WG. 1.2.
Validation of a non-target method: a practical approach

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Program

• Introduction of the participants
• Presentation by Annemieke Kolkman
  • Non-target screening in (drinking)water – practices in the Netherlands
• Questions from the audience

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Audience

• Universities (80%)
• Metrology background (ca 10)
• Industry (5-7)

• How many are using non-targeted methods?
  • Ca 10 people
• Is it validated?
  • ....
• Areas represented
  • Environmentals, metabolomics, food, ....

Q1: Are the classical validation parameters relevant for non-targeted and suspect screening?

• Selectivity, Identification, Scope
• False positive rate, False negative rate
• Repeatability & Reproducibility
• Robustness
• LoD & LoQ
• Stability
• Accuracy, Trueness
• Working range
What is non-targeted analysis?

- Fingerprinting
- Aiming to identify compounds present

Techniques
- LC/HRMS
- GC/HRMS
- Other methods

Terminology

- Scope
  - Analytes
  - Research question
- Selectivity vs False positive/negative rate
  - Chemical space
  - Focus of the method
- Working range
  - Concentration vs scope
- Sampling
  - Taking the sample, storing the sample, stability, contamination
Spiking

• Scope
• Working range (concentration)
• Interferences

Validation

• The non-targeted method is ultimately validated when combined with targeted method
  • Serves as validation for non-targeted
• The big difference is that non-targeted analysis need more replicates
Standardization of validation

• How much can validation be standardized?
• Is relevant to make most of them

Data processing

• Should it be validated?
• How can it be validated?
• Vendor software vs own script
• Preprocessing – how much is too much?
Materials

• Reference materials
• What is a blank?
• What is a quality control sample?
• What do you monitor for QC?
  • Instrument control
  • How similar between targeted and non-targeted methods
• Collaborative trials