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Chemical fingerprinting and cluster-based evaluation of vegetable oils for biodiesel applications

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ABSTRACT

This study evaluates the biodiesel potential of five vegetable oils—safflower, flaxseed, rapeseed, niger seed, and perilla through detailed analysis of their fatty acid composition and key fuel properties. Gas chromatography mass spectrometry (GC-MS/MS) was used to characterize the oils and quantify their saturated, monounsaturated, and polyunsaturated fatty acid contents. The impact of fatty acid profiles on cetane number, oxidative stability, viscosity, and cold-flow behavior was assessed. Hierarchical and K-Means clustering techniques identified chemical similarities and guided the development of optimized blending strategies. Results showed that rapeseed and safflower oils, with high monounsaturated fatty acid content, provided superior oxidative stability and combustion performance. In contrast, flaxseed and perilla oils offered improved cold-flow properties but required stabilization to enhance storage life. Based on these findings, nine biodiesel blend formulations were proposed to balance fuel quality and adapt to different operational conditions. This research demonstrates that integrating chemical fingerprinting and clustering analysis can effectively support feedstock selection and biodiesel optimization.

1. Introduction

The growing global energy demand and environmental concerns make the transition to renewable energy sources essential. In this context, biofuels have gained prominence as alternative energy sources due to their renewability and lower carbon footprint. Biodiesel is a renewable fuel produced from vegetable oils or animal fats. It is biodegradable, emits fewer greenhouse gases than fossil fuels, and can be used in diesel engines without major modifications. This study explores the significance of biodiesel and its advantages over fossil fuels in terms of sustainability and environmental impact. Furthermore, the role and potential of biodiesel within the scope of renewable energy sources will be assessed.

The environmental impacts of fossil fuels and the need for sustainable energy sources are increasingly recognized. Fossil fuel depletion and their combustion products contribute to global issues like greenhouse effects, ozone layer depletion, and pollution [1]. Transitioning to renewable energy sources is crucial for mitigating climate change, ensuring energy security, and promoting social and economic development. However, challenges such as market failures, lack of information, and access to raw materials hinder this transition [2]. The hydrogen energy system, produced from renewable sources, is proposed as a clean and efficient alternative to fossil

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fuels [1]. Additionally, blockchain technology shows potential in enhancing energy market efficiency and integrating renewable resources [3]. Despite challenges like high initial costs and political barriers, the shift to sustainable energy offers economic benefits, including improved energy security and potential job creation [3,4]. In recent years, studies on alternative fuels have become increasingly popular due to their potential to reduce dependence on conventional fossil fuels and mitigate environmental impacts [5, 6].

Biodiesel, a renewable alternative to petroleum diesel, offers several advantages including carbon neutrality, biodegradability, and reduced toxic emissions [7,8]. It is produced from various renewable resources such as vegetable oils, animal fats, and algae through transesterification, with methanol being a common alcohol used [9,10]. Biodiesel exhibits superior properties like higher flash point, cetane number, and lubricity compared to conventional diesel [7,8]. However, challenges include higher viscosity, lower energy content, and poor cold-flow properties. To address feedstock concerns, alternative non-food oilseed crops like camelina and field pennycress are being explored. Production methods have evolved from batch processes to continuous reactors, with the selection of an effective catalyst being crucial for efficiency [7–9].

Biodiesel, a renewable alternative to petroleum-based diesel, offers several advantages including carbon neutrality, biodegradability, and reduced emissions [9,10]. It is primarily produced through transesterification of vegetable oils, animal fats, and other renewable feedstocks. The evolution of biodiesel production has seen four generations, with algae-based third-generation feedstocks showing promise due to high energy content and lower environmental impact [11]. Palm oil and its by-products have emerged as excellent raw materials for biodiesel production, offering properties similar to conventional diesel. However, the food versus fuel debate has led to increased research on utilizing palm oil by-products and mill effluent as alternative feedstocks [12]. Biodiesel can be used in pure form or blended with petroleum diesel, making it suitable for various applications such as vehicles, generators, and heaters [9].

Various vegetable oils have been explored as potential feedstocks for biodiesel production due to their availability, sustainability, and chemical composition. Among them, safflower (Carthamus tinctorius), flaxseed (Linum usitatissimum), rapeseed (Brassica napus), niger seed (Guizotia abyssinica), and perilla (Perilla frutescens) oils have gained attention due to their unique fatty acid profiles and widespread cultivation.

Safflower (*Carthamus tinctorius*) is an oilseed crop widely grown in arid and semi-arid regions. Its seeds contain a high proportion of oleic acid and are rich in monounsaturated fatty acids (MUFA), making safflower oil a promising feedstock for biodiesel production. Its high oxidative stability enhances the shelf life and combustion properties of safflower oil-based biodiesel. Flaxseed (*Linum usitatissimum*) is known for its high polyunsaturated fatty acid (PUFA) content, particularly linolenic acid, and is widely used in industrial applications and nutritional supplements. However, its high PUFA content makes biodiesel more prone to oxidation, requiring stabilizers to prevent degradation. Rapeseed (*Brassica napus*) is among the most commonly used oil crops for biodiesel production, particularly in Europe, due to its balanced MUFA and PUFA composition. With significant levels of oleic acid and linoleic acid, rapeseed oil produces high-quality biodiesel with excellent cold-flow properties and efficient combustion performance. Niger seed oil is rich in linoleic acid and similar to safflower oil but may cause oxidation issues in biodiesel. Perilla (*Perilla frutescens*) contains a high percentage of alpha-linolenic acid, a type of PUFA known for its health benefits. While primarily used in the food and pharmaceutical industries, its high degree of unsaturation makes it a potential biodiesel feedstock, though its oxidation susceptibility remains a challenge.

The suitability of an oil for biodiesel production largely depends on its fatty acid composition, oxidative stability, and combustion properties. Oils with high monounsaturated fatty acid (MUFA) content, such as safflower and rapeseed oils, are the most advantageous in terms of biodiesel stability, cetane number, and fuel efficiency. In contrast, PUFA-rich oils, including flaxseed, niger seed, and perilla, are more prone to oxidative degradation and may require antioxidant additives to enhance biodiesel performance.

One of the most commonly used methods for biodiesel production is the transesterification reaction, where vegetable oils react with methanol and a base catalyst (typically NaOH or KOH) to produce biodiesel (fatty acid methyl esters, FAME) and glycerol as a by-product. The fatty acid profile of the oil directly influences the properties of the resulting biodiesel. Biodiesel derived from safflower and rapeseed oils exhibits high oxidative stability and superior combustion efficiency, making these oils more suitable for long-term fuel storage and high-performance applications. Conversely, biodiesel produced from flaxseed, niger seed, and perilla oils is more susceptible to oxidation, requiring additional processing to improve stability. Moreover, blending different oils can help balance biodiesel's oxidation resistance, viscosity, and combustion performance, leading to an optimized fuel formulation with enhanced properties.

In this study, five different vegetable oils safflower, flaxseed, rapeseed, niger seed, and perilla were investigated for their biodiesel production potential. These oils differ significantly in their proportions of saturated, monounsaturated (MUFA), and polyunsaturated (PUFA) fatty acids, enabling the examination of structural differences that influence key biodiesel fuel properties. One of the main objectives of this study was to evaluate the impact of fatty acid composition on biodiesel characteristics such as cetane number, oxidative stability, viscosity, and cold-flow behavior. The selected oils represent a balance between widely studied feedstocks (e.g., rapeseed and flaxseed) and less commonly explored but agriculturally promising and regionally accessible alternatives (e.g., niger seed and perilla). While some of these crops can be cultivated in arid or marginal lands, others are traditionally used in sectors such as food and health. Thus, the study incorporates not only chemically diverse but also practically viable oil sources. Moreover, the inclusion of underutilized oils aligns with the global trend toward moving beyond food-based feedstocks in biodiesel research. Several studies have also indicated that these oils are suitable feedstocks for biodiesel production. In conclusion, the selected oils were not chosen arbitrarily; rather, they were strategically selected to enable meaningful comparisons, support cluster analyses, and facilitate the development of optimized blending strategies.

2. Material and method

2.1. Fatty acid composition analysis and biodiesel feedstock evaluation

Safflower, flaxseed, rapeseed, niger seed, and perilla oils were examined in this study as potential feedstocks for biodiesel production. These oils were selected due to their chemical composition and the advantages they offer in biodiesel production. Fig. 1 Workflow diagram illustrating the sequential methodology applied in this study, including seed sampling and extraction, fatty acid composition analysis by GC–MS/MS, multivariate statistical evaluation (PCA, hierarchical clustering, K-means clustering), biodiesel fuel property scoring, and blend formulation.

The oils were extracted from their seeds using the cold-press method, a mechanical extraction process that preserves the natural properties of the oil without the use of heat or chemical solvents. This method helps maintain the stability and purity of the extracted oils, making them more suitable for biodiesel applications. Following extraction, the oils were separated from solid residues and filtered to remove any remaining particulates, ensuring a cleaner and more refined oil. This refining process enhances the quality of the oils, minimizing impurities that could affect the efficiency of biodiesel production. By preserving the natural characteristics of the oils and ensuring their purity, the cold-press method provides a sustainable and efficient approach to obtaining high-quality feedstocks for biodiesel production. Fig. 2 shows the seed samples and the corresponding oil samples obtained from them. This image demonstrates the originality of the raw materials at the beginning of the experimental process and provides a visual representation of the materials used.

The efficiency of biodiesel production largely depends on the oil content of the feedstock. In this study, five different oilseeds were analyzed: flaxseed, perilla, niger seed, rapeseed, and safflower, each with varying crude oil content. The oil content of the seeds was determined as follows: perilla (51 %), flaxseed (47 %), niger seed (46 %), rapeseed (46 %), and safflower (35 %). Perilla seeds exhibited the highest oil yield, making them a potentially rich source for biodiesel production. Flaxseed and rapeseed also demonstrated significant oil content, contributing to efficient oil extraction and transesterification processes. Niger seed, despite having a slightly lower oil content, is still considered a viable option. Safflower, with the lowest oil yield among the studied seeds, may require additional processing or blending with higher-yielding oils to optimize biodiesel production. The variation in oil content among these seeds highlights the importance of selecting appropriate feedstocks to maximize biodiesel efficiency and yield. While high oil content is desirable for increased biodiesel output, the fatty acid composition and oxidative stability of these oils must also be considered to ensure optimal fuel properties.

The fatty acid profile of each oil was determined using gas chromatography-mass spectrometry (GC-MS/MS), and their chemical fingerprint was analyzed. GC-MS/MS was employed to determine the composition of fatty acid methyl esters (FAMEs). GC-MS/MS is

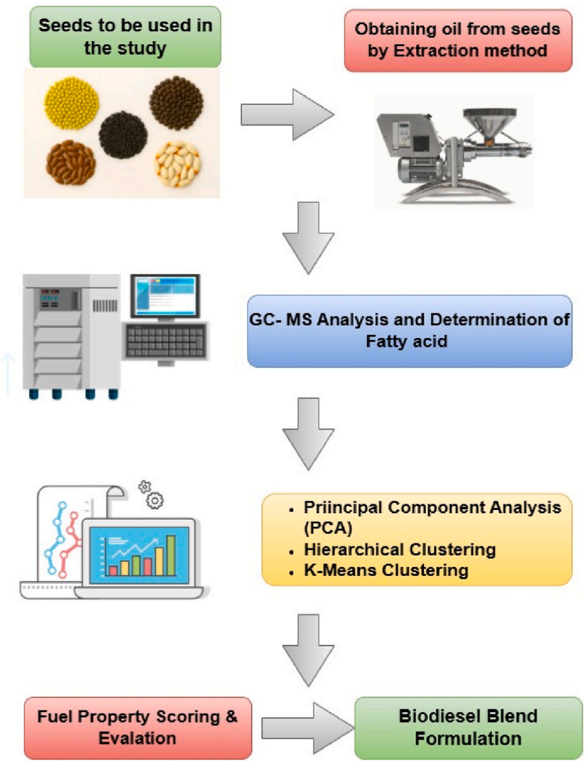

Fig. 1. Workflow diagram of the study methodology.

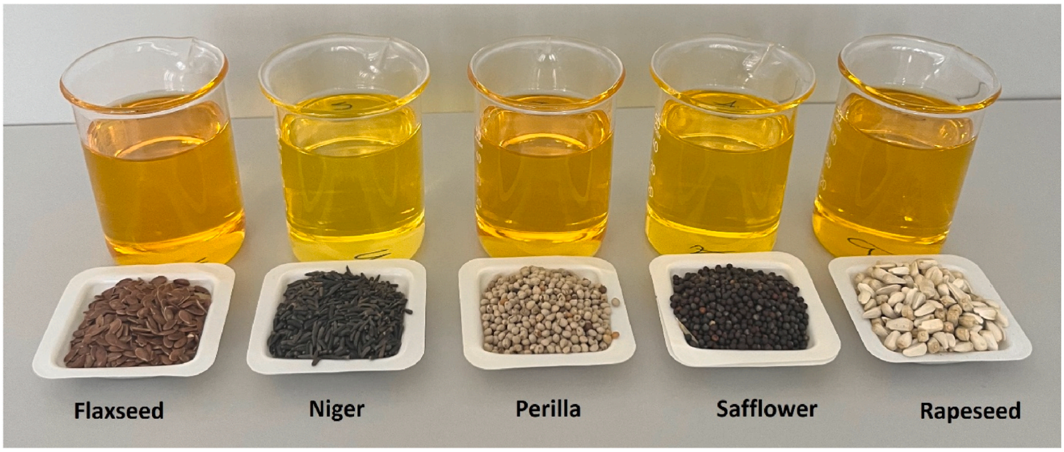

Fig. 2. Oilseeds used in this study and the cold-pressed oil samples obtained from them.

Table 1
Results of fatty acid distribution of seeds.

Component Name	Safflower	Flaxseed	Rapeseed	Niger	Perilla	
	%	%	%	%	%	
Tridecanoic acid (C13:0)	0.00	0.00	0.00	0.00	0.00	**Saturated fatty acids**
Lauric acid (C12:0)	0.00	0.00	0.02	0.00	0.00	
Butyric acid (C4:0)	0.00	0.00	0.00	0.00	0.00	
Undecanoic acid (C11:0)	0.00	0.00	0.00	0.00	0.00	
Pentadecanoic acid (C15:0)	0.04	0.04	0.04	0.04	0.01	
Tricosanoic acid (C23:0)	0.06	0.01	0.02	0.06	0.13	
Heneicosanoic acid (C21:0)	0.02	0.02	0.03	0.01	0.01	
Arachidic acid(C20:0)	2.12	1.59	2.57	2.65	2.98	
Capric acid (C10:0)	0.00	0.00	0.08	0.00	0.00	
Heptadecanoic acid (C17:0)	0.00	0.14	0.11	0.00	0.00	
Caproic acid (C6:0)	0.00	0.01	0.01	0.00	0.01	
Behenic acid (C22:0)	0.00	0.60	1.65	0.00	0.00	
Myristic acid (C14:0)	0.28	0.08	0.11	0.15	0.04	
Lignoceric acid (C24:0)	0.66	0.00	0.85	2.02	0.05	
Palmitic acid (C16:0)	10.72	8.81	7.72	11.62	10.16	
Caprylic acid (C8:0)	0.00	0.00	0.00	0.00	0.00	
Stearic acid (C18:0)	6.08	9.67	2.91	11.79	3.48	
Total	**19.97**	**20.97**	**16.12**	**28.33**	**16.87**	
Nervonic acid (C24:1)	0.82	0.13	0.00	0.05	0.01	**Monounsaturated fatty acids**
Palmitoleic acid (C16:1)	0.08	0.08	0.12	0.08	0.07	
Pentadecenoic acid (C15:1)	0.00	0.00	0.00	0.00	0.00	
Heptadecenoic acid (C17:1)	0.18	0.13	0.21	0.03	0.06	
Eicosenoic acid (C20:1)	1.43	0.90	4.72	1.53	1.01	
Myristoleic acid (C14:1)	0.00	0.00	0.00	0.00	0.00	
Oleic acid (C18:1n9c)	31.09	19.94	40.92	21.97	19.03	
Elaidic acid (C18:1n9t)	0.99	0.72	1.48	0.84	0.92	
Erucic acid (C22:1n9)	0.50	0.05	1.99	0.10	0.09	
Total	**35.10**	**21.95**	**49.44**	**24.61**	**21.19**	
Linolelaidic acid (C18:2n6t)	0.04	0.60	0.15	0.07	0.02	**Polyunsaturated fatty acids**
Eikosapentaenoik acid (C20:5n3)	0.06	0.02	0.02	0.06	0.13	
Linoleic acid (C18:2n6c)	43.00	20.19	19.20	44.06	18.71	
Eikosatrienoik acid (C20:3n6)	0.00	0.03	0.00	0.00	0.00	
Dokosadienoik acid (C22:2)	0.15	0.01	0.02	0.00	0.00	
Arasidonic acid (C20:4n6)	0.00	0.26	0.08	0.00	0.01	
Eikosadienoik acid (C20:2)	0.20	0.00	0.02	0.13	0.31	
Alpha linolenic acid (C18:3n3)	1.28	35.88	14.04	2.69	42.71	
Dokosahegzaenoik acid (C22:6n3)	0.01	0.02	0.02	0.00	0.01	
Eikosatrienoik acid (C20:3n3)	0.01	0.03	0.04	0.00	0.00	
Gamma linolenic (C18:3n6)	0.16	0.00	0.27	0.03	0.02	
Total	**44.91**	**57.05**	**33.84**	**47.04**	**61.93**	

widely used in biodiesel research due to its high specificity, sensitivity, and ability to separate and quantify complex mixtures with precision. It enables the accurate identification of saturated, monounsaturated, and polyunsaturated fatty acids, which are key parameters influencing biodiesel quality. The detailed fatty acid profiles obtained via GC-MS/MS analysis played a crucial role in comparing the biodiesel suitability of the selected vegetable oils. The content of saturated, monounsaturated, and polyunsaturated fatty acids was evaluated to assess their suitability for biodiesel production. Safflower and rapeseed oils, which have a high proportion of monounsaturated fatty acids, emerged as the most suitable options for biodiesel due to their high oxidative stability and superior combustion properties. In contrast, flaxseed, niger seed, and perilla oils, with their high polyunsaturated fatty acid content, may be more prone to oxidation, requiring additional stabilization measures. The results obtained from these analyses provide a critical foundation for identifying the most suitable raw materials for biodiesel production and optimizing biodiesel fuel properties. Table 1 shows the results of fatty acid distribution of the seeds. The summary of saturated, monounsaturated, and polyunsaturated fatty acid contents is shown in Fig. 3.

Table 1 shows the fatty acid composition of safflower, flaxseed, rapeseed, niger seed, and perilla oils, which were analyzed to assess their suitability for biodiesel production (see Fig. 4). The composition of each oil was determined using GC-MS/MS and classified into three major categories: saturated, monounsaturated, and polyunsaturated fatty acids. Since the fatty acid profile directly influences the physicochemical properties of biodiesel, identifying these compositions is crucial for optimizing biodiesel quality and performance.

The saturated fatty acid group includes palmitic acid, stearic acid, and arachidic acid, which enhance oxidative stability and improve the long-term storage capacity of biodiesel. However, high levels of saturated fatty acids can negatively affect the cold-flow properties of biodiesel, making it more prone to solidification at low temperatures. Therefore, maintaining a balanced composition of saturated fatty acids is essential to ensure biodiesel performance under varying climatic conditions.

The monounsaturated fatty acid category consists of oleic acid, eicosenoic acid, and nervonic acid, which contribute to enhanced oxidative stability and improved combustion efficiency. Oils with a high monounsaturated fatty acid content, such as rapeseed and safflower oils, offer superior stability and better fuel properties. Rapeseed oil, with its high oleic acid content, is considered one of the most stable options for biodiesel production, while safflower oil also provides improved oxidation resistance and prolonged storage stability, making it a highly suitable biodiesel feedstock.

The polyunsaturated fatty acid category includes linoleic acid, alpha-linolenic acid, and eicosapentaenoic acid, which improve biodiesel lubricity, reducing engine component wear. However, high polyunsaturated fatty acid content increases oxidative susceptibility, leading to biodiesel degradation over time. Flaxseed and perilla oils have the highest alpha-linolenic acid content, making them highly prone to oxidation. Similarly, safflower and niger seed oils, with their high linoleic acid content, may require additional stabilization to prevent oxidative deterioration during storage.

The results presented in the table serve as a foundation for identifying the most suitable oils for biodiesel production and optimizing fuel formulations. Oils with high monounsaturated fatty acid content, such as safflower and rapeseed, were identified as the most suitable options for biodiesel production due to their superior stability and combustion characteristics. Meanwhile, oils with high polyunsaturated fatty acid content, such as flaxseed, niger seed, and perilla, may require antioxidant additives to enhance oxidation resistance and improve biodiesel quality. These findings provide valuable insights into blending different oils to develop biodiesel formulations with balanced oxidation resistance, viscosity, and combustion efficiency. The experimental procedures, analytical techniques, and evaluated parameters are summarized in Table 2.

Table 2 provides a comprehensive summary of the experimental procedures and conditions applied throughout this study. It includes information on the selected vegetable oils, the extraction and characterization methods, the clustering analysis techniques used for classifying chemical profiles, and the key biodiesel fuel properties evaluated. This overview ensures clarity and transparency of the experimental design, enabling reproducibility and facilitating comparison with similar studies.

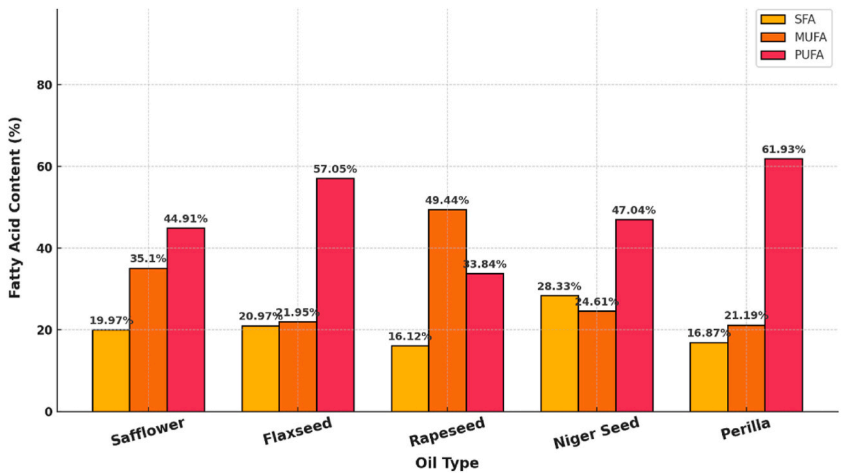

Fig. 3. Fatty acid composition of the tested vegetable oils.

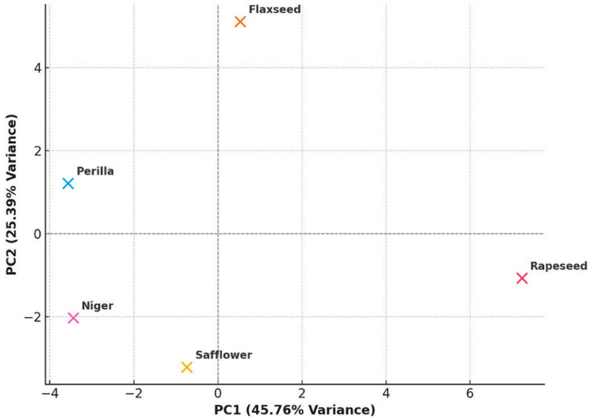

Fig. 4. Hierarchical clustering of fatty acids (Dendrogram).

Table 2
Summary of experimental procedures, parameters, and analytical techniques.

Parameter	Description
Tested Vegetable Oils	Safflower, Flaxseed, Rapeseed, Niger Seed, Perilla
Extraction Method	Cold-press mechanical extraction
Fatty Acid Profiling Method	Gas Chromatography–Mass Spectrometry (GC–MS/MS)
Analyzed Fatty Acid Categories	Saturated Fatty Acids (SFA), Monounsaturated Fatty Acids (MUFA), Polyunsaturated Fatty Acids (PUFA)
Clustering Analysis Techniques	Hierarchical Clustering (Ward's Linkage, Euclidean Distance), K-Means Clustering
Optimal Cluster Determination	Elbow Method
Evaluated Biodiesel Properties	Cetane Number, Oxidative Stability, Viscosity, Cold-Flow Performance, Combustion Efficiency
Output Visualizations	Dendrogram, K-Means Cluster Plot, Heat Map, Blend Formulation Table

3. Results and discussion

3.1. Chemical fingerprinting and cluster analysis

The chemical composition of vegetable oils plays a crucial role in determining their suitability for biodiesel production. Fatty acid composition directly affects key fuel properties such as oxidative stability, viscosity, ignition quality, and cold flow behavior. To classify and compare different oil sources, chemical fingerprinting techniques are employed to analyze their structural characteristics [13–15]. In this study, GC-MS/MS was used to determine the fatty acid profile of safflower, flaxseed, rapeseed, niger seed, and perilla oils. The obtained data were then subjected to cluster analysis, including hierarchical clustering (dendrogram) and K-Means clustering, to identify similarities and differences between the oils. These clustering techniques provide insights into the grouping patterns of oils based on their chemical composition, allowing for the selection of the most suitable feedstocks for biodiesel production [16,17]. In this study, both Hierarchical Clustering and K-Means Clustering methods were employed together. Hierarchical Clustering progressively reveals the multidimensional similarity relationships among the oil samples through the dendrogram output and demonstrates the natural formation of classes. This method is particularly effective for exploring the data structure in cases where the number of clusters is not predetermined. In contrast, K-Means Clustering partitions the samples into more compact groups based on a predefined number of clusters and highlights the average chemical profiles of each cluster by determining their centroids. By applying these methods in combination, the validity and reliability of the results were enhanced through comparative analysis. The optimal number of clusters was objectively determined using the Elbow method, ensuring that the analyses were based on sound methodological grounds. Thus, by integrating the advantages of different clustering approaches, the biodiesel suitability of the oil samples was evaluated in a more comprehensive manner. Hierarchical clustering was performed to visualize the degree of similarity between different oils, while K-Means clustering was used to classify the oils into distinct groups based on their fatty acid profiles. These analyses help optimize biodiesel formulation by identifying which oils can be blended to enhance fuel stability and performance. Fig. 2 shows the hierarchical clustering of fatty acids (Dendrogram).

Hierarchical clustering is a powerful unsupervised machine learning method that groups data points based on their similarity [18,19]. In this study, hierarchical clustering was applied to categorize different seed oils according to their fatty acid compositions, particularly their saturated (SFA), monounsaturated (MUFA), and polyunsaturated (PUFA) fatty acid content. The dendrogram visually represents these relationships and provides insight into how closely related each oil type is in terms of chemical composition. The dendrogram in this study was generated using Ward's linkage method, which minimizes the variance within clusters to ensure more compact and meaningful groupings. The Euclidean distance metric was used to measure similarity between the oils. Oils that merge at lower distances in the dendrogram are chemically more similar, while those merging at higher distances are more distinct from each other.

From the hierarchical clustering results:

- Rapeseed oil is distinctly located on the positive PC1 axis in the PCA score plot, indicating a statistically significant separation from the other oils. This differentiation primarily results from its high monounsaturated fatty acid (MUFA) proportion and low saturated fatty acid content. Such a profile enhances oxidative stability and renders rapeseed oil a promising feedstock with superior combustion characteristics for biodiesel production.
- Flaxseed oil exhibits a high positive PC2 score, demonstrating a unique chemical composition driven by its substantial polyunsaturated fatty acid (PUFA) content. The elevated PUFA level adversely affects oxidative stability, implying a potential need for antioxidant additives or blending strategies when utilized as biodiesel feedstock.
- Safflower oil occupies a moderately negative position on both PC1 and PC2 axes, indicating a composition characterized by a high oleic acid MUFA profile. This distinctive fatty acid pattern contributes to a higher cetane number and improved combustion efficiency, underscoring safflower oil's potential as a high-performance biodiesel precursor.
- Niger seed oil is positioned within the negative PC1 and negative PC2 quadrant, clustering closely with Perilla oil. This spatial proximity suggests a balanced MUFA/PUFA ratio and moderate oxidative stability, making it a candidate for biodiesel blends aiming to balance fuel stability and cold flow properties.
- Perilla oil shows negative PC1 and positive PC2 scores, reflecting compositional similarities to Niger seed oil. This profile indicates a relatively high proportion of unsaturated fatty acids and moderate stability potential, supporting its consideration as an alternative biodiesel feedstock.

Additionally, the percentage values indicated on the PC1 and PC2 axes represent the proportion of total variance in the dataset explained by each principal component. The PC1 axis accounts for 45.76 % of the variability in the fatty acid profiles, while the PC2 axis explains 25.39 %. Together, the first two components capture 71.15 % of the total variance, demonstrating that the plotted positions effectively reflect the compositional differences among the seed oils.

Hierarchical clustering provides valuable insights into the suitability of different oils for biodiesel production. Oils that are chemically similar can be considered for blending, while those that are significantly different may require additional processing or formulation adjustments. This method also helps to identify potential substitutions for biodiesel feedstocks, ensuring optimal fuel quality while maintaining cost efficiency. By analyzing the hierarchical clustering results, the study provides a scientific basis for selecting and optimizing biodiesel feedstocks. Oils with high MUFA content (such as Safflower oil) may be preferred due to their superior oxidative stability and better combustion properties. On the other hand, PUFA-rich oils (such as Flaxseed oil) may require antioxidants or blending with more stable oils to enhance biodiesel performance. These findings are critical for the renewable energy sector, as biodiesel quality is heavily influenced by the chemical structure of its feedstocks. Hierarchical clustering serves as a data-driven approach to refining feedstock selection, ensuring that biodiesel production is both efficient and sustainable. Hierarchical Clustering of Fatty Acids (Dendrogram) is given in Fig. 3.

Findings from the Hierarchical Clustering Analysis:

This dendrogram presents the results of the hierarchical clustering analysis performed based on the fatty acid profiles of five different seed oils. The analysis was conducted using Ward's linkage method and the Euclidean distance metric. The seed oils displayed along the horizontal axis are arranged according to their chemical composition, while the vertical axis represents the Euclidean distance, indicating the magnitude of dissimilarity between clusters. As shown in the figure, flaxseed and perilla oils are merged at a low distance, demonstrating a high degree of similarity in their fatty acid profiles. These two oils form a chemically similar group, primarily due to their high proportions of polyunsaturated fatty acids (PUFA). In contrast, rapeseed oil is separated at a much higher distance near the top of the dendrogram, indicating the most pronounced compositional difference among all the samples. This separation can be attributed to its high monounsaturated fatty acid (MUFA) content. Safflower and niger oils are grouped together at a moderate distance, reflecting their balanced composition with comparable MUFA and PUFA ratios, which makes them more homogeneous as a cluster. This clustering structure provides a valuable basis for understanding the potential blendability and functional properties of the oils in biodiesel production. Overall, hierarchical clustering analysis systematically classifies the similarities and differences among the fatty acid profiles of the examined seed oils, offering a scientific reference for feedstock selection in biodiesel applications.

The dendrogram results obtained in this study are fully consistent with the fatty acid distribution presented in Fig. 3. The separation and clustering patterns observed in the dendrogram are based on the overall proportions of saturated, monounsaturated (MUFA), and polyunsaturated (PUFA) fatty acids in each oil sample. Notably, the distinct positioning of safflower oil due to its high MUFA content and the grouping of flaxseed oil driven by its elevated PUFA proportion directly corroborate the chemical profile findings shown in Fig. 3. This consistency highlights the accuracy and scientific validity of the hierarchical clustering analysis conducted.

Significance of Hierarchical Clustering for Biodiesel Applications: Hierarchical clustering plays a crucial role in determining which oils are most suitable for biodiesel production. Oils with similar chemical structures can be blended to optimize fuel properties, while those with different characteristics may require additional processing or stability enhancement. The chemical structure of the feedstock directly influences biodiesel stability, viscosity, and combustion efficiency. Oils rich in MUFA (e.g., safflower oil) are considered ideal options for biodiesel due to their stability and high cetane number, whereas PUFA-rich oils (e.g., flaxseed oil) may need antioxidants or blending with more stable oils to improve their oxidative resistance. This analysis provides a data-driven approach for selecting the best biodiesel feedstocks, ensuring that biodiesel production is both efficient and sustainable. The insights from hierarchical clustering can also be used to detect potential adulteration in biodiesel by comparing the fatty acid fingerprint of commercial biodiesel samples against known profiles. In conclusion, hierarchical clustering serves as a powerful analytical tool for biodiesel research, helping to classify, optimize, and enhance fuel quality based on the chemical properties of different feedstocks. K-Means Clustering of Fatty Acid Profiles is given in Fig. 6.

K-Means clustering is a widely used unsupervised machine learning technique that groups data into a predefined number of clusters based on similarity (see Fig. 7). In this study, K-Means clustering was applied to classify different seed oils based on their fatty acid composition and to determine the most suitable oils for biodiesel production [20,21]. The analysis presented in this figure focuses on the quantification and comparison of saturated fatty acids (SFA), monounsaturated fatty acids (MUFA), and polyunsaturated fatty acids (PUFA) across the investigated seed oils. This approach enables a clear understanding of the chemical profiles of the oils and their suitability for biodiesel production.

Findings from the K-Means Clustering Analysis:

- Safflower oil exhibited a high MUFA content (~44.91 %), highlighting its potential as an ideal biodiesel feedstock due to improved oxidative stability and combustion performance.
- Flaxseed oil displayed the highest PUFA proportion (~57.05 %), indicating increased susceptibility to oxidative degradation. Consequently, stabilization measures, such as antioxidant addition or blending with more stable oils, may be necessary.
- Rapeseed oil had the highest MUFA content (~49.44 %) among all samples, supporting its classification as a preferred biodiesel feedstock with superior cetane number and storage stability.
- Niger seed oil and Perilla oil demonstrated a more balanced MUFA-PUFA profile, with PUFA content exceeding 47 %, suggesting moderate oxidative stability and potential blending compatibility.

Importance of Fatty Acid Profiling for Biodiesel Applications:

The comparative evaluation of fatty acid composition provides critical insights into the performance characteristics of biodiesel derived from different feedstocks. Specifically:

- MUFA-rich oils, such as safflower and rapeseed, are associated with higher oxidative stability, lower viscosity, and improved cold flow properties, making them preferable for biodiesel production.
- PUFA-dominant oils, notably flaxseed and perilla, may require additional processing or formulation strategies to enhance stability and fuel quality.
- The relative abundance of oleic acid (MUFA) emerges as the most influential factor determining the oxidative stability and cetane number of biodiesel fuels.

The clustering analyses performed in this study further confirmed that fatty acid composition is the principal determinant of chemical similarity among the oils. Oils with higher oleic acid content were distinctly separated from PUFA-rich oils in both hierarchical and K-Means clustering. This finding reinforces the significance of MUFA content as a critical parameter for selecting, blending, and optimizing biodiesel feedstocks. Overall, the fatty acid composition analysis presented here offers a scientific foundation for the development of efficient, stable, and high-performance biodiesel fuels, supporting more sustainable bioenergy production.

The clustering analyses performed in this study revealed that the fatty acid composition was the main determinant of the chemical similarity among the investigated oils. Specifically, the oleic acid content, representing the proportion of monounsaturated fatty acids (MUFA), emerged as the principal component driving the clustering patterns. Oils with higher oleic acid concentrations, such as safflower and rapeseed oils, were distinctly separated from PUFA-rich oils like flaxseed and perilla. This observation was consistent across both hierarchical and K-Means clustering methods.

In hierarchical clustering, the first division (largest dissimilarity) corresponded to the differentiation between oils dominated by MUFA (notably oleic acid) and those with elevated levels of polyunsaturated fatty acids, particularly linolenic acid. Similarly, in K-

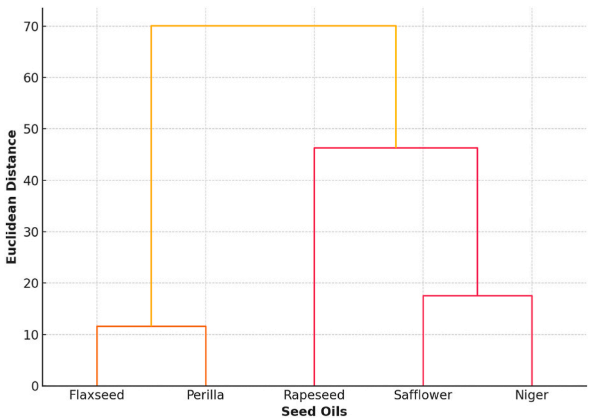

Fig. 5. Hierarchical clustering of fatty acids (dendrogram).

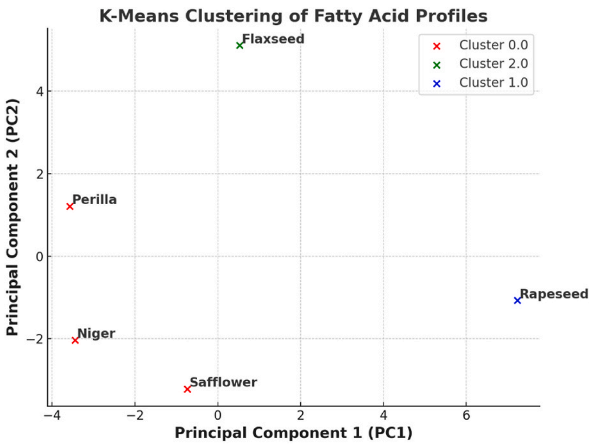

Fig. 6. K-means clustering of fatty acid profiles.

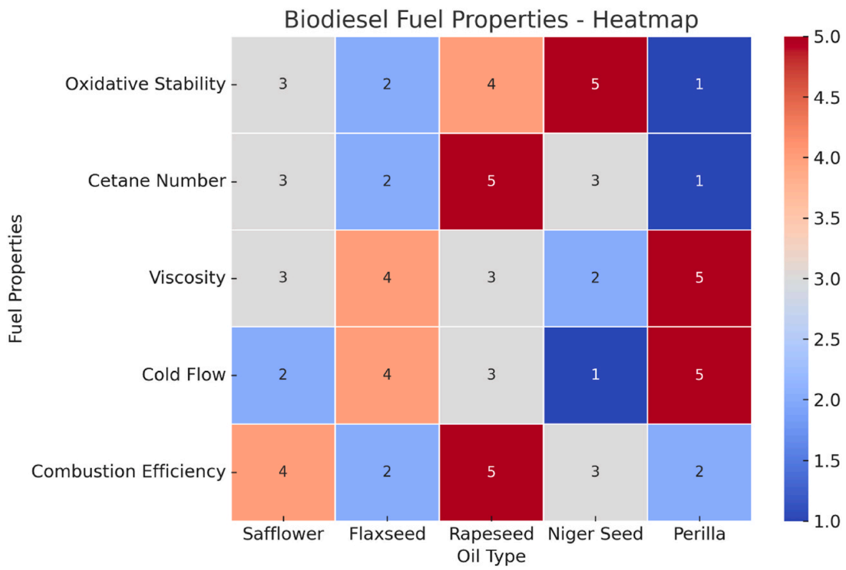

Fig. 7. Heat map of biodiesel fuel properties of oils.

Means clustering, the cluster containing safflower and rapeseed oils demonstrated significantly higher MUFA percentages, confirming that oleic acid was the most influential factor in defining the principal component that accounted for the majority of variance among samples. Therefore, the principal component can be identified as the relative abundance of oleic acid, which not only dictates the chemical fingerprint of the oils but also correlates strongly with key biodiesel properties, including oxidative stability and cetane number. This finding underscores the importance of MUFA content as a critical parameter in selecting and blending feedstocks for biodiesel production.

3.2. Evaluation of fuel properties

This heatmap visually represents the biodiesel fuel properties of different vegetable oils. Darker red colors indicate better performance, while darker blue colors represent weaker performance. Each oil has been evaluated based on oxidative stability, cetane number, viscosity, cold flow properties, and combustion efficiency, with ratings ranging from 1 to 5 points. Below is a detailed explanation of the safflower, flaxseed, rapeseed, niger seed, and perilla oils, focusing on their individual fuel characteristics. Heat map of biodiesel fuel properties of oils given in Fig. 5.

Safflower oil is a moderately suitable feedstock for biodiesel production. Oxidative stability is rated at 3 points, indicating moderate performance. Compared to oils with higher saturated fat content, it has a shorter shelf life but still offers reasonable oxidation resistance. Cetane number is rated at 3 points, meaning its combustion efficiency in diesel engines is average neither outstanding nor poor. Viscosity is also rated at 3 points, meaning it is thick enough to prevent excessive injector wear but not too thick to cause clogging issues. However, cold flow properties are rated at 2 points, meaning it tends to solidify at lower temperatures, making it less suitable for cold climates. Combustion efficiency is rated at 4 points, which means it provides a relatively clean burn with minimal carbon buildup. Overall, safflower oil is a decent biodiesel option with good combustion properties but poor cold flow performance.

Flaxseed oil has some advantages but is weak in oxidative stability. With an oxidative stability rating of 2 points, it is prone to degradation due to its high polyunsaturated fatty acid (PUFA) content, making it unsuitable for long-term storage. Cetane number is also rated at 2 points, which means it has a lower ignition quality and may result in delayed combustion. Viscosity is rated at 4 points, meaning it has a lower viscosity, making it ideal for fuel injectors and ensuring smooth flow through the engine. Cold flow properties receive a rating of 4 points, indicating that it remains fluid even in lower temperatures, reducing the risk of fuel gelling. Combustion efficiency is rated at 2 points, meaning it burns less efficiently and produces more NO_x emissions. Overall, flaxseed oil performs well in cold conditions but has poor oxidative stability, requiring antioxidants to prevent degradation.

Rapeseed oil is one of the best biodiesel feedstocks due to its balanced properties. Oxidative stability is rated at 4 points, meaning it has a good balance between saturated and unsaturated fatty acids, ensuring better storage stability. Cetane number is rated at 5 points, making it the best oil for combustion efficiency, as it ignites quickly and cleanly. Viscosity is rated at 3 points, meaning it has a moderate flow rate and works well in fuel injection systems. Cold flow properties are rated at 3 points, indicating that while it is not the best choice for extremely cold climates, it still performs adequately in moderate temperatures. Combustion efficiency is rated at 5 points, meaning it burns cleanly with minimal residue and improves engine longevity. Overall, rapeseed oil is the most well-rounded biodiesel feedstock with excellent cetane number, stable oxidation, and high combustion efficiency.

Niger seed oil is one of the most oxidation-resistant biodiesel feedstocks. With an oxidative stability rating of 5 points, it has the highest oxidation resistance due to its high saturated fat content, allowing for longer storage without degradation. Cetane number is rated at 3 points, meaning it offers a balanced combustion performance. Viscosity is rated at 2 points, indicating that it is thicker than most other oils and may cause clogging issues in fuel injectors. Cold flow properties are rated at 1 point, making it the least suitable oil for low temperatures as it solidifies quickly. Combustion efficiency is rated at 3 points, providing moderate burning performance. Overall, niger seed oil is highly stable for long-term storage but is not recommended for cold environments due to its poor flow properties.

Perilla oil is one of the best-performing oils in cold weather conditions but has some major drawbacks. With an oxidative stability rating of 1 point, it is the least stable oil due to its extremely high PUFA content, making it highly prone to oxidation and degradation. Cetane number is rated at 1 point, meaning it has the lowest ignition quality and is not an efficient fuel. Viscosity is rated at 5 points, making it highly fluid and ideal for fuel injectors as it reduces clogging risks. Cold flow properties are rated at 5 points, making it the best oil for extremely cold conditions as it remains fluid even at low temperatures. Combustion efficiency is rated at 2 points, meaning it produces more carbon buildup and has a lower overall burning efficiency. Overall, perilla oil is a great choice for cold weather applications but has very poor oxidative stability and combustion efficiency.

The heatmap constructed in this study provides a comparative analysis of biodiesel fuel properties based on the fatty acid composition of each vegetable oil. Each oil was evaluated according to five key parameters: cetane number, oxidative stability, viscosity, cold flow performance, and combustion efficiency, and scored on a scale from 1 (poor performance) to 5 (excellent performance). This scoring system was visualized through color intensities on the heatmap, where darker red shades indicate superior fuel characteristics and blue tones represent weaker performance. This approach not only enables individual evaluation of each oil but also highlights their relative strengths and limitations. As such, it offers valuable insights for selecting optimal combinations in biodiesel formulations. By integrating visual and numerical data, this method facilitates multidimensional assessment of fuel quality and serves as a practical tool for designing sustainable and efficient biodiesel blends.

3.3. Biodiesel blend formulations

Research has shown a clear relationship between the fatty acid composition of biodiesel and its cetane number (CN), a key indicator of ignition quality. As the content of saturated fatty acids, particularly palmitic and stearic acid, increases, the CN value rises, improving ignition quality [22]. This correlation is attributed to the influence of fatty acid alkyl moiety on ignition delay, with longer chain lengths and higher degrees of saturation reducing delay duration [23]. Studies have demonstrated that biodiesel derived from palm oil, rich in saturated fatty acids, exhibits higher CN values compared to other feedstocks. Furthermore, researchers have developed methods to synthesize stearic acid derivatives as potential CN improvers, with some showing superior performance to traditional additives [24]. These findings highlight the importance of fatty acid composition in determining biodiesel quality and engine performance. Polyunsaturated fatty acids (PUFA) improve the cold flow properties of biodiesel, overcoming a major drawback of this alternative fuel. Linoleic and linolenic acids contribute to better cold weather performance by reducing the cloud point, pour point and cold filter plugging point of biodiesel. Researchers have investigated various methods to increase PUFA content and improve the cold flow properties of biodiesel, including the synthesis of fatty acid derivatives and the use of additives [25,26]. The oxidative stability of biodiesel decreases with increasing polyunsaturated fatty acid (PUFA) content. Higher monounsaturated fatty acid (MUFA) content, especially oleic acid, increases stability [27,28]. The viscosity of biodiesel increases with fatty acid chain length and saturation, affecting fuel properties and engine performance [23,29]. Longer chain lengths and higher saturation levels lead to increased viscosity, boiling point, and cetane number, but may negatively impact low-temperature properties. However, balancing fatty acid composition is crucial, as different fatty acids have varying effects on biodiesel properties. Genetic modification of feedstocks could potentially address multiple fuel property issues simultaneously by altering fatty acid profiles [30]. Biodiesel's oxidative stability is a critical factor affecting its commercial viability and long-term use in engines. Unsaturated fatty acid components significantly influence oxidation deterioration and stability [31]. Oxidation can alter biodiesel properties, including viscosity, acid value, and cetane

Table 3
Biodiesel blend formulations.

Formulation Code	Oil Blend Ratios (%)	Theoretical Advantages	Suggested Application Area
F1	Rapeseed (60 %) + Flaxseed (40 %)	High cetane number, good cold-flow balance and low NO_x emissions	Light vehicles, urban diesel engines
F2	Safflower (50 %) + Perilla (30 %) + Niger (20 %)	MUFA/PUFA balance; fluidity and combustion compatibility	Cold climate engines, agricultural machinery
F3	Rapeseed (40 %) + Niger (30 %) + Perilla (30 %)	Oxidative stability and cold-flow balance	Generators, mid-sized vehicles
F4	Safflower (40 %) + Flaxseed (30 %) + Rapeseed (30 %)	Good stability and low-temp flow	Rural transport, farm equipment
F5	Flaxseed (60 %) + Perilla (40 %)	High cold-flow performance; low viscosity	Emergency vehicles in cold regions
F6	Rapeseed (70 %) + Safflower (30 %)	High cetane number; long shelf life	Long-distance transport, hot climate engines
F7	Rapeseed (50 %) + Perilla (25 %) + Flaxseed (25 %)	Moderate cold-flow and stability, balanced combustion	Commercial vehicles, minibuses
F8	Niger (40 %) + Safflower (30 %) + Flaxseed (30 %)	High combustion efficiency, engine protection, compatible viscosity	Light-duty vehicles, short-range logistics
F9	Perilla (50 %) + Niger (25 %) + Rapeseed (25 %)	High cold resistance, moderate combustion performance	Public transport in winter conditions

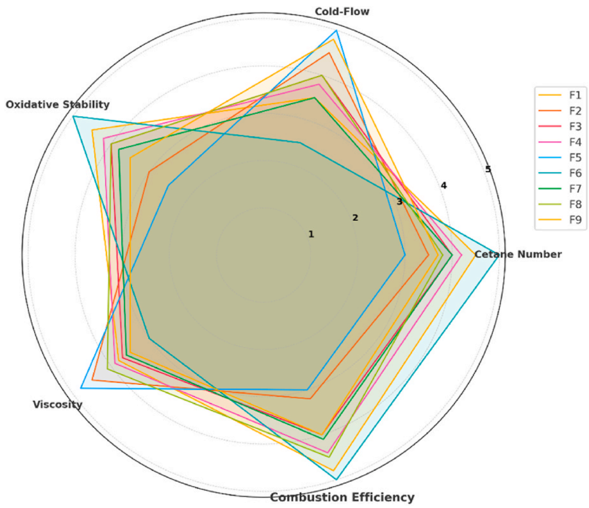

Fig. 8. Fuel properties of biodiesel blend formulations.

number, potentially impacting engine performance and emissions [31,32].

The detailed analysis of individual oils has highlighted the critical influence of fatty acid composition on key biodiesel properties such as cetane number, oxidative stability, viscosity, and cold-flow behavior. However, while each oil exhibits unique advantages, none alone provides an ideal balance of all desired fuel characteristics. For this reason, strategic blending of different oils emerges as a promising approach to synergize the strengths of multiple feedstocks and compensate for their individual limitations. By leveraging complementary fatty acid profiles, it becomes possible to formulate biodiesel blends that meet the performance demands of specific applications and environmental conditions. In this context, Table 3 presents a set of optimized biodiesel blend formulations derived from the oils examined in this study. Each blend is designed to enhance critical fuel properties, offering targeted benefits such as improved combustion efficiency, enhanced oxidative stability, or superior cold-weather performance. These formulations represent practical pathways for producing high-quality biodiesel with balanced characteristics, contributing to both engine compatibility and environmental sustainability.

The primary objective of these formulations was to mitigate the individual limitations of each oil such as poor oxidative stability, high viscosity, or weak cold-flow properties by leveraging the complementary advantages of others. For example, flaxseed and perilla oils possess high degrees of unsaturation, which can hinder oxidative stability, but these drawbacks can be compensated by blending with rapeseed or safflower oils that exhibit better cetane numbers and thermal resistance. Similarly, oils with high viscosity were balanced with more fluid oils to ensure compliance with fuel standards and engine requirements. Each formulation was tailored to optimize specific biodiesel performance characteristics such as ignition quality, storage stability, and seasonal adaptability. The suggested application areas for each blend ranging from light vehicles in urban settings to generators and agricultural equipment were identified based on the theoretical fuel properties and practical feasibility. This blend-based approach enables the development of high-quality biodiesel fuels that are chemically balanced, functionally versatile, and more aligned with real-world operational and environmental conditions. The performance scores of these formulations across major fuel quality indicators are visually summarized in Fig. 8.

4. Conclusion

This study comprehensively assessed the biodiesel potential of safflower, flaxseed, rapeseed, niger seed, and perilla oils by evaluating their fatty acid composition and key fuel properties relevant to combustion and storage stability. Among the tested feedstocks, rapeseed and safflower oils exhibited the most favorable profiles, with high monounsaturated fatty acid content contributing to improved oxidative stability, cetane number, and overall combustion performance. In contrast, flaxseed and perilla oils showed better cold-flow properties, which can be advantageous in colder climates but may necessitate antioxidant treatment to mitigate oxidation risks during storage.

Clustering and comparative analyses further indicated that blending different oils could balance positive attributes, enhancing biodiesel quality and performance across a range of applications. Based on these findings, it is recommended that biodiesel producers explore strategic blending formulations tailored to regional climatic conditions and specific engine requirements. Further research focusing on long-term storage stability, economic feasibility, and engine performance testing will help optimize the use of these non-edible feedstocks as sustainable biodiesel sources.

Future studies could focus on the long-term storage stability and oxidative degradation of blended biodiesel formulations under different environmental conditions. Additionally, engine performance and emission tests with various blend ratios will be valuable to validate the practical applicability of these feedstocks. Economic assessments and life cycle analyses are also recommended to evaluate the sustainability and commercial viability of large-scale biodiesel production from non-edible oils.

CRediT authorship contribution statement

Hüseyin Söyler: Writing – review & editing, Writing – original draft, Validation, Resources, Methodology, Formal analysis, Conceptualization. **Mustafa Kemal Balki:** Software, Methodology, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Nomenclature

GC–MS/MS	Gas Chromatography–Mass Spectrometry
MUFA	Monounsaturated Fatty Acids
PUFA	Polyunsaturated Fatty Acids
SFA	Saturated Fatty Acids
FAME	Fatty Acid Methyl Esters
PCA	Principal Component Analysis
PC1	Principal Component 1
PC2	Principal Component 2
CN	Cetane Number
NO_x	Nitrogen Oxides
NaOH	Sodium Hydroxide
KOH	Potassium Hydroxide
F1–F9	Biodiesel Blend Formulation Codes (Formulation 1 to Formulation 9)

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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