



**Analytisches Forschungsinstitut für Non-Target
Screening GmbH**

AFIN-TS

AFIN-TS is an independent research institute in the novel area of 'mass spectrometric non-target screening' (NTS), as well as other related analytical sciences, using chromatographic separation techniques hyphenated with (tandem-) mass spectrometric detection.

AFIN-TS offers a broad spectrum of services, including education in chromatography, spectroscopy, mass spectrometry and NTS, consulting for analytical institutions as well as the transfer of NTS -knowledge and -technologies to analytical institutions and also the NTS analysis of samples. Furthermore AFIN-TS supports basic analytical research, creating workflow strategies and process optimization therein.

Expand analysis towards the unknown and unexpected

Non-target screening can answer analytical questions in many areas and disciplines, such as food, pharma and environmental analysis, metabolomics or foodomics. It can be applied to characterize samples by molecular fingerprinting, to compare different samples, or to detect trends among samples. But NTS is also well suitable for the identification of new, unexpected or unknown organic compounds.

Even well characterized samples can contain relevant and not yet detected compounds. Depending on the nature of the sample and the aim of the analytics, the presence of such unknown compounds can be of concern and relevance. The occurrence of unexpected molecules (e.g. industrial chemicals, pharmaceuticals, compounds of daily use, and others) cannot be monitored with classical (quantitative) 'multi residue monitoring' (MRM) analytical approaches. Non-target screening can be conducted in parallel to already implemented approaches, allowing to monitor the presence or to determine the concentration of known hazardous compounds in samples and to simultaneously screen for unexpected or unknown compounds. This can be beneficial for all kinds of food safety analytics, where samples are regularly screened for the



presence of pesticides, biocides, or (from packaging) migrating compound. NTS can here be applied for the screening for non-intentionally added substances (NIAS) in food analysis, or the screening and identification of unexpected compound residues of anthropogenic origin in environmental samples. But NTS can also be used to monitor industrial production processes and help to identify unexpected by-products, or side-reactions. The following described NTS techniques often allow here to identify novel unexpected contaminants and to compare samples.

Analytical challenges

There is –as stated above- a significant difference between non-target screening and commonly conducted, targeted and quantitative single- or multi-compound analytics (like MRM). Instead of focusing on specific compounds in a sample, using non-target screening a large number of signals can be recorded in an unfocused detection process. The data, which can easily contain several thousands of data points (Figure 1) has to be evaluated thoroughly.

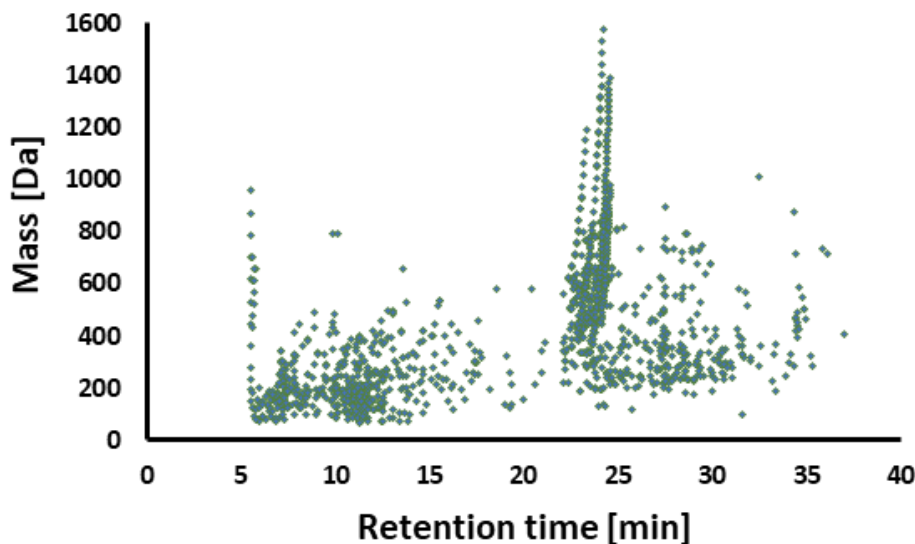
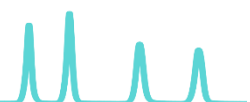


Figure 1: Retention time - mass plot of a complex sample, analyzed with non-target screening using (LC-)LC-MS/MS.

To gain a most comprehensive view on investigated samples, all steps of the analytical process have to be adjusted and validated. Since complex samples often contain a broad spectrum of organic compounds with very different characteristics, powerful chromatographic techniques and mass spectrometric detection are required. Depending on the composition of a sample, **gas chromatography (GC)**, **liquid chromatography (LC)**, and/or **supercritical fluid chromatography (SFC)**, all coupled to high resolution mass spectrometry can be applied in tailored workflows answering specific analytical questions. With samples containing non-polar, polar and/or very



polar compounds, the use of **reversed phase liquid chromatography (RPLC)** and/or **hydrophilic interaction liquid chromatography (HILIC)**, respectively as separation technique can be necessary. If the full range of non-polar to very polar compounds is needed to be separated at once, polarity extended separation techniques, such as the **coupling of RPLC and HILIC** or polar SFC can be utilized.

Subsequently to a successful separation of molecules, an accurate and sensitive mass spectrometric detection is required. The range of detectable masses should be chosen as broad as possible. Thus, high resolution and highly accurate tandem-mass spectrometers, such as Orbitrap instruments or Q-TOF systems are mostly used. These instruments allow to scan very large mass ranges and to provide **molecular weight** and **molecular structure information** of most detected molecules. Data recording is unrestricted, allowing to scan the full mass range during the total analytical experiment. This typically results in a large amount of data, which have thoroughly and transparently been evaluated in the following workflows. Each recorded data point (like shown in Figure 1), consists of retention time, molecular mass, fragment spectra and signal intensities, derived from the analysis, but there are also further information levels, which play an important role in non-target data evaluation. Examples are the **elemental composition and elemental formula**, obtained from the accurately detected mass, **structural information**, the **hydrophobicity** of a compound and **meta-information** (see Figure 2), such as the origin and nature of the sample or its pre-treatment. All this data and information can be combined in innovative and robust workflows, allowing to identify relevant data points.

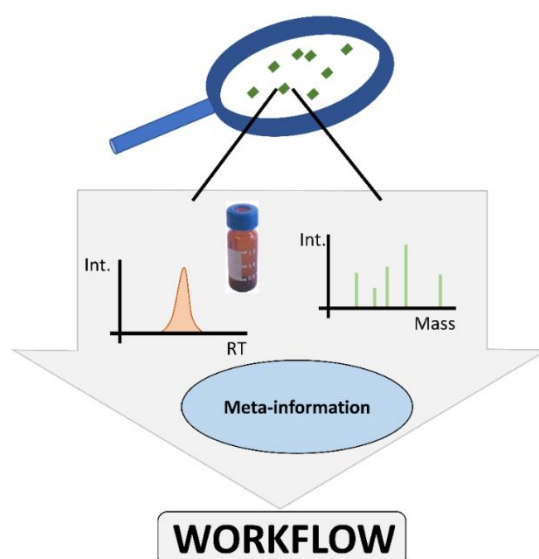


Figure 2: Typical Non-Target Screening scheme, highlighting the essential data analysis in specific workflows.

Intensive and professional support

The services of AFIN-TS cover all aspects of mass spectrometric NTS (including chromatography), from education and training, over consulting for the development of customer-specific NTS strategies, to the creation of tailor-made NTS workflows. In our well-equipped lab, we offer NTS analysis, customer-specific method development and capacities to conduct basic research.

Education (personal and institutional):

Concepts, seminars, and in-house workshops as well as virtual reality solutions covering the following topics:

- Separation techniques, such as RPLC, HILIC, SFC and polarity extended separation techniques
- Mass spectrometry
- Non-target screening (general and specific)

Consulting (personal and institutional):

Comprehensive consulting and support for the establishment of NTS:

- Development of operational procedures
- Optimization of existing analytical processes
- Perspective establishment and NTS applications for future scenarios

Workflows:

Development and adjustment of data evaluation strategies in close collaboration with clients, ensuring a highly efficient implementation and usage of NTS workflows and strategies.

For further information about the services of AFIN-TS and more details about the benefits of NTS, please feel free to contact us:

AFIN-TS GmbH Am Mittleren Moos 48 D-86167 Augsburg Germany

www.afin-ts.de

info@afin-ts.de

