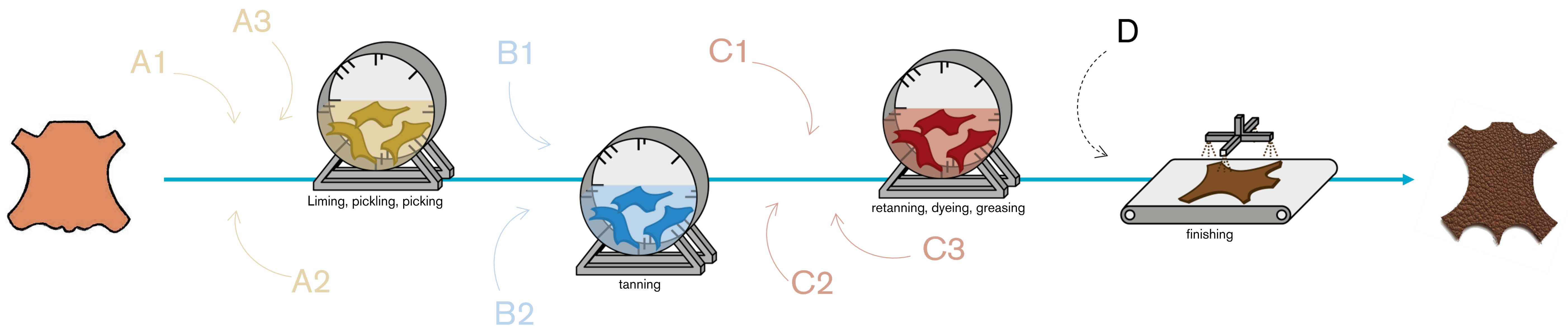


MS SIMILARITY FACTOR A TOOL FOR DATA EVALUATION

Introduction

Quality assurance and control are essential tools in the manufacturing industry in order to identify deviations from reference values and potential material defects at an early stage of production. This not only ensures a high quality standard, but also guarantees customer satisfaction. Py-GC/MS has proven to be a suitable test method for the monitoring (continuous control of the production steps) of such production chains. However, the quick and easy evaluation and interpretation of the complex (Py-)GC/MS data is quite complicated. This inevitably results in the need for trained, scientific staff. For this reason, we have developed an evaluation tool that automatically compares two Py-GC/MS data sets, resulting in a similarity factor at the end.

Simplified production chain of leather



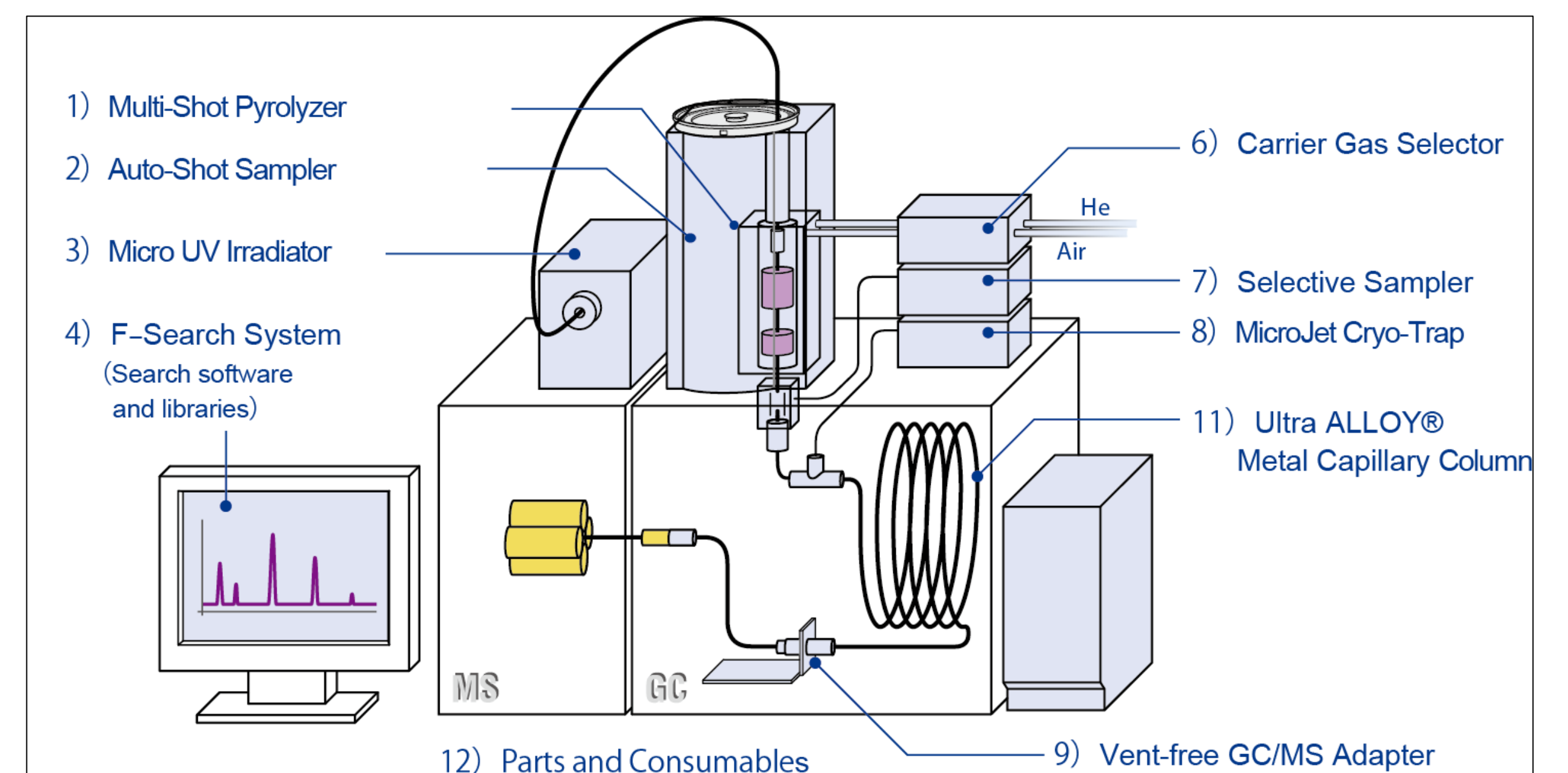
Monitoring means that quality control can be carried out after each manufacturing step. For this reason basic materials (A-D), intermediates and end products must be analyzed.

The problem/dilemma of simple evaluation and interpretation of complex data in the industry

- you have to make decisions **quickly** (e.g. is the quality of the basic material high enough to be put into the production?)
- you have to analyze **process-accompanying** (there is no time to send the samples to a testing laboratory)
- you need **trained scientific staff** during the **whole** production
- often you need **more than one** analysis method to get all your required information

Many small and medium-sized companies do not have the financial resources to create conditions for on-site analysis and evaluation of their products. The result is an analysis of only the end product.

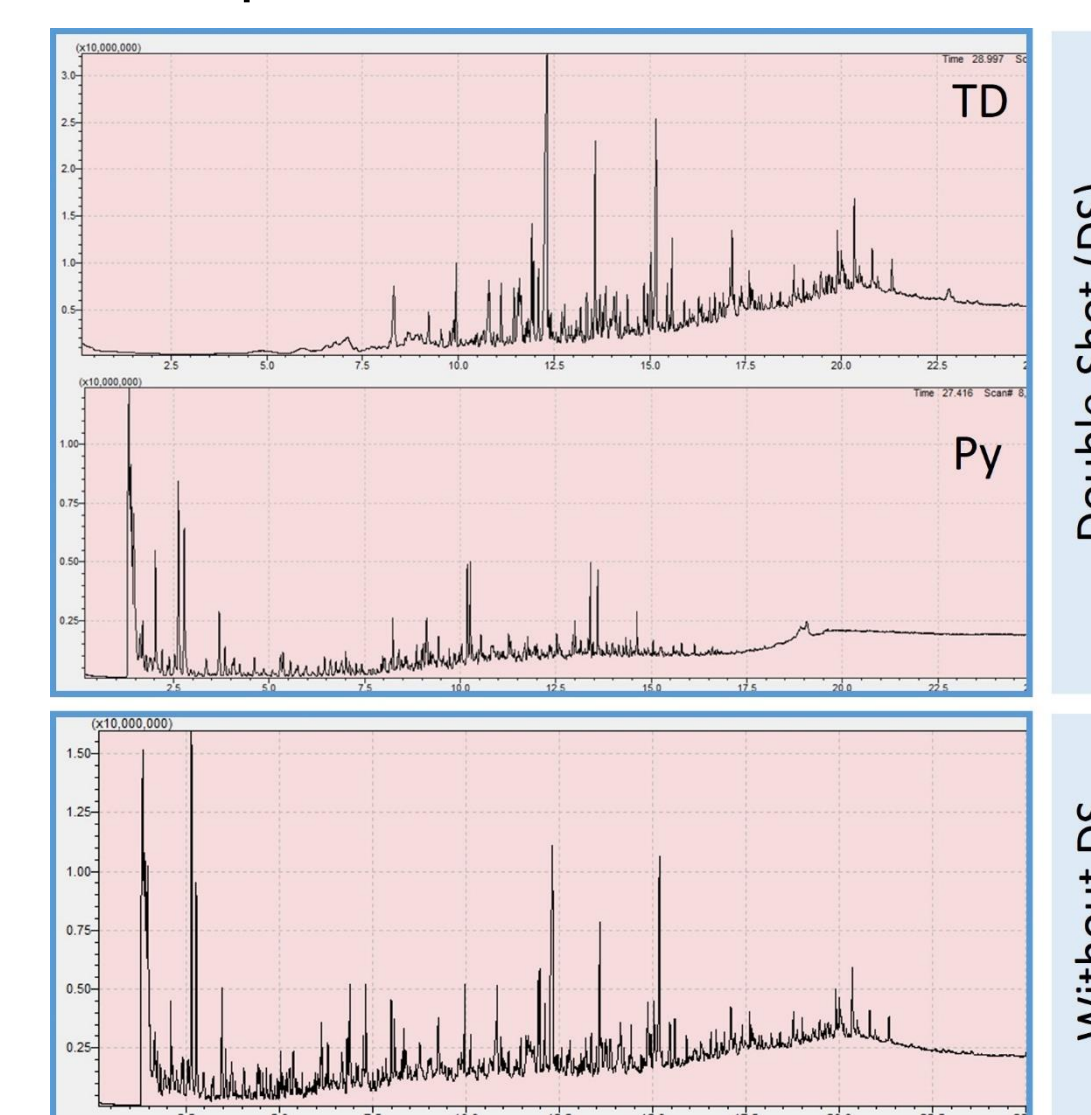
Py-GC/MS – a method for (almost) everything



Multi-Functional Pyrolysis System Configuration [1]. The modules 3), 6), 8) and 9) are not necessarily required.

Advantages of Py-GC/MS:

- user friendly, simple sample preparation without previous extraction
- applicable for lots of materials (e.g. leather, coated textiles, polymers)
- solid, insoluble and non-volatile samples can be analyzed
- high informative content because of the double-shot modus (detailed information about additives (volatiles) AND high molecular compounds (non-volatiles) in ONE analysis



Thermodesorption-phase (TD):

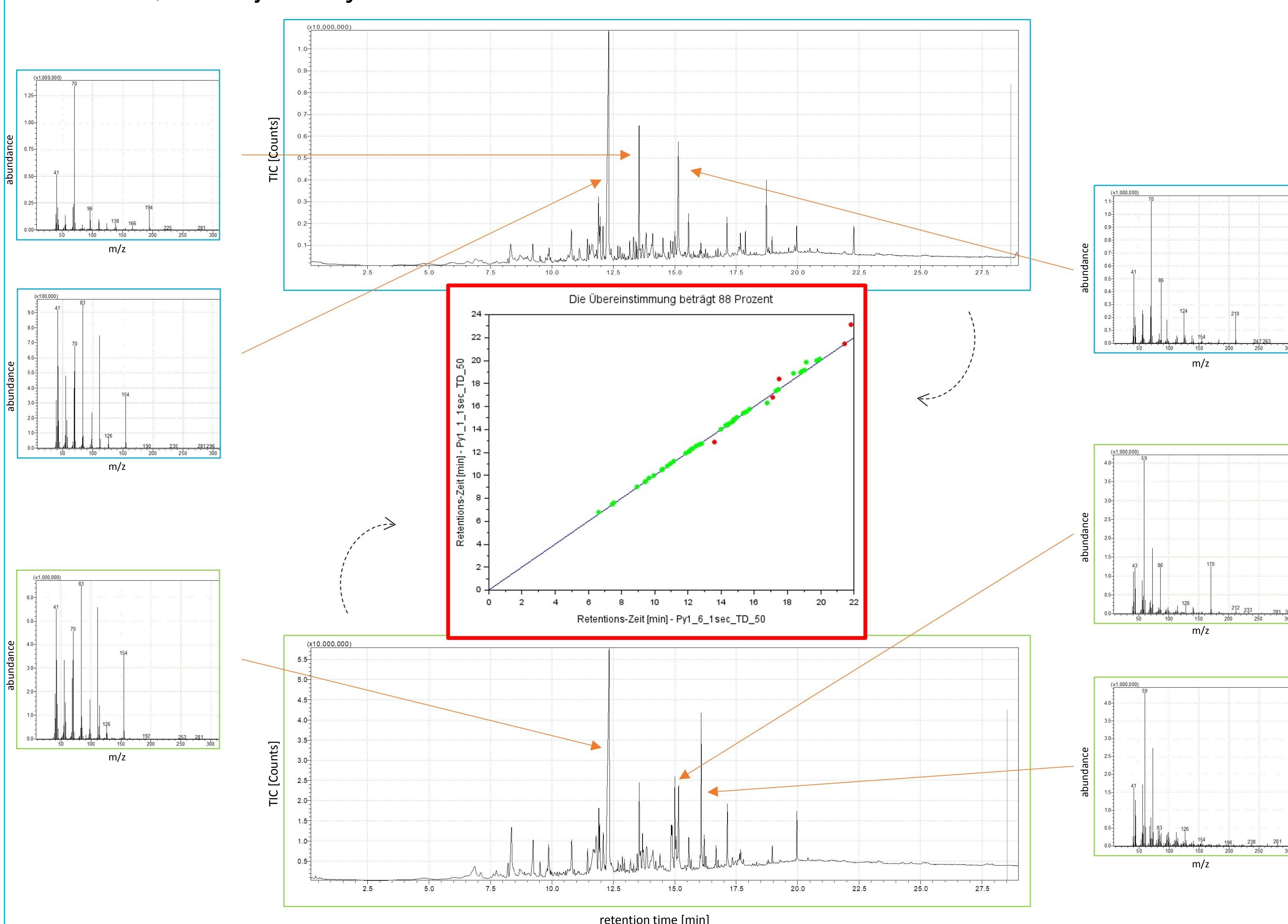
- Heating the sample using a temperature gradient up to approx. 350°C
- Analysis of volatile components using GC/MS

Pyrolysis-phase (Py):

- Thermal decomposition of the sample at a defined temperature (up to 800°C)
- Analysis of the fragments using GC/MS

MS similarity factor

The final evaluation in the daily routine is often carried out via manual chromatogram comparison. At that point, the mass spectra of compliant peaks are compared. That's not trivial, because the chromatograms can consist of numerous peaks depending on the sample matrix. In addition, this form of data evaluation is very subjective. With our developed tool, this data comparison is also carried out, but objectively.



With the developed evaluation methodology, we want to give a simple and everyday option to the industry to compare (Py-)GC/MS data for quality assurance and control. This means, that non-specialist employees can also be included in the interpretation of complex data sets.

MS Tool

Our tool is based on the freely accessible software package Scilab. The peak integration is initially carried out automatically via the measurement software. After that, the exported data sets are imported into the evaluation tool. In a first step, the algorithm compares the retention time of each peak including a defined tolerance. Peaks with retention times that do not appear in the other data set are ignored in further consideration. Compliant peaks are compared again, but this time via their mass spectra. At the end, the tool creates a list of all peaks with the same retention times and mass spectra and uses this to calculate a percentage agreement (the similarity factor). To verify the evaluation tool, we compared a manual judgement by an expert with the automatic generated valuation and it works very well.

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Literature:

[1] Frontier Laboratories Ltd. <https://www.frontier-lab.com/products/multi-functional-pyrolysis-system/200599/>. Accessed 21 March 2024.

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