ISSN: 3144-1890

Wissen PUBLICATION GROUP

Journal of
Advanced Physics and Interdisciplinary Science

Review Article

Volume: 1 | Issue: 1 | November 2026 | Pages 01–12

Beyond Chemical Fingerprinting: Raman Photonics, Molecular Spectroscopy and Explainable Artificial Intelligence for Palm Oil Authentication, Quality Assessment and Transferable Optical Sensing

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Submitted: 27 October 2026 **Accepted:** 02 November 2026 **Published:** 10 November 2026

Citation: Judijanto, L. (2026). Beyond Chemical Fingerprinting: Raman Photonics, Molecular Spectroscopy and Explainable Artificial Intelligence for Palm Oil Authentication, Quality Assessment and Transferable Optical Sensing. Journal of Advanced Physics and Interdisciplinary Science, 1(1), 01-12. DOI: doi.org/10.67927/jadvphysintersci/2026(1)110.

Abstract

Authenticity verification and quality control in palm oil increasingly require rapid, defensible measurements across heterogeneous supply chains. This critical qualitative literature review examines the molecular physics, analytical performance, and interpretability challenges associated with Raman photonics and complementary optical spectroscopies. Drawing on journal evidence published between 2020 and 2026, it distinguishes chemically grounded measurement from statistical identification that may depend on correlated pigments, processing conditions, or instrument characteristics. Recent handheld Raman studies demonstrate geographical discrimination of West African palm oils, while machine learning-assisted Raman analysis has reported promising prediction of peroxide, iodine, and acid values. However, high within-study accuracy does not establish causal provenance markers, robustness across refining states, or transferability to new instruments and regions. The review compares Raman, Fourier transform infrared, near-infrared, fluorescence, and multimodal approaches; critically evaluates spectral preprocessing, variable selection, explainable AI, calibration transfer, and uncertainty management; and proposes an evidence-gated framework for deployment. Key recommendations include chemically verified band assignments, hierarchical out-of-domain validation, metrological controls, prediction intervals, standardized acquisition metadata, and reference-laboratory confirmation of consequential decisions. The resulting framework positions explainable spectroscopy as a powerful screening and process-monitoring capability while maintaining clear boundaries between compositional inference, product authentication, geographic attribution, and certified sustainability traceability.

Keywords: Palm Oil Authenticity, Raman Spectroscopy, Molecular Photonics, Vibrational Spectroscopy, Explainable Artificial Intelligence, Chemometrics, Spectral Data Fusion, Calibration Transfer, Uncertainty Quantification, Quality Assurance.

Introduction

Background and Analytical Problem

Palm oil is simultaneously a major food ingredient, an industrial feedstock, and the object of increasing scrutiny concerning authenticity, safety, and supply-chain transparency. The resulting analytical problem is not a single classification task. A mill may need to know whether crude oil has deteriorated before refining; a trader may need to identify dilution with another edible oil; a regulator may need to test a label claim; and a buyer may ask whether an oil originated from a specified production zone. These decisions differ in reference standard, acceptable error, and evidentiary burden. A spectral signature that supports chemical similarity cannot automatically verify the ownership or history of a supply chain [1-3].

Conventional analytical chemistry provides indispensable reference measurements. Chromatographic profiling, titration, nuclear magnetic resonance, and other established laboratory techniques can quantify composition or specific quality markers, although the necessary reagents, operator expertise, preparation steps, and laboratory logistics restrict their usefulness for immediate decisions in geographically dispersed settings. Optical methods offer a different division of labor: fast measurements may help screen samples and prioritize confirmatory assays, while definitive enforcement or certification claims still require validated reference evidence. The principal challenge is therefore to construct a reliable bridge between optical observations, underlying molecular chemistry, and the decisions being made [4-7].

Raman spectroscopy is attractive because it probes changes in molecular polarizability associated with vibrational motion. It can be nondestructive, often requires limited sample preparation, and supports miniaturized instruments. Unlike a generic visual color assessment, an adequately resolved Raman spectrum contains information about specific molecular bonds and their local environment. Nevertheless, the scattering signal is intrinsically weak, and the final measurement is a joint outcome

of the sample, the excitation source, the optical collection system, detector response, fluorescence background, and acquisition protocol. Practical analytical validity consequently depends on both chemistry and photonic engineering [7-9].

Contemporary Evidence and Urgency

A particularly important empirical anchor is the 2025 investigation of 171 West African palm oil samples acquired from five countries using a handheld 1064 nm Raman instrument. Multivariate scores revealed geographical patterns, but the dominant first principal component was strongly linked to beta-carotene-associated signals. The result is genuinely promising for targeted screening, yet its most important scientific implication is also a warning: a geographic grouping can be mediated by pigment concentration, maturity, handling, or processing rather than by an exclusive marker of geographical origin. Verification of provenance thus requires sampling designs that intentionally separate these plausible alternatives [10-12].

A second anchor is the 2026 report of Raman-based prediction of crude palm oil peroxide and iodine values using 200 samples drawn from five Ghanaian markets. In that study, a genetic algorithm–random forest model achieved reported prediction correlations of 0.9831 for peroxide value and 0.9752 for iodine value. A separate 2025 Food Chemistry study investigated deep learning for acid-value estimation during thermal oxidation of palm oil. Both demonstrate that contemporary algorithms can capture useful multivariate associations, but neither finding removes the need to challenge new processing conditions, external reference methods, or instruments not represented in the original calibration [13-15].

Applications already extend beyond conventional composition. Surface-enhanced Raman scattering has been tested for acetamiprid residue detection in crude palm oil, while attenuated-total-reflectance infrared spectroscopy has been evaluated for adulteration with lard and with bleached used cooking oil. These examples reveal the breadth of possible target definitions and the potential danger of treating them as interchangeable. The same feature can be informative for one task and a nuisance variable for another: bleaching may reduce pigments, heating alters oxidation chemistry, and an impurity can change the baseline without uniquely identifying its source [16-19].

Research Gap, Aims and Contribution

The knowledge gap is not a lack of sophisticated classifiers. It is the absence of a sufficiently integrated framework for determining when a learned spectral relation is molecularly defensible, transferable to a new domain, and reliable enough for a stated operational use. Reviews of edible-oil authentication and spectroscopy show rapid methodological growth, while research on explainable machine learning and calibration transfer warns that a persuasive feature map or high held-out score is not sufficient evidence of robustness. This article connects those literatures to the concrete physical and chemical challenges of crude and refined palm oil. Recent methodological research additionally demonstrates that repeated-measurement leakage and model-selection leakage can create overly optimistic reported performance, making independent test units a substantive requirement rather than an optional reporting convention [5,20-24].

The review addresses seven linked questions: the physical origin of informative Raman features; the effects of pigments and deterioration on those features; the strength of contemporary evidence for quality and provenance tasks; the confounding caused by instruments and sample structure; the value and limitations of explainable AI; the requirements for external validation and uncertainty-aware calibration; and the role of complementary sensing. Its contribution is a proposed evidence-gated optical quality-assurance pathway that distinguishes proof-of-concept, laboratory validation, field validation, and decision-readiness. It neither reports new measurements nor presents a novel calibrated product as already demonstrated [10,13,15,25].

Literature Review

Molecular Photonics: Inelastic Scattering and Spectral Resolution

Raman scattering arises when incident photons exchange energy with molecular vibrational modes. Most scattered photons undergo elastic Rayleigh scattering, whereas the smaller inelastic fraction acquires a shifted frequency. In the Stokes process, the scattered photon has lower energy because vibrational energy is deposited in the molecule; in anti-Stokes scattering, thermally populated vibrational states can transfer energy to the scattered photon. For incident and scattered wavelengths, λ_0 and λ_s, respectively, the conventional signed Raman shift is defined by Equation (1), with both wavelengths expressed in nanometers. This shift is principally determined by molecular structure rather than by the laser wavelength, while the observed intensity is strongly instrument-dependent [7-9].

$$\Delta\tilde{\nu} = 10^7 \times (1/\lambda_0 - 1/\lambda_s)\ \mathrm{cm}^{-1} \quad (1)$$

For Stokes scattering, λ_s exceeds λ_0 and Equation (1) yields a positive Raman shift; the sign is reversed for anti-Stokes scattering. The spectral shift locates molecular vibrational features, whereas intensity additionally depends on concentration, optical collection efficiency, and sample-dependent background [7,10].

A vibrational mode is Raman-active when motion along its normal coordinate changes the molecular polarizability tensor. In simplified form, the scattered intensity depends on concentration, excitation power, collection efficiency, and the squared polarizability derivative for the relevant mode; it is not a direct universal measure of analyte concentration. Resonance enhancement, polarization, absorption, temperature, optical path length, and intermolecular interactions may change relative peak intensities. Consequently, a peak assignment should describe a plausible mode and measurement context instead of asserting that a single narrow wavenumber unambiguously represents an entire compound class [7,12,26]. Practical detection also involves spectral resolution and sampling physics. Lower-resolution portable devices can merge nearby vibrational bands; noise suppression may alter weak features; and strong fluorescence backgrounds may exceed the magnitude of useful Raman scattering. Excitation wavelength therefore introduces a meaningful tradeoff: near-infrared excitation often helps suppress fluorescence relative to shorter wavelengths, yet Raman efficiency and detector sensitivity may change. Handheld configurations further depend on vial geometry, sample homogeneity, and temperature. The 2025 West African study heated samples to approximately 50 °C and used 1064 nm excitation, emphasizing that even an on-site-oriented method may require explicit sample conditioning [4,9,10].

The physically meaningful Raman spectrum should be separated from a visualization of an idealized spectrum. Baseline subtraction, normalization, derivative transforms, and smoothing may increase modeling convenience, but these operations are not neutral with respect to band shape, noise correlation, or chemical interpretability. Aggressive second derivatives can sharpen overlaps while amplifying noise; normalization can reduce concentration-linked total intensity; and an inaccurate baseline model can create artifactual shoulders. A scientifically auditable workflow retains raw spectra, records preprocessing, and tests whether claimed diagnostic bands survive plausible alternative analytical treatments [8,13,20]. Figure 1 summarizes the Raman energy-transfer principle and the principal spectral regions discussed in palm oil studies. These positions are illustrative rather than universal constants: lipid composition, laser wavelength, spectral resolution, pigment resonance, and sample conditioning can alter the observed features. The correct interpretation is therefore band-centered and experimentally calibrated, not a deterministic lookup table of isolated peaks [4,11,13].

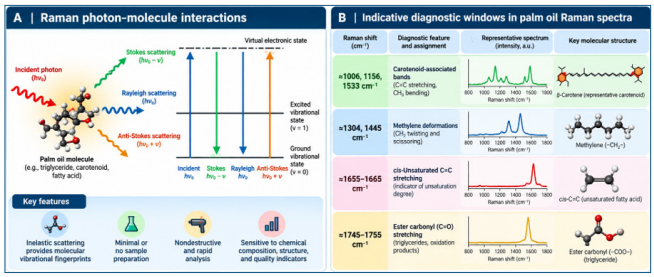


Figure 1: Conceptual Raman Interactions and Selected Palm-Oil-Relevant Spectral Regions; Not an Experimental Spectrum.

The energy-level schematic depicts the difference between elastic and inelastic scattering, while the adjacent list identifies commonly discussed carotenoid, methylene, unsaturation, and ester-associated regions. These assignments direct attention toward chemically plausible mechanisms but do not themselves demonstrate that a measured change originates from geographical provenance, hydroperoxide formation, or adulteration. Independent reference chemistry is necessary to test those more specific claims.

Palm Oil Chemistry and Target-Specific Authenticity Claims

Palm oil consists largely of triacylglycerols whose acyl chains differ in length and unsaturation, with variable minor constituents including carotenoids, tocopherols, tocotrienols, and other compounds depending on the product stream. Crude palm oil, refined bleached deodorized palm oil, palm olein, and palm stearin cannot be treated as a spectrally homogeneous matrix. Fractionation redistributes acyl-chain populations; refining can eliminate or reduce pigments; and thermal exposure modifies minor constituents and oxidation state. A robust analytical domain must specify product stream, composition range, and treatment history before model training begins [1,5,6]. Common palm oil Raman regions include skeletal carbon–carbon vibrations, methylene deformations around the 1300–1450 cm^{-1} region, cis-carbon–carbon double bond stretching near 1660 cm^{-1}, and ester carbonyl stretching around 1750 cm^{-1}. Carotenoid-associated features near approximately 1006, 1156, and 1533 cm^{-1} can be especially influential in crude oil. These positions are useful chemical cues, but overlapping vibrational contributions and changing optical response prevent a simplistic one-band–one-property rule. The value of an assignment increases when it co-varies with a chemically independent reference measurement under controlled sample conditions [10,12,27,28].

The iodine value expresses an operational measure of unsaturation, traditionally obtained through a chemical reference procedure. Changes in cis-unsaturation-related Raman features can therefore support an interpretable calibration, especially when a model is constructed and tested across deliberately varied fatty acid compositions. In contrast, peroxide value quantifies primary oxidation products using a specified reference assay, and a bulk carbonyl band is not uniquely a hydroperoxide band because native triacylglycerol esters already contain strong carbonyl functionality. Interpreting a carbonyl-region predictor as direct peroxide detection without controls risks overstating molecular specificity [13,27-29]. Acid value and free fatty acid content are related but distinct quantities defined through analytical procedures. Hydrolysis, heating, oxidation, and sample storage can affect their associations with spectral signals. During thermal oxidation, a regression model might perform well because several degradation-related changes occur together, not because its selected peak uniquely measures one target. The acid-value work by Liang and colleagues provides an important demonstration of task-specific prediction, while broader studies on thermally oxidized edible oils suggest that Raman–infrared combinations can provide complementary information about chemical changes [14,28,29].

Geographical authenticity poses an additional inferential challenge. Carotenoid content may correlate with harvest maturity, genotype, extraction practice, storage, or processing intensity, all of which vary within and across origins. Therefore, the discovery of reproducible geographic clusters in an observational sample set does not identify geographic causation. The relevant validation question is whether the origin signal remains after matching or stratifying samples by maturity, refining status, storage exposure, and pigment concentration. That task is more demanding than showing that previously sampled regions occupy distinct locations in a principal-component plot [3,10,11,].

Optical Modalities as Complementary Measurements

Fourier transform infrared and Raman spectroscopy both interrogate molecular vibrations but obey different intensity-selection rules. Infrared absorption is associated with a changing dipole moment, while Raman scattering requires a changing polarizability. The techniques therefore provide overlapping but nonidentical information on lipid functional groups. Attenuated-total-reflectance FTIR offers convenient sample contact measurements, whereas Raman can be especially useful for particular conjugated structures and handheld interrogation. Neither modality has a universal advantage across all palm oil products, instruments, contaminants, or target concentrations [5,6,28]. Near-infrared methods primarily exploit higher-order vibrational overtones and combination bands. These broad, overlapping responses usually require multivariate calibration but can be attractive where rapid, mature, commercially supported process sensors already exist. Studies involving peanut oil demonstrate how NIR models can estimate acid and peroxide-related reference properties, but transferring those reported errors directly to crude palm oil would be unjustified because the matrix, target ranges, and validation conditions differ. Selection between Raman and NIR should be driven

by actual cross-sample performance, throughput, cleaning requirements, and the final application [5,15,29].

Fluorescence may be an interference term in Raman acquisition and a useful analytical modality when measured intentionally. Pigment-sensitive fluorescence, UV–visible absorption, and excitation–emission data can provide complementary information that assists fraud screening or compositional analysis. However, color-bearing signals may be less transferable across bleaching, lighting conditions, and storage than structural lipid features. A fused sensor may improve calibration within a trial while becoming more sensitive to differences between field instruments or processing conditions. The joint model must consequently be challenged with precisely the same external domains as its individual components [25,30,31].

Surface-enhanced Raman scattering addresses low analyte sensitivity through electromagnetic enhancement near suitable nanostructures. Palm oil residue research indicates potential for detecting selected contaminants, but SERS measurements introduce substrate variability, adsorption selectivity, enhancement hot spots, and substrate-lot effects. Such devices may eventually complement bulk lipid characterization rather than replace it: a chemically targeted contaminant sensor and a bulk authenticity classifier solve different problems. Reference concentrations, matrix recovery, standard addition, and sensor stability must be established before field deployment [7,16,22].

Chemometrics, Explainable Artificial Intelligence and Generalization

Chemometric modeling begins with an explicitly defined response variable. Principal component analysis is exploratory and captures directions of variation in the spectra, whereas partial least squares regression relates spectra to quantitative references. PLS discriminant analysis, support vector machines, random forests, and deep neural networks can estimate classes or numerical values, but increasing complexity does not automatically confer chemical validity. Edible-oil studies show that supervised algorithms may outperform simple unsupervised separation on their chosen test sets; the relevant question is whether the extra apparent performance persists on new independent lots and devices [9,32-34]. Explainable AI is often proposed as a solution to black-box modeling. SHAP, spectral masking, surrogate models, and gradient-based attribution can rank the parts of a spectrum associated with a prediction. For optical sensing, a useful interpretation must be checked at the spectral-band level and connected to reference chemistry. Adjacent Raman variables are strongly correlated, so a method may assign the same physical contribution to different neighboring wavenumbers after minor preprocessing changes. The correct goal is not merely an attractive attribution heatmap but a stable and experimentally falsifiable chemical explanation [20,35-37].

Transferability is a separate issue from interpretability. A model may emphasize chemically plausible bands yet perform poorly when detector response, laser wavelength, probe geometry, sample temperature, or product stream changes. Conversely, a highly transferable model could exploit reliable but indirect correlations without proving a unique physical mechanism. Reviews on calibration transfer distinguish correction of measurement shifts from more difficult changes in the underlying chemical or label relationships. Instrument standardization can reduce some sources of variation, but it cannot recover an authenticity marker whose relationship to origin disappears in a new production system [15,21,38]. Recent applications of explainability in agricultural materials, optical emission, and biomedical spectral imaging provide methodological analogs. Cottonseed cultivar work illustrates the use of Raman with interpretable learning, while studies in pollen scattering, wine-grape spectroscopy, and imaging demonstrate feature attribution across diverse optical data. These papers show that explanations can be generated and interrogated; they do not constitute direct evidence that any particular attribution is valid for palm oil. The applicability of such methods should be tested against palm-specific molecular assignments and confounders [31,36,39,40].

Spectral processing advances also include compressed representations, deep architectures, and fused sensor features. Such approaches can be beneficial where physical modes overlap or signals are weak, as illustrated in other food matrices and spectral domains. Nevertheless, the apparent benefit of a pretrained network, latent representation, or augmented dataset must be measured against a transparent PLS baseline using identical external test units. An informative comparison controls for acquisition cost and model maintenance, not only prediction accuracy. This prevents complexity from masquerading as improved scientific understanding [41-44].

Methodology: Critical Qualitative Literature Review

Research Design and Evidence Boundaries

This article uses a critical qualitative literature review (QLR), not a systematic literature review, evidence meta-analysis, bibliometric census, or experimental validation study. Its purpose is analytical interpretation: to examine the internal consistency of claims, relate observed spectral features to molecular physics, compare competing explanations, and synthesize requirements for trustworthy deployment. No PRISMA flow, exhaustive count of database records, pooled detection limit, or universal ranking of technologies is claimed. This distinction is especially important because the published studies differ markedly in oil matrices, sampling systems, instruments, metrics, and target properties [5,8,20]. The review considers peer-reviewed journal work published from January 2020 through October 2026, supplemented by general theoretical relationships that do not require historical source expansion. The concept-driven literature mapping covers palm oil quality and authenticity, Raman and infrared photonics, portable spectroscopy, spectral data fusion, explainable AI, metrology, and calibration transfer. Direct palm oil results receive first attention; closely related edible-oil studies illustrate transfer hypotheses; and papers from agricultural or biomedical spectroscopy inform method design without being mischaracterized as palm oil experiments [10,13,22,25].

Source Appraisal and Qualitative Coding

Each selected article was interpreted using a common set of questions: what product matrix was measured; whether samples were crude, refined, oxidized, blended, or otherwise manipulated; how the analyte or class was defined; which spectral acquisition and preprocessing choices were used; what the underlying chemical mechanism could plausibly be; and how the prediction was validated. The review gives explicit attention to the unit of independence, distinguishing replicate spectra from separate vials, physical samples, production lots, locations, acquisition dates, instruments, and laboratories [10,13,15].

Evidence was organized into three tiers. Tier A consists of direct palm oil measurements with accessible methodological details and references to analytical targets. Tier B contains studies involving other edible oils or comparable optical and chemometric operations; it supports methodological plausibility but cannot establish the numerical performance of palm oil models. Tier C contains broader photonics, explainable learning, data fusion, and calibration-transfer studies; it informs design principles and testable propositions. This tier system is an interpretive guide, not a numerical quality score or a claim to formal risk-of-bias assessment [20,21,28,33].

Thematic coding focused on five linked domains: molecular band specificity; confounding from matrix and acquisition; model construction and explanation; independent validation and calibration stability; and intended industrial decision. Findings were treated as convergent when multiple sources supported a common principle with different methods, and as unresolved when explanations or validation settings were insufficient. In particular, the review rejects direct comparison of numerical correlations or accuracy values across studies whose target ranges, sample independence, reference procedures, or prevalence differ. The appraisal also treated longitudinal sample aging, spectral acquisition campaign, and batch-level independence as separate sources of heterogeneity because these variations can determine whether a spectral calibration generalizes beyond its development set [13,15,24,27,30,45].

A qualitative synthesis cannot determine pooled diagnostic sensitivity, economic return, or real-world environmental impact from heterogeneous published reports. Nor can it test whether a particular causal diagram accurately describes every palm oil source. The proposed framework is therefore formulated as a research and validation agenda, supported by literature-derived considerations rather than by new experimental proof. Source papers reporting excellent performance are described using their own measured setting, while statements about cross-country utility, universal traceability, and continuous process monitoring are explicitly conditional [3,10,21]. Interpretive bias was reduced by seeking discrepant evidence and highlighting tests that might disconfirm appealing hypotheses. For example, a carotenoid origin proxy must be challenged using matched carotenoid distributions, a peroxide predictor must be tested against oxidation pathways and interfering esters, and a fusion system must be compared with simpler single-sensor models under domain shift. These counterfactual checks are central to the article because they convert a narrative review from descriptive enthusiasm into a critical evaluation of how scientific claims might fail [10,18,25,28].

Results: Thematic Findings from the Literature

Raman Evidence for Palm Oil Identity and Provenance

The strongest immediately relevant geographical result is the handheld Raman study by Stradling and colleagues. It included samples from Ghana, Côte d'Ivoire, Liberia, Sierra Leone, and Togo, with repeated spectral acquisition and subsequent multivariate exploration. Important carotenoid-related signals occurred near 1006, 1156, and 1533 cm^{-1}, and the primary principal-component direction was dominated by pigment differences. A beta-carotene calibration constructed in a coconut-oil matrix showed strong predictive statistics for that prepared calibration. What the study most securely establishes is that the sampled oils were spectrally distinguishable in the tested setting, not that pigment differences are exclusive geographic labels [10,12]. A related fresh-fruit Raman study associated carotenoid-sensitive vibrational structure with ripeness classification. That result matters for finished-oil provenance because it supplies a plausible alternative pathway through which geographically clustered oils might appear different: harvesting practices and fruit maturity can affect pigments before extraction. The same molecular signal could therefore reflect an agronomic process rather than geographic location itself. Studies designed to infer geographic origin should include harvest maturity or its proxies as explicit nuisance factors and should compare origins under balanced maturity and refining conditions [10,11].

Authentication need not always involve country of origin. A portable Raman investigation directly assessed palm oil as an adulterant in other edible oils, demonstrating an application to mixture recognition. Such a task is conceptually easier to define than traceability because composition can be manipulated in known blending ratios and compared with prepared standards. Nonetheless, the relevant detection threshold depends on matrix similarity, instrument noise, adulterant concentration, and the held-out brands or samples. Findings from spiked mixtures should not be assumed to capture complex commercial fraud involving bleaching, deodorization, or unknown multiple adulterants [33,34,46]. Infrared studies further clarify the difference between identifying an adulterant and reconstructing a complete product history. A 2026 study investigated lard in palm oil exposed to controlled heating, while another examined bleached used oil blended into fresh palm cooking oil. These reports demonstrate the feasibility of targeted classification and concentration estimation for defined laboratory mixtures. Their results should be understood in the context of imposed adulteration mechanisms, reference labels, and sample treatment. Extension to unknown industrial blends will require wider negative controls and prospective performance assessment [17-19].

Quality-Index Prediction and the Chemistry of Interpretation

The 2026 Raman quality study reported an optimized genetic algorithm–random forest combination for peroxide and iodine value prediction using 200 samples from five Ghanaian markets. Reported prediction correlation coefficients approached 0.98 for both targets, and the authors identified features related to unsaturation and oxidation. These findings provide compelling within-study analytical evidence. Nevertheless, predictive accuracy is conditional on the concentration range and reference variability of the tested dataset; an RPD or correlation coefficient cannot be transferred numerically to a different sampling frame without a corresponding evaluation [13,15]. The most chemically plausible portion of iodine-value prediction is the association between unsaturation and vibrational features, especially cis-C=C stretching and related modes. Portable Raman experiments with mixed edible oils support the general concept that iodine value can be estimated using spectral calibration. Still, natural fatty-acid distributions, refining fractions, and oxidation history can change the mapping between specific spectral bands and chemically measured iodine value. A useful model should perform beyond a narrow set of recipes or regional samples and report absolute error in the original reference units [13,27,28].

Peroxide-value prediction warrants more cautious assignment. The ester carbonyl band of native triacylglycerols is already

strong, and secondary oxidation chemistry can modify spectral profiles in ways not exclusive to hydroperoxides. Accordingly, when selected features lie around 1748–1840 cm^{-1}, they should be described as predictive carbonyl-region information unless independent evidence demonstrates direct molecular specificity for primary oxidation products. A suitable falsification experiment would vary oxidation and hydrolysis separately, quantify reference peroxide and acid values, and test whether a learned predictor can distinguish their joint and independent effects [13,28,29]. The 2025 palm-oil acid-value study investigated thermal oxidation with deep learning, making it a useful complement to the simultaneous peroxide/iodine work. Deep networks may capture nonlinear features that linear PLS models miss, but there is no guarantee that the extra fitted structure reflects a single analyte. A comparison should therefore report performance under new heating protocols, unobserved oil batches, and independent acid-value assays. Explanations can help generate mechanistic hypotheses only when they remain consistent across preprocessing alternatives and with the chemically plausible response of hydrolysis and oxidation [14,20,42].

Other edible-oil studies reinforce the potential but emphasize conditionality. Raman and machine learning have classified market oils and estimated adulteration; a handheld Raman study assessed iodine value; an NIR peanut-oil study predicted acid and peroxide values; and handheld Raman work examined saponification value. These results show that fast optical estimation is not confined to a single laboratory task. The numbers cannot be pooled because oil matrices, reference methods, modeling structures, and sample ranges differ. Their legitimate contribution is to suggest feasible methodological options for rigorous palm-specific benchmarking. An independently published reference resource involving 19 naturally aged edible-oil types and repeated multi-instrument measurement campaigns offers a particularly relevant basis for future validation experiments, although its results are not a substitute for palm-specific external testing [29,32,33,45,47].

Data Preprocessing, Feature Selection and Interpretable Modeling

The published palm quality models illustrate the strengths and hazards of variable selection. Competitive adaptive reweighted sampling, genetic algorithms, and other procedures can reduce the dimensionality of a correlated spectral space, making regression more efficient. However, selecting features using data later treated as an independent test would invalidate the test. All feature selection, baseline optimization, spectral normalization parameters, and hyperparameter tuning must be fitted within training folds. Only a genuinely untouched, grouped external dataset can provide a credible estimate of performance in a new decision environment. A recent examination of chemometric validation specifically identifies leakage from repeated observations and hyperparameter or variable selection as routes by which apparent predictive ability may be inflated [9,13,15,23,24]. The possibility of nonchemical shortcuts is particularly important in geographical analysis. If each country is represented by distinct processing practices, bottle conditions, or measurement sessions, a classifier may accurately predict the country for the wrong reason. Likewise, replicate spectra from a single physical sample are correlated observations and cannot safely be distributed across both training and testing sets to create artificial independence. Random splitting at the spectrum level is therefore inappropriate when the deployed use involves new samples, lots, sites, instruments, or seasons. The analysis unit should match the intended use [10,15,21].

Contemporary XAI provides a practical starting point for interrogating such models. Reviews of spectroscopy-specific XAI describe SHAP, masking, and surrogate approaches, while examples in cottonseed classification and limited spectral datasets show how attributions can be calculated and visualized. Yet an attribution plot describes model behavior, not the ground-truth identity of a molecule. High correlation among neighboring wavelengths can redistribute importance across a band, and baseline artifacts can become salient predictors. Explanation faithfulness should be assessed through grouped-band perturbation, alternate preprocessing, and independent chemical confirmation [20,35,36]. Applications outside palm oil illuminate the same methodological risk. Optical emission spectroscopy studies have visualized features used by neural models to estimate conductivity or volatile compounds, while mass-spectrometry imaging has explored localized Shapley-based biomarker discovery. These are relevant analogs for identifying instrument and context effects, although their optical physics and matrices differ from palm oil. A defensible Raman framework should borrow the testing philosophy, not the physical assignments. Similarly, interpretable optical models for chromophores support the value of connecting attribution patterns to established photophysics rather than trusting statistical saliency alone [26,37,48,49].

A key thematic finding is that physically constrained models need not be fully mechanistic to improve scientific credibility. Restricting candidate predictors to preregistered spectral bands, penalizing unstable attributions, and comparing with measured fatty-acid or carotenoid data can make the fitted relation easier to evaluate. These strategies should be compared with unrestricted baselines on external tests, since an overly restrictive model could miss real interactions or degrade precision. The scientific outcome is an empirical tradeoff between accuracy, interpretability, stability, and error under distribution shift, not a single maximal accuracy score [9,20,39,50].

Multimodal Sensing and Industrial Feasibility

Evidence from edible oils shows that fused infrared and Raman inputs can support analysis of chemical quality during thermal oxidation, while broader food studies compare fusion at raw-feature, selected-feature, and decision levels. A multimodal sensor may reveal chemistry that is partly invisible to a single channel, particularly if the modalities respond differently to polar functional groups, unsaturation, or fluorescence-active compounds. However, data fusion also increases acquisition complexity and creates new opportunities for model leakage when preprocessing and data selection are not nested properly [25,28,30]. Investigations involving thermally treated food matrices, contamination analysis, and machine learning-assisted spectroscopy provide examples of handling complex overlapping signals. Pork-batter Raman modeling, NIR/Raman fusion for chicken-mince quality, and optical sensor fusion for heavy metals demonstrate the technical breadth of multivariate signal integration. These are Tier B or C methodological analogs, not empirical evidence for crude palm oil performance. Their relevance lies in how they motivate reference assays, intervention controls, and cross-condition validation for challenging food matrices [42,43,51].

Portable instruments introduce a useful but nontrivial operational tradeoff. A handheld device can reduce the delay between sample collection and screening, but its lower signal-to-noise ratio, temperature dependence, calibration stability, and user handling can materially influence performance. A laboratory reference method remains necessary at least for initial calibration, independent validation, and periodic drift checks. Economic usefulness depends on avoided laboratory tests and faster decisions, balanced against instrument maintenance, calibration samples, personnel training, rejected or uncertain scans, and the cost of false alarms [4,10,21]. The evidence also distinguishes portability from autonomous traceability. A portable spectrum can report chemical similarity or a probability of belonging to a defined reference class; it cannot independently establish land ownership, certified conservation compliance, absence of deforestation, or the integrity of every intermediary transaction. Such claims require documentary traceability, governance, and potentially other information systems. The strongest immediate contribution of optical analysis is thus an independently auditable quality and fraud-screening layer embedded within, rather than substituted for, broader supply-chain assurance [1,3,4].

Figure 2 presents the most consequential synthesis of the empirical literature: a measured spectrum depends jointly on composition, origin-associated factors, processing history, and instrument context. It explains why a classifier that works on a geographically structured dataset could fail when refining, temperature, or acquisition conditions change. The arrows are a conceptual causal hypothesis to be challenged experimentally, not a fitted causal model or quantitative evidence of particular effect sizes [10,17,21].

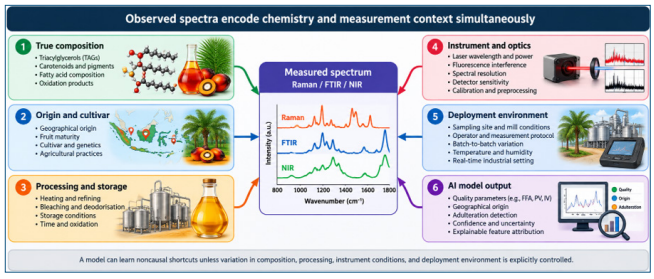


Figure 2: Conceptual Sources of Causal and Noncausal Variation in Observed Optical Spectra and AI Predictions.

The model-output node receives its information through the observed spectrum, but a spectrum is not a pure readout of geographic location. Oil chemistry, storage, processing, and device response may all shape measured intensity and band structure. A study seeking stable geographic classification should therefore cross or balance origin with these other factors, while an industrial quality model should measure whether the target remains identifiable after nuisance variables are varied.

Discussion and Analysis

Interpreting Spectral Accuracy as Scientific Evidence

The first research question concerns the role of photon scattering and lipid vibrations in making palm oil measurable. The evidence supports the presence of chemically plausible Raman information about pigments, acyl-chain structure, and certain quality-related changes. Yet the existence of a measurable molecular vibration is not equivalent to a validated assay for a chosen quality index. Spectroscopy measures an optical response, whereas the target may be an operational reference quantity derived by titration or chromatography. A defensible calibration must explicitly demonstrate that the optical relation remains stable over the plausible sources of sample variation [7,10,13,27]. A second distinction concerns authentication versus quality. An authentic sample may have deteriorated through oxidation or hydrolysis, while a chemically fresh sample may be adulterated or incorrectly labeled. Conversely, an oil whose pigments match a geographical reference class need not actually come from that region. Each inferential claim requires a separate target, validation design, and policy decision threshold. Reporting one generic authenticity score obscures these differences and creates the risk that users will interpret a correlational classification output as legal evidence of origin or sustainability [2,3,5].

The 2025 pigment-centered geographic result is especially informative because it is a concrete, falsifiable scientific hypothesis. If beta-carotene intensity principally drives apparent origin groups, experiments can remove, equalize, or independently measure carotenoid differences and determine whether origin discrimination survives. A matched study should compare crude and refined streams, oils with similar carotenoid concentrations from different origins, and multiple harvest seasons. Results could support pigment-informed screening under specific market conditions while demonstrating that the marker is not universally transferable. Both outcomes would advance knowledge more than another unchallenged accuracy report [10-12]. For iodine and peroxide values, orthogonal reference assays offer a similar falsification strategy. Manipulating unsaturation independently of oxidation should reveal whether a model truly differentiates target-related chemistry. Controlled oxidation series should quantify primary peroxides, secondary carbonyl products, acid value, and loss of unsaturation over time, rather than using thermal treatment as an unobserved proxy for all degradation. Such experiments would clarify why a model succeeds, the limits of its calibration, and the conditions under which its selected band assignments should be revised [13,14,28,29].

Conditions for Faithful Explainable Artificial Intelligence

Explainability should be assessed at three levels: descriptive, mechanistic, and interventionally robust. Descriptive attribution indicates which spectral variables influence a fitted output. Mechanistic interpretation offers a physically justified hypothesis linking those variables with molecular bonds, constituents, or instrumental effects. Interventionally robust explanation requires that the hypothesized relation respond appropriately when concentration, chemical state, or nuisance conditions are intentionally changed. Most off-the-shelf feature attribution addresses only the first level. Conflating these three levels makes models appear scientifically more settled than they are [20,26,35,36]. A good explanation protocol would define a limited set of plausible band families in advance, report the sensitivity of attribution to adjacent-wavenumber grouping, and compare at least two explanation methods with different assumptions. Band-level permutation or masking should not create physically impossible spectra without a caveat; where feasible, actual mixture or chemical-perturbation experiments should be preferred. Model explanations must also be tested across calibration folds, held-out sites, and instruments. A feature that repeatedly disappears or changes sign under small benign changes has limited value as a transferable chemical interpretation [20,31,37,39].

It is helpful to treat instrumental artifacts as candidate explanatory variables rather than as invisible measurement noise. Baseline slopes, saturated fluorescence, focal errors, laser-power drift, and sample-container effects can generate systematic patterns learned by flexible algorithms. The proposed solution is not necessarily to remove every nuisance factor from the training data; it is to measure them, deliberately vary them, and ask whether the model is invariant to changes irrelevant to its target. Spectroscopy-based XAI therefore becomes most scientifically useful when embedded in a metrological experiment with clearly specified controls [38,21,48,49]. Prediction stability should be evaluated using both physically constrained baselines and more flexible models. A band-restricted PLS model could be easier to audit than a deep convolutional network, but it may fail if important broad spectral interactions are neglected. Conversely, a neural network might outperform simpler models within a development dataset while providing unstable or misleading explanations. Researchers should preregister the comparison metric, use identical held-out domain partitions, and state when the added complexity yields a clinically or industrially meaningful improvement. Interpretability is a performance dimension, not a decorative appendix [9,15,33,42].

A Transferable Calibration and Validation Framework

The strongest answer to the generalization question is a hierarchical evaluation design. Samples should be grouped by physical oil specimen, then by production lot, origin or mill, season, and instrument. A random held-out spectrum is only a test of repeat-acquisition reproducibility, not deployment to an unseen mill or geography. Where the proposed application concerns new devices, leave-one-instrument-out validation is essential; where it concerns origin claims, leave-one-origin-out or leave-one-season-out tests reveal how strongly the decision rule depends on the initial reference population. Metrics should be interpreted in the context of their target decision [15,21,38]. Model transfer must distinguish correctable instrument shifts from changes in underlying chemistry. Wavenumber alignment, intensity standardization, transfer samples, and instrument-specific corrections can reduce optical differences when the chemical relationship is stable. Domain adaptation might further improve predictive fit when new labeled samples are limited, but using target-domain labels during adaptation alters the validation question. A transparent report should identify all target-domain material used during calibration and retain an untouched final test set. When the underlying link between carotenoid and location changes, no amount of detector standardization can guarantee geographic validity [10,21,38].

Uncertainty quantification supplies the missing connection between model scores and decisions. A quality regression should report prediction intervals with empirically checked coverage over independent domains, not just a point estimate and an R^2 value. A geographic classifier should communicate calibrated class probabilities or an explicit rejection option, especially when a new sample does not resemble any training class. An operational system should define when the result triggers release, process adjustment, remeasurement, or reference-laboratory confirmation. These thresholds depend on the cost of wrong decisions and on changing product requirements. Recent food-adulteration work demonstrates how conformal prediction can provide sample-level uncertainty intervals for mid-infrared calibrations, but analogous coverage must be verified rather than assumed for new palm oil domains [15,21,52,53]. A further risk is the use of synthetic mixtures or simulated spectra as though they represented future commercial samples. Digital spectral-library studies offer valuable feasibility checks for designed adulteration tasks, while multitask Raman models in olive oil demonstrate computational flexibility. However, virtual mixtures may not reproduce physical mixing, matrix effects, aging, or undocumented fraud methods. Calibration sets should include realistic production variability and independent commercial samples. Challenges should be selected to expose foreseeable deployment failures rather than merely to confirm the interpolation accuracy of a conveniently generated training distribution [34,52,54].

Figure 3 translates these principles into a proposed eight-stage research-to-deployment sequence. The steps must be read as evidence gates: a completed model is not deployment-ready until each relevant gate has been passed, documented, and rechecked when circumstances change. The model is not a reported field-tested palm oil product, but an actionable design specification for a multicenter validation program [15,21,25].

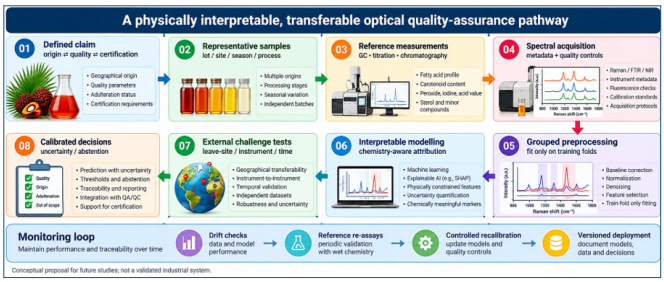


Figure 3: Proposed Evidence-Gated Pathway from Claims and Reference Assays to Explainable, Uncertainty-Aware, Transferable Optical Sensing.

The sequence begins with choosing the exact inferential claim and collecting representative samples with reliable reference values. It then calls for controlled acquisition, leakage-free model development, externally challenged explanations, and calibrated decision policies. A monitoring loop closes the process through drift detection and reference re-assays. This structure is designed to prevent an excellent single-site training result from being mistaken for a validated industrial quality-assurance system.

Comparative Technology Choices and Sensor Fusion

A technology decision should begin with the analyte and operational setting rather than with a preference for a particular instrument. Raman is attractive for specified vibrational features and potentially portable interrogation, but weak scattering and fluorescence are material constraints. ATR-FTIR often offers strong functional-group signals and economical contact measurement, while NIR can support rapid prediction of broader bulk properties when extensive calibration data are available. Fluorescence may add pigment sensitivity but can be highly dependent on optical context. SERS is relevant when low-concentration target analytes justify additional nanostructured substrates and associated controls [5,6,16,29]. Table 1 summarizes qualitative strengths and tradeoffs. The judgments describe analytical tendencies, not universal rankings of cost, sensitivity, or accuracy. In particular, an expensive sensor may be cost-effective if it eliminates large delays at a mill, while a low-cost portable system may be inappropriate when

uncertainty near a regulatory threshold is unacceptable. Head-to-head comparison should use matched samples, independent references, identical domain splits, and the same definition of acceptable error [4,25,30].

Table 1: Qualitative Comparison of Optical Modalities for Palm Oil Applications (Context-Dependent, not Empirical Rankings).

Modality	Most plausible strengths	Principal caveats	Indicative use
Raman	Distinct vibrational bands; portable instruments possible	Weak scatter, fluorescence, matrix overlap	Oil identification; unsaturation and pigment-informed screening
ATR-FTIR	Strong functional-group response; practical contact interface	Sample contact, surface effects, overlaps	Defined adulteration or processing-state assays
NIR	Fast bulk-property predictions; industrial sensor availability	Broad bands; calibration-intensive	Bulk quality screening and continuous process trend
Fluorescence / UV–Vis	Sensitive response to selected pigment/chromophore changes	Photophysical and treatment confounding	Complementary pigments or fraud flags
SERS	Potential trace-analyte enhancement	Substrate reproducibility and adsorption chemistry	Selected contaminant/residue testing
Multimodal fusion	Complementary features and potential robustness	Higher cost; integration and shift risk	Escalated screening where single modality is inadequate

Multimodal systems should be assessed according to incremental value. If a low-level fusion model adds substantial performance only in random splits and loses its advantage on an independent mill, its complexity is unjustified. A staged approach may be more robust: a cheap primary sensor screens all samples, and a complementary sensor or laboratory assay is activated when predictions are uncertain or high-stakes. Such cascaded sensing converts the technology comparison into a decision problem and may lower total cost while preserving analytical defensibility. It also preserves the ability to audit each modality separately [25,28,30,51].

Evidence Grading, Operational Governance and Future Research

The evidence matrix in Table 2 clarifies why the review avoids treating all recent spectroscopy papers as proof of industrial readiness. Direct palm oil studies answer concrete questions about sampled matrices; edible-oil comparisons provide transferable methods; and XAI or instrument-transfer research supplies evaluation tools. These forms of evidence are complementary but not substitutable. An application should advance toward deployment only when the direct evidence includes reference chemistry, grouped external validation, plausible spectral attribution, and an operational error policy. Current calibration guidance likewise emphasizes that model tuning and unbiased testing serve different purposes; independent external samples are especially important when models may be used to justify consequential quality or authenticity decisions [10,13,20,21,23,24].

Table 2: Evidence-Type Matrix and Inferential Limits in the Reviewed Research.

Evidence tier	Representative sources	Supported inference	Critical remaining test
A — palm oil direct	Stradling, Adade, Liang, Nazri [13,14,17].	Feasible measurement and modeling within reported samples	Unseen origins, processes, and instruments
B — edible-oil analogs	Zhao, Pulassery, Liu, Ozen [5,27,28,33].	Methods and feature families worth adapting	Palm-specific performance and reference chemistry
C — methods and optics	Contreras, Guo, Roger, [20,21,25].	Explanations, fusion designs, and shift-handling options	Experimentally tested palm oil implementations

A priority study would assemble a multi-origin, multiseason collection including at least several production systems, both crude and refined streams, and deliberately controlled storage and heating histories. It would obtain independent measurements of fatty acid distribution, pigments, peroxide value, acid value, and other targeted properties. Laboratory and portable instruments should measure overlapping specimens using standardized metadata such as laser wavelength, power, integration time, temperature, container, and preprocessing version. Most importantly, evaluation domains should be declared before modeling, and the final unseen datasets should remain unavailable to all feature selection and model tuning [10,13,15,21].

A second program should test whether molecularly meaningful attributions are more stable than unconstrained models. Studies could preregister expected carotenoid, methylene, unsaturation, and carbonyl regions; acquire targeted chemical perturbations; and compare band-level explanation consistency, external prediction errors, and calibration maintenance costs. The intervention must distinguish primary oxidation from hydrolysis and pigment loss. The outcome would be valuable even if an explainable model performs no better numerically, because it would define the limits of mechanism-based interpretation rather than silently favoring a more complex learner [12,13,20,35]. Third, practical deployment research should document decision consequences. A mill-level model designed to detect rapid changes in acid value should be evaluated against process

delays and reference-laboratory throughput, whereas a market-fraud model should optimize false-positive burden and recall for realistic adulterants. Geographic authenticity claims demand especially strong safeguards because error can affect producers, purchasers, and regulators. Publicly documented confidence thresholds, reference confirmation pathways, drift monitoring, and periodic retraining are necessary to prevent predictive labels from acquiring unwarranted evidentiary authority [2,10,21,22].

The economic and environmental contribution of optical quality assurance is plausible but unquantified by this review. Faster screening can potentially reduce reagents, sample transport, waste, and processing delays; on the other hand, instruments consume power, require replacement parts, and must be recalibrated using physical standards. Claims of greener or cheaper operation should therefore be supported by prospective cost and life-cycle comparisons in actual mill settings. More broadly, optical measurements can complement documentary sustainability traceability but cannot replace the geographic, legal, and governance information necessary for certification [1,3,4]. Finally, cross-disciplinary collaboration must connect photonics experts, analytical chemists, palm-oil process scientists, statisticians, and regulatory users. Each group defines a different failure mode: instrumental drift, chemically ambiguous bands, poorly representative sampling, data leakage, or incorrect operational action. Open and de-identified reference spectra with acquisition metadata, documented sample provenance where permissible, versioned processing scripts, and externally verified reference values would make future comparisons more useful than a new series of isolated single-laboratory accuracy claims. The end goal is reproducible measurement science in which AI improves accessibility without reducing accountability [8,15,21,25].

Conclusions

This critical qualitative review finds that Raman spectroscopy provides chemically meaningful access to palm oil constituents and selected quality-associated variations. Recent palm oil studies substantiate the practical promise of handheld geographical screening and machine learning-assisted estimation of iodine, peroxide, and acid values. However, the strongest scientific interpretation is conditional: a spectroscopic correlation reflects the measured sample and the conditions under which it was acquired. Neither a high classification score nor a prominent attribution peak alone demonstrates a universally valid authenticity marker. The substantive answer to the central research questions is that molecular physics, representative sampling, external validation, and explicit decision logic must be evaluated together. Pigment-sensitive bands may help distinguish particular origins but are vulnerable to confounding from maturity and processing. Unsaturation-related vibrations provide plausible routes to iodine-value prediction, whereas oxidation-related spectral regions require careful chemical controls before assigning analyte specificity. Explainable AI can strengthen scientific scrutiny when spectral attributions are stable, physically justified, and subjected to independent experimental challenge.

Raman, FTIR, NIR, fluorescence, and SERS should be viewed as complementary rather than universally competing technologies. A single sensor may be sufficient for an appropriately bounded screening application; more elaborate fusion is justified only when its incremental benefit survives cross-domain testing and outweighs additional costs. For high-consequence authenticity, safety, or compliance decisions, optical predictions should support a documented escalation pathway to calibrated reference methods rather than substitute for all confirmatory evidence. The recommended implementation pathway begins with an explicit claim and reference procedure, proceeds through broad sample coverage and controlled data collection, and requires leakage-free learning, independent challenge tests, explanation auditing, calibrated uncertainty, and versioned monitoring. Future research priorities include multi-origin and multicenter benchmarks, laboratory-to-handheld transfer experiments, chemically intervened attribution studies, out-of-distribution rejection policies, and prospective evaluation of operating costs and errors.

A credible next generation of palm oil spectroscopy will not be defined only by more accurate classification algorithms. It will be defined by knowing what the light actually measures, why the model responds, how far the calibration can be trusted, and when the correct scientific decision is to request another measurement. This provides a practical basis for more transparent and defensible optical quality assurance across the palm oil value chain.

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