SURVEY OF CHEMICAL COMPOSITION TOWARDS ANTIOXIDANT EFFECTS OF *MURDANNIA BRACTEATA* GROWN IN CAN THO CITY

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ABSTRACT

Murdannia bracteata is a wild plant in Can Tho City in particular and in Vietnam in general. This is a rich source of raw materials, easy to find, but up to now, domestic and world research on this plant is limited. Therefore, the project was carried out to study the chemical composition according to antioxidant orientation of total and fractional extracts (diethyl ether, ethyl acetate, n-butanol, water) from Murdannia bracteata using DPPH test (1,1-diphenyl-2-picrylhydrazyl) with vitamin C as reference. The results of the project have determined that the ethyl acetate fraction of Murdannia bracteata has the strongest antioxidant activity, with IC_{50} = 881.66 µg/mL. From the ethyl acetate fraction of Murdannia bracteata, after repeated chromatography and purification, we have isolated and identified the structures of 4 compounds: apigenin (compound 1), kaempferol-3-O-rhamnoside (compound 2), pimaric acid (compound 3) and quercetin (compound 4). Compounds (2) and (3) were found for the first time in the species Murdannia bracteata grown in Can Tho City, Vietnam compared to previous studies. The results of this study provide a database for further research on biological effects in Murdannia bracteata.

Keywords: *Antioxidant, Can Tho, DPPH, Murdannia bracteata, .*

1. INTRODUCTION

Vietnam has rich and diverse sources of medicinal herbs and has long-standing experience in using medicinal plants to treat diseases in traditional medicine. Hundreds of medicinal plants have been proven by modern science to have medicinal effects. The trend of in-depth research to verify the experience of traditional medicine and search for natural compounds with high biological activity from medicinal herbs to make medicine is of increasing interest in our country as well as around the world. Taking advantage of popular local plants that do not have high economic value, but have the potential to become herbs used as raw materials for the production of pharmaceuticals with high economic value, has always been of interest and concern. exploit. Nowadays, as the demand for drugs of medicinal origin is increasing, delving into research, verifying the experience of traditional medicine and searching for natural compounds with high biological activity is being conducted. the world cares.

The *Murdannia bracteata* tree belongs to the genus *Murdannia*, one of the largest genera of the Commelinaceae family. This genus is mainly distributed in tropical and humid temperate regions (de Oliveira Pellegrini M. O. et al., 2016), suitable for hot and humid climates; In Vietnam there are 16 species, of which 7 species are used as medicine. *Murdannia bracteata* is found in China, Laos, Thailand, and Vietnam (Wu Z. and Al-Shehbaz I.A., 2000). Some studies around the world have recorded that this plant has antibacterial effects (Wang Y. C. & Huang T. L., 2005), anti-inflammatory (Wang G. J. et al., 2007), and liver protection (Yam M. F. et al., 2010).), supporting the treatment of

liver cancer and diabetes (Ooi K. L. et al., 2015). In traditional medicine in some countries, *Murdannia bracteata* is used to treat coughs (Li D. L. et al., 2017), anti-inflammatory, and treat liver and kidney diseases (Ooi K. L. et al., 2015). However, up to now, specific research on the chemical composition and biological effects of *Murdannia bracteata* in Vietnam is still very limited. In order to provide scientific data for further research on the medicinal properties and active ingredients of *Murdannia bracteata* to promote the value of this herb, the research project was conducted on whole extracts. and fractional extracts aimed at creating natural products for the protection of public health.

2. MATERIALS AND METHODS

Materials

The medicinal herb of the whole plant *Murdannia bracteata* was collected at coordinates 10°14'58.5"N 105°34'47.2"E, Tan Loc ward, Thot Not district, Can Tho city identified by Dr. Thieu Van Duong, Faculty of Pharmacy and Nursing, Tay Do University. Raw materials are identified by observing plant morphology, microbiological surveys and comparison with plant classification documents. Researched medicinal herbs are mainly whole plants. The whole plant material is dried and ground into powder for research.

Methods

Preliminary analysis of phytochemical composition

Follow the modified Ciulei method (Ciulei, 1982) Extract the test sample with three solvents of increasing polarity (diethyl ether, ethanol, water) to obtain a diethyl ether extract containing groups of less polar substances. Alcohol and aqueous extracts contain more polar groups of substances. Confirm the presence of groups of compounds in the extracts by coloration or precipitation reactions. Carry out hydrolysis by heating the extracts with 10% HCl acid to investigate the aglycon fraction.

High preparation of total ethanol and high fractions

From the whole plant powder of *Murdannia bracteata*, it is extracted by soaking with 96% ethanol at a ratio of 1/10 (w/v), at room temperature for 24 hours. The powder of *Murdannia bracteata* is soaked 3 times, the extract from the soaks is collected, the solvent is removed using a vacuum rotary evaporator under low pressure at 50 ^{o}C to obtain concentrated extracts of *Murdannia bracteata*. Take a little bit of total extract to test for antioxidant activity. The remaining portion is mixed with a sufficient amount of water to obtain a liquid form. The diluted extract is shaken to distribute liquid - liquid in turn with solvents of different concentrations. with increasing polarity such as petroleum ether, ethyl acetate, *n*-butanol to obtain petroleum ether, ethyl acetate, *n*-butanol and aqueous solutions, evaporation recovers the solvent under reduced pressure to correspondingly high levels. These extracts were used to test the antioxidant and isolation effects.

Investigation of total and fractional high antioxidant activity

Prepare a 0.6 mM DPPH solution in methanol by dissolving 5.915 mg of DPPH with an adequate amount of methanol, then transfer to a volumetric flask and add 25 mL of methanol. After mixing, use immediately, store in colored glass bottles. Investigation of DPPH free radical scavenging activity of total extracts from samples of medicinal materials. The extracts were dissolved with methanol to obtain an initial concentration of 1 mg/mL for the dried medicinal plant. If it is difficult to dissolve, you can use DMSO to help dissolve. The positive control used was vitamin C. Prepare a solution of DPPH with a concentration of 1 mM in methanol. This solution is not stable to light, only prepared before use. Test solution: Take a sample for the phase in MeOH according to table 1:

Table 1. DPPH test response

Tube	Test solution (mL)	MeOH solution (mL)	DPPH solution (mL)
White	0	4	0
Control	0	3.5	0.5
Test	0.5	3	0.5

Shake the tubes well for 15s, stabilize at room temperature for 30 min, and photometrically at λ = 517 nm.

The HTCO free radical scavenging activity (%) was calculated by the formula:

$$HTCO\ (\%) = [(OD_{control} - OD_{test})/ OD_{control}\ ] \times 100$$

Test results are expressed as the mean of three different independent measurements. From HTCO (%) and sample concentration, a standard curve was constructed. Based on the standard curve, calculate IC_{50} (capability of catching 50% of the DPPH of the sample) by replacing y = 50 into the logarithmic linear regression equation of the form y = aln(x) + b. The lower IC_{50} value corresponds to a higher HTCO and vice versa (Chanda and Dave, 2009; Huang *et al*., 2005). Select the part used and the extract with the strongest antioxidant effect for isolation and purification.

Methods of isolation and structure determination

The extract with the highest antioxidant activity was carried out by column chromatography (silica gel, Sephadex LH-20), fractional crystallization, repeated filtration and washing of the precipitate with different solvents to obtain pure compounds. Determine the structures of the isolated compounds by means of UV, MS, NMR spectroscopy and compare with reference materials.

3. RESULTS AND DISCUSSION

Preliminary analysis results of chemical composition

Analytical results showed that the whole plant extracts of *Murdannia bracteata* reacted positively to the following groups of compounds: Flavonoids, saponins, tannins, organic acids, alkaloids, reducing sugars, sterols and carotenes. Among them, flavonoids are the most reactive components of the species *Murdannia bracteata*.

Investigation results of antioxidant activity by DPPH in vitro test

Investigate the antioxidant activity of extracts by measuring UV-Vis spectral absorbance. To confirm the antioxidant capacity of the extracts of Murdannia bracteata, evaluate the antioxidant activity based on the IC_{50} value. Survey 5 was high at concentrations of 2000 µg/mL, 1000 µg/mL. Calculate the average HTCO (%) of each peak. Then, select the extract with the highest HTCO (%), construct a logarithmic curve and calculate IC_{50} at 5 different concentrations. Compare the results with the IC_{50} of the sample with the vitamin C control.

Table 2. Results of investigating the antioxidant capacity of 5 *Murdannia bracteata* extracts

No	Ingredient name	Abs medium	Anti-oxidation (%)
1	DPPH	0.806	0
2	Ethanol 96% extract 2000 μg/mL	0.512	36.476
3	Ethanol 96% extract 1000 μg/mL	0.619	23.201
4	Petrolium ether extract 2000 µg/mL	0.623	22.705
5	Petrolium ether extract 1000 µg/mL	0.670	16.915
6	Ethyl acetat extract 2000 µg/mL	0.061	92.473
7	Ethyl acetat extract 1000 µg/mL	0.311	61.414
8	*n*-butanol extract 2000 µg/mL	0.457	43.259
9	*n*-butanol extract 1000 µg/mL	0.576	28.577
10	Water extract 2000 µg/mL	0.691	14.227
11	Water extract 1000 µg/mL	0.755	6.286

Based on the results, ethyl acetate extract 2000 µg/mL (92.473%), ethyl acetate extract 1000 µg/mL (61.414%) have HTCO > 50%, so we should continue to survey HTCO to find IC_{50}. Results of building a logarithmic equation and replacing y = 50 to find IC_{50}.

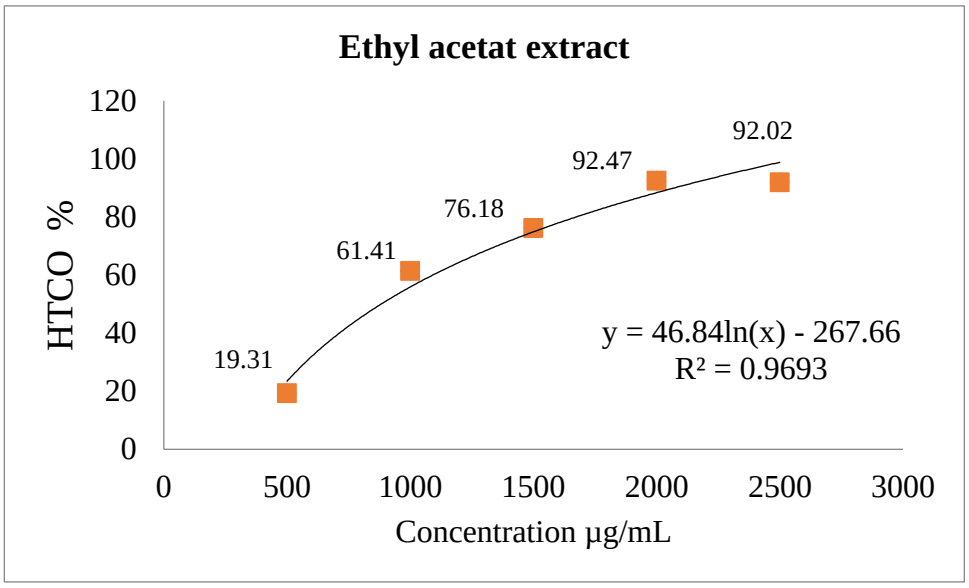

Figure 1. Log graph of ethyl acetate extract

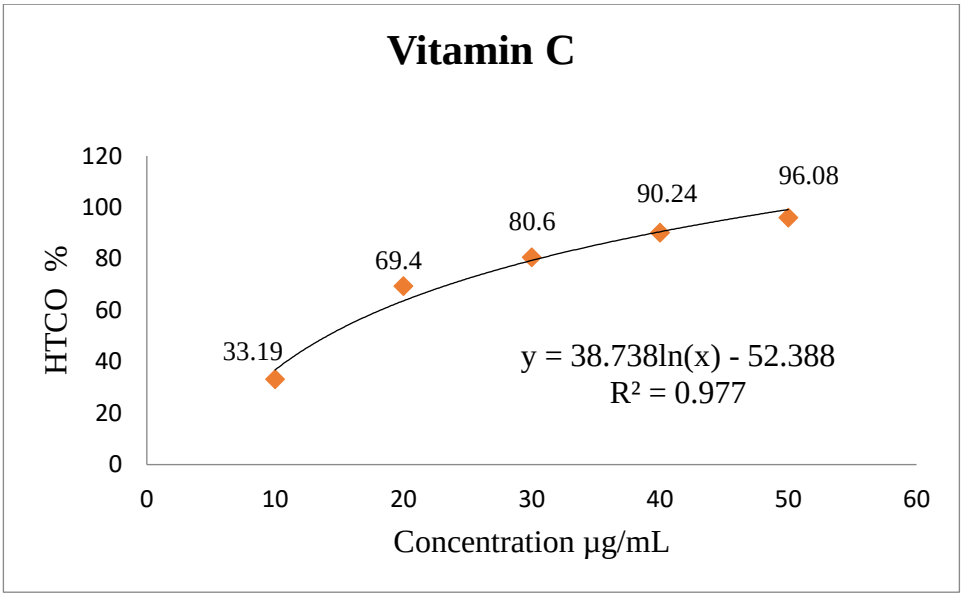

Figure 2. Logarithmic graph of Vitamin C

Table 3. IC_{50} results of Vitamin C and ethyl acetate extract

Sample	**Equation** y= aln(x)+b	**IC_{50} µg/mL**
Vitamin C	y = 38.738ln(x) – 52.388	14.06
Ethyl acetat extract	y = 46.84ln(x) – 267.66	881.66

Screening results show that ethyl acetate extract of *Murdannia bracteata* has the strongest antioxidant effect, with IC_{50} = 881.66 µg/mL. However, the activity of this extract is much lower than the positive control vitamin C, IC_{50} = 14.06 µg/mL.

Results of isolation and structure determination

The project selected the ethyl acetate fraction of *Murdannia bracteata* with the strongest antioxidant effect (IC_{50} = 881.66 µg/mL) and conducted column chromatography on the ethyl acetate (EA) fraction (EA, 20 g) with the solvent system. Solve *n*-hexane-EA (100:0→0:100) to obtain 6 fractions EA1 (950 mg), EA2 (510 mg), EA3 (920 mg), EA4 (1140 mg), EA5 (1.8 g), EA6 (930 mg). Multiple column chromatography fractionated EA5 (1.8 g) on silica gel with the solvent system $CHCl_3$-MeOH (10:2→5:5) to obtain 5 fractions EA5.1 (120 mg), EA5.2 (500 mg), EA5.3 (450 mg), EA5.4 (350 mg), EA5.6 (150 mg). Continue to purify the EA5.2 fraction (500 mg) by column chromatography on silica gel with the solvent system $CHCl_3$-MeOH (3:7→2:8) and purify it many times to obtain compound 1 (23 mg). Continue to purify fraction EA5.3 (450 mg) by column chromatography on RP18 with the solvent system MeOH-H_2O (30:70) to obtain compound 2 (25 mg). Fraction EA5.4 (350 mg) was further subjected to Sephadex LH-20 gel chromatography with MeOH solvent and purified several times to obtain compound 3 (27 mg) and compound 4 (15 mg).

Compound 1: Light yellow powder. ESI-MS spectrum: *m/z* 270.9 $[M+H]^+$ → CTPT: $C_{15}H_{10}O_5$ (M = 270). The ESI-MS spectrum of compound 1 shows a molecular ion peak at *m/z* 270.9 $[M+H]^+$ corresponding to molecular mass M = 270, consistent with the molecular formula $C_{15}H_{10}O_5$. In the ^{1}H-NMR spectrum of compound 1, there is an aromatic proton signal of two paired doublets at δ_H 6.19 and 6.47 (J = 2.0 Hz) showing HSQC correlation with the corresponding carbon resonance at δ_C 98.8 (d) and 94.0 (d), assigned to H-6 and H-8 of ring A. Two directly coupled doublets at δ_H 7.92

and 6.82 (2H, J = 2.0 Hz) shows distant bindings to the ^{13}C-NMR signal at δ_C 161.3 (C-4'). Therefore, assigned H-2'/6' and H-3'/5' of ring B, respectively. Additionally, a singlet at δ_H 6.76 was assigned to H-3. The H-3 assignment is confirmed by distant correlations with C-2. (δ_C 161.0) and C-1' (δ_C 120.9). ^{13}C-NMR at δ_C 164.0 shows correlation of HMBC with H-6 and H-8, assigned to C-7. ^{13}C-NMR and DEPT spectra showed signals of 8 quaternary carbons and 7 CH groups. Based on the data analyzed above and compared with the ^{1}H-NMR and ^{13}C-NMR spectra in the reference document (Alwahsh M.A.A. et al., 2015), the structure of compound 1 was determined to be apigenin with the formula structure is as follows:

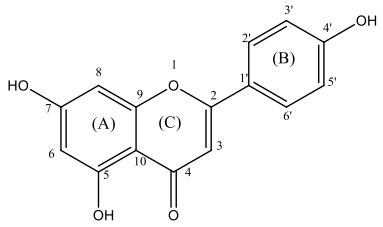

Figure 3. Structural formula of apigenin

Table 3. Comparison of ^{13}C-NMR (125 MHz) and ^{1}H-NMR (500 MHz) spectral data of compound 1 and apigenin measured in DMSO

Location C	Apigenin (Alwahsh M.A.A. et al., 2015)		Compound 1	
	δ_C (ppm)	δ_H (ppm) (*J*, Hz)	δ_C (ppm)	δ_H (ppm) (*J*, Hz)
2	147.9		146.7	
3	135.9		135.6	
4	176.0		175.7	
5	160.9		160.6	
6	98.4	6.17 (d; J = 2.0)	98.1	6.18 (d; J = 2.5)
7	164.1		163.8	
8	93.5	6.39 (d; J = 2.0)	93.3	6.40 (d; J = 2.5)
9	156.3		156.1	
10	103.2		102.9	
1'	122.1		121.9	
2'	115.2	7.66 (d; J = 2.0)	115.0	7.67 (d; J = 3.0)
3'	145.2		145.0	
4'	147.0		147.6	
5'	115.8	6.87 (d; J = 8.5)	115.5	6.88 (d; J = 9.5)
6'	120.2	7.53 (dd; J = 8.0; 2.0)	119.9	7.53 (dd; J = 8.5; 3.0)

Apigenin isolated from different species also showed anti-cancer effects on a variety of cell lines. For example, apigenin isolated from *Lycopodium clavatum* activates apoptosis in A375 skin cancer and A549 human lung carcinoma cells, mainly through the mechanism of stimulating free radical generation, causing mitochondrial dysfunction bodies and caspase activation (Das S. et al., 2012); apigenin isolated from *Macaranga gigantifolia* was toxic to mouse P-388 leukemia cells with IC_{50} 14.13 μg/mL (Fajriah S. et al., 2016); apigenin isolated from *Eriocephalus africanus* inhibits the growth of HepG2 liver cancer cells with EC_{50} = 11.93 μg/mL (Magura J. et al., 2021).

Compound 2: Compound 2 was obtained as a pale yellow powder, easily soluble in acetone. The HR-ESI-MS spectrum shows the molecular ion tip $[M+Na]^+$ at *m/z* 455.0930 (theoretical 455.0954), allowing the molecular formula to be determined as $C_{21}H_{20}O_{10}$. ^{1}H-NMR spectrum of compound 2 in the weak magnetic field region, showing the presence of 1 -OH group at δ_H 12.71 (s, 1H) and 2 aromatic proton signals at δ_H 6.48 (d, 1H , J = 2.0 Hz, H-8), δ_H 6.27 (d, 1H, J = 2.0 Hz, H-6) meta-pairing together characterizes the A aromatic nucleus of the flavonoid framework. The ^{1}H–NMR spectrum also shows two aromatic proton signals at δ_H 7.86 (d, 2H, J = 8.5 Hz), δ_H 7.02 (d, 2H, J = 9.0 Hz) demonstrating the presence of an aromatic nucleus with 2 substituents at position 1,4 (B nucleus).

The ^{1}H-NMR spectrum also shows signals of 5 oxymethine groups at δ_H 5.54 (brs, 1H), δ_H 4.23 (brs, 1H), δ_H 3.70 (dd, 1H, J = 9.0, 2 ,5 Hz), δ_H 3.33 (m, 1H), δ_H 3.30 (m, 1H) and 1 double nasal methyl group at δ_H 0.90 (d, 3H, J = 5.5 Hz), confirm presence of α-L-rhamnopyranosyl sugar molecule in the structure of compound 2. ^{13}C-NMR spectrum combined with HSQC spectrum helps identify 21 carbon signals of compound 2, including 15 carbon signals of flavonoids (including 1 carbonyl group at δ_C 179.3; there are 6 sp^2 carbon signals directly bonded to oxygen atoms at δ_C 165.0; 163.2; 160.9; 158.5; 158.0 and 135, 6; there are 5 aromatic carbon signals at δ_C 131.7; 116.3; 105.8; 99.8; 94.3) and 6 signals of α-L-rhamnopyranosyl sugar molecules (5 methine signals at δ_C 102.8; 73.0; 72.2; 71.5; 71.4 and 1 signal of methyl group at δ_C 17.7). Investigation of HMBC spectral data helped confirm that compound 2 is a flavonoid glycoside compound. Besides, the correlation between the anomer proton signal at δ_H 5.54 (H-1") and the carbon signal at δ_C 135.6 (C-3) proves the connection of sugar molecules at C-3 of the aglycon part. From the analysis of HR-ESI-MS, ^{1}H, ^{13}C-NMR spectral data, combined with HMBC, HSQC spectra and comparison with the literature (Do V. M. et al., 2021), it shows that there are similarities. Therefore, the structure of compound 2 was determined to be kaempferol-3-O-rhamnoside with the following structure:

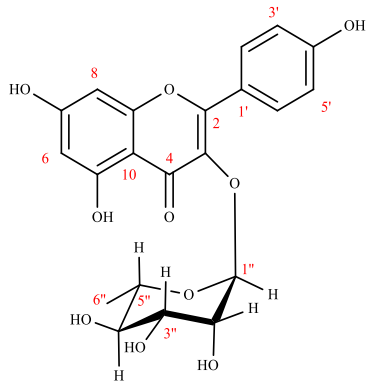

Figure 4. Structural formula of kaempferol-3-O-rhamnoside

Table 4. Comparison of ^{13}C-NMR (125 MHz) and ^{1}H-NMR (500 MHz) spectral data of compound 2 and kaempferol-3-O-rhamnoside

Location C	Kaempferol-3-*O*-rhamnosid (Do V. M. *et al*., 2021)		Compound 2	
	δ_C (ppm) (Aceton-d_6, 125 MHz)	δ_H (ppm) (*J*, Hz) (Aceton-d6, 500 MHz)	δ_C (ppm) (MeOD-d_4, 150 MHz)	δ_H (ppm) (*J*, Hz) (MeOD-d_4, 600 MHz)
2	158.5		159.3	
3	135.6		136.2	
4	179.3		179.6	
5	163.2		163.2	
6	99.8	6.27 *d* (2.0)	99.8	6.30 *d* (1.9)
7	165.0		165.9	
8	94.3	6.48 *d* (2.0)	94.7	6.48 *d* (1.9)
9	158.0		158.5	
10	105.8		105.9	
5-OH		12.71 *s*		
1'	122.7		122.6	
2'	131.7	7.86 *d* (8,5)	131.9	7.86 *d* (8.5)
3'	116.3	7.02 *d* (9.0)	116.5	7.03 *d* (8.7)
4'	160.9		161.6	
5'	116.3	7.02 *d* (9.0)	116.5	7.03 *d* (8.7)
6'	131.7	7.86 *d* (8.5)	131.9	7.86 *d* (8.5)
1''	102.8	5.54 *brs*	103.5	5.47 *d* (1.6)
2''	71.5	4.23 *m*	71.9	4.31 *dd* (3.3; 1.6)
3''	72.2	3.70 *dd* (9.0; 2.5)	72.1	3.80 *dd* (9.0; 3.4)
4''	73.0	3.33 *m*	73.1	3.42 *m*
5''	71.4	3.30 *m*	72.0	3.40 *m*
6''	17.7	0.90 *d* (5.5)	17.6	1.01 *d* (5.5)

Kaempferol-3-O-rhamnoside (afzelin) is a flavonoid compound with an aglycon part of the flavonol group. This is a flavonoid compound that has been shown to have antioxidant activity (Akter M. et al., 2022). Publications show that afzelin inhibits the growth of breast cancer cells by stimulating apoptosis (Diantini A. et al., 2012), has the ability to remove superoxide anion radicals in RAW264.7 cells and shows Significant anti-prostate cancer activity against two cancer lines PC-3 and LNCaP (Mao Y. W. et al., 2011).

Compound 3: Needle-shaped crystals. Shows gray color with Vaniline/H_2SO_4 reagent. ESI-MS *m/z*: 303.6 $[M+H]^+$. Has molecular formula $C_{20}H_{30}O_2$ (M=302). The ^{1}H-NMR spectrum of compound 3 shows a vinyl group at the end of the chain [δ_H 5.78 (1H, dd, J = 17.0, 10.5 Hz, H-15); 4.91 (1H, dd, J = 17.0, 1.5 Hz, H-16a); 4.89 (1H, dd, J = 10.5, 1.5 Hz, H-16b); δ_C 148.9 (C-15); 110.2 (C-16), a proton of the triple-substituted olefin group at δ_H 5.23 (1H, s, H-14); δ_C 136.6 (C-8); 129.1 (C-14)] and 3 methyl groups at δ_H 0.85; 1.05; 1.22. In addition, the ^{13}C-NMR and HSQC spectra show resonance signals of 20 carbons: 3 methyl groups (3×CH_3), 8 methylene groups (7×CH_2), 4 methine groups (3×CH) and 5 quaternary carbons. (3×Cq), including 1 carboxyl group at δ_C 184.9. By spectral analysis and comparison with previously published data, it was confirmed that compound 3 is a pimarane diterpenoid. Combining the above spectral data with comparison of the published spectral data of the compound pimaric acid (Hau D. V. et al., 2017), it can be confirmed that compound 3 is pimaric acid with the following structural formula:

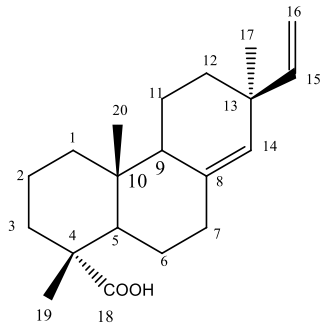

Figure 5. Structural formula of pimaric acid

Table 5. Comparison of ^{13}C-NMR (125 MHz) and ^{1}H-NMR (500 MHz) spectral data of compound 3 and pimaric acid measured in $CDCl_3$

Location C	Acid pimaric (Hau D. V. et al., 2017)		Compound 3	
	δ_C (ppm)	δ_H (ppm) (J, Hz)	δ_C (ppm)	δ_H (ppm) (J, Hz)
1	38.4		38.3	
2	18.3		18.2	
3	37.1		37.1	
4	47.2		47.3	
5	48.7		48.8	
6	24.9		24.9	
7	35.6		35.5	
8	136.2		136.6	
9	50.7		50.6	
10	38.1		37.7	
11	18.8		18.6	
12	34.6		34.5	
13	37.4		37.4	
14	129.3	5.22 (s)	129.1	5.23 (s)
15	149.9	5.71 (dd, J=17.0; 10)	148.91	5.78 (dd, J=17.0; 10.5)
16	110.5	4,91 (dd, J=17.0; 1.7) 4,95 (dd, J=10; 1.7)	110.2	4,91 (dd, J=17.0; 1.5) 4,89 (dd, J=10.5; 1.5)
17	26.2	1.04 (s)	26.0	1.05 (s)
18	185.3		184.9	
19	16.8	1.21 (s)	16.8	1.22 (s)
20	15.3	0.84 (s)	15.2	0.85 (s)

Pimaric acid is an organic acid, belonging to the group of resin acids. The isolation results are consistent with the qualitative results of the presence of organic acids in *Murdannia bracteata*. Pimaric acid is often found in pine resin (López-Goldar X. et al., 2020). In addition, it also appears in some other tree species such as Aralia cordatac (Suh S. J. et al., 2012) and Dacrycarpus imbricatus (Hau D. V. et al., 2017). Regarding biological effects, pimaric acid in Aralia cordatac has been shown to inhibit metalloproteinase-9 production and inhibit the migration of human aortic smooth muscle

cells. Since then, this substance has shown potential to reduce the risk of atherosclerosis in humans (Suh S. J., et al., 2012).

Compound 4: Needle-shaped crystal, yellow. ESI-MS spectrum: *m/z* 302.8 $[M+H]^+$ with molecular formula $C_{15}H_{10}O_7$ (M = 302). The ESI-MS spectrum of compound 4 shows a molecular ion peak at *m/z* 302.8 $[M+H]^+$ corresponding to molecular mass M = 302, consistent with the molecular formula $C_{15}H_{10}O_7$. ^{1}H-NMR spectrum shows 2 doublet signals of 2 aromatic protons at δ_H 6.18 (1H, d, J = 2.5 Hz; H-6) and 6.40 (1H, d, J = 2.5 Hz; H-8). There are also 3 aromatic proton signals at 7.67 (1H, d, J = 3.0 Hz; H-2'); 6.88 (1H, d, J = 9.5 Hz; H-5'); 7.53 (1H, dd, J = 8.5; 3.0 Hz; H-6') shows an ABX-type signal. The ^{13}C-NMR and DEPT spectrum of compound 4 shows the signal of 15 C of the flavonoid framework between the range δ_C 93.3 – 175.7 ppm, with 5 CH aromatic at δ_C 98.1 (C-6); 93.3 (C-8); 115.0 (C-2'); 115.5 (C-5') and 119.9 (C-6'); 10 C in which the signal δ_C 175.7 ppm characterizes the carbonyl group, 4 carbons have a shift δ_C 145.0; 147.6; 160.6; 163.8 ppm characterizes the bond form of the aromatic ring with the OH group of carbons C-3', C-4', C-5, C-7. In addition, the carbon signal at δ_C 135.6 (C-3) characterizes the carbon of the double bond bonded to a hydroxyl group. Based on the above analysis and comparison of spectral data of compound 4 with the literature (Liu H. et al., 2010), it is confirmed that compound 4 is quercetin.

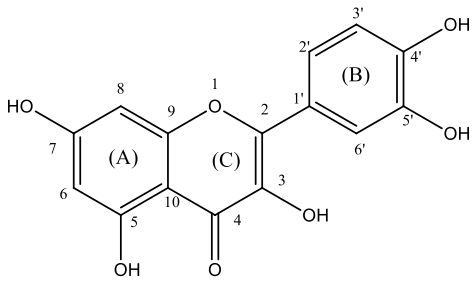

Figure 6. Structural formula of quercetin

Table 6. Comparison of ^{13}C-NMR (125 MHz) and ^{1}H-NMR (500 MHz) spectral data of compound 4 and quercetin measured in DMSO

Location C	Quercetin (Liu H. et al., 2010)		Compound 4	
	δ_C (ppm)	δ_H (ppm) (*J*, Hz)	δ_C (ppm)	δ_H (ppm) (*J*, Hz)
2	147.9		146.7	
3	135.9		135.6	
4	176.0		175.7	
5	160.9		160.6	
6	98.4	6.17 (d; J = 2.0)	98.1	6.18 (d; J = 2.5)
7	164.1		163.8	
8	93.5	6.39 (d; J = 2.0)	93.3	6.40 (d; J = 2.5)
9	156.3		156.1	
10	103.2		102.9	
1'	122.1		121.9	
2'	115.2	7.66 (d; J = 2.0)	115.0	7.67 (d; J = 3.0)
3'	145.2		145.0	
4'	147.0		147.6	
5'	115.8	6.87 (d; J = 8.5)	115.5	6.88 (d; J = 9.5)
6'	120.2	7.53 (dd; J = 8.0; 2.0)	119.9	7.53 (dd; J = 8.5; 3,0)

In 2011, quercetin was isolated from *Vaccinium arctostaphylos* by Barman Nickavar and his colleagues for pancreatic α-amylase inhibitory activity with IC_{50} = 0.16 - 0.17 mM (Nickavar B. & Amin G., 2011). According to research by Choi So Jin and colleagues in 2012, quercetin isolated from *Cratoxylum formosum* has the ability to inhibit NO production in RAW 264.7 cells stimulated by LPS, through regulating iNOS expression (Choi S. J. et al. al., 2012). That is the mechanism for the anti-inflammatory effect, similar to the anti-inflammatory mechanism of *Murdannia bracteata* extract reported in the study of Wang Guei Jane and colleagues in 2006 (Wang G. J. et al., 2007). Besides the above effects, quercetin also has many other activities such as antioxidant, cardiovascular protection, anti-hypertension, antiviral, immune regulation, etc. (David A. V. A. et al., 2016).

4. CONCLUSION

Screening results on the antioxidant activity of total and fractionated extracts showed that ethyl acetate extract of *Murdannia bracteata* has the strongest antioxidant effect, with IC_{50} = 881.66 µg/mL. From the ethyl acetate fraction of *Murdannia bracteata*, after repeated chromatography and purification, we have isolated and identified the structures of 4 compounds: apigenin (compound 1), kaempferol-3-O-rhamnoside (compound 2), pimaric acid (compound 3) and quercetin (compound 4). Compounds (2) and (3) were found for the first time in the species *Murdannia bracteata* grown in Can Tho City, Vietnam compared to previous studies. The results of this study provide a database for further research on biological effects in *Murdannia bracteata.*

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