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Data Article

Dataset of Phytochemical and secondary metabolite profiling of holy basil leaf (*Ocimum sanctum* Linn) ethanolic extract using spectrophotometry, thin layer chromatography, Fourier transform infrared spectroscopy, and nuclear magnetic resonance

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ABSTRACT

Holy basil (*Ocimum sanctum* Linn) or known also as "kemangi" in Indonesia is a plant commonly used as a herb in Asian countries. It is also medicinal with antipyretic, anti-inflammatory, anti-cancer, and neuroprotective properties. This dataset article provides broad screening of the phytochemical component of *Ocimum sanctum* ethanolic extract (EEOS) as well as a secondary metabolite profile of EEOS. Analyses were done qualitatively and quantitatively using a combination of spectrophotometer, thin layer chromatography, Fourier transform infrared spectroscopy (FTIR), and ^{1}H-nuclear magnetic resonance (^{1}H-NMR). Results showed that *Ocimum sanctum* ethanolic extract contains phytochemical compounds, including flavonoids, phenols, tannins, saponins, alkaloids, steroids, and terpenoids. In addition, a secondary metabolite was found and classified into metabolite groups including alcohol, amine, carboxylic acid, alkane, alkene,

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aldehyde, phenol, ether, sulfur, halogen, benzene, nitrogen, sterol, amino acid, carbohydrate, and nitrogen.

Specifications Table

Subject	Food science and technology
Specific subject area	Food composition, food analysis
Type of data	Table Picture or graphic
How data were acquired	The ethanolic extract of *Ocimum sanctum* Linn was obtained by maceration into an extract that was analyzed for phytochemical compounds, and secondary metabolic profiles were analyzed by UV-Vis spectrophotometry, thin layer chromatography (TLC), Fourier transform infrared spectroscopy (FTIR), and ^{1}H-nuclear magnetic resonance (NMR).
Data format	Raw data Analyzed data
Parameters for data collection	Variable of analysis including of non-targeted active compound or phytochemicals and a secondary metabolic contained by the ethanolic extract *Ocimum sanctum* Linn.
Description of data collection	Triplicate samples of ethanolic extract from the leaves of *Ocimum sanctum* Linn were prepared for spectrophotometry analysis, and a duplicate sample was analyzed by TLC, FTIR, and ^{1}NMR.
Data source location	Institution: Integrated Laboratory for Research and Testing, Universitas Gadjah Mada City/Town/Region: Yogyakarta/ Special Region of Yogyakarta Country: Indonesia
Data accessibility	Within the article and in raw supplementary material as Mendeley dataset. DOI:10.17632/r8xx9wsjp9.1 (https://data.mendeley.com/drafts/r8xx9wsjp9; Raw analysis of *Ocimum sanctum* leaves ethanolic extract by spectrophotometry and thin layer chromatography", Mendeley Data, V1)
Related research article	Mataram, M.B.A., Hening P., Harjanti, F.N., Karnati, S., Wasityastuti, W., Nugrahaningsih, D.A., Kusindarta, D.L., Wihadmadyatami, H. The neuroprotective effect of ethanolic extract *Ocimum sanctum* Linn in the regulation of neuronal density in hippocampus areas as a central autobiography memory on the rat model of Alzheimer's disease, J. Chem. Neuroanat. 111 (2021) 101–885, https://doi.org/10.1016/j.jchemneu.2020.101885.

Value of the Data

- The dataset contributed to the identification and characterization of phytochemicals and metabolites found in *Ocimum sanctum* Linn ethanolic extract.
- The data improves our understanding of several reliable methods that can used for food compound characterization and standardization.
- The dataset from the active phytochemical and secondary metabolite analysis of *Ocimum sanctum* Linn ethanolic extract may lead to the discovery of specific compounds for the development of novel food nutrition, medication, and therapeutics.

1. Data Description

Holy basil (*Ocimum sanctum* Linn) is a plant found in almost all Asian countries but especially in Southeast Asia and South Asia. Currently, *Ocimum sanctum* is used not only used as a basic herb in food but also as a herbal remedy to treat various disorders due to its antipyretic, anti-inflammatory, anti-cancer, neuroprotective, antioxidant, and antimicrobial properties [1–3].

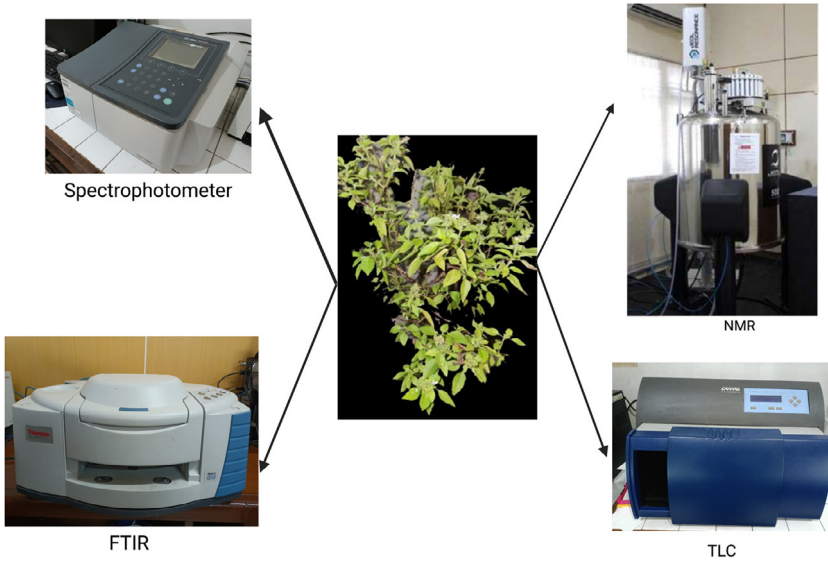

Fig. 1. Schematic illustration of the procedure analysis of the phytochemical and secondary metabolite characterization of the *Ocimum sanctum* Linn ethanolic extract.

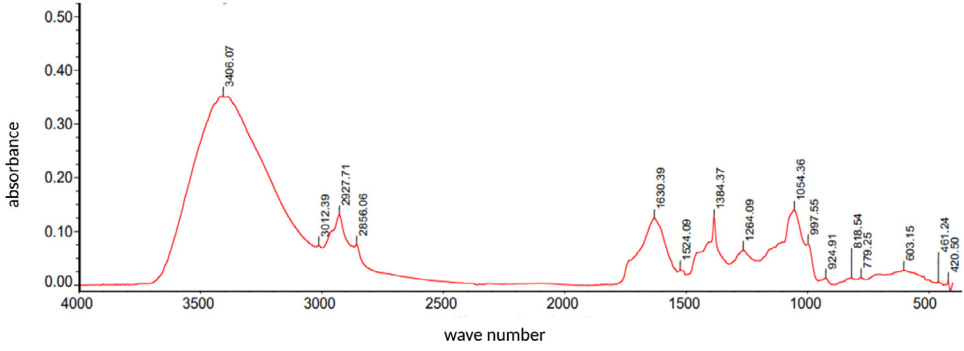

Fig. 2. Specific peaks (wave number in cm^{-1}) on Fourier transform infrared (FTIR) of *Ocimum sanctum* Linn ethanolic extract (leaves).

With the widespread use of *Ocimum sanctum*, increasing research has analyzed the phytochemical compounds in its leaves. The extraction procedures were done using ethanol, an organic solvent. The following data are a complete screening dataset of the active phytochemical compounds as well as secondary metabolite profiling of the ethanolic extract of *Ocimum sanctum* leaves. The leaves were converted into ethanolic extracts using the maceration method, then the extracts were analyzed by spectrophotometry and thin layer chromatography to determine the phytochemical composition. Data from spectrophotometry were analyzed quantitatively while data from thin layer chromatography were analyzed qualitatively. Furthermore, Fourier transform infrared spectroscopy (FTIR) and ^{1}H-nuclear magnetic resonance (^{1}H-NMR) were applied to determine the types of secondary metabolites and types of chemical bonds between the chemical molecules of the EEOS compounds (Figs. 1–5; Tables 1–4; raw data in the Mendeley doi: 10.17632/r8xx9wsjp9.1 (https://data.mendeley.com/drafts/r8xx9wsjp9; Raw analysis of *Ocimum sanctum* leaves ethanolic extract by spectrophotometry and thin layer chromatography", Mendeley Data, V1).

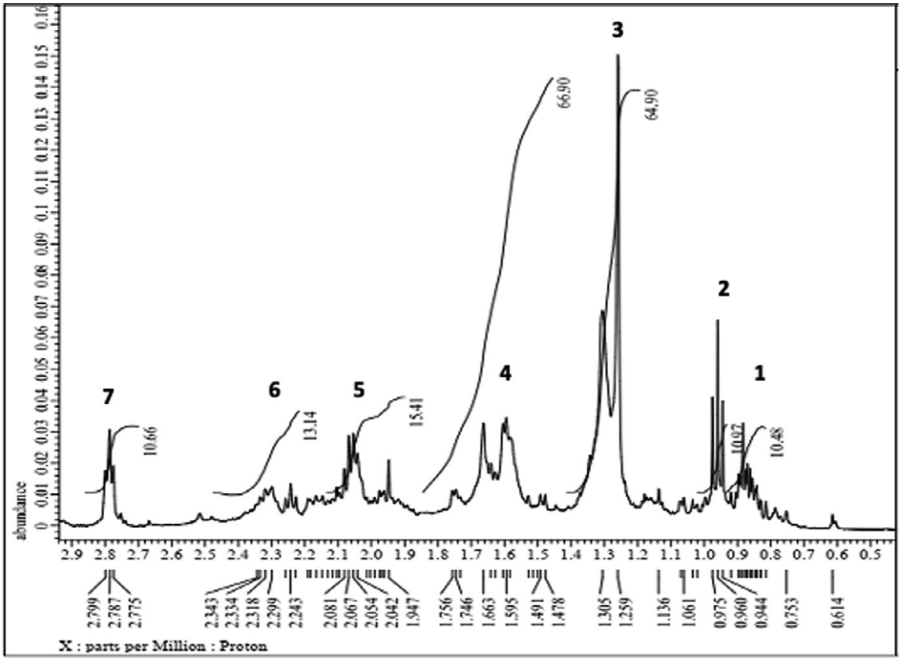

Fig. 3. [1]H nuclear magnetic resonance spectrum of *Ocimum sanctum* Linn ethanolic extract: part A; sterol (peak 1); valin, leusin, isoleusin (peak 2); threonine (peak 3); alanine (peak 4); glutamine, glutamate (peak 5), proline (peak 6); citric acid, aspartate (peak 7).

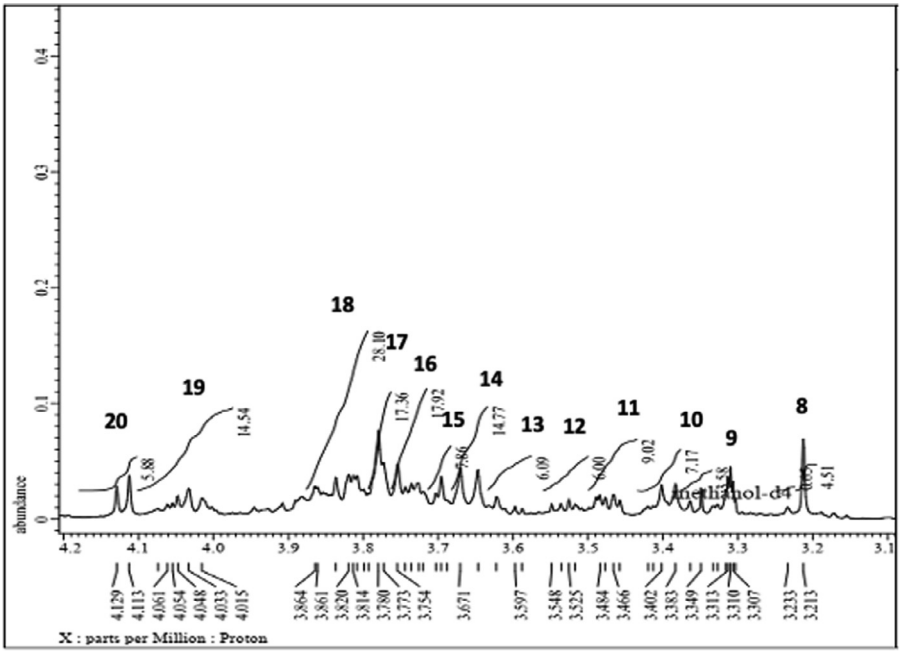

Fig. 4. [1]H nuclear magnetic resonance spectrum of *Ocimum sanctum* Linn ethanolic extract: part B; methanol (peak 8, 9, 10, 11, 12); glycine, inositol (peak 13); glycerol (peak 14); glucose (peak 15, 16, 17, 18, 19); proline, sucrose (peak 20).

Table 1
Different structural functional group of Ethanolic extract Ocimum sanctum Linn based on specific peaks in Fourier Transform Infrared Spectrophotometry.

Functional group	Absorbance	Appearance	Spesific Peaks
Alcohol			
O – H stretching	3550–3200	Strong[1]	3406,07
	3200–2700	Strong[1]	3012,39
O – H bending			
C – O stretching	1085–1050	Strong[1]	1054,36
Amine			
N – H stretching	3400–3300	Medium[2]	3406,07
	3500–3400	Medium[2]	3406,07
	3000–2800	Medium[2]	2927,71
	3000–2800	Medium [2]	2856,06
N – H bending amine	1650–1580	Medium[2]	1630,39
C – N stretching	1342–1266	Strong[1]	1264,09
Carbocyclic acid			
O – H stretching	3300–2500	Strong[1], board	3012,39
Alkane			
C – H stretching	3100–3000	Medium [2]	3012,39
	3000–2800	Medium [2]	2927,71
	3000–2800	Medium[2]	2858,06
C – H bending	1385–1380	Medium[2]	1384,37
Alkene			
C – H stretching	3100–3000	Medium [2]	3012,39
C = C stretching	1662–1626	Strong[1]	1630,39
	1650–1600		
	1650–1566		
C = C Bending	995–985	Strong[1]	997,55
	915–905	Strong[1]	924,91
	840–790	Medium[2]	818,54
Aldehyde			
C – H bending	1390–1380	Medium[2]	1384,37
Ester			
C – O stretching	1310–1250	Strong[1]	1264,09
Ether			
C – O stretching	1275–1200	Strong[1]	1264,09
Sulfur compound			
S = O stretching	1070–1030	Strong [1]	1054,36
Halogen compound			
C – Cl stretching	850–550	Strong [1]	818,54
	850–550	Strong [1]	779,25
	850–550	Strong [1]	603,30
C – Br stretching	690–515	Strong[1]	603,16
Benzene derivative			
C – H bending	810 ± 20	Strong[1]	818,54
	780 ± 20	Strong[1]	779,25
Nitro compound			
N – O stretching	1550–1500	Strong[1]	1524,09

[1] Strong : sharp intensity absorption probably double or triple bound.
[2] Medium : predicted as single bond.

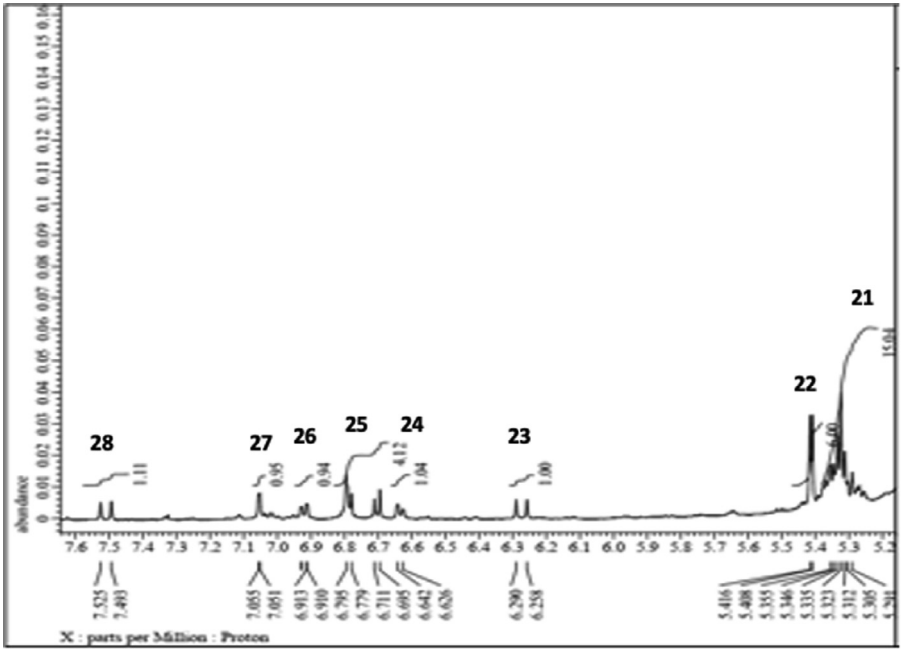

Fig. 5. ^{1}H nuclear magnetic resonance spectrum of *Ocimum sanctum* Linn ethanolic extract: part C; sucrose (peak 21, 22); uridine, naringenin, glycoside (peak 23); kaempferol (peak 24); tyrosine (peak 25, 26); tryptophan (peak 27); phenol (peak 28).

Table 2
Identification of the Phytochemical Compound of Ethanolic Extract Ocimum sanctum Linn using Spectrophotometry UV-Vis and Thin Layer Chromatography.

No	Name of compound	Concentration	Unit	Metode
1.	Total flavonoid	47,23	%b/b	Spectrophotometry UV-Vis
2.	Total Fenol	12,14	%b/b	Spectrophotometry UV-Vis
3.	Total Tannin	21,68	%b/b	Spectrophotometry UV-Vis
4.	Total Saponin	128	%b/b	Spectrophotometry UV-Vis
5.	Total Alkanoid	022	%b/b	Spectrophotometry UV-Vis
6.	Steroid	173	%b/b	Thin Layer Chromatography
7.	Terpenoid	Positif	–	Thin Layer Chromatography

2. Experimental Design, Materials and Methods

2.1. Preparation of Ocimum sanctum *Linn ethanolic extract*

Dried simplicia was obtained from CV Merapi Farma Herbal, Yogyakarta, then made into ethanolic extract at the Integrated Research and Testing Laboratory (LPPT), Universitas Gadjah Mada. Leaf extract was made using the maceration technique, then an ethanolic extract of *Ocimum sanctum* was obtained in the form of a paste.

Table 3
Identification of secondary metabolite of Ethanolic Extract Ocimum sanctum screening by ^{1}H Nuclear Magnetic Resonance.

Peak No.	Chemichal Shift (ppm)	Metabolit Compound	Integration	Multiplicity
1	0.684	sterols	10.48	multiplet
2	1.015	valine, leucine, isoleucine	10.97	triplet
3	1.282	Palmitic acid, threonin	64.90	doublet
4	1.622	alanine	66.90	multiplet
5	2.105	glutamine, glutamate	15.41	multiplet
6	2.335	GABA, proline	13.14	multiplet
7	2.787	citric acid, aspartate	10.66	triplet
8	3.223	methanol	4.51	doublet
9	3.328	methanol	3.58	multiplet
10	3.405	methanol	7.17	doublet of doublet
11	3.471	methanol	9.00	doublet of doublet
12	3.541	methanol	6.00	doublet of doublet
13	3.603	glycine, inositol	6.09	multiplet
14	3.659	glycerole	14.77	doublet
15	3.7	glucose	7.86	doublet
16	3.739	glucose	17.92	multiplet
17	3.777	glucose	17.36	singlet
18	3.839	glucose	28.10	multiplet
19	4.043	fructose	14.54	ultiplet
20	4.121	proline, sucrose	5.88	doublet
21	5.324	sucrose, malic acid	15.04	multipel
22	5.412	sucrose, malic acid	6.00	doublet
23	6.274	uridine	1.00	doublet
24	6.634	naringenin dan glycoside (dihidro)campherol	1.04	doublet
25	6.745	tyrosine	4.12	doublet
26	6.92	tyrosine	0.94	doublet
27	7.053	glicosida (dihidro) campherol	0.95	doublet
28	7.509	tryptophan, phenol	1.11	doublet

Table 4
The Prediction of Chemistry Binding Structure containing on Ethanolic extract Ocimum sanctum Linn. generated by ^{1}H Nuclear Magnetic Resonance.

Chemistry Binding	Chemichal Shift Range (ppm)
CH>CH2>CH3	0,5 - 2
amine N - H	1 - 2
alcohol - O - H	1 - 5
amide N - H	1 - 6
thiol, SH	1,3 - 1,5
allylic C - H	1,5 - 2,5
thiol, sulfide	2 - 2,5
amine N - C - H	2,3 - 3
benzylic C - H	2 - 3
carbonil alfa C - H	2 - 3
≡C - H	2 - 3
epoxide C - H	2,5 - 3,5
X (F, Cl, Br) - C - H	3 - 5
alcohol, eter, ester	3,3 - 5
alkene C - H	4 - 7
aromatic C - H	6 - 8
aldehide C - H	9 - 10
carbocylate O - H	10 - 12

2.2. Spectrophotometry UV-Vis

2.2.1. Flavonoids

A 50 mg sample of *Ocimum sanctum* ethanolic extract (EEOS) was placed into a 10 ml test tube followed by 0.3 ml of 5% sodium nitrite. Next, 5 min 0.6 ml of 10% aluminum chloride was added, and the mixture was left for 5 min before 2 ml of 1 M sodium hydroxide was added. Finally, 10 ml of distilled water was added. The mixture was then diluted as needed and transferred to a cuvette; it was read at a wavelength of 510 nm.

2.2.2. Phenols

A 50 mg sample of EEOS, 0.5 ml of Folin–Ciocalteu reagent, and 7.5 ml of aquabides were mixed together. The mixture was then allowed to stand for 10 min at room temperature before 1.5 ml of 20% sodium carbonate was added. Sufficient water to increase the volume to 10 ml was then added. The mixture was then diluted as needed, transferred to a cuvette, and read at a wavelength of 760 nm.

2.2.3. Tannins

A 50 mg sample of EEOS was put into 10 mL of diethyl ether for 20 h, then filtered. The remaining diethyl ether was evaporated, then distilled water was added to bring the volume of the mixture up of 10 mL; 1 mL of the sample solution was taken then added to 0.1 mL of Folin–Ciocalteu reagent, vortexed, then incubated for 5 min. The mixture was added to 2 mL of 20% sodium carbonate and vortexed, then brought to a volume of 10 ml with aquades, and diluted 10 times. The absorbance was read at 760 nm after the mixture was incubated for 30 min at room temperature.

2.2.4. Alkaloids

A 50 mg sample of EEOS was added to 5 mL of 2 N hydrochloric acid, then homogenized. The solution was then washed three times with 10 mL of chloroform in a separating funnel, with the chloroform phase being discarded. The solution was then neutralized by adding 0.1 M of sodium hydroxide. Then 5 mL of Bacillus Calmette-Guerin (BCG) solution and 5 mL of phosphate buffer were added. The solution was extracted with 5 mL of chloroform, then stirred with a magnetic stirrer at 500 rpm for 15 min. The extraction with chloroform was repeated twice. The chloroform phase was collected, evaporated with nitrogen gas, then chloroform was added to bring the volume up to 5 mL. The absorption was read at a wavelength of 470 nm.

2.2.5. Saponins

A 50 mg sample of EEOS was added to 2 ml of 25% sulfuric acid. The mixture was then autoclaved for 120 min at 110 °C, extracted with ether, and the filtrate dried. Then 1 ml of water was added and extraction by vortex occurred for 5 min. Then 50 ml of anisaldehyde was added, and the mixture was homogenized and left to stand for 10 min. Then 2 ml of 50% sulfuric acid was added and the mixture was heated in a water bath at 60 °C for 10 min. Water was then added to bring the volume up to 10 ml with a measuring flask, and the mixture was diluted five times. The absorption was read at a wavelength of 435 nm.

2.3. Thin layer chromatography

Thin layer chromatography was used to analyze any steroid and terpenoid. A 50 mg sample of EEOS was added to 1 ml of ethanol. Sonication was applied to the mixture for 60 min, then it was vortexed and centrifuged. Maceration then occurred for 24 h. A spot sample was placed on silica gel 60 F254, including standard betasitosterol (60% purity). It was then put into the saturated chamber with mobile phase toluene and ethyl acetate (80:20), sprayed with Lieberman–Burchard reagent, then finally heated at 110 °C for 2 min. The wavelength was analyzed at 340 nm.

2.4. Fourier transform infrared spectroscopy (FTIR)

For the FTIR analysis, a powder sample and potassium bromide were mixed at an appropriate ratio (1:50). The mixture formed pellets. Pellets were prepared with the same pressure to maintain a constant thickness for each pellet. FTIR spectra were recorded in the 400–4000 cm^{-1} spectral region with a FTIR spectrophotometer (Shimadzu 8201, Tokyo, Japan). The spectra were collected at a resolution of 4 cm^{-1}. Each spectrum was the average of 10 scans.

2.5. ^{1}H nuclear magnetic resonance

A 30 mg sample of EEOS was mixed with methanol-d6 and homogenized at 20–25 °C. A ^{1}H nuclear magnetic apparatus (JNM-ECZ500R/S1, Jeol, Japan) was then operated at a frequency of 500 MHz for hydrogen. This frequency was used for acquisition of NMR spectra. The spectra were acquired in a spinning mode at a calibrated probe temperature of room temperature. Free induction decay (FID) was acquired with a spectral width of 15 ppm, 128 scan, acquisition time of 1.74588 s, recycle delay of 5 s, and a flip angle of 45 [deg]. Manual phase and baseline correction were performed prior to integration. Data derived were analyzed based on a study of the literature [4,5].

Ethical Approval

The datasets was approved by the Ethics Committee of Faculty of Veterinary Medicine, Universitas Gadjah Mada, Yogyakarta, Indonesia (00053/EC/FKH/Int./2021).

Declaration of Competing Interest

All authors declare there are no competing interests.

CRediT Author Statement

Ulayatul Kustiati: Formal analysis, Investigation, Validation, Data curation; **Hevi Wihadmadyatami:** Methodology, Resources, Conceptualization, Supervision, Project administration, Writing – original draft; **Dwi Liliek Kusindarta:** Conceptualization, Software, Writing – review & editing, Funding acquisition.

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