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Efficiency of NIR spectroscopy and chemometrics to assess mislabeling of fish fillets

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ABSTRACT

Mislabeling and species substitution are widely affecting the fishery sector, especially considering fish fillets. It is difficult for both consumers and official control authorities to ascertain the identity information provided in the label. For this reason, there is a constant need of innovative, fast, and reliable instruments to improve the detection of such frauds. The present study explores how near-infrared (NIR) spectroscopy coupled with chemometric tools can identify fillets from five different fish species, namely: Atlantic cod (*Gadus morhua*), Goldblotch grouper (*Epinephelus costae*), Tub gurnard (*Chelidonichthys lucerna*), Guinean sole (*Synaptura cadenati*), and European plaice (*Pleuronectes platessa*). Fifty fresh samples of each species were collected and analyzed using three NIR devices: the portable MicroNIR by VIAVI, the handheld SCiO by Consumer Physics, and the benchtop MPA by Bruker. The acquired spectra were processed and analyzed to build classification models. Results showed high accuracy: SCiO performed with over 93 % accuracy in both cross-validation and test set prediction; MPA followed with accuracy over 83 %, while MicroNIR showed accuracy slightly lower than 81 %. These results suggest great reliability of the approach combining NIR spectroscopy and chemometric methods, in the context of food authenticity and fight against seafood frauds.

1. Introduction

Fraud in seafood production is a widespread issue, and seafood products are often ranked among the top three most vulnerable food categories that are subject to fraud (Reilly, 2018). Recent investigations from the non-profit organization Oceana and the Food and Agriculture Organization (FAO) show that about a third of all fish and seafood products sold worldwide is mislabeled (Acutis et al., 2019; FAO, 2021; Lawrence et al., 2022; Reilly, 2018; Thurston, 2021; Warner et al., 2019). Thus, there is an increase in seafood fraud across the world firstly due to the heterogeneity of seafood and to the large variety of commercial species (150–200 species) as well. The main forms of seafood fraud include the labelling of low-value species as more expensive ones. In fact, it is not easy to reliably identify a fish, especially if it is commercialized in the form of a skinless fillet (FAO, 2022; Reilly, 2018).

The reasons why the fishing industry is so affected by mislabeling are not always predictable; sometimes they can be referred to simple misinterpretation of regulations or mistranslations from foreign languages. However, in most cases the underlying rationale is economic gain since profits from selling lower-priced fish labelled as higher priced fish can be very significant (Donlan and Luque, 2019; Reilly, 2018). When economic gain is involved, these actions are considered as commercial frauds. Indeed, fish products can be relatively easy to counterfeit and it is also quite common that large price (and value) variability in

Abbreviations: FT, Fourier transform; NIR, near-infrared; PCA, principal component analysis; PLS-DA, partial least squares-discriminant analysis; SNV, standard normal variate; VIP, variable importance in projection.

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different species does not reflect any substantial morphological diversity (FAO, 2022; The State of World Fisheries and Aquaculture, 2020 - Sustainability in action, 2020).

Even though species substitution and mislabeling usually only represent commercial fraud, sometimes impacts can be even more dangerous, with consequences both on species conservation and on human health. This is the case of species with temporary fishing bans, which are illegally caught and then deliberately mislabeled. Also, it occurs that harmful species (e.g., poisonous, or tropical species) are consciously sold with fake descriptions, putting consumers at risk of becoming intoxicated or infected (Donlan and Luque, 2019; Kusche and Hanel, 2021).

To prevent these risks and to set up trustworthy methods for official controls, genetic techniques, such as DNA barcoding and nucleotide sequencing (Acutis et al., 2019; Calosso et al., 2020; Carvalho et al., 2017), have been developed, whereas traditional methods are based on protein analysis like electrophoresis, chromatography, or immunological techniques (Civera, 2003). Notwithstanding that these reference techniques are accurate and precise, frauds are still rampant in the seafood industry also because these traditional techniques are expensive, destructive, and require long analysis times, thus resulting in only about 1 % of the production getting inspected.

Therefore, beside DNA analysis, alternative and innovative analytical procedures must be investigated, such as hyperspectral imaging, Raman spectroscopy and near-infrared (NIR) spectroscopy (Grassi et al., 2018; Hu et al., 2023; O'Brien et al., 2013; Qin et al., 2020). NIR spectroscopy has the advantage to be a rapid, non-destructive, and rather affordable technique. It is based on the evaluation of the biochemical properties of tissues, such as: the presence and content of proteins, fat, water, total volatile basic nitrogen (TVB-N), trimethylamine (TMA), and the pH (Prabhakar et al., 2020). This technology has already been used to evaluate the freshness and wholesomeness of fish products and to discriminate fresh fillets from thawed ones, as well as farmed from wild-caught fish (Kimiya et al., 2013; Pennisi et al., 2021; Sivertsen et al., 2011; Trocino et al., 2012; Uddin et al., 2005; Zhou et al., 2019). Furthermore, spectra obtained through NIR spectroscopy are highly informative since multiple analytical signals are recorded at the same time (Trocino et al., 2012). For this reason, multivariate data analysis becomes pivotal, and chemometric tools are often used to model NIR spectra and to extract valuable information from spectral data (Blanco and Villarroya, 2002).

To guarantee the most comprehensive scenario, in this study three types of NIR instruments were used and their performance evaluated: a handheld and low-cost tool (SCiO, by Consumer Physics), a portable instrument (MicroNIR Pro Es, by VIAVI Solutions), and a benchtop spectrophotometer (Multi Purpose Analyzer–MPA, by Bruker). Fillets from five different fish species were scanned and compared, leading to the discovery of large variability of the resulting spectra. The aim of the present study was to evaluate the performances of NIR spectroscopy and chemometrics to assess mislabeling of fish fillets, in the case of multiple available classes/species. Furthermore, the accuracy and performances of three different NIR instruments were calculated and compared, to inspect their reliability.

2. Materials and methods

2.1. Study design and NIR instrumentation

Five different fish species were included in this study (Fig. 1): "MN" (*Gadus morhua* – Atlantic cod), "CE" (*Epinephelus costae* – Goldblotch grouper), "GL" (*Chelidonichthys lucerna* – Tub gurnard), "SO" (*Synaptura cadenati* – Guinean sole), "PL" (*Pleuronectes platessa* – European plaice). For each species, 50 individual fillets were selected, resulting in a total of 250 fillets analyzed. The fillets were selected and prepared following standardized commercial processing protocols, ensuring consistency in size, thickness, and anatomical orientation across all specimens.

Spectral data were collected in reflectance mode using three near-infrared (NIR) instruments: two portable devices—SCiO pocket molecular sensor (v1.2, Consumer Physics Inc., Tel Aviv, Israel) and MicroNIR 1700 Pro ES (VIAVI Solutions, San Jose, CA, USA)—and one benchtop Fourier transform-NIR (FT-NIR) spectrophotometer (Multi Purpose Analyzer–MPA, Bruker Optics, Ettlingen, Germany). The SCiO sensor acquires spectra in the 740–1070 nm range with a spectral resolution of approximately 10 nm, while the MicroNIR 1700 Pro ES captures spectra from 908 to 1676 nm, with higher spectral resolution of ~6 nm. The Bruker MPA FT-NIR spectrometer operates in the 800–2500 nm range, with a spectral resolution of 8 cm^{-1} (approximately 2–4 nm depending on the region of the spectrum). A representation of the averaged SNV-preprocessed and mean centered spectra of all five fish species is provided in Fig. 2a-c. The spectra were reported in their preprocessed version to enhance the differences among the species. A more detailed representation of the whole (preprocessed) datasets is provided as

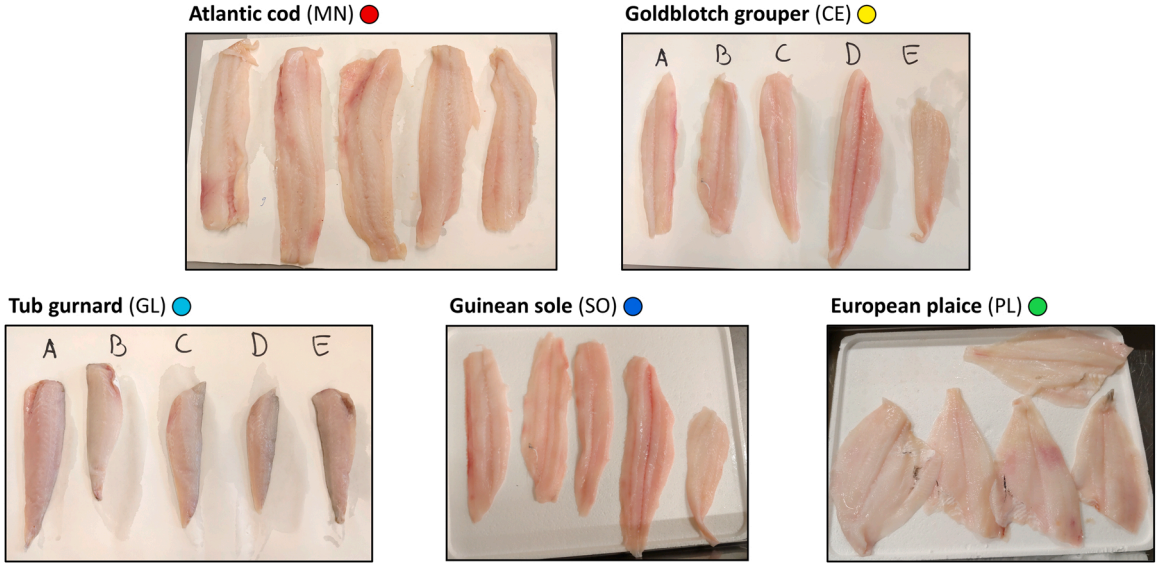

Fig. 1. Example photos of the five fish species analyzed. The codes in brackets and the assigned colors match with the notation used throughout the main text and the PCA scores colors of Fig. 3.

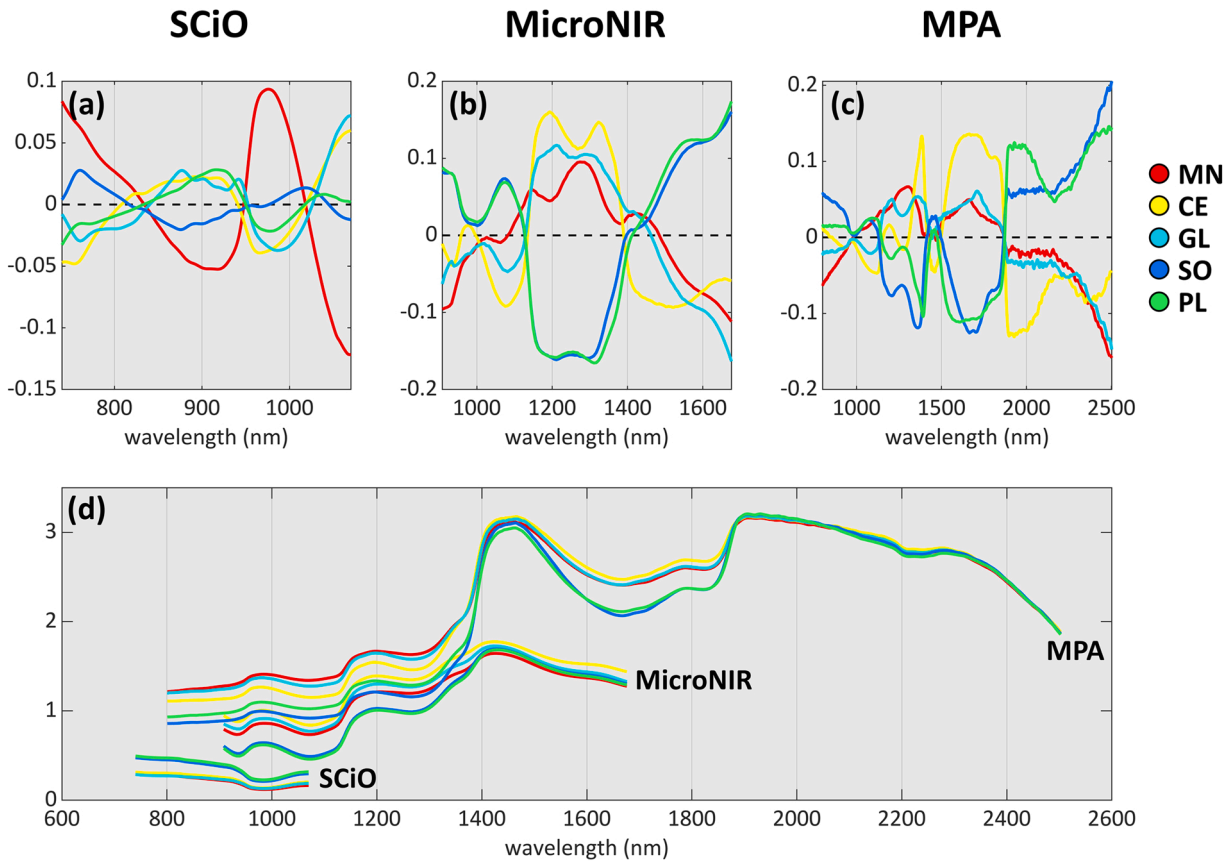

Fig. 2. Averaged profiles of the five fish classes analyzed in this study. The data in (a-c) were preprocessed with SNV and mean center, to enhance the differences among the species, and are detailed for each NIR instrument: (a) SCiO, (b) MicroNIR, (c) MPA. The plot in (d) reports the averaged profiles of the raw data all together, to provide a global representation of how the three instruments' wavelength ranges overlap.

Figure S1 in the Supplementary Materials. Also, the averaged profiles of the raw data all together are reported in Fig. 2d, to provide a global representation of how the three instruments' wavelength ranges overlap.

All portable scans were performed in-field immediately after filleting, at room temperature of about 10–15 °C. To ensure anatomical consistency, spectra were acquired from the same anatomical location on each fillet – the mid-dorsal muscle region. To capture within-sample variability, each fillet was scanned three times with the SCiO sensor and the MicroNIR instrument, and at least four times with the MPA benchtop instrument.

After field measurements, the fillets were stored in a transportation box at 2 ± 2 °C to maintain cold chain integrity and were transferred to a laboratory, where they were scanned using the FT-NIR benchtop instrument at room temperature of about 15–20 °C. The same anatomical region was analyzed in all specimens with the different instruments. All devices were calibrated prior to the initial scan and subsequently recalibrated after every ten samples according to manufacturer-specific guidelines. For detailed specifications and technical configurations of each instrument please refer to Cavallini et al. (2022) and Pennisi et al. (2021).

2.2. Data analysis

One spectral dataset for each NIR instrument was obtained. The initial data quality inspection allowed removing all spectral acquisitions affected by experimental problems, as well as spectra showing significant deviation among replicates. This process ensured data reliability and minimized variability not ascribable to biological differences. Subsequently, the datasets were explored by principal component analysis (PCA (Bro and Smilde, 2014; Jolliffe, 2002)), to check whether grouping tendencies related to the five fish species were present, but also to detect possible effects related to the acquisition date, which can be detrimental for the subsequent classification modelling. No relevant acquisition time effects were detected. After data quality inspection all acceptable replicates were averaged, yielding one dataset of 250 representative spectra for each NIR instrument: each spectrum corresponded to one individual fish fillet.

Prior to chemometric modelling (exploratory and classification analyses) all datasets were pre-processed using standard normal variate (SNV (Sun et al., 2009)), followed by mean centering. For the SCiO instrument, the same spectral dataset was considered to perform a parallel data analysis, which involves the use of different pre-processing methods explored through the Consumer Physics online platform, *The Lab*. More in detail, the four available options available on this platform, i.e., "Processed," "Normalize", "Processed & Normalize", and "(log) R and Normalize" were evaluated and the best-performing model was retained based on the corresponding classification metrics.

Regarding the classification modelling, the partial least squares-discriminant analysis (PLS-DA (Ballabio and Consonni, 2013)) method was chosen and consistently applied to all datasets. Each dataset was split into a calibration (training) and a test (validation) set and processed under MATLAB environment using the Duplex algorithm (Daszykowski et al., 2002), which was individually applied to each fish species class, to obtain balanced calibration and test sets, with a 33 % split ratio. All calibration sets counted 165 samples, and all test sets consisted of the remaining 85 samples. It is important to consider that the actual samples selected for each test sets are not – by definition – the same across the three spectral datasets. The classification results are reported as two confusion matrices: for each fish species the

cross-validated (CV) the test set prediction results are reported.

To keep the results exposition and interpretation as simple as possible and considering that the classification problem under examination concerns five classes, only accuracy will be discussed as the performance parameter. The model accuracy (Ballabio et al., 2018) basically is an estimation of the model error, and it is computed as the sum of the true positives (i.e., the correctly classified samples of each class) divided by the total number of samples. By looking at the confusion matrix (for more details please refer to Table S1, Table S2 and Table S3 in the Supplementary Materials) computing the accuracy means taking the sum of the values of the diagonal of the matrix and dividing the result by the total number of samples. For each dataset, the calibration and test set prediction accuracy values were computed.

Concerning the interpretation of the most influent NIR signals in the classification models, it was decided to plot and interpret the variable importance in projection (VIP) scores (Farrés et al., 2015), which allow identifying the most influent spectral variables with a simple plot.

Concerning the SCiO models built using directly *The Lab* online platform, classification performance of the four pre-processing options was compared using both confusion matrix accuracy and the F1 score, a widely accepted performance metric that balances precision and recall (Ballabio et al., 2018). The accuracy of the validation set for the best SCiO model was then reported as the percentage of fillets correctly identified, providing an objective measure of real-world model performance (Pennisi et al., 2021).

2.3. Software and toolboxes

All datasets were processed and analyzed under MATLAB environment (version 2021a, The Mathworks, MA, USA). PCA exploratory analysis and PLS-DA classification modelling were performed using the functions of the PLS_Toolbox (version 8.9, Eigenvector Research Inc., Manson, WA, USA) software package. Dataset splitting into calibration and test sets was performed using the Duplex algorithm by Michał Daszykowski (https://www.researchgate.net/publication/305536996, MATLAB code for the Duplex uniform subset selection algorithm, last accessed 19/06/2025). In-house routines were developed to import, manage, and assess the raw data and organize the data analysis workflow under MATLAB environment.

The smartphone app "The Lab" (version 1.2.1; https://play.google.com/store/apps/details?id=com.consumerphysics.researcher or https://apps.apple.com/us/app/the-lab-dev-toolkit-for-scio/id965758603, last accessed 19/06/2025) was used to control the SCiO sensor and was installed on an Android phone. The SCiO spectra were managed, downloaded, and analyzed (in parallel to the MATLAB data analysis workflow) using the web interface of *The Lab*.

3. Results and discussion

3.1. Exploratory analysis

The exploratory analysis by PCA highlighted rather clear separation tendencies for all spectral datasets, as shown in Fig. 3, where only the most relevant combinations of principal components are reported. In all cases clear groupings can be seen, even if some fish species appear more overlapped: for both the MicroNIR and MPA data the species of MN, GL and CE tend to be overlapped (Fig. 3b-c), but separated from the species of PL and SO (Fig. 3b-c). More specifically, in the MicroNIR case PL and SO appear to be indistinguishable – i.e., completely overlapped – at least for what concerns the information described by PC1 and PC2 (Fig. 3b). These two species appear much less overlapped in the MPA case (Fig. 3c).

The loadings plots (Fig. 3, panels d–f) offer essential insights into which spectral regions most influence the separation among fish species observed in the PCA scores plots. In the SCiO dataset (Fig. 3d), prominent loading peaks appear between 875–925 nm and 1040–1070 nm, corresponding to NIR absorption bands typically associated with water and protein content (i.e., O–H and N–H overtones or combination bands). These suggest that interspecies differences in muscle composition, particularly in terms of moisture and protein levels, contribute

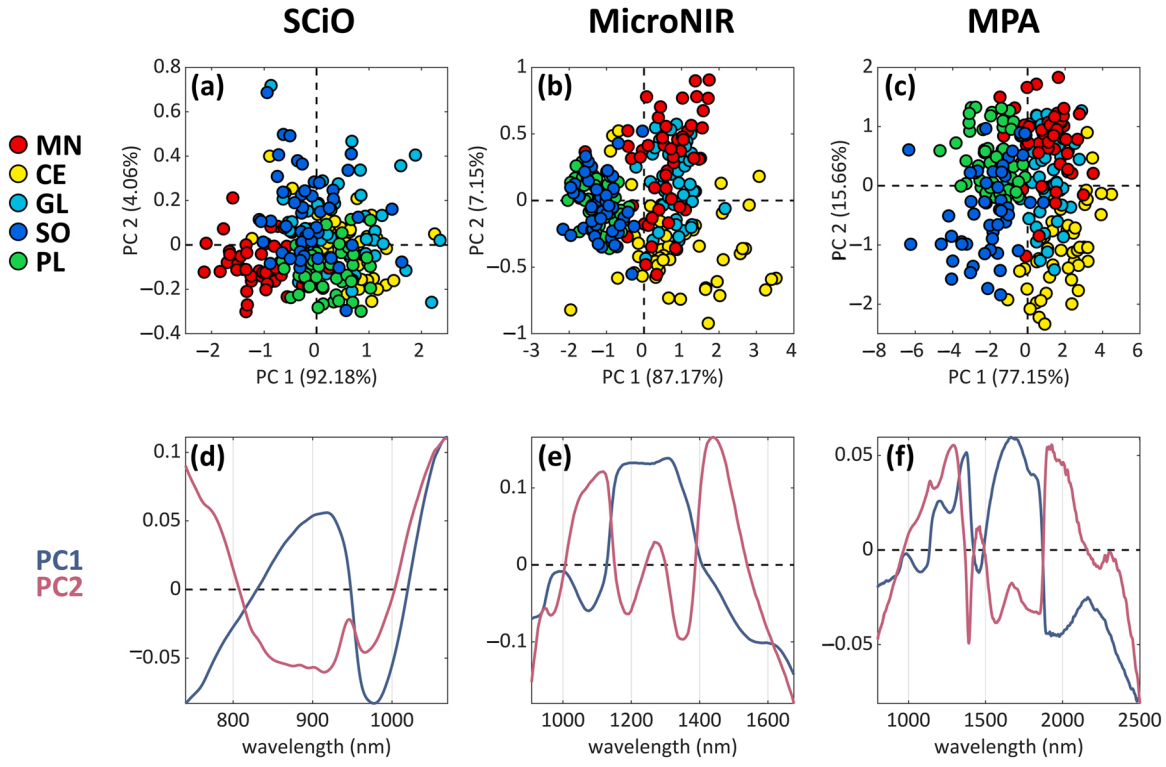

Fig. 3. Most relevant PCA scores plots (a – SCiO, b – MicroNIR, c – MPA) in terms of fish species separations. On the bottom row (d–f) the corresponding loadings plots are reported.

significantly to the observed clustering. For the MicroNIR dataset (Fig. 3e), the reported PCs show strong contributions in the 1100–1300 nm region, as well as around 1450 nm, which are characteristic of water second overtone and aliphatic compounds. Similarly, the loadings in the MPA dataset (Fig. 3f) emphasize the 1400–1600 nm region, often attributed to N–H and C–H stretching vibrations related to proteins and lipids.

Overall, the loadings plots confirm that the spectral separation observed in the PCA scores plots reflect underlying biochemical differences among the fish species. These findings are further supported by the VIP scores analysis discussed in 3.3, highlighting the central role of water, protein, and aliphatic content in NIR-based species discrimination.

3.2. Classification analysis: overall results

The classification modelling was done with PLS-DA on all datasets, and additionally with the classification tools provided by *The Lab* web application by Consumer Physics, in the case of the SCiO data. Across all models, high accuracy was achieved. The overall classification accuracy, intended as the mean of the specific accuracy values obtained for each fish species (see Table 1), was highest for the handheld SCiO device: 93.9 % (CV, 10 samples misclassified) and 94.1 % (test set, 5 samples misclassified). The MPA achieved an overall accuracy of 83.6 % (CV, 27 samples misclassified) and 83.5 % (test set, 14 samples misclassified), followed by MicroNIR with 81.2 % (CV, 31 samples misclassified) and 82.3 % (test set, 15 samples misclassified).

Regarding the accuracy in prediction (test set prediction), the trend is confirmed, with the SCiO instrument still showing the best performances, followed by the MicroNIR and MPA instruments, both with comparable performances: over 94 % for SCiO, over 82 % for MicroNIR and over 83 % for MPA. All results obtained for each species and for each instrument are reported in Table 1.

All PLS-DA models provided rather good classification performances. However, the multi-class problem at hand was approached with a discriminant analysis method, which forces each sample to be assigned to one class with no chance of unassigned samples, so a higher error rate can in general be expected, and we would argue that, in the perspective of a proof-of-concept study, the obtained results are acceptable and promising.

3.3. Classification analysis with PLS-DA: interpretation of the most influential signals

To inspect the most influential wavelengths of each PLS-DA classification model it is possible to plot the VIP scores, which are reported in Fig. 4. From this representation, the spectral bands reported in Table 2 were inspected and largely assigned to classes of compounds.

Table 1
Classification results: accuracy values expressed in percentage. Each instrument's accuracy in prediction is reported, both in Cross-Validation (CV) set and in Test set prediction.

Prediction in Cross-Validation (CV)					
	CE	**GL**	**MN**	**PL**	**SO**
SCiO	84.8 %	93.9 %	97.0 %	93.9 %	100 %
SCiO (The Lab)	93.4 %	96.9 %	96.9 %	96.9 %	96.9 %
Micro NIR	90.9 %	93.9 %	87.9 %	78.8 %	54.5 %
MPA	78.8 %	90.0 %	75.8 %	93.8 %	78.8 %
Prediction in Test set					
	CE	**GL**	**MN**	**PL**	**SO**
SCiO	82.3 %	100 %	88.2 %	100 %	100 %
SCiO (The Lab)	100 %	100 %	91.7 %	86.8 %	91.9 %
Micro NIR	82.3 %	100 %	82.3 %	82.3 %	64.7 %
MPA	82.3 %	88.2 %	76.5 %	88.2 %	82.3 %

Water is the main constituent of fish flesh, roughly accounting for about 66–81 % of the weight of a fresh fish fillet (Grassi et al., 2018). A range of possible signal interpretations emerged across the three NIR instruments, as deduced from the VIP plot interpretation (Fig. 4). All the discussed signal interpretations are also reported in Table 2, together with those signals and bands that could not be interpreted (bottom row marked "Unassigned").

Signals related to water emerged as important in the SCiO and MPA datasets, with the 2nd and 3rd overtones. Unexpectedly, the overtone at 1440 nm (Alamprese and Casiraghi, 2015; Grassi et al., 2018; Liu et al., 2013) related to water did not result of importance in any datasets. Then, still focusing on the SCiO and MPA datasets, the proteins are represented with some complementary signals between the two techniques: for the SCiO instrument three main bands are reported (875 nm, 925 nm, 1050–1070 nm), while for the MPA instrument two main bands were found (1100 nm, 1600–1750 nm). Regarding the aliphatic compounds, no signals were identified in the SCiO data, while some bands could be spotted for the MicroNIR and MPA datasets: two bands for the MicroNIR (1120 nm, 1210 nm (Alamprese and Casiraghi, 2015; Grassi et al., 2018)) and signals in the range 1700–1910 nm (1st overtone C–H stretching of fats (Grassi et al., 2018; Liu et al., 2013)).

In accordance with a previous study carried out by the authors of this work (Cavallini et al., 2022), the SCiO dataset shows a signal at wavelengths < 750 nm, i.e., in the visible radiation zone corresponding to red absorption, suggesting that for this dataset also the color information could be important in discriminating among the different fish species, even if based on color shades not perceptible by naked eye.

The most difficult fish species to distinguish and correctly classify proved to be the SO and PL samples, even if the SCiO sensor performed particularly good in this case. To this aim, a parallel study focused on these two classes alone was carried out by the authors and has been already published (Cavallini et al., 2022), proving that by considering the PL and SO classes alone it is possible to efficiently distinguish them. In this perspective, a potential development of the classification modelling presented in the present work could encompass the use of hierarchical models, i.e., considering first a four-classes model in which PL and SO samples would be treated as one class alone. When a sample would be assigned to this class, a second classification model would be used to further distinguish between the SO and PL classes.

3.4. Classification analysis with The Lab web application

Concerning the SCiO data analyzed with *The Lab* web application the F1 score resulted equal to 0.801, and it was obtained using the "Processed" pre-processing method. The percentage of correctly identified fish fillets was found higher than 94 %, more specifically: CV 96.2 % (6), test set 94.1 % (4). This model was validated using an external dataset, i.e., it was not used for building the model. The obtained results showed good capability of the model to correctly identify the five species. More details are provided in Supplementary materials, with the confusion matrix of the cross-validation and test set results (Table S4).

The accuracy values obtained with the online *The Lab* analysis resulted comparable to those obtained with the classic chemometric approach applied to the same SCiO acquisitions. In fact, only small differences were observed between the two "versions" of the SCiO analysis. These outcomes suggest that this cloud-based device may also assist non-expert users in obtaining reliable and satisfactory results. An important limitation during the training phase of this modelling approach is that no signal inspection or validation can be performed, since the proprietary nature of Consumer Physics' *The Lab* prevents access to its algorithms: no VIP or other signal visualization can therefore be performed, in this case.

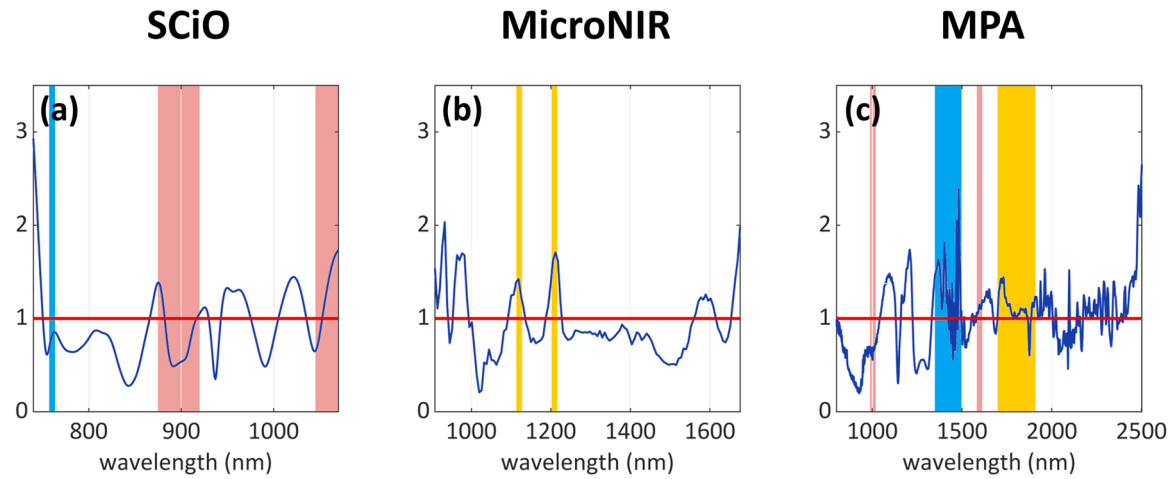

Fig. 4. VIP scores of the three PLS-DA classification models: (a) SCiO, (b) MicroNIR, and (c) MPA results. The signal assignments of Table 2 are reported in colors: blue = water, red = proteins, yellow = aliphatics.

Table 2
Signal assignments of the most influential variables identified using the VIP scores of the three PLS-DA models.

	SCiO	MicroNIR	MPA
Water	760 nm, 3rd overtone	/	1350–1500 nm, 2nd overtone
Proteins	875–920 nm 1045–1070 nm	/	1010 nm, RNH_2 3rd overtone 1600 nm, N–H 1st and 2nd overtones + N–H and C═O combination band (Grassi et al., 2018; Liu et al., 2013)
Aliphatics	/	1120 nm 1210 nm C–H stretching 2nd overtone (Alamprese and Casiraghi, 2015; Grassi et al., 2018)	1700–1910 nm 1st overtone C–H stretching (Grassi et al., 2018) of fats (Liu et al., 2013)
Other	< 750 nm, related to red adsorption	/	/
Unassigned	960 nm, 1020 nm	920–1000 nm 1590 nm 1650–1675 nm	1200 nm 1900–2000 nm > 2150 nm

4. Conclusions

The purpose of this study was to investigate an innovative and quick method based on the combination of NIR spectroscopy and chemometrics, as an alternative to traditional techniques such as DNA and protein analysis. NIR spectroscopy has been lately used with considerable success in several fields of the food industry: by combining handheld NIR instruments with pre-trained chemometric models, many samples can be acquired in a short time and easily classified. In this perspective, the added value of the study lies in demonstrating that a pre-configured and accessible device can perform efficiently and cost-effectively.

NIR spectroscopy is proving to be an efficient technique, because of its quick and simple usage, cost effectiveness, and very reduced need for sample preparation, to the point in which the sample remains intact and it is minimally handled during the analysis. Indeed, all instruments tested in this study provided good accuracy results, both in calibration and cross-validation, but also in testing with external datasets. The lower performance in species discrimination reported for MicroNIR and MPA could be ascribed to the complexity of the spectral signal, which made it more difficult to extract and process the useful information. Nevertheless, the classification accuracy values still demonstrate remarkable prediction capability for these instruments. This confirms the applicability of NIR spectroscopy in the fish sector as a replacement for more expensive and complex analyses in control activities. Despite the different instrumental characteristics, the performances of the three NIR devices are comparable, suggesting potentially high interchangeability.

Based on these results, it is likely that these kinds of tools will be used to detect food fraud directly on the market, both by authorities and companies or even by consumers, through small portable devices with pre-trained models. Furthermore, this study suggests the possibility for competent control authorities to make use of this analytical system (i.e., NIR and chemometrics), which can be validated for official controls.

CRediT authorship contribution statement

Francesco Geobaldo: Writing – review & editing, Supervision. **Giovanna Esposito:** Writing – original draft, Software, Methodology, Data curation. **Alberto Pianezzola:** Resources. **Luca Magnani:** Resources. **Francesco Pennisi:** Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation. **Francesco Savorani:** Writing – review & editing, Validation, Supervision, Software, Project administration, Conceptualization. **Alessandro Giraudo:** Validation, Software, Methodology, Formal analysis. **Nicola Cavallini:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Formal analysis. **Elena Bozzetta:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization. **Marzia Pezzolato:** Writing – review & editing, Methodology, Formal analysis.

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Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests. Luca Magnani reports a relationship with Esselunga S.p.A. that includes: employment. Alberto Pianezzola reports a relationship with Esselunga S.p.A. that includes: employment. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jfca.2025.108630.

Data availability

Data will be made available on request.

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