ARTIFICIAL INTELLIGENCE IN FOURIER TRANSFORM INFRARED (FTIR) SPECTRAL DATA ANALYSIS: A MINI REVIEW

Aakanksha C. Pawar[1], Ashlesh A. Chikte[1], Lalit G. Gawande[1], Mayuri S. Kolhe[1], Disha W. Bandre[1]*, Komal M. Masaram[2], Nilesh V. Gandhare[1]*
[1]Department of Chemistry, Nabira Mahavidyalaya, Katol, 441302, Maharashtra, India.
[2]Department of Chemistry, Government Institute of Science, Nagpur-440001, India.
*E-mail Addresses: bandredisha@gmail.com , nilkanth81@gmail.com

Abstract: Fourier Transform Infrared (FTIR) spectroscopy is a powerful and widely used spectroscopic technique, and accurate interpretation of its spectra provides essential insights into molecular structure. Interpreting FTIR spectra can be time-consuming and requires expert knowledge. However, recent advances in computer science, particularly in cheminformatics and machine learning, have significantly simplified large-scale spectral analysis. Computer-aided expert systems and automated pattern recognition tools now enable rapid, accurate, and high-throughput identification of functional groups and molecular structures, improving both efficiency and reliability in spectral interpretation. The integration of artificial intelligence with FTIR spectroscopy enables rapid, automated, and highly accurate spectral interpretation, transforming molecular identification and accelerating innovation in research and industry. This review highlights the application of artificial intelligence (AI) techniques in FTIR spectroscopy, including machine learning, deep learning, traditional chemometric algorithms, advanced neural networks, and support vector machines for improved spectral analysis and molecular identification.

Keywords: Artificial Intelligence, ATR-FTIR, Cheminformatics, Machine Learning

I. INTRODUCTION

Fourier transform infrared (FTIR) spectroscopy is an experimental technique used to analyze organic substances qualitatively and quantitatively. It provides information on molecular structure, chemical bonding, and environment [1]. FTIR is based on the fact that molecules absorb infrared radiation at characteristic frequencies corresponding to vibrational transitions. The spectrum obtained is the molecular fingerprint. It can be used for qualitative and quantitative analysis. FTIR is being used in a wider range of fields than just pharmaceuticals, including environmental studies, polymer, agriculture, materials science, food analysis and biomedical diagnostics [2]. Mid-infrared (IR) spectroscopy is a widely used technique for identifying and analyzing chemical substances. The peaks in a sample's IR spectrum represent the excitation of vibrational modes of the molecules in the sample, and hence correspond to the various chemical bonds and functional groups present in the molecules. Thus, a compound's IR spectrum is one of its most distinguishing physical qualities, serving as its fingerprint. Infrared spectroscopy is also an effective method for quantitative analysis since the amount of infrared energy absorbed by a substance is proportional to its concentration [3].

However, FTIR spectra can contain overlapping bands and complicated background noise, making interpretation problematic, especially in multiple components and biological substances. As a result, a variety of chemometric techniques are employed, such as Principal Component Analysis (PCA), Hierarchical Cluster Analysis (HCA), Artificial Neural Network (ANN), and Partial Least Squares Regression (PLSR). These techniques offer preliminary data modelling but are limited

in their ability to handle nonlinear patterns. The most widely used techniques include Convolution Neural Network (CNNs), Support Vector Machines (SVMs), ANN and ensemble learning methods have demonstrated significant potential in extracting meaningful information directly from raw or minimally preprocessed spectral data [4].

Artificial Intelligence (AI) has been a revolutionary tool in analytical chemistry and spectroscopy in recent years. AI is the term for computer programs that can simulate human intelligence in order to carry out tasks like learning, pattern recognition, prediction, categorization, and decision-making. AI-based methods such as chemometrics, machine learning and, deep learning are promising tools that lead to a clearer and more profound understanding of data [5]. In the context of FTIR spectroscopy, AI-based technologies and machines have the capacity to learn by doing and make better decisions as more data is entered into the system, handling of noisy, flawed, and imperfect data, the capacity to address non-linear issues and after the tool has been taught, rapid prediction and generalization. AI provides a powerful alternative through algorithms that can discover hidden patterns, improve classification accuracy, and enable rapid quantitative predictions. Large spectral datasets may be processed effectively by AI algorithms, which can also identify hidden patterns, minimize human interaction, and increase analytical precision and repeatability [6].

Conventional FTIR spectrum interpretation frequently relies on specialist knowledge and manual peak assignment. Conventional approaches are limited in terms of speed and precision due to growing spectral complexity and the availability of big datasets. Advanced computer techniques that can uncover hidden patterns and correlations in spectral data are made possible by AI. Manual interpretation becomes inefficient and less reliable when handling multidimensional datasets, nonlinear spectral relationships, and subtle variations between similar samples. In addition, baseline drift, instrumental fluctuations, sample heterogeneity, and variations in measurement conditions further complicate FTIR spectral analysis, reducing the accuracy, precision, and reproducibility of traditional spectral interpretation methods [7].

In recent years, the convergence of FTIR spectroscopy and AI has transformed the way spectral data are analyzed and interpreted. This review explores the role of AI in FTIR spectral data analysis, highlighting current applications, challenges, and future prospects. By examining recent developments in AI-driven spectral analytics, this review aims to provide a comprehensive understanding of how intelligent algorithms can enhances the performance, efficiency, and reliability of FTIR spectroscopy in modern scientific research and industrial applications.

II. AI in FTIR

i) Analysis of Polymers

Villegas Camacho, O., *et al.* studied six polymers (PET, HDPE, PVC, LDPE, PP, and PS) using the FTIR-PLASTIC-c4 dataset, a core component of deep learning (DL). To predict the fingerprint region of FTIR spectra a multilayer perceptron (MLP) architecture was evaluated. The coefficient of determination (R^2) was used to evaluate performance. Results suggest model captures spectral variability, but some polymers show lowest performance recommend model optimization for some polymers [8].

Aeint Shune Thar *et al.* emphasized the necessity of developing innovative and accurate approaches as the global prevalence of microplastics continues to increase. The ability of ML and DL models to categorize microplastics using FTIR spectra distorted by membrane filter noise was compared in this study. They thoroughly evaluated many machine learning algorithms and CNNs using an FTIR dataset from various sources. Support Vector Classification (SVC) and K-Nearest Neighbors (KNN), two ML models, had accuracies of 95.99% and 95.55%, respectively, however LeNet5, a DL model, outperformed both with 96.93%. On the other hand, several DL models performed poorly, which highlighted the complexity of the identification problem [9].

Xinyu Yan, *et al.* studied many ML based approach for marine microplastic (MP) identification, using Attenuated Total Reflection Fourier Transform Infrared Spectroscopy (ATR-FTIR). The unbalanced and insufficient samples in MP datasets are currently a significant obstacle to training MP identification models, particularly when these conditions are paired with copolymers and

multiple components. The data augmentation method is a useful strategy to enhance the ML performance in MP identification. Explainable Artificial Intelligence (XAI) and Gaussian Mixture Models (GMM) are used in this work to show how FTIR spectral regions affect the identification of each type of MP. This research suggests a Fingerprint Region based Data Augmentation (FRDA) technique to produce fresh FTIR data to complement MP datasets based on the detected regions. According to the evaluation results, FRDA performs better than the current spectral data augmentation techniques [10].

ii) Bio-Medical Applications

Catalin Negoita *et al.* evaluated various artificial intelligence (AI) approaches for the classification of synthetic cannabinoids and hallucinogenic amphetamines based on ATR-FTIR spectral data. Partial Least Squares Regression applied on the most relevant absorptions chosen by a genetic algorithm has been used to construct the initial application. Next, tests were conducted on the Random Forest and K-Nearest Neighbors algorithms. From the perspective of the classification rates, the outcomes have been compared. The evaluation of these forensic applications' sensitivity and selectivity has received particular attention due to the legal implications of the analytical results. There is also discussion of these class identification assignment systems' limitations [11].

Renee George *et al.* determined estrogen receptor (ER) and progesterone receptor (PR) status in formalin-fixed paraffin-embedded (FFPE) breast cancer tissues using artificial intelligence (AI) combined with ATR-FTIR spectroscopy. Their approach enabled the label-free classification of ER and PR status without the need for conventional labeling procedures. A genetic algorithm was used to train and optimize seven AI models: logistic regression, support vector machine (SVM), decision tree, XGBoost, feed forward neural network (FNN), recurrent neural network (RNN), and convolutional neural network (CNN). AUC-ROC, accuracy, sensitivity, specificity, PPV, NPV, and F1 score were used to evaluate the model's performance by repeated cross-validation. CNN achieved the highest classification performance for both ER and PR. FNN, RNN, and XGBoost also demonstrated strong performance, whereas SVM yielded the lowest accuracy and F1 scores[12].

Riccardo Di Santo *et al S*tudied 278 biological samples, for the FTIR spectroscopy and Autoencoder based detection of Cancer Biomarkers in Extracellular Vesicles(EV). Whole blood was processed to obtain plasma, red blood cells (RBCs), RBC-ghosts (RBC-G), and extracellular vesicles (EVs). A Bruker Alpha II FTIR spectrometer fitted with an Eco-ATR was used to conduct spectroscopic measurements. An autoencoder neural network was implemented in R v4.4.0 using the keras3 package. With minimal reconstruction error, the autoencoder preserved spectral information while compressing spectra into 12 latent characteristics. This work offers the first demonstration that an autoencoder can be used to extract physiologically significant latent features from EV FTIR spectra, potentially useful for cancer detection[13].

Ahmed Fadlelmoula *et al.* conducted a review discussing the application of FTIR spectroscopy combined with ML for human blood analysis. Their study demonstrated that SVMs are among the most effective machine learning classifiers for analyzing high-dimensional biological data. The review highlighted that SVMs exhibit excellent classification performance, particularly for binary classification problems, making them well suited for the analysis of FTIR spectral data obtained from biological samples such as human blood. The majority of biological genomic data are noisy, diverse, and high-dimensional. Because of this characteristic, some techniques including SVMs, PCA, and RFsare more appropriate for usage in the biological domain than others, like DL and PCC. Despite their benefits and meticulous planning, machine learning techniques nevertheless have a number of drawbacks that call for further research. Because researchers are restricted to recorded data, retrospective database studies were shown to be especially susceptible to the absence of relevant variables [14].

P. I. Haris *et al.* used artificial intelligence to measure the average length and percentages of secondary structures using neural network analysis on normalized sections of FTIR (1700-1600 cm^{-1}) and CD (180-259 nm) spectral data, both with and without boxcar averaging. The protein secondary structure was quantified using

a hybrid genetic algorithm/neural network approach that automatically chooses structure-sensitive wavelength/frequency. When specific wavelengths were employed, CD spectroscopic analysis outperformed FTIR spectroscopy; however, FTIR performed better when neural network analysis was applied to the whole region between 1700-1600 cm^{-1} (FTIR) and 180-259 nm (CD). When the spectrum data was analyzed using the Adaptive Neuro-Fuzzy Inference System (ANFIS) with fuzzy subtractive clustering, the average helix/sheet length for FTIR spectroscopy was predicted somewhat more accurately than with CD [15].

O. K. Gasymov *et al.* observes despite the great successes in various cancer types, effective and accepted screening techniques do not exist for lung cancer. A model developed using the biomarker module of the Metabo Analyst 4.0 software was used to predict human lung cancer using artificial intelligence. Linear SVM, PLS-DA, and Random Forest algorithms were used on unknown samples to predict the classification of lung carcinoma and healthy samples using the model enhanced by removing outlier samples. AI based on FTIR spectra of human blood plasma can be developed as a widespread screening method for the identification of patients at high risk, according to prediction accuracy (80–90%). This screening technique is inexpensive, quick, and minimally intrusive [16].

Qiang Chen *et al.* utilized machine learning methods along with ATR-FTIR spectroscopy technology to methodically describe the spectrum evolution characteristics of corneal tissues under various post-mortem interval (PMI). ElasticNet, Ridge, Lasso, PLSR, GPR, SVR, GBDT, XGBoost, RF, and MLP were among the ten regression models that were built and compared in the study. According to the findings, the ElasticNet model performed the best in terms of prediction and generalization. Additionally, the SHapley Additive explanations (SHAP) framework was established for interpretive analysis in order to overcome the algorithm's "black box" problem, and 20 important spectral properties were chosen. This work developed a corneal PMI prediction method based on ATR-FTIR spectroscopy and machine learning in conjunction with SHAP interpretative analysis for the first time, offering a quick, non-destructive, and comprehensible new tool for forensic medicine's inference of death time [17].

iii) Food and Agricultural Analysis

Agustin E. Lopez-Rosas *et al.* employed artificial intelligence to recognize patterns in spirit beverages based on their spectroscopic characteristics. A Nicolet iS5 FTIR spectrometer with a diamond-tipped Attenuated Total Reflectance (ATR) device was utilized for this purpose. Tequila 100% agave (n= 20), Mezcal (n = 20), Raicilla (n = 20), Aguardiente (n = 20), and Vodka (n = 20) were analyzed. The results demonstrated that the suggested artificial intelligence algorithm is an excellent choice method that is creative, quick, and inexpensive, enhancing food quality evaluations by machine learning decision-making. It is able to correctly identify 100% of the samples [18].

Ellison H. de Paulo *et al.* used ATR-FTIR spectroscopy to detect water adulteration in soymilk samples. Using ATR-FTIR along with chemometric techniques can be a rapid and beneficial solution to this issue. For one-class modeling, the unequal dispersed classes (UNEQ), data-driven soft independent modeling of class analogies (DD-SIMCA), soft independent modeling of class analogies (SIMCA), and one-class random forest (OC-RF) approaches were employed. The non-adulterated samples were used as the target class (TA) in the models, whereas the adulterated samples were used as the non-target class (NT). Multiclass modelling was done using the k-nearest neighbours (k-NN), dual class random forest (DC-RF), dual class random forest with Monte Carlo sampling (DC-RF-MC), and partial least squares discriminant analysis (PLS-DA) techniques [19].

E. S. Estracanholl i*et al.* reported the development of an integrated system that combined three analytical techniques with signal processing for monitoring the mashing process during beer production. Carbohydrates produced by enzymatic reactions between barley malt enzymes and starch during the saccharification step are quantified in real time. This is typically accomplished through spectral analysis using FTIR absorption in the mid-infrared region through real-time sample collection and referral. In the process, machine learning methods will be applied through real-time spectroscopy [20].

Yu-Tang Wang *et al.* developed an FTIR spectroscopy-based analytical tool for the simultaneous determination of five artificial sweeteners, namely sodium cyclamate, sucralose, sodium saccharin, acesulfame-K, and aspartame. A total of 131 characteristic wavenumbers were selected from the full spectral range for model development. By combining spectral pre-processing with principal component analysis (PCA), the proposed method enabled both qualitative classification and quantitative determination of the sweeteners. The support vector machine (SVM) model demonstrated superior identification performance and predictive capability compared with random forest (RF), k-nearest neighbor (KNN), and linear discriminant analysis (LDA) models [21].

Thomas A. Teklemariam *et al.* applied ATR-FTIR spectroscopy combined with machine learning to detect sugar adulteration in coconut water. The collection includes infrared spectra from samples of coconut water that have been contaminated with fifteen different kinds of possible sugar alternatives, including as sugars, artificial sweeteners, and sugar alcohols. Principal component analysis (PCA) and t-distributed stochastic neighbor embedding (t-SNE) were employed to develop an interactive application for the non-targeted identification of sugar adulterants through enhanced data visualization and pattern recognition. On the same dataset, targeted analysis using ensemble learning random forest (RF) and deep learning 1-dimensional convolutional neural network (1D CNN) produced higher classification accuracies (95% and 96%, respectively) than support vector machine (SVM) at 88% and sparse partial least squares discriminate analysis (sPLS-DA) at 77% [22].

Sinem Colak *et al.* investigated buffalo milk adulteration using FTIR spectroscopy. The adulteration detection performance of six artificial intelligence (AI) models was evaluated and compared with those of soft independent modelling of class analogies (SIMCA) and data-driven SIMCA (DD-SIMCA) chemometric approaches. Additionally, using particle swarm optimization (PSO) to reduce the number of FTIR spectroscopy measurements has been examined as a way to attain good performance with fewer measurements. In the Ensemble Bagged Tree technique, it was found that the features chosen using PSO achieved an accuracy value of 90.38%. Experts in the field of food adulteration are expected to benefit from the quick outcomes of artificial intelligence-assisted systems [23].

Manish M. Paradkar et al. determined the caffeine content in soft drinks using FTIR spectroscopy. Quantitative estimation was performed using principal component regression (PCR) and partial least squares (PLS) regression over the spectral region of 2800–3000cm¹. The combination of FTIR spectroscopy with chemometric analysis, particularly PLS applied to first-derivative spectra, accurately predicted caffeine concentrations, achieving a coefficient of determination (R^2) greater than 0.97 and a standard error of prediction (SEP) of less than 2.43 using prediction models with four to six latent components. In about five minutes, the generated model was used to forecast the amount of caffeine in four commercial fizzy drinks [24].

Gaoqiang Lvet *al.* were the first to characterize *in situ* residues of the broad-spectrum fungicide boscalid on plant surfaces using portable ATR-FTIR spectroscopy. Tomato fruits with pre-established boscalid residue concentrations were subjected to ATR-FTIR scanning without any pre-treatment, and the resulting spectra were subsequently analyzed using chemometric techniques. This study emphasizes the potential of portable ATR-FTIR for both on-site and in-situ qualitative and quantitative pesticide residue monitoring [25].

Xuebin Xu *et al.* synergistically combined laser-induced breakdown spectroscopy (LIBS) and FTIR spectroscopy to develop a rapid analytical framework. To comprehensively characterize organic fertilizers, the authors integrated spectral fusion, machine learning techniques, two-dimensional correlation spectroscopy (2D-COS), and variable selection methods. Partial least squares regression (PLSR) exhibited the best predictive performance for nitrogen (N) and potassium (K) quantification using individual FTIR and LIBS spectra, respectively. With significant speed and cost savings over conventional techniques, this improved FTIR-LIBS approach creates a practical and environmentally friendly analytical framework for thorough organic fertilizer testing [26].

Sanja Duvnjak *et al.* reported that the rapid and accurate identification of intracellular pathogenic *Brucella* species and biovars is essential for effective public health surveillance, outbreak control, and the protection of both human and animal health. The IR Biotyper software incorporates many machine learning algorithms, such as ANN, support vector machine with linear kernel (linear SVM), and support vector machine with radial basis function (RBF SVM), all of which were examined in order to create an automated classifier. In terms of classification accuracy, the Support Vector Machine (RBF SVM) algorithm performed better than ANN throughout the machine learning model selection process [27].

III. CHALLENGES AND FUTURE PERSPECTIVE

FTIR spectra often contain baseline offset, noise, atmospheric interference (CO_2, H_2O), and instrument variability. Baseline distortion misleads ML models. Noise can reduce classification/regression accuracy. Many polymer functional groups have overlapping peaks in the fingerprint region (~1500–400 cm^1), making human interpretation difficult and ML feature extraction challenging. Different preprocessing (normalization, derivatives, smoothing) significantly impacts model performance. Choosing the right sequence (e.g., baseline correction → normalization → Savitzky-Golay smoothing) is non - trivial. Inappropriate preprocessing can introduce artifacts. Large, well-annotated FTIR datasets for specific polymer systems are limited. Lack of ground truth makes supervised ML difficult. Mislabeling or mixed sample spectra degrade model training quality. Heterogeneous polymer blends complicate class boundaries [28]. High dimensionality increases: CNNs and auto encoders can effectively analyze raw spectral maps without extensive feature engineering. However, they require substantial memory, long training times, and high GPU resources. Additionally, these deep learning models are more susceptible to over fitting, particularly when trained on limited datasets. Real time spectral analysis on embedded devices is still challenging.

DL models, such as CNNs and deep artificial neural networks (ANNs), generally provide high classification accuracy; however, their limited interpretability remains a significant challenge. The complex decision-making process of these models makes it difficult to associate predictions with specific chemical features or spectral bands, thereby reducing confidence among domain experts who require physically meaningful explanations. In contrast, traditional ML techniques, including SVMs and partial least squares (PLS) regression, offer greater interpretability but may exhibit lower predictive accuracy than deep learning models. Future research should focus on the development of explainable artificial intelligence (XAI) approaches that enhance model transparency while maintaining high predictive performance. In addition, active learning strategies, in which AI selectively queries experts to label uncertain samples, can substantially improve model performance while minimizing the effort required for data annotation. Transfer learning, which involves fine-tuning pretrained models developed on large spectral datasets for specific polymer systems, represents another promising approach. This strategy reduces the need for extensive labeled datasets, improves model generalizability, and facilitates the application of AI to diverse spectroscopic analyses [29].

IV. CONCLUSION

In conclusion, the integration of AI with FTIR spectroscopy has emerged as a powerful approach for enhancing spectral analysis, prediction, and classification capabilities. Machine learning and deep learning algorithms, including CNNs, have demonstrated significant potential in extracting complex spectral patterns, improving analytical accuracy, and enabling rapid data interpretation across diverse applications. Although challenges such as data availability, model interpretability, and standardization remain, advancements in explainable AI, transfer learning, and automated data processing are expected to further strengthen the reliability and applicability of AI-assisted FTIR spectroscopy. Overall, the combination of spectroscopy and AI represents a promising direction toward more efficient, accurate, and intelligent analytical systems for scientific research and industrial applications.

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