

Novel data handling strategies for the analysis of dissolved organic matter in wastewater using high resolution mass spectrometry



fazafra@icra.cat

Zafra F.A.^{1,2}, Čelić M.^{1,2}, Aguilar P.^{1,2}, Petrović M.^{1,3}, Perez-Lopez C.⁴, José Farré M.^{1,2}

¹Catalan Institute for Water Research (ICRA), C. Emili Grahit 101, 17003 Girona, Spain

²University of Girona, Plaça de Sant Domènec 3, 17004 Girona, Spain

³Catalan Institution for Research and Advanced Studies (ICREA), C. Emili Grahit 101, 17003 Girona, Spain

⁴Institute of Environmental Assessment and Water Studies (IDAEA-CSIC), Department of Environmental Chemistry, Jordi Girona 18–26, 08034 Barcelona, Spain

What?

Dissolved organic matter (DOM) is a heterogeneous mixture of water-soluble organic compounds of different natural or anthropogenic origin.

Why?

Understanding the composition and fate of DOM in wastewater treatment processes may help predict optimal water treatments and minimize side effects, such as the formation of byproducts.

How?

High-resolution mass spectrometry (HRMS) is employed in non-target strategies to analyze mixtures of organic compounds in water, which may assist in DOM characterization.

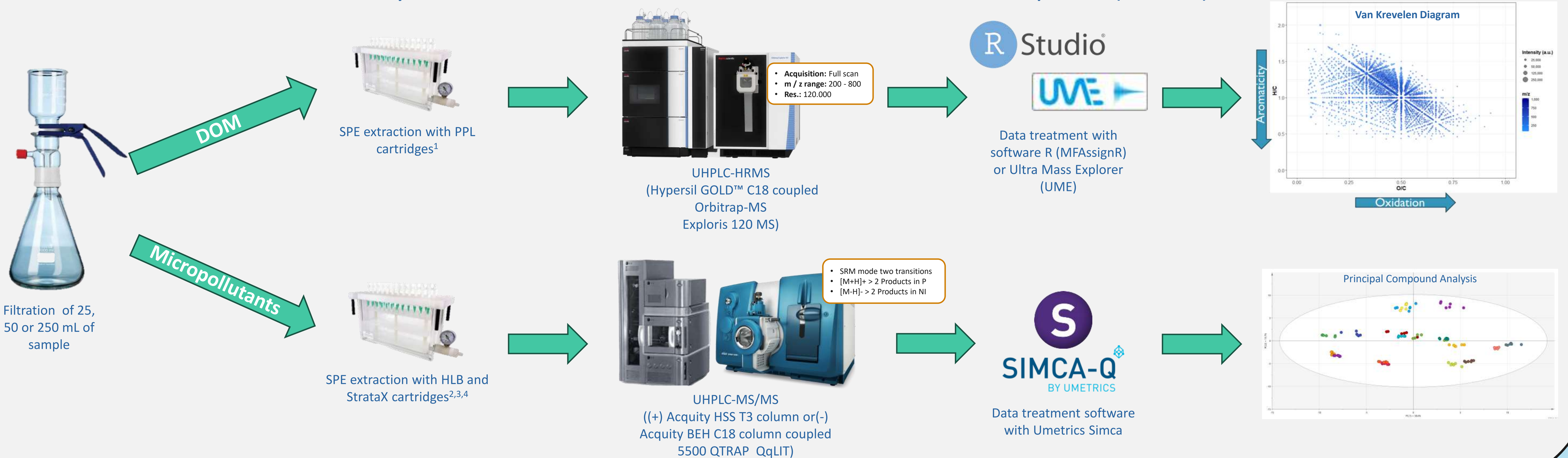
Research Questions?



- Are non target strategies suitable for DOM characterization to evaluate wastewater treatment processes?
- Can DOM serve as a reliable indicator of the efficiency of wastewater treatment?
- Is there any correlation between targeted micropollutants present in wastewater and DOM analyzed with HRMS?

Methodology

Analysis of effluents and influents of wastewater treatment plants (WWTP)



First results

Analysis of effluent and influent in:

3 WWTPs

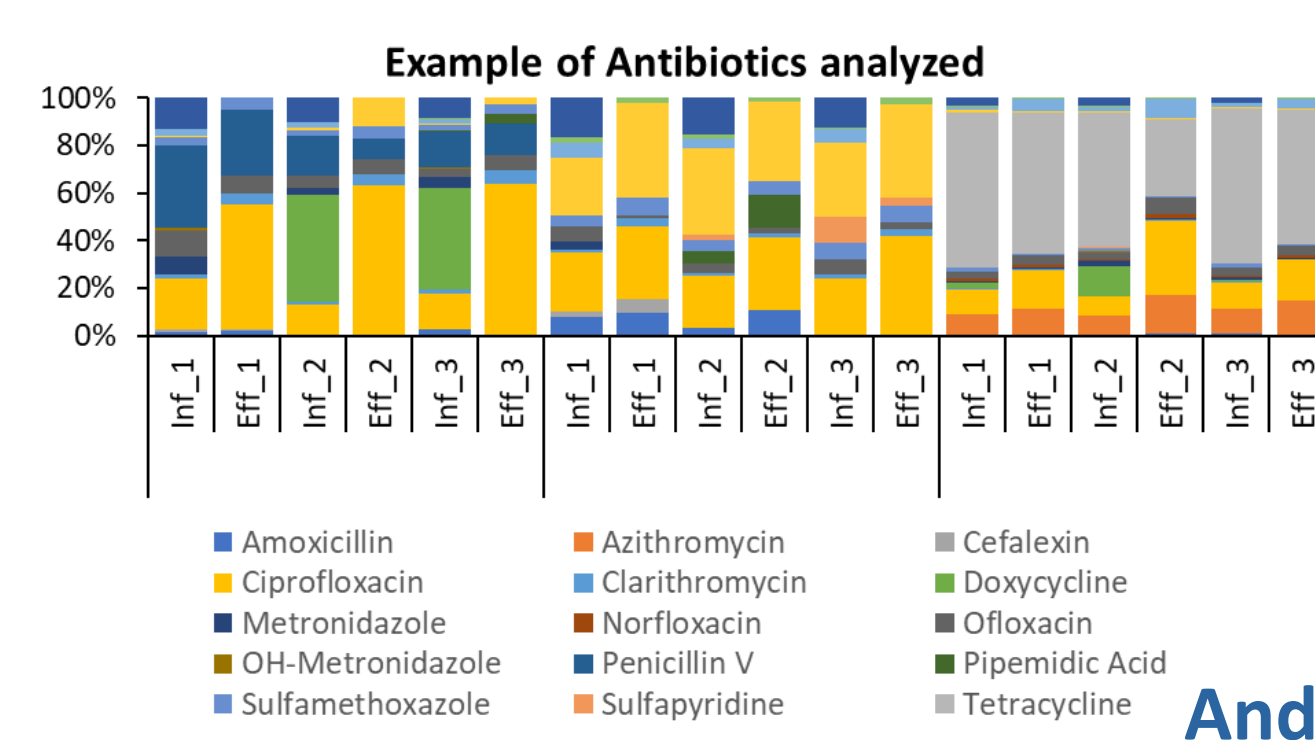


3 Campaigns

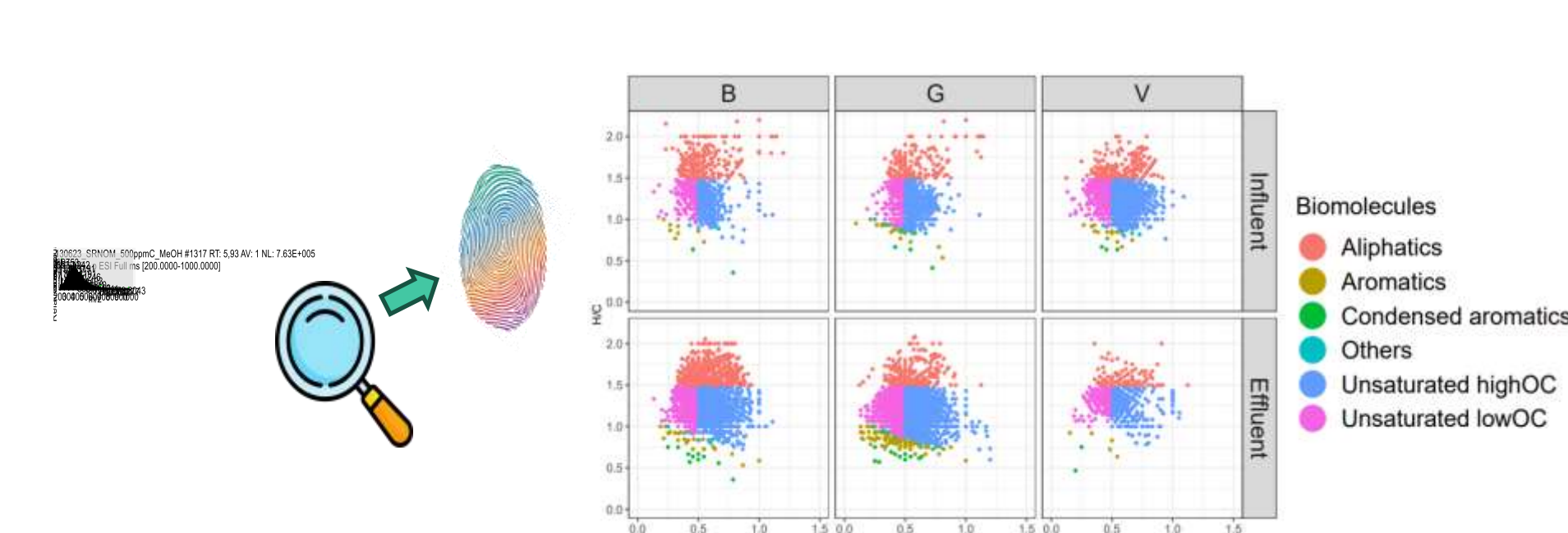


Total 54 samples

A total of 140 micropollutants analysed

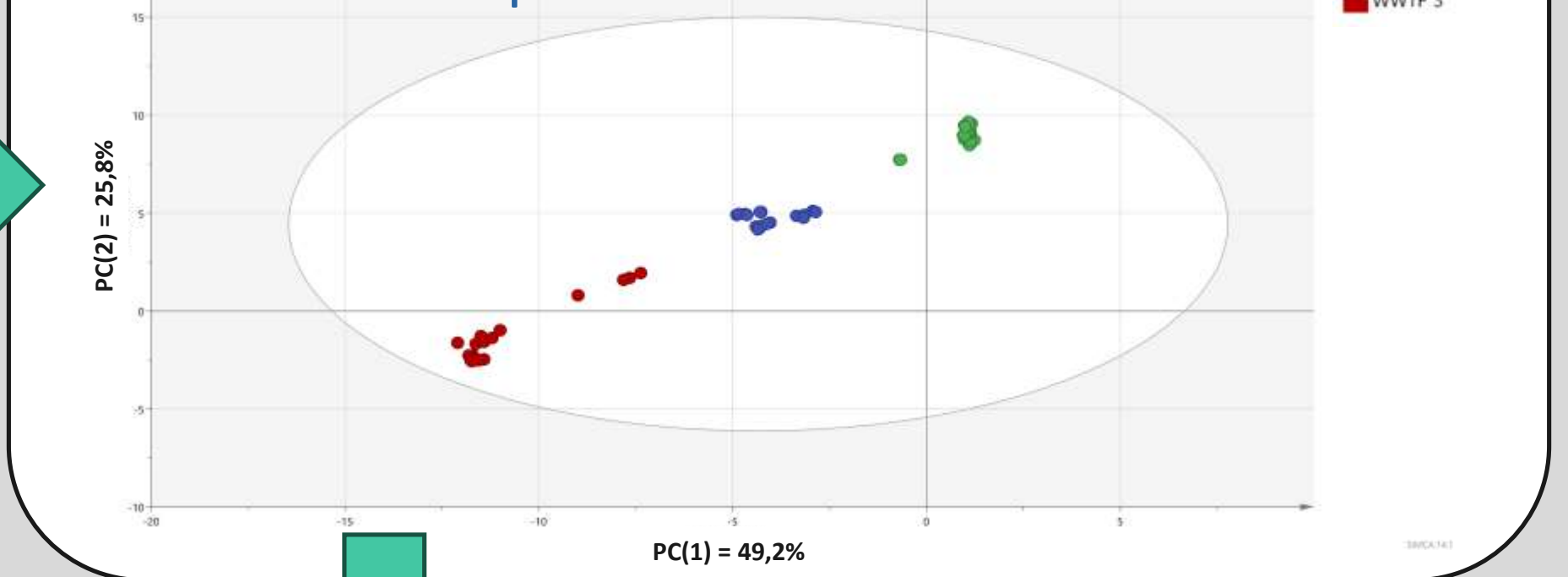


Fingerprinting DOM

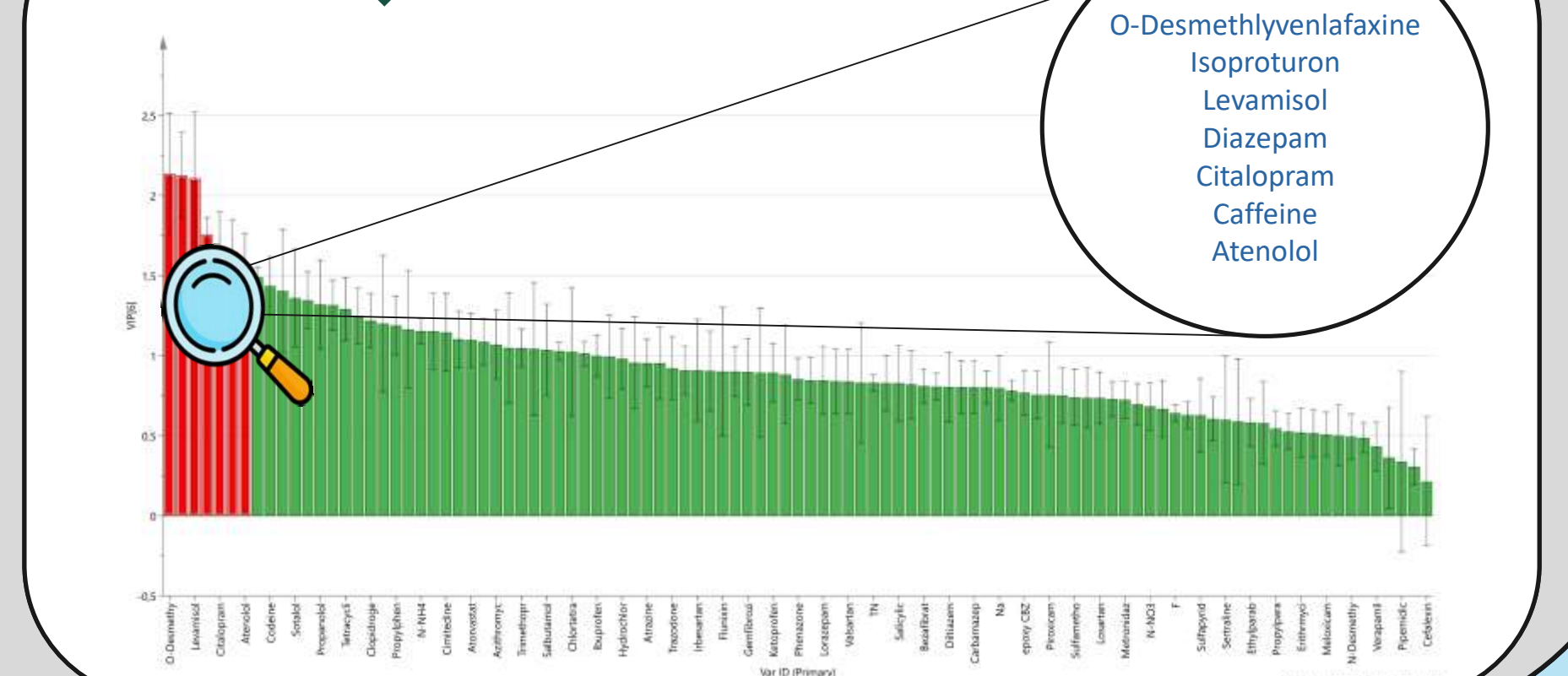


Partial Least Squares Discriminant Analysis (PLS-DA)

Effluent samples



VIPs of PLS-DA



Conclusions

- DOM analysis in WWTP influent samples suffer from signal suppression, as there are more m/z features in the effluent than in the influent samples. Nevertheless, DOM fingerprinting can be used to characterize WWTP effluents.
- A correlation among the detected micropollutants across the various samples analyzed was observed.
- The potential for utilizing statistical tests to identify characteristic compounds in wastewater treatment plants based on the seasonal or the geographical variations was confirmed.

Bibliography

¹(Dittmar et al., 2008) ²(Gros et al., 2012) ³(Jakimska et al., 2013) ⁴(Gros et al., 2013)

Francisco Zafra acknowledges the Spanish State Research Agency of the Spanish Ministry of Science and Innovation and European Social Fund+ for his Predoctoral Fellowship PRE2021-099897 funded by MCIN/AEI/10.13039/501100011033 and FSE+

