Integrated machine learning-based approach to evaluate authenticity in various food matrices via MALDI-TOF-MS technology

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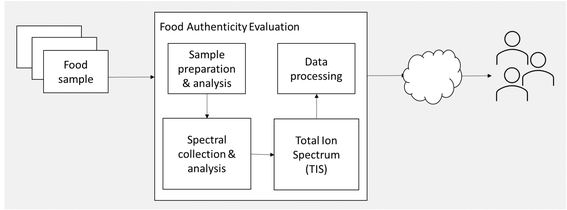
Introduction

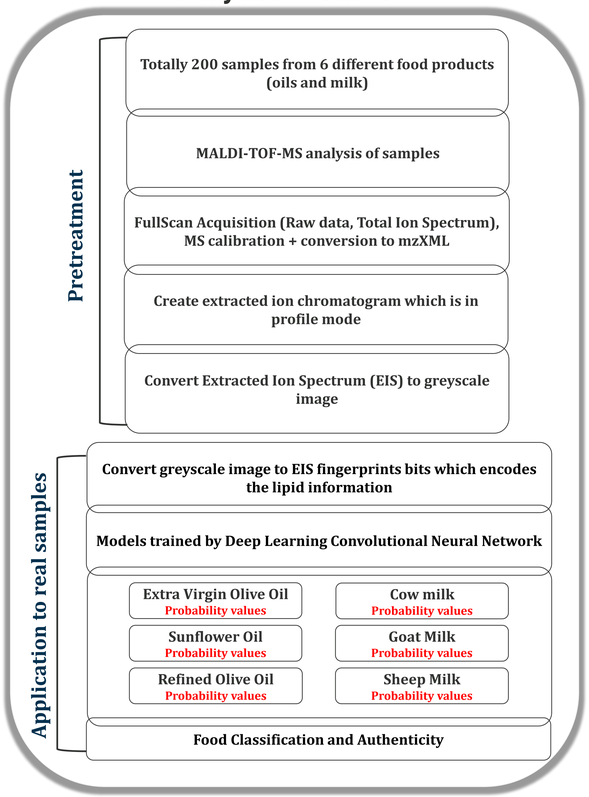
During the last decades, food authenticity has been found in the frontline of scientific research, to ensure high nutritional value, superior quality and food safety. Global recognition of food products, known for their unique nutritional properties, such as olive oil and dairy products, has raised awareness for quality assurance. However, the financial importance of these food products leads producers to several fraudulent practices, such as mislabelling or adulteration of products with illegal substances for profit purposes [1]. In the present study, a holistic machine learning- based approach was developed, to evaluate the origin of food products via Matrix-Assisted Laser Desorption/Ionization - Time of Flight Mass Spectrometry (MALDI-TOF-MS), investigating the lipid profile of olive oil and milk as case studies.

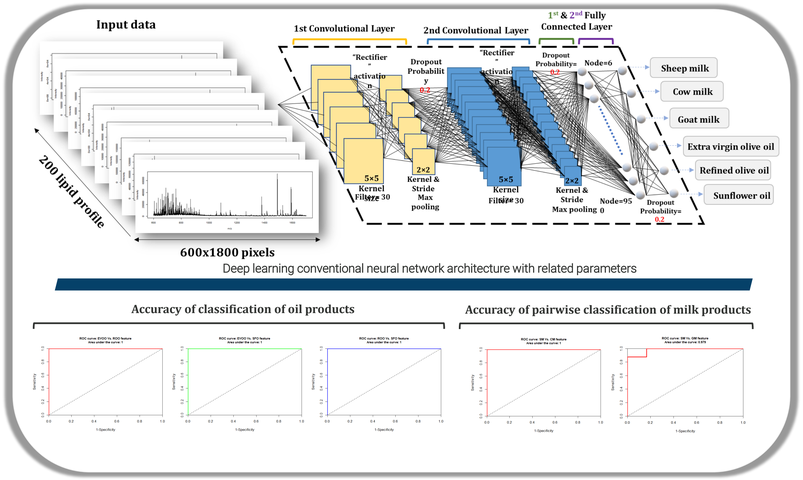
Methods

The presented methodology exploits the lipid content of food matrices of plant and animal origin to investigate the authenticity and detect potential adulteration. Sample preparation was based on a simple extraction using chloroform and methanol, while a-cyano-hydroxycinnamic acid was used as MALDI matrix [2]. For the spotting procedure, a double layer method was applied in a ground steel target plate. Data from MALDI-TOF-MS analysis were processed by a deep learning (DL) model to predict the origin of each food (i.e., olive oil, milk). The model uses the total lipid profile of food, obtained from MALDI-TOF-MS, as learning input, by searching for Region of Interest (ROIs) that are specific for each food product, adjusting the layers according to the data collection. To evaluate the applicability of the developed workflow, the methodology was applied in both food of animal and plant origin, using milk and olive oil per case. For this purpose, a common fraudulent practice of substitution was investigated, discriminating the animal origin of milk, as well as the detection of extra virgin olive oil adulteration wither lower quality oils, respectively. The parameters were adjusted and optimized based on cross validation techniques to overcome overfitting issues during the training of the DL model. Regarding MALDI-TOF analysis, a microfleX LRF (Bruker Daltonics, Bremen, Germany) was used, operated in reflector mode.

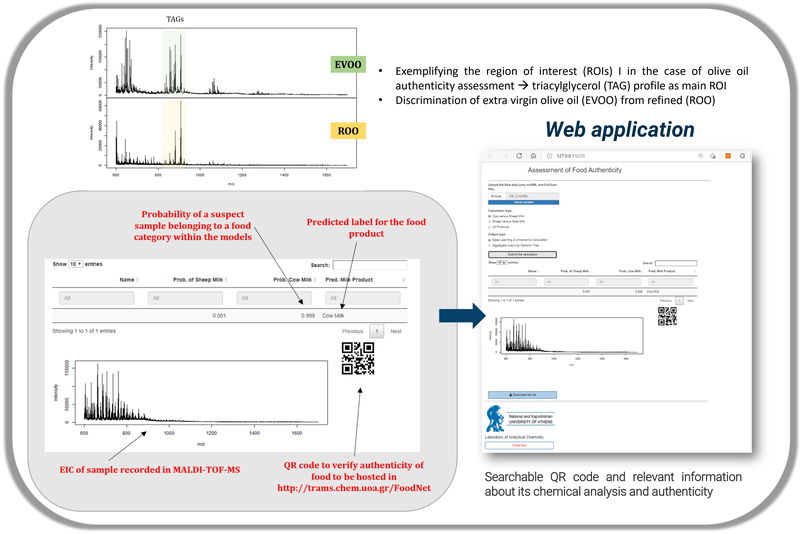


Analytical workflow





Outcome



Summary

A novel fast & reliable screening MALDI-TOF-MS methodology was developed to investigate food authenticity based on a machine learning workflow. The workflow successfully detected the origin of each sample matrix (oil and milk as case studies), while detection of adulteration was achieved down to 1%. The authenticity outcome can potentially interpreted into a digital mark, which communicates the authenticity results, and their adulteration probability values with consumers or food products manufacturers to ensure traceability in the production line.

Regarding the developed workflow, a European Patent application has been submitted by the authors: European Patent EP22201755.0 entitled "A method for evaluating the authenticity of food products and a system thereof", Nikolaos S. Thomaidis, Reza Aalizadeh, Anastasia S. Kritikou, Sofia K. Drakopoulou (submitted October 14th, 2022)

References

[1] https://doi.org/10.1016/j.foodchem.2021.131057

[2] https://doi.org/10.1016/j.foodchem.2012.02.154

Conclusion

- Universal approach for food assessment exploiting the total lipid profile via MALDI-TOF-MS.
- The workflow is based on an in-house nature inspired computational workflow based on convolutional neural network deep learning model.
- The model uses the lipid profile of foods, obtained from MALDI-TOFMS, as learning input.
- The algorithm creates Region of Interest (ROIs) for each extracted lipid mass spectra and correlates these ROIs to their food origin/label in a supervised manner.
- The model dynamically searches for ROIs that are specific for each food product and it adjusts its output layer based on number of food labels.
- The output is also interpreted into a QR code which communicates the authenticity results, and their adulteration probability values with consumers or food products manufacturers.
- The simplicity of sample preparation, the speed of data collection and analysis, and low per-sample costs support the use of MALDI-TOF-MS for the implementation of the developed strategy in a plethora of food matrices.

MALDI: Applications