

Review

Research Progress of Fourier-Transform Infrared Spectroscopy in Oat Quality Control

Bharani Kumar Palani, Joanna Bryś , Eliza Gruczyńska-Sękowska  and Piotr Koczoń * 

Department of Chemistry, Institute of Food Sciences, Warsaw University of Life Sciences (SGGW),
Nowoursynowska St. 159c, 02-787 Warsaw, Poland; bharani_palani@sggw.edu.pl (B.K.P.);
joanna_brys@sggw.edu.pl (J.B.); eliza_gruczynska@sggw.edu.pl (E.G.-S.)

* Correspondence: piotr_koczon@sggw.edu.pl; Tel.: +48-22-59-37616

Abstract

Oats (*Avena sativa* L.) are an analytically demanding cereal. They carry a lipid fraction of roughly 5–9% together with high lipase and lipoxygenase activity, a protein fraction dominated by globulins, a high-molecular-weight (1→3), (1→4)-β-D-glucan, and avenan-thramides that occur in no other grain. Each of these fractions changes during kilning, milling, storage, and fermentation, and each change affects a quality attribute of commercial consequence. Fourier-transform infrared (FT-IR) spectroscopy, interpreted with chemometric models, offers a rapid and non-destructive route to several of these attributes from a single measurement. This review draws the oat-specific literature together. It covers the identification, classification and authentication of oat material, including: the separation of oats from gluten-containing cereals, the discrimination of cultivars and of commercial milled forms, and the grading of grain; the prediction of quality parameters and the compositional analysis of moisture, β-glucan, protein, starch and lipid; the molecular changes that accompany processing and storage—β-glucan depolymerisation, lipid oxidation and hydrolysis, thermally induced protein aggregation, avenan-thramide degradation and starch retrogradation—and the spectral features by which sound and deteriorated oat material can be discriminated; and the portable and handheld instruments now bringing the measurement closer to the production line. Reported calibrations are frequently accurate but rest on limited sample sets, and multi-site validation together with shared reference spectra remains the principal requirement before routine industrial use.

Keywords: FT-IR spectroscopy; chemometrics; oats; molecular characterization; food quality



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1. Introduction

Oats (*Avena sativa* L.) are a unique cereal, offering immense potential in various fields and providing a substantial nutrient content that can offer health benefits to consumers, serve as animal feed, and find applications in cosmetics [1]. Oats (*Avena sativa* L.) have a long history of use in both human nutrition and animal feed. They are one of the first crops used by human civilization [2]. Through archaeological research in southeastern Italy, scientists have discovered traces of the oat plant in a cave occupied by Upper Palaeolithic hunter–gatherers, which is well before 32,000 years ago, before the domestication of plants [3].

Oats (*Avena sativa* L.) occupy an unusual position among the cereals. They carry a lipid fraction of roughly 5–9%, several times that of wheat, together with markedly higher lipase and lipoxygenase activity; their principal soluble fibre, (1→3),(1→4)-β-D-glucan, is

a high-molecular-weight polysaccharide concentrated in the cell walls of the endosperm and aleurone; their protein fraction is dominated by globulins rather than by the prolamins typical of other cereals; and they contain avenanthramides, a group of phenolic alkaloids not found in other grains. This combination is what gives oats their nutritional standing and also makes them difficult to control analytically. Each of these constituents' changes during kilning, storage, milling and fermentation, and each change alters a quality attribute of commercial consequence, whether viscosity, oxidative stability, texture or shelf life. Any method proposed for routine oat quality control, therefore, has to report on several chemically distinct fractions at once, and preferably without consuming the sample.

Fourier-transform infrared spectroscopy is a highly versatile technique. This technique is applicable to a wide range of materials. This includes gases, liquids, and solids. The primary principle of this tool is to allow the infrared beam to pass through the sample and then analyse the information about the molecular components of the sample from the beam that has passed through it. This is possible because the infrared beam passing through the samples creates a unique molecular fingerprint for each sample [4], thereby enabling FT-IR analysis to study the chemical bonds and functional groups across different samples. Unlike dispersive IR spectroscopy, FT-IR uses an interferometer, a component absent from conventional instruments. This interferometer is usually of the Michelson design, which allows the FT-IR to record all the wavelengths simultaneously. It collects data from the samples and converts it mathematically into a spectral form via the Fourier transform, displaying it in the software monitor for the naked eye to view [5]. Due to these advantages, FT-IR is easy to use, covers a wide wavelength range, and provides precise, rapid results. FT-IR is used across many fields, including the food industry and pharmaceutical companies.

FT-IR responds directly to molecular structure. Absorption in the mid-infrared region occurs when the frequency of the incident radiation matches the frequency of a molecular vibration and that vibration produces a change in dipole moment; bonds between atoms of differing electronegativity, such as C=O, O-H, and C-O, therefore absorb strongly, while symmetric non-polar bonds absorb weakly or not at all. Vibrations are broadly of two kinds: stretching modes that alter bond length and bending modes that alter bond angle, and the two respond differently to their local environment. Stretching frequencies shift with hydrogen bonding and conformation, which is why the polysaccharide C-O-C region is sensitive to chain order, whereas the carbonyl stretching frequency is governed largely by the substituents on the carbonyl carbon, which makes it diagnostic for the chemical identity of an oxidation product.

One of the advantages of FT-IR in food analysis is the ability of the equipment to analyse various nutrient factors in food. This includes protein, carbohydrates, fat content, and vitamins. This was made possible because of the attenuated total reflectance (ATR) cells present inside the FT-IR instrument [6]. Due to this, the nutrient analysis capability of FT-IR enables the monitoring of changes occurring in food during processing, such as chemical and compositional alterations. FT-IR can also be used efficiently for a food authentication device. There are many studies we will discuss below in Table 1 that show the usage of FT-IR applied in the determination of various agricultural products back to their origin of growth, thus maintaining the authenticity of the food products, especially value-added products, because of their origin. FT-IR can be utilised in many ways, especially in the food industry.

Oats contain many chemical components, among which the following are always present: Lipids, proteins, and carbohydrates. They generate characteristic bands in the IR spectra: C=O ester bond at around 1745 cm^{-1} , C=O stretching; Amide I bond at around 1650 cm^{-1} , and Amide II bond as well as C-N stretching around 1540 cm^{-1} ; and C-O-C and

C-O stretching in the fingerprint region at around 900 cm^{-1} , respectively. Their position and intensity can serve as markers of the quality of oat grain. Other components, e.g., β -glucans, which are the most significant bioactive fraction of the soluble fibre in oats, give diagnostic bands in the region of around $1020\text{--}1040\text{ cm}^{-1}$ (stretching vibrations of C-O in primary alcohols) or at $890\text{--}900\text{ cm}^{-1}$ generated by deformations of anomeric carbon. A decrease in intensity or a shift in the band at 1020 cm^{-1} indicates depolymerisation of the fibre, and hence a decrease in its quality. This is the most important fraction of the soluble fibre in the oats. Its degradation dramatically decreases the quality of the oats in terms of technological and healthy value. Another compound is free fatty acids, which form very quickly when the grain is destroyed or damp. The lipase, whose level is quite high in oat grains, is released, and in its presence, free fatty acids are formed from lipids. Their presence indicates a decrease in oat quality, as indicated by a band at around 1710 cm^{-1} , which is assigned to C=O vibrations in free fatty acids. Phenolic compounds (e.g., phenolic acids and avenanthramides) can serve for the spectral quantification of the oat quality. Oats are rich in antioxidants, including avenanthramides and acids (e.g., ferulic acid), which are unique to this grain. They protect the grain from oxidation. During prolonged or improper storage (e.g., at high temperatures), these compounds degrade, fighting free radicals. A decrease in the intensity of these bands indicates the exhaustion of the grain's natural antioxidant potential. For quality diagnosis, a broad band of stretching vibrations of the OH groups attached to the benzene ring, occurring around 3200 cm^{-1} , can be used, as well as stretching vibrations of the conjugated C=C bonds in the aromatic rings, occurring around 1600 cm^{-1} . Too high moisture is also a factor decreasing the oats' quality. Its level can be evaluated by the intensity of the band at 1640 (which, unfortunately, often overlaps with the Amide I band). A band with very high intensity indicates an environment conducive to the development of yeasts and moulds.

Two further assignments are worth stating explicitly because they are used later in this review. Protein conformation is followed through the contour of the amide I band between approximately 1670 and 1634 cm^{-1} , in which the appearance of intermolecular β -sheet features near 1682 and $1624\text{--}1626\text{ cm}^{-1}$ at the expense of α -helical content reports the thermally induced aggregation of oat globulins that reduces protein extractability. Starch order is followed more narrowly still, through the intensity ratios of the 995 , 1022 and 1047 cm^{-1} bands: a rise in the $995/1022\text{ cm}^{-1}$ ratio reports gelatinisation, while a rise in the $1047/1022\text{ cm}^{-1}$ ratio reports the short-range order restored during retrogradation, 1047 cm^{-1} reflecting ordered crystalline domains and 1022 cm^{-1} the amorphous regions.

In practice, however, individual bands seldom separate good material from poor on their own: the bands overlap, the matrix is chemically crowded, and the differences in interest are often small relative to the variation between samples. Discrimination comes instead from treating the spectrum as a multivariate signal and applying chemometric methods, which is the combination this review examines.

This review examines how that combination has been applied to oats. It covers the identification and classification of oat material, including: geographical origin, category and grade; the quantification of moisture and of the major biochemical constituents; the molecular changes that β -glucan, lipids, proteins, avenanthramides and starch undergo during processing and storage, and the spectral signatures by which those changes are detected; and the emergence of portable and handheld FT-IR instruments that move the measurement towards the point of production. Existing reviews of infrared spectroscopy in cereals treat oats alongside other grains and, in doing so, pass over the compositional features that make oats a distinct analytical case. The aim here is to bring together the oat-specific literature, assess what FT-IR can currently deliver for oat quality control, and identify where the method still falls short.

2. Identification, Classification, and Quality Evaluation

Significant similarities are found between oat varieties. Thus, very sophisticated technologies are required to accurately identify and classify oats. During the processing of oats, physical defects and chemical changes can occur in the oats. Therefore, identification and classification of oats is necessary to ensure the quality of oats. This process of identification and classification includes the geographical origin, grade, variety, category, and year of production. The quality of the oats is mainly determined by the quality of their fat. Examples of IR spectra of high- and low-quality oat oil are shown in Figures 1–3.

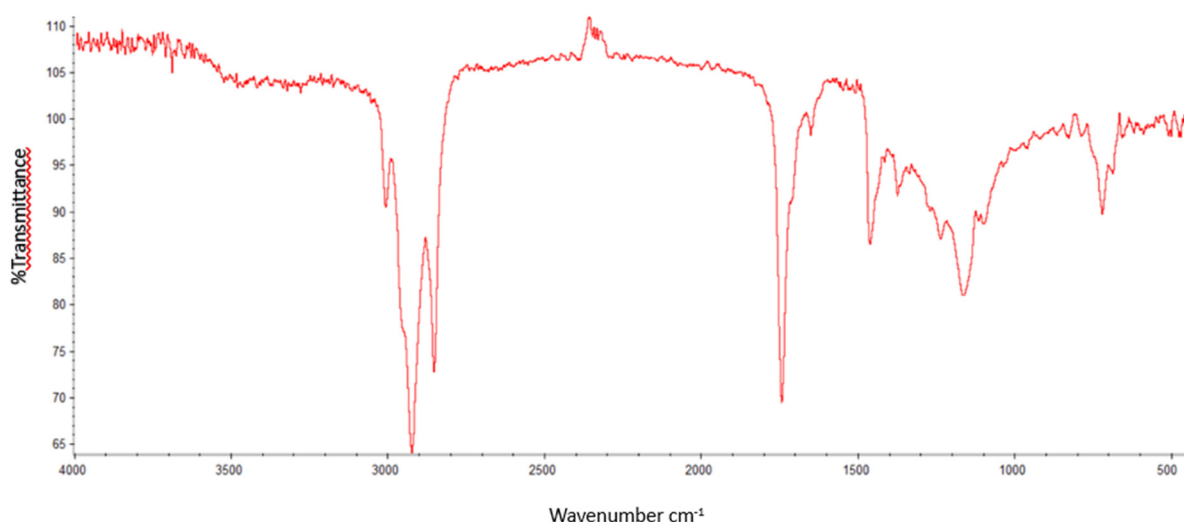


Figure 1. FT-IR spectrum of high-quality oat oil (low peroxide value). Spectrum recorded in the authors' laboratory on oil from the sample set used to calibrate the chemometric models reported in [7]; not previously published.

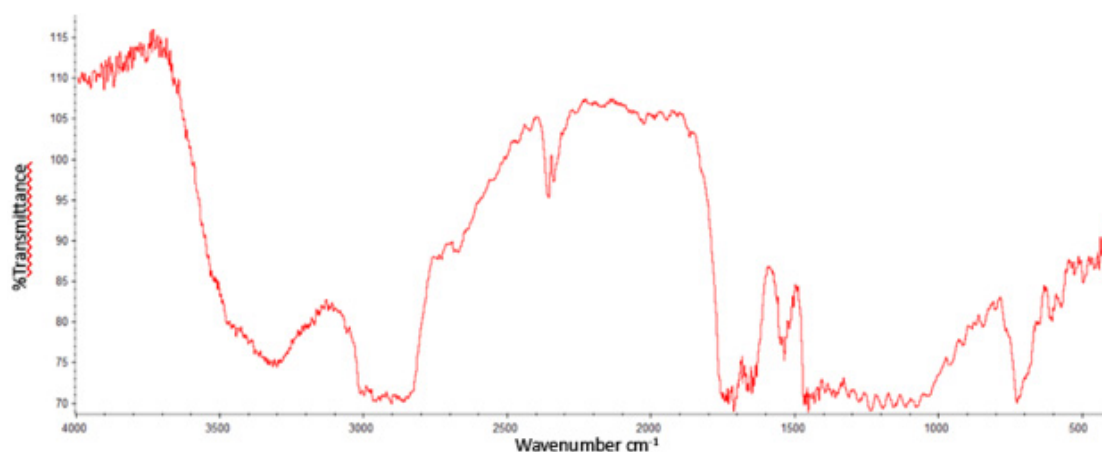


Figure 2. FT-IR spectrum of low-quality oat oil (high peroxide value). Spectrum recorded in the authors' laboratory on oil from the sample set used to calibrate the chemometric models reported in [7]; not previously published.

Figures 1 and 2 show the mid-infrared spectra of two oat oil samples that differ in oxidative state, and Figure 3 presents the same two spectra overlaid, with the good-quality sample in blue and the poor-quality sample in red. The spectra were recorded on oil extracted from oat grain and were acquired as part of the calibration set used to build the chemometric models reported earlier by the present authors [7]. They have not been published previously and are presented here to illustrate, specifically on oat material, the spectral contrasts that underpin those models. The comparison below is deliberately

descriptive and is confined to the features visible in the three figures. The reaction pathways that generate these features, and the quantitative relationships between spectral change and oxidation indices, are treated separately in Section 4.2.

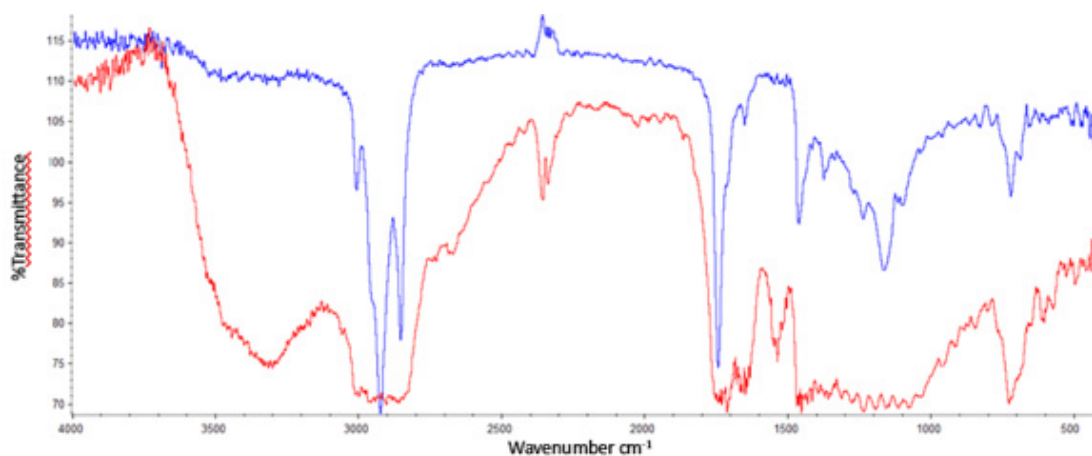


Figure 3. Overlaid FT-IR spectra of high-quality (blue) and low-quality (red) oat oil, plotted from the spectra shown in Figures 1 and 2.

The clearest difference between the two samples lies in the hydroxyl stretching region, approximately $3600\text{--}3100\text{ cm}^{-1}$. In the good-quality oil (Figure 1), this region is essentially featureless, running close to the baseline, as would be expected of an oil in which neither hydroperoxides nor appreciable moisture has accumulated. In the poor-quality oil (Figure 2), a broad, intense absorption dominates the same interval. The breadth of the band is itself diagnostic: O–H oscillators in hydroperoxides and hydroxy fatty acids are extensively hydrogen-bonded, and the resulting distribution of bond strengths smears what would otherwise be a narrow stretching mode across several hundred wavenumbers. Because hydroperoxides are the primary products of the autoxidation of unsaturated acyl chains, growth in this region is among the earliest spectral indications that an oil has begun to deteriorate, and it has been shown to track peroxide value closely in edible oils oxidised under controlled conditions [8]. In oat oil, where the linoleic acid content is high and lipoxygenase activity in the grain is considerable, this region is correspondingly informative.

The $3050\text{--}2800\text{ cm}^{-1}$ interval carries two distinct pieces of information. The weak band near 3006 cm^{-1} arises from the stretching of C–H bonds attached directly to cis-carbon-carbon double bonds, and its intensity therefore scales with the degree of unsaturation of the acyl chains; it is well established as a spectroscopic proxy for iodine value in vegetable oils [9,10]. In Figure 1, this band is sharp and clearly resolved, consistent with an intact complement of oleic and linoleic acids. In Figure 2, it is weaker and less well defined, which is the expected consequence of the consumption of double bonds during oxidation and of the partial isomerisation of the remaining cis bonds to the trans configuration. The much stronger bands near 2925 and 2855 cm^{-1} , from the asymmetric and symmetric stretching of methylene and methyl groups, report on the aliphatic chains themselves. These remain sharp and well-proportioned in the good-quality sample. In the poor-quality sample, they are broadened and sit on a displaced baseline, which is consistent with scission of the long acyl chains into shorter fragments and with the general loss of homogeneity in the lipid matrix. It should be noted, however, that baseline displacement of this kind can also arise from differences in sample presentation and optical path, and it is therefore weaker evidence than the band-shape changes that accompany it.

The ester carbonyl band near 1745 cm^{-1} behaves in the way that has been described repeatedly for oxidising oils. In the good-quality sample, it is narrow, symmetric and isolated,

as expected of the triacylglycerol ester linkages of an unaltered oil. In the poor-quality sample, it is broadened and visibly asymmetric. The distortion reflects the appearance of additional carbonyl species whose absorptions lie close to, but not coincident with, the ester band: free fatty acids released by hydrolysis absorb near 1711 cm^{-1} , while the aldehydes and ketones formed on decomposition of the hydroperoxides absorb in the region of 1728 cm^{-1} [11,12]. Since these components are not resolved from one another at ordinary resolution, the practical signal is a change in the contour and width of the composite band rather than the appearance of separate peaks, and it is precisely this behaviour that makes the carbonyl region suited to multivariate rather than single-band treatment [8,13].

In the fingerprint region between 1500 and 1000 cm^{-1} , the good-quality oil retains the sharp, well-resolved profile characteristic of an unaltered vegetable oil, with the C–O and C–O–C stretching modes of the glycerol ester backbone clearly distinguishable. The corresponding region of the poor-quality oil is noticeably degraded: bands overlap, individual features become ill-defined, and the overall contour is noisier. This is consistent with the structural breakdown of the glycerolipid core and with the accumulation of a heterogeneous mixture of oxidation products, each contributing its own weak absorption to an already crowded region. The diagnostic value of this region lies less in any individual band than in the loss of resolution across it, which is why it is normally exploited through pattern-based rather than peak-based analysis [6].

Taken together, the overlaid spectra in Figure 3 show that the two quality classes are separated not by a single marker but by a set of concurrent changes: the emergence of a broad hydroxyl absorption, the weakening of the cis olefinic band, the broadening of the aliphatic and carbonyl bands, and the loss of definition in the fingerprint region. Each of these has an established chemical interpretation, and each moves in the same direction as oxidation proceeds, which is what allows a spectrum to be assigned to a quality class with reasonable confidence. The practical consequence for oat quality control is that a single measurement requiring no solvent, no titration and little sample preparation carries information equivalent to that obtained from peroxide value and free fatty acid determination, and can be acquired in minutes; instrumentation suitable for this purpose outside the laboratory is now available [14]. Two qualifications should be stated. First, the assignment of quality classes to the samples in Figures 1 and 2 rests on the accompanying wet-chemistry determinations rather than on the spectra alone, and spectral interpretation of this kind should not be divorced from reference analysis. Second, the contrast shown here is between two samples at opposite ends of the quality range; discriminating intermediate material, where the spectral differences are small relative to the variation between cultivars and growing seasons, requires the chemometric treatment discussed in the sections that follow.

2.1. Geographical Origin

The geographical origin of the oat is a major factor to consider in determining the quality of the nutrients because the agricultural factors, like the quality of soil and climatic conditions, have a direct impact on the production of bioactive compounds in the growth of crops. Studies have found that oats grown and cultivated in colder regions, such as in Canada and Scandinavian countries, possess a comparatively higher β -glucan percentage (5–7%) [15,16]. The soil and bedrock quality may have a substantial effect on the nitrogen cycle [17]. The regional soil factors were influenced by the essential trace elements, such as selenium [18]. The secondary metabolites also fall under this category, and their production is influenced by soil factors. For example, avenanthramides are influenced by UV radiation and elevation gradient factors [19]. This can be explained by the Finnish-grown oats, which are known for their higher β -glucan content, in contrast to the Australian varieties that often have higher mineral densities in their oat products [20]. This proves that the quality

and nutrition differ based on the geographical distinction. Geographical authentication of oat material, therefore, serves three purposes:

1. Nutritional valuation (functional food).
2. Transparency of the supply chain (PDO certification, premium pricing).
3. Safety assurance.

Future studies might measure these associations with the use of more sophisticated spectral fingerprinting (e.g., FT-IR-PLSR) combined with geospatial modelling.

The molecular fingerprint of plants and food products of plant origin also differs in response to the geographical origin of the oat, since it is affected by the geographical growing conditions, including weather and elevation. Using the molecular fingerprint of plants and foods, FT-IR spectroscopy has emerged as a useful technique for identifying and determining their geographic origins. The bands that would carry such information are well characterised in oats— β -glucan near 1040 cm^{-1} , lipid ester carbonyl near 1740 cm^{-1} and amide I near 1650 cm^{-1} [21]—but they have so far been used to describe composition rather than to classify samples by growing region. Reports of this kind remain scarce for oats, however, and the evidence currently available is thin.

Current progress in technology leads to the advancement of FT-IR devices, which pave the way to improve the application of FT-IR in various fields, causing rapid, non-destructive geographical origin verification without laboratory preprocessing [22]. In the case of FT-IR being combined with machine learning algorithms, e.g., support vector machines (SVM), it may become a promising method of enhancing the traceability of the supply chain. This application can be potentially used for detecting the adulteration or mislabelling of premium oat varieties, as these different varieties have distinct molecular and chemical differences that can be identified using FT-IR through spectral patterns. No systematic study of this kind has yet been carried out on oats, which is one of the clearer gaps in the present literature.

A distinction has to be drawn at this point between what has been demonstrated for other commodities and what has been demonstrated for oats. Geographical-origin authentication by mid-infrared FT-IR is well established for other cereal and oil matrices [23–25], where classification accuracies approaching 100% have been reported. No equivalent study exists for oats. A systematic search of the literature returned no FT-IR investigation in which oat samples of declared provenance were classified by growing region or country of origin. The oat-specific work that does exist addresses authenticity in a different sense, namely the separation of oats from gluten-containing cereals and the discrimination of commercial oat forms, and it rests largely on near-infrared rather than mid-infrared measurement. Table 1 sets out that evidence and explicitly records the provenance gap.

Table 1. Application of FT-IR spectroscopy for the identification, classification, and tracing of the geographic origin of oats.

Instruments	Samples	Sample Sizes	Spectral Range (cm^{-1})	Parameters & Key Findings	Model (s) & Accuracy (%)	Reference
NIR diffuse reflectance	Oat flour from groats, steel-cut and rolled oats; gluten-containing adulterants (wheat, farro, triticale, barley, rye, ryegrass)	NR	NIR	Authentication of oat flour and detection of adulteration with gluten-containing cereals	PCA, SIMCA, OPLS-DA; sensitivity 100%, specificity 97.78% (SIMCA) and 100% (OPLS-DA)	[26]

Table 1. Cont.

Instruments	Samples	Sample Sizes	Spectral Range (cm ⁻¹)	Parameters & Key Findings	Model (s) & Accuracy (%)	Reference
NIR hyperspectral imaging	Oat, dehulled oat, barley, dehulled barley, wheat and rye grains	NR	900–1700 nm	Discrimination of gluten-free oats from gluten-rich contaminants; five key wavelengths (1069, 1126, 1189, 1243, 1413 nm)	PCA, PLS-DA; 99% correct prediction for dehulled oat	[27]
FT-IR (mid-infrared)	Oats of declared geographical origin	-	-	No study identified. Geographical provenance of oats has not been addressed by mid-infrared FT-IR, unlike other food matrices [23–25]	-	-

FT-IR—Fourier-Transform Infrared Spectroscopy; NIR—Near-Infrared; OPLS-DA—Orthogonal Partial Least Squares Discriminant Analysis; PCA—Principal Component Analysis; SIMCA—Soft Independent Modelling of Class Analogy.

Within-species varietal differences, by contrast, are beginning to be documented in the mid-infrared. Cozma et al. [28] recorded ATR-FT-IR spectra (4000–500 cm⁻¹, 32 scans, 4 cm⁻¹ resolution) of black oat (*Avena strigosa*) alongside three *Avena sativa* cultivars grown under a single, uniform set of agronomic conditions. The overall spectral envelope was common to all four samples, as would be expected of a shared cereal matrix, but the relative intensities of the carbohydrate fingerprint bands near 1150, 1076 and 997 cm⁻¹, together with the β -glycosidic marker around 860 cm⁻¹, differed systematically between cultivars and allowed the samples to be ranked by their apparent β -glucan contribution. Two points follow for the present review. First, cultivar discrimination in oats is carried mainly by the 1200–900 cm⁻¹ region rather than by the amide or lipid bands because it is the non-starch polysaccharide fraction that varies most between genotypes grown side by side. Second, the assignment is semi-quantitative: starch and other hemicelluloses absorb across the same interval, so band-intensity ratios report relative rather than absolute β -glucan content unless the spectra are calibrated against an enzymatic or chromatographic reference. Because the material in that study was grown under one set of pedoclimatic conditions, the observed differences can be attributed to genotype rather than to environment—the converse of the design needed to establish provenance, and this is a useful illustration of why variety and origin have to be treated as separate experimental questions.

The absence of any provenance study on oats is itself a finding of this review. Oats are traded internationally in volume, are marketed on regional identity in several European and North American markets, and carry a lipid, β -glucan and avenanthramide profile that is known to respond to growing conditions, which is precisely the kind of compositional variation that mid-infrared spectroscopy is able to register. The methodological groundwork therefore exists, and the demonstrations on other matrices [23–25] show that the approach transfers. What is missing is the authenticated sample set: geographical classification models require material of verified origin collected across several harvest years, and no such collection appears to have been assembled for oats. Establishing one is the obvious next step and a prerequisite for any of the traceability applications discussed above.

2.2. Type and Categories

Adulteration of the milled product has been addressed in the same way. Fourier-transform near-infrared spectroscopy coupled with partial least squares regression was applied to oat flour and detected and quantified adulteration across a range of 5–50%,

with a root mean square error of prediction of approximately 1.98% *w/w* [29]. The result indicates that vibrational spectroscopy can support authenticity control in cereal flours at the levels of adulteration likely to be encountered commercially.

Mislabelling of oat quality or grade category frequently results in the oat market and food industry dealing with adulterated oat products with degraded or low-quality oats. As a result, low-quality final products are sometimes accidentally produced and released to consumers, rather than the premium-quality product intended. In the oat market and food industry, this mislabelled raw oat was generally identified by conventional methods, such as expert physical inspection and the use of wet chemistry methods, which require a significant amount of laboratory work, preprocessing, and time. This is where the FT-IR comes into application, as it can be utilised to quickly and cost-effectively grade and categorise the oat samples. Numerous studies have demonstrated the ability of FT-IR to distinguish oat varieties and types. These studies in particular [28,30,31] found that FT-IR can be successfully utilised for distinguishing between oat types and varieties based on their unique spectral fingerprints.

Research has established that infrared (IR) technology could be employed to forecast important nutritional parameters in oats. As an example, [32] used FT-NIR combined with PLS regression to predict total starch, protein, β -glucan, and fat in oat grain, obtaining coefficients of determination for prediction ranging from 0.76 to 0.90 depending on the parameter. Another study [33] used FT-IR coupled with principal component analysis (PCA) to successfully demonstrate the technique's capability in distinguishing oat products from other cereal products based on the chemical profiles of the samples. All the above studies demonstrate that the FT-NIR spectroscopy tool, combined with chemometrics techniques, can be used as an effective method to identify adulteration, determine the variety and categories of oat grains, as well as oat-related food products. FT-NIR can measure spectral data from individual samples; these data contain sufficient information to determine and extract all the valuable details needed for food product authentication and the determination of nutrient parameters. This technology offers us a valuable opportunity to utilise this method for detecting adulteration in cereal-based products [29]. The reason FT-IR is a fantastic and effective tool in various fields is not only because it is fast and precise, but also because it can accurately read the molecular fingerprint of a wide variety of foods. There are multiple studies that utilised the ability of the FT-IR to determine the nutritional parameters of their subject food samples. In these studies [34,35], the authors used FT-IR to determine the nutritional parameters of oat products, including calorific value, fat content, and fatty acid composition, by analysing the spectral region near 1740 cm^{-1} of the samples. The applications of FT-IR in the food industry are very wide and varied, with potential uses in both quality inspection and regulation [34,35].

The given studies indicate a developing range of research that recognises the significance of spectroscopic techniques in the study of the intricate biochemical character of oats and in improving the quality and nutritional worth of oat-based foods. Table 2 summarises the oat studies in which vibrational spectroscopy has been used for type and category identification: the separation of hulled from naked genotypes, the discrimination of cultivars, the distinction between intact kernels and groats, and the exclusion of other cereal grains from oat and groat streams. Studies whose primary objective is authentication or the detection of adulteration are collected in Table 1 instead, so that each study appears once. Because the mid-infrared literature on these questions is sparse, near-infrared, FT-NIR, and hyperspectral imaging studies are also included; the technique used is stated for each entry so that mid-infrared and near-infrared evidence are not conflated.

Table 2. Vibrational spectroscopic techniques applied to the identification of oat type, category and authenticity.

Instruments	Samples	Spectral Range (cm ⁻¹)	Sample Sizes	Parameters & Key Findings	Model (s) & Accuracy (%)	Reference
NIR hyperspectral imaging	Intact oat kernels & groat	10,000–6000	150	Obtained almost complete classification of oat	PCA+ PLS-DA – 100% correct discrimination	[36]
NIR	Hulled and naked oat genotypes from China, Canada and the United States	NIR	NR	Discrimination of naked from hulled oats; prediction of total phenolic content and antioxidant capacity	PCA of second-derivative spectra; PLSR	[37]
Multispectral imaging	Seeds of 16 oat cultivars	405–970 nm	NR	Cultivar identification from combined morphological and spectral features	LDA 89.69%, SVM 92.71%	[38]
NIR (single-kernel and high-speed sorter)	Oat and groat kernels against barley, wheat, rye and triticale	904–1685 nm	NR	Exclusion of gluten-containing grains from oat and groat streams	94.5–100% correct classification (single-kernel); 95.0–99.4% (automated sorter)	[39]

LDA—Linear discriminant analysis; NIR—Near-infrared; NR—Not reported; PCA—Principal component analysis; PLS-DA—Partial least squares discriminant analysis; PLSR—Partial least squares regression; SVM—Support vector machine.

2.3. Storage and Year of Production

During storage, oats undergo numerous physicochemical transformations; for instance, their quality parameters such as moisture and fat content change. It also depends on the condition and duration of the storage [32]. In the long-term storage, it leads to lipid oxidation, accumulation of free fatty acids and peroxide in the products, rancidity, and reduction in the nutritional value. At the same time, the functional qualities of oat-based products are more affected by protein denaturation. Despite this, there are still very few systematic studies available on the topic of comparing the quality degradation under storage conditions.

There are studies from [40,41] that show that the traditional analytical techniques, such as HPLC, GC, and NMR, have been employed to investigate the storage effect on the antioxidant and lipid profiles of oat storage, as well as other quality changes. However, these methods are, most of the time, very expensive to perform, labour-intensive, and time-consuming. As such, there is a need for a rapid, non-destructive, and cost-effective analytical tool. When compared with conventional wet chemistry employed to investigate the storage effect on the antioxidant and lipid profiles of oat storage analyses, FT-IR spectroscopy, a rapid and non-destructive technique, has shown good results in tracking compositional changes such as protein, carbohydrate, and starch structure in the oat grains, producing strong correlations (R^2 up to 0.998) [42]. The same principle applies to stored oat flour, where the growth of hydroperoxide and secondary oxidation bands offers a route to detecting early rancidity before it becomes apparent by sensory assessment [43].

As an example, ref. [44] showed that storage-induced changes in the composition of oats can be detected using multivariate analysis techniques, including principal component analysis (PCA), by using the results of PCA on the lipidomic data of oat flour before and after storage, which clearly show a separation using chemical shifts. These investigations indicate the possibilities of FT-IR as a valid method of the analysis of oats and oat-product quality.

2.4. Grade

To create a quality oat-related product, the first and most important process is to select high-grade (quality) oat grains as the raw material for the product. The quality of this grade depends on several factors such as the type of oat variety, processing quality, nutritional quality, and the number of defects in the oat grains. Producing a high-quality product not only ensures a higher nutritional quality intake for the consumers, but also determines the product range. This grading process is very significant in identifying these factors of importance. Numerous research studies have successfully implemented wet chemistry methods for the grading procedure. However, the complexity of the procedure and the time it takes for the lengthy process are clear in their studies. For example, in the study by [45], the importance of the grading procedure is discussed, but the complexity of the wet chemistry involved in this procedure is also evident. Thus, there is a need for a faster and more cost-effective tool for the grading procedure in the food industry, particularly for grading oat products.

Several analytical approaches have been explored to improve oat grading. Several studies have used FT-IR to determine the nutritional value of oats. For example, in [31], the authors evaluated the nutritional parameters of the oat sample, which included protein content, moisture content, oil, and starch content, with a remarkable correlation coefficient (r) of 0.80 or greater. This indicates that FT-IR spectroscopy can be used to evaluate oat grading and determine the nutrient parameters, too.

In commercial practice, however, the primary grading criterion applied to oats is not composition but groat percentage, that is, the proportion of hull-less kernel recovered after dehulling, which predicts milling yield more reliably than test weight does. Redaelli and Berardo [46] developed near-infrared calibrations for this parameter directly on whole kernels of oat cultivars, reaching a coefficient of determination of 0.80 and dispensing with the grinding step entirely. The same problem has since been taken down to single-kernel resolution. Serranti et al. [36] applied near-infrared hyperspectral imaging over 1006–1650 nm with PLS-DA and separated oat from groat kernels with an accuracy approaching 100%, and further showed that three wavelengths alone (1132, 1195 and 1608 nm) retained correct classification rates of 97.1% and 99.0% for groat and oat respectively—a finding of direct relevance to on-line sorting. Armstrong and Maghirang [39] extended the same logic to the exclusion of foreign grain, discriminating oats and groats from barley, wheat, rye and triticale with 94.5–100% correct classification on a single-kernel near-infrared instrument and 95.0–99.4% on an automated high-speed sorter, with fewer than 4% of non-oat kernels misassigned. Grading in this narrower sense—dehulling efficiency and freedom from gluten-containing contaminants—is thus already tractable instrumentally, and underpins the certification of gluten-free oat streams.

It should be stated plainly that this body of work is almost entirely near-infrared. The mid-infrared contribution to oat grading runs through composition rather than through kernel sorting: the amide I and II bands, the ester carbonyl near 1745 cm^{-1} and the $1200\text{--}900\text{ cm}^{-1}$ carbohydrate region supply the fundamental absorptions that the near-infrared exploits only as overtones and combinations, and they are correspondingly easier to assign. What is missing from the literature is a study in which oat lots of documented commercial grade are classified from their mid-infrared spectra alone. Until such work appears, FT-IR is best presented as a compositional and structural tool that informs grading decisions, not as a validated substitute for the physical criteria on which grading currently rests. This is arguably the clearest single opportunity for mid-infrared research on oats.

The incorporation of the FT-IR spectroscopic method with other molecular spectroscopic methods may provide a better understanding of the molecular physicochemical and nutritional profiles of the study. As an illustration, the physicochemical and nutritional

properties of *Avena sativa* grain have been examined through a combination of molecular spectroscopic methods, including synchrotron radiation-based Fourier-transform infrared (SR-FT-IR) spectroscopy, X-ray fluorescence (XRF) and attenuated total reflectance Fourier-transform infrared (ATR-FT-IR) spectroscopy [47]. Used alongside these complementary techniques, ATR-FT-IR can support more effective and more precise grading of oats.

2.5. Quality-Parameter Prediction

Advances in modern technology and recent research have contributed to improved understanding of FT-IR spectroscopy and its remarkable applicability in determining the physicochemical and sensory characteristics of oat-based products. As an example, research by [48] looked at modifications that take place in oat products at different stages of oat processing. The paper found that the protein and carbohydrate structures were altered through the different stages of processing. This shows that FT-IR spectroscopic methods can be used to analyse the physicochemical transformations during the stages of the process, and to determine the sensorial property transformations of oat products during processing.

Therefore, the FT-IR that is coupled with the sophisticated chemometrics methods may serve as a more useful tool in the process of identifying and analysing various quality parameters of oat grains. One such application is reported in [49], where FT-IR spectroscopy was combined with multivariate modelling—principal component analysis (PCA) and PLS regression—to compare the physical and compositional variation in oat-based beverages. That work concentrated on β -glucan content and starch degradation as the quality parameters of interest. Their study findings reveal the applicability of spectroscopic methods in quantifying the quality and nutritional characteristics of such oat-based drinks. This method might be relevant to other plant-based drinks, which may result in the development of the product and the better formulation of such drinks.

A related study [32] addressed the determination of quality parameters in oat grain. A non-destructive method was developed using near-infrared spectroscopy with PLS regression, and eight spectral pre-treatments were screened against four feature-wavelength selection algorithms, including Competitive Adaptive Reweighted Sampling (CARS) and the Successive Projections Algorithm (SPA). Performance varied by parameter: fat was predicted best ($R^2_p = 0.903$), followed by protein ($R^2_p = 0.853$, MSC-CARS), total starch ($R^2_p = 0.768$) and β -glucan ($R^2_p = 0.759$). The results indicate that no single pre-treatment and wavelength selection combination is optimal across all constituents, and that the accuracy achievable depends strongly on which parameter is targeted.

3. Chemical Composition Analysis

Oats have gained much attention due to their unique nutritional and sensory properties because of their valuable bioactive constituents, such as β -glucans, polyphenols (phenolic acids and avenanthramides), unsaturated lipids, and high-quality proteins. These compounds add flavour to the oat-based products and help to increase their health-promoting effects, and oats play a critical role in diverse dietary applications [50].

Among the components of oats, β -glucans are the focus of the most extensive research due to their significant physiological benefits. In a comprehensive meta-analysis conducted by [51], it was found that consuming at least 3 g of oat β -glucans per day may reduce low-density lipoprotein (LDL) cholesterol and total cholesterol levels. The outcome validates the significance of β -glucans in the prevention of heart diseases and emphasises their beneficial effect on the decrease in cardiovascular risk [52]. Moreover, oat-specific avenanthramides have strong anti-inflammatory and antioxidant effects, which is the reason for the unique flavour of oat and its health-promoting effects. The complicated structure of oats and the outstanding nutritional values of oats serve as the reasons for the growing interest in the

usage of oats as a functional food, and hence, causing the correct quality assessment of oats and their chemical structure. In such a way, oat lipids, which are rich sources of unsaturated fatty acids, have two purposes: they contribute to the formation of the flavour and the nutritional value of the food product. Considering the importance of these components, evaluating the quality of oats, their nutritional efficiency, and the performance of processed oat products is impossible without a complete chemical analysis.

In recent years, FT-IR has been a highly effective, fast, and non-destructive analytical technique for identifying the biochemical composition of oat products when coupled with chemometric techniques [53]. The approach has a number of advantages, such as effective authentication of oat-based products and quality control. This strategy benefits the industry by increasing traceability, product consistency, and processing parameter optimisation. It will be essential to use the latest analytical methods to exploit the full potential of oats as a functional food and meet the needs of consumers with high-quality products as their interest in them increases.

3.1. Moisture Content and Water Activity

Water activity and moisture content are the two main factors that can be used to define the effectiveness of oat grain storage. Oats that have just been harvested have an ascribed moisture of 16–18%. To maintain the stability of the conditions in the storage, the level of humidity should be no more than 13%. These critical threshold measures prevent a series of deleterious biochemical reactions, including the enzymatic degradation of nutrients important in oats, lipid rancidity caused by oxidation, and the growth of storage fungi in oats. The rapid breakdown of oat lipids and β -glucans caused by lipase and lipoxygenase enzymatic activity significantly reduces the nutritional value and sensory qualities of oats [54].

Water activity (a_w) is a more precise measure of storage stability than moisture content because it directly reflects the amount of water available for microbial and enzymatic activity. Research has established that fungal species such as *Aspergillus* and *Fusarium* are metabolically active at a_w above 0.65, and their growth rates are much higher in high environmental humidity [55]. This microbial activity predisposes the risk of mycotoxin contamination and exacerbates the degradation of the oat components because of enhanced enzymatic hydrolysis. It is important to control both factors simultaneously to maintain oat quality during extended storage periods, since high a_w and high moisture content interact to create conditions conducive to the growth of microorganisms, resulting in oat quality degradation [56].

Rapid, non-destructive determination of moisture in cereal grains is now routine, and contemporary applications combine FT-IR and FT-NIR measurements with multivariate calibration to determine moisture, along with protein and starch attributes, from a single spectrum [53]. For oats specifically, however, dedicated moisture calibrations remain scarce: the compositional models reviewed in Section 3.2 report moisture only as one output among several, and no independently validated oat moisture calibration was identified in the present review. The gap is worth naming, because moisture and water activity are the two parameters on which safe storage most directly depends. Portable spectrometers make the measurement feasible at intake and during storage, so that corrective action can be taken as either parameter approaches its critical value rather than after it has been crossed.

Used in this way, spectroscopic monitoring supports a preventive rather than a reactive approach to storage management. The measurement is unobtrusive and can be repeated as often as required, so moisture and water activity can be followed across the supply chain and interventions timed before either parameter reaches the threshold at which

enzymatic and microbial degradation accelerates. Applied consistently, this preserves both the nutritional and the sensory quality of oat products between harvest and consumption.

3.2. Biochemical Constituents

FT-IR has also been applied to oat material whose composition has been deliberately altered. In a study of solid-state fermented oat grain [42], FT-IR combined with partial least squares regression was used to track the nutritional and chemical changes brought about by fermentation. Protein, fibre, tannin and phytic acid contents, spanning a range of 0.15–9.5%, were predicted with coefficients of determination between 0.954 and 0.998, which demonstrates that the technique retains its accuracy in a matrix undergoing active biochemical change.

Recent advances in FT-IR spectroscopy have cemented it as a viable method of analysis in the rapid and non-destructive determination of various nutritional constituents in oats and other grains. An essential study conducted by [57] revealed the ability of portable FT-IR to determine the key nutritional values, such as β -glucan, protein, starch, and lipid content in oat groats with high accuracy when coupled with partial least squares. Based on the research, FT-IR can recognise unique molecular vibration patterns related to proteins, carbohydrates, and lipids, and the error of prediction is usually less than 1 per cent. The accuracy of compositional assessment in actual oat quality assessment procedures is greatly improved by this capability.

The same study also reported that oat protein and lipid concentrations in both ground and intact oat groats can be precisely estimated using portable FT-IR and PLSR, with predictive R^2 values greater than 0.90. This is a methodological technique that can be used to perform non-destructive quality measurements in an efficient and fast manner by allowing screening of different oat cultivars with different nutritional profiles in a high-throughput manner.

In addition to the analysis of macronutrients, FT-IR spectroscopy proved to be highly effective in determining the bioactive composition of cereals. As an example, ref. [58] applied PLSR models and attenuated total reflectance FT-IR (ATR-FT-IR) to 14 various plant powders, such as various cereals, and yielded impressive predictive R^2 values of 0.962 for total phenolic content, 0.911 for Ferric-Reducing Antioxidant Power (FRAP), and 0.829 for Cupric-Reducing Antioxidant Capacity, a spectrophotometric assay (CUPRAC) antioxidant activity. These results suggest that FT-IR can be used in quality control processes of oats and oat functional foods, as it is appropriate in the fast and non-destructive determination of valuable bioactive compounds, including phenolics and antioxidants.

The study by [59] highlighted the potential of FT-IR for detecting nutritional differences among various oat cultivars. The analysis revealed some distinct spectral features in carbohydrate-lignin fingerprint areas, especially at 1023, 1152, and 1080 cm^{-1} , which were linked to the variations in the nutritional content of CDC oat cultivars. This finding is a good indication that FT-IR can be used to identify various types of grains according to their biochemical content. These findings demonstrate that FT-IR spectroscopy is a fast, precise, and robust method for measuring oat quality when combined with advanced chemometric methods, such as PLS regression, principal component analysis (PCA), and support vector machines (SVM). The flexibility of FT-IR has contributed to its significance in agricultural research and industry in general, facilitating the simplification of quality control while minimising reliance on traditional, resource-intensive methods. Table 3 summarises the published FT-NIR calibrations for the chemical composition of oats; the mid-infrared studies discussed above are treated in the text rather than tabulated, since no comparable body of tabulated FT-IR calibration data exists for this grain.

Table 3. FT-NIR spectroscopy for chemical composition analysis of oats.

Instruments	Samples	Spectral Range (cm ⁻¹)	Sample Sizes	Parameters & Key Findings	Model(s) & Accuracies (%)	Reference
FT-NIR	Whole naked oat grain	12,500–4000	90: Cal 45: Val	Protein: Good predictive ability; good for quality control and breeding selection.	PLS regression: RMSECV = 0.40%, RMSEP = 0.46%, RPD = 5.38	[21]
FT-NIR	Whole naked oat grain	12,500–4000	90: Cal 45: Val	Starch: Accurate prediction, suitable for screening	PLS regression: R ² = 0.97, RMSECV = 0.59%, RMSEP = 0.68%, RPD = 5.07	[21]
FT-NIR	Whole naked oat grain	12,500–4000	90: Cal 45: Val	Lipid: Very good prediction Good screening.	PLS regression: RMSECV = 0.27%, RMSEP = 0.26%, RPD = 6.06	[21]
FT-NIR	Whole naked oat grain	12,500–4000	90: Cal 45: Val	β-Glucan: Reliable for screening	PLS regression: R ² = 0.98, RMSECV = 0.09%, RMSEP = 0.10%, RPD = 5.13	[21]
FT-NIR	Whole naked oat grain	12,500–4000	90: Cal 45: Val	Avenanthramides: It can only be used for rough screening because of the skewed distribution.	PLS regression: R ² = 0.90, RMSECV = 60.4 mg/kg, RMSEP = 47.7 mg/kg, RPD = 3.37	[21]
FT-NIR	Milled naked oat grain	12,500–4000	90: Cal 45: Val	Protein: more homogeneity and more accurate prediction.	PLS regression: R ² = 0.98, RMSECV = 0.35%, RMSEP = 0.40%, RPD = 6.30	[21]
FT-NIR	Milled naked oat grain	12,500–4000	90: Cal 45: Val	Starch: Accurate; can be milled for more accuracy than whole grain.	PLS regression: R ² = 0.98, RMSECV = 0.52%, RMSEP = 0.63%, RPD = 5.15	[21]
FT-NIR	Milled naked oat grain	12,500–4000	90: Cal 45: Val	Lipid: Excellent predictive power; accurate and reproducible	PLS regression: R ² = 0.97, RMSECV = 0.24%, RMSEP = 0.26%, RPD = 6.24	[21]
FT-NIR	Milled naked oat grain	12,500–4000	90: Cal 45: Val	β-Glucan: Excellent accuracy, surpassing the accuracy of whole-grain models.	PLS regression: R ² = 0.98, RMSECV = 0.06%, RMSEP = 0.09%, RPD = 6.17	[21]
FT-NIR	Milled naked oat grain	12,500–4000	90: Cal 45: Val	Avenanthramides: Utilised for screening only; prediction is less well established.	PLS regression: R ² = 0.90, RMSECV = 59.2 mg/kg, RMSEP = 46.3 mg/kg, RPD = 3.56	[21]
FT-NIR	Whole naked oat grain	~7400–5400	113	Total polyphenols: Good accuracy and robustness in predicting total phenolics in oats	PLS regression: Calibration: R ² = 0.895, RMSECV = 0.0665; Validation: R ² = 0.924, RMSEV = 0.0457	[60]
FT-NIR	Whole oat groats & ground oat groats	10,000–4000	150	β-Glucan content: Predict β-glucan with high accuracy	Modified PLS regression: R ² = 0.93, SEC = 0.18, SECV = 0.23; Ground groats: R ² = 0.94, SEC = 0.16, SECV = 0.22	[61]

Cal—Calibration set; DPPH—2,2-diphenyl-1-picrylhydrazyl (antioxidant assay); r—Pearson Correlation Coefficient; R²—Coefficient of Determination; RMSECV—Root Mean Square Error of Cross-Validation; RMSEP—Root Mean Square Error of Prediction; RMSEV—Root Mean Square Error of Validation; RPD—Ratio of Performance to Deviation; SEC—Standard Error of Calibration; SECV—Standard Error of Cross-Validation; SEP—Standard Error of Prediction; Val—Validation set.

4. Molecular Changes in Oats and FT-IR Detection

Processing, storage, and fermentation result in changes at the molecular level in the oat constituents—including depolymerisations of β -glucan, oxidation of lipids, denaturation and aggregation of proteins, degradation of phenolic antioxidants, and reorganisation of starch crystallinity—which collectively contribute to the final nutritional quality, bioactivity, and shelf life of the final product. Because each of these transformations affects the vibrational behaviour of certain functional groups, Fourier-transform infrared (FT-IR) spectroscopy can be used as a rapid, non-destructive tool to link molecular structure to quality assessment. Specific spectral regions are selectively affected by these changes: the carbohydrate fingerprint region ($1000\text{--}1200\text{ cm}^{-1}$), the carbonyl stretch region ($\sim 1740\text{ cm}^{-1}$), the protein amide I and II bands (~ 1650 and $\sim 1550\text{ cm}^{-1}$), and the starch order-sensitive bands at 1047 and 1022 cm^{-1} [62,63]. The following subsections discuss each of these classes of molecular changes and the corresponding FT-IR markers used to detect the change.

4.1. β -Glucan Molecular Structural Changes

The high-molecular-weight polysaccharide, oat $(1\rightarrow3)$, $(1\rightarrow4)$ - β -D-glucan, is very sensitive to solubility and chain length during processing. In general, the normal oat β -glucan weight is around $1.4\text{--}2.3 \times 10^6\text{ g/mol}$, and this weight can be decreased through the occurrence of thermal processing, extrusion, fermentation, and baking procedures [64]. By adjusting the severity of extrusion, ref. [65] showed that the oat bran cereal could be decreased in β -glucan molecular weight (MW) down to $251,000\text{ g/mol}$ from an initial $1,930,000\text{ g/mol}$, leading to a resulting drop in apparent viscosity of the extracts from 2900 to $131\text{ mPa}\cdot\text{s}$, respectively; because the cholesterol-lowering activity of β -glucan depends on viscosity, this loss is functionally significant [65]. In the presence of prolonged dough fermentation and baking, the polymer exposes itself to endogenous β -glucanases, and aggregation of depolymerized chains may occur with storage: low-MW β -glucan (less than $\sim 50\text{ kDa}$) is stable as dispersions, and only larger fragments may agglomerate with storage above that size [66]. The polymer is also cleavable by enzymatic hydrolysis (e.g., using lichenase), and acid degradation and oxidative degradation will introduce new carbonyl and carboxyl groups—measurable by FT-IR as a new absorption band at 1723 cm^{-1} , which changes rheological and bioactive properties [67].

These structural changes are followed by FT-IR in the carbohydrate fingerprint region between 1000 and 1200 cm^{-1} , where C-O-C and C-O-H backbone stretching vibrations generate the characteristic absorption pattern of the polymer [68]. Hydrothermal treatment at varying temperatures and durations alters the profile of this region, in parallel with the microstructural changes seen by SEM [68]. The same region has been used to confirm the presence of β -glucan in extracted gum pellets [69], while chemical modification such as sulfation introduces readily identified bands at 1250 and 810 cm^{-1} (S=O and C-O-S), demonstrating the sensitivity of the method to structural alteration [70]. Combined with PCA, the $1000\text{--}1200\text{ cm}^{-1}$ window further allows β -glucan to be distinguished from co-extracted polysaccharides such as arabinoxylans in complex cereal matrices, which makes it a convenient means of tracking compositional and structural change through processing [68].

4.2. Lipid Oxidation Pathways

The carbonyl stretching region, whose broadening and increasing asymmetry distinguished the sound from the deteriorated oat oil in the spectral comparison introduced in Section 2 (Figures 1–3), has also been exploited quantitatively on oat lipids. Working with oil extracted from oats, ATR-FT-IR spectra were used to model peroxide value over the carbonyl stretching range between 1852 and 1685 cm^{-1} , obtaining a calibration correlation

of $r = 0.967$ and a prediction correlation of $r = 0.819$ by partial least squares regression [7]. This confirms that the carbonyl region carries enough information to follow oxidative stability in the oat lipid fraction itself, and not only in the simpler edible-oil systems in which the approach was first established.

Oats are unusually vulnerable to lipid oxidation. Their lipid fraction of roughly 5–9% is about five times that of wheat, and their lipase and lipoxygenase activities are 10–15 times higher [71]. Milling brings enzyme and substrate together: lipase liberates free fatty acids (FFA), and the unsaturated species among them, chiefly linoleic and oleic acid, are rapidly attacked by lipoxygenase and peroxygenase to give hydroperoxides and epoxy fatty acids as primary products. In non-heat-treated oat flour, non-volatile oxidised fatty acid (NVOFA) content rose to 1700–2000 $\mu\text{g g}^{-1}$ during storage, epoxy fatty acids appearing first and hydroxy fatty acids subsequently [71]. These primary products decompose in turn to secondary volatile carbonyls, of which hexanal and 2-pentylfuran are the most commonly reported markers and the source of the paint-like off-flavour characteristic of stored raw oat flour [72]. Kilning inactivates the lipases, but it does not settle the matter: bran heat-treated to zero lipase activity generated five to seven times more headspace hexanal after twelve months of storage than untreated bran [73], indicating that polar membrane lipids continue to oxidise slowly once the enzymatic route has been closed [11].

FT-IR reports on this cascade at several diagnostic positions. The carbonyl region between 1740 and 1850 cm^{-1} is the most informative: the band near 1743 cm^{-1} grows as hydroperoxides decompose on the residual ester fragments, and within the same region ester bonds, free carboxylic acids and aldehydic carbonyls can be resolved from one another [11]. The technique is also sensitive to hydroxyl and hydroperoxyl groups, the earliest oxidation intermediates, thereby enabling detection of oxidative damage before secondary volatiles accumulate [12]. Across the wider edible-oil literature, both primary products, expressed as peroxide value, and secondary carbonyls have been quantified from spectral change, most reliably with PLS regression or multivariate curve resolution [13].

4.3. Protein Molecular Structural Changes

Oat proteins, 70–80% of which are globulins, undergo pronounced structural change during thermal processing and storage. The most complete FT-IR characterisation of oat globulin shows a native amide I envelope between 1670 and 1634 cm^{-1} arising from β -turns, β -sheets, α -helices and random coils; under aggregating conditions, the α -helix contribution falls while intermolecular β -sheet bands at 1682 and 1624–1626 cm^{-1} grow, the signature of thermally induced aggregation through β -strand formation [74]. Industrial kilning of oat groats reproduces this pattern, reducing α -helix and random-coil content and promoting intramolecular β -sheet formation and aggregation via noncovalent interactions and disulfide bonds [75]. Notably, that aggregation proceeds without classical denaturation as measured by DSC, which accounts for the fall in protein extractability from 67% to 23% and for the resulting limits on the use of kilned material in liquid oat applications.

The Maillard reaction adds a further layer to these changes. Under prolonged heating or storage, lysine and cysteine residues react with reducing sugars or with β -glucan to form covalent conjugates that alter the secondary structure of the protein. Maillard conjugation of oat protein isolate with β -glucan shifts the C=O stretching and C-H/N-H deformation features in the FT-IR spectrum, and circular dichroism shows a matching loss of α -helix and β -sheet with a gain in β -turn and random coil [76]. Stir-frying at 230 °C drives a progressive conversion of β -turns to β -sheets together with an increase in disulfide content, producing aggregation, larger particles, and reduced digestibility, all traceable through the amide I ($\sim 1650 \text{ cm}^{-1}$) and amide II ($\sim 1550 \text{ cm}^{-1}$) profiles [77]. Dry roasting and microwave irradiation likewise give distinct α -helix to β -sheet and amide I to starch area ratios by

ATR-FT-IR, and these ratios correlate directly with rumen degradability of protein and dry matter [78].

4.4. Avenanthramide and Phenolic Changes

Avenanthramides (AVNs), a class of N-cinnamoylanthranilic acids unique to oats, respond to processing in a structure-dependent way. AVN-C, the caffeic acid conjugate carrying a catechol moiety, is labile at neutral and alkaline pH in combination with heat, whereas the p-coumaric (AVN-A) and ferulic (AVN-B) conjugates are more stable [19,79]. Processing route matters as much as severity: drum drying of steamed rolled oats removed almost all tocopherols and substantially reduced avenanthramides and cinnamic acids, while autoclaving largely preserved tocopherols but still lowered AVNs and left essentially no caffeic acid [79]. Enzymatic loss is a separate pathway. Polyphenol oxidase (PPO), present in oats as in wheat, barley and rye, oxidises avenanthramides when non-heat-treated milled oats are steeped in water [80]. Germination works in the opposite direction, with a 3.6-fold rise in AVN concentration reported in organically grown oats after 96 h, most likely through de novo biosynthesis catalysed by hydroxycinnamoyl transferases [81].

Quantifying individual avenanthramides in whole oat grain by mid-infrared spectroscopy is, however, difficult, even though chemometric FT-IR and NIR models for total phenolic content have been developed successfully. The concentrations involved are very low against a dominant carbohydrate and protein matrix: HPLC profiling of ten oat cultivars, with and without mass spectrometry, returned total AVN concentrations of only 36–303 $\mu\text{g g}^{-1}$ dry weight [82]. The three principal forms are esters of 5-hydroxyanthranilic acid with p-coumaric, ferulic or caffeic acid [83] and differ only in the hydroxylation and methoxylation pattern of the cinnamic acid moiety. Trace concentration and near-identical structure together leave FT-IR with little discriminatory power at the level of the individual compound. NIR-PLS models built specifically for oat polyphenols reach calibration R^2 values around 0.90 [60], but that performance describes the prediction of a total polyphenol pool rather than the resolution of individual avenanthramides. The same limited sensitivity of FT-IR to trace phenolics has been reported elsewhere and identified as a principal constraint on its use in real food matrices [84].

4.5. Starch Retrogradation and Gelatinisation

Gelatinisation and retrogradation are the dominant crystallinity transitions in oat processing, and FT-IR provides a sensitive non-destructive window on both. During gelatinisation, hydrated granules swell and lose semicrystalline order, which registers in the 995–1022 cm^{-1} region: the 995/1022 cm^{-1} ratio follows the transition between 59 and 70 °C accurately, and the magnitude of the change correlates closely with the enthalpy of gelatinisation measured by DSC ($R^2 = 0.988$) [85]. On cooling and storage, the process reverses in two stages, with amylose reassociating within hours and amylopectin recrystallizing over days to weeks, restoring short-range order that is seen as a rise in the 1047/1022 cm^{-1} intensity ratio, where the band near 1047 cm^{-1} reflects ordered domains and that near 1022 cm^{-1} reflects the amorphous fraction [63]. In oat starch specifically, dual autoclaving-retrogradation treatment raised the 1047/1022 cm^{-1} ratio, consistent with the formation of resistant starch (RS3), although XRD additionally revealed V-type crystallinity from amylose–lipid complexes, a contribution of particular relevance in a grain as lipid-rich as oats [86].

Oat starch retrogrades less than wheat starch, with reported degrees being ~28–30% against 42% [87], which has been attributed to its higher gelatinisation temperature and to the inhibitory effect of oat protein and lipid on amylopectin recrystallisation. Oat protein in particular retards short-term retrogradation and weakens the water-binding

capacity of the starch gel; after seven days, appropriate protein levels produced an ordered honeycomb porous gel with a higher resistant starch content [88]. The spectroscopic indices themselves have been validated against thermal analysis, the retrogradation ratios $IRAD_{1047} = H_{1047}/H_{1022}$ and $IRAD_{995} = H_{995}/H_{1022}$ agreeing well with the degree of retrogradation determined by DSC [63]. Over a 28-day period, FT-IR-derived short-range order tracked XRD crystallinity closely throughout long-term retrogradation [89], establishing the technique as a reliable real-time probe of the crystallinity changes that govern textural quality and enzymatic digestibility in processed oat products.

5. Portable FT-IR

Micro-electromechanical systems (MEMS) have made compact FT-IR spectrometers practical outside the laboratory. Designs built on translational micromirror actuators and micromachined silicon interferometers achieve sub-millisecond scan times, high resistance to vibration and mechanical shock, and signal-to-noise ratios adequate for quantitative work in packages of a few cubic centimetres, with analytical performance approaching that of benchtop systems [90–93]. What matters for the present review is the consequence for oats: the measurement can now be taken to the intake point, the mill and the fermentation vessel rather than the sample being brought to the instrument.

In food science, portable and handheld mid-infrared instruments operating in attenuated total reflectance (ATR) mode have been applied to the non-destructive assessment of cereal grains, oats among them. A review of this literature found that portable devices combined with chemometric models returned detection limits, coefficients of determination and discrimination accuracies sufficient for the assessment of food authenticity and composition [22].

Two oat-specific applications illustrate the range. Fermentation of oat-based yoghurt has been monitored by FT-IR of the protein and carbohydrate bands, which tracked pH closely enough to support a predictive model with $R^2 = 0.941$ and $RMSEP = 0.247$ against conventional pH measurements [94]. A portable ATR spectrometer applied to oat groats gave PLSR calibrations across 148 ground samples measured over $4000\text{--}650\text{ cm}^{-1}$, with standard errors of prediction of 0.20% for β -glucan, 0.6% for protein, 1.0% for starch and 0.3% for lipid, accuracies comparable to those obtained on benchtop NIR and FT-IR instruments [57]. Taken together, these results indicate that portable FT-IR-ATR is now dependable enough for on-site screening, fermentation monitoring and routine quality control of oats.

6. Conclusions

This review has brought together the published work on FT-IR spectroscopy as a tool for oat quality control, covering the identification and classification of oat material, the quantification of its principal constituents, and the molecular changes that accompany processing and storage. Read as a whole, the literature supports a consistent conclusion: a single non-destructive measurement, interpreted with a suitable chemometric model, can answer questions that would otherwise require several separate wet chemistry determinations. Oats are a particularly informative matrix in this respect, because their unusually high and highly unsaturated lipid fraction and their soluble β -glucan both give strong, well-separated mid-infrared signatures.

For identification and classification, the evidence assembled in Sections 2.1–2.5 shows that vibrational spectroscopy combined with multivariate classification can separate hulled from naked genotypes, distinguish cultivars and the different milled forms, and detect the adulteration of oat flour with cheaper or gluten-containing material. Classification accuracies reported for these tasks are generally high. Grading draws on the same spectral

information, although the demonstrated instrumental work on groat percentage and kernel sorting is near-infrared, and mid-infrared models at present inform, rather than replace, the physical criteria on which commercial grading currently rests. Where mid-infrared measurements have been combined with complementary techniques such as synchrotron-based FT-IR or X-ray fluorescence, the resulting picture of grain quality is more complete than any single method provides.

For chemical composition, Section 3 shows that FT-IR calibrations for moisture, β -glucan, protein, starch and lipid in oats reach accuracies close to those of the reference methods they are intended to replace, with reported errors of prediction in the range of a few tenths of one per cent for β -glucan and lipid and around one per cent for starch. Moisture, which together with water activity governs storage stability, is among the parameters most readily followed, although the published oat calibrations for it are still few. These calibrations are no longer confined to benchtop instruments: portable and handheld ATR systems built on micro-electromechanical mirror designs now deliver prediction errors comparable to laboratory spectrometers, moving the technique from the analytical laboratory towards the point of intake, the mill, and the processing line.

The molecular basis of these applications is set out in Section 4. Depolymerisation of β -glucan, oxidation and hydrolysis of the lipid fraction, thermally induced protein aggregation, degradation of avenanthramides and starch retrogradation each produce a characteristic and interpretable change in the spectrum, in the carbohydrate fingerprint region ($1000\text{--}1200\text{ cm}^{-1}$), the carbonyl stretching region ($\sim 1740\text{ cm}^{-1}$), the amide I and II bands (~ 1650 and $\sim 1550\text{ cm}^{-1}$) and the order-sensitive starch bands at 1047 and 1022 cm^{-1} . The practical consequence is that sound and deteriorated oat material can be told apart directly from the spectrum. A sound sample shows sharp aliphatic CH_2 stretching bands between 2850 and 3000 cm^{-1} , a symmetric and isolated ester carbonyl peak near 1745 cm^{-1} and a flat hydroxyl region. As deterioration proceeds, hydroperoxide accumulation broadens the band near 3450 cm^{-1} , free fatty acids distort the low-wavenumber side of the ester peak around 1710 cm^{-1} , and, in advanced rancidity, the ester peak is depleted, while aldehydic and ketonic secondary oxidation products contribute an additional absorption near 1728 cm^{-1} . Because these shifts track peroxide value and free fatty acid content, they provide a spectral criterion for accepting or rejecting a lot that does not depend on titration.

Several limitations qualify these conclusions. Most published calibrations rest on modest numbers of samples drawn from a single cultivar set, growing region or season, and their performance on independent material is rarely reported, so the transferability of the models remains largely untested. Part of the evidence on cultivar and category discrimination comes from near-infrared, FT-NIR or hyperspectral measurements rather than from the mid-infrared, and the two should not be treated as interchangeable. There is as yet no agreed protocol for sample presentation and spectral acquisition in oats, and no shared spectral library against which laboratories could validate their own models. The most useful next steps are therefore practical rather than instrumental: multi-site validation on independent harvests, open reference spectra for oat grain and oat products, and model-building software that a quality control operator can use without specialist chemometric training. If those are put in place, FT-IR is well positioned to move from a research technique to a routine element of oat quality assurance.

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Abbreviations

The following abbreviations are used in this manuscript:

ATR	Attenuated total reflectance
FT-IR	Fourier-transform infrared spectroscopy
PLSR	Partial least squares regression
PCA	Principal component analysis
PLS-DA	Partial least squares discriminant analysis
OPLS-DA	Orthogonal partial least squares discriminant analysis
FT-NIR	Fourier-transform near-infrared spectroscopy
RMSEP	Root mean square error of prediction
PDO	Protected designation of origin
SR-FT-IR	Synchrotron radiation-based Fourier-transform infrared
XRF	X-ray fluorescence
ATR-FT-IR	Attenuated total reflectance Fourier-transform infrared
PLS	Partial least squares
NIR	Near-infrared
CARS	Competitive adaptive reweighted sampling
LDL	Low-density lipoprotein
FRAP	Ferric-reducing antioxidant power
CUPRAC	Cupric-reducing antioxidant capacity
SEP	Standard error of prediction
RMSECV	Root mean square error of cross-validation
RPD	Ratio of performance to deviation
RMSEV	Root mean square error of validation
DPPH	2,2-Diphenyl-1-picrylhydrazyl
SEC	Standard error of calibration
SECV	Standard error of cross-validation
MW	Molecular weight
SEM	Scanning electron microscopy
NVOFA	Non-volatile oxidised fatty acid
DSC	Differential scanning calorimetry
AVN	Avenanthramide(s)
AVN-A	Avenanthramide-A (p-coumaric acid conjugate)
AVN-B	Avenanthramide-B (ferulic acid conjugate)
AVN-C	Avenanthramide-C (caffeic acid conjugate)
PPO	Polyphenol oxidase
MS	Mass spectrometry
NIR-PLS	Near-infrared partial least squares
XRD	X-ray diffraction
MEMS	Micro-electromechanical systems

FFA	Free fatty acid
SIMCA	Soft independent modelling of class analogy
LDA	Linear discriminant analysis
SVM	Support vector machine
MSC	Multiplicative scatter correction
VSM	Variable selection method
HPLC	High-performance liquid chromatography
GC	Gas chromatography
NMR	Nuclear magnetic resonance
DDGS	Distillers dried grains and solubles
RS3	Type 3 resistant starch
NR	Not reported

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