1989-2019 Eurachem
A focus for analytical chemistry in Europe

WG. 1.3. Recent instrumental developments in targeted and non-targeted analysis.

Chair

Ivo Leito

20.-21. May 2019, Tartu, Estonia

Validation of a non-target method: a practical approach

1989-2019 Eurachem
A focus for analytical chemistry in Europe

- Introduction
  - 31 participants, close to 20 countries
  - From universities, institutes, authorities, labs, industry

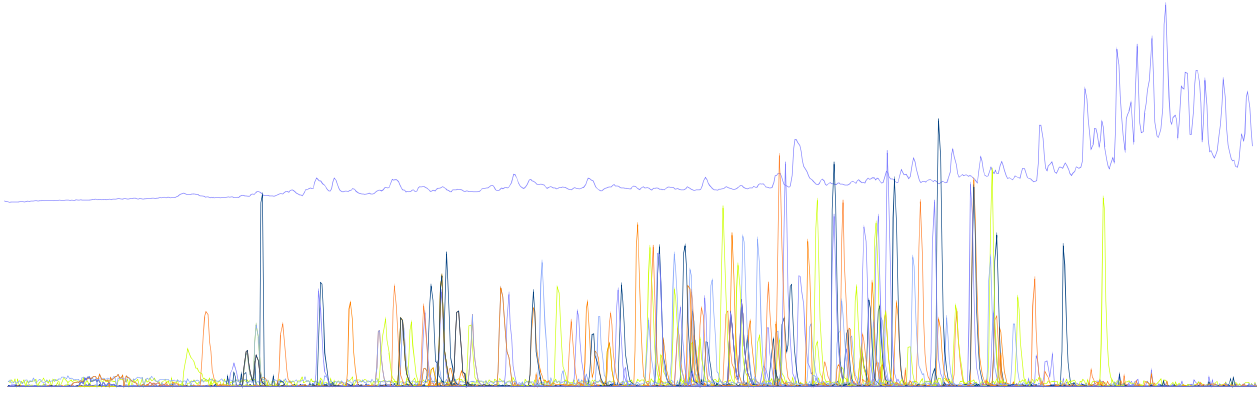
- How was workshop arranged: any deviation into groups? **No**
  how many questions for discussion? **Mostly from chair**

20.-21. May 2019, Tartu, Estonia

1989-2019 Eurachem 30
A focus for analytical chemistry in Europe

A typical picture:

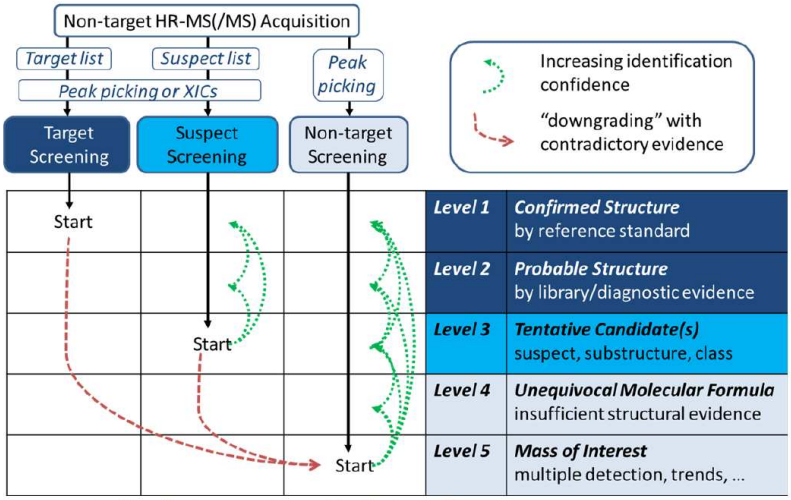
Food Safety Screening, QuEChers Extract



Scheme: Sven Vedder, Shimadzu

Non-target screening with high resolution mass spectrometry: Critical review using a collaborative trial on water analysis

Emma L. Schymanski1*, Heinz P. Singer1, Jaroslav Slobodnik2, Ildiko M. Ipolyi2, Peter Oswald2, Martin Krauss3, Tobias Schulze3, Peter Haglund4, Thomas Letzel5, Sylvia Grosse5, Nikolaos S. Thomaidis6, Anna Bletsou6, Christian Zwiener7, María Ibáñez8, Tania Portolés8, Ronald de Boer9, Malcolm J. Reid10, Matthias Onghena11, Uwe Kunkel12, Wolfgang Schulz13, Amélie Guillon14, Naïke Noyon14, Gaëla Leroy15, Philippe Bados16, Sara Bogialli17, Draženka Stipaničev18, Pawel Rostkowski19, Juliane Hollender1,20*.



Analytical and Bioanalytical Chemistry
August 2015, Volume 407, Issue 21, pp 6237–6255

Figure 1: Matrix of identification approach versus identification confidence.

Scheme: Sahun Bilsborough, Agilent

Workflow

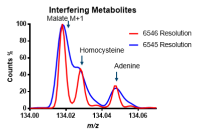
- **Reproducibility, robustness**
- **Sample preparation**

- **As routine as possible**
  - Suspect list
    - That defines the method
    - E.g. 300 pecticides on the list

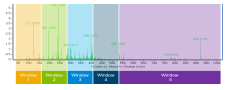
- **Identification**
  - RT, m/z accuracy, isotoope ratio accuracy, MS/MS spectral match

Possible workflow:

High resolving power even at high acquisition speeds



QRAI workflow to acquire MS and MS/MS spectra in a single run with increased separation and LOQ

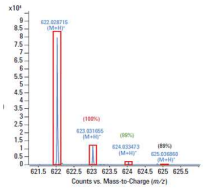


Software workflows to maximise productivity in your laboratory

4 confirmation criteria for suspect screen

Wide in spectrum dynamic range to enable ID of high and low abundance compounds in a single analysis

High quality isotopic fidelity to increase confidence in identifications



Scheme: Sahun Bilsborough, Agilent

Instrumental

- **When targeted at low LoD**: **QqQ**
- **When non-targeted, complex samples: Q-TOF, triple-TOF** seem most practical
  - ***HRAM, Resolution*** n x 10 000
  - ***Wider dynamic range*** > 4 orders
    - Form one run vastly ifferent
  - ***Accurate isotopic patterns***
    - Ca 95% false positiive scan be eliminated
  - ***Advanced acquisition***
- Ion sources
- LC

Acquisition and software

- **Software is BIG**
- Handling **large number of components**
  - In LC mode
  - Algorithms for detecting peaks
  - Advanced data acquisition strategies (SWATH, …)
  - Open software, open platforms
  - Identification
    - RT, m/z accuracy, isotoope ratio accuracy, MS/MS spectral match
- **Databases**
  - Curation (removal of imperfections)
- **Statistical analysis**

Nothing is perfect!