# Mass Spectrometric Non-Target Screening – Interdisciplinary Solutions and Data Handling

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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 analyst, performing the analysis).

In our days, the analytical performances are challenging in using various chromatographic separation techniques, (ion mobility) as well as (tandem)mass spectrometric detection. On the other hand, these systems are mostly quality-assured and robust useable. The subsequent data evaluation and data interpretation steps are ongoing research topics to realize flexible but reproducible data handling. Workflow steps like the so-called peak picking, componentization, alignment and others [1] as well as their combination are under development 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. However, there are solutions available that can be used in interdisciplinary context.

This lecture will present and include the similarities and differences of NTS concepts and workflows in different disciplines. Such NTS data handling pipelines are presented for real life solutions in environmental analysis (with the identification of emerging compounds like PFAS in water samples [2]), in plant metabolomics samples (with the molecular reflection of metabolomics pathways [3]), in food analysis (with focus on authenticity check), in process analysis (with salty waters) and in clinical analysis (with a view on disease biomarkers).

The state-of the art reflection gives direct consequences for the future of NTS in research and in practice; both will be discussed.

References:

[1] S. Minkus, S. Bieber and T. Letzel: Spotlight on mass spectrometric non-target screening analysis: Advanced data processing methods recently communicated for extracting, prioritizing and quantifying features. *Analytical Science Advances*, **2022**, 1-10.
[2] H. Ulrich, A. Macherius, U. Kunkel, M. Sengl, T. Letzel: Novel PFAS-specific monitoring approach for highly impacted surface waters. *Chemosphere*, **2024**, 349 (2), 140893.
[3] R. Wahman, C. Cruzeiro, J. Graßmann, P. Schröder, and T. Letzel: The changes in Lemna minor metabolomic profile: a response to diclofenac incubation. Chemosphere, **2022**, 287(1), 132078.