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Nutritional Composition and Volatile Compounds of Black Cumin (*Nigella sativa* L.) Seed, Fatty Acid Composition and Tocopherols, Polyphenols, and Antioxidant Activity of Its Essential Oil

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Abstract: This study was to assess the nutritional quality and bioactive properties of black cumin (*Nigella sativa* L.) seeds and oil commonly found in the Chinese market. The results showed that black cumin seeds contain 5.02, 21.07, 39.02, 3.02, 6.01, and 25.86% moisture, crude proteins, crude fat, ash, fiber, and carbohydrates, respectively. It also contains substantial amounts of minerals, namely calcium, potassium, phosphorus, magnesium, sodium, iron, zinc, and copper. Glutamic acid (4.10 g/100 g protein) is the major amino acid of black cumin seeds. The major volatile components in black cumin seeds were thymoquinone (21.01%), o-cymene (18.23%), and β-thujene (17.22%). Cumin seed oil extracted by the soxhlet method contains high quantities of unsaturated fatty acids (UFA; 85.16%) and low amounts of saturated fatty acids (SFA; 15.02%). The major fatty acid of black cumin seed oil was linoleic acid (57.71%), followed by oleic acid (24.46%). The most prominent TAG of black cumin seed oils was oleoyl-dilinoleoyl-glycerol (OLL; 38.87%). In addition, the levels of α-tocopherol, β-tocopherol, γ-tocopherol, and total polyphenols in the black cumin seed oil were 25.59, 14.21, and 242.83 mg/100 g, and 315.68 mg GAE/kg, respectively, and possessed high antioxidant activity (DPPH $IC_{50\%}$, of 4.02 mg/mL). These findings demonstrate that black cumin seeds are nutritionally rich with high potential applications in the food, pharmaceutical, and cosmetic industries.

Keywords: amino acids; bioactive properties; black cumin seed (*Nigella sativa* L.); fatty acids; nutritional quality; tocopherols

1. Introduction

The supply of nutritional and functional products may be enhanced by non-conventional seeds, whose components possess unique chemical properties [1]. For this reason, looking for new unconventional plant-derived oils, such as black seed oils, has caught the attention of researchers. Black cumin (*Nigella sativa* L.) is an annual herb that belongs to the

Ranunculaceae family. Despite its Mediterranean origins, this important plant is widely grown in other areas. Nigella seeds have a black color and a small size similar to sesame seeds [2], and the oil and seeds are used as nutritional supplements. Seeds are added as a natural flavoring agent to some food products, including pasta, pastries, cheese, pickles, and bakery items, [3]. It is also used to prepare functional cosmetic and medicinal products. There has been much attention given to the study of seeds and their oils since they contain a wide number of chemical constituents and biological activities that play imperative roles in helping to promote human health and nutrition and are of unique medicinal significance against diseases [4]. Black cumin seeds are used as a natural remedy for asthma, hypertension, diabetes, inflammation, cough, bronchitis, headache, eczema, fever, dizziness, and influenza [1,5]. The seeds of black cumin are an important source of carbohydrates (40.0%), fat (28.5%), and protein (26.7%) [6]. It has also been reported that Turkish black cumin contains 39.37% fat, 21.65% protein, 32.58% carbohydrates, and 5.14% ash [7], and high levels of linoleic acid (C18:2, 57.49%) [3]. In addition, black cumin seeds are rich sources of calcium, potassium, phosphorus, magnesium, sodium, copper, zinc, iron, and manganese [1]. Black cumin seed oil plays a significant part in human nutrition and health. It is considered one of the newest sources of edible oils. Moreover, the chemical diversity and functional properties of volatile compounds in cumin seeds have attracted significant attention [8]. The main aroma compounds in black cumin seeds are thymoquinone (38.23%), p-cymene (28.61%), 4-isopropyl-9-methoxy-1-methyl-1-cyclohexene (5.74%), longifolene (5.33%), -thujene (3.88%), and carvacrol (2.31%), and these compounds have shown antimicrobial and pharmacological properties [9]. Literature data on the chemical composition of black cumin seeds is limited. The objective of this study was to assess the nutritional composition, volatile compounds, fatty acid profile, and bioactive properties of oil extracted from black cumin seeds. This study is trying to supply information on whether black cumin seeds are suitable as a nutritional addition to the human diet.

2. Materials and Methods

The black cumin seeds were obtained from the local market in Yiwu city, Zhejiang Province, China, in December 2021. The Nigella seeds were separately milled in a heavy-duty grinder for 3 min, passed through 1.0–2.0 mm screens, and were then preserved in hermetically sealed bags at −20 °C until analysis. 2,2-Diphenyl-1-picrylhydrazyl (DPPH), standards for determinations of tocopherols (α, γ, and β-tocopherol), and a standard mixture of 37 kinds of fatty acid methyl esters (C4~C24, 18919-1AMP) were purchased from Sigma-Aldrich Co., Ltd. (Shanghai, China). The 22 amino acid standards were procured from Agilent Technologies (Santa Clara, CA, USA). Chemicals used in the experiments were of high purity and used throughout the experiments without additional purification.

2.1. Methods

2.1.1. Proximate Analysis

The black cumin seeds' fat, ash, moisture, and fiber contents were determined with AOAC methods 932.06, 923.03, 925.09, and 985.29, respectively [10]. While the crude protein content of black cumin seeds was determined using FOSS (DK-3400 Hilleroed, Denmark) with a protein factor of 6.25. Carbohydrates are calculated as the difference between the mean values [100 − (proteins + lipids + ash + moisture)].

2.1.2. Mineral and Amino Acid Analysis

The black cumin seeds' mineral content was determined as described by Karrar et al. [11]. Results are expressed in mg/100 g sample. The amino acid contents of black cumin seed powder were digested using (6 M HCl) for 24 h at 110 °C under a nitrogen ambiance. Separation of amino acids was performed with a reverse phase HPLC (Agilent1100, Agilent Technologies, Inc., CA, USA) on a Zorbax 80 A C18 column (4.6 mm × 180 mm, Agilent) at a temperature of 40 °C with detection at 338 nm, as described by Jarrett et al. [12].

2.1.3. Determination of Volatile Compound

Volatile compounds were determined according to the method described by Karrar et al. [11]. In this study, volatile compounds were separated using GC-MS (Bruker-Scion SQ 456-GC, Bruker Corporation, Markham, ON, Canada) using a DBWAX column (30 m × 0.25 mm × 0.25 m) at 250 °C for 3 min. Volatile compounds were identified by comparing them with those in Wiley's and NIST's libraries. A peak area was used to define the quantities.

2.1.4. Fatty Acids (FA) Composition

The fatty acid composition of cumin seed oil was determined following the method described by Karrar et al. [13]. The oil of the black cumin seeds was extracted using the Soxhlet method. Then, the FAME of the extracted oil was prepared by mixing 60 mg of oil with 2 mL n-hexane and 500 µL of KOH-CH_3OH. FAMEs were analyzed using a GC (Agilent 7820A) equipped with a flame ionization detector and a BPX capillary column (0.25 m × 60.0 m × 0.22 mm). Identification of FA composition was based on comparing the peak retention times of the samples with those of FAMEs authentic standards treated and run under the same conditions.

2.1.5. Determination of the Triacylglycerol Profile Using UPLC-Q-TOF-MS

About 0.3 mg/mL concentration of the black seed oil was determined by dissolving it in n-hexane. The triacylglycerol levels were determined using ultra-performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UPLC-Q-TOF-MS) (Waters, Milford, MA, USA) as described previously [13,14]. The TAGs were identified using Waters MassLynx 4.1 software (Waters, Milford, MA, USA) and quantified using Progenesis QI QI software (Waters, Milford, MA, USA).

2.1.6. Tocopherols and Total Phenolic Content of Black Seed Oil

The tocopherols and total phenolic contents of black cumin seeds were determined using the method designated previously [13]. Briefly, 0.1 g of black cumin seed oil was dissolved in 10 mL of n-hexane and filtered using a 0.45 m organic filter. Analyses of tocopherols were conducted on an HPLC (Agilent, 1260, Agilent Technologies, USA) equipped with a C18 column (4.6 mm × 250 mm × 5 µm) and a UV detector. 20 µL of the samples were injected into the high-performance liquid chromatographic system using hexane as a mobile phase with a flow rate of 1.0 mL/min and the column temperature at 30 °C. Results are expressed in mg/100 g sample. The retention time and standard curve were used to determine the tocopherol content of black cumin seed oil. The Folin–Ciocalteu method was used to determine the total phenolic content [13]. Each sample was expressed as mg of gallic acid equivalent (GAE)/kg.

2.1.7. DPPH Radical Scavenging Ability

A DPPH assay was conducted according to our previous study [13]. The antioxidant activity of test compounds was expressed as an antioxidant IC_{50}, which is the number of antioxidative compounds that caused 50% scavenging of DPPH radicals over the defined period.

2.1.8. Fourier Transform Infrared (FT-IR) Spectroscopy

Based on our previous studies, the infrared absorption spectra of black cumin seed oil were determined [13,15]. The oil sample was analyzed using a Nicolet 5700 spectrometer (Thermo Nicolet Co., Waltham, MA, USA) with a wavenumber range of 4000–400 cm^{-1}.

2.1.9. Statistical Analysis

The sample determination was performed in triplicate, and the results were reported as mean ± standard deviation (SD). Statistical analysis was performed using SPSS 20.0,

and significant differences between the variables of the test black seeds were assessed by Duncan's test at $p < 0.05$.

3. Results

3.1. Proximate Composition of Black Seed Powder

As shown in Table 1, the moisture, crude proteins, crude fat, ash, fiber, and carbohydrate contents of black cumin seed were 5.02, 21.07, 39.02, 3.02, 6.01, and 25.86%, respectively. These results showed that the fat represents the major component in the black cumin seed, followed by carbohydrates, then protein. In a literature study, approximate moisture analysis of black cumin seed found that crude protein ranged from 20.6 to 31.2%, ash ranged from 3.9 to 4.8%, fats ranged from 22.6 to 53.4%, carbohydrates varied from 24.9 to 34%, and moisture ranged 3.8 to 7.4% [2,4,6,16,17]. The black seed had higher fat content than corn (10%) [18] and soybean (20%) [19], suggesting that the black seed would be a suitable source for oil industry applications. Additionally, the black seed is an excellent source of fats and proteins for humans. The black seed contained significant amounts of important minerals. Also shown in Table 1 is the amount of minerals in black seed essential for human nutrition. In the study, calcium was the most abundant mineral in the black seeds. It was followed by potassium, phosphorus, and magnesium. Additionally, in decreasing order of quantity, other minerals are sodium, iron, zinc, and copper. Compared to literature, calcium and potassium are the main differences in the mineral contents of black seeds. The amounts of calcium and potassium reported by [4] were 579.33 mg/100 g and 510.30 mg/100 g, respectively. Calcium (Ca) was found to be high (810.54 mg/100 g), while potassium was low (716.47 mg/100 g). These differences may be associated with variations in cultivation and climate differences within the region [20]. The minerals in black seeds (sodium, iron, zinc, and copper) are relatively high. The amount of black seed consumed will not predict the nutritional status of these minerals [6].

Table 1. Chemical characteristics (dry weight) of black seed (*Nigella sativa*).

Component	Values *
Moisture [a]	5.02 ± 0.01
Crude protein [a]	21.07 ± 0.01
Crude fat[a] (Petroleum ether extract lipid)	39.02 ± 0.09
Ash [a]	3.02 ± 0.02
Fiber [a]	6.01 ± 0.06
Carbohydrates [a]	25.86 ± 0.10
Sodium (Na) [b]	27.60 ± 0.20
Magnesium (Mg) [b]	276.87 ± 0.05
Potassium (K) [b]	716.47 ± 0.18
Calcium (Ca) [b]	810.54 ± 0.36
Iron (Fe) [b]	0.95 ± 0.68
Copper (Cu) [b]	0.25 ± 0.03
Zinc (Zn) [b]	0.43 ± 0.02
Phosphorus (P) [b]	358.62 ± 0.17

* All values given are means of three determinations means ± SD deviation. [a] % (*w*/*w*) dry matter basis. [b] mg/100 g of dry weight flour.

3.2. Amino Acid Composition

Amino acids are organic compounds necessary for life and an important nitrogen source [21]. The seeds of black cumin are generally considered an excellent source of amino acids. Table 2 shows the amino acid composition as grams per 100 g, listing the concentrations of 16 amino acids. Results showed that the major amino acid was glutamic (4.10 g/100 g), followed by aspartic acid (1.59 g/100 g), arginine (1.40 g/100 g), leucine (0.93 g/100 g), and glycine (0.91 g/100 g). Over 58% of the total amino acids were the major amino acids in the black cumin seeds. Valine and proline were the most minor amino acids in the black seed. Black cumin seeds contain relatively high amounts of amino acids,

namely alanine, isoleucine, serine, threonine, phenylalanine, lysine, tyrosine, and histidine. The content of cysteine is low. Black cumin seeds contain more non-essential amino acids than their corresponding essential amino acids. Differences in the amino acid composition of black cumin seeds were observed between the results of this study and that reported by [22], which may be due to genotypic variation or environmental factors.

Table 2. Amino acid composition of black seeds (*Nigella sativa*).

Amino Acids	Black Seed	FAO/WHO/UNU [b]	
Essential Amino Acids (EAAs)		**Adult**	**Child**
Leucine [a]	0.93 ± 0.02	6.60	1.90
Valine [a]	0.84 ± 0.01	3.50	1.30
Lysine [a]	0.55 ± 0.05	5.80	1.60
Threonine [a]	0.57 ± 0.03	3.40	0.90
Phenylalanine [a]	0.57 ± 0.03	6.30	1.90
Methionine [a]	0.29 ± 0.01	2.70	1.70
Histidine [a]	0.40 ± 0.09	1.90	1.60
Isoleucine [a]	0.63 ± 0.07	2.80	1.30
Tyrosine [a]	0.52 ± 0.05	6.30	1.90
Cystine [a]	0.09 ± 0.01	-	-
Total essential amino acids	5.39 ± 0.37		
Non-essential amino acids (NEAAs)			
Glutamic acid [a]	4.10 ± 0.12	-	0.99
Arginine [a]	1.40 ± 0.08	-	0.46
Aspartic acid [a]	1.59 ± 0.10	-	0.65
Glycine [a]	0.91 ± 0.02	-	0.55
Proline [a]	0.83 ± 0.04	-	0.55
Serine [a]	0.61 ± 0.01	-	0.55
Alanine [a]	0.67 ± 0.02	-	0.26
Total non-essential amino acids	10.11 ± 0.39		
Total amino acids	15.50 ± 0.76		
E/N	0.53		

All values given are means of three determinations means ± SD deviation. [a] (g/100 g protein). [b] Lists of FAO/WHO/UNU: daily requirements for human child and adult.

3.3. Volatile Organic Compounds

Characterizing the volatile components of black seed essential oil is crucial for understanding its impact on flavor and food industry applications [8]. A further investigation of its role in traditional medicine requires the characterization of volatile components [8]. In this study, 31 volatile compounds were identified from black seed extract, as shown in Table 3. Thymoquinone (21.01%), o-cymene (18.23%), β-thujene (17.22%), cis-4-methoxythujane (7.04%), longifolene (6.43%), β-pinene (5.08%), D-limonene (3.46%), (E)-longipinene (2.19%), and phenol, 2-methyl-5-(1-methylethyl) (2.07%) were the major volatile components of black seed in this study. The results were similar to those obtained from seeds cultivated in countries such as Bangladesh, India, Poland, and Tunisia [8,23–25], with some variations in the quantitative compositions. Several studies have reported that thymoquinone has therapeutic potential [26,27]. In a study conducted by Oz [28] to determine the effect of black cumin use in meatball production on the formation of heterocyclic aromatic amines, which are mutagenic and/or carcinogenic compounds, and lipid oxidation in meatballs, it was determined that the use of black cumin in the production of meatballs reduced both the individual and total HAA content of meatballs and the lipid oxidation level of meatballs. The researcher attributed black seed's inhibitory effect on heterocyclic aromatic amines and lipid oxidation to the antioxidant activity of black seed phenolic compounds.

Table 3. GC–MS analysis of volatile compounds, retention time (RT) and their amounts detected in the extract of black seed.

RT	Compound Name	Content % *
3.41	β-Thujene	17.22 ± 0.25
4.64	β-Pinene	5.08 ± 1.05
6.05	α-Terpinolene	0.41 ± 0.07
6.44	D-Limonene	3.46 ± 0.98
7.45	gamma-Terpinene	0.77 ± 0.05
8.04	o-Cymene	18.23 ± 1.09
8.61	cis-4-methoxy thujane	7.04 ± 0.81
11.20	p-Mentha-1,5,8-triene	0.12 ± 0.03
11.46	p-Cymenene	0.19 ± 0.09
11.67	Acetic acid	0.28 ± 0.02
12.21	(E)-Longipinene	2.19 ± 0.06
12.55	Ylangene	0.04 ± 0.01
12.97	trans-2-Caren-4-ol	0.69 ± 0.11
13.80	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	1.69 ± 0.05
14.01	D-Verbenone	0.02 ± 0.01
14.23	Longifolene	6.43 ± 0.16
15.26	Butanoic acid	0.26 ± 0.03
16.08	Estragole	0.07 ± 0.01
17.25	(-)-Carvone	0.18 ± 0.02
17.63	Thymoquinone	21.01 ± 0.09
18.97	Anethole	0.39 ± 0.01
19.34	p-Cymen-8-ol	0.23 ± 0.05
22.39	(-)-Isolongifolol, acetate	0.22 ± 0.02
24.31	(Z)-18-Octadec-9-enolide	0.21 ± 0.01
24.47	9(E),11(E)-Conjugated linoleic acid	0.32 ± 0.04
24.71	Nonanoic acid	0.22 ± 0.01
25.21	Phenol, 2-methyl-5-(1-methylethyl)-	2.07 ± 0.12
26.19	5-Hepten-3-yn-2-ol, 6-methyl-5-(1-methylethyl)-	0.08 ± 0.01
28.94	p-Cymene-2,5-diol	0.82 ± 0.04
29.79	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	0.38 ± 0.01
30.64	Benzo[b]thiophene, 3,6-dimethyl-	0.10 ± 0.03

*All values given are means of three determinations means ± SD deviation.

3.4. Fatty Acid and Triacylglycerol (TAG) Composition

In vivo, fatty acids play various roles and are an important component of biological matter [29]. Table 4 shows the fatty acid composition of black seed. In this study, the levels of linoleic acid (57.71%), oleic acid (24.46%), palmitic acid (12.17%), eicosadienoic acid (2.52%), and stearic acid (2.31%) were high in the black cumin seed. These results agree with previous studies reporting that linoleic acid is the predominant polyunsaturated fatty acid (PUFA) in oil from black seed [2,5,28,29]. Arachidic (0.33%), γ-Linolenic (0.19%), myristic (0.19%), palmitoleic (0.12%), α-linolenic (0.12%), and myristoleic (0.02%) acids were also found in trace contents. Unsaturated fatty acids (UFA) and saturated fatty acids (SFA) accounted for 85.16% and 15.02%, respectively. Black cumin oil has a higher quantity of unsaturated fatty acids than other vegetable oils, indicating benefits to human health [30,31]. There is evidence that linoleic acid is beneficial in preventing vascular embolism diseases [32]. The content of linoleic acid in black cumin seed oil was higher than that in a large number of vegetable oils, such as oil from flaxseed (13.02%) and oil from olive (11.72%) [33,34]. In addition, oleic acid offered nutritional benefits and oxidative stability to oil [35]. As a result of the high oleic acid content and palmitic acid content of black cumin seed oil, its application in cosmetics could be feasible due to the appropriate texture and spreadability properties of this oil [36]. The fatty acid profile of black cumin seed oil suggests that it might serve as a valuable source for food and cosmetics.

Table 4. Fatty acid composition of black seed (*Nigella sativa*) oil extracted by Soxhlet method.

FAs	Nomenclature	Content (%) *
C14:0	Myristic acid	0.19 ± 0.02
C14:1	Myristoleic acid	0.02 ± 0.01
C16:0	Palmitic acid	12.17 ± 0.04
C16:1	Palmitoleic acid	0.14 ± 0.02
C18:0	Stearic acid	2.31 ± 0.07
C18:1	Oleic acid	24.46 ± 0.10
C18:2	Linoleic acid (LA)	57.71 ± 0.15
C18:3n-6	γ-Linolenic (GLA)	0.19 ± 0.03
C18:3n-3	α-Linolenic (ALA)	0.12 ± 0.02
C20:0	Arachidic acid	0.33 ± 0.01
C20:2	Eicosadienoic acid	2.52 ± 0.08
SFA		15.02 ± 0.15
UFA		85.16 ± 0.41
Triacylglycerol (TAG)		
LLL		22.79 ± 1.78
OLL		38.87 ± 0.67
POL		30.82 ± 0.48
OOO		7.52 ± 0.12
Tocopherols (mg/100 g oil)		
α-tocopherol		25.59 ± 0.09
β-tocopherol		14.21 ± 0.21
γ-tocopherol		242.83 ± 0.13
Total tocopherols		282.63 ± 0.43
Polyphenols (mg GAE/kg oil)		315.68 ± 0.56
DPPH (IC_{50}, mg/mL)		4.02 ± 0.04

* Means of three determinations ± SD. *SFA* saturated fatty acid, *UFA* unsaturated fatty acid. TAG: structure of triacylglycerols, for example, C18:2/C18:2/C18:2 stands for the structure of palmitoyl-stearoyl-oleoyl-glycerol. Abbreviations: GAE, (gallic acid equivalent)/kg of oil; IC_{50}, sample concentration providing 50% activity.

Oils and fats can be evaluated for functional characteristics by assessing their relative amounts and types of triacylglycerol (TAG) [13]. Table 4 and Supplementary material Figure S1 show the TAG distribution determined through UPLC-Q-TOF-MS. The most prominent TAG of black cumin seed oils was oleoyl-dilinoleoyl-glycerol (OLL; 38.87%), followed by palmitoyl-oleoyl-linoleoyl-glycerol (POL; 30.82%) and trilinoleic (LLL; 22.79%), while trioleic (OOO; 7.52%) was low. It has been reported in a previous study [2] that the major TAG in nigella seeds was LLL, followed by OLL and PLL (palmitoyl-dilinoleoyl-glycerol). The differences between the results of these studies may be due to genotypic variation or environmental factors.

3.5. Tocopherol, Polyphenols, and Antioxidant Activity

Tocopherols are found primarily in oils and are extremely beneficial to human health [13,37]. Seed oils contain tocopherols, which are extremely important. Naturally occurring lipophilic antioxidants are found mainly in seed oils. The high biological activity of α-tocopherol makes it suitable for human consumption [37]. As antioxidants, tocopherols are used in foods such as frying oil, fried snacks, and margarine. The tocopherol content of black cumin seed was illustrated in Table 4. It was found that the levels of α-tocopherol, β-tocopherol, and γ-tocopherol in the black cumin seed oil were 25.59, 14.21, and 242.83 mg/100 g, respectively. Black cumin seed oil in this study contained higher levels of α, γ, and β-tocopherol than that reported in the previous studies [38]. This study provides useful information about using black cumin seed oil in the industry. Many natural antioxidants are found in edible oils, including polyphenols, tocopherols, and phytosterols, that may reduce the risk of chronic diseases such as cancer and heart disease [13]. The polyphenols from black seed was 315.68 mg GAE/kg oil (Table 4). Black seed oil contains more polyphenols than most edible oils, except olive oil, which has high amounts (19–380 mg/kg) of total polyphenols [39–42]. Previously, a high amount

(245–309 mg GAE/kg oil) of total polyphenol content was also reported in black cumin seed oil [6]. In this sense, black cumin seed oil could be a potential natural polyphenol source that may help prevent heart disease and cancer. DPPH radical scavenging ability was used to determine the antioxidant activity of black seed oil (Table 4). Results showed that black seed oil has the strongest DPPH radical scavenging ability (IC_{50}, 4.02 mg/mL). The low IC_{50} level indicates strong antioxidant activity. Food oils are thought to have radical scavenging properties due to their total phenolic content, especially thymol, which has been linked to oil lipid oxidation [13]. Previously, DPPH inhibition (IC_{50}) of black cumin seed oil extracted by supercritical fluid extraction and the cold press was found to be 1.58 mg/mL and 2.30 mg/mL, respectively [39]. The variation between these studies could be due to the difference in cumin genotype, growing conditions, and oil extraction methods.

3.6. Infrared Spectral Characterization

Black cumin seed oil was analyzed using Fourier transform infrared spectroscopy to determine its functional groups and bonding structure. As shown in Supplementary material Figure S2, two strong absorption peaks at 2800–3000 cm^{-1} can be attributed to the C–H stretching vibrations of the methyl ($–CH_3$) and methylene ($–CH_2$) backbones of the oils [39,40]. Carbonyl groups (C=O), commonly found in long-chain fatty acids, were attributed to the prominent peak at 1750 cm^{-1} in the low-wavenumber region [32]. Asymmetry between C–O–C bonds and the asymmetric stretching of C–C(=O)–O bonds is responsible for the overlapped peaks located at around 1000–1500 cm^{-1}. Those peaks corresponded to the functional groups in the oil, like alcohols, esters, and ethers. Furthermore, a peak at 730 cm^{-1} was associated with the cis C=C plane external bending, corresponding to the aliphatic chains of fatty acids [32].

4. Conclusions

In this study, black cumin seed was an excellent source of high-quality oil and protein and a valuable source of compounds with positive impacts on health, such as calcium, potassium, linoleic acid, tocopherols, polyphenols, and thymoquinone. It is possible to utilize black cumin seeds as an oil and as a nutritional source for meeting the daily dietary requirements of humans. A high total polyphenol concentration/content was found in black cumin seed oil. Additionally, the results showed high DPPH radical scavenging ability and low IC_{50} concentrations. These findings demonstrate that black cumin seeds may be used for food, pharmaceutical, and cosmetic purposes.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/horticulturae8070575/s1, Figure S1: HPLC chromatogram of triacylglycerol of black seed oil using Soxhlet method. Figure S2: Spectroscopic bands were obtained from black seed oil.

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