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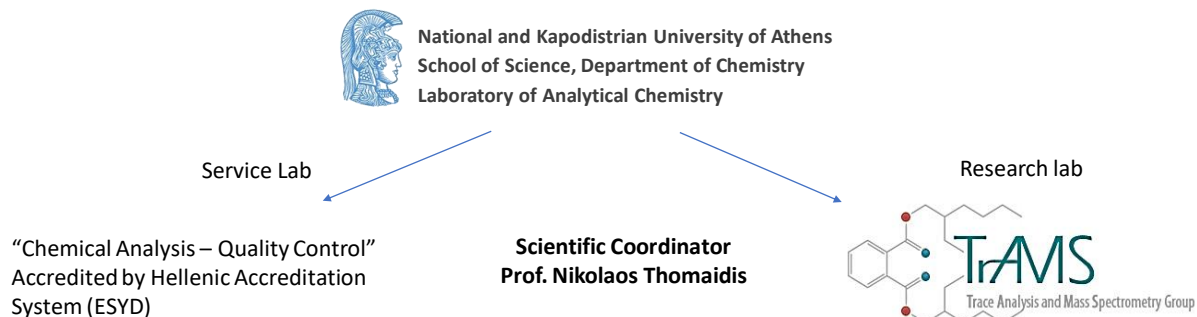


Validation of wide-scope method with mass spectrometry Problems and perspectives

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Instrumentation

Other Instrumentations

HPLC- DAD
GC-FID/ECD/NPD
Ion Chromatography
Atomic Absorption Spectrometry (ETAAS, FAAS)
Atomic Emission Spectrometry (MPAES, FAES)

Mass Spectrometry

LC-MS/MS
LC-qTOF-MS
MALDI-TOF
GC-MS/MS

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Mass Spectrometry

Determination of thousand compounds with a single run

Combined with Gas and Liquid Chromatography

Low resolution
(Triple
Quadrupole)

- Widespread between laboratories
- Low Detection Limits
- Guidelines for validation (SANTE-2002/657/EC)

High Resolution
(qTOF, orbitrap)

- High mass accuracy
- Not widespread yet
- More and more accessible (institutions – Universities)
- Studies for –omics

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High Resolution Mass Spectrometry



Capable of identification of millions of compounds with a single run



Generic pre-treatment methods in order to include as much compounds as it possible



a wide-scope databases

Metabolomic studies

Emerging Contaminants



In Literature, very well-established criteria for the identification of a compound



Quantification, questions about its capability

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Is it possible to be validated a single method with 2000 analytes?

Problems with wide-scope analytical methods

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Single method with wide-scope analytes

Current State

- No guideline
- In literature, validation a low percentage of representative compounds with same structure and physicochemical properties

Problems

- It is impossible to validate all the analytes
- Time consuming and huge cost

Questions

- Is it so important to validate all the analytes?
- Has to be the same criteria as in a method with a single analyte?
- How to be accredited a such a method?

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Thoughts

Preliminary Screening

- Validation only the compounds after screening

“Risk-based” validation

- The level of concentration and number of replicates depending on the compound (toxicity, legislation limits)

Accreditation

- Strict criteria for identification
- The procedure of laboratory to choose the appropriate criteria for validation of quantification

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Thank you very
much



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