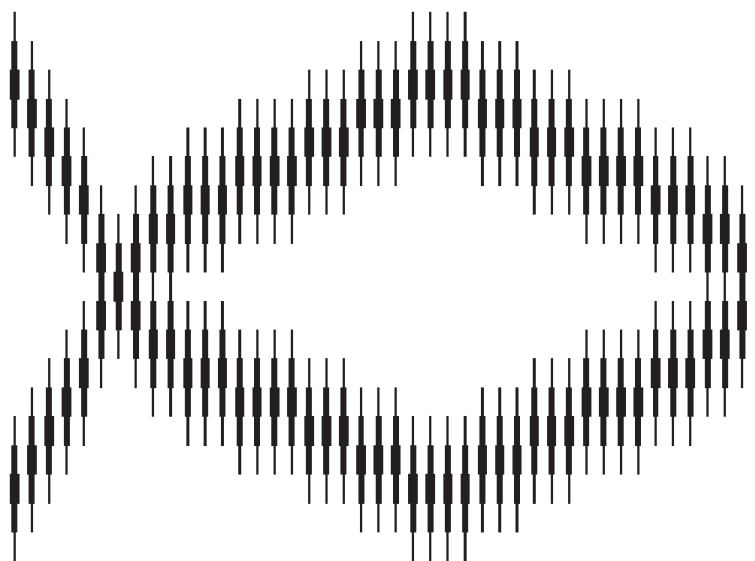


Toxicometabolomics and biotransformation product screening in single zebrafish embryos



Slides available from:
DOI: [10.5281/zenodo.4042005](https://doi.org/10.5281/zenodo.4042005)

Image: Magnus Edblom.
Source: Anton Ribbenstedt.

Assoc. Prof. Dr. Emma L. Schymanski

FNR ATTRACT Fellow and PI in Environmental Cheminformatics

Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg

Email: emma.schymanski@uni.lu and @ESchymanski

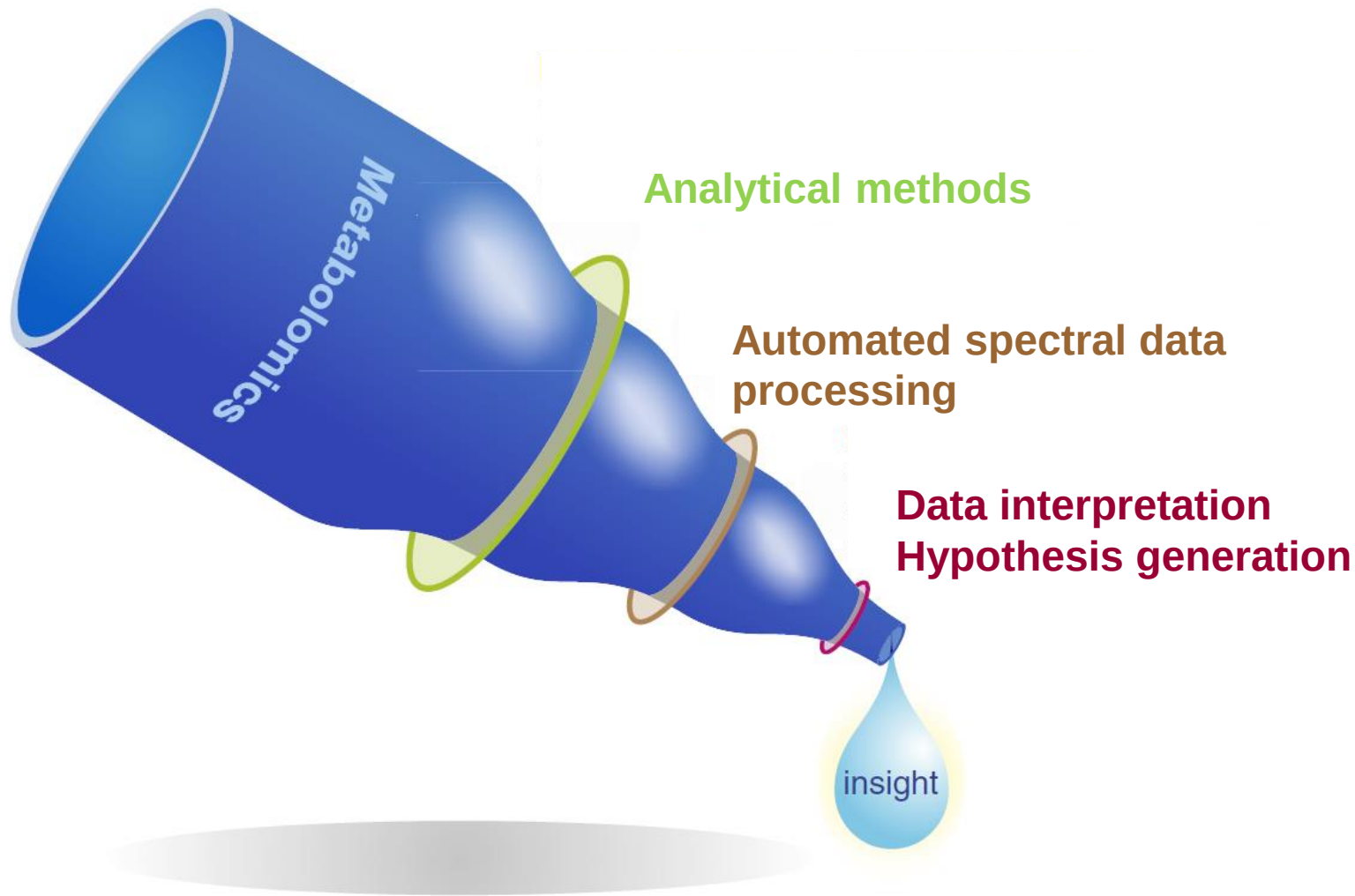


Luxembourg National
Research Fund

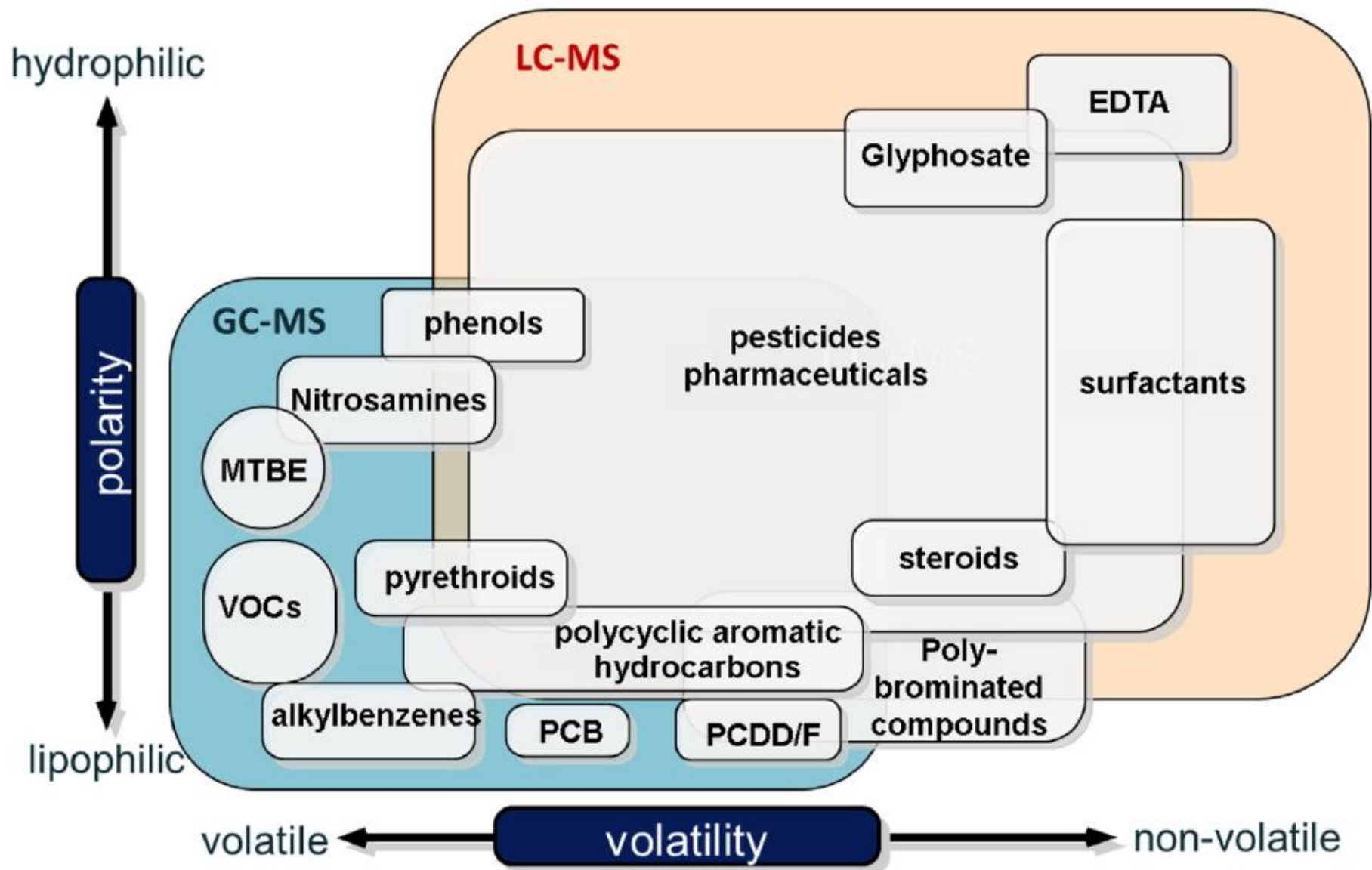
“Opponent” of Anton Ribbenstedt



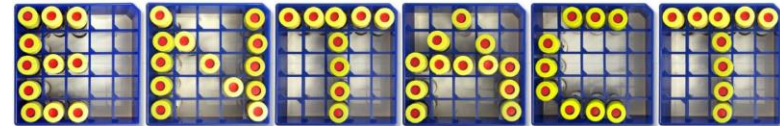
Critical Bottlenecks in Biological Interpretation



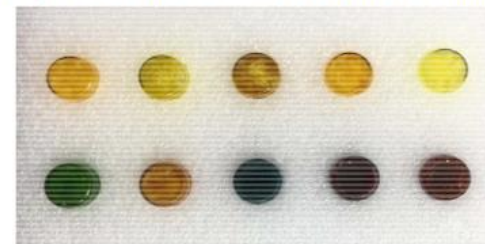
Analytical Methods: LC vs GC?



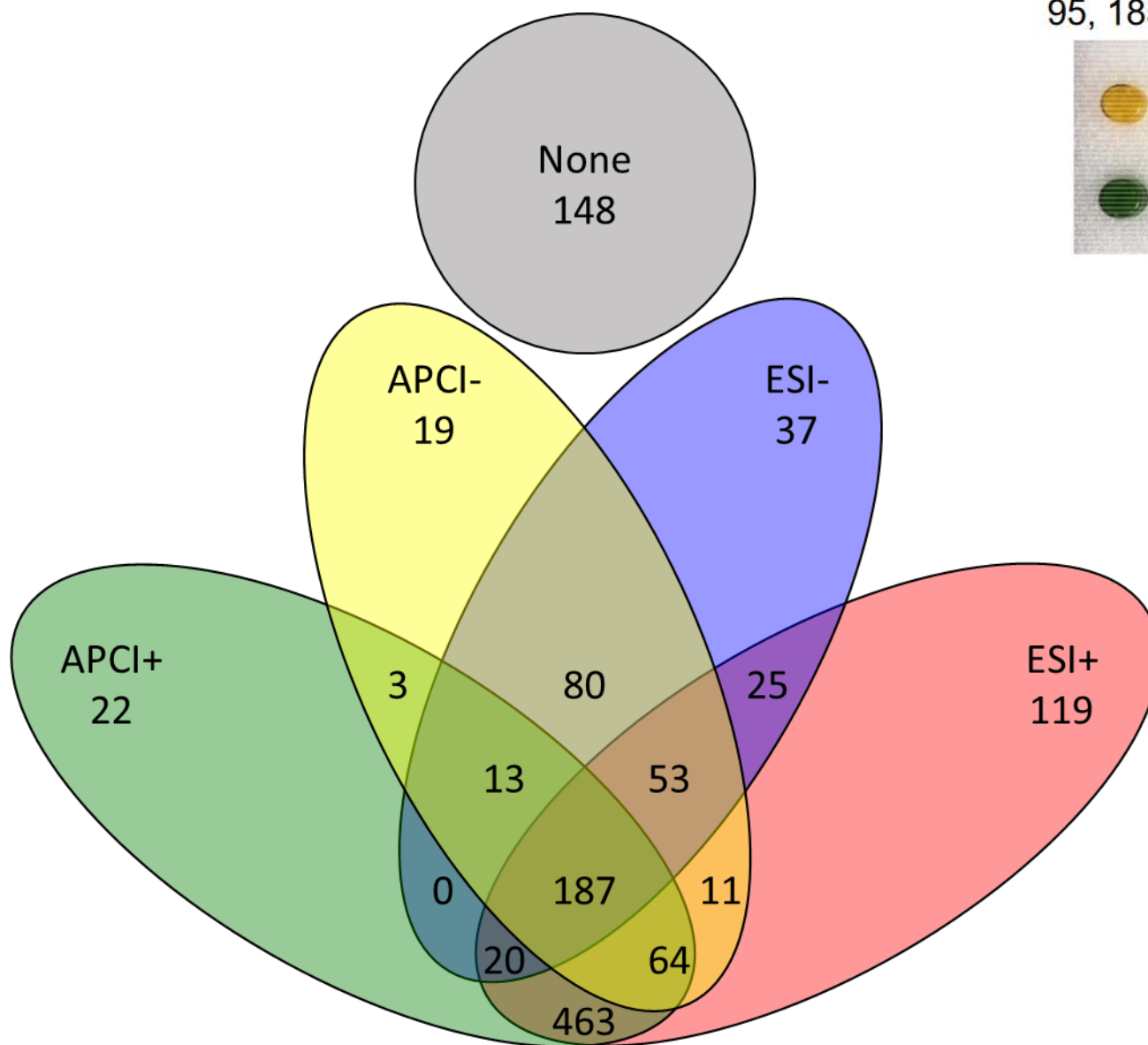
Analytical Methods: Ionisation



95, 185 or 365 substances/mixture

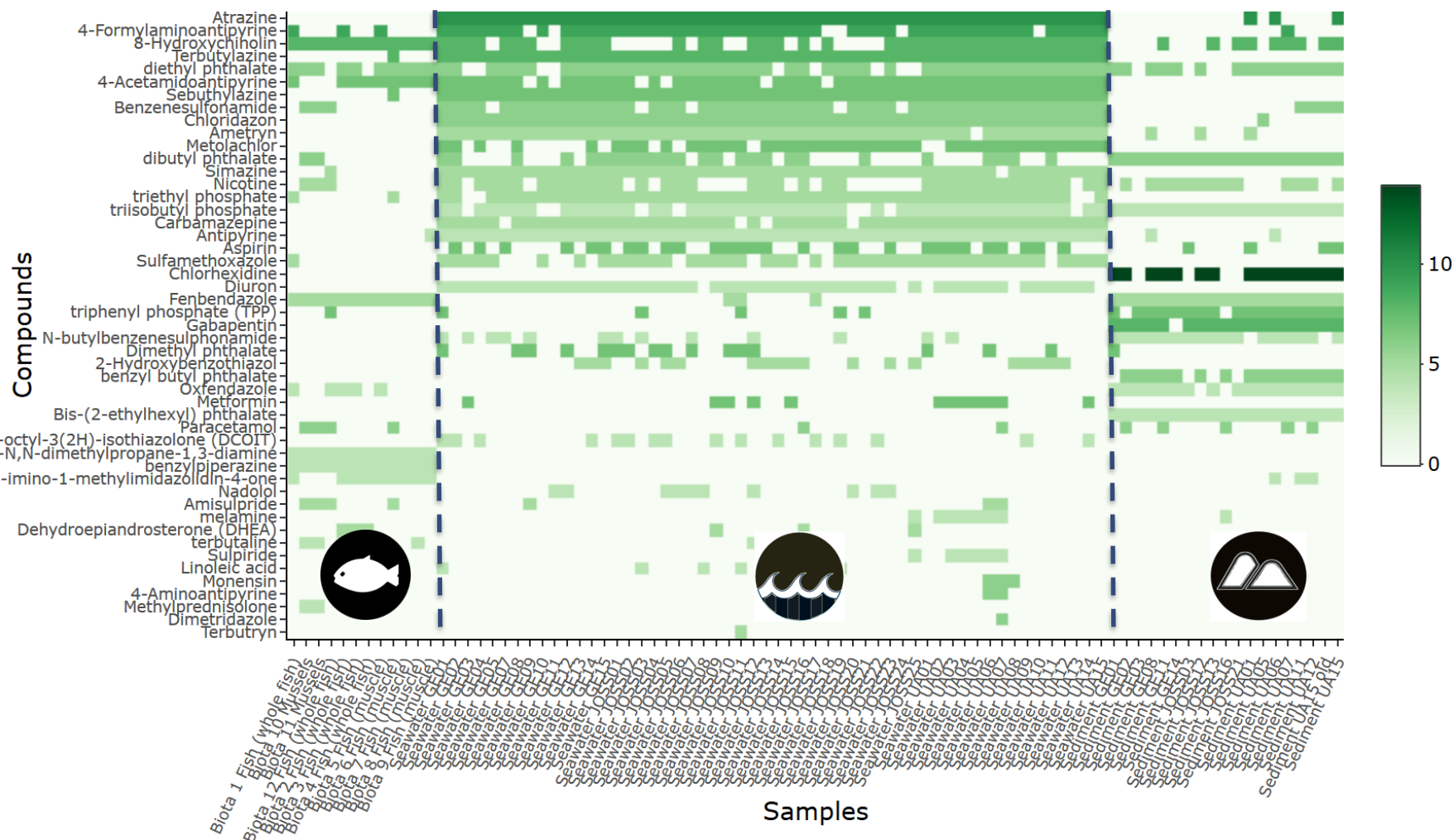


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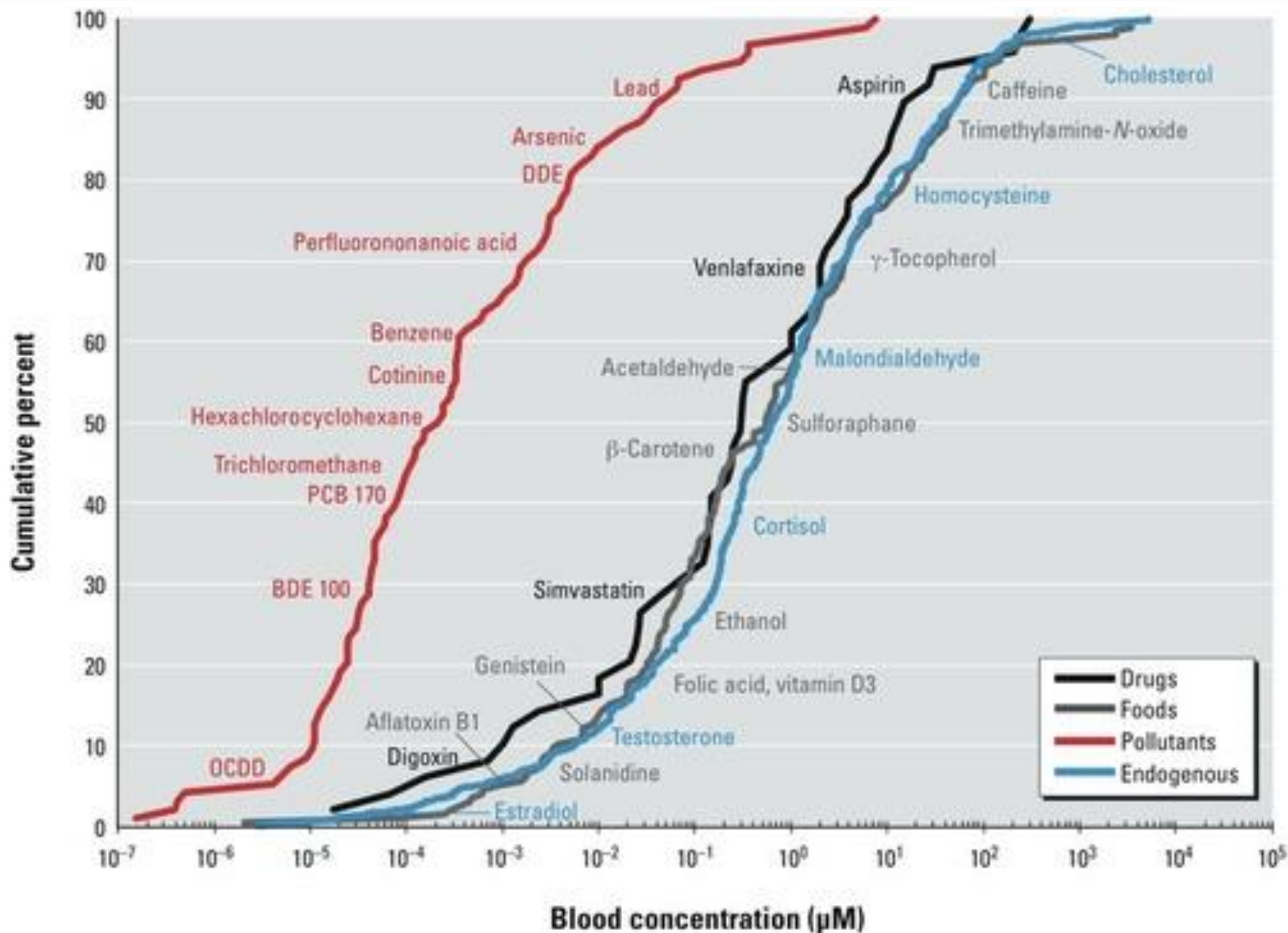


Retrospective screening of REACH chemicals in Black Sea samples (various matrices)

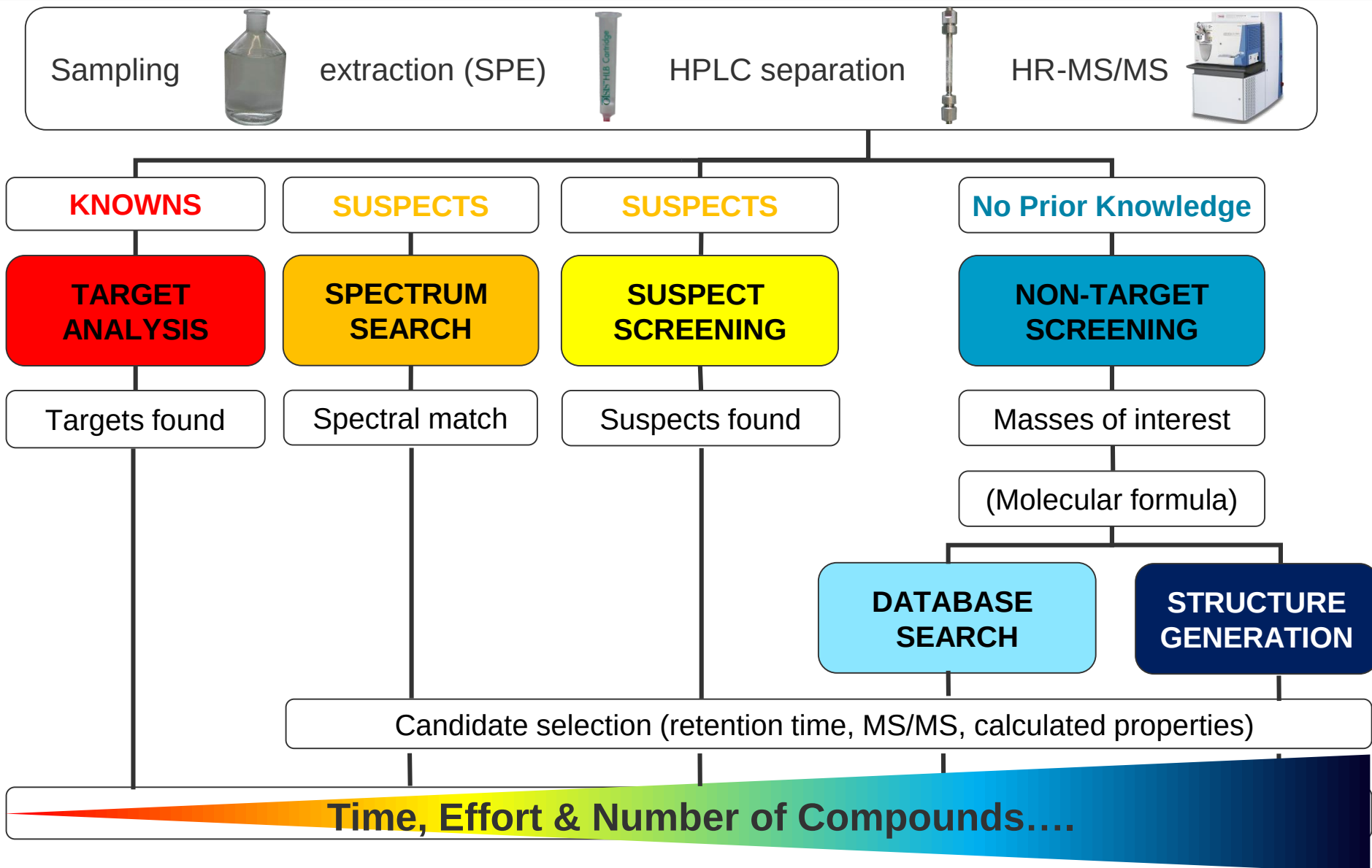
Occurrence Results



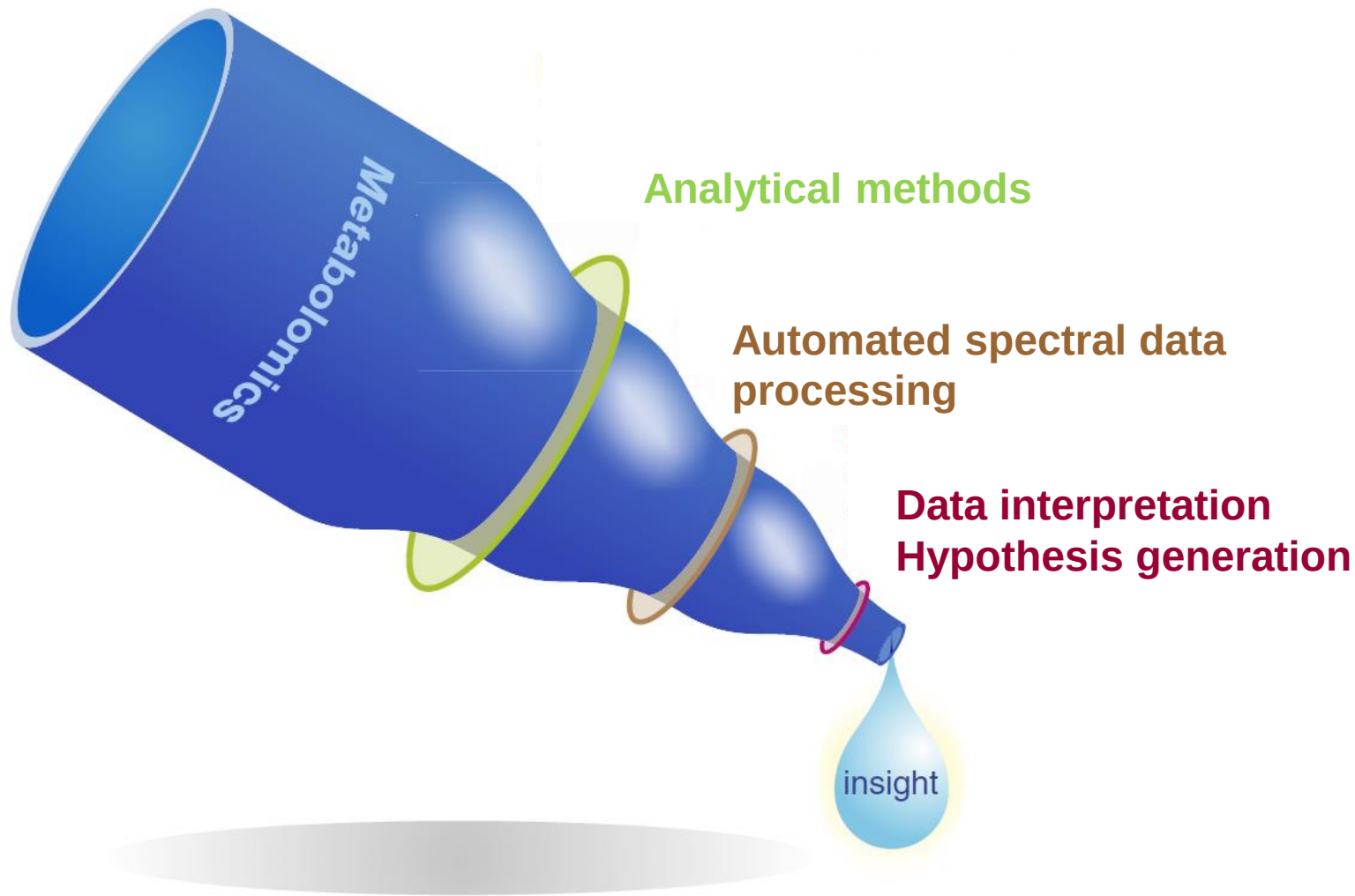
Analytical Methods: Widely Varying Concentrations



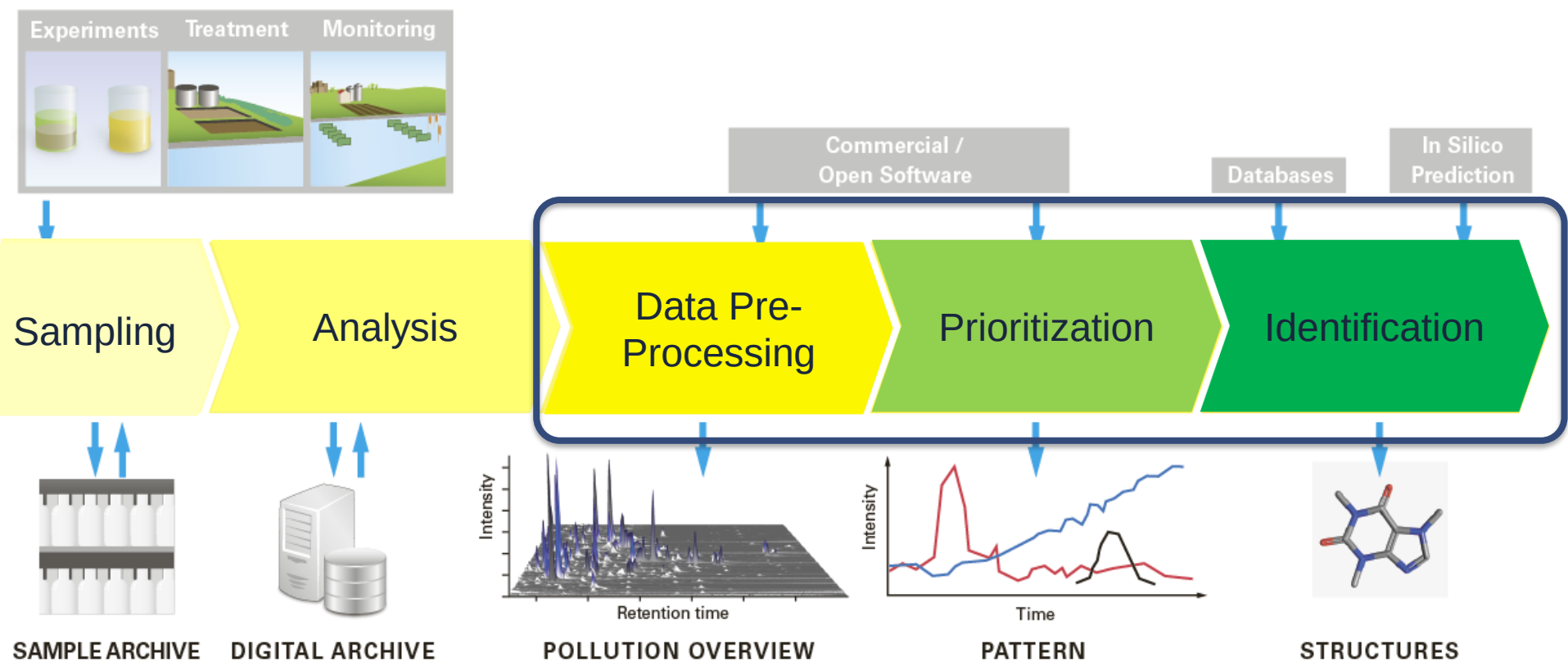
Analytical Methods: Target vs Non-target



Critical Bottlenecks in Biological Interpretation

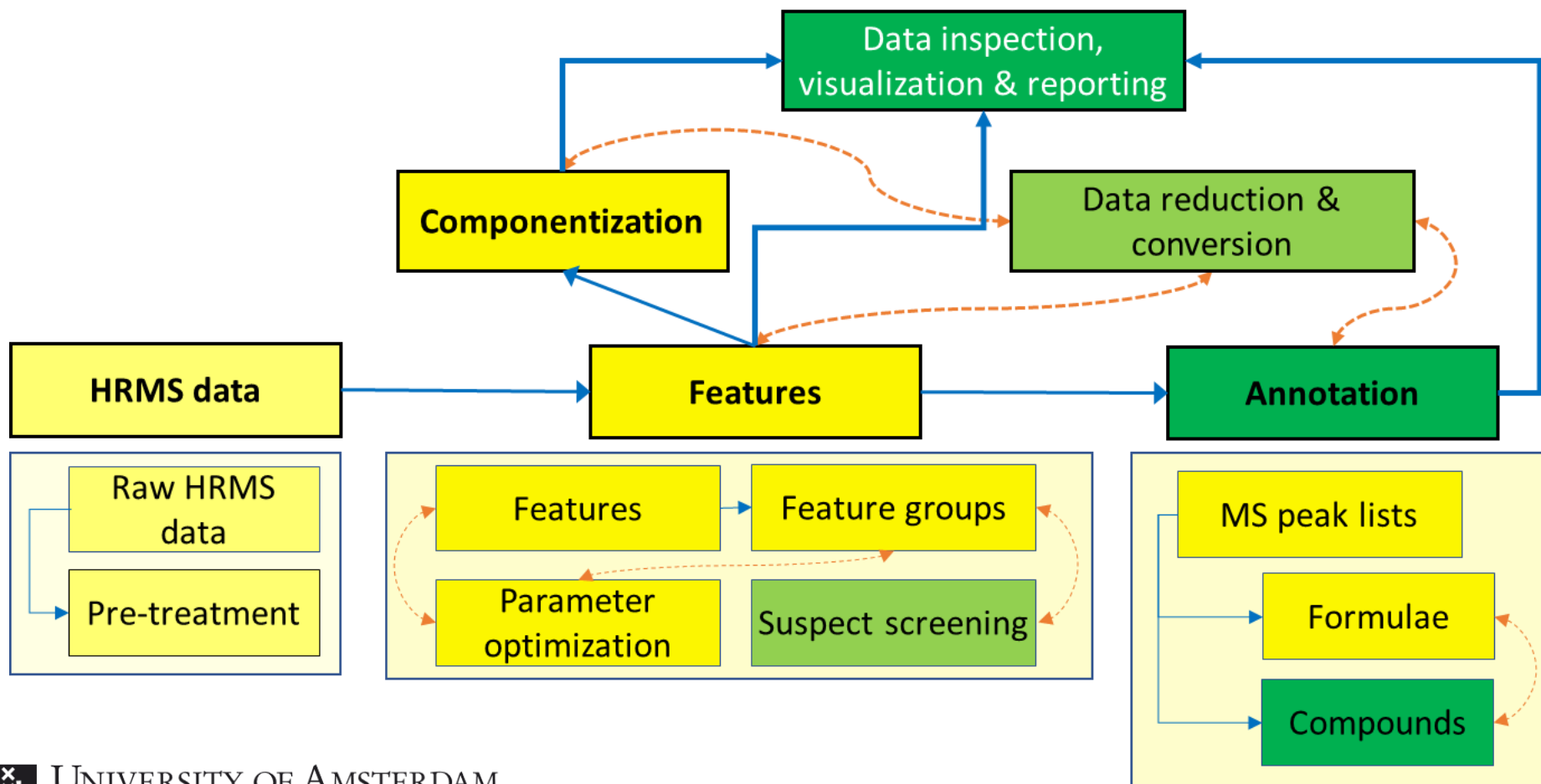


Automated Processing: Looks so simple ...



Automated Processing: ... but isn't ...

- One (current) example:
- patRoon: <https://rickhelmus.github.io/patRoon/>



Automated Processing: ... even meta"R"bolomics ...

MS data handling & processing

- Centroiding
- Direct infusion MS
- Hyphenated MS
- Targeted MS
- Additional dimensionality
- Isotope labelling using MS
- Data structure & meta-data
- Feature grouping
- Feature annotation

NMR data handling & processing

- Data pre-processing
 - Fourier transformation
 - Apodization
 - Zero filling
 - Phase and baseline correction
 - Bucketing
- Annotation & identification

UV data handling & processing

- Alignment
- Baseline correction
- Componentization

Multifunctional workflows

- Data processing workflows
- Multiple statistics and network analysis
- User interfaces and workflow engines

Ion species grouping & annotation

- Grouping of related species
- Molecular formula and isotope analysis
- Adduct/fragment annotation

MS/MS data

- MSⁿ and libraries
- Spectral matching and clustering
- *In silico* fragmentation

Molecule structures & chemical structure databases

- Structure representation and manipulation
- Database queries

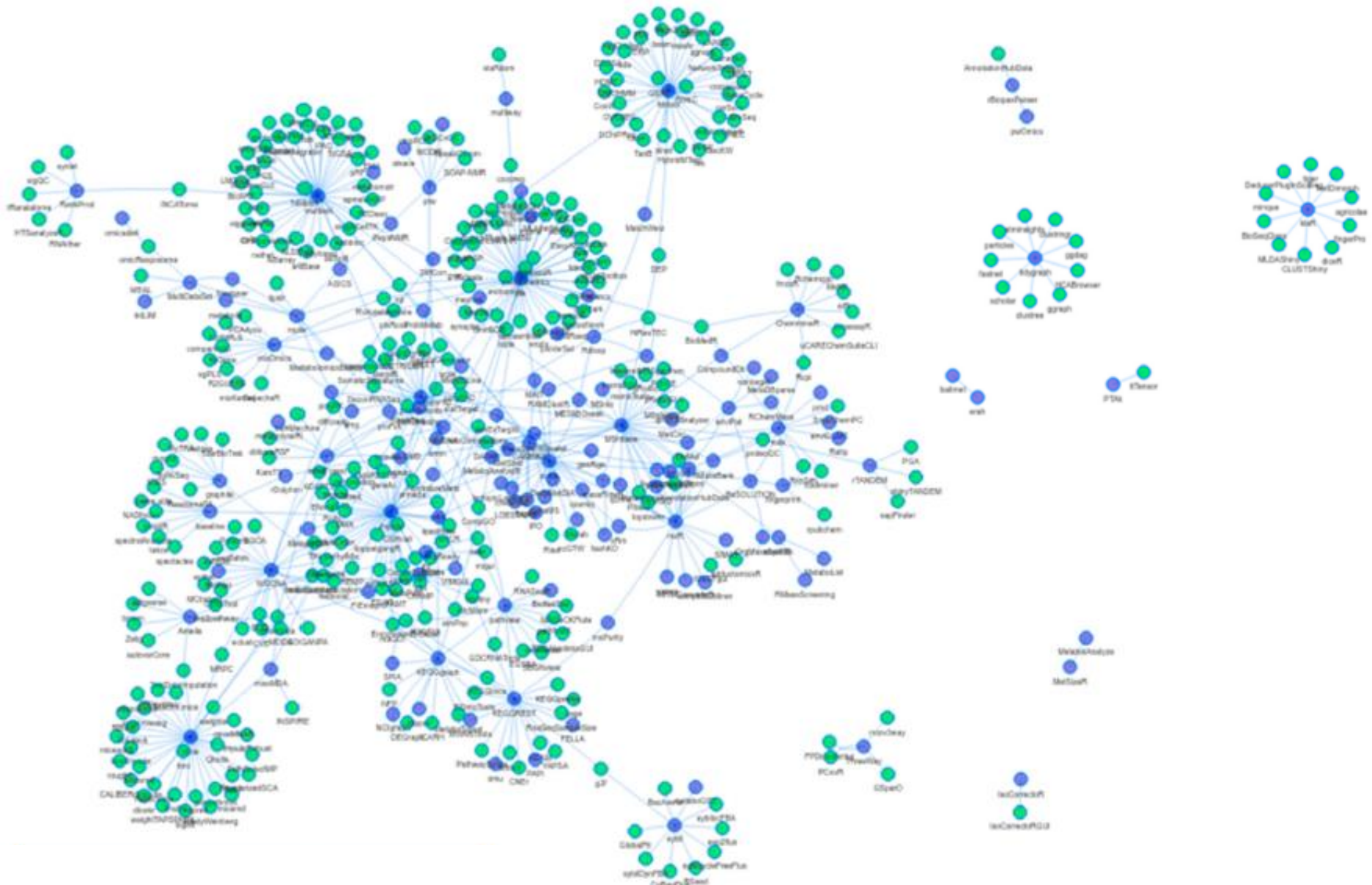
Statistics

- Sample size
- Normalization
- Exploratory data analysis
- Univariate hypothesis testing
- Multivariate modelling and feature selection
- Omics data integration
- Missing value imputation

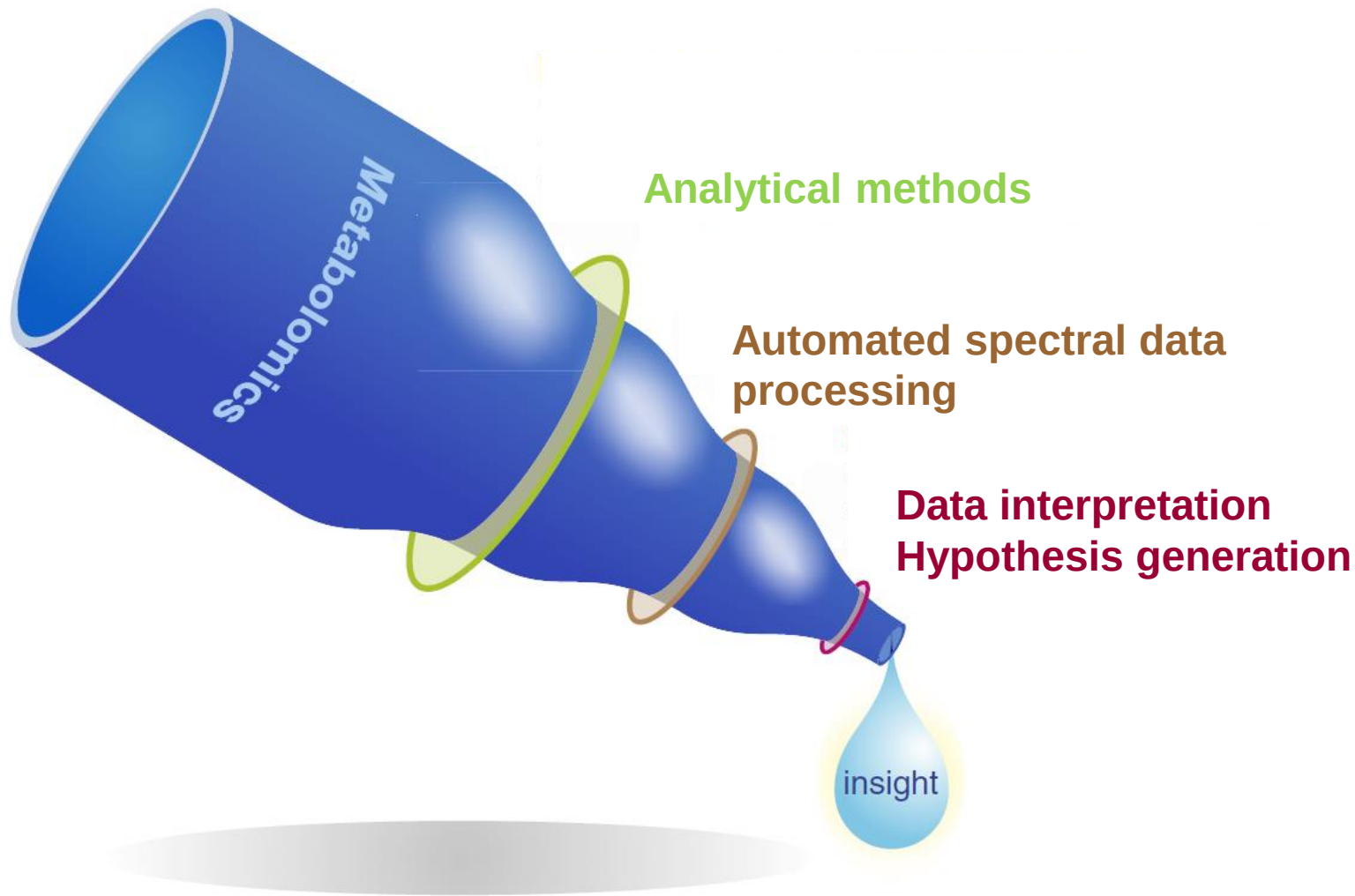
Network analysis & Biochemical pathways

- Network infrastructure and analysis
- Annotation
- Metabolite networks
- Pathway analysis
- Pathway resources and interfaces

Automated Processing: ... even meta”R”bolomics ...

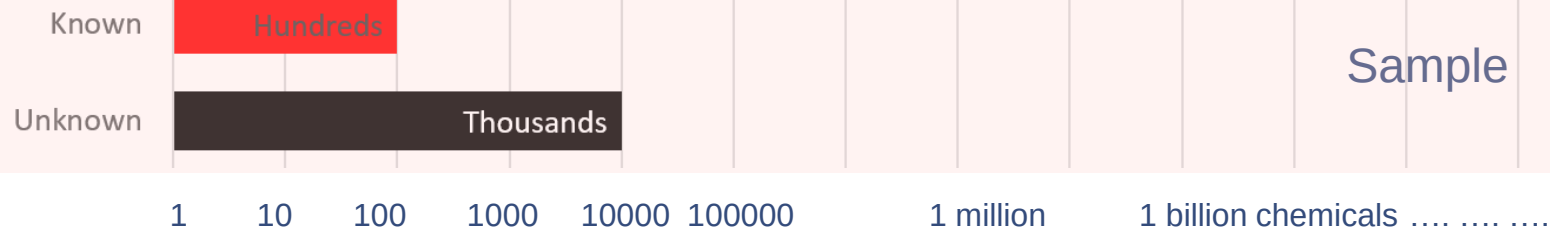
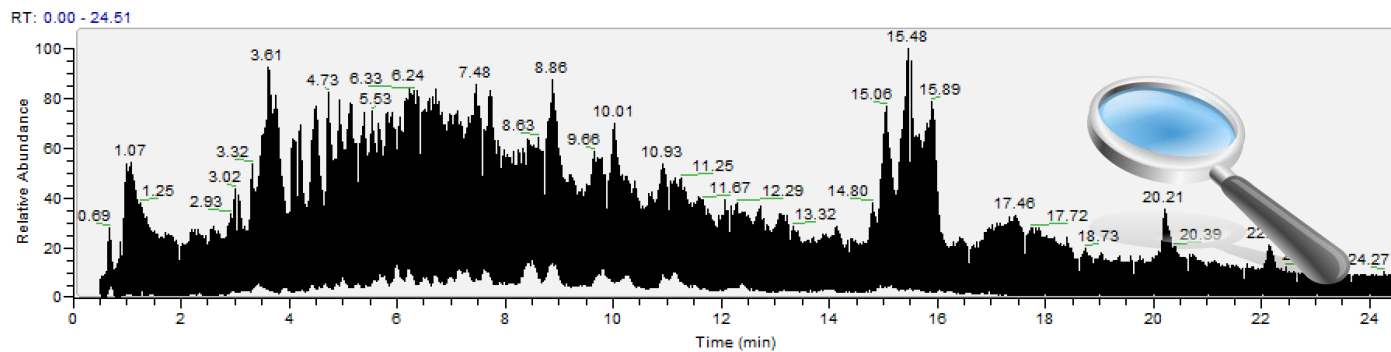


Critical Bottlenecks in Biological Interpretation



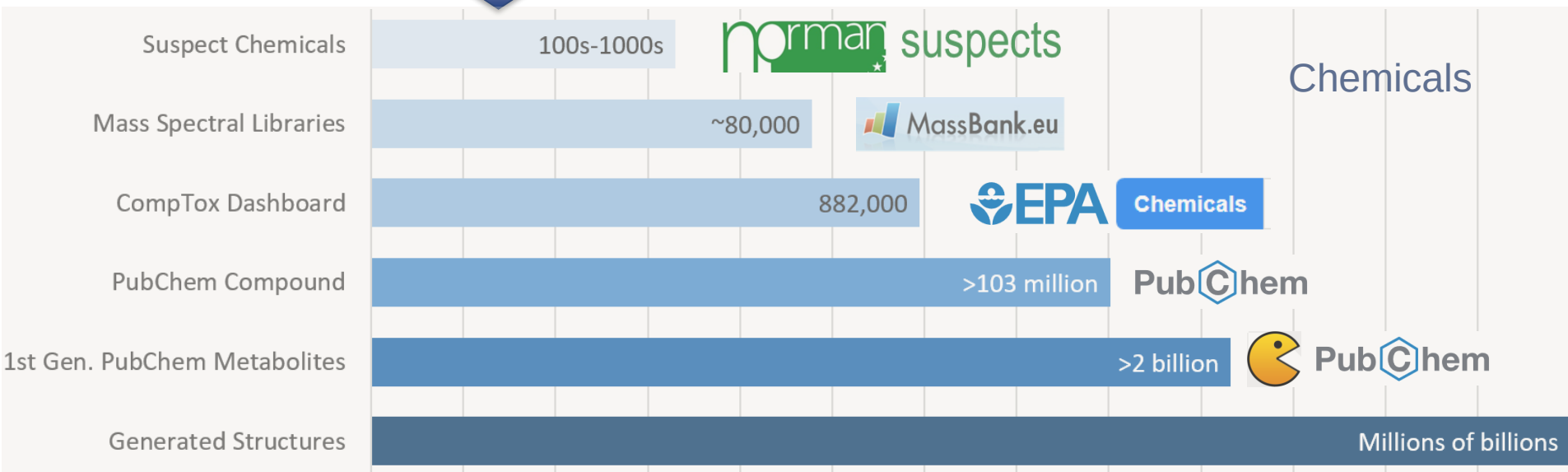
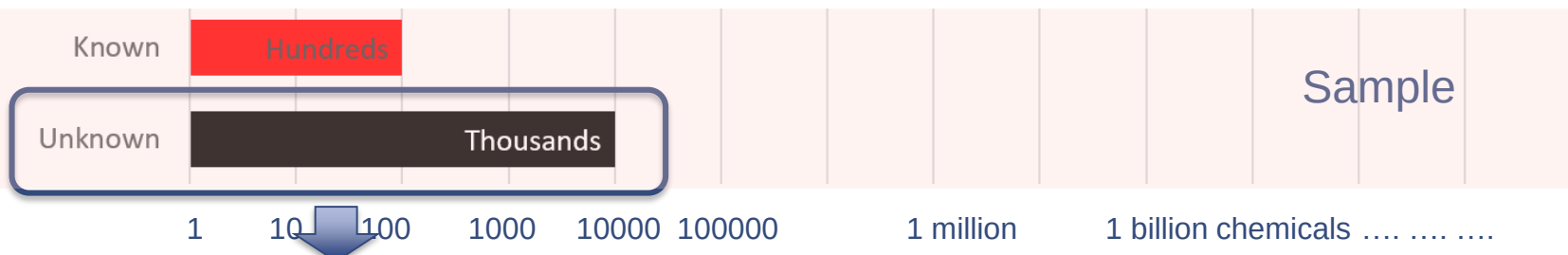
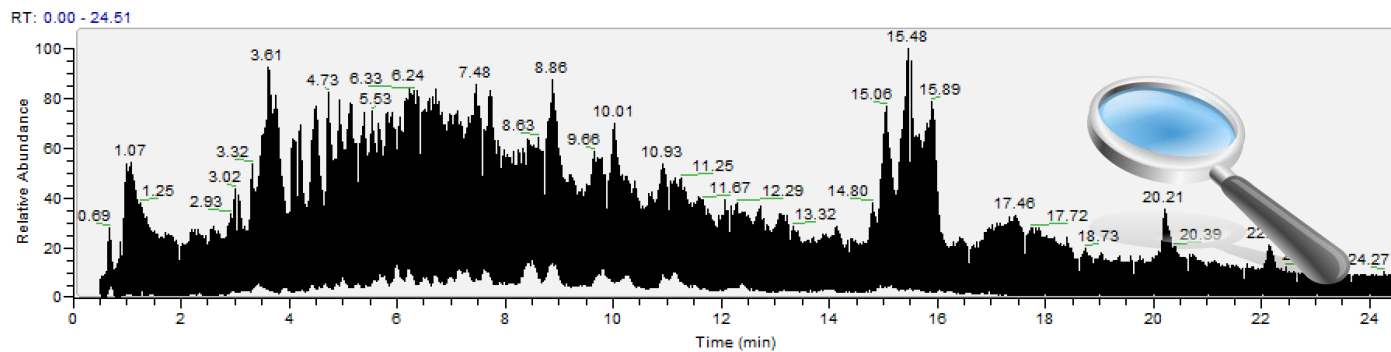
Data interpretation: Identifying Chemicals

High resolution
mass spectrometry

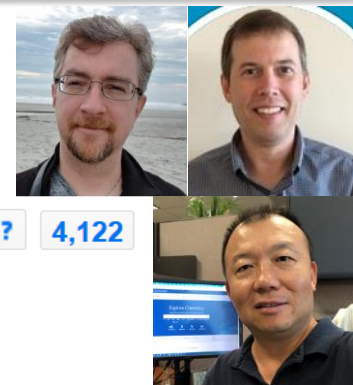


Data interpretation: Identifying Chemicals

High resolution
mass spectrometry
AND connecting
chemical knowledge



Data interpretation: Filling the TP Data Gaps!



PubChem NORMAN Suspect List Exchange

▼ NORMAN Suspect List Exchange Classification ? 117,037

▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 4,122

▶ S25 | OECDPFAS | List of PFAS from the OECD ? 3,680

▶ S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ? 647

▶ S60 | SWISSPEST19 | Swiss Pesticides and Metabolites ? 1,358

▶ S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? 574

▶ S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag ? 258

▶ S68 | HSDBTPS | Transformation Products Extracted from HSDB Content in PubChem ? 97

▶ S69 | LUXPEST | Pesticide Screening List for Luxembourg ? 386

▶ S72 | NTUPHTW | Pharmaceutically Active Substances from PubChem Terbutylazine (Compound)

S00 | SUSDAT | Merged NORMAN Suspect List: SusDat ?

S01 | MASSBANK | NORMAN Compounds in MassBank EU

S02 | STOFFIDENT | HSWT/LfU STOFF-IDENT Database of W

S03 | NORMANCT15 | NORMAN Collaborative Trial Targets an

S04 | UJIBADE | Target List from UJI used in Bade et al 2015

S05 | KWRSJERPS | KWR Drinking Water Suspect List ?

S06 | ITNANTIBIOTIC | Antibiotic List from the ITN MSCA ANS

S07 | EAWAGSURF | Eawag Surfactants Suspect List ? 1

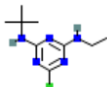
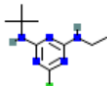
S08 | ATHENSSUS | University of Athens Surfactants and Susp

S09 | PFASTRIER | PFAS Suspect List of fluorinated substance

8.5 Transformations

Page 3 of 25 items View More Rows & Details

Download

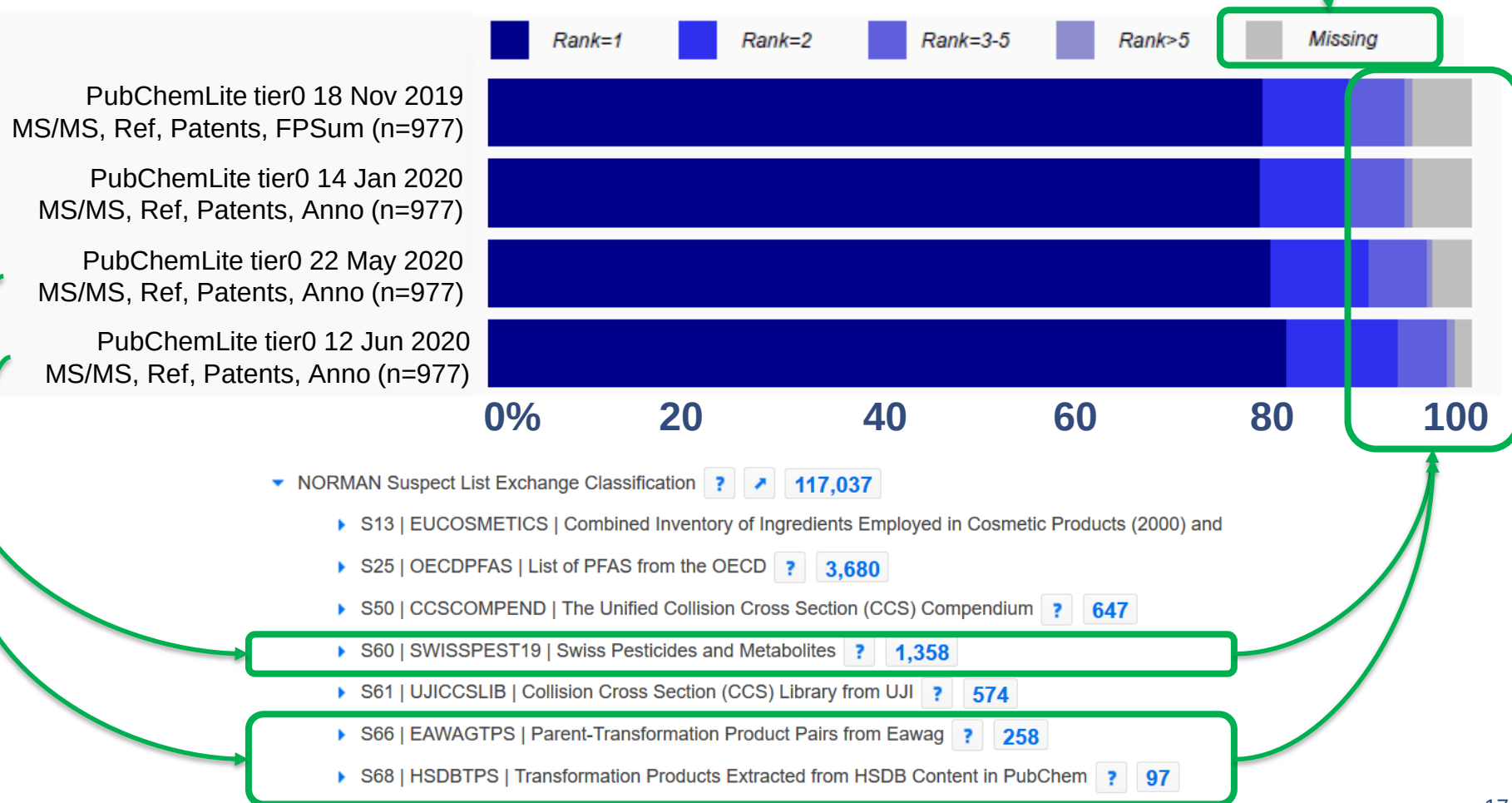
SORT BY Please Choose One					
Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Evidence DOI
	Terbutylazine	Mammalian metabolism		6-Chloro-1,3,5-triazine-2,4-diamine	10.5281/zenodo.3827
	Terbutylazine	Deethylation		Terbutylazine-desethyl	10.1007/s13361-017-

Data interpretation: Filling the TP Data Gaps!

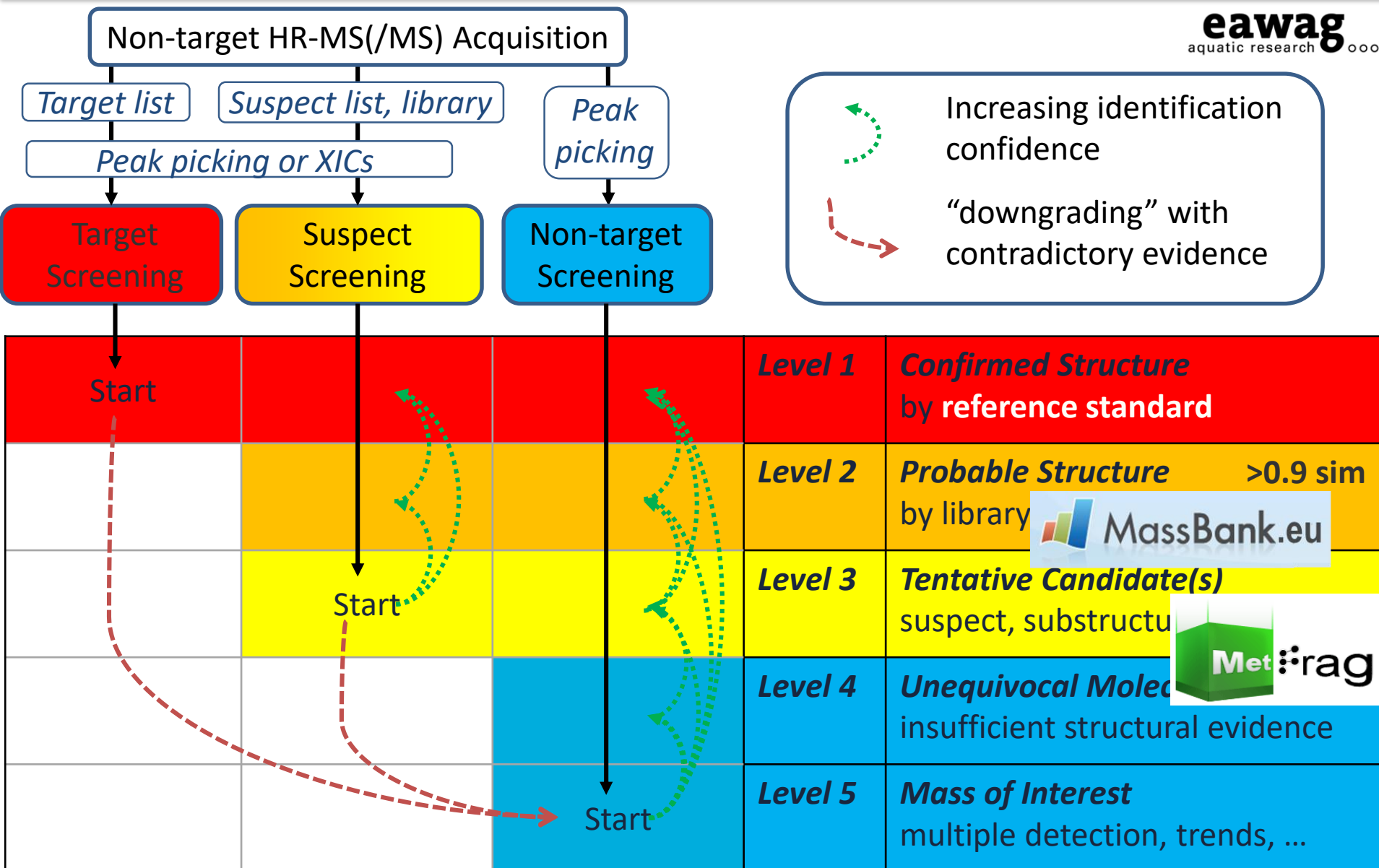


U.S. National Library of Medicine
National Center for Biotechnology Information

○ Assessing (filling) the missing entries ...

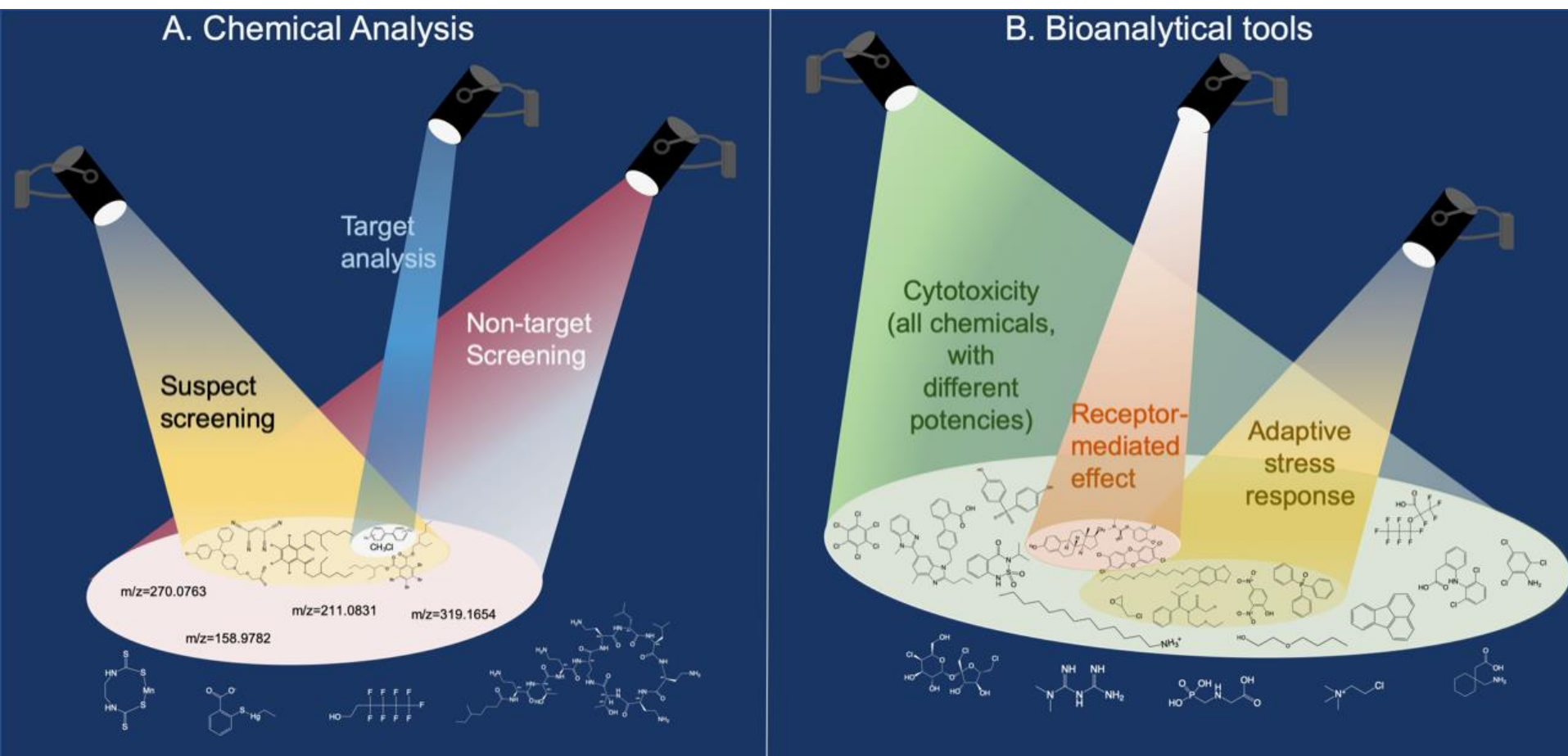


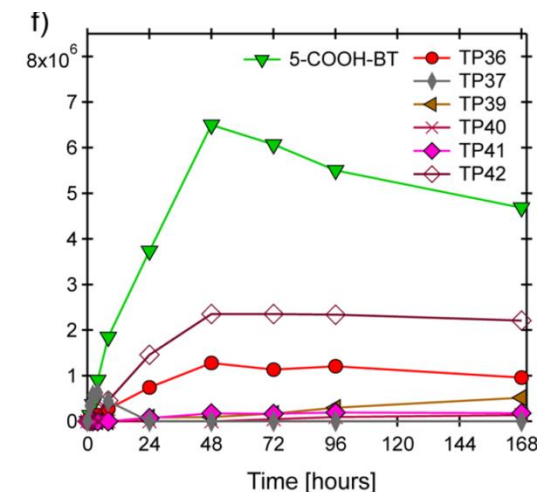
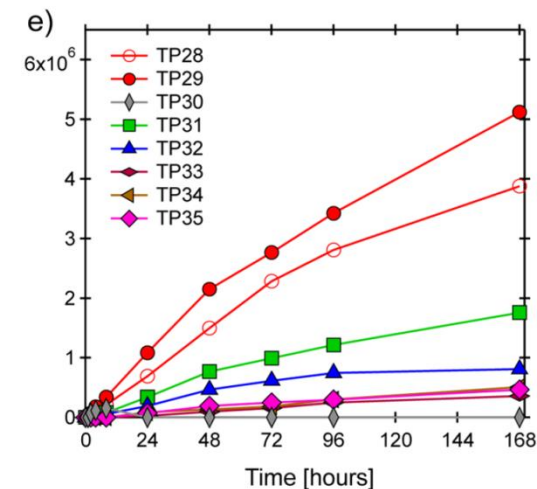
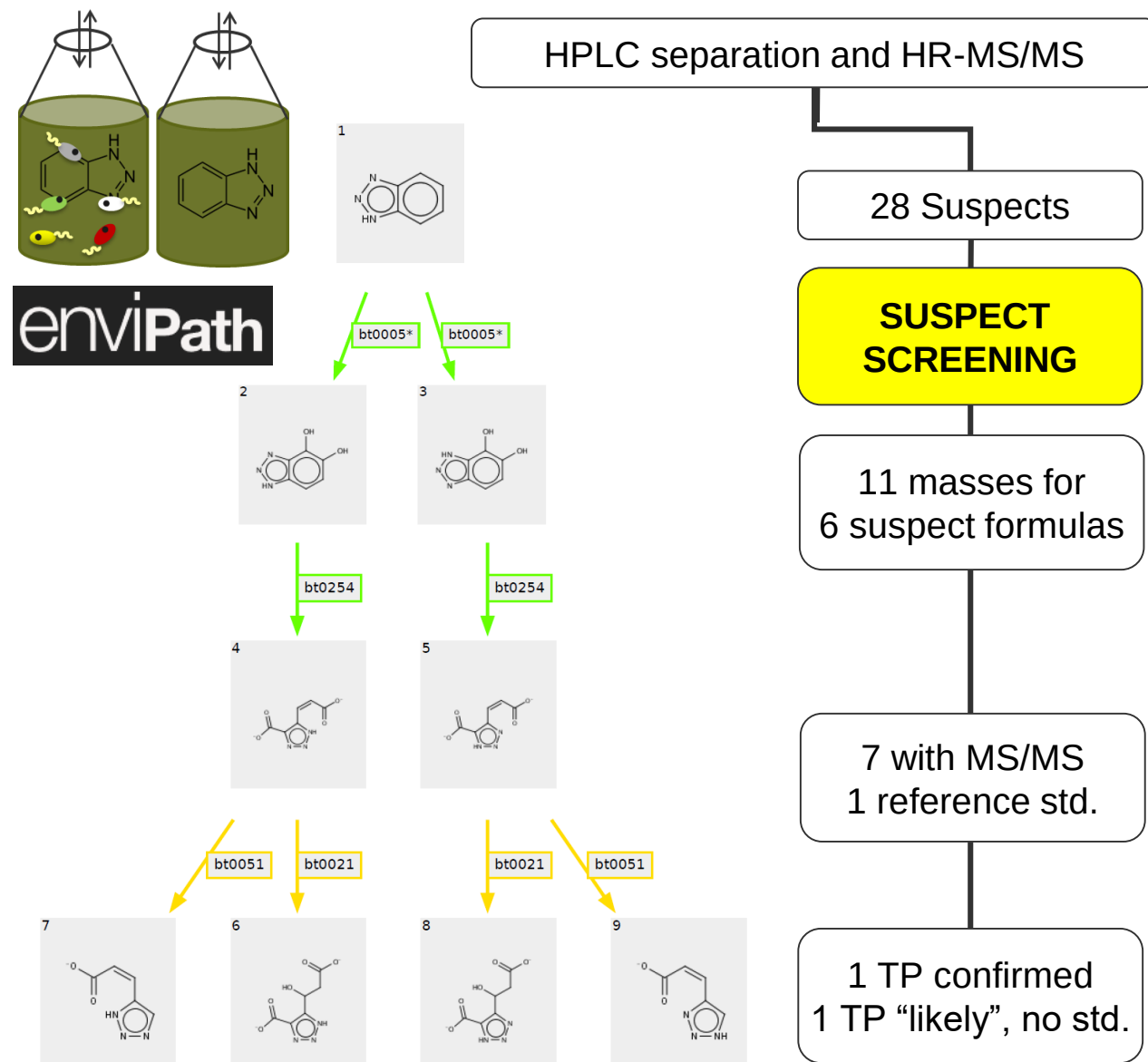
Data interpretation: ID Strategies and Confidence



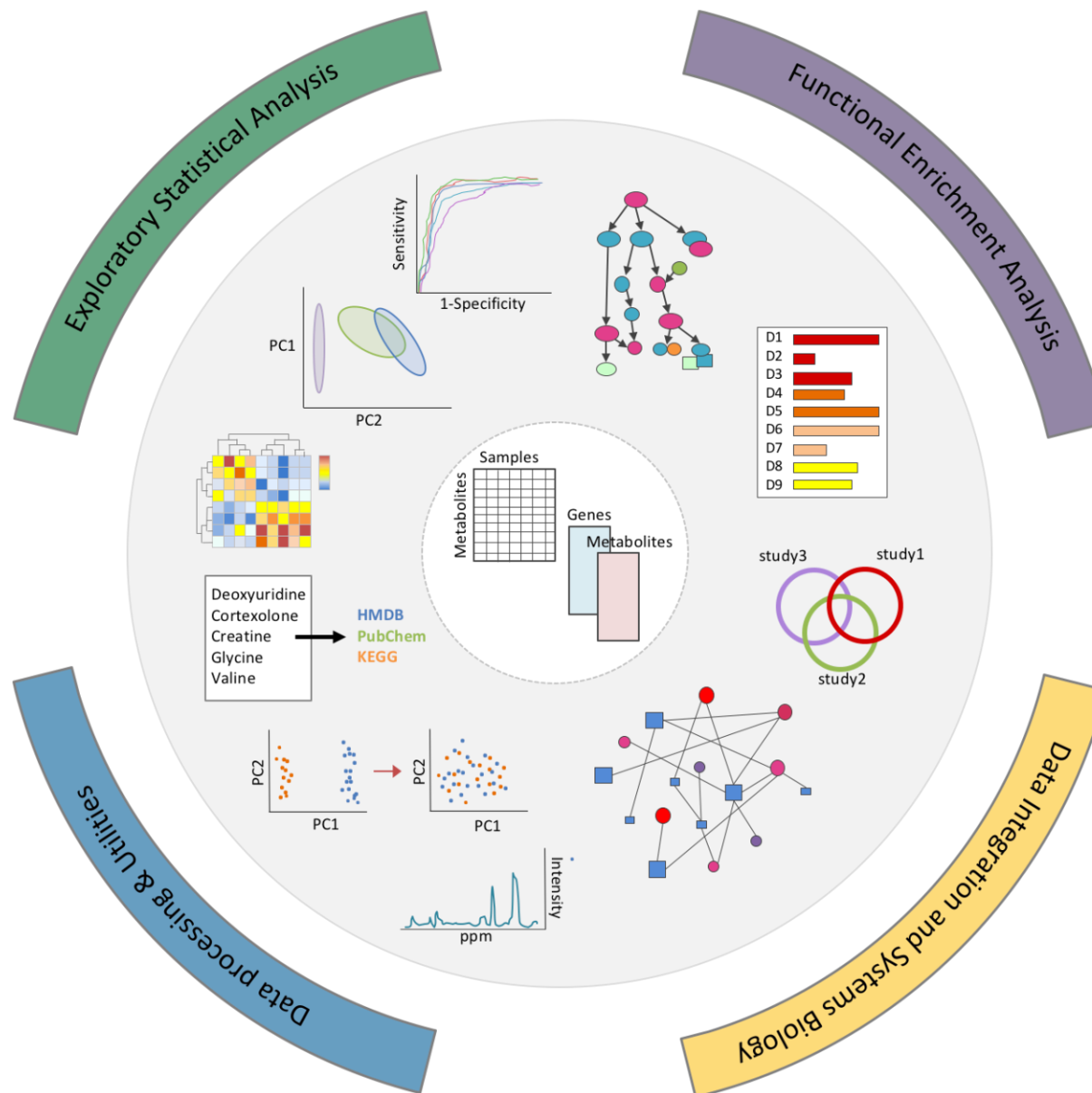
Data interp: Toxicometabolomics ... two worlds collide?

- Metabolomics vs environmental ... chemicals vs effects ...

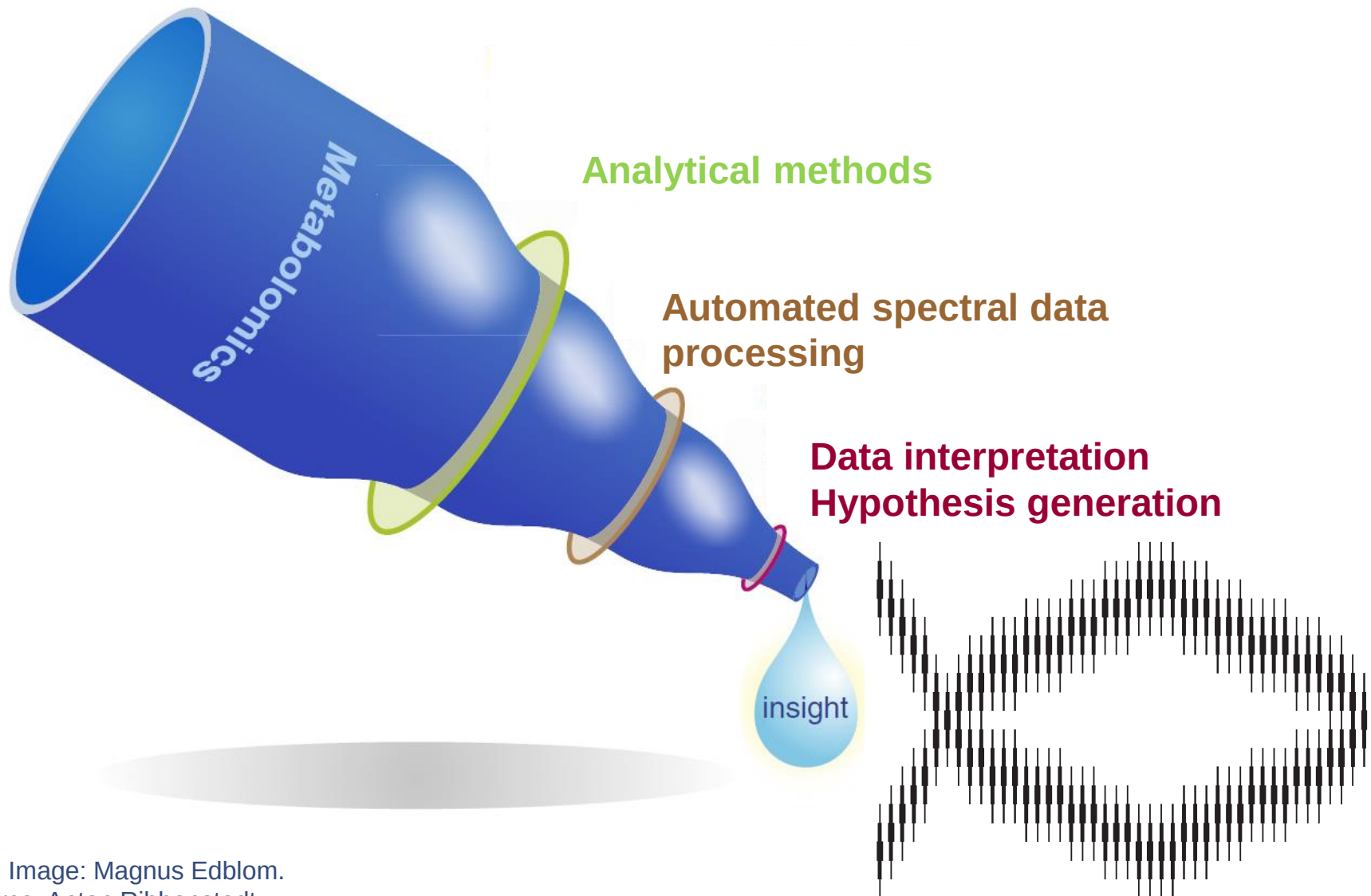




Data interpretation: Metabolomics World ...



Critical Bottlenecks in Biological Interpretation



Fish Image: Magnus Edblom.
Source: Anton Ribbenstedt.