



*A focus for analytical chemistry in Europe*



## WG. 2.2. Tools for analytical quality control for non-targeted methods.

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20.-21. May 2019, Tartu, Estonia

### Validation of a non-target method: a practical approach



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- Introduction
  - 30 participants, 19 countries
  - Universities, research institutes
  - Different authorities
  - Fields: food, environment
- First a discussion circle on the topic and then discussion of different questions.

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## Working Group Session



### Tools for analytical quality control for non-targeted methods



- Focus: data quality control in connection with classificatory non-target methods
- Many participants raised the question whether this can be meaningfully distinguished from instrumental or sample prep. QC
- Question was raised whether the real question shouldn't rather be: how can we ensure that the validation samples are sufficiently representative?
- Question whether classificatory non-target methods can be expected to perform at an acceptable level in different laboratories
- Questions whether data quality requirements should be specified as part of the method itself
- Validation samples should be described
- Suggestions for QC parameters:
  - Mass bank workflow for uploading specifies data quality parameters
  - Metadata
  - QC criterion for QC samples

In connection with non-targeted methods, what standards or guides do you use for validation and for quality control?



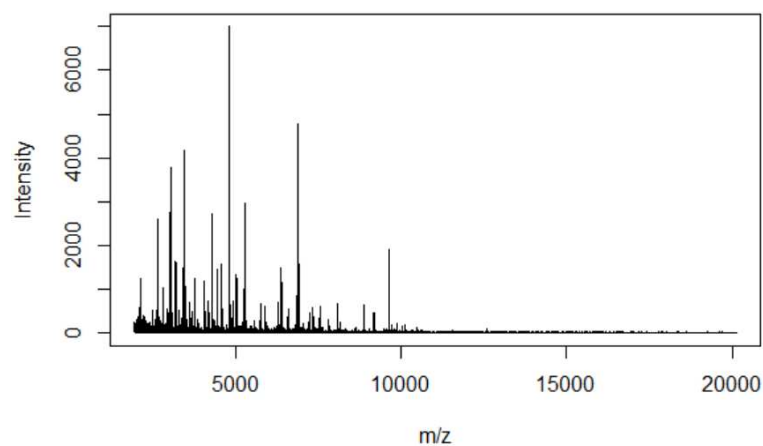
No  
Except for: EN 15768 (nontargeted GC-MS for drinking water)

Are there any accreditation requirements for non-targeted methods? What are the challenges for you in applying ISO 17025 to non-targeted methods?



- ISO 17025 definitely provides the correct framework. Its requirements are applicable, e.g. software validation

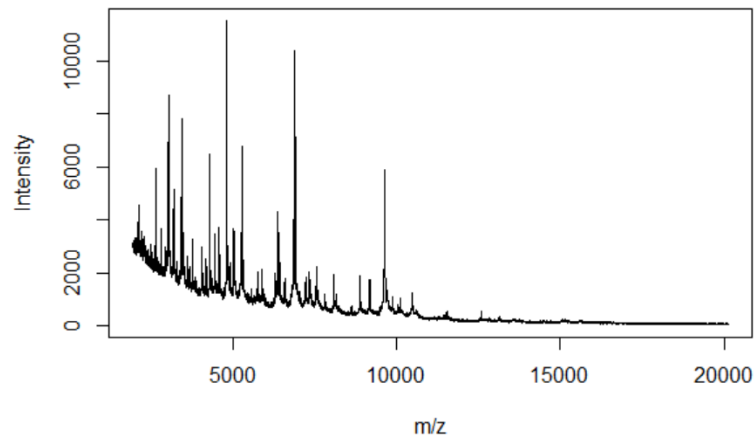
Consider the following spectrum. Would you analyze this dataset?



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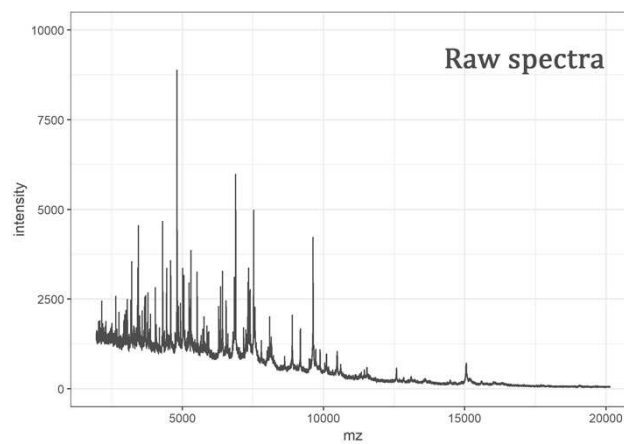
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How can you measure the success of pre-processing?



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How much pre-processing is too much pre-processing?



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