



A focus for analytical chemistry in Europe



Joint Eurachem/AOAC-E webinar

Trends & challenges for Non-Targeted Methods
2. "NTMs – qualitative or quantitative?"
June 6th 2022, 13:00-17:00 CEST • Online (Webex)


"'FINGER-PRINTS' – BY USE OF A MULTITUDE OF ANALYTICAL PRINCIPLES"



Baden-Württemberg

06.06.2023

Stephan G Walch, PhD
Executive Director, Chemisches und Veterinäruntersuchungsamt Karlsruhe, Germany

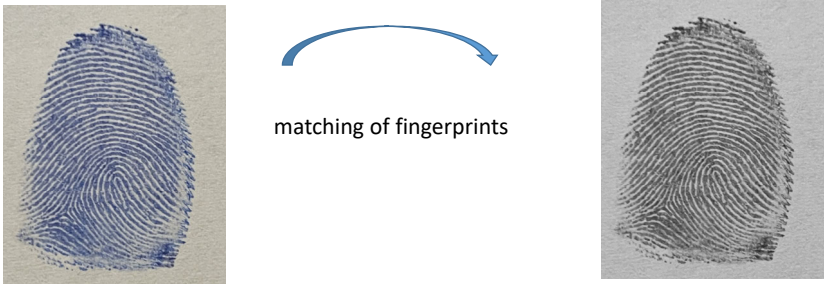



definitions

- 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.)

2 06.06.2023 Baden-Württemberg

definitions





fingerprint of sample

fingerprint of reference

- "Yes" (match) or "no" (no match) decision
- one sample vs. one reference

3 06.06.2023 Baden-Württemberg

definitions



fingerprint of sample

fingerprint data base

- still "yes" (match) or "no" (no match) decision
- one sample vs. reference data base

4 06.06.2023 Baden-Württemberg

fingerprint - definitions

- a method that determines the similarity of a sample to a reference or reference set
- it uses no specific markers, but the full spectrum recorded
- it has a binary output—the sample is atypical or typical with respect to the known reference or reference sample set

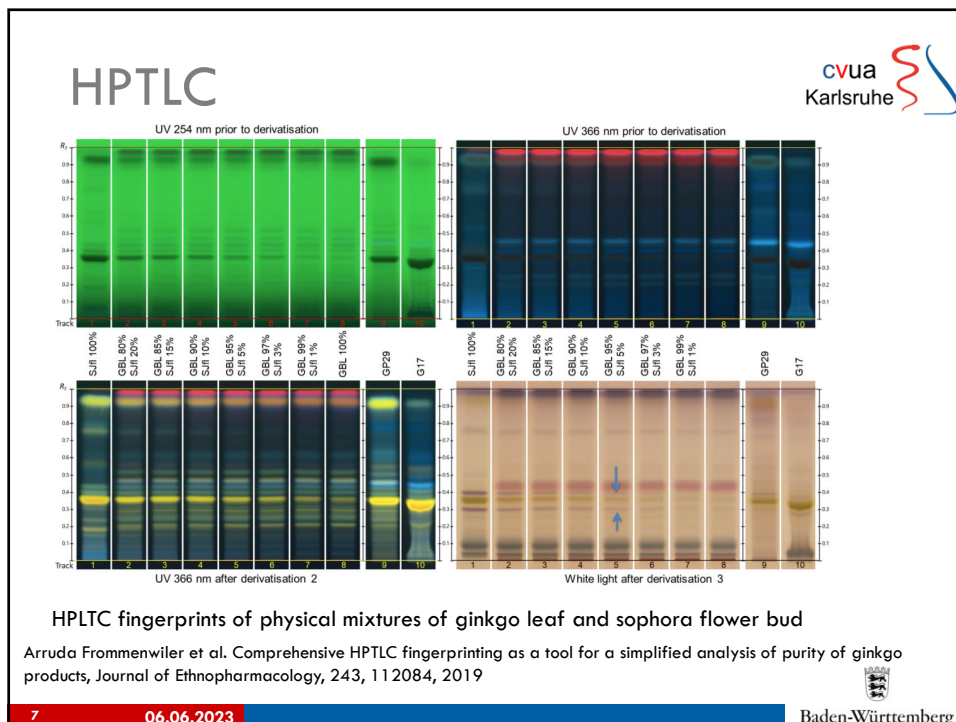
fingerprinting – analytical methods

- recording characteristic full spectra (fingerprints) using spectroscopic or spectrometric analytical techniques




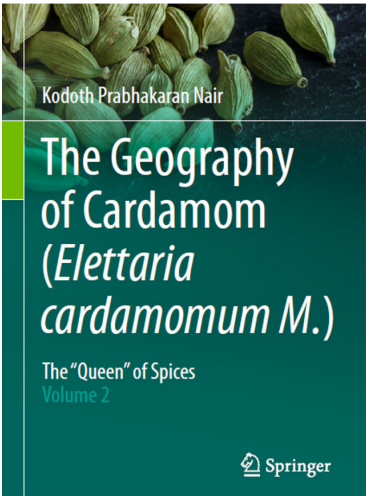
and many more:
HPTLC, ICP-MS,
Raman, etc.





MALDI-TOF MS






Chapter 14
False Cardamom

- Alpinia* sp.
- Amomum* sp.
- Lanxangia* sp.
- Aframomum* sp.
- Elettaria* sp.


In addition to true cardamom and large cardamom, all other crops that produce aromatic seeds are lumped together as false cardamom. They do not have much commercial importance, except for *Aframomum corrorima* (*Anomum melegueta*, the Korarima cardamom or "grains of paradise"), which is cultivated on a small scale in some West African countries. Still, most of these false cardamoms are important locally as spices and flavorants and as remedies for various ailments. Detailed studies of these species are lacking, although a few have been subjected to chemical analysis. This chapter briefly considers false cardamoms.




Data and pictures courtesy of Landeslabor Berlin-Brandenburg, Dr. Martin Kaufmann

8
06.06.2023
Baden-Württemberg


MALDI-TOF MS




Aframomum sp.




Alpinia sp.



Amomum sp.




Elettaria sp.



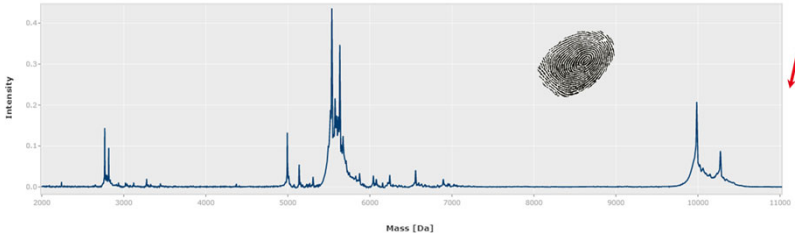
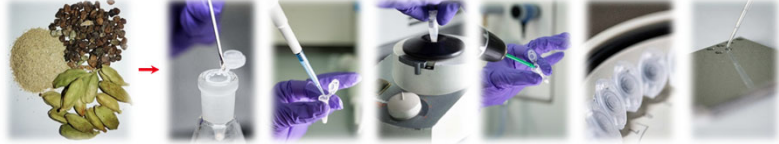
Data and pictures courtesy of Landeslabor Berlin-Brandenburg, Dr. Martin Kaufmann

9 06.06.2023 Baden-Württemberg

MALDI-TOF MS

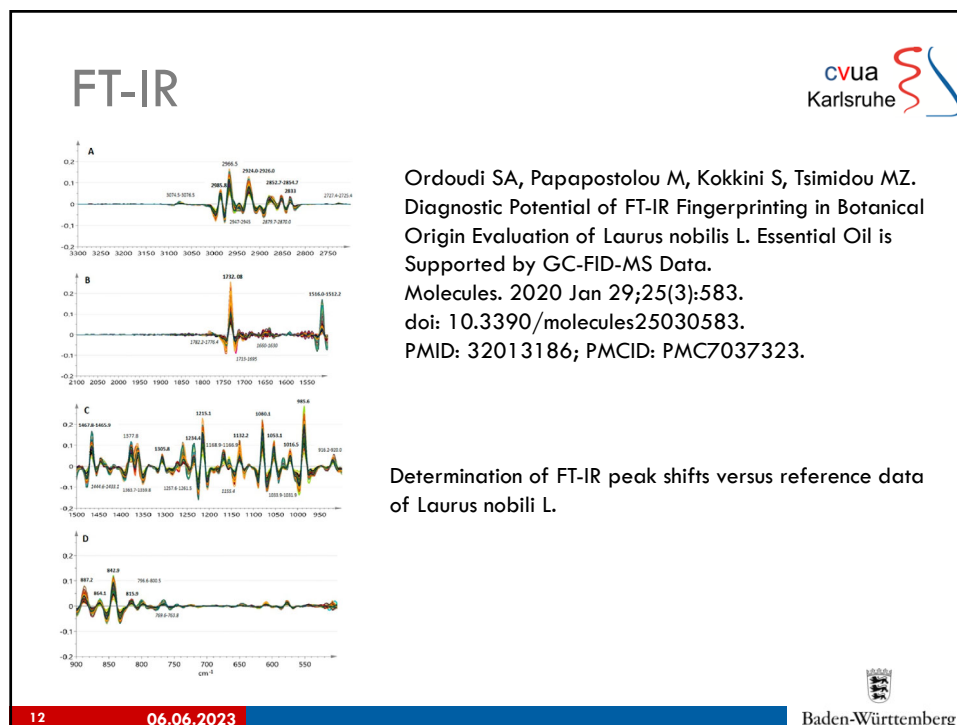
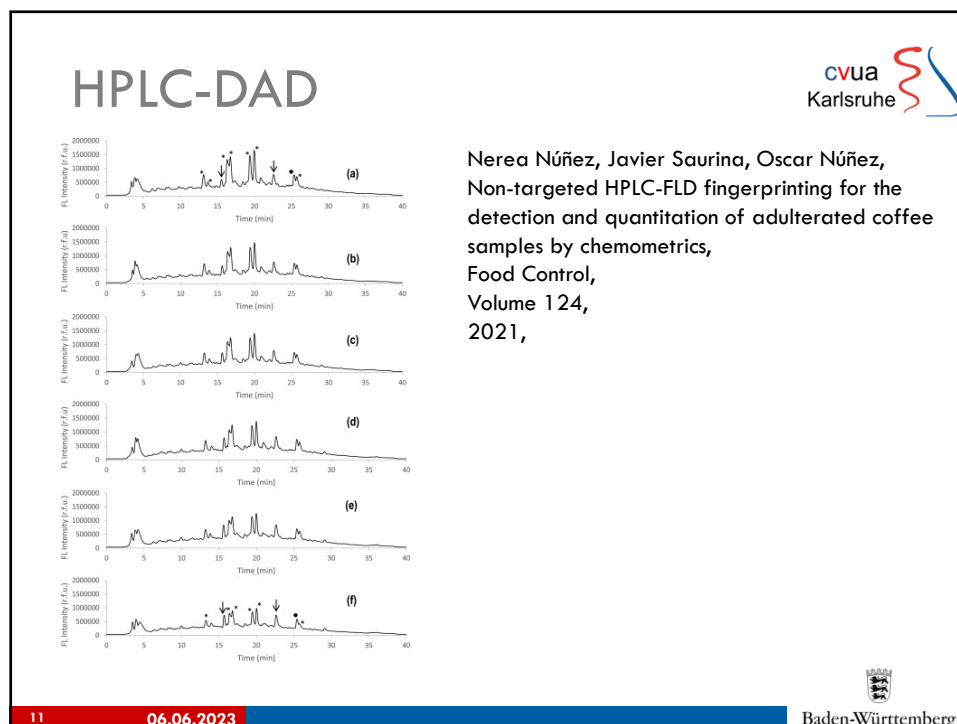


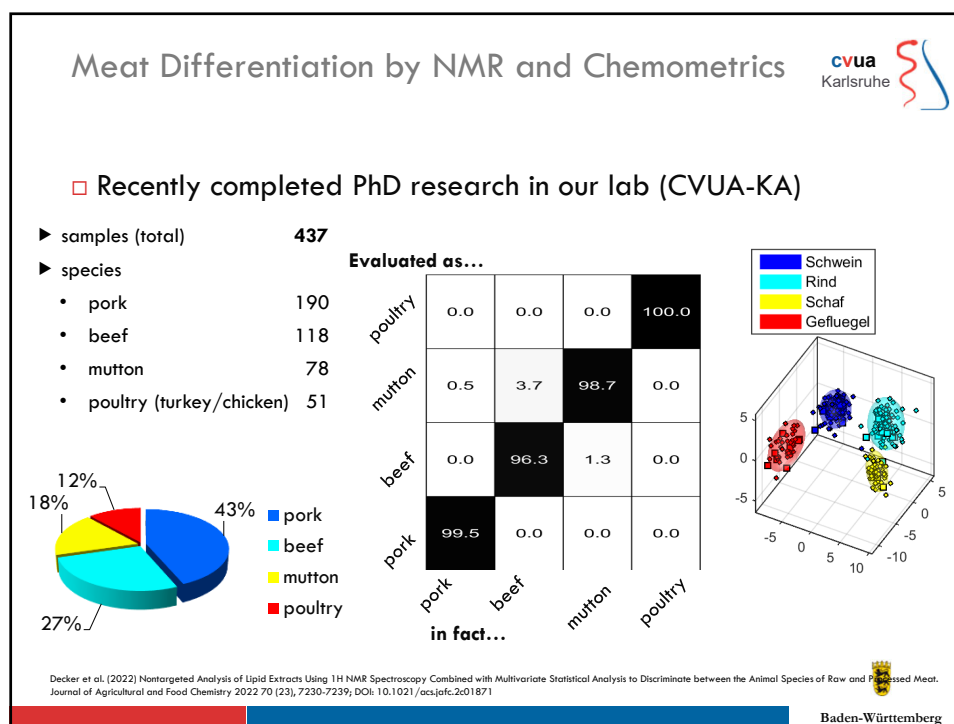
Application: authenticity of cardamom



Data and pictures courtesy of Landeslabor Berlin-Brandenburg, Dr. Martin Kaufmann

10 06.06.2023 Baden-Württemberg





Conclusion

- fingerprint analysis in non target analysis is widely used and applied
- quality of results depends on quality of reference (either single reference or reference data base)
- quality (especially measurement uncertainty) of analytical technique/method has high impact on quality of results
- comparability between laboratories depends on reliable validation and realistic determination of measurement uncertainty

Conclusion



- the transition from fingerprint to marker based analysis is fluent in the majority of published papers
- True "fingerprint" methods seem to be limited for the users (or regulators/enforcement)

15

Baden-Württemberg

Thanks



- CVUA Karlsruhe, Germany, NMR Team: Jan Teipel, Sandra Weber, Thomas Kuballa
- Landeslabor Berlin Brandenburg, Germany: Martin Kaufmann

16

06.06.2023

Baden-Württemberg



THANK YOU FOR YOUR
ATTENTION – QUESTIONS?



Baden-Württemberg

contact: stephan.walch@cvuaka.bwl.de