


Joint Eurachem/AOAC-E webinar

Trends & challenges for Non-Targeted Methods
1. Quo Vadis? What, How and Who?
November 15 2022, 13:00-17:00 CET • Online (Webex)

THE CONCEPT OF NT (TERMINOLOGY AND POSSIBLE APPROACHES)




Baden-Württemberg


16.11.2022

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Agenda



- ❑ The challenge on the topic
- ❑ Targeted methods
- ❑ Non-targeted methods
- ❑ Conclusion



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The challenge and the topic



- What is target and non-target analysis?
- Different definitions, from different contexts and different use

NTS offers several opportunities for chemical water monitoring. Firstly, for the prioritization of environmental and health-relevant chemicals for more detailed analyses. Secondly and perhaps more importantly, NTS allows for the identification of previously unknown environmental contaminants by searching for substance or source-specific patterns in the data sets.

- NTS - a large list of suspect compounds ($n \gg 1$) is checked for presence or absence
- Non-target methods, non-target workflow, non-targeted approach, etc.

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The challenge and the topic



- Food and feed authenticity, environmental monitoring, food contact materials
- Not restricted to „chemical methods“
- What are profiling, signature, non-targeted profiling and fingerprinting?
- Non target screening – identification of compounds?
- Necessary to have a broad discussion and set definitions - without the claim to be always right
- Set of definitions for the „right“ application area

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Targeted methods



- A targeted analysis covers detection or quantification of one or more pre-defined analytical target(s).
- The analytical targets are chemically or biologically characterized and annotated with established importance prior to data acquisition.
- They can be either primary or secondary markers.

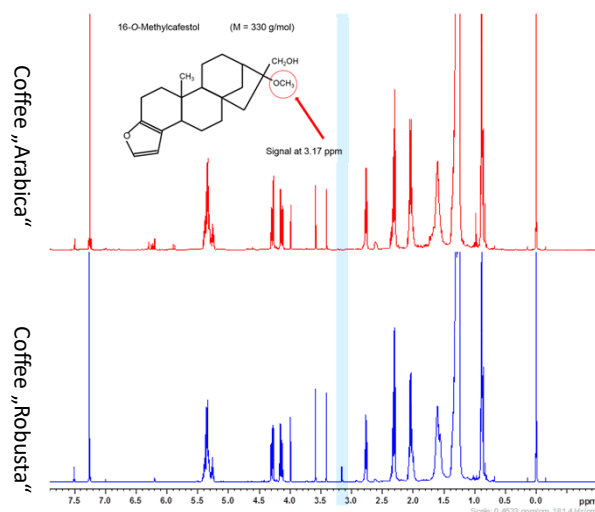
Bolln, N. Z., & Laurusen, K. H. (2019). To target or not to target? Definitions and nomenclature for targeted versus non-targeted analytical food authentication. Trends in Food Science and Technology, 86(June 2018), 537–543. <https://doi.org/10.1016/j.tifs.2018.09.025>

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Arabica or Robusta OPSON VIII - Coffee



Okaru et al. (2020). Validation of a Quantitative Proton Nuclear Magnetic Resonance Spectroscopic Screening Method for Coffee Quality and Authenticity (NMR Coffee Screener). In: Foods 9 (1), S. 47. DOI: 10.3390/foods9010047.

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Non-Targeted method



- A method that determines the similarity of a sample (U) to a reference standard or set (S_n).
- It has a binary output—the sample is Atypical or Typical with respect to the known sample set. The concept of non-targeted methods covers a spectrum from truly non-targeted (largely theoretical) to semi-targeted (most practical applications), but for the purposes of this paper any broadly nonspecific adulterant detection method is treated as nontargeted, as the same principles are applicable.

2021 USPC: Appendix XVIII: Guidance on Developing and Validating Non-Targeted Methods for Adulteration Detection



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Non Target methods



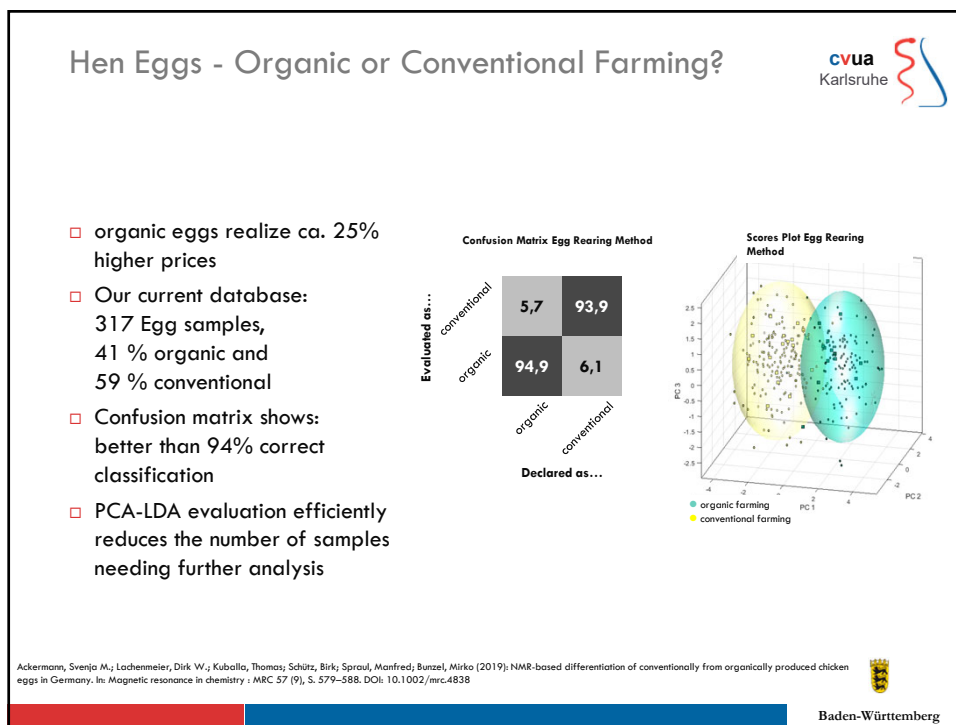
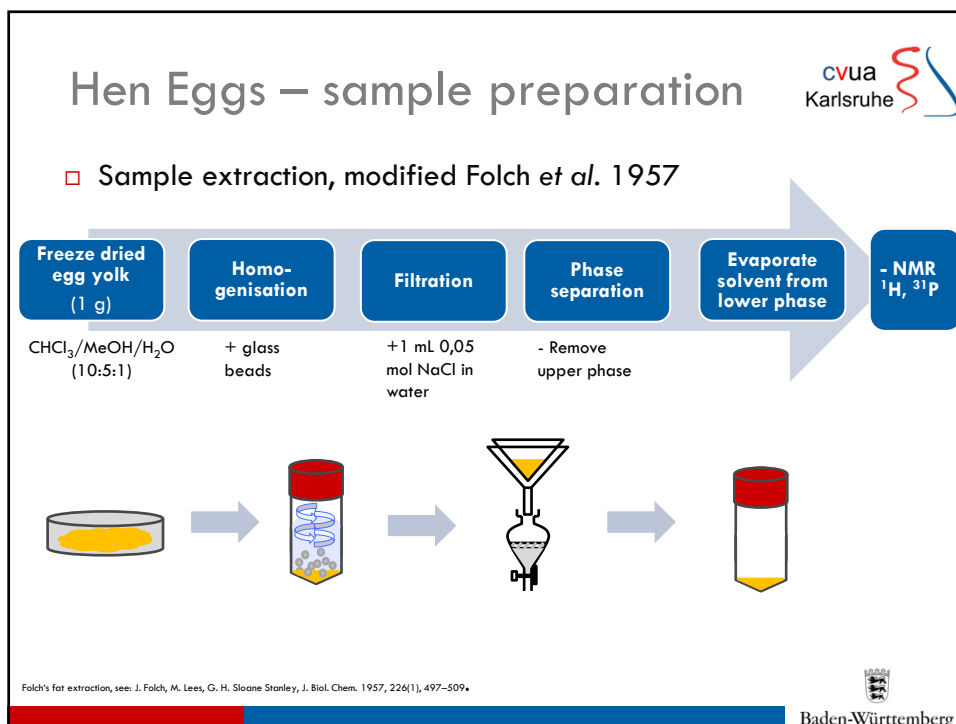
- Definition ensures horizontal applicability to a wide range of methods
- remains limited to a subset of methods for food authenticity testing, namely: one-class classification methods for testing adulteration or mixing
- other somewhat differing definitions are available in literature
- a comprehensive approach to a broad definition can be expected to be published by CEN/TC 460 WG 5

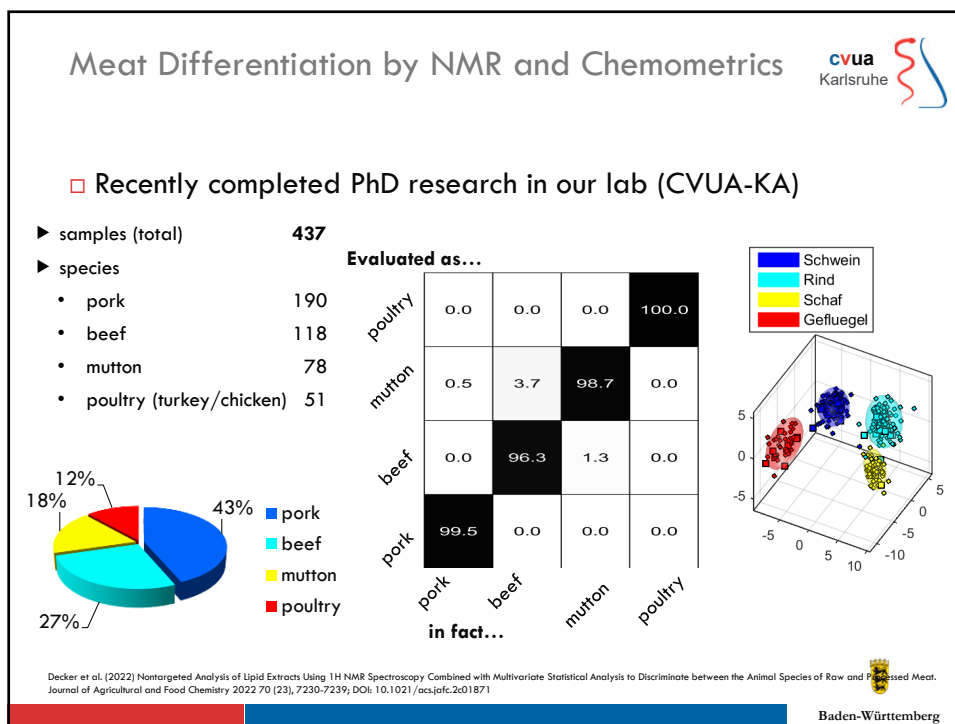


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Questions

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- Is the definition limited to the analytical method?
- No - should include the „analytical pipeline“ and quality criteria for validation

Components of NTM

Analytical method (Wet lab)

Reference database

Statistical model (Dry lab)

Decision criteria

- “database” may refer to the entire technology behind the storage and management of data
- “database” could only refer to the collection of data stored in it

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Questions



- What about Fingerprinting and profiling?
- Are they NTM because both both require a statistical model (dry lab) and a reference database for decision making?
- Fingerprints of a material are electronic records (e.g., whole or part of chromatograms or spectra) produced by an instrument without further information regarding the identities or quantities of entities represented by the record.
- A **profile** constitutes of quantity values of defined entities of a material (e.g., elements, fatty acids, sugars, etc.)

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Conclusion



- Currently projects in different organizations are underway (CEN, AOAC, etc.)
- Aim of this cooperation and webinars is to create a setting for discussion within the interested scientific community
- Create a common ground of understanding and commonly accepted definitions
- Without such a common ground much money, time, resources and credibility will be wasted
- I turn over to the following speakers for more details and answers

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THANK YOU FOR YOUR
ATTENTION – QUESTIONS?



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