

# Prediction of Fuel-related Properties of *papaya* Seed Oil and Lard Oil Methyl esters from their fatty acid methyl ester compositions-based models

Ezekannagha C. B.<sup>1\*</sup>, Onukwuli O. D.<sup>2</sup>

<sup>1\*</sup>Department of Chemical Engineering, Madonna University, Nigeria

<sup>2</sup>Department of Chemical Engineering, Nnamdi Azikiwe University, Awka, Anambra State, Nigeria

Corresponding Author: \*contactchy20@gmail.com

Received 15 July 2025; revised 19 August 2025; accepted 30 October 2025

## Abstract

This work aims to establish a correlation between the compositions of fatty acid methyl ester (FAME) and the key fuel properties of methyl ester. The experimental data of the analysis was obtained from the methyl esters of calcined hybrid-banana-plantain-peel ash (CHBPPA)-catalyzed methanolysis of *papaya* seed oil (PSO) and lard oil (LO) produced at the optimal reaction conditions of temperature 60°C:57°C, catalyst amount 2.5 wt.:%:2.5 wt.%, time 1 h:1.5 h, and methanol/oil molar ratio 9:1:10.5:1, respectively. PSO and LO methyl esters were characterized using American Society for Testing and Materials (ASTM) methods, as well as Fourier-Transform-Infrared-Spectroscopy (FTIR) and Gas Chromatography-Mass Spectrometry (GC-MS) to determine their physicochemical properties, functional groups, and FAME compositions. Methyl Oleate (C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>) was identified as the dominant ester in PSO (48.01%) and LO (31.63%) methyl esters. PSO methyl ester was found to possess 54% monounsaturated fatty acids, while LO methyl ester was predominantly composed of 58% saturated fatty acids. The predicted fuel properties included cetane number (CN), higher heating value (HHV), iodine value (IV), and saponification value (SV). These predicted values, derived from the FAME profiles, were compared with experimental values obtained through ASTM standard testing. The average absolute deviations (AAD) between predicted and experimental values for PSO and LO methyl esters were 3.64:4.85, 0.83:1.92, 11.66:10.46, and 2.16:3.29% for CN, HHV, IV, and SV, respectively, indicating a good correlation. Hence, a satisfactory prediction of the fuel-related properties based on the FAME composition can be given by the models, signaling the possibility of establishing a cost-effective and improved efficiency process.

**Keywords:** fatty acid methyl ester (FAME), fuel properties, lard oil, models, *papaya* seed oil, prediction

## 1. Introduction

In the pursuit of sustainable energy sources and the mitigation of environmental impacts associated with fossil fuels, methyl ester, commonly known as biodiesel, has emerged as a promising alternative for transportation and industrial fuels (Ezekannagha et al., 2025; Wang et al., 2025). Derived from renewable feedstocks such as vegetable oils, waste cooking oils, and animal fats, methyl ester offers the potential for reduced greenhouse gas emissions and decreased reliance on finite petroleum resources (Guimaraes, 2025). Amongst the available feedstocks for methyl ester synthesis, lard oil (LO) and *papaya* seed oil (PSO) stand out due to their abundance, oil content, low cost and potential as viable sources. Feedstock selection plays a vital role in determining the sustainability of methyl ester production (Ansari et al., 2025). In addition, understanding and predicting the fuel-related properties of

methyl ester derived from these feedstocks are crucial steps towards their sustainability and efficient utilization in the transportation sector. Lard oil is a by-product of the pork rendering process and is among the least expensive feedstocks available for methyl ester synthesis (Ezekannagha et al., 2024). On the other hand, papaya seeds are not consumed and have sufficient oil content ranging from 30% – 34%, which makes them useful as feedstock for biodiesel production.

Triglycerides, the main constituents of vegetable oils and animal fats, undergo transesterification reaction to yield fatty acid methyl esters (FAMES), the key components of biodiesel (Ezekannagha et al., 2023). The fatty acid composition of biodiesel is directly derived from its parent oil or fat, and this composition significantly impacts the fuel's properties, implying that the characteristics of biodiesel are largely dependent on the fatty acid structure of the source oil utilized (Ezekannagha et al., 2017, Knothe 2009). As the chemical composition of these FAMES, characterized by the types and proportions of fatty acids present, greatly influences the fuel properties of biodiesel, factors such as cetane number, higher heating value, viscosity, density, and oxidative stability play pivotal roles in determining biodiesel's performance in internal combustion engines (Bamgboye and Hansen 2008).

Prior research has elucidated correlations between the fatty acid composition of biodiesel feedstocks and their resulting fuel properties. For instance, saturated fatty acids tend to enhance oxidative stability, but they can also elevate viscosity, while unsaturated fatty acids often contribute to improved cold flow properties but may compromise oxidative stability. These complicated interaction patterns underscore the importance of understanding how the compositions of lard oil and papaya seed oil, specifically their FAME compositions influence the fuel-related properties of the resulting methyl esters (Esonye et al., 2018).

While predictive models exist for estimating biodiesel properties based on FAME compositions of common feedstocks like soybean oil and palm oil, there remains a gap in utilizing these comprehensive models tailored to predict the fuel-related properties of lard oil and papaya seed oil methyl esters. Employing accurate predictive models for these feedstocks (lard oil, papaya seed oil, etc.) and their methyl esters is essential for biodiesel producers, researchers, and policymakers to make informed decisions regarding feedstock selection and process optimization. Leveraging models to predict the key fuel properties of lard oil and papaya seed oil methyl esters will enhance understanding of the relationship between their chemical compositions and the fuel-related properties. Ultimately, there will be facilitation of the efficient utilization of these alternative feedstocks in methyl ester production, thereby promoting sustainability and reducing reliance on fossil fuels.

Notably, Tong et al., (2011) and Gopinath (2009) have demonstrated the feasibility of using FAME compositions to predict some key fuel properties of biodiesel derived from different feedstocks. However, to the best of our knowledge, there is limited research specifically on predicting the fuel-related properties of papaya seed oil methyl ester (PSOME) and waste lard oil methyl ester (WLOME) based on their FAME compositions.

Therefore, this study aims to address this gap in literature by employing models to predict some fuel-related properties (cetane number-CN, higher-heating-value-HHV, saponification value-SV and iodine value-IV) of PSO and WLO methyl esters based on their FAME compositions as determined by GC-MS. This will contribute to the advancement of utilizing models in biodiesel research and the sustainable development of the biodiesel industry. It will also facilitate the transition to a more environmentally friendly transportation sector. In addition, the influence of fatty acid composition on the fuel-related properties of PSOME and WLOME was ascertained.

## **2. Materials and Methods**

### **2.1 Materials**

Discarded *papaya* seeds and waste pork lard obtained from Ariaria market, Enugu, and home-based waste were utilized to extract *papaya* seed oil and lard oil, respectively. Calcined hybrid banana-plantain peel ash (CHBPPA) synthesized from a prior experiment by Ezekannagha et al., (2024) was utilized. Extractive solvent (n-hexane), methanol (CH<sub>3</sub>OH, 99.8% purity) and other chemicals/reagents were purchased from Conraws Company Ltd, Enugu. All the chemicals and reagents employed were of superior purity.

## 2.2 Analytical Methods

The PSO, WLO, and the methyl esters of *papaya* seed oil and lard oil obtained at the optimum reaction conditions of temperature 60°C: 57°C, catalyst amount of 2.5 wt.%, 2.5 wt.%, time of 1 h: 1.5 h, and methanol/oil molar ratio of 9:1: 10.5:1 in prior experiments of Ezekannagha et al., (2024) and Ezekannagha et al., (2024a), respectively, were subjected to ASTM methods, FTIR, and GC-MS characterization techniques. The physico-chemical properties, FTIR-based functional groups and the GC-MS-based fatty acid compositions of the papaya seed oil (PSO), waste lard oil (WLO), *papaya* seed oil methyl ester (PSOME) and waste lard oil methyl ester (WLOME) were ascertained.

### 2.2.1 American Society for Testing and Materials (ASTM) Methods

The PSOME and WLOME fuel-related properties, saponification value (SV), and iodine value (IV) were determined using standard laboratory techniques as stipulated by the ASTM International standard (Equations (1-2)) while cetane number (CN) and higher heating value (HHV) were ascertained from Equations (3-4) suggested by Mohibbe et al., (2025) by substituting the experimental values of IV and SV in Equations (3) and (4), respectively.

$$\text{Iodine value-IV} = \frac{V_b - V_a \times 12.69 \times 0.1}{\text{Wt.}(g) \text{ of sample}} \quad (1)$$

$$\text{Saponification value-SV} = \frac{56.1 \times N \times (V_b - V_a)}{\text{Wt.}(g) \text{ of sample}} \quad (2)$$

w= weight of oil taken in grams, N= normality of HCl solution, V<sub>a</sub>= volume of HCl solution used in the test in millilitres, V<sub>b</sub>= volume of HCl solution used in the blank in millilitres.

$$\text{Cetane number-CN} = 46.3 + \left(\frac{5458}{\text{SV}}\right) - 0.225(\text{IV}) \quad (3)$$

$$\text{Higher heating number-HHV} = 49.43 - [0.041(\text{SV}) + 0.015(\text{IV})] \quad (4)$$

### 2.2.2 Fourier Transform Infrared (FTIR) Spectroscopy Analysis

Papaya seed oil (PSO), papaya seed oil methyl ester (PSOME), waste lard oil (WLO) and waste lard oil methyl ester (WLOME) samples were subjected to FTIR spectroscopy analysis (Model: Agilent-Cary 630) for functional group identification in the wavelength region of 4000 - 650 cm<sup>-1</sup>.

### 2.2.3 Gas Chromatography -Mass Spectrometry (GC-MS) analysis

The fatty acid compositions of PSOME and WLOME were examined using GC-MS (Model: Agilent 6890 gas chromatograph, CA, USA).

### 2.2.4 Prediction of PSO and WLO methyl ester fuel properties from their fatty acid methyl ester compositions-based models

Based on the compositions of the different compounds present in the PSOME and WLOME determined by GC-MS, the saponification value (SV), iodine value (IV), cetane number (CN), and higher heating value (HHV) of the biofuels were calculated.

The saponification and iodine values of the PSOME and WLOME were calculated, respectively, via the model expressions (Equations 5-6) adopted by Ezekannagha et al., (2017).

$$\text{IV} = \sum \frac{(254 \times D_i \times A_i)}{MW_i} \quad (5)$$

$$\text{SV} = \sum \frac{(560 \times A)}{MW_i} \quad (6)$$

where *IV* is the iodine value, *SV* is the saponification value, *D* is the number of double bonds; *A<sub>i</sub>* and *MW<sub>i</sub>* are the percentage composition and molecular mass of a particular ester, respectively.

The cetane number and higher heating values of PSOME and WLOME based on the GC-MS data were calculated by substituting the empirical values of Equations 5 and 6 in Equation 3 and Equation 4, respectively, as applied by Ezekannagha et al., 2017.

Degree of unsaturation (DU) was determined based on percentages of monounsaturated and polyunsaturated FAMES of the PSOME and WLOME, respectively, with Equation (7).

$$\text{DU} = (\text{monounsaturated Cn} : 1 \text{ wt}\%) + 2 (\text{polyunsaturated Cn} : 2, 3 \text{ wt}\%) \quad (7)$$

Saturated fatty acid methyl esters (FAMES) have single bonds between carbon atoms e.g. (Cn:0). Monounsaturated FAMES have one double bond between carbon atoms, e.g., (Cn:1); and Polyunsaturated FAMES have multiple double bonds between carbon atoms e.g., (Cn:2, 3).

### 2.3 Comparison of the ASTM experimental and model-predicted values

The error functions- absolute relative error (ARE), average absolute deviation (AAD), variance  $S^2$ , and residual root mean square error (RMSE) were used to perform the error analysis and variability of the experimental and predicted datasets. The metrics are shown in Equations (8-11).

(i) The absolute relative error (ARE):

$$ARE = \left| \frac{(\text{predicted} - \text{experimental})}{\text{experimental}} \right| \quad (8)$$

(ii) The average absolute deviation (AAD):

$$AAD = \frac{100}{n} \sum_{i=1}^n \left| \frac{\phi_{cal} - \phi_{exp}}{\phi_{exp}} \right| \quad (9)$$

(iii) The variance ( $S^2$ ):

$$S^2 = \sum \frac{(\phi_{cal} - \phi_{exp})^2}{n-1} \quad (10)$$

(iii) The residual root mean square error (RMSE):

$$RMSE = \sqrt{\frac{1}{n-2} \sum_{i=1}^n (\phi_{exp} - \phi_{cal})^2} \quad (11)$$

where n is the number of data points,  $\phi_{exp}$ ,  $\phi_{cal}$  are the respective experimental and calculated/predicted property values

## 3. Results and Discussion

### 3.1 Physicochemical properties of PSO and PSO methyl ester

Table 1 comprises the results of the physicochemical characterization of the PSO and optimum PSO methyl ester. The PSOME results are compared with the ASTM D6751 and EN14214 international standards. The acid value, free fatty acid and kinematic viscosity reduced to a large extent, followed by specific gravity, saponification and iodine values, water content and flash point, which also reduced moderately after the transesterification reaction. This shows that the transesterification reaction has a great influence on the PSO conversion to PSO methyl ester. A great conformity was noted on comparing the PSO methyl ester with the international standards for fuel (ASTM D6751; EN14214), which indicates its aptness to be consumed in a diesel engine.

**Table 1:** PSO and PSOME fuel-related properties

Properties	Units	PSO	PSOME	ASTM D6751	EN14214
Acid-value	MgKOH/g oil	5.3	0.46	0.50 max.	0.50 max
Free-Fatty-Acid	%	2.7	0.23	-	-
Specific-gravity@30°C	-	0.902	0.855	0.86 – 0.90	0.85
Kinematic-viscosity@40°C	mm <sup>2</sup> /s	44.860	3.56	1.9 – 6.0	3.5 – 5.0
Saponification-value	MgKOH/g oil	215.384	188.6	-	-
Iodine-value	gI <sub>2</sub> /100g oil	46.192	40.30	-	3 min
Water-content	%	0.5	-	-	-
Peroxide-value	MEq/kg	43.91	-	-	-
Cetane-number	-	-	67	47 min	51 min
Higher-heating-value	MJ/kg	-	41.2	40 – 42	-
Flash-point	°C	228	126	130 min	120 min
Cloud-point	°C	-	+3	-3 to 12	-
Pour-point	°C	-	+2	-15 to 10	-

### 3.2 Physicochemical Properties of WLO and WLO Methyl Ester

Table 2 depicts the physicochemical properties of the WLO and WLO methyl ester. The acid value, free fatty acid, and kinematic viscosity decreased drastically when compared with the values obtained from the waste lard oil. This indicates the CHBPPA-catalyzed transesterification reaction has a great impact on the process with improved fuel quality. Though the physicochemical properties of the WLO methyl ester compared positively with other researchers' findings, they are contained in the ASTM D6751 and EN-14214 limits.

**Table 2:** WLO and WLOME fuel-related properties

Properties	Units	WLO	LOME	ASTM-D6751	EN-14214
Acid-value	mgKOH/g oil	2.2	0.28	0.50 max	0.50 max
Free-fatty-acid	%	1.1	0.14	-	-
Specific-gravity@30 °C	-	0.915	0.873	0.86 – 0.90	0.85
Kinematic-viscosity@40 °C	mm <sup>2</sup> /s	80.994	4.63	1.9 – 6.0	3.5 – 5.0
Saponification-value	mgKOH/g oil	226.459	199.7	-	-
Iodine-value	gI <sub>2</sub> /100g oil	34.491	32.42	-	3 min
Water-content	%	0.53	-	-	-
Peroxide-value	MEq/kg	81.40	-	-	-
Cetane-number	-	-	68	47 min	51 min
Higher-heating-value	MJ/kg	-	41.1	40 - 42	-
Flash-point	°C	240	135	130 min	120 min
Cloud-point	°C	-	+9	-3 to 12	-
Pour-point	°C	-	+6	-15 to 10	-

### 3.3 PSO and PSO methyl ester functional groups

The PSO and PSO methyl ester samples were analyzed via FTIR to determine the functional groups present in the samples, which exhibited a high level of similarities, as could be seen in Figs. 1-2. This could be as a result of the inherent high-level chemical similarities that exist between triglyceride and methyl ester emanating from the C=O and C-O ester functional groups present in the analyzed samples. However, functional group modification was observed in the FTIR spectrum of the PSO after the transesterification process whereby it was converted to biodiesel. The significant modifications were observed in the FTIR spectra region of 1500 – 1000cm<sup>-1</sup>, which is due to the replacement of the CH<sub>2</sub> functional group in the triglyceride by the CH<sub>3</sub> functional group in the methyl ester. The peak at 1241.2cm<sup>-1</sup> in the PSOME spectrum suggests the asymmetric stretching of the group C-O-C. The nonexistence of a peak in the region of 1650 -1540cm<sup>-1</sup> implies the absence of soap formation, commonly referred to as saponification, in the synthesized biodiesel. Niju *et al.*, (2018) and Salaheldeen *et al.*, (2015) obtained similar results to the results recorded in this study.

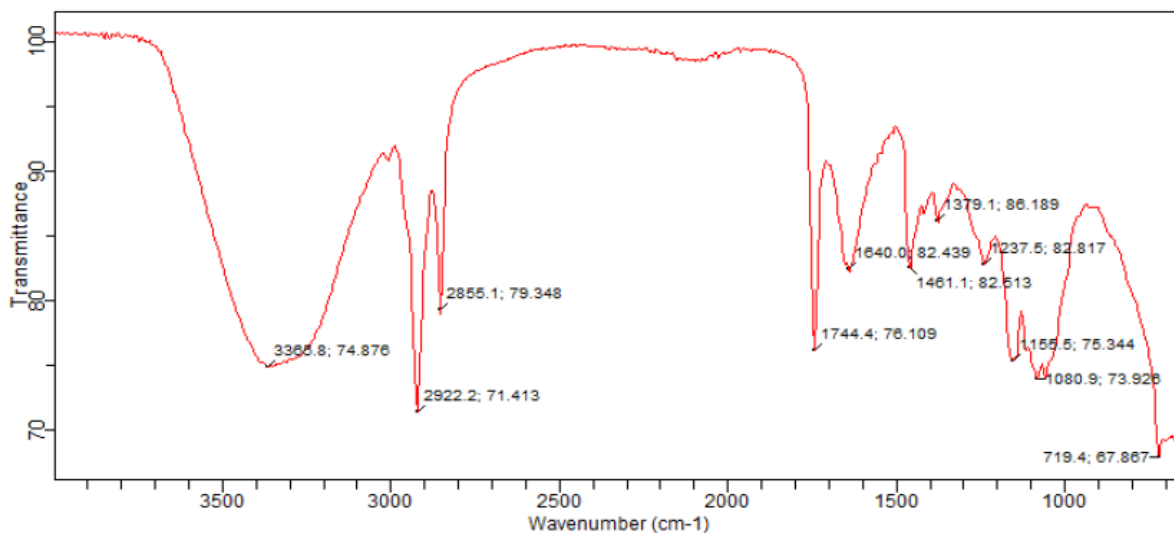


Fig. 1: FTIR spectrum of PSO.

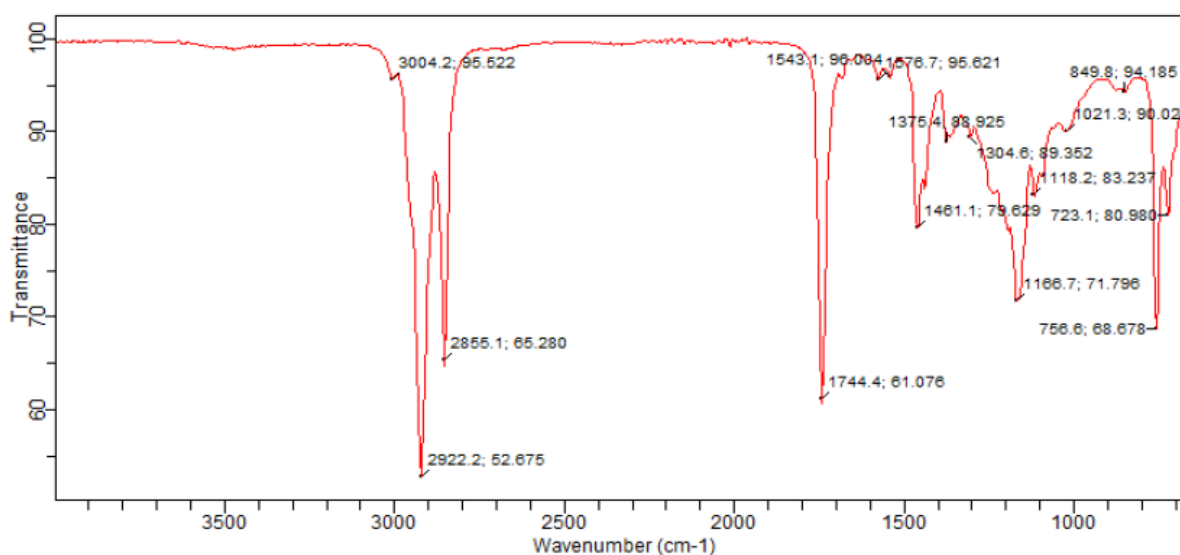


Fig. 2: FTIR spectrum of PSO methyl ester.

### 3.4 WLO and WLO methyl ester functional groups

WLO and WLO methyl ester samples were analyzed using FTIR to determine the functional groups present in the samples. The FTIR spectra of the WLO and transesterified lard oil-WLO methyl ester were carried out in the range of 4000 - 650 cm<sup>-1</sup> to study the effect of transesterification on the lard oil. The FTIR spectra results of WLO and WLO methyl ester are shown in Figs. 3 - 4, respectively. Changes were observed in the (%) transmission and the functional groups, which indicate the modifications that occurred during the transesterification process. The FTIR spectra of the WLO and WLO methyl ester are very similar because of high chemical similarities that exist between triglycerides and methyl ester. However, a small difference is observed in these three regions: C=O ester, CH<sub>3</sub> and C-O ester, as WLO methyl ester has a different compound/functional group bonded, methyl - CH<sub>3</sub>, compared to the lard oil, which has CH<sub>2</sub> bonded to it. In Figs. 3 - 4, the strong ester peaks at 1744cm<sup>-1</sup> (C=O ester) and at 1170 - 1200 cm<sup>-1</sup> (C-O ester) are clearly present in the WLO and WLO methyl ester spectra, which is where the high similarities between the triglyceride and methyl ester emanate from. According to Meyer *et al.*, (2000), the wave frequencies (cm<sup>-1</sup>); for C=O ester and C-O ester functional groups are 1750 - 1725cm<sup>-1</sup> and 1170 - 1200cm<sup>-1</sup> respectively. This compared favorably with the wavenumber ranges found in the WLO and WLO methyl ester spectra, in this study for the C=O and C-O ester groups. Outside these two regions, another characteristic peak which indicates the presence of CH<sub>3</sub> group in the

mixtures of methyl ester can be observed at  $1445\text{cm}^{-1}$ . A similar finding was reported by Yun Hin *et al.*, (2011).

It should also be noted that triglycerides irrespective of the natural source they are derived from, like animal fats, vegetable oil, plant oil etc. contain the same functional groups. This could be seen in Fig. 1 and Fig. 3 for PSO and WLO, respectively. Similar functional groups in PSO and WLO were also recorded by several other researchers, such as Niju *et al.*, (2018) and Salaheldeen *et al.*, (2015), confirming the observation made.

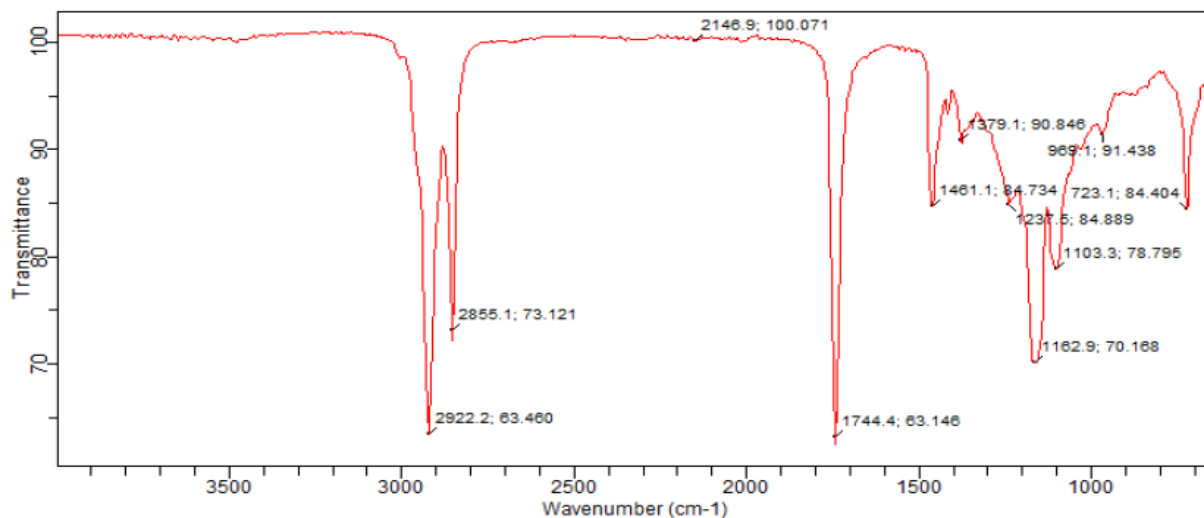


Fig. 3: FTIR spectrum of WLO.

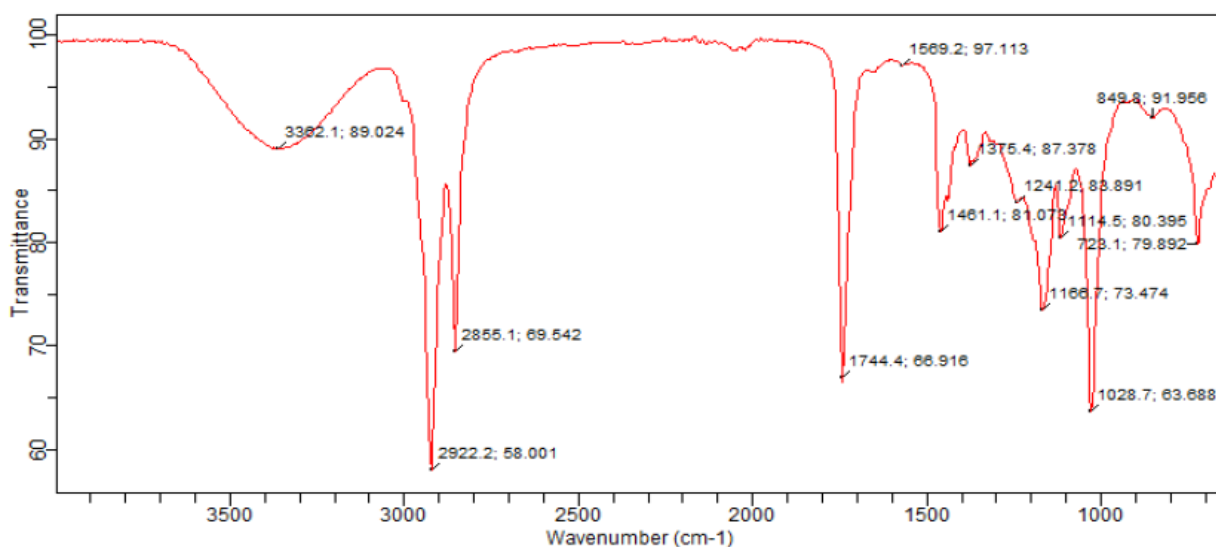


Fig. 4: FTIR spectrum of WLO methyl ester.

### 3.5 PSO Methyl Ester Fatty Acid Content

The fatty acid methyl ester (FAME) content of the analyzed PSO methyl ester was summarized in Table 3, while the chromatogram was depicted in Figure 5. The profile results of the analyzed sample shown in Table 3 revealed 9-octadecenoic acid, methyl ester (E)- (methyl oleate:  $\text{C}_{18}\text{H}_{34}\text{O}_2$ ) as the predominant fatty acid compound with the highest percentage of 48.6%, followed by hexadecanoic acid, methyl ester (methyl palmitate:  $\text{C}_{16}\text{H}_{32}\text{O}_2$ ) with 27.44%, and are monounsaturated fatty acid (MUFA) and saturated fatty acid (SFA), respectively. The result infers that the unsaturated compound is more than the saturated compound. This implies that the synthesized PSOME will not solidify easily when used in engines rather it will flow just like the conventional diesel fuel. The findings of Agunbiade *et al.*, (2014)

corroborate with the results of this study. The palmitic and oleic acids in the analyzed sample resulted in 75.45% of the fatty acid methyl ester composition which suggests good fuel properties. A similar order of FAME compounds was also observed in the LOME sample analyzed. Polyunsaturated fatty acids (PUFA's), also termed essential fatty acids, which are compounds with more than one carbon double bond, are not present in the analyzed sample. The methyl esters with area (%) less than 0.10 were unpublished in Table 3.

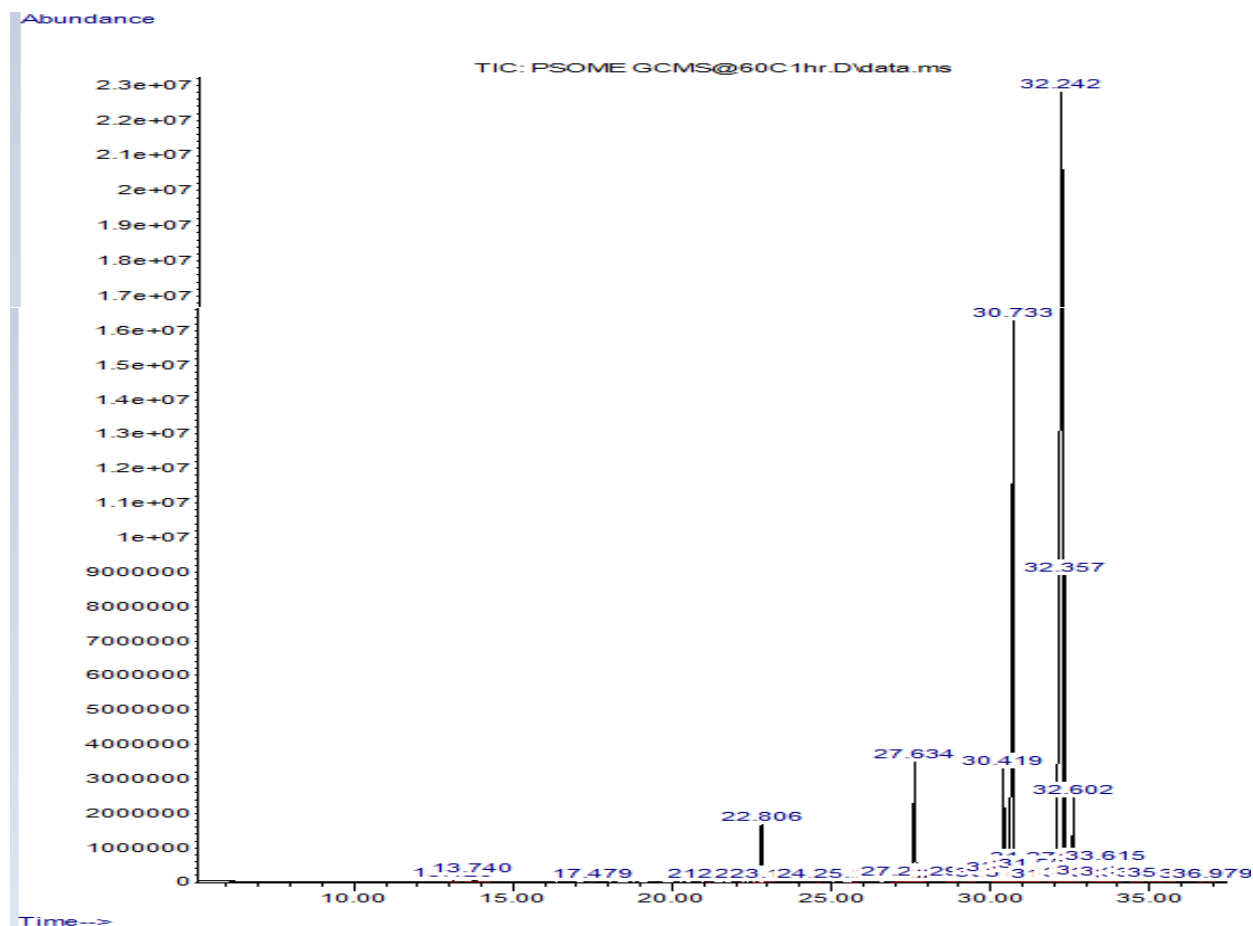


Fig. 5 GC-MS chromatogram of FAME of PSO methyl ester

Table 3: Fatty acid methyl ester content of PSO methyl ester

Retention Time (Mins)	wt. (%)	Compound	Structure	Formula
22.806	2.37	Dodecanoic acid, methyl ester (lauric acid)	C13:0	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>
27.257	0.14	Methyl myristoleate	C15:1	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>
27.634	6.13	Methyl tetradecanoate (myristic acid)	C15:0	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>
30.419	3.12	9-Hexadecenoic acid, methyl ester, (z)-(palmitoleic acid)	C17:1	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>
30.733	27.44	Hexadecanoic acid, methyl ester (palmitic acid)	C16:0	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>
32.242	48.01	9-Octadecenoic acid, methyl ester (E)- (oleic acid)	C19:1	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>
32.357	6.88	Methyl stearate (stearic acid)	C19:0	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>
33.458	0.52	cis-11-Eicosenoic acid, methyl ester (gondoic acid)	C21:1	C <sub>21</sub> H <sub>40</sub> O <sub>2</sub>
33.615	0.42	Eicosanoic acid, methyl ester (arachidonic acid)	C20:0	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>

### 3.6 WLO methyl ester fatty acid content

The values of the fatty acid methyl ester compositions and the chromatogram of the lard oil methyl ester (LOME) were presented in Table 4 and Figure 6, respectively. Only methyl ester peaks were seen on the chromatogram, with the nonexistence of other characteristic peaks, which ascribes that the synthesized methyl ester is of top quality. Table 4 shows that the lard oil methyl ester produced consists mainly of hexadecanoic acid, methyl ester, (palmitic acid: 27.84%) and 9-octadecenoic acid (z)-, methyl ester (oleic acid; 31.63%) which are saturated and monounsaturated compounds, respectively. The implication of this is that the biodiesel will have less affinity to oxygen, which leads to quick peroxidation. The synthesized LOME is also of high quality with respect to stability, as a higher degree of unsaturation in FAME limits the suitability for use as a fuel due to a high polymerization tendency resulting from peroxidation.

The methyl esters with area (%) less than 0.10 were not published.

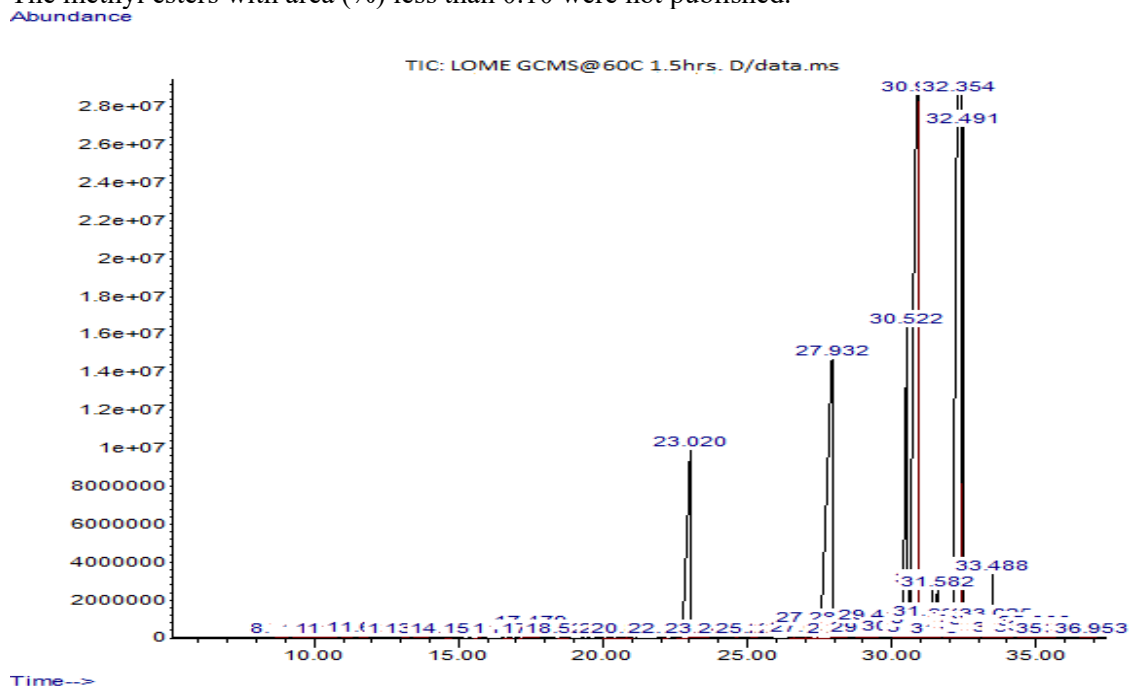


Fig. 6: GC-MS chromatogram of FAME of WLO methyl ester

Table 4: Fatty acid methyl ester content of LO methyl ester

Retention wt. Time (Mins) (%)	Compound	Structure	Formula
23.020 7.04	Dodecanoic acid, methyl ester (lauric acid)	C13:0	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>
27.286 0.36	Methyl myristoleate	C15:1	
	C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>		
27.932 14.95	Methyl tetradecanoate (myristic acid)	C15:0	
	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>		
30.522 7.31	9-Hexadecenoic acid, methyl ester, (z)- (palmitoleic acid)	C17:1	
	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>		
30.895 27.84	Hexadecanoic acid, methyl ester (palmitic acid)	C16:0	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>
31.405 0.45	cis-10-Heptadecenoic acid, methyl ester	C18:1	
	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>		
31.582 0.39	Heptadecanoic acid, methyl ester (margaric acid)	C17:0	
	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>		
32.354 31.63	9-Octadecenoic acid (z)-, methyl ester (oleic acid)	C19:1	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>
32.491 6.80	Methyl stearate (stearic acid)	C19:0	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>
32.674 0.20	9,12-Octadecadienoic acid, methyl ester (linoleic acid)	C18:2	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>

33.488	0.75	cis-11-Eicosenoic acid, methyl ester (gondoic acid)	C21:1
$C_{21}H_{40}O_2$			
33.625	0.13	Eicosanoic acid, methyl ester (arachidonic acid)	C20:0 $C_{20}H_{40}O_2$

### 3.7 Prediction of Fuel Properties from the Models Based on the Fatty Acid Content

The compositions of PSO methyl ester and WLO methyl ester synthesized at optimum reaction conditions of temperature 60 °C:60 °C, catalyst content 2.5 wt%:2.5 wt%, time 1 h:1.5 h, and methanol/oil molar ratio of 9:1:10.5:1, respectively, were determined with GC-MS. Based on the compositions of the different compounds present in the PSO methyl ester (Table 3) and WLO methyl ester (Table 4), and the model expressions as given in Equations (3-6), the cetane number (CN), higher heating value (HHV), saponification value (SV), and iodine value (IV) of the fuel were calculated.

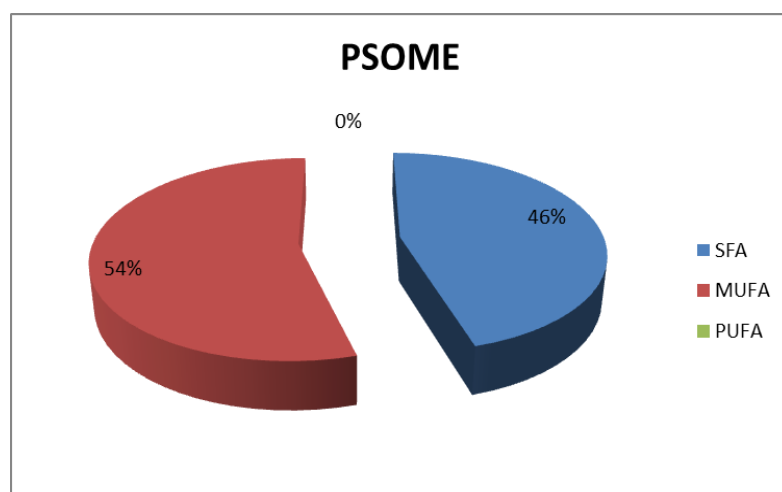
#### 3.7.1 Prediction of PSO Methyl Ester Fuel Properties

The predicted values of the fuel properties, saponification value (SV), iodine value (IV), cetane number (CN) and the higher heating value (HHV) of the GC-MS-based fatty acid content of PSO methyl ester are summarized in Table 5. It could be visualized in Table 5 and Figure 7 that the percentage composition of the unsaturated fatty acid methyl ester of PSOME is more than the saturated percentage composition. This suggests that the synthesized PSOME will flow easily in a diesel engine.

The experimental values of the physicochemical properties of PSOME shown in Table 5 were found to be very close to the predicted values of these properties determined with the ASTM method, as confirmed by the low absolute relative error, thus in good agreement. This confirms the reliability of the listed fuel properties prediction from its fatty acid composition based on the model expressions, which looks very promising in mitigating laboratory cost and time spent.

**Table 5:** Predicted and experimental values of the PSO methyl ester fuel properties

Parameter	Experimental values	Predicted values	Absolute relative error
Saponification value (mgKOH)	188.6	192.68	0.0216
Iodine value (gI <sub>2</sub> /100g)	40.30	45	0.1166
Cetane number (CN)	67	64.56	0.0364
Higher heating value (HHV) MJ/kg	41.2	40.86	0.0083
Saturated FAME (%)	-	43.24	-
Monounsaturated FAME (%)	-	51.79	-
Polyunsaturated FAME (%)	-	-	-
Degree of unsaturation	-	51.79	-



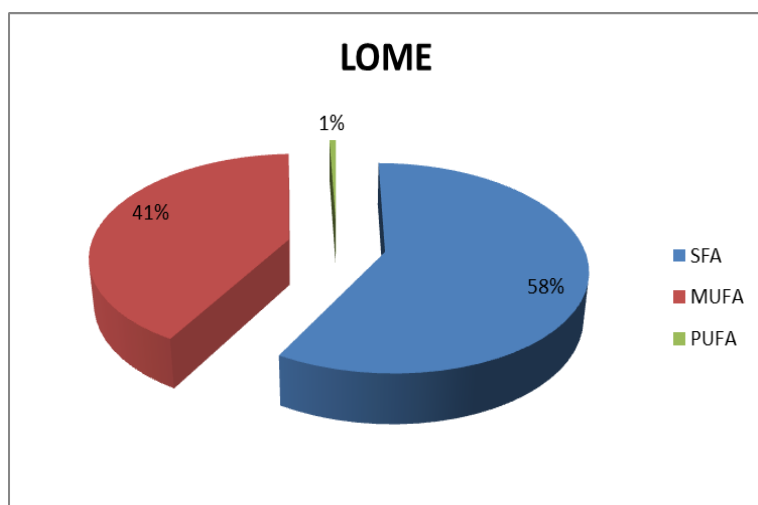
**Fig. 7:** Fatty acid distribution in PSO methyl ester

### 3.7.2 Prediction of WLO Methyl Ester Fuel Properties

Table 6 illustrates the predicted values of the fuel properties of WLO methyl ester. It could be seen from Table 6 and Figure 8 that the percentage composition of the saturated compound outweighs that of monounsaturated and polyunsaturated, hence the degree of unsaturation. This observation is typical of methyl ester synthesized from animal fats, which have a high content of saturated compounds. This implies that LOME may be more stable to deterioration than FAME compositions of samples with a higher degree of unsaturation and could also solidify at low temperature characteristics of cold and temperate regions of the globe. As could be visualized in Table 6, the predicted values of the fuel properties of WLO methyl ester determined via the models based on the GC-MS fatty acid compositions are in reasonable agreement with the experimental values of these properties determined with the ASTM method as confirmed by the low absolute relative error values. The results obtained in this study suggest that the fuel properties of the methyl esters could be satisfactorily estimated from their fatty acid composition, thus alleviating laboratory cost, time and energy.

**Table 6:** Predicted and experimental values of the WLO methyl ester fuel properties

Parameter	Experimental values	Predicted values	Absolute relative error
Saponification value (mgKOH)	199.7	206.28	0.0329
Iodine value (gI <sub>2</sub> /100g)	32.42	35.81	0.1046
Cetane number (CN)	68	64.70	0.0485
Higher heating value (HHV) MJ/kg	41.1	40.31	0.0192
Saturated FAME (%)	-	57.15	-
Monounsaturated FAME (%)	-	40.5	-
Polyunsaturated FAME (%)	-	0.2	-
Degree of unsaturation	-	40.7	-



**Fig. 8:** Fatty acid distribution in PSO methyl ester

### 3.7.3 Comparison of PSO methyl ester and WLO methyl ester fuel-related properties

The degree of unsaturation of PSO methyl ester was observed to be higher than WLO methyl ester which suggests less stability than WLO methyl ester. This observation is supported by the iodine value of PSOME (45%), which was found to be greater than that of LOME (35.8%), corroborating its unsaturation property. The larger the iodine value, the larger the degree of unsaturation (UKEssays, 2025). Cetane number measures how easily ignition occurs and the smoothness of combustion. PSOME and LOME showed relatively high cetane numbers of 64.56 and 64.70, respectively, indicating better ignition quality. According to Meher et al., (2006), the higher the cetane number, the better the ignition quality and efficiency of the fuel, and vice versa. Fuels with low cetane numbers show an increase in gaseous and particulate exhaust emissions due to incomplete combustion. Higher heating value (HHV)

or heat of combustion denotes the quantity of heat discharged by the complete combustion of a unit quantity of fuel and it is an important parameter for approximating fuel consumption. The greater the heat of combustion, the lower the fuel consumption. The ASTM D6751 standard for fuel specifies 40-42 as the limit for the HHV, while according to the EN14213, the minimum specification for the heating value is 35 MJ/kg. Both the PSOME and LOME HHV fall within this specification, indicating good fuel quality. Methyl Oleate (C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>) was found to be the dominant ester in PSO and LO methyl esters with percentage weights of 48.01% and 31.63%, respectively. However, PSO methyl ester consists of 54% monounsaturated fatty acids, while LO methyl ester is mainly composed of saturated fatty acids, totaling 58%. PSOME is likely to possess poor storage stability, enhanced cold flow properties (cloud and pour points) at low temperatures, and low thermal efficiency, deciphering to lower CO and HC emissions when compared with saturated LOME with better storage stability and poor low-temperature flow properties. This observation is also in accordance with the works of Agunbiade (2014). The fuel properties, cetane number (CN), higher heating value (HHV), iodine value (IV), and saponification value (SV) recorded an average absolute deviation (AAD) of 3.64:4.85, 0.83:1.92, 11.66:10.46, and 2.16:3.29% for PSO and LO methyl esters, respectively. The absolute relative error of the properties for each of the methyl esters was found to be very low, depicting a good correlation in existence between the predicted and experimental data. This was derived from the application of the error functions and subsequently comparing the fuel properties experimental data obtained from the ASTM method with the predicted data from the model based on the fatty acid composition of the PSO and WLO methyl esters, respectively.

#### **4. Conclusion**

The predicted values of the fuel-related properties, cetane number (CN), higher heating value (HHV), iodine value (IV), and saponification value (SV) of the PSO and WLO methyl esters via models based on their fatty acid methyl ester compositions indicated a good correlation with the experimental values derived from the ASTM methods. Hence, a satisfactory prediction of the fuel-related properties from the FAME compositions could be given by the models. Methyl Oleate (C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>) was found to be the dominant ester in PSO and LO methyl esters, with percentage compositions of 48.01% and 31.63%, respectively. PSO methyl ester possesses 54% monounsaturated fatty acids, while LO methyl ester has 58% saturated fatty acids. It is established from the results that the choice of feedstock can significantly impact the fatty acid content of the methyl esters and hence, the fuel properties. The methyl esters of PSO and WLO physicochemical properties established are within the EN14214 and ASTM D6751 allowable limits; hence, they are fitting for utilization in an internal combustion engine.

#### **Acknowledgements**

Special thanks to the staff of Biochem Analytics Ltd. Enugu; the National Research Institute for Chemical Technology (NARICT) Zaria; and Isa Yakubu of Ahmadu Bello University, Zaria, for granting me access to their laboratory equipment.

#### **Competing interests**

On behalf of all authors, the corresponding author states that there is no conflict of interest.

#### **Funding**

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

#### **Data availability**

The manuscript has no associated data.

#### **References**

- Ansari M., Jamali H., Ghanbari R., Ehrampoush M.H., Zamani P., Hatami B., (2025). Heterogeneous solid acid catalysts for sustainable biodiesel production from wastewater-derived sludge: A systematic and critical review. *Chemical Engineering Journal Advances*, 22: 100718. <https://doi.org/10.1016/j.ceja.2025.100718>
- Bamgboye A.I., Hansen A.C., (2008). Prediction of cetane number of biodiesel fuel from the fatty acid methyl ester (FAME) composition. *International Agrophysics* 22, 21-29

- Esonye C., Onukwuli O.D., Ofoefule A.U., (2018). The influence of fatty acid composition and functional groups on fuel related properties of sweet almond (*Prunus Amygdalus Dulcis*) seed oil methyl esters. *Der Pharma Chemica*, 10(7): 207 – 214. <http://www.derpharmachemica.com/archive.html>
- Etim A.O., Musonge P., (2025). The potential of waste avocado-banana fruit peels catalysts in the transesterification of non-edible Mafura kernel oil: Process Optimization by Taguchi. *Cleaner Chemical Engineering*. <https://doi.org/10.1016/j.clce.2025.100158>
- Ezekannagha, C.B., Onukwuli, O.D., Ude, C.N., Obiora-Okafo I.A., Udunwa D.I., (2025). Effects of process parameters on the yield of methyl esters derived from fruit-peel ash catalyzed lard oil methanolysis. *UNIZIK Journal of Engineering and Applied Sciences* 4(2), 1841-1851. <https://journals.unizik.edu.ng/ujears/article/view/5637/4684>
- Ezekannagha C. B., Ude C.N., Onukwuli O.D. (2017). Estimation of pork lard biodiesel properties from its fatty acid methyl ester profile by GC-MS. *Sigma Journal of Engineering and Natural Sciences*. 35 (3), 2017, 457-469
- Ezekannagha C.B., Onukwuli O.D. Uzoh C.F. Eze C.N., 2023. Kinetic modeling of bio based heterogeneously catalyzed lard oil methanolysis in methyl ester production. *Reaction Kinetics, Mechanisms and Catalysis*, 136(5): 2617-2638. <https://doi.org/10.1007/s11144-023-02478-w>
- Ezekannagha C.B., Onukwuli O.D. Obibuenyi J.I., Udunwa D.I. (2023). Kinetic modeling of papaya seed triglyceride transesterification catalyzed by calcined banana peel ash in methyl ester production. *Chemical Engineering Research and design*, 200: 256-265. <https://doi.org/10.1016/j.cherd.2023.10.006>
- Ezekannagha C.B., Onukwuli O.D., Nnanwube I.A., Ezeamaku U.L., Ohaegbulam C.M., (2024). Green hetero-alkali catalyst in optimized waste lard oil transesterification for biodiesel synthesis. *Results in Chemistry*, 11:101797. <https://doi.org/10.1016/j.rechem.2024.101797>.
- Ezekannagha C.B., Onukwuli O.D, Nwabueze H.O., Nnanwube I.A. (2024a). Heterogeneous base catalyst from hybrid banana and plantain peels in papaya seed oil (*Carica papaya*) methyl ester synthesis. *Chemistry Africa*, 7: 1935 – 1950 <https://doi.org/10.1007/s42250-024-00884-8>
- Gopinath, A., Puhan, S. and Nagarajan, G., (2009). Theoretical modeling of iodine value and saponification value of biodiesel fuels from their fatty acid composition. *Renewable Energy*, 34, 1806 – 1811.
- Knothe, G. (2009). Improving biodiesel fuel properties by modifying fatty esters composition. *Journal of Energy and Environmental Science*, 10,1039-1054.
- Mohibbe, A., Amtul, W., Nahar, N.M., (2005). Prospect and potential of fatty acid methyl esters of some non-traditional seeds oils for use as biodiesel in India. *Biomass Bioenergy* 29: 293 – 302.
- Onukwuli O.D., Esonye C., Ofoefule A.U., Eyisi R., (2021). Comparative analysis of the application of artificial neural network-genetic algorithm and response surface methods-desirability function for predicting the optimal conditions for biodiesel synthesis from chrysophyllum albidum seed oil. *Journal of the Taiwan Institute of Chemical Engineers*, 125: 153-167. <https://doi.org/10.1016/j.jtice.2021.06.012>
- Onukwuli O.D., Esonye C., Ofoefule A.U., (2021). Combustion exhaust release impact, diesel engine performance, and optimization studies of green diesel- petro diesel blend in a high compression ratio direct-injection compression-ignition engine. *Advances in Mechanical Engineering*, 13(5): 1–25. DOI: 10.1177/16878140211018778
- Tong D., Hu C., Jiang K., Li Y., (2011). Cetane number prediction of biodiesel from the composition of the fatty acid methyl esters. *Journal of American Oil Chemical Society*, 88: 415–423. DOI 10.1007/s11746-010-1672-0

- UKEssays, (2025). Vegetable oils determining degree of unsaturation and viscosity biology essay. Retrieved from <https://www.ukessays.com/essays/biology/vegetable-oils- determining degree-of-unsaturation-and-viscosity-biology-essay.php?vref=1> on April 8, 2025.
- Wang Y., He C., Li G., Liu X., Liu L., Jiao, Y., (2025). Sustainable hollow spherical CaO derived from waste eggshells for transesterification of lard: Catalytic characterization, performance, and thermodynamics. *Renewable Energy*, 250: 123302 <https://doi.org/10.1016/j.renene.2025.123302>