CHAPTER III

RESULTS AND DISCUSSION

3.1 Highly volatile constituents of *Vetiveria zizanioides* roots grown under different cultivation conditions

3.1.1 Extraction by Likens-Nickerson simultaneous distillation and extraction (SDE) apparatus

Essential oils of the dry vetiver roots were extracted by SDE apparatus for only 5 h to prevent loss of volatiles and obtain high recoveries without thermal degradation of oil samples. All obtained essential oils appeared as a brown-yellow viscous liquid with percentage yields of 0.18, 0.27, and 0.06 w/w from dried vetiver which were cultivated in normal soil, normal soil with added microbes, and semi-hydroponic condition, respectively. This result revealed the activity of the intracellular bacteria that was involved with the essential oil cells in the glands of vetiver roots, which has been reported in the study of Adams and co-workers.[30] Their results showed that an unidentified biotic factor, apparently bacteria or fungi, appeared to enhance the oil production in normal soil by increasing yield. This result of endogenous microbial transformation of plant chemicals may have broader physiological implications, especially among monocotyledons including cereals. In contrast, vetiver oil from semi-hydroponic cultivation, which contained no fertilizer and no effective microbes, gave the lowest yield. The loss of volatile oil from the dried vetiver roots obtained from this

cultivation system was quite high and was possibly due to the continual evaporation of volatiles as the roots were exposed to the atmosphere during the growing stage. By performing sensory evaluation of all the oils, the results indicated similar aroma description which was burned and woody. This meant that the methods of cultivation have no effect on overall aroma character of the oils.

3.1.2 GCΔGC and SPME-GCΔGC analysis

The technique of GCΔGC was used for analysis of the overall volatile constituents in the vetiver root essential oils whereas the SPME-GCΔGC was utilized to investigate the highly volatile fractions of the oils. The vetiver oil obtained from normal soil cultivation system was a representative of all samples employed in this experiment because its raw material being planted and studied extensively. The two systems employed a column set of DB-5×BP-20. DB-5, a non polar column, was chosen as the first column separating the monoterpene hydrocarbon region and a similar region at higher first dimensional retention time comprising the sesquiterpene hydrocarbons which played an important role in the aroma of the vetiver essential oils. All components were separated and demonstrated in first dimensional plane. Unfortunately, the oxygenated derivatives of both of these groups were generally found to elute closely after the main group in the first dimension. However, owing to their wide range of component polarity, they were found to spread throughout a wider region of the second dimensional plane by using a BP-20 polar column. The comprehensive GCΔGC contour plots shown in Figure

3.1A and 3.1B exhibit volatile constituents in the crude essential oil and in its highly volatile fraction obtained by GCΔGC and SPME-GCΔGC, respectively. The peaks appeared in these GCΔGC and SPME-GCΔGC profiles revealed at least 156 and 48 volatile constituents, respectively. The profiles of GCΔGC obtained by direct injection of the vetiver essential oil revealed the overall of components comprising light and high molecular weight sesquiterpenes while the profile of SPME-GCΔGC was richer in light sesquiterpenes of which some components obtained in SPME-GCΔGC profiles were tentatively recognized as the key odor volatiles of vetiver oil. The results in this experiment indicated that SPME is a selective and highly efficient extraction device for low molecular weight sesquiterpenes, which included the key odors of the vetiver essential oils.

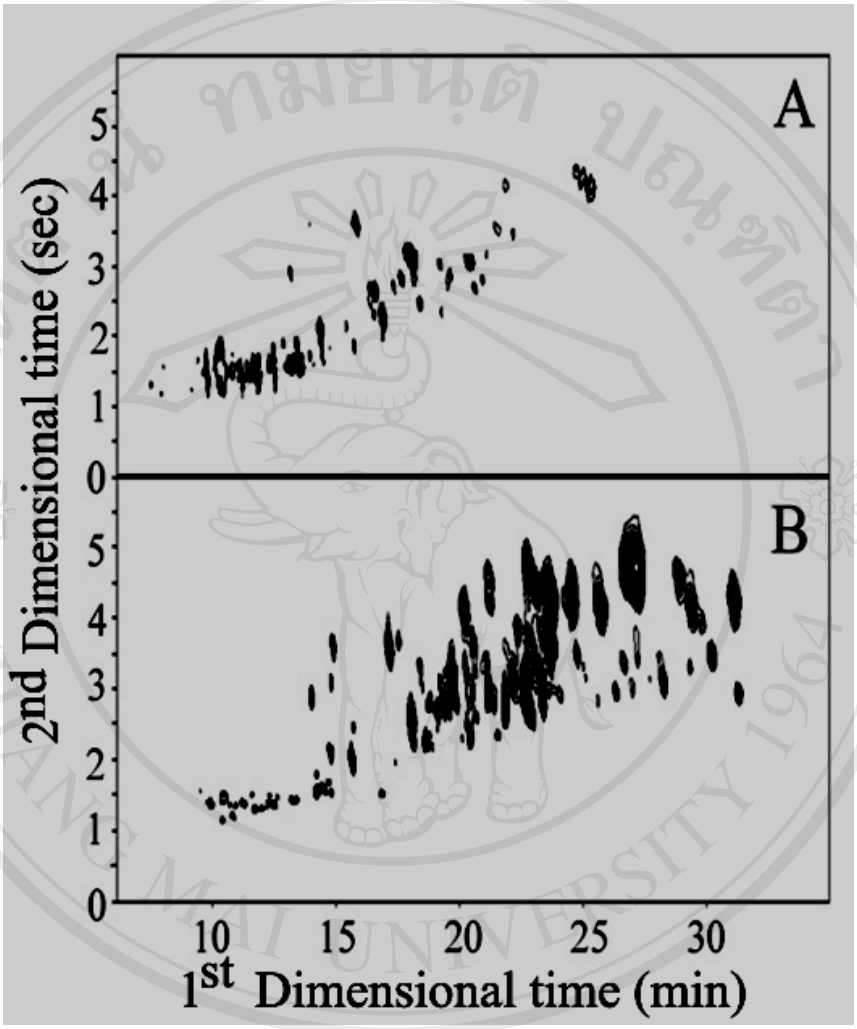


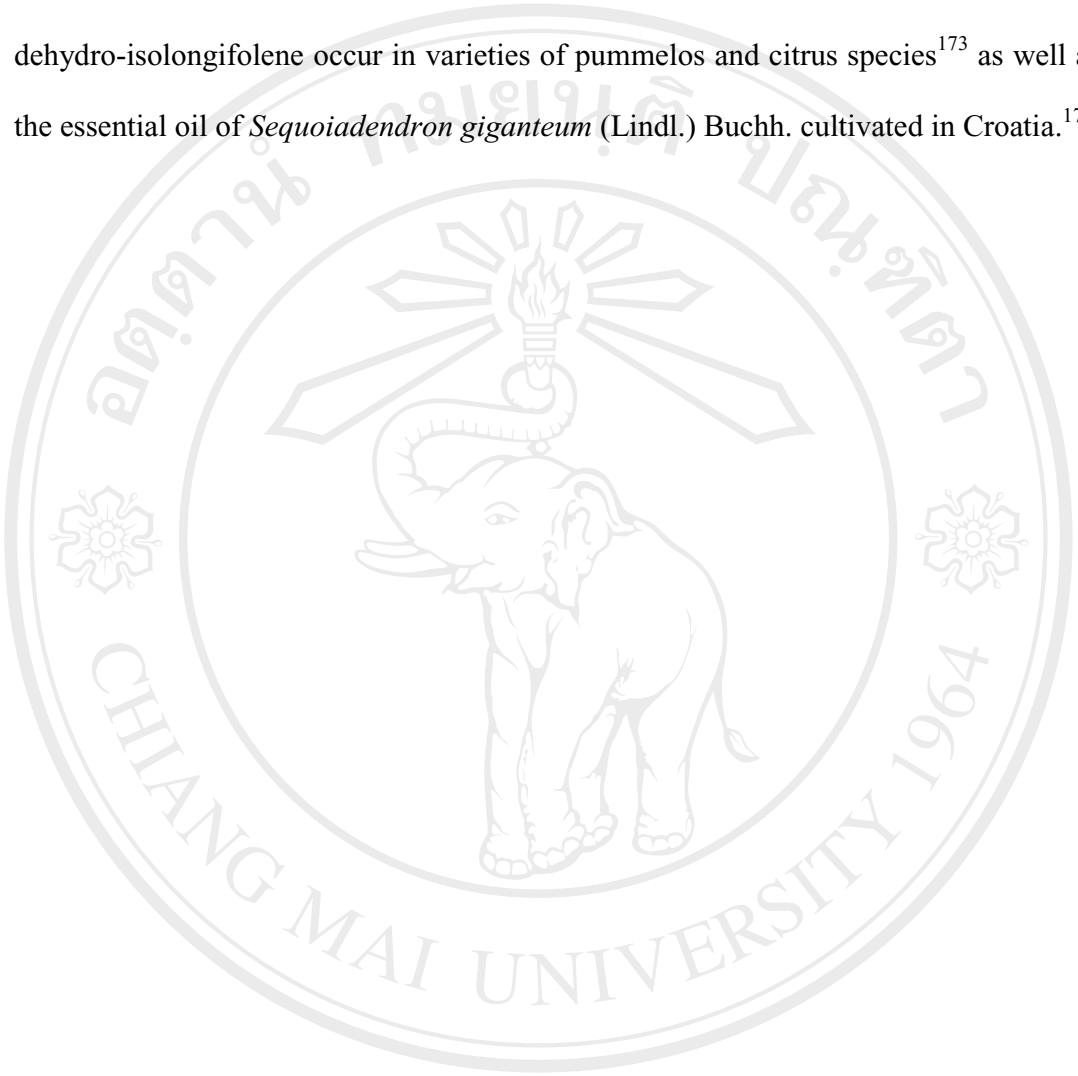
Figure 3.1 The contour plots of volatile component profiles of vetiver essential oils obtained from normal soil cultivation using A. SPME-GCΔGC and B. GCΔGC

3.1.3 SPME-GC-MS analysis

All SPME-GC-MS chromatograms and the identified volatile components, as well as their relative peak area percents, are shown in Figure 3.2 and Table 3.1, respectively. Apart from the mass spectral comparison with the mass spectral library software, the volatile components were identified by comparing their Kovát indices with those reported data.[22,25,29,30]

Thirty-seven volatiles in the oil obtained by vetiver cultivated in normal soil were identified. Among these components, (Z)-9,10-dehydro-2-norzizaene (20.78%), khusimone (20.57%) and khusimol (11.11%) were the majority. For the oil obtained from vetiver cultivated in normal soil with added microbes, 39 volatile components were observed, with only (Z)-9,10-dehydro-2-norzizaene (46.03%) predominant. In addition, sesquicineole and delta-cadinene were detected only in the oil derived from vetiver cultivated in normal soil with added microbes, which probably resulted from an unidentified biotic factor.[30] However, Weyerstahl and co-workers reported the presence of sesquicineole and δ-cadinene in vetiver oil derived from vetiver cultivated in normal soil.[25] But in our study, these components were not present in the oil derived from vetiver cultivated in normal soil or they were present at concentration below the detection limits of our techniques. It is remarkable that three volatile components, (+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one, cadina-1(10),6,8-triene, and 9,10-dehydro-isolongifolene were identified in essential oil of vetiver root for the first time in this report. The compound (+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one is a isomer of 2(3H)-naphthalenone constituents and it has been found to contribute to the

distinctive flavor of grapefruit and citrus paradise.[172] Cadina-1(10),6,8-triene and 9,10-dehydro-isolongifolene occur in varieties of pummelos and citrus species[173] as well as in the essential oil of *Sequoiadendron giganteum* (Lindl.) Buchh. cultivated in Croatia.[174]



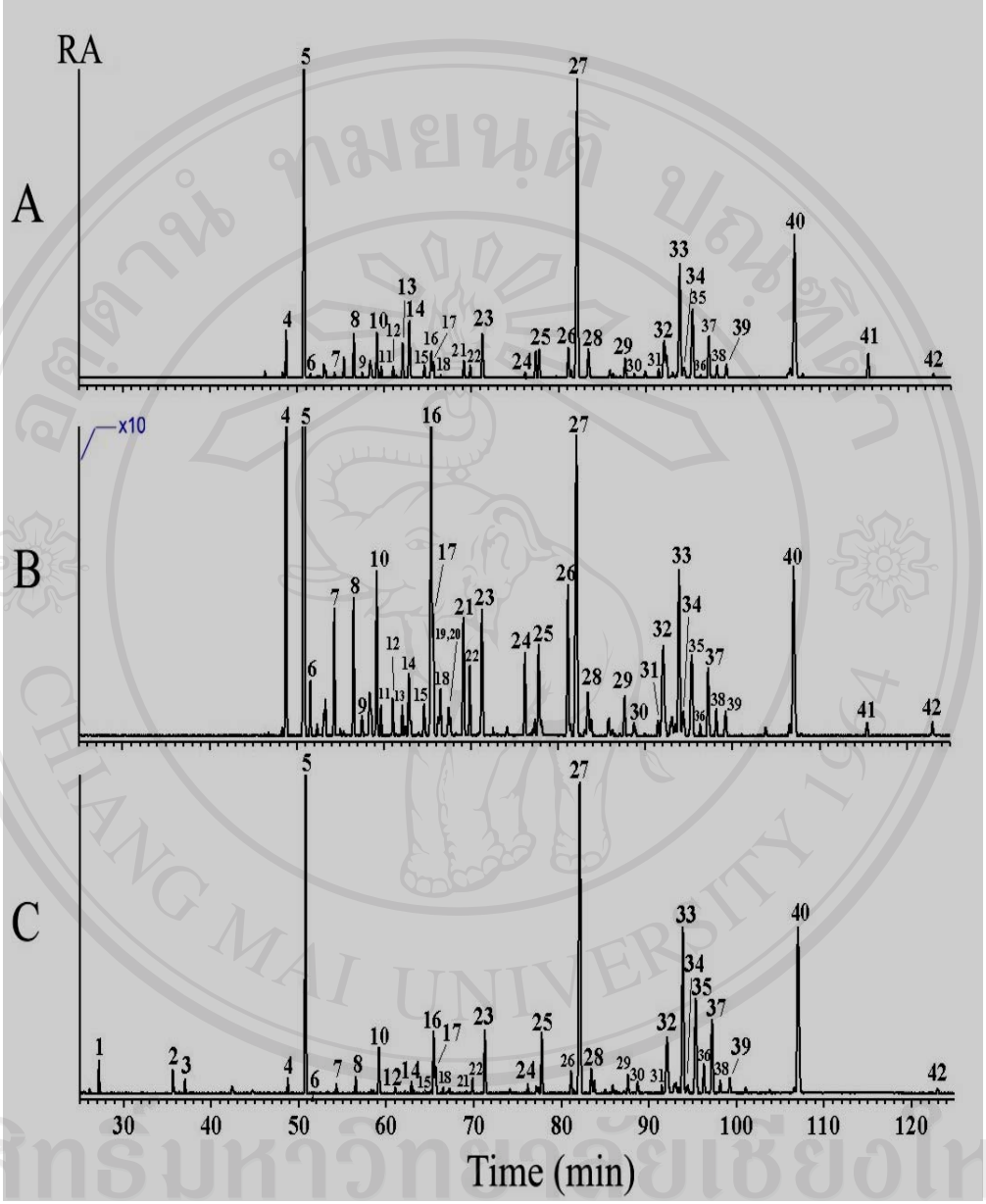


Figure 3.2 SPME-GC-MS chromatograms of vetiver essential oils obtained from root cultivated in three different systems. A. normal soil B. normal soil with added microbes C. semi-hydroponic system.

Table 3.1 Structural assignment and relative peak area percent of the volatile components in essential oils obtained from root of vertiver grass cultivated in three different systems

No.[a]	*KI*[b]	Structural Assignment[c]	Reference[d]	Average relative peak area (%) ± SD		
				Normal soil	Normal soil with added microbes	Semi-hydroponic
1	1294	1-nonanal[1,3]	179			1.06 ± 0.01
2	1345	nonanoic acid[1,3]	180			0.99 ± 0.01
3	1352	1-decanal[1,3]	181			0.45 ± 0.02
4	1393	(*E*)-9,10-dehydro-2-norzizaene[1]	182	1.87 ± 0.06	5.30 ± 0.01	0.46 ± 0.01
5	1405	(*Z*)-9,10-dehydro-2-norzizaene[1]	182	20.78 ± 0.05	46.03 ± 0.02	14.71 ± 0.02
6	1406	alpha-funebrene[1,2,3]	25	0.14 ± 0.02	0.60 ± 0.02	0.02 ± 0.01
7	1417	2-norzizaene[1]	25	0.20 ± 0.02	1.56 ± 0.03	0.29 ± 0.01
8	1425	acora-2,4-diene[1]	25	1.93 ± 0.02	1.73 ± 0.02	0.65 ± 0.01
9	1430	alpha-cedrene[1]	25	0.19 ± 0.01	0.28 ± 0.02	

Table 3.1 (continued)

No.[a]	*KI*[b]	Structural Assignment[c]	Reference[d]	Average relative peak area (%) ± SD		
				Normal soil	Normal soil with added microbes	Semi-hydroponic
10	1436	cascarilladiene[1]	25	2.16 ± 0.04	2.27 ± 0.04	2.04 ± 0.01
11	1442	11,12,13-tri-*nor*-eremophil-1(10)-en-7-one[1]	25	0.43 ± 0.02	0.34 ± 0.02	
12	1451	gamma-elemene[1,2]	25	0.48 ± 0.02	0.47 ± 0.02	0.18 ± 0.01
13	1459	prezizaene[1,2]	25	1.55 ± 0.03	0.35 ± 0.01	
14	1462	khusimene[1,2]	25	3.04 ± 0.39	0.89 ± 0.02	0.42 ± 0.02
15	1468	*ar*-curcumene[1,2]	25	0.60 ± 0.01	0.44 ± 0.01	0.09 ± 0.01
16	1471	4,7-epoxy-spirovetiva-2,11-diene[1]	25	1.35 ± 0.04	5.59 ± 0.02	2.94 ± 0.02
17	1474	alpha-amorphene[1,2]	25	0.76 ± 0.01	1.47 ± 0.01	1.30 ± 0.01
18	1490	*cis*-eudesma-6,11-diene[1,2]	25	0.07 ± 0.02	0.65 ± 0.02	0.14 ± 0.01
19	1502	sesquicineole[1]	25		0.34 ± 0.03	

Table 3.1 (continued)

No.[a]	*KI*[b]	Structural Assignment[c]	Reference[d]	Average relative peak area (%) ± SD		
				Normal soil	Normal soil with added microbes	Semi-hydroponic
20	1508	delta-cadinene[1,2]	25		0.22 ± 0.01	
21	1518	gamma-vetivenene[1,2]	25	0.83 ± 0.13	1.83 ± 0.01	0.07 ± 0.01
22	1538	(+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one[1]	25	0.56 ± 0.02	0.95 ± 0.05	0.55 ± 0.02
23	1550	dimethylbicyclo[4.4.0]dec-1-en-3-one[1]	183	2.44 ± 0.02	2.00 ± 0.09	3.21 ± 0.01
24	1566	beta-calacorene[1,2]	25	0.22 ± 0.01	1.18 ± 0.01	0.30 ± 0.01
25	1574	15-*nor*-funebran-3-one[1]	25	1.45 ± 0.02	1.46 ± 0.01	2.91 ± 0.01
26	1579	*cis*-eudesm-6-en-11-ol[1]	25	1.58 ± 0.04	2.37 ± 0.01	1.09 ± 0.03
27	1598	khusimone[1,2]	25	20.57 ± 0.01	6.13 ± 0.07	20.91 ± 0.01
28	1602	13-*nor*-*cis*-eudesm-6-en-11-one[1]	25	1.80 ± 0.02	0.66 ± 0.02	1.35 ± 0.01

Table 3.1 (continued)

No.[a]	*KI*[b]	Structural Assignment[c]	Reference[d]	Average relative peak area (%) ± SD		
				Normal soil	Normal soil with added microbes	Semi-hydroponic
29	1612	*trans*-dracunculifoliol[1]	25	1.07 ± 0.02	0.63 ± 0.02	0.77 ± 0.01
30	1618	13-*nor*-eremophila-1(10)-en-11-one[1]	25	0.18 ± 0.02	0.21 ± 0.02	0.55 ± 0.01
31	1638	eudesm-4(15),7-dien- -ol[1]	25	0.43 ± 0.02	0.22 ± 0.02	0.27 ± 0.01
32	1644	beta-eudesmol[1,2]	25	2.61 ± 0.02	2.37 ± 0.02	4.48 ± 0.01
33	1651	(*E*)-opposita-4(15),7(11)-dien-12-al[1]	25	7.71 ± 0.02	3.00 ± 0.06	10.55 ± 0.01
34	1660	prezizaan-15-al[1]	25	0.67 ± 0.01	0.41 ± 0.02	0.51 ± 0.03
35	1665	2-epi-ziza-6(13)-en-3 -ol[1]	25	5.31 ± 0.02	1.83 ± 0.03	6.85 ± 0.16
36	1671	zizanal[1,2]	25	0.09 ± 0.01	0.12 ± 0.01	1.40 ± 0.01
37	1687	khusian-2-ol[1]	25	2.74 ± 0.02	1.24 ± 0.01	4.65 ± 0.01
38	1690	(*E*)-opposita-4(15),7(11)-dien-12-ol[1]	25	0.59 ± 0.02	0.41 ± 0.02	0.56 ± 0.01

Table 3.1 (continued)

No.[a]	*KI* [b]	Structural Assignment[c]	Reference[d]	Average relative peak area (%) ± SD		
				Normal soil	Normal soil with added microbes	Semi-hydroponic
39	1694	cadina-1(10),6,8-triene[1]	25	0.83 ± 0.03	0.43 ± 0.02	0.79 ± 0.01
40	1762	khusimol[1,2]	25	11.11 ± 0.05	3.55 ± 0.04	12.21 ± 0.02
41	1798	9,10-dehydro-isolongifolene[1]	184	1.43 ± 0.01	0.19 ± 0.01	
42	1804	nootkatone[1,2,3]	25	0.21 ± 0.02	0.21 ± 0.01	0.31 ± 0.01
total number of volatile components				**37**	**39**	**36**

[a] Identification: 1, mass spectrum; 2, Kovát indices; 3, standard compound. [b] Kovát indices on DB-5 column. [c] Compounds in Figure 3.2.

[d] Reference having same mass spectrum

Thirty-six volatiles were detected in the oil obtained from semi-hydroponically cultivated vetiver root. Khusimone (20.91%), (Z)-9,10-dehydro-2-norzizaene (14.71%), khusimol (12.21%), and (E)-opposita-4(15),7(11)-dien-12-al (10.55%) were present as the major odors. In comparison with those obtained from various soil cultivations, the odor volatile profile was similar to that cultivated in normal soil but strikingly different from that cultivated in normal soil with added microbes. Additionally, two low molecular weight aldehydes, 1-nonanal and decanal, and one fatty acid, nonanoic acid, were observed and present in trace amounts. These aldehydes have never been observed in the vetiver oil compositions reported in early studies. It was also suggested that these components have a limited effect on aroma character of the vetiver oil. On the other hand, six volatile components, alpha-cedrene, 11,12,13-tri-nor-eremophil-1(10)-en-7-one, prezizaene, sesquicineole, delta-cadinene, and 9,10-dehydro-isolongifolene, were absent from the oil of vetiver root samples obtained using semi-hydroponic cultivation. Although the semi-hydroponic cultivation has several advantages, such as being simple to plant and requiring a small space and budget, this system yielded vetiver root with a much lower percentage yield of essential oil than those obtained by the other cultivation systems.

3.2 Comparative study on volatile constituents of Thai vetiver root essential oils subjected to different extraction methods and analyzed by comprehensive two-dimensional gas chromatography-mass spectrometry

3.2.1 Comparison of extraction techniques

The percentage yields (w/w) of vetiver root oil obtained by different extraction methods are summarized in Table 3.2. In SFE, MAE and SE, three solvents with different polarity, toluene, dichloromethane, and methanol, were utilized in order to extend the extraction efficiency of each technique. The general aim was to obtain the highest yield of the essential oil. SE was found to provide the highest yields of vetiver root oil, followed by MAE, SFE and SDE, respectively, although some of lists may not be pure essential oil. Colors of the oils varied from yellow to dark brown. All vetiver root extracts obtained are shown in Figure 3.3. The dark brown color was observed mostly in the oils obtained from SE and MAE technique. The higher yield was achieved with the oils having dark color. This can be explained by the presence of increasing amounts of nonvolatile compounds in the extract. In contrast, the color of the oils obtained by SFE using toluene or dichloromethane as modifier was rather similar to those extracted by SDE, being light yellow-orange in color. The absence of nonvolatile or high molecular weight components such as fatty acids and waxes in these oils was probably due to the lower extraction temperature used. The result from aroma evaluation test of vetiver oil samples revealed the same aroma description between the oils extracted by SFE with toluene or dichloromethane, and those obtained by SDE. However, the SFE technique was much faster and provided

approximately three times the amount of oil yield than those obtained by SDE. Therefore, SFE with toluene or dichloromethane should be an alternative way to obtain vetiver root oils suitable for perfumery and fragrance uses.

Table 3.2 Percentage yield of vetiver root oil obtained by different extraction methods

Method	Solvent	Extraction time	Yield (%) ∂ SD
SDE	dichloromethane	24 h	1.04 ± 0.05
SFE	dichloromethane	15 min	3.15 ± 0.03
	toluene	10 min	3.23 ± 0.04
	methanol	30 min	3.42 ± 0.03
MAE	dichloromethane	20 min	3.45 ± .021
	toluene	25 min	5.53 ± 0.45
	methanol	15 min	6.06 ± 0.05
SE	dichloromethane	24 h	6.50 ± 0.08
	toluene	24 h	7.09 ± 0.02
	methanol	24 h	13.30 ± 0.04

1 2 3 4 5 6 7 8 9 10

Figure 3.3 Vetiver root extracts obtained from three different extraction methods; vial No. 1-3 obtained by SE with toluene, dichloromethane and methanol, respectively, vial No. 4-6 obtained from MAE with toluene, methanol and dichloromethane, respectively, vial 7-9 obtained by SFE with methanol, dichloromethane and toluene, respectively, and vial No. 10 obtained by SDE.

3.2.2 Selection of GCΔGC-FID and GCΔGC-qMS column set and conditions

In general, GCΔGC systems consist of non-polar and polar phase columns in first and second dimensions, respectively. This arrangement is commonly applied for separation of the components in most essential oils. In this study, apart from this conventional combination (BPX5×BP20), an inverse phase combination (Solgel wax×BP1) and a combination applying an enantioselective first dimension column (EtTBS-ηCD×BP20) were also investigated. The vetiver root essential oil obtained by SDE was used for optimization of the GCΔGC conditions for all column sets. The resulting GCΔGC-FID contour plots obtained by the three column sets are shown in Figure 3.4.

The component separations in the first column of the column set 1 and 3 were based primarily on boiling point with the latter offering additional enantioselective selectivity. The enantioselective column has a cyclodextrin derivative dispersed in a polymer phase of 14% cyanopropylphenyl-86% methylpolysiloxane, and so this is slightly more polar than the BPX5 phase. The separation in 1st-dimension (1D) space of column set 3 was similar to that obtained from column set 1 although polarity of column was increased. It can be noted that most components were separated under the mechanism controlled by boiling point rather than polarity. However, polarity separation mechanism will dominate in the second dimension of both column sets. It may therefore be expected that the two GCΔGC contour plots for column set 1 and 3 should have similar presentation of components in the 2nd-dimension (2D) space (Figure 3.4A and 3.4C, respectively) and this seems to be borne out. However, better

resolution leading to an increased number of resolved components was observed by the use of column set 1 compared to column set 3. Although an enantioselective column is a good choice for separation of essential oil isomeric components, ready observation of enantiomers will be partly obscured due to the high complexity of the vetiver oil constituents (and the possible large ratio difference between the enantiomers). The separation using the polar/non-polar column set, shown in Figure 3.4B**,** contains broadened peaks, probably due to longer 2D retention times in the second dimension as a relatively thick stationary phase was chosen for the second column. Component wrap-around also appears to be substantial, and the tailing of some components is also observed which adversely affects quantitative and qualitative results. Thus, column set 1, with non-polar and polar phase was selected for further use in quantification studies

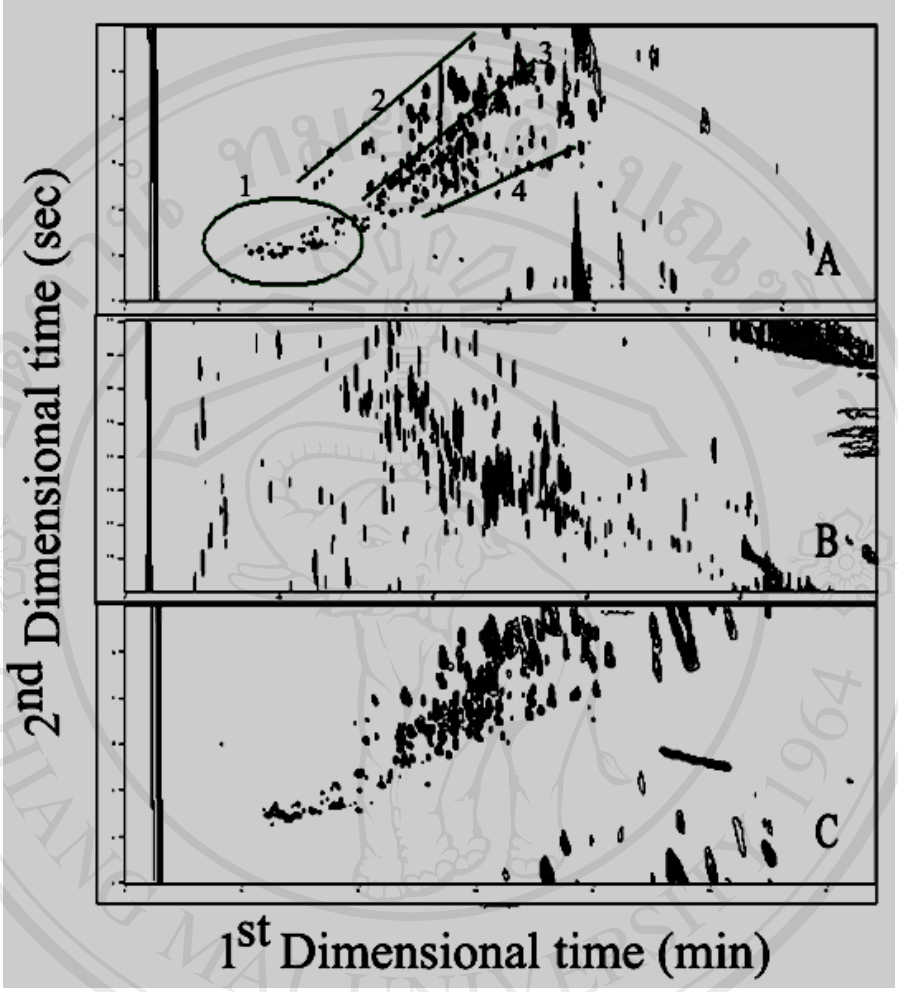


Figure 3.4 GCΔGC-FID contour plots obtained by the three column sets A. BPX-5×BP-20 B. Solgel wax×BP-1 C. EtTBS-ηCD×BP20

3.2.3 Separation and identification of volatile components in vetiver root oils by GC-MS and GC×GC-qMS

Identification of volatile constituents in the vetiver root oils was performed using GC-MS and GCΔGC-qMS. Apart from a minor difference in the column set, the same chromatographic conditions were applied for both GC-MS and GCΔGC-qMS operation. It is noted that peak identification of volatile constituents was mainly based on mass spectral data comparison with database libraries including Adams 2001, NIST 98, and Wiley 275. The linear temperature program retention indices (LTPRI) data which were calculated from retention times on the first column was also utilized. Some sample spectra were compared with the literature reference data in the references, in which their structural information were present.[22,25,29,30] The similar GC-MS chromatograms were found in all vetiver root oils obtained from all extraction methods as shown in Figure 3.5. The results obtained by GC-MS showed the separation of at least 95 components in all vetiver oil samples but only 64 components were tentatively identified through reasonable LTPRI and spectral data. Identification of the oil components by GC-MS was especially difficult due to the complex nature of vetiver root oils that contain many isomeric compounds. These compounds are often closely eluted and provide similar mass fragmentation patterns, which compromise the mass spectral matching protocol. Thus, most of the component identifications were achieved and confirmed by the GCΔGC-MS experiment where many co-eluted peaks from 1D-GC could be entirely resolved on the ^{2}D column. As a result, 43 more constituents were additionally identified by using GCΔGC-MS. Among the three column sets, a 2D contour plot obtained by GCΔGC

analysis using the non-polar/polar column combination showed the best resolution in the first dimension. Many components were well resolved throughout the 2D plane, and some minor components, which were unapparent in the first column, were spread out within the 2D separation plane. All identified components obtained by GC-MS and GC×GC-qMS are shown in Table 3.3 and 3.4, respectively. An increase in sensitivity and resolution in GCΔGC-qMS resulted generally in higher and more precise match qualities of mass spectra than those obtained with GC-MS. In addition, the modulated peaks obtained from the individual components in GCΔGC-qMS provided a number of deconvolution by the separation of the peaks on the ^{2}D column, which facilitated more accurate identification results. The GC×GC-qMS analysis revealed at least 245 components found in all vetiver oil samples. Among them, 107 components were tentatively identified. All GC×GC contour plots of all extracts are demonstrated in Figure 3.6. In addition, peak assignment of components in the vetiver root oil obtained from SDE method were labeled in GC×GC-qMS contour plots shown in Figure 3.7. A typical analysis of vetiver oils obtained by different extraction methods indicated that sesquiterpenes and its derivatives were found to be the major components of vetiver oil. An existence of a group-type separation of some major components is shown in Figure 3.4A. Components identified as sesquiterpenes having a molecular weight of 204 were found in region 1. In addition, sesquiterpenols, sesquiterpenones and sesquiterpenes having molecular weights of 220, 218, and 222 were found approximately aligned along the lines 2, 3, and 4, respectively. Most of the identified components were also identified in the report of Weyerstahl et al.[25] The chemical profiles of all vetiver oils were almost the same, which showed the predominant component of khusinic acid in a large amount, followed by khusimol,

khusimone, and nootkatone, respectively. Vetiver oil obtained by SDE gave a more distinct pattern of the compositional content as compared to that obtained by the other extraction methods, namely, SFE, MAE, and SE, which yielded similar patterns. Some components, such as 9,10-dehydro-2-norzizaene, -copaene, and trans-calamenene, were found in the oil obtained by SDE with much higher contents than those found in other techniques. However, some non-terpenoid components were also identified in trace amounts such as 2,3-dihydrobenzofuran, 1,2,3,4,5,6-hexahydro-1-methyl-2,2'-bipyridine, tris(1-methylethyl)-benzene, and 7,8-dihydro-8,8-dimethyl-5(6H)-benzocyclooctenone.

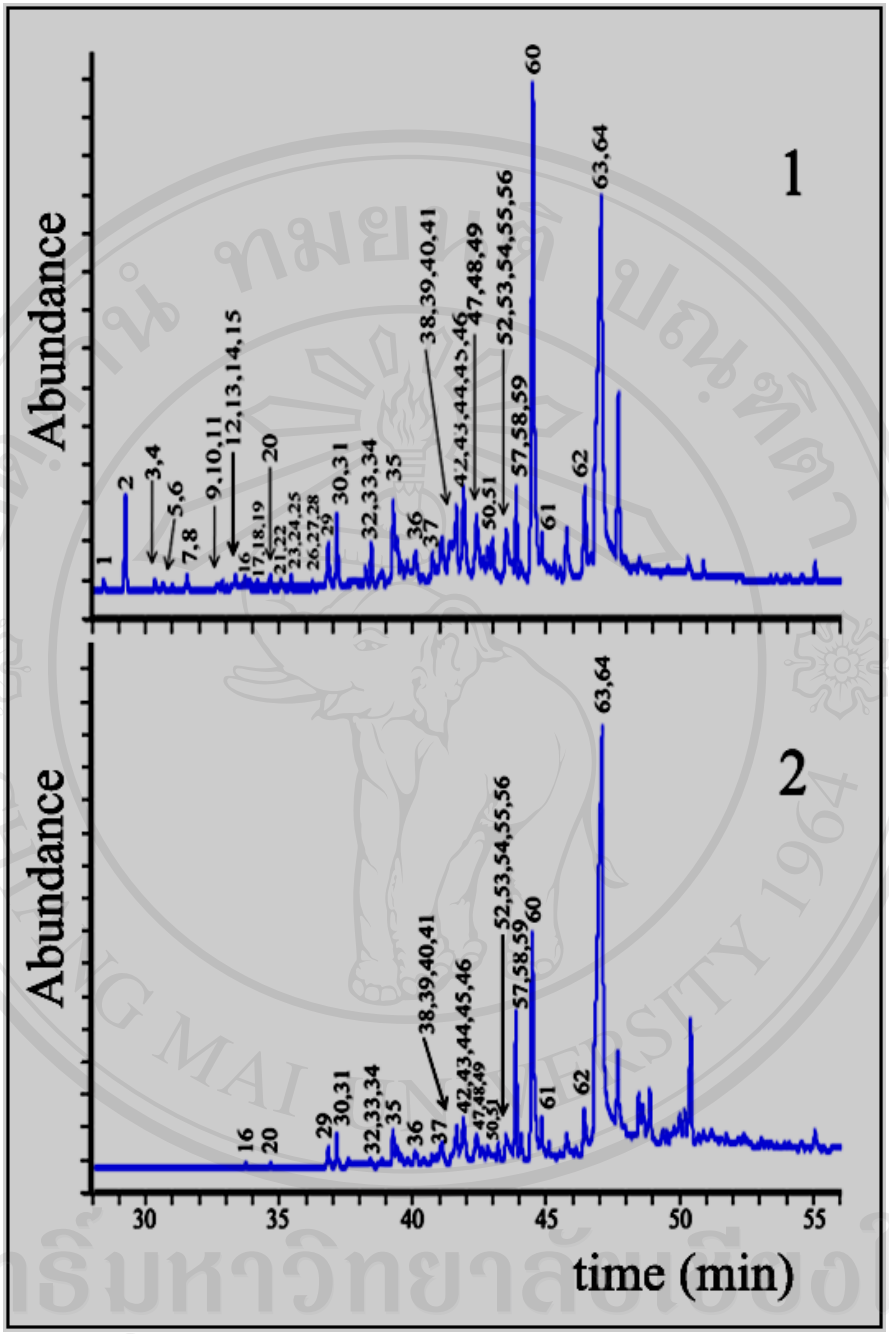


Figure 3.5 GC-MS chromatograms of vetiver root essential oils obtained from 1. SDE 24 hrs and 2. SFE with DCM

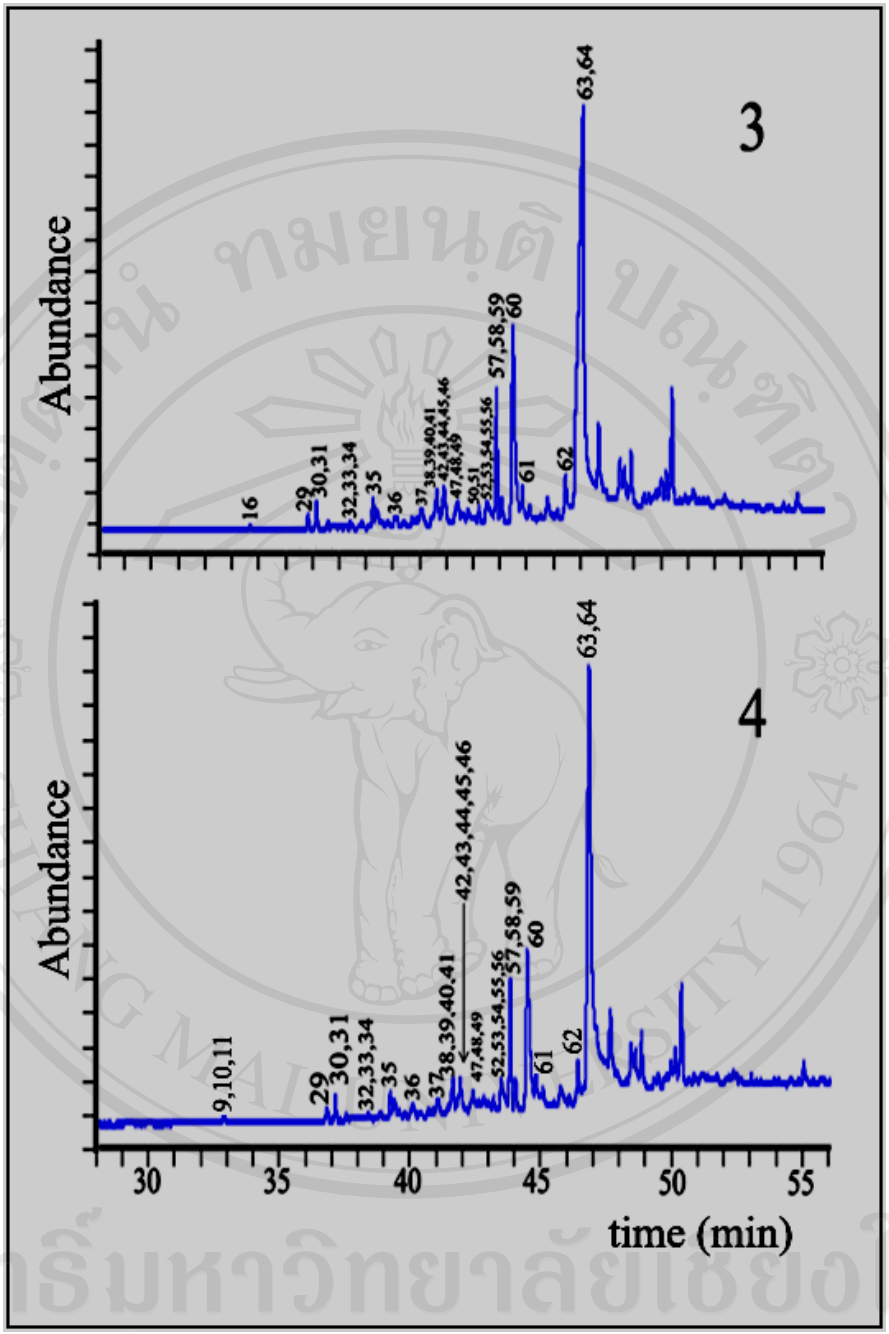


Figure 3.5 (continued) GC-MS chromatograms of vetiver root essential oils obtained from 3. SFE with methanol and 4. SFE with toluene

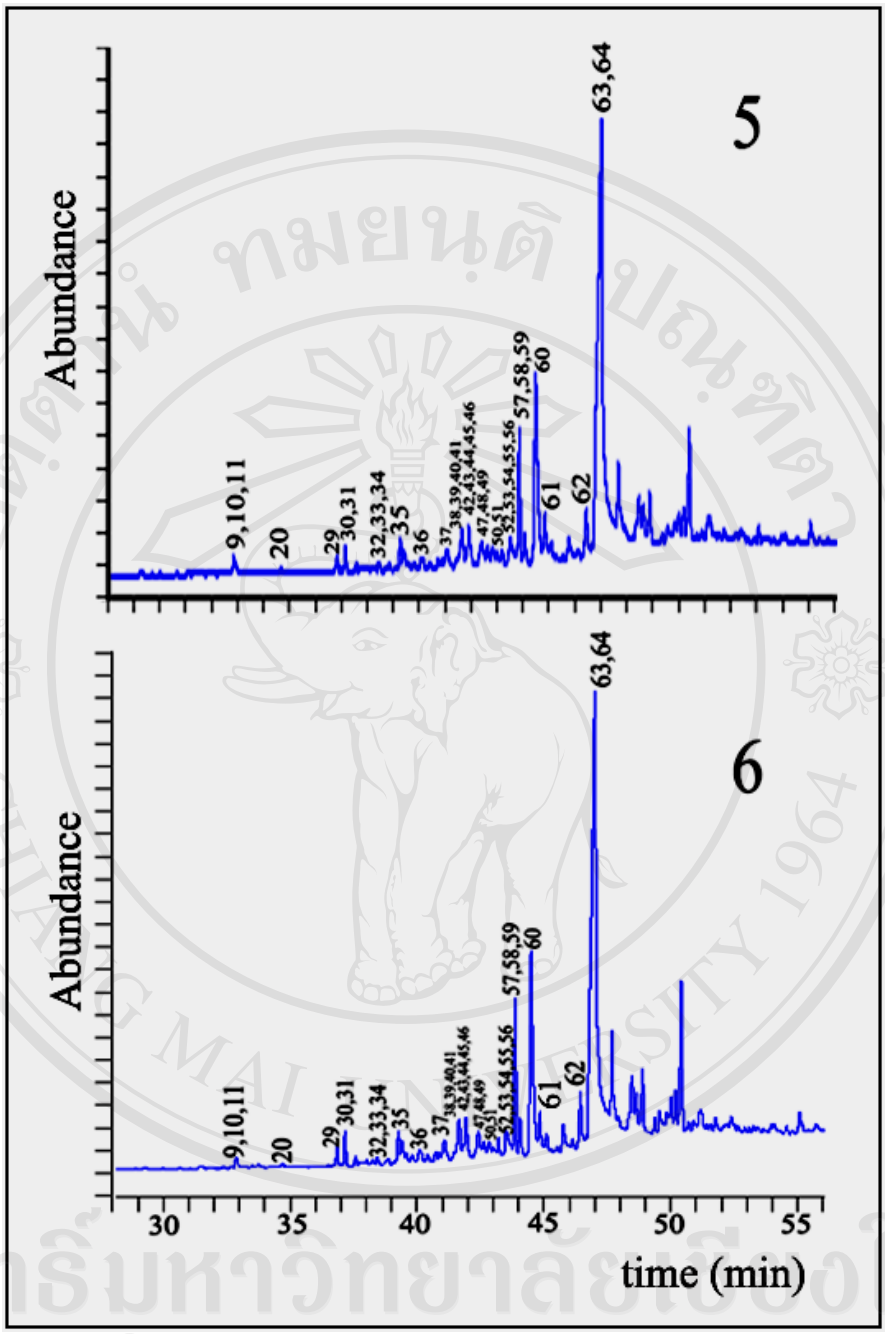


Figure 3.5 (continued) GC-MS chromatograms of vetiver root essential oils obtained from 5. soxhlet with methanol and 6. soxhlet with toluene

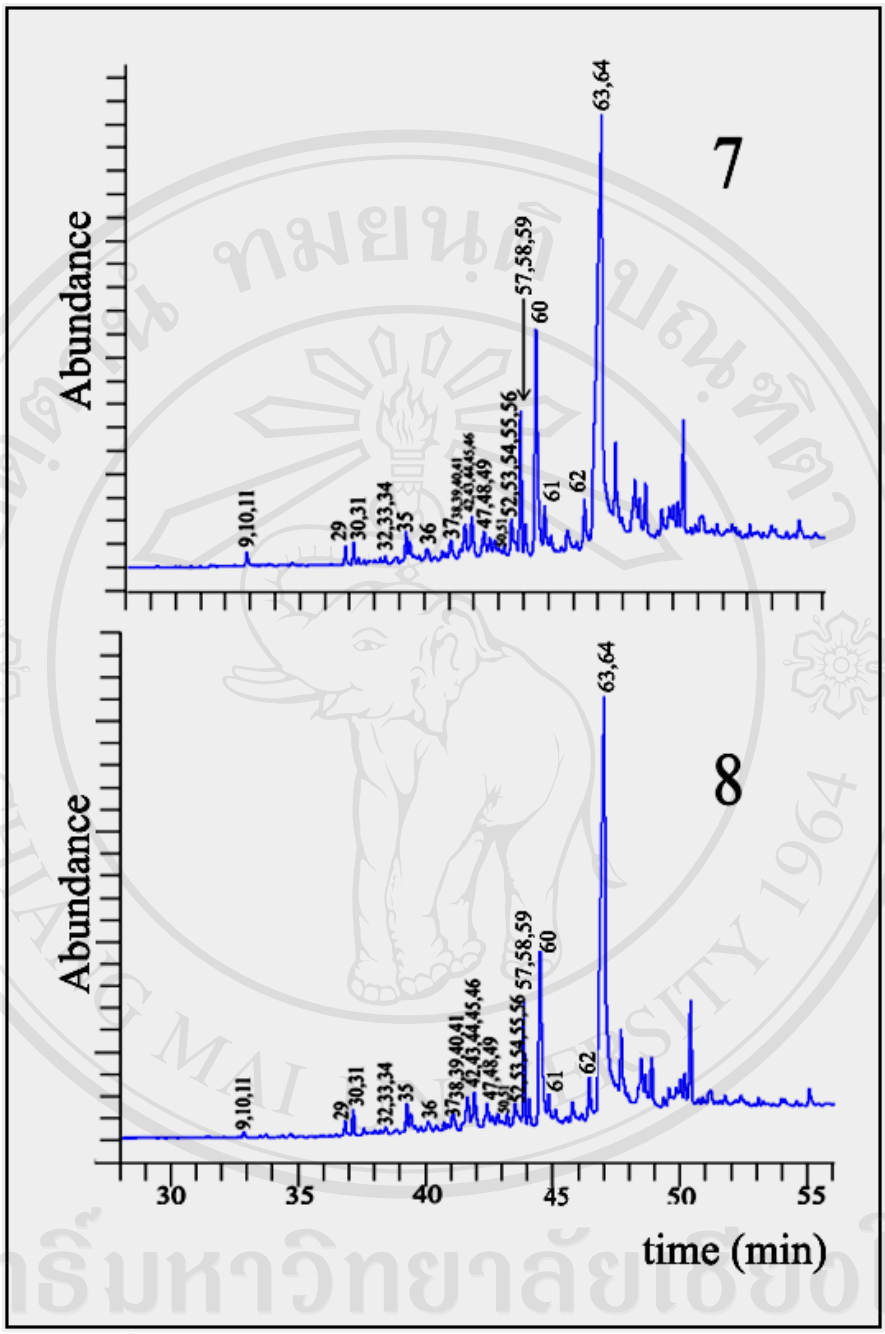


Figure 3.5 (continued) GC-MS chromatograms of vetiver root essential oils obtained from 7. soxhlet with DCM and 8. microwave with toluene

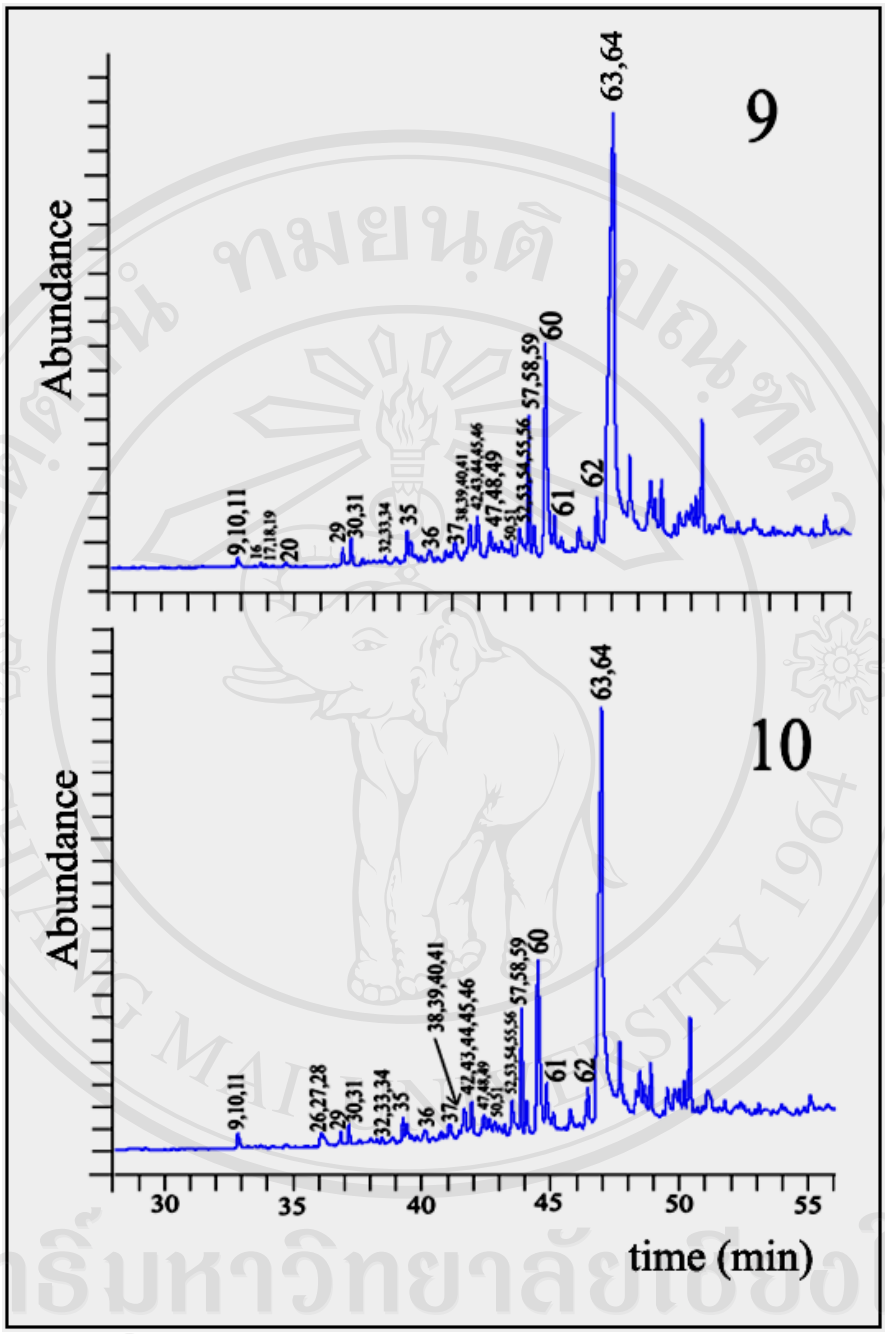


Figure 3.5 (continued) GC-MS chromatograms of vetiver root essential oils obtained from 9. microwave with DCM and 10. microwave with methanol

Table 3.3 Structural assignment and electron impact (EI) mass spectra of vetiver root essential oils obtained from all extraction methods and analyzed by GC-MS

No.	Structural assignment	m/z (%RA)	MW	Extraction Method								
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
1	9,10-dehydro-2 -norzizaene	41(38), 53(24), 67(32), 77(56), **91(100)**, 105(34), 118(84), 131(38), 145(86), 159(17), 173(75), 188(60)	188	*									
2	alpha-funebrene	43(19), 55(44), **69(100)**, 79(36), 93(64), 105(40), 120(38), 133(40), 147(17), 161(73), 189(16), 204(18)	204	*									
3	2-norzizaene	41(25), 55(18), 67(28), 79(60), 91(64), 105(40), **120(100)**, 133(26), 147(42), 162(18), 175(27), 190(21)	190	*									
4	7,8-dihydro-8,8-dimethyl-5(6H)-benzocyclooctenone	115(58), 127(34), **129(100)**, 143(55), 157(74), 172(66), 185(40), 200(58)	200	*									
5	(R)- 1,5,5,9-tetramethylSpiro[5.5] undeca-1,8-diene	27(16), 41(18), 53(10), 67(9), 79(22), 93(65), 107(59), 121(95), **136(100)**, 161(15), 189(13), 204(24)	204	*									
6	alpha-cedrene	41(24), 55(18), 69(22), 77(19), 93(45), 105(35), **119(100)**, 136(15), 147(19), 161(26), 175(8), 189(12), 204(26)	204	*									
7	beta-copaene	41(38), 55(22), 69(20), 81(38), 93(57), 105(94), **119(100)**, 136(18), 147(12), 161(18), 175(7), 189)12), 204(38)	204	*									

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method								
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
8	gamma-elemene	41(60), 55(40), 93(75), 1o7(50), **121(100)**, 136(20), 147(15), 161(20), 189(10), 204(10)	204	*									
9	prezizaene	41(18), 55(21), 69(17), 81(30), 91(41), 108(40), 119(46), **133(100)**, 147(28), 161(30), 175(18), 189(42), 204(23)	204	*			*	*	*	*	*	*	*
10	dehydroaromadendrene	41(62), 55(20), 67(23), 77(22), 91(48), 105(50), 117(37), 131(40), 145(43), **159(100)**, 173(10), 187(24), 202(41)	202	*			*	*	*	*	*	*	*
11	khusimene	41(60), 56(50), 67(40), 77(40), 91(60), 105(50), 119(55), **134(100)**, 161(20), 189(38), 204(20)	204	*			*	*	*	*	*	*	*
12	ar-curcumene	27(20), 41(50), 55(20), 69(20), 91(50), 105(60), **119(100)**, 132(90), 145(30), 159(10), 189910), 202(20)	202	*									
13	alpha-amorphene	41(40), 55(20), 79(40), 91(60), 105(78), 119(63), 133(46), 148(17), **161(100)**, 176(10), 189(15), 204(39)	204	*									

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method								
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
14	cyclocopacamphan-12-al	67(35), 79(51), 105(75), 118(32), 121(31), 133(27), 145(84), 159(22), **160(100)**, 161(33), 203(4), 218(23)	218	*									
15	delta-silenene	55(18), 69(20), 77(15), 93(43), 105(32), **119(100)**, 136(15), 147(17), 161(23), 175(9), 189(14), 204(24)	204	*									
16	gamma-amorphene	41(28), 55(18), 69(17), 81(26), 94(66), **105(100)**, 119(32), 133(20), 147(15), 161(55), 189(18), 204(38)	204	*	*	*						*	
17	delta-amorphene	27(38), 41(70), 55(28), 69(38), 79(65), 91(68), 105(70), 119(68), 133(43), **161(100)**, 204(34)	204	*								*	
18	11,12,13-tri-nor-cis-eudesma-5,8-dien-7-one	51(26), 55(31), 65(26), 77(41), 79(29), **91(100)**, 92(32), 105(79), 119(25), 120(33), 121(94), 133(84), 134(27), 147(25), 161(38), 176(57)	176	*								*	
19	8-isopropenyl-3,3,7-trimethylbicyclo[5.1.0] oct-5-en-2-one	41(48), 55(24), 69(24), 77(28), 91(60), 105(92), **119(100)**, 134(90), 149(22), 161(38), 176(18), 189(15), 204(34)	204	*								*	

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method								
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
20	gamma-vetivenene	53(21), 67(20), 77(40), 91(70), **103(100)**, 117(44), 131(66), 145(84), 159(86), 187(57), 202(90)	202	*	*			*	*			*	
21	trans-calamenene	41(18), 53(8), 65(9), 77(12), 91(14), 105(15), 115(13), 129(16), 144(13), **159(100)**, 202(20)	202	*									
22	1a,2,6,7,7a,7b-hexahydro-1,1,7,7a-tetramethyl-1H-cyclopropa[a]naphthalene	41(94), 53(26), 65(22), 77(42), 91(66), 105(60), 117(53), 131(64), 145(63), 159(66), 187(44), **202(100)**	202	*									
23	beta-calacorene	28(25), 41(10), 115(27), 128(18), 142(65), **157(100)**, 200(24)	218	*									
24	zingiberene	41(45), 69(58), 93(60), 105(20), 119(57), 133(55), 147(25), **161(100)**, 189(10), 204(80)	204	*									
25	6,12-epoxy-elema-1,3-diene	55(69), 69(52), 77(24), 81(100), 91(31), 95(30), 109(30), 137(20), 151(24), 163(17), 177(11), 205(23), 220(4)	220	*									

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
26	13-nor-eudesm-5 -en-11-one	55(10), 67(10), 77(6), 79(8), **81(100)**, 91(10), 93(25), 95(4), 105(6), 107(6), 119(2), 147(2), 163(10), 206(3)	206	*									*
27	elemol	**41(100)**, 55(58), 59(90), 66(70), 81(60), 93(64), 105(43), 120(45), 136(40), 147(38), 161(59), 189(30)	204	*									*
28	alpha-agarofuran	55(22), **82(100)**, 91(24), 105(24), 109(26), 123(36), 147(41), 187(22), 205(43), 220(83)	220	*									*
29	(+)(6S,10R)-6,10-dimethylbicyclo[4.4.0] dec-1-en-3-one	41(60), 79(55), 93(50), 109(52), 122(63), 136(78), 150(60), 163(38), **178(100)**	178	*	*	*	*	*	*	*	*	*	*
30	15-nor-prezizaan -7-one	55(27), 67(53), 79(46), 82(40), 93(50), 95(35), 107(75), 121(31), 135(93), 150(37), 177(16), 191(75), **206(100)**	206	*	*	*	*	*	*	*	*	*	*
31	cascarilladienol	55(23), 77(21), 93(35), 195(31), 107(29), 135(45), 145(55), 159(16), **177(100)**, 187(10), 205(8), 220(15)	220	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
32	12-nor-2,3-epoxy -ziza-6(13)-ene	55(24), 67(26), 77(40), 79(40), 105(52), 117(29), 121(31), 133(37), 143(31), **161(100)**, 189(52), 204(19)	204	*	*	*	*	*	*	*	*	*	*
33	cis-eudesm-6-en-11-ol	**59(100)**, 67(21), 81(24), 95(24), 108(30), 135(19), 164(60), 175(14), 189(21), 204(22), 222(18)	222	*	*	*	*	*	*	*	*	*	*
34	2-acetyl-5,6,7,8-tetrahydroquinoxaline	39(20), 43(71), 53(20), 79(40), 106(36), 119(20), **133(100)**, 148(42), 161(16), 176(84)	176	*	*	*	*	*	*	*	*	*	*
35	4-(2,2-dimethyl-6-methylenecyclohexylidene)-3-methylidene-2-one	29(18), 43(80), 55(38), 69(50), 79(36), 93(53), 107(81), 121(40), 133(22), 149(19), **163(100)**, 191(52), 206(18)	206	*	*	*	*	*	*	*	*	*	*
36	clovane	26(10), 43(44), 55(24), 67(20), 81(24), 95(30), 121(24), **135(100)**, 150(21), 163(25), 191(26), 206(20)	206	*	*	*	*	*	*	*	*	*	*
37	cyclocopacamphan -12-ol	53(16), 65(16), 77(40), **95(100)**, 119(82), 121(40), 145(31), 161(87), 189(29), 202(16), 205(8), 220(37)	220	*	*	*	*	*	*	*	*	*	*
38	khusimone	**41(100)**, 55(68), 67(50), 77(51), 91(74), 108(78), 119(64), 133(60), 145(22), 164(39), 173(24), 189(44), 204(62)	204	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
39	trans-dracunculifoliol	55(11), 67(11), 81(21), 93(24), 95(27), **109(100)**, 133(18), 135(26), 151(26), 161(19), 179(32), 189(31), 204(2), 222(8)	222	*	*	*	*	*	*	*	*	*	*
40	10-epi-cubenol-12-nor -ziza-6(13)-en- -ol	41(93), 59(64), 67(42), 81(56), 93(62), 105(65), **119(100)**, 135(22), 147(21), 161(94), 179(22), 189(25), 204(46)	204	*	*	*	*	*	*	*	*	*	*
41	12-nor-ziza-6(13) -en- -ol	55(59), 77(40), 79(55), **91(100)**, 93(36), 105(36), 109(34), 117(62), 118(38), 159(9), 173(14), 188(17), 205(10), 220(3)	220	*	*	*	*	*	*	*	*	*	*
42	epoxy-allo-alloaromadendrene	**41(100)**, 55(37), 67(38), 91(64), 105(51), 121(32), 135(23), 147(34), 159(22), 177(23), 189(31), 202(21), 220(18)	220	*	*	*	*	*	*	*	*	*	*
43	eremophila-1(10),6-dien-12-al	81(20), 91(40), 105(47), 119(50), 133(17), **147(100)**, 161(93), 176(32), 189(22), 203(52), 204(13), 218(28)	218	*	*	*	*	*	*	*	*	*	*
44	13-nor-eremophila-1(10), 6-dien-11-one	53(16), 55(20), 77(27), 91(67), 105(56), 119(58), 131(16), 135(15), 147(56), **161(100)**, 189(21), 204(41)	204	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
45	-funebren-15-al	69(32), 79(44), 91(69), 105(68), 119(23), 121(21), **133(100)**, 147(32), 162(26), 175(40), 189(15), 203(12), 218(25)	218	*	*	*	*	*	*	*	*	*	*
46	tris(1-methylethyl)-benzene	27(15), 39(21), 51(18), 65(15), 77(24), 91(23), **105(100)**, 120(38)	120	*	*	*	*	*	*	*	*	*	*
47	13-nor-trans-eudesma-4(15),7-dien-11-one	77(21), 79(20), 91(39), 93(27), 105(35), 108(20), 119(23), 133(24), 135(26), 147(10), 161(50), 189(74), **204(100)**	204	*	*	*	*	*	*	*	*	*	*
48	eudesm-4(15),7-dien--ol	81(38), **91(100)**, 105(80),119(55), 131(52),145(30), 159(60), 177(17), 187(18), 202(19), 220(17)	220	*	*	*	*	*	*	*	*	*	*
49	allo-khusiol	55(33), 69(48), **71(100)**, 91(65), 105(40), 109(52), 119(46), 133(44), 161(26),189(30), 204(16), 222(7)	222	*	*	*	*	*	*	*	*	*	*
50	acorenone	41(80), 55(53), 69(51), 82(68), 93(41), **109(100)**, 121(44), 135(84), 149(38), 177(59), 220(80)	220	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
51	prezizaan-15-al	67(40), 77(46), 91(78), **109(100)**, 121(45), 135(60), 159(20), 177(90), 189(23),202(20), 205(25), 220(27)	220	*	*	*	*	*	*	*	*	*	*
52	2-epi-ziza-6(13)-en -3-one	67(25), 79(63), 94(82), 105(45), 121(63), 133(28), 147(61), **148(100)**, 161(28), 175(46), 190(25), 203(10), 218(45)	218	*	*	*	*	*	*	*	*	*	*
53	khusian-2-ol	**55(100)**, 69(72), 81(60), 93(50), 95(38), 105(52), 109(65), 121(53), 149(29), 161(62), 177(34), 204(16), 220(22)	220	*	*	*	*	*	*	*	*	*	*
54	ziza-6(13)-en-3-one	79(95), 93(93), 105(74), **121(100)**, 133(41), 148(95), 161(42), 175(44), 190(38), 218(64)	218	*	*	*	*	*	*	*	*	*	*
55	eudesma-4(15),7-dien- -ol	77(19), 91(34), 105(37), 117(32), 119(32), 131(31), 145(32), **159(100)**, 173(5), 187(35), 202(19), 220(35)	220	*	*	*	*	*	*	*	*	*	*
56	13-nor-eudesma-4,6-dien-11-one	55(26), 77(29), 81(32), 91(67), 105(83), 117(25), 119(38), 133(23), 145(27), 147(30), 161(80), **189(100)**, 204(93)	204	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
57	cadina-1(10),6,8-triene	27(9), 41(12), 77(12), 91(15), 105(15), 115(17), 128(18), 145(17), 159(54), **187(100)**, 202(43)	202	*	*	*	*	*	*	*	*	*	*
58	eudesma-3,5-dien- -ol	55(10), 67(10), 77(14), 81(15), 91(24), 105(23), 117(46), 131(29), 145(13), **159(100)**, 191(40), 202(13), 220(26)	220	*	*	*	*	*	*	*	*	*	*
59	prezizanol	43(40), 55(24), 71(91), 82(75), 95(53), 109(65), 123(38), 137(42), **179(100)**, 189(41), 204(25), 222(45)	222	*	*	*	*	*	*	*	*	*	*
60	khusimol	91(34), 117(22), 131(66), **150(100)**, 159(53), 187(24), 202(44), 220(16)	220	*	*	*	*	*	*	*	*	*	*
61	9,10-dehydro-isolongifolene	27(20), 41(38), 55(20), 77(23), 91(24), 105(22), 119(50), **131(100)**, 145(44), 159(82), 173(15), 187(25), 202(41)	202	*	*	*	*	*	*	*	*	*	*
62	nootkatone	41(68), 67(30), 79(64), 91(65), 105(58), 121(74), 133(78), **147(100)**, 161(82), 175(64), 190(59), 203(61), 218(24)	218	*	*	*	*	*	*	*	*	*	*

Table 3.3 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
63	beta-vetivone	41(64), 55(41), 91(44), 105(43), 121(50), 147(43), **185(100)**, 203(24), 218(44)	218	*	*	*	*	*	*	*	*	*	*
64	khusenic acid	41(71), 67(40), 79(45), 91(62), 105(38), 119(78),131(34), **145(100)**, 164(65), 173(24), 191(30), 219(50), 234(26)	234	*	*	*	*	*	*	*	*	*	

* Existence

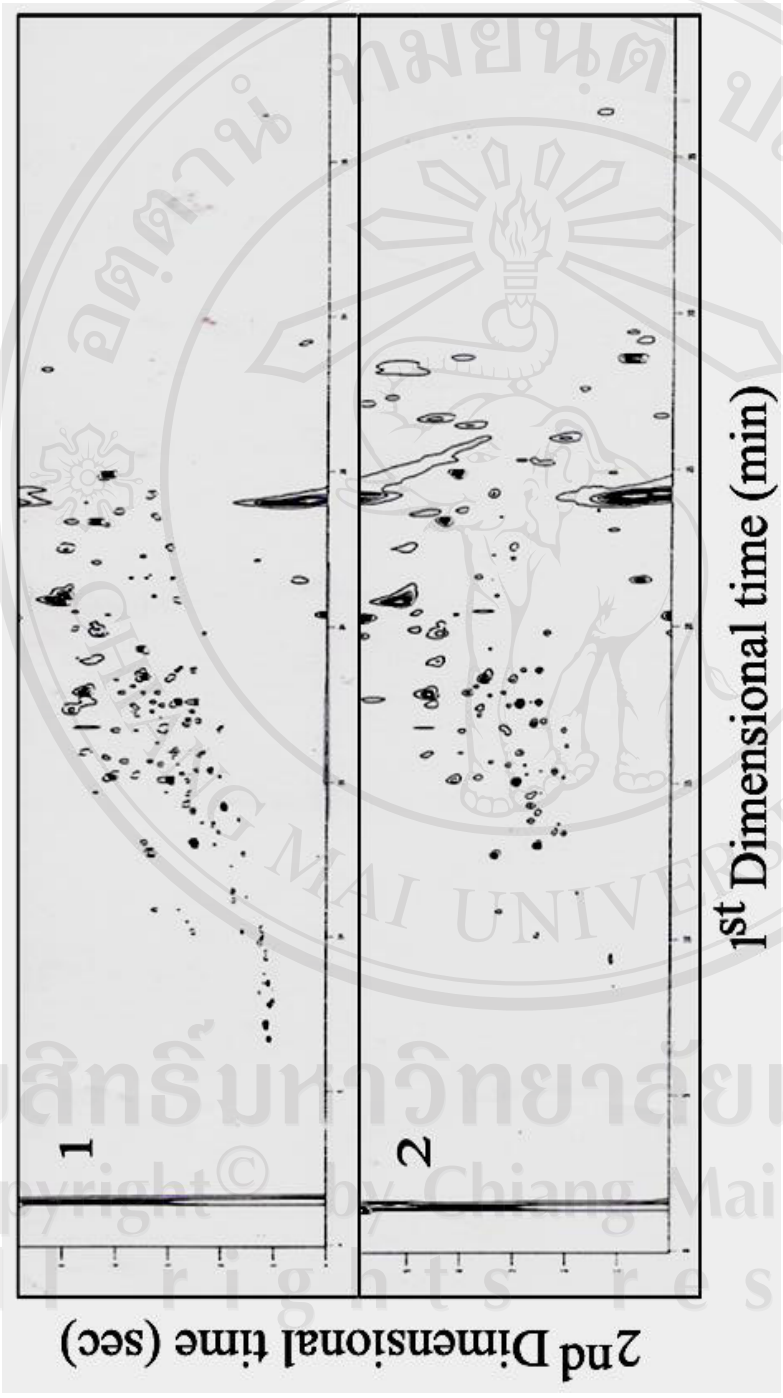


Figure 3.6 GC×GC-qMS contour plot of vetiver root essential oils obtained from 1. SDE 24 hrs and 2. SFE with DCM

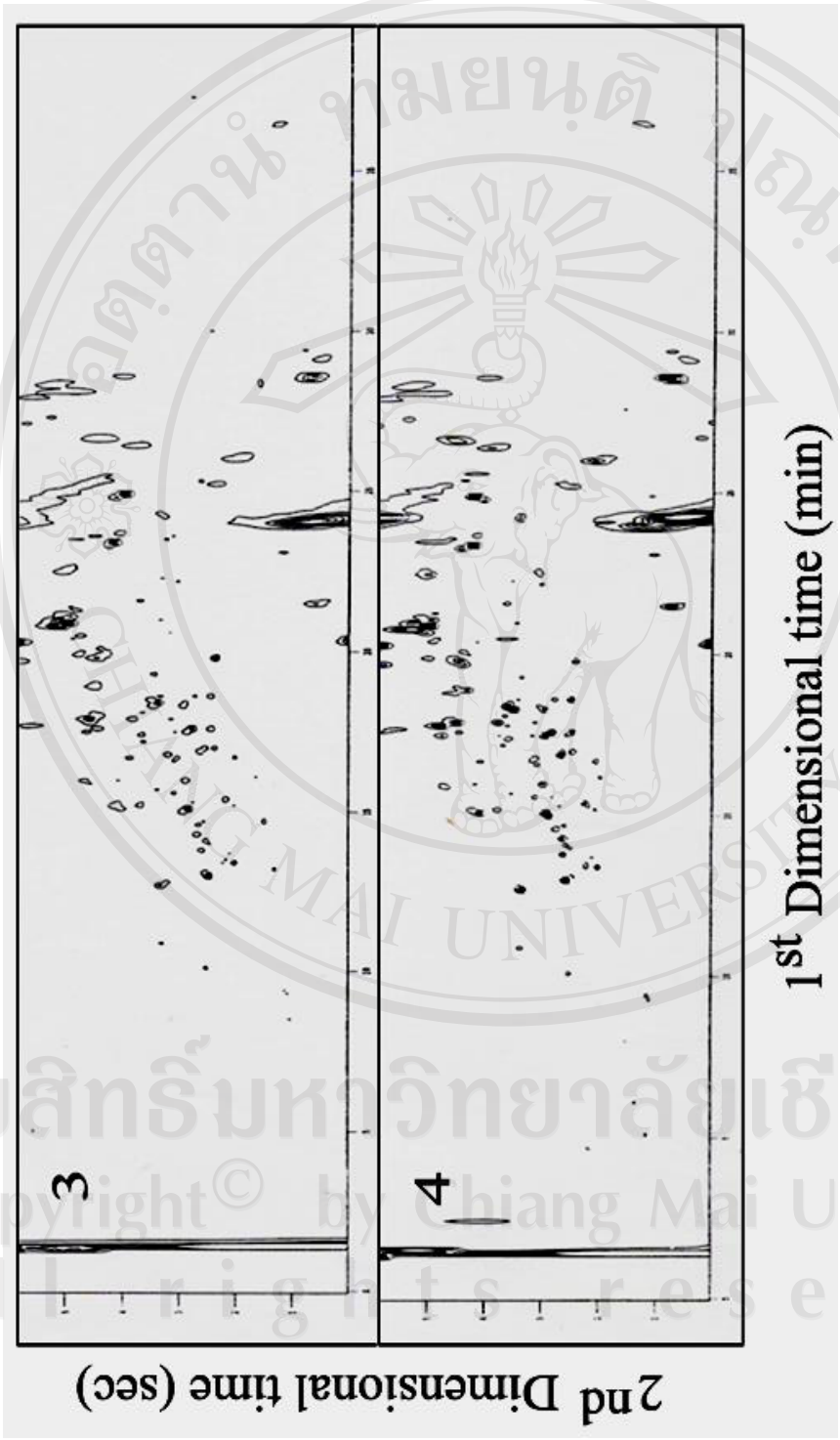


Figure 3.6 (continued) GC×GC-qMS contour plot of vetiver root essential oils obtained from 3. SFE with methanol and 4. SFE with toluene

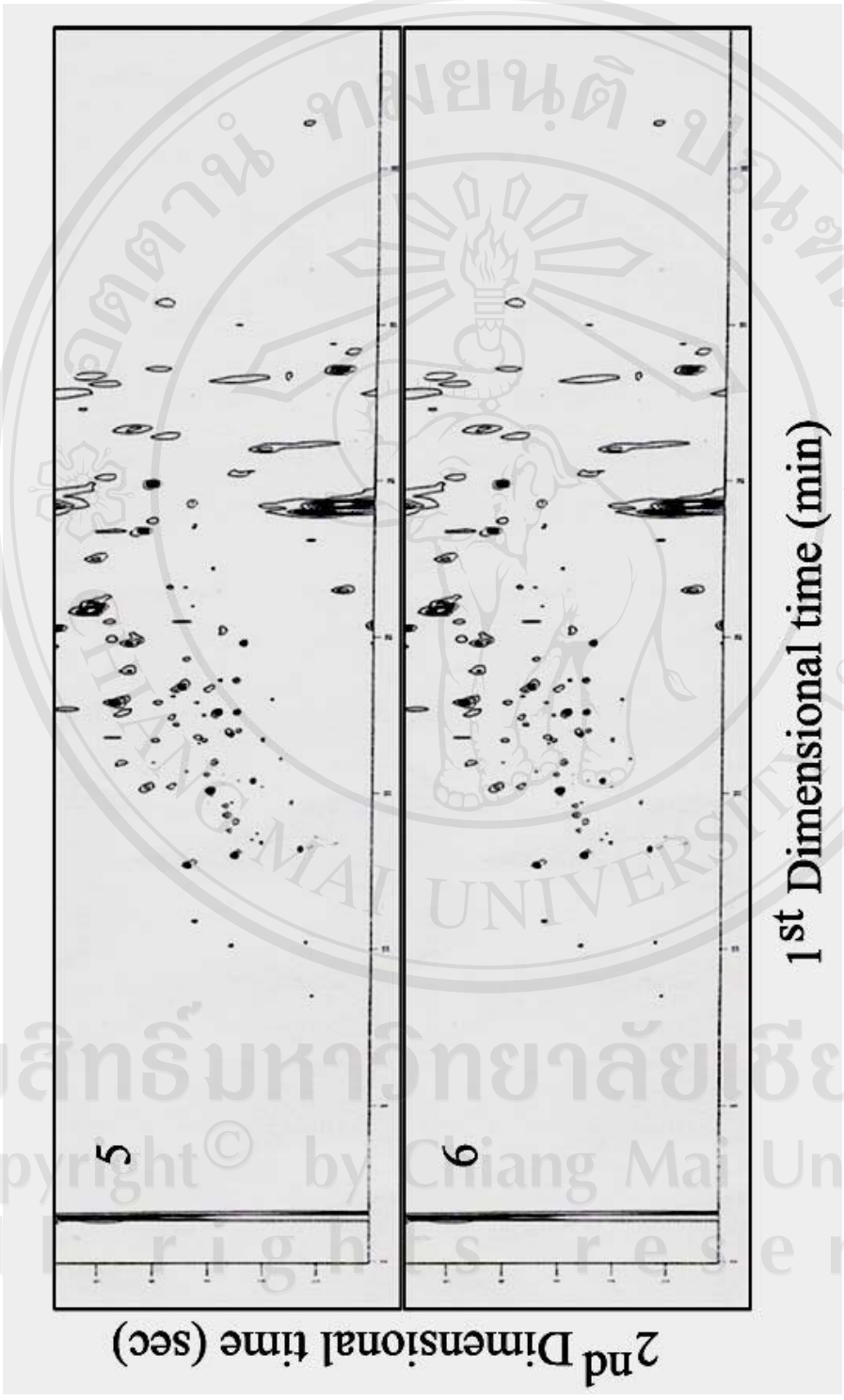


Figure 3.6 (continued) GC×GC-qMS contour plot of vetiver root essential oils obtained from 5. soxhlet with methanol and 6. soxhlet with toluene

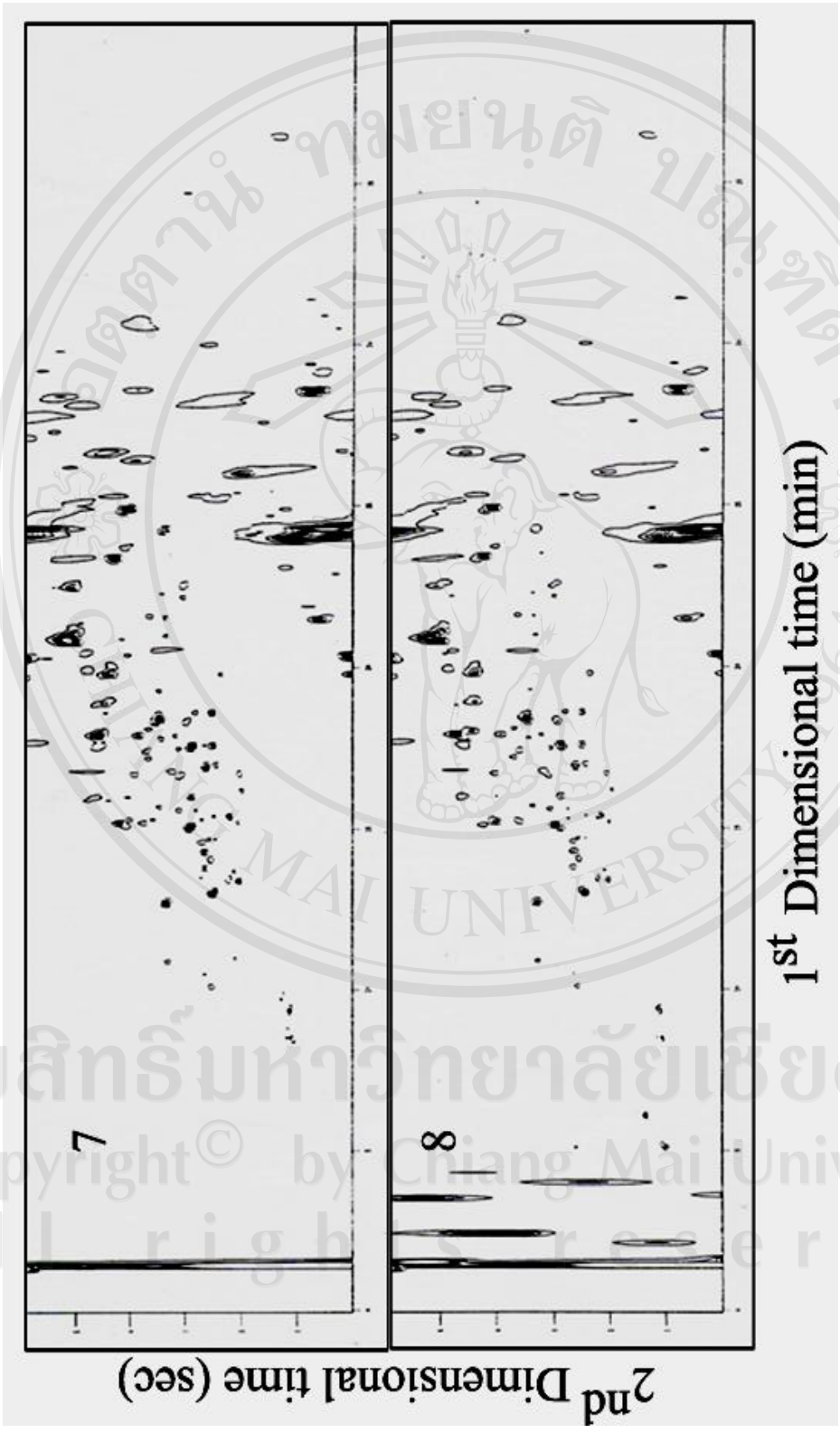


Figure 3.6 (continued) GC×GC-qMS contour plot of vetiver root essential oils obtained from 7. soxhlet with DCM and 8. microwave with toluene

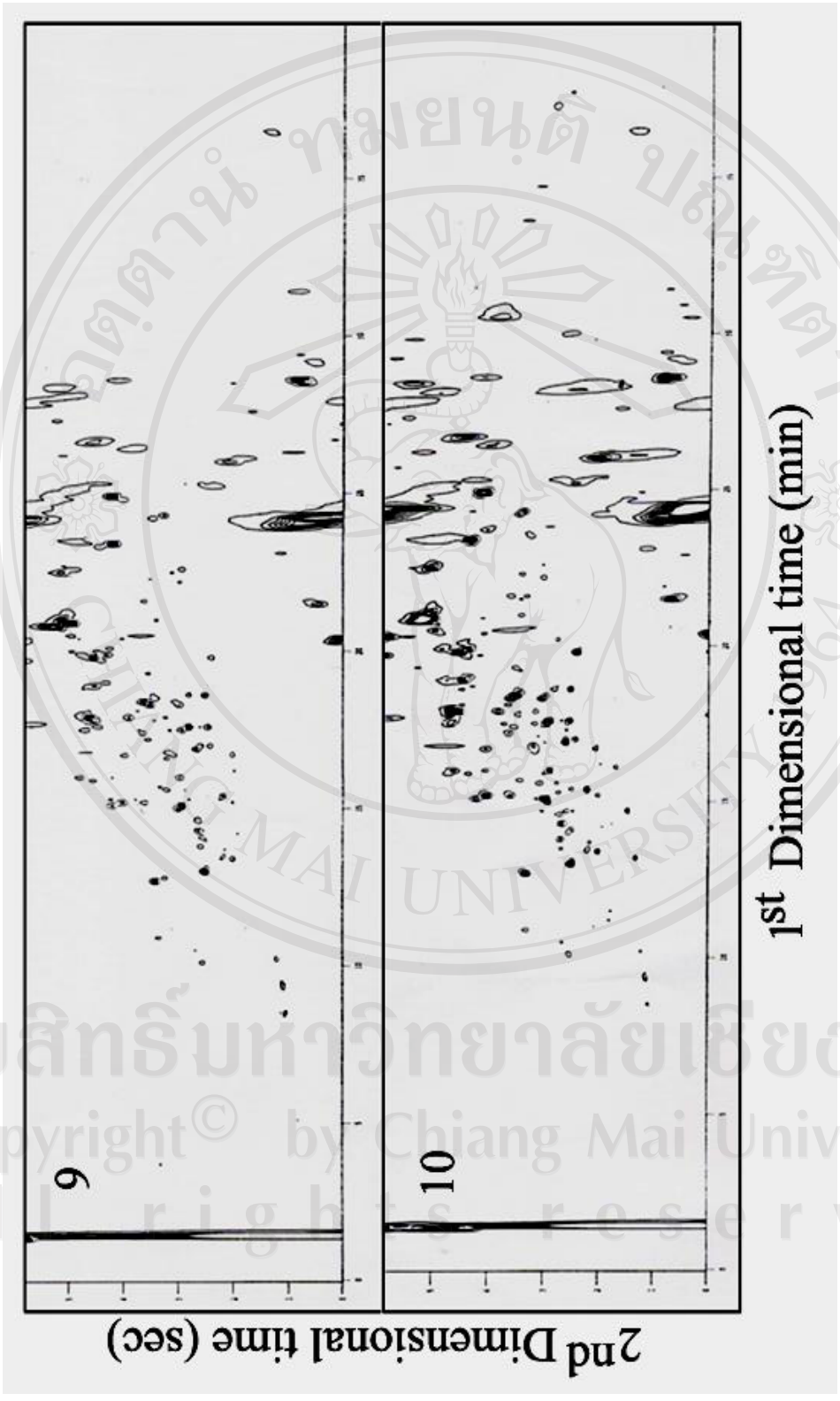


Figure 3.6 (continued) GC×GC-qMS chromatograms of vetiver root essential oils obtained from 9. microwave with DCM and 10. microwave with methanol

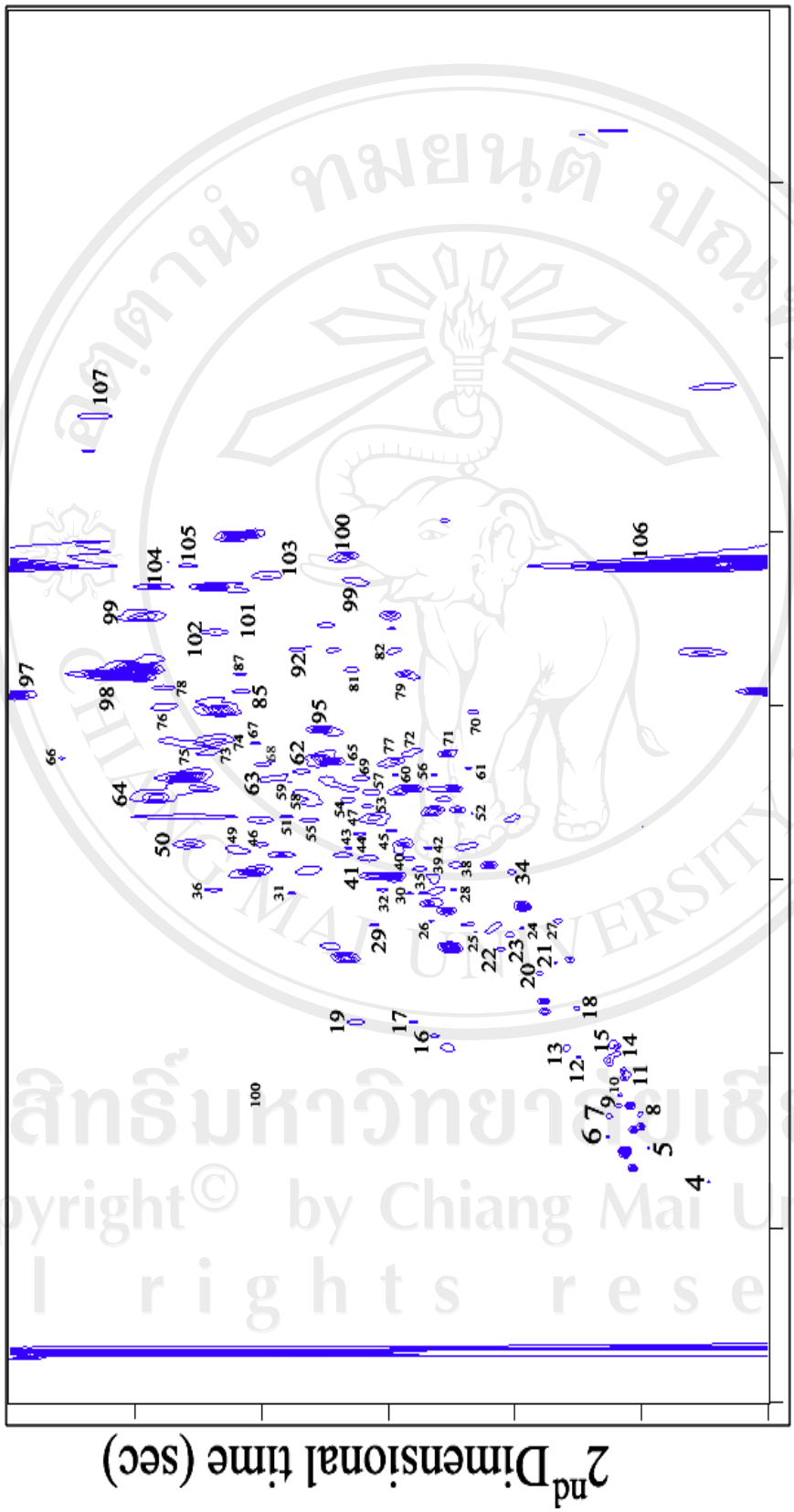


Figure 3.7 GC×GC contour plot of vetiver root essential oil obtained from SDE method showing peak assignment

Table 3.4 Structural assignment and electron impact (EI) mass spectra of vetiver root essential oils obtained from all extraction methods and analyzed by GC×GC-qMS

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
1	2,3-dihydrobenzofuran	27(18), 29(21), 39(70), 40(40), 41(95), 42(38), 69(60), **70(100)**	70								*		
2	2,3-dihydro-4,7-dimethyl-1H-indene	51(12), 65(13), 77(12), 91(24), 102(8), 105(9), 115(23), 128(20), **131(100)**, 146(64)	146		*		*	*				*	
3	1,2,3,4-tetrahydro-1,1,6-trimethylnaphthalene	27(10), 41(12), 51(9), 65(10), 77(12), 91(11), 105(13), 115(14), 128(12), 143(12), **159(100)**, 174(24)	174		*			*			*		
4	alpha-cubebene	41(40), 55(28), 69(18), 91(40), **105(100)**, 119(90), 133(16), 147(9), 161(89), 175(6), 189(7), 204(22)	204	*									
5	9,10-dehydro-2-norzizaene	41(38), 53(24), 67(32), 77(56), **91(100)**, 105(34), 118(84), 131(38), 145(86), 159(17), 173(75), 188(60)	188	*	*	*		*		*	*	*	*
6	alpha-ylangene	41(58), 55(32), 69(21), 81(38), 93(83), **105(100)**, 119(94), 136(24), 147(18), 161(81), 189(9), 204(26)	204	*									
7	alpha-funebrene	43(19), 55(44), **69(100)**, 79(36), 93(64), 105(40), 120(38), 133(40), 147(17), 161(73), 189(16), 204(18)	204	*				*			*		
8	6-butyl-1,2,3,4-tetrahydronaphthalene	51(23), 65(21), 78(19), 91(53), **104(100)**, 128(21), 132(60), 156(45), 170(23), 184(32), 202(23)	202	*				*	*		*		

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
9	2-norzizaene	41(25), 55(18), 67(28), 79(60), 91(64), 105(40), **120(100)**, 133(26), 147(42), 162(18), 175(27), 190(21)	190	*	*	*		*		*	*	*	
10	7,8-dihydro-8,8-dimethyl-5(6H)-benzocyclooctenone	115(58), 127(34), **129(100)**, 143(55), 157(74), 172(66), 185(40), 200(58)	200	*				*	*	*	*	*	
11	(R)- 1,5,5,9-tetramethylSpiro[5.5] undeca-1,8-diene	27(16), 41(18), 53(10), 67(9), 79(22), 93(65), 107(59), 121(95), **136(100)**, 161(15), 189(13), 204(24)	204	*	*		*	*		*		*	*
12	4b,5,6,7,8,8a,9,10-octahydro-1-methylphenanthrene	77(12), 91(18), 105(16), 115(24), 128(40), 143(66), 153(12), 157(71), 172(24), 185(28), 192(12), **200(100)**	200	*				*	*		*		
13	alpha-cedrene	41(24), 55(18), 69(22), 77(19), 93(45), 105(35), **119(100)**, 136(15), 147(19), 161(26), 189(12), 204(26)	204	*	*	*	*	*	*	*	*	*	*
14	beta-copaene	41(38), 55(22), 69(20), 81(38), 93(57), 105(94), **119(100)**, 136(18), 147(12), 175(7), 189)12), 204(38)	204	*	*	*	*	*	*	*	*	*	*
15	2-[(Z)-3-hexenyl]-1-methyl-3-methylen-1-cyclohexene	79(56), **93(100)**, 105(91), 121(92), 134(21), 147(31), 161(34), 175(21), 190(33)	190	*				*	*		*	*	*
16	gamma-elemene	41(60), 55(40), 93(75), 1o7(50), **121(100)**, 136(20), 147(15), 161(20), 189(10), 204(10)	204	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
17	prezizaene	55(21), 69(17), 91(41), 108(40), 119(46), **133(100)**, 147(28), 161(30), 175(18), 189(42), 204(23)	204	*	*	*	*	*	*	*	*	*	*
18	dehydroaromadendrene	41(62), 55(20), 67(23), 77(22), 91(48), 105(50), 117(37), 131(40), 145(43), **159(100)**, 187(24), 202(41)	202	*				*	*	*			*
19	khusimene	41(60), 56(50), 67(40), 77(40), 91(60), 105(50), 119(55), **134(100)**, 161(20), 189(38), 204(20)	204	*	*	*	*	*	*	*	*	*	*
20	1,2,3,4,5,6-hexahydro-1-methyl-2,2'-bipyridine	29(10), 40(12), 43(14), 52(24), 56(12), 60(12), 64(13), 78(23), 110(11), 128(41), **156(100)**	156	*			*	*			*		
21	beta-acoradiene	**44(100)**, 57(12), 76(11), 93(11), 105(10), 141(14), 156(13), 170(12), 189(14), 204(13)	204	*	*	*	*	*	*	*		*	*
22	4,7-epoxy-spirovetiva-2,11-diene	55(12), 68(60), **84(100)**, 108(63), 121(28), 137(64), 161(23), 176(21), 190(22), 203(24), 218(64)	218	*	*	*			*				
23	ar-curcumene	27(20), 41(50), 55(20), 69(20), 91(50), 105(60), **119(100)**, 132(90), 145(30), 159(10), 189910), 202(20)	202	*				*	*				
24	alpha-amorphene	41(40), 55(20), 79(40), 91(60), 105(78), 119(63), 133(46), 148(17), **161(100)**, 176(10), 189(15), 204(39)	204	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
25	cyclocopacamphan-12-al	53(32), 79(51), 94(32), 105(75), 118(32), 133(27), 145(84), 159(22), **160(100)**, 161(33), 203(4), 218(23)	218	*	*	*	*	*	*		*	*	*
26	delta-silenene	41(22), 55(18), 69(20), 93(43), 105(32), **119(100)**, 136(15), 161(23), 175(9), 189(14), 204(24)	204	*	*	*	*	*	*	*	*	*	*
27	beta-vetispirene	55(13), 68(62), **84(100)**, 108(62), 121(24), 137(63), 161(24), 176(24), 190(28), 203(24), 218(66)	218	*									
28	gamma-amorphene	41(28), 55(18), 69(17), 81(26), 94(66), **105(100)**, 119(32), 133(20), 147(15), 161(55), 189(18), 204(38)	204	*	*			*	*	*	*		*
29	cis-eudesma-6,11-diene	55(50), 67(50), 81(38), **91(100)**, 107(43), 119(35), 131(52), 145(30), 177(17), 187(18), 202(19), 220(17)	220	*	*	*	*	*	*	*	*	*	*
30	trans-beta-guaiene	41(76), 55(51), 67(28), 91(62), 105(90), 119(63), 133(41), 149(68), **161(100)**, 175(12), 189(48), 204(89)	204	*		*		*					
31	delta-amorphene	27(38), 41(70), 55(28), 69(38), 79(65), 91(68), 105(70), 119(68), 133(43), **161(100)**, 204(34)	204	*	*	*	*	*	*	*	*	*	
32	beta-curcumene	41(56), 55(31), 69(22), 77(21), 91(24), 105(46), **119(100)**, 132(78), 145(28), 159(11), 187(9), 202(34)	202	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE	SFE			Soxhlet			MAE		
				24 hrs	toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
33	11,12,13-tri-nor-cis-eudesma-5,8-dien-7-one	55(31), 65(26), 77(41), **91(100)**, 105(79),120(33), 121(94), 133(84), 134(27), 147(25), 161(38), 176(57)	176		*	*		*	*	*	*	*	*
34	5H-3a,7-methanoazulen-6-one	68(38), 80(64), 92(25), **107(100)**, 120(60), 164(44)	164	*									
35	(+-)-2-methyl-6-p-tolyl-4-heptanol	91(18), 105(19), **119(100)**, 132(24), 145(20), 159(9), 187(7), 202(20), 220(8)	220	*				*	*	*		*	
36	cis-dihydroagarofuran	**29(100)**, 41(36), 55(21), 67(20), 95(20), 109(40), 124(21), 137(43), 164(21), 189(23), 207(66), 222(12)	222	*	*	*	*	*	*	*	*	*	*
37	3,4-dihydro-4,6,7-trimethyl-1(2H)-naphthalenone	39(24), 51(21), 63(24), 77(13), 90(80), 104(12), 115(22), **118(100)**, 131(19), 146(63)	146		*	*							
38	8-isopropenyl-3,3,7-trimethylbicyclo[5.1.0] oct-5-en-2-one	41(48), 69(24), 77(28), 91(60), 105(92), **119(100)**, 134(90), 161(38), 176(18), 189(15), 204(34)	204	*	*	*	*	*	*	*	*	*	*
39	delta-cadinene	41(21), 55(18), 69(18), 81(24), 105(46), 119(44), 134(65), 147(15), **161(100)**, 176(9), 189(21), 204(62)	204	*		*		*	*				
40	gamma-vetivenene	53(21), 67(20), 77(40), 91(70), **103(100)**, 117(44), 131(66), 145(84), 159(86), 187(57), 202(90)	202	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
41	trans-calamenene	41(18), 53(8), 65(9), 77(12), 91(14), 105(15), 115(13), 129(16), 144(13), **159(100)**, 202(20)	202	*	*	*	*	*	*	*	*	*	*
42	1a,2,6,7,7a,7b-hexahydro-1,1,7,7a-tetramethyl-1H-cyclopropa[a]naphthalene	41(94), 53(26), 65(22), 77(42), 91(66), 105(60), 117(53), 131(64), 145(63), 159(66), 187(44), **202(100)**	202	*	*	*	*	*		*	*	*	*
43	3-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-2-propenal	27(21), 43(44), 55(20), 69(18), 81(24), 95(21), **109(100)**, 121(21), 151(60), 179(15), 194(21)	194	*	*	*	*	*	*	*	*	*	*
44	beta-calacorene	28(25), 41(10), 115(27), 128(18), 142(65), **157(100)**, 200(24), 218(56)	218	*	*	*	*	*	*	*	*	*	*
45	zingiberene	41(45), 69(58), 93(60), 105(20), 119(57), 133(55), 147(25), **161(100)**, 189(10), 204(80)	204	*	*	*	*	*	*	*	*	*	*
46	6,12-epoxy-elema-1,3-diene	55(69), 69(52), 79(39), **81(100)**, 97(70), 109(30), 137(20), 151(24), 163(17), 177(11), 205(23), 220(4)	220	*	*	*	*	*	*	*	*	*	*
47	13-nor-eudesm-5-en-11-one	55(10), 67(10), 77(6), **81(100)**, 93(25), 95(4), 105(6), 107(6), 119(2), 147(2), 163(10), 206(3)	206	*	*	*	*	*	*	*	*	*	*
48	elemol	**41(100)**, 59(90), 66(70), 81(60), 93(64), 105(43), 120(45), 136(40), 147(38), 161(59), 189(30), 204(20)	204				*			*			*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
49	alpha-agarofuran	55(22), **82(100)**, 91(24), 105(24), 109(26), 123(36), 147(41), 187(22), 205(43), 220(83)	220	*	*	*	*	*	*	*	*	*	*
50	(+)(6S,10R)-6,10-dimethylbicyclo[4.4.0] dec-1-en-3-one	41(60), 79(55), 93(50), 109(52), 122(63), 136(78), 150(60), 163(38), **178(100)**	178	*	*	*	*	*	*	*	*	*	*
51	15-nor-prezizaan-7-one	55(27), 67(53), 79(46), 93(50), 94(47), 107(75), 121(31), 135(93), 150(37), 177(16), 191(75), **206(100)**	206	*	*	*	*	*	*	*	*	*	*
52	cascarilladienol	55(23), 77(21), 91(42), 107(29), 121(26), 135(45), 145(55), 159(16), **177(100)**, 187(10), 205(8), 220(15)	220	*	*	*	*	*	*	*	*	*	*
53	12-nor-2,3-epoxy-ziza-6(13)-ene	79(40), 105(52), 117(29), 121(31), 133(37), 147(37), **161(100)**, 175(16), 189(52), 204(19)	204	*	*	*	*	*	*	*	*	*	*
54	cis-eudesm-6-en-11-ol	**59(100)**, 67(21), 81(24), 95(24), 108(30), 123(26), 149(64), 164(60), 175(14), 189(21), 204(22), 222(18)	222	*	*	*	*	*	*	*	*	*	*
55	2-acetyl-5,6,7,8-tetrahydroquinoxaline	39(20), 43(71), 53(20), 79(40), 106(36), 119(20), **133(100)**, 148(42), 161(16), 176(84)	176	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
56	12-nor-preziza-7(15)-en-2-one	55(37), 79(55), 91(80), 119(61), 133(59), 147(88), **161(100)**, 175(30), 189(42), 204(95)	204	*	*	*	*	*	*	*	*	*	*
57	15-nor-funebran-3-one	55(36), 69(38), 79(32), 91(28), 93(49), 107(26), 121(50), 136(37), 149(11), **163(100)**, 191(7), 206(21)	206	*	*	*	*	*	*	*	*	*	*
58	4-(2,2-dimethyl-6-nethylenecyclohexylidene)-3-methylidene-2-one	43(80), 55(38), 69(50), 79(36), 93(53), 107(81), 133(22), 149(19), **163(100)**, 191(52), 206(18)	206	*	*	*	*	*	*	*	*	*	*
59	clovane	26(10), 43(44), 55(24), 67(20), 81(24), 95(30), 121(24), **135(100)**, 150(21), 163(25), 191(26), 206(20)	206	*	*	*	*	*	*	*	*	*	*
60	cyclocopacamphan-12-ol	55(23), 65(16), 79(42), **95(100)**, 119(82), 131(40), 145(31), 161(87), 189(29), 202(16), 205(8), 220(37)	220	*	*	*	*	*	*	*		*	*
61	13-nor-eremophil-1(10)-en-11-one	55(48), 67(38), 79(55), 81(40), **91(100)**, 107(66), 121(98), 135(38), 147(23), 163(33), 191(14), 206(35)	206	*	*	*			*	*	*	*	*
62	khusimone	**41(100)**, 55(68), 67(50), 77(51), 91(74), 108(78), 133(60), 145(22), 164(39), 173(24), 189(44), 204(62)	204	*	*	*	*	*	*	*	*	*	*
63	trans-dracunculifoliol	55(11), 79(21), 95(27), **109(100)**, 133(18), 135(26), 151(26), 161(19), 179(32), 189(31), 204(2), 222(8)	222	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
64	10-epi-gamma-eudesmol	41(20), **59(100)**, 81(23), 95(24), 123(23), 135(21), 149(63), 164(52), 175(7), 189(21), 204(23), 222(12)	222	*	*	*	*	*	*	*	*	*	*
65	10-epi-cubenol-12-nor-ziza-6(13)-en- -ol	59(64), 67(42), 81(56), 93(62), 105(65), **119(100)**, 135(22), 161(94), 179(22), 189(25), 204(46)	204	*	*	*	*	*	*	*	*	*	*
66	12-nor-ziza-6(13)-en- -ol	55(59), 67(47), 79(55), **91(100)**, 105(36),, 117(62), 118(38), 159(9), 173(14), 188(17), 205(10), 220(3)	220	*	*	*	*	*	*	*	*	*	*
67	epoxy-allo-allo aromadendrene	**41(100)**, 55(37), 82(53), 91(64), 105(51), 135(23), 147(34), 159(22), 177(23), 189(31), 202(21), 220(18)	220	*	*	*	*	*	*	*	*	*	*
68	eremophila-1(10),6-dien-12-al	55(17), 81(20), 91(40), 105(47), 119(50), **147(100)**, 161(93), 176(32), 189(22), 203(52), 218(28)	218	*	*	*	*	*	*	*	*	*	*
69	13-nor-eremophila-1(10), 6-dien-11-one	55(20), 65(17), 77(27), 91(67), 105(56), 119(58), 131(16), 147(56), **161(100)**, 189(21), 204(41)	204	*	*	*	*	*	*	*	*	*	*
70	-funebren-15-al	55(18), 79(44), 91(69), 105(68), 119(23), **133(100)**, 147(32), 175(40), 189(15), 203(12), 218(25)	218	*	*	*	*	*	*	*	*	*	*
71	tris(1-methylethyl)-benzene	27(15), 39(21), 51(18), 65(15), 77(24), 91(23), **105(100)**, 120(38)	120	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
72	13-nor-trans-eudesma-4(15),7-dien-11-one	77(21), 91(39), 105(35), 108(20), 119(23), 133(24), 135(26), 147(10), 161(50), 189(74), **204(100)**	204	*	*	*	*	*	*	*	*	*	*
73	eudesm-4(15),7-dien--ol	55(50), 67(50), 79(51), **91(100)**, 53), 105(80), 119(55), 131(52), 159(60), 177(17), 187(18), 202(19), 220(17)	220	*	*	*	*	*	*	*	*	*	*
74	valerianol	79(53), 85(98), 105(80), 119(55), 134(42), 145(50), **177(100)**, 187(18), 202(19), 220(17)	220	*	*	*	*	*	*	*	*	*	*
75	7,15-epoxy-prezizaane	53(38), 77(62), **91(100)**, 105(73), 119(74), 133(75), 161(34), 175(28), 188(15), 191(30), 205(38), 220(10)	220	*	*	*	*	*	*	*	*	*	*
76	4,8-dimethyl-1-(1-methylethyl)-spiro[4.5] dec-8-en-7-ol	41(84), 55(65), 69(48), 84(93), 95(67), 109(72), 138(95), **151(100)**, 166(32), 179(38), 207(18), 222(84)	222	*	*	*	*	*	*	*	*	*	*
77	allo-khusiol	55(33), 67(53), **71(100)**, 82(66), 91(65), 109(52), 119(46), 133(44), 161(26), 189(30), 204(16), 222(7)	222	*	*	*	*	*	*	*	*	*	*
78	acorenone	41(80), 55(53), 69(51), 82(68), 93(41), **109(100)**, 121(44), 135(84), 149(38), 177(59), 220(80)	220	*	*	*	*	*	*	*	*	*	*
79	prezizaan-15-al	69(30), 91(78), 94(32), **109(100)**, 121(45), 135(60), 147(20), 159(20), 202(20), 205(25), 220(27)	220	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
80	E-opposita-4(15),7(11)-dien-12-al	79(84), **91(100)**, 93(82), 105(60), 119(38), 133(61), 161(37), 175(37), 185(34), 189(27), 203(60), 218(42)	218		*				*		*		
81	zizanal	59(43), **73 (100)**, 105(60), 119(38), 122(44), 133(81), 147(62), 161(47), 189(23), 203(68), 218(59)	218	*	*	*	*	*	*	*	*	*	*
82	2-epi-ziza-6(13)-en-3-one	67(25), 94(82), 105(45), 119(59), 121(63), 147(61), **148(100)**, 175(46), 190(25), 203(10), 218(45)	218	*	*	*	*	*	*	*	*	*	*
83	khusian-2-ol	**55(100)**, 69(72), 81(60), 95(38), 105(52), 119(60), 135(60), 149(29), 161(62), 177(34), 204(16), 220(22)	220	*	*	*	*	*	*	*	*	*	*
84	ziza-6(13)-en-3-one	79(95), 93(93), 105(74), **121(100)**, 133(41), 148(95), 161(42), 175(44), 190(38), 218(64)	218	*	*	*	*	*	*	*	*	*	*
85	eudesma-4(15),7-dien--ol	77(19), 91(34), 105(37), 119(32), 131(31), 145(32), **159(100)**, 173(5), 187(35), 202(19), 220(35)	220	*	*	*	*	*	*	*	*	*	*
86	13-nor-eudesma-4,6-dien-11-one	55(26), 77(29), 81(32), 91(67), 105(83), 119(38), 133(23), 145(27), 147(30), 161(80), **189(100)**, 204(93)	204	*	*	*	*	*	*	*	*	*	*
87	eudesma-3,5-dien--ol	55(10), 67(10), 77(14), 91(24), 117(46), 131(29), **159(100)**, 191(40), 202(13), 220(26)	220	*	*	*	*	*		*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
88	(E)-opposita-4(15), 7(11)-dien-12-ol	55(47), 79(81), 91(95), 105(60), 119(37), 131(52), 145(32), 177(11), **187(100)**, 202(40), 205(18), 220(6)	220	*	*	*	*	*	*	*	*	*	*
89	cadina-1(10),6,8-triene	27(9), 41(12), 77(12), 91(15), 105(15), 115(17), 128(18), 145(17), 159(54), **187(100)**, 202(43)	202	*	*	*	*	*	*	*	*	*	*
90	preziza-7(15)-en- -ol	53(26), 77(34), 91(58), 108(47), 117(23), **131(100)**, 145(21), 159(21), 187(24), 202(15), 220(15)	220	*	*	*	*	*	*	*	*	*	*
91	13-nor-7,8-epoxy-trans-eudesm-4(15)-en-11-one	79(45), 93(64), 105(45), 121(40), 133(34), 145(35), 159(100), 177(78), 187(80), 202(68), 220(2)	220		*	*	*	*	*	*	*	*	*
92	ziza-6(13)-en- -ol	53(59), 65(31), 79(57), 91(79), 105(53), 131(67), 133(69), 159(91), 173(26), **187(100)**, 202(59), 220(2)	220	*	*	*	*			*	*	*	*
93	eudesma-3,5-dien- -ol	55(10), 77(14), 91(24), 105(23), 117(46), 131(29), **159(100)**, 191(40), 202(13), 220(26)	220	*	*	*	*	*	*	*	*	*	*
94	2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-1H-3a,7-methanoazulene-6-methanol	41(80), 69(48), 79(81), 91(56), 105(46), **135(100)**, 159(17), 177(21), 189(12), 202(10), 220(19)	220	*	*	*	*	*	*	*	*	*	*
95	oplopanone	59(46), 79(80), 95(76), 105(46), 121(22), 135(60), 147(61), 159(35), **189(100)**, 202(70), 220(35)	220	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
96	1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(2-propenyl)-1-naphthalenol	69(76), 79(38), 83(68), 95(78), **109(100)**, 123(61), 150(58), 177(21), 187(64), 202(45), 220(24)	220	*	*	*	*	*	*	*	*	*	*
97	prezizanol	43(40), 55(23), 71(92), 82(76), 95(48), 109(64), 123(37), 137(41), **179(100)**, 189(42), 204(24), 222(43)	222	*	*	*	*	*	*	*	*	*	*
98	khusimol	91(34), 117(22), 131(66), **150(100)**, 159(53), 187(24), 202(44), 220(16)	220	*	*	*	*	*	*	*	*	*	*
99	bicyclovetivenol	55(65), 47(64), 79(42), 93(54), 105(42), 119(50), 133(37), 145(44), **159(100)**, 173(15), 187(55), 202(41),220(13)	220	*	*	*	*	*	*	*	*	*	*
100	9,10-dehydro-isolongifolene	27(20), 41(38), 55(20), 77(23), 91(24), 105(22), 119(50), **131(100)**, 145(44), 159(82), 173(15), 187(25), 202(41)	202	*	*	*	*	*	*	*	*	*	*
101	nootkatone	53(28), 79(64), 91(65), 121(74), 133(78), **147(100)**, 161(82), 175(64), 190(59), 203(61), 218(24)	218	*	*	*	*	*	*	*	*	*	*
102	1-O-acetyl-2-methyl-naphthalene-1,4-diol	43(78), 51(18), 77(21), 91(21), 105(24), 115(23), 131(21), 145(18), **174(100)**, 216(24)	216	*	*	*	*	*	*	*	*	*	*
103	2,2,4-trimethylfuro[6,7-c]-1,3,8H-azulene	131(38), 145(39), 173(21), 187(25), 201(61), **216(100)**	216	*	*	*	*	*	*	*	*	*	*

Table 3.4 (continued)

No.	Structural assignment	m/z (%RA)	MW	Extraction Method									
				SDE 24 hrs	SFE			Soxhlet			MAE		
					toluene	DCM	methanol	toluene	DCM	methanol	toluene	DCM	methanol
104	(+)-decahydro-4,8,8,9-tetramethyl-1,4-methanoazulen-7-ol	**41(100)**, 55(63), 79(77), 95(78), 107(65), 121(56), 136(44), 148(84), 165(24), 189(21), 204(22), 222(22)	222	*	*	*	*	*	*	*	*	*	*
105	beta-vetivone	41(64), 55(41), 91(44), 105(43), 121(50), 147(43), **185(100)**, 203(24), 218(44)	218	*	*	*	*	*	*	*	*	*	*
106	khusenic acid	29(19), 41(71), 55(42), 67(40), 79(45), 91(62), 105(38), 119(78),131(34), **145(100)**, 164(65), 173(24), 191(30), 219(50), 234(26)	234	*	*	*	*	*	*	*	*	*	*
107	alpha-vetivone	41(64), 55(43), 91(51), 105(41), 121(54), 147(41), **185(100)**, 203(23), 218(57)	218	*	*	*	*	*	*	*	*	*	*

* Existenece

3.2.4 Quantitative analysis using GCΔGC-FID

Quantitative determination of the identified vetiver oil components obtained from all extraction techniques was performed by using GCΔGC-FID. All integration profiles were exported as *.csv files, then analyzed using an in-house Matlab program. Similar contour was achieved in all extracts. The quantitation results of all vetiver oil components were listed in Table 3.5. In the absence of a suitable internal standard that could be added to the sample and guarantee to produce a peak that was well resolved from the matrix, peak area normalization was utilized to determine the relative proportions of individual components. The advantage of GCΔGC-FID in terms of separation power has made quantitation of the components of the highly complex sample more accurate than that obtained by GC-FID. In GCΔGC-FID analysis, many components co-eluted in the first dimension were distributed throughout the second dimension plane, resulting in a much higher number of components identified in pure form rather than as overlapped peaks. Consequently, peaks could be reliably detected and matched with the library spectra at lower amounts than that possible by GC-FID analyses where some overlaps existed. Additionally, the greater sensitivity provided by GCΔGC-FID facilitated the quantitation of some minor volatile constituents.

Table 3.5 Relative contents of the identified component in Thai vetiver root oils obtained from different extraction methods using GC×GC-FID

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
1	2,3-dihydrobenzofuran	a	1354																	0.02				
2	2,3-dihydro-4,7-dimethyl-1H-indene	a	1356					0.02				0.01		0.01								0.03		
3	1,2,3,4-tetrahydro-1,1,6-trimethylnaphthalene	a	1356					0.02						0.04						0.02				
4	alpha-cubebene	a	1382	1351		0.09																		
5	9,10-dehydro-2-norzizaene	b	1393		2.33	2.31	0.05	0.05	0.07	0.05			0.09	0.01			0.03	0.03	0.08	0.03	0.07	0.04	0.07	0.01
6	alpha-ylangene	a	1402	1375		0.05																		
7	alpha-funebrene	b	1405	1403	0.10	0.08							0.08	0.03					0.05	0.03				
8	6-butyl-1,2,3,4-tetrahydronaphthalene	b	1406		0.10	0.07							0.04	0.02		0.02			0.04	0.02				
9	2-norzizaene	b	1417		0.05	0.05	0.03	0.03	0.04	0.04			0.04	0.02			0.02	0.02	0.04	0.02	0.05	0.02		
10	7,8-dihydro-8,8-dimethyl-5(6H)-benzocyclooctenone	b	1418		0.09	0.04							0.02	0.02		0.01	0.05	0.03	0.03	0.03	0.03	0.03		
11	(R)- 1,5,5,9-tetramethylSpiro[5.5]undeca-1,8-diene	a	1423		0.21	0.08	0.02	0.02				0.01	0.04	0.02			0.09	0.03			0.06	0.03	0.08	0.05
12	4b,5,6,7,8,8a,9,10-octahydro-1-methylphenanthrene	a	1429		0.09	0.05							0.03	0.03		0.03			0.03	0.03				
13	alpha-cedrene	b	1436	1412	0.09	0.04	0.05	0.02	0.05	0.02		0.06	0.11	0.10	0.09	0.01	0.05	0.08	0.12	0.08	0.08	0.08	0.12	0.10

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
14	beta-copaene	b	1436	1432	0.37	0.21	0.06	0.05	0.07	0.06	0.07	0.03	0.06	0.03	0.10	0.03	0.06	0.05	0.08	0.03	0.10	0.02	0.07	0.02
15	2-[(Z)-3-hexenyl]-1-methyl-3-methylen-1-cyclohexene	b	1442		0.05	0.04							0.05	0.01	0.03	0.02			0.09	0.05	0.02	0.03		0.05
16	gamma-elemene	b	1454	1437	0.07	0.03	0.05	0.03	0.05	0.04	0.08	0.05	0.06	0.04	0.05	0.06	0.07	0.04	0.07	0.05	0.08	0.05	0.06	0.04
17	prezizaene	b	1459	1450	0.09	0.09	0.06	0.05	0.07	0.06	0.05	0.07	0.06	0.09	0.08	0.08	0.09	0.04	0.07	0.06	0.07	0.07	0.09	0.02
18	dehydroaromadendrene	b	1462		0.07	0.05							0.03	0.04	0.02	0.01	0.07	0.02						0.05
19	khusimene	b	1462	1455	0.21	0.06	0.09	0.05	0.08	0.04	0.58	0.12	0.82	0.12	0.48	0.12	0.59	0.11	0.23	0.12	0.45	0.13	0.66	0.12
20	1,2,3,4,5,6-hexahydro-1-methyl-2,2'-bipyridine	a	1464			0.07						0.03		0.06						0.06				
21	beta-acoradiene	a	1467	1471		0.05		0.06		0.06		0.01		0.09		0.02		0.04				0.03		0.04
22	4,7-epoxy-spirovetiva-2,11-diene	a	1468			0.09		0.05		0.04						0.04								
23	ar-curcumene	b	1471	1481	0.30	0.09							0.05	0.02	0.05	0.01								
24	alpha-amorphene	b	1474	1485	0.10	0.09	0.08	0.06	0.06	0.06	0.07	0.04	0.11	0.07	0.10	0.05	0.06	0.06	0.10	0.05	0.10	0.06	0.07	0.05
25	cyclocopacamphan-12-al	b	1476		0.20	0.08	0.14	0.08	0.13	0.10	0.09	0.08	0.11	0.05	0.14	0.04			0.15	0.01	0.11	0.06	0.08	0.04
26	delta-silenene	b	1477	1493	0.27	0.07	0.09	0.02		0.07		0.08	0.09	0.04	0.10	0.04	0.10	0.04	0.08	0.07	0.06	0.08	0.10	0.09
27	beta-vetispirene	a	1479	1495		0.02																		
28	gamma-amorphene	b	1484	1496	0.05	0.04	0.02	0.02					0.04	0.03	0.04	0.04	0.02	0.03	0.10	0.05			0.05	0.04

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
29	cis-eudesma-6,11-diene	a	1484	1490		0.08		0.07		0.05		0.10		0.11		0.11		0.11		0.10		0.11		0.13
30	trans-beta-guaiene	a	1490	1503		0.06				0.08				0.07										
31	delta-amorphene	b	1491	1512	0.31	0.07	0.14	0.07	0.16	0.09	0.12	0.12	0.14	0.12	0.15	0.13	0.16	0.12	0.13	0.15	0.13	0.04		
32	beta-curcumene	a	1493	1514		0.06		0.05		0.05		0.08		0.09		0.08		0.06		0.05		0.04		0.05
33	11,12,13-tri-nor-cis-eudesma-5,8-dien-7-one	b	1496	w(1517)			0.07	0.03	0.04	0.02			0.06	0.05	0.08	0.06	0.02	0.02	0.05	0.03	0.12	0.06	0.08	0.06
34	6H-3a,7-methanoazulen-6-one	a	1500			0.07																		
35	(+-)-2-methyl-6-p-tolyl-4-heptanol	b	1501		0.04	0.04							0.03	0.03	0.02	0.02	0.02	0.02			0.04	0.03	0.05	
36	cis-dihydroagarofuran	a	1501	1520		0.11		0.09		0.11		0.05		0.05		0.06		0.04		0.04		0.05		0.07
37	3,4-dihydro-4,6,7-trimethyl-1(2H)-naphthalenone	a	1503					0.02		0.04														
38	8-isopropenyl-3,3,7-trimethylbicyclo[5.1.0]oct-5-en-2-one	b	1508		0.34	0.05	0.10	0.03	0.25	0.10	0.11	0.06	0.06	0.07	0.03	0.07	0.03	0.05	0.14	0.04	0.03	0.07	0.02	0.07
39	delta-cadinene	a	1508	1523		0.02				0.02				0.02		0.02								
40	gamma-vetivenene	b	1527	1533	0.13	0.05	0.14	0.03	0.13	0.10	0.13	0.08	0.14	0.04	0.13	0.03	0.10	0.05	0.13	0.11	0.14	0.05	0.14	0.06
41	trans-calamenene	b	1534	1529	0.36	0.25	0.07	0.04	0.07	0.03	0.06	0.06	0.06	0.01	0.04	0.05	0.05	0.05	0.07	0.07	0.04	0.06	0.04	0.05
42	1a,2,6,7,7a,7b-hexahydro-1,1,7,7a-tetramethyl-1H-cyclopropa[a]naphthalene	b	1534		0.05	0.04	0.03	0.03	0.03	0.03	0.01	0.01	0.06	0.02			0.04	0.02	0.05	0.03	0.04	0.03	0.03	0.03

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																			
					SDE 24 hrs		SFE						SE						MAE					
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
43	3-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-2-propenal	b	1536		0.11	0.09	0.07	0.09	0.10	0.06	0.09	0.08	0.13	0.10	0.10	0.08	0.09	0.08	0.11	0.09	0.10	0.08	0.09	0.05
44	beta-calacorene	b	1538	1546	0.21	0.11	0.16	0.10	0.14	0.12	0.12	0.07	0.16	0.15	0.11	0.16	0.16	0.06	0.15	0.10	0.15	0.06	0.16	0.13
45	zingiberene	b	1538		0.10	0.08	0.11	0.04	0.10	0.04	0.08	0.04	0.04	0.05	0.03	0.04	0.03	0.05	0.04	0.06	0.04	0.07	0.04	0.08
46	6,12-epoxy-elema-1,3-diene	b	1540	w(1547)	0.15	0.07	0.12	0.04	0.10	0.08	0.11	0.09	0.11	0.07	0.16	0.10	0.12	0.11	0.09	0.09	0.10	0.10	0.12	0.10
47	13-nor-eudesm-5-en-11-one	b	1542	w(1547)	2.23	2.20	1.18	1.10	1.03	0.98	0.93	0.70	0.88	0.82	1.04	1.02	0.66	0.63	1.00	0.91	0.89	0.50	7.00	0.64
48	elemol	b	1542	1550							0.13	0.06					0.19	0.15					0.17	0.06
49	alpha-agarofuran	a	1547	1550	0.30	0.25	0.31	0.22	0.21	0.21	0.22	0.23	0.25	0.22	0.27	0.22	0.30	0.23	0.32	0.21	0.24	0.20	0.25	0.21
50	(+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one	b	1550		1.45	1.02	0.71	0.63	0.72	0.55	0.74	0.56	0.80	0.59	0.66	0.57	0.65	0.58	0.70	0.54	0.70	0.56	0.79	0.43
51	15-nor-prezizaan-7-one	a	1558	w(1540)	0.20	0.14	0.21	0.15	0.22	0.13	0.25	0.11	0.12	0.12	0.15	0.12	0.21	0.15	0.24	0.14	0.23	0.14	0.22	0.12
52	cascarilladienol	a	1559	w(1551)	0.10	0.05	0.09	0.04	0.14	0.07	0.08	0.02	0.09	0.04	0.12	0.06	0.04	0.01	0.08	0.03	0.07	0.04	0.09	0.06
53	12-nor-2,3-epoxy-ziza-6(13)-ene	b	1564	w(1551)	0.13	0.12	0.10	0.14	0.12	0.12	0.10	0.12	0.12	0.14	0.15	0.04	0.14	0.07	0.15	0.08	0.13	0.05	0.12	0.08
54	cis-eudesm-6-en-11-ol	b	1565	w(1566)	0.14	0.14	0.15	0.14	0.20	0.16	0.14	0.15	0.20	0.17	0.15	0.12	0.15	0.13	0.16	0.14	0.15	0.12	0.20	0.15
55	2-acetyl-5,6,7,8-tetrahydroquinoxaline	a	1565		0.25	0.21	0.24	0.24	0.23	0.23	0.30	0.25	0.32	0.24	0.25	0.25	0.28	0.22	0.21	0.22	0.25	0.22	0.26	0.27
56	12-nor-preziza-7(15)-en-2-one	b	1567	w(1566)	0.45	0.12	0.24	0.13	0.23	0.12	0.21	0.11	0.24	0.14	0.20	0.13	0.24	0.12	0.21	0.11	0.21	0.13	0.29	0.12

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
57	15-nor-funebran-3-one	b	1568	w(1562)	1.34	1.11	0.33	0.25	0.35	0.34	0.37	0.31	0.37	0.32	0.31	0.25	0.33	0.30	0.34	0.33	0.37	0.32	0.35	0.34
58	4-(2,2-dimethyl-6-methylenecyclohexylidene)-3-methylidene-2-one	b	1576		0.82	0.50	0.52	0.41	0.53	0.44	0.52	0.44	0.52	0.45	0.56	0.54	0.55	0.55	0.51	0.52	0.57	0.46	0.59	0.44
59	clovane	b	1587		0.11	0.08	0.10	0.05	0.13	0.04	0.15	0.07	0.11	0.06	0.11	0.05	0.08	0.02	0.10	0.08	0.06	0.04	0.14	0.05
60	cyclocopacamphan-12-ol	a	1590	w(1643)	0.11	0.06	0.09	0.03	0.07	0.03	0.08	0.02	0.05	0.03	0.08	0.02	0.10	0.07			0.14	0.05	0.10	0.02
61	13-nor-eremophil-1(10)-en-11-one	a	1590	w(1598)	0.15	0.08	0.10	0.02	0.08	0.02					0.04	0.03	0.04	0.01	0.05	0.02	0.10	0.01	0.07	0.01
62	khusimone	b	1598	1604	2.37	2.10	1.24	1.11	1.20	1.15	1.25	1.05	1.26	1.04	1.24	1.06	1.26	1.17	1.20	1.05	1.20	1.16	1.35	1.22
63	trans-dracunculifoliol	b	1600	w(1582)	0.34	0.28	0.41	0.39	0.32	0.38	0.26	0.16	0.25	0.22	0.20	0.19	0.16	0.09	0.28	0.21	0.16	0.13	0.19	0.12
64	10-epi-gamma-eudesmol	a	1602	1624	0.45	0.36	0.35	0.30	0.41	0.31	0.42	0.31	0.48	0.32	0.45	0.35	0.35	0.30	0.41	0.29	0.29	0.28	0.29	0.25
65	10-epi-cubenol-12-nor-ziza-6(13)-en- -ol	a	1604	w(1598)	0.10	0.05	0.14	0.06	0.15	0.07	0.13	0.04	0.09	0.05	0.09	0.06	0.10	0.05	0.11	0.06	0.14	0.04	0.10	0.07
66	12-nor-ziza-6(13)-en- -ol	a	1606	w(1603)	0.14	0.09	0.12	0.09	0.20	0.13	0.14	0.08	0.15	0.09	0.18	0.10	0.21	0.11	0.14	0.09	0.24	0.12	0.25	0.14
67	epoxy-allo-alloaromadendrene	a	1611	1641	0.21	0.14	0.18	0.11	0.24	0.12	0.24	0.14	0.28	0.14	0.22	0.10	0.21	0.10	0.23	0.11	0.15	0.08	0.24	0.10
68	eremophila-1(10),6-dien-12-al	a	1616	w(1625)	0.30	0.24	0.35	0.22	0.36	0.23	0.33	0.24	0.32	0.26	0.36	0.21	0.33	0.22	0.24	0.23	0.26	0.22	0.28	0.20
69	13-nor-eremophila-1(10),6-dien-11-one	a	1616	w(1617)	0.15	0.09	0.16	0.10	0.14	0.11	0.13	0.12	0.15	0.15	0.11	0.12	0.15	0.13	0.12	0.14	0.14	0.14	0.12	0.15
70	-funebren-15-al	a	1618	w(1625)	0.15	0.10	0.18	0.13	0.11	0.06	0.18	0.10	0.08	0.04	0.24	0.13	0.17	0.09	0.19	0.11	0.10	0.08		0.12
71	tris(1-methylethyl)-benzene	a	1618		1.40	1.10	1.23	1.09	1.32	1.00	1.14	0.93	1.18	0.98	1.14	1.08	1.22	0.97	1.15	1.03	1.25	0.91		0.96

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
72	13-nor-trans-eudesma-4(15),7-dien-11-one	b	1632	w(1645)	0.10	0.08	0.79	0.50	0.74	0.45	0.77	0.47	0.72	0.48	0.71	0.42	0.70	0.41	0.68	0.42	0.70	0.47	0.69	0.49
73	eudesm-4(15),7-dien- -ol	b	1638	w(1638)	0.71	0.10	0.45	0.10	0.42	0.12	0.46	0.15	0.45	0.14	0.40	0.15	0.42	0.15	0.41	0.10	0.43	0.12	0.40	0.13
74	valerianol	b	1645	1654	2.04	0.10	1.30	0.12	1.10	0.13	1.20	0.19	1.30	0.12	1.32	0.11	1.22	0.17	1.33	0.17	1.25	0.16	1.25	0.11
75	7,15-epoxy-prezizaane	a	1646	w(1628)	0.10	0.06		0.04		0.07		0.04		0.06		0.04		0.02		0.10		0.03		0.03
76	4,8-dimethyl-1-(1-methylethyl)-spiro[4.5]dec-8-en-7-ol	a	1647		1.32	1.17	1.23	1.00	1.25	1.03	1.20	1.07	1.40	1.05	1.12	0.91	1.22	1.07	1.25	1.06	1.26	1.07	1.25	1.18
77	allo-khusiol	a	1655	w(1628)	0.25	0.18	0.28	0.18	0.30	0.25	0.24	0.26	0.35	0.21	0.25	0.17	0.30	0.21	0.21	0.21	0.28	0.22	0.32	0.20
78	acorenone	b	1667	1693	0.63	0.25	0.15	0.23	0.13	0.21	0.11	0.22	0.25	0.16	0.22	0.13	0.28	0.15	0.38	0.25	0.25	0.22	0.29	0.26
79	prezizaan-15-al	a	1667	w(1663)	0.41	0.31	0.33	0.23	0.32	0.21	0.30	0.26	0.35	0.23	0.41	0.26	0.36	0.29	0.32	0.23	0.33	0.25	0.39	0.24
80	E-opposita-4(15),7(11)-dien-12-al	b	1671	w(1679)			0.33	0.23							0.21	0.15			0.15	0.17				
81	zizanal	b	1671	1697	0.22	0.22	0.25	0.20	0.22	0.21	0.25	0.22	0.28	0.23	0.22	0.22	0.20	0.23	0.25	0.23	0.29	0.22	0.25	0.20
82	2-epi-ziza-6(13)-en-3-one	b	1673	w(1657)	0.30	1.23	0.19	1.22	0.36	1.22	0.22	1.22	0.37	1.23	0.15	1.11	0.12	1.12	0.17	1.24	0.25	1.22	0.25	1.23
83	khusian-2-ol	b	1678	w(1668)		0.23	1.03	0.23	0.99	0.27	1.00	0.24	0.96	0.27	0.88	0.27	0.63	0.27	0.98	0.28	1.16	0.26	0.87	0.25
84	ziza-6(13)-en-3-one	a	1678			0.15	0.23	0.05	0.25	0.20	0.23	0.18	0.26	0.15	0.19	0.18	0.17	0.14	0.26	0.16	0.29	0.20	0.31	0.24
85	eudesma-4(15),7-dien- -ol	b	1684	w(1679)	0.80	0.14	0.47	0.14	0.44	0.19	0.44	0.11	0.52	0.13	0.53	0.12	0.50	0.13	0.64	0.11	0.82	0.13	0.68	0.11
86	13-nor-eudesma-4,6-dien-11-one	b	1685	w(1692)		0.31	0.23	0.25	0.11	0.25	0.19	0.25	0.34	0.23	0.33	0.23	0.26	0.24	0.40	0.20	0.48	0.24	0.38	0.20

Table 3.5 (continued)

No.	Component		LTP RI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
87	eudesma-3,5-dien- -ol	b	1685	w(1704)	0.11	0.09		0.02		0.04		0.01		0.02				0.04		0.01		0.02		0.01
88	(E)-opposita-4(15),7(11)-dien-12-ol	a	1685	w(1687)		0.24		0.22		0.20		0.23		0.21		0.22		0.22		0.21		0.22		0.22
89	cadina-1(10),6,8-triene	b	1694			0.14	1.04	1.11	1.35	1.51	1.05	1.06	1.48	1.45	1.16	1.14	1.40	1.20	1.00	1.05	1.19	1.00	1.35	1.30
90	preziza-7(15)-en- -ol	a	1694	w(1663)		0.11		0.12		0.12		0.13		0.11		0.12		0.13		0.11		0.12		0.15
91	13-nor-7,8-epoxy-trans-eudesm-4(15)-en-11-one	a	1705	w(1653)				0.44		0.46		0.41		0.41		0.40		0.40		0.42		0.40		0.43
92	ziza-6(13)-en- -ol	a	1711	w(1663)	0.22	0.16		0.03		0.01		0.01						0.02		0.01		0.01		0.01
93	eudesma-3,5-dien- -ol	a	1719	w(1708)		0.50	0.55	0.41	0.48	0.43	0.44	0.45	0.43	0.41	0.52	0.39	0.41	0.28	0.40	0.41	0.42	0.40	0.36	0.40
94	2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-1H-3a,7-methanoazulene-6-methanol	a	1725			0.17		0.18		0.14		0.11		0.12		0.10		0.10		0.14		0.12		0.14
95	oplopanone	b	1728	1740	2.44	1.36	5.11	1.15	4.96	1.16	5.05	1.16	4.27	1.15	4.53	1.15	4.60	1.15	4.27	1.15	4.37	1.14	4.34	1.15
96	1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(2-propenyl)-1-naphthalenol	a	1734			1.23		1.02		1.03		1.03		1.04		1.03		1.02		1.03		1.03		1.04
97	prezizanol	b	1748		0.34	0.90	1.12	0.88	1.01	0.85	1.10	0.81	1.75	0.80	1.46	0.80	1.84	0.81	1.20	0.87	1.05	0.94	1.27	0.85
98	khusimol	b	1762	1743	19.26	5.59	11.39	3.25	11.02	3.26	10.82	3.25	10.08	3.27	10.08	3.29	10.79	3.46	10.11	3.47	10.10	3.45	9.27	3.46
99	bicyclovetivenol	b	1790	1793	2.06	2.10	1.19	1.14	1.02	1.12	0.90	1.17	0.94	1.13	1.12	1.14	1.13	1.13	1.24	1.13	1.26	1.13	1.02	1.15

Table 3.5 (continued)

No.	Component		LTPRI	Adams' RI	% Relative content																	
					SDE 24 hrs		SFE						SE						MAE			
							toluene		DCM		methanol		toluene		DCM		methanol		toluene		DCM		methanol	
					A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
100	9,10-dehydro-isolongifolene	b	1798		0.74	0.54	0.62	0.48	0.54	0.40	0.52	0.44	0.58	0.42	0.55	0.46	0.52	0.42	0.60	0.45	0.62	0.45	0.54	0.46
101	nootkatone	b	1804	1807	2.43	1.12	1.49	1.12	1.39	1.14	1.38	1.14	1.56	1.13	1.51	1.14	1.58	1.10	1.46	1.03	1.71	1.17	1.51	1.17
102	1-O-acetyl-2-methyl-naphthalene-1,4-diol	a	1819			0.88		0.74		0.71		0.70		0.71		0.74		0.74		0.71		0.71		0.70
103	2,2,4-trimethylfuro[6,7-c]-1,3,8H-azulene	a	1828			0.44		0.34		0.32		0.36		0.31		0.32		0.34		0.32		0.38		0.35
104	(+)-decahydro-4,8,8,9-tetramethyl-1,4-Methanoazulen-7-ol	a	1834			0.60		0.58		0.57		0.52		0.51		0.50		0.52		0.53		0.58		0.57
105	beta-vetivone	b	1843	1823	0.34	0.25	0.31	0.26	0.38	0.29	0.32	0.25	0.33	0.21	0.31	0.25	0.30	0.27	0.31	0.25	0.32	0.26	0.36	0.23
106	khusenic acid	b	1849		24.10	22.85	37.64	31.20	39.73	30.50	30.95	29.50	31.27	28.52	31.36	30.98	34.86	31.24	35.48	31.16	36.03	31.32	32.15	30.24
107	alpha-vetivone	b	1856	1843	1.66	1.05	1.88	1.08	0.12	1.09	1.07	1.08	2.50	1.07	2.23	1.08	1.46	1.05	2.20	1.08	2.24	1.07	1.68	1.06
	ea a ea o e iden i ied co onen s				89.16	61.37	80.08	58.99	79.08	58.82	70.42	56.43	73.97	56.34	72.22	58.15	75.51	58.17	76.16	58.90	77.35	58.33	76.86	57.87

[a] found in GC×GC not GC

[b] found in GC×GC and GC

A %relative content in GC

B %relative content in GC×GC

w(xxxx); Weyerstashl *et al.*[22] (LTPRI on 100% dimethyl polysiloxane phase)

LTPRI; linear temperature program retention indices

Different extraction techniques were found to play an important role in the relative contents of the vetiver oil components. Summation of the percentage peak areas of the identified components in all vetiver oil samples, compared with the total response of all peaks in the chromatogram calculated for the GCΔGC-FID analysis varied from 56.4 to 61.4 %. Thus, the residual unidentified composition is of the order of 40-45%. This fraction of the identified components can be increased through the optimization of the modulation time. According to the work of Davis and co-workers[182] on the statistic overlap theory (SOT), for the same standard deviations, changing of modulation time had a little effect on maxima single component peak (SCP) numbers. This is due to many wrapped around components lay in an otherwise virtually empty region of GC×GC-FID contour plot. As can be seen in Figure 3.4A, many polar components had a longer retention time in second column which were being overlapped and wrapped around in 2D plane although the optimum condition of 6 s modulation period was employed. This may result in the decreasing of the resolution and the maxima SCP. Table 3.6 demonstrates the average % relative contents of the identified components in all samples with their variation and total numbers of time detected of each component in GC-FID and GC×GC-FID chromatogram. Wide range variation of % relative content of each component was observed with the compounds such as (+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one (0.43-1.02), 15-nor-funebran-3-one (0.25-1.34), trans-dracunculifoliol (0.09-0.41) and eudesm-4(15),7-dien- -ol (0.10-0.71). The relation between numbers of times detected and % relative content of each component in GC-FID and GC×GC-FID are shown in Figure 3.8 and Figure 3.9, respectively. Similar plots were illustrated in both figures. Most of components were found in all different extracts by

using GC-FID and GC×GC-FID. Many identified components with trace amounts were also detected in both techniques. Frequency of components detected 3, 5, 6, 8 and 9 times in GC-FID was the same as those obtained by GC×GC-FID analysis. However, frequency of components detected 2, 4, 7 and 10 times by GC×GC-FID was higher than those obtained by GC-FID while number of components observed 1 time by GC-FID showed contrary result. In overall, twenty components were not detected by GC-FID (0 times). Average relative content of some components detected 1 and 9 times by GC-FID such as 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(2-propenyl)-1-naphthalenol and tris(1-methylethyl)-benzene were much greater in content of 1.09 % and 1.11 % than those obtained by GC×GC-FID. In addition, the relation between numbers of times detected and average % relative content of all identified components by GC-FID and GC×GC-FID are displayed in Figure 3.10 and Figure 3.11, respectively. A similar plot was achieved in GC-FID and GC×GC-FID. It is remarkable that these graphs are not simply a linear increase of number of times versus amount. Amount of most components detected by GC×GC-FID was reduced compared to GC-FID. However, some peaks detected by GC-FID for 0 or 1 time had reasonable areas when analyzed by GC×GC-FID which provided greater sensitivity. The obtained results seem to suggest that peak identification frequency across the different extracts is not really related to component amount in GC×GC-FID. However, GC×GC-FID technique gives successful detection across the total range of solute amounts.

Table 3.6 Average relative contents of the identified component in all samples with its variation and total numbers of time detected in GC and GC×GC

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
1	2,3-dihydrobenzofuran	0.02	0.02	1	0.001	0	1
2	2,3-dihydro-4,7-dimethyl-1H-indene	0.02	0.01-0.03	4	0.004	0	4
3	1,2,3,4-tetrahydro-1,1,6-trimethylnaphthalene	0.03	0.02-0.04	3	0.004	0	3
4	alpha-cubebene	0.09	0.09	1	0.005	0	1
5	9,10-dehydro-2-norzizaene	0.33	0.01-2.33	16	0.266	8	8
6	alpha-ylangene	0.05	0.05	1	0.003	0	1
7	alpha-funebrene	0.06	0.03-0.10	6	0.019	3	3
8	6-butyl-1,2,3,4-tetrahydronaphthalene	0.04	0.02-0.10	7	0.016	3	4
9	2-norzizaene	0.03	0.02-0.05	14	0.024	7	7
10	7,8-dihydro-8,8-dimethyl-5(6H)-benzocyclooctenone	0.03	0.01-0.09	11	0.019	5	6
11	(R)- 1,5,5,9-tetramethylSpiro[5.5]undeca-1,8-diene	0.06	0.03-0.21	13	0.037	6	7
12	4b,5,6,7,8,8a,9,10-octahydro-1-methylphenanthrene	0.04	0.03-0.09	7	0.014	3	4
13	alpha-cedrene	0.07	0.01-0.12	19	0.068	9	10
14	beta-copaene	0.08	0.02-0.37	20	0.078	10	10
15	2-[(Z)-3-hexenyl]-1-methyl-3-methylen-1-cyclohexene	0.04	0.01-0.09	11	0.022	5	6

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
16	gamma-elemene	0.05	0.03-0.08	20	0.054	10	10
17	prezizaene	0.07	0.02-0.09	20	0.068	10	10
18	dehydroaromadendrene	0.04	0.02-0.07	9	0.018	4	5
19	khusimene	0.26	0.04-0.82	20	0.259	10	10
20	1,2,3,4,5,6-hexahydro-1-methyl-2,2'-bipyridine	0.06	0.03-0.07	4	0.011	0	4
21	beta-acoradiene	0.04	0.01-0.09	9	0.020	0	9
22	4,7-epoxy-spirovetiva-2,11-diene	0.06	0.04-0.09	4	0.011	0	4
23	ar-curcumene	0.09	0.01-0.09	6	0.026	3	3
24	alpha-amorphene	0.07	0.04-0.11	20	0.072	10	10
25	cyclocopacamphan-12-al	0.09	0.04-0.15	18	0.085	9	9
26	delta-silenene	0.08	0.02-0.10	18	0.075	8	10
27	beta-vetispirene	0.02	0.02	1	0.001	0	1
28	gamma-amorphene	0.04	0.02-0.05	14	0.028	7	7
29	cis-eudesma-6,11-diene	0.10	0.05-0.13	10	0.049	0	10
30	trans-beta-guaiene	0.07	0.06-0.08	3	0.010	0	3
31	delta-amorphene	0.13	0.04-0.31	18	0.118	9	9

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
32	beta-curcumene	0.06	0.04-0.06	10	0.031	0	10
33	11,12,13-tri-nor-cis-eudesma-5,8-dien-7-one	0.05	0.02-0.07	16	0.043	8	8
34	6H-3a,7-methanoazulen-6-one	0.07	0.07	1	0.004	0	1
35	(+-)-2-methyl-6-p-tolyl-4-heptanol	0.03	0.02-0.04	11	0.017	6	5
36	cis-dihydroagarofuran	0.07	0.04-0.11	10	0.034	0	10
37	3,4-dihydro-4,6,7-trimethyl-1(2H)-naphthalenone	0.03	0.02-0.04	2	0.003	0	2
38	8-isopropenyl-3,3,7-trimethylbicyclo[5.1.0]oct-5-en-2-one	0.09	0.03-0.11	20	0.086	10	10
39	delta-cadinene	0.02	0.02	4	0.004	0	4
40	gamma-vetivenene	0.10	0.03-0.14	20	0.096	10	10
41	trans-calamenene	0.08	0.04-0.36	20	0.077	10	10
42	1a,2,6,7,7a,7b-hexahydro-1,1,7,7a-tetramethyl-1H-cyclopropa[a]naphthalene	0.03	0.01-0.06	18	0.028	9	9
43	3-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-2-propenal	0.09	0.05-0.11	20	0.090	10	10
44	beta-calacorene	0.13	0.06-0.21	20	0.129	10	10
45	zingiberene	0.06	0.03-0.10	20	0.058	10	10
46	6,12-epoxy-elema-1,3-diene	0.10	0.07-0.15	20	0.102	10	10

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
47	13-nor-eudesm-5-en-11-one	1.32	0.63-2.23	20	1.317	10	10
48	elemol	0.13	0.06-0.19	6	0.038	3	3
49	alpha-agarofuran	0.24	0.20-0.31	20	0.244	10	10
50	(+)(6S,10R)-6,10-dimethylbicyclo[4.4.0]dec-1-en-3-one	0.70	0.43-1.02	20	0.698	10	10
51	15-nor-prezizaan-7-one	0.17	0.11-0.22	20	0.169	10	10
52	cascarilladienol	0.07	0.04-0.14	20	0.066	10	10
53	12-nor-2,3-epoxy-ziza-6(13)-ene	0.11	0.04-0.15	20	0.111	10	10
54	cis-eudesm-6-en-11-ol	0.15	0.12-0.20	20	0.153	10	10
55	2-acetyl-5,6,7,8-tetrahydroquinoxaline	0.25	0.21-0.32	20	0.247	10	10
56	12-nor-preziza-7(15)-en-2-one	0.19	0.11-0.45	20	0.187	10	10
57	15-nor-funebran-3-one	0.42	0.25-1.34	20	0.417	10	10
58	4-(2,2-dimethyl-6-methylenecyclohexylidene)-3-methylidene-2-one	0.52	0.41-0.82	20	0.522	10	10
59	clovane	0.08	0.02-0.11	20	0.082	10	10
60	cyclocopacamphan-12-ol	0.06	0.02-0.14	18	0.057	9	9
61	13-nor-eremophil-1(10)-en-11-one	0.05	0.01-0.15	16	0.041	8	8
62	khusimone	1.28	1.05-2.37	20	1.284	10	10

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
63	trans-dracunculifoliol	0.24	0.09-0.41	20	0.237	10	10
64	10-epi-gamma-eudesmol	0.35	0.25-0.45	20	0.349	10	10
65	10-epi-cubenol-12-nor-ziza-6(13)-en- -ol	0.09	0.04-0.14	20	0.085	10	10
66	12-nor-ziza-6(13)-en- -ol	0.14	0.08-0.25	20	0.141	10	10
67	epoxy-allo-alloaromadendrene	0.17	0.10-0.24	20	0.167	10	10
68	eremophila-1(10),6-dien-12-al	0.27	0.20-0.36	20	0.270	10	10
69	13-nor-eremophila-1(10),6-dien-11-one	0.13	0.10-0.15	20	0.131	10	10
70	-funebren-15-al	0.12	0.06-0.24	19	0.119	9	10
71	tris(1-methylethyl)-benzene	1.11	0.93-1.32	19	1.055	9	10
72	13-nor-trans-eudesma-4(15),7-dien-11-one	0.58	0.42-0.77	20	0.576	10	10
73	eudesm-4(15),7-dien- -ol	0.29	0.10-0.71	20	0.290	10	10
74	valerianol	0.73	0.10-2.04	20	0.734	10	10
75	7,15-epoxy-prezizaane	0.05	0.03-0.10	11	0.029	1	10
76	4,8-dimethyl-1-(1-methylethyl)-spiro[4.5]dec-8-en-7-ol	1.16	0.91-1.32	20	1.156	10	10
77	allo-khusiol	0.24	0.17-0.32	20	0.244	10	10
78	acorenone	0.24	0.11-0.63	20	0.238	10	10

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
79	prezizaan-15-al	0.30	0.21-0.41	20	0.302	10	10
80	E-opposita-4(15),7(11)-dien-12-al	0.21	0.15-0.33	6	0.062	3	3
81	zizanal	0.23	0.20-0.29	20	0.231	10	10
82	2-epi-ziza-6(13)-en-3-one	0.72	0.30-1.24	20	0.721	10	10
83	khusian-2-ol	0.68	0.23-2.58	20	0.682	10	10
84	ziza-6(13)-en-3-one	0.20	0.05-0.31	20	0.204	10	10
85	eudesma-4(15),7-dien- -ol	0.36	0.11-0.82	20	0.358	10	10
86	13-nor-eudesma-4,6-dien-11-one	0.31	0.11-1.01	20	0.307	10	10
87	eudesma-3,5-dien- -ol	0.04	0.01-0.11	10	0.018	1	9
88	(E)-opposita-4(15),7(11)-dien-12-ol	0.22	0.20-0.28	11	0.124	1	10
89	cadina-1(10),6,8-triene	1.20	1.04-2.05	20	1.202	10	10
90	preziza-7(15)-en- -ol	0.12	0.11-0.15	11	0.069	1	10
91	13-nor-7,8-epoxy-trans-eudesm-4(15)-en-11-one	0.42	0.40-0.46	9	0.189	0	9
92	ziza-6(13)-en- -ol	0.05	0.01-0.22	9	0.023	1	8
93	eudesma-3,5-dien- -ol	0.43	0.28-0.55	20	0.430	10	10

Table 3.6 (continued)

No.	Structural assignment	Average relative content (%)	% Relative content variations	Total No. of times detected	Norm average amount (amnt/n) max =20	Total No. of times detected (1DGC)	Total No. of times detected (GC×GC)
94	2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-1H-3a,7-methanoazulene-6-methanol	0.14	0.10-0.23	11	0.078	1	10
95	oplopanone	2.78	1.14-5.05	20	2.782	10	10
96	1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(2-propenyl)-1-naphthalenol	1.09	1.02-1.50	11	0.599	1	10
97	prezizanol	1.03	0.34-1.84	20	1.033	10	10
98	khusimol	7.43	3.25-19.26	20	7.433	10	10
99	bicyclovetivenol	1.21	0.90-2.10	20	1.210	10	10
100	9,10-dehydro-isolongifolene	0.52	0.40-0.74	20	0.518	10	10
101	nootkatone	1.36	1.12-2.43	20	1.364	10	10
102	1-O-acetyl-2-methyl-naphthalene-1,4-diol	0.74	0.70-0.88	10	0.368	0	10
103	2,2,4-trimethylfuro[6,7-c]-1,3,8H-azulene	0.35	0.31-0.44	10	0.174	0	10
104	(+)-decahydro-4,8,8,9-tetramethyl-1,4-Methanoazulen-7-ol	0.55	0.50-0.60	10	0.274	0	10
105	beta-vetivone	0.29	0.21-0.36	20	0.290	10	10
106	khusenic acid	31.55	22.85-39.73	20	31.554	10	10
107	alpha-vetivone	1.39	1.02-2.50	20	1.388	10	10

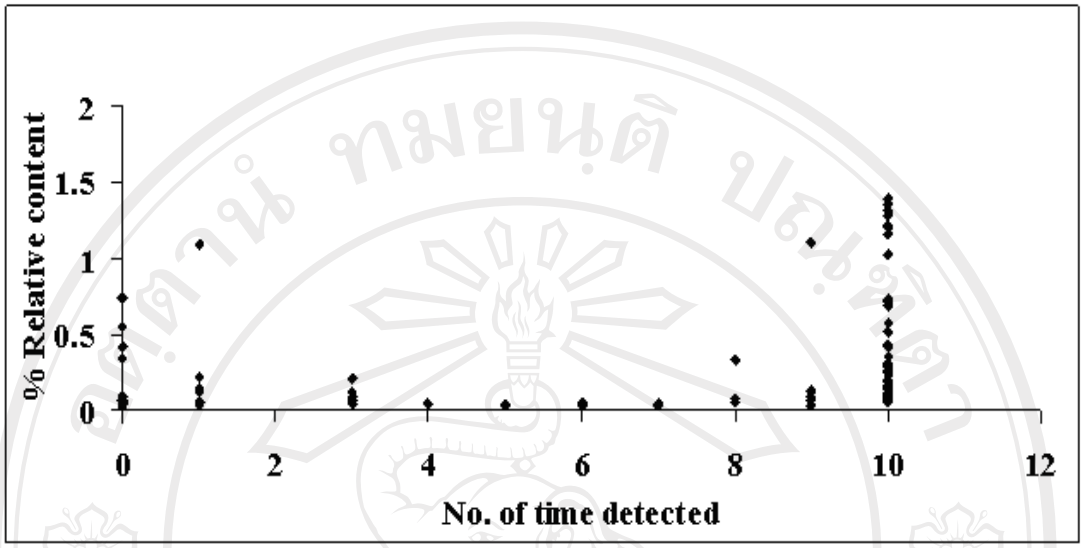


Figure 3.8 The relation between number of times detected and % relative content of all identified components in GC plot

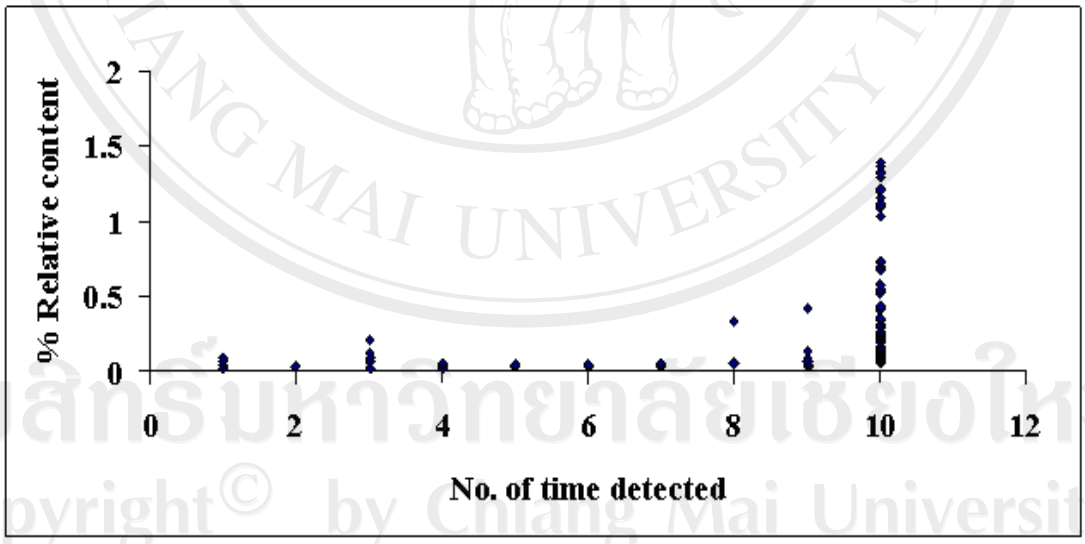


Figure 3.9 The relation between number of times detected and % relative content of all identified components in GC×GC plot

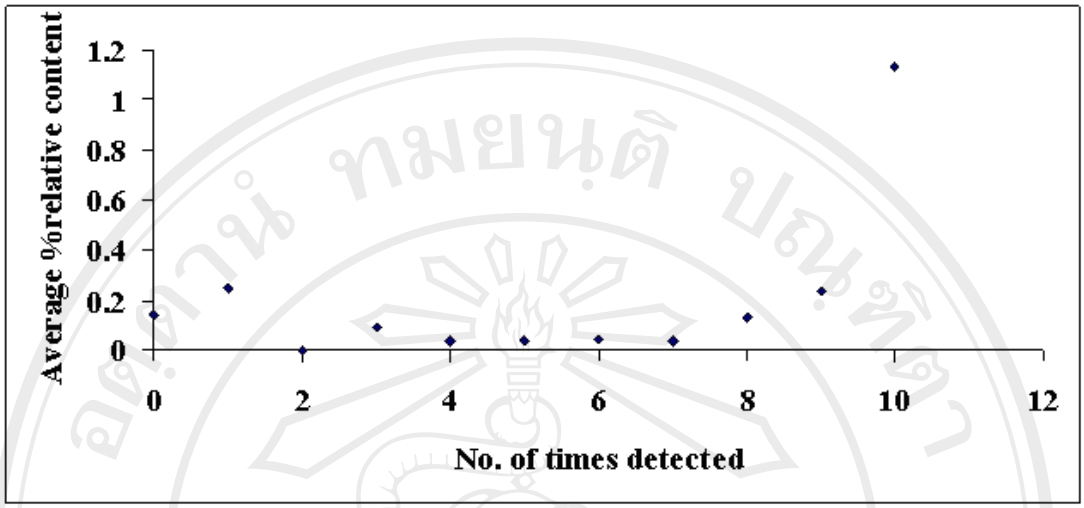


Figure 3.10 The relation between number of times detected and average % relative content of all identified components in GC plot

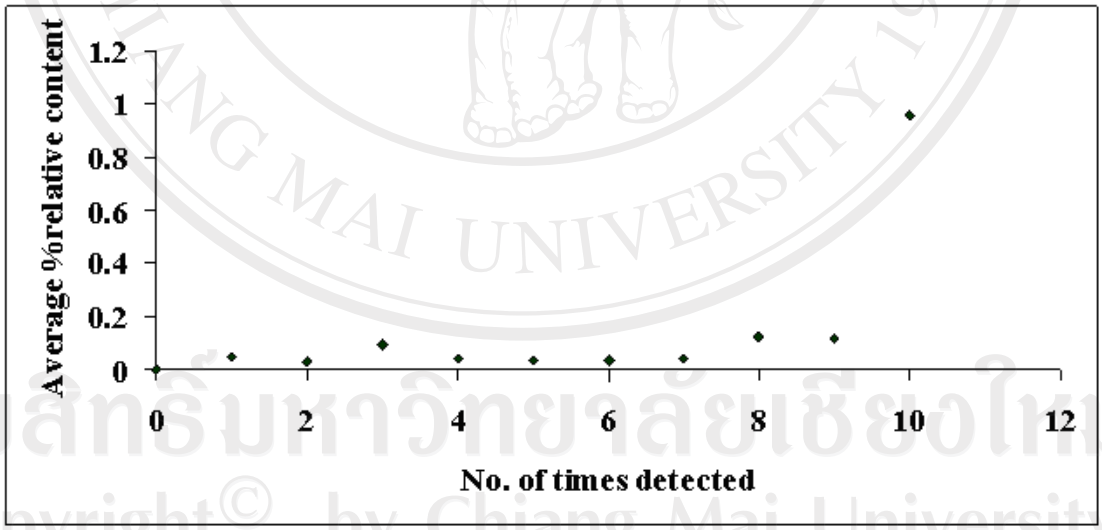


Figure 3.11 The relation between number of times detected and average % relative content of all identified components in GC×GC plot