Mass Spectrometric Non-Target Screening in Practice – Quo Vadis?
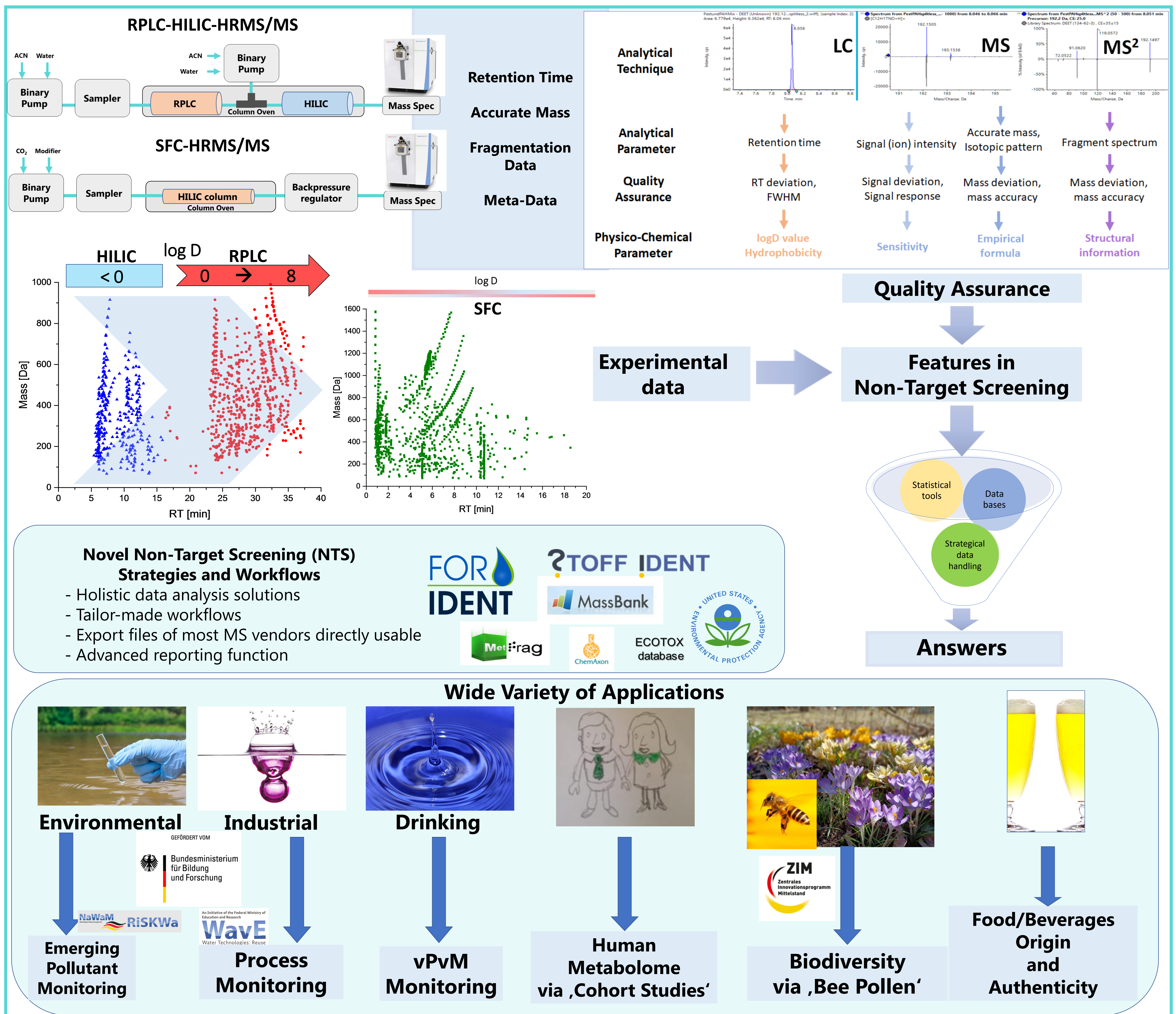
Stefan Bieber and Thomas Letzel

Introduction - Mass spectrometric non-target screening (NTS), non-target analysis and untargeted screening are synonyms for the fact that mass spectrometric driven ion extraction, fragmentation and fragment detection is leading to new insights into very complex samples (sometimes without former molecular knowledge of the experiment-performing analyst).

The analytical performances are wide-spread in using various chromatographic separation, (ion mobility) as well as (tandem)mass spectrometric detection and mostly quality-assured. The subsequent data evaluation and data interpretation steps are ongoing research topics to realize flexible but reproducible data handling as steps like the so called peak picking, componentization, alignment and others. These developments are ongoing but on a good way.

However, new challenges in NTS come up, if one wants to answer specific questions in different disciplines which is mostly very application specific and needs adjusted but robust holistic solutions. On the other hand, there are solutions available that can be used in interdisciplinary context.

This poster presentation includes the similarities and differences of NTS concepts and workflows in different disciplines.

This has direct consequences for the future of NTS in research and in practice; both is shown below.

RPLC-HILIC-HRMS/MS

ACN — Water
Binary Pump — Sampler — RPLC — Column Oven — HILIC — Binary Pump (ACN / Water) — Mass Spec

SFC-HRMS/MS

CO_2 — Modifier
Binary Pump — Sampler — HILIC column (Column Oven) — Backpressure regulator — Mass Spec

Retention Time

Accurate Mass

Fragmentation Data

Meta-Data

	LC	MS	MS^2
Analytical Technique			
Analytical Parameter	Retention time	Signal (ion) intensity	Accurate mass, Isotopic pattern	Fragment spectrum
Quality Assurance	RT deviation, FWHM	Signal deviation, Signal response	Mass deviation, mass accuracy	Mass deviation, mass accuracy
Physico-Chemical Parameter	logD value Hydrophobicity	Sensitivity	Empirical formula	Structural information

HILIC log D **RPLC**
< 0   0 → 8

SFC

Mass [Da] vs RT [min]

Quality Assurance

Experimental data → **Features in Non-Target Screening**

Statistical tools | Data bases | Strategical data handling

Answers

Novel Non-Target Screening (NTS) Strategies and Workflows
- Holistic data analysis solutions
- Tailor-made workflows
- Export files of most MS vendors directly usable
- Advanced reporting function

FOR IDENT | STOFF IDENT | MassBank | MetFrag | ChemAxon | ECOTOX database | UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

Wide Variety of Applications

Environmental | **Industrial** | **Drinking**

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung

NaWaM RiSKWa | WavE Water Technologies: Reuse

ZIM Zentrales Innovationsprogramm Mittelstand

Emerging Pollutant Monitoring | **Process Monitoring** | **vPvM Monitoring** | **Human Metabolome via 'Cohort Studies'** | **Biodiversity via 'Bee Pollen'** | **Food/Beverages Origin and Authenticity**

Create new paradigms in complex sample analysis using Non-Target Screening workflows !

Get **answers for YOUR analytical questions** and conduct molecule or sample characterization and/or statistical data interpretation

Reference:
S. Bieber, G. Greco, S. Grosse, T. Letzel: RPLC-HILIC and SFC with mass spectrometry: Polarity-extended organic molecule screening in environmental (water) samples. Analytical Chemistry 2017, 89 (15), 7907-7914 (DOI: 10.1021/acs.analchem.7b00859).