Fifty Shades of Filth, 23rd January 2020

The Next Big Thing in Environmental Chemistry?

Future challenges and opportunities

Andrea Mizzi Brunner

KWR

Bridging Science to Practice

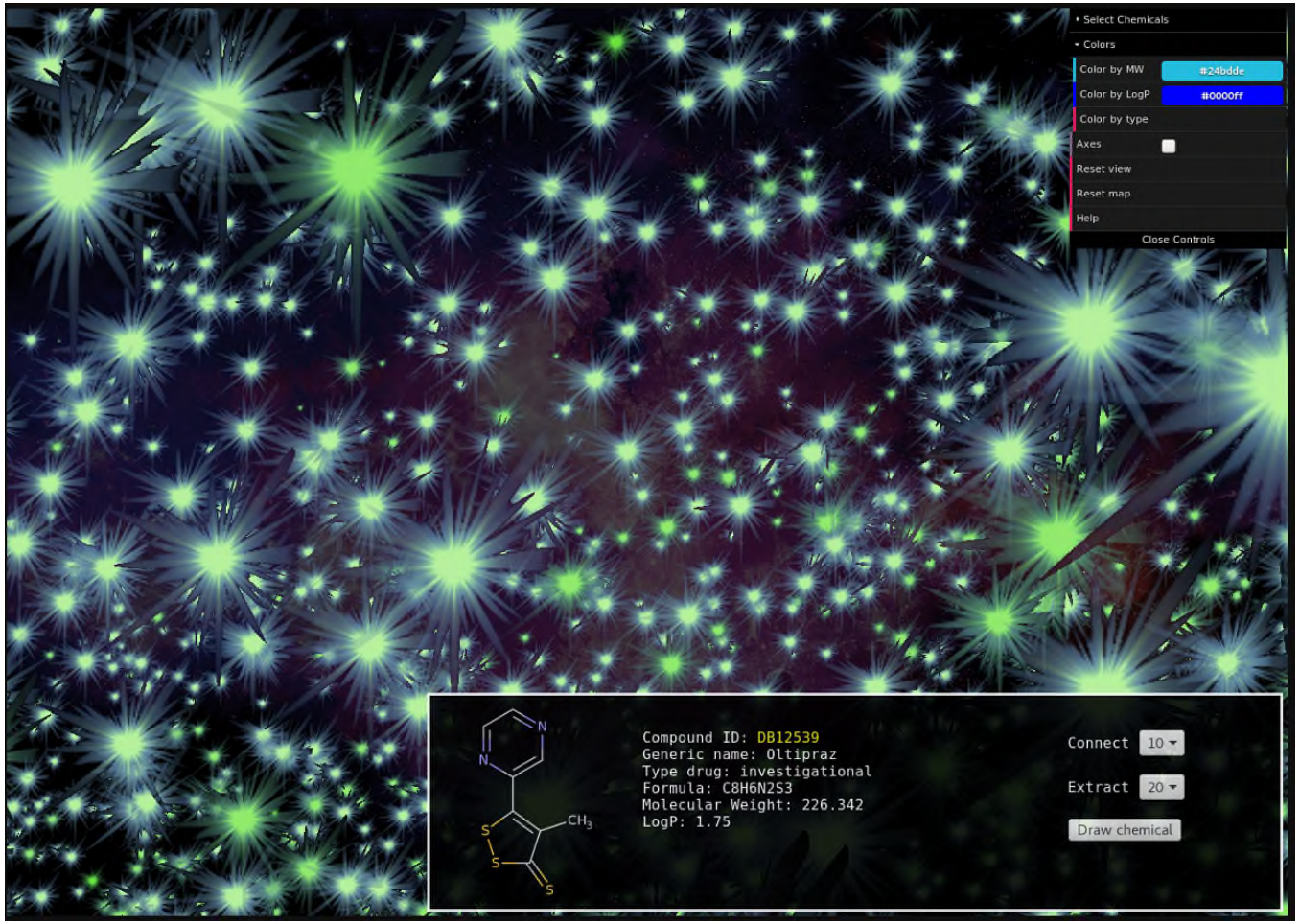
On-site monitoring of chemicals with automatic risk assessment

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



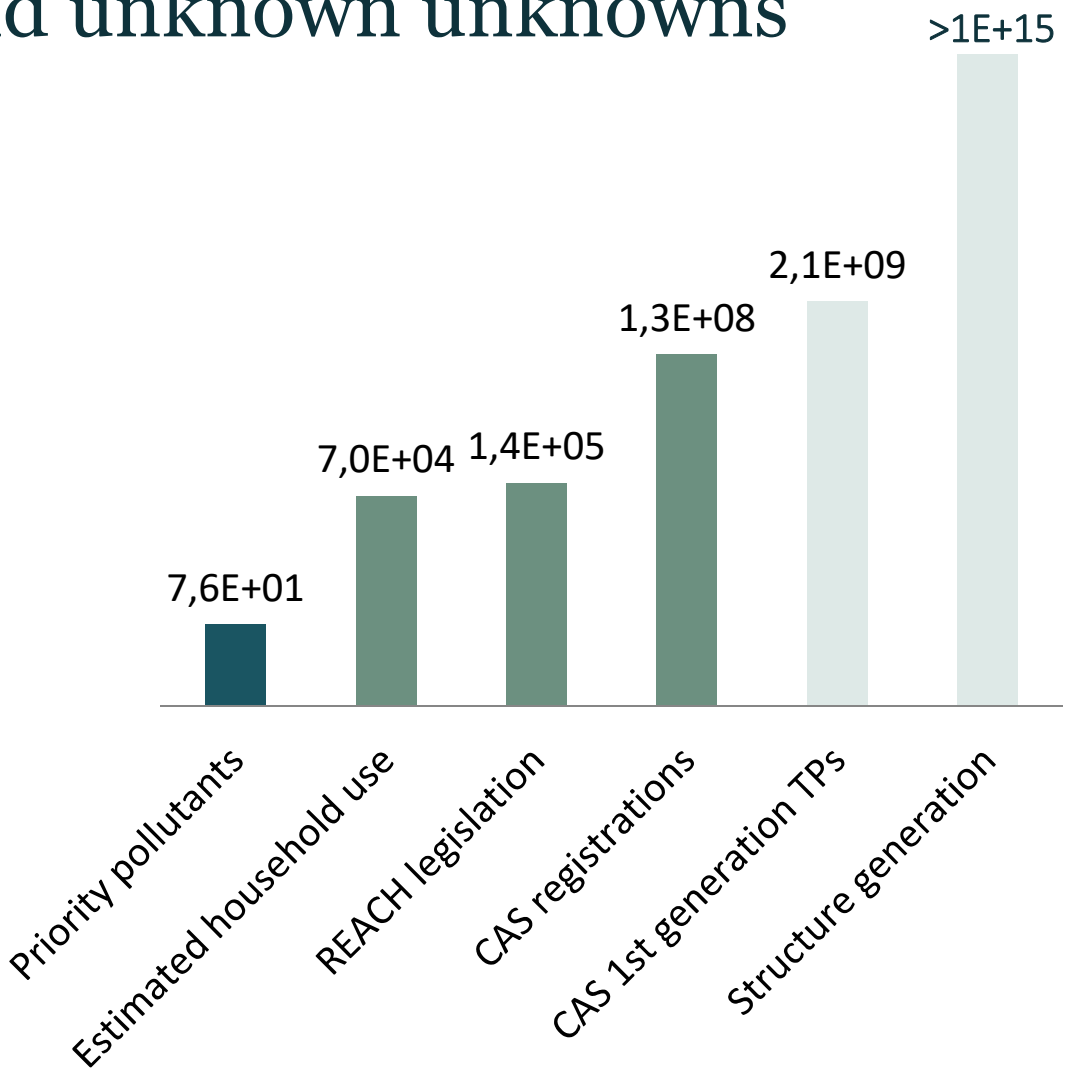
Borrel et al. (2018) Exploring drug space with ChemMaps.com. Bioinformatics
https://doi.org/10.1093/bioinformatics/bty412

Knowns, known unknowns and unknown unknowns

Target Screening

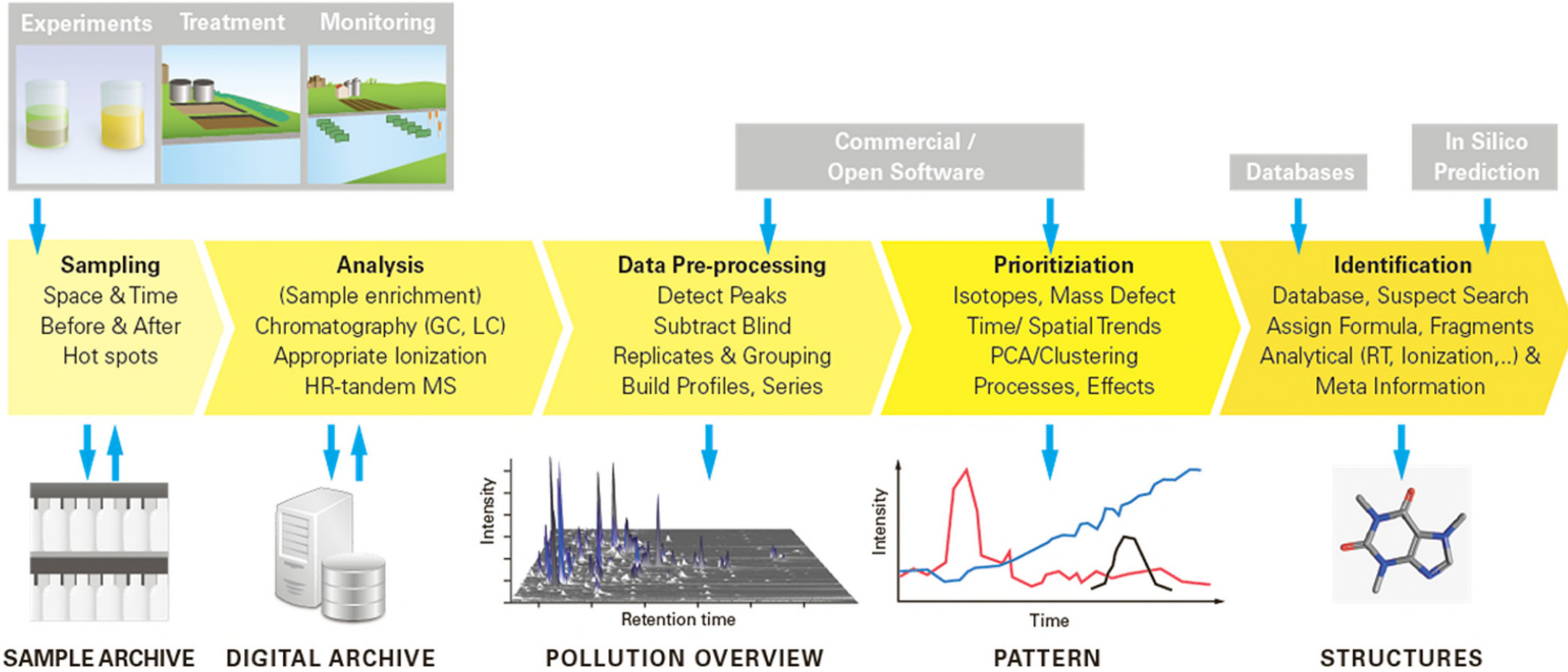
Suspect Screening

Non-target Screening



Hollender et al. (2017) ES&T
https://doi.org/10.1021/acs.est.7b02184

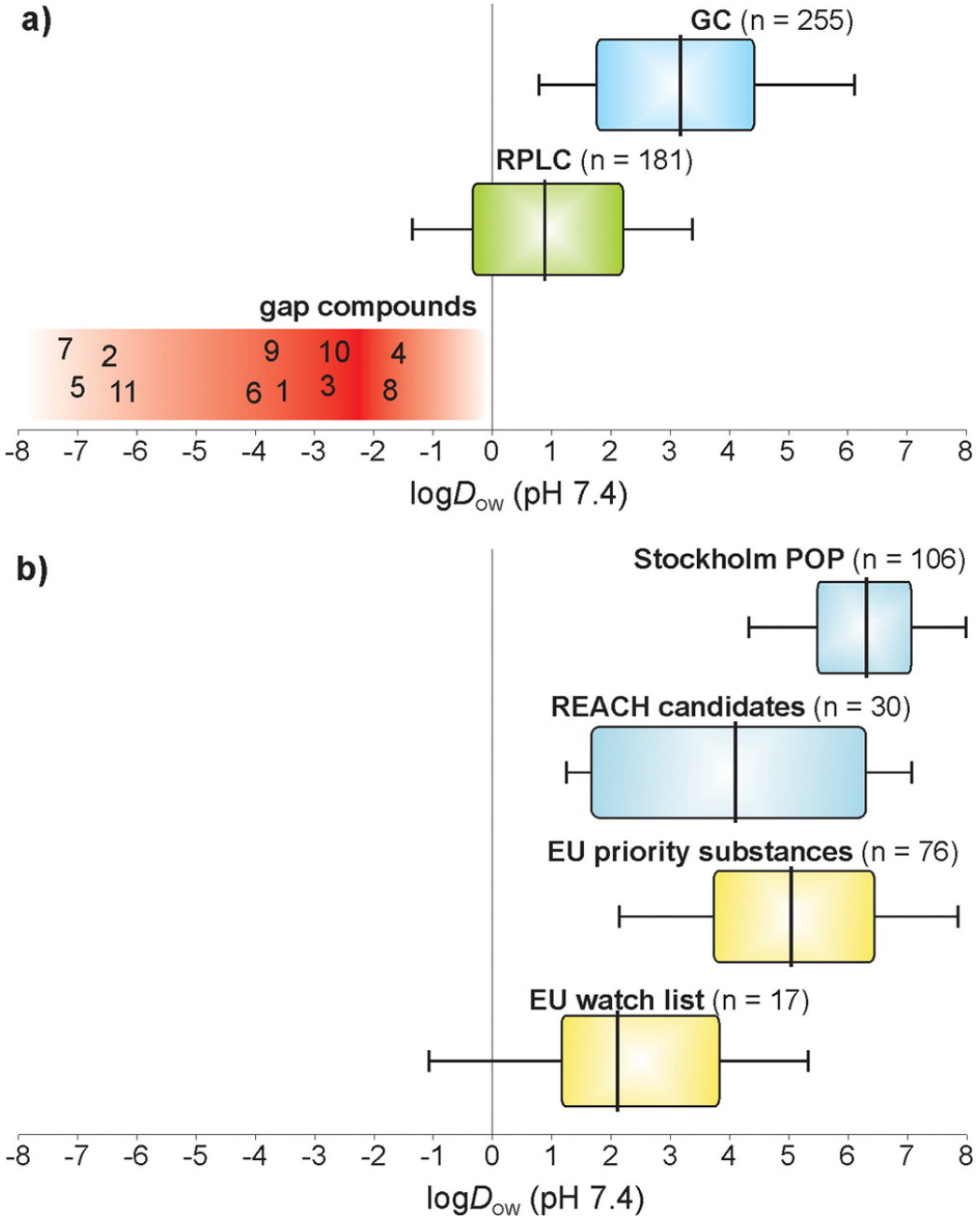
Non-target screening with High Resolution Mass Spectrometry in the Environment



Hollender et al. (2017) ES&T
https://doi.org/10.1021/acs.est.7b02184

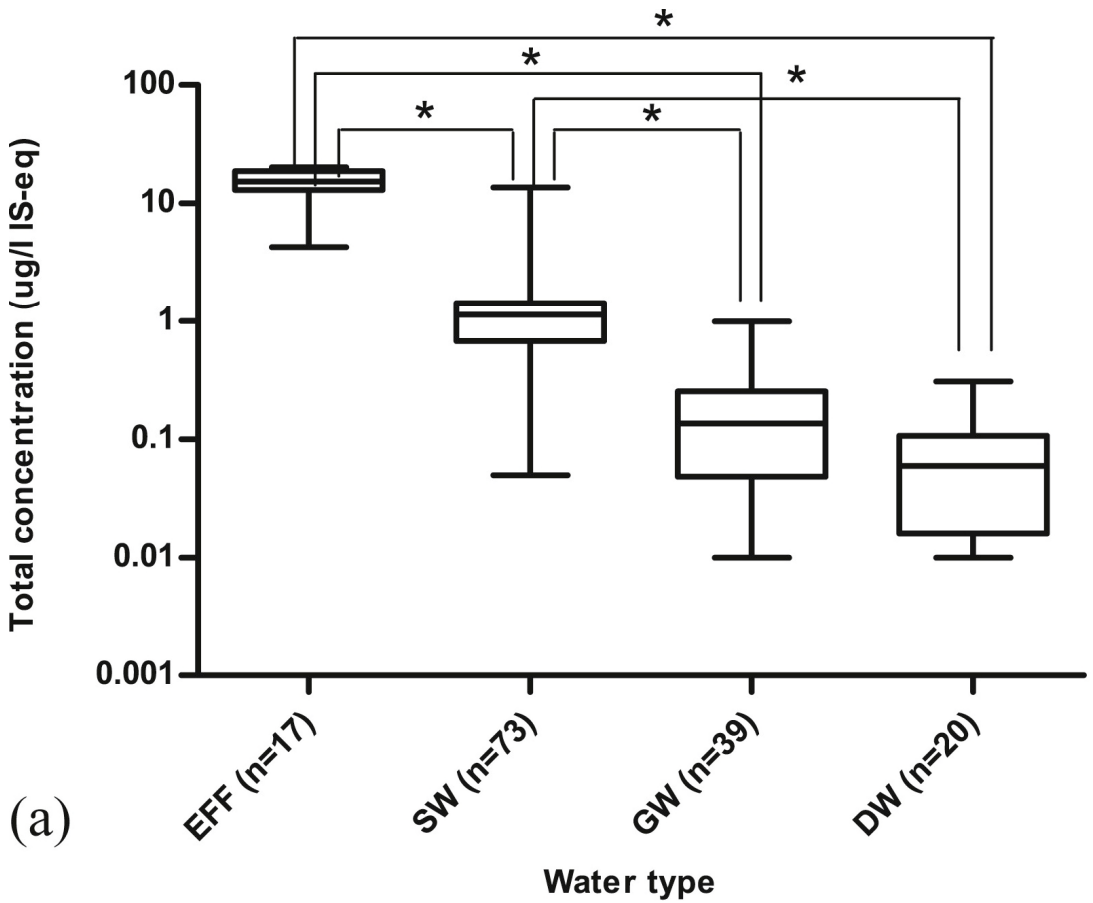
Mind the gap

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

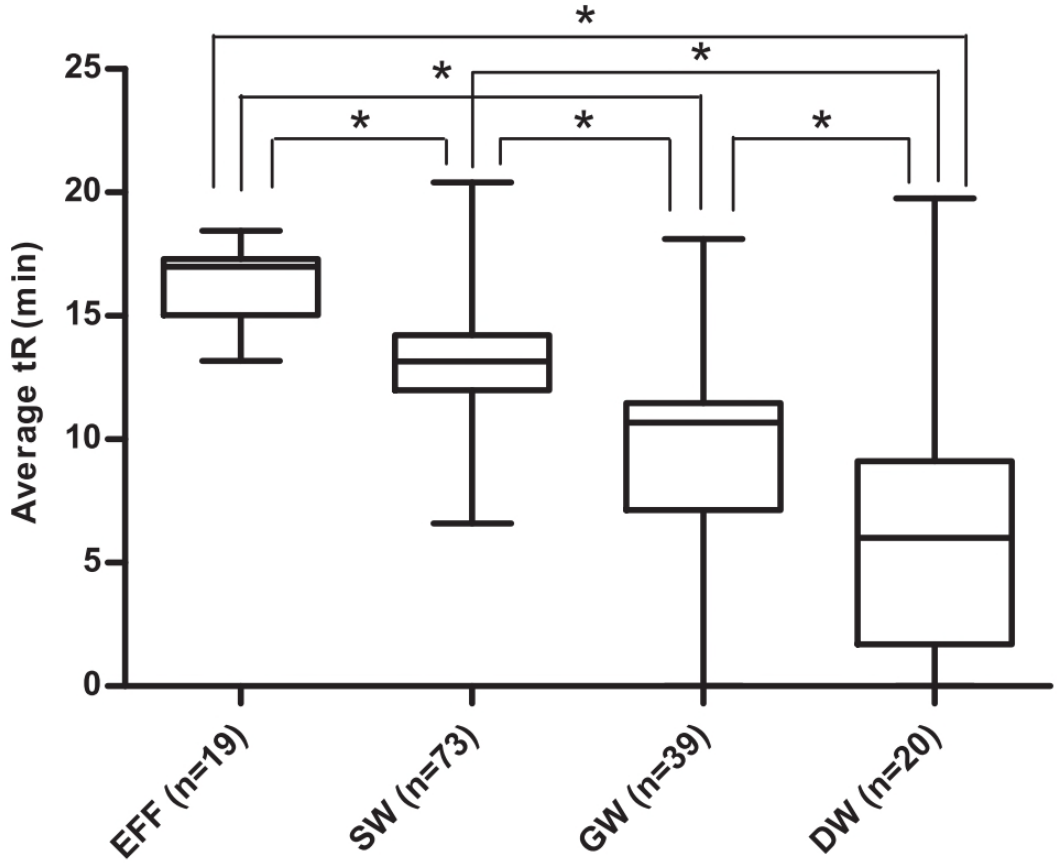


Reemtsma et al. (2016) ES&T
https://doi.org/10.1021/acs.est.6b03338

Shift from non-polar to polar environmental contaminants

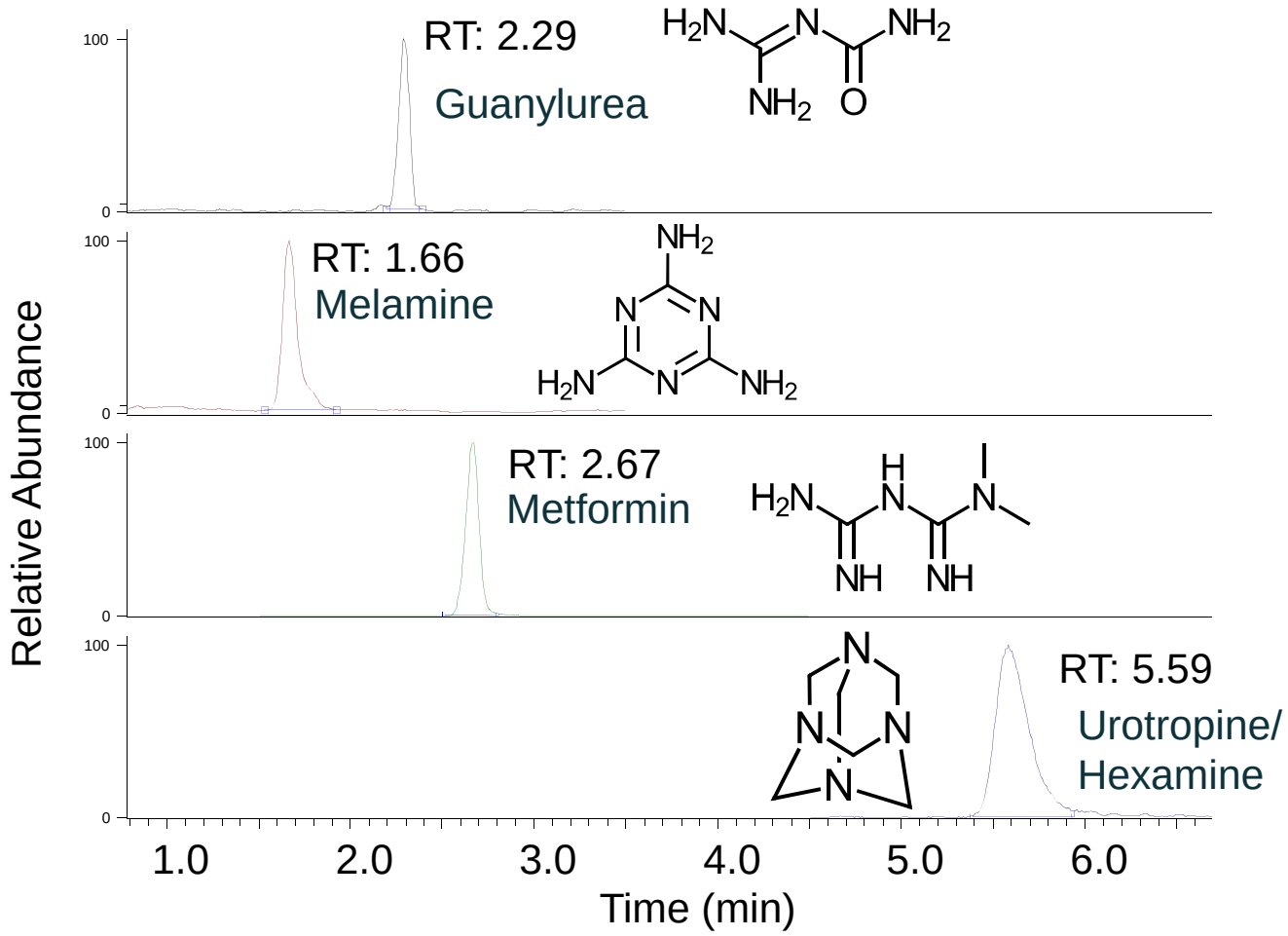


(a)



Sjerps et al. (2016) Water Research
https://doi.org/10.1016/j.watres.2016.02.034

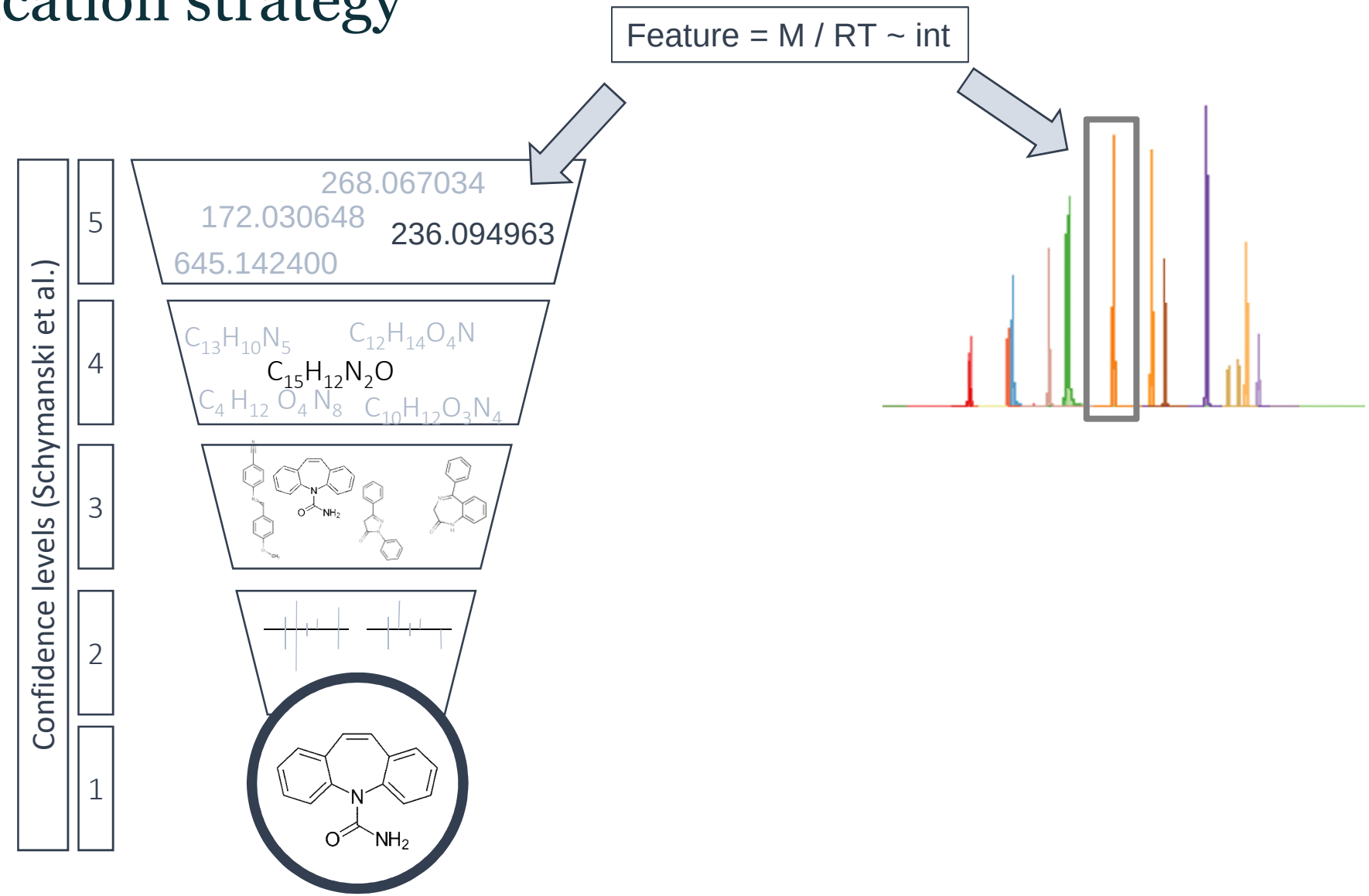
Screening for very polar compounds



Alternative chromatographies:

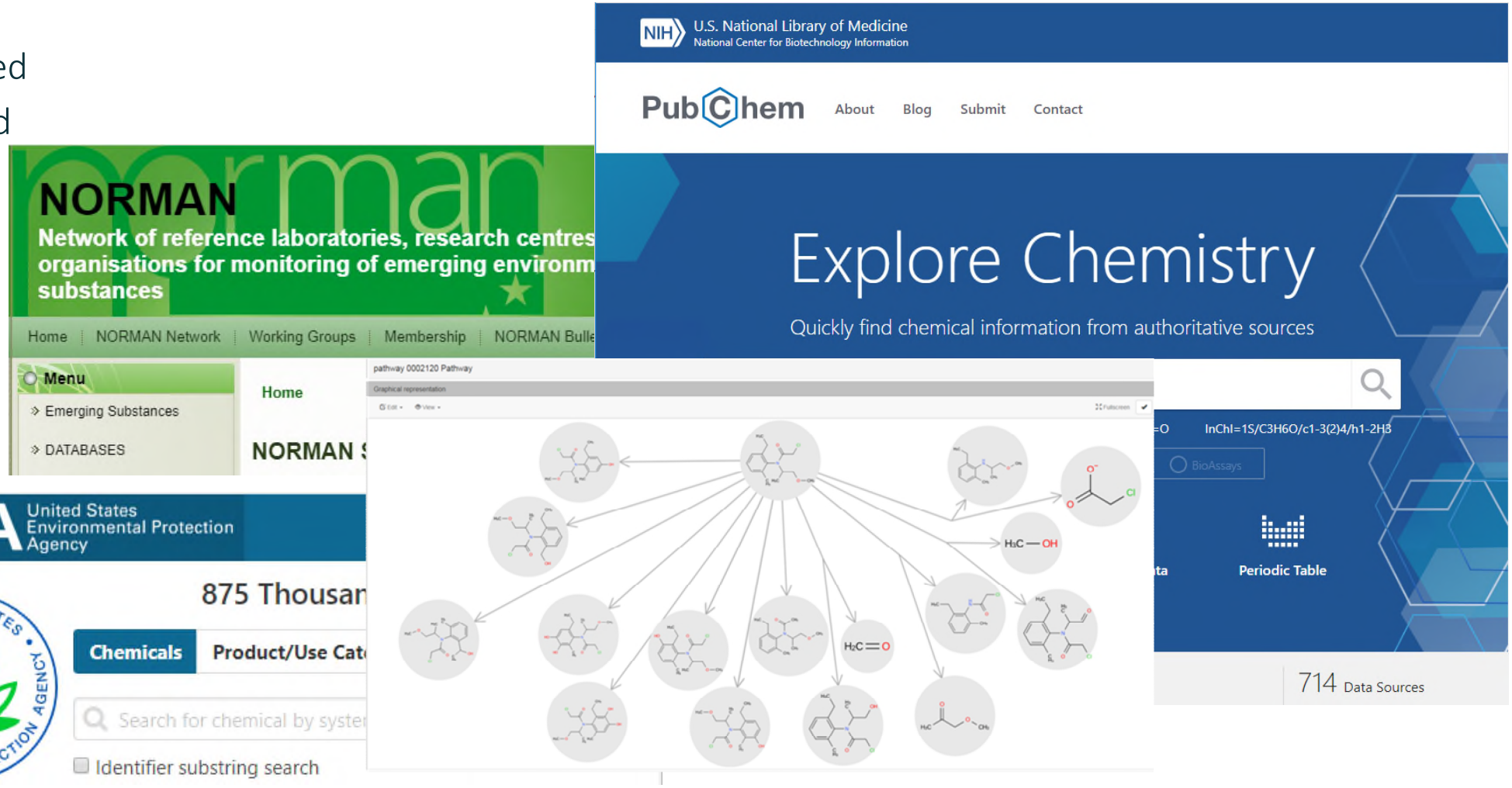
- HILIC
- Mixed mode

Identification strategy

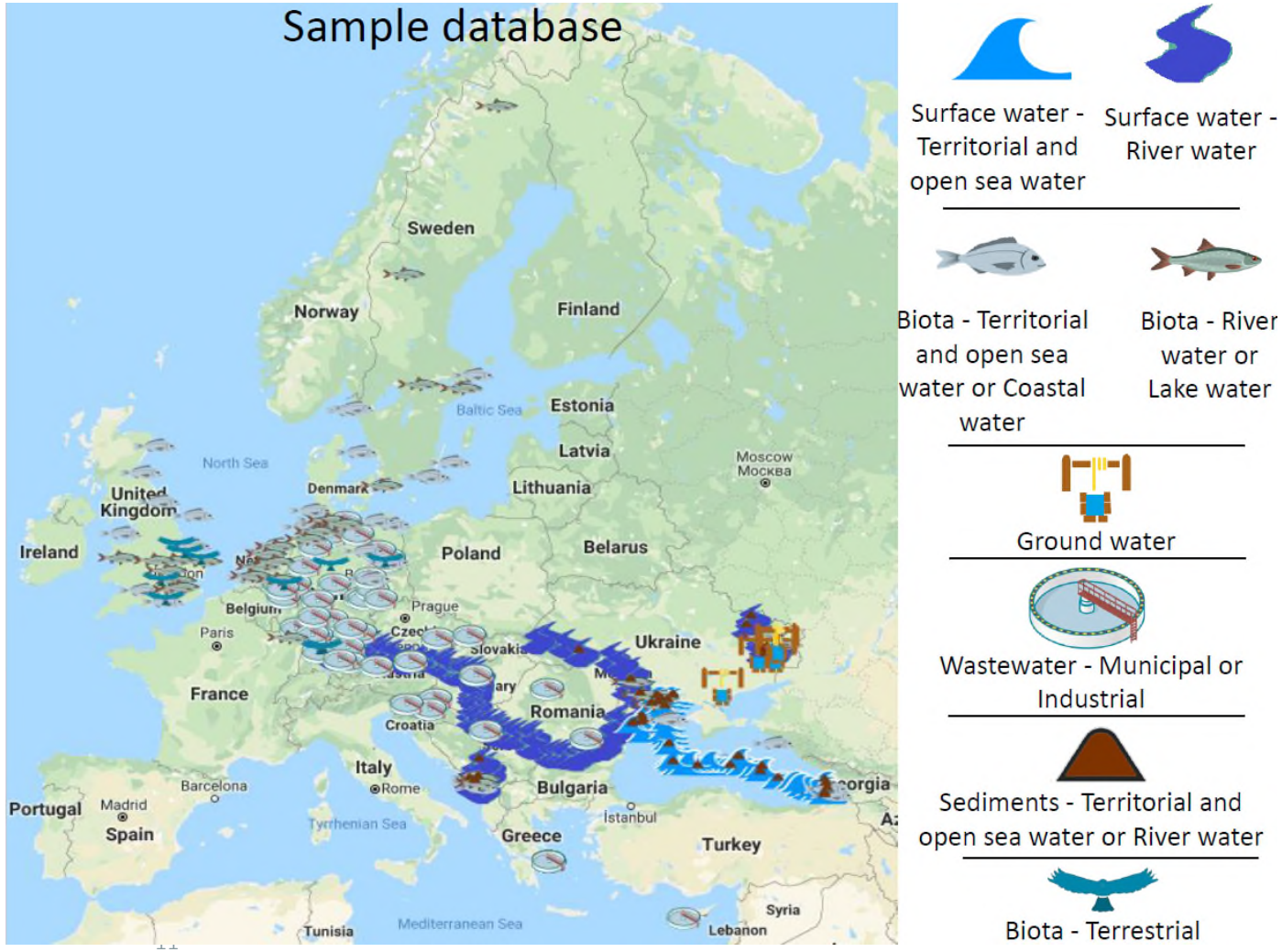


Suspect screening meets non-target screening through larger and larger suspect lists

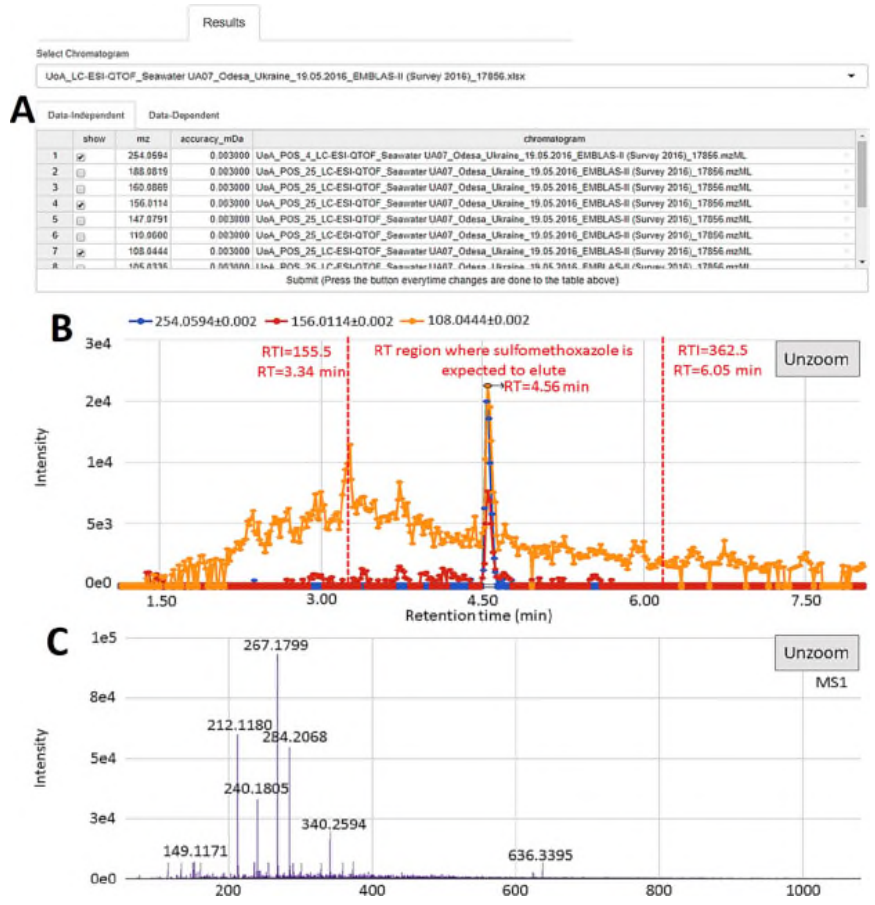
- Registered
- Predicted



Automated suspect screening in data repositories



Digital Sample Freezing Platform (NORMAN)

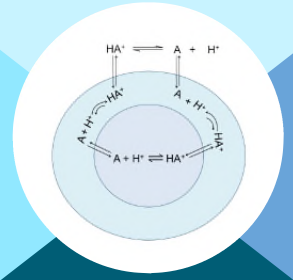


Alygizakis et al. (2010) TrAC
https://doi.org/10.1016/j.trac.2019.04.008

Making non-target screening quantitative

Solvent
Organic solvent %
pH
Additive type

Compound
Hydrophibicity
pKa

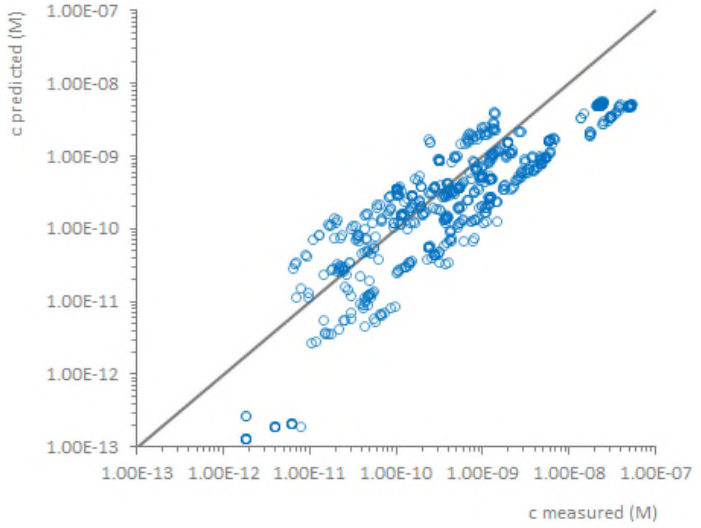


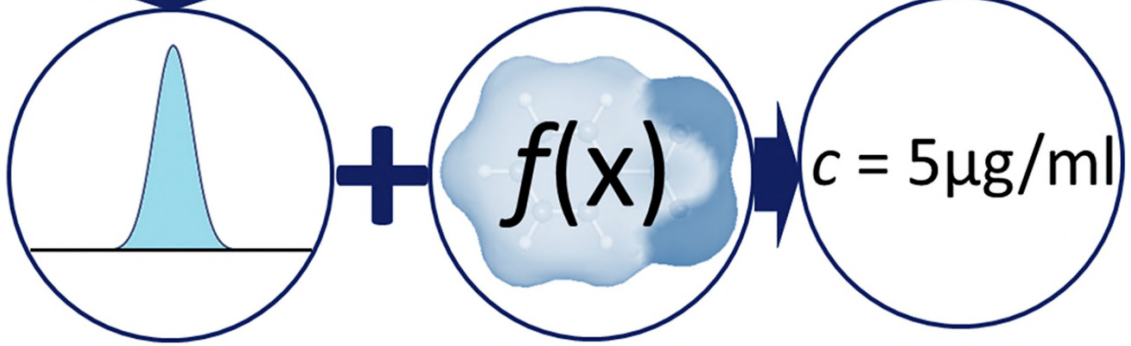
Matrix
Similar order of compounds
Good correlation

Instrument
Similar order of compounds
Good correlation

Ionization Efficiency (IE)

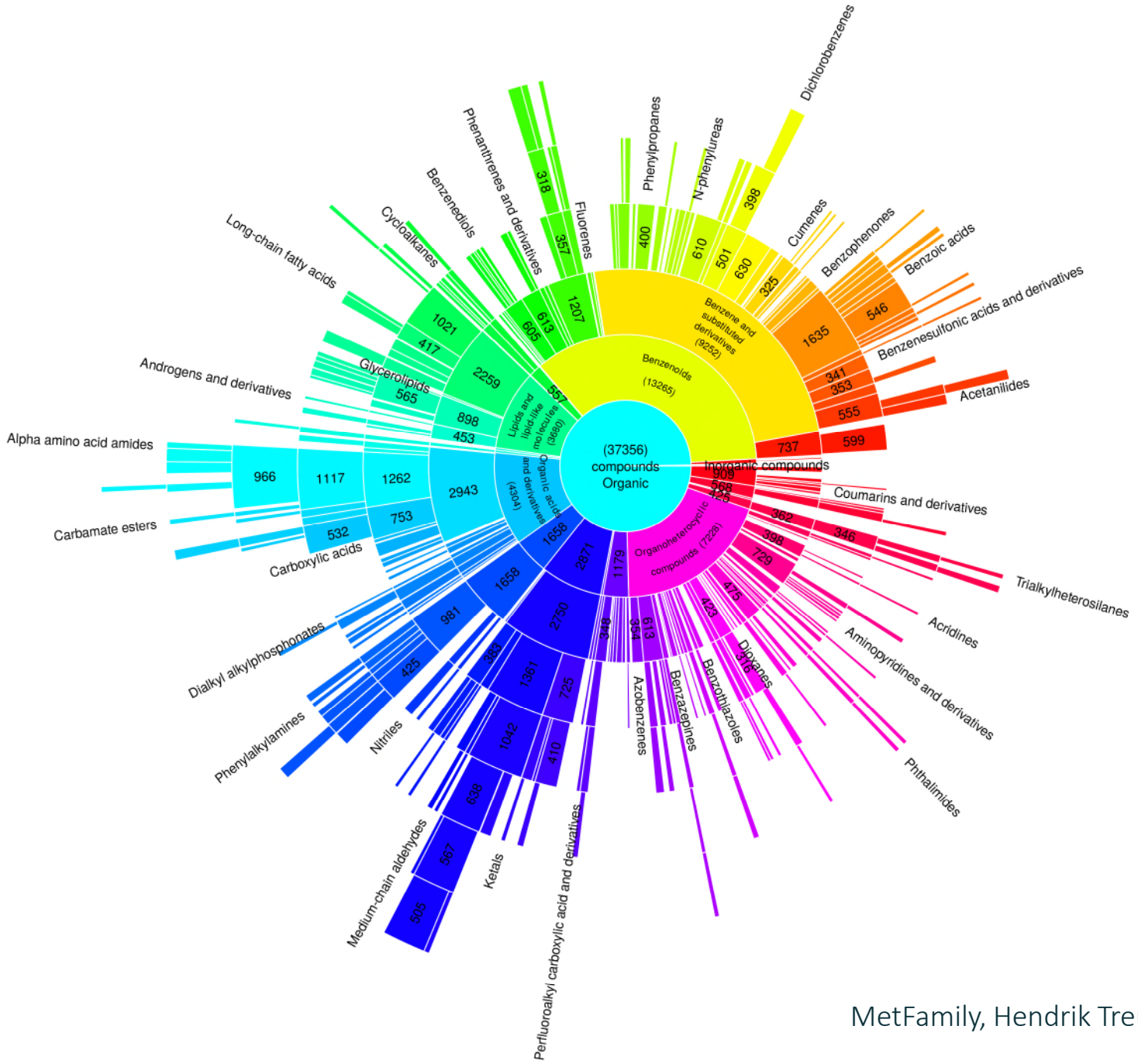
PRELIMINARY RESULTS



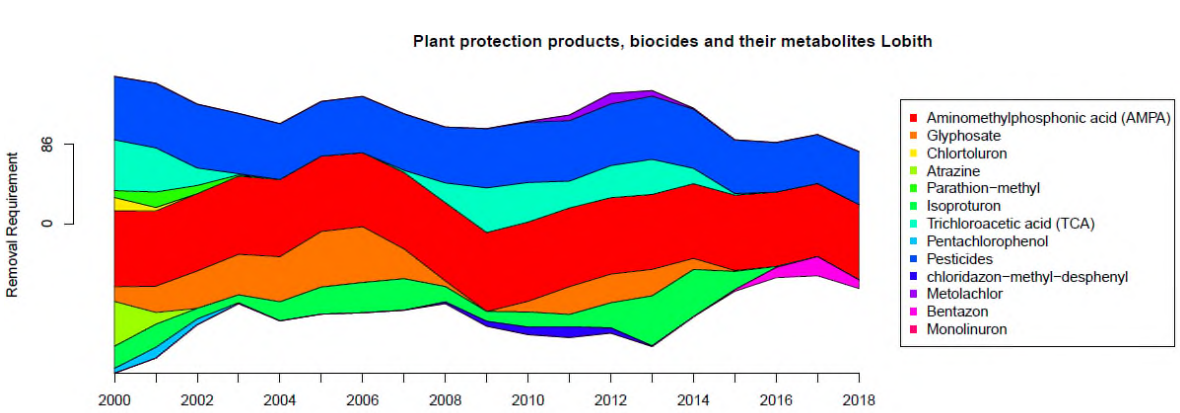


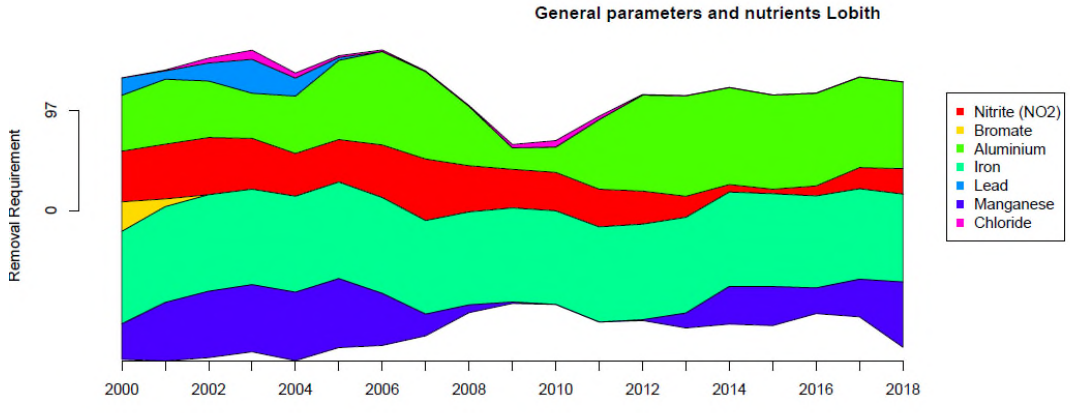
Kruve (2019) Rapid Communications in Mass Spectrometry
https://doi.org/10.1002/rcm.8208

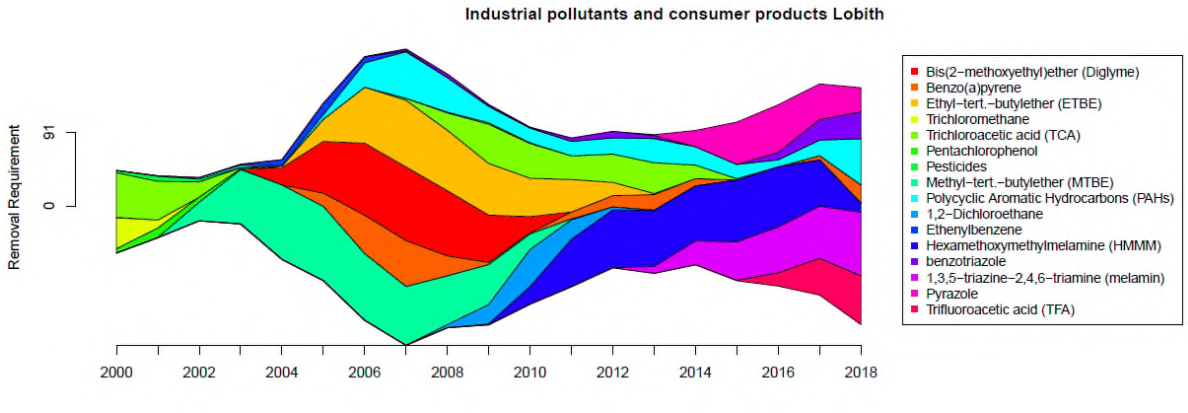
Cheminformatics

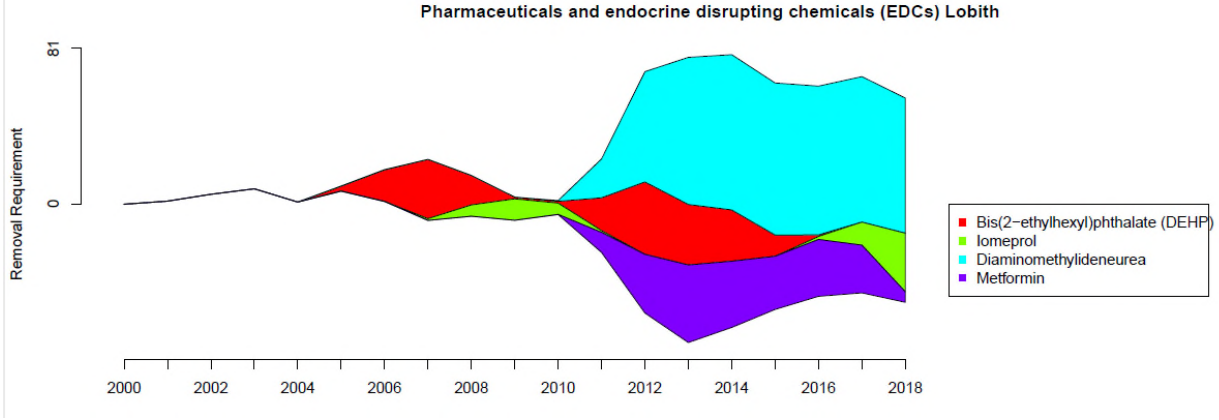


Data science



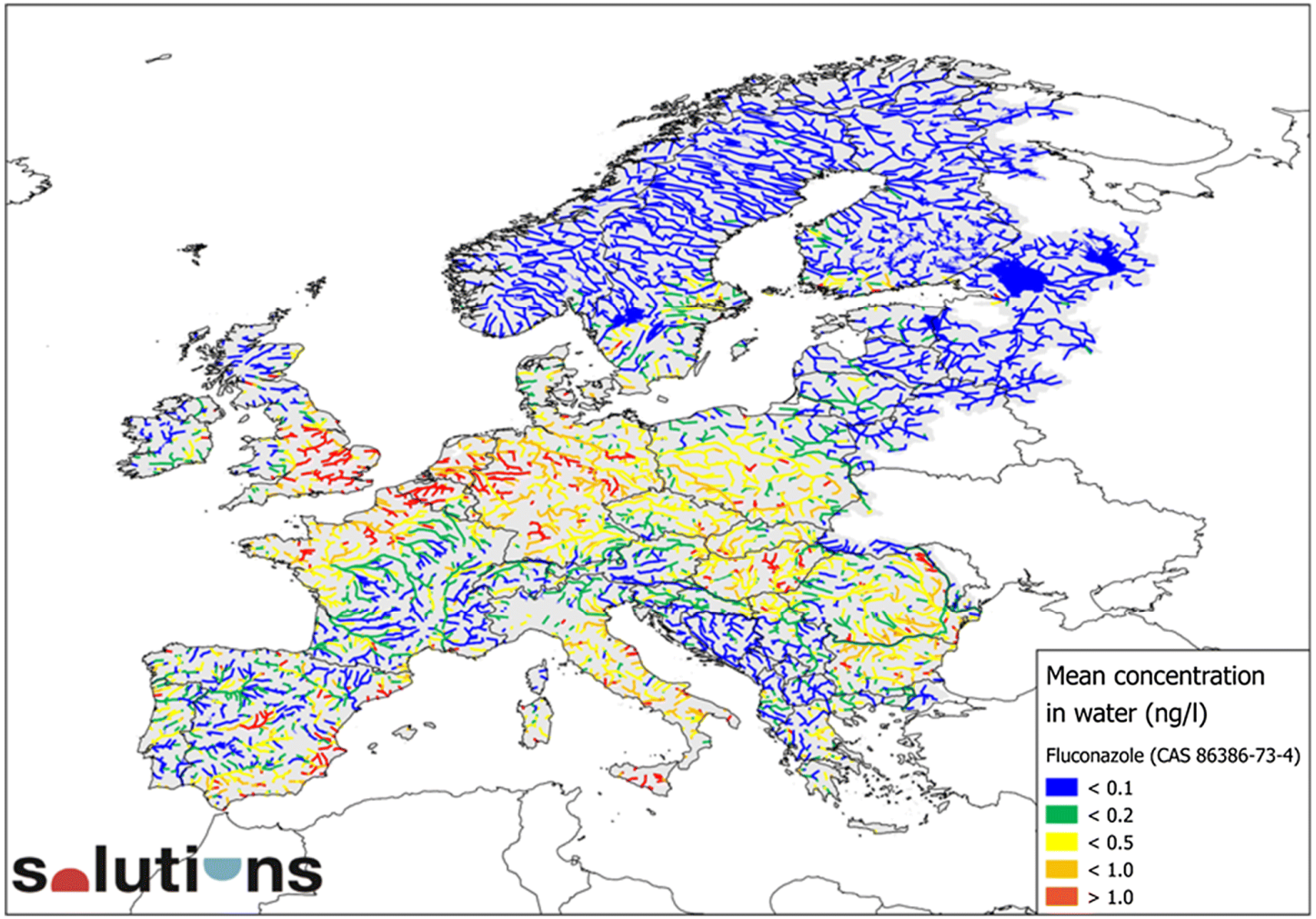






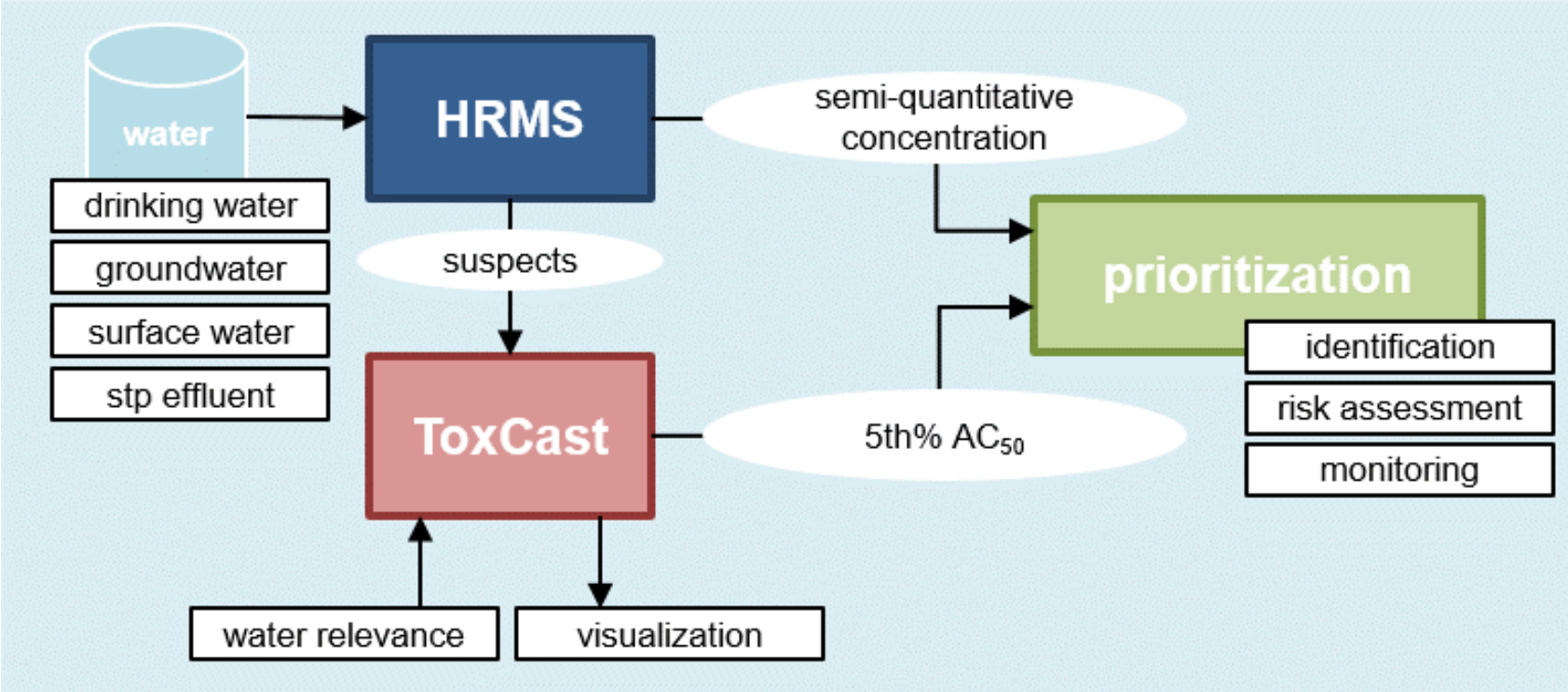
Water purification index, Tessa Pronk

Modelling instead of measurement data



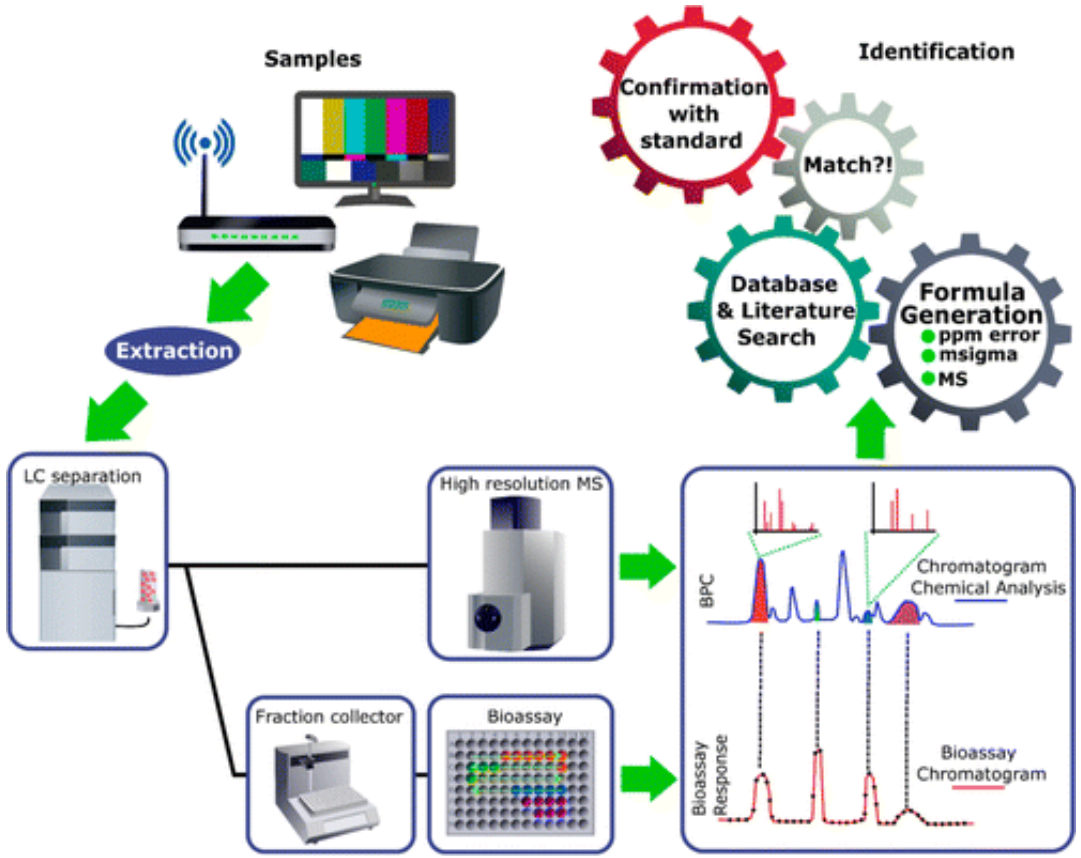
Van Gils et al. (2019) Environ Sci Eur
https://doi.org/10.1186/s12302-019-0248-3

Focus on compounds that pose a risk

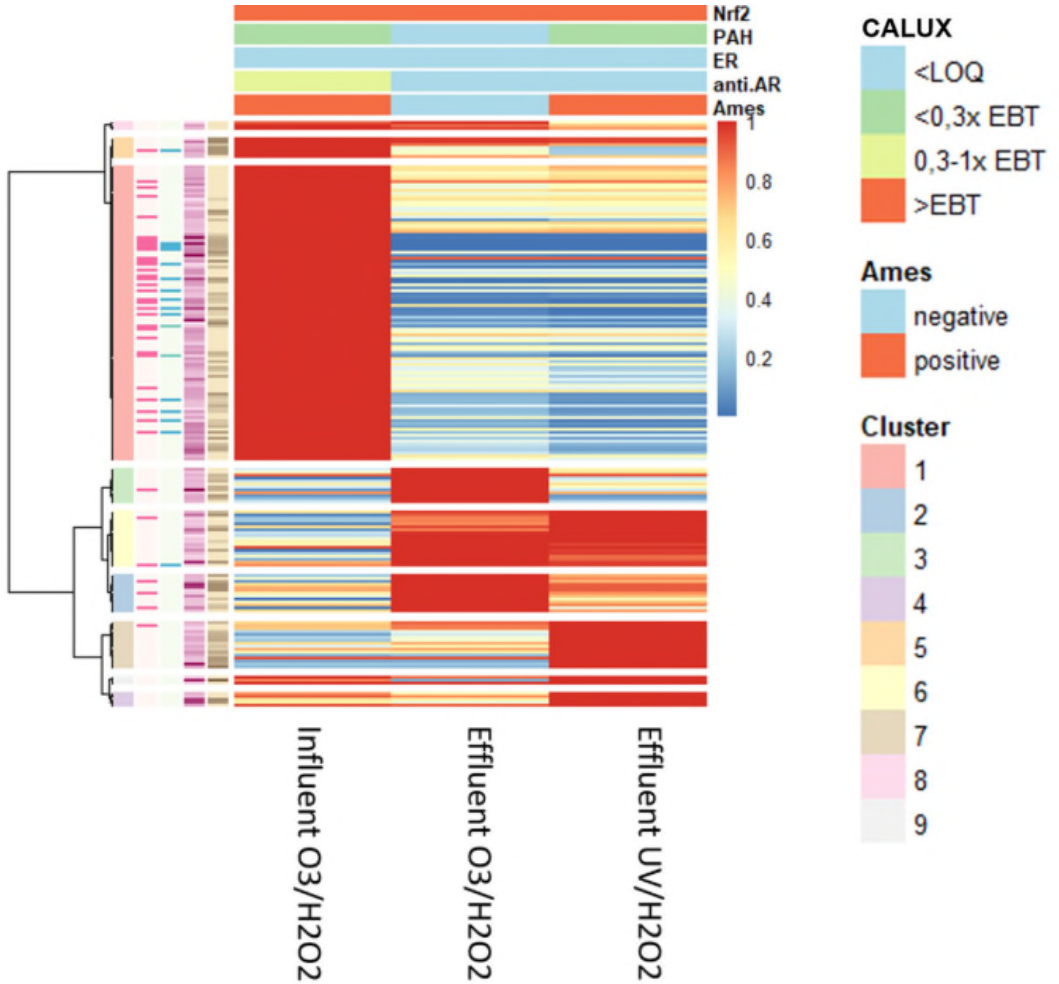


Brunner et al. (2018) JHazMat
https://doi.org/10.1016/j.jhazmat.2018.10.044

(Virtual) effect directed analysis

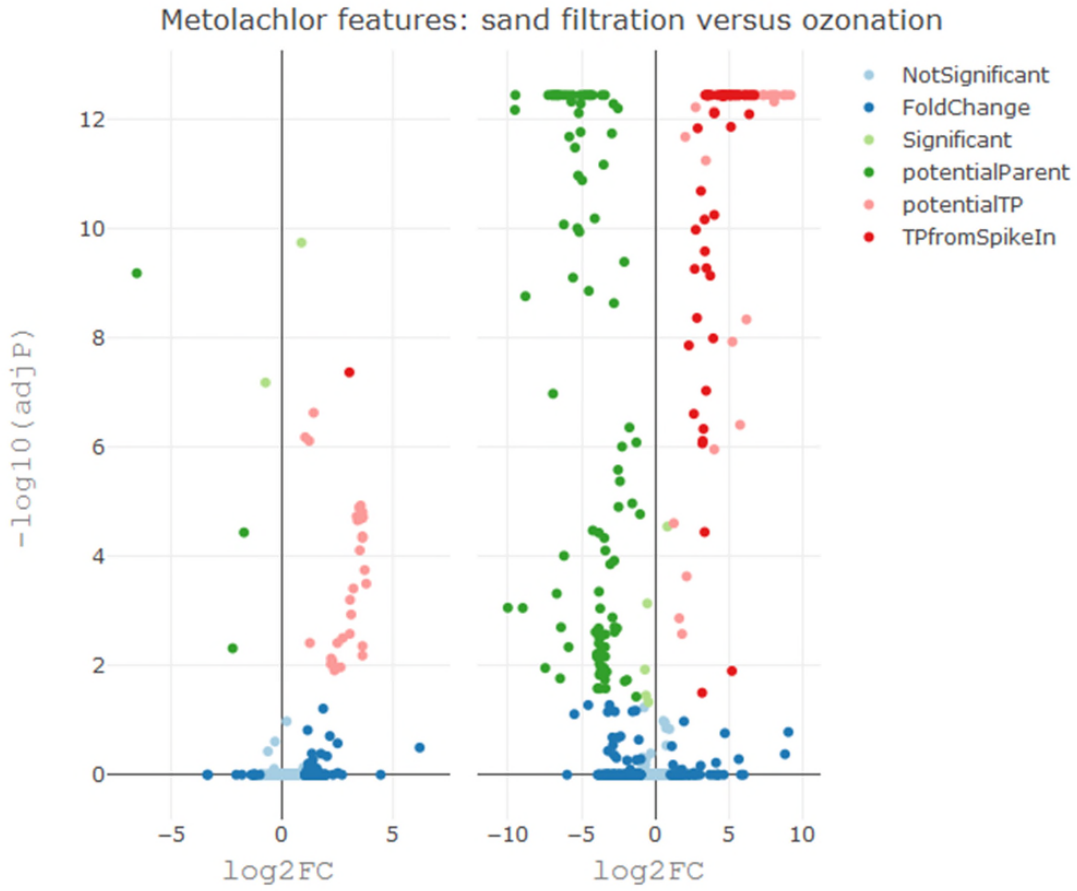


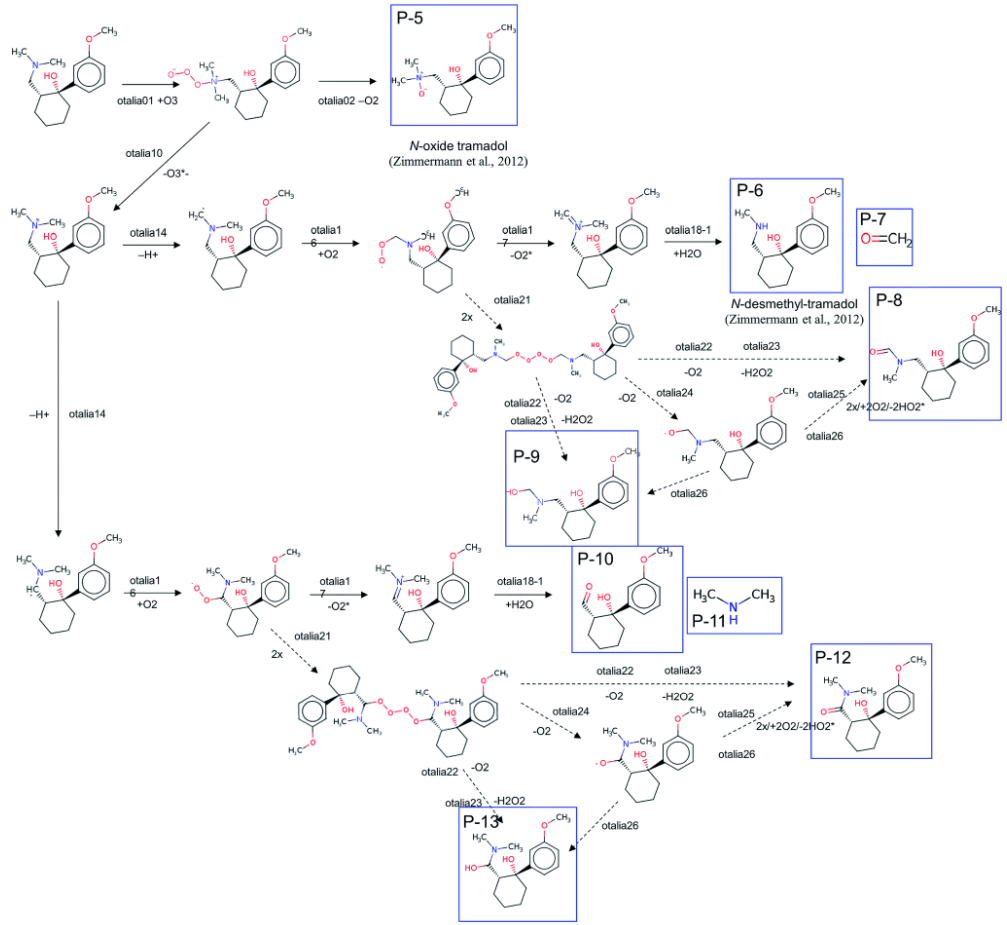
Jonker et al. (2016) ES&T
https://doi.org/10.1021/acs.est.6b03762



Brunner et al. (2016) STOTEN
https://doi.org/10.1016/j.scitotenv.2019.135779

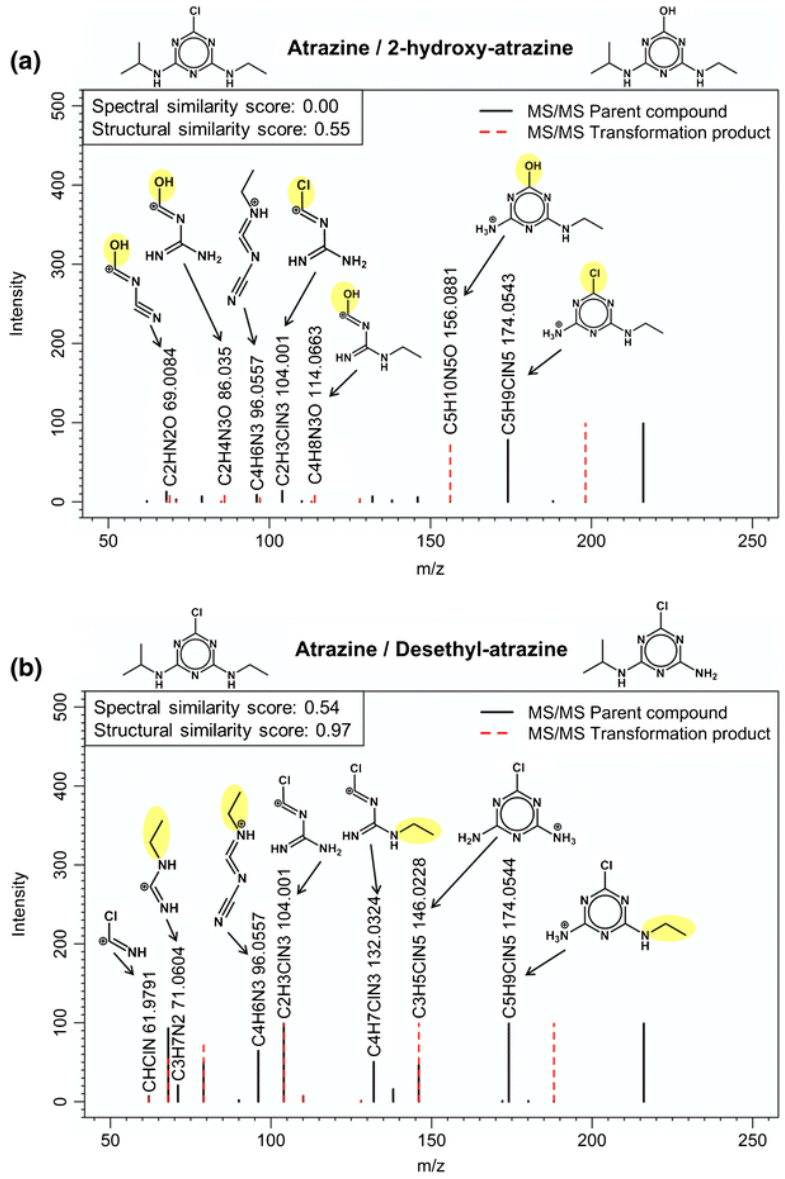
True unknown unknowns – Transformation products





Lee et al. (2017) Env Science:Proc & Impacts
https://doi.org/10.1039/C6EM00584E

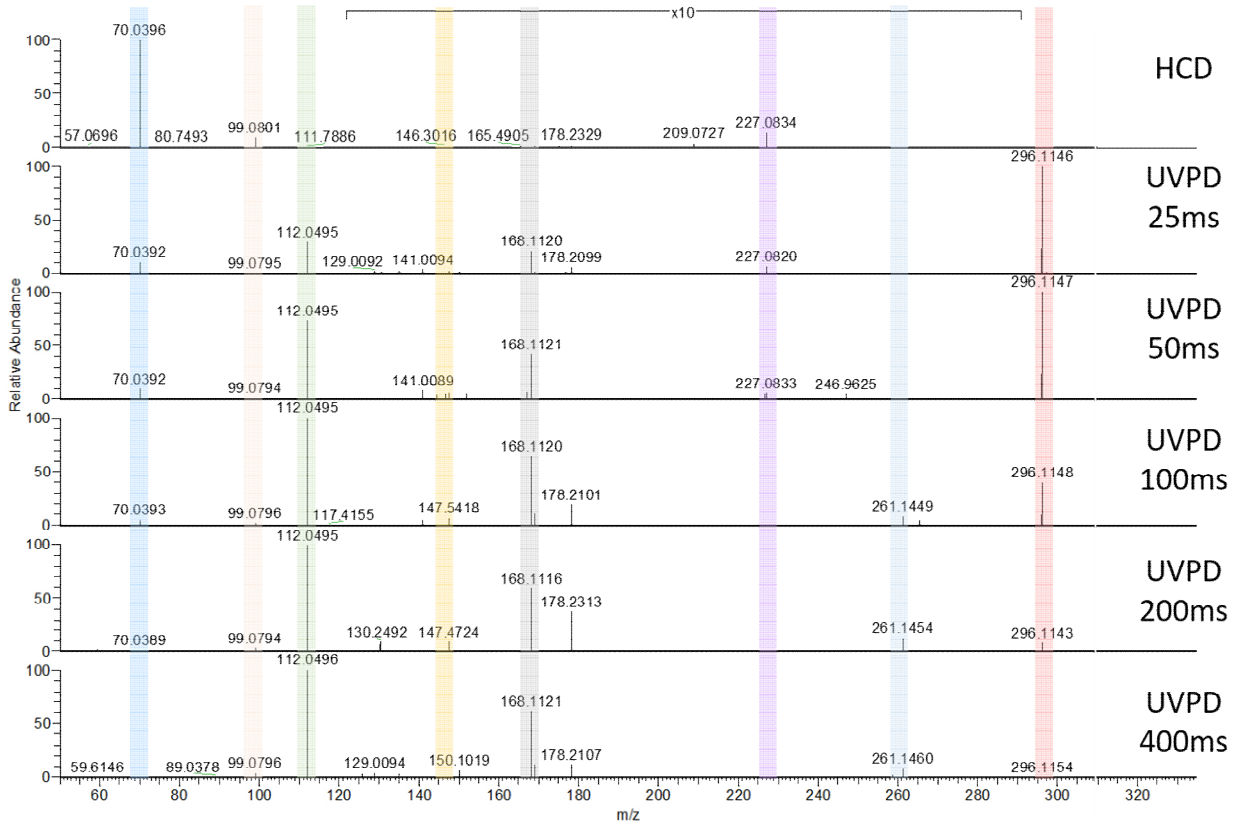
Structural ~ spectral similarity

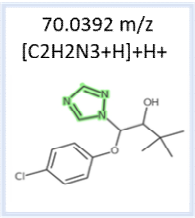


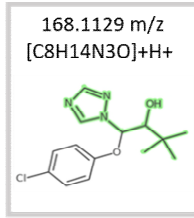
Schollee et al (2017) J Am Soc Mass Spec
10.1007/s13361-017-1797-6

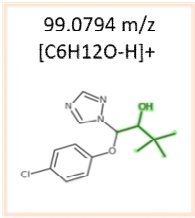
Novel methods:
Alternative fragmentation ultraviolet photodissociation

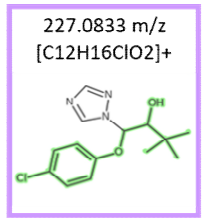
- 213nm laser implemented in Orbitrap Fusion Lumos
- potential to structurally elucidate compounds that cannot be identified by HCD
- Triadimenol

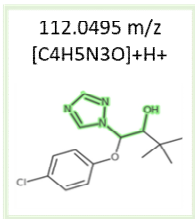


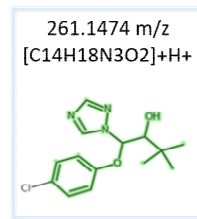


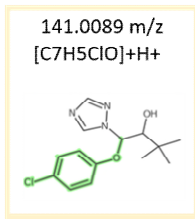


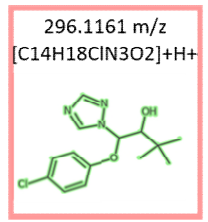






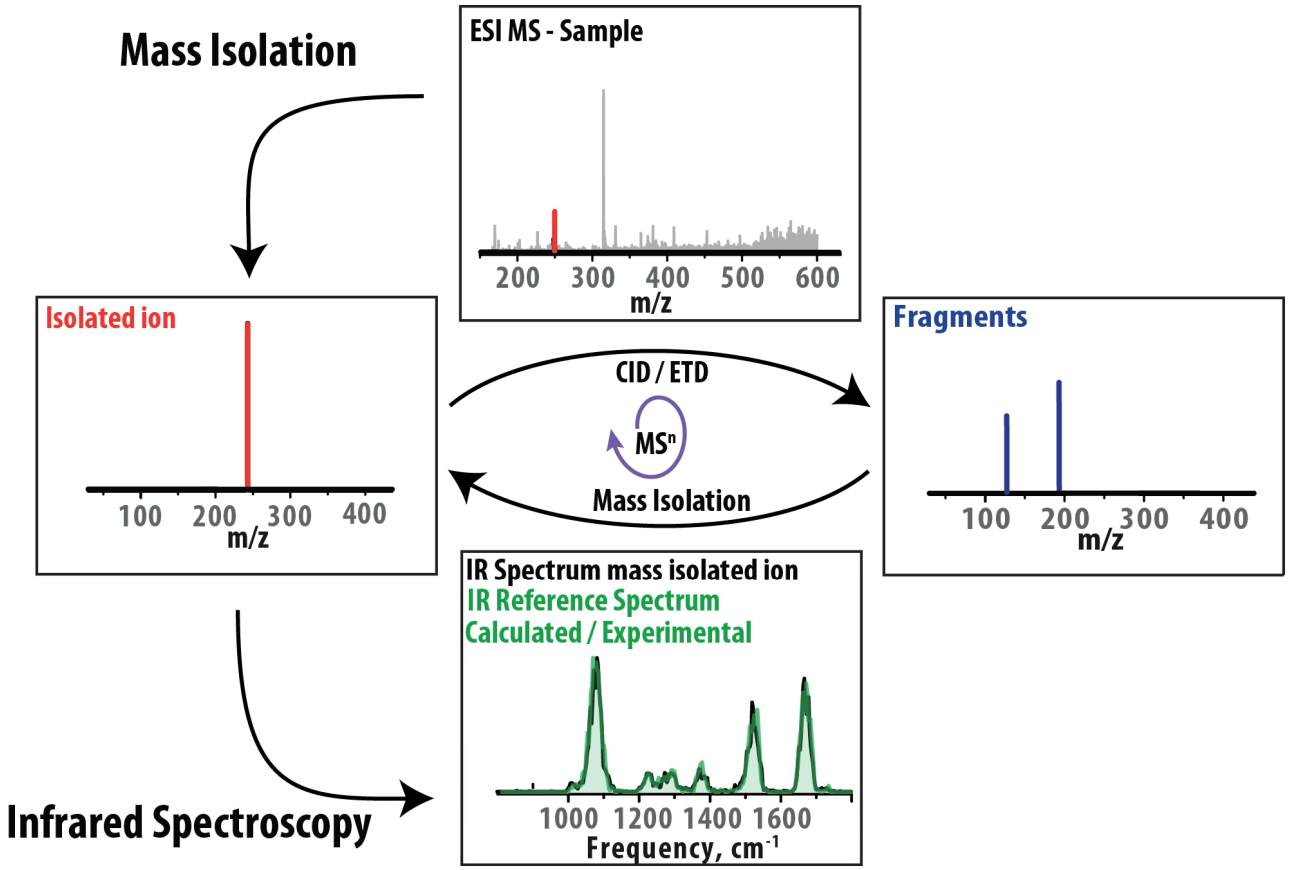


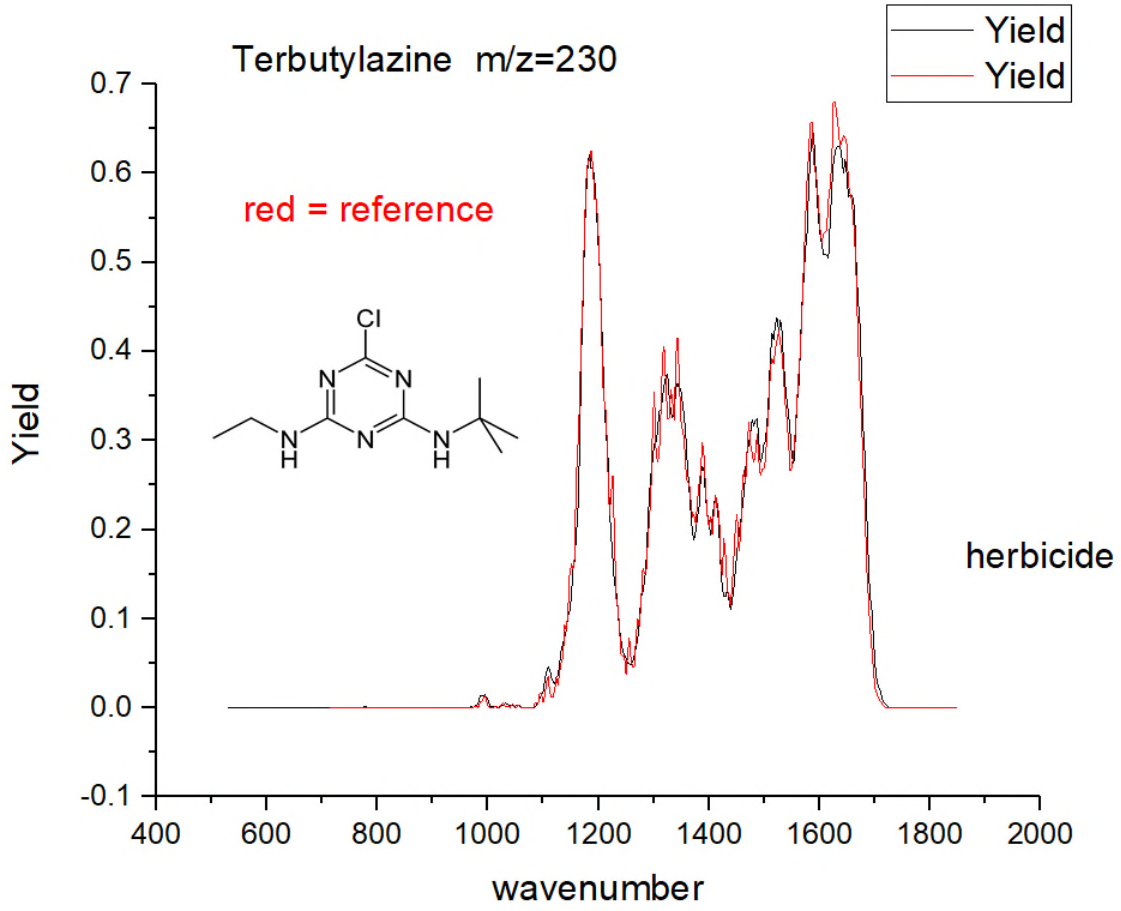




Christian Panse, Functional Genomics Center Zurich

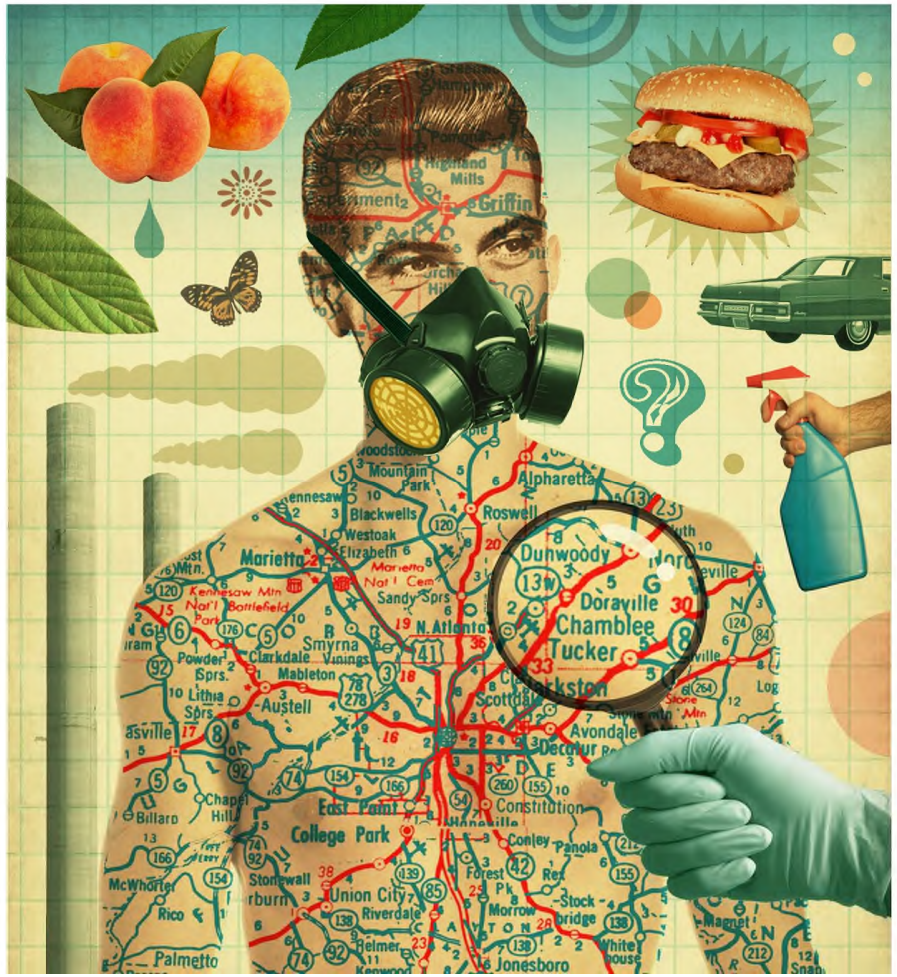
Novel methods:
Infrared Ion Spectroscopy coupled to MS



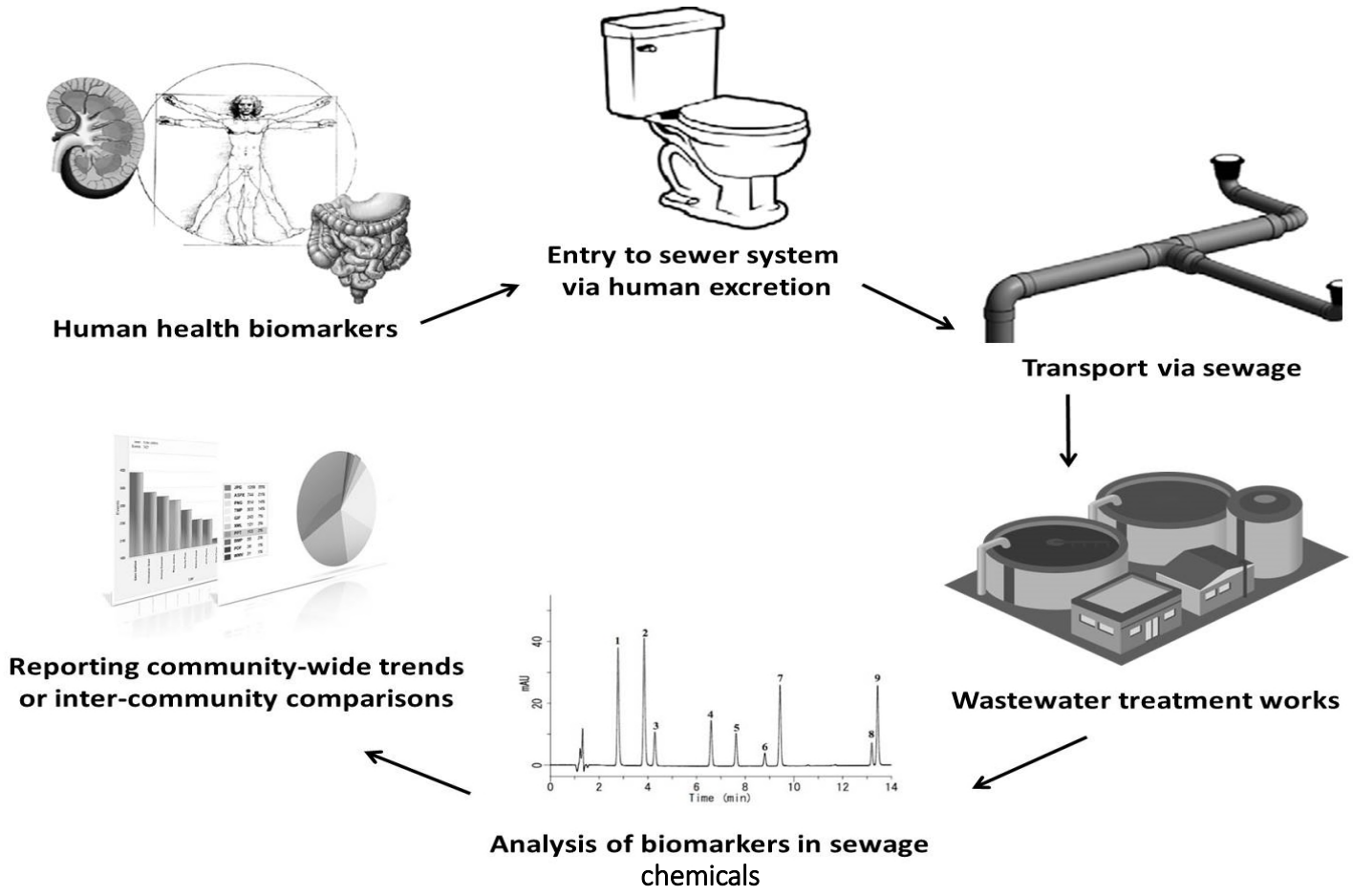


Jos Oomens et al. FELIX

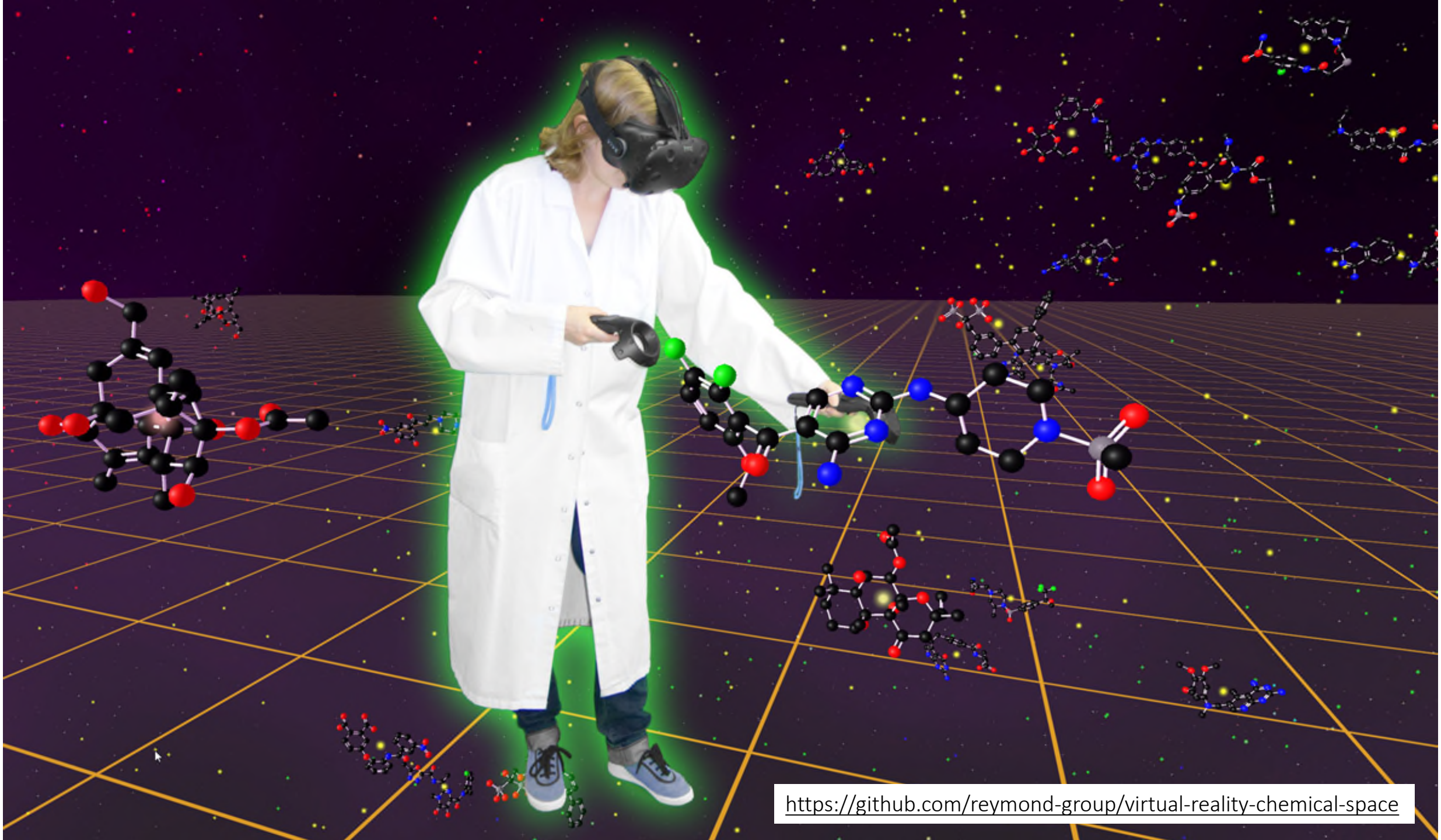
Exposome – One Health



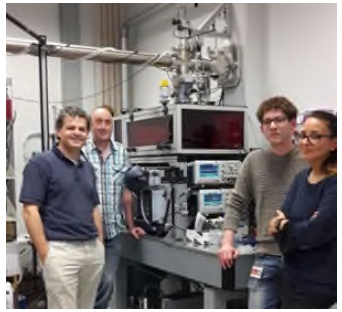
Mapping the exposome - Atlanta Magazine, Michael Waraksa



Yeonsuk Ryu, NIVA


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

Thank you!



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Andrea.brunner@kwrwater.nl

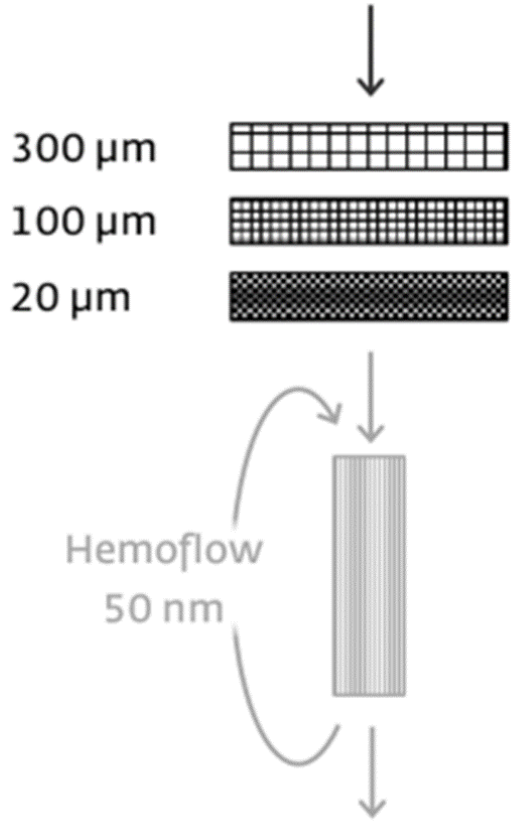
Microplastics to nanoplastics

500 µm metal sieve

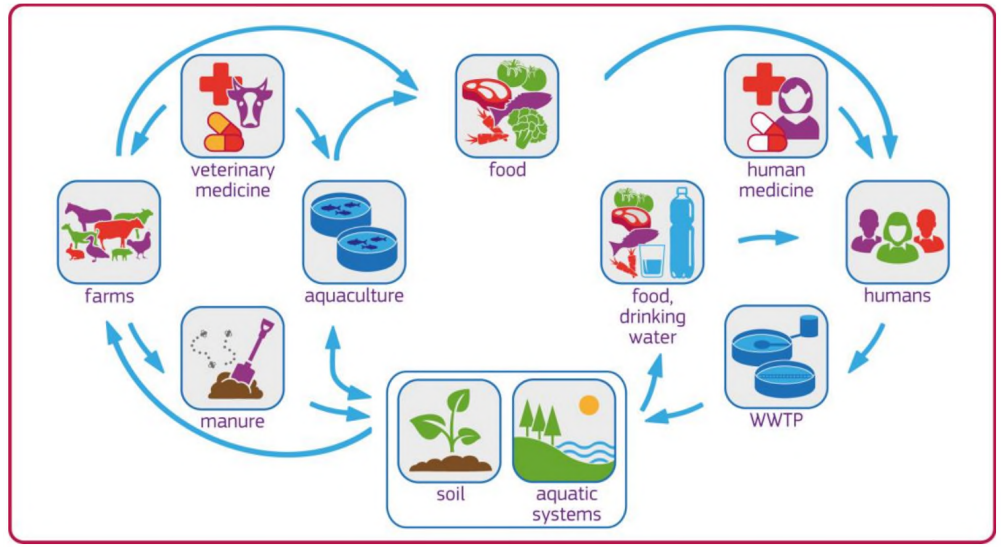
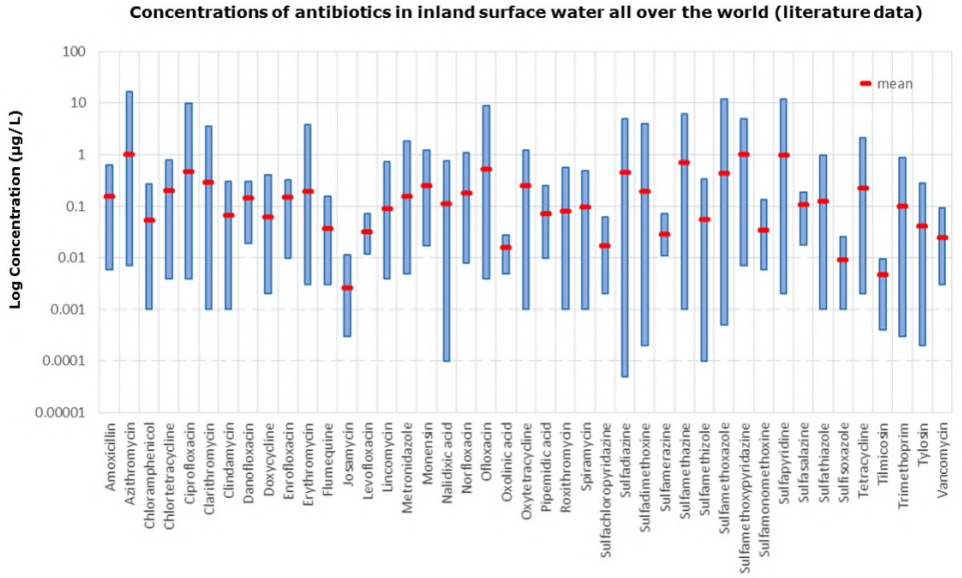
100 µm metal sieve

10 µm plankton net

Laser directed infrared light



TGA GC-MS

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