

Fifty Shades of Filth, 23rd January 2020

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# The Next Big Thing in Environmental Chemistry?

## Future challenges and opportunities

Andrea Mizzi Brunner

**KWR**

Bridging Science to Practice

# On-site monitoring of chemicals with automatic risk assessment



Tricoder  
Star Trek Next generation

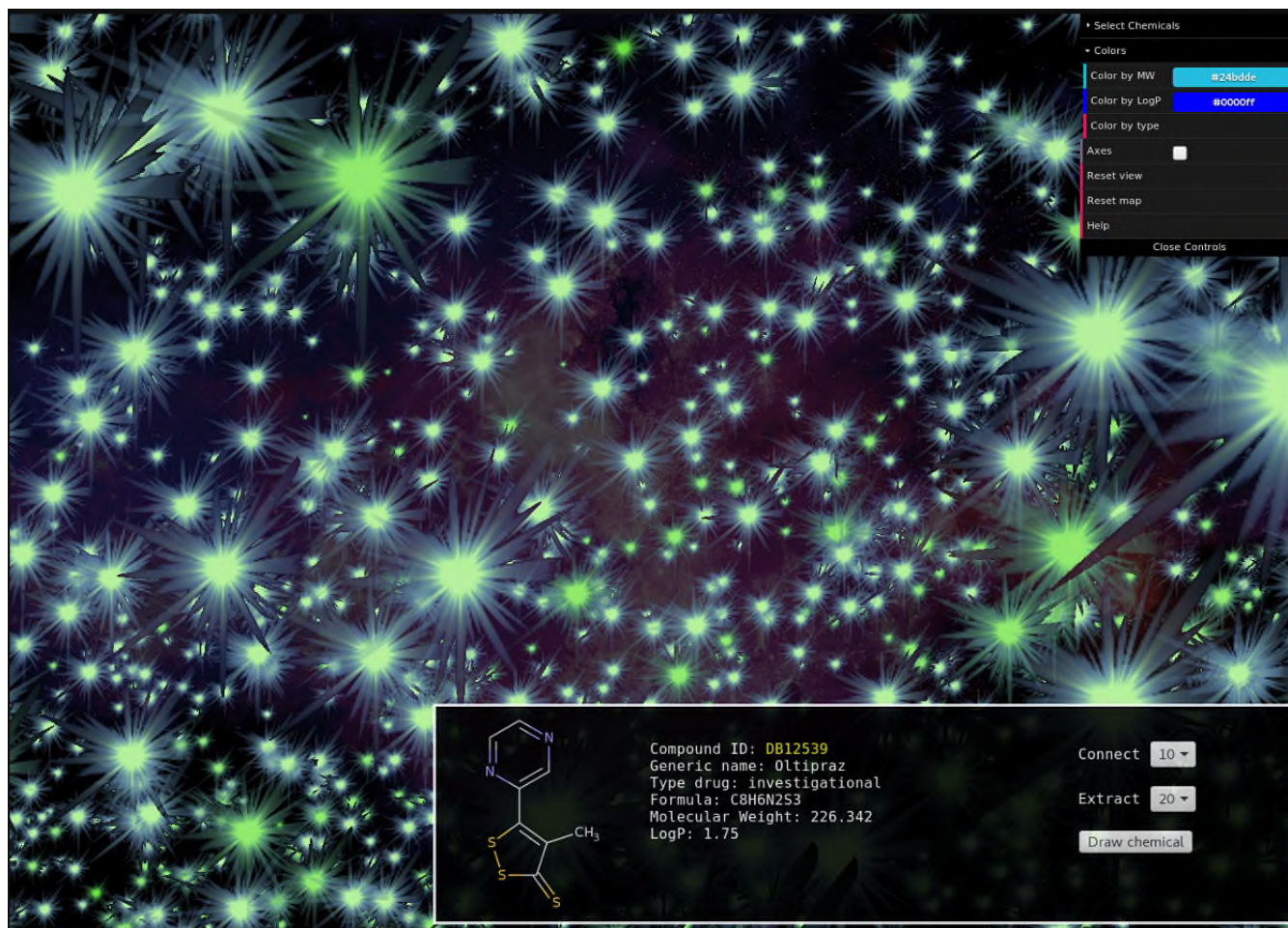


Ion mobility spectrometer for trace detection  
NASA



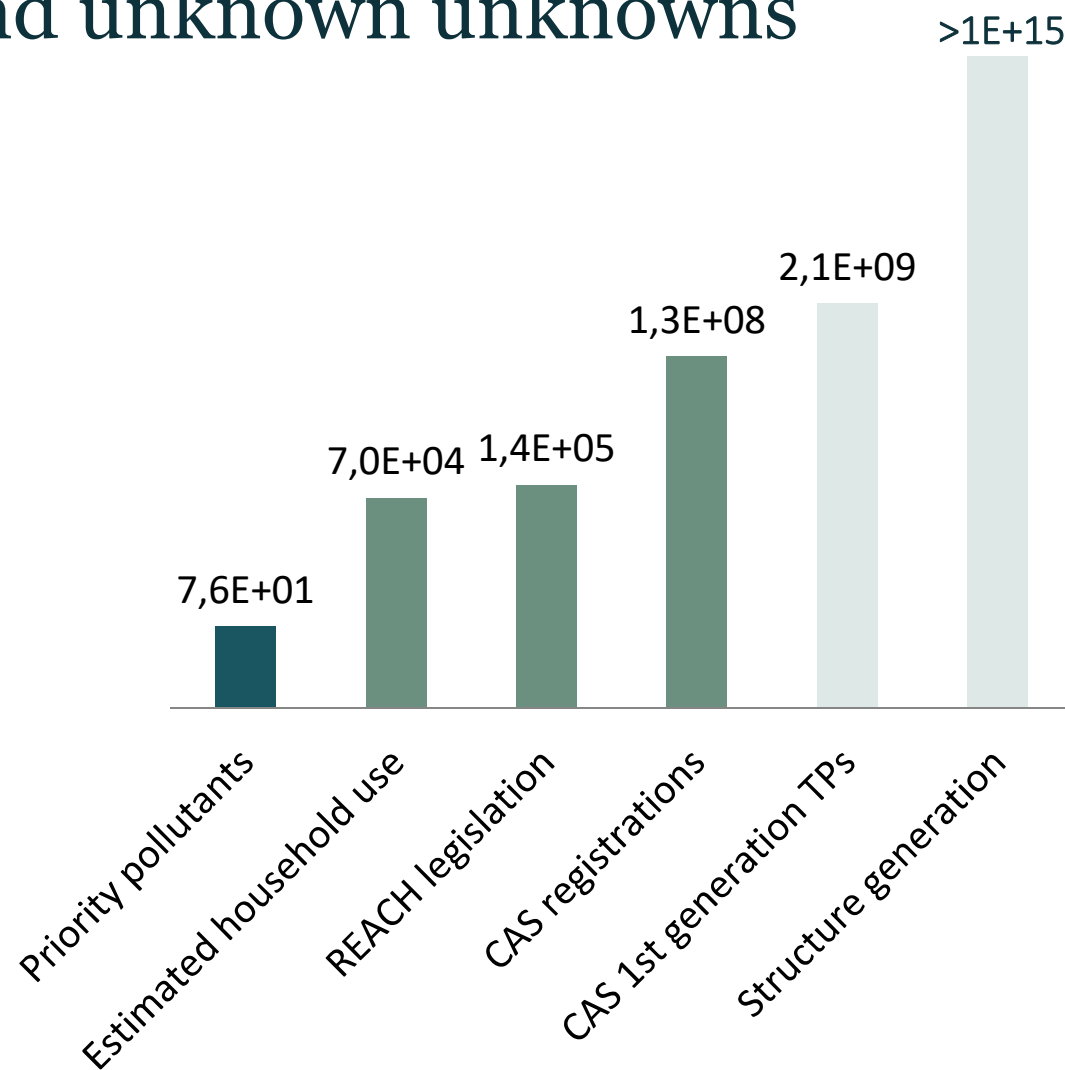
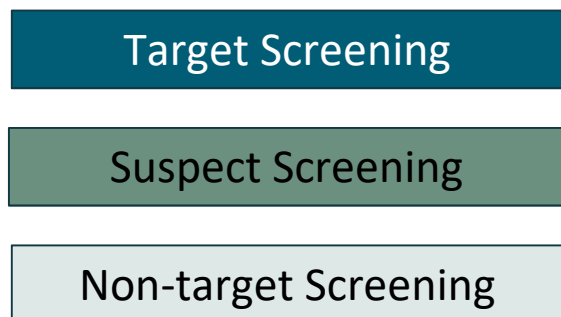
Portable mass spectrometer for on-site OMP analysis  
EAWAG

# Towards covering the whole chemical space

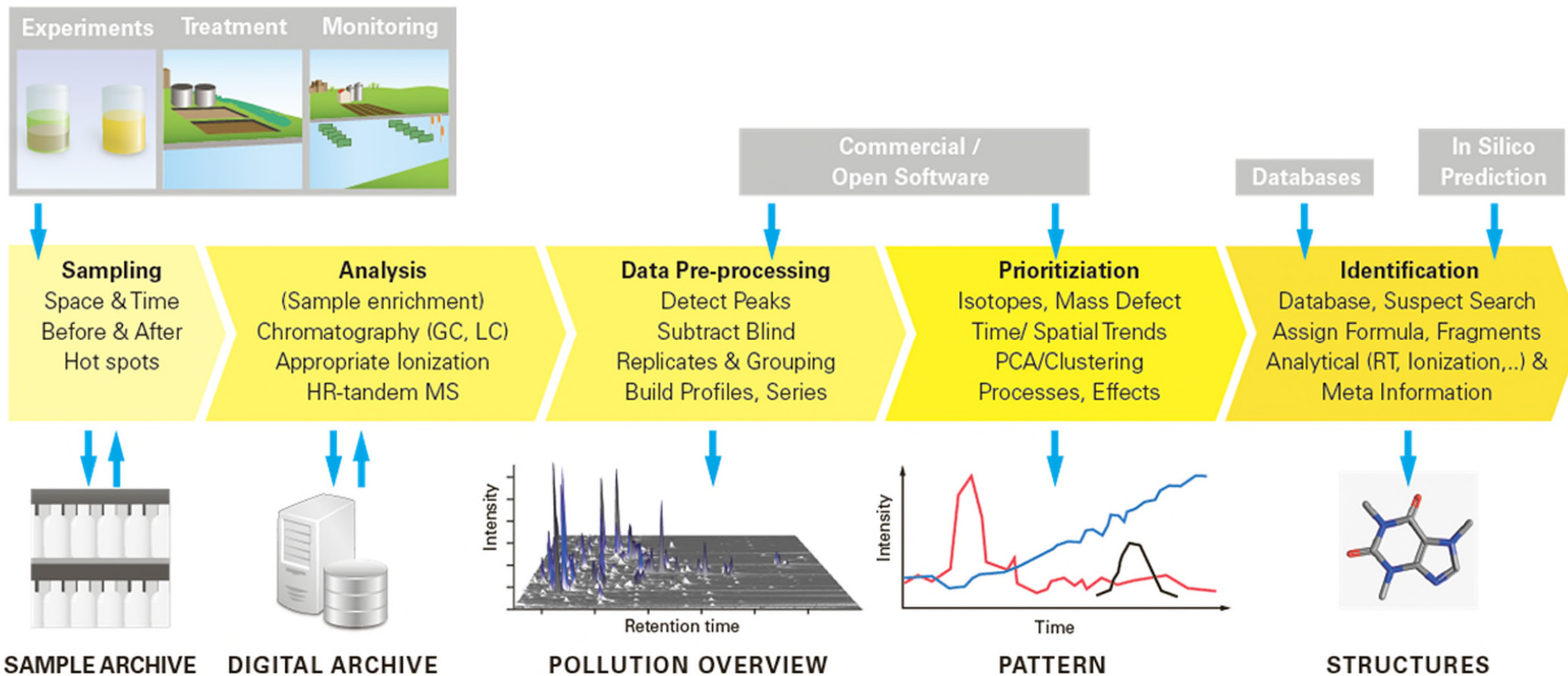


Borrel et al. (2018) Exploring drug space with ChemMaps.com. *Bioinformatics*  
<https://doi.org/10.1093/bioinformatics/bty412>

# Knowns, known unknowns and unknown unknowns



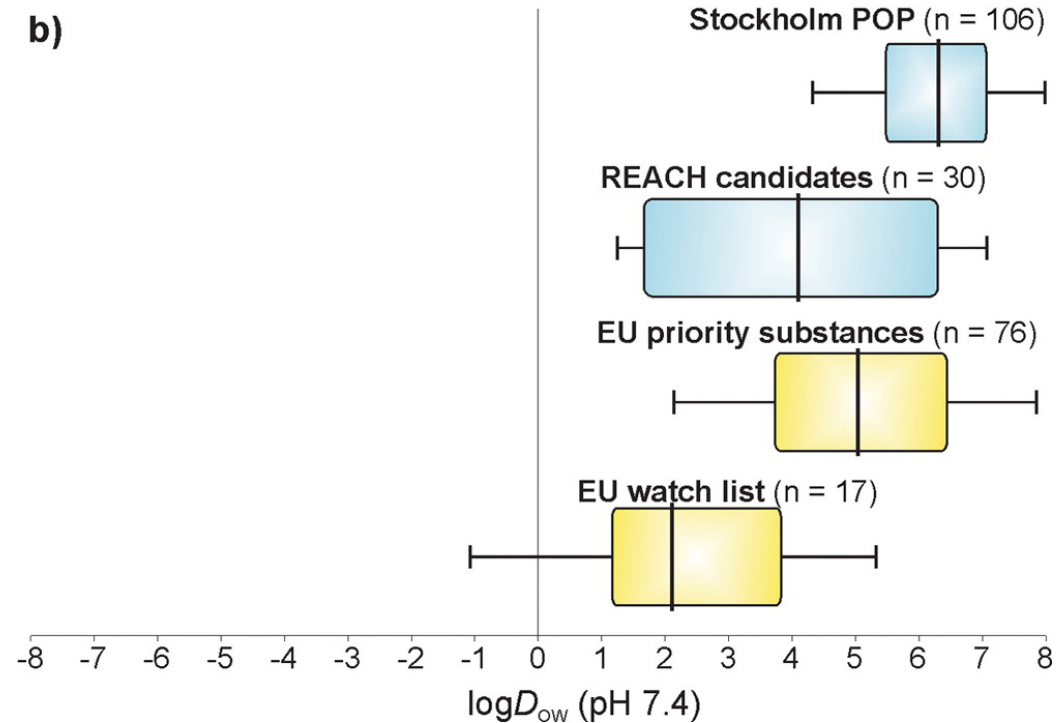
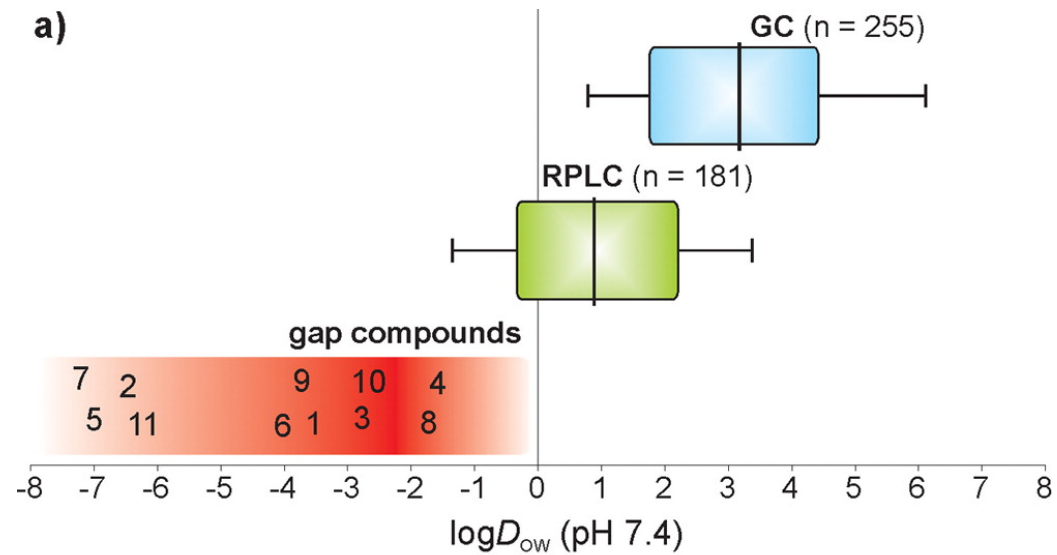
# Non-target screening with High Resolution Mass Spectrometry in the Environment



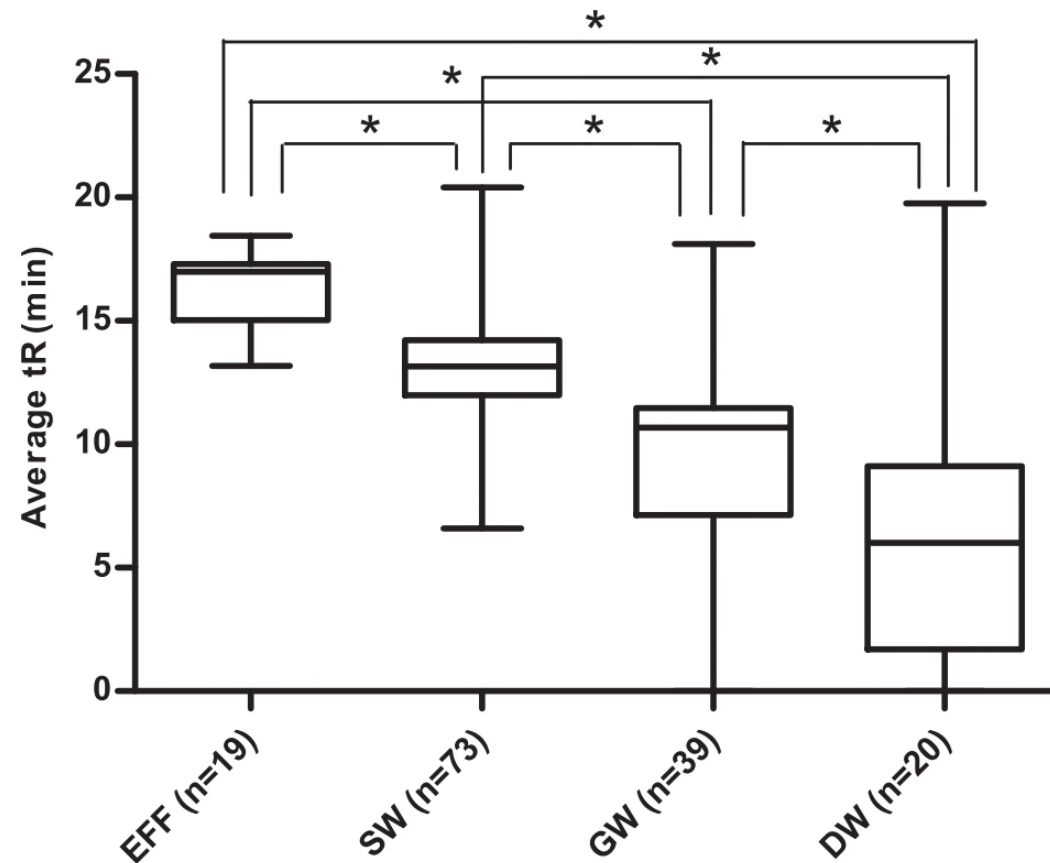
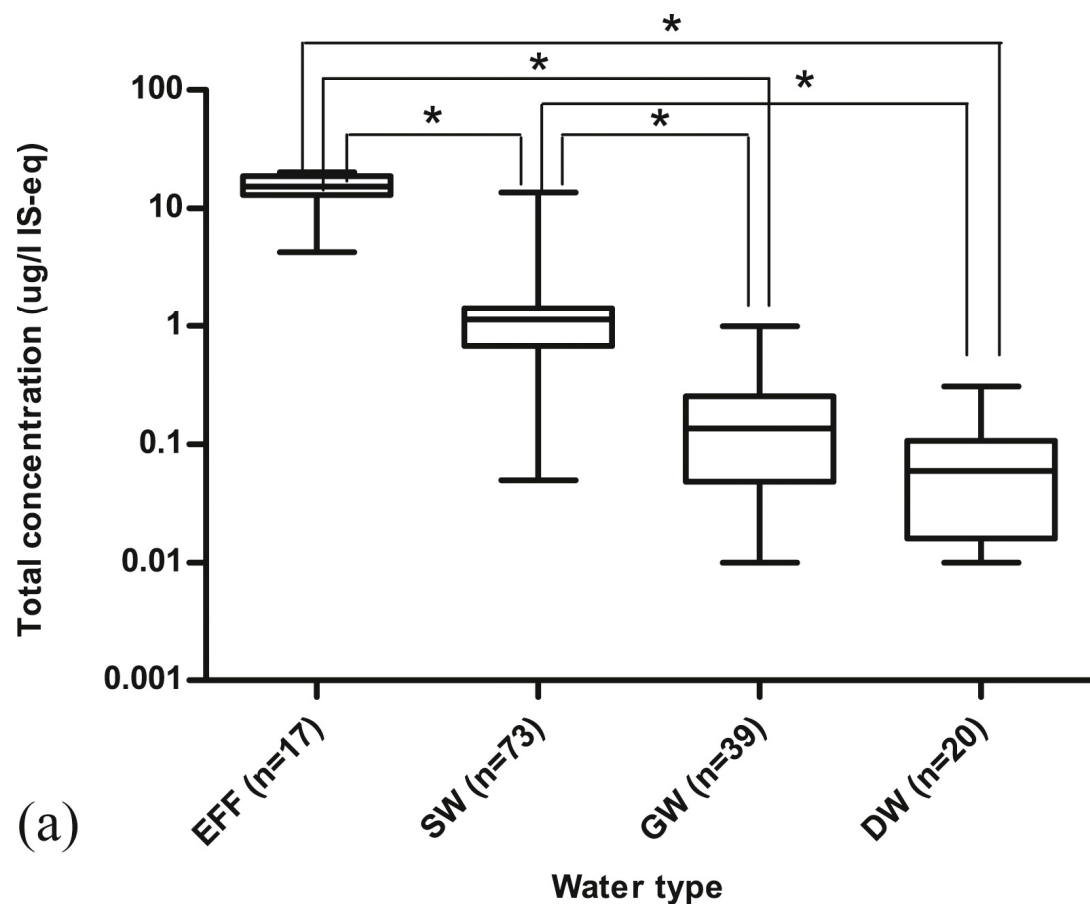
# Mind the gap

- 1: AMPA
- 2: Paraquat
- 3: Cyanuric acid
- 4: DMS
- 5: Diquat
- 6: 5-Fluorouracil
- 7: Glyphosate
- 8: Melamine
- 9: Metformin
- 10: Perfluoroacetic acid
- 11: EDTA

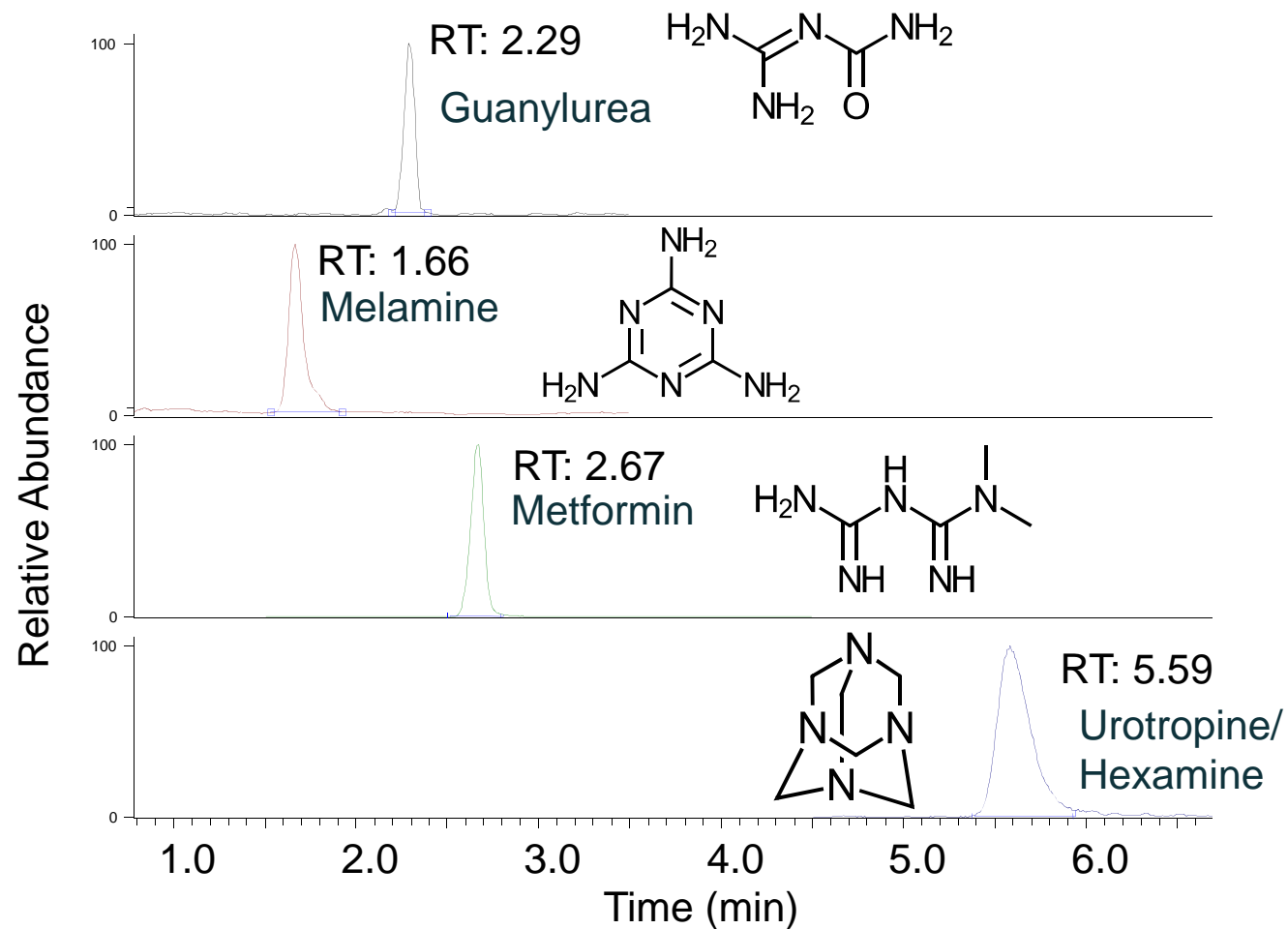
Reemtsma et al. (2016) ES&T  
<https://doi.org/10.1021/acs.est.6b03338>



# Shift from non-polar to polar environmental contaminants



# Screening for very polar compounds

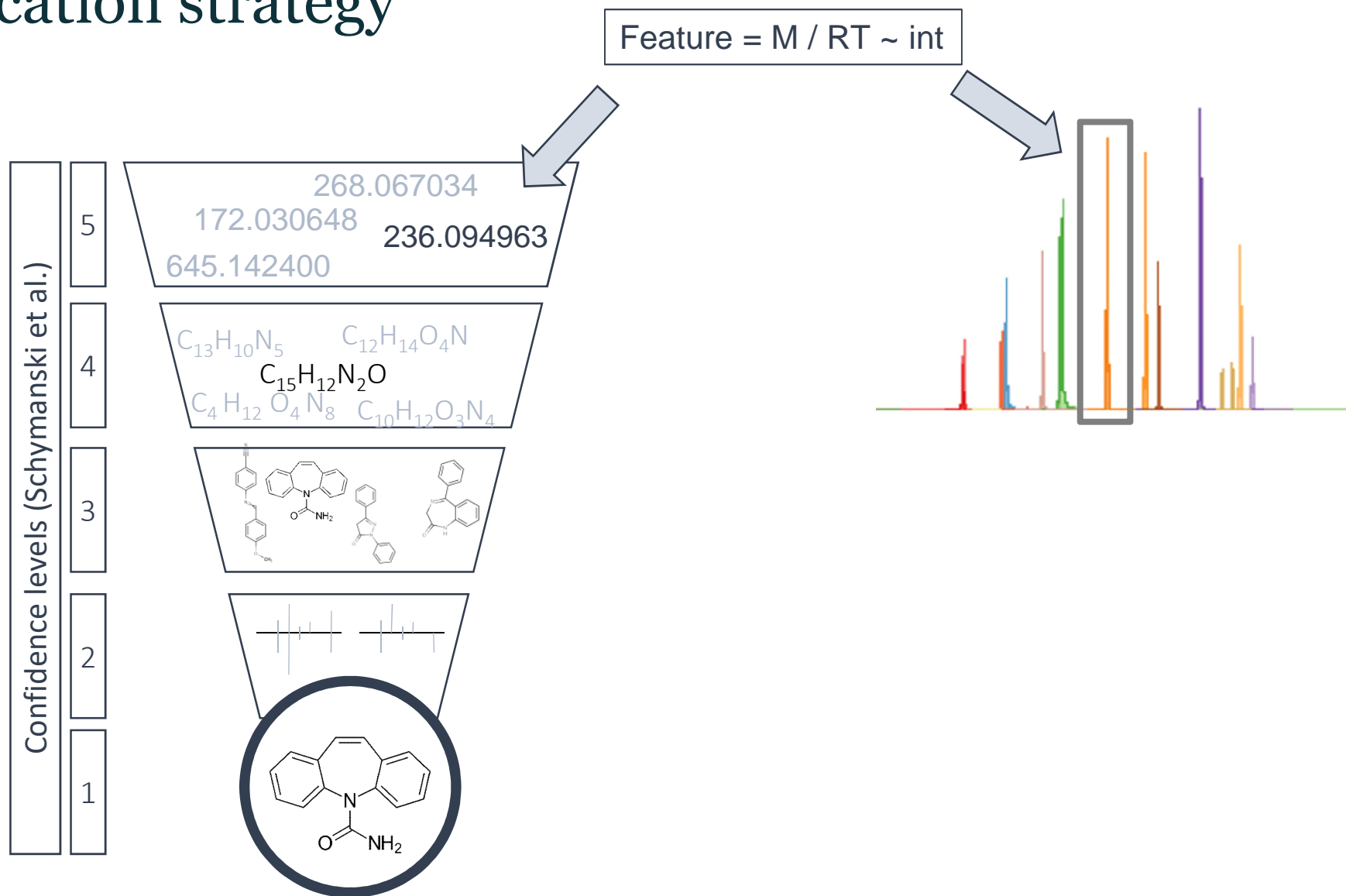


Alternative chromatographies:

- HILIC
- Mixed mode



# Identification strategy



# Suspect screening meets non-target screening through larger and larger suspect lists

- Registered
- Predicted

**NORMAN**  
Network of reference laboratories, research centres  
organisations for monitoring of emerging environmental  
substances

Home | NORMAN Network | Working Groups | Membership | NORMAN Bulletin

**Menu**

- › Emerging Substances
- › DATABASES

NIH U.S. National Library of Medicine  
National Center for Biotechnology Information

PubChem About Blog Submit Contact

**Explore Chemistry**  
Quickly find chemical information from authoritative sources

Search: InChI=1S/C3H6O/c1-3(2)4/h1-2H3

BioAssays

Periodic Table

714 Data Sources

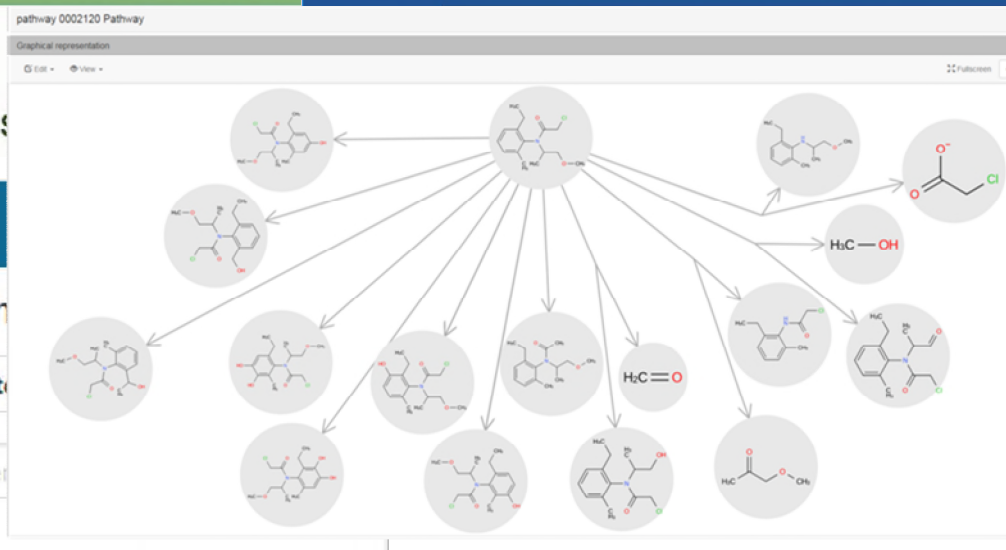
**EPA** United States Environmental Protection Agency

875 Thousand

Chemicals Product/Use Categories

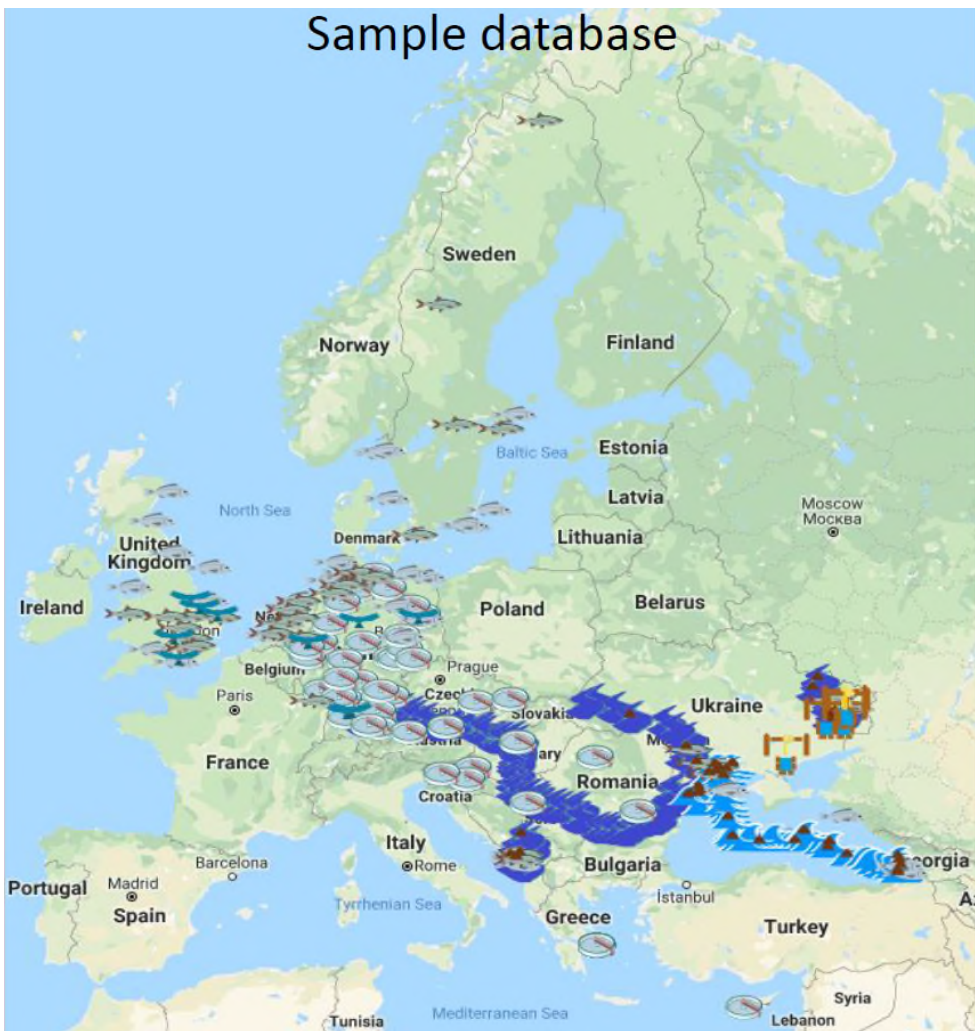
Search for chemical by system

Identifier substring search



# Automated suspect screening in data repositories

Sample database



Surface water -  
Territorial and  
open sea water



Surface water -  
River water



Biota - Territorial  
and open sea  
water or Coastal  
water



Biota - River  
water or  
Lake water



Ground water



Wastewater - Municipal or  
Industrial



Sediments - Territorial and  
open sea water or River water



Biota - Terrestrial

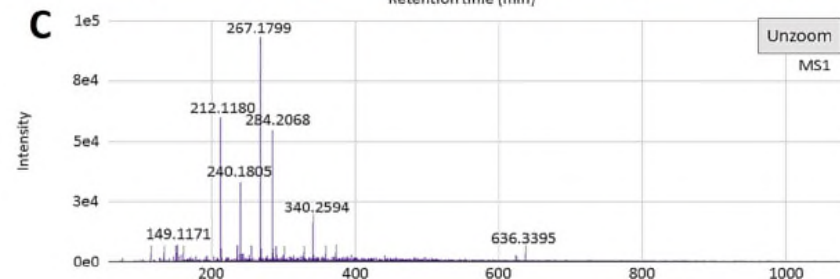
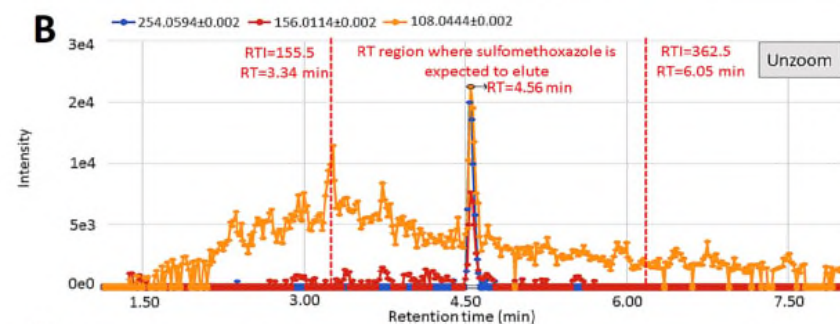
Digital Sample Freezing Platform (NORMAN)

Results

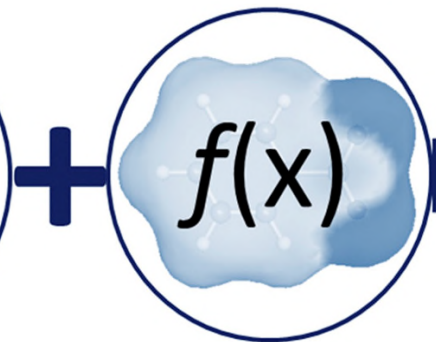
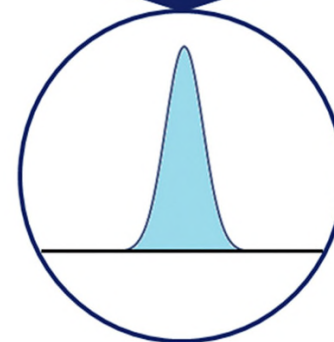
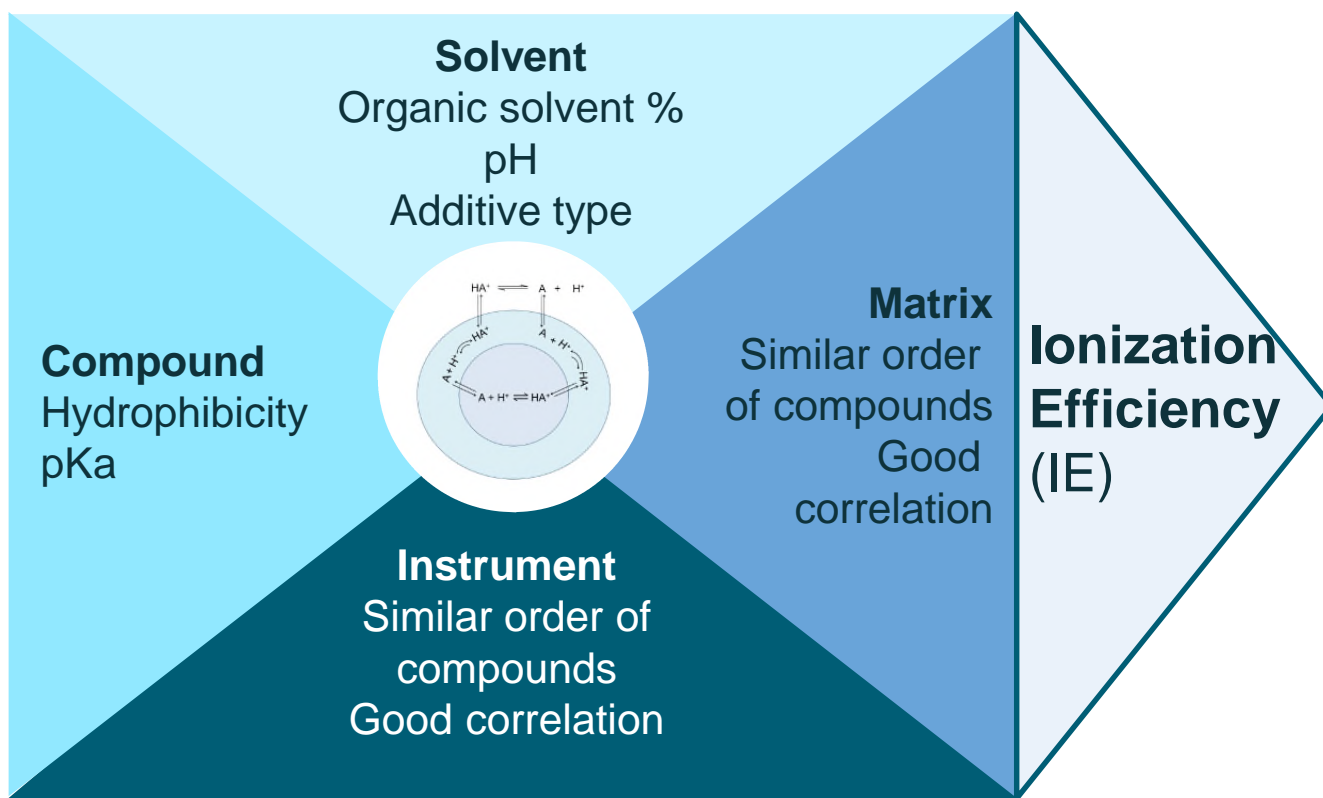
Select Chromatogram  
UoA\_LC-ESI-QTOF\_SeaWater\_UA07\_Odesa\_Ukraine\_19.05.2016\_EMBLAS-II (Survey 2016)\_17856.mzML

Data-Independent		Data-Dependent		chromatogram
show	mz	accuracy_mDa		
1	254.0594	0.003000	UoA_POS_4_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
2	188.0619	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
3	160.0889	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
4	156.0114	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
5	147.0791	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
6	119.0600	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
7	108.0444	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	
8	106.0114	0.003000	UoA_POS_25_LC-ESI-QTOF_SeaWater_UA07_Odesa_Ukraine_19.05.2016_EMBLAS-II (Survey 2016)_17856.mzML	

Submit (Press the button everytime changes are done to the table above)

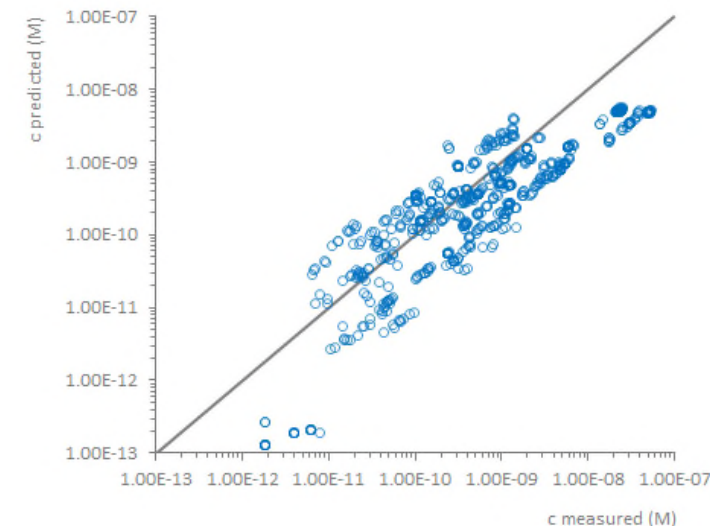


# Making non-target screening quantitative

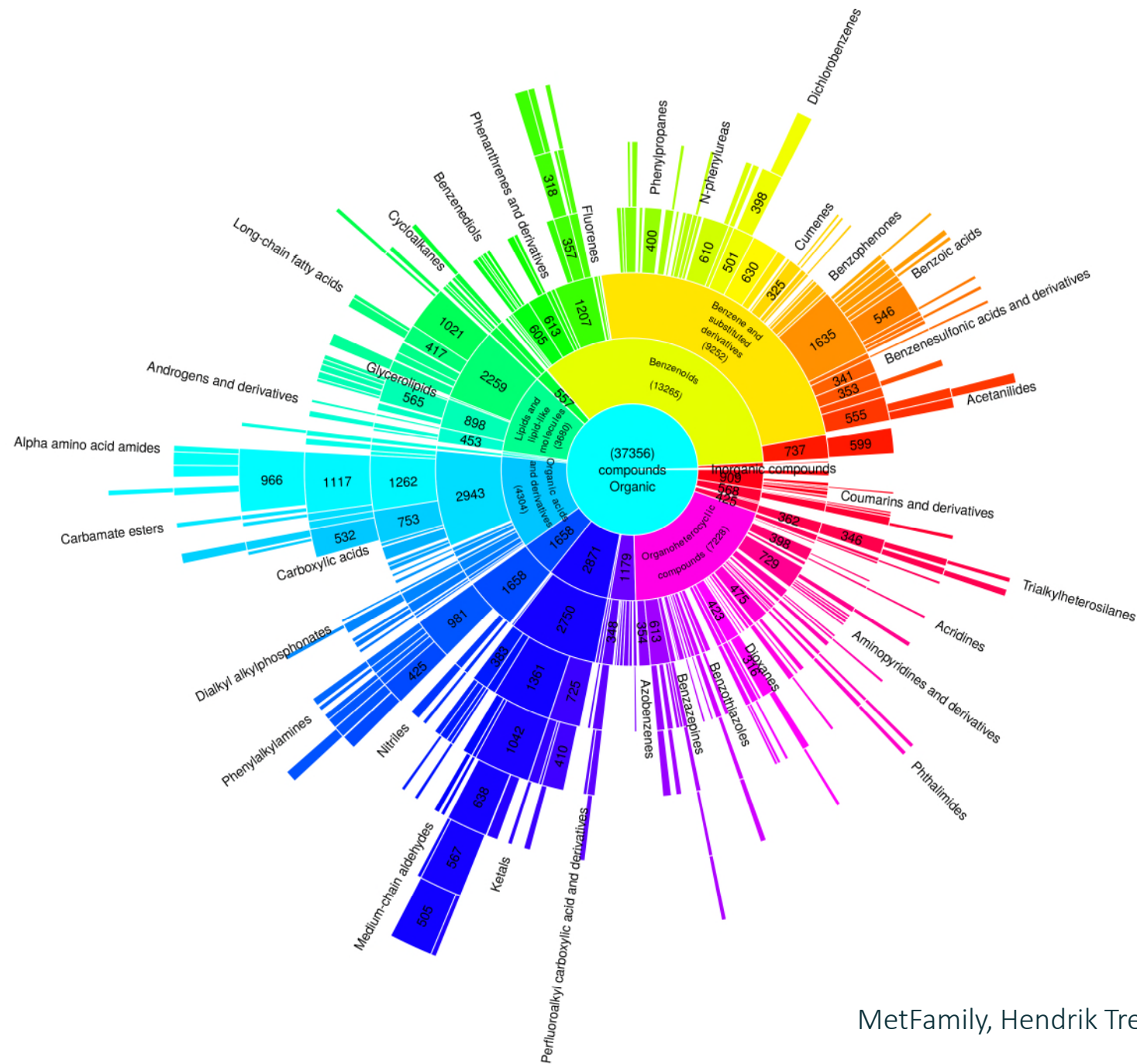


$c = 5 \mu\text{g/ml}$

## PRELIMINARY RESULTS

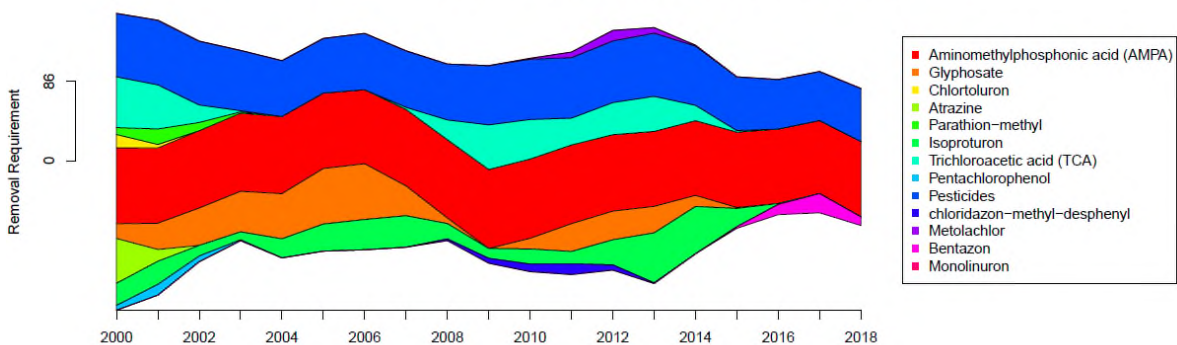


# Cheminformatics

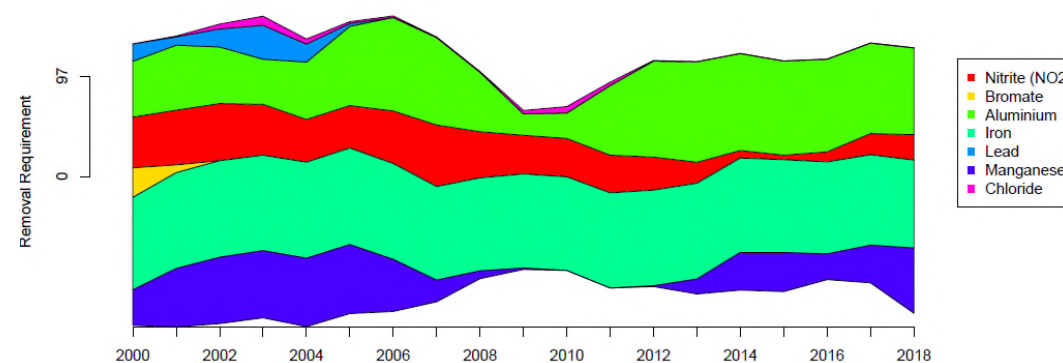


# Data science

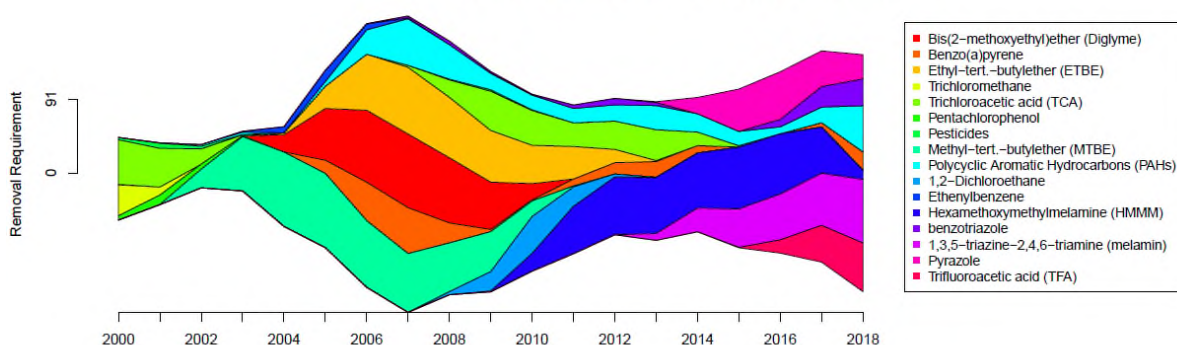
Plant protection products, biocides and their metabolites Lobith



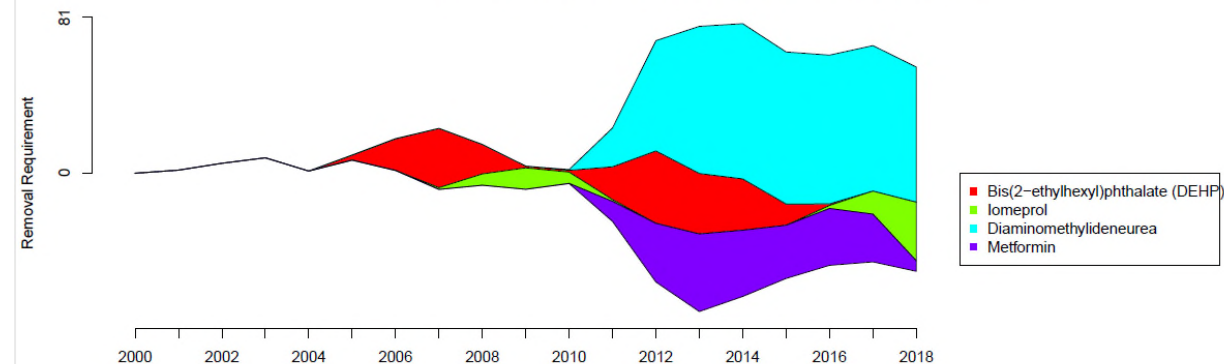
General parameters and nutrients Lobith



Industrial pollutants and consumer products Lobith

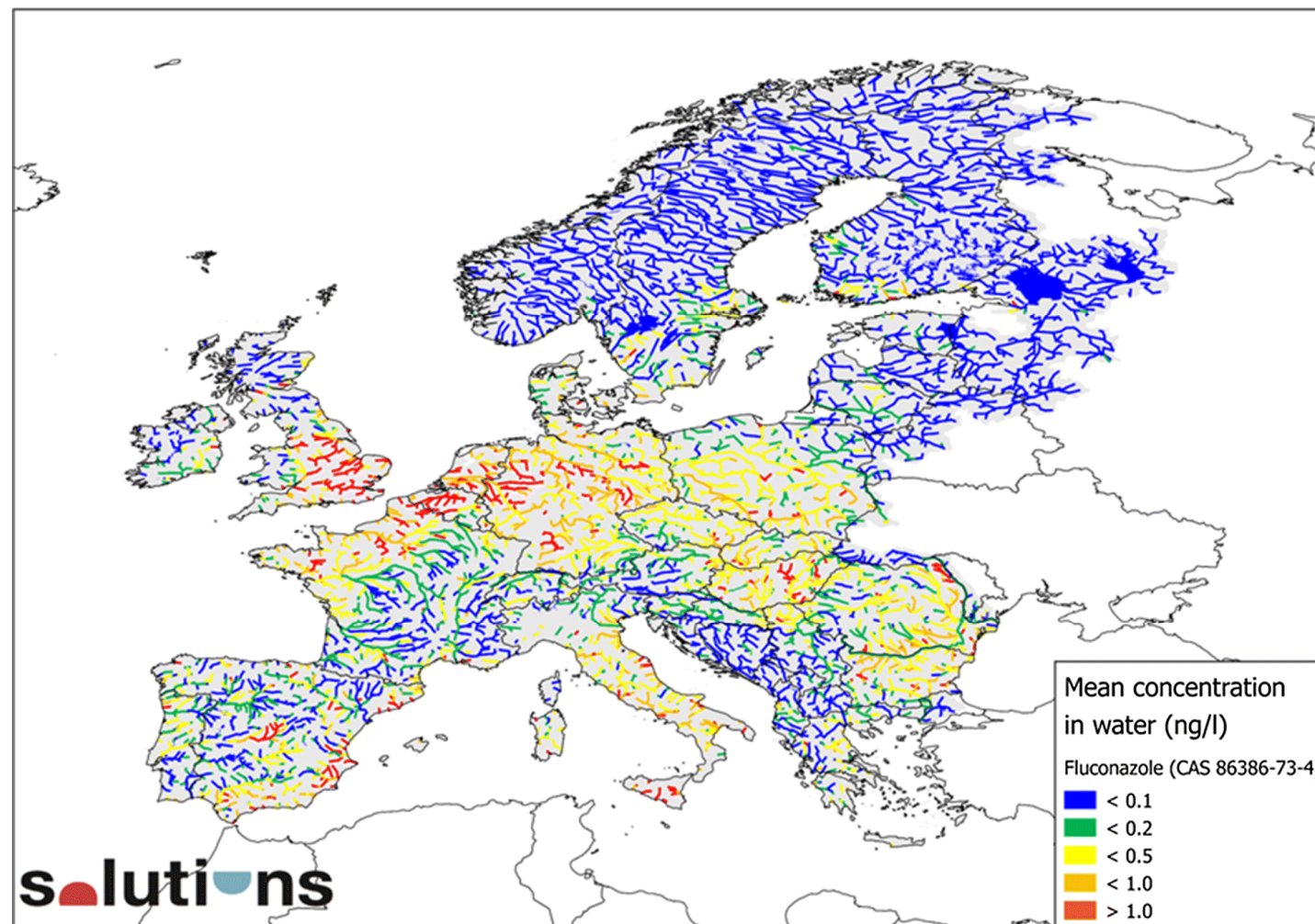


Pharmaceuticals and endocrine disrupting chemicals (EDCs) Lobith

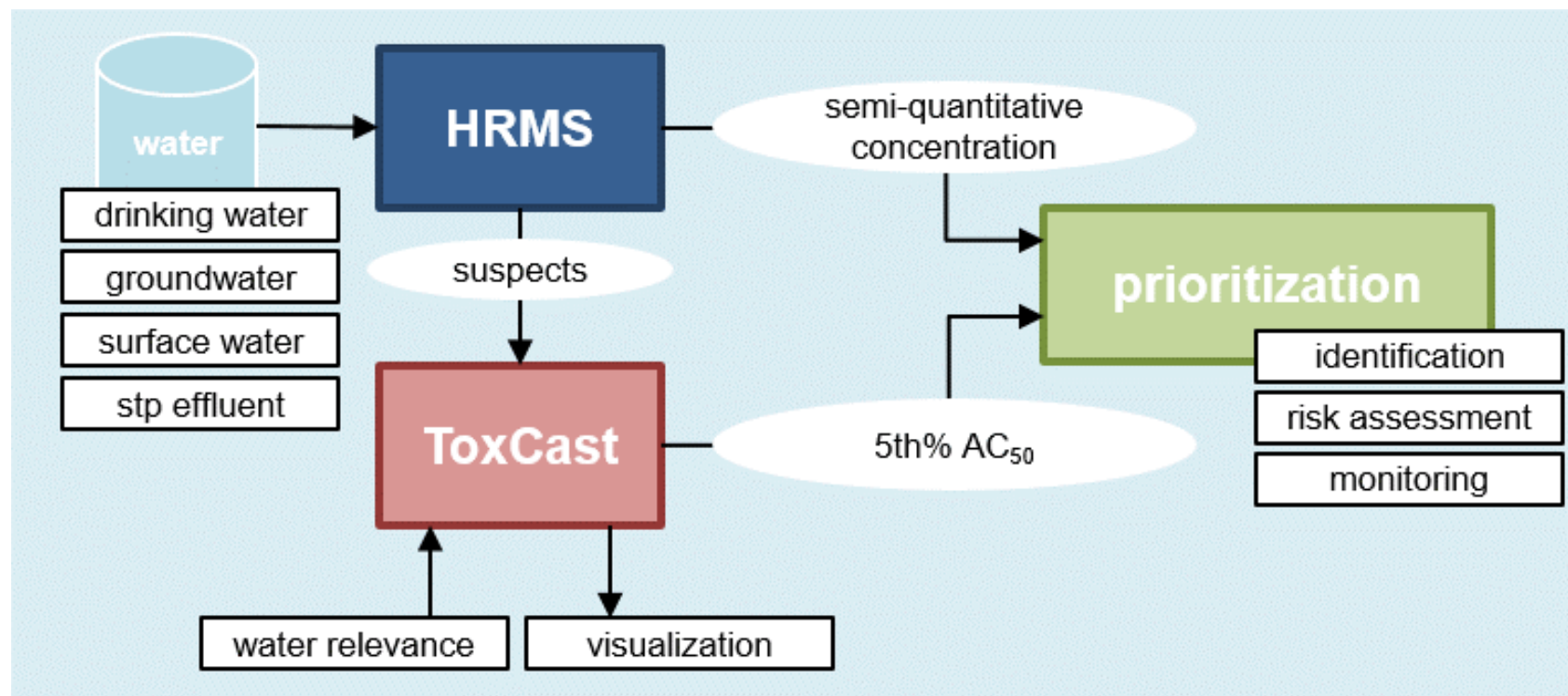


Water purification index, Tessa Pronk

# Modelling instead of measurement data



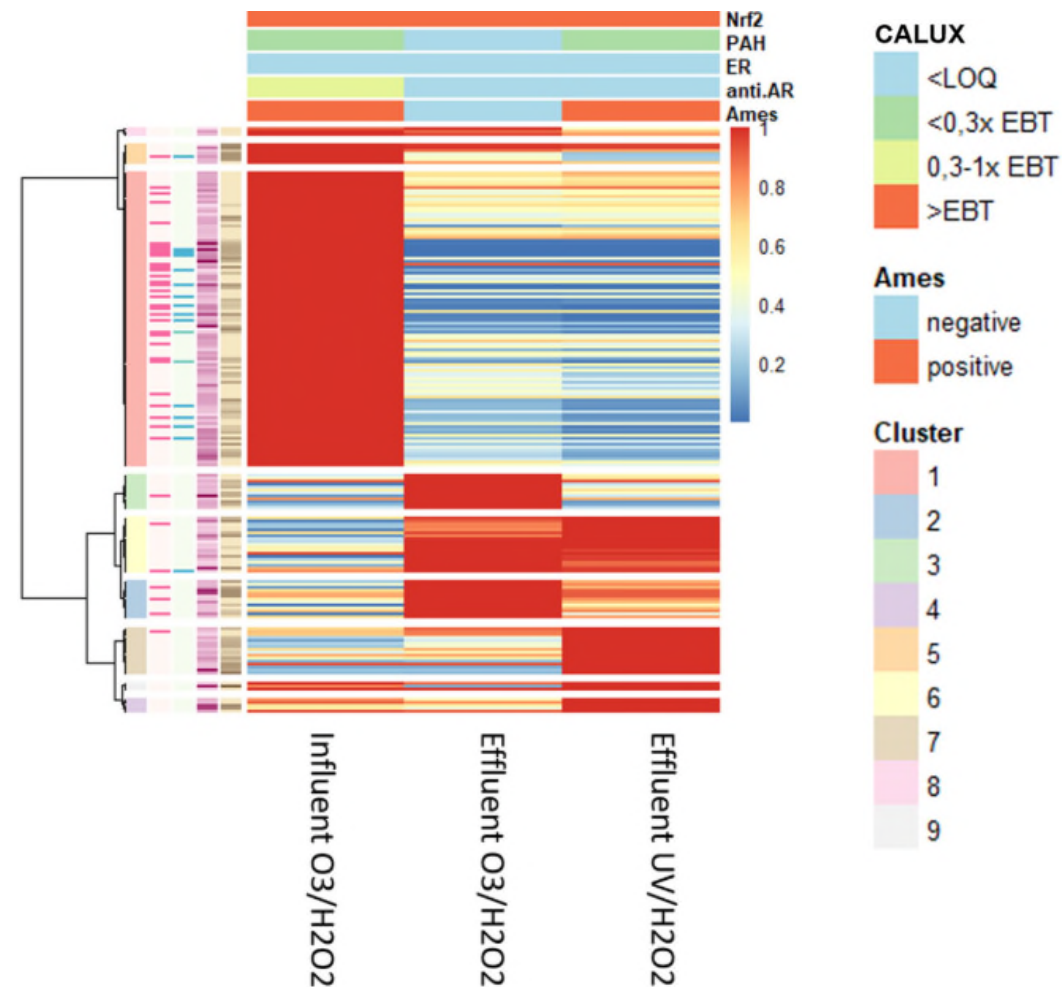
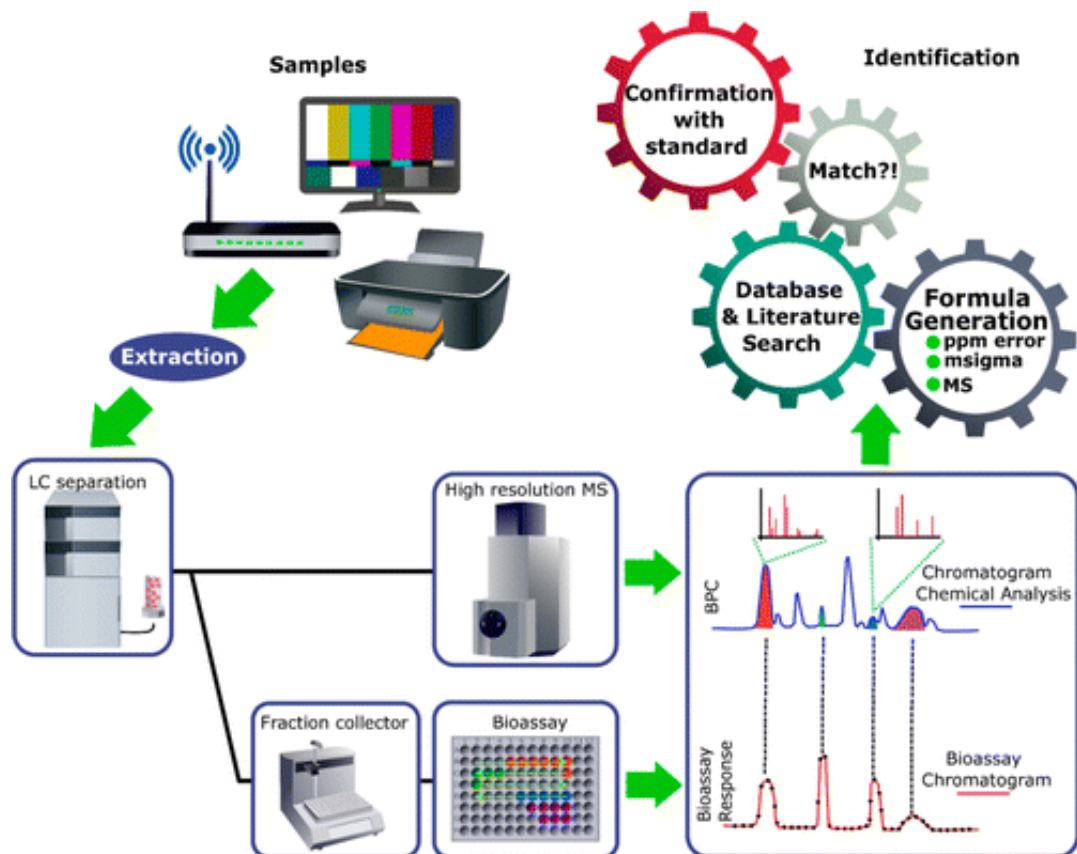
## Focus on compounds that pose a risk



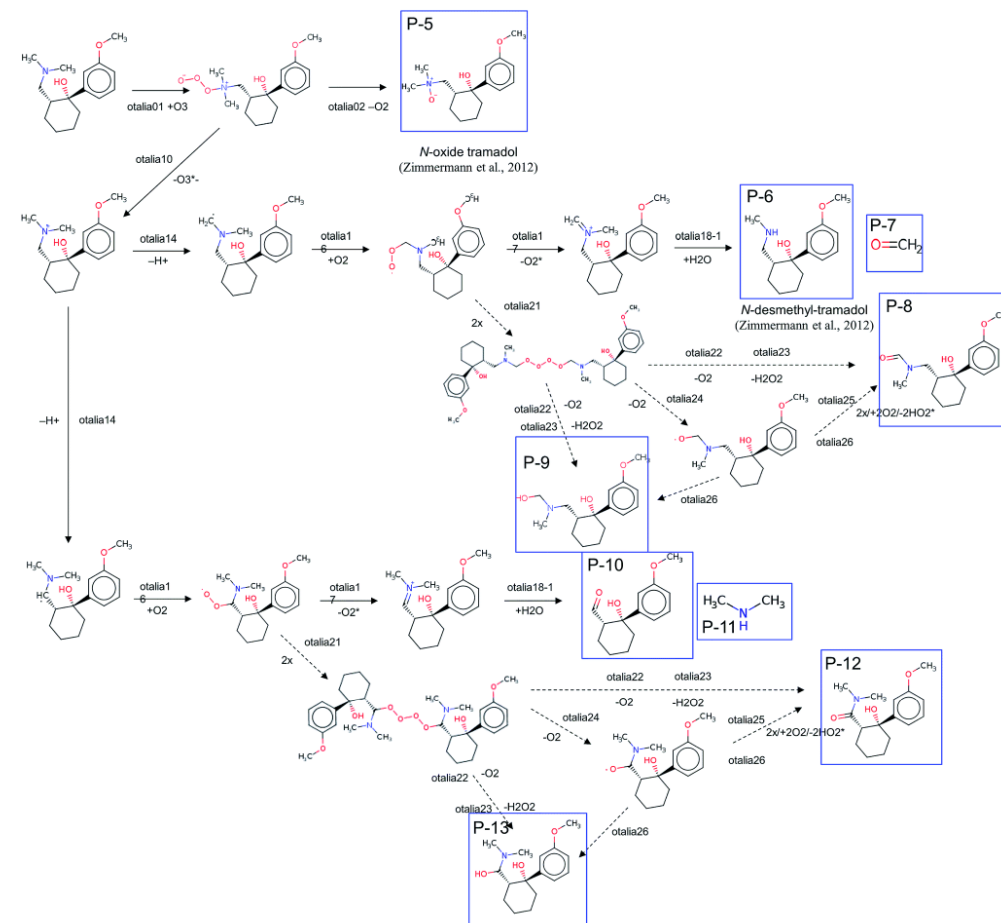
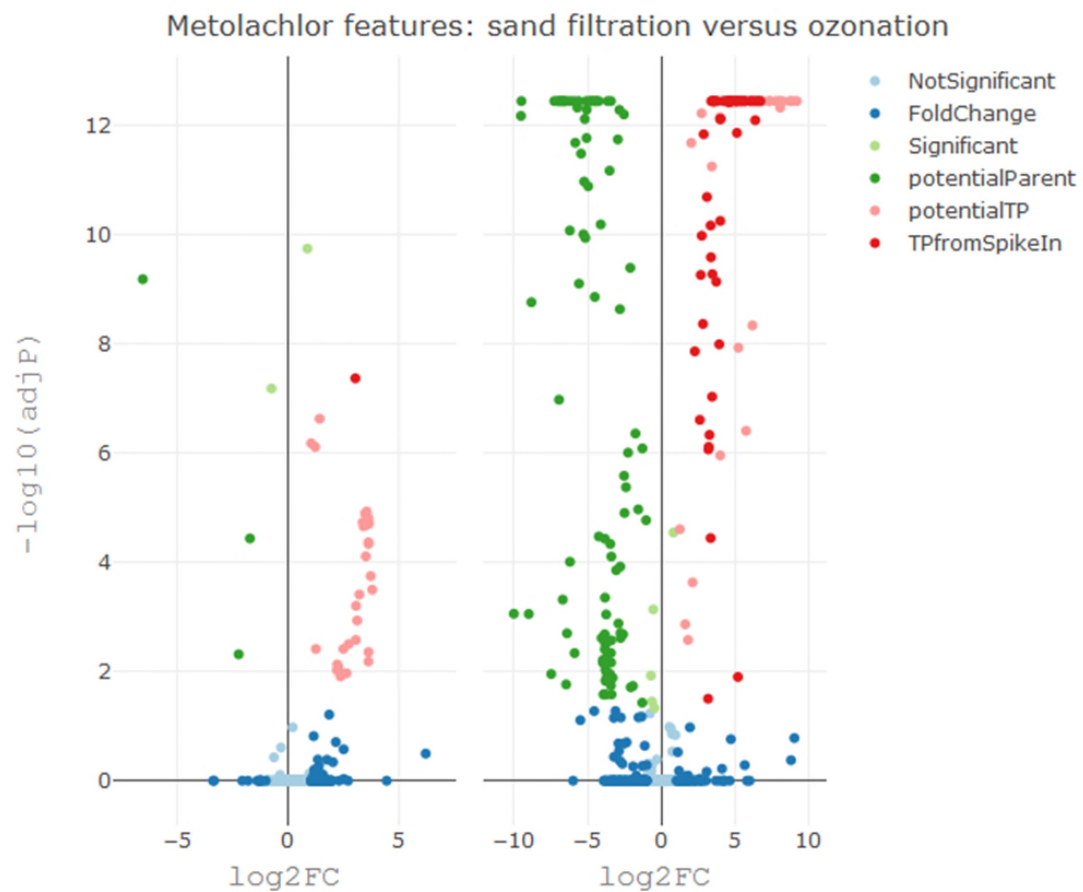
Brunner et al. (2018) JHazMat  
<https://doi.org/10.1016/j.jhazmat.2018.10.044>



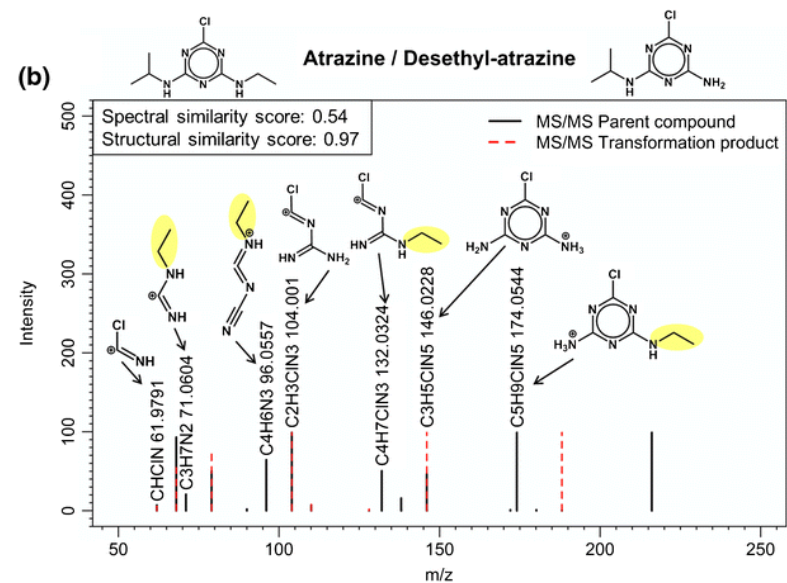
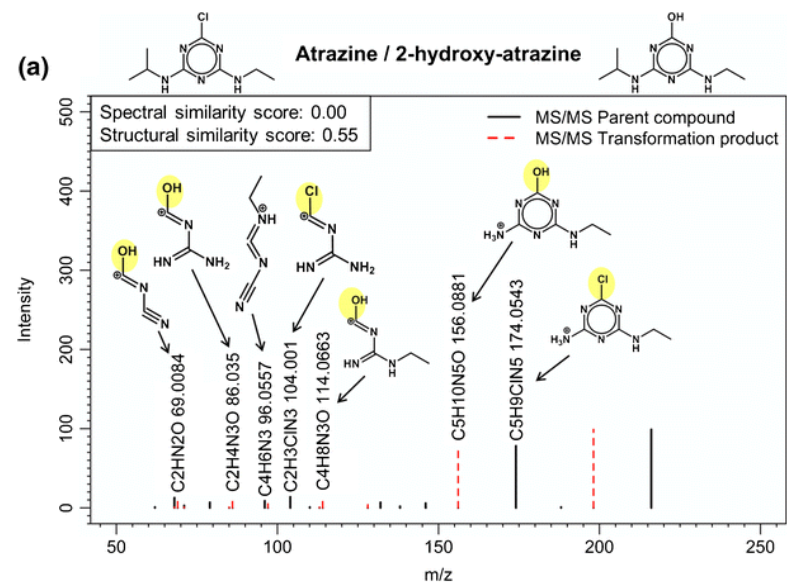
# (Virtual) effect directed analysis



# True unknown unknowns – Transformation products

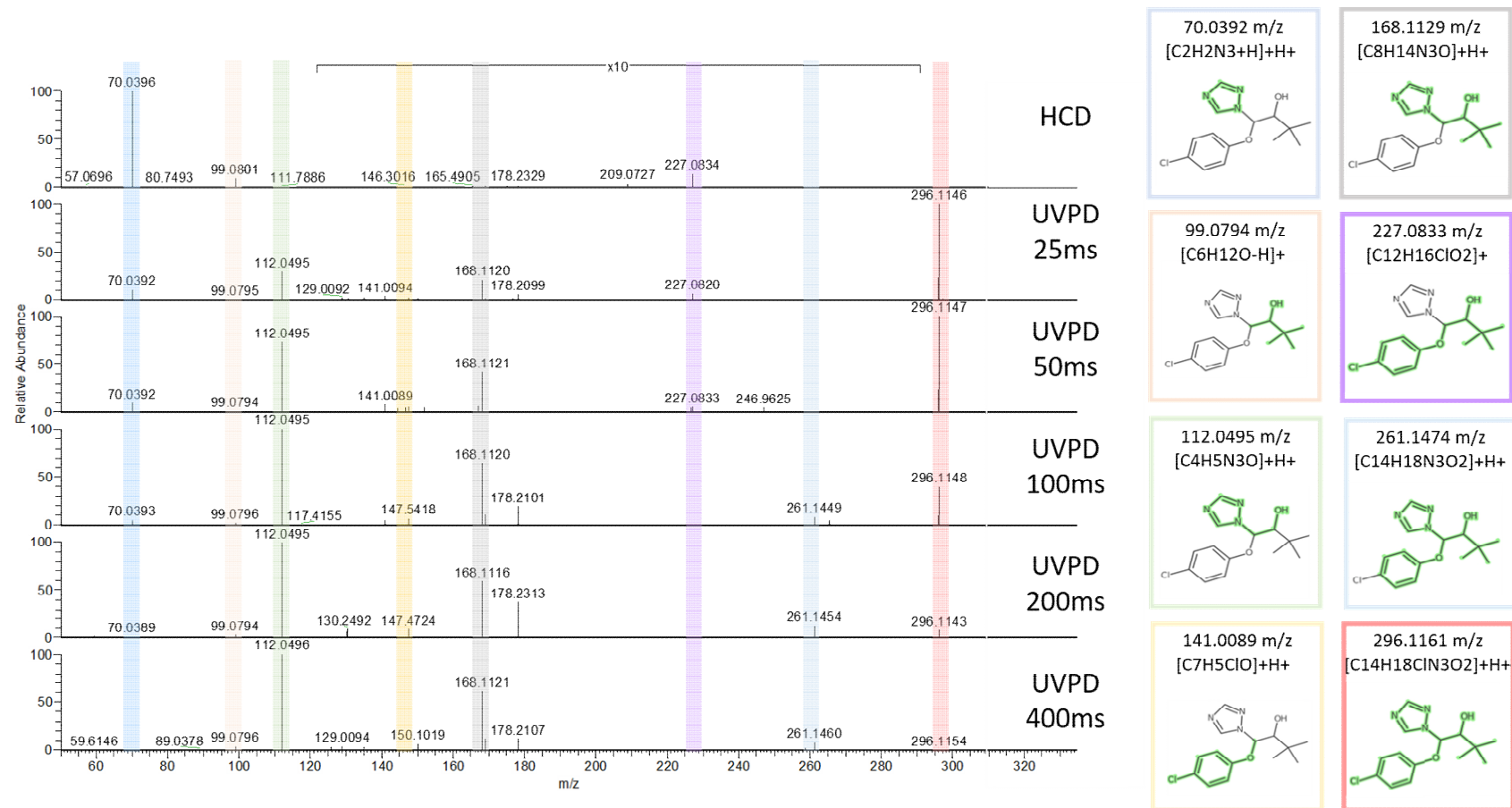


# Structural ~ spectral similarity

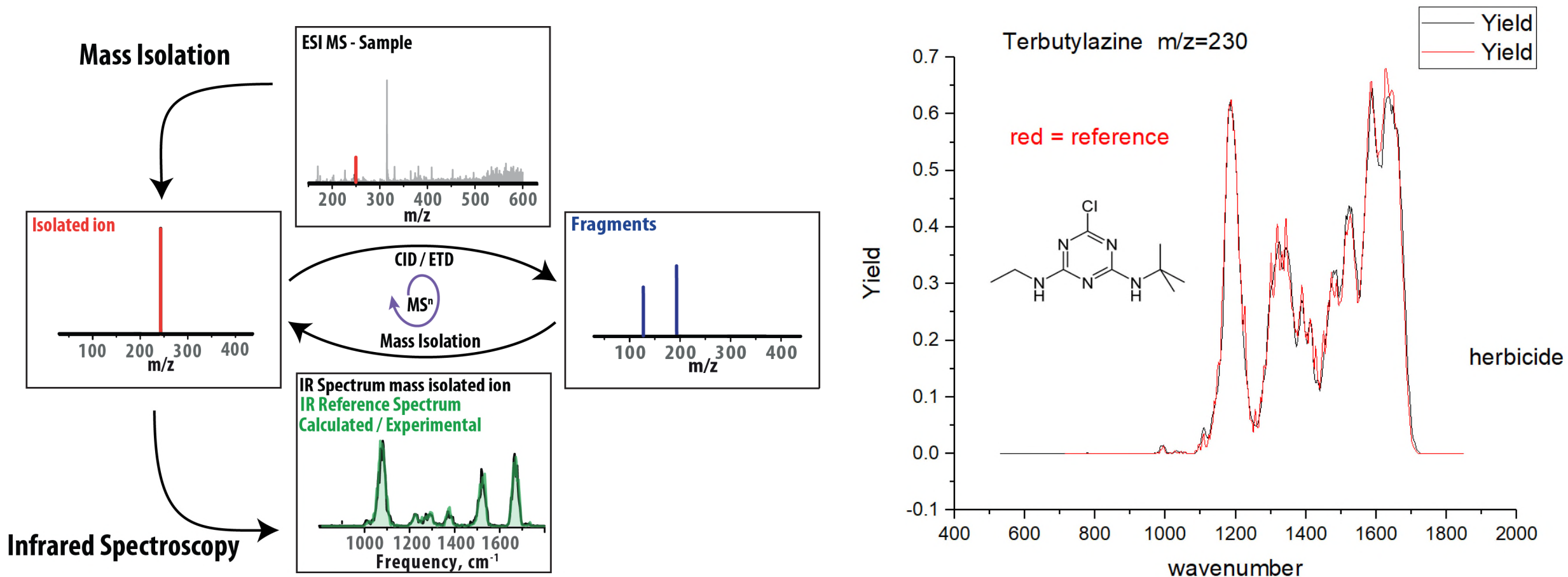


# Novel methods: Alternative fragmentation ultraviolet photodissociation

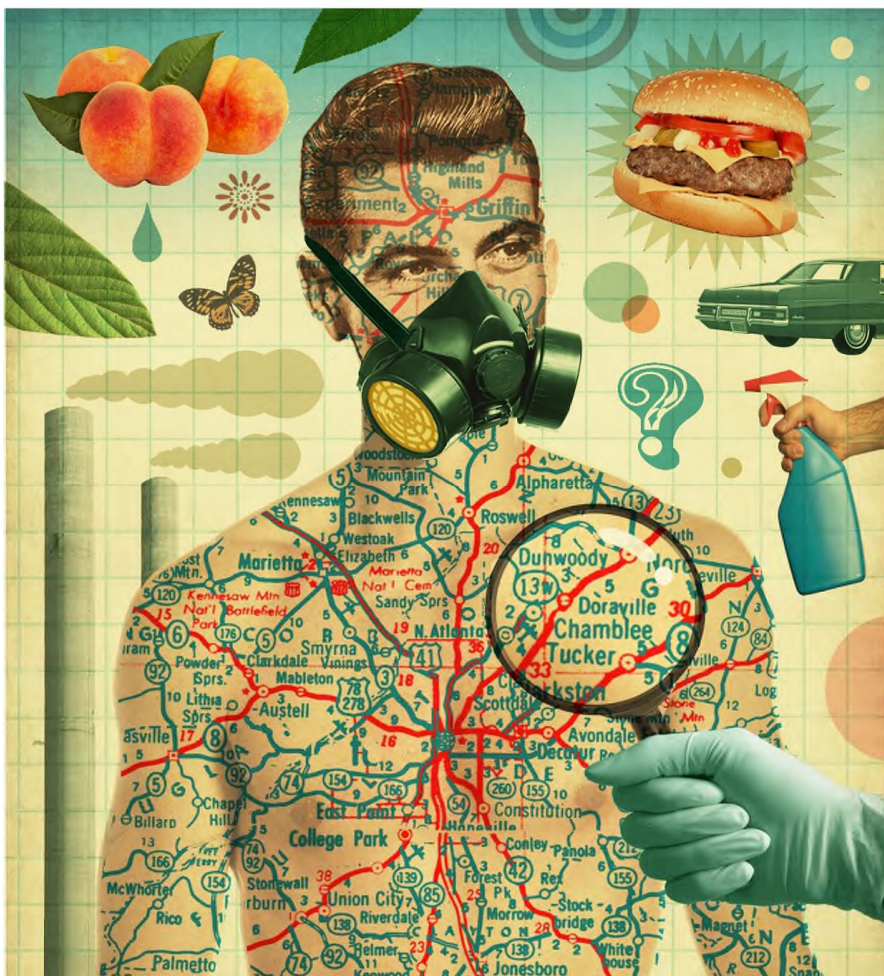
- 213nm laser implemented in Orbitrap Fusion Lumos
- potential to structurally elucidate compounds that cannot be identified by HCD
- Triadimenol



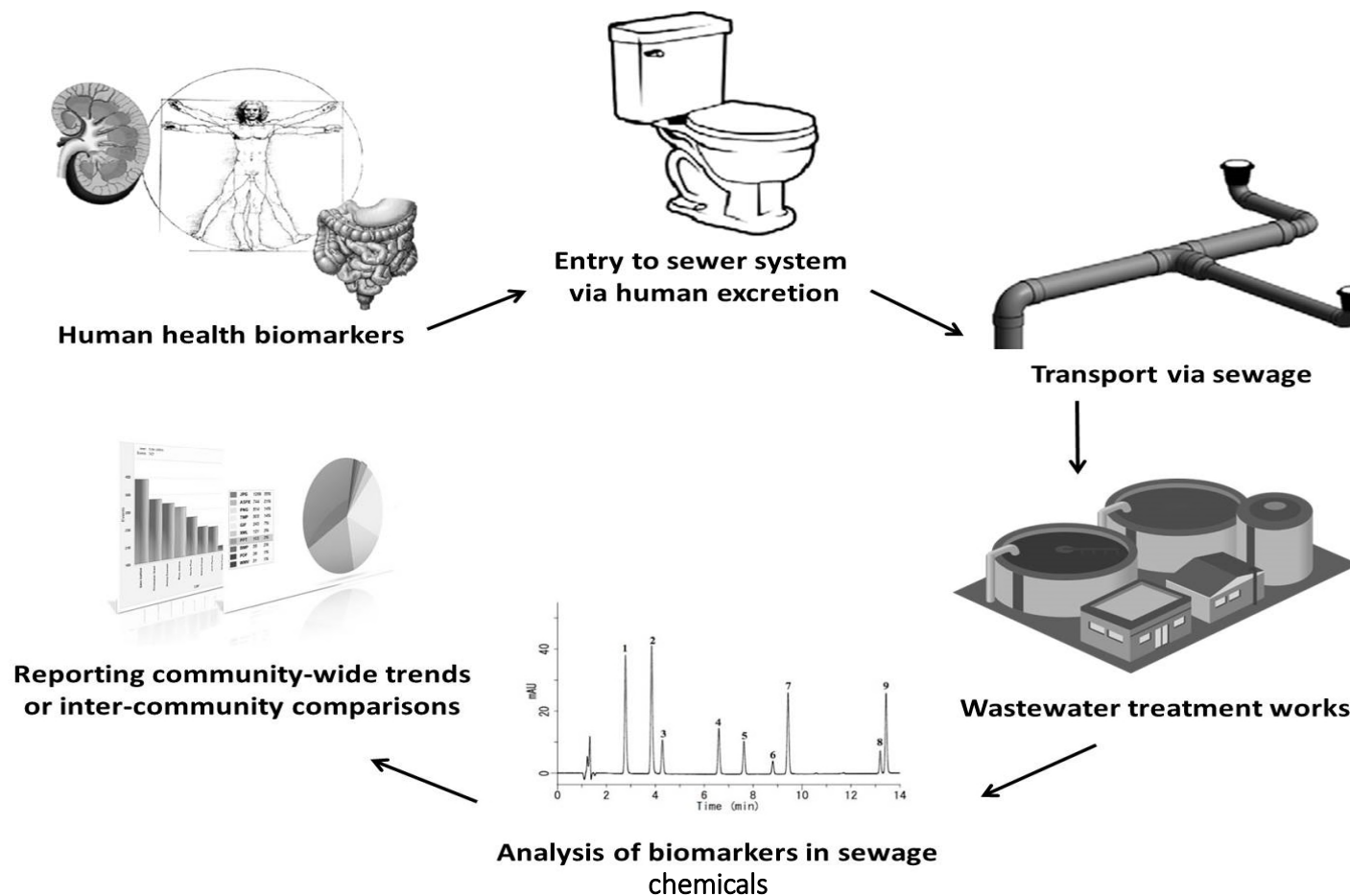
# Novel methods: Infrared Ion Spectroscopy coupled to MS

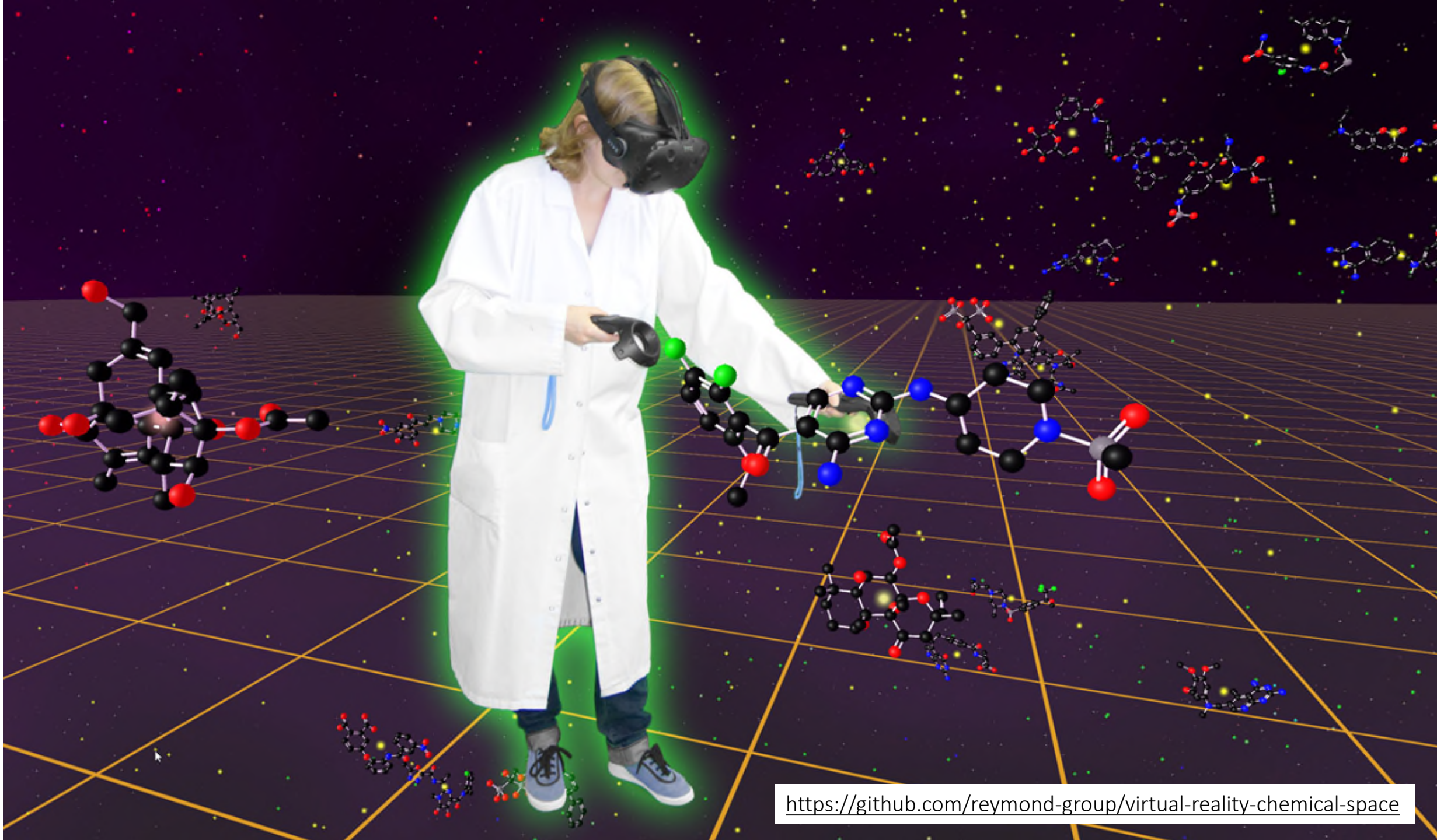


# Exposome – One Health



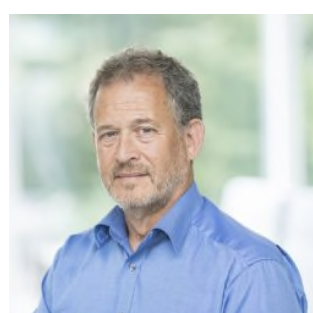
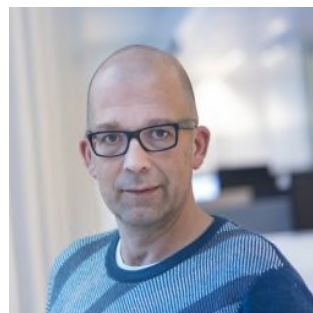
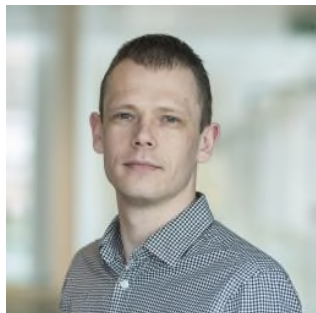
Mapping the exposome - Atlanta Magazine, Michael Waraksa





<https://github.com/reymond-group/virtual-reality-chemical-space>

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Thank you!







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[@KWR\\_Water](https://twitter.com/KWR_Water)



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 Andrea Mizzi Brunner

[Andrea.brunner@kwrwater.nl](mailto:Andrea.brunner@kwrwater.nl)

# Microplastics to nanoplastics



500 µm metal sieve



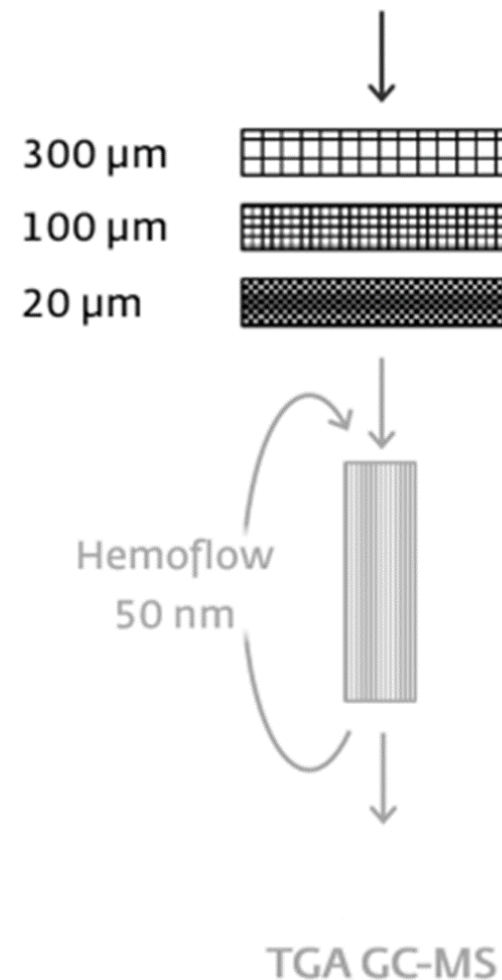
100 µm metal sieve



10 µm plankton net

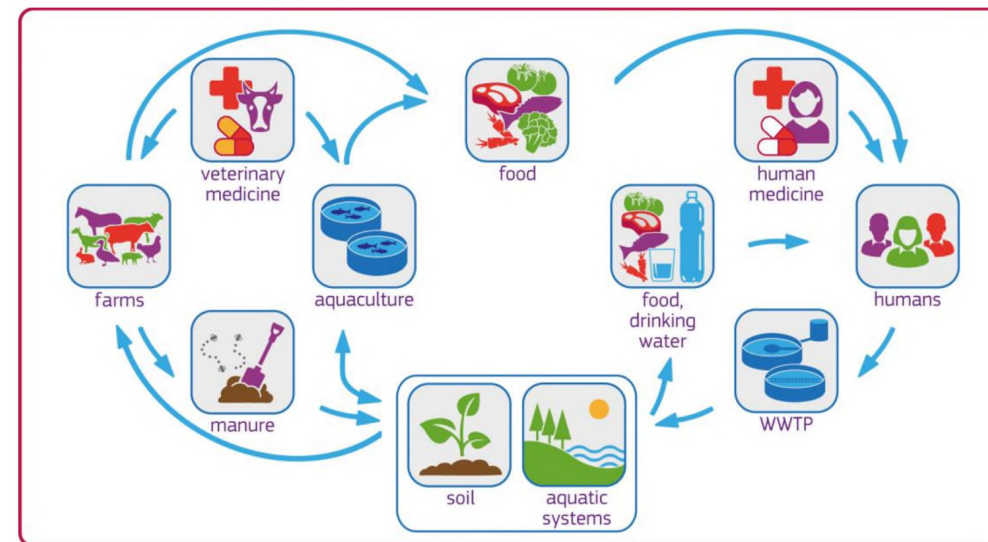
Laser directed infrared light

438 001  
438 030



# Antibiotics and antibiotics resistance

- Overuse and misuse of human and veterinary antimicrobials → selective pressure
- Main cause of death by 2050 (WHO)
- Spread of resistant bacteria and resistance genes
- Threat for the environment, including drinking water production



Concentrations of antibiotics in inland surface water all over the world (literature data)

