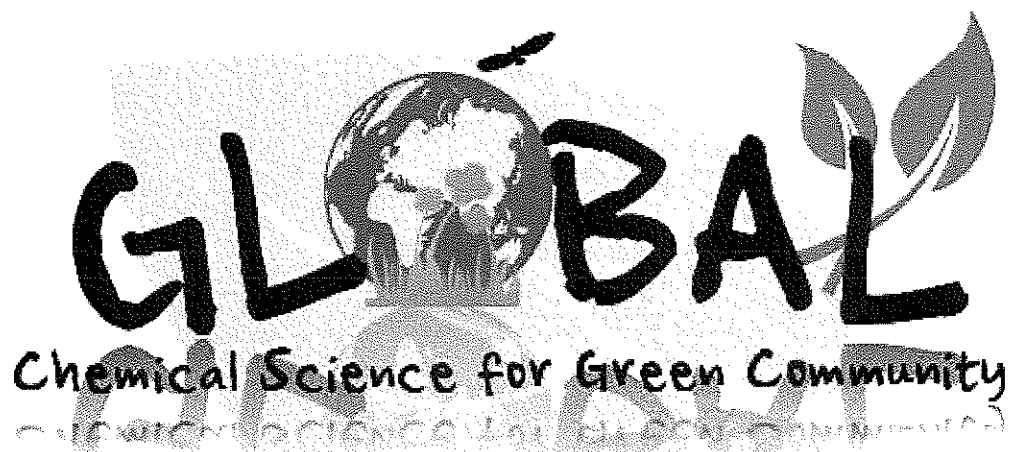


PROCEEDINGS
PURE AND APPLIED CHEMISTRY INTERNATIONAL
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CHEMICAL COMPOSITIONS AND ANTIBACTERIAL ACTIVITY OF *PLECTRANTHUS ROTUNDIFOLIUS* EXTRACTS

Chalida Phungpanya¹, Theeraphan Machan^{1*}, Patcharee Pripdeevech¹, Chalernporn Thongpoon²,
Kanlaya Jumpatong³

¹Program of Applied Chemistry, School of Science, Mae Fah Luang University, Chiang Rai 57100, Thailand

²Program of Chemistry, Faculty of Sciences and Technology, Pibulsongkram Rajabhat University, Phitsanulok 65000, Thailand

³Department of Chemistry, School of Science, University of Phayao, Phayao 56000, Thailand

* Author for correspondence; E-Mail: t.machan@sci.mfu.ac.th, Tel. +66 53 916769, Fax. +66 53 916776

Abstract: This work reported the study of chemical compositions and antibacterial activity of the extracts from aerial part and tubers of *Plectranthus rotundifolius*. The chemical constituents of both extracts were analyzed by GC-MS technique. Five major components of aerial extract were γ -muurolene (21.68%), α -humulene (12.68%), *E*-caryophyllene (5.67%), *n*-dodecane (5.55%), and 1-octen-3-ol (4.63%) while the main components in tuber extract were *epi*- α -cadinol (15.52%), sesquiceneole (9.36%), cyperene (4.88%), *epi*- α -bisabolol (3.00%), and α -santalene (2.25%). The aerial hexane extract showed antibacterial activity in microtiter plates with two-fold serial dilution assay against *Bacillus subtilis*, *Escherichia coli*, and *Staphylococcus aureus* with MIC values of 10.00, 1.25, and 1.25 mg/mL, respectively. The hexane extract of tubers also showed significant antibacterial activity in paper disc diffusion method against *Bacillus subtilis*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus* with MIC values of 75.00, 125.00, and 500.00 mg/mL, respectively.

1. Introduction

P. rotundifolius (Poir.) Spreng (synonyms: *P. tuberosus* Blume, *Coleus dysentericus* Buk., *C. rotundifolius* (Poir.) A. Chev. & E. Perrot, *C. parviflorus* Benth., and *Solenostemon rotundifolius* (Poir.) J.K. Morton) [1] is a green perennial aromatic herb that belongs to the family Lamiaceae (Labiatae) and locally known in Thai as "Man Khi-Nu" and "Man Nu". This plant is widely distributed in Asia and tropical areas, especially in the Southern part of Thailand [2]. Leaves of the plant present a light scent. Tubers can be eaten as vegetable and often used in Southern Thai cuisine such as curry and grill. The tubers can also be fermented to the alcoholic beverages [3,4]. In addition, this plant is used in the traditional medicine for treatment of dysentery, blood in the urine as well as eye disorders [5]. There have no reports on an organic solvent extraction except the hydrodistillation method from this plant. In this study, the aerial part and tubers of *P. rotundifolius* are extracted by hexane, moreover, then analyzed by GC-MS technique, the identification of components, and the

investigation of antibacterial activity are also the highlight of this study.

2. Materials and Methods

2.1 Plant Materials

Fresh aerial part and tubers were collected from Surat Thani, Thailand in July, 2011. The plant was identified and deposited at CMU herbarium, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand. Mixtures of *n*-alkanes (C_8 - C_{22}) analogue were purchased from Merck (Darmstadt, Germany).

2.2 Extraction

The 1.10 kg of aerial part and tubers were chopped into small pieces and then separately macerated in 1.50 L hexane for 3 days at room temperature in 2 times, afterwards, solvent removal under reduced pressure was evaporated to obtain 0.048 and 0.19% of aerial and tuber hexane extracts, respectively.

2.3 Gas Chromatography-Mass Spectrometry (GC-MS)

The hexane extracts of both parts of the plant were analyzed by a Hewlett Packard model HP6890 gas chromatograph (Agilent Technologies, Palo Alto, CA, USA). The HP-5MS (5% phenylpolymethylsiloxane) capillary column (30 m $\times$ 0.25 mm i.d., film thickness 0.25 μ m; Agilent Technologies, USA) was equipped and interfaced to an HP model 5793 mass-selective detector. The oven temperature was initially held at 60°C and then increased by 3°C/min to 250°C. The injector and detector temperatures were 250°C and 280°C, respectively. Purified helium was used as the carrier gas at a flow rate of 1 mL/min. EI mass spectra were collected at 70 eV ionization voltages over the range of *m/z* 29–300. The electron multiplier voltage was 1150 V. The ion source and quadrupole temperatures were set at 230°C and 150°C, respectively. The identification of hexane extracts were performed by comparison of their Kovats retention indices, relative to C_8 - C_{22} *n*-alkanes, and comparison of the mass spectra of individual components with the

reference mass spectra in the NIST 98 and Wiley 275 databases at the present quality match greater than 90%. The relative quantity of the components of all samples was determined directly from the GC peak areas. The percentage compositions of hexane extracts of *P. rotundifolius* were reported in **Table 1**.

Table 1 Chemical compositions of fresh aerial part and tuber hexane extracts from *P. rotundifolius*

Chemical compounds	%RA ^a		RI ^d (Exp)	RI ^e (Lit)
	AH ^b	TH ^c		
<u>Acyclic monoterpene</u>				
Myrcene	0.56		998	990
Limonene	0.36		1025	1029
<u>Cyclic monoterpene</u>				
α -Thujene	tr		931	930
ρ -Cymene		tr	1021	1024
β -Phellandrene		tr	1026	1029
<u>Oxygenated monoterpene</u>				
Camphor	1.51	tr	1141	1146
Menthol		tr	1170	1171
Eugenol		0.20	1355	1359
<u>Acyclic sesquiterpene</u>				
<i>Z</i> - β -Farnesene		0.73	1438	1442
<u>Cyclic sesquiterpene</u>				
α -Copaene	0.91	tr	1371	1376
β -Elemene	0.98	0.38	1387	1390
Cyperene		4.88	1387	1390
Sibirene		tr	1394	1398
α -Gurjunene		0.74	1409	1409
<i>E</i> -Caryophyllene	5.67		1414	1419
α -Santalene		2.25	1415	1417
α - <i>trans</i> -Bergamotene		0.98	1431	1438
α -Humulene	12.68		1448	1454
<i>cis</i> -Muurolo-3,5-diene		1.24	1466	1450
<u>Oxygenated sesquiterpene</u>				
Sesquicineole		9.36	1511	1516
<i>E</i> -Nerolidol		0.13	1560	1563
<i>trans</i> -Sesquisabinene hydrate		0.48	1576	1579
α -Acorenol		tr	1629	1633
<i>epi</i> - α -Cadinol		15.52	1641	1640
<i>epi</i> - α -Bisabolol		3.00	1681	1684
<i>trans</i> -Muurolo-3,5-diene		0.34	1458	1453
β -Chamigrene		0.35	1469	1477

Table 1 (Cont.) Chemical compositions of fresh aerial part and tuber hexane extracts from *P. rotundifolius*

Chemical compounds	%RA ^a		RI ^d (Exp)	RI ^e (Lit)
	AH ^b	TH ^c		
β -Bisabolene		0.31	1505	1505
γ -Cadinene	tr		1511	1513
δ -Cadinene	0.31		1518	1523
α -Cadinene		tr	1533	1538
<u>Cyclic diterpene</u>				
3 <i>E</i> -Cembrene A		0.24	1952	1948
<u>Oxygenated diterpene</u>				
Phytol	3.18		2112	2111
<u>Acyclic hydrocarbon</u>				
n -Nonane	0.20		897	900
n -Decane	2.37		997	1000
n -Dodecane	5.55	0.42	1196	2000
n -Tridecane	0.62	tr	1295	1300
n -Tetradecane	3.59		1395	1400
n -Pentadecane	1.01		1494	1500
n -Hexadecane	1.87	0.20	1594	1600
n -Heptadecane	0.65	tr	1694	1700
n -Octadecane	0.67		1793	1800
n -Nonadecane	0.67		1893	1900
n -Eicosane	0.83		1993	2000
n -Docosane	0.51		2194	2200
<u>Aromatic hydrocarbon</u>				
1,2,4-Trimethylbenzene	0.29		1020	1025
Naphthalene	0.24		1180	1181
<u>Alcohol</u>				
2 <i>Z</i> -Hexenol	0.25	tr	884	867
1-Octen-3-ol	4.63		976	979
Benzyl alcohol		tr	1034	1031
Phenylethyl alcohol		0.11	1113	1116
p -vinyl-Guaiacol		0.15	1313	1309
<u>Phenylpropene</u>				
Elemicin		tr	1554	1557
<u>Ketone</u>				
Cyperotundone		0.30	1689	1695
<u>Ester</u>				
cis -2- <i>tert</i> -butyl-Cyclohexanol acetate	0.58		1289	1293
Myrtenyl acetate		tr	1321	1326
Methyl- <i>o</i> -anisate		tr	1338	1337
Benzyl salicylate		0.56	1863	1865
Methyl hexadecanoate	0.47	0.43	1921	1921

Table 1 (Cont.) Chemical compositions of fresh aerial part and tuber hexane extracts from *P. rotundifolius*

Chemical compounds	%RA ^a		RI ^d (Exp)	RI ^e (Lit)
	AH ^b	TH ^c		
Methyl linoleate		0.50	2094	2095
(Z,Z,Z)-9,12,15-Octadecatrienoic acid, methyl ester	1.05		2098	2105

%RA^a, Relative peak area (raw peak area relative to total peak area)

AH^b, Aerial part hexane extract of *P. rotundifolius*

TH^c, Tuber hexane extract of *P. rotundifolius*

RI (Exp)^d, Programmed temperature retention indices as determined on HP-5MS column using a homologous series of *n*-alkanes (C₈–C₂₂) as internal standard and H₂ as a carrier gas

RI (Lit)^e, Values from literature data using He as a carrier gas

tr^f, Trace amount (%RA < 0.10)

2.4 Antibacterial activity

The aerial hexane extract was used to determine the MIC inhibition by microtiter plates with two-fold serial dilution assay against *Bacillus subtilis*, *Bacillus cereus*, *Escherichia coli*, *Staphylococcus aureus*, *Salmonella typhimurium*, *Pseudomonas aeruginosa*, *Pseudomonas fluorescens*, and *Micrococcus luteus* whereas disc diffusion assay was tested for tuber hexane extract against *Bacillus subtilis*, *Escherichia coli*, *Staphylococcus aureus*, *Salmonella typhimurium*, *Pseudomonas aeruginosa*, *Micrococcus luteus*, and Methicillin-resistant *Staphylococcus aureus* (MRSA). The results were presented as follows in Table 2.

Table 2 The MIC of antibacterial activity of crude extracts from *P. rotundifolius*

Bacteria	MIC of <i>P. rotundifolius</i> (mg/mL)	
	AH ^a	TH ^b
<i>B. subtilis</i>	10.00	75.00
<i>B. cereus</i>	10.00	- ^c
<i>E. coli</i>	1.25	ND ^d
<i>S. aureus</i>	1.25	500.00
MRSA	-	ND
<i>S. typhimurium</i>	ND	ND
<i>Ps. aeruginosa</i>	ND	125.00
<i>Ps. fluorescens</i>	ND	-
<i>M. luteus</i>	ND	ND

AH^a, Aerial hexane extract of *P. rotundifolius*

TH^b, Tuber hexane extract of *P. rotundifolius*

ND^c, Not detected

-^d, Not tested

3. Results and Discussion

The aerial and tuber hexane extracts of *P. rotundifolius* were analyzed and identified the chemical components by GC–MS technique. Five major

compounds of aerial hexane extract were γ -muurolene (21.68%), α -humulene (12.68%), *E*-caryophyllene (5.67%), *n*-dodecane (5.55%), and 1-octen-3-ol (4.63%) while *epi*- α -cadinol (15.52%), sesquicineole (9.36%), cypere (4.88%), *epi*- α -bisabolol (3.00%), and α -santalene (2.25%) were also five main components of tuber hexane extract. From the results, the chemical components of both parts were significantly difference presented chemotypes, although there were in same major groups (cyclic sesquiterpene and oxygenated sesquiterpene group).

In antibacterial activity study, three microbes, *B. subtilis*, *E. coli*, and *S. aureus*, were exhibited by aerial hexane extract with MIC values of 10.00, 1.25, and 1.25 mg/mL, respectively. The tuber hexane extract inhibited the growth of *B. subtilis*, *Ps. aeruginosa*, and *S. aureus* with MIC values of 75.00, 125.00, and 500.00 mg/mL, respectively. From these results, major compositions of the extracts were monoterpenes and sesquiterpenes and they could be the compounds that showed antibacterial activity against bacteria and fungi [6].

4. Conclusions

In this present study, the aerial part and tubers of *P. rotundifolius* were extracted with hexane, analyzed by GC–MS technique, and investigated the MIC of antibacterial activity. The most abundant group of major compounds were cyclic sesquiterpenes in an aerial extract while the oxygenated sesquiterpenes were the major group of compounds in the tuber extract. In addition, terpenoid compositions in both crude extracts had ability to inhibit some microbes in this study.

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