COMPLETE STATISTICAL WORKFLOW FOR OPTIMIZED USED OF GC × GC-TOFMS

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Key points

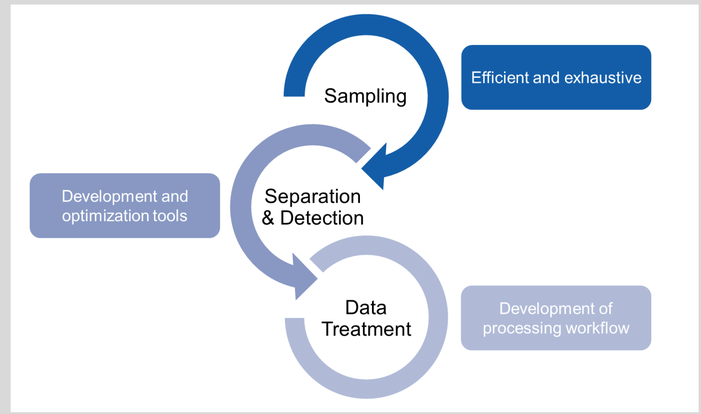
In the last years, multidimensional chromatography methods have undergone numerous developments on the technical side. Several commercial systems of two dimensional gas chromatography coupled to high-resolution mass spectrometer (GC × GC-HRTOFMS) are now commercially available. However, the users are still facing **challenges for method optimization and data processing steps.**

This research aims to develop a complete optimization and processing workflows for GC × GC-TOFMS application. **The simplification of the technique would be a game change for broader transfer of this technology to the industry.**

- GC × GC-TOFMS offers a powerful solution for non-targeted studies but it is challenging to implement for non-expert users
- There is a clear lack of defined workflow for optimization and data processing
- The establishment of standard workflow will facilitate method transferability and implementation

Context

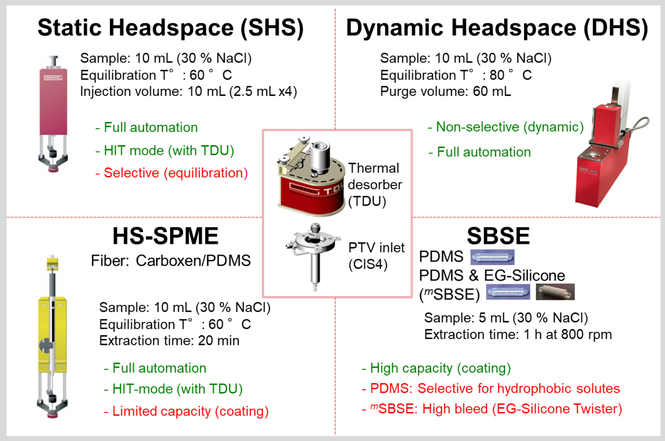
The development of analytical workflow for GC × GC-TOFMS application can be separated in three main steps. For the **sampling and the Separation & Detection** different tools are already available to demonstrate the robustness and help to optimized the experimental conditions. However, a major part of the users still rely on empirical approaches to establish the analytical conditions. In addition, there is no minimum reporting standards for data publication. This situation is generating bias when a established method has to be replicated in another lab.



Results & Discussion

Application of statistical experimental design for sampling and separation optimization

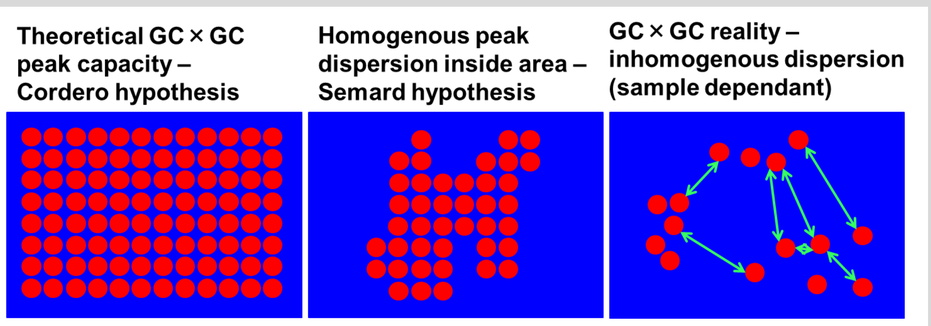
1. Sampling and separation methods selection

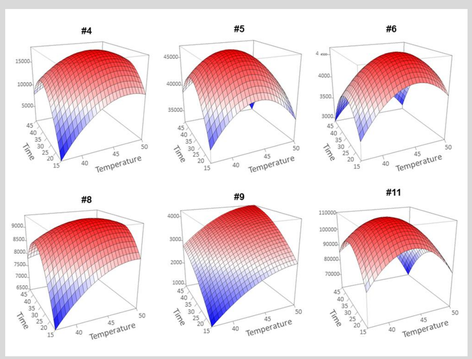


Currently: Selection of the sampling and analytical approaches are mainly based on users' experience and available data.

Development: Selection based on statistical models build on appropriate sample and method descriptors.

2. Statistical optimization





Following the selection, there is the need of conditions optimization

Currently:
- Also based on users experience
- Statistical tools are available but not routinely used due to lack of systematic approaches

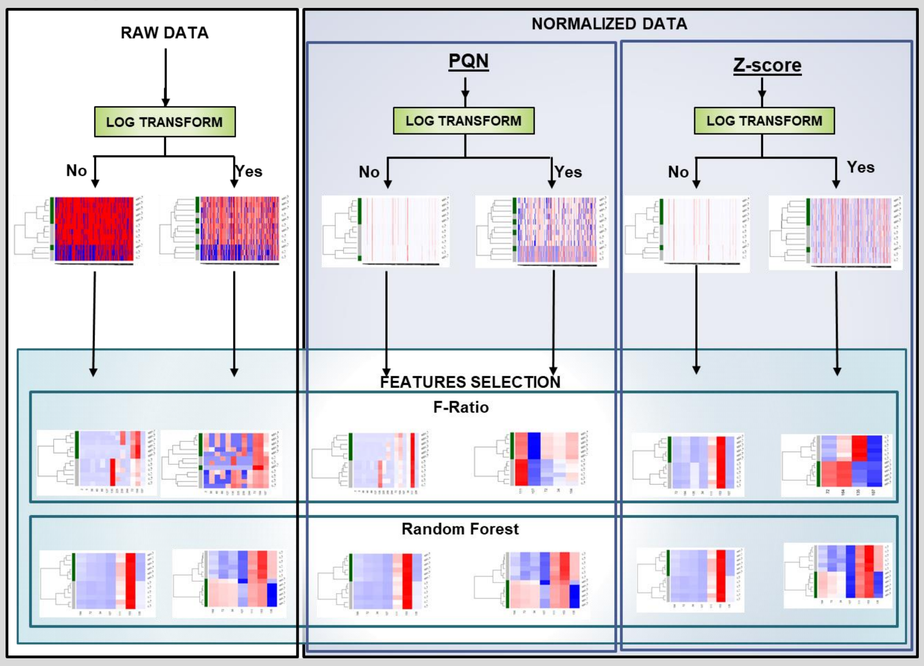
Development:
- Establishment of the key optimization parameters and descriptors for each sampling and analytical methods
- Development of universal workflow for statistical optimization of the analytical conditions

3. Data processing workflow

Currently: there is an overlap between the work of the analytical chemist and the data scientist. This overlap is usually called the "pre-processing"
Development: universal data pre-processing workflow which are able to generate robust data for subsequent model building.

Example: Effect of the pre-processing approach on classification

→ The pre-processing can have a crucial influence on the resulting model efficiency



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