Analytisches Forschungsinstitut für Non-Target Screening GmbH

AFIN-TS

Retrospective Data Evaluation and Data Handling in Non-Target Screening

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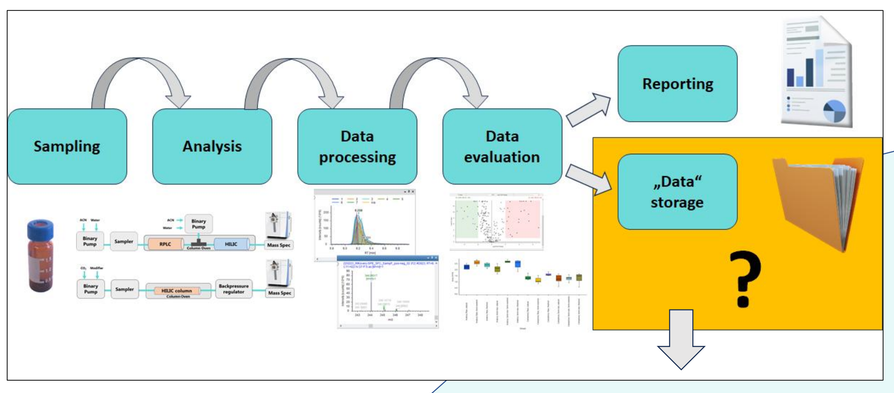
Introduction - Until now, a large part of the working time spent on evaluating NTS data has been devoted to the use and transfer of data between individual NTS software solutions. Since these are mainly standalone proprietary or open-source software tools, it makes sense to bring them together on one platform and combine them into workflows known as pipeline solutions. For this purpose, a demonstrator was developed based on the **Open Semantic Lab** (OSL), which is based on the open-source software modules called **NTS-Hive**. The 'OSL' concept now enables, for the first time, the active, functional and flexible integration of the tools used on the basis of standardised interfaces, as well as the consistent use of intelligent data analysis to improve analytical NTS results on an innovative digital platform with the integration of device, data processing, data interpretation and report-specific components. This means that individual solutions are still possible, but for the first time, a wide range of components can be used, adapted and expanded in an innovative, secure, sustainable and FAIR-compliant digital environment for all NTS work.



Retention Time

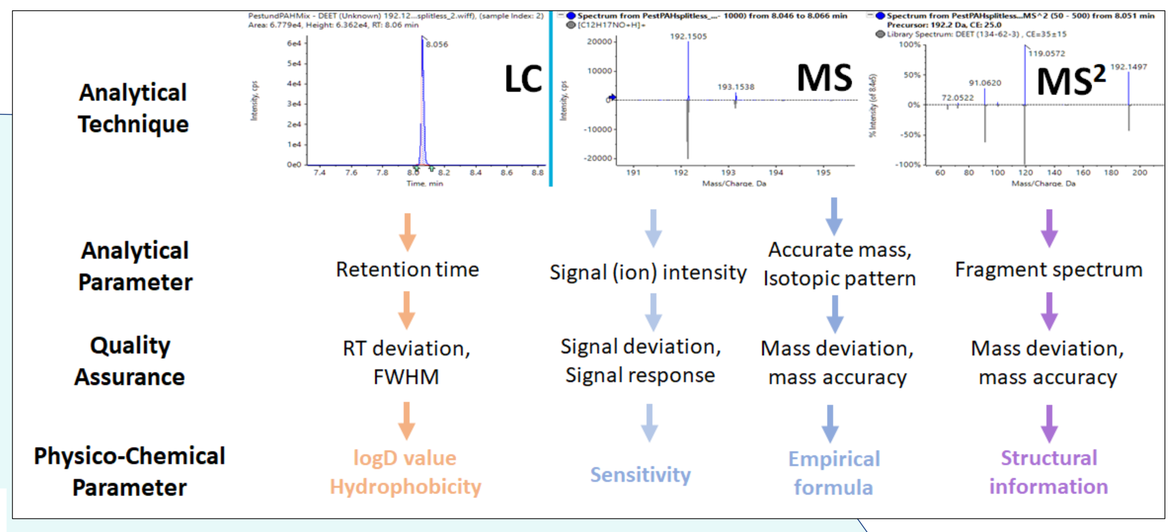
Accurate Mass

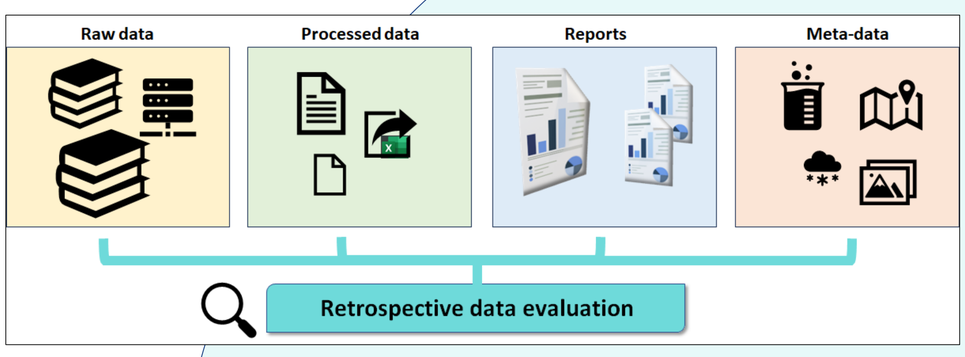
Signal Intensity

Fragmentation Data

&

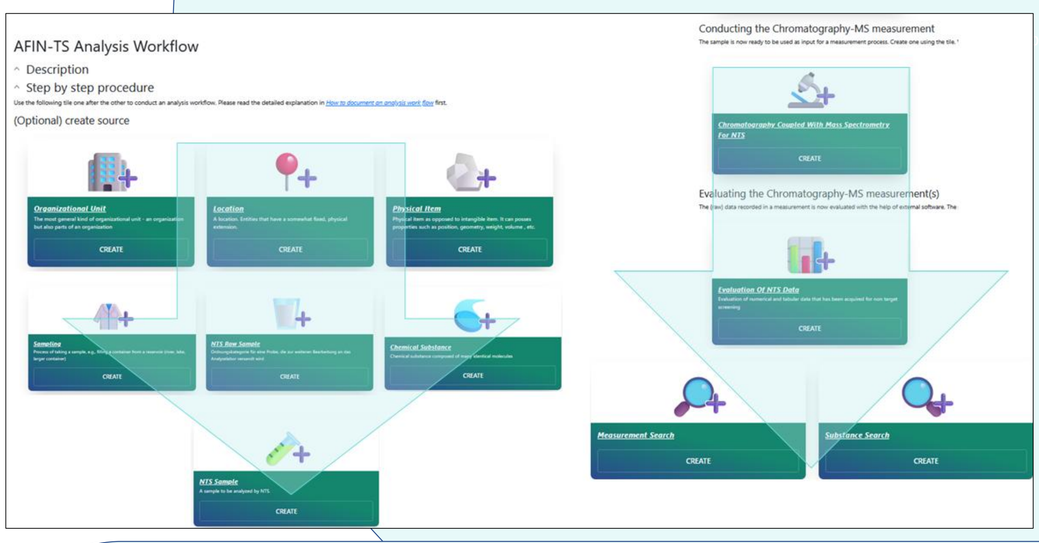
Meta-Data

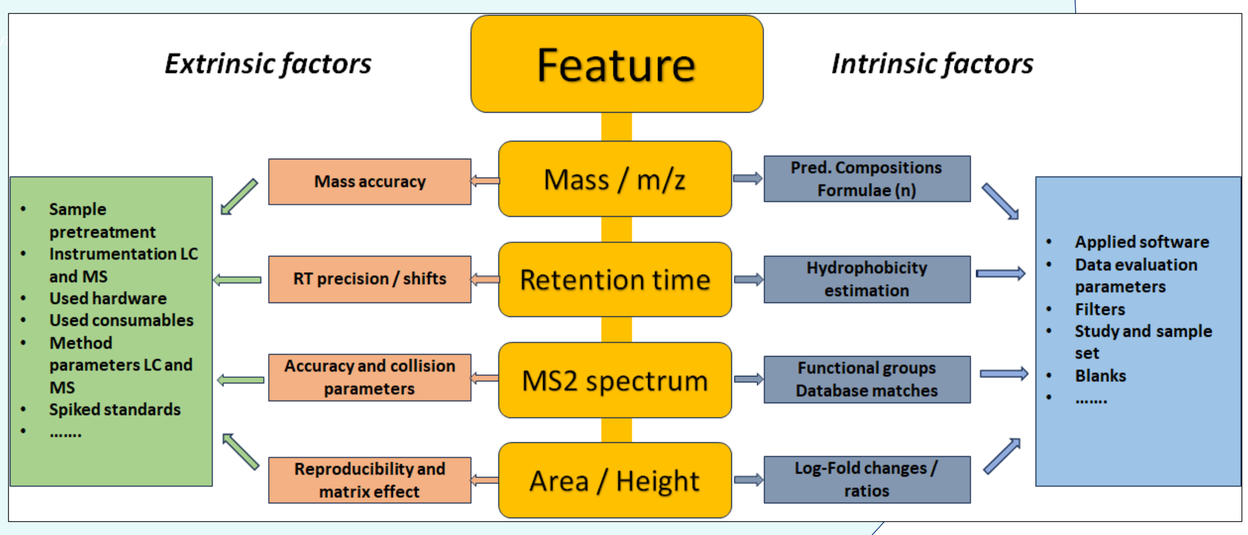




NTS Hive

Holistic NTS data management platform

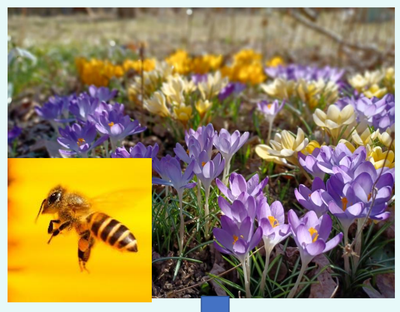




Environmental

Industrial

Drinking



https://de.freepik.com/

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

NaWaM RiSKWa

An Initiative of the Federal Ministry of Education and Research 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/ e.g. Coffee/ Oil Origin and Authenticity

Create new paradigms in complex sample analysis using
Non-Target Screening and restrospective data analysis concepts !
Get **YOUR NTS data prepared for retrospective analysis and actively available for machine learning tools as well as AI-ready** !

German References:
S. Bieber und T. Letzel: Analytik neu gedacht. Nachrichten aus der Chemie (GDCh), 2025, 73 (1), 47-49;
S. Bieber und T. Letzel: Retrospektiver Einsatz von Non-Target Screening: Moderne Datenspeicherung, -nutzung und -interpretation. Wasserforum- Sonderpublikation zum 16. Langenauer Wasserforum 2025, 11.

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