1989-2019 Eurachem
A focus for analytical chemistry in Europe

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

Chair

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20.-21. May 2019, Tartu, Estonia

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 valdiation 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

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- 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