



Inhibitory activity of the ethyl acetate extract of *Desmanthus virgatus* (L.) Willd. leaves against α -glucosidase enzyme: *In silico* and *in vitro* studies

[Actividad inhibitoria del extracto de acetato de etilo de hojas de *Desmanthus virgatus* (L.) Willd. contra la enzima α -glucosidasa: Estudios *in silico* e *in vitro*]

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Abstract

Context: The α -glucosidase enzyme plays a key role in postprandial hyperglycemia in diabetes mellitus. This condition results in elevated blood glucose levels that exceed physiological limits in patients with diabetes mellitus. *Desmanthus virgatus* is a wild plant that contains various secondary metabolite compounds that can inhibit the activity of the α -glucosidase enzyme.

Aims: To evaluate the inhibitory activity of the ethyl acetate extract of *D. virgatus* leaves against α -glucosidase enzyme through *in silico* and *in vitro* approaches.

Methods: The content of secondary metabolite compounds of the ethyl acetate extract of *D. virgatus* leaves was analyzed using an LC-MS instrument, which was then continued with molecular docking analysis. Research on the inhibitory activity of the α -glucosidase enzyme using the ethyl acetate extract of *D. virgatus* leaves was conducted at five concentrations: 1.25, 6.25, 25.00, 50.00, and 100.00 μ g/mL.

Results: LC-MS analysis identified 182 phytochemicals with 25 dominant flavonoids. Nineteen compounds fulfilled Lipinski's rule of five and were subjected to molecular docking, where luteolin-7-glucoside showed the strongest binding affinity (-9.52 kcal/mol) compared to acarbose (-9.25 kcal/mol). *In vitro* assays revealed a strong inhibitory effect with an IC_{50} of 7.14 ± 0.42 μ g/mL, comparable to acarbose (4.64 ± 0.21 μ g/mL).

Conclusions: These findings suggest that the ethyl acetate extract of *D. virgatus* exhibits promising α -glucosidase enzyme inhibitory activity and could be developed as a potential antidiabetic agent.

Keywords: *Desmanthus virgatus*; α -glucosidase enzyme; *in vitro* assay; luteolin-7-glucoside; molecular docking.

Resumen

Contexto: La enzima α -glucosidasa desempeña un papel clave en la hiperglucemia posprandial en la diabetes mellitus. Esta condición provoca niveles elevados de glucosa en sangre que superan los límites fisiológicos en pacientes con diabetes mellitus. *Desmanthus virgatus* es una planta silvestre que contiene diversos metabolitos secundarios que pueden inhibir la actividad de la enzima α -glucosidasa.

Objetivos: Evaluar la actividad inhibitoria del extracto de acetato de etilo de hojas de *D. virgatus* contra la enzima α -glucosidasa mediante métodos *in silico* e *in vitro*.

Métodos: Se analizó el contenido de metabolitos secundarios del extracto de acetato de etilo de hojas de *D. virgatus* mediante un equipo de LC-MS, seguido de un análisis de acoplamiento molecular. Se realizó una investigación sobre la actividad inhibitoria de la enzima α -glucosidasa utilizando el extracto de acetato de etilo de hojas de *D. virgatus* a cinco concentraciones: 1,25; 6,25; 25,00; 50,00 y 100,00 μ g/mL.

Resultados: El análisis LC-MS identificó 182 fitoquímicos con 25 flavonoides dominantes. Diecinueve compuestos cumplieron la regla de cinco de Lipinski y se sometieron a acoplamiento molecular, donde la luteolina-7-glucósido mostró la mayor afinidad de unión (-9,52 kcal/mol) en comparación con la acarbosa (-9,25 kcal/mol). Los ensayos *in vitro* revelaron un fuerte efecto inhibitorio con una CI_{50} de $7,14 \pm 0,42$ μ g/mL, comparable a la de la acarbosa ($4,64 \pm 0,21$ μ g/mL).

Conclusiones: Estos hallazgos sugieren que el extracto de acetato de etilo de *D. virgatus* exhibe una prometedora actividad inhibitoria de la α -glucosidasa y podría desarrollarse como un posible agente antidiabético.

Palabras Clave: acoplamiento molecular; *Desmanthus virgatus*; ensayo *in vitro*; enzima α -glucosidasa; luteolina-7-glucósido.

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INTRODUCTION

Diabetes mellitus (DM) is a chronic and complex metabolic disorder with multiple etiologies and profound risks, both acute and chronic (Salehi et al., 2019). Type 2 diabetes mellitus (T2DM) is a chronic metabolic disorder characterized by insulin resistance and persistent hyperglycemia, leading to multiple organ complications (Tanty et al., 2018). Postprandial hyperglycemia can be managed by inhibiting α -glucosidase enzyme, a key enzyme in carbohydrate digestion (Khin et al., 2023). Although synthetic inhibitors such as acarbose are effective, they often cause gastrointestinal side effects, driving the search for safer, plant-derived alternatives (Juneja et al., 2022).

The search for herbal plants on a global scale continues due to its perceived safety and effectiveness. One of the herbal plants as a potential antidiabetic agent candidate is *Desmanthus virgatus* (L.) Willd. leaves. *D. virgatus* is a foreign plant from Tropical America in the *Mimosae* tribe, which has a fairly wide distribution and is often used as animal feed (Azani et al., 2017). Plants from the *Fabaceae* family offer a range of benefits, including antidiabetic, antifertility, anti-inflammatory, and antioxidant properties (Maroyi, 2018). In ethnomedical practice, plants from the *Fabaceae* family are used to treat basic health problems, such as fever, constipation, and muscle pain. Thus, ethnomedical practices provide valuable initial clues in directing scientific research to explore and prove the biological activities of species in this family (Sutjaritjai et al., 2022). The leaves of *D. virgatus* were chosen as the object of study due to their abundant presence in various tropical regions, including Indonesia, making them a potential source of medicinal material for natural material-based research (Wirawan et al., 2021). In addition, the active compounds that are widespread in the *Fabaceae* family, especially the *D. virgatus* plant, are known to be effective in the treatment of diabetes (Tukiran et al., 2025).

D. virgatus leaf extract by phytochemical test is reported to have abundant tannin compounds (Wirawan et al., 2021). Tannins are polyphenolic substances with varying molecular weight and complexity (Ajebli and Eddouks, 2019). Polyphenols are a group of secondary metabolites that are widespread in plants (Suybeng et al., 2021). Due to its structure with polyhydroxy groups on the aromatic ring, it has the potential to scavenge free radicals, regulate enzymes, bind with metal ions, and perform other functions, which have been applied to improve health (Mukai et al., 2005). Tannins are divided into two types: hydrolysed tannins (HT), which are polyesters of gallic acid and various sugars, and condensed tannins (CT), which

are polymers of flavonoids. Tannins are widely distributed in the plant kingdom and have been demonstrated to have neuroprotective benefits in diabetic complications due to their anti-inflammatory and antioxidant properties (Omar et al., 2022). The mechanism of tannins in reducing blood glucose levels involves inducing pancreatic β -cells, which in turn affect adipose cells, thereby strengthening insulin activity. In addition, tannins can reduce the absorption of nutrients by inhibiting glucose absorption in the intensive care unit (Sun et al., 2020). Tannins also exhibit antidiabetic effects, with a mechanism of action that enhances cell recovery and propagation, as well as reduces carbohydrate absorption by inhibiting α -glucosidase enzyme activity (Ajebli and Eddouks, 2019).

The diverse secondary metabolites in *D. virgatus* leaves, coupled with the lack of prior studies on its antidiabetic potential, justify the necessity of this research. Ethyl acetate was chosen as a solvent because it is effective for extraction, has an easy evaporation process, and has a lower level of toxicity compared to methanol, ethanol, and chloroform (Kumar et al., 2023). The ethyl acetate fraction is a polyphenol-rich extract containing catechin and epicatechin compounds that potentially inhibit α -glucosidase enzyme activity and affect glucose absorption (Olaokun et al., 2016). This study investigates the α -glucosidase enzyme inhibitory activity of the ethyl acetate extract of *D. virgatus* leaves through LC-MS profiling, molecular docking, and *in vitro* assays.

MATERIAL AND METHODS

Chemicals

The chemical compounds employed in this study included the α -glucosidase enzyme 3.2.1.20 (BRENDA, IUBMB), *p*-nitrophenyl- α -D-glucopyranoside (Merck, Germany), Na_2CO_3 (Sigma-Aldrich), ethanol pro analyses (Sigma Aldrich), ethyl acetate pro analyses (Sigma-Aldrich), and acarbose (HY-B0089). Data on bioactive compounds of ethyl acetate extract of *D. virgatus* leaves were obtained from the PubChem website (<https://pubchem.ncbi.nlm.nih.gov/>) in (.sdf) format, while the 3D protein structure was downloaded from the Protein Data Bank website (<http://www.rcsb.org/>) namely the crystal structure of isomaltase from *Saccharomyces cerevisiae* (3A4A) which has a structure and function similar to hom sapiens, there is a co-crystallized alpha-D-glucopyranose ligand in the structure which was downloaded in (.pdb) format.

Extraction and partition

D. virgatus leaf samples were collected from Kedunglungkem Village, Benjeng Subdistrict, Gresik Regency, East Java, located between latitude -7.2918593° and longitude 112.4490716° East, Indonesia, in March 2024. Plant material was authenticated at Genbnesia Herbarium, Indonesia (Voucher No. BT-02/035/24). A total of 6.8 kg of *D. virgatus* leaves were cleaned of dirt using water drainage, then dried in the sun for 3 days. The dried leaves were then ground to obtain a powder sample of 3.8 kg. The *D. virgatus* leaf powder was macerated using an ethanol solvent for two days, and the process was repeated four times. The filtrate and macerate were filtered using a Buchner funnel and evaporated using a Buchi vacuum rotary evaporator to produce 478 g of ethanol extract. The ethanol extract was fractionated using an ethyl acetate solvent in a separatory funnel to produce two layers, which were then separated. The fractionation process was repeated until a colorless solution of ethyl acetate solvent was obtained. The fractionated ethyl acetate solution was evaporated using a vacuum rotary evaporator, resulting in 1.4 g of concentrated extract. LC-MS profiling was conducted on a Shimadzu LC-MS-8040 with specified parameters.

Bioavailability analysis

Dominant compounds from LC-MS analysis results with a composition of more than 1% are used in the analysis to determine the permeability and solubility of a compound when it passes through biological membranes, such as the intestines or skin. The bioavailability test method utilizes Lipinski's rule of five parameters, as accessed through the SwissADME website (<https://www.swissadme.ch/>). Lipinski's rule of five includes hydrogen bond donors, Log P value, molecular weight, molar refraction value, and hydrogen bond acceptors. Ligands that fulfil Lipinski's rule of five reflect the oral bioavailability of the ligand.

Molecular docking analysis

Data on bioactive compounds of ethyl acetate extract of *D. virgatus* leaves were obtained from the PubChem website (<https://pubchem.ncbi.nlm.nih.gov/>) in (.sdf) format, while the 3D protein structure was downloaded from the Protein Data Bank website (<http://www.rcsb.org/>), namely the crystal structure of isomaltase from *Saccharomyces cerevisiae* (PDB ID: 3A4A), which was downloaded in (.pdb) format. Ligands are prepared by adding hydrogen atoms, and proteins are prepared by removing residues and water molecules. After preparing the ligands and receptors, docking molecular analysis is performed using

Autodock 4.2.6. MGLTools software. Next, the grid is adjusted to a grid distance of 0.375 Å, with the dimensions of the grid boxes X, Y, and Z set to 60 × 60 × 60 Å. The center grid parameters are at x, y, and z with values 21.243, -7.756, and 24.341. The Lamarckian Genetic Algorithm approach is used to find the smallest binding affinity value by applying minimization to the genetic algorithm and managing the gene population. Other parameters of molecular docking are as follows: Rate of Gene Mutation: 0.02; Population Size: 150; Maximum Number of Evals: 2500000; Maximum Number of Generations: 27000; Number of GA Runs: 100; and Rate of Crossover: 0.8. Molecular docking was validated by re-docking the co-crystallized ligand to ensure RMSD < 2 Å.

Absorption, distribution, metabolism, excretion, and toxicity (ADMET)

The pharmacokinetic properties of the compound in terms of absorption, oral bioavailability, toxicity potential, and P-glycoprotein inhibitors were evaluated using the pkCSM server (<https://biosig.lab.uq.edu.au/pkcsml/>).

In vitro α -glucosidase enzyme inhibition assay

The α -glucosidase enzyme inhibition test using the extract was performed according to standard methods with slight modifications (Etsassala et al., 2020). A total of 50 μ L of phosphate buffer was added to a 96-well plate, which was then supplemented with 10 μ L of α -glucosidase enzyme 3.2.1.20 (BRENDA, IUBMB) derived from *S. cerevisiae* (yeast) with a purity level of 98%. *D. virgatus* extract was added to the plate with varying concentrations of 31.25 to 500 μ g/mL, which was then incubated at 37°C for 15 minutes. After that, 20 μ L of *p*-nitrophenyl- α -D-glucopyranoside substrate, with a concentration of 5 mM, was added to each well and incubated at 37°C for 20 minutes. The ongoing reaction was stopped by adding 50 μ L Na₂CO₃. Using a multiplate reader instrument, *p*-nitrophenyl released from the reacting mixture with enzyme inhibitory activity was measured at a wavelength of 405 nm. In this study, acarbose was used as a control drug with varying concentrations from 0.7813 to 50.00 μ g/mL. Readings were taken three times using a multiplate reader instrument (Allsheng FlexA-200 Microplate Reader), and inhibition presentations were obtained as equation [1].

$$\text{Inhibitory activity (\%)} = \left(1 - \frac{A}{b}\right) \times 100 \quad [1]$$

where A is the absorption in the presence of extract and b is the absorbance in the presence of the phosphate buffer (control).

Statistical analysis

Statistical analysis of the IC₅₀ value of *D. virgatus* leaf extract was performed using one-way ANOVA followed by the LSD post-hoc test in IBM SPSS Statistics software version 26. *In vitro* α -glucosidase enzyme inhibition was measured in triplicate at concentrations of 1.53, 6.25, 25, 50, and 100 μ g/mL, expressed as the mean $\pm$ standard deviation. Statistical significance was determined by one-way ANOVA followed by LSD post-hoc test (p<0.01).

RESULTS

LC-MS analysis

LC-MS analysis identified 182 phytochemicals with 25 dominant flavonoids (>1% composition) ethyl

acetate extract of *D. virgatus* leaves (Table 1, Table S1, and Fig. 1).

Lipinski’s rule of five

The dominant compounds from the ethyl acetate extract of *D. virgatus* leaves were analyzed for bioavailability before conducting molecular docking tests using Lipinski's rule of five. The results of the analysis showed that the average of the dominant compounds is hydrophilic with hydrogen donor and acceptor values exceeding 5 and 10.

This was reinforced by the negative log P values in some of the dominant compounds, but the log P values of the twenty-five dominant compounds were in accordance with Lipinski's rule of five which ranged a maximum of log P value (-4) (as seen in Table 2).

Table 1. LC-MS results of 25 dominant compounds in the ethyl acetate extract of *D. virgatus* leaves, with a percentage composition greater than 1.00000%.

Identified compounds	Retention time	Composition (%)
Quercetagenin	11.520	1.05621
Demethyltorosaflavone C	12.757	1.18708
5,7,4'-trihydroxy-3'-C-methylflavone 4'-rhamnoside	19.786	1.02174
Kaempferol-3-rhamnoside	21.429	1.16639
Kaempferol-3-galactoside	22.178	1.36700
Kaempferol-5-glucoside	22.185	1.46965
Calycosin-7-O- β -D-glucoside	22.216	1.22516
Quercetin-3-rhamnoside	22.616	1.23425
Kaempferol-3-glucoside	22.623	1.83824
Kaempferol-7-O-glucoside	22.624	1.42567
Luteolin-7-glucoside	22.628	1.47147
Quercitrin	23.194	1.54232
Quercetin 7-O- β -D-glucoside	23.311	1.54421
Hirsutin	23.977	1.10346
Isoquercitrin	24.018	1.32544
Hyperoside	24.020	1.07007
Querciturone	25.835	1.32175
Luteolin 7,3'-dimethylether 5-rhamnoside	25.844	1.35226
Glucotricin	27.973	1.05163
Kaempferide-3-rhamnoside-7-xyloside	33.442	1.11664
Naringin	33.563	1.11574
Kaempferol 3-neohesperidoside	33.625	1.40847
Kaempferol-7-rhamnoside-4'-glucoside	34.003	1.89019
Kaempferol-3(5''-feruloylapioside)	34.016	1.74381
Desmanthin 1	35.520	1.18836

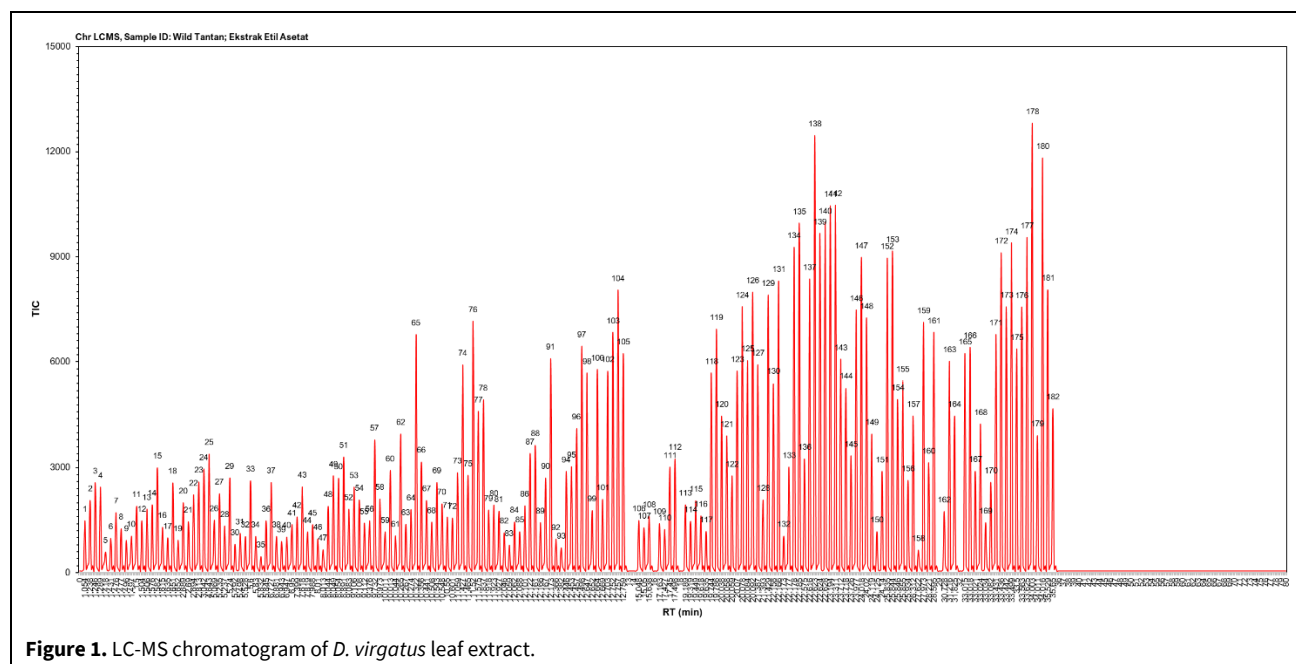


Figure 1. LC-MS chromatogram of *D. virgatus* leaf extract.

The results of the analysis, based on Lipinski's rule of five, showed that the dominant compounds are hydrophilic, with an average negative log P value. The dominant compounds also have donor and acceptor hydrogen bonds that exceed the rule limits, which can affect solubility and permeability in the body. There are several dominant compounds that are difficult for the body to absorb because they have molecular weights exceeding 500 Da, making it challenging for them to pass through cell membranes. Thus, absorption in the intestine is not optimal and difficult to excrete through the kidneys, which can result in toxic properties. Of these, 19 fulfilled Lipinski's rule of five and were subjected to docking analysis.

Molecular docking analysis

Validation of molecular docking is done by re-docking natural ligands and calculating the average RMSD value, which must be below 2 Å, indicating the accuracy of this method. The validation results of the molecular docking method in this study yielded an average RMSD value of 0.788 Å, indicating that this method has high validity and can be considered accurate, as evidenced by the RMSD value below 2 Å, which suggests that the copy ligand is similar to the natural ligand (Fig. 2).

The molecular docking validation was continued by docking the dominant compounds of *D. virgatus* leaf extract with the target protein to determine the bond conformation in inhibiting the α -glucosidase enzyme. This study employed a positive control, namely the synthetic drug acarbose, to compare the effectiveness of the dominant compounds in inhibit-

ing the α -glucosidase enzyme. The results of the molecular docking are presented in Table 3.

Based on the results of molecular docking analysis, luteolin-7-glucoside exhibited the strongest binding affinity (-9.52 kcal/mol), surpassing that of acarbose (-9.25 kcal/mol). Hydrogen bonding interactions were observed with GLN279, ASP69, GLN182, GLU277, ASP215, ASP352, ARG442, and TYR158. This strong interaction suggests its potential as a natural α -glucosidase enzyme inhibitor (Fig. 3).

ADMET prediction

The results of *in silico* predictions for the pharmacokinetic (ADMET) properties and toxicity of luteolin-7-glucoside and the control drug acarbose are presented in Table 4.

In silico predictions of pharmacokinetic (ADME) properties and toxicity indicate that luteolin-7-glucoside from *D. virgatus* extract has a good safety profile and promising pharmacokinetic properties, with intestinal absorption of 37.56%, non-toxic according to the AMES test, and does not inhibit major cytochrome P450 enzymes, making it a potential candidate for a safe antidiabetic drug.

Inhibition of the α -glucosidase enzyme

To determine the effect of *D. virgatus* leaf extract, which contains as many as 182 compounds, including 25 potential dominant compounds, further testing was carried out to assess its effectiveness in inhibiting the α -glucosidase enzyme *in vitro* (Table 5). Acarbose, used as a positive control, showed an IC₅₀ value of 4.64 ± 0.21 μ g/mL in the concentration range of 0.7813

to 50.0000 $\mu\text{g/mL}$. The IC_{50} value of acarbose is a strong inhibitor because acarbose is a synthetic drug that is often used by people with type 2 diabetes to reduce blood sugar levels.

In vitro testing of the ethyl acetate extract on α -glucosidase enzyme inhibition is highly significant, with concentration variations ranging from 1.53 to 100 $\mu\text{g/mL}$. The IC_{50} value of the ethyl acetate extract of *D. virgatus* leaves also shows strong inhibition, with

an IC_{50} value of $7.14 \pm 0.42 \mu\text{g/mL}$, as shown in Table 6 and Fig. 4.

In vitro assays demonstrated concentration-dependent α -glucosidase enzyme inhibition, with an IC_{50} of $7.14 \pm 0.42 \mu\text{g/mL}$, comparable to acarbose ($4.64 \pm 0.21 \mu\text{g/mL}$). It can be concluded that *D. virgatus* leaf extract falls into the same inhibitory category as acarbose; however, the effectiveness of inhibition against the α -glucosidase enzyme, as indicated by the IC_{50} value, is significantly different ($p < 0.01$).

Table 2. Lipinski's rule of five analysis of 25 dominant compounds of the ethyl acetate extract of *D. virgatus* leaves.

Identified compounds	H-donor (<10)	H-acceptor (<5)	Log P (<5)	Molar refractivity (40-130)	Molecular weight (500 g/mol)
Quercetagenin	6	8	0.92	80.06	318.24
Demethyltorosaflavone C	4	8	1.94	101.74	394.33
5,7,4'-trihydroxy-3'-C-methylflavone 4'-rhamnoside	5	9	1.46	109.92	430.40
Kaempferol-3-rhamnoside	5	10	0.63	110.58	446.40
Kaempferol-3-galactoside	7	11	-0.12	108.13	448.38
Kaempferol-5-glucoside	7	11	-0.12	108.13	448.38
Calycosin-7-O- β -D-glucoside	5	10	0.63	110.58	446.40
Quercetin-3-rhamnoside	7	11	0.22	109.00	448.38
Kaempferol-3-glucoside	7	11	-0.12	108.13	448.38
Kaempferol-7-O-glucoside	6	11	-0.12	106.13	432.38
Luteolin-7-glucoside	7	11	-0.12	108.13	448.38
Quercitrin	7	11	0.01	109.00	448.38
Quercetin-7-O- β -D-glucoside	8	12	-0.59	110.16	464.38
Hirsutrin	8	12	-0.48	110.16	462.40
Isoquercitrin	8	12	-0.48	110.16	464.38
Hyperoside	8	12	-0.38	110.16	464.38
Querciturone	8	13	-0.47	110.77	478.36
Luteolin-7,3'-dimethyl ether-5-rhamnoside	4	10	1.46	115.91	460.43
Glucotricin	6	12	0.58	119.10	492.43
Kaempferide-3-rhamnoside-7-xyloside	7	14	-0.27	137.59	578.52
Naringin	8	14	-0.87	134.91	580.53
Kaempferol-3-neohesperidoside	9	15	-1.64	139.36	594.52
Kaempferol-7-rhamnoside 4'-glucoside	6	10	0.48	106.97	432.38
Kaempferol-3(5''-feruloylapioside)	6	14	2.69	150.07	594.52
Desmanthin 1	10	16	0.32	146.73	616.48

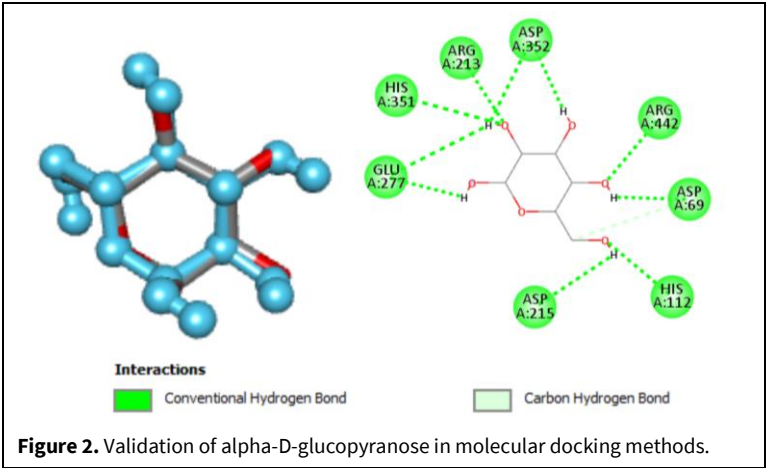


Table 3. Molecular docking results of dominant compounds of *D. virgatus* extract.

Compound	Binding affinity (kcal/mol)				Inhibition constant (μM)
	I	II	III	Average	
Acarbose	-9.25	-9.15	-9.22	-9.20 ± 0.05	0.013 ± 0.050
Quercetagenin	-7.03	-7.16	-7.07	-7.08 ± 0.07	6.420 ± 0.670
Demethyltorosaflavone C	-8.50	-8.56	-8.57	-8.54 ± 0.04	0.051 ± 0.001
5,7,4'-Trihydroxy-3'-C-methylflavone 4'-rhamnoside	-8.53	-8.59	-8.51	-8.54 ± 0.04	0.052 ± 0.004
Kaempferol-3-rhamnoside	-7.21	-7.04	-7.06	-7.10 ± 0.09	5.440 ± 0.334
Kaempferol-3-galactoside	-9.00	-9.11	-8.93	-9.01 ± 0.09	0.020 ± 0.012
Kaempferol-5-glucoside	-8.21	-8.07	-8.20	-8.16 ± 0.08	0.470 ± 0.650
Calycosin-7-O-β-D-glucoside	-8.90	-8.88	-8.86	-8.88 ± 0.02	0.027 ± 0.006
Quercetin-3-rhamnoside	-7.28	-7.49	-7.52	-7.43 ± 0.12	3.646 ± 0.847
Kaempferol-3-glucoside	-6.87	-6.96	-7.04	-6.95 ± 0.08	8.050 ± 1.177
Kaempferol-7-O-glucoside	-8.25	-8.20	-8.13	-8.19 ± 0.06	0.092 ± 0.010
Luteolin-7-glucoside	-9.52	-9.62	-9.42	-9.52 ± 0.12	0.010 ± 0.071
Quercitrin	-7.63	-7.41	-7.56	-7.53 ± 0.11	2.780 ± 1.034
Quercetin 7-O-β-D-glucoside	-7.64	-7.94	-7.71	-7.76 ± 0.15	2.050 ± 0.534
Hirsutrin	-6.15	-6.07	-6.92	-6.38 ± 0.46	25.086 ± 12.768
Isoquercitrin	-6.48	-6.19	-6.51	-6.39 ± 0.17	30.553 ± 0.944
Hyperoside	-7.83	-8.32	-8.03	-8.06 ± 0.24	1.069 ± 0.899
Querciturone	-5.64	-5.88	-6.07	-5.86 ± 0.21	52.593 ± 19.209
Luteolin-7,3'-dimethyl ether 5-rhamnoside	-7.82	-7.79	-7.58	-7.73 ± 0.12	2.196 ± 0.516
Glucotricin	-8.55	-8.57	-8.77	-8.63 ± 0.12	0.041 ± 0.01

DISCUSSION

The primary objective of this study was to determine the content of potential dominant phytochemicals in the ethyl acetate extract of *D. virgatus* leaves and to evaluate their inhibitory activity against the α -glucosidase enzyme. In this study, leaf samples of *D. virgatus* were collected from remote rural areas in Indonesia, and the content of all phytochemicals was

evaluated using an LC-MS instrument. The LC-MS profiling revealed 25 dominant flavonoids, most of which were glycosides of quercetin, kaempferol, and luteolin. The dominant flavonoid compounds with levels of more than 1% were analyzed *in silico* to determine the interaction of ligand molecules with target proteins in *in vitro* assays. Docking studies indicated luteolin-7-glucoside had superior binding affinity compared to acarbose.

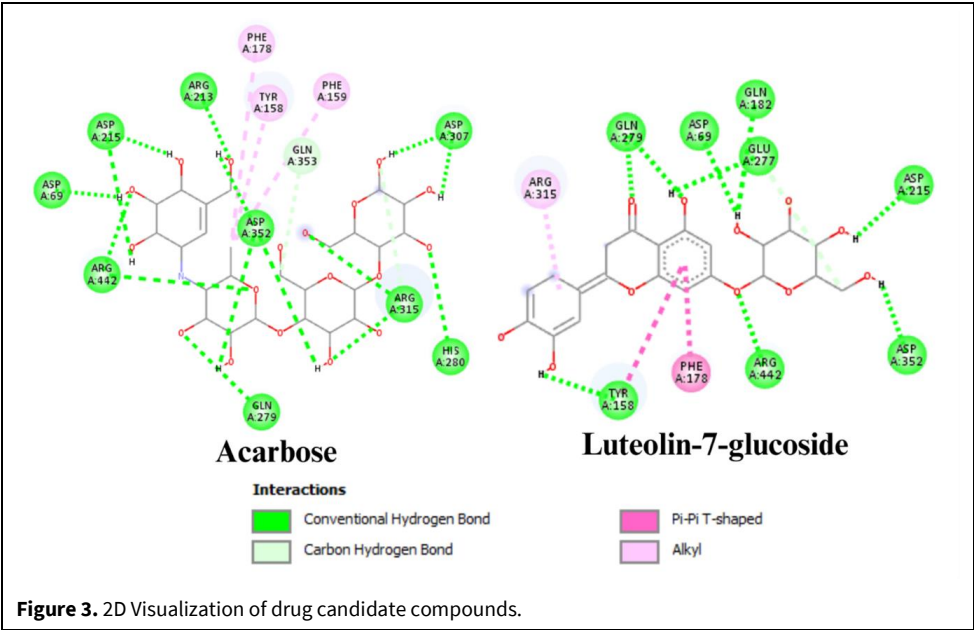


Table 4. ADMET prediction of luteolin-7-glucoside and acarbose.

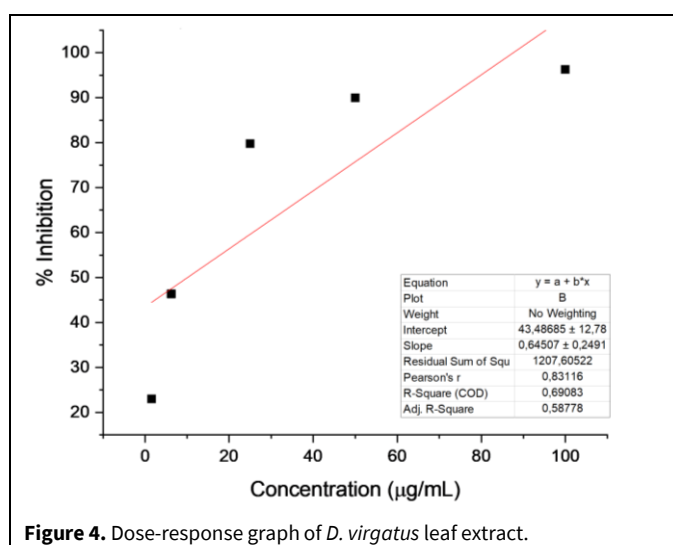
Parameter	Pharmacokinetic property	Predicted value	
		Luteolin-7-glucoside	Acarbose
Absorption	Water solubility (log mol/L)	-2.716	-1.361
	CaCO ₂ permeability (log Papp in 10 ⁻⁶ cm/s)	0.248	-0.717
	Human intestinal absorption (%)	37.556	0
	P-glycoprotein substrate	Yes	Yes
	P-glycoprotein I/II inhibitor	No/No	No/No
Distribution	VDss (human) (log L/kg)	0.884	-0.833
	Fraction unbound (human) (Fu)	0.224	0.569
	BBB permeability (log BB)	-1.564	-1.841
Metabolism	CYP2D6 substrate	No	No
	CYP3A4 substrate	No	No
	CYP1A2 inhibitor	No	No
	CYP2C19 inhibitor	No	No
	CYP2C9 inhibitor	No	No
	CYP2D6 inhibitor	No	No
	CYP3A4 inhibitor	No	No
Excretion	Total clearance (log mL/min/kg)	0.478	0.619
	Renal OCT2 substrate	No	No
Toxicity	AMES toxicity	No	No
	Max. tolerated dose (human) (log mg/kg/day)	0.584	0.613
	hERG I/II inhibitor	No/No	No/No
	Oral rat acute toxicity (LD ₅₀) (mol/kg)	2.547	2.673
	Oral rat chronic toxicity (LOAEL) (log mg/kg_bw/day)	4.279	4.466
	Hepatotoxicity	No	No
	<i>T. pyriformis</i> toxicity (log µg/L)	0.285	0.285

Table 5. IC₅₀ value of acarbose against α -glucosidase enzyme.

Conc. (μ g/mL)	Log [Conc.]	Inhibition (%)			Average	IC ₅₀ (μ g/mL)
		I	II	III		
0.7813	-0.1072	14.04	20.15	27.45	20.55 $\pm$ 6.72	
1.5625	0.1938	21.38	26.73	32.89	27.00 $\pm$ 5.76	
3.1250	0.4949	32.55	44.73	42.01	39.76 $\pm$ 6.40	
6.2500	0.7959	54.66	58.40	58.23	57.10 $\pm$ 2.11	4.64 $\pm$ 0.21
12.5000	1.0969	66.29	63.75	60.27	63.44 $\pm$ 3.30	
25.0000	1.3979	64.38	64.77	65.66	64.94 $\pm$ 0.65	
50.0000	1.6990	72.70	65.66	65.87	68.36 $\pm$ 3.78	

Table 6. IC₅₀ value of *D. virgatus* leaf extract against α -glucosidase enzyme.

Conc. (μ g/mL)	% inhibition			Average	IC ₅₀ (μ g/mL)
	I	II	III		
1.53	25.28	18.05	25.71	23.01 $\pm$ 4.31	
6.25	45.64	49.34	44.12	46.37 $\pm$ 2.69	
25.00	80.92	80.60	77.72	79.75 $\pm$ 1.76	7.14 $\pm$ 0.42
50.00	90.03	89.85	90.01	89.96 $\pm$ 0.10	
100.00	96.78	96.36	95.60	96.25 $\pm$ 0.60	

**Figure 4.** Dose-response graph of *D. virgatus* leaf extract.

On the other hand, the ethyl acetate extract of *D. virgatus* leaves tested against the α -glucosidase enzyme had a very strong IC₅₀ value, equivalent to that of the synthesized drug, acarbose. The dominant compounds contained in the ethyl acetate extract of *D. virgatus* leaves are dominated by flavonoid glycosides, particularly quercetin, kaempferol, and luteolin derivatives conjugated with glucose, rhamnose, or galactose. These compounds encompass various classes of flavonoids, including flavonols, flavones, flavanones, isoflavones, C-methyl flavonoids, and des-

manthin, which are characteristic compounds of the *Desmanthus* species.

In testing the bioavailability of a drug candidate compound, Lipinski's rule of five is used to analyze parameters such as the number of acceptor-donor bonds with fewer than 5 and 10 hydrogen bonds, molar refraction values ranging from 40 to 130, log P values less than 5, and molecular weight less than 500 g/mol. Hydrogen bonding plays an important role in drug partitioning and permeability. However, the presence of too many hydrogen bond donors and

acceptors can damage drug partitioning and membranes (Coimbra et al., 2021). Compounds with higher molecular weights are less likely to be orally active compared to those with lower molecular weights (Doak et al., 2014). The log P value expresses solubility in fat (hydrophobic) or water (hydrophilic) with a range of values less than 5; the ligand cannot be too negative because it cannot pass through the lipid bilayer membrane, and the log P value cannot be too positive because the molecule is increasingly hydrophobic (Ruswanto et al., 2020). Molar refraction is a value of the total polarizability of drug molecules that is highly dependent on temperature, refractive index, and pressure. This parameter indicates the ability of a drug to interact with receptors and cause biological activity (Lipinski, 2004). In this study, nineteen dominant compounds in the *D. virgatus* leaf extract were identified as potential drug candidates. The molecular docking results showed that the luteolin-7-glucoside had a more negative binding affinity value than acarbose. The more negative the binding affinity value obtained, the more stable the bond complex formed between the receptor protein and the compound (Lipinski et al., 2001). The luteolin-7-glucoside has similarities to acarbose through the binding of amino acid residues ASP69, ASP215, ASP352, ARG442, ARG315, GLN279, PHE178, and TYR158. Visualization of 2D interactions between luteolin-7-glucoside and the amino acid residues of the enzyme can be shown in Fig. 3. The similarity and coverage of the binding area of amino acid residues that are close to the positive control compound, acarbose, are predicted as potential inhibitors in inhibiting target proteins (Amini et al., 2025).

ADME predictions for compounds indicate human intestinal absorption (HIA) scores, which predict a compound's ability to be absorbed in the gastrointestinal tract, with higher values indicating excellent absorption. The blood-brain barrier (BBB) penetration score, with lower values indicating limited central nervous system (CNS) permeability. This prediction aids in assessing the pharmacokinetics of a potential compound that is active both peripherally and centrally (Tong et al., 2022). The prediction for luteolin-7-glucoside in Table 4 shows a relatively low HIA score (37.556%), indicating promising intestinal absorption, while its BBB penetration score (-1.564 log BB) indicates limited CNS permeability. Despite its limited direct penetration into the CNS, luteolin-7-glucoside remains a potential candidate due to its well-documented antidiabetic properties.

The results of the *in vitro* analysis showed that the ethyl acetate extract of *D. virgatus* leaves had an IC_{50} value of 7.14 ± 0.42 g/mL, equivalent to a very strong category, similar to the synthetic drug acarbose. *D.*

virgatus leaf extract contains many dominant compounds, such as kaempferol, which is a flavonol group. Kaempferol can increase plasma insulin levels and reduce blood glucose levels. Kaempferol exhibits antidiabetic activity through various molecular mechanisms. This compound inhibits the α -glucosidase enzyme by binding to its active site and disrupting the enzyme's catalytic center, resulting in a change in the enzyme's conformation (Peng et al., 2016). Additionally, kaempferol activates autophagy, enhances intracellular lipid degradation, and protects pancreatic β cells from lipotoxicity and endoplasmic reticulum stress (Ashrafizadeh et al., 2020; Kim et al., 2021). Its antioxidant activity is demonstrated through increased levels of reduced glutathione, superoxide dismutase, and glutathione peroxidase, thereby suppressing lipid and glucose peroxidation (Al-Numair et al., 2015). Kaempferol also inhibits the ASK1/MAPK signaling pathway, prevents myocardial hypertrophy, and improves cardiac function (Feng et al., 2017). Kaempferol glycosides have been reported to increase renal glucose excretion and improve insulin resistance (Rossetti et al., 1987).

Luteolin-7-glucoside is a potential flavonoid with various benefits, especially its effectiveness as an antidiabetic agent. Luteolin can prevent the formation of reactive oxygen species (ROS) by inhibiting enzymes that produce these species and thereby protecting other components of the antioxidant system. The antioxidant activity of luteolin combined with its hypoglycemic potential protects the pancreas as well as increases insulin secretion (Han et al., 2023). In the ethyl acetate extract of *D. virgatus*, there is a quercetin compound that can significantly increase the expression of phosphorylated glycogen synthase kinase 3 β (GSK-3 β), namely Ser9, and Akt phosphorylation increases the expression of glucokinase (GCK) protein, thereby increasing hepatic glycogen synthesis and alleviating glucose metabolism disorders (Peng et al., 2017).

Several flavonoid glycoside compounds exhibit antidiabetic potential through various molecular mechanisms. Desmanthin-1 inhibits both aldose reductase and α -glucosidase enzymes, reducing sorbitol accumulation and preventing cell damage caused by diabetic complications. It also helps control postprandial blood sugar levels (Matsuda et al., 2002). Naringin can lower lipid and blood glucose levels and enhance antioxidant enzyme activity, which has been clinically proven to aid in weight loss (Hartogh et al., 2019). Kaempferide-3-rhamnoside-7-xyloside acts through the XRA/ABCA1 and PI3K/AKT signaling pathways mediated by PPAR γ to address metabolic disorders and insulin resistance (Tang et al., 2021). Glucotrisin acts as a competitive inhibitor of the ERK

receptor, thereby helping to regulate glucose balance in the body (Pathak and Kim, 2024). The compound hyperoside offers protection against diabetic nephropathy by enhancing kidney function, mitigating oxidative stress, stimulating extracellular signal-regulated protein kinase activity, and preventing pyroptosis in human renal tubular epithelial cells (Zhang et al., 2023). Hirsutrin reduces osmotic stress caused by hyperglycemia by inhibiting RLAR activity and galactitol formation (Kasali et al., 2021). Calycosin-7-O- β -D-glucoside can reduce endothelial cell apoptosis triggered by increased advanced glycation end products, thereby potentially reducing diabetes complications (Han et al., 2022). Compounds 5,7,4'-trihydroxy-3'-C-methylflavone-4'-rhamnoside and demethyltorosaflavone C are flavonoids that are often found in medicinal plants. In general, flavonoids function to inhibit PTP1B by increasing insulin sensitivity (Koren and Fantus, 2007). Quercetagenin non-competitively inhibits α -glucosidase and α -amylase enzymes by reducing the breakdown of carbohydrates into glucose (Wang et al., 2016).

The strong inhibitory activity of *D. virgatus* extract correlates with its high content of flavonoid glycosides, particularly luteolin-7-glucoside. Similar to acarbose, luteolin-7-glucoside forms multiple hydrogen bonds within the α -glucosidase catalytic site, explaining its potent activity. These results are consistent with other plant-derived α -glucosidase enzyme inhibitors reported in the literature. However, bioavailability predictions indicate potential absorption limitations, suggesting that formulation strategies may be needed. Future studies should include *in vivo* validation and toxicity profiling to assess clinical feasibility.

CONCLUSION

The ethyl acetate extract of *D. virgatus* leaves exhibits potent α -glucosidase enzyme inhibitory activity, mediated mainly by luteolin-7-glucoside. These findings support its potential as a natural antidiabetic agent; however, *in vivo* studies and safety evaluations are required before clinical application.

CONFLICT OF INTEREST

The authors declare no conflicts of interest.

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GENERATIVE ARTIFICIAL INTELLIGENCE (AI)

The authors declare that no generative artificial intelligence (AI) or AI-assisted technologies were used in the preparation, writing, or editing of this manuscript. All content was developed solely by the authors, who take full responsibility for its accuracy and integrity.

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AUTHOR CONTRIBUTION:

Contribution	Tukiran T	Syahrul LH	Andika PW
Concepts or ideas	x	x	x
Design	x		x
Definition of intellectual content		x	x
Literature search	x	x	x
Experimental studies	x	x	x
Data acquisition	x	x	x
Data analysis		x	x
Statistical analysis	x	x	x
Manuscript preparation	x	x	
Manuscript editing	x	x	x
Manuscript review	x	x	x

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Supplementary Data

Annex 1. LC-MS chromatogram result, sample id: *D. virgatus*; ethyl acetate extract.

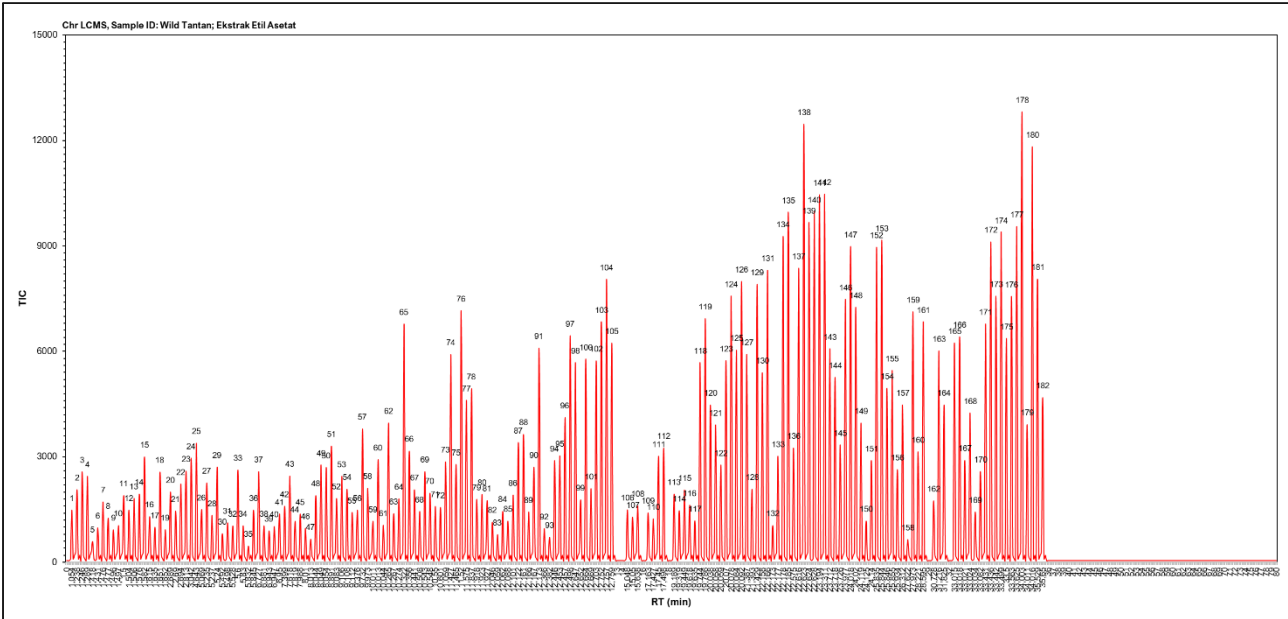
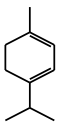
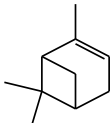
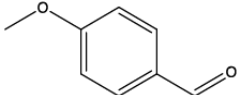
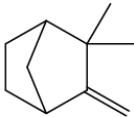
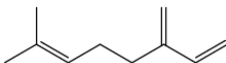
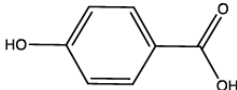
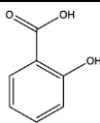
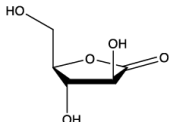
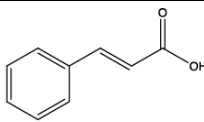
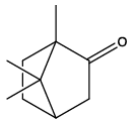
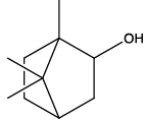
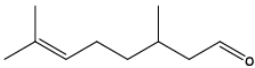
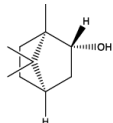
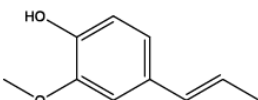
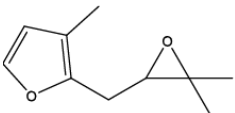
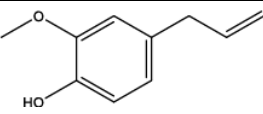
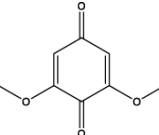
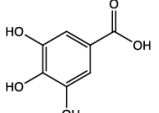
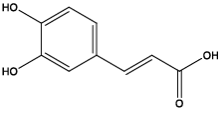
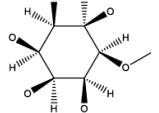
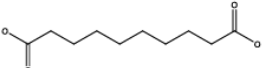
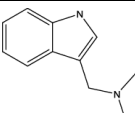
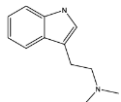
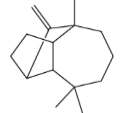
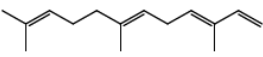
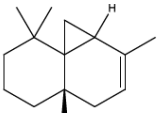
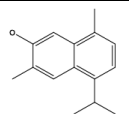
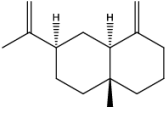
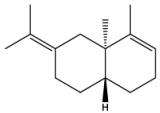
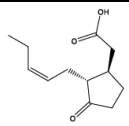
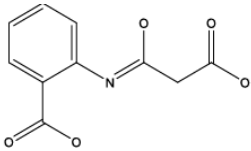
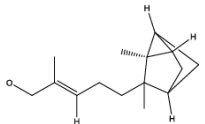
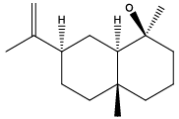
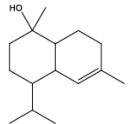
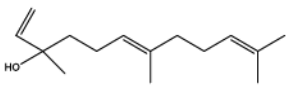
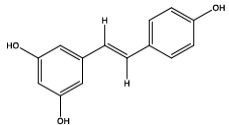
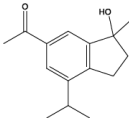
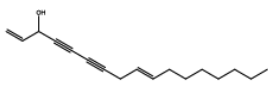
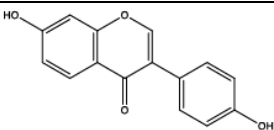


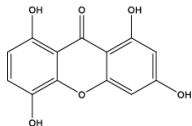
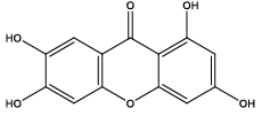
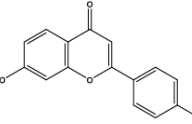
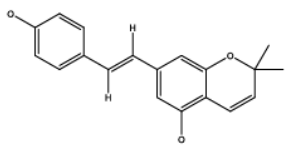
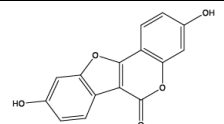
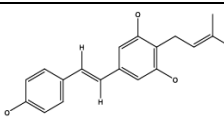
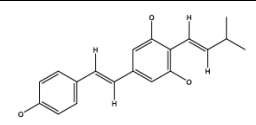
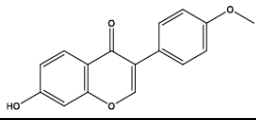
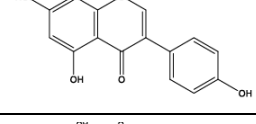
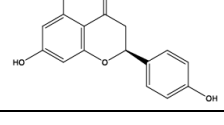
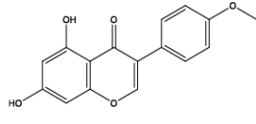
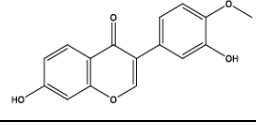
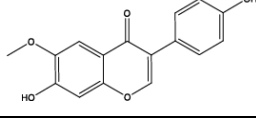
Table S1. Chromatogram result.

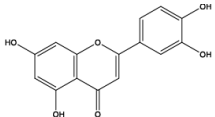
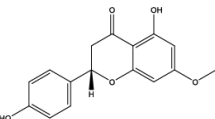
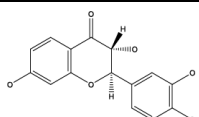
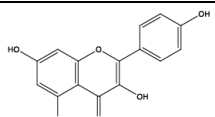
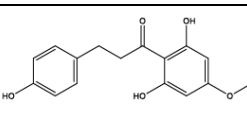
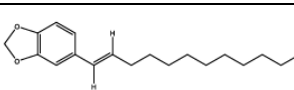
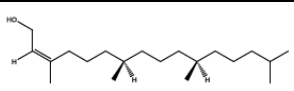
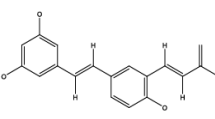
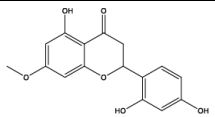
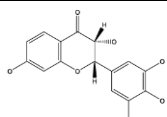
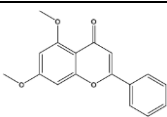
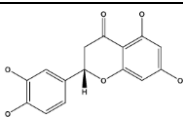
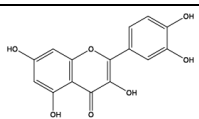
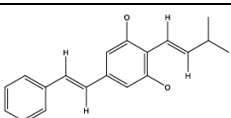
Peak number	RT (min)	Similarity index (%)	Curve area	Composition (%)	Compound result	
					Analysis	Structure
1	1.054	92	1482.40435	0.21877	glyoxylic acid Chemical Formula: C ₂ H ₂ O ₃ Exact Mass: 74.00 Molecular Weight: 74.04 m/z: 74.00 (100.0%), 75.00 (2.3%)	
2	1.238	92	2066.08442	0.30491	fumaric acid Chemical Formula: C ₄ H ₄ O ₄ Exact Mass: 116,0110 Molecular Weight: 116,0720 m/z: 116.0110 (100.0%), 117.0143 (4.3%)	
3	1.246	92	2574.39597	0.37993	succinic acid Chemical Formula: C ₄ H ₆ O ₄ Exact Mass: 118,0266 Molecular Weight: 118,0880 m/z: 118.0266 (100.0%), 119.0300 (4.3%)	
4	1.289	92	2443.74352	0.36064	benzoic acid Chemical Formula: C ₇ H ₆ O ₂ Exact Mass: 122,0368 Molecular Weight: 122,1230 m/z: 122.0368 (100.0%), 123.0401 (7.6%)	
5	1.418	92	590.27064	0.08711	agmatine Chemical Formula: C ₅ H ₁₄ N ₄ Exact Mass: 130,1218 Molecular Weight: 130,1950 m/z: 130.1218 (100.0%), 131.1252 (5.4%), 131.1189 (1.5%)	
6	1.431	92	978.70835	0.14444	cinnamaldehyde Chemical Formula: C ₉ H ₈ O Exact Mass: 132,0575 Molecular Weight: 132,1620 m/z: 132.0575 (100.0%), 133.0609 (9.7%)	

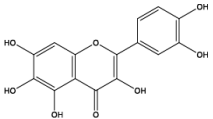
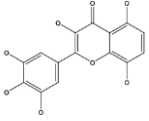
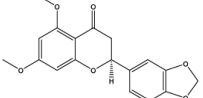
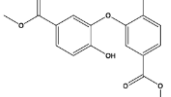
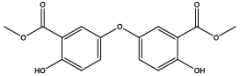
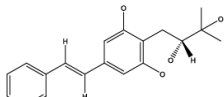
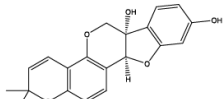
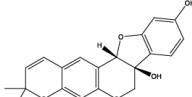
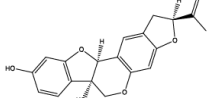
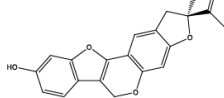
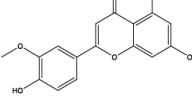
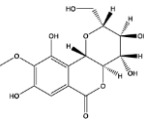
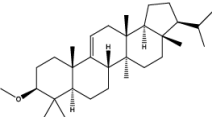
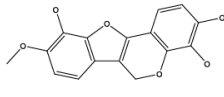
7	1.476	92	1713.29458	0.25285	α-terpinene Chemical Formula: $C_{10}H_{16}$ Exact Mass: 136,1252 Molecular Weight: 136,2380 m/z: 136.1252 (100.0%), 137.1286 (10.8%)	
8	1.477	92	1257.75711	0.18562	α-pinene Chemical Formula: $C_{10}H_{16}$ Exact Mass: 136,1252 Molecular Weight: 136,2380 m/z: 136.1252 (100.0%), 137.1286 (10.8%)	
9	1.496	92	923.03923	0.13622	p-anisaldehyde Chemical Formula: $C_8H_8O_2$ Exact Mass: 136,0524 Molecular Weight: 136,1500 m/z: 136.0524 (100.0%), 137.0558 (8.7%)	
10	1.497	92	1043.58381	0.15401	camphene Chemical Formula: $C_{10}H_{16}$ Exact Mass: 136,1252 Molecular Weight: 136,2380 m/z: 136.1252 (100.0%), 137.1286 (10.8%)	
11	1.500	92	1897.13778	0.27998	β-myrcene Chemical Formula: $C_{10}H_{16}$ Exact Mass: 136,1252 Molecular Weight: 136,2380 m/z: 136.1252 (100.0%), 137.1286 (10.8%)	
12	1.504	92	1483.36515	0.21891	p-hydroxybenzoic acid Chemical Formula: $C_7H_6O_3$ Exact Mass: 138,0317 Molecular Weight: 138,1220 m/z: 138.0317 (100.0%), 139.0350 (7.6%)	
13	1.506	92	1817.86391	0.26828	salicylic acid Chemical Formula: $C_7H_6O_3$ Exact Mass: 138,0317 Molecular Weight: 138,1220 m/z: 138.0317 (100.0%), 139.0350 (7.6%)	
14	1.576	92	1939.13091	0.28617	D-arabino-1,4-lactone Chemical Formula: $C_8H_8O_5$ Exact Mass: 148,0372 Molecular Weight: 148,1140 m/z: 148.0372 (100.0%), 149.0405 (5.4%), 150.0414 (1.0%)	
15	1.582	92	2997.80659	0.44241	cinnamic acid Chemical Formula: $C_9H_8O_2$ Exact Mass: 148,0524 Molecular Weight: 148,1610 m/z: 148.0524 (100.0%), 149.0558 (9.7%)	
16	1.615	92	1296.43696	0.19133	camphor Chemical Formula: $C_{10}H_{16}O$ Exact Mass: 152,1201 Molecular Weight: 152,2370 m/z: 152.1201 (100.0%), 153.1235 (10.8%)	
17	1.635	92	999.83955	0.14755	borneol Chemical Formula: $C_{10}H_{18}O$ Exact Mass: 154,1358 Molecular Weight: 154,2530 m/z: 154.1358 (100.0%), 155.1391 (10.8%)	
18	1.651	92	2564.93203	0.37853	citronellal Chemical Formula: $C_{10}H_{18}O$ Exact Mass: 154,1358 Molecular Weight: 154,2530 m/z: 154.1358 (100.0%), 155.1391 (10.8%)	
19	1.652	92	924.07882	0.13637	isoborneol Chemical Formula: $C_{10}H_{18}O$ Exact Mass: 154,1358 Molecular Weight: 154,2530 m/z: 154.1358 (100.0%), 155.1391 (10.8%)	
20	2.689	92	1999.01135	0.29501	isoeugenol Chemical Formula: $C_{10}H_{12}O_2$ Exact Mass: 164,0837 Molecular Weight: 164,2040 m/z: 164.0837 (100.0%), 165.0871 (10.8%)	

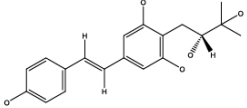
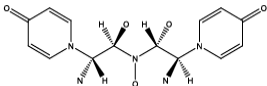
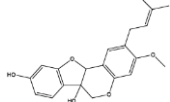
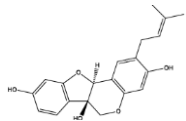
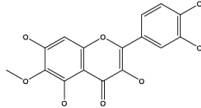
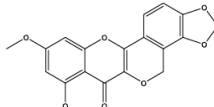
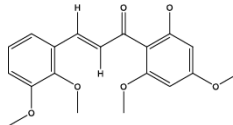
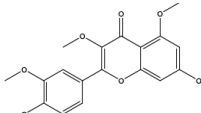
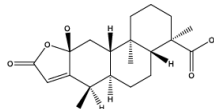
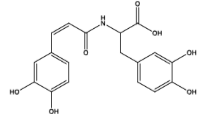
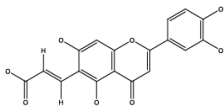
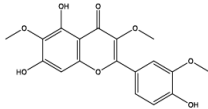
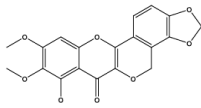
21	2.690	92	1455.69451	0.21483	2-(2',3'-epoxy-3'-methylbutyl)-3-methylfuran Chemical Formula: C ₁₀ H ₁₄ O ₂ Exact Mass: 166,0994 Molecular Weight: 166,2200 m/z: 166.0994 (100.0%), 167.1027 (10.8%)	
22	2.694	92	2222.92899	0.32806	eugenol Chemical Formula: C ₁₀ H ₁₂ O ₂ Exact Mass: 164,0837 Molecular Weight: 164,2040 m/z: 164.0837 (100.0%), 165.0871 (10.8%)	
23	2.813	92	2591.29488	0.38242	2,6-dimethoxy-1,4-benzoquinone Chemical Formula: C ₈ H ₆ O ₄ Exact Mass: 168,0423 Molecular Weight: 168,1480 m/z: 168.0423 (100.0%), 169.0456 (8.7%)	
24	3.042	92	2963.24358	0.43731	gallic acid Chemical Formula: C ₇ H ₆ O ₅ Exact Mass: 170,0215 Molecular Weight: 170,1200 m/z: 170.0215 (100.0%), 171.0249 (7.6%), 172.0258 (1.0%)	
25	4.643	92	3383.44432	0.49932	caffeic acid Chemical Formula: C ₉ H ₈ O ₄ Exact Mass: 180,0423 Molecular Weight: 180,1590 m/z: 180.0423 (100.0%), 181.0456 (9.7%)	
26	5.069	92	1502.67971	0.22176	ononitol Chemical Formula: C ₇ H ₁₄ O ₆ Exact Mass: 194,0790 Molecular Weight: 194,1830 m/z: 194.0790 (100.0%), 195.0824 (7.6%), 196.0833 (1.2%)	
27	5.235	92	2255.60525	0.33288	sebacic acid Chemical Formula: C ₁₀ H ₁₈ O ₄ Exact Mass: 202,1205 Molecular Weight: 202,2500 m/z: 202.1205 (100.0%), 203.1239 (10.8%)	
28	5.237	92	1332.36010	0.19663	gramine Chemical Formula: C ₁₁ H ₁₄ N ₂ Exact Mass: 174,1157 Molecular Weight: 174,2470 m/z: 174.1157 (100.0%), 175.1191 (11.9%)	
29	5.240	92	2710.24714	0.39997	N,N-dimethyltryptamine Chemical Formula: C ₁₂ H ₁₆ N ₂ Exact Mass: 188,1313 Molecular Weight: 188,2740 m/z: 188.1313 (100.0%), 189.1347 (13.0%)	
30	5.492	92	815.61711	0.12037	longifolene Chemical Formula: C ₁₅ H ₂₄ Exact Mass: 204,1878 Molecular Weight: 204,3570 m/z: 204.1878 (100.0%), 205.1912 (16.2%), 206.1945 (1.2%)	
31	5.498	92	1122.58467	0.16567	α-farnesene Chemical Formula: C ₁₅ H ₂₄ Exact Mass: 204,1878 Molecular Weight: 204,3570 m/z: 204.1878 (100.0%), 205.1912 (16.2%), 206.1945 (1.2%)	
32	5.528	92	1034.96284	0.15274	thujopsene Chemical Formula: C ₁₈ H ₂₄ Exact Mass: 204,1878 Molecular Weight: 204,3570 m/z: 204.1878 (100.0%), 205.1912 (16.2%), 206.1945 (1.2%)	
33	5.600	92	2623.57232	0.38718	7-hydroxycadalene Chemical Formula: C ₁₅ H ₁₈ O Exact Mass: 214,1358 Molecular Weight: 214,3080 m/z: 214.1358 (100.0%), 215.1391 (16.2%), 216.1425 (1.2%)	
34	5.830	92	1037.85154	0.15316	β-eudesmene Chemical Formula: C ₁₅ H ₂₄ Exact Mass: 204,1878 Molecular Weight: 204,3570 m/z: 204.1878 (100.0%), 205.1912 (16.2%), 206.1945 (1.2%)	

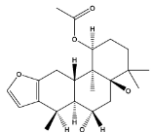
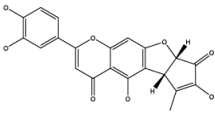
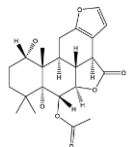
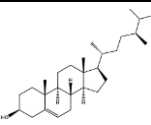
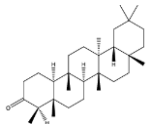
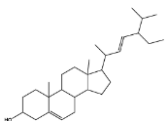
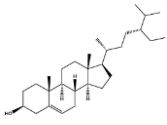
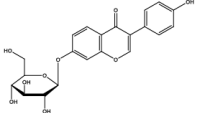
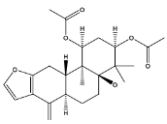
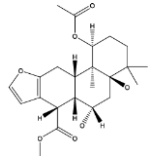
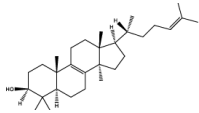
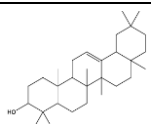
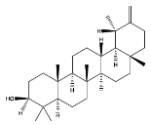
35	5.832	92	460.23932	0.06792	eudesma-3,7(11)-diene Chemical Formula: C ₁₅ H ₂₄ Exact Mass: 204,1878 Molecular Weight: 204,3570 m/z: 204.1878 (100.0%), 205.1912 (16.2%), 206.1945 (1.2%)	
36	5.845	92	1483.31738	0.21891	jasmonic acid Chemical Formula: C ₁₂ H ₁₈ O ₃ Exact Mass: 210,1256 Molecular Weight: 210,2730 m/z: 210.1256 (100.0%), 211.1289 (13.0%)	
37	6.727	92	2577.63635	0.38040	2-[[[carboxyacetyl]amino]benzoic acid Chemical Formula: C ₁₀ H ₉ NO ₅ Exact Mass: 223,0481 Molecular Weight: 223,1840 m/z: 223.0481 (100.0%), 224.0514 (10.8%), 225.0523 (1.0%)	
38	6.881	92	1038.29638	0.15323	α-santalol Chemical Formula: C ₁₅ H ₂₄ O Exact Mass: 220,1827 Molecular Weight: 220,3560 m/z: 220.1827 (100.0%), 221.1861 (16.2%), 222.1894 (1.2%)	
39	6.943	92	893.36903	0.13184	neo-intermedeol Chemical Formula: C ₁₅ H ₂₆ O Exact Mass: 222,1984 Molecular Weight: 222,3720 m/z: 222.1984 (100.0%), 223.2017 (16.2%), 224.2051 (1.2%)	
40	6.947	92	1015.96077	0.14993	α-cadinol Chemical Formula: C ₁₅ H ₂₆ O Exact Mass: 222,1984 Molecular Weight: 222,3720 m/z: 222.1984 (100.0%), 223.2017 (16.2%), 224.2051 (1.2%)	
41	6.950	92	1376.51058	0.20314	nerolidol Chemical Formula: C ₁₅ H ₂₆ O Exact Mass: 222,1984 Molecular Weight: 222,3720 m/z: 222.1984 (100.0%), 223.2017 (16.2%), 224.2051 (1.2%)	
42	7.399	92	1595.31683	0.23543	resveratrol Chemical Formula: C ₁₄ H ₁₂ O ₃ Exact Mass: 228,0786 Molecular Weight: 228,2470 m/z: 228.0786 (100.0%), 229.0820 (15.1%), 230.0854 (1.1%)	
43	7.618	92	2453.25290	0.36205	cylindrene Chemical Formula: C ₁₈ H ₃₀ O ₂ Exact Mass: 232,1463 Molecular Weight: 232,3230 m/z: 232.1463 (100.0%), 233.1497 (16.2%), 234.1530 (1.2%)	
44	7.819	92	1166.43898	0.17214	7,10,13-hexadecatrienal Chemical Formula: C ₁₆ H ₂₆ O Exact Mass: 234,1984 Molecular Weight: 234,3830 m/z: 234.1984 (100.0%), 235.2017 (17.3%), 236.2051 (1.4%)	
45	7.988	92	1374.42971	0.20284	falcarinol Chemical Formula: C ₁₇ H ₃₄ O Exact Mass: 244,1827 Molecular Weight: 244,3780 m/z: 244.1827 (100.0%), 245.1861 (18.4%), 246.1894 (1.6%)	
46	8.010	92	968.52880	0.14293	heptadeca 8,11,14 trienal Chemical Formula: C ₁₇ H ₂₈ O Exact Mass: 248,2140 Molecular Weight: 248,4100 m/z: 248.2140 (100.0%), 249.2174 (18.4%), 250.2207 (1.6%)	
47	8.013	92	653.64358	0.09646	daidzein Chemical Formula: C ₁₅ H ₁₀ O ₄ Exact Mass: 254,0579 Molecular Weight: 254,2410 m/z: 254.0579 (100.0%), 255.0613 (16.2%), 256.0646 (1.2%)	

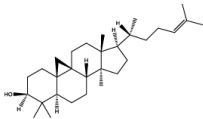
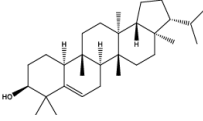
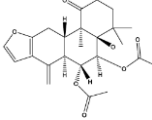
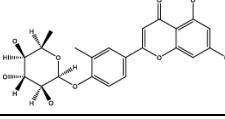
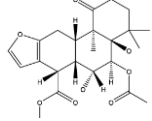
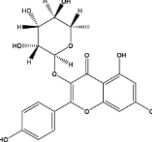
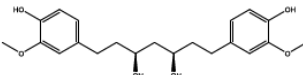
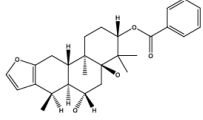
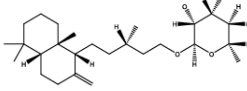
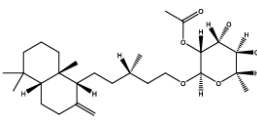
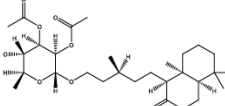
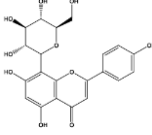
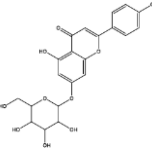
48	8.044	92	1896.46959	0.27988	1,3,5,8-tetrahydroxyxanthone Chemical Formula: C ₁₃ H ₈ O ₆ Exact Mass: 260.0321 Molecular Weight: 260.2010 m/z: 260.0321 (100.0%), 261.0354 (14.1%), 262.0363 (1.2%)	
49	8.049	92	2770.12418	0.40881	1,3,6,7-tetrahydroxyxanthone Chemical Formula: C ₁₃ H ₈ O ₆ Exact Mass: 260.0321 Molecular Weight: 260.2010 m/z: 260.0321 (100.0%), 261.0354 (14.1%), 262.0363 (1.2%)	
50	8.054	92	2696.17341	0.39790	7,4'-dihydroxyflavone Chemical Formula: C ₁₅ H ₁₀ O ₄ Exact Mass: 254.0579 Molecular Weight: 254.2410 m/z: 254.0579 (100.0%), 255.0613 (16.2%), 256.0646 (1.2%)	
51	8.891	92	3307.68829	0.48814	5-hydroxy-7-[2-(4-hydroxyphenyl)ethenyl]-2,2-dimethyl-2H-1-benzopyran Chemical Formula: C ₁₉ H ₁₈ O ₃ Exact Mass: 294.1256 Molecular Weight: 294.3500 m/z: 294.1256 (100.0%), 295.1289 (20.5%), 296.1323 (2.0%)	
52	9.083	92	1812.16688	0.26744	coumestrol Chemical Formula: C ₁₅ H ₈ O ₅ Exact Mass: 268.0372 Molecular Weight: 268.2240 m/z: 268.0372 (100.0%), 269.0405 (16.2%), 270.0439 (1.2%), 270.0414 (1.0%)	
53	9.106	92	2443.08326	0.36055	4-prenylresveratrol Chemical Formula: C ₁₈ H ₂₀ O ₃ Exact Mass: 296.1412 Molecular Weight: 296.3660 m/z: 296.1412 (100.0%), 297.1446 (20.5%), 298.1480 (2.0%)	
54	9.108	92	2079.52701	0.30689	4-(3-methyl-but-1-enyl)-3,4,5-trihydroxystilbene Chemical Formula: C ₁₉ H ₂₀ O ₃ Exact Mass: 296.1412 Molecular Weight: 296.3660 m/z: 296.1412 (100.0%), 297.1446 (20.5%), 298.1480 (2.0%)	
55	9.112	92	1418.03686	0.20927	formononetin Chemical Formula: C ₁₆ H ₁₂ O ₄ Exact Mass: 268.0736 Molecular Weight: 268.2680 m/z: 268.0736 (100.0%), 269.0769 (17.3%), 270.0803 (1.4%)	
56	9.376	92	1481.24685	0.21860	genistein Chemical Formula: C ₁₅ H ₁₀ O ₆ Exact Mass: 270.0528 Molecular Weight: 270.2400 m/z: 270.0528 (100.0%), 271.0562 (16.2%), 272.0595 (1.2%), 272.0571 (1.0%)	
57	9.732	92	3791.50480	0.55954	naringenin Chemical Formula: C ₁₅ H ₁₂ O ₅ Exact Mass: 272.0685 Molecular Weight: 272.2560 m/z: 272.0685 (100.0%), 273.0718 (16.2%), 274.0752 (1.2%), 274.0727 (1.0%)	
58	9.973	92	2105.21482	0.31068	malvalic acid Chemical Formula: C ₁₈ H ₃₂ O ₂ Exact Mass: 280.2402 Molecular Weight: 280.4520 m/z: 280.2402 (100.0%), 281.2436 (19.5%), 282.2469 (1.8%)	
59	10.011	92	1166.71526	0.17218	biochanin A Chemical Formula: C ₁₆ H ₁₂ O ₅ Exact Mass: 284.0685 Molecular Weight: 284.2670 m/z: 284.0685 (100.0%), 285.0718 (17.3%), 286.0752 (1.4%), 286.0727 (1.0%)	
60	10.013	92	2923.68771	0.43147	calycosin Chemical Formula: C ₁₆ H ₁₂ O ₅ Exact Mass: 284.0685 Molecular Weight: 284.2670 m/z: 284.0685 (100.0%), 285.0718 (17.3%), 286.0752 (1.4%), 286.0727 (1.0%)	
61	10.044	92	1052.40787	0.15531	glycitein Chemical Formula: C ₁₆ H ₁₂ O ₅ Exact Mass: 284.0685 Molecular Weight: 284.2670 m/z: 284.0685 (100.0%), 285.0718 (17.3%), 286.0752 (1.4%), 286.0727 (1.0%)	

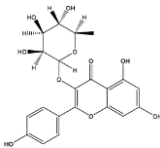
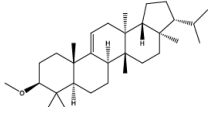
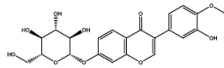
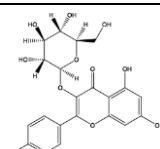
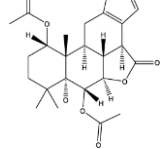
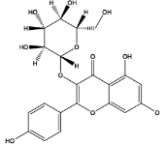
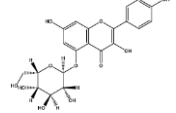
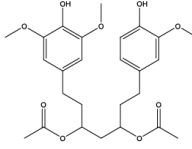
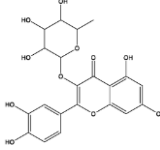
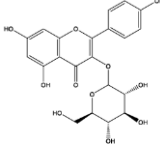
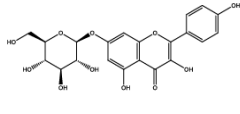
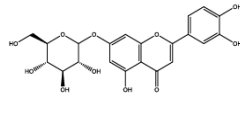
62	10.265	92	3956.96685	0.58396	luteolin Chemical Formula: $C_{15}H_{10}O_6$ Exact Mass: 286,0477 Molecular Weight: 286,2390 m/z: 286.0477 (100.0%), 287.0511 (16.2%), 288.0520 (1.2%), 288.0544 (1.2%)	
63	10.267	92	1385.50864	0.20447	sakuranetin Chemical Formula: $C_{16}H_{14}O_5$ Exact Mass: 286,0841 Molecular Weight: 286,2830 m/z: 286.0841 (100.0%), 287.0875 (17.3%), 288.0908 (1.4%), 288.0884 (1.0%)	
64	10.274	92	1803.19526	0.26611	fustin Chemical Formula: $C_{15}H_{12}O_6$ Exact Mass: 288,0634 Molecular Weight: 288,2550 m/z: 288.0634 (100.0%), 289.0667 (16.2%), 290.0676 (1.2%), 290.0701 (1.2%)	
65	10.322	92	6773.25968	0.99959	kaempferol Chemical Formula: $C_{15}H_{10}O_6$ Exact Mass: 286,0477 Molecular Weight: 286,2390 m/z: 286.0477 (100.0%), 287.0511 (16.2%), 288.0520 (1.2%), 288.0544 (1.2%)	
66	10.356	92	3161.11030	0.46651	asebogenin Chemical Formula: $C_{16}H_{16}O_5$ Exact Mass: 288,0998 Molecular Weight: 288,2990 m/z: 288.0998 (100.0%), 289.1031 (17.3%), 290.1065 (1.4%), 290.1040 (1.0%)	
67	10.441	92	2060.39869	0.30407	pipataline Chemical Formula: $C_{19}H_{28}O_2$ Exact Mass: 288,2089 Molecular Weight: 288,4310 m/z: 288.2089 (100.0%), 289.2123 (20.5%), 290.2156 (2.0%)	
68	10.508	92	1446.72682	0.21351	phytol Chemical Formula: $C_{20}H_{40}O$ Exact Mass: 296,3079 Molecular Weight: 296,5390 m/z: 296.3079 (100.0%), 297.3113 (21.6%), 298.3146 (2.2%)	
69	10.543	92	2580.68253	0.38085	3-isopentadienyl-3',4,5'-trihydroxystilbene Chemical Formula: $C_{19}H_{18}O_3$ Exact Mass: 294,1256 Molecular Weight: 294,3500 m/z: 294.1256 (100.0%), 295.1289 (20.5%), 296.1323 (2.0%)	
70	10.548	92	1962.63203	0.28964	artocarpانون Chemical Formula: $C_{16}H_{14}O_6$ Exact Mass: 302,0790 Molecular Weight: 302,2820 m/z: 302.0790 (100.0%), 303.0824 (17.3%), 304.0857 (1.4%), 304.0833 (1.2%)	
71	10.55	92	1586.79882	0.23418	dihydrorobinetin Chemical Formula: $C_{16}H_{12}O_7$ Exact Mass: 304,0583 Molecular Weight: 304,2540 m/z: 304.0583 (100.0%), 305.0617 (16.2%), 306.0625 (1.4%), 306.0650 (1.2%)	
72	10.601	92	1561.00682	0.23037	5,7-dimethoxyflavone Chemical Formula: $C_{17}H_{14}O_4$ Exact Mass: 282,0892 Molecular Weight: 282,2950 m/z: 282.0892 (100.0%), 283.0926 (18.4%), 284.0959 (1.6%)	
73	11.059	92	2855.88208	0.42147	eriodictyol Chemical Formula: $C_{18}H_{12}O_6$ Exact Mass: 288,0634 Molecular Weight: 288,2550 m/z: 288.0634 (100.0%), 289.0667 (16.2%), 290.0676 (1.2%), 290.0701 (1.2%)	
74	11.427	92	5908.26448	0.87193	quercetin Chemical Formula: $C_{15}H_{10}O_7$ Exact Mass: 302,0427 Molecular Weight: 302,2380 m/z: 302.0427 (100.0%), 303.0460 (16.2%), 304.0469 (1.4%), 304.0494 (1.2%)	
75	11.465	92	2782.99971	0.41071	2-(3-methyl-1-butenyl)-5-(2-phenylethenyl)-1,3-benzenediol Chemical Formula: $C_{19}H_{20}O_2$ Exact Mass: 280,1463 Molecular Weight: 280,3670 m/z: 280.1463 (100.0%), 281.1497 (20.5%), 282.1530 (2.0%)	

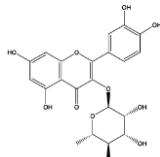
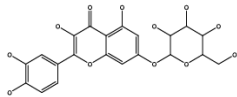
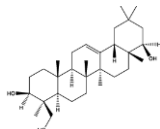
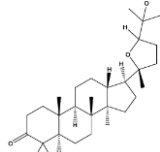
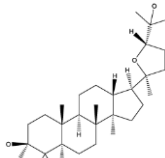
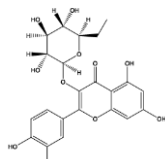
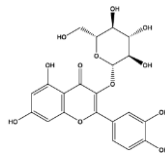
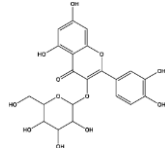
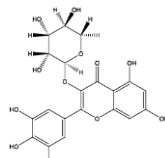
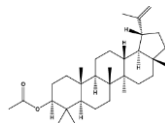
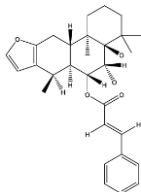
76	11.520	92	7156.95187	1.05621	quercetagetin Chemical Formula: C ₁₅ H ₁₀ O ₈ Exact Mass: 318,0376 Molecular Weight: 318,2370 m/z: 318.0376 (100.0%), 319.0409 (16.2%), 320.0418 (1.6%), 320.0443 (1.2%)	
77	11.575	92	4607.50835	0.67997	3,5,8,3',4',5'-hexahydroxyflavone Chemical Formula: C ₁₅ H ₁₀ O ₈ Exact Mass: 318,0376 Molecular Weight: 318,2370 m/z: 318.0376 (100.0%), 319.0409 (16.2%), 320.0418 (1.6%), 320.0443 (1.2%)	
78	11.837	92	4939.36691	0.72894	(2S)-5,7-dimethoxy-3',4'-methylenedioxyflavanone Chemical Formula: C ₁₈ H ₁₆ O ₆ Exact Mass: 328,0947 Molecular Weight: 328,3200 m/z: 328.0947 (100.0%), 329.0980 (19.5%), 330.1014 (1.8%), 330.0989 (1.2%)	
79	11.918	92	1791.43408	0.26438	cylindol A Chemical Formula: C ₁₆ H ₁₄ O ₇ Exact Mass: 318,0740 Molecular Weight: 318,2810 m/z: 318.0740 (100.0%), 319.0773 (17.3%), 320.0782 (1.4%), 320.0807 (1.4%)	
80	11.923	92	1926.93232	0.28437	cylindol B Chemical Formula: C ₁₆ H ₁₄ O ₇ Exact Mass: 318,0740 Molecular Weight: 318,2810 m/z: 318.0740 (100.0%), 319.0773 (17.3%), 320.0782 (1.4%), 320.0807 (1.4%)	
81	11.927	92	1759.59898	0.25968	2-(2,3-dihydroxy-3-methylbutyl)-5-(2-phenylethenyl)-1,3-benzenediol Chemical Formula: C ₁₉ H ₂₂ O ₄ Exact Mass: 314,1518 Molecular Weight: 314,3810 m/z: 314.1518 (100.0%), 315.1552 (20.5%), 316.1585 (2.0%)	
82	12.046	92	1141.25552	0.16842	glyceollin I Chemical Formula: C ₂₀ H ₁₈ O ₅ Exact Mass: 338,1154 Molecular Weight: 338,3590 m/z: 338.1154 (100.0%), 339.1188 (21.6%), 340.1221 (2.2%), 340.1197 (1.0%)	
83	12.059	92	786.87085	0.11613	glyceollin II Chemical Formula: C ₂₀ H ₁₈ O ₅ Exact Mass: 338,1154 Molecular Weight: 338,3590 m/z: 338.1154 (100.0%), 339.1188 (21.6%), 340.1221 (2.2%), 340.1197 (1.0%)	
84	12.062	92	1449.70003	0.21394	glyceollin III Chemical Formula: C ₂₀ H ₁₈ O ₅ Exact Mass: 338,1154 Molecular Weight: 338,3590 m/z: 338.1154 (100.0%), 339.1188 (21.6%), 340.1221 (2.2%), 340.1197 (1.0%)	
85	12.088	92	1170.08813	0.17268	glyceollin VI Chemical Formula: C ₂₀ H ₁₆ O ₄ Exact Mass: 320,1049 Molecular Weight: 320,3440 m/z: 320.1049 (100.0%), 321.1082 (21.6%), 322.1116 (2.2%)	
86	12.101	92	1913.16326	0.28234	chrysoeriol Chemical Formula: C ₁₆ H ₁₂ O ₆ Exact Mass: 300,0634 Molecular Weight: 300,2660 m/z: 300.0634 (100.0%), 301.0667 (17.3%), 302.0701 (1.4%), 302.0676 (1.2%)	
87	12.122	92	3409.86960	0.50322	bergenin Chemical Formula: C ₁₄ H ₁₆ O ₉ Exact Mass: 328,0794 Molecular Weight: 328,2730 m/z: 328.0794 (100.0%), 329.0828 (15.1%), 330.0837 (1.8%), 330.0861 (1.1%)	
88	12.161	92	3635.15267	0.53647	cylindrin Chemical Formula: C ₃₁ H ₅₂ O Exact Mass: 440,4018 Molecular Weight: 440,7560 m/z: 440.4018 (100.0%), 441.4052 (33.5%), 442.4085 (2.7%), 442.4085 (2.7%)	
89	12.166	92	1428.51283	0.21082	aracarpene 1 Chemical Formula: C ₁₆ H ₁₂ O ₆ Exact Mass: 300,0634 Molecular Weight: 300,2660 m/z: 300.0634 (100.0%), 301.0667 (17.3%), 302.0701 (1.4%), 302.0676 (1.2%)	

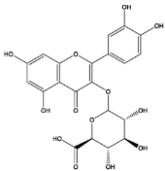
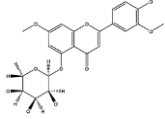
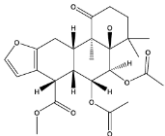
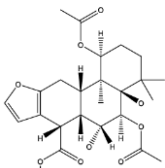
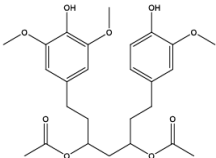
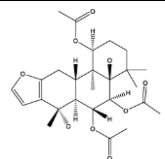
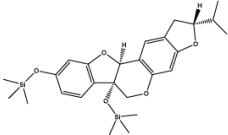
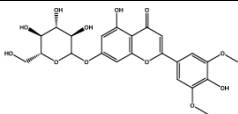
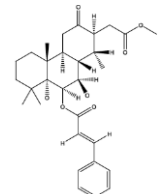
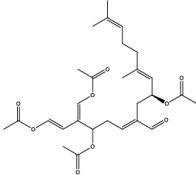
90	12.167	92	2708.23085	0.39968	2-(2,3-dihydroxy-3-methylbutyl)-5-[2-(4-hydroxyphenyl)ethenyl]-1,3-benzenediol Chemical Formula: C ₁₉ H ₂₂ O ₅ Exact Mass: 330,1467 Molecular Weight: 330,3800 m/z: 330.1467 (100.0%), 331.1501 (20.5%), 332.1534 (2.0%), 332.1510 (1.0%)	
91	12.173	92	6091.36362	0.89895	mimopudine Chemical Formula: C ₁₄ H ₁₉ N ₅ O ₅ Exact Mass: 337,1386 Molecular Weight: 337,3360 m/z: 337.1386 (100.0%), 338.1420 (15.1%), 338.1357 (1.8%), 339.1453 (1.1%), 339.1429 (1.0%)	
92	12.366	92	956.30832	0.14113	glyceollin IV Chemical Formula: C ₂₁ H ₂₂ O ₅ Exact Mass: 354,1467 Molecular Weight: 354,4020 m/z: 354.1467 (100.0%), 355.1501 (22.7%), 356.1534 (2.5%), 356.1510 (1.0%)	
93	12.382	92	713.54992	0.10530	glyceocarpin Chemical Formula: C ₂₀ H ₂₀ O ₅ Exact Mass: 340,1311 Molecular Weight: 340,3750 m/z: 340.1311 (100.0%), 341.1344 (21.6%), 342.1378 (2.2%), 342.1353 (1.0%)	
94	12.446	92	2895.63987	0.42733	patuletin Chemical Formula: C ₁₆ H ₁₂ O ₈ Exact Mass: 332,0532 Molecular Weight: 332,2640 m/z: 332.0532 (100.0%), 333.0566 (17.3%), 334.0575 (1.6%), 334.0599 (1.4%)	
95	12.453	92	3028.27686	0.44691	pulcherrimin Chemical Formula: C ₁₈ H ₁₂ O ₇ Exact Mass: 340,0583 Molecular Weight: 340,2870 m/z: 340.0583 (100.0%), 341.0617 (19.5%), 342.0650 (1.8%), 342.0625 (1.4%)	
96	12.457	92	4118.38282	0.60778	2'-hydroxy-2,3,4',6'-tetramethoxychalcone Chemical Formula: C ₁₉ H ₂₀ O ₈ Exact Mass: 344,1260 Molecular Weight: 344,3630 m/z: 344.1260 (100.0%), 345.1293 (20.5%), 346.1327 (2.0%), 346.1302 (1.2%)	
97	12.498	92	6443.33322	0.95090	quercetin 3,5,3'-trimethyl ether Chemical Formula: C ₁₈ H ₁₆ O ₇ Exact Mass: 344,0896 Molecular Weight: 344,3190 m/z: 344.0896 (100.0%), 345.0930 (19.5%), 346.0963 (1.8%), 346.0938 (1.4%)	
98	12.647	92	5677.80045	0.83792	neocaesalpin H Chemical Formula: C ₂₀ H ₂₆ O ₅ Exact Mass: 348,1937 Molecular Weight: 348,4390 m/z: 348.1937 (100.0%), 349.1970 (21.6%), 350.2004 (2.2%), 350.1979 (1.0%)	
99	12.652	92	1774.07526	0.26182	clovamide Chemical Formula: C ₁₈ H ₁₇ NO ₇ Exact Mass: 359,1005 Molecular Weight: 359,3340 m/z: 359.1005 (100.0%), 360.1039 (19.5%), 361.1072 (1.8%), 361.1047 (1.4%)	
100	12.664	92	5778.12368	0.85273	demethyltorosaflavone D Chemical Formula: C ₁₈ H ₁₂ O ₈ Exact Mass: 356,0532 Molecular Weight: 356,2860 m/z: 356.0532 (100.0%), 357.0566 (19.5%), 358.0599 (1.8%), 358.0575 (1.6%)	
101	12.669	92	2091.69014	0.30869	jaceidin Chemical Formula: C ₁₈ H ₁₆ O ₈ Exact Mass: 360,0845 Molecular Weight: 360,3180 m/z: 360.0845 (100.0%), 361.0879 (19.5%), 362.0912 (1.8%), 362.0888 (1.6%)	
102	12.703	92	5724.62822	0.84483	6-methoxypulcherrimin Chemical Formula: C ₁₉ H ₁₄ O ₈ Exact Mass: 370,0689 Molecular Weight: 370,3130 m/z: 370.0689 (100.0%), 371.0722 (20.5%), 372.0756 (2.0%), 372.0731 (1.6%)	

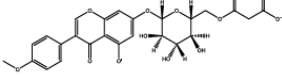
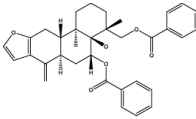
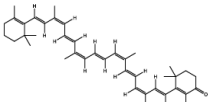
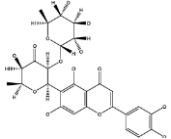
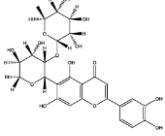
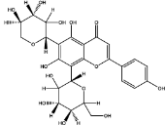
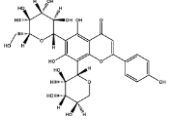
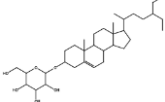
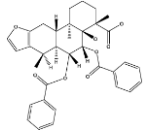
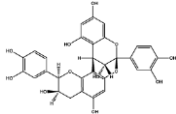
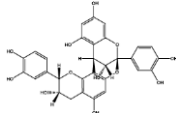
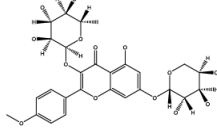
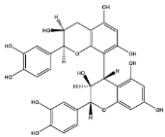
103	12.752	92	6836.97325	1.00899	caesalpinin K Chemical Formula: $C_{22}H_{32}O_5$ Exact Mass: 376,2250 Molecular Weight: 376,4930 m/z: 376.2250 (100.0%), 377.2283 (23.8%), 378.2317 (2.7%), 378.2292 (1.0%)	
104	12.757	92	8043.72877	1.18708	demethyltorosaflavone C Chemical Formula: $C_{21}H_{14}O_8$ Exact Mass: 394,0689 Molecular Weight: 394,3350 m/z: 394.0689 (100.0%), 395.0722 (22.7%), 396.0756 (2.5%), 396.0731 (1.6%)	
105	12.759	92	6229.32323	0.91931	caesalpinin H Chemical Formula: $C_{22}H_{28}O_7$ Exact Mass: 404,1835 Molecular Weight: 404,4590 m/z: 404.1835 (100.0%), 405.1869 (23.8%), 406.1902 (2.7%), 406.1877 (1.4%)	
106	15.048	92	1490.86822	0.22002	campesterol Chemical Formula: $C_{28}H_{48}O$ Exact Mass: 400,3705 Molecular Weight: 400,6910 m/z: 400.3705 (100.0%), 401.3739 (30.3%), 402.3772 (2.7%), 402.3772 (1.7%)	
107	15.050	92	1287.46758	0.19000	3-friedelanone Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426,3862 Molecular Weight: 426,7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	
108	15.638	92	1603.62768	0.23666	stigmasterol Chemical Formula: $C_{29}H_{48}O$ Exact Mass: 412,3705 Molecular Weight: 412,7020 m/z: 412.3705 (100.0%), 413.3739 (31.4%), 414.3772 (2.7%), 414.3772 (2.0%)	
109	17.163	92	1407.50480	0.20772	β-sitosterol Chemical Formula: $C_{29}H_{50}O$ Exact Mass: 414,3862 Molecular Weight: 414,7180 m/z: 414.3862 (100.0%), 415.3895 (31.4%), 416.3929 (2.7%), 416.3929 (2.0%)	
110	17.427	92	1233.74845	0.18207	daidzin Chemical Formula: $C_{21}H_{20}O_9$ Exact Mass: 416,1107 Molecular Weight: 416,3820 m/z: 416.1107 (100.0%), 417.1141 (22.7%), 418.1174 (2.5%), 418.1150 (1.8%)	
111	17.450	92	3015.82845	0.44507	caesalpinin C Chemical Formula: $C_{26}H_{32}O_8$ Exact Mass: 416,2199 Molecular Weight: 416,5140 m/z: 416.2199 (100.0%), 417.2232 (26.0%), 418.2266 (2.7%), 418.2241 (1.2%)	
112	17.498	92	3249.42832	0.47955	bonducellpin C Chemical Formula: $C_{23}H_{32}O_7$ Exact Mass: 420,2148 Molecular Weight: 420,5020 m/z: 420.2148 (100.0%), 421.2182 (24.9%), 422.2215 (2.7%), 422.2190 (1.4%)	
113	19.189	92	1937.33615	0.28591	lanosterol Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426,3862 Molecular Weight: 426,7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	
114	19.319	92	1468.76406	0.21676	β-amyrin Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426,3862 Molecular Weight: 426,7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	
115	19.449	92	2053.26580	0.30302	taraxerol Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426,3862 Molecular Weight: 426,7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	

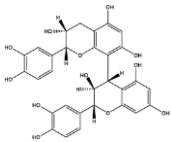
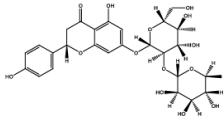
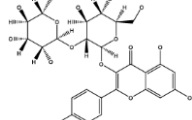
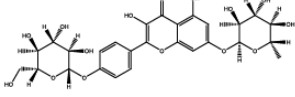
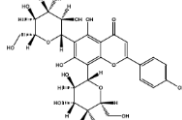
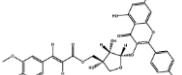
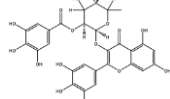
116	19.618	92	1621.90832	0.23936	cycloartenol Chemical Formula: C ₃₀ H ₅₀ O Exact Mass: 426.3862 Molecular Weight: 426.7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	
117	19.635	92	1179.01398	0.17400	simiarenol Chemical Formula: C ₃₀ H ₅₀ O Exact Mass: 426.3862 Molecular Weight: 426.7290 m/z: 426.3862 (100.0%), 427.3895 (32.4%), 428.3929 (2.7%), 428.3929 (2.4%)	
118	19.744	92	5679.49286	0.83817	1-deacetoxy-1-oxocaesalmin C Chemical Formula: C ₂₄ H ₃₀ O ₇ Exact Mass: 430.1992 Molecular Weight: 430.4970 m/z: 430.1992 (100.0%), 431.2025 (26.0%), 432.2059 (2.7%), 432.2034 (1.4%)	
119	19.786	92	6923.37315	1.02174	5,7,4'-trihydroxy-3'-C-methylflavone 4'-rhamnoside Chemical Formula: C ₂₂ H ₂₂ O ₉ Exact Mass: 430.1264 Molecular Weight: 430.4090 m/z: 430.1264 (100.0%), 431.1297 (23.8%), 432.1331 (2.7%), 432.1306 (1.8%)	
120	20.038	92	4476.29293	0.66060	bonducellpin B Chemical Formula: C ₂₃ H ₃₀ O ₈ Exact Mass: 434.1941 Molecular Weight: 434.4850 m/z: 434.1941 (100.0%), 435.1974 (24.9%), 436.2008 (2.7%), 436.1983 (1.6%)	
121	20.058	92	3907.14419	0.57661	afzelin Chemical Formula: C ₂₁ H ₂₆ O ₁₀ Exact Mass: 432.1056 Molecular Weight: 432.3810 m/z: 432.1056 (100.0%), 433.1090 (22.7%), 434.1124 (2.5%), 434.1099 (2.1%)	
122	20.059	92	2767.63505	0.40844	(3S,5S)-3,5-diacetoxy-1,7-bis(3,4-dihydroxyphenyl)heptane Chemical Formula: C ₂₁ H ₂₆ O ₈ Exact Mass: 376.1886 Molecular Weight: 376.4490 m/z: 376.1886 (100.0%), 377.1919 (22.7%), 378.1953 (2.5%), 378.1928 (1.2%)	
123	20.07	92	5736.17331	0.84653	pulcherrin B Chemical Formula: C ₂₃ H ₃₄ O ₅ Exact Mass: 438.2406 Molecular Weight: 438.5640 m/z: 438.2406 (100.0%), 439.2440 (29.2%), 440.2473 (2.7%), 440.2473 (1.4%), 440.2449 (1.0%)	
124	20.078	92	7569.76803	1.11713	mimosaside A Chemical Formula: C ₂₈ H ₄₆ O ₅ Exact Mass: 438.3345 Molecular Weight: 438.6490 m/z: 438.3345 (100.0%), 439.3379 (28.1%), 440.3412 (2.7%), 440.3412 (1.1%), 440.3388 (1.0%)	
125	20.084	92	6030.88842	0.89003	mimosaside C Chemical Formula: C ₂₈ H ₄₆ O ₆ Exact Mass: 480.3451 Molecular Weight: 480.6860 m/z: 480.3451 (100.0%), 481.3484 (30.3%), 482.3518 (2.7%), 482.3518 (1.7%), 482.3493 (1.2%)	
126	20.092	92	7985.67443	1.17851	mimosaside B Chemical Formula: C ₃₀ H ₅₀ O ₇ Exact Mass: 522.3557 Molecular Weight: 522.7230 m/z: 522.3557 (100.0%), 523.3590 (32.4%), 524.3624 (5.1%), 524.3599 (1.4%)	
127	21.387	92	5909.29168	0.87208	vitexin Chemical Formula: C ₂₁ H ₂₀ O ₁₀ Exact Mass: 432.1056 Molecular Weight: 432.3810 m/z: 432.1056 (100.0%), 433.1090 (22.7%), 434.1124 (2.5%), 434.1099 (2.1%)	
128	21.393	92	2075.63587	0.30632	cosmosiin Chemical Formula: C ₂₁ H ₂₀ O ₁₀ Exact Mass: 432.1056 Molecular Weight: 432.3810 m/z: 432.1056 (100.0%), 433.1090 (22.7%), 434.1124 (2.5%), 434.1099 (2.1%)	

129	21.429	92	7903.52842	1.16639	kaempferol-3-rhamnoside Chemical Formula: $C_{21}H_{20}O_{10}$ Exact Mass: 432,1056 Molecular Weight: 432,3810 m/z: 432.1056 (100.0%), 433.1090 (22.7%), 434.1124 (2.5%), 434.1099 (2.1%)	
130	22.158	92	5390.51824	0.79552	arundoin Chemical Formula: $C_{31}H_{52}O$ Exact Mass: 440,4018 Molecular Weight: 440,7560 m/z: 440.4018 (100.0%), 441.4052 (33.5%), 442.4085 (2.7%), 442.4085 (2.7%)	
131	22.166	92	8301.76691	1.22516	calycosin-7-O-β-D-glucoside Chemical Formula: $C_{22}H_{22}O_{10}$ Exact Mass: 446,1213 Molecular Weight: 446,4080 m/z: 446.1213 (100.0%), 447.1247 (23.8%), 448.1280 (2.7%), 448.1255 (2.1%)	
132	22.173	92	1044.83654	0.15420	astragalin Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
133	22.177	92	3017.22442	0.44528	caesalpinin D Chemical Formula: $C_{24}H_{30}O_8$ Exact Mass: 446,1941 Molecular Weight: 446,4960 m/z: 446.1941 (100.0%), 447.1974 (26.0%), 448.2008 (2.7%), 448.1983 (1.6%)	
134	22.178	92	9262.89158	1.36700	kaempferol-3-galactoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
135	22.185	92	9958.47091	1.46965	kaempferol-5-glucoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
136	22.575	92	3248.41997	0.47940	3,5-diacetoxy-7-(3,4-dihydroxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)heptane Chemical Formula: $C_{26}H_{34}O_9$ Exact Mass: 490,2203 Molecular Weight: 490,5490 m/z: 490.2203 (100.0%), 491.2236 (28.1%), 492.2270 (2.7%), 492.2245 (1.8%), 492.2270 (1.1%)	
137	22.616	92	8363.33267	1.23425	quercetin-3-rhamnoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
138	22.623	92	12456.04682	1.83824	kaempferol-3-glucoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
139	22.624	92	9660.39882	1.42567	kaempferol-7-O-glucoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
140	22.628	92	9970.76592	1.47147	luteolin-7-glucoside Chemical Formula: $C_{21}H_{20}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	

141	23.194	92	10450.82928	1.54232	quercitrin Chemical Formula: $C_{21}H_{26}O_{11}$ Exact Mass: 448,1006 Molecular Weight: 448,3800 m/z: 448.1006 (100.0%), 449.1039 (22.7%), 450.1073 (2.5%), 450.1048 (2.3%)	
142	23.311	92	10463.62925	1.54421	quercetin 7-O-β-D-glucoside Chemical Formula: $C_{21}H_{20}O_{12}$ Exact Mass: 464,0955 Molecular Weight: 464,3790 m/z: 464.0955 (100.0%), 465.0988 (22.7%), 466.0997 (2.5%), 466.1022 (2.5%)	
143	23.712	92	6068.94832	0.89565	soyasapogenol B Chemical Formula: $C_{30}H_{50}O_3$ Exact Mass: 458,3760 Molecular Weight: 458,7270 m/z: 458.3760 (100.0%), 459.3794 (32.4%), 460.3827 (2.7%), 460.3827 (2.4%)	
144	23.718	92	5260.43283	0.77633	kapurone Chemical Formula: $C_{30}H_{50}O_3$ Exact Mass: 458,3760 Molecular Weight: 458,7270 m/z: 458.3760 (100.0%), 459.3794 (32.4%), 460.3827 (2.7%), 460.3827 (2.4%)	
145	23.726	92	3339.65235	0.49286	ocotillol II Chemical Formula: $C_{30}H_{52}O_3$ Exact Mass: 460,3916 Molecular Weight: 460,7430 m/z: 460.3916 (100.0%), 461.3950 (32.4%), 462.3984 (2.7%), 462.3984 (2.4%)	
146	23.977	92	7477.08464	1.10346	hirsutrin Chemical Formula: $C_{22}H_{26}O_{11}$ Exact Mass: 462,1162 Molecular Weight: 462,4070 m/z: 462.1162 (100.0%), 463.1196 (23.8%), 464.1229 (2.7%), 464.1205 (2.3%)	
147	24.018	92	8981.26512	1.32544	isoquercitrin Chemical Formula: $C_{21}H_{20}O_{12}$ Exact Mass: 464,0955 Molecular Weight: 464,3790 m/z: 464.0955 (100.0%), 465.0988 (22.7%), 466.0997 (2.5%), 466.1022 (2.5%)	
148	24.020	92	7250.86787	1.07007	hyperoside Chemical Formula: $C_{21}H_{20}O_{12}$ Exact Mass: 464,0955 Molecular Weight: 464,3790 m/z: 464.0955 (100.0%), 465.0988 (22.7%), 466.0997 (2.5%), 466.1022 (2.5%)	
149	24.119	92	3956.97331	0.58396	myricitrin Chemical Formula: $C_{21}H_{26}O_{12}$ Exact Mass: 464,0955 Molecular Weight: 464,3790 m/z: 464.0955 (100.0%), 465.0988 (22.7%), 466.0997 (2.5%), 466.1022 (2.5%)	
150	24.125	92	1172.96691	0.17310	lupeol acetate Chemical Formula: $C_{32}H_{52}O_2$ Exact Mass: 468,3967 Molecular Weight: 468,7660 m/z: 468.3967 (100.0%), 469.4001 (34.6%), 470.4034 (3.1%), 470.4034 (2.7%)	
151	24.14	92	2895.50835	0.42731	pulcherrin A Chemical Formula: $C_{29}H_{36}O_5$ Exact Mass: 464,2563 Molecular Weight: 464,6020 m/z: 464.2563 (100.0%), 465.2596 (31.4%), 466.2630 (2.7%), 466.2630 (2.0%), 466.2605 (1.0%)	

152	25.835	92	8956.29264	1.32175	querciturone Chemical Formula: $C_{21}H_{18}O_{13}$ Exact Mass: 478.0747 Molecular Weight: 478.3620 m/z: 478.0747 (100.0%), 479.0781 (22.7%), 480.0790 (2.7%), 480.0815 (2.5%)	
153	25.844	92	9163.01200	1.35226	luteolin 7,3'-dimethyl ether 5-rhamnoside Chemical Formula: $C_{23}H_{24}O_{10}$ Exact Mass: 460.1369 Molecular Weight: 460.4350 m/z: 460.1369 (100.0%), 461.1403 (24.9%), 462.1437 (2.7%), 462.1412 (2.1%)	
154	25.846	92	4950.02963	0.73052	caesalpinin J Chemical Formula: $C_{26}H_{32}O_9$ Exact Mass: 476.2046 Molecular Weight: 476.5220 m/z: 476.2046 (100.0%), 477.2080 (27.0%), 478.2113 (3.5%), 478.2089 (1.8%)	
155	25.855	92	5458.03834	0.80549	bonducellpin A Chemical Formula: $C_{25}H_{34}O_9$ Exact Mass: 478.2203 Molecular Weight: 478.5380 m/z: 478.2203 (100.0%), 479.2236 (27.0%), 480.2270 (2.7%), 480.2245 (1.8%)	
156	25.934	92	2636.97558	0.38916	3,5-diacetoxy-1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)heptane Chemical Formula: $C_{28}H_{34}O_9$ Exact Mass: 490.2203 Molecular Weight: 490.5490 m/z: 490.2203 (100.0%), 491.2236 (28.1%), 492.2270 (2.7%), 492.2245 (1.8%), 492.2270 (1.1%)	
157	26.312	92	4476.07846	0.66057	caesalmin E Chemical Formula: $C_{28}H_{36}O_9$ Exact Mass: 492.2359 Molecular Weight: 492.5650 m/z: 492.2359 (100.0%), 493.2393 (28.1%), 494.2426 (3.8%), 494.2402 (1.8%)	
158	27.622	92	644.93235	0.09518	glyceollin V Chemical Formula: $C_{26}H_{38}O_5Si_2$ Exact Mass: 484.2101 Molecular Weight: 484.7390 m/z: 484.2101 (100.0%), 485.2135 (28.1%), 485.2097 (10.2%), 486.2070 (6.7%), 486.2131 (2.9%), 486.2168 (2.7%), 487.2103 (1.9%), 486.2168 (1.1%), 486.2144 (1.0%)	
159	27.973	92	7125.90845	1.05163	glucotricin Chemical Formula: $C_{23}H_{24}O_{12}$ Exact Mass: 492.1268 Molecular Weight: 492.4330 m/z: 492.1268 (100.0%), 493.1301 (24.9%), 494.1335 (2.7%), 494.1310 (2.5%)	
160	28.221	92	3143.68400	0.46394	pulcherralin Chemical Formula: $C_{30}H_{40}O_7$ Exact Mass: 512.2774 Molecular Weight: 512.6430 m/z: 512.2774 (100.0%), 513.2808 (32.4%), 514.2841 (5.1%), 514.2816 (1.4%)	
161	28.595	92	6836.97331	1.00899	4-(acetyloxy) 2 [3,6 bis(acetyloxy) 4 [(acetyloxy)methylene] 5 hexenylidene] 6,10 dimethyl 5,9 undecadienal Chemical Formula: $C_{33}H_{50}O_9$ Exact Mass: 518.2516 Molecular Weight: 518.6030 m/z: 518.2516 (100.0%), 519.2549 (30.3%), 520.2583 (4.4%), 520.2558 (1.8%)	

162	30.728	92	1749.28954	0.25816	biochanin A-7-O-β-D-glucoside-6"-O-malonate Chemical Formula: C ₂₈ H ₃₂ O ₁₃ ²⁻ Exact Mass: 530,1071 Molecular Weight: 530,4391 m/z: 265.0536 (100.0%), 265.5552 (27.0%), 266.0569 (2.7%), 266.0557 (2.7%)	
163	31.216	92	6006.02413	0.88636	isovouacapenol E Chemical Formula: C ₃₄ H ₃₆ O ₈ Exact Mass: 540,2512 Molecular Weight: 540,6560 m/z: 540.2512 (100.0%), 541.2545 (36.8%), 542.2579 (6.6%), 542.2554 (1.2%)	
164	31.825	92	4476.45629	0.66063	echinenone Chemical Formula: C ₄₀ H ₅₄ O Exact Mass: 550,4175 Molecular Weight: 550,8710 m/z: 550.4175 (100.0%), 551.4208 (43.3%), 552.4242 (9.1%)	
165	33.015	92	6228.37286	0.91917	cassiaoccidentalin B Chemical Formula: C ₂₇ H ₂₆ O ₁₄ Exact Mass: 576,1479 Molecular Weight: 576,5070 m/z: 576.1479 (100.0%), 577.1513 (29.2%), 578.1522 (2.9%), 578.1546 (2.7%), 578.1546 (1.4%)	
166	33.018	92	6410.66448	0.94608	2"-O-α-L-rhamnosyl-6-C-fucosyl-luteolin Chemical Formula: C ₂₇ H ₃₀ O ₁₄ Exact Mass: 578,1636 Molecular Weight: 578,5230 m/z: 578.1636 (100.0%), 579.1669 (29.2%), 580.1678 (2.9%), 580.1703 (2.7%), 580.1703 (1.4%)	
167	33.021	92	2897.28435	0.42758	vicenin 1 Chemical Formula: C ₂₈ H ₂₈ O ₁₄ Exact Mass: 564,1479 Molecular Weight: 564,4960 m/z: 564.1479 (100.0%), 565.1513 (28.1%), 566.1546 (3.8%), 566.1522 (2.9%)	
168	33.024	92	4244.83651	0.62645	vicenin 3 Chemical Formula: C ₂₈ H ₂₈ O ₁₄ Exact Mass: 564,1479 Molecular Weight: 564,4960 m/z: 564.1479 (100.0%), 565.1513 (28.1%), 566.1546 (3.8%), 566.1522 (2.9%)	
169	33.034	92	1428.87242	0.21087	daucosterol Chemical Formula: C ₃₄ H ₅₈ O ₈ Exact Mass: 562,4233 Molecular Weight: 562,8320 m/z: 562.4233 (100.0%), 563.4267 (36.8%), 564.4300 (6.6%), 564.4276 (1.2%)	
170	33.082	92	2585.58835	0.38158	pulcherrimin C Chemical Formula: C ₃₄ H ₃₆ O ₈ Exact Mass: 572,2410 Molecular Weight: 572,6540 m/z: 572.2410 (100.0%), 573.2444 (36.8%), 574.2477 (6.6%), 574.2453 (1.6%)	
171	33.431	92	6773.39267	0.99961	procyanidin A2 Chemical Formula: C ₃₀ H ₂₄ O ₁₂ Exact Mass: 576,1268 Molecular Weight: 576,5100 m/z: 576.1268 (100.0%), 577.1301 (32.4%), 578.1335 (2.7%), 578.1310 (2.5%), 578.1335 (2.4%)	
172	33.436	92	9109.18515	1.34432	proanthocyanidin A1 Chemical Formula: C ₃₀ H ₂₄ O ₁₂ Exact Mass: 576,1268 Molecular Weight: 576,5100 m/z: 576.1268 (100.0%), 577.1301 (32.4%), 578.1335 (2.7%), 578.1310 (2.5%), 578.1335 (2.4%)	
173	33.442	92	7566.44381	1.11664	kaempferide 3-rhamnoside-7-xyloside Chemical Formula: C ₂₇ H ₃₀ O ₁₄ Exact Mass: 578,1636 Molecular Weight: 578,5230 m/z: 578.1636 (100.0%), 579.1669 (29.2%), 580.1678 (2.9%), 580.1703 (2.7%), 580.1703 (1.4%)	
174	33.499	92	9387.37334	1.38537	procyanidin B3 Chemical Formula: C ₃₀ H ₂₆ O ₁₂ Exact Mass: 578,1424 Molecular Weight: 578,5260 m/z: 578.1424 (100.0%), 579.1458 (32.4%), 580.1491 (2.7%), 580.1467 (2.5%), 580.1491 (2.4%)	

175	33.5	92	6364.32803	0.93924	procyanidin B4 Chemical Formula: C₃₀H₂₆O₁₂ Exact Mass: 578.1424 Molecular Weight: 578.5280 m/z: 578.1424 (100.0%), 579.1458 (92.4%), 580.1491 (2.7%), 580.1467 (2.5%), 580.1491 (2.4%)	
176	33.563	92	7560.31523	1.11574	naringin Chemical Formula: C₂₇H₃₀O₁₄ Exact Mass: 580.1792 Molecular Weight: 580.5390 m/z: 580.1792 (100.0%), 581.1826 (29.2%), 582.1835 (2.9%), 582.1859 (2.7%), 582.1859 (1.4%)	
177	33.625	92	9543.88205	1.40847	kaempferol 3-neohesperidoside Chemical Formula: C₂₇H₃₀O₁₅ Exact Mass: 594.1585 Molecular Weight: 594.5220 m/z: 594.1585 (100.0%), 595.1618 (29.2%), 596.1627 (3.1%), 596.1652 (2.7%), 596.1652 (1.4%)	
178	34.003	92	12808.04358	1.89019	kaempferol-7-rhamnoside 4' glucoside Chemical Formula: C₂₇H₃₀O₁₅ Exact Mass: 594.1585 Molecular Weight: 594.5220 m/z: 594.1585 (100.0%), 595.1618 (29.2%), 596.1627 (3.1%), 596.1652 (2.7%), 596.1652 (1.4%)	
179	34.011	92	3915.33158	0.57782	vicenin 2 Chemical Formula: C₂₇H₃₀O₁₅ Exact Mass: 594.1585 Molecular Weight: 594.5220 m/z: 594.1585 (100.0%), 595.1618 (29.2%), 596.1627 (3.1%), 596.1652 (2.7%), 596.1652 (1.4%)	
180	34.016	92	11816.13299	1.74381	kaempferol-3(5''-feruloylapioside) Chemical Formula: C₃₀H₂₆O₁₃ Exact Mass: 594.1373 Molecular Weight: 594.5250 m/z: 594.1373 (100.0%), 595.1407 (92.4%), 596.1441 (2.7%), 596.1416 (2.7%), 596.1441 (2.4%)	
181	35.529	92	8052.37286	1.18836	desmanthin 1 Chemical Formula: C₂₈H₂₄O₁₆ Exact Mass: 616.1064 Molecular Weight: 616.4840 m/z: 616.1064 (100.0%), 617.1098 (30.3%), 618.1131 (4.4%), 618.1107 (3.3%)	
182	35.65	92	4684.33987	0.69131	myricetin 3-(4''-galloylrhamnoside) Chemical Formula: C₂₈H₂₄O₁₆ Exact Mass: 616.1064 Molecular Weight: 616.4840 m/z: 616.1064 (100.0%), 617.1098 (30.3%), 618.1131 (4.4%), 618.1107 (3.3%)	