



Compound Databases in Official Food Control – Thoughts and Challenges for Validation and Verification

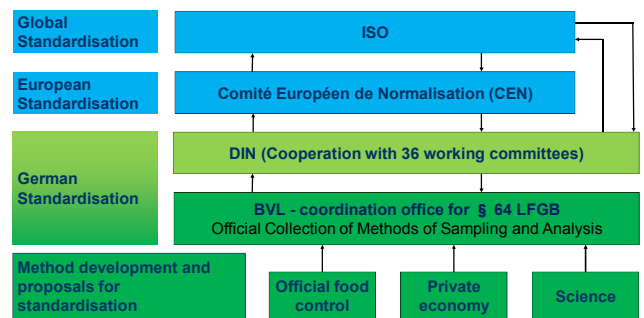
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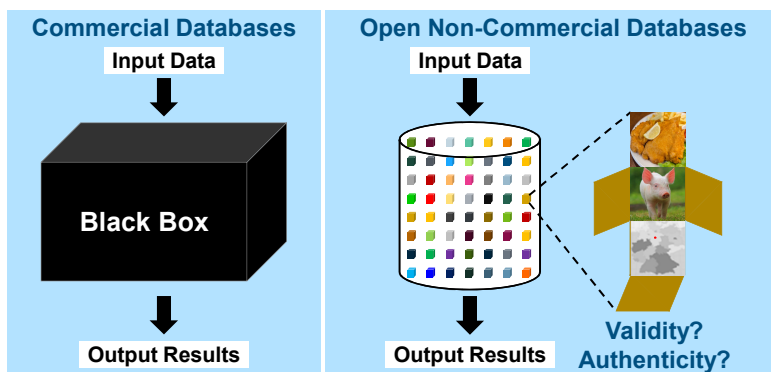
Introduction

In recent years, new analytical methods with high potential have reached the food surveillance sector. The new methods include, among others, peptidomics with liquid chromatography (LC) mass spectrometry (MS), fingerprinting with matrix-assisted laser desorption and ionisation (MALDI) time-of-flight (TOF) MS, or nuclear magnetic resonance (NMR) spectroscopy. In order to harness these methods for official food control, the coordination office for § 64 LFGB (German Food and Feed Act) of the Federal Office of Consumer Protection and Food Safety (BVL) is constituting several new working groups for the standardisation of the new methods^[1-3].

Since the new methods generally target more than one parameter for analysis or even use an untargeted approach, intentional deception of the methods is particularly difficult. However, due to the large number of parameters, usage of compound databases is often mandatory for the new methods. Here, we discuss possible challenges regarding validation and verification of databases for official food control.



Compound Databases in Official Food Control



Compound databases utilised by the new food forensic methods mainly divide into two groups; free-access, relatively open databases, and restricted, commercially licensed databases. Since the latter group often generates high costs and dependencies on commercial providers, usage of such databases is problematic for official food control. Moreover, commercial databases are usually not transparent, as providers keep their source code and algorithms secret for economic reasons.

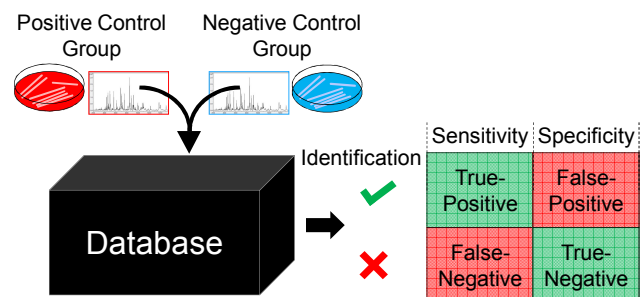
The non-commercial, open group of databases offers high transparency in their source codes and algorithms. The database entries, however, are often not traceable and valid, as usually anyone can make new entries into the databases. Moreover, there is still a lack of non-commercial databases for food commodities. Assembling such databases for official food control is a difficult task due to the need for reference and authentic materials. The unsupervised use of public databases is also not feasible, as fraudsters would have access too.

Parameter-based Validation Strategy of Baden-Württemberg

Due to the lack of alternatives, the use of commercial databases for official food control is still mandatory in some areas. In order to ensure quality even when using commercial databases, the official food control laboratories of the German state of Baden-Württemberg (BW) have developed their own validation concept for MALDI-TOF-MS databases for the identification of microorganisms and other applications^[4].

Rather than validating the entire database, the laboratories switched to a parameter-based validation strategy, meaning they focus only on microorganisms that are key for their official expert opinions. The validation of a database parameter is achieved by application to a sufficiently large authentic sample group of the selected microorganism. The database entry is also validated against a negative control group. The experiments are moreover performed in all five official food control laboratories of BW. The identification results can then be used to calculate false-negative and false-positive rates and therefore draw conclusions about the sensitivity and the specificity of the database output.

With the help of this validation concept for databases, the official laboratories of BW obtained a flexible accreditation by the German accreditation body for their microorganism identification with MALDI-TOF. Their validation concept will also be a validation topic in the recently founded § 64 LFGB working group "MALDI-TOF".



Acknowledgements

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References

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