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Molecules and Their functions

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Abstract

Pterocarpus and Pterocarpus products have certain human health function. In this paper, Diospyros celebica Bakh as an example, we study its human health components by using PY–GC–MS, TDS–GC–MS and GC–MS. The composition of known human health functions was studied by reviewing the literature. 3-O-Methyl-d-glucose has a certain conservation property, and it can protect the pancreatic B cells against the toxicity of alloxan. P-Cresol plays a role in endothelial dysfunction in uremic patients, and it can repair wounds and reduce endothelial pro-gression. 2(3H)-Furanone, 5-methyl- has certain biological resistance, and has high antimicrobial activity against NCIM 2501 and NCIM 5021.

1. Introduction

Diospyros celebica Bakh is mainly grown in Sulawesi, Indonesia, belonging to Ebenaceae, Diospyros. Diospyros celebica Bakh is the best of the Diospyros ebum Koenig, and the par-adise bird, the red dragon fish collectively known as the three national treasures of Indonesia, known as “the black pearl in the wood”. Diospyros celebica Bakh grows mainly in the annual drought, rare rain cliff; Because of its poor growth environment, Diospyros celebica Bakh has a long period of material, generally take hundreds or even thousands of years. Diospyros celebica Bakh is evergreen broad-leaved trees, with tree height up to 40 m and DBH up to 1 m. Diospyros celebica Bakh wood for the hollow material, heartwood and sapwood are significantly different, heartwood was black, the surface with shiny and deep and white stripes. Wood with high strength, big hardness, corrosion resistance and strong insect resistance, air dry density of 1.09 g/cm^3 . Diospyros celebica Bakh can emit fungal and antibiotics and other natural molecules and it enter the body to inhibit and kill the body of native viruses and bacteria, with human health function. In this paper, the Diospyros celebica Bakh powder was analyzed by PY–GC–MS, TDS–GC–MS, TG and FT-IR; The extracts of ethanol, ethanol/benzene and ethanol/methanol in the Diospyros celebica Bakh were analyzed by GC–MS and FT-IR. To determine the active molecules of Diospyros celebica Bakh, figurative effect of human care function.

2. Materials and methods

2.1. Materials

Diospyros celebica used in the experiment was produced in Indonesia. When we do the experiment, the Diospyros celebica Bakh are first pulverized and then tested with the obtained wood powder. The ethanol, benzene and methanol used in the experiments were purely chromatographed. Quantitative filter paper should be extracted with ethanol for 12 h. The three



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extracts used in the experiment were ethanol, ethanol/benzene (volume ratio of 1:2) and ethanol/methanol (volume ratio of 1:1).

2.2. Experimental methods

2.2.1. Extraction method

The crushed and processed *Diospyros celebica* Bakh's powder was weighed 3 parts and the mass was 10 g (accuracy was 1.0 mg). A well-weighed powder and 250 mL of ethanol, ethanol/benzene (1:2 by volume) and ethanol/methanol (1:1 by volume) were added in the three round bottom flasks respectively. And then refluxed at 85 LC, 82 LC and 80 LC for 4.5 h. The obtained extract was subjected to suction filtration on a circulating water type vacuum pump (YUHUA SHZ-D (III)) using a quantitative filter paper subjected to ethanol extraction treatment for 12 h. Finally, the obtained extract was steamed and concentrated by a rotary evaporator (YUHUA RE-2000A).

2.2.2. Ft-ir method

Diospyros celebica's powder and the concentrated extract refluxed by three kinds of extractants were subjected to FT-IR detection (ThermoFisher Nicolet, 670FT-IR). The scanning of each powder was collected at a spectral resolution of 4 cm⁻¹ and the spectral range was 400–4000 cm⁻¹.

2.2.3. TG method

The powder of *Diospyros celebica* was analyzed by thermo-gravimetric analyzer (TGA Q50 V20.8 Build 34). The carrier gas used in the experiment was high purity nitrogen and the nitrogen release rate was 60 mL/min. The temperature program of TG starts at 30 LC and rises to 250 LC at a rate of 5 LC/min. During the test, the sample's weight (%), Deriv. Weight (%/LC) were recorded.

2.2.4. GC–Ms method

The three extracts were analyzed using a gas chromatography-mass spectrometer (Agilent GC–MS 7890B 5977A). Column HP-5MS (30 m 250 μ m 0.25 mm). Elastic quartz capillary column, the carrier gas used for high purity helium, flow rate of 1 mL/min. The split ratio is 20:1. The temperature program of the GC starts at 50 LC, rises to 250 LC at a rate of 8 LC/min, and then rises to 300 LC at a rate of 5 LC/min. MS program scan mass range of 30–600 amu, ionization voltage of 70 eV, ionization current of 150 μ A electron ionization (EI). The ion source and the quadrupole temperature were set at 230 LC and 150 LC, respectively.

2.2.5. TDS–GC–MS method

The *Diospyros celebica*' powder was analyzed with thermal desorption–gas chromatography–mass spectrometry. TDS starting temperature of 30 LC, for 1 min, at 10 LC/min rate rose to 100 LC, keep 5 min, then 10 LC/min rate rose to 200 LC, the transmission line temperature of 230 LC. CIS starting temperature of 50 LC, hold 0.1 min, and then 10 LC/s rate rose to 230 LC, keep 1 min. Gas Chromatography-Mass Spectrometer (Agilent GC–MS 7890B 5977A). The temperature program of the GC starts at 50 LC, rises to 250 LC at a rate of 8 LC/min, and then rises to 300 LC at a rate of 5 LC/min. MS program scan mass range of 30–600 amu, ionization voltage of 70 eV, ionization current of 150 μ A electron ionization (EI). The ion source and the quadrupole temperature were set at 230 LC and 150 LC, respectively. The analytical standard library was analyzed by NIST14.L.

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2.2.6. PY–GC–MS method

The powder of *Diospyros celebica* was analyzed by thermal cracking–gas chromatography–mass spectrometry (CDS5200-trace1310 ISQ). The carrier gas used for high purity helium, the pyrolysis temperature was 500 LC, the heating rate was 20 LC/ms, and the pyrolysis time was 15 s. The pyrolysis pro-duct transfer line and the injection valve temperature are set to 300 LC; Column TR-5MS; Capillary column (30 m 0.25

mm 0.25 lm); Shunt mode, split ratio of 1:60, shunt rate of 50 mL/min. The temperature of the GC program starts at 40 LC for 2 min, rises to 120 LC at a rate of 5 LC/min, and then rises to 200 C at a rate of 10 LC/min for 15 min. Ion source (EI) temperature of 280 LC, scanning range of 28–500 amu.

3. Results and analysis

3.1. Ft-ir analysis

Fig. 1 shows the infrared contrast spectra of the *Diospyros celebica* Bakh powder and the three extracts. The infrared

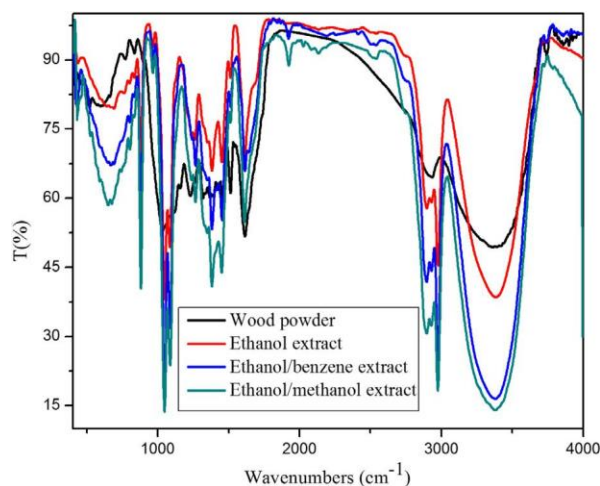


Fig. 1 FT-IR comparison spectra of *Diospyros celebica* Bakh powders and three extracts.

spectrum of 3360 cm^{-1} is the OAH stretching vibration in the cellulose, phenol, alcohol, carboxylic acid compounds (Iwaki and Dlott, 2000; Shamsudin et al., 2017). The infrared spec-trum of 2900 cm^{-1} is CAH stretching vibration and CAH bending vibration in cellulose and hemicellulose. The infrared spectrum of 1738 cm^{-1} is C,O stretching vibration in hemicellulose, lipid, ketone compounds (Gomti et al., 2004; Rahman et al., 2017; Khan et al., 2017); There is the lignin aromatic carbon skeleton vibration at 1600 cm^{-1} , 1510 cm^{-1} . The infrared spectrum of 1425 cm^{-1} is the CH_2 bending vibration and the CH_2 shear vibration in the lignin, the cellulose (Ito and Nakanaga, 2010). The infrared spectrum of 1370 cm^{-1} is the CAH stretching vibration in the cellulose and hemicellu-lose. Infrared spectrum of 1266 cm^{-1} is the G-ring CAH out-side

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the bending vibration (Schlemmer et al., 2005; Ghafar et al., 2017). The infrared spectra of 1126 cm^{-1} and 1033 cm^{-1} are CAH aromatic in-plane bending vibrations (Maroni et al., 2005; Aziz and Hanafiah, 2017).

3.2. Tg analysis

Fig. 2 shows the TG curve of the *Diospyros celebica* Bakh. 40– 80 LC temperature section in the figure, the quality of *Diospyros celebica* Bakh change faster, mainly for water and a small amount of oil evaporation; 120–180 LC temperature section is

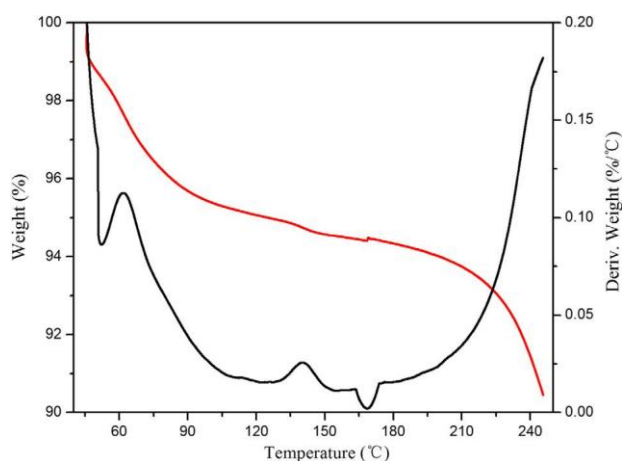
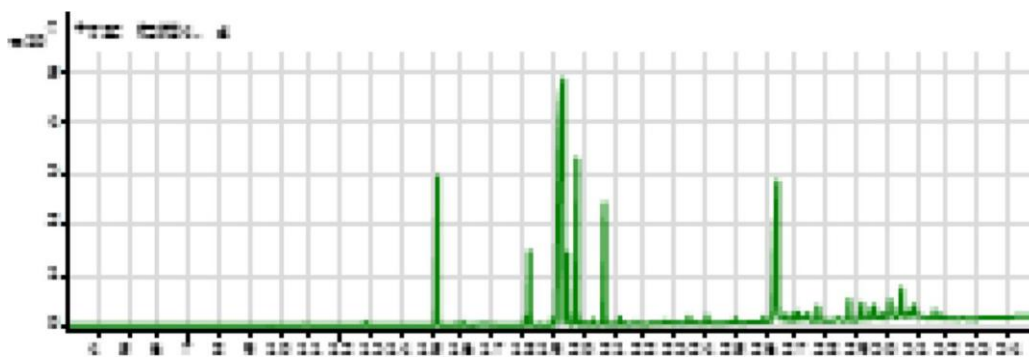


Fig. 2 *Diospyros celebica* bakh's tg curve.





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the continuous endothermic process of wood flour; Diospyros celebica Bakh powder more violent pyrolysis reaction in the 190–250 LC temperature, making the quality of wood powder decreased faster.

3.3. GC–MS analysis

Figs. 3–5 show the total ion chromatograms of the extracts of ethanol, ethanol/benzene and ethanol/methano, respective.

The chemical constituents of three extracts of Diospyros cel-ebica Bakh were determined by GC–MS qualitative analysis technique (Jiye et al., 2005; Halim and Phang, 2017). A total of 34 peaks were isolated by GC–MS gas chromatographic analysis of the ethanol extract of Diospyros celebica Bakh, and 8 compounds were identified; A total of 45 peaks were iso-lated by GC–MS gas chromatographic analysis of the Ethanol/ benzene extract, and 7 compounds were identified; A total of 39 peaks were isolated by GC–MS gas chromatographic anal-ysis of the Ethanol/methanol extract, and 10 compounds were identified. Tables 1–3 were the results of GC–MS analysis of extracts of ethanol, ethanol/benzene and ethanol/methanol of Diospyros celebica Bakh.

3.4. TDS–GC–MS analysis

There is the total ion chromatogram of the Diospyros celebica Bakh powder in Fig. 6.

The chemical constituents of Diospyros celebica Bakh pow-der were determined by TDS–GC–MS qualitative analysis technique (Shao et al., 2015; Hassan et al., 2017). A total of 39 peaks were isolated by TDS–GC–MS gas chromatographic analysis of Diospyros celebica Bakh powder, and 7 compounds were identified; Table 4 shows the results of TDS–GC–MS analysis of Diospyros celebica Bakh powder.

3.5. PY–GC–MS analysis

There is the Relative abundance curve of the Diospyros cele-bica Bakh powder in Fig. 7.

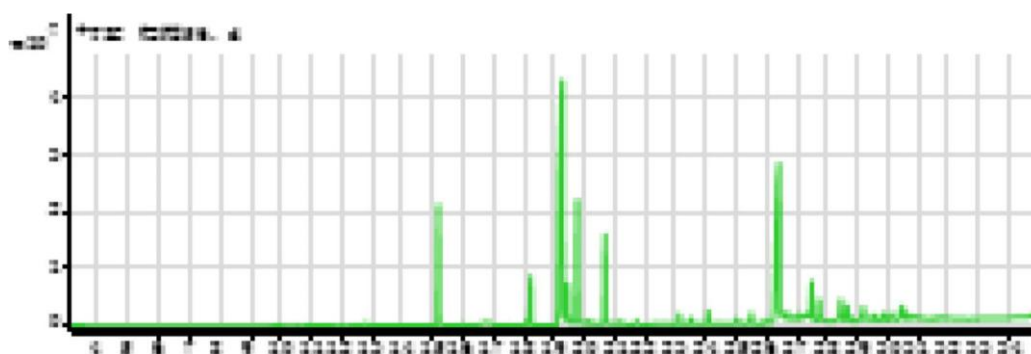
The chemical constituents of Diospyros celebica Bakh pow-der were determined by PY–GC–MS qualitative analysis tech-nique (Gao et al., 2013; Sukor et al., 2017). A total of 50 peaks were isolated by PY–GC–MS gas chromatographic analysis of Diospyros celebica Bakh powder, and 9 compounds were Retention time (min)

Fig. 3 Total ion chromatogram of ethanol extract of Diospyros celebica bakh.



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Retention time (min)

Fig. 4 Total ion chromatogram of ethanol/benzene extract of *Diospyros celebica* bakh.

Retention time (min)

Fig. 5 Total ion chromatogram of ethanol/methano extract of *Diospyros celebica* bakh.

Table 1 Ethanol extract of GC-MS analysis results.

No.	Retention time (min)	Peak area (%)	Compounds
1	15.203	15.11	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
2	18.231	6.63	Naphthalene, 2,3-dimethoxy-
3	19.486	6.16	2-Acetyl-3,5-dimethylbenzo(b)thiophene
4	20.702	13.49	Quinolin-8-amine, 5,6-dimethoxy-4-methyl-
5	21.193	0.6	Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-
6	22.12	0.4	3-O-Methyl-d-glucose
7	26.388	34.91	Ethanone, 2-hydroxy-1,2-bis(4-methoxyphenyl)-
8	28.749	2.33	6a,12a-Dihydro-6H-(1,3)dioxolo(5,6)benzofuro(3,2-c)chromen-3-ol
9	29.176	2.23	6a,12a-Dihydro-6H-(1,3)dioxolo(5,6)benzofuro(3,2-c)chromen-3-ol



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Table 2 Ethanol/Benzene extract of GC-MS analysis results.

No.	Retention time (min)	Peak area (%)	Compounds
1	15.19	14.35	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
2	18.217	6.44	Naphthalene, 2,3-dimethoxy-
3	20.152	1.5	2-Acetyl-3,5-dimethylbenzo(b)thiophene
4	20.676	12.71	Quinolin-8-amine, 5,6-dimethoxy-4-methyl-
5	22.31	1.21	1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-
6	24.072	1.77	Benzene, 1,3-dimethoxy-5-[(1E)-2-phenylethenyl]-
7	27.726	5.83	S-Indacene-1,7-dione, 2,3,5,6-tetrahydro-3,3,4,5,5,8-hexamethyl-

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Table 3 Ethanol/Methanol extract of GC–MS analysis results.

No.	Retention time (min)	Peak area (%)	Compounds
1	15.19	15.67	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
2	18.101	0.67	5-(4-Methylphenyl)furan-2-carboxylic acid
3	18.224	6.46	Naphthalene, 2,3-dimethoxy-
4	19.44	4.17	2-Acetyl-3,5-dimethylbenzo(b)thiophene
5	20.676	12.1	Quinolin-8-amine, 5,6-dimethoxy-4-methyl-
6	21.23	1.01	p-Cresol
7	24.072	1.66	Benzene, 1,3-dimethoxy-5-[(1E)-2-phenylethenyl]-
8	26.21	1.22	9-Octadecenoic acid (Z)-, methyl ester
9	27.727	3.01	S-Indacene-1,7-dione, 2,3,5,6-tetrahydro-3,3,4,5,5,8-hexamethyl-
10	28.438	3.33	10,11-Dihydro-10-hydroxy-2,3,6-trimethoxydibenz(b,f)oxepin

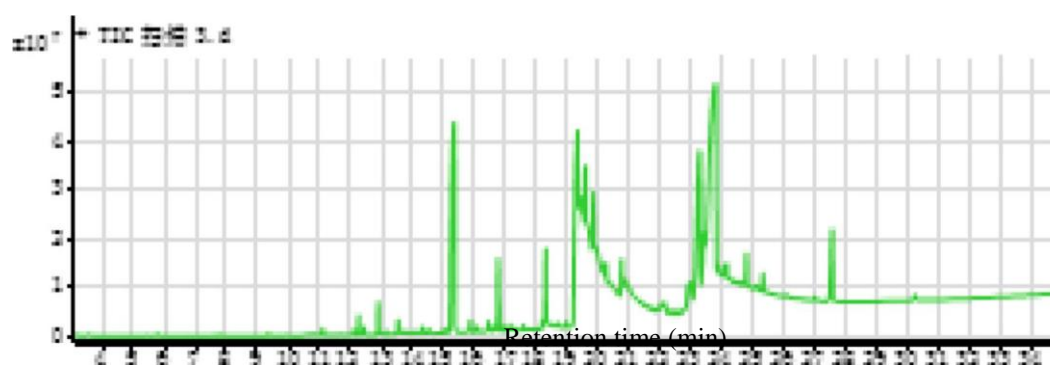


Fig. 6 Total ion chromatogram of Diospyros celebica bakh powder.

Table 4 Diospyros celebica bakh powder of TDS–GC–MS analysis results.

No.	Retention time (min)	Peak area (%)	Compounds
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1	12.262	1.03	Ethanol, 2-(2-butoxyethoxy)-, acetate
2	12.892	1.84	Methyleugenol
3	13.535	1.1	4-Methoxybenzene-1,2-diol
4	15.35	40.98	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
5	16.762	5.75	2-Naphthalenemethanol, decahydro-.alpha., .alpha.,4a-trimethyl-8-methylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-
6	18.312	6.77	Naphthalene, 2,3-dimethoxy-
7	25.117	1.33	Phenol, 4-methyl-2-[5-(2-thienyl)pyrazol-3-yl]-

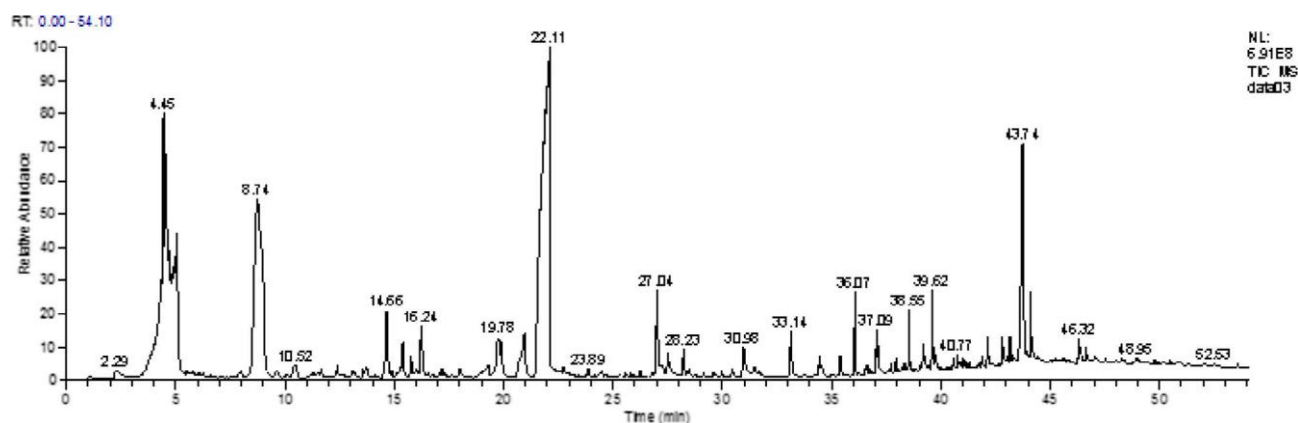


Fig. 7 Relative abundance curve of the *Diospyros celebica* bakh powder.



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Table 5 Diospyros celebica bakh powder of PY–GC–MS analysis results.

No.	Retention time (min)	Peak area (%)	Compounds
1	4.53	55.34	Acetic acid, oxo-, methyl este
2	10.52	2.16	2(3H)-Furanone, 5-methyl-
3	14.66	12.56	2-Furancarboxaldehyde, 5-methyl-
4	19.31	3.85	Pentanoic acid, 4-oxo-
5	21.83	120.01	Levoglucosenone
6	22.13	47.78	Levoglucosenone
7	27.04	10.86	1,4:3,6-Dianhydro- α -d-glucopyranose
8	27.51	22.47	5-Hydroxymethylfurfural
9	33.14	32.24	Phenol, 2,6-dimethoxy- 2-Propanone, 1-(4-hydroxy-3-
10	38.55	17.09	methoxyphenyl)-



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identified; Table 5 shows the results of PY–GC–MS analysis of Diospyros celebica Bakh powder.

3.6. Functional analysis

Pterocarpus is a high-end, expensive furniture materials collectively. Pterocarpus and Pterocarpus products have a certain human health function. The PY–GC–MS, TDS–GC–MS and GC–MS techniques were used to qualitatively analyze the Diospyros celebica Bakh, and the related compounds were obtained. By reviewing the relevant literature and reports, we have obtained the proven, human health function composition. 6a,12a-Dihydro-6H-(1,3)dioxolo(5,6)benzofuro(3,2-c)chromen-3-ol is a biologically active molecule with anti-angiogenic activity (Mathi et al., 2016). Benzene, 1,2,3-trimethoxy-5-(2-propenyl)- has medicinal value, with antioxidant, anti-inflammatory, anti-thrombosis and hypolipidemic effect (Naheer et al., 2013). 3-O-Methyl-d-glucose has a certain conservation properties, and it can protect the pancreatic B cells against the toxicity of alloxan (Malaisse-Lagae et al., 1983; Norris et al., 2006). P-Cresol plays a role in endothelial dysfunction in uremic patients, and it can repair wounds and reduce endothelial progression (Dou et al., 2004). 2-Naphthalenemethanol, decahydro-. alpha., .alpha., 4a-trimethyl-8-methylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]- with medicinal efficacy of cough and phlegm, detoxification (Tu et al., 2009). 1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,7a,7b-octahydro-1, 1,4,7-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a. beta.,7b.alpha.)]- has protective effect on acetaminophen-induced necrosis of renal tissue (Sarumathy et al., 2011). 2(3H)-Furanone, 5-methyl- has certain biological resistance, and has high antimicrobial activity against NCIM 2501 and NCIM 5021 (Jadhav et al., 2010).

4. Conclusion

GC–MS analysis, a total of 34 peaks were isolated by GC–MS gas chromatographic analysis of the ethanol extract of Diospyros celebica Bakh, and 8 compounds were identified; a total of 45 peaks were isolated by GC–MS gas chromatographic analysis of ethanol/benzene extract, and 7 were identified; a total of 39 peaks were isolated by GC–MS gas chromatographic analysis of ethanol/methanol extract, and 10 compounds were identified.

TDS–GC–MS analysis, a total of 39 peaks were isolated by TDS–GC–MS gas chromatographic analysis of Diospyros celebica Bakh powder, and 7 compounds were identified.

PY–GC–MS analysis, a total of 50 peaks were isolated by PY–GC–MS gas chromatographic analysis of Diospyros celebica Bakh powder, and 9 compounds were identified.

Through access to the literature and related reports, we clear the Diospyros celebica Bakh contains human health ingredients and functions. 6a,12a-Dihydro-6H-(1,3)dioxolo(5,6)benzofuro(3,2-c)chromen-3-ol is a biologically active molecule with anti-angiogenic activity. Benzene, 1,2,3-trimethoxy-5-(2-propenyl)- has medicinal value, with antioxidant, anti-inflammatory, anti-thrombosis and hypolipidemic effect. 3-O-Methyl-d-glucose has a certain conservation properties, and it can protect the pancreatic B cells against the toxicity of alloxan. P-Cresol plays a role in endothelial dysfunction in uremic patients, and it can repair wounds and reduce endothelial progression. 2-Naphthalenemethanol, decahydro-. alpha., .alpha.,



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4a-trimethyl-8-methylene-, [2R-(2.alpha., 4a.alpha., 8a.beta.)]- with medicinal efficacy of cough and phlegm, detoxification.

Acknowledgments

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