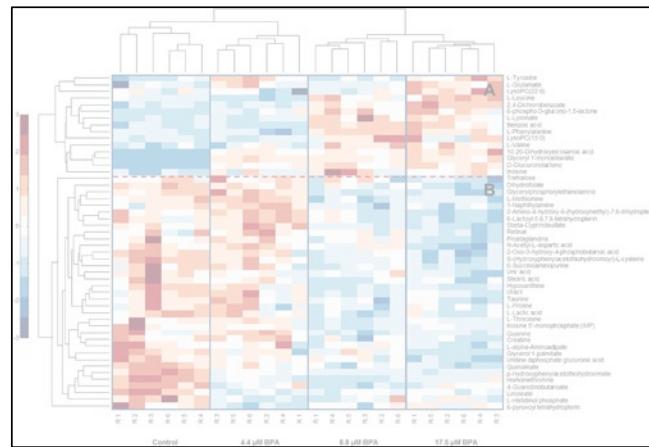
## Metabolites

- Triglycerides
- Cholesterol esters
- Diacylglycerols
- Sphingomyelines
- Phosphatidylcholines
- Phosphatidylethanolamines
- Other phospholipids
- Fatty acids
- Eicosanoids & metabolites
- Bile acids
- Bilirubin
- Amino acids, amines
- Organic acids
- Sugars
- Other polar: e.g. purines & pyrimidines

Polarity



LC(+/-) and IC(-) with sample preparation: **61% coverage**



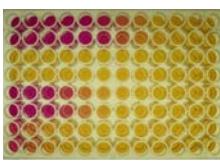
# Aquatic environment



+17 internal standards

500x enrichment

## Toxicity evaluation

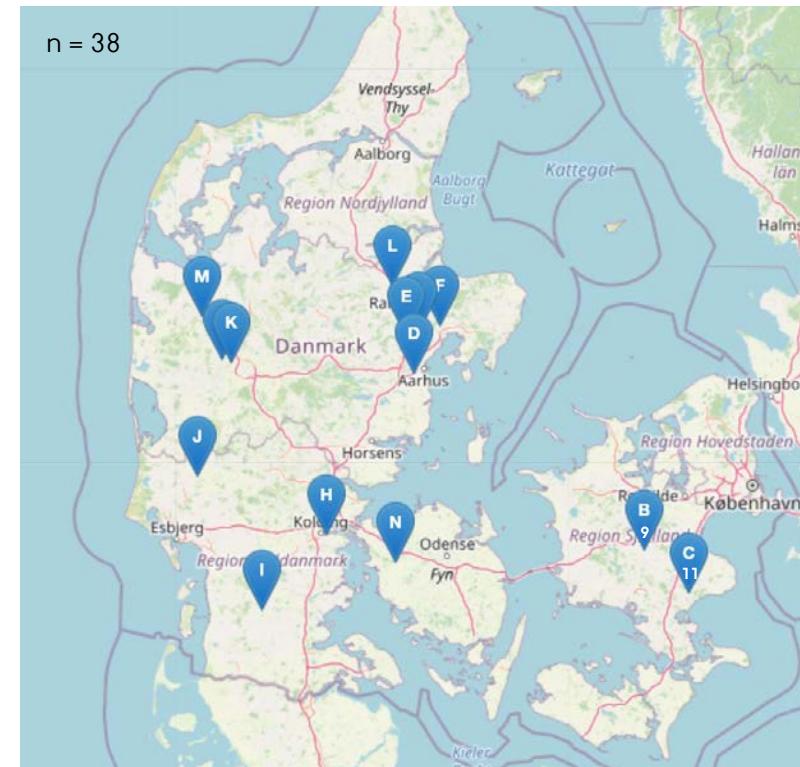


Estrogen receptor  
Androgen receptor



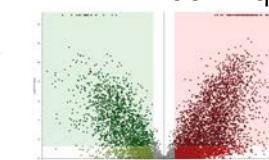
DTU Food  
National Food Institute

AARHUS  
UNIVERSITY  
DEPARTMENT OF ENVIRONMENTAL SCIENCE



Anion exchange chromatography - HRMS/MS (-)  
Liquid chromatography - HRMS/MS (+/-)

Data analysis pipelines

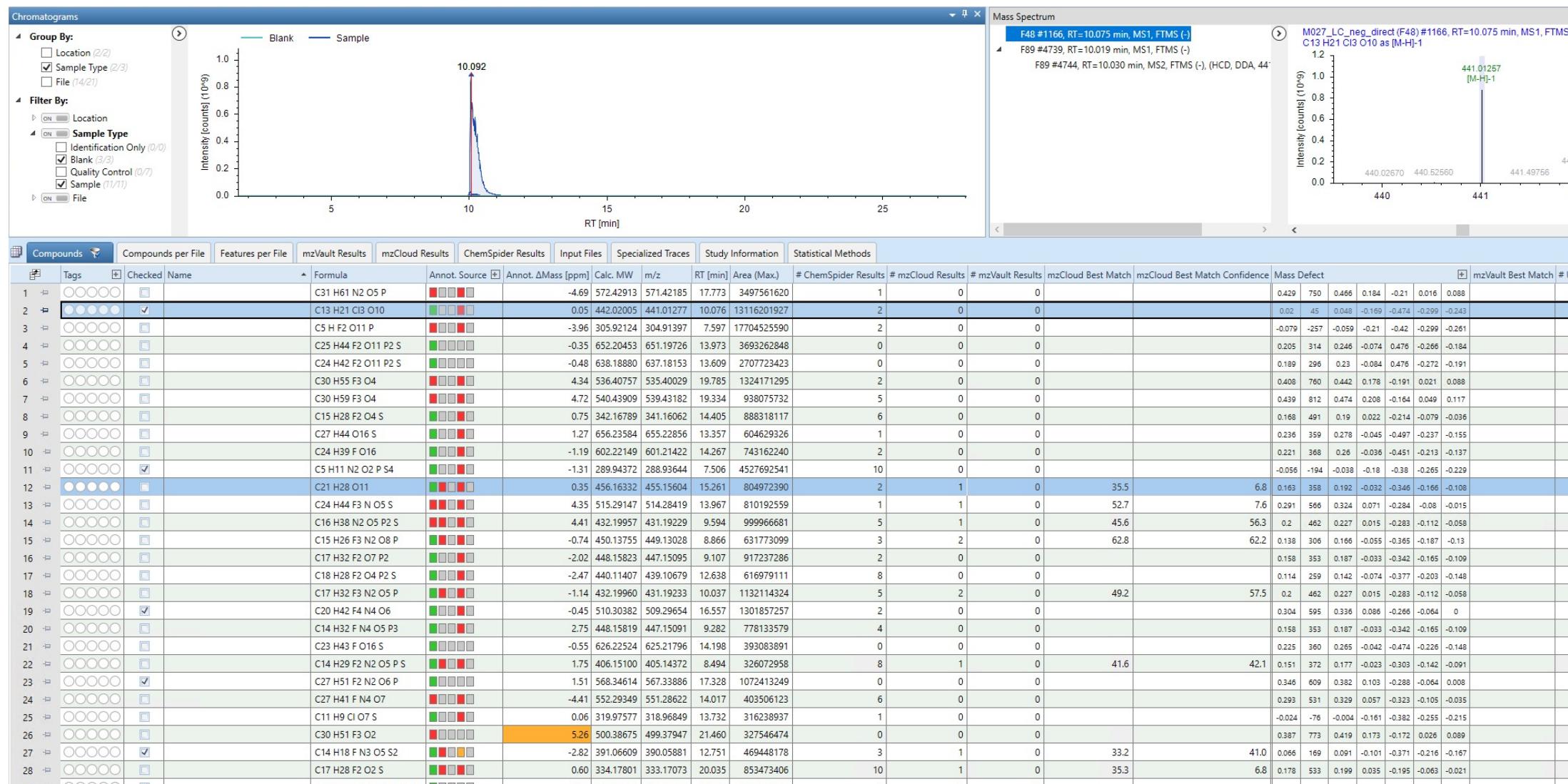


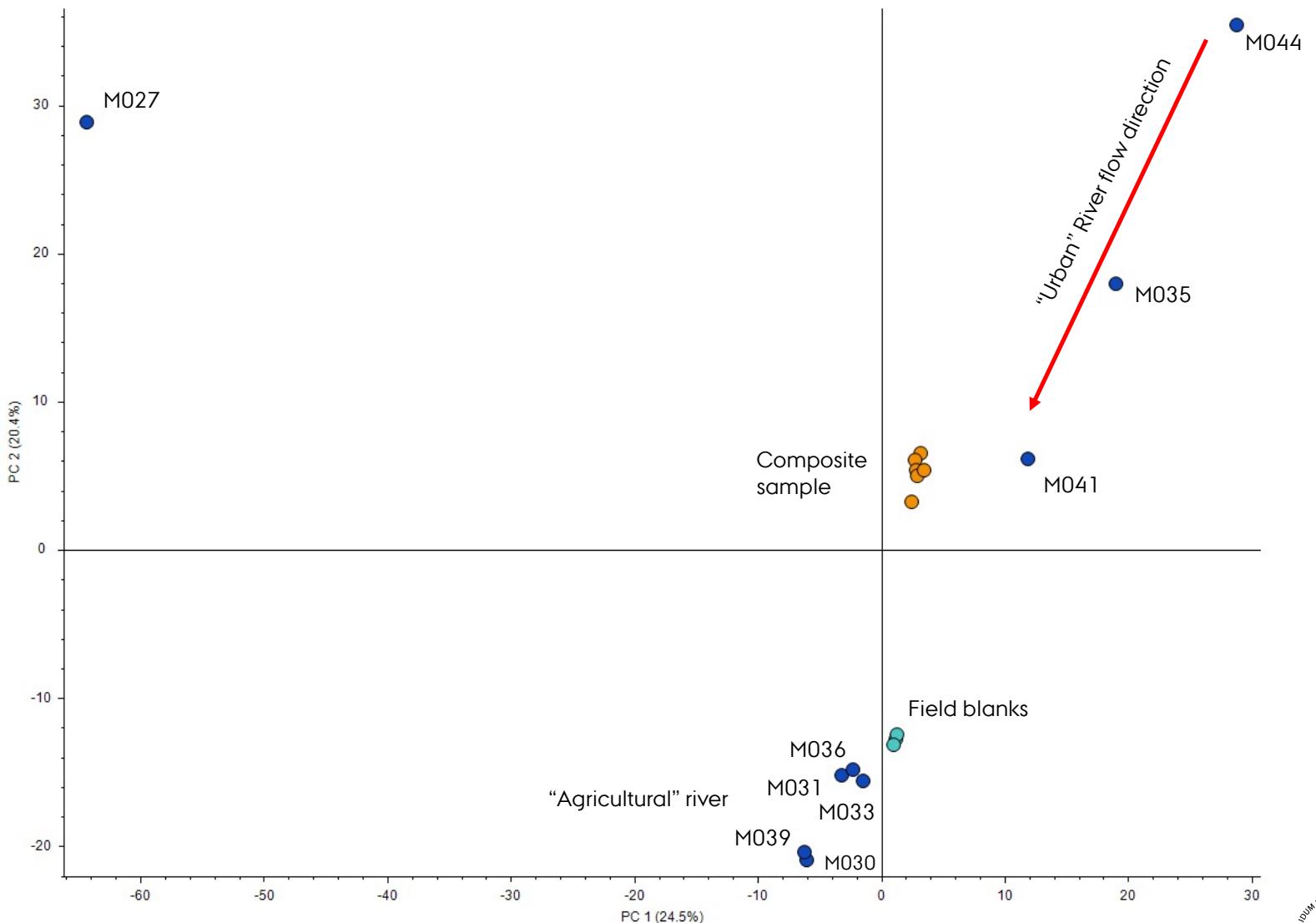
Semi-quantification

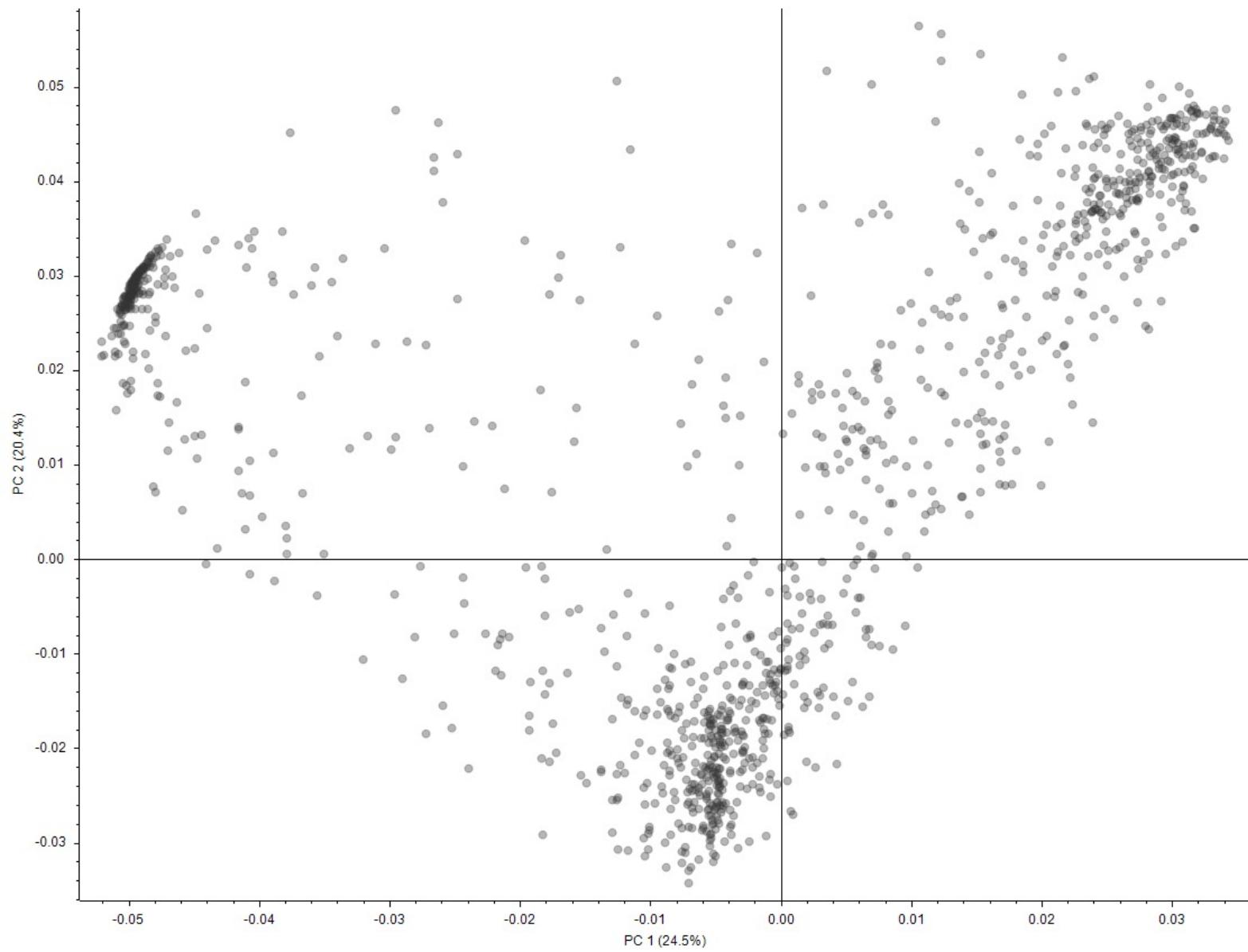


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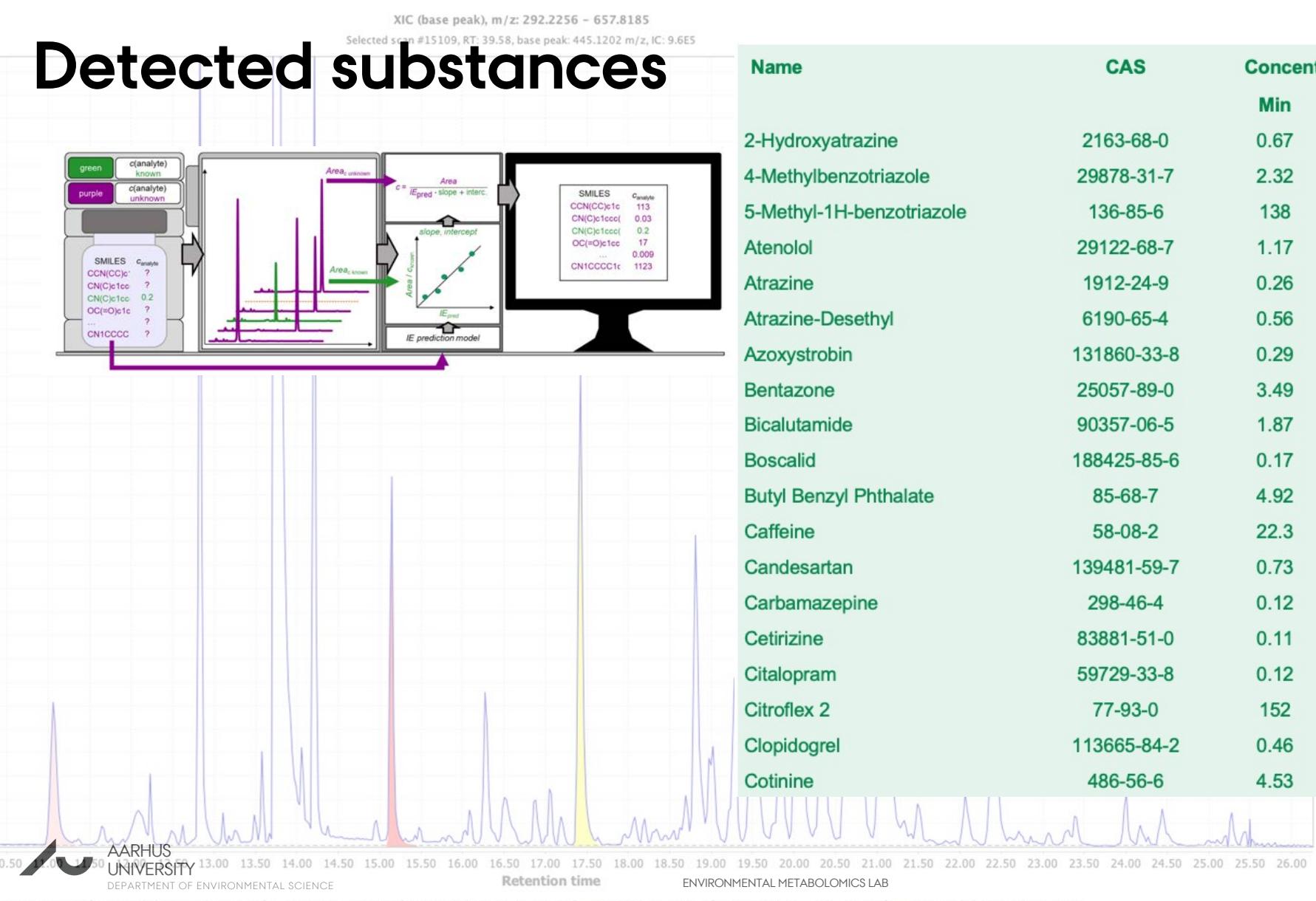


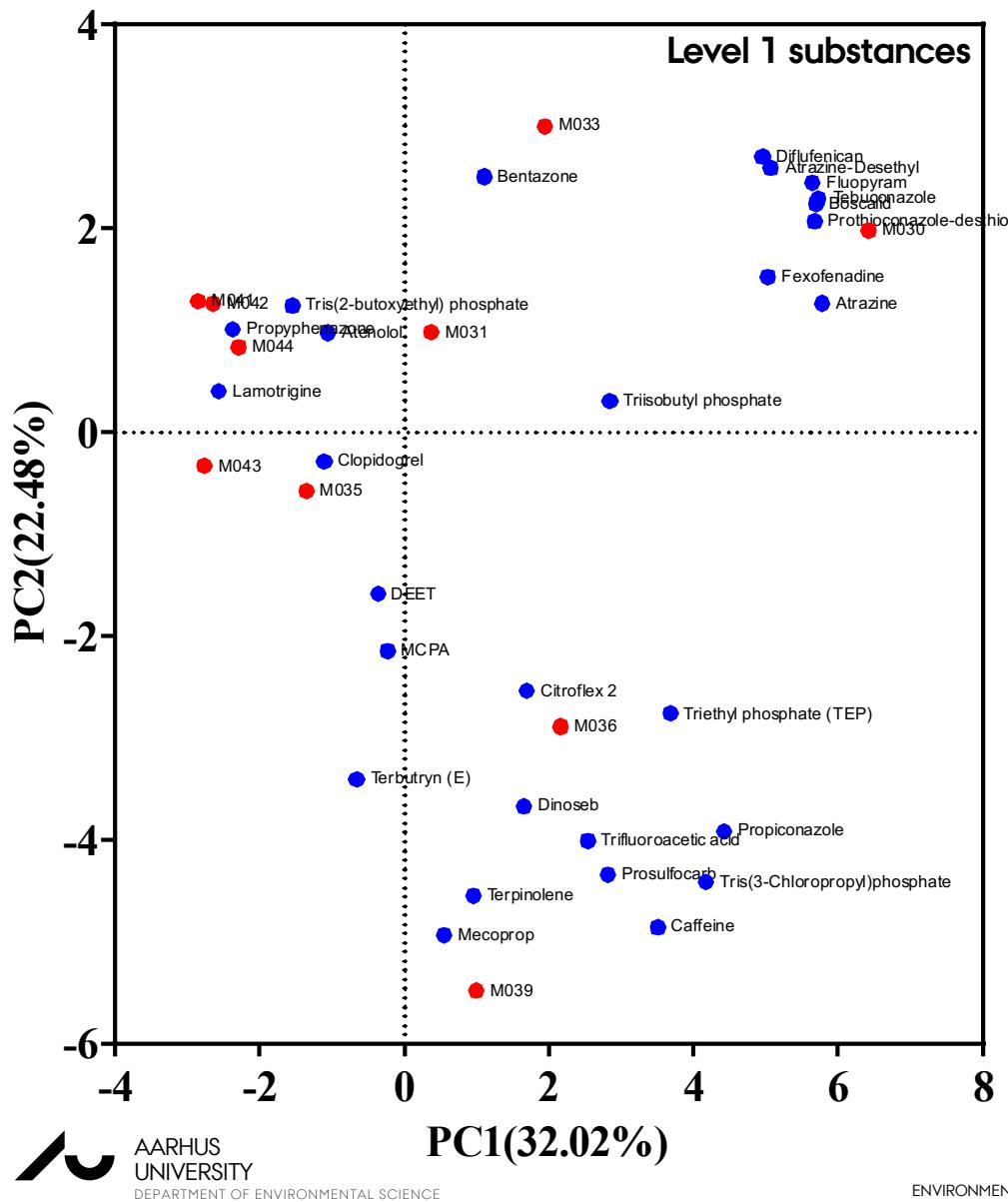










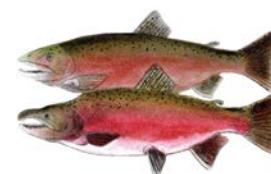
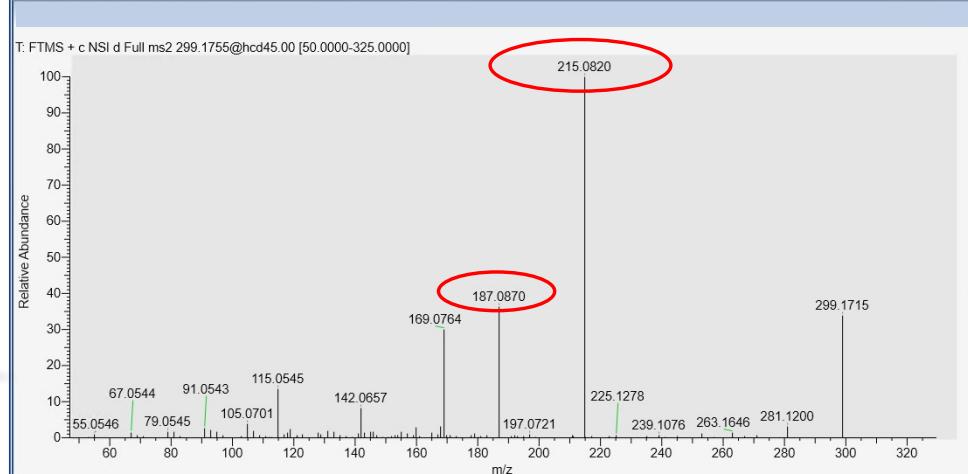
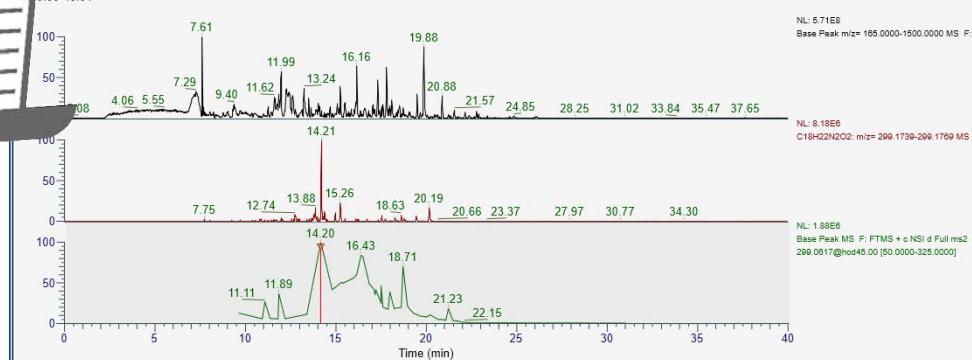


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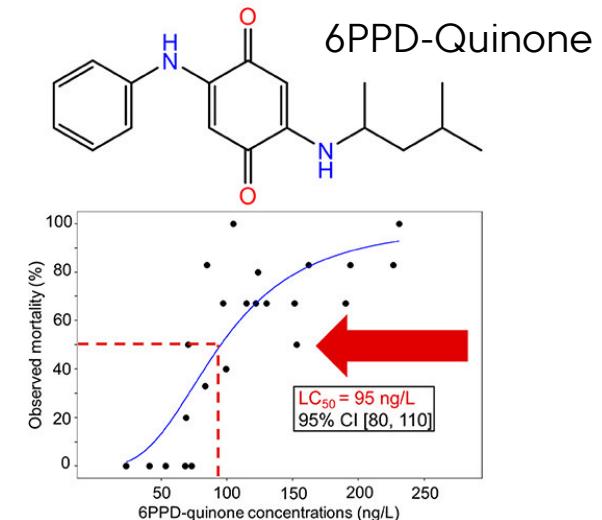




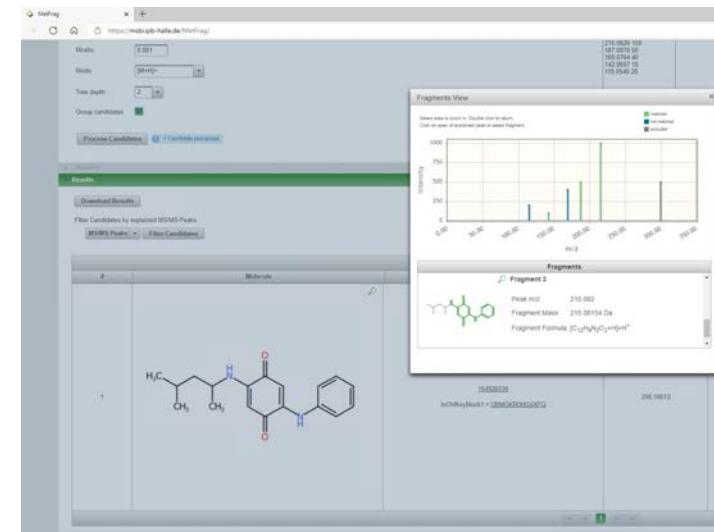
# Retrospective analysis



Coho Salmon



Tian et al., Environ. Sci. Technol. Lett. 2022, 9, 2, 140–146

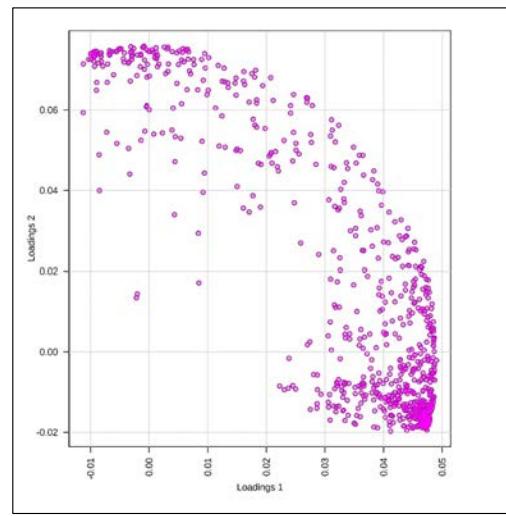
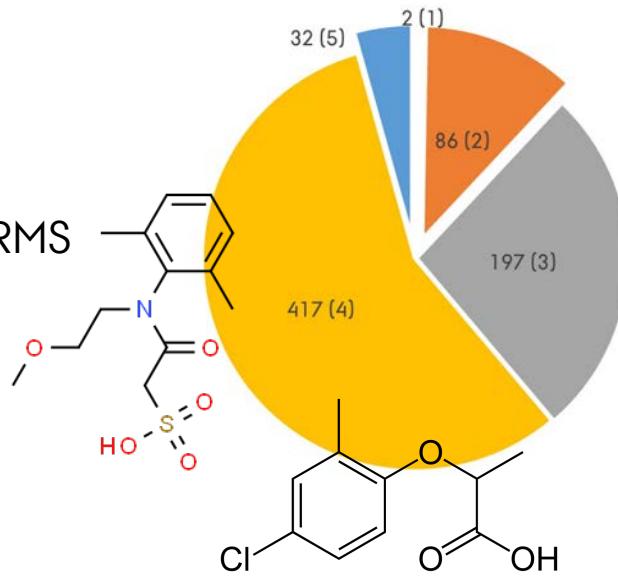
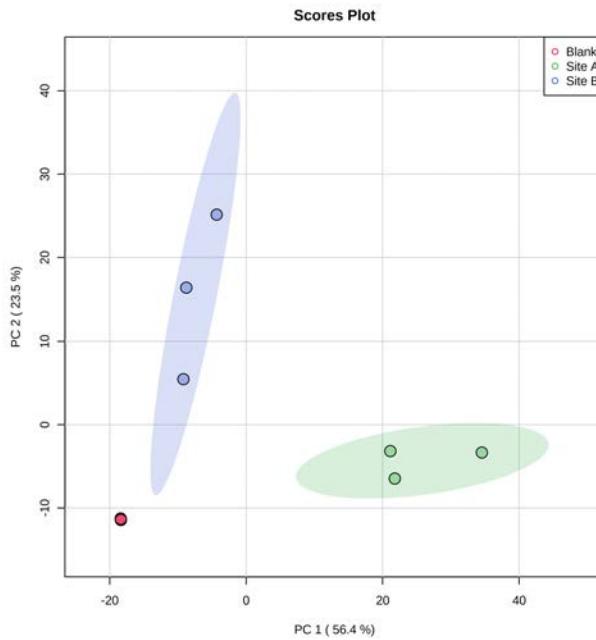


# Drinking water

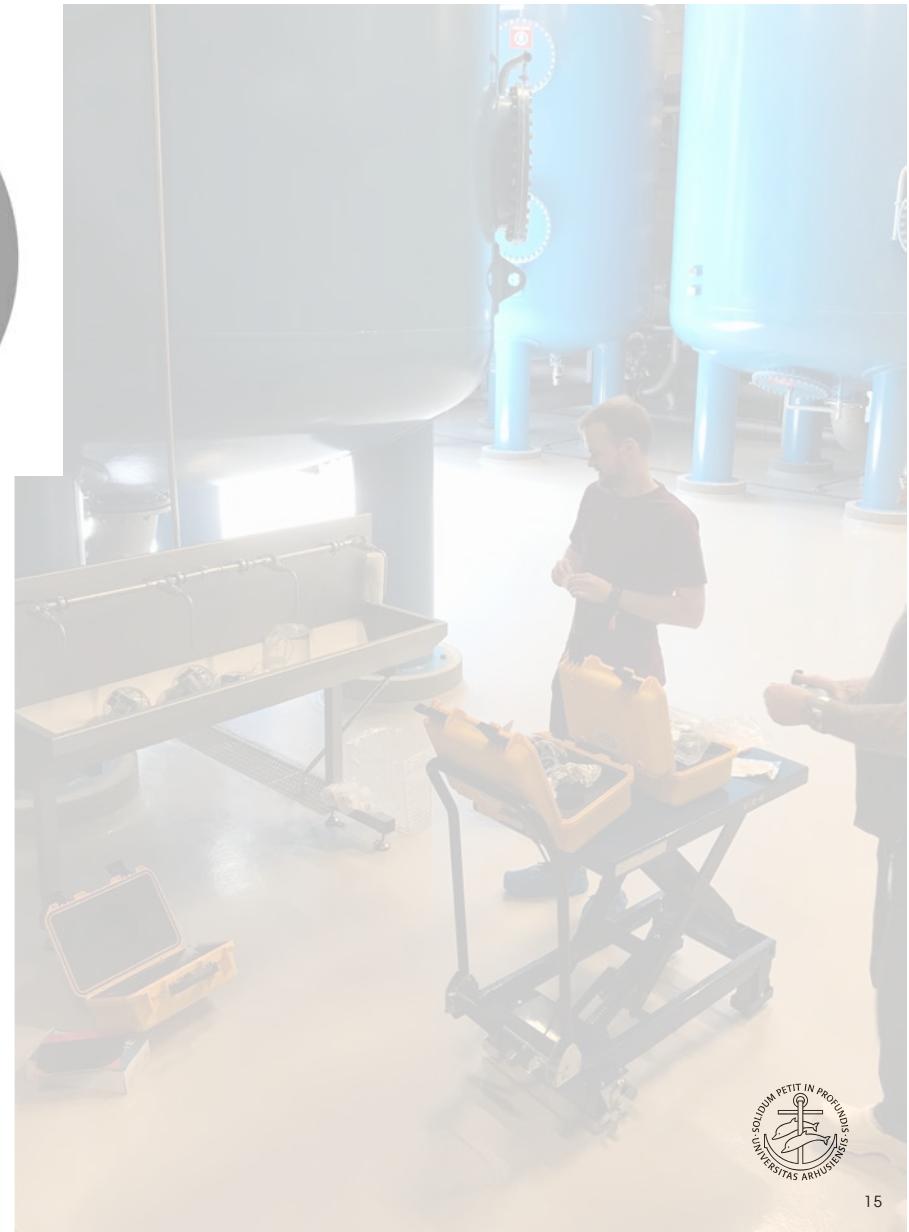


Enriched >300 L water  
Ion chromatography HRMS  
>700 substances

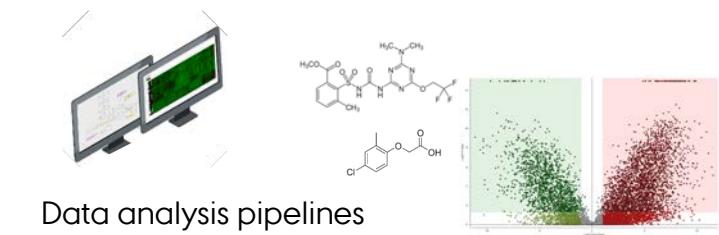
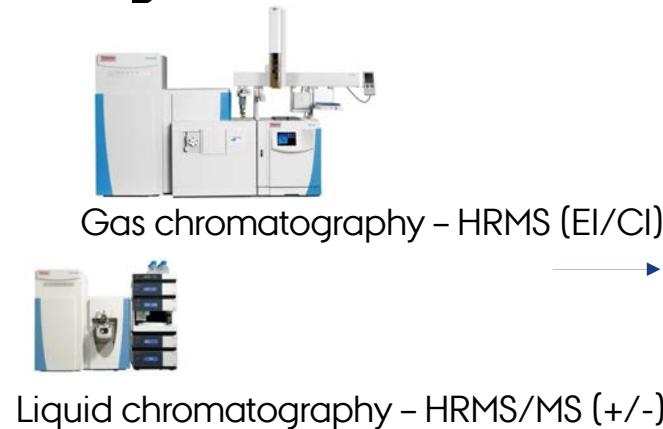
Dimethachlor ESA  
Mecoprop  
Trifluoroacetic acid



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# Wastewater sludge



Chemosphere 280 (2021) 130582

Contents lists available at ScienceDirect

Chemosphere

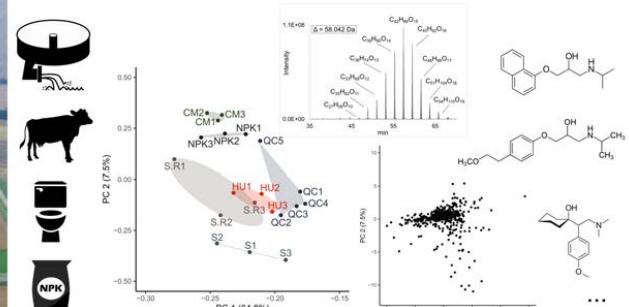
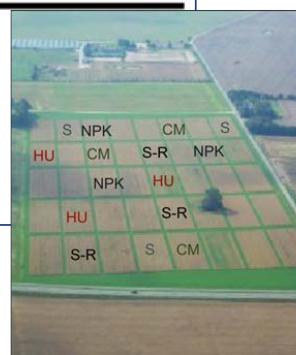
journal homepage: [www.elsevier.com/locate/chemosphere](http://www.elsevier.com/locate/chemosphere)

Non-target analysis of organic waste amended agricultural soils:  
Characterization of added organic pollution

Thorsten Klaus Otto Gravert <sup>a,\*</sup>, Jeanne Vuaille <sup>b</sup>, Jakob Magid <sup>b</sup>, Martin Hansen <sup>a,\*\*</sup>

<sup>a</sup> Aarhus University, Department of Environmental Science, Environmental Metabolomics Lab, Roskilde, Denmark

<sup>b</sup> University of Copenhagen, Department for Plant and Environmental Sciences, Copenhagen, Denmark

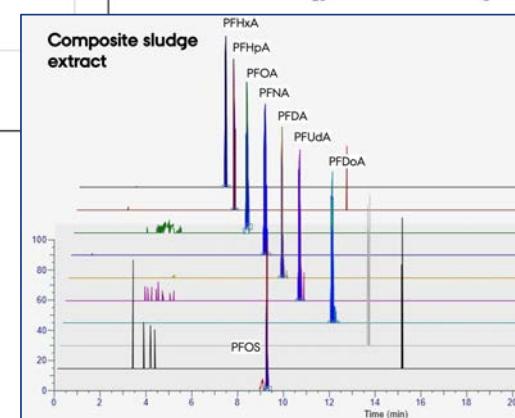
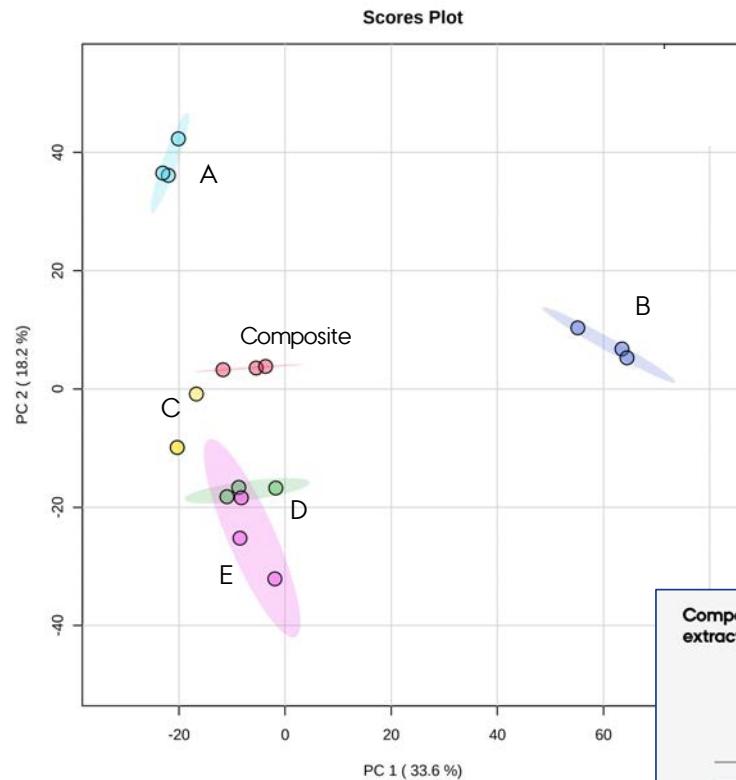


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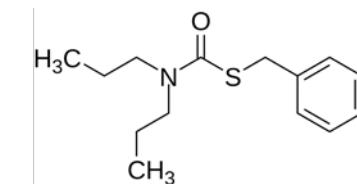
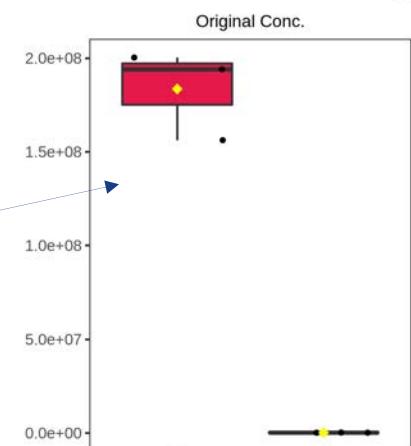
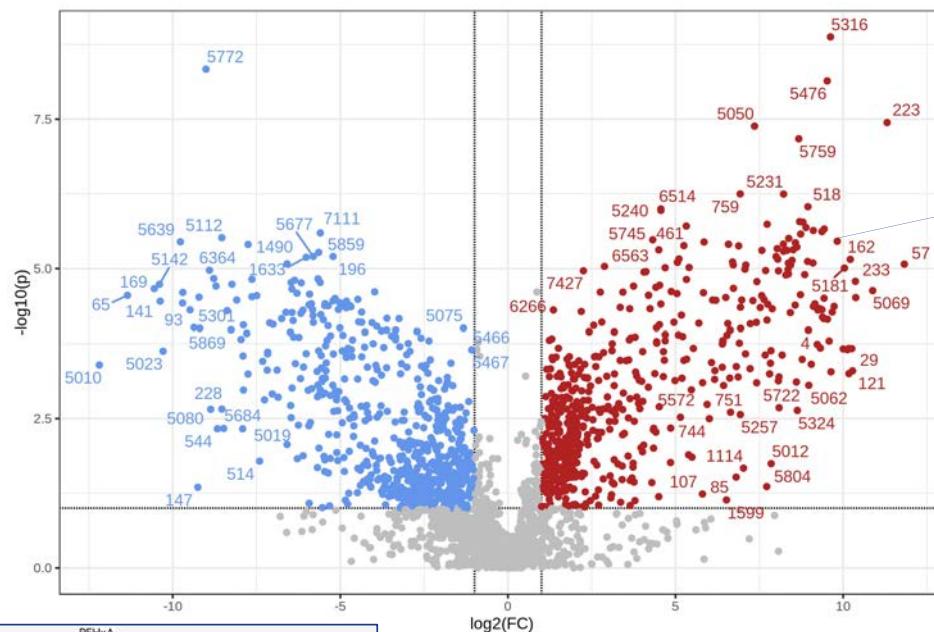


Pressurized liquid extraction

>15,000 substances



### Site A vs Site E



Prosulfocarb

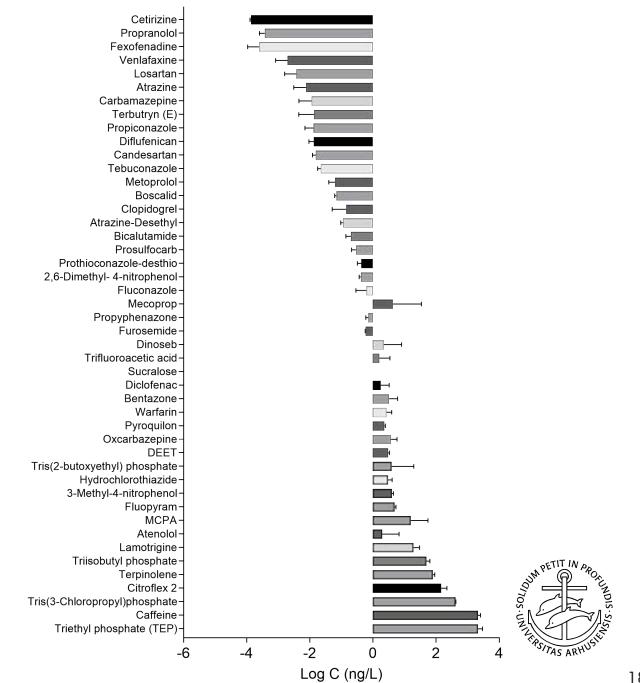
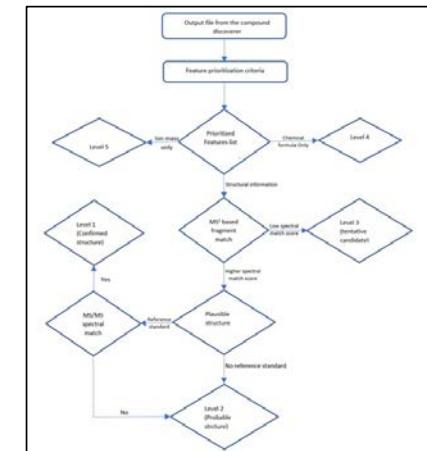
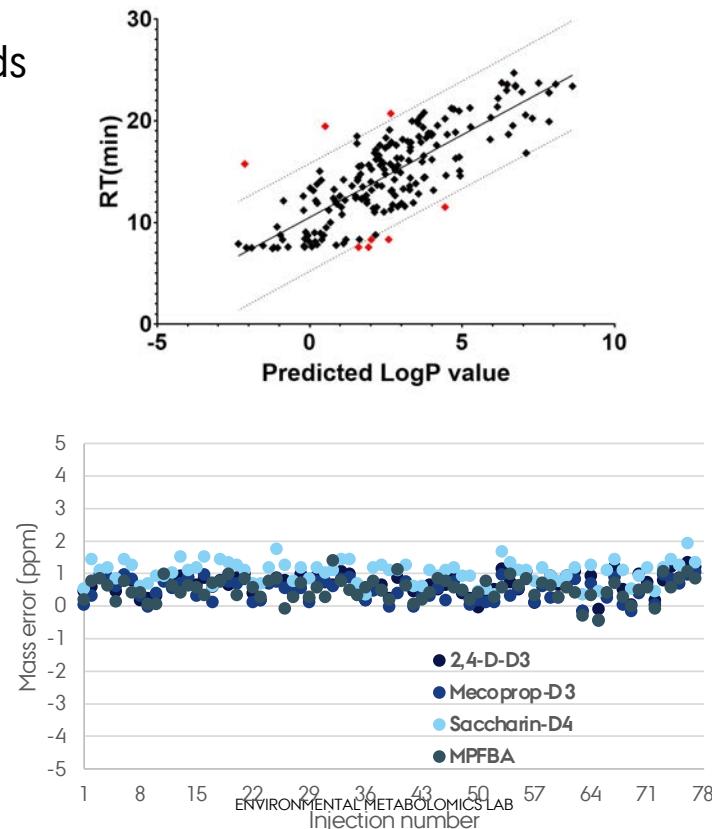
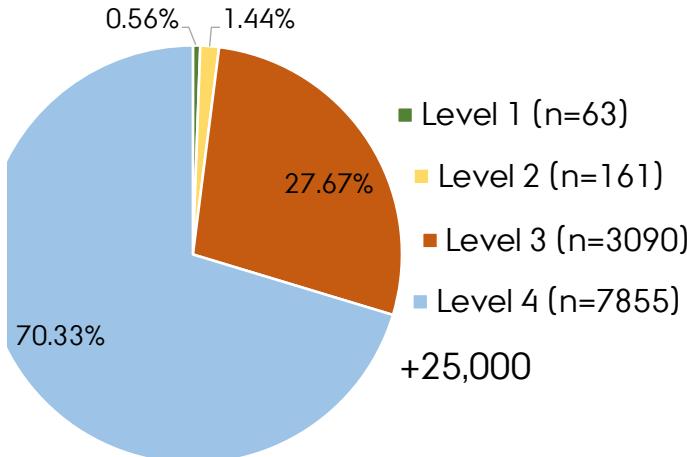
80-300 µg/kg  
In 3 out of 5 sites

Name	Formula	Calcd. MW	Annotation MW
Ciprofloxacin	C17 H18 FN3 O3	331.13311	331.13322
Sertaline	C17 H17 Cl2 N	305.07375	305.0738
Cetirizine	C21 H25 Cl N2 O3	388.15532	388.15537
Tris(3-Chloropropyl)phosphate	C9 H18 Cl3 O4 P	326.00079	326.00083
Citalopram	C20 H21 F N2 O	324.16376	324.16493
Epitestosterone	C19 H28 O2	288.20891	288.20893
Losartan	C22 H23 Cl N6 O	422.16217	422.16219
Clomazone	C12 H14 Cl N O2	239.0713	239.07131
Tris(2-butoxyethyl) phosphate	C18 H39 O7 P	398.24337	398.24441
Aspartame	C14 H18 N2 O5	294.1216	294.12271
Prosulfocarb	C14 H21 N O S	251.13442	251.13438
Amlodipine	C20 H25 Cl N2 O5	408.14525	408.1452
Terbutryn	C10 H19 N5 S	241.13615	241.13612
Lamotrigine	C9 H7 Cl2 N5	255.00789	255.00785
Imazilil	C14 H14 Cl2 N2 O	296.04836	296.04832
Metoprolol	C15 H25 N O3	267.18349	267.18344
Daidzein	C15 H10 O4	254.05795	254.05791

# Challenges?

## Harmonize reporting

- Methods, workflows and decision trees
- Replicates really needed?
- Complete description of dataset and number of detected substances
- Use ID levels
- Support ID with *in silico* methods
- Use internal standards
- Archiving of raw data





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European Union



**Ministry of Environment  
of Denmark**

Environmental  
Protection Agency



**Ministry of Higher  
Education and Science  
Denmark**



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