An automated machine-learning approach for detecting fish species and body parts using Rapid Evaporative Ionization Mass Spectrometry

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***Abstract*—Marine biomass composition analysis traditionally requires time-consuming processes and domain expertise. This study demonstrates the effectiveness of Rapid Evaporative ionization Mass Spectrometry (REIMS) combined with advanced machine learning techniques for accurate marine biomass composition determination. Using fish species and body parts as model systems representing diverse biochemical profiles, we investigate various machine learning methods, including unsupervised pre-training strategies for transformers. The deep learning approaches consistently outperformed traditional machine learning across all tasks. We further explored the explainability of the best-performing and mostly black-box models using Local Interpretable Model-agnostic Explanations (LIME). We found important features driving decisions behind each of the top-performing classifiers. REIMS analysis with machine learning is an accurate and explainable technique for automated marine biomass compositional analysis. It has potential applications in marine-based industry quality control, product optimization, and food safety monitoring.**

***Index Terms*—AI applications, explainable AI, machine learning, marine biomass, mass spectrometry, multidisciplinary AI**

I. Introduction

THE fish processing industry forms a critical component of the global seafood supply chain, transforming raw marine biomass into consumer products through multiple stages. This process typically involves species sorting, cleaning, filleting, packaging, and quality control at various checkpoints. Each stage presents unique challenges that can benefit from artificial intelligence and machine learning (AI/ML) solutions. The traditional fish processing workflow begins with the arrival of catch, where workers must rapidly sort different species - a task prone to human error particularly with similar-looking fish. The catch then moves through cleaning and filleting stations, where different body parts are separated for various products - from premium fillets to processed fish meal. Quality control occurs throughout, checking for freshness, proper handling, and accurate labeling. Finally, products are packaged and prepared for distribution. Several critical challenges exist within this workflow:

1) Quality control: Mislabeling and fraud remain persistent issues in the seafood industry [1], with economic and food safety implications. Studies have shown significant rates of species substitution in various markets [2].
2) Product Optimization: Different fish body parts have varying commercial values and uses, with some parts commanding premium prices in specific markets. Accurate classification of these parts ensures optimal resource utilization and maximizes economic value across the supply chain [3].
3) Safety Monitoring: Accurate tracking of processed species volumes is essential for both regulatory compliance and stock management [4].

To address these challenges, we explore the application of machine learning to Rapid Evaporative Ionization Mass Spectrometry (REIMS) data across two critical classification tasks: fish species identification and body part classification. REIMS technology, combined with ML algorithms, offers a promising solution for real-time, accurate analysis during processing operations. Our focus on these specific tasks is driven by their direct impact on industry pain points:

(1) Species classification helps combat fraud and ensures proper resource management. (2) Body part identification optimizes processing efficiency and product value. (3) Accurate species counting supports both regulatory compliance and sustainability efforts.

This paper demonstrates how machine learning techniques applied to REIMS data can enhance the efficiency and accuracy of these critical fish processing operations, while supporting broader goals of sustainability and food security in the seafood industry.

This study utilizes datasets provided by New Zealand Plant and Food Research as part of the Cyber-Marine project, which focuses on developing a flexible factory for quality assurance in marine biomass analysis. The factory uses Rapid Evaporative Ionization Mass Spectrometry (REIMS) to optimize the value obtained from seafood resources. The dataset consists of mass spectrometry samples collected using REIMS, where an electrosurgical knife is used to create an aerosol from the samples. This aerosol is then directed into a mass spectrometer, where ionization occurs, allowing for mass-to-charge ratio analysis. Each sample undergoes multiple incisions lasting 3-5 seconds, providing detailed chemometric data in the mass range of m/z 77.04 - 999.32.

REIMS marine biomass analysis faces several challenges: time-consuming manual ”offline” analysis, costly domain expertise required, high-dimensionality, [5] and few training

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samples, and the need for automated "online" inference. Note, "online" inference in the domain of chemistry and fish processing, not to be confused with "online" learning from machine learning. The rapid nature of REIMS necessitates equally rapid inference of its results, as traditional analytical chemistry techniques which take several hours are too slow [6]. Furthermore, current analytical methods for REIMS data often require domain expertise in chemistry and fish processing, which does not match the speed of REIMS. Traditionally, samples would be sent away for "offline" analysis by domain experts in chemistry, we look to develop methods capable of automated inference for "online" analysis on the production line of a fish processing factory. REIMS also produces high-dimensional data, with this particular dataset having 2080 mass-to-charge ratios as features, but there are limited training instances due to the time-consuming and expensive task of sample preparation. Additionally, industry applications require fast, accurate, and interpretable models that can be verified and troubleshooted in real-world scenarios.

To address the above challenges, this paper proposes several innovative machine learning approaches that provide automated inference, eliminating the need for domain expertise in fish processing. To handle the high-dimensionality of REIMS data, this paper utilizes deep learning [7], [8] and evolutionary computation [9], [10] that are well-suited for complex feature interactions in mass spectra with limited training instances. Techniques like BERT [7] and attention mechanisms [8] can capture complex, non-linear relationships between features in high-dimensional data. Evolutionary Computation via Genetic programming [9]–[11] can efficiently search large feature spaces to identify important feature combinations and interactions. To mitigate the limited number of training samples, we implement data augmentation and unsupervised pretraining. Data augmentation artificially increases the size of the training dataset by creating modified versions of existing samples. For example, in image processing, you might flip, rotate, or add noise to existing images to create new, slightly different samples. This helps the model learn to be more robust and generalizable, even with a limited initial dataset. The unsupervised pretraining approach involves training the model on a large amount of unlabeled data before fine-tuning it on the limited labelled dataset. The model learns general features and patterns from the unlabeled data, which can then be transferred to the specific task at hand. This can significantly improve performance when labelled data is scarce. Finally, we employ Local Interpretable Model-agnostic Explanations (LIME) [12] to provide interpretable outputs that identify important features and quantify their impact, making our models more accessible to domain experts in chemistry and fish processing.

The main contributions of the paper are:

1) **Real-time Marine Biomass Analysis:** The paper demonstrates the use of Rapid Evaporative Ionization Mass Spectrometry (REIMS) combined with advanced machine learning techniques to enable automated analysis of marine biomass. This represents a significant improvement over traditional, time-consuming methods.
2) **Machine learning on sequential data:** Developed and analysed different machine learning models, including traditional methods, deep learning and evolutionary computation approaches. The deep learning methods consider the sequential nature of the data.
3) **Feature importance:** Identify the important mass-to-charge ratios for the best performing models. This enhances domain knowledge in fish processing and chemistry.

II. Related works

Building upon the foundation laid in the introduction, this section delves deeper into the existing body of research on marine biomass analysis, exploring both traditional methods and recent advancements in REIMS technology, while highlighting the gaps and challenges that our proposed approach aims to address. We also provide the necessary background on deep learning and evolutionary computation required.

A. Marine Biomass

Mislabelling is a significant issue in the global seafood industry, with a meta-analysis of genomic profiling methods finding an average mislabelling rate of 30% worldwide [2]. Machine learning methods using Rapid Evaporative Ionization Mass Spectrometry (REIMS) data offer a promising solution to this problem by enabling more accurate fish species classification. For example, in 2016, a restaurant in Melbourne was accused of serving catfish instead of dory [13], highlighting the need for better species detection techniques. REIMS technology, which works on both raw and cooked biomass, can combat fraud by ensuring species authenticity. Approximately 40% of a fish is edible fillet, while the remaining 60% can be repurposed into products like fertilizers or high-value pharmaceutical-grade omega-3 concentrates. Fish oil, rich in omega-3 polyunsaturated fatty acids [14], is nutritionally essential but increasingly scarce in Western diets [15]. REIMS-based machine learning methods in fish processing also help identify high-value parts for repurposing into valuable products, contributing to the rising consumer demand for omega-3 supplements made from diverse marine biomass [16].

B. REIMS

Traditional approaches for analyzing marine biomass composition have long been the cornerstone of research and quality control in the seafood industry. These methods include Gas Chromatography-Mass Spectroscopy [17], Nuclear Magnetic Resonance Spectroscopy [18], and Genomic Profiling [2]. While these techniques have proven valuable, they often come with significant drawbacks. They are typically time-consuming, requiring extensive sample preparation and analysis time. Additionally, they are labour-intensive, demanding skilled technicians to operate complex equipment and interpret results. Perhaps most importantly, these methods necessitate substantial domain expertise, limiting their accessibility and scalability in real-world applications. These limitations have spurred the search for rapid techniques for marine biomass analysis in fish processing.

In recent years, Rapid Evaporative ionization Mass Spectrometry (REIMS) has emerged as a promising technique for

rapid and accurate analysis of biological samples, addressing many of the limitations of traditional methods. Since its introduction in the original paper by Balog et al. [19], REIMS has demonstrated its versatility and effectiveness across various applications. For instance, it has been successfully employed to detect horse offal mixed into beef mince at concentrations as low as 1%-5%, showcasing its potential in addressing food fraud [1]. In the realm of seafood, REIMS has been applied to binary classification tasks for detecting fish species and catch methods, further illustrating its utility in combating fish fraud [20]. Historically, REIMS biomass analysis has primarily relied on Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) [21]–[23] with Principal Component Analysis (PCA) for dimensionality reduction [24]. However, this PCA-OPLS-DA approach has limitations, particularly in its reliance on outlier thresholding for adulteration detection, which requires manually defined hyperparameters set by domain experts in chemistry. This work proposes automated methods with learnable parameters that don't require domain expertise in chemistry to be configured. Additionally, this work proposes deep learning and evolutionary computation methods from machine learning that outperform the traditional OPLS-DA approach.

C. Deep Learning

These models were selected for Rapid Evaporative Ionization Mass Spectrometry (REIMS) marine biomass analysis because of their ability to handle complex, high-dimensional data with sequential or structured dependencies, which are inherent in REIMS data. Transformers [7], [8], known for their powerful self-attention mechanisms, excel at weighing the importance of different features in sequential data, making them well-suited for identifying patterns in REIMS spectra. Since REIMS data, like sequences in language, consists of ordered data points (mass-to-charge ratios) with varying degrees of importance, the transformer's attention mechanism allows it to dynamically focus on critical parts of the spectrum for classification or prediction. Long Short-Term Memory (LSTM) networks [25], a type of recurrent neural network (RNN), are also effective for REIMS data because they capture long-term dependencies in sequential data. This is crucial for REIMS analysis, as spectral data might contain dependencies across distant mass-to-charge values. LSTM's ability to store and retrieve information over long sequences enhances its performance in such tasks, especially when the signal patterns may not be immediately adjacent. Variational Autoencoders (VAE) [26] offer an effective approach to handling the complexity and variability of REIMS data by learning a compressed, latent representation of the spectral information. VAEs can also reconstruct this data, making them ideal for tasks like species and body parts classification, where they can model and detect small anomalies or deviations in the spectral data. Kolmogorov-Arnold Networks (KAN) [27] are highly efficient at approximating complex functions, which is essential in REIMS data analysis, where subtle differences in spectra can indicate different classes such as species and body parts. KAN's ability to improve function approximation makes it especially powerful for handling non-linear patterns in mass spectrometry data, which traditional models may struggle to capture. Convolutional Neural Networks (CNN) [28]–[31], although primarily used in image processing, are highly effective for REIMS data due to the spatial connectivity in mass spectra. Just as neighbouring pixels in images share spatial relationships, neighbouring mass-to-charge ratios in REIMS data also exhibit dependencies. CNNs can exploit this structure to identify patterns in one-dimensional data, treating mass spectra similarly to 1D images. Finally, Mamba [32], a state-space model, offers an efficient alternative to transformers for sequential data processing. Mamba is designed for high-performance handling of complex time-series data, making it an excellent fit for REIMS analysis, where both computational efficiency and the ability to model sequential dependencies are essential for automated or large-scale biomass analysis.

D. Evolutionary Computation

Evolutionary computation, particularly genetic programming (GP), offers a powerful paradigm for automated feature construction and selection in complex classification tasks. The seminal work by Koza [11] established genetic programming as a method for evolving computer programs through simulated evolution, demonstrating its effectiveness across a wide range of problem domains. In GP, solutions are represented as tree structures that undergo evolutionary processes including crossover and mutation to iteratively improve their fitness for a given task. Building on this foundation, recent advances have focused on applying GP specifically to feature construction for high-dimensional data classification. Tran et al. [9] proposed a GP-based approach for feature construction and selection that effectively handles high-dimensional datasets. Their method constructs multiple features simultaneously while performing feature selection, showing improved performance compared to traditional feature selection methods. This work was extended in [10] to develop multiple class-independent feature construction (MCIFC), which constructs features specific to each class in a dataset. MCIFC employs a multi-tree representation where each tree corresponds to a different class, allowing the algorithm to learn class-specific feature transformations. The MCIFC approach is particularly relevant for REIMS data analysis as it can capture complex, non-linear relationships between mass-to-charge ratios that may be characteristic of different fish species or body parts. The method's ability to construct multiple features simultaneously while considering class-specific information makes it well-suited for handling the high dimensionality and complex class structures present in marine biomass analysis.

III. Methods

With the background established, this section moves on to the heart of our analytical approach: the classification methods that extract meaningful insights from the REIMS spectra. This paper evaluates a diverse range of machine learning techniques to classify the REIMS spectra:

- **Traditional machine learning methods:** Random Forest (RF) [33], K-Nearest Neighbors (KNN) [34], Decision

Trees (DT) [35], Naive Bayes (NB) [36], Logistic Regression (LR) [37], Support Vector Machines (SVM) [38], and Linear Discriminant Analysis (LDA) [23].
- **Ensemble method:** [39]: A combination of the above traditional methods.
- **Benchmark method:** Orthogonal Partial Least Squares Disrciminant Analysis (OPLS-DA) [22].
- **Deep neural networks:** Transformer [7], [8], Long Short-Term Memory (LSTM) [25], Variational Autoencoder (VAE) [26], Convolutional Neural Network (CNN) [28]–[31], Kolmogorov-Arnold Networks (KAN) [27] and Mamba [32].
- **Evolutionary computation:** Multiple Class Independent Feature Construction (MCIFC) [9], [10]

A. Transformer

1) Architecture: The transformer model, originally proposed in the seminal paper by Vaswani et al. [8], revolutionized natural language processing and other tasks involving sequence data by relying entirely on self-attention mechanisms instead of recurrent or convolutional layers. Our transformer model consists of an encoder only structure, where encoders are stacked as layers. Each encoder layer comprises multi-head self-attention followed by position-wise feed-forward layers. We implement a transformer without positional embeddings (NoPE) [40].

In the architecture used for this work (Figure 1), the encoder blocks are equipped with residual connections [41], allowing gradients to flow efficiently during backpropagation. These residual connections act as "gradient superhighways," enabling deeper models without the risk of vanishing or exploding gradients, thus allowing better training stability.

A notable aspect of the transformer architecture used in this work is the choice of pre-norm layer normalization [42], [43], where the layer normalization is applied before multi-head attention and feed-forward layers. This approach contrasts with post-norm layer normalization (used after the attention block), as it stabilizes training and improves the convergence of deep transformers by ensuring more consistent gradients across layers. By normalizing before the main components of each layer, the pre-norm structure helps maintain better gradient flow across the network, contributing to more effective training of the encoder layers.

2) Progressive masking: Figure 2 illustrates the concept of progressive masking in pre-training transformer models. At the bottom right we see the original mass spectra. On the top left, we see the first mask, which applies a mask to all spectra except the first one. On from that we see masks that slowly shrink down until we reach the original spectra. These patterns demonstrate how the masking process evolved, starting with masking just one spectra and progressively unmasking more spectra in the sample. Mask 1 shows only the first spectra, with the rest masked. Mask 2 reveals two spectra, masking the remainder. Mask 3 unmasks one more spectra, showing three spectra. The final mask shows all the spectra except the final one. This progressive masking technique creates multiple training examples from a single spectra, effectively increasing

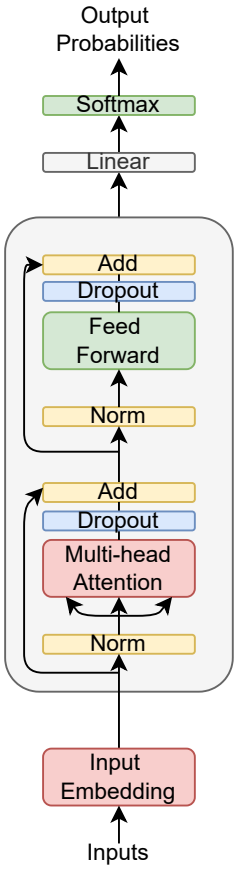


Fig. 1: Transformer Architecture.

the amount and diversity of training data for the transformer model. In this work, we apply left-to-right progressive masking to Rapid Evaporative Ionization Mass Spectrometry data. Instead of sentences in natural language processing, we are masking mass spectra, and pre-training has the model predict the masked spectra. This amortized the limited number of training samples by creating 2080 masked spectra per instance to train from, resulting in a training set of 2080 features $\times$ 72 samples = 149,760 instances.

3) Pre-trained Transformers: Pre-training is an extension of transformers that allows them to be pre-trained on a general task, then transfer the pretrained weights to a transformer model to be fine-tuned on a downstream task. This paper adopts unsupervised pre-training inspired by BERT [7] to improve the performance of transformer models on mass spectrometry tasks. Unsupervised pre-training offers significant benefits, particularly for models working with limited labelled data. By training on large-scale, unlabeled datasets, the model learns general patterns that capture the underlying structure of the data, resulting in useful embeddings that can be fine-tuned for specific downstream tasks with smaller, labelled datasets. This approach mitigates the need for extensive labelled data while still providing high-quality results.

This approach is an adaptation of the masked language modelling (MLM) task used in BERT to handle mass spectrometry data. In MLM, tokens in a sentence are progressively

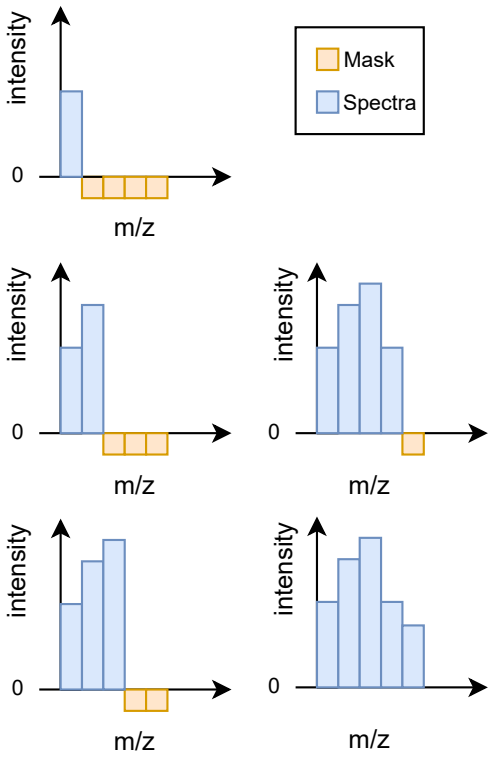


Fig. 2: Masked language modelling.

masked, and the model is trained to predict these masked tokens. Analogously, in masked spectra modelling (MSM), mass-to-charge ratios in spectra are progressively masked, and the model learns to predict the missing values. This is framed as a regression task, where the loss function is the mean squared error (MSE). By learning to predict missing mass-to-charge ratios, the model develops a robust understanding of the relationships between features in the spectra, making it well-suited for downstream tasks. We use left-to-right progressive masking to amortize the limited number of training instances.

By pre-training on this task, the transformer network learns valuable domain-specific representations. When fine-tuned on smaller, labelled datasets, the model can leverage these pre-trained weights, resulting in improved accuracy, faster convergence, and better generalization. This approach is particularly advantageous in fields like mass spectrometry, where labeled data is limited but large amounts of unlabeled data are readily available.

B. Evolutionary Computation

Complementing the deep learning approach of transformers, we now explore multi-tree genetic programming as an alternative paradigm for feature construction and classification in marine biomass analysis using REIMS. This approach, known as multiple class independent feature construction (MCIFC) [10], offers a novel application in this domain. Here we extend MCIFC for classification with a winner-takes-all strategy. The MCIFC algorithm, detailed in Algorithm 1, represents candidate solutions as multiple trees, with one subtree per class. This structure serves feature construction and classification purposes, employing a winner-takes-all strategy for class prediction. In our fish species classification task, MCIFC uses a two-tree representation for the two classes (Hoki and Mackerel), while the fish body parts classification task utilizes a six-tree representation for its six classes (fillet, heads, livers, skins, guts, and frames).

Algorithm 1 GP-based multiple feature construction.

Input : train_set, m;
Output : Best set of m trees;
Initialise a population of GP individuals. Each individual is an array of m trees;
best_inds $\leftarrow$ the best e individuals;
while Maximum generation is not reached **do**
  for $i = 1$ to Population Size **do**
    $transf\_train \leftarrow$ Calculate constructed features of individual i on train_set;
    $fitness \leftarrow$ Apply fitness function on $transf\_train$;
    Update best_inds the best e individuals from elitism and offspring combined;
  end for
  Select parent individuals using tournament selection for breeding;
  Create new individuals from selected parents using crossover or mutation;
  Place new individuals into population for next generation;
end while
Return best individual in best_inds;

The genetic operators in MCIFC [9], [10] include crossover (80% probability) and mutation (20% probability), adapted from conventional genetic programming [11]. Genetic programming, popularized by John Koza in 1994 [11], is a type of evolutionary algorithm that simulates the process of natural selection to solve problems by evolving computer programs. It operates by generating a population of potential solutions, each represented as a tree structure. Over successive generations, these solutions are refined through genetic operations such as mutation and crossover. Mutation involves making small, random changes to parts of an individual solution to explore new possibilities. Crossover combines portions of two parent solutions to produce offspring. These processes, along with selection mechanisms, guide the population toward better solutions over time. Tournament selection with a size of 7 is used for parent selection. Importantly, crossover only occurs between trees of the same class, while mutation randomly alters one subtree. The fitness evaluation in MCIFC combines accuracy with a distance term:

$$\alpha \cdot \textit{balanced\_accuracy} + (1-\alpha)(\beta \cdot \textit{inter} + (1-\beta) \cdot (1-\textit{intra}))$$

Where $\alpha = 0.8$ (prioritising accuracy) and $\beta = 0.5$ (balancing inter and intra-class distances). The interclass and intraclass distances are calculated as:

$$\textit{inter} = \frac{1}{|S|} \sum_{i,j} d(i,j) \quad \forall \quad i \neq j \quad \text{and} \quad \text{class}(i) \neq \text{class}(j)$$

$$\textit{intra} = \frac{1}{|S|} \sum_{i,j} d(i,j) \quad \forall \quad i \neq j \quad \text{and} \quad \text{class}(i) = \text{class}(j)$$

Here, $d(i,j)$ represents the Euclidean distance between two instances i and j, and $|S|$ is the total number of pairs of instance. This approach aims to maximize interclass distances while minimizing intraclass distances, thereby promoting better class separation in the constructed feature space.

IV. Experimental setup

Having outlined our various machine learning approaches for analyzing REIMS data, we now describe the experimental setup used to evaluate these methods, including the benchmark technique, datasets, and parameter settings used in our evaluation

A. Benchmark technique

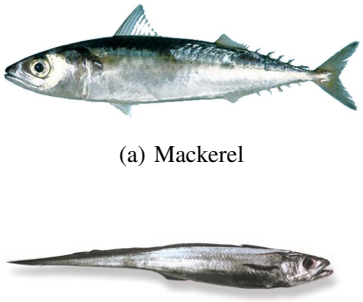
To evaluate the performance of the proposed methods, OPLS-DA is used as a benchmark to compare new approaches to the existing methods for REIMS analysis. Each method is evaluated and the average is given over 30 independent runs. Stratified k-fold cross-validation, with $k = 5$ for fish species and $k = 3$ for body parts, is particularly beneficial for evaluating model performance on datasets with limited training samples and imbalanced classes. This method ensures that each fold maintains a class distribution similar to the entire dataset, which helps the model learn effectively from both majority and minority classes. By doing so, it reduces the variance of performance estimates, leading to more stable and reliable metrics. Additionally, it maximizes the use of available data, allowing each sample to contribute to both training and validation, which is crucial for small datasets. With three and five-fold cross-validation, the model is tested across various scenarios, improving its generalization to unseen data and providing a comprehensive evaluation of its performance.

B. Datasets

Figure 3 gives the two wild-caught fish species - Hoki and Mackerel - that are the subject of this study. These are two important fish in New Zealand's seafood industry, especially given New Zealand's largest fishery is hoki [44].

For illustrative purposes, the different fish body parts, which are shared across both species of fish, are given in Figure 4.

The dataset used consists of REIMS spectra collected from two fish species and seven body parts. Particularly, we will have four different datasets corresponding to four different (following) tasks:



(a) Mackerel

(b) Hoki

Fig. 3: Mackerel (left) Hoki (right) fish species.

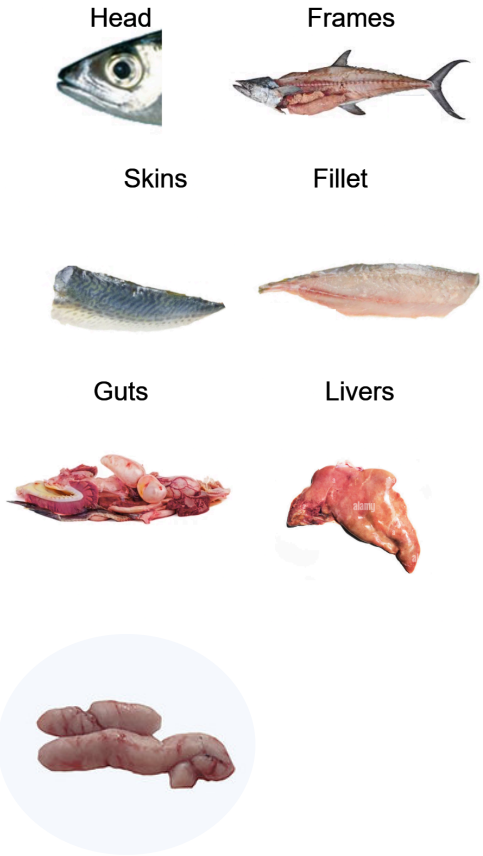


Fig. 4: Fish body parts.

1) **Species classification:** The task is to distinguish between two species of fish (Hoki and Mackerel) based on 2080 features derived from REIMS analysis. This classification is crucial for food authentication and quality control in the seafood industry, helping prevent species substitution fraud and ensure accurate product labeling. We focus on pure (non-contaminated/non-mixed) samples to establish a reliable baseline for species identification. The dataset contains 106 samples, with a relatively balanced distribution of 44.44% Hoki and 55.56% Mackerel. These proportions reflect the natural availability of samples while maintaining sufficient representation for both species to train a robust classifier.
2) **Body parts classification:** This multi-class classification task aims to identify seven distinct fish parts (fillets, heads, livers, skins, gonads, guts, and frames) using REIMS data. The classification supports process automation by enabling automated sorting and processing in seafood production lines, while helping maximize the value of each fish part, such as using fillets for premium products and frames for fish meal. Furthermore, precise classification ensures proper tracking and documentation of different fish components throughout the supply chain. The dataset contains 33 samples with a distribution of 16.66% each for fillets, heads, livers, skins, and guts, and 8.33% each for gonads and frames. The relatively small sample size per class is attributed to a limited number of annotated samples for each class of body part.

The REIMS spectra were normalised to be within $x \in [0, 1]$, fitted to the training set of each fold. Let $X = \{x_1, x_2, \ldots, x_n\}$ be a dataset containing n elements. The normalized value x_i' for each element x_i is given by:

$$x_i' = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} \tag{1}$$

Where:

- $x_{\min}$ is the minimum value in the dataset X
- $x_{\max}$ is the maximum value in the dataset X

C. Parameter settings

Experiments use the default settings from sklearn [45], except SVM with a linear kernel, and LR set to 2,000 for the maximum number of iterations. The ensemble voting classifier combines all the traditional machine learning methods into one mode. The ensemble uses hard voting, i.e. uses predicted class labels for majority rule voting.

The deep learning models all use the following parameters. The AdamW optimizer [46] decouples weight decay from the learning rate, an improvement over the popular Adam optimizer [47]. Dropout [48] turns off neurons at random during training to efficiently approximate a bagged ensemble of sub-neural networks. Label smoothing [49] softens class labels by combining the one-hot encodings with a uniform distribution, adding noise to the class labels. The deep learning networks uses Gaussian error linear units (GELU) [50] for activation functions. Data augmentation replicates each instance five times and injects noise [51] expanding the training set five-fold - data augmentation inflates the number of training instances. Early stopping [52] is one of the most common forms of regularization which saves the model parameters when the validation loss improves, it tunes the hyperparameter of epochs [53]. To allow fair comparison, each model has the same hyperparameters; a hidden dimension of 128, trained for 100 epochs, a learning rate of 1e-5, a batch size of 64, 4 layers (where applicable), dropout of $p = 0.2$ and label smoothing of 0.1.

TABLE I: Transformer parameter settings.

Learning rate	1E-5
Epochs	100
Dropout	0.2
Label smoothing	0.1
Early stopping patience	5
Optimiser	AdamW
Loss: MSM	MSE
Loss: Speciation	CCE
Input dimensions	2080
Hidden dimensions	128
Output dimensions: MSM	2080
Output dimensions: Speciation	2
Output dimensions: Part	7
Number of layers	4
Number of heads	4

TABLE II: MCFIC parameter settings.

Function Set	$+, -, \times$, protectedDiv
Terminal Set	$x_1, x_2, ..., x_n$
Maximum Tree Depth	6
Population size	1 * 2080 (= 1× #features)
Initial Population	Ramped Half-and-Half
Generations	400
Crossover	0.8
Mutation	0.2
Elitism	0.1
Selection	Tournament
Tournament Size	7
Construction ratio	1
Fitness weighting α	0.8
Distance weighting β	0.5

D. Transformer parameters

Table I gives the configuration of hyperparameters for the transformer - these settings were derived through trial and error via experimentation.

E. Genetic Programming parameters

Table II provides a comprehensive overview of the parameter settings used in the MCIFC method, including the construction ratio, which denotes the number of trees per class.

V. Results and Discussion

Having outlined our classification strategies, this section now presents and interprets the outcomes of applying these various machine learning techniques to the REIMS datasets. Table III and Table IV gives the results of the classifiers on the training and test set, with the best-performing model on the test set given in **bold**, and the second-best are given in *italics*.

Method	Train	Test
KNN	95.76% ± 0.00%	79.37% ± 0.00%
DT	100.00% ± 0.00%	99.17% ± 0.00%
LR	100.00% ± 0.00%	85.21% ± 0.00%
LDA	98.54% ± 0.00%	92.29% ± 0.00%
NB	89.17% ± 0.00%	66.67% ± 0.00%
RF	100.00% ± 0.00%	90.05% ± 0.56%
SVM	100.00% ± 0.00%	84.58% ± 0.00%
Ensemble	100.00% ± 0.00%	87.84% ± 0.40%
OPLS-DA	98.91% ± 0.74%	96.39% ± 4.44%
Transformer	100.00% ± 0.00%	*99.17% ± 1.67%*
Pre-trained	100.00% ± 0.00%	**99.62% ± 1.15%**
LSTM	100.00% ± 0.00%	*98.84% ± 1.76%*
VAE	100.00% ± 0.00%	98.64% ± 1.94%
KAN	100.00% ± 0.00%	97.41% ± 2.45%
CNN	100.00% ± 0.00%	96.87% ± 3.24%
Mamba	100.00% ± 0.00%	98.27% ± 2.14%
MCIFC	100.00% ± 0.00%	97.89% ± 2.59%

TABLE III: Classification results for fish species identification.

Method	Train	Test
KNN	43.06% ± 0.00%	39.17% ± 0.00%
DT	100.00% ± 0.00%	35.50% ± 4.35%
LR	100.00% ± 0.00%	59.58% ± 0.00%
LDA	74.31% ± 0.00%	52.92% ± 0.00%
NB	100.00% ± 0.00%	48.33% ± 0.00%
RF	100.00% ± 0.00%	61.67% ± 0.00%
SVM	100.00% ± 0.00%	52.33% ± 2.57%
Ensemble	100.00% ± 0.00%	52.33% ± 2.57%
OPLS-DA	80.11% ± 2.86%	51.17% ± 22.16%
Transformer	100.00% ± 0.00%	**84.06% ± 6.42%**
Pre-trained	100.00% ± 0.00%	*83.94% ± 7.12%*
LSTM	100.00% ± 0.00%	82.11% ± 9.15%
VAE	85.43% ± 6.28%	74.81% ± 13.84%
KAN	100.00% ± 0.00%	73.06% ± 9.58%
CNN	100.00% ± 0.00%	70.41% ± 13.75%
Mamba	100.00% ± 0.00%	80.67% ± 8.73%
MCIFC	97.95% ± 1.61%	55.45% ± 19.19%

TABLE IV: Classification results for fish body parts identification.

Note that the method pre-trained indicates the transformer with progressive left-to-right masked pre-training.

Our study employed a diverse range of machine learning techniques to classify REIMS spectra for various tasks related to marine biomass analysis. The results demonstrate varying levels of success across different models and tasks, providing insights into the strengths and limitations of each approach.

A. Fish Species Classification

For the task of fish species classification, the best-performing models were the pre-trained Transformer (99.62%). This model excels in capturing the intricate patterns in the Rapid Evaporative Ionization Mass Spectrometry (REIMS) data, which provides distinct signatures for different fish species. The high performance of the decision tree model (99.17%) shows that even traditional machine learning methods are highly effective in this domain. The tree-based models like Decision Trees and Random Forests work well because they can split the data based on highly discriminative features, capturing non-linear relationships effectively. For a decision tree, while individual splits are linear (axis-parallel), their combination creates non-linear decision boundaries.

The consistently high test accuracy across all models suggests that the REIMS dataset for fish species contains strong, distinguishable signals that can be effectively exploited by various machine learning techniques. This makes the classification task easier for both deep learning models and traditional methods. The models excel at this task because the REIMS data likely provides clear, consistent, and high-dimensional representations of species differences, which can be leveraged by the deep architectures for feature extraction and by traditional methods for decision-making.

The deep learning models consistently outperform the traditional OPLS-DA method (96.39%) from the literature for REIMS analysis. The research field of REIMS analysis should consider deep learning methods for other applications, as they offer superior performance.

B. Fish Body Part

The transformer without pre-training performed the best in the task of classifying fish body parts, achieving a test accuracy of 84.06%. These models are well-suited for this task because they can handle complex and multi-dimensional input data like REIMS, capturing the subtle differences between body parts through advanced feature extraction and context awareness. LSTMs, with their ability to capture sequential dependencies, also perform well (82.11%), suggesting some temporal or positional dependencies in the ionization patterns that relate to specific body parts.

Traditional machine learning methods, however, show lower performance compared to the fish species classification task. This suggests that classifying fish body parts is inherently more complex due to less distinct signal differences between body parts, making it harder for simpler models to differentiate between classes. This increased difficulty likely arises from overlapping chemical compositions between different parts of the same species. Previous work [17] on fish species and body parts classification with gas chromatography data illustrated the increased difficulty of body parts classification.

Again, deep learning methods (84.06%) outperform the OPLS-DA method (51.17%). For the second task, deep learning methods have proven to be superior to the traditional approaches from the literature.

C. Summary:

Across all tasks, the deep learning methods offered superior performance to the OPLS-DA method that dominates the literature [1], [6], [19], [20] on REIMS analysis. Future work in the field for other applications of REIMS analysis should consider deep learning methods as a viable alternative. The varying performance of different models across tasks highlights the importance of selecting appropriate algorithms for specific analytical challenges in marine biomass analysis. While the transformer model consistently excelled, simpler models like decision trees demonstrated competitive performance in certain tasks, offering potential advantages in terms of interpretability and computational efficiency. The challenges faced in body part classification, point to areas where further research is needed. This might include exploring more advanced feature extraction

techniques, increasing the size and diversity of the training dataset, or developing specialised model architectures tailored to these specific tasks. Overall, our results demonstrate the potential of combining REIMS with machine learning for automated and accurate marine biomass analysis, while also highlighting areas for future improvement and research.

VI. Further Analysis on the Explainability

While the performance of our vanilla and pretrained transformers is promising, understanding how they arrive at their predictions is crucial for building trust and gaining insights. It is important to identify important features driving decisions made by black-box models, such that these models can be understood, trusted, and verified by domain experts in chemistry and fish processing. To address this, we employ Local Interpretable Model-agnostic Explanations (LIME), a technique used to explain predictions made by complex black-box machine learning models [54]. We analyze the top 5 most important features of the top-performing models that have been identified by LIME. LIME approximates a complex model's behaviour with a simpler and interpretable model (e.g. linear regression) for a specific instance in a local area to be understood. LIME creates and evaluates many altered versions through perturbations of an instance in the input data to see how those perturbations change the prediction. Through perturbations and their observed changes to the prediction, this information is used to generate a local explanation that highlights which features influenced the prediction. LIME charts are used to explain the predictions of machine learning models by showing which features (in this case, specific mass-to-charge ratios) are most influential for a particular prediction. In these LIME charts:

- **Green bars:** These represent features (mass-to-charge ratios) that contribute positively towards the predicted class. In other words, the presence or higher intensity of these features increases the likelihood of the sample being classified as the predicted class.
- **Red bars:** These represent features that contribute negatively towards the predicted class. The presence or higher intensity of these features decreases the likelihood of the sample being classified as the predicted class.
- **The x-axis:** The length of each bar indicates the magnitude of the feature's importance. Longer bars (whether green or red) signify that the corresponding feature strongly influences the model's prediction. The x-axis represents the feature importance.
- **The y-axis:** This represents the mass-to-charge (m/z) ratios and their intensity thresholds from the mass spectrometry data. The y-axis represents the important features.

A. Fish Species Classification

The pre-trained transformer is one of the models that achieves the best classification accuracy (99.62%) for fish species classification. Figure 5 gives the LIME explanation for the pre-trained transformer for the fish species Mackerel. The most important feature, and the strongest green bar, is when the mass-to-charge ratio 121.0934 m/z is within the normalized intensity range $0.01 < y \leq 0.04$. Suggesting that small amounts of this molecule are present in the fish species Mackerel.

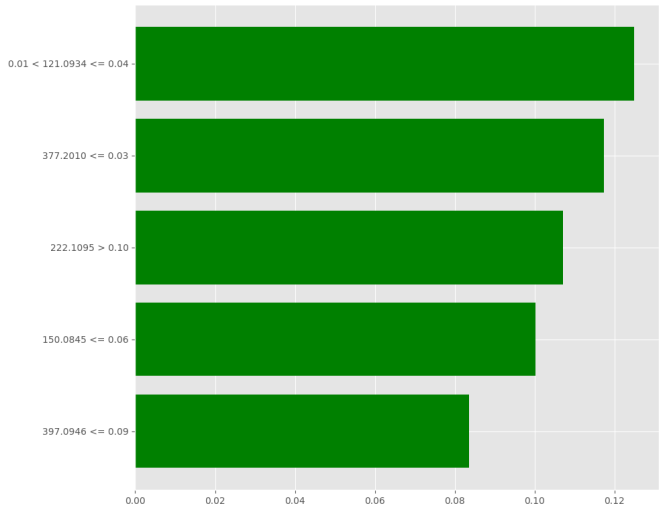


Fig. 5: Lime explanation for transformer for classification of fish species Mackerel.

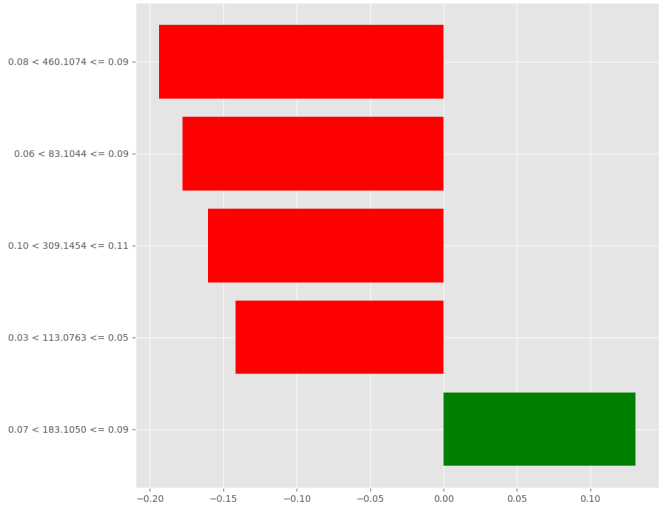


Fig. 6: Lime explanation for transformer for classification of fish species Hoki.

Figure 6 gives the LIME explanation for the pre-trained transformer for the fish species Hoki. The most important feature, and the strongest red bar, is when the mass-to-charge ratio 460.1074 m/z is within the normalized intensity range $0.08 < y \leq 0.09$. Suggesting that large amounts of this molecule indicate a sample does not belong to the fish species Hoki.

Figure 7 gives the decision tree with near-perfect accuracy, showing how a simple model with two splits, can classify fish species, giving both a highly accurate and interpretable model. The figure shows the two mass-to-charge ratios and their intensity thresholds for which they based their decision boundaries on.

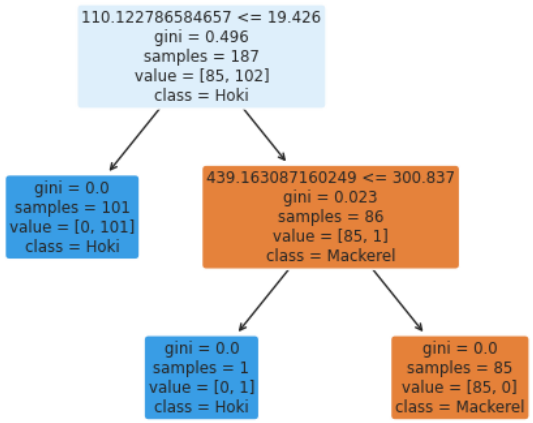


Fig. 7: Decision tree for fish species.

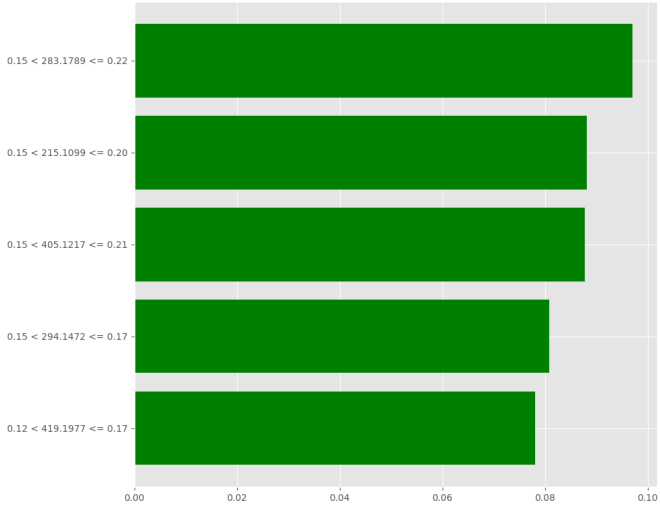


Fig. 8: Lime explanation for transformer for classification of fish part head.

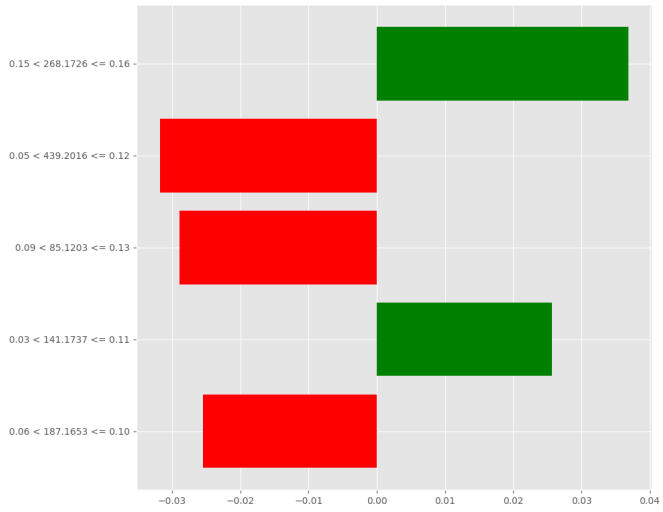


Fig. 9: Lime explanation for transformer for classification of fish part fillet.

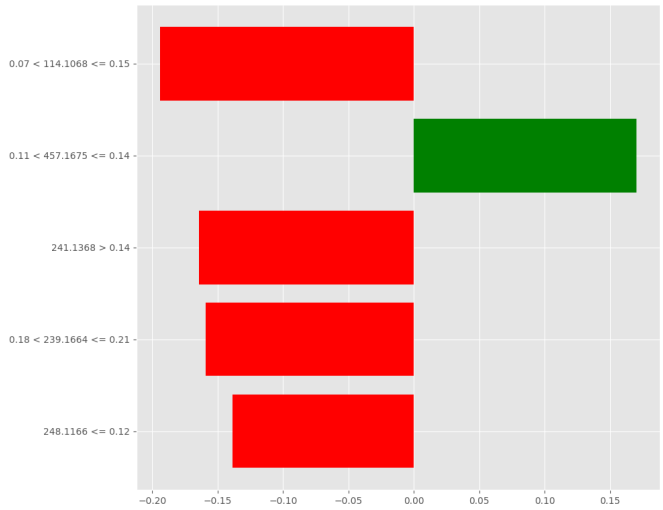


Fig. 10: Lime explanation for transformer for classification of fish part liver.

B. Fish Body Part

The transformer performs the best (83.94%) on the fish parts dataset. Figure 8 gives the LIME explanation for the transformer for the fish parts classification for fish heads. The most important feature, and the strongest green bar, is when the mass-to-charge ratio 283.1789 m/z is within the normalized intensity range $0.15 < y \leq 0.22$. This indicates that large amounts of this molecule are likely present in fish heads.

Figure 9 gives the LIME explanation for the transformer for the fish body part of the fillet. The most important feature, and strongest green bar, is when the mass-to-charge ratio 268.1726 m/z is within the normalized intensity range $0.15 < y \leq 0.16$. This suggests that large amounts of this molecule are present in fish fillets.

Figure 10 gives the LIME explanation for the transformer for the fish body part of the liver. The most important feature, and strongest red bar, is when the mass-to-charge ratio 114.1068 m/z is within the normalized intensity range of $0.14 < y \leq 0.15$. This indicates that large amounts of this molecule are not likely to be found in fish liver.

Figure 11 gives the LIME explanation for the transformer for the fish body part of the skins. The most important feature, and the strongest green bar, is when the mass-to-charge ratio 464.1736 m/z is within the normalized intensity range $0.14 < y \leq 0.19$. This indicates that large amounts of this molecule can be found in fish skins.

Figure 12 gives the LIME explanation for the transformer for the fish body part of the guts. The most important feature, and the strongest green bar, is when the mass-to-charge ratio 114.1430 m/z is within the normalized intensity range $0.13 < y \leq 0.19$. This suggests that large amounts of this molecule can be found in fish guts.

Figure 13 gives the LIME explanation for the transformer for the fish body part of frames. The most important feature, and strongest red bar, is when the mass-to-charge ratio 389.1507 m/z is less than or equal to the normalized intensity

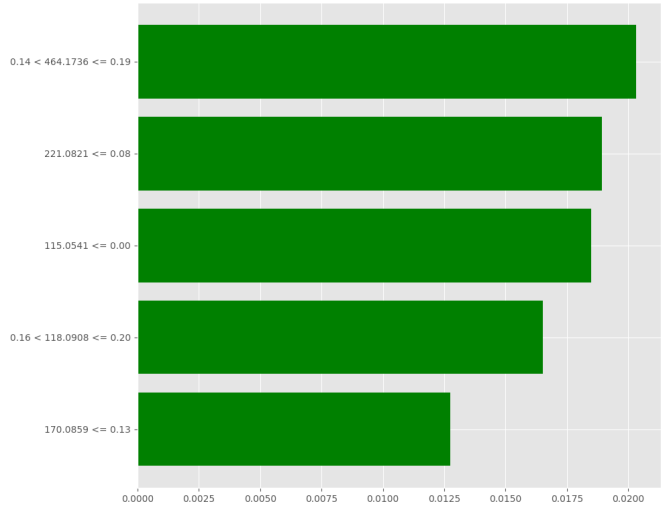


Fig. 11: Lime explanation for transformer for classification of fish part skins.

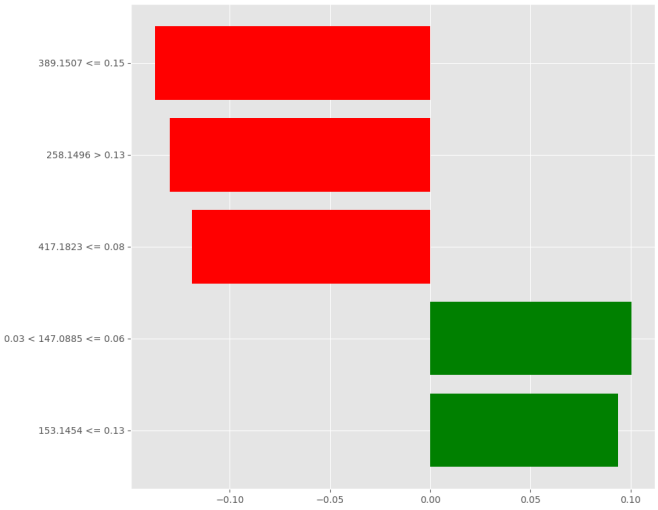


Fig. 13: Lime explanation for transformer for classification of fish part frames.

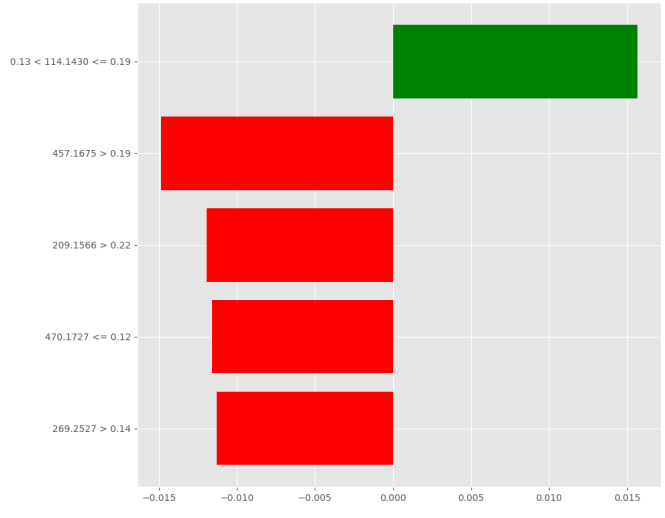


Fig. 12: Lime explanation for transformer for classification of fish part guts.

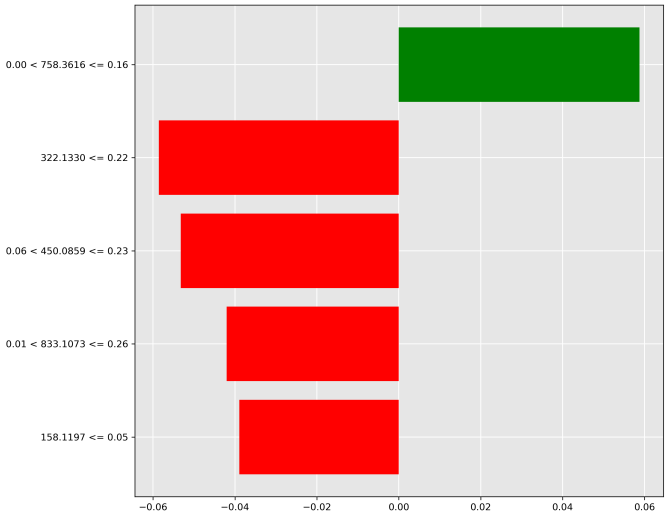


Fig. 14: Lime explanation for transformer for classification of fish part gonads.

threshold of 0.15. This indicates that small to average amounts of this molecule are not likely to be found in fish frames.

Figure 14 gives the LIME explanation for the transformer for the fish body part of gonads. The most important feature, and strongest green bar, is when the mass-to-charge ratio 758.3616 m/z is less than or equal to the normalized intensity threshold of $0.00 < y \leq 0.16$. Biochemically, this could suggest that m/z 758.3616 might correspond to a compound that's characteristically abundant in fish gonads, while the other peaks might be more characteristic of other fish parts.

VII. Conclusion and Future Work

The results from these classification tasks demonstrate that deep learning models, particularly Transformer, VAE, KAN and LSTM, are well-suited for handling the complex, high-dimensional data generated by Rapid Evaporative Ionization Mass Spectrometry (REIMS). These models consistently outperform traditional machine learning methods, especially for tasks involving subtle or overlapping signal differences, such as body parts detection. The pre-trained transformer outperforms the regular transformer on fish species classification, suggesting that pre-training captures meaningful embeddings that improve the performance of downstream classification tasks. While traditional models like decision trees show excellent performance in simpler tasks like fish species classification, their performance drops significantly for more challenging tasks, highlighting the need for advanced feature extraction and representation learning that deep models provide. The overall strong performance across the board suggests that REIMS data provides rich, discriminative information, particularly for fish species classification. However, body part identification requires more sophisticated modelling approaches, where deep learning shines due to its ability to capture complex patterns and subtle signal deviations.

The application of explainable AI techniques, particularly LIME (Local Interpretable Model-agnostic Explanations), provided valuable insights into the decision-making processes of our models. These explanations revealed specific mass-to-charge ratios that strongly influence classifications, enhancing our understanding of the biochemical markers associated with different fish species and body parts. For instance, the LIME analysis for fish speciation highlighted distinct spectral regions that differentiate Mackerel from Hoki. This interpretability not only increases confidence in the model's predictions but also opens up possibilities for new scientific insights into the biochemical composition of marine biomass. It demonstrates that our approach can provide both accurate classifications and meaningful, chemically relevant explanations for those classifications.

Overall, this research opens up new possibilities for automated, accurate, and interpretable analysis in marine biomass compositional studies, with significant implications for quality control, product optimization, and food safety in marine-based industries.

While our study has yielded promising results, it also opens up numerous avenues for further research and development. These are potential directions for expanding and refining our approach. Those directions for future work include: (1) develop a system for real-time REIMS data acquisition and analysis, allowing for immediate classification results in industrial settings, and (2) work with regulatory bodies to ensure that the developed methods meet or exceed current standards for marine biomass analysis and food safety monitoring.

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