The ‚Analytisches Forschungsinstitut für Non-Target Screening' vs. AFIN-TS GmbH is an independent educational, consulting, supporting, technological-transfering institution performing also analytical research with an overall focus in the novel field of mass spectrometric Non-Target Screening (NTS).

Find the 'Unknowns' close to the 'Knowns'

Mass spectrometric NTS is well suitable for the identification of new, unexpected or unknown organic compounds. This provides special benefits for the investigation of complex samples in various disciplines. Even well characterized samples can contain relevant and yet not 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.

Non-target screening is a universal technique that can be applied in many areas, such as food analysis and the screening for MOSH/MOAH or Non-Intentionally Added Substances (NIAS). The occurrence of unexpected molecules (e.g. industrial chemicals, pharmaceuticals, 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, such as beverages, vegetable and organic food samples, which are regularly screened for the presence of pesticides, biocides, or (from packaging) migrating compounds. The following described

NTS techniques often allow here to identify novel unexpected contaminants and to compare samples (like in authenticity tests).

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, a large number of signals can be recorded in an unfocussed detection process using non-target screening. The data, which can easily contain several thousands of data points (see Fig. 1) has to be evaluated thoroughly.
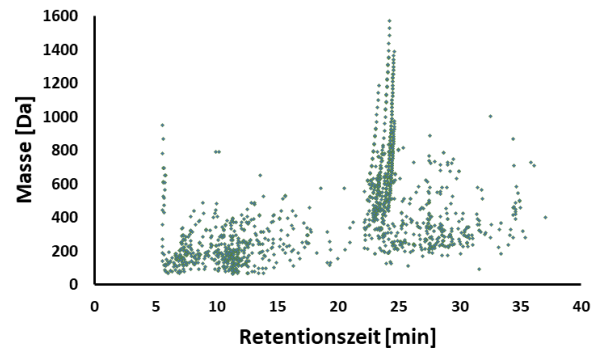

Figure 1: Retention time- mass plot presenting a Non-Target Screening measurement of a complex sample

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. 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

supercritical fluid chromatography (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. 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.
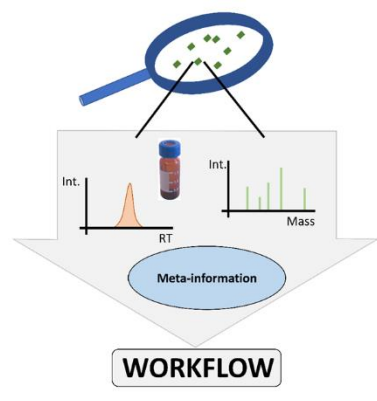

Figure 2: Typical Non-Target Screening Scheme highlighting the essential data analysis in specific workflows.

Intensive and professional Support

AFIN-TS provides comprehensive, professional and general support in all areas of non-target screening. This includes NTS education, NTS consulting, support in establishing as well as in transferring non-target screening strategies and the development of workflows, fitting for individual analytical challenges.

AFIN-TS operates its own N-TS laboratory where you can commission sustainable studies as well as projects. With this you can also start a long-term analytical product support.

Further key focuses are on:

Education (personal and institutional):
Concepts, seminars, and in-house workshops as well as augmented reality and virtual reality solutions covering the following topics:

- 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.

Contact:
AFIN-TS GmbH
Am Mittleren Moos 48
D - 86167 Augsburg, Germany
E-Mail: info@afin-ts.de; Web: www.afin-ts.de