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Artificial neural network predictive modelling of *luffa cylindrica* seed oil antioxidant yield

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Keywords

ANN

Terpineol

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Abstract

This study applied artificial neural network (ANN) in evaluating the models for terpineol and polyphenol yield from *luffa cylindrica* seed oil. The experiment was carried out at a temperature (60-80ºC), time (4-6 hours), and solvent/seed ratio (8-12 ml/g) with response as antioxidant yield. FTIR (Fourier Transform Infra-red Spectroscopy) revealed the presence of terpineol and polyphenol at peaks of 1461.1cm^{-1} and 3008.0cm^{-1} respectively. The ANN prediction indices are thus; terpineol (R^2= 9.9999E-1, MSE=2.25766E-9) and polyphenol (R^2=9.9999E-1, MSE=4.42588E-10). This study reveals that the ANN technique can successfully predict antioxidants from *luffa cylindrica* seed oil.

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1. INTRODUCTION

Antioxidants occur naturally in vegetables and fruits, prevents free radical attack and reduce carcinogenic disease risk (Karadžić Banjac et al., 2018). In addition, studies have revealed that food rich in antioxidants (flavonoids, polyphenols, vitamins and minerals) has positive health impacts. Hence, their regular consumption reduces cardiovascular diseases, vision problems, high blood cholesterol and cancer. (Ohlsson & Bengtsson, 2002; Liyana-Pathirana et al., 2006; Gonçalves et al., 2012).

Luffa cylindrica is a non-edible fibrous vegetable with fruits containing black seeds found in the tropics, a *Cucurbitaceae*, intensifying considerable attention from researchers to harness its potentials (Oboh &Aluyor, 2009). However, antioxidants in leaves and fruits of *luffa cylindrica* have been revealed to offer interesting economic values. (Oyetayo & Ojo, 2012).

Reports have shown that *luffa*-based derivatives constitute antioxidants such as terpineol, polyphenol present in our food, applied in the treatment of various ailments, and cosmetics production. (Vladimir-Knežević et al. 2011; Park et al., 2012; Zengin & Baysal, 2014; Akinsanmi et al., 2015; Shendge & Belemkar, 2018; Yu et al., 2018; Okla et al., 2019). (Vladimir-Knežević et al. (2011), Zengin & Baysal (2014), and Campone et al. (2020) have researched extensively on terpineol and polyphenol extraction from plants. However, the relationship between factors that affect the extraction process and its response (polyphenol/terpineol yield)) is uncertain and complex from earlier reports (Khaleel et al., 2018; Molina et al., 2019; Sales et al., 2020).

ANN has shown its capability of controlling imprecise relationships among variables (Maosudi et al., 2018); ANN comprises mathematical models that apply biological neurons in solving intricate and uncertain processes, hence can be relied upon than linear and multivariate statistical procedures that have shown their

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inefficiency in handling nonlinear trends in data. (Almeida, 2002; Soto et al., 2019; Ojediran et al., 2020; Oke et al., 2020; 2021).

ANN modeling approach has been proven as a reliable technique in antioxidant yield estimation of plants, thus, the antioxidant properties of bananas (Guiné et al., 2015), beet-root (Kovacević et al., 2015), tea (Cimpoiu et al., 2011), polyphenols from green tea (Xi et al., 2013), essential oils (Cabrera & Prieto, 2010), polyphenols from pine fallen foliage (Vats & Negi, 2013), blueberries (Guiné et al., 2018) and lettuce (Karadžić Banjac et al., 2018) have been predicted successfully by ANN. However, there is sparse literature on antioxidant yield from vegetable seed oil. Thus, this study predicts polyphenol and terpineol yield from *luffa cylindrica* seed oil using the ANN model.

2. MATERIAL AND METHOD

2.1. Sample Preparation

Luffa cylindrica fruits were procured from nearby bushes at Amawom, Umuahia, Nigeria. The seed was winnowed, husks and dirt removed, after which it was sun-dried for easy removal of the shell and was also oven-dried at 60^{o}C to constant weight before grinding to increase the surface area for oil extraction.

The experimental matrix was designed using Design-Expert version 10, where Box-Behnken implementing response surface methodology on a three factors and three-level basis was employed to generate seventeen runs. The factors include time, temperature, and seed/solvent ratio, and the response is polyphenol/terpineol yield. The summary is shown in Table 1.

Table 1. *Design of Experiment*

Factors	**Units**	**Level**		
		-1	**0**	**1**
Temperature	^{o}C	60	70	80
Time	Hour	4	5	6
Solvent/seed	ml/g	8	10	12

2.2. Experimental Procedure

Luffa oil extraction process was carried out at Chemical Engineering Department laboratory, Michael Okpara University of Agriculture Umudike, Abia State, Nigeria, using the method described by (Afolabi et al., 2014). 40 g of grounded *luffa* seed was utilized for each experimental run. 250 cm^3 capacity Soxhlet apparatus and *n*-hexane of analytical grade was employed for the process. The solvent was recovered at every interval and the obtained oil was weighed, the oil yield was calculated using the equation below.

$$Y = \frac{M_o}{M_s} \times 100 \qquad (1)$$

Where: Y : oil yield (%)

M_o : mass of oil extracted (g)

M_s : mass of *luffa* seed (g)

2.2.1. Terpineol Concentration Determination

The terpineol concentration was determined using a method modified by Ghorai et al. (2017). 0.1g of the *luffa* oil was introduced into a test tube, 1 ml methanol was added, placed in a water bath, it was stirred for 30minutes at a temperature of 100°C, 1 ml sulphuric acid was introduced, the colour turned to reddish-brown, it was allowed to stand for 30minutes then the absorbance was taken in a UV spectrophotometer, the standard curve was generated by treating the linalool as the sample with serial dilution.

2.2.2. Polyphenol Yield Determination

The total polyphenol content was determined using the Folin Ciocalteu method by Singleton & Rossi (1965). About 0.1g of the oil extract was weighed in a test tube, 1ml of methanol was introduced into a water bath and shaker, where it was allowed to shake for 30minutes at 40^0C. Next, the sample was removed, and 1ml of Folin-Ciocalteu and 2ml of 20% Na_2CO_3 were introduced; the mixture was allowed to stand for 10 minutes before it was stirred in a centrifuge for 20minutes at 400rpm; the absorbance was taken using a UV spectrophotometer at 625nm. The standard curve was generated by preparing different concentrations ranging from 10mg/l of Gallic acid.

2.2.3. FT-IR Analysis

Fourier transform infrared (FTIR) analysis was carried out to determine the functional groups present on *luffa oil* using the FTIR spectroscope (PerkinElmer Spectrum one v3.02 Spectrometer, India).

2.3. ANN Model Development

ANN modeling of the extraction process was developed using the neural fitting toolbox of MATLAB R2014b. The architecture consists of 3 input layers (temperature, time and solute/solvent ratio), two output layers (polyphenol and terpineol yield) and a hidden layer. The dataset obtained from the extraction process was split into (training, validation and testing) with 70%, 15%, and 15%. The ANN structure is presented in Figure 1. To determine the best algorithm for the prediction, MSE and R^2 were used as the statistical criteria to assess the algorithm's performance. (Uzuner & Cekmecelioglu, 2016; Masoudi et al., 2018; Nwosu-Obieogu et al., 2020).

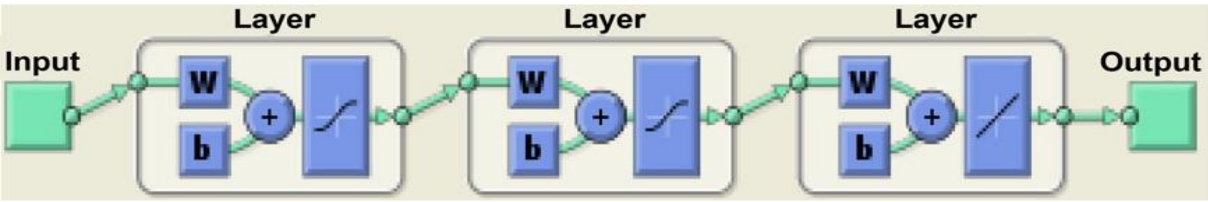

Figure. 1. *ANN Structure*

3. RESULTS AND DISCUSSION

3.1. Antioxidant Yields from *luffa* oil

The maximum terpineol yield of 2657 ml/g was obtained at a solvent/ solute concentration of 12mol/g, temperature of 80ºC, and a time of 5hours, while polyphenol yield of 609.37 ml/g was obtained at a solvent/solute ratio concentration of 10mol/g, the temperature of 80ºC and time of 6 hours as shown in Table 2, increase in process parameters led to an increase in terpineol and polyphenol yield, indicating that the factors had a significant effect on the antioxidant product (Afolabi et al.,2014; Oniya et al., 2017; Yu et al., 2018). The data were utilised in ANN prediction of terpineol and polyphenol yield (Nwosu-Obieogu et al., 2020).

The ANN-based model was developed based on the feed-forward, backpropagation (BP) algorithms. The hidden layer comprises ten neurons; the coefficient of determination (R^2) value at training, validation and testing is 1 for terpineol yield, while the polyphenol yield prediction gave 1 for training and testing, and 0.99996 for confirmation, as shown in Figure 2 and 3; these indicate the level of variability of the experimental results captured by the predicted. As shown in Table 3 and 4, the Bayesian regularization was the best of the algorithms for terpineol and polyphenol yield, having the smallest MSE of 2.25766E-9 and 4.42588E-10, respectively; the optimal results were obtained at epoch 901 and 701 for terpineol and polyphenol yield as shown in Figure 4 and 5, these comparisons indicate that the model predicted antioxidants yield from *luffa oil* appropriately; The effectiveness of the expected ANN model results is in agreement with reports from (Uzuner & Cekmecelioglu, 2016; Karadžić Banjac et al., 2018; Oke et al., 2020; Adeniyi et al., 2021).

***Table 2**. Experimental Values for the Total Terpineol/Polyphenol Yield*

Runs	Time (hours)	Temperature (°C)	Solvent/seed ratio (ml/g)	Terpineol yield (g/ml)	Polyphenol yield (g/ml)
1	5	70	10	1613	258.43
2	5	70	10	1613	258.43
3	4	80	10	1091	266.67
4	4	70	12	1109	183.82
5	4	60	10	713	107.43
6	5	70	10	1613	258.43
7	6	80	10	1724	609.37
8	5	60	8	978	340.1
9	6	60	10	1858	228.35
10	5	80	8	1639	128.57
11	5	80	12	2657	393.16
12	5	70	10	1613	258.43
13	5	60	12	1700	156.86
14	5	70	10	1613	258.43
15	4	70	8	668	151.72
16	6	70	8	1534	145.35
17	6	70	12	2172	126.92

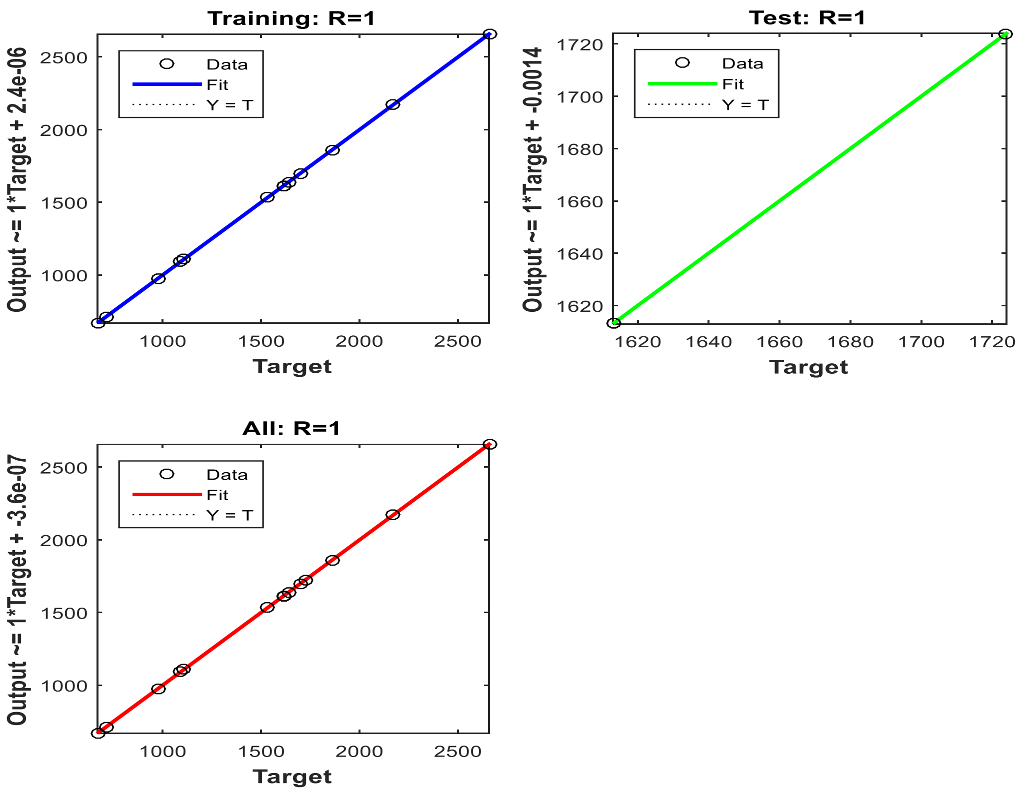

***Figure 2**. ANN Regression Graph for Terpineol Yield Prediction*

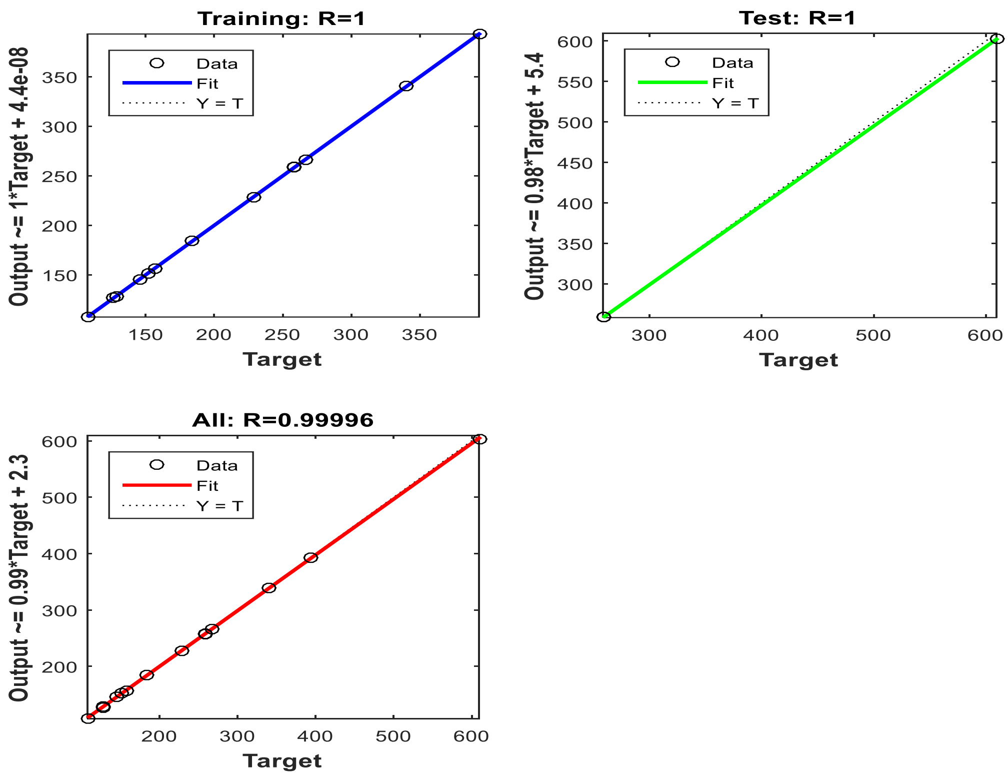

Figure 3*. ANN Regression Graph for Polyphenol Yield Prediction*

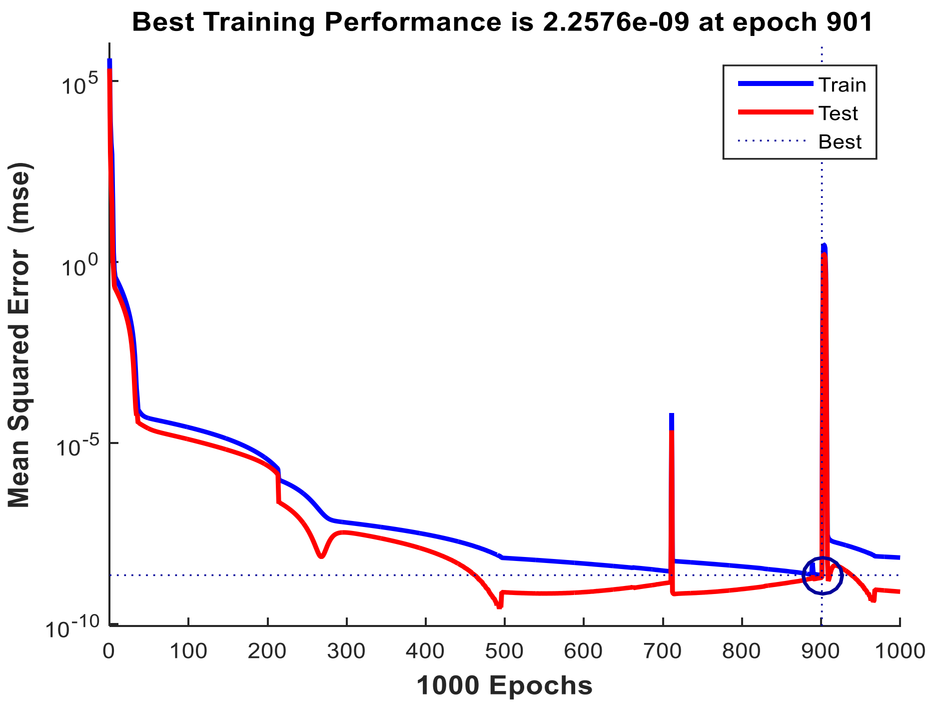

Figure 4. *Training Error (mean squared error, MSE) Curve for Terpineol Yield Prediction*

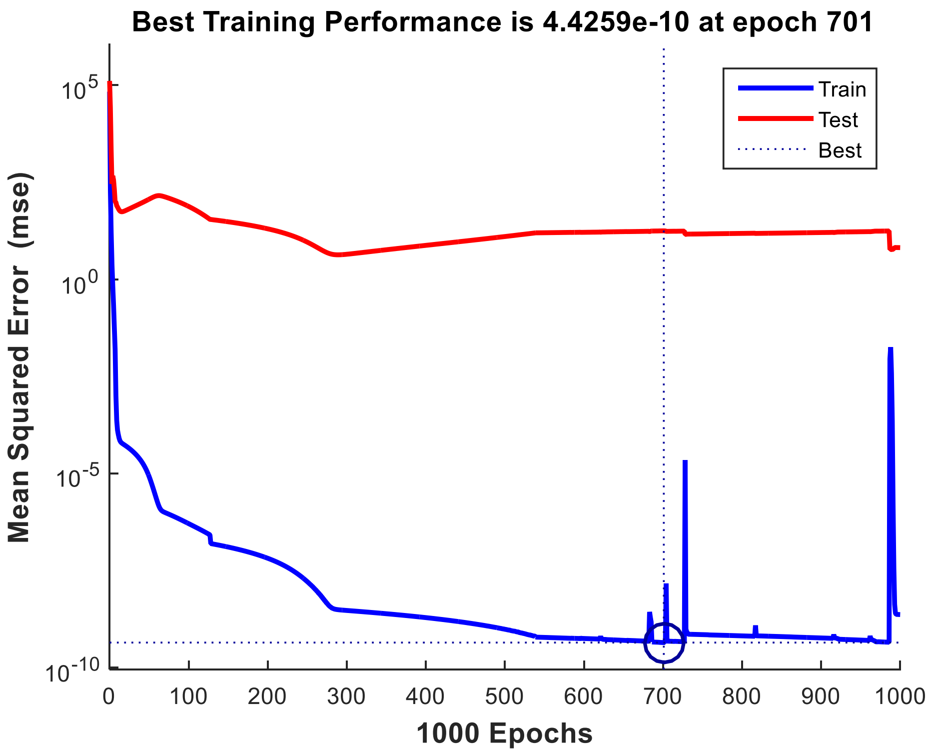

Figure 5. *Training Error (mean squared error, MSE) Curve for Polyphenol Yield Prediction*

Table 3. *Comparison of the ANN Algorithm for Terpineol Yield*

S/N	Algorithm	MSE	R^2
1	Levenberg-Marquardt	4523.36933E-0	0.9935
2	**Bayesian Regularization**	**2.25766E-9**	**0.9999**
3	Scaled Conjugate Gradient	401381.42860E-0	0.0011
4	*trainrp*	5.0602E4	0.9436
5	*traincgf*	1.1738E05	0.9998
6	*traincgp*	1.4700E05	0.9732
7	*traincgb*	1.2690E04	0.9889
8	*trainbfg*	1.3758E05	0.9829
9	*trainoss*	1.5833E04	0.9971
10	*traingd*	1.5693E06	0.3644
11	*traingdx*	2.0683E05	0.9433
12	*traingdm*	2.6889E06	0.8609

Table 5 shows the antioxidant yield of *luffa* oil compared to guava plant, lemon plant, Sorghum Moench and apple pomace; the yield of 2657mg/l for terpineol compared to the result of 348ml/g and 97ml/g for guava and lemon plant respectively and, 609.37ml/g of polyphenol compared to 313ml/g and 775 ml/g for sorghum Moench and apple pomace, respectively, indicates that *luffa* oil contains plenty of antioxidants that can be harnessed to proper use.

Table 4. *Comparison of the ANN Algorithm for Polyphenol Yield*

S/N	Algorithm	MSE	R^2
1	Levenberg-Marquardt	4.75287E-1	0.9998
2	**Bayesian Regularization**	**4.42588E-10**	**0.9999**
2	Scaled Conjugate Gradient	4220.33975E-0	0.8912
3	*trainrp*	1.2821E04	0.9315
4	*traincgf*	400.1718	0.9980
5	*traincgp*	3.2516E03	0.9998
6	*traincgb*	9.4288E03	0.9921
7	*trainbfg*	1.7404E04	0.5519
8	*trainoss*	648.1305	0.9924
9	*traingd*	2.7824E05	0.8954
10	*traingdx*	2.4738E03	0.8351
11	*traingdm*	1.4876E05	0.9994

Table 5*. Comparison of Terpineol and Polyphenol Present in Some Seed Oils with Luffa Seed Oil*

Oils	Terpineol yield (g/ml)	Polyphenol yield (g/ml)
Luffa seed oil (present study)		
Guava plant	348 (de Lima et al., 2010)	-
Lemon plant	97 (Ferhat et al., 2007)	
Sorghum Moench	-	313 (Liu et al., 2018)
Apple pomace		775 (Skrypnik &Novikova, 2020)

3.2. FTIR Result

The FT-IR results of the oil yield from *luffa cylindrica* is shown in Figure 6, the peak at 3008.0cm^{-1} can be ascribed to –OH stretching, which indicates the presence of polyphenol, two sharp-pointed peaks at 2922.2 cm^{-1} and 2855.1cm^{-1} indicated alkane group, another sharply pointed peak with value 1744 cm^{-1} indicates the presence of esters (6-membered lactone) with the structure C=O, hence the oil has high saponification value and could be recommended for soap production. The shorter, smaller pointed peak with a vibrational mode at 1461.1 cm^{-1} indicates the presence of terpineol (Agatonovic-Kustrin et al., 2020), while a medium sharp peak was observed with a value of 1379 cm^{-1}, indicating an alkane of gem dimethyl group. The peak at 1237.5cm^{-1} indicates an alkyl aryl ether with structure C – O – C, while 987.7cm^{-1} and 723.1cm^{-1} peaks indicated alkene compounds. The presence of unsaturated hydrocarbons makes oil suitable for plastic and paint industries, as a drying agent in the production of cosmetics, and may be edible for animal feed (Oli et al., 2014).

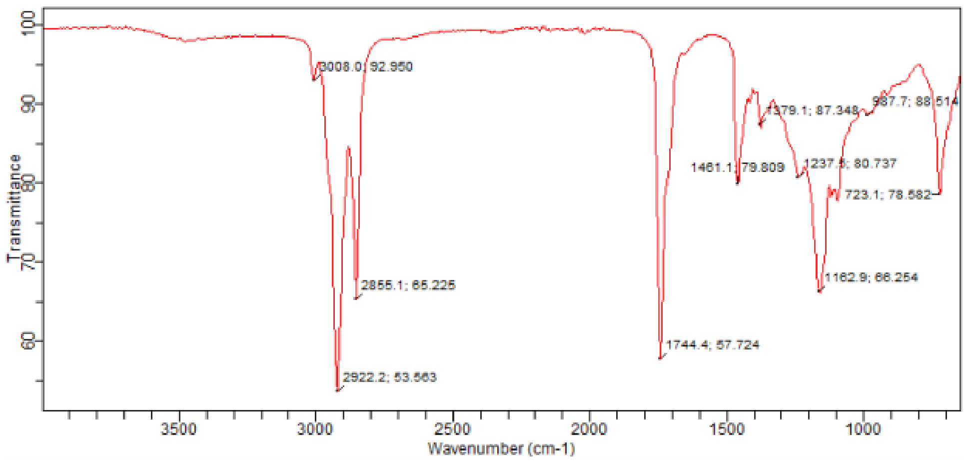

Figure 6 *FT-IR Result of the Oil Yield*

4. CONCLUSION

In this study, ANN has been applied to model antioxidant yields from *luffa* oil. Various conclusions were drawn from the findings. The coefficient of determination (R^2) value at validation was 1 for terpineol yield with optimal results obtained at epoch 901 and 0.99996 for polyphenol yield with optimal results obtained at epoch 701, the accuracy of the model was validated with experimental results. The study's findings are relevant in designing and developing a dynamic neural network controller for antioxidant production from vegetable seed oils.

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CONFLICT OF INTEREST

The author declares no conflict of interest.

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