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The scientific challenges in moving from targeted to non-targeted mass spectrometric methods for food fraud analysis: a proposed validation workflow to bring about a harmonized approach

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Abstract

Background

Detecting and measuring food fraud is a challenging analytical task since a very wide range of food ingredients and types may be adulterated by numerous potential adulterants, many of which are yet unknown. To date most of the methods applied for the control of food fraud are targeted methods, which are focused on the detection of one or a few classes of known compounds.

Scope and Approach

There is an increasing availability of solutions and applications based on high resolution mass spectrometry (HRMS), allowing parallel non-targeted approaches, novel compound identification and retrospective data analysis. For these types of methods sample-handling must be minimal to allow the inclusion of as many as possible chemical categories. However data-handling of such methods is much more demanding, together with the potential requirement to integrate multiplatform data as well as conducting data fusion. To allow the processing of massive amounts of information based on the separation techniques and mass spectrometry approaches employed, effective software tools capable of rapid data mining procedures must be employed and metabolomics based approaches does appear to be the correct way forward.

To verify the relevance of modelling results, appropriate model validation is essential for non-targeted approaches, confirming the significance of the chemical markers identified.

Key Findings and Conclusions

The present paper is devoted to review and assess the current state of the art with regards non- targeted mass spectrometry in food fraud detection within many food matrices and to propose a harmonized workflow for all such applications.

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