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A focus for analytical chemistry in Europe

WG. 1.1.
Traceability and uncertainty for quantitative targeted and non-targeted analysis
Summary of the discussion

Chair

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20.-21. May 2019, Tartu, Estonia

Eurachem publications
Traceability

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Traceability in order to get comparability of results

- Eurachem Guide on Traceability - New version 2019 with minor updates to be published this week.
- Traceability leaflet

20.-21. May 2019, Tartu, Estonia

Eurachem A FOCUS FOR ANALYTICAL CHEMISTRY IN EUROPE CITAC Cooperation on International Traceability in Analytical Chemistry

Metrological Traceability of Analytical Results

In order for results to be comparable we need metrological traceability.

From the LEAFLET

Traceability in the 19th century

Once a dairymaid bought one kilo of flour from the local shop. Next day she returned to sell one kilo of butter to the shopkeeper. He then complained that 50 grams of the kilo were missing.

— *Oh that is odd,* the dairymaid said, *to get the correct weight I used the kilo of flour you sold to me yesterday to weigh the butter!*

Eurachem publications Uncertainty

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Uncertainty in order to know the quality of the result

- **Analysis**
  - Eurachem Guide – Analytical uncertainty – Latest version 2012
  - Eurachem Guide – Setting Target Uncertainty – First version 2015
  - Leaflet on uncertainty– old version from 2001
  - Leaflet on Setting Target Uncertainty – to be published this week
  - Leaflet on difficult issues 1) Square root and 2) Treatment of bias
- **Sampling**
  - Eurachem Guide – Sampling uncertainty – New version with major updates to be published this week – One major update is working with uncertainty > 30 %

Participants

29 participants from:

- Universities
- State agencies
- Environment, food, clinical
- Statistics, PT provider

Definition

- Targeted analysis
  - I want to determine x in matrix y
- Non targeted analysis
  - I want to screen for y e.g. organic impurities
  - I want to determine the composition of sample xe
  - I want to know if this waste is hazardous
  - I want to know if there are features that have a trend in my sample
  - I would like to classify my sample.
    - Is that really a non-targeted analysis?

Matrix?

- How to define the matrix?
  - Depending on a method, the definition of matrix depends. Sometimes it is very important if low/high fat content etc.
  - It is important when expanding a method.
- Uncertainties can depend on the matrix

- Definition of matrix - What is wastewater?
  - Depends on the industry as well.

Q1: Difficulties with traceability

- Variability of reference materials
- Operational methods:
  - Eg moisture. Possible to use other methods but then then the first method is the reference method.
- Databases for reference materials:
  - COMAR
- CRM with defined measurement uncertainty for certain method:
  - Need to use the methods determined
  - Sample preparation technique is important!

Q1: Difficulties with traceability

- Read the certificate!
- Problems depend on a field you are working at.

Q3: Traceability for non-target methods

- Important to divide into Screening or fingerprinting.
- Traceability not relevant?
  - Always relevant!
- We need some kind of traceability but we are very far from it.
- Qualitative analysis.
  - France and not-France
  - Role of traceability?
  - Traceability is relevant here.
    - What was reference used to determine that is from France.
- Whenever you measure something, you are traceable to something.

Q4: What are you traceable to?

- What are the links in traceability.
- Your method is traceable to your calibration and the conditions specified
- CRM is a higher level.

Q5: Uncertainty problems

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- High uncertainty
  - We assume that the data is normally distributed but this is only valid for low uncertainty. The issue of high uncertainty will be treated the Eurachem Berlin workshop 19-20 November
- Definition av measurand
  - Sampling uncertainty:
    - Define the object you are analyzing
    - River at the 300 m range or one sample at one point in one time.