

# Measuring the chemical exposome: delusion or next frontier?

Benedikt Warth

**Global Exposomics & Biomonitoring Laboratory**

**Department of Food Chemistry and Toxicology, Faculty of Chemistry**

**University of Vienna**

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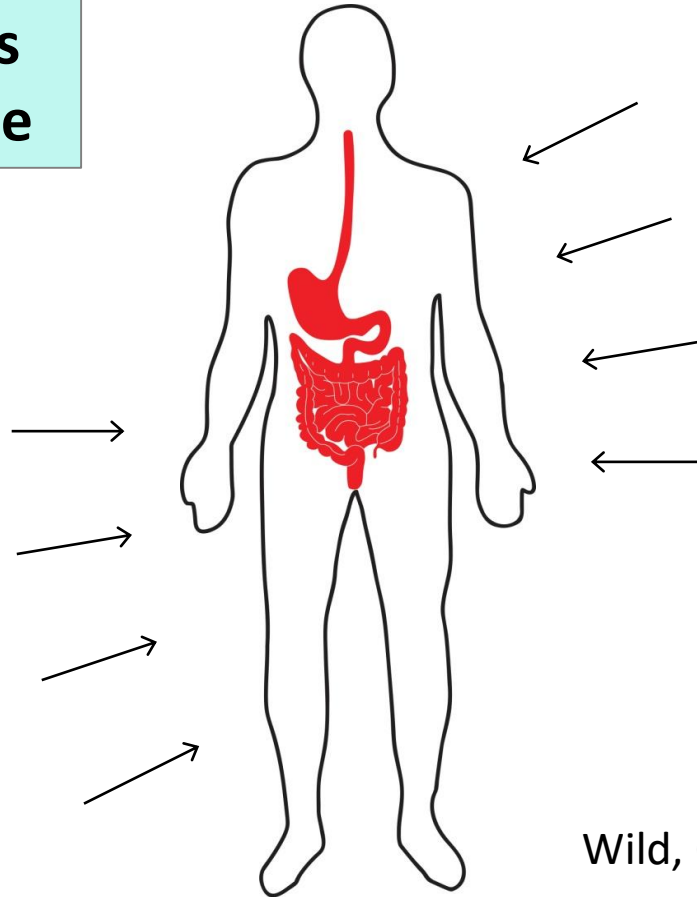
HEAP Symposium Graz - June 1<sup>st</sup> 2022

**Multiple exposures  
throughout lifetime**

## External exposures

Diet  
Toxicants  
Drugs  
Radiation  
Infectious agents

Lifestyle  
Behaviour  
Stress



## Internal exposures

Metabolism  
Hormones  
Microbiome  
Oxidative stress  
Inflammation

Wild, C. P. (2012) *Int. J. Epidemiol.*  
Rappaport & Smith (2010) *Science*

Niedzwiecki et al. (2019) *Ann. Rev. Pharmacol. Toxicol.*

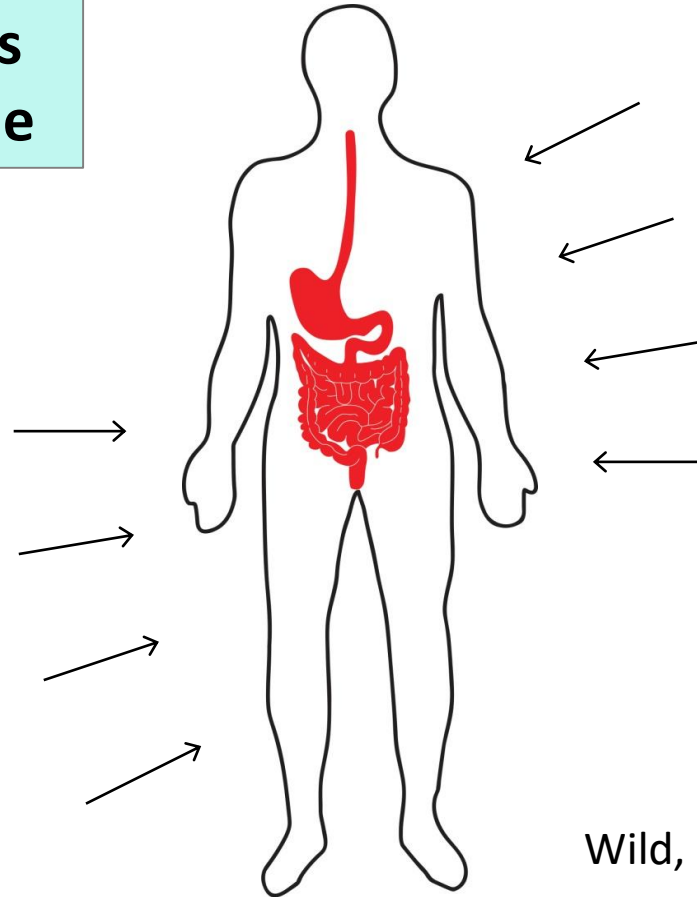
**Multiple exposures  
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## External exposures

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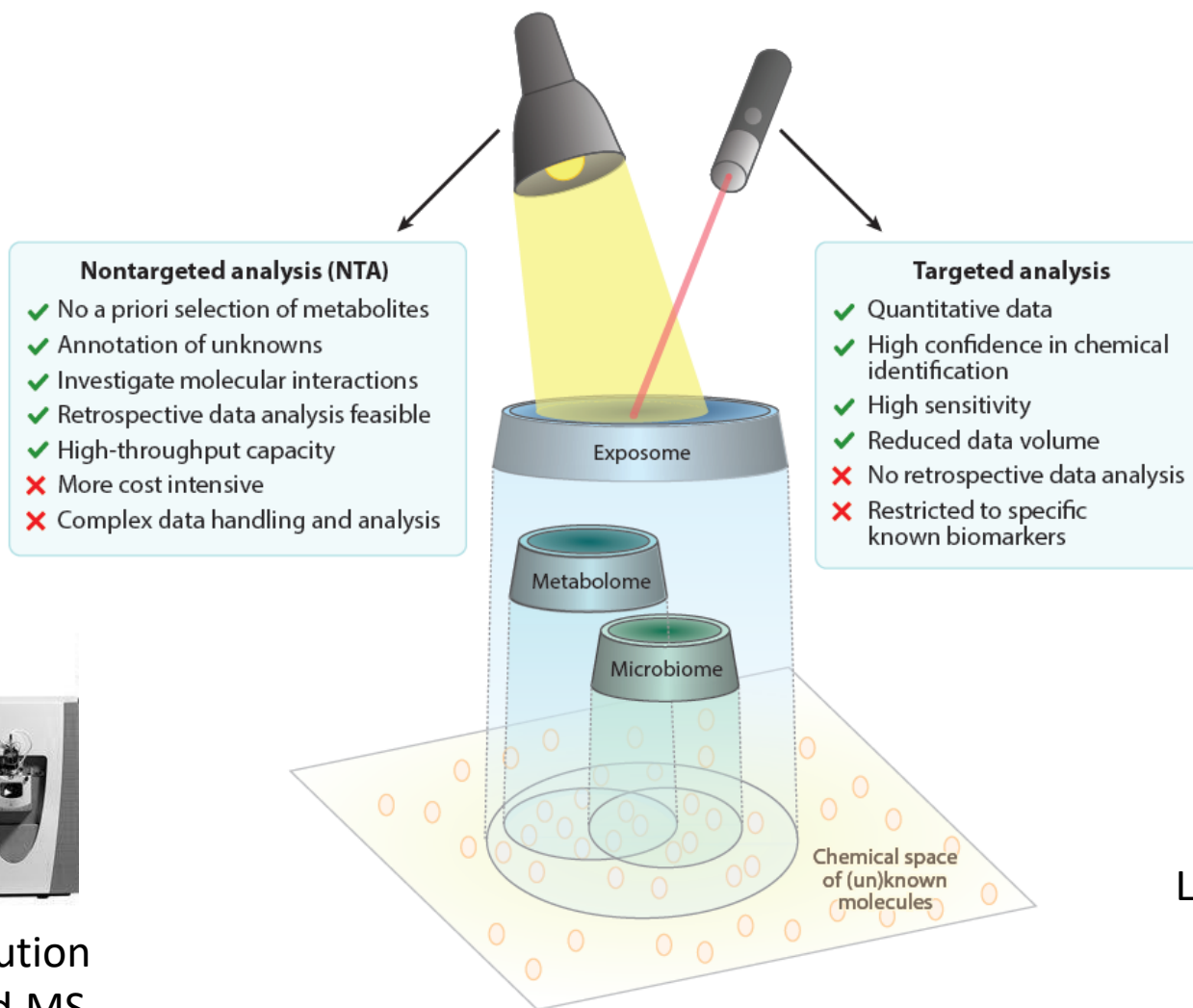
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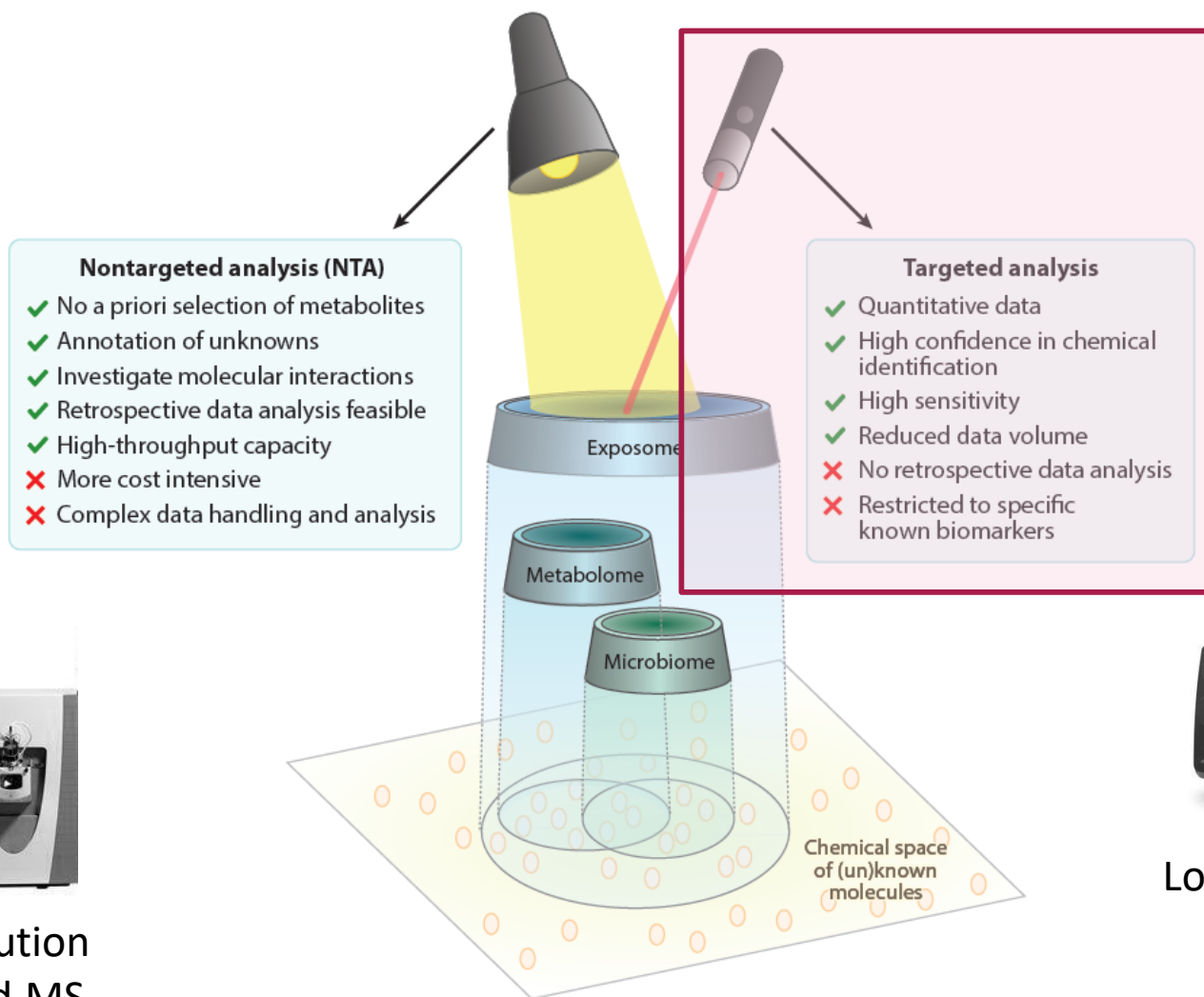


High-resolution  
Untargeted MS



Low-resolution  
Targeted MS

# The Exposome – Targeted approaches



High-resolution  
Untargeted MS

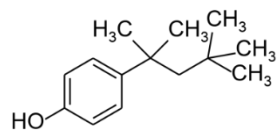


Low-resolution  
Targeted MS

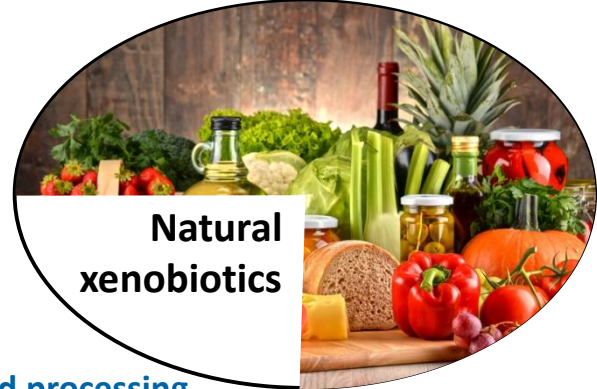
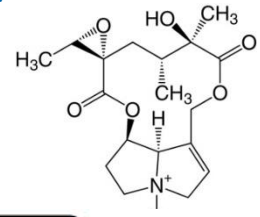
# Multi-xenobiotics method



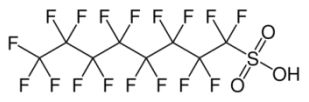
## Alkylphenols



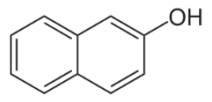
## Phytotoxins



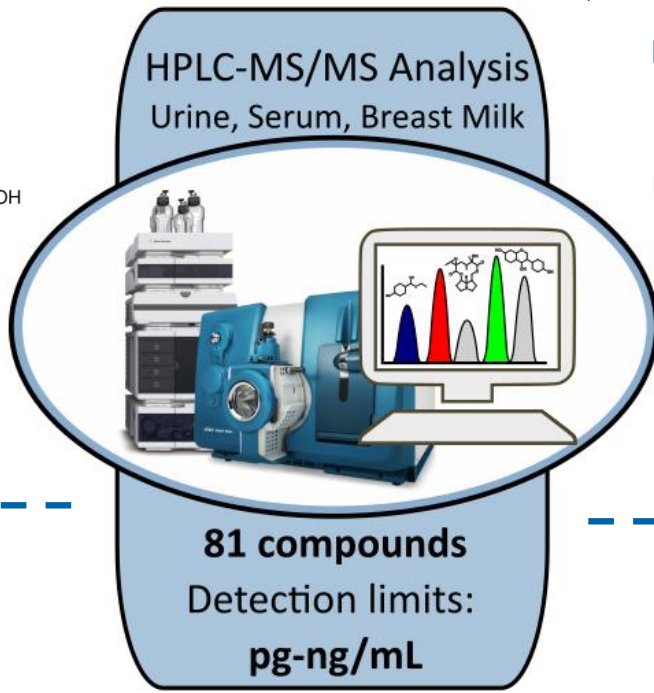
## Perfluorinated alkylated substances



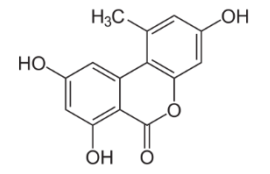
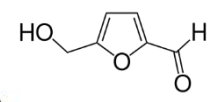
## Polycyclic aromatic hydrocarbons



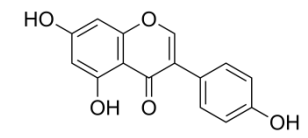
HPLC-MS/MS Analysis  
Urine, Serum, Breast Milk



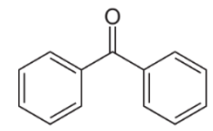
## Food processing carcinogens



## Mycoestrogens



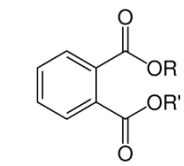
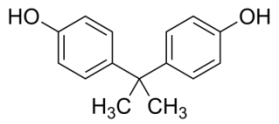
## Phytoestrogens



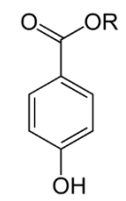
## Benzophenones



## Bisphenols



## Phthalates



## Parabens



## Personal care products



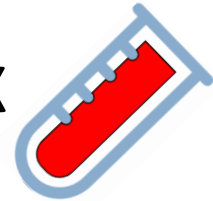
MEDICAL UNIVERSITY  
OF VIENNA

Extremely premature infants  
< 1 kg at birth



Plasma sampling  
4 weeks postpartum

21 x



Qtrap 6500+ Triple Quadrupol  
(AB Sciex)

1) Liquid-Liquid extraction

2) Protein precipitation

3) Targeted analysis

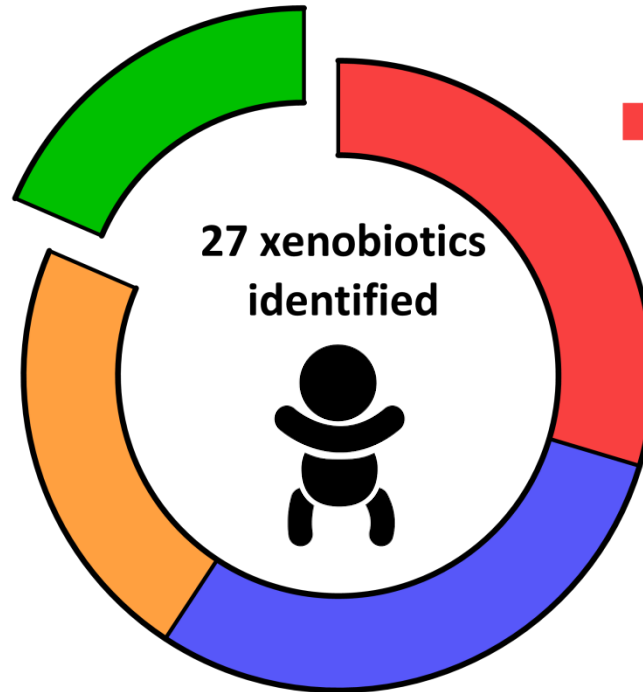




■ 5 Natural xenobiotics

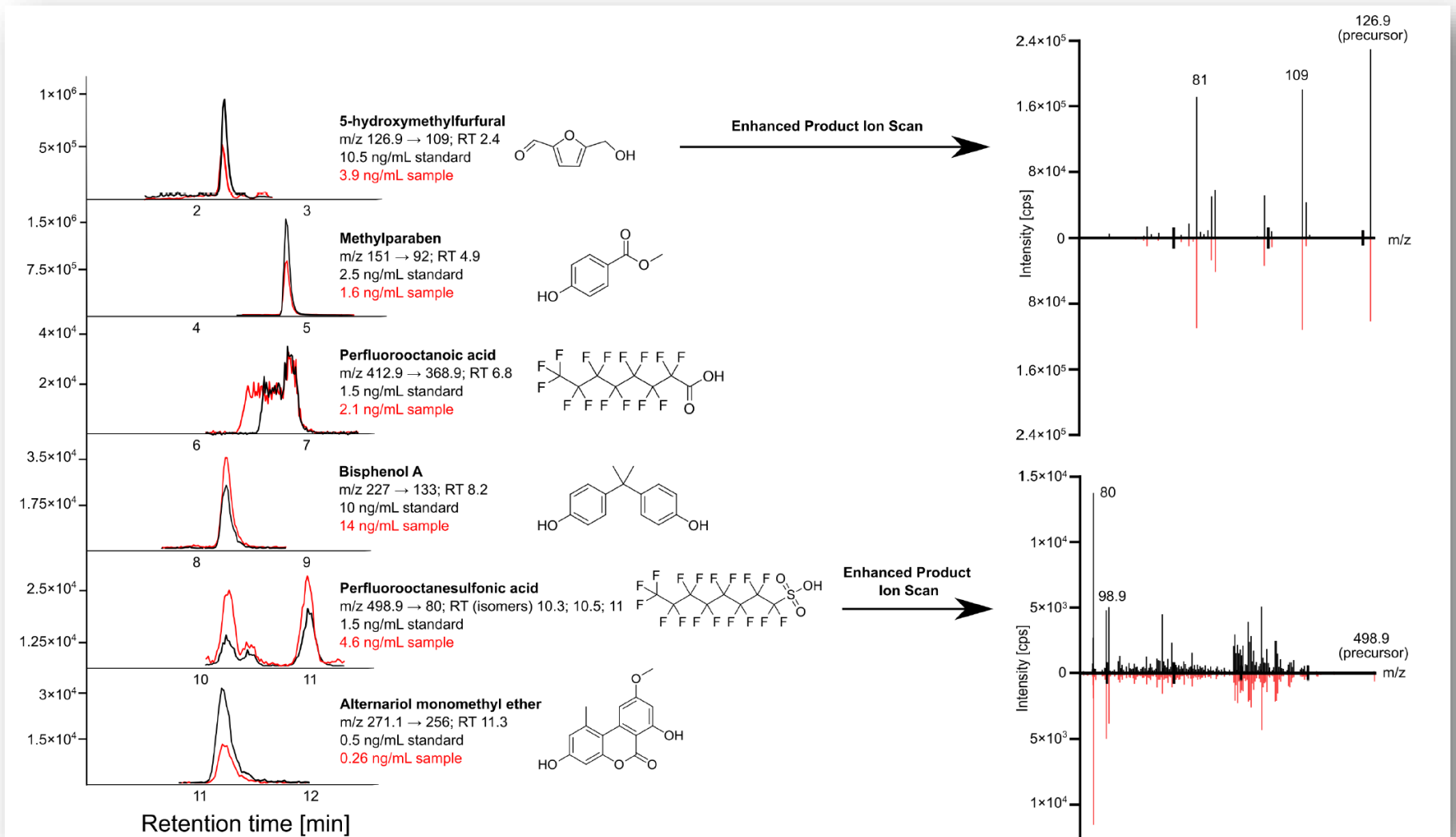
■ 8 Plasticizers and plastic components

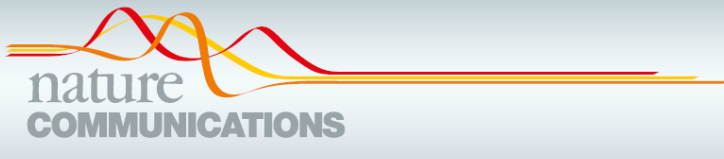
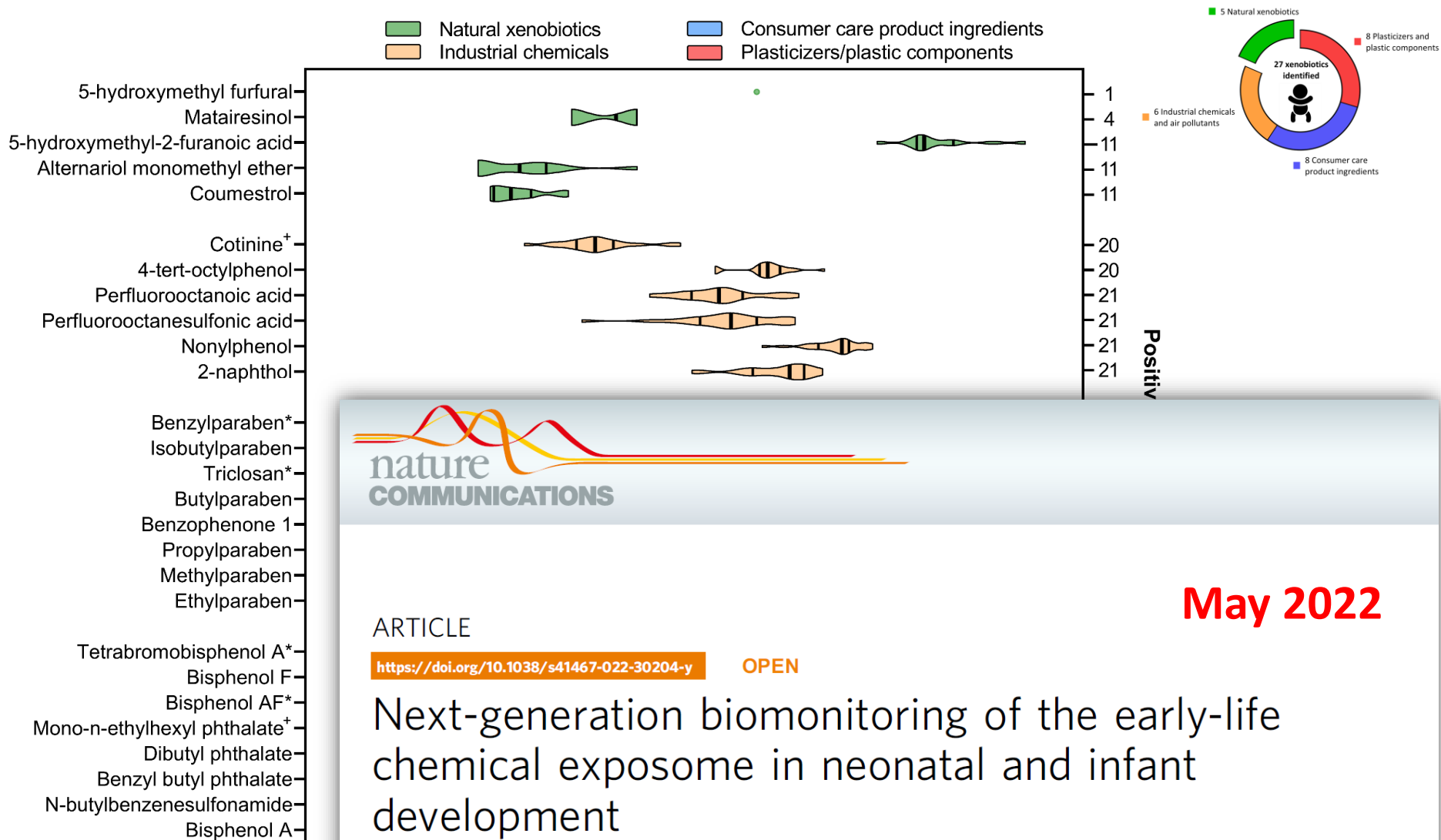
■ 6 Industrial chemicals and air pollutants



■ 8 Consumer care product ingredients







ARTICLE

<https://doi.org/10.1038/s41467-022-30204-y>

OPEN

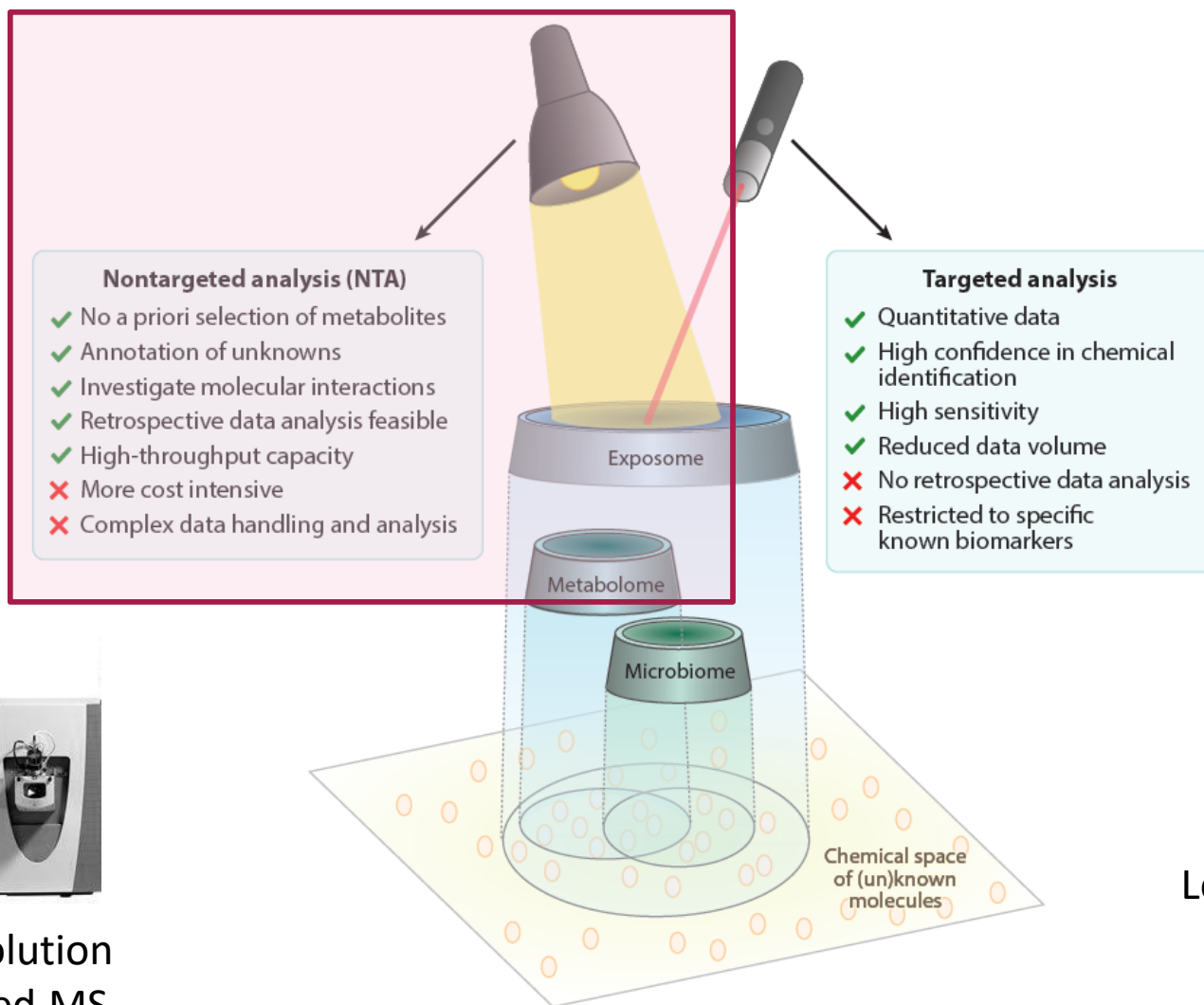
May 2022

## Next-generation biomonitoring of the early-life chemical exposome in neonatal and infant development

Thomas Jamnik<sup>1</sup>, Mira Flasch<sup>1</sup>, Dominik Braun<sup>1</sup>, Yasmin Fareed<sup>1</sup>, Daniel Wasinger<sup>1</sup>, David Seki<sup>2,3</sup>, David Berry<sup>3</sup>, Angelika Berger<sup>2</sup>, Lukas Wisgrill<sup>2,4</sup> & Benedikt Warth<sup>1,4</sup>✉

Benedikt Warth

# The Exposome – Non-targeted approaches



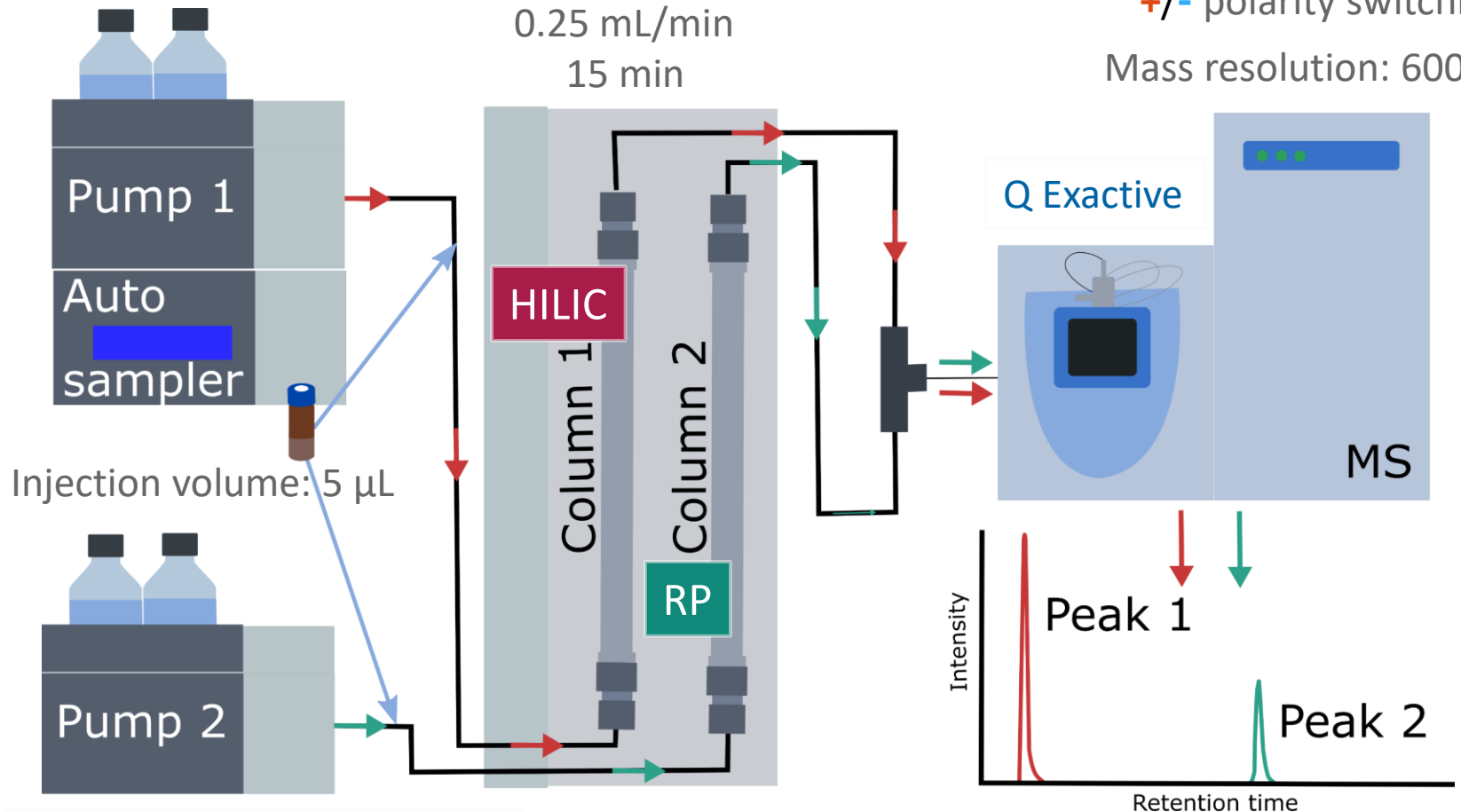
High-resolution  
Untargeted MS



Low-resolution  
Targeted MS

# Non-targeted: Dual-column approach

**Aim: Combined workflow for xenobiotics & endogenous metabolites ('exposure & effect')**



Vanquish Duo UHLC System

w/ Gunda Koellensperger, Univ. Vienna

# Non-targeted: Dual-column approach

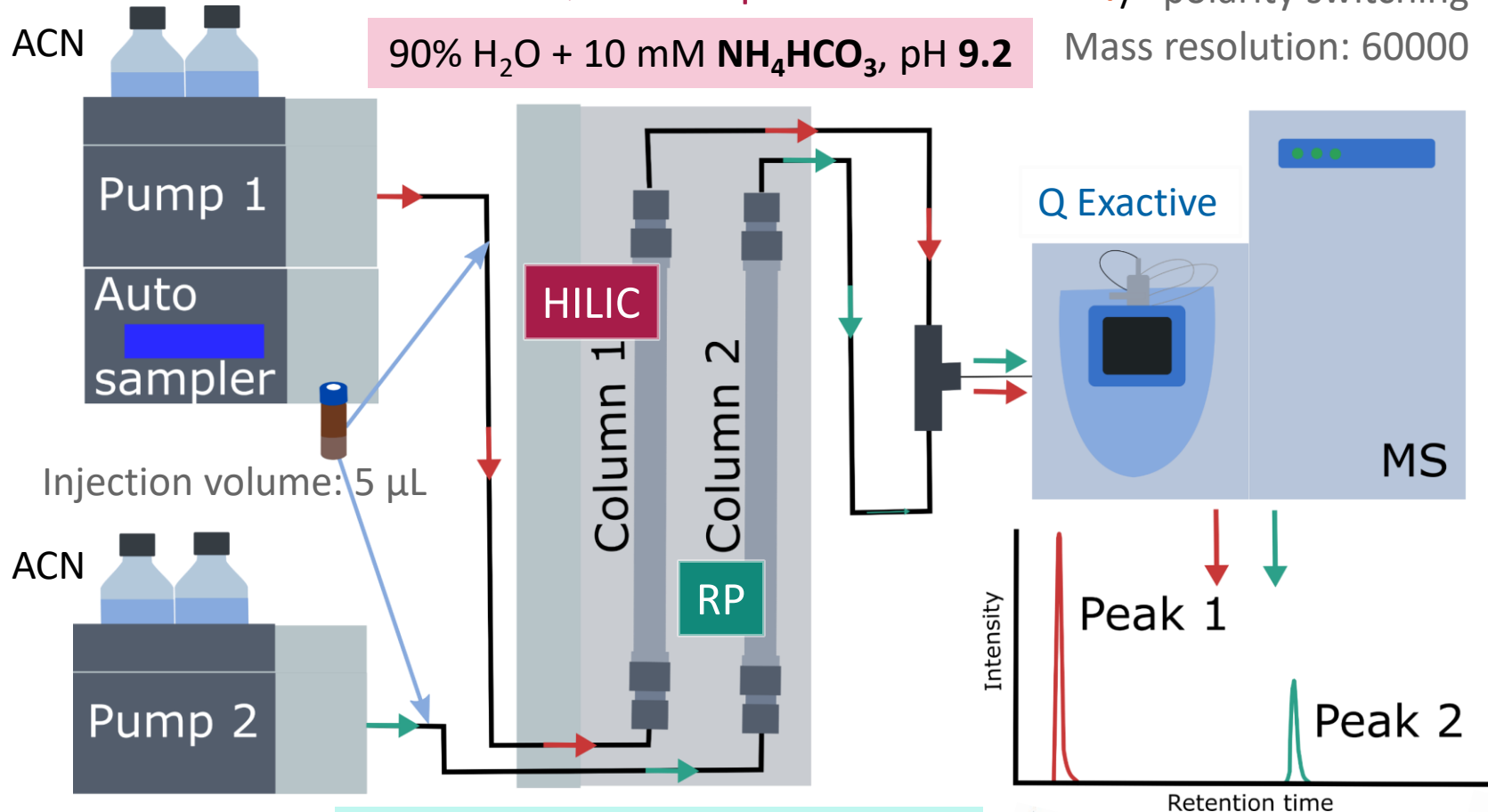
Schwaiger (2019) *Analyst*

SeQuant ZIC pHILIC

+/- polarity switching

Mass resolution: 60000

90% H<sub>2</sub>O + 10 mM NH<sub>4</sub>HCO<sub>3</sub>, pH 9.2

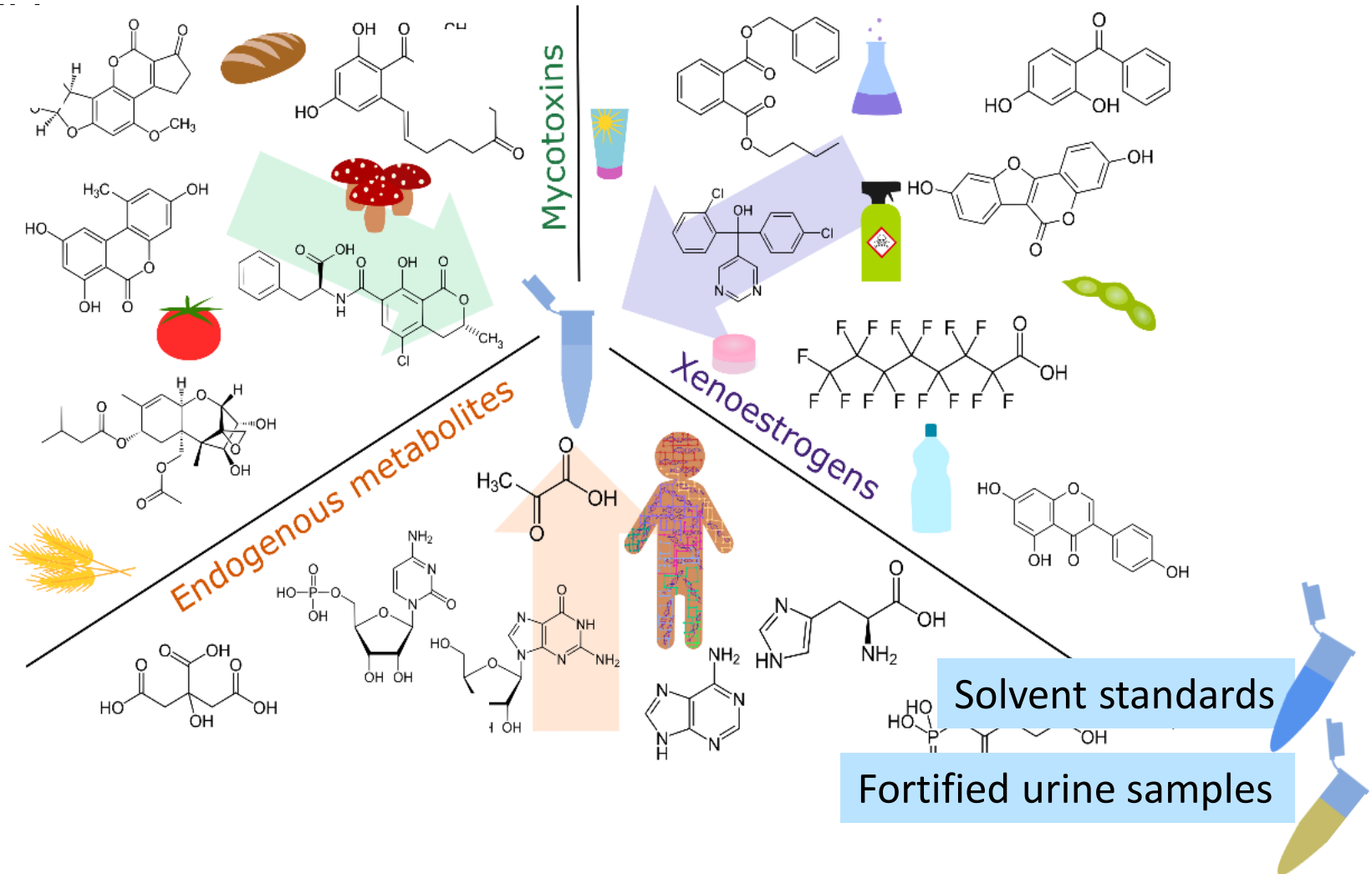


H<sub>2</sub>O + 0.3 mM Ammonium fluoride

Acquity HSS T3



# Non-targeted: Dual-column approach



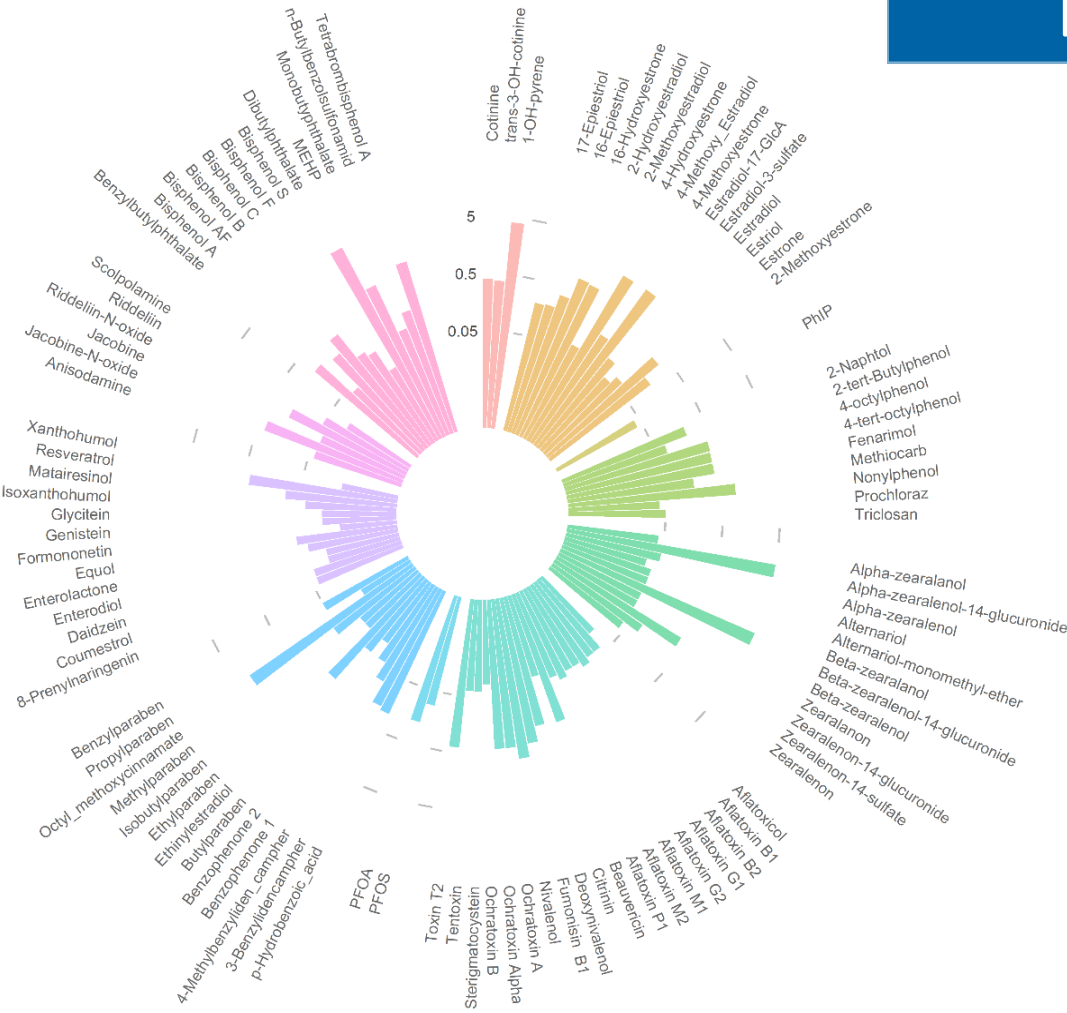
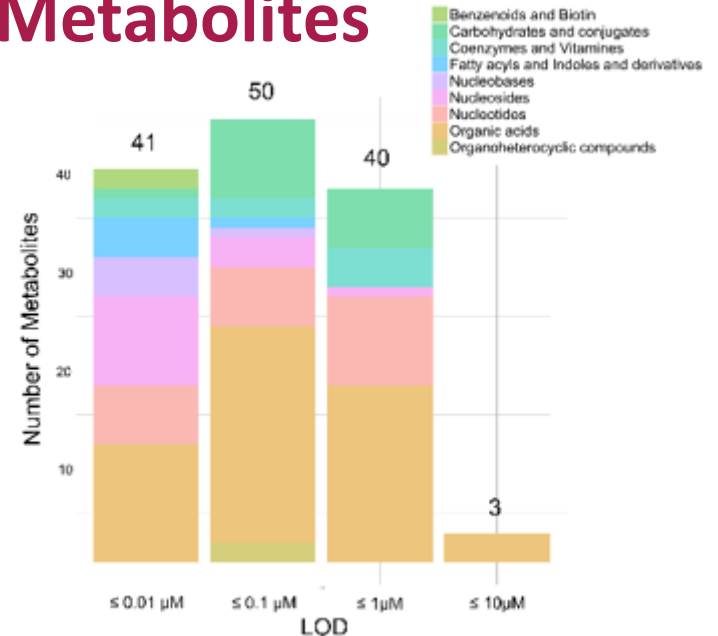
# Non-targeted: Dual-column approach

## Limit of Detection (LOD)

**Xenobiotics**  
median 0.7 ng/mL

- Air pollutants and food processing by-product
- Endogenous estrogens
- Industrial side products and pesticides
- Mycoestrogens and mycotoxins
- Perfluorinated alkylated substances
- Personal care product ingredients, pharmaceuticals and metabolites
- Phytoestrogens and phytochemicals
- Plastizer/Plastic components and metabolites

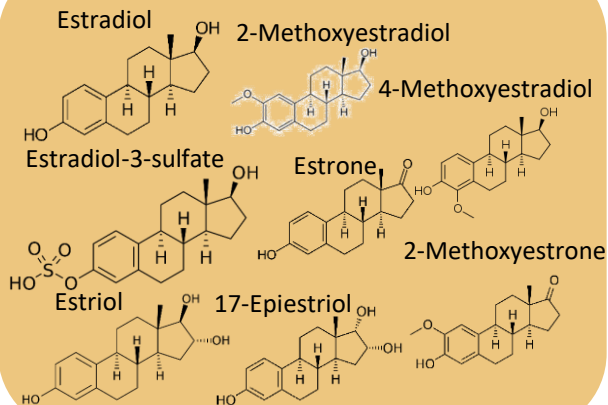
## Metabolites



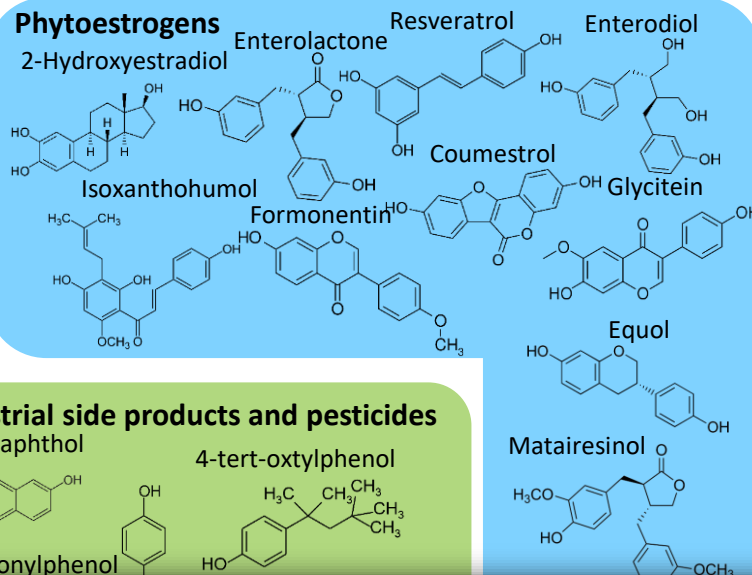


## Unknown samples

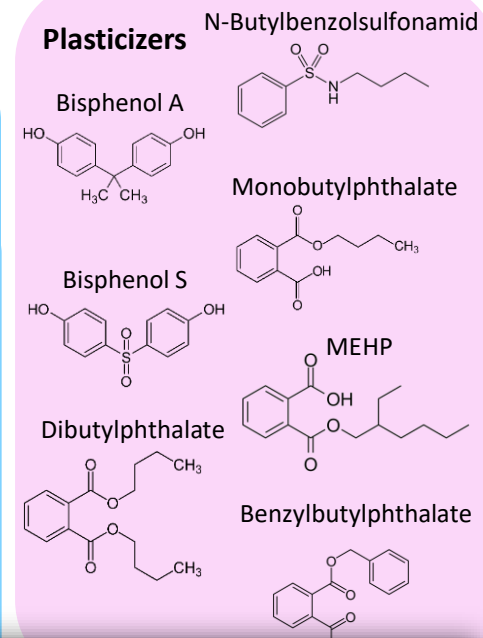
### Endogenous estrogens



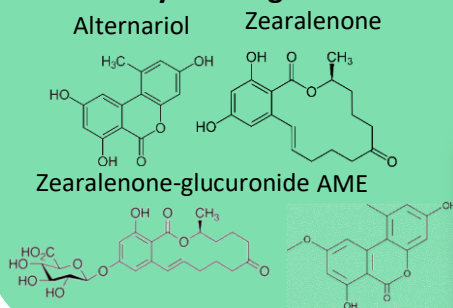
### Phytoestrogens



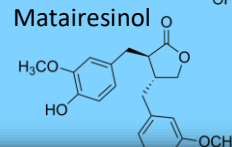
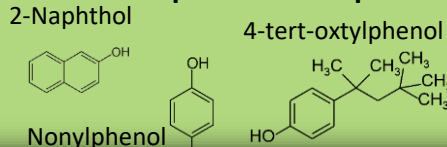
### Plasticizers



### Mycoestrogens



### Industrial side products and pesticides



## Analytical Chemistry

### Air pollutant



## Integrated exposomics/metabolomics for rapid exposure and effect analyses

WORKING PAPER

**Mira Flasch** University of Vienna,  
**Veronika Fitz** University of Vienna,  
**Evelyn Rampler** University of Vienna,  
**Chibundu N. Ezekiel** Babcock University,  
**Gunda Koellensperger** University of Vienna,  
**Benedikt Warth** University of Vienna

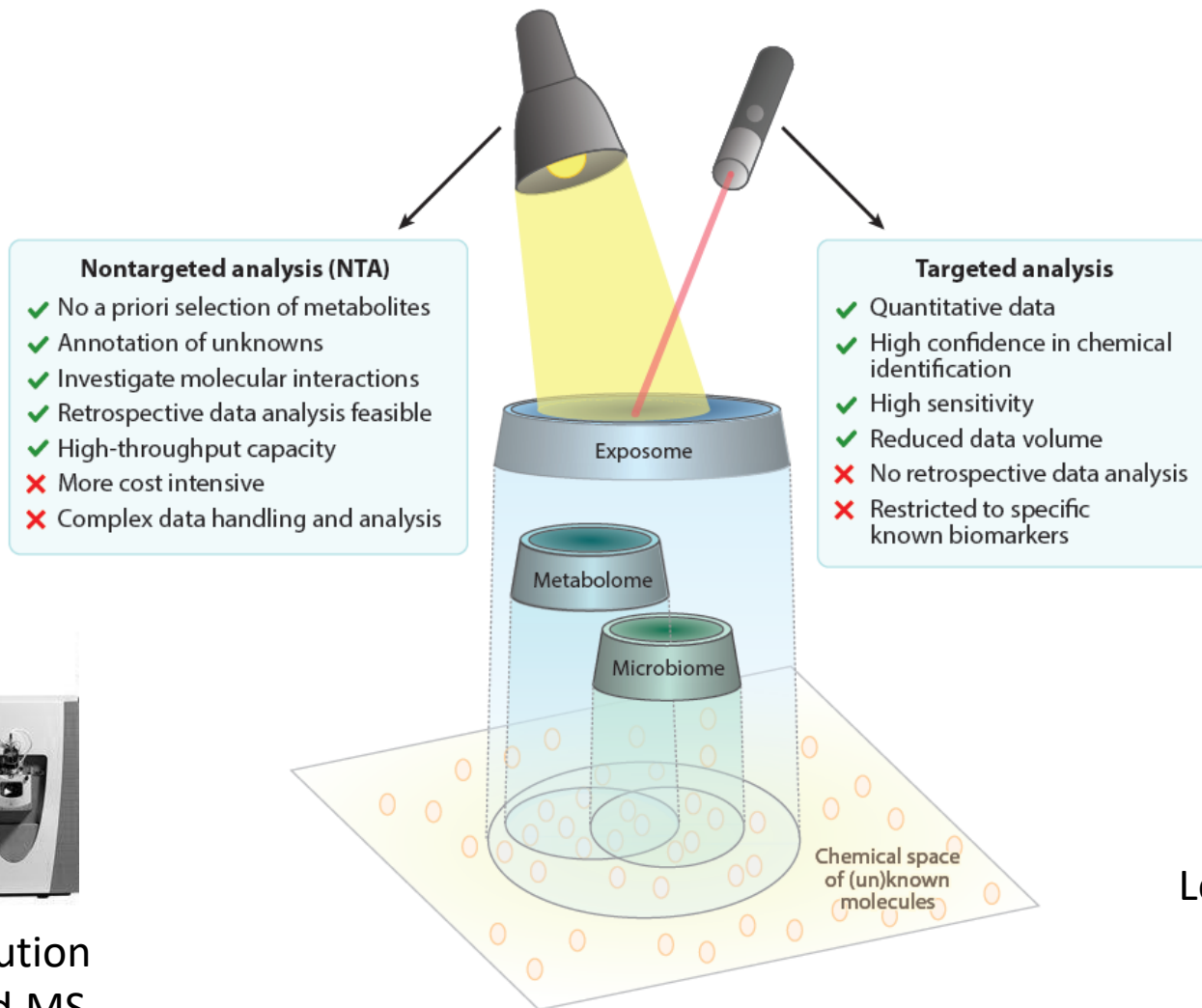
DOWNLOAD

# ChemRxiv™





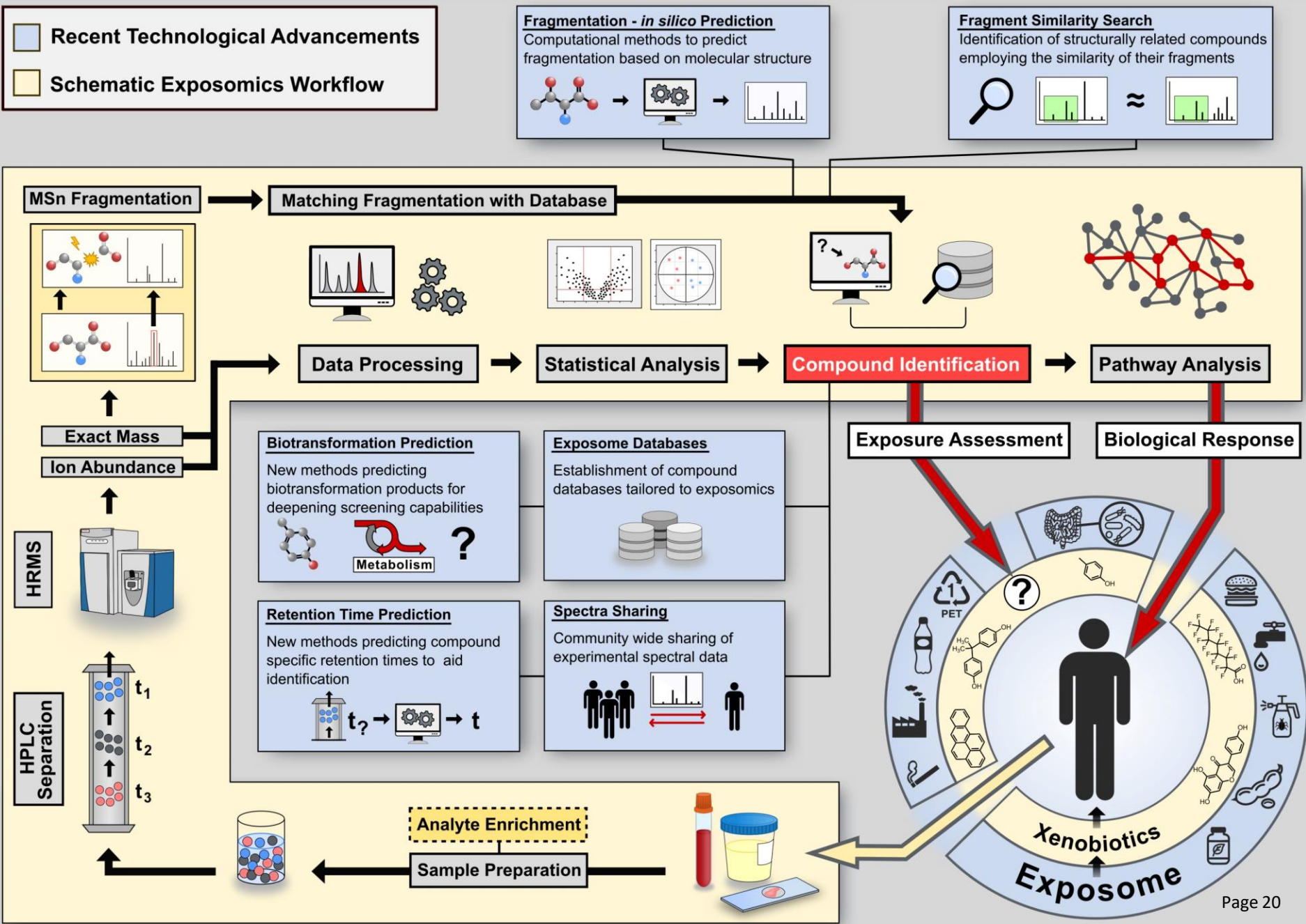
***Measuring the chemical exposome:  
delusion or next frontier?***



High-resolution  
Untargeted MS



Low-resolution  
Targeted MS



# Need to overcome scientific 'silos'

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# Need to overcome scientific 'silos'

ESFRI



The poster features a white silhouette of a human figure with arms outstretched, centered against a background of blue and grey dots of varying sizes. A red dotted line with a white arrowhead points from the left towards the figure's chest. The top left corner contains the University of Vienna logo and 'Fakultät für Chemie'. The top right corner features the 'Exposome Austria' logo, which includes a circular network diagram and the text 'Research Infrastructure National EIRENE Hub'. A dark blue horizontal band across the middle contains the event title 'Exposome Austria - Launch Event' in white. Below this band, the event details are listed: 'Dienstag, 31. Mai 2022, 10:00 Uhr' and 'Kleiner Festsaal, Universitätsring 1, 1010 Wien'. At the bottom left, there is a vertical copyright notice: '© Global Exposomics & Biomonitoring Laboratory'. At the bottom center, there is a navigation bar with icons for back, home, search, and other presentation controls, along with a 140% zoom indicator.

universität  
wien  
Fakultät für Chemie

Exposome Austria  
Research Infrastructure  
National EIRENE Hub

**Exposome Austria - Launch Event**

Dienstag, 31. Mai 2022, 10:00 Uhr  
Kleiner Festsaal, Universitätsring 1, 1010 Wien

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**EIRENE RI**



**Exposome Austria**  
Research Infrastructure  
National EIRENE Hub

<https://exposome.at>  
<https://www.eirene-ri.eu>

# Acknowledgements



# Measuring the chemical exposome: delusion or next frontier?

*Thank you for the attention*

## Contact

Email: [benedikt.warth@univie.ac.at](mailto:benedikt.warth@univie.ac.at)

Web: [exposomics.univie.ac.at](http://exposomics.univie.ac.at)

Twitter: [@ben\\_warth](https://twitter.com/ben_warth)