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Review

Artificial Intelligence-Assisted FT-IR Spectral Sensing: From Molecular Fingerprints to Quantitative and Interpretable Chemical Information

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Abstract

Fourier-transform infrared (FT-IR) spectroscopy provides rapid, accessible, and chemically informative molecular fingerprints, but quantitative analysis of complex samples is often hindered by band overlap, baseline variation, matrix effects, and nonlinear relationships between spectra and target properties. This review examines how artificial intelligence (AI), including machine learning, deep learning, and explainable artificial intelligence (XAI), can convert FT-IR fingerprints into quantitative and interpretable chemical information. Recent studies were organized according to analytical function and examined with respect to spectral acquisition and data organization, preprocessing and input preparation, model development, validation, uncertainty, transferability, and chemical interpretation. AI-assisted FT-IR has been applied to composition and concentration prediction, adulteration and contamination-level estimation, physicochemical and material-attribute prediction, and process-, time-, and state-dependent prediction. Across these applications, robust performance depends on representative independent samples, leakage-free validation, transparent preprocessing, uncertainty assessment, calibration transfer, and spectroscopically plausible interpretation of model-relevant regions. Data augmentation, transfer learning, and XAI may improve model robustness and interpretability, but they require validation with independent real samples. Overall, AI can extend FT-IR from qualitative fingerprinting to quantitative and predictive spectral sensing, provided that future studies emphasize method-centered validation, reproducibility, transferability, and chemically meaningful explanation rather than relying solely on classification accuracy and regression error metrics.

Keywords: FT-IR spectroscopy; artificial intelligence; spectral sensing; quantitative analysis; chemical interpretability

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1. Introduction

Fourier-transform infrared (FT-IR) spectroscopy is a well-established molecular spectroscopic technique that probes vibrational absorption and provides characteristic fingerprints of molecules, materials, and complex mixtures [1]. Its rapid measurement, minimal sample preparation, relatively low cost, and compatibility with sampling modes such as attenuated total reflection (ATR), transmission, and diffuse reflectance have supported broad applications in chemical analysis, materials characterization, biomedical research, environmental monitoring, pharmaceutical quality control, and food authentication. Beyond conventional molecular characterization, FT-IR can be regarded as an optical spectral

sensing platform that translates variations in chemical composition, molecular interactions, structural organization, and material state into measurable vibrational responses. Functional-group bands provide relatively localized structural information, whereas the fingerprint region encodes broader compositional and matrix-dependent characteristics.

The analytical scope of FT-IR has been reviewed across diverse fields. Koczoń et al. summarized its capabilities in molecular characterization, quantitative analysis, technological processes, environmental monitoring, and food analysis [2], while Cherniienko et al. examined ex situ and in situ applications in chemical and pharmaceutical analysis, including substance identification, quantification, impurity analysis, and process monitoring [3]. Application-oriented reviews have further addressed biological tissues [4], quantitative pharmaceutical, biomedical, and clinical analysis [5], food and edible-oil authentication using chemometrics [6], and inorganic-material characterization [7]. Together, these reviews establish FT-IR as a versatile platform for qualitative and quantitative chemical analysis, materials characterization, and process monitoring.

Despite this versatility, FT-IR spectra from real samples are often difficult to interpret or quantify using individual absorption bands alone. Overlapping bands, matrix effects, baseline and scattering variations, water and atmospheric interference, particle-size effects, and sampling variability can obscure target-related information [1,8]. Chemically relevant information may instead be distributed across multiple weak and correlated spectral features, with relationships to target properties that are nonlinear or matrix-dependent. Reliable analysis therefore often requires preprocessing and multivariate modeling beyond visual interpretation or single-band calibration [8,9]. Artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL), provides an extended framework for modeling these complex spectral–property relationships, while explainable artificial intelligence (XAI) can help identify the spectral regions contributing to predictions. Preprocessing remains integral to this workflow because it changes the spectral representation presented to the model and must therefore be selected and validated in relation to both predictive performance and chemical meaning.

Previous reviews have examined AI-assisted spectral analysis from complementary perspectives. Mokari et al. described the workflow from spectral preprocessing and classical data modeling to DL [8], whereas Fadlelmoula et al. focused on ML applications to FT-IR data from human blood cells [10]. Cai et al. reviewed the benefits, limitations, transfer-learning strategies, and interpretability of DL across vibrational-spectroscopic platforms [11], and Luo et al. addressed FT-IR-based molecular monitoring from static characterization to dynamic trend analysis [12]. Recent methodological studies have extended AI-assisted FT-IR to functional-group recognition, spectral reconstruction, transformer-based modeling, grouped spectral interpretation, and chemically informed data augmentation [13–17]. Applications have likewise expanded across composition analysis, contamination and safety assessment, physicochemical-property prediction, and process- or state-dependent monitoring [18–26]. These advances demonstrate the growing analytical capabilities of AI-assisted FT-IR but also highlight the need for rigorous validation, transferability assessment, prediction-uncertainty evaluation, and chemically plausible interpretation.

Existing reviews have generally focused on specific sample domains, selected methodological aspects, or broader developments in AI-assisted vibrational spectroscopy [8,10–12]. However, relatively few cross-domain reviews have organized conventional one-dimensional (1D) FT-IR applications by analytical function while examining predictive performance and the extent to which validation, generalizability across sample populations and matrices, inter-instrument transferability, prediction uncertainty, and chemically grounded interpretation have been addressed. The present review therefore evaluates AI-assisted FT-IR as an analytical

sensing methodology rather than merely cataloguing applications or comparing algorithms. Recent studies are examined according to four analytical functions: composition-related screening and concentration prediction; adulteration, contamination, and safety-related detection or level estimation; physicochemical-property and material-attribute prediction; and process-, time-, and state-dependent prediction and monitoring. XAI and chemically grounded model interpretation are treated as cross-cutting topics.

A focused literature search was conducted primarily in Web of Science, supplemented by Scopus and Google Scholar. The core search combined "FT-IR" or "FTIR" with "artificial intelligence," "machine learning," or "deep learning" and covered studies published from 2020 through July 2026. Original research articles were retained when conventional 1D FT-IR or ATR-FTIR was a principal analytical input and predictive modeling was applied directly to the spectra. Studies using FT-IR only for supplementary characterization, applying AI to unrelated data, or relying primarily on another analytical platform were generally excluded, although selected classical chemometric, multimodal, or cross-platform studies were retained as methodological comparators. Representative studies were selected according to analytical function, methodological relevance, and validation design, with chemical or model interpretation considered where reported. Accordingly, this focused narrative review emphasizes representative sampling, preprocessing, leakage-free validation, uncertainty assessment, calibration transfer, robustness, and spectroscopically plausible interpretation to assess the conditions required for AI-assisted FT-IR to progress toward reliable chemical sensing.

2. FT-IR Spectral Data and the Need for AI-Assisted Analysis

FT-IR spectra contain direct information on molecular vibrations, but analytical targets in complex samples are rarely represented by a single, isolated absorption band. The analytical challenge is therefore to distinguish chemically meaningful variation from matrix-, sampling-, and instrument-related variation and to convert multivariate spectral responses into reliable classifications, quantitative estimates, or state assessments. This section considers how chemical information is encoded in FT-IR spectra, why spectra from real samples are analytically complex, and how AI-assisted analysis can extract useful information from these responses.

2.1. Chemical Information Encoded in FT-IR Spectral Responses

Infrared absorption occurs when a molecular vibration produces a change in dipole moment. Band positions are governed by factors such as bond strength, atomic mass, molecular structure, and the local chemical environment, whereas band intensities are influenced by concentration, transition strength, molecular interactions, and measurement conditions [1,2]. Functional-group bands can provide relatively localized information for molecular identification and structural comparison. By contrast, the fingerprint region contains numerous coupled and overlapping vibrations that collectively reflect molecular architecture, composition, intermolecular interactions, and physicochemical state.

In mixtures and other complex matrices, the measured spectrum represents the combined responses of multiple constituents. These responses may be approximately additive, but hydrogen bonding, molecular association, matrix effects, and physical differences among samples can alter band positions, shapes, and intensities [1–3]. Consequently, a spectral variable cannot always be assigned uniquely to a single compound or structural feature.

For analytical sensing, target-related information may therefore be encoded through several complementary forms: relatively distinct analyte bands, ratios or combinations of band intensities, broad compositional patterns, derivative features, and subtle variations within the fingerprint region. In some cases, the relevant spectral response is directly

associated with the target compound; in others, it arises indirectly through correlated changes in the surrounding matrix. FT-IR spectra should thus be treated as ordered, chemically structured multivariate signals rather than as collections of independent peak intensities [6,8,9]. This distributed information provides the basis for chemometric and AI-assisted classification, calibration, and property prediction.

2.2. Analytical Complexity of Real FT-IR Sensing Data

The same chemical richness that makes FT-IR useful also complicates its interpretation. Absorptions from different molecular species frequently overlap, while broad O–H and N–H bands, multiple carbonyl contributions, and densely populated fingerprint-region features can limit direct band assignment and single-band quantification [1,8]. Minor target-related changes may also be obscured by stronger matrix signals or appear as small variations in band position, width, shape, or relative intensity.

Spectral responses are additionally affected by the sample–instrument interface. In ATR measurements, effective penetration depth, sample–crystal contact, applied pressure, surface roughness, refractive index, moisture, and sample heterogeneity can influence the measured intensity and band profile. Transmission measurements are sensitive to path length, sample thickness, and dilution, whereas diffuse-reflectance spectra can be strongly affected by particle size, packing, and light scattering. Baseline drift, atmospheric water and carbon dioxide, detector noise, temperature, and inter-instrument variation introduce further sources of variability [1,2,8]. Adsorption of surface-active or strongly retained analytes and matrix components onto ATR crystals, transmission windows, or flow-cell surfaces can cause incomplete sample removal and carryover, thereby biasing band intensities and downstream model predictions. Appropriate cleaning procedures, blank measurements, and replicate checks are therefore needed to identify and control these effects [1].

Preprocessing methods—including baseline correction, smoothing, normalization, scatter correction, spectral alignment, and derivative transformation—are commonly applied to reduce such variation [8,9]. However, preprocessing is not a chemically neutral operation. Normalization may reduce or remove absolute intensity information related to concentration, derivatives can emphasize weak or overlapping features while amplifying noise, and aggressive baseline or scatter correction can alter genuine matrix-dependent patterns. Preprocessing should therefore be regarded as part of the analytical method and selected within the validation process rather than treated as a routine computational step applied independently of the prediction objective.

The relationship between FT-IR responses and analytical targets may also be indirect or nonlinear. Band overlap, intermolecular interactions, scattering, detector saturation, and correlated compositional variation can generate spectral–property relationships that are difficult to represent using a single wavelength or a simple linear response [8,11]. Moreover, a model may obtain apparently high predictive performance by exploiting spectral differences associated with sample origin, batch, preparation procedure, or measurement conditions rather than the intended chemical target. Distinguishing direct target-related information from correlated proxy information is therefore essential when assessing the analytical validity, generalizability, and chemical meaning of AI-assisted predictions.

2.3. AI-Assisted Conversion of Spectral Responses into Chemical Information

Classical chemometric approaches established the use of FT-IR spectra for multivariate classification, calibration, and quality assessment [6,8,9]. Modern ML and DL methods extend these capabilities by modeling nonlinear relationships, interactions among spectral variables, and distributed patterns that may not be captured adequately by individual

bands or linear latent-variable models [8,11,12]. Convolutional models can learn local spectral patterns such as band shapes and neighboring-variable relationships, whereas transformer-based models can represent interactions across more widely separated spectral regions [11,15].

AI-assisted FT-IR analysis can serve several analytical functions. These include spectral recognition and sample classification [13,15,18,21,22]; quantitative prediction of chemical composition, contamination levels, biochemical parameters, and material properties [19–21,23–25]; reconstruction or augmentation of spectral data [14,17]; and monitoring of time- or state-dependent chemical changes [12,26]. These functions rely on information distributed across the spectrum rather than exclusively on isolated marker bands.

The analytical value of AI nevertheless extends beyond obtaining high classification accuracy or low prediction error. Model performance should be evaluated together with the representativeness of the samples, independence of the validation data, robustness to measurement variation, applicability to new matrices or instruments, and consistency of model-relevant regions with spectroscopic knowledge. XAI and feature-attribution methods can help identify which spectral regions influence a prediction and whether a model relies on chemically plausible information [16,17,22]. Such attribution results, however, describe the behavior of a fitted model; they do not by themselves demonstrate that the highlighted bands are causally or uniquely related to the target.

AI is therefore most valuable when it converts overlapping, variable, and matrix-dependent FT-IR responses into quantitative or decision-relevant information within a validated analytical workflow. Its contribution should be judged not only by predictive performance but also by the reliability, transferability, and chemical interpretability of the resulting analysis.

3. AI Workflow for Quantitative FT-IR Spectral Sensing

AI-assisted FT-IR spectral sensing is an integrated analytical workflow rather than an algorithm-selection exercise. It includes representative sample selection, spectral acquisition and data organization, preprocessing and input preparation, model development, and performance validation. Although all major stages should be considered and documented, the specific sub-steps within each stage are not universally required and should be selected according to the analytical objective, sample matrix, data characteristics, and intended application. Decisions made at each stage determine whether a model captures generalizable chemical information or sample-, batch-, and instrument-specific correlations. Errors at one stage can propagate through the workflow: unrepresentative sampling may restrict applicability, inconsistent acquisition or unsuitable preprocessing may introduce nonchemical variation, inappropriate optimization may promote overfitting, and non-independent validation may produce optimistically biased performance estimates. These errors may ultimately result in quantitative bias, misclassification, poor transferability, misleading spectral interpretation, and underestimated uncertainty. The complete workflow and rationale for each selected step should therefore be specified and validated as part of the analytical method. Figure 1 summarizes the principal stages and distinguishes core considerations from conditionally selected methodological options.

3.1. Spectral Acquisition and Data Organization

Reliable modeling begins with spectra that are reproducible and representative of the intended application. ATR, transmission, and diffuse-reflectance measurements differ in sampling depth, sample preparation, and sensitivity to physical variation; the measurement mode should therefore be selected according to the matrix and analytical objective [1,8]. Spectral range, resolution, number of scans, background collection, temperature, sample

presentation, and—where relevant—ATR pressure should be standardized and reported. Repeated measurements can characterize instrumental and sampling repeatability, but they cannot compensate for insufficient diversity among independent samples.

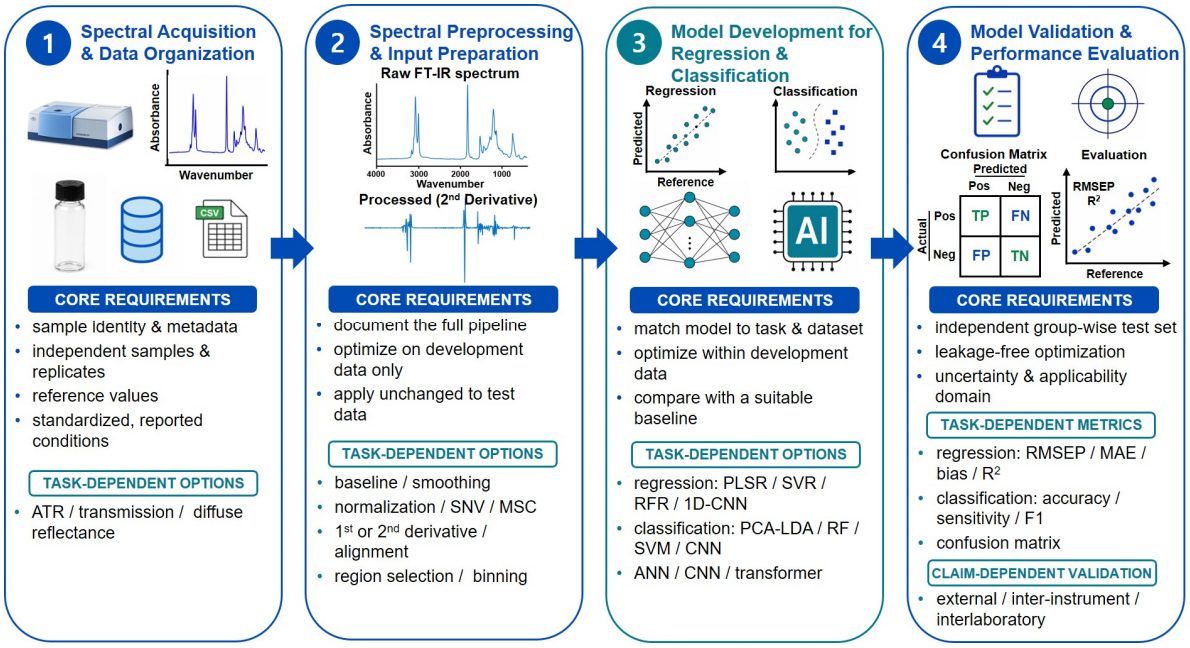


Figure 1. General workflow of AI-assisted quantitative FT-IR spectral sensing, showing core requirements, task-dependent options and metrics, and claim-dependent validation procedures.

Calibration samples should span the intended concentration or property range and include relevant sources of nuisance variation, such as product type, raw-material origin, batch, preparation day, operator, environmental condition, and instrument. Reference values should be obtained using appropriate analytical methods, with their precision and uncertainty considered when interpreting achievable prediction error. Here, analytical precision refers to the agreement among replicate measurements obtained under specified conditions, whereas accuracy refers to agreement with an accepted reference value. If the intended use includes threshold-based decisions, sample density near the decision boundary is particularly important.

Each spectrum should be linked to the independent sample, batch, reference value, acquisition conditions, preprocessing history, and replicate structure. The independent physical sample—not the individual spectrum—should be treated as the primary analytical unit. Technical replicates and repeated scans from the same sample should remain in the same data partition; otherwise, near-duplicate spectra can occur in both model development and testing and produce optimistically biased performance.

3.2. Spectral Preprocessing and Input Preparation

Preprocessing is used to reduce unwanted spectral variation and present target-relevant information in a form suitable for modeling. In complex spectra, distinguishing unwanted spectral variation from target-related chemical variation is not always straightforward and generally requires comparisons among replicate, reference, or quality-control spectra. Spectral overlays, difference spectra, and multivariate score and loading plots, interpreted together with measurement metadata, can reveal baseline shifts, intensity scaling, peak displacement, noise, or clustering associated with measurement conditions, batches, or instruments [27,28]. Common operations include baseline correction, smoothing, normalization, standard normal variate (SNV) transformation, multiplicative scatter

correction (MSC), spectral alignment, and first- or second-derivative transformation [27,28]. Savitzky–Golay smoothing and differentiation are widely used to calculate derivative spectra while preserving local spectral structure when window length, polynomial order, and derivative order are selected appropriately [29].

Input preparation may also involve removal of atmospheric, water-dominated, saturated, noisy, or instrumentally unreliable regions, together with spectral binning or downsampling. Region exclusion based on predefined spectroscopic or instrumental criteria is distinct from data-driven variable selection. When regions or variables are selected using the target response, selection forms part of model optimization and must be performed within the training and validation workflow.

Preprocessing is not chemically neutral. Normalization can suppress concentration-related intensity differences, derivatives can resolve overlapping features but amplify noise, and aggressive baseline or scatter correction can alter genuine matrix-dependent signals. The preprocessing sequence and all parameters should therefore be specified, fitted or optimized using training data only when they are data-dependent, and then applied unchanged to validation and test samples [30,31]. Comparisons among raw and processed representations should use identical sample partitions so that any performance gain can be attributed to the spectral transformation rather than to differences in data splitting.

3.3. Model Development for Regression and Classification

Model selection should reflect the analytical objective, number and diversity of independent samples, spectral complexity, expected nonlinearity, and required level of interpretability. Regression models predict continuous variables such as concentrations, adulteration levels, physicochemical properties, or process parameters, whereas classification models assign samples to predefined categories or decision classes. Some applications, particularly adulteration and contamination assessment, may use classification for screening and regression for level estimation.

Common approaches include linear and latent-variable chemometric methods, distance- and kernel-based algorithms, tree-based ensembles, and neural networks [8–11]. Partial least squares regression (PLSR) remains an important baseline for quantitative calibration of highly collinear spectra. Principal component analysis followed by linear discriminant analysis (PCA–LDA) and partial least squares discriminant analysis (PLS-DA) provide comparatively transparent classification approaches. K-nearest neighbors (KNN), support vector machine (SVM), and support vector regression (SVR) use sample similarity or kernel-based learning, whereas decision trees, random forest (RF), and gradient-boosting models can represent nonlinear relationships and interactions among spectral variables.

Artificial neural networks (ANNs) and convolutional neural networks (CNNs) can model more complex spectral relationships. One-dimensional CNNs (1D-CNNs) learn local patterns such as band shapes and neighboring-wavenumber relationships directly from ordered spectral inputs. Transformer-based architectures can additionally model interactions among more widely separated spectral regions [11,15]. These models may be valuable for complex tasks, but their higher flexibility also increases the need for adequate sample diversity, regularization, and independent validation.

Full-spectrum modeling is appropriate when chemically relevant information is broadly distributed, whereas region selection or dimensionality reduction may improve robustness and interpretation when substantial irrelevant or noisy variation is present. Hyperparameters, feature-selection rules, and preprocessing alternatives should be optimized only within the model-development data. Because no model family is universally superior, complex models should be compared with suitable chemometric or ML baselines under the same sample partitions and evaluation criteria.

3.4. Model Validation and Performance Evaluation

Validation should estimate performance for genuinely unseen samples. Internal cross-validation (CV) is useful for model and hyperparameter selection, whereas an independent test set provides a more realistic final assessment. When sample size is limited, nested CV can separate inner-loop optimization from outer-loop performance estimation. In all cases, partitioning should be performed at the level of independent samples or, when appropriate, batches, products, preparation days, or acquisition sessions. Preprocessing optimization, target-informed variable selection, and hyperparameter tuning must remain within the training and validation workflow to prevent information leakage [30,31].

Regression performance is commonly summarized using the root mean square error of prediction (RMSEP), mean absolute error (MAE), bias, and coefficient of determination (R^2). These metrics should be reported for independent samples and interpreted relative to the calibration range, reference-method precision, and intended analytical use. Classification performance should not rely on overall accuracy alone; sensitivity, specificity, precision (positive predictive value), recall, F1 score, balanced accuracy, and confusion matrices are particularly important when class sizes or decision costs are unequal.

Uncertainty in AI-assisted FT-IR analysis should not be represented by classification accuracy or regression error alone. Confidence intervals for these metrics describe variability in overall performance estimates, whereas the reliability of an individual prediction may also be affected by spectral repeatability, sample presentation, reference-measurement uncertainty, calibration-data coverage, model fitting, and extrapolation. Depending on the task, uncertainty can be assessed using replicate measurements, resampling, prediction intervals, calibrated class probabilities, and applicability-domain evaluation. These estimates should be evaluated using independent data, and predictions with large uncertainty or outside the represented domain should be flagged for confirmatory analysis [32].

A final test set should remain untouched until model development is complete and should not subsequently be reused for model selection. Stronger evidence of generalization is provided by external samples that differ in batch, source, preparation time, operator, instrument, or laboratory in ways relevant to the intended application. Accordingly, the credibility of an AI-assisted FT-IR method depends not only on numerical performance but also on transparent sample organization, leakage-free optimization, uncertainty-aware evaluation, and validation under realistic sources of variation.

Overall, reliable AI-assisted FT-IR analysis requires representative acquisition, chemically justified preprocessing, task-appropriate modeling, and validation based on independent analytical units. Broader challenges related to uncertainty, robustness, transferability, and deployment are discussed in Section 6.

4. Quantitative and Predictive Applications of AI-Assisted FT-IR Spectral Sensing

AI-assisted FT-IR applications are organized here by analytical function rather than sample type. The four groups are composition-related screening and concentration prediction; adulteration, contamination, and safety-related detection or level estimation; physicochemical-property and material-attribute prediction; and process-, time-, and state-dependent prediction or monitoring. This function-centered structure also separates fundamentally different outputs—continuous estimates, class assignments, threshold-based decisions, and dynamic predictions—that require different validation designs and performance metrics.

Some studies span more than one group. For example, an adulteration workflow may first classify the adulterant and then estimate its level, while a process model may predict both composition and reaction state. Placement therefore follows the intended analytical

decision rather than the mathematical form of the output alone. Across all groups, the target should be defined independently by an appropriate reference method, data splitting should preserve the true independent-sample or batch structure, and performance should be evaluated under conditions representative of the intended use.

4.1. Composition-Related Screening and Concentration Prediction

Continuous concentration prediction is the most direct extension of conventional quantitative FT-IR analysis: spectra are calibrated against values from an independent reference method and used to estimate native constituents or composition-related parameters in unknown samples. Composition-related screening is included in this subsection when biochemically measured traits are converted into decision classes rather than predicted as continuous values. The distinction is important because a classifier for high, medium, or low content is not equivalent to a quantitative calibration.

Gao et al. calibrated FT-IR spectra against gas chromatography–mass spectrometry (GC–MS) measurements and used PLSR to quantify six volatile compounds in beer [33]. Herath et al. analyzed 270 colored-rice accessions and used RF and SVM, together with other classifiers, to assign biochemically quantified phenolic and antioxidant traits to screening classes with reported accuracies of 93.5–100%; this was high-throughput composition-related classification rather than continuous concentration regression [34]. Siregar et al. used PCA and PLSR to estimate protein, lipid, moisture, ash, and carbohydrate in seven rice varieties [35]. However, Gaussian-distributed target values were generated around a small number of reference measurements to match the much larger number of spectra, illustrating why repeated spectra or generated targets should not be treated as additional independent chemical samples. Holden et al. developed PLSR models that linked ATR-FTIR spectra of xylem sap and freeze-dried leaves to hormone concentrations measured by mass spectrometry [36]. Chechekina et al. further demonstrated regression of multiple serum biochemical parameters, with RF regression performing strongly in a complex biofluid [19].

Across these studies, validation relied mainly on CV, internal training–test splits, or randomly selected validation subsets [19,33–36]. However, the number of spectra did not always represent the number of independent analytical units, particularly when data augmentation [19] or repeated spectra paired with generated target values [35] were used. Evaluation using wholly independent beer batches, germplasm populations, plant experiments, or clinical cohorts was not described in [33,34,36] and [19], respectively. Reported performance should therefore be interpreted within the sampled matrices, reference ranges, and preprocessing conditions. FT-IR outputs should be regarded as calibrated estimates or screening decisions linked to their reference methods rather than universal replacements for compound-specific analyses. Table 1 summarizes the analytical targets and modeling approaches together with the reported validation scope and limitations.

Table 1. Representative studies on composition-related screening and concentration prediction using AI-assisted FT-IR spectral sensing.

Sample/ Matrix	Target/Analytical Purpose	Modeling Approach	Validation and Limitations	Ref.
Beer	Discrimination and quantification of six volatile compounds	PCA and PLSR	80/20 split using GC–MS reference concentrations; no independent batch or instrument validation	[33]
Colored-rice germplasm	Classification of phenolic and antioxidant traits for high-throughput screening	RF and SVM, ANN, KNN, Naïve Bayes	70/30 split with 10-fold CV; no external season-, site-, or instrument-level validation	[34]

Table 1. *Cont.*

Sample/ Matrix	Target/Analytical Purpose	Modeling Approach	Validation and Limitations	Ref.
Seven rice varieties	Prediction of protein, lipid, moisture, ash, and carbohydrate contents	PCA and PLSR	CV only; generated target values were based on five replicate reference measurements per variety; no external validation	[35]
Plant xylem sap and freeze-dried leaves	Quantitative prediction of plant hormone concentrations	PCA, PCA-LDA, SVM, PLSR	1000-run Monte Carlo CV using UHPLC–HRMS reference concentrations; no external population, season, or instrument validation	[36]
Blood serum	Quantitative prediction of 12 routine biochemical parameters	Linear/Lasso Regression, DTR, RFR, GBR/XGBoost, SVR	Ninety-one sera with a 70:20:10 split and 10-fold CV; augmentation timing relative to data partitioning was not clearly reported	[19]

4.2. Adulteration, Contamination, and Safety-Related Detection or Level Estimation

Adulteration and contamination analysis is analytically distinct from ordinary composition prediction because the intended decision concerns a non-native, fraudulent, or hazardous component in an otherwise expected matrix. The output may be binary detection, adulterant-type classification, concentration regression, or classification relative to a safety threshold. These outputs should not be conflated: level estimation requires continuous reference values and regression validation, whereas screening requires sensitivity, specificity, and performance near the relevant decision boundary.

Because adulteration often changes the global molecular fingerprint without producing a single isolated marker band, models can exploit distributed differences across the spectrum. Representative studies include detection and level estimation of wheat flour in gluten-free cornbread [37]; classification of 15 sugar, sugar-alcohol, and artificial-sweetener adulterants in coconut water [38]; prediction of sawdust adulteration in coriander powder [39]; classification and quantitative detection of adulteration in Panax notoginseng using a CNN–transformer framework [40]; interpretable classification and prediction of deoxynivalenol (DON) in wheat flour [21]; screening of aflatoxin B1 (AFB1) in chili powder [41]; and chemometric screening with micro-FT-IR imaging for turmeric adulteration [42]. The coconut-water and AFB1 studies are principally detection or classification examples, whereas the cornbread, coriander, *Panax notoginseng*, and DON studies include quantitative level estimation.

Across these studies, validation relied mainly on internal data splitting or CV, often using laboratory-prepared mixtures, without independent validation across sample sources, preparation batches, brands, or instruments [21,37–40]. Market samples were evaluated using sample-level leave-one-out cross-validation (LOOCV) for chili-powder screening [41], whereas turmeric screening included external validation and a 20-sample interlaboratory comparison, with 80% agreement [42]. These findings support validation using independent preparation batches, multiple authentic-source populations, low-level samples near decision thresholds, and, where possible, external market and interlaboratory samples. Classical chemometric screening is retained as a methodological comparator rather than uniformly categorized as modern AI [42]. Table 2 summarizes the analytical targets and modeling approaches together with the reported validation procedures and limitations, while distinguishing detection or classification from quantitative level estimation.

Table 2. Representative studies on adulteration, contamination, and safety-related detection or level estimation.

Sample/ Matrix	Target/Analytical Purpose	Modeling Approach	Validation and Limitations	Ref.
Gluten-free cornbread/corn flour	Detection and quantification of wheat-flour contamination	KNN, RF, SVC/SVR, DT, PLSR, and voting ensemble	70/30 split with training-set CV; 13 single-source formulations and no external validation	[37]
Coconut water	Classification of 15 sugar, sugar-alcohol, and artificial-sweetener adulterants	RF, 1D-CNN, sPLS-DA, SVM	Laboratory-spiked mixtures evaluated internally; no independent coconut-source, brand, or batch validation reported	[38]
Coriander powder	Quantitative prediction of sawdust adulteration level	LR, DT, SVR, ANN	Internal validation using 28 laboratory mixtures; single material sources and no external samples	[39]
Panax notoginseng	Identification of three adulterants and prediction of adulteration level	CNN, Transformer, PLS-DA, RBFNN, and LSSVM	Prediction-set evaluation of laboratory mixtures; no external retail-product or inter-instrument validation reported	[40]
Wheat flour	Classification by DON safety level and quantitative prediction of DON concentration	XGBoost, RF, TabPFN, CatBoost	Five-fold CV and a held-out test set; no external batch or instrument validation reported	[21]
Chili powder	Classification of Aflatoxin B1 contamination	Logistic regression, RF, SVM, KNN	Sample-level LOOCV on 73 market samples; best accuracy was 73%; no external-region or instrument validation was reported	[41]
Turmeric powder	Non-targeted detection of multiple adulterants and screening of commercial samples	PCA, OPLS-DA, PLS-DA	External validation and a 20-sample interlaboratory comparison; 80% agreement was reported	[42]

4.3. Physicochemical-Property and Material-Attribute Prediction

Physicochemical-property prediction differs from concentration analysis because the target may arise from molecular architecture, functional-group distribution, structural modification, or bulk material behavior rather than the amount of a single compound. FT-IR can therefore serve as a surrogate sensor when reproducible multivariate spectral patterns correlate with independently measured structural or performance attributes. The strength of such a model depends on whether the calibration set spans the chemical and physical variability expected in use.

Rhein et al. predicted the degree of substitution of cellulose acetate from ATR-FTIR spectra using nuclear magnetic resonance-derived reference values [20]. Chen et al. modeled unsaturation, effective hydrogen-to-carbon ratio, lower heating value, and elemental composition of biomass pyrolysis oils [43]. Two studies extended this concept to sustainable aviation fuel (SAF). Comesana et al. used non-negative matrix factorization (NMF) to derive additive spectral features and ensemble regressors to predict final boiling point, flash point, freezing point, density, and kinematic viscosity (Figure 2) [44], whereas Tao et al. compared PCA-assisted SVR, ANN, and RF models for rapid SAF characterization [45]. He et al. provided a particularly informative validation example for soil properties: random CV suggested useful interpolation, but leave-one-prefecture-out validation revealed weak extrapolation, including negative R^2 values for some targets [46]. This contrast demon-

strates that performance within a sampled domain does not establish transferability to a new region or sample population.

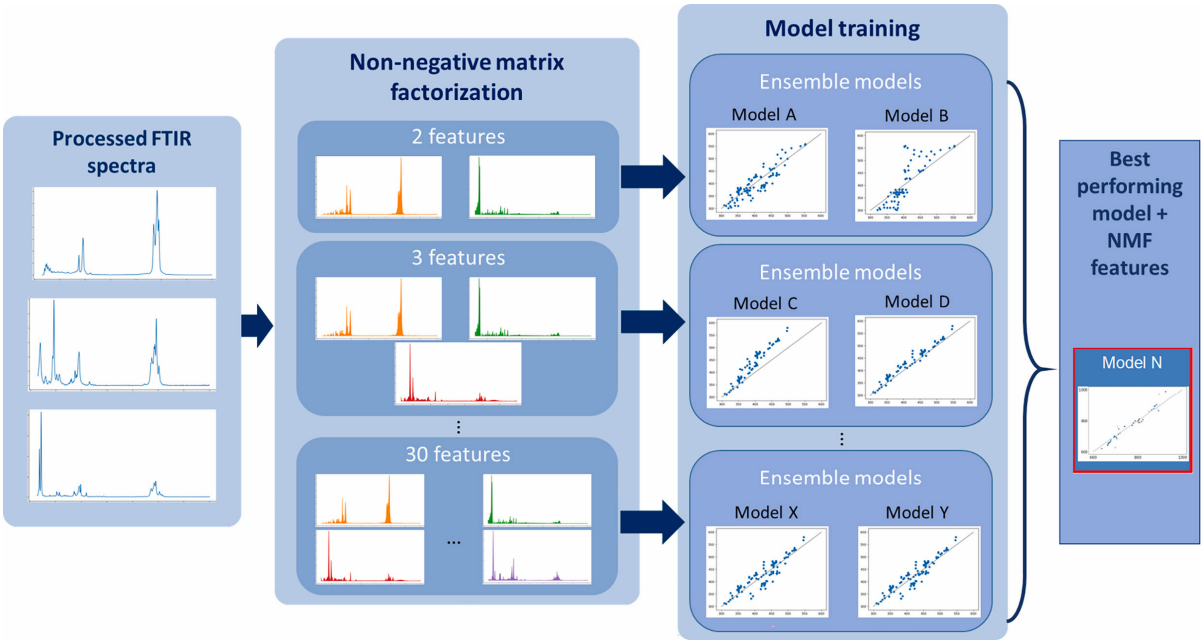


Figure 2. Schematic of the model-development process for predicting sustainable aviation fuel properties. Reprinted from Comesana et al. [44] under the CC BY 4.0 license.

Applicability domain is therefore central to property prediction. A model trained on one polymer family, fuel formulation space, soil region, or processing route may rely on composition–property relationships that do not extend to chemically related but unseen samples. Validation should accordingly span relevant property ranges and preparation routes and include grouped or external tests aligned with the intended axis of transfer. The studies in Table 3 illustrate different validation scopes: repeated CV and evaluation on additional cellulose-ester datasets were conducted within a single laboratory [20]; the bio-oil and SAF studies used held-out test sets but were based on laboratory-prepared model mixtures rather than authentic fuels [43,45]; the aviation-fuel study used a separate test set, although the property-specific datasets were relatively small [44]; and the soil study used prefecture-level holdouts, under which performance decreased for regional transfer in a geographically imbalanced dataset [46]. Table 3 summarizes the predicted properties, modeling approaches, and reported validation procedures and limitations, thereby indicating the applicability domains within which the reported results were established.

Table 3. Representative studies on physicochemical-property and material-attribute prediction.

Sample/ Matrix	Predicted Property	Modeling Approach	Validation and Limitations	Ref.
Cellulose acetate	Degree of substitution	Multiple linear regression	Repeated 8-fold CV (1000 runs) plus other cellulose-ester datasets; all data came from one laboratory	[20]
Bio-oil model mixtures	Unsaturation, effective H/C ratio, lower heating value, and C/H/O contents	SVR, PCA-SVR	CV and a test set were used; laboratory model mixtures only, with no authentic bio-oil validation	[43]

Table 3. *Cont.*

Sample/ Matrix	Predicted Property	Modeling Approach	Validation and Limitations	Ref.
Neat molecules, aviation fuels, and blends	Final boiling point, flash point, freezing point, density, and viscosity	NMF with Extra Trees and RF regression	68:12:20 split with held-out testing; property-specific datasets contained 31–72 samples	[44]
Sustainable aviation fuel mixtures	Flash point, H/C ratio, lower heating value, C and H content	PCA-assisted SVR, ANN, RF	CV and an independent test set; model mixtures only, without real-SAF validation	[45]
Japanese agricultural soils	Soil pH, mineralizable nitrogen, and K_2O	PLSR, RF, 1D-CNN	Random-CV and prefecture-level holdouts; some regional-holdout R^2 values were negative, and sampling was geographically imbalanced	[46]

4.4. Process-, Time-, and State-Dependent Prediction and Monitoring

In process-, time-, and state-dependent applications, the analytical target changes with reaction, treatment, storage, aging, or another controlled condition. The output may be a continuously varying concentration or yield, a process curve, elapsed-time class, or processing stage. These cases differ from static calibration because measurements are ordered or clustered within runs, specimens, products, or time series; random splitting of individual spectra can therefore leak trajectory- or specimen-specific information.

Syauqi et al. predicted carbon dioxide loading and monoethanolamine composition in carbon-capture solvents, providing a basis for process-relevant solvent analysis [47]. Zhang et al. quantified 3-nitro-1,2,4-triazol-5-one (NTO) during heating–cooling crystallization cycles using ATR-FTIR and multiple regression models [48], while Liu et al. used FT-IR features with RF and ANN models to predict food freeze-drying curves [49]. Time or ordered state was the analytical target in skeletal-muscle wound-age estimation [50]. Ma et al. classified the repeated steaming-and-drying stages of Polygonatum kingianum using parallel FT-NIR and ATR-FTIR deep-learning workflows; it is retained as a comparative multimodal example because ATR-FTIR was a direct model input, but its results should not be attributed to FT-IR alone [51]. Zaharulill et al. treated monthly ages of black gel inks measured for 12 months under three environmental conditions as classification targets [52]. At the most integrated level, Ashikari et al. generated mimicked reaction-mixture spectra by linearly combining pure-component spectra, trained a neural-network yield model, and coupled real-time inline FT-IR prediction to closed-loop optimization of a Suzuki–Miyaura reaction [53].

Validation across these studies was based mainly on CV or held-out testing. Extrapolative concentrations or levels excluded from calibration were additionally evaluated for carbon-capture solvent and NTO monitoring [47,48]. Experimental freeze-drying tests included nine market-sourced food types, although all measurements were conducted within a single laboratory and instrument setting [49]. Independent forensic cases or processing batches were not described for wound-age estimation and steaming-and-drying stage classification, respectively [50,51], while the data-splitting or CV procedure was not clearly reported for ink-age classification [52]. Predictions for prepared mixtures and 63 additional flow reactions were compared with GC measurements within a single Suzuki–Miyaura reaction system [53]. Table 4 brings together these applications, their prediction targets and modeling approaches, and the reported validation procedures and limitations, thereby indicating the scope within which the reported results were established.

Table 4. Representative studies on process-, time-, and state-dependent prediction and monitoring.

Sample/ Matrix	Prediction Target/Analytical Purpose	Modeling Approach	Validation and Limitations	Ref.
Carbon-capture solvent system	Quantification of CO_2 loading and monoethanolamine composition for solvent monitoring	LASSO-LARS, PLSR, SVR, RF, XGBoost, and AdaBoost	Held-out testing included 10 wt% MEA outside the training range; only prepared solutions, not real process samples, were evaluated	[47]
NTO in ethanol solution	Quantification of NTO during heating–cooling crystallization cycles	PLSR, SVR, RF, XGBoost, ANN, LightGBM	k-fold CV and three concentrations excluded from calibration; all samples came from one NTO/ethanol system	[48]
Liquid and semi-solid food samples	Prediction of pre-freezing, sublimation, and desorption temperatures and times	ANN, RF, KNN	Five-fold CV and experimental freeze-drying tests of nine market-sourced food types were performed; no independent-site or inter-instrument validation was reported	[49]
Skeletal muscle	Estimation of wound age under early postmortem interference	GA-Ridge, GA-Lasso, GA-PLS	CV and held-out testing were used; no independent specimen batch or forensic case validation was reported	[50]
Processed *Polygonatum kingianum*	Classification of stages across nine steaming-drying cycles	PCA, PLS-DA, OPLS-DA, ResNet	Separate train/test sets achieved 100% accuracy; reported results involved parallel FT-NIR and ATR-FTIR workflows, with no independent batch validation reported	[51]
Black gel inks	Classification of monthly ink age over 12 months	DA, SVM, KNN, DT	Multiple brands and environments were included, but split or CV procedures were unreported; replicate independence remains unclear	[52]
Flow reaction mixtures	Real-time yield prediction for closed-loop reaction optimization	Neural network with Bayesian optimization	Prepared mixtures and 63 additional reactions agreed with GC; all validation used one Suzuki–Miyaura reaction system	[53]

Overall, the studies in Tables 1–4 show that AI-assisted FT-IR is expanding from conventional multivariate calibration to composition-related screening, safety decisions, surrogate property measurement, and dynamic process monitoring. The categories are linked by a common requirement: performance must be demonstrated at the level of the intended analytical decision using independent samples, batches, regions, instruments, or process runs as appropriate. Model accuracy without such alignment can describe interpolation within a study-specific dataset but does not by itself establish reliable chemical sensing.

5. Explainable AI for Chemically Meaningful FT-IR Spectral Sensing

As AI-assisted FT-IR models move from proof-of-concept classification toward quantitative and decision-relevant sensing, interpretation becomes part of analytical validation. Although FT-IR bands are chemically assignable in principle, a fitted model may exploit direct analyte signals, correlated matrix variation, sample-presentation effects, preprocessing artifacts, or instrument-specific patterns. XAI can reveal which parts of a spectrum influence a prediction, but it cannot by itself determine why those regions covary with the analytical target. This section therefore considers both the capabilities and limitations of

XAI, representative FT-IR applications, and the additional evidence required to convert spectral attribution into chemically grounded interpretation. The conceptual workflow is summarized in Figure 3.

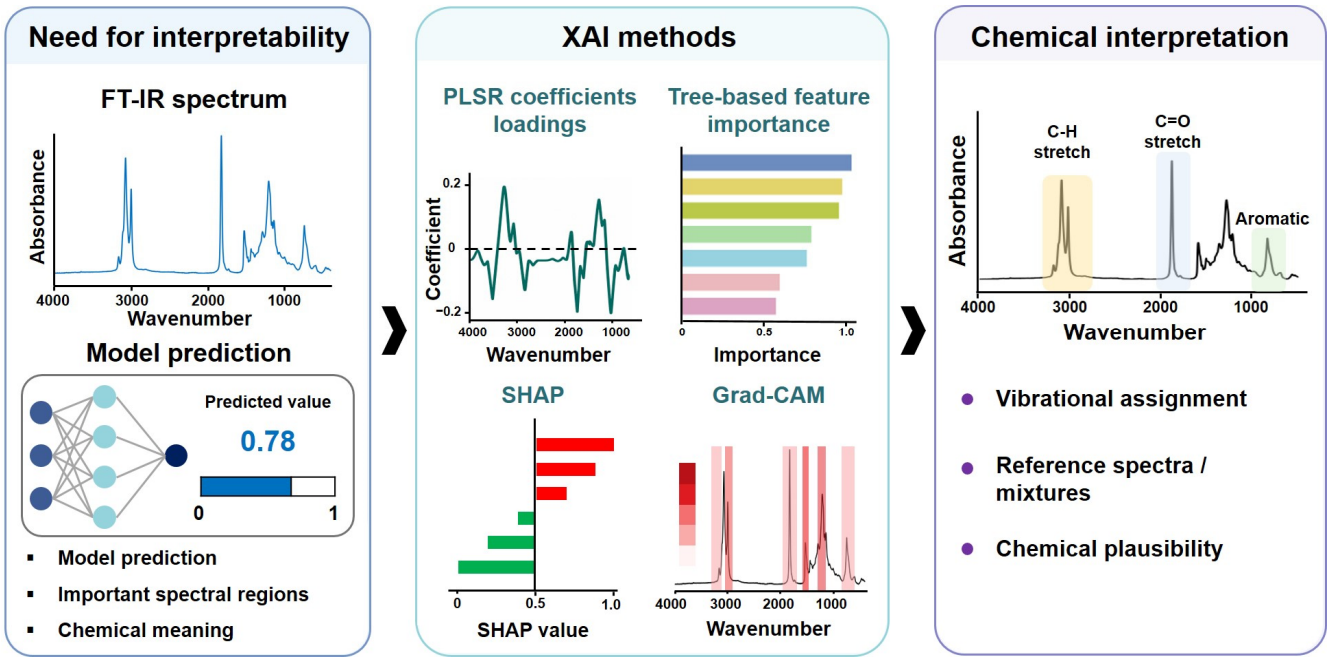


Figure 3. General workflow from model prediction and XAI-based spectral attribution to chemical interpretation in AI-assisted FT-IR spectral sensing.

5.1. Why Model Interpretation Is Analytically Necessary

High predictive performance does not establish that an FT-IR model has learned target-specific chemical information. In a regression task, a model may predict a concentration or material property from matrix features that covary with the target rather than from direct analyte bands. In classification, it may distinguish sample origin, preparation batch, measurement session, or another confounder instead of the intended chemical class. Such proxy relationships may support interpolation within the development dataset yet fail when sample populations or measurement conditions change.

Model interpretation has three complementary analytical roles: identifying possible proxy or artifact-driven predictions, assessing whether model-relevant regions agree with known vibrational information, and examining whether the learned spectral basis remains stable across samples and validation conditions. These roles require a clear distinction among model explanation, chemical interpretation, and causal evidence. An influential spectral region is evidence about the behavior of the fitted model; it becomes a chemically defensible marker only when supported by independent spectroscopic or experimental evidence.

5.2. XAI Methods for One-Dimensional Spectral Models

FT-IR model interpretation can draw on conventional chemometric outputs, model-specific importance measures, and post hoc XAI methods. Loadings, regression coefficients, scores, and variable-importance summaries can relate latent-variable models to spectral structure [8,9]. Tree ensembles provide split- or permutation-based importance measures, but attribution may be divided among strongly correlated neighboring variables and can change with the selected importance definition. These outputs should therefore be examined as model-dependent summaries rather than as direct band assignments.

Shapley additive explanations (SHAP) express an individual prediction relative to a reference output as additive feature contributions; aggregation across samples can provide class- or dataset-level summaries [54]. The result depends on the explainer, reference distribution, and treatment of feature dependence, which is especially important for highly correlated spectra. Gradient-weighted class activation mapping (Grad-CAM) weights convolutional feature maps using gradients of a target output and projects the resulting activation onto the input domain [55]. For a 1D-CNN, this procedure can highlight spectral intervals influencing a class score or regression output.

Because FT-IR spectra are ordered, continuous, and highly collinear, isolated wavenumber explanations can fragment a single vibrational band or redistribute importance among adjacent variables. Grouping neighboring variables into spectroscopically meaningful zones can produce more stable and interpretable summaries [16]. Reports should therefore specify the input representation and preprocessing, the explanation method and reference distribution, the level of spectral grouping, and whether the displayed result is local or aggregated.

5.3. Representative FT-IR Applications of SHAP and Grad-CAM

Recent studies illustrate several analytical uses of SHAP. In edible-oil classification, SHAP was used to compare spectral regions contributing to decisions from absorbance and second-derivative inputs [18]. In wheat-flour safety analysis, SHAP identified regions influencing DON level prediction [21], while a CNN–SHAP framework linked microplastic classifications to chemically relevant FT-IR regions [22]. XAI has also been used prospectively: Yan et al. identified polymer-specific fingerprint regions and used them to guide FT-IR data augmentation [17]. Thus, attribution can support model auditing, spectral interpretation, and chemically focused input design, although each use requires separate validation.

Grad-CAM has been adapted to both classification and regression with one-dimensional infrared spectra. For printing-paper origin classification, Grad-CAM-based data-point attribution mapped 1D-CNN decisions to ATR-IR regions associated with carbonyl and cellulose vibrations [56]. For multilayer composite plastic films, Grad-CAM identified regions influencing layer-thickness prediction and supported construction of a more compact FT-IR–1D-CNN regression model [57]. These studies demonstrate that convolutional activation maps can be projected onto the wavenumber axis, but the resulting regions still require testing beyond the dataset used to derive them.

The interpretation method should match both the predictive architecture and the analytical claim. Latent-variable outputs are natural for chemometric models, feature-importance measures for tree ensembles, SHAP for local or aggregated attribution across several model families, and Grad-CAM for convolutional representations. These outputs are not interchangeable: agreement among methods can increase confidence in a region, but disagreement may reflect different explanation targets or assumptions rather than an error in one method.

5.4. From Spectral Attribution to Chemically Grounded Interpretation

Feature attribution should not be equated with chemical identification or causality. A large SHAP value, regression coefficient, tree importance, or activation signal indicates that changing or using a spectral variable affects the model output under a particular explanation procedure. The signal may nevertheless represent a correlated matrix component, baseline structure, water contribution, scattering pattern, preprocessing effect, or instrument response rather than the target compound itself.

Chemically grounded interpretation should proceed at the band or region level. Model-relevant intervals should first be mapped to plausible vibrational assignments and checked

against the original and preprocessed spectra. The sign or direction of the contribution should then be evaluated for consistency with the analytical target. Explanation stability should be assessed across resampling, independent samples, preprocessing choices, and reasonable model alternatives. Finally, the proposed interpretation should be evaluated, where possible, against pure-component or reference spectra, controlled mixtures, spectral responses to controlled changes in target composition or measurement conditions, or an independently supported chemical mechanism [16,26,48].

XAI is therefore most valuable as a model-auditing and hypothesis-generating component of analytical validation. A defensible explanation should be chemically plausible, reproducible across validation conditions, and consistent with independent evidence; it should also reveal when a model relies on nonchemical or dataset-specific information. Broader requirements for representative validation, uncertainty assessment, robustness, and transferability are considered in the next section.

6. Current Challenges and Future Directions Toward Robust FT-IR Spectral Sensing

The studies reviewed above demonstrate the breadth of quantitative and predictive information that can be extracted from FT-IR spectra. Translation to routine analytical use, however, requires validation against the conditions and decisions for which the model is intended. The principal barriers are limited diversity among independent samples, leakage or mismatch in validation design, incomplete treatment of uncertainty, sensitivity to preprocessing and measurement variation, weak inter-instrument transfer, and overinterpretation of model attribution. These are method-level challenges and cannot be resolved by algorithmic complexity alone.

6.1. Data Representativeness, Validation, Uncertainty, and Spectral Augmentation

A major limitation of many AI-assisted FT-IR studies is the small number of genuinely independent analytical units. Repeated scans, technical replicates, spectral crops, and measurements from the same sample or batch can increase the number of spectra without increasing chemical diversity. If related spectra are divided across training and test sets, performance can be inflated by sample-specific or session-specific similarity. Controlled mixtures are valuable for calibration, but they may not represent authentic products, unknown adulterants, new raw-material sources, or realistic processing histories.

The validation design should match the claimed use. Sample-level splits estimate performance for new samples drawn from the represented population, whereas grouped splits by product, batch, region, preparation day, or instrument test more demanding axes of generalization. All target-informed preprocessing, variable selection, augmentation, and hyperparameter optimization must remain within the training workflow [30,31]. A final test set should remain untouched, and claims of external applicability should be based on genuinely independent samples that challenge the intended deployment boundary.

Uncertainty arises from spectral repeatability, sample presentation, reference measurements, calibration data, model fitting, and extrapolation beyond the represented domain. The magnitude and interdependence of these contributions vary with the matrix, sampling and acquisition procedure, reference method, model, and intended use; therefore, a numerical uncertainty budget should be constructed for each defined quantitative analytical method using representative replicate, reference, and validation data. Quantitative studies should therefore report RMSEP or MAE together with bias, calibration range, and the precision of the reference method, rather than relying mainly on correlation coefficients. Confidence or prediction intervals and applicability-domain checks are particularly im-

portant near regulatory or operational thresholds [32]. A model should flag, rather than silently quantify, samples that are insufficiently represented by its calibration domain.

Spectral augmentation can improve tolerance to plausible variation, but it should be applied only to model-development data and should preserve the chemistry and measurement physics of the original spectrum. Chemically focused augmentation has been guided by XAI-defined fingerprint regions [17], while physically motivated intensity, baseline, and scattering transformations have improved infrared classification in small datasets [58]. Luo et al. used a conditional generative model to augment plastic spectra from FT-IR, Raman, and laser-induced breakdown spectroscopy [59], and broader generative and augmentation strategies have been reviewed across spectroscopic modalities [60]. Nevertheless, improved internal accuracy after augmentation does not demonstrate external validity. Test samples should remain experimentally measured and unaugmented, and synthetic spectra should complement rather than replace independent chemical diversity. Where broader applicability is claimed, independent interlaboratory comparisons are also needed to determine whether the observed performance is reproducible beyond the development laboratory.

These methodological recommendations are grounded in established chemometric validation principles and recurring limitations identified across the reviewed literature, rather than in the performance of a single dataset. They should be regarded as evaluation criteria, not as universally sufficient conditions; their adequacy for a specific application must be demonstrated through validation that reflects the intended analytical use and relevant sources of variation, including representative independent samples when external applicability is claimed [30,31].

6.2. Spectral Variability, Preprocessing Robustness, Calibration Transfer, and Transfer Learning

FT-IR spectra combine chemical information with variation introduced by sampling and instrumentation. Baseline drift, atmospheric water and carbon dioxide, scattering, particle size, ATR contact and pressure, surface roughness, pathlength, temperature, resolution, wavenumber-axis registration, and detector response can all alter spectral patterns independently of the analytical target. Among these factors, temperature deserves particular attention because it can introduce systematic spectral variation unrelated to the analytical target [1]. Sample temperature should therefore be controlled where possible or otherwise recorded and considered when evaluating model robustness. A model developed under one combination of these conditions may therefore lose accuracy or acquire bias when transferred to another batch, accessory, instrument, or laboratory.

Preprocessing can reduce unwanted variation but can also suppress concentration-related intensity, amplify noise, shift model emphasis, or remove matrix information that is relevant to the target [11,21,60]. The complete pipeline and its parameters should be fitted or selected using development data and then fixed before external testing. Robustness should be assessed through sensitivity analyses across scientifically defensible preprocessing choices and through repeated measurements under realistic nuisance conditions. Stability of both predictive performance and model-relevant spectral regions is more informative than the single best result from extensive preprocessing optimization.

Calibration transfer addresses systematic differences between a model-development instrument and one or more receiving instruments. When paired spectra of common transfer standards are available, and the shift is mainly instrumental, standardization, direct or piecewise direct standardization, and slope and bias correction provide appropriate initial approaches and baselines for more flexible learning-based transfer [61].

Beyond these conventional procedures, transfer learning adapts learned representations or model parameters to a target domain. Retaining a pretrained feature extractor and retraining only the output layer may be suitable for closely related domains with

few labeled target spectra. Partial or full fine-tuning permits greater adaptation to matrix or instrumental differences but requires more labeled target data and careful regularization. Domain-adaptation methods may be useful when target spectra are available, but labels are limited, whereas parameter-efficient methods such as low-rank adaptation can reduce the retraining burden for large models [11,62]. Selection should therefore consider source–target similarity, the origin of the shift, and the availability of paired spectra and target labels. Each method should be compared with simple calibration-transfer baselines and evaluated using independent target-domain samples. Because comparative evidence remains limited for FT-IR, no strategy can currently be considered universally superior; the Raman application in [62] provides a methodological precedent rather than direct FT-IR evidence.

6.3. Chemical Interpretability, Standardized Reporting, and Practical Deployment

Model attribution does not by itself establish chemical causality. Chemometric coefficients, tree-based importance, SHAP, and Grad-CAM can identify influential regions, but the highlighted signal may originate from correlated matrix variation, preprocessing artifacts, water or atmospheric bands, or instrument-specific responses [16,18,21,22,54–57]. Interpretation should therefore remain explicitly linked to what the fitted model uses, rather than being presented as automatic compound identification.

Chemically meaningful interpretation should connect model-relevant bands or regions with known vibrational assignments, reference or pure-component spectra, controlled mixtures, and plausible chemical mechanisms. The direction and stability of the attribution should be tested across independent samples, validation folds, preprocessing strategies, and reasonable model alternatives. Explanations that are unstable, dominated by nonchemical regions, or inconsistent with the observed spectral change should be reported as evidence of model dependence rather than forced into a chemical narrative.

Transparent and standardized reporting is equally important. Studies should state the number of independent samples and technical replicates, sample and batch structure, acquisition conditions, excluded spectral regions, preprocessing sequence and parameters, model architecture or settings, data-partitioning unit, optimization procedure, and final validation design. Performance metrics should be accompanied by sample counts and, where feasible, variability estimates. Internal, external, and inter-instrument validation should be distinguished, as should statistical attribution and spectroscopic interpretation. Shared spectra, reference values, and analysis code would further improve reproducibility.

Practical deployment should begin with a defined analytical use. Screening models require sensitivity, specificity, and false-decision behavior near the relevant threshold; quantitative models require a calibrated range, bias and precision assessment, prediction uncertainty, and an applicability domain. Routine use also requires quality-control samples, monitoring of spectral and prediction drift, version control for preprocessing and models, predefined recalibration criteria, and a procedure for referring out-of-domain or ambiguous samples for confirmatory analysis. AI should support, rather than obscure, the analytical decision process.

Emerging approaches include multimodal learning, transformer spectral models, chemistry-informed augmentation, and parameter-efficient model transfer [11,15,17,60,62]. These approaches may reduce data requirements or improve portability, but their value should be demonstrated through comparison with suitable baselines and validation on new sample populations and measurement systems. A more complex representation is useful only when it improves the reliability or scope of the analytical method.

The future development of AI-assisted FT-IR spectral sensing should therefore be method-centered rather than model-centered. Representative data and claim-aligned

validation are needed to establish generalization; robust preprocessing and calibration-transfer strategies are needed to maintain performance across measurement conditions; and chemically grounded interpretation, uncertainty-aware decision rules, and transparent reporting are needed for defensible deployment. These three priorities are summarized in Figure 4 and provide a practical pathway from successful dataset modeling to reliable chemical sensing.

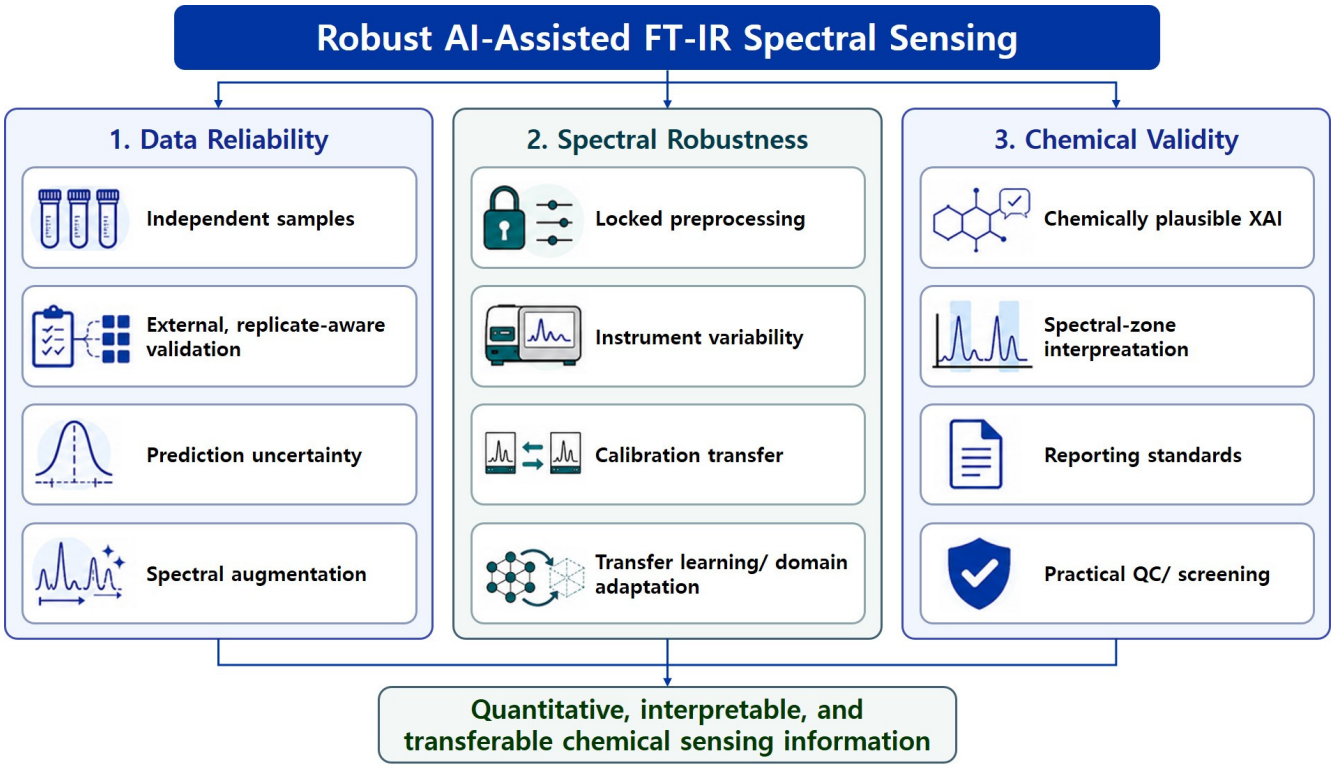


Figure 4. Major challenges and development priorities for robust AI-assisted FT-IR spectral sensing.

7. Conclusions

FT-IR spectroscopy is a rapid and accessible optical spectral sensing platform whose molecular fingerprints encode composition, intermolecular interactions, structural organization, and material state. AI extends this information from qualitative comparison to classification, quantitative calibration, property prediction, and dynamic monitoring. Across the representative studies reviewed here, these capabilities were organized by analytical function: composition-related screening and concentration prediction; adulteration, contamination, and safety assessment; physicochemical-property and material-attribute prediction; and process-, time-, and state-dependent prediction.

The central finding is that predictive performance alone is insufficient evidence of analytical reliability. Samples and data partitions must represent the intended use, technical replicates must remain within independent sample groups, and preprocessing and model optimization must be contained within a leakage-free validation workflow. Quantitative outputs should be interpreted with prediction error, bias, reference uncertainty, and the model's applicability domain, while claims of robustness or transferability should be demonstrated across relevant batches, populations, instruments, or laboratories. XAI can strengthen this evaluation by identifying the spectral basis of predictions, but attribution should be interpreted at the band or region level and should not be treated as proof of chemical causality.

Future progress should therefore be method-centered rather than model-centered. More complex architectures, synthetic spectra, pretrained models, and transfer-learning

strategies will be valuable only when they improve performance on genuinely new samples and under realistic measurement conditions. By combining representative sampling, transparent preprocessing, independent validation, uncertainty-aware prediction, robust calibration transfer, and chemically constrained interpretation, AI-assisted FT-IR can convert molecular fingerprints into quantitative, interpretable, and transferable chemical sensing information.

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Abbreviations

The following abbreviations are used in this manuscript:

AI	Artificial intelligence
ML	Machine learning
DL	Deep learning
FT-IR	Fourier-transform infrared spectroscopy
ATR	Attenuated total reflection
PCA	Principal component analysis
PLS-DA	Partial least-squares discriminant analysis
PCA-LDA	Principal component analysis–linear discriminant analysis
PLSR	Partial least-squares regression
SVM	Support vector machine
SVR	Support vector regression
RF	Random forest
RFR	Random forest regression
KNN	K-nearest neighbors
CNN	Convolutional neural network
1D-CNN	One-dimensional convolutional neural network
XAI	Explainable artificial intelligence
SHAP	Shapley additive explanations
Grad-CAM	Gradient-weighted class activation mapping
RMSEP	Root mean square error of prediction
SNV	Standard normal variate
MSC	Multiplicative scatter correction
ANN	Artificial neural network
DT	Decision tree
XGBoost	Extreme gradient boosting
MAE	Mean absolute error

GC–MS	Gas chromatography–mass spectrometry
CV	Cross-validation
LOOCV	Leave-one-out cross-validation
AFB1	Aflatoxin B1
DON	Deoxynivalenol
SAF	Sustainable aviation fuel
NMF	Non-negative matrix factorization
NTO	3-Nitro-1,2,4-triazol-5-one

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