CHAPTER III

RESULTS AND DISSCUSSIONS

This work was emphasized on the isolation of aroma compounds of scented vetiver root (*Vetiveria zizanioides* Nash). It consisted of two parts. First part involved the investigation of volatiles in scented vetiver root that contributed to aroma character of the root. According to this, extraction of volatiles from the raw root was performed using SPME technique employing a PDMS fiber for adsorption of the volatiles. Separation and structural identification of the volatile components was then performed by GC-MS. The volatile compounds were identified by comparing their mass spectra with the Wiley 275 mass spectral library. The SPME-GC-MS analysis was studied at room temperature (30°C) and also at higher temperature.

In the second part, the volatile components that involved in aroma character of the scented vetiver root were isolated for further investigation on their chemical structures. The components were first extracted by maceration in dichloromethane. Then, the components in a crude extract were separated using chromatographic techniques utilizing spectroscopic detectors. The fractions and components obtained from each separation were tested for aroma quality by sensory evaluation method. The aroma-active component isolated was finally analyzed by GC-MS.

3.1 Investigation of the aroma components in scented vetiver roots using SPME-GC-MS

3.1.1 SPME-GC-MS analysis at room temperature (30 °C)

Extraction of volatile compounds in scented vetiver root by SPME was performed using a polydimethylsiloxane (PDMS) fiber followed by separation and identification by GC-MS. The procedures of this experiment were presented in **Fig. 2.1**. All extracted volatile compounds were resolved showing the SPME-GC-MS chromatograms in **Fig. 3.1A, B, C** and **D**. Mass spectral data were summarized in **Table 3.1**.

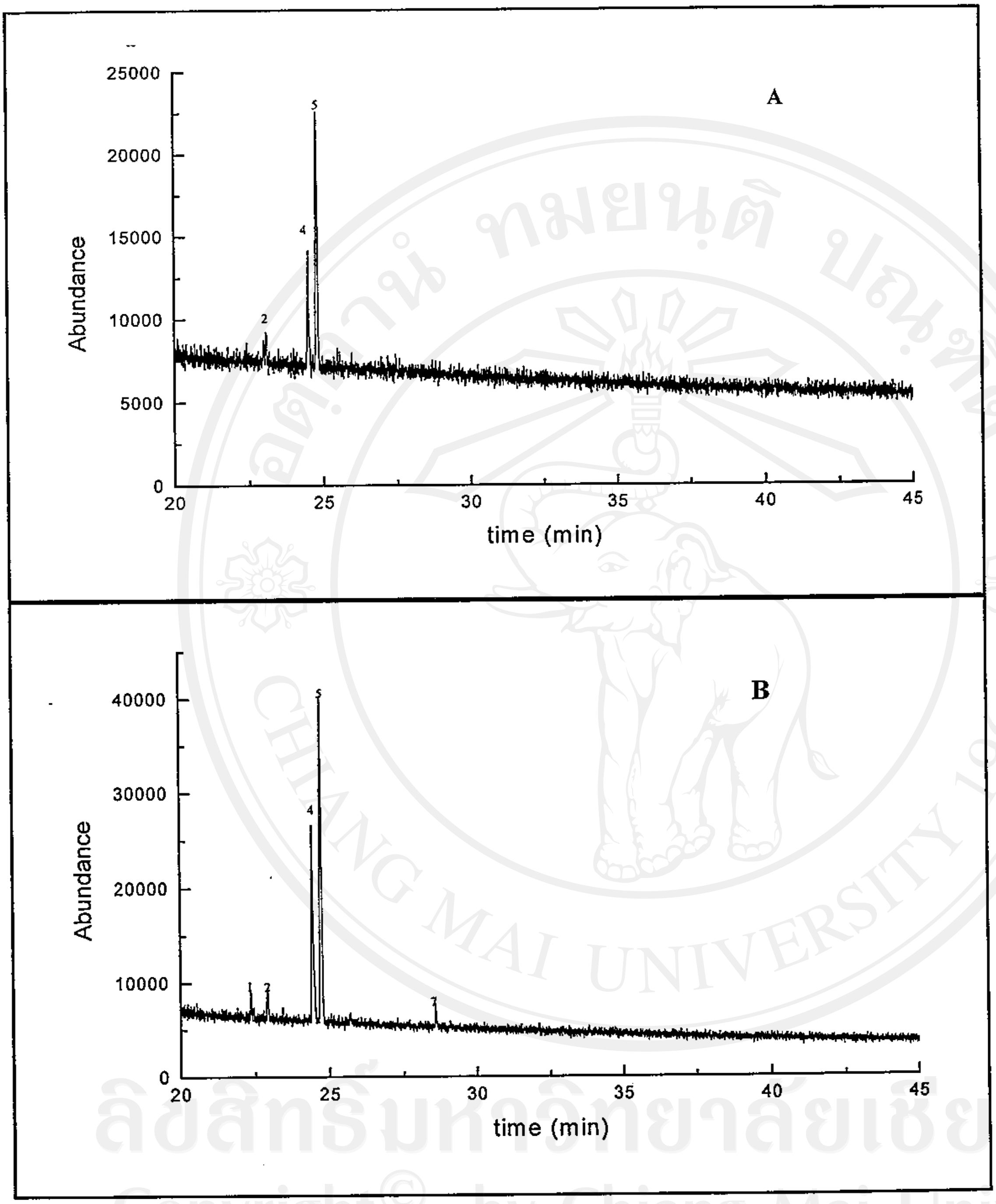


Fig. 3.1 Comparison of SPME-GC-MS chromatograms of volatiles at room temperature (30 °C). **A.** Extraction time 10 min, **B.** 20 min, **C.** 30 min and **D.** 60 min.

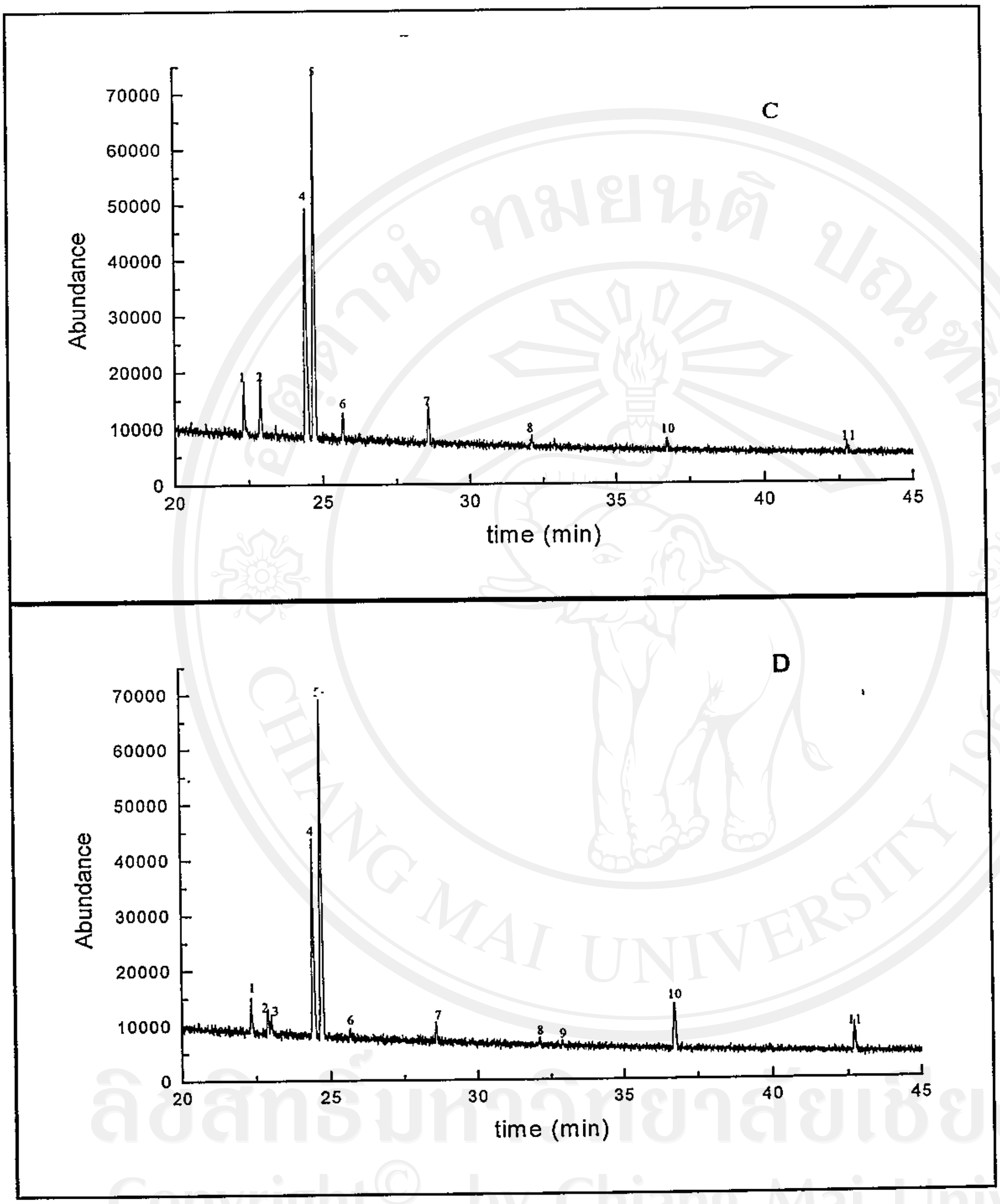


Fig. 3.1 (continued)

Table 3.1 Mass spectral data of volatile components obtained at room temperature.

No.	Structure	% Matching	m/z (%relative abundance)
1	Unknown	-	**41(100)**, 55(60), 69(89), 77(53), 91(71), 93(66), 161(96)
2	Unknown	-	29(32), 41(29), 91(32), 105(44), 119(30), **161(100)**
3	Unknown	-	29(40), **73(100)**, 147(53), 326(51)
4	?(-)-5-Epizizaene	85	29(23), 41(54), 55(36), 67(37), 77(42), 81 (41), 93(68), 103(11), 108(73), 115(12), 119(60), 133(100), 147(30), 161(37), 175 (14), 189(57), 204(30)
5	Khusimene	95	29(14), 41(39), 51(7), 55(26), 67(28), 79 (33), 91(50), 95(11), 105(25), 109(6), 115 (6), 119(36), **134(100)**, 147(8), 161(17), 189(17), 204(9)
6	Unknown	-	91(69), **105(100)**, 161(67)
7	Unknown	-	29(63), 41(78), 91(84), 105(59), 119(66), **161(100)**, 204(78)
8	Unknown	-	59(93), **149(100)**
9	Unknown	-	**152(100)**
10	Unknown	-	41(82), 67(51), 77(68), **91(100)**, 96(52), 108(90), 119(75), 133(79), 161(59), 189 (66), 204(77)
11	Unknown	-	41(78), 55(63), **79(100)**, 91(83), 95(60), 120(63), 147(62)

Fig. 3.1 and **Table 3.1** depicted some volatile components extracted from the raw root at room temperature. As aroma compounds normally possesses volatility property, they were readily subjected to extraction by SPME at room temperature. The obtained chromatograms presented an increase of numbers of volatile compounds when an extraction time was increased as shown in chromatogram A, B, C and D respectively. However, a number of volatiles were not increase when extraction time was greater than 60 min. The components obtained were identified using Wiley 275 mass spectral library. Low content of volatile components in sample headspace effected their total ion chromatogram and mass spectra accordingly. This results in unidentification of some volatile components. Compound 4 and 5 were the major volatile components in this kind of scented vetiver root. The compound 4 was tentatively being (-)-5-epizizaene and compound 5 was khusimene. The chemical structure of khusimene had been studied by Nigam[14] and was shown in **Fig. 3.3.**

3.1.2 SPME-GC-MS analysis at higher temperature

In this experiment, extraction of volatile components in scented vetiver root was performed using a polydimethylsiloxane (PDMS) fiber followed by separation and identification by GC-MS. The procedures of this experiment were presented in **Fig. 2.2**. SPME-GC-MS chromatograms obtained were shown in **Fig. 3.2A, B** and **C**. Mass spectral data were summarized in **Table 3.2**.

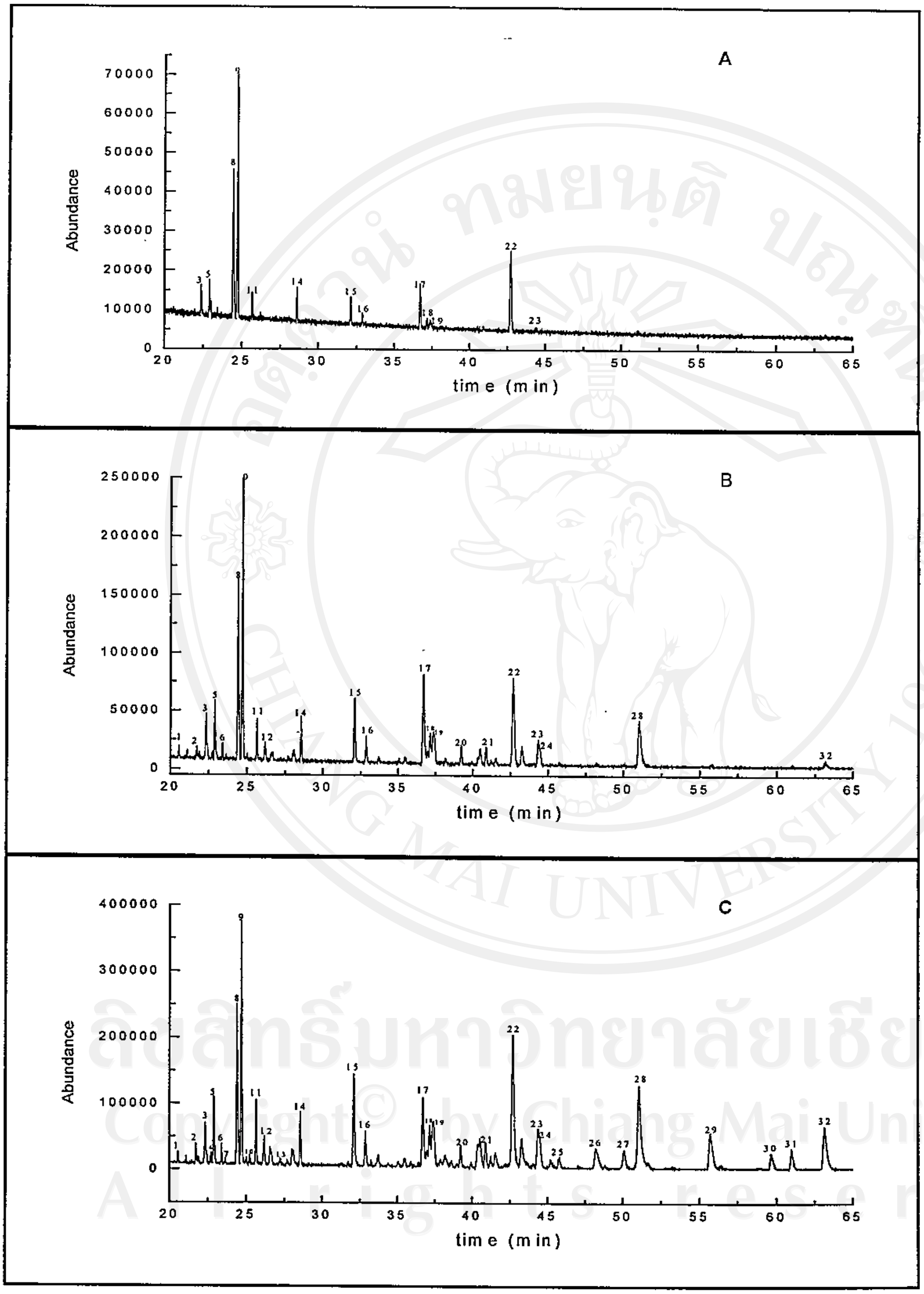


Fig. 3.2 SPME-GC-MS chromatograms of volatiles at higher temperature. **A.** extraction temperature 50°C, **B.** 70°C and **C.** 90°C.

Table 3.2 Mass spectral data of volaties at higher temperature (50, 70 and 90 °C).

No.	Structure	%Matching	m/z (%relative abundance)
1	Unknown	-	41(40), 55(24), 69(29), 77(21), 93(57), 105(34), **119(100)**, 161(22)
2	α-Chamigrene	91	29(18), 41(29), 55(18), 77(21), 93(65), 105(18), 121(92), **136(100)**, 204(32)
3	?β-Funebrene	81	29(20), 43(17), 55(42), 65(17), 69(99), 77(40), 82(30), 93(65), 105(42), 109(19), 120(36), 133 (47), **161(100)**, 204(25)
4	Unknown	-	41(46), 81(29), 91(46), 105(87), **119(100)**, 121 (50), 161(72)
5	Calarene	94	29(7), 41(22), 55(12), 65(5), 69(13), 77(15), 81 (14), 91(28), 105(35), 115(6), 119(26), 129(5), 133(14), **161(100)**, 190(5), 204(8)
6	Unknown	-	29(27), 41(54), 55(27), 79(29), 91(62), **105(100)**, 119(43), 133(39), 161(55), 175(29), 190(41)
7	Unknown	-	41(58), 55(28), 79(39), 91(74), 95(27), 105(62), 119(37), 133(41), 147(24), 161(88), 175(19), **189 (100)**, 204(91)
8	?(-)-5-Epizizaene	87	29(29), 41(56), 55(33), 67(31), 79(46), **91(100)**, 95(35), 108(57), 115(14), 119(47), 133(99), 147 (25), 161(28), 189(49), 204(20)
9	Khusimene	95	29(14), 41(39), 51(7), 55(26), 67(28), 79(33), 91 (50), 95(11), 105(25), 109(6), 115(6), 119(36), **134(100)**, 147(8), 161(17), 189(17), 204(9)
10	Unknown	-	29(34), 41(40), 91(48), 117(39), 131(45), **145 (100)**, 159(60), 187(56), 202(90)

Table 3.2 (continued)

No.	Structure	% Matching	m/z (%relative abundance)
11	α-Muurolene	92	29(20), 41(45), 51(10), 55(23), 67(10), 81(35), 94 (60), **105(100)**, 115(10), 119(30), 133(15), 147 (10), 161(80), 189(10), 204(40)
12	Unknown	-	29(21), 41(42), 55(25), 67(19), 77(22), 81(30), 91 (53), 95(24), 105(30), 119(29), 133(360, 145(19), 161(79), **189(100)**, 204(82)
13	Unknown	-	41(51), 91(48), 105(66), 119(62), 134(52), **161 (100)**, 204(66)
14	Unknown	-	29(20), 41(56), 55(35), 67(24), 79(34), 83(12), 91 (57), 95(11), 105(49), 115(15), 119(48), 133(31), 147(47), **161(100)**, 189(33), 204(76)
15	Unknown	-	29(17), 39(15), **43(100)**, 55(33), 59(84), 67(22), 79 (25), 81(38), 93(34), 97(23), 108(38), 121(19), 135 (15), 149(92), 164(42), 189(17), 207(25)
16	Unknown	-	29(19), 43(18), 55(25), 67(15), 81(17), 91(23), 105 (14), 109(43), 137(25), **152(100)**, 161(12), 222(13)
17	Unknown	-	29(33), 41(93), 51(29), 55(54), 67(63), 77(69), 81 (28), **91(100)**, 96(51), 103(19), 108(80), 115(25), 119(93), 133(75), 143(18), 147(37), 161(66), 189 (75), 204(88)
18	Unknown	-	29(17), 39(19), 43(82), 55(41), 69(28), 77(26), **81 (100)**, 91(30), 105(44), 109(22), 119(25), 161(56), 204(27)
19	Unknown	-	29(32), 41(92), 55(56), 59(19), 67(41), 71(18), 77 (39), 81(80), 91(62), 95(48), 105(52), **109(100)**, 121(38), 133(39), 137(22), 147(21), 161(76), 179 (32), 189(68), 204(65)

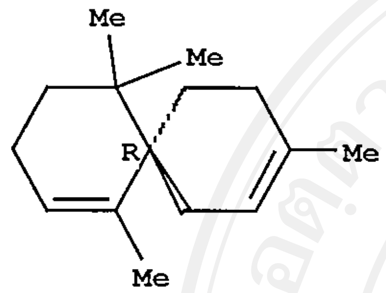
Table 3.2 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
20	Unknown	-	29(55), **41(100)**, 55(67), 79(65), 91(82), 105(63), 119 (61), 133(75), 161(43), 205(48)
21	Unknown	-	29(27), 39(22), **43(100)**, 55(34), 67(42), 71(65), 77(26), 82(41), 91(29), 95(40), 105(22), 109(37), 119(21), 135 (20), 161(25), 179(48), 189(23), 204(18)
22	Unknown	-	29(25), 41(96), 55(52), 67(46), **79(100)**, 94(80), 105(51), 115(12), 120(60), 133(32), 148(64), 161(28), 175(35), 190(26), 203(16), 218(48)
23	Unknown	-	29(33), 41(83), 55(64), 69(32), 77(26), 81(36), 95(35), 107(48), 122(41), 135(25), 151(29), 161(28), **177(100)**, 189(15), 207(18), 222(47)
24	Unknown	-	29(38), **41(100)**, 55(59), 67(55), 79(81), 83(38), 91(78), 95(56), 105(60), 121(46), 148(42), 177(59), 218(38)
25	Unknown	-	43(58), 55(66), 69(53), 79(68), 93(62), 105(74), 131 (60), **159(100)**, 187(83)
26	Unknown	-	29(30), 41(75), 55(59), 67(38), 79(60), **91(100)**, 95(31), 105(76), 119(48), 133(63), 147(34), 161(71), 189(65), 205(76)
27	Unknown	-	29(40), **41(100)**, 55(72), 67(48), 79(60), 91(77), 105 (53), 119(74), 131(38), 145(44), 161(53), 177(35), 187 (75), 202(39), 220(54)
28	Unknown	-	31(23), 41(61), 51(80), 55(36), 67(41), 71(46), 79(53), 91(99), 95(19), 105(47), 109(10), **119(100)**, 129(10), 133(68), 145(24), 150(83), 159(51), 173(9), 189(83), 202(7), 205(7), 220(6)
29	Unknown	-	41(98), 55(51), 67(47), 79(71), **91(100)**, 105(84), 119 (56), 160(48), 187(86), 202(98)

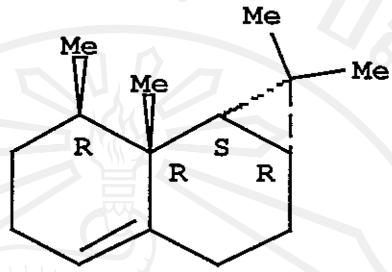
Table 3.2 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
30	Unknown	-	41(73), 55(44), 67(55), 79(49), 83(47), 91(67), 136(63), 161(41), **218(100)**
31	Unknown	-	29(52), 41(87), 55(53), 77(64), **91(100)**, 105(84), 119 (56), 161(65), 176(38), 203(35), 218(76)
32	β-Nootkatone	91	41(45), 55(20), 67(20), 77(30), 91(30), 105(25), 121 (20), 133(20), 147(30), 157(20), 161(35), 175(15), **185 (100)**, 203(30), 218(50)

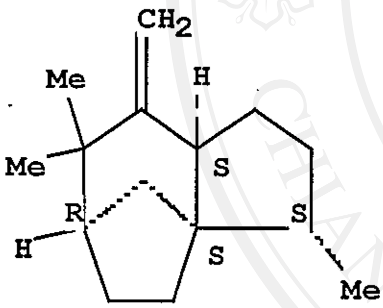
The SPME-GC-MS chromatogram of volatile components in **Fig. 3.1** showed that some volatile components were extracted at room temperature. However, more volatile components were extracted at higher temperature, which means that the efficiency of extraction at higher temperature is better than at room temperature. Increasing the extraction temperature from 50 to 90 °C resulted in an increase amounts and numbers of volatile components extracted. However, a number of volatile components were not increased when temperature was higher than 90 °C. The aroma quality of volatile components would be changed when a temperature was changed because generally aroma of the sample is resulted from overall odors of volatile components in the sample. In this experiment, all volatile compounds extracted by SPME fiber were assumed to play an important role in scent of vetiver root. Among them, there were seven identified compounds and more than 20 unknown compounds. The identified compounds named α-chamigrene, calarene, khusimene, α-muurolene and β-nootkatone. Chemical structures of identified compounds were shown in **Fig. 3.3**. Due to the overlapping of other components in the extract, some compounds could not completely be identified such as β-funebrene and (-)-5-epizizaene.



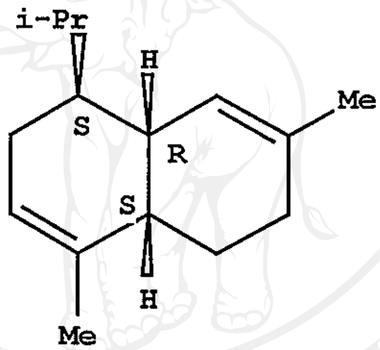
α-Chamigrene



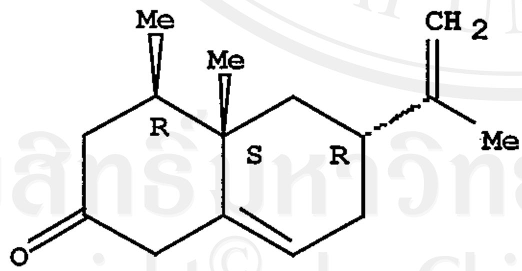
Calarene



Khusimene



α-Muurolene



β-Nootkatone

Fig. 3.3 Chemical structures of some volatile components in raw scented vetiver root extracted by SPME at higher temperature.

3.2 Isolation and purification of aroma component in scented vetiver root

3.2.1 Analysis of the dichloromethane crude extract by GC-MS

Extraction of the scented vetiver root was performed by maceration in dichloromethane. The obtained crude extract was diluted in small amount of dichloromethane and then investigated by GC-MS. Conditions of GC-MS were shown in **Table 2.1**. Chromatogram of the extract and mass spectral data of its components were demonstrated in **Fig.3.4**, **Fig 3.5** and **Table 3.3**, respectively.

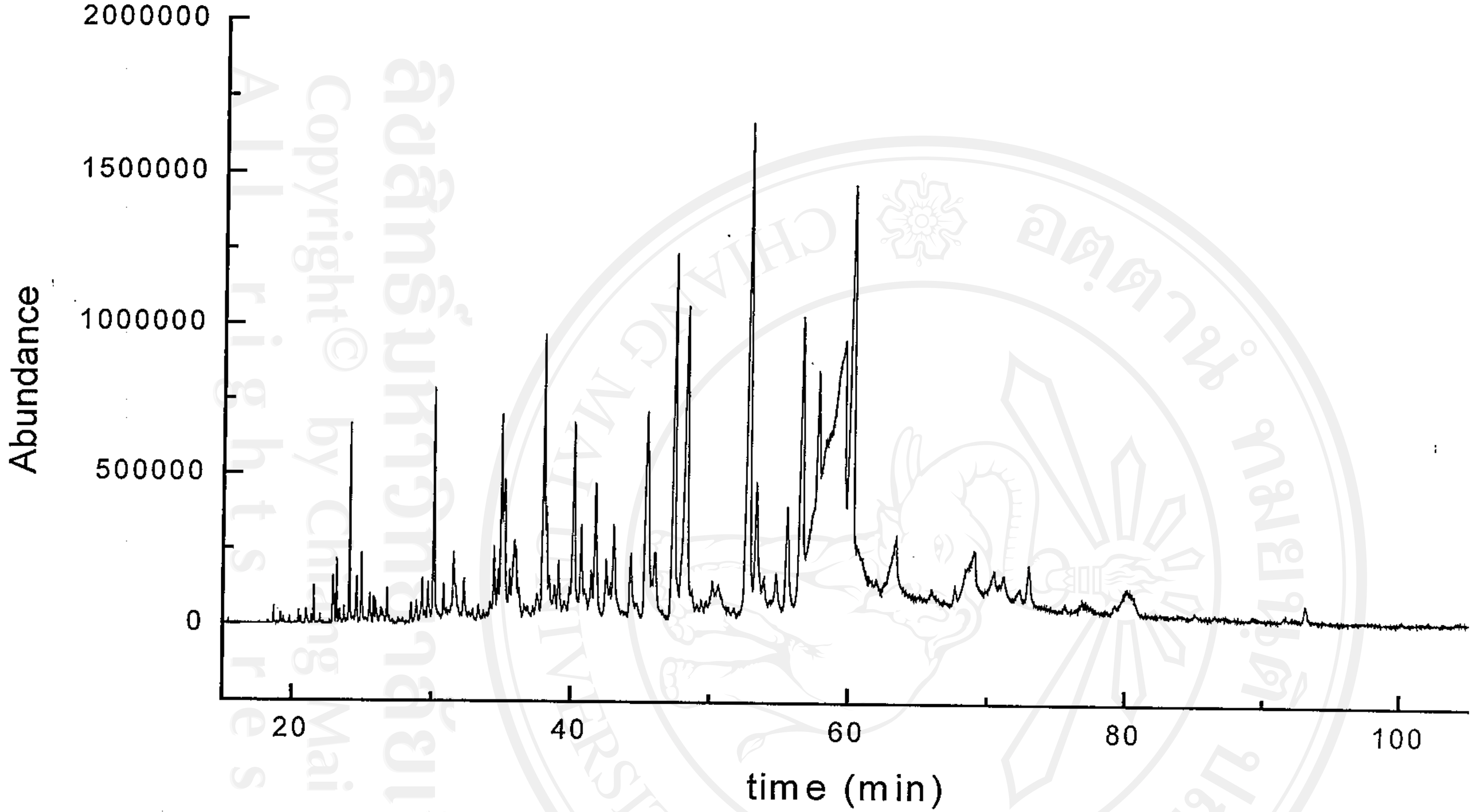


Fig. 3.4 GC-MS chromatotogram of dichloromethane crude extract of scented vetiver root.

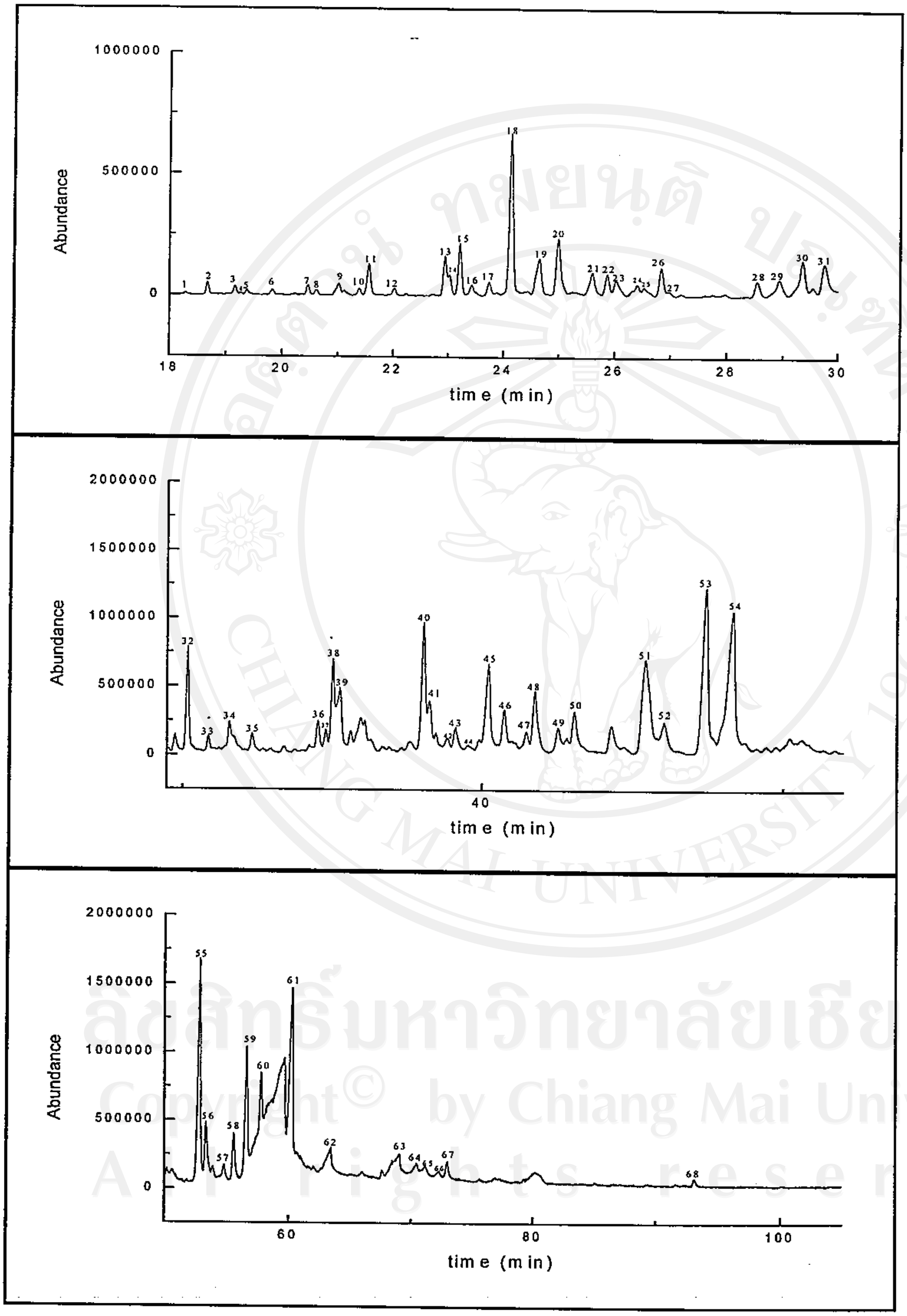


Fig. 3.5 Expansion of GC-MS chromatogram of **Fig. 3.4** and its labeled components.

Table 3.3 Mass spectral data of labeled components in dichloromethane crude extract.

No.	Structure	%Matching	m/z (%relative abundance)
1	Unknown	-	51(14), 55(19), 67(22), 79(50), 91(84), 105(42), 109 (20), **117(100)**, 131(22), 145(46), 149(31), 188(26)
2	α-Ylangene	98	55(19), 69(12), 77(24), 93(64), **105(100)**, 119(80), 131(10), 136(15), 147(10), 161(57), 189(6), 204(22)
3	Unknown	-	53(3), 65(6), 77(10), 81(4), 91(19), 105(9), 115(11), **119(100)**, 128(12), 134(37), 141(3), 145(9), 159(40), 187(13), 202(23)
4	Unknown	-	51(6), 55(32), 67(24), 79(30), 83(10), 91(62), 95(15), 105(60), 109(15), 115(13), 119(61), 133(35), 147 (52), **161**(100), 175(4), 189(42), 204(80)
5	α-Cedrene	90	55(17), 65(7), 69(22), 77(23), 81(10), 93(44), 105 (34), 109(5), 115(5), **119(100)**, 123(5), 133(9), 147 (9), 161(19), 204(13)
6	2-Norzizaene	90	51(10), 55(29), 67(23), 79(44), 91(49), 95(15), 105 (30), **120(100)**, 133(12), 147(36), 175(15), 190(10)
7	α-Chamigrene	92	55(11), 67(10), 79(20), 93(60), 107(42), 115(5), 121 (81), **136(100)**, 189(6), 204(30)
8	?Germacrene D	81	55(18), 67(14), 77(27), 91(54), 96(6), 105(57), 115 (14), 120(48), 128(12), 133(30), 145(16), **161(100)**, 187(21), 204(11)
9	?β-Funebrene	85	55(17), 65(14), 69(70), 79(39), 83(6), 91(61), 95(14), 105(47), 109(22), 115(9), 120(41), 133(10), 147(14), **161(100)**, 175(5), 189(10), 204(23)
10	?Cadina-1,4-diene	83	55(17), 65(9), 69(12), 77(17), 81(24), 91(35), 95(7), 105(79), 115(11), **119(100)**, 123(6), 131(9), 136(22), 147(8), 161(51), 189(4), 204(10)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
11	?Epibicyclosesquiphellandrene	86	55(7), 65(4), 69(6), 77(10), 81(11), 91(19), 105 (31), 145(5), 119(21), 133(9), **161(100)**, 204(5)
12	Unknown	-	55(18), 65(11), 69(15), 79(30), 91(59), 95(9), **105 (100)**, 109(6), 115(14), 119(59), 128(7), 133(36), 147(20), 161(55), 175(21), 190(33), 204(17)
13	?(-)-5-Epizizaene	89	51(6), 55(26), 67(27), 79(40), 91(88), 95(35), 103 (6), 108(69), 115(9), 119(47), 123(5), 129(5), **133 (100)**, 147(20), 161(28), 175(10), 189(37), 204 (19)
14	α-Gurjunene	96	51(9), 55(29), 67(30), 79(44), 91(72), 95(23), **105 (100)**, 109(11), 115(16), 119(44), 128(15), 133 (55), 147(16), 161(90), 175(11), 189(45), 204(65)
15	Khusimene	98	55(16), 67(21), 79(32), 91(44), 95(11), 105(23), 109(7), **134(100)**, 147(8), 161(13), 175(5), 189 (15), 204(6)
16	Unknown	-	55(11), 67(11), 77(12), 83(31), 91(21), 105(16), 115(8), **119(100)**, 131(10), 145(16), 159(19), 177 (2), 187(6), 202(17)
17	Unknown	-	51(6), 55(11), 65(13), 69(6), 77(22), 81(9), 91 (35), 95(5), 105(26), 117(31), 131(36), 141(14), **145(100)**, 159(58), 173(11), 187(41), 202(81)
18	α-Muurolene	94	55(12), 65(7), 69(8), 79(22), 94(53), **105(100)**, 115(8), 119(30), 128(5), 133(15), 147(9), 161(48), 189(10), 204(35)
19	Cadinene	92	55(18), 67(14), 77(24), 91(50), 105(51), 119(32), 128(13), 133(36), 145(18), 160(7), 161(89), 175 (12), **189(100)**, 204(77)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
20	γ-Cadinene	91	55(5), 69(9), 79(25), 93(42), 105(40), 119(33), 133 (23), 148(5), **161(100)**, 175(3), 189(8), 204(1)
21	δ-Cadinene	90	55(17), 69(10), 81(25), 91(50), 105(66), 119(69), 128(11), 134(59), 145(17), **161(100)**, 189(21), 204 (58)
22	?8,9-Dehydro-neoisolongifolene	80	55(8), 65(6), 77(14), 91(29), 105(24), 115(18), 120 (9), **131(100)**, 145(55), 159(17), 173(7), 187(2), 202(51)
23	Unknown	-	55(20), 67(11), 77(16), 77(16), 83(40), 91(24), 105 (25), **119(100)**, 131(25), 139(10), 145(11), 159 (12), 187(6), 202(16)
24	Unknown	-	55(27), 67(29), 79(30), 83(18), 91(52), 95(16), 105 (53), **121(100)**, 133(18), 147(32), 161(27), 177(4), 189(25), 204(51)
25	Unknown	-	51(7), 55(20), 65(10), 69(16), 77(30), 81(31), 91 (54), 105(65), 119(92), 134(68), 145(17), **161 (100)**, 176(5), 189(19), 204(55)
26	Unknown	-	51(6), 55(32), 67(24), 79(30), 83(10), 91(62), 95 (15), 105(60), 109(15), 115(13), 119(61), 133(35), 147(52), **161(100)**, 175(4), 189(42), 204(80)
27	Cis-calamenene	91	55(7), 67(5), 77(11), 91(18), 105(16), 119(14), 128 (14), 133(7), 145(10), **159(100)**, 202(15)
28	α-Calacorene	92	55(2), 63(2), 69(1), 77(4), 83(1), 91(4), 105(3), 115 (10), 121(10), 128(8), 142(49), 152(4), **157(100)**, 165(2), 183(3), 200(19)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
29	Unknown	-	55(12), 67(14), 71(5), 77(24), 81(14), 91(47), 95 (23), 105(36), 117(33), 131(56), 145(78), 159(81), 173(5), 187(40), **202(100)**
30	?1, 2, 9, 10,-Tetradehydro aristolane	80	53(7), 67(9), 77(16), 91(31), 105(26), 117(26), 131 (49), 145(72), 159(74), 187(37), **202(100)**
31	Unknown	-	55(33), 59(89), 67(37), 77(30), 81(54), **93(100)**, 107(63), 121(42), 133(29), 147(24), 161(43), 175 (10), 189(25), 204(16)
32	?β-Eudesmol	85	53(8), 59(67), 67(16), 81(36), 93(31), 108(39), 115 (5), 121(23), 128(3), 135(15), 142(5), **149(100)**, 157(11), 164(40), 189(18), 207(25), 222(3)
33	Unknown	-	55(22), 67(13), 81(21), 91(27), 97(6), 109(57), 115 (6), 121(19), 131(4), 137(22), 147(8), **152(100)**, 161(29), 177(6), 189(10), 204(12), 222(10)
34	Unknown	-	53(5), 65(4), 77(9), 91(14), 105(12), 115(14), 121 (5), 131(25), 145(21), 159(14), 173(15), 187(89), **202(100)**, 222(1)
35	?α-Copaene	86	55(34), 65(14), 69(23), 77(36), 81(40), 91(52), 105 (83), 119(81), 134(13), 145(10), **161(100)**, 189 (15), 204(46)
36	Khusimone	98	55(40), 67(41), 77(57), 81(28), 96(45), 103(13), **108(100)**, 117(34), 135(48), 147(39), 161(62), 173 (18), 189(67), 204(84)
37	?(+)-8(15)-Cedren-9-ol	85	55(37), **69(100)**, 81(34), 91(42), 96(5), 108(49), 118(42), 123(12), 131(18), 136(23), 149(16), 159 (36), 164(5), 177(23), 187(5), 205(4), 220(9)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
38	Unknown	-	55(31), 59(26), 67(25), 71(32), 79(51), 91(56), **95 (100)**, 105(58), 109(38), 121(74), 135(27), 149 (26), 161(86), 177(10), 189(15), 204(48), 220(13)
39	?Eudesmol	86	55(21), **59(100)**, 67(23), 71(8), 77(18), 81(31), 93 (34), 105(28), 109(34), 121(34), 135(18), 149(66), 161(34), 189(30), 204(27), 222(4)
40	Unknown	-	55(29), 65(10), 71(31), 79(50), **95(100)**, 105(54), 115(7), 121(73), 128(5), 135(25), 149(25), 161 (81), 177(9), 189(13), 204(48), 220(13)
41	α-Eudesmol	93	53(11), **59(100)**, 67(23), 81(31), 93(64), 109(34), 115(4), 121(24), 135(18), 147(66), 161(34), 175 (5), 189(30), 204(27), 222(4)
42	Unknown	-	55(20), 59(5), 65(7), 69(21), 77(14), **81(100)**, 91 (21), 95(17), 105(19), 109(20), 115(7), 121(19), 135(20), 149(14), 157(20), 161(14), 177(18), 189 (7), 203(6), 207(2), 220(14)
43	Unknown	-	55(59), 65(14), 69(51), 79(45), **84(100)**, 91(54), 95 (58), 105(65), 109(58), 119(62), 123(42), 133(17), 138(62), 147(11), 151(59), 161(35), 166(16), 175 (6), 179(18), 189(11), 204(13), 222(30)
44	Unknown	-	55(15), 59(2), 65(7), 69(12), 77(16), 81(16), 91 (25), 95(11), 105(22), 109(7), 115(17), 119(19), 128(10), 133(11), 142(33), **157(100)**, 161(9), 175 (29), 185(2), 189(7), 200(25), 204(6), 218(6)
45	?3-Zizanone	84	55(47), 67(46), **49(100)**, 93(88), 105(65), 115(16), 120(71), 128(8), 133(37), 148(86), 161(35), 175 (47), 189(24), 203(18), 204(9), 218(49)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
46	?Zizanol	88	91(52), 117(24), 131(67), **150(100)**, 159(40), 181 (16), 202(18), 220(9)
47	Unknown	-	55(12), 67(8), 77(14), 81(12), 91(27), 95(30), 105(22), 109(5), 115(10), 119(19), 129(8), 133 (16), 147(11), 162(9), 175(10), **189(100)**, 202(2), 218(20)
48	Unknown	-	55(40), 65(8), 69(27), 77(21), 81(33), 91(35), 95 (41), 107(44), 141(15), 122(36), 135(22), 139(8), 147(14), 151(27), 161(24), **177(100)**, 189(20), 207(12), 222(37)
49	Unknown	-	55(25), 67(29), 81(50), 93(39), 105(33), 121(35), 135(3), 149(16), 161(35), 179(2), **189(100)**, 204 (29), 222(30)
50	?3-Epizizanol	89	83(9), 95(27), 131(65), 146(35), 159(94), **178 (100)**, 202(35), 220(5)
51	Unknown	-	55(29), 67(29), 79(49), 91(78), 95(51), 105(81), 119(48), 133(71), 147(30), 161(72), 189(83), **205 (100)**, 220(14)
52	Unknown	-	55(50), 67(54), 79(48), 83(49), 91(78), 95(38), 105(65), 109(35), 117(20), 121(96), 131(33), **136 (100)**, 145(30), 159(30), 163(15), 177(9), 187 (10), 202(48), 220(26)
53	1-Naphthalene ethanol	91	81(30), 95(32), 105(47), 119(52), 133(25), 147 (16), 161(45), 173(6), **187(100)**, 202(50), 220 (67)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
54	Unknown	-	55(27), 67(32), 79(47), 91(84), 105(50), **119(100)**, 133(68), 150(91), 159(56), 189(87), 202(10), 220(5)
55	Unknown	-	55(28), 67(22), 77(34), 79(38), 83(8), 91(65), 95(26), 105(59), 109(18), 115(14), 119(48), 123(19), 131 (28), 135(8), 145(33), 161(43), 187(54), **202(100)**, 220(12)
56	Unknown	-	51(6), 55(36), 67(26), 79(49), 83(22), 93(87), 98(30), 105(77), 109(26), 117(18), **121(100)**, 131(22), 145 (36), 161(27), 173(8), 187(19), 202(25), 220(13)
57	Nootkatone	90	55(38), 67(37), 79(86), 91(86), 108(55), 121(83), 133 (73), **147(100)**, 161(72), 175(52), 190(51), 203(52), 218(25)
58	?5(1H)-Azulenone	88	55(31), 65(23), 77(40), 83(45), 91(68), 105(41), 119 (35), 133(45), 147(37), 161(52), 176(38), 189(7), 203 (15), **218(100)**
59	Unknown	-	55(29), 67(53), 77(39), 83(46), 91(65), 107(50), 115 (14), 121(57), 131(12), 136(93), 147(36), 161(52), 176(37), 185(7), 190(8), 203(14), **218(100)**
60	?β-Nootkatone	85	55(17), 67(16), 77(2), 91(38), 105(26), 121(22), 147 (27), 161(25), 175(10), **185(100)**, 203(21), 218(50)
61	Zizanoic acid	91	55(40), 67(37), 79(59), 91(64), 105(74), 119(97), 131 (33), **145(100)**, 164(66), 173(17), 191(26), 219(59), 234(10)

Table 3.3 (continued)

No.	Structure	%Matching	m/z (%relative abundance)
62	Unknown	-	55(54), 67(420, 79(70), **91(100),** 95(54), 105 (80), 119(49), 133(48), 145(48), 159(39), 173 (19), 187(85), 202(86), 207(16), 220(14)
63	Unknown	-	55(41), 67(34), 79(59), **91(100)**, 105(82), 119 (91), 131(39), 135(34), 145(58), 161(55), 173 (28), 189(40), 201(28), 205(9), 219(37), 234(82)
64	Unknown	-	55(50), 68(83), 79(88), 91(71), 105(74), 109(31), 123(46), 133(33), **149(100)**, 191(31), 203(11), 219(90, 234(5)
65	Unknown	-	59(31), 65(24), 94(18), 108(20), 113(25), 119 (29), 134(88), 140(25), 150(50), 161(22), 171 (17), 177(25), **192(100)**, 203(6), 218(22), 236 (16)
66	Unknown	-	55(35), 69(29), 79(49), 91(72), 95(24), 105(59), 109(22), 117(30), **121(100)**, 131(28), 145(41), 161(34), 173(18), 189(19), 201(12), 219(24), 234 (31)
67	Unknown	-	55(61), 67(33), 79(49), 93(57), 107(45), 121(67), 137(53), 148(19), 161(30), **165(100)**, 175(58), 191(10), 201(9), 206(13), 234(54)
68	Unknown	-	55(10), 67(10), 79(20), 91(34), 105(18), 117(32), 133(30), 145(66), 159(15), 173(48), **188(100),** 216(12), 233(9), 275(35)

Dichloromethane was employed to extract the components in scented vetiver root because it was generally able to extract both of nonpolar and polar components while the other common solvents, such as ethanol and hexane were suitable for polar and nonpolar extraction respectively. Moreover, evaporation of dichloromethane is simply performed. In this experiment, the maceration technique was used due to its ability to remain original sample components. However, there are other extraction techniques such as steam distillation but it is not suitable because this technique gives additional oxidation products. Thus, the use of dichloromethane was proven to be suitable for use as extracting solvent in this experiment.

Mass spectrum of each component was analyzed by comparing with the Wiley 275 mass spectral library in which the matching quality was resulted. Typically, if the percent of a matching quality is in a range of 90-99%, it is revealed that the analyte is proven to be similar to the standard. If the percent of matching quality is in a range of 80-89%, it will be prefixed by " ? " which revealed that this analyte is not properly proven to be similar to a standard. And if the percent of matching quality is less than 70%, it will be identified as "unknown" which revealed that this analyte is not found in the Wiley 275 mass spectral library.

The mass spectral presented in the obtained chromatogram were more than 140 components. Mass spectral data were unambiguously obtained for only 68 components. Among these, chemical structures of 33 components were identified by comparing their mass spectra with the mass spectral library. Majority of the identified components were in a group of sesquiterpene, sesquiterpene ketone, sesquiterpene alcohol and sesquiterpene acid.

3.2.2 Separation of the aroma fraction using classical liquid column chromatography (CC)

The dichloromethane crude extract was subjected to CC using silica gel as stationary phase. Three eluents were used which were 150 mL of toluene and ethyl acetate (4:1), then 100 mL of ethyl acetate and finally excess absolute ethanol. Ten milliliters of effluent were collected for each fraction. The whole separation resulted in eight separated fractions (code: A1-A8). Fraction A1 to A5 were eluted by the first eluent. The elution of fraction A6 and A7 were then followed by the second eluent, ethyl acetate. The last fraction, A8, was eluted by absolute ethanol. All fractions were analyzed using GC-MS. The GC-MS conditions were listed in **Table 2.1**. Comparison of GC-MS chromatograms of each fraction was shown in **Fig. 3.6**. Detailed separation of each chromatogram as well as its labeled components was shown in **Fig. 3.7**, **3.8**, **3.9**, **3.10**, **3.11**, **3.12**, **3.13** and **3.14**, respectively. Mass spectral data of the labeled components was summarized in **Table 3.4**. Comparison of the components obtained from each fraction was shown in **Table 3.5**. After solvent was evaporated, the aroma quality of each fraction was evaluated. The method was performed by asking for odor description of each fraction from 12 judges. It was found that all of the judges evaluated the fraction A6 as having the best aroma quality among all.

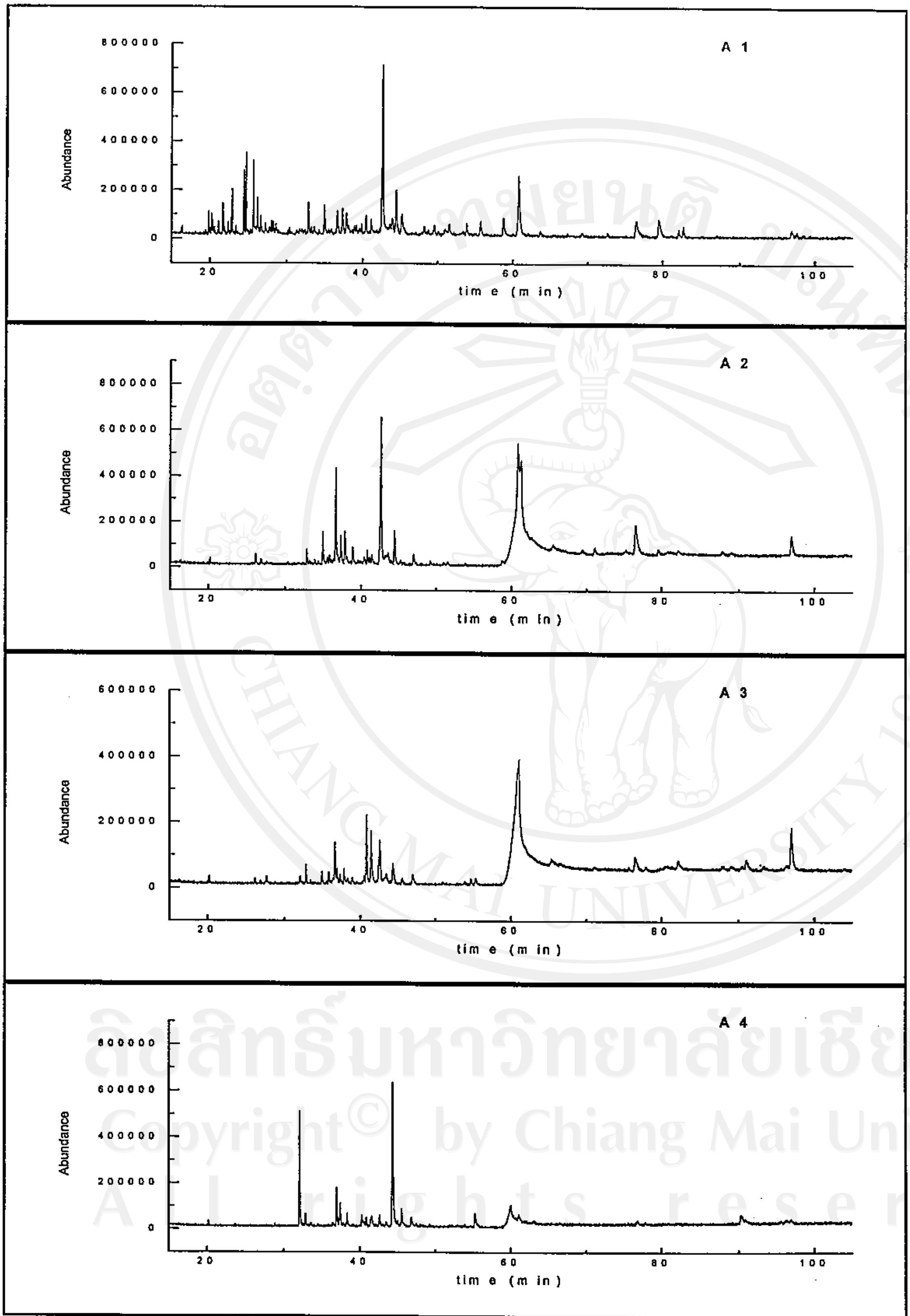


Fig. 3.6 Comparison of GC-MS chromatograms of 8 separated fractions of scented vetiver root crude extract.

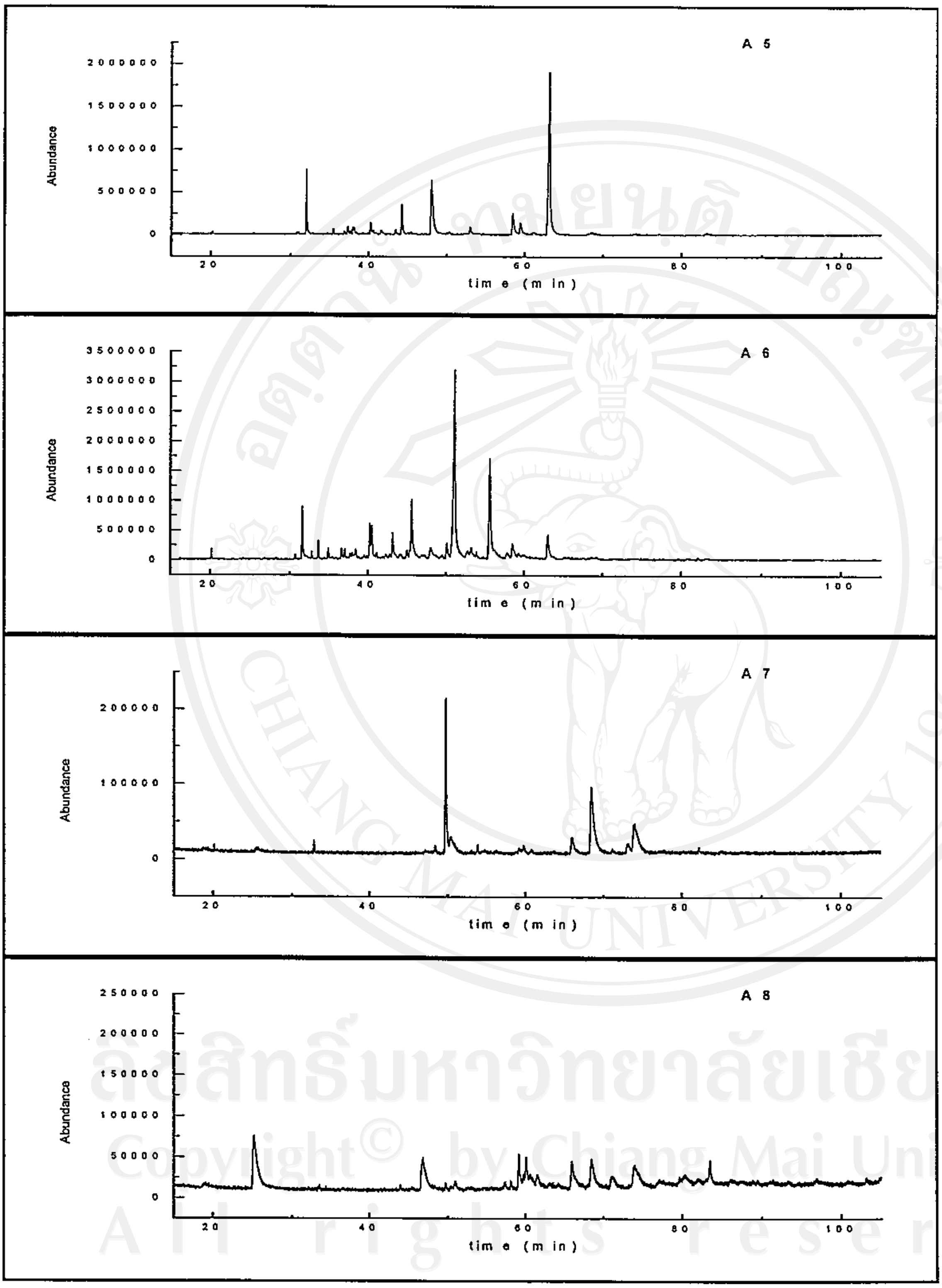


Fig. 3.6 (continued)

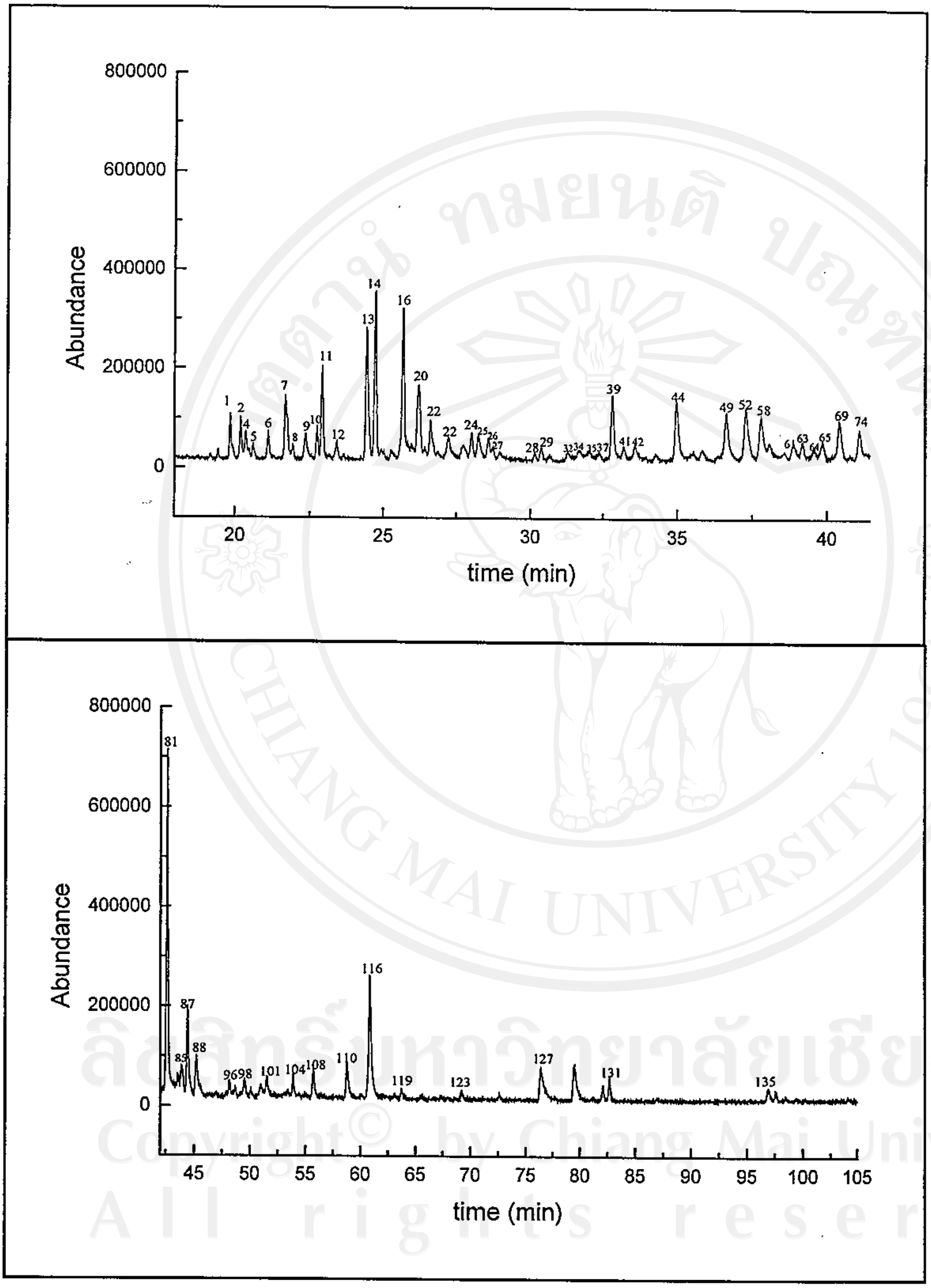


Fig. 3.7 Expansion of GC-MS chromatogram and its labeled components of fraction A1.

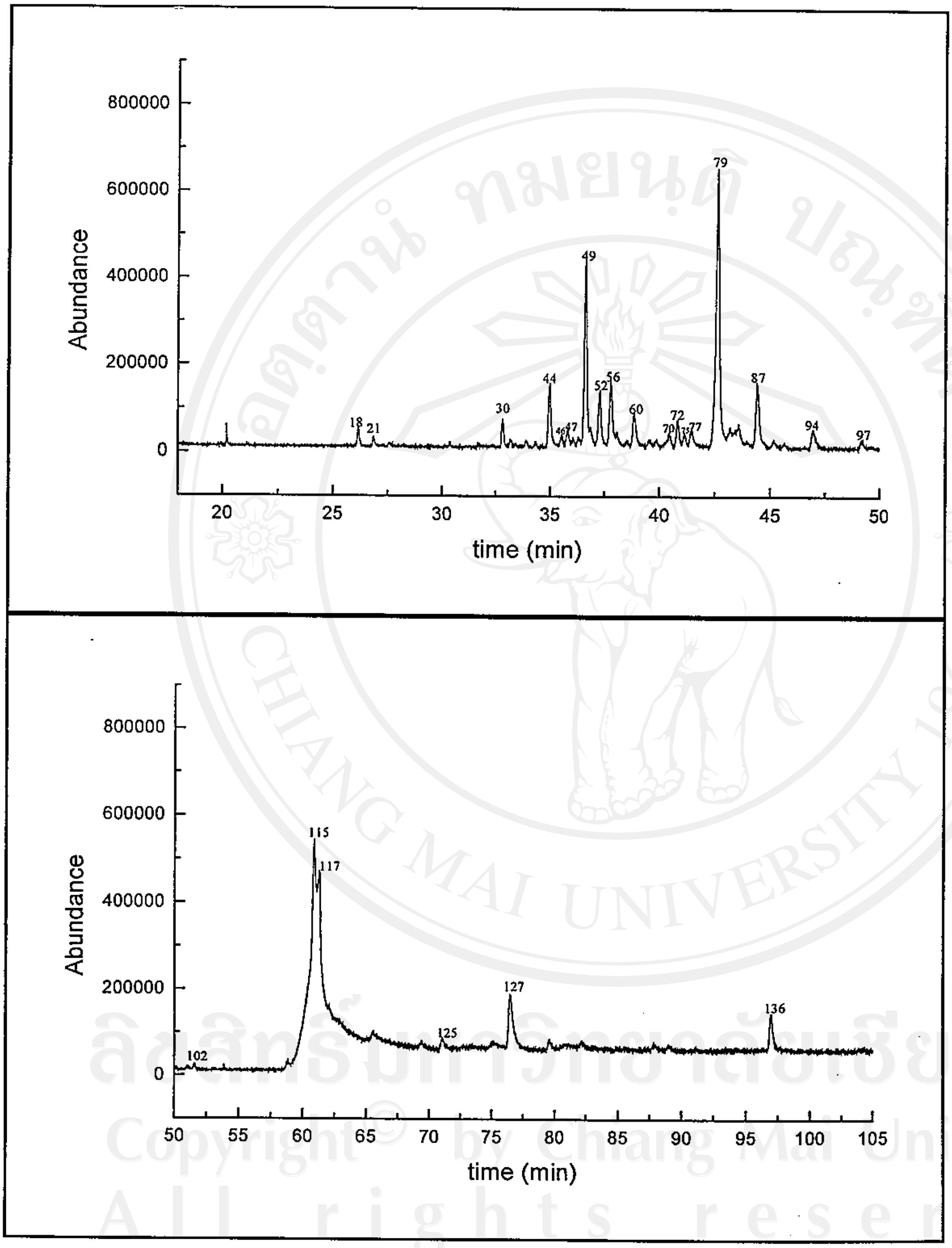


Fig. 3.8 Expansion of GC-MS chromatogram and its labeled components of fraction A2.

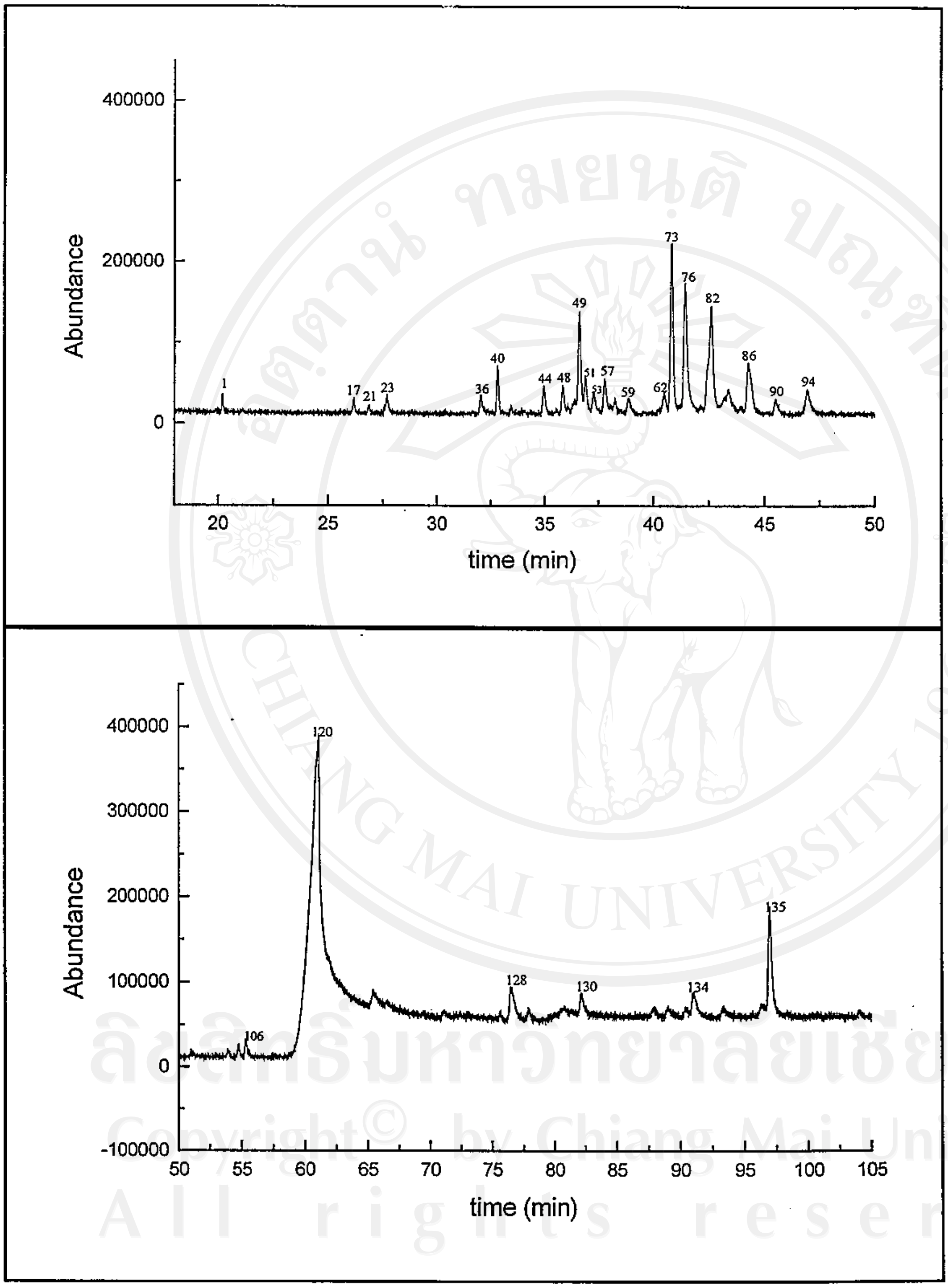


Fig. 3.9 Expansion of GC-MS chromatogram and its labeled components of fraction A3.

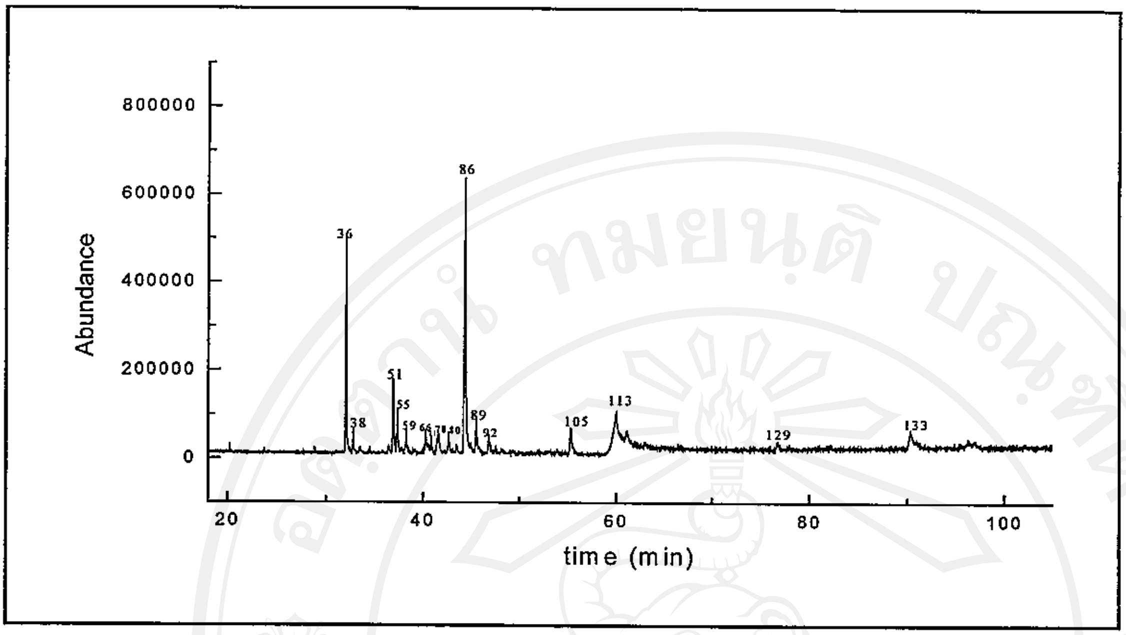


Fig. 3.10 Expansion of GC-MS chromatogram and its labeled components of fraction A4.

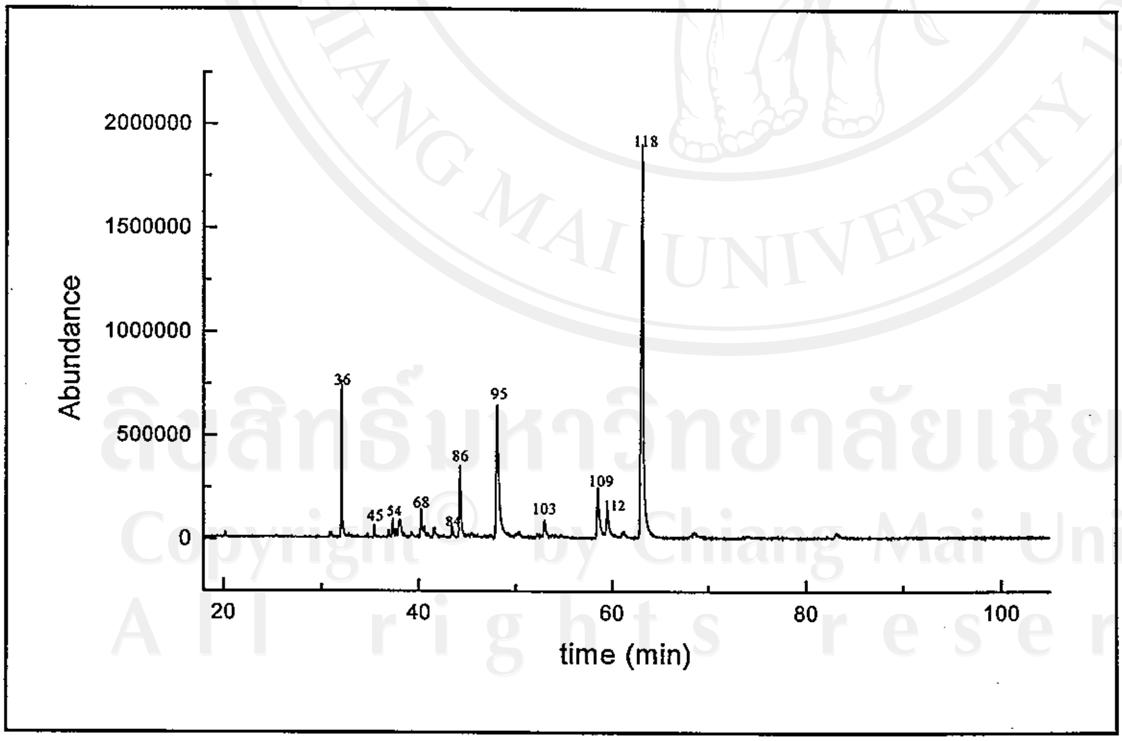


Fig. 3.11 Expansion of GC-MS chromatogram and its labeled components of fraction A5.

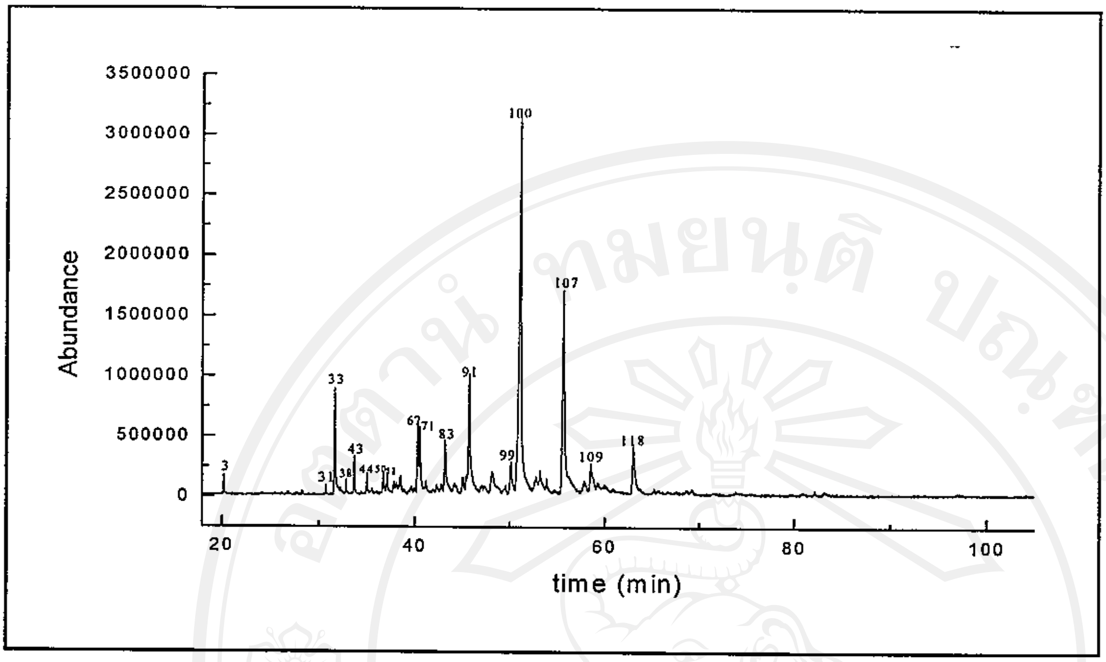


Fig. 3.12 Expansion of GC-MS chromatogram and its labeled components of fraction A6.

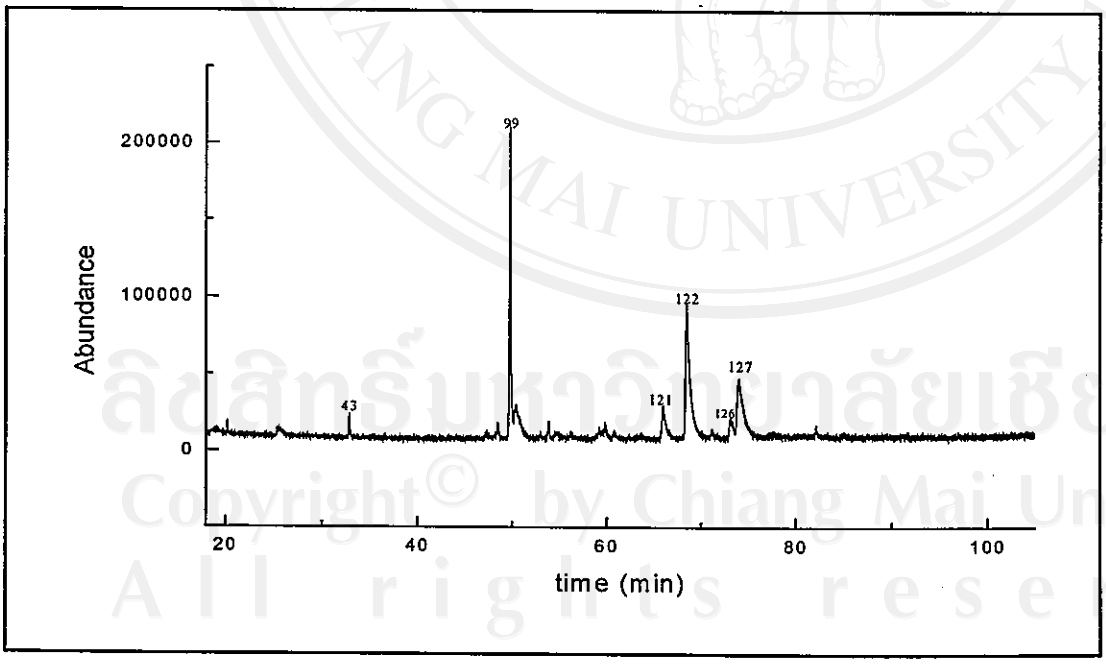


Fig. 3.13 Expansion of GC-MS chromatogram and its labeled components of fraction A7.

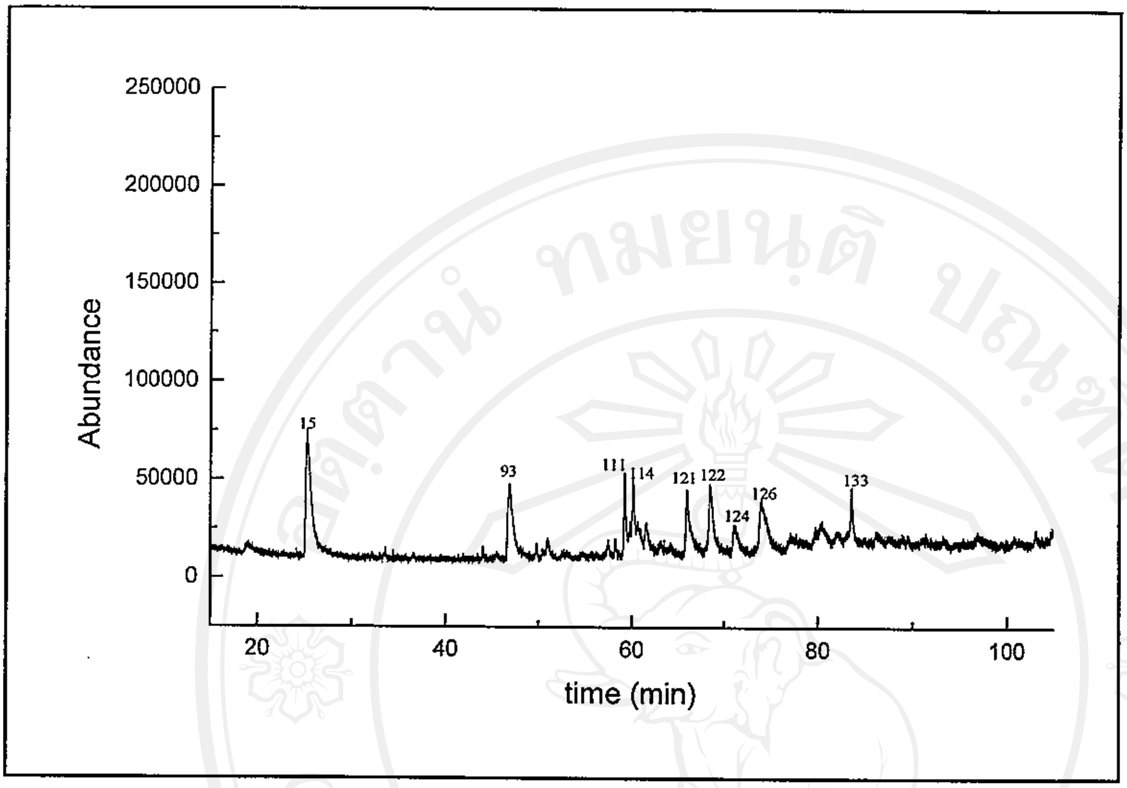


Fig. 3.14 Expansion of GC-MS chromatogram and its labeled components of fraction A8.

Table 3.4 Mass spectral data of labeled components obtained by CC.

No.	Structure	%Matching	m/z (% relative abundance)
1	?α-Ylangene	88	29(14), 41(38), 51(6), 55(20), 65(14), 69(15), 77(31), 81(24), 93(74), **105(100)**, 115(14), 119 (92), 129(8), 133(17), 147(9), 161(67), 189(9), 204(24)
2	Unknown	-	29(17), 39(8), 43(81), **57(100)**, 67(4), 71(56), 85(38), 99(8), 113(5), 127(3), 198(7)
3	Unknown	-	29(21), 43(83), **57(100)**, 71(54), 85(29), 99(6), 113(4), 127(3), 141(1), 170(6)
4	Unknown	-	29(9), 41(18), 53(8), 57(20), 67(9), 71(11), 77 (19), 81(7), 91(31), 105(14), 115(16), **119(100)**, 128(15), 134(37), 141(6), 145(29), 159(51), 173 (17), 188(23), 202(26)
5	? α-Cedrene	81	41(12), 55(11), 65(10), 69(23), 77(18), 81(13), 93(43), 105(35), 109(8), **119(100)**, 133(9), 147 (8), 161(21), 204(17)
6	2-Norzizaene	92	41(33), 55(22), 67(26), 79(50), 91(47), 105(28), **120(100)**, 133(15), 147(35), 175(14), 190(14)
7	Cyperene	94	29(6), 41(20), 51(4), 55(16), 65(6), 69(7), 79 (15), 91(28), 95(8), 105(36), 109(3), 119(34), 133(23), 147(16), 161(31), 175(15), 189(60), **204(100)**
8	Unknown	-	29(72), 41(43), 55(1), 77(69), 91(67), 105(25), 119(25), **159(100)**, 187(54), 202(62)
9	?(+)-β-Funebrene	81	51(10), 55(26), 65(14), 69(72), 79(38), 93(68), 105(50), 109(28), 120(46), 133(47), 147(12), **161(100)**, 189(17), 204(32)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
10	?Cadina-1,4-diene	84	29(23), 41(33), 55(29), 65(15), 69(19), 77(30), 81(38), 93(31), 105(86), 115(16), **119(100)**, 136(28), 161(58), 204(16)
11	?Epi-bicyclosesquiphellandrene	87	29(4), 41(16), 51(2), 55(7), 69(8), 77(12), 81(13), 91 (20), 95(3), 105(31), 119(21), 133(12), 145(3), **161 (100)**, 175(3), 190(5), 204(8)
12	Unknown	-	41(55), 55(42), 65(19), 69(30), 79(47), 91(65), 95(22), **105(100)**, 109(16), 115(26), 119(74), 128(17), 132 (62), 148(28), 161(58), 175(44), 190(78)
13	?(-)-5-Epizizaene	89	41(43), 55(26), 69(13), 81(29),91(76), 108(52), 119 (39), **133(100)**, 147(17), 161(24), 175(10), 189(35), 204(19)
14	Khusimene	98	41(32), 67(22), 77(20), 91(44), 95(11), 105(23), 109 (6), 119(32), **134(100)**, 147(7), 161(13), 189(19), 204 (7)
15	?Isoeugenol	88	39(14), 51(11), 55(20), 65(10), 77(31), 81(51), 91(28), 103(27), 107(6), 121(18), 131(23), 137(6), 149(35), **164(100)**
16	α-Muurolene	96	29(10), 41(34), 55(16), 67(11), 79(28), 91(44), 95(16), **105(100)**, 115(9), 119(34), 133(17), 147(11), 161(68), 204(36)
17	Unknown	-	39(55), 43(49), 55(55), 67(34), **79(100)**, 91(99), 105 (71), 121(49), 136(51), 163(51), 178(61)
18	α-Muurolene	94	29(18), 41(68), 51(21), 55(41), 65(27), 69(18), **79 (100)**, 93(84), 105(45), 109(17), 121(46), 136(52), 145(22), 150(15), 163(41), 178(95)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
19	Unknown	-	29(19), 41(69), 585(54), 67(29), 77(52), 81(41), 93(74), 105(85), 109(30), 121(44), 133(55), 147(37), 161(99), 175(16), 189(97), **204(100)**
20	Unknown	-	41(46), 51(8), 55(21), 67(20), 79(45), 91(53), 95(15), 105 (68), 115(10), 119(62), 133(31), 148(9), **161(100)**, 189 (15), 204(38)
21	Unknown	-	41(50), 55(28), 67(27), 79(47), 93(72), **107(100)**, 122 (50), 178(36)
22	Unknown	-	41(38), 53(20), 65(20), 69(23), 79(36), 91(45), 95(13), 105(80), 115(22), 119(80), 131(35), 145(51), **161(100)**, 189(15), 204(45)
23	Unknown	-	29(50), 41(61), 51(31), 55(54), 67(81), **79(100)**, 91(86), 95(40), 105(62), 119(48), 133(90), 148(80), 161(44), 176 (54)
24	α-Amorphene	94	29(8), 41(37), 51(8), 55(17), 67(21), 79(37), 83(11), 105 (49), 115(9), 119(51), 128(10), 133(21), 148(7), **161 (100)**, 189(7), 204(24)
25	Unknown	-	29(27), 41(43), 53(19), 57(11), 65(15), 69(38), 79(36), 83 (12), 93(30), 105(45), 109(28), 115(16), 119(92), 123 (20), 128(12), **134(100)**, 145(16), 149(50), 161(38), 176 (11), 189(16), 204(19)
26	Unknown	-	41(58), 55(26), 67(41), 77(21), 81(38), 91(60), 95(19), 105(53), 109(34), 119(35), 133(45), 147(67), **161(100)**, 189(41), 204(64)
27	Unknown	-	115(4), 129(16), 144(11), **159(100)**, 202(16)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
28	Unknown	-	41(71), 55(50), 69(49), 79(59), 93(54), 105(52), **119 (100)**, 131(30), 147(37), 159(33), 177(39), 205(97)
29	?α-Calacorene	82	29(8), 41(4), 69(7), 107(6), 115(12), 128(9), 142(43), **157(100)**, 200(24)
30	Unknown	-	29(8), 43(38), 57(30), 65(4), 71(18), 77(10), 85(11), 95(13), 99(4), 109(49), 121(5), 137(20), **152(100)**, 222(10)
31	?Elemol	88	29(17), 43(49), 55(34), **59(100)**, 67(41),81(41), 93 (64), 107(47), 121(34), 135(24), 149(14), 161(50), 189(22), 204(9)
32	?1,2,9,10-Tetradehydro aristolane	86	41(25), 55(7), 65(21), 77(37), 91(62), 105(48), 117 (31), 131(56), 145(71), 159(65), 187(40), **202(100)**
33	2(3H)-Naphtha lenone	94	29(19), 41(49), 51(19), 55(32), 67(29), 79(75), 93 (65), 107(59), 121(64), **135(100)**, 150(60), 163(43), 178(90)
34	Unknown	-	41(59), 53(33), 65(26), 69(33), 77(52), 81(33), 91 (48), 95(26), 105(61), 109(31), 117(46), 121(26), 133 (66), 135(25), 145(86), 159(49), 187(60), **202(100)**
35	Unknown	-	69(4), 95(14), 129(19), 142(53), **157(100)**, 200(25)
36	Unknown	-	29(10), 43(81), 59(78), 67(16), 81(32), 93(26), 97 (23), 108(31), 121(18), 135(14), **149(100)**, 164(44), 189(16), 207(29), 222(5)
37	Unknown	-	43(42), 53(65), 56(85), 69(95), 83(83), 97(75), 115 (72), **161(100)**
38	?Hexadecane	87	29(17), 43(76), **57(100)**, 71(63), 85(39), 99(10), 113 (5), 127(4), 135(3), 154(2), 178(2), 226(6)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
39	Unknown	-	29(18), 43(84), 57(85), 71(50), 85(34), 95(12), 109(50), 137(19), **152(100)**, 165(3), 179(3), 189(3), 222(11)
40	Unknown	-	29(26), **43(100)**, 57(70), 71(52), 81(35), 91(35), 105 (42), 121(32), 137(17), 152(34), 161(46), 189(10), 207 (21)
41	Unknown	-	29(24), 41(88), 53(40), 57(49), 67(83), 71(26), 77(52), 81(78), 93(72), 107(96), 121(54), 131(28), **135(100)**, 150(31), 159(27), 163(37), 191(82), 206(96)
42	Unknown	-	53(26), 67(32), 77(24), 81(60), 95(25), 107(25), 115 (33), 119(35), 131(50), 145(27), 159(30), **187(100)**, 202 (80)
43	Unknown	-	29(4), 43(27), 55(13), 67(80, 77(9), 81(15), 93(19), 105 (27), 109(10), 121(35), 133(6), **161(100)**, 179(19), 189 (2), 195(3), 204(2)
44	Unknown	-	43(56), 53(9), 65(10), 77(16), 91(29), 105(13), 115(10), 119(73), 131(6), 135(6), 147(47), **162(100)**, 189(6), 204 (33)
45	Unknown	-	41(54), 55(60), 69(75), 79(39), 81(66), **95(100)**, 105 (32), 109(42), 119(62), 123(25), 135(42), 151(49), 161 (36), 204(31)
46	Unknown	-	29(50), 39(75), **43(100)**, 53(49), 77(27), 82(39), 91(85), 95(58), 107(76), 115(48), 123(87), 133(66), 147(43), 161(29), 189(45), 204(93)
47	Unknown	-	**43(100)**, 53(22), 65(18), 69(6), 77(21), 81(41), 91(38), 95(19), 105(17), 109(41), 119(13), 123(37), 135(19), 147(16), 163(36), 191(51), 206(68)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
48	Unknown	-	41(55), 55(59), 69(68), 79(58), 93(75), 107(37), 121 (55), 136(34), **163(100)**, 191(25), 206(40)
49	Unknown	-	29(15), 41(74), 51(21), 55(50), 67(53), 79(57), 83 (20), 91(95), 96(44), 108(99), 119(78), 133(90), 147 (46), 161(61), 173(16), 189(71), **204(100)**
50	Unknown	-	29(14), 41(68), 55(48), 67(50), 79(47), 91(84), 95 (35), 105(45), 119(89), 135(76), 145(93), 159(21), 173(88), **188(100)**
51	(+)-8(15)-Cedren-9-ol	91	29(14), 41(60), 55(41), **69(100)**, 81(43), 91(37), 108 (50), 118(33), 136(21), 149(20), 159(32), 177(26), 187(7), 220(12)
52	?1-Naphthalenol	84	29(17), 41(44), 55(34), 67(27), 81(39), 91(25), 95 (30), **109(100)**, 121(16), 133(15), 135(19), 149(6), 153(17), 161(37), 179(29), 189(16), 204(30), 222(8)
53	Unknown	-	29(7), 43(52), 53(20), 57(19), 67(45), 77(33), 81(50), 93(48), 105(46), **109(100)**, 121(30), 133(33), 147 (19), 161(57), 179(27), 189(33), 204(41)
54	Unknown	-	41(66), 55(47), 59(39), 69(41), 77(31), 81(57), 91 (71), 105(57), 119(37), 133(50), 161(57), **189(100)**, 204(78)
55	Unknown	-	29(16), 43(74), 79(55), 69(68), 81(68), 91(47), 105 (64), 119(44), 133(51), 149(30), 161(96), **189(100)**, 204(75)
56	?Eremo philene	80	29(20), **41(100)**, 55(52), 67(45), 79(96), 91(95), 96 (58), 107(83), 119(56), 128(9), 134(70), 147(35), 161 (67), 176(28), 189(43), 204(70)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
57	?Alloaroma dendrene	87	29(34), 41(82), 51(26), 55(41), 67(50), 77(68), 81(95), **91(100)**, 95(53), 107(74), 119(68), 133(68), 147(58), 161(80), 176(23), 189(68), 204(80)
58	Unknown	-	29(24), **43(100)**, 53(49), 65(28), 69(37), 77(52), 81(53), 91(80), 108(56), 119(33), 134(44), 147(26), 175(35), 204(79), 218(11)
59	Unknown	-	29(28), 39(32), 43(68), 55(5), 79(31), 91(53), 105(22), 115(21), 119(29), 131(21), 135(19), 147(52), **161(100)**, 189(32), 204(67)
60	Unknown	-	29(8), **43(100)**, 55(11), 65(12), 77(18), 91(35), 105(33), 119(38), 128(9), 133(13), 147(47), 161(93), 189(37), 204(66)
61	Unknown	-	43(76), 53(15), 65(13), 69(13), 77(12), 81(16), 91(30), 105(16), 115(20), 119(46), 131(21), 135(15), 147(46), **161(100)**, 189(31), 204(56)
62	Unknown	-	39(40), 53(39), **59(100)**, 69(65), 71(47), 81(48), 93(57), 109(82), 119(52), 135(32), 149(73), 161(31), 189(25), 204(33)
63	Unknown	-	**41(100)**, 53(54), 67(85), 82(57), 95(64), 105(29), 109 (62), 119(65), 133(84), 149(43), 159(32), 173(47), 177 (53), 188(40), 205(72)
64	Unknown	-	41(74), 51(22), 55(32), 65(37), 69(70), 77(45), 91(40), 95(30), 105(69), 109(37), 117(33), 121(41), **133(100)**, 147(41), 162(35), 175(35), 187(28), 218(28)
65	Unknown	-	29(16), **41(100)**, 55(53), 67(60), 79(72), 91(91), 95(39), 105(57), 119(90), 133(84), 149(38), 161(49), 175(33), 191(31), 205(56), 220(19)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
66	Unknown	-	29(30), 41(65), 55(73), 67(57), 79(74), 91(96), 105(98), 119(63), 131(46), 145(54), **159(100)**, 177(61), 187(50), 220(69)
67	Unknown	-	29(7), 43(36), 55(16), 59(54), 67(12), 71(9), 79(23), 95 (30), 105(26), 121(20), 135(27), 149(15), **161(100)**, 189 (13), 204(37), 222(1)
68	Unknown	-	29(29), 41(78), 55(46), 67(48), 79(58), **91(100)**, 105 (73), 119(45), 131(40), 147(38), 159(73), 177(44), 187 (36), 220(34)
69	Unknown	-	29(14), **41(100)**, 55(53), 69(76), 77(22), 81(40), 93(43), 105(16), 121(51), 135(78), 145(12), 149(43), 161(30), 177(83), 205(14), 220(78)
70	Unknown	-	29(45), 41(69), 53(55), 69(49), 82(51), 91(66), **109 (100)**, 119(51), 123(29), 133(53), 149(47), 159(29), 177 (29), 191(29), 205(41), 220(46)
71	Unknown	-	31(8), 43(23), 55(15), **59(100)**, 67(16), 77(11), 81(23), 93(24), 109(26), 122(18), 135(12), 149(59), 161(26), 189(23), 204(20), 222(5)
72	Unknown	-	**43(100)**, 55(43), 65(12), 71(96), 77(32), 82(56), 95(47), 109(49), 119(29), 137(31), 148(11), 161(36), 179(71), 189(39), 207(16), 222(20)
73	?(-)-Prezizanol	86	29(12), **43(100)**, 55(32), 67(45), 71(97), 82(52), 95(43), 109(45), 119(22), 137(31), 148(9), 161(30), 179(65), 189(39), 204(12), 222(20)
74	Unknown	-	29(34), 41(99), 55(43), 69(77), 81(46), 93(32), 109(87), 121(61), 135(96), 149(44), 161(35), **177(100)**, 205(13), 220(91)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
75	Unknown	-	29(28), **41(100)**, 55(72), 69(84), 81(60), 91(45), 109 (87), 121(80), 135(87), 149(58), 161(36), 177(88), 220 (75)
76	Unknown	-	29(14), 41(53), 55(51), 69(38), **84(100)**, 91(28), 95(51), 109(48), 119(32), 138(59), 151(59), 161(26), 179(16), 189(6), 207(6), 222(30)
77	Unknown	-	29(21), 41(92), 55(61), 69(68), 77(39), **84(100)**, 95(65), 105(58), 111(40), 119(56), 138(66), 151(41), 161(32), 222(30)
78	Unknown	-	**43(100)**, 55(68), 69(44), 81(66), 95(55), 109(46), 119 (57), 138(41), 145(16), 151(40), 161(40), 179(16), 189 (31), 204(32), 222(20)
79	3-Zizanone	91	29(20), 41(81), 55(53), 67(50), **79(100)**, 94(93), 105 (54), 120(69), 133(29), 148(82), 161(29), 175(46), 190 (33), 203(16), 218(51)
80	Unknown	-	29(19), 41(74), 55(54), 69(44), 79(83), 91(73), 105(58), 121(72), 133(90), 145(25), **159(100)**, 176(89), 202(40), 220(25)
81	Unknown	-	29(22), 41(87), 55(53), 67(51), **79(100)**, 93(84), 105 (56), 121(73), 133(33), 148(85), 161(26), 175(46), 190 (28), 203(23), 218(53)
82	Unknown	-	41(73), 55(47), **79(100)**, 93(76), 105(59), 109(38), 121 (63), 133(46), 148(59), 159(30), 175(37), 190(21), 203 (12), 218(39)
83	Unknown	-	29(13), 41(41), 55(31), 67(28), 79(35), 91(43), 107(32), 119(23), 131(54), 145(11), **150(100)**, 159(29), 177(6), 187(12), 202(17), 220(8)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
84	Unknown	-	29(6), 39(12), **43(100)**, 53(8), 65(9), 77(15), 91(23), 107(14), 119(42), 135(21), 147(26), 162(13), 177(29), 205(5), 220(31)
85	Unknown	-	41(39), 51(18), 55(27), 65(20), 77(36), 82(19), 91(41), 95(14), 107(38), 116(16), 121(90), 131(22), 136(36), 145(8), 149(21), **162(100)**, 175(95), 189(29)
86	Unknown	-	29(16), 41(56), 55(43), 69(26), 81(31), 95(35), 107 (40), 122(36), 135(19), 151(27), 161(21), **177(100)**, 189(9), 207(13), 222(43)
87	Unknown	-	29(16), 41(76), 53(51), 67(56), **79(100)**, 93(90), 97 (30), 105(54), 115(21), 120(84), 133(24), 148(85), 161 (32), 175(45), 190(25), 203(19), 218(67)
88	Unknown	-	29(43), 41(90), 55(45), 67(58), 79(78), 91(80), 95(64), 107(62), **119(100)**, 133(53), 148(54), 161(26), 175(28), 185(19), 189(79), 203(30), 218(41)
89	?Zierone	82	29(11), 41(32), 55(20), 67(12), 77(24), 91(31), 105 (27), 119(29), 133(29), 147(38), 161(29), 175(43), 189 (9), 203(13), **218(100)**
90	Unknown	-	29(36), 39(38), 53(24), 69(36), 77(51), 81(33), 93(33), 105(52), 119(43), 133(46), 147(63), 161(39), 175(50), 189(25), **218(100)**
91	Unknown	-	29(12), 41(43), 55(29), 67(26), 79(30), 91(40), 105 (32), 119(21), 131(51), 146(2), 159(76), 173(18), **187 (100)**, 202(37), 220(2)
92	Unknown	-	41(44), 55(26), 69(29), 81(36), 91(15), 105(43), 121 (34), 133(23), 145(16), **159(100)**, 177(32), 202(24), 220(38)

Table 3.4 (continued)

No.	Structure	%Mathing	m/z (% relative abundance)
93	Unknown	-	29(7), **43(100)**, 55(36), 69(28), 81(40), 91(27), 99 (67), 109(23), 117(23), 123(28), 137(17), 149(10), 154(11), 163(11), 175(10), 183(9), 193(16), 236(21)
94	Unknown	-	29(26), **43(100)**, 53(16), 67(21), 77(32), 81(32), 91 (35), 105(48), 117(21), 119(33), 129(17), 133(24), 147(19), 161(55), 175(18), 189(92), 204(94)
95	Unknown	-	31(18), 41(43), 55(29), 67(29), 79(46), 91(67), 95 (45), 105(70), 119(40), 133(64), 147(28), 161(71), 189(83), **205(100)**, 220(13)
96	Unknown	-	29(20), 43(81), 55(40), 69(40), 79(44), 91(62), 98 (61), **105(100)**, 121(41), 133(40), 147(30), 161(47), 192(22), 219(38), 234(46)
97	Unknown	-	43(88), 53(34), 67(54), 82(60), 93(44), 107(40), 135 (38), 150(30), 163(32), **191(100)**, 206(62), 234(33)
98	Unknown	-	41(55), 55(43), 65(27), 79(47), 91(63), 98(60), **105 (100)**, 121(40), 133(40), 145(43), 161(69), 192(22), 219(48), 234(36)
99	?7-Acetyl-2-hydroxy-2-methyl-5-isopropylbicycl[4.3.0] nonane	81	**43(100)**, 55(11), 71(23), 81(9), 93(11), 111(15), 135 (68), 153(95), 177(7), 187(2), 205(10), 220(2), 238 (11)
100	Unknown	-	1(13), 41(47), 55(28), 67(32), 79(45), 91(83), 105 (48), **119(100)**, 133(69), 150(98), 159(53), 189(96), 202(9), 220(6)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
101	Unknown	-	41(77), 55(37), 68(92), 77(78), 91(94), **105(100)**, 121 (36), 133(73), 147(54), 161(26), 175(43), 203(25), 218 (45)
102	Unknown	-	39(67), 53(58), 67(78), 79(84), **91(100)**, 105(92), 133 (71), 175(46), 218(49)
103	Unknown	-	29(31), 41(61), 55(40), 67(29), 79(55), 91(77), 105 (73), 119(37), 133(29), 145(33), 161(42), 177(28), 189 (18), 201(12), 219(55), **234(100)**
104	?Octadecane	87	29(20), 43(74), **57(100)**, 71(63), 85(40), 99(15), 113 (8), 119(5), 155(5), 254(5)
105	?Aristolone	82	29(14), 41(24), 55(13), 65(10), 77(24), 91(35), 105 (36), 119(39), 133(27), 147(45), 161(28), 175(58), 190 (23), 203(55), **218(100)**
106	Unknown	-	29(30), 39(26), 55(22), 67(23), 77(35), 91(23), 105 (49), 119(45), 133(32), 147(50), 161(37), 175(65), 190 (32), 203(54), **218(100)**
107	Unknown	-	29(15), 41(47), 55(32), 67(22), 79(39), 91(63), 95(26), 105(54), 109(18), 119(45), 131(24), 145(29), 161(41), 173(8), 187(52), **202(100)**, 220(14)
108	Unknown	-	29(21), 41(55), 55(36), 67(48), 77(46), 81(18), 91(87), 95(30), 105(49), 109(18), 115(16), 119(44), 131(97), 145(39), 159(83), 173(20), 187(79), **202(100)**
109	Nootkatone	-	29(20), 41(84), 55(44), 67(36), 79(90), 91(89), 105 (65), 121(89), 133(80), **147(100)**, 161(71), 175(61), 190(51), 203(53), 218(26)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
110	Unknown	-	29(41), 41(68), 53(44), 67(38), 77(70), 81(33), 91(99), 95(59), 105(98), 119(65), 128(27), 133(41), 143(21), 148(48), 161(83), 176(65), 185(14), 189(40), 203(72), **218(100)**
111	Unknown	-	29(31), 41(83), 51(14), 55(43), 67(29), 77(58), 81(31), **91(100)**, 105(82), 115(24), 119(59), 133(39), 145(46), 161(82), 176(40), 189(33), 203(58), 218(90)
112	Unknown	-	29(14), 41(530, 55(29), 67(130, 79(46), 91(59), 107 (48), 121(54), 136(87), 147(41), 161(48), 176(37), 185(9), 190(11), 203(18), **218(100)**
113	Unknown	-	41(54), 51(18), 67(31), 79(33), 91(59), 105(31), 119 (77), 131(14), **145(100)**, 164(88), 173(21), 191(38), 219(88), 234(21)
114	Unknown	-	43(95), **59(100)**, 71(48), 79(39), 91(30), 95(46), 105 (28), 109(57), 119(23), 123(50), 135(27), 145(18), 149(95), 164(47), 189(19)
115	Unknown	-	29(23), 41(86), 55(48), 67(43), 79(62), 91(96), 105 (65), 119(95), 133(34), **145(100)**, 164(82), 176(21), 189(37), 203(29), 219(74), 234(16)
116	Unknown	-	29(31), 41(83), 51(14), 55(43), 67(29), 77(58), 81(31), **91(100)**, 105(82), 115(24), 119(59), 133(39), 145(46), 161(82), 176(40), 189(33), 203(58), 218(90)
117	Unknown	-	60(62), 81(20), 89(5), 108(11), 122(11), 133(15), **144 (100)**, 151(66), 166(5), 174(13), 193(7), 205(64), 216 (77), 234(7)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
118	β-Nootkatone	97	41(28), 55(15), 67(14), 77(17), 91(31), 105(20), 121 (20), 133(13), 147(24), 161(23), 175(10), **185(100)**, 203(23), 218(55)
119	Unknown	-	43(61), 55(35), 67(11), 77(45), 81(30), 91(57), 107 (36), 119(47), 131(73), 145(36), 159(81), 187(83), **202(100)**
120	Khusenic acid	91	29(19), 41(55), 55(29), 67(36), 79(41), 91(61), 105 (34), 119(79), 131(25), **145(100)**, 164(87), 173(27), 191(29), 219(73), 234(19)
121	Unknown	-	**43(100)**, 55(38), 67(29), 81(29), 93(48), 105(36), 119 (55), 135(27), 147(23), 159(47), 177(19), 187(14), 238(19)
122	Unknown	-	31(9), 43(68), 55(26), 69(17), 77(24), 91(23), 105(18), 117(19), 131(20), 149(61), 159(30), 177(36), **192 (100)**, 216(11), 234(10)
123	Unknown	-	29(65), 43(42), 53(37), 57(40), 69(60), 79(69), 91(50), 95(37), 105(72), 119(86), 131(56), 145(55), 160(59), 187(97), **202(100)**
124	Unknown	-	**43(100)**, 55(38), 69(43), 71(59), 91(68), 105(64), 119 (45), 135(44), 149(30), 161(38), 189(65), 205(54), 220(44)
125	Unknown	-	42(27), 51(31), 68(29), 80(35), 88(27), 97(29), 106 (30), 122(38), 132(10), 136(19), 148(53), 162(42), 175(32), 203(36), **218(100)**
126	Unknown	-	43(50), 59(47), 67(47), 79(48), 92(32), 105(39), 117 (37), 121(31), 135(33), 145(29), 149(45), 161(44), **177(100)**, 192(46), 219(43)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
127	Unknown	-	29(25), 41(56), 67(55), 79(62), 93(58), 109(43), 121 (41), 131(15), 137(58), 145(24), **165(100)**, 175(57), 191(26), 206(16), 219(68), 234(72)
128	Unknown	-	55(61), 67(33), 79(49), 93(57), 107(45), 121(67), 137 (53), 148(19), 161(30), **165(100)**, 175(58), 191(10), 201(9), 206(13), 234(54)
129	Unknown	-	41(51), 53(13), 57(31), 65(39), 77(18), 81(45), 91(32), 95(33), 107(43), **118(100)**, 131(61), 146(54), 161(29), 189(30)
130	Unknown	-	**29(100)**, 41(48), 54(47), 69(53), 81(27), 91(50), 106 (38), 122(40), 137(44), 149(61), 159(44), 164(29), 173 (8), 189(8), 217(21), 232(52)
131	?Hexadeca noic acid	89	29(21), 43(39), 55(31), 61(12), 69(22), 81(6), **88(100)**, 95(10), 101(58), 115(8), 143(8), 157(13), 199(6), 213 (6), 241(14), 284(20)
132	Unknown	-	29(19), 43(64), **57(100)**, 71(73), 79(19), 91(22), 105 (20), 113(26), 119(12), 135(14), 145(13), 173(10), 225 (10)
133	Unknown	-	41(47), 53(49), 65(23), 71(16), 79(47), 91(69), 107 (55), 112(45), 121(65), 131(31), 147(31), 159(25), 171 (26), 189(34), 199(17), 217(38), **232(100)**
134	Unknown	-	29(47), 39(26), 54(33), 65(16), 77(35), 91(42), 106 (26), 121(39), 128(22), 137(18), 143(22), 159(31), 171 (25), 187(28), 217(34), **232(100)**
135	Unknown	-	43(36), 53(22), 69(25), 79(31), 91(55), 105(30), 119 (44), 133(30), 145(79), 159(20), 173(51), **188(100)**, 275(34)

Table 3.4 (continued)

No.	Structure	%Matching	m/z (% relative abundance)
136	Unknown	-	29(18), 41(50), 55(41), 67(28), 79(31), 91(54), 105 (30), 119(45), 133(31), 145(78), 164(21), 173(51), **188 (100)**, 202(10), 219(13), 233(10), 256(4), 275(35)

Table 3.5 Comparison the detail of separated components obtained from CC.

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
1	?α-Ylangene	*	-	-	-	-	-	-	-
2	Unknown	*	-	-	-	-	-	-	-
3	Unknown	-	-	-	-	-	*	-	-
4	Unknown	*	-	-	-	-	-	-	-
5	? α-Cedrene	*	-	-	-	-	-	-	-
6	2-Norzizaene	*	-	-	-	-	-	-	-
7	Cyperene	*	-	-	-	-	-	-	-
8	Unknown	*	-	-	-	-	-	-	-
9	?(+)-β-Funebrene	*	-	-	-	-	-	-	-
10	Cadina-1,4-diene	*	-	-	-	-	-	-	-
11	?Epi-bicyclosesqui phellandrene	*	-	-	-	-	-	-	-
12	Unknown	*	-	-	-	-	-	-	-
13	?(-)-5-Epizizaene	*	-	-	-	-	-	-	-
14	Khusimene	*	-	-	-	-	-	-	-
15	?Isoeugenol	-	-	-	-	-	-	-	*
16	α-Muurolene	*	-	-	-	-	-	-	-
17	Unknown	-	-	*	-	-	-	-	-

Table 3.5 (continued)

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
18	Unknown	-	*	-	-	-	-	-	-
19	Unknown	*	-	-	-	-	-	-	-
20	Unknown	*	-	-	-	-	-	-	-
21	Unknown	-	*	*	-	-	-	-	-
22	Unknown	*	-	-	-	-	-	-	-
23	Unknown	-	-	*	-	-	-	-	-
24	α-Amorphene	*	-	-	-	-	-	-	-
25	Unknown	*	-	-	-	-	-	-	-
26	Unknown	*	-	-	-	-	-	-	-
27	Unknown	*	-	-	-	-	-	-	-
28	Unknown	*	-	-	-	-	-	-	-
29	?α-Calacorene	*	-	-	-	-	-	-	-
30	Unknown	-	*	-	-	-	-	-	-
31	?Elemol	-	-	-	-	-	*	-	-
32	?1,2,9,10-Tetra dehydroaristolane	*	-	-	-	-	-	-	-
33	2(3H)-Naphtha lenone	-	-	-	-	-	*	-	-
34	Unknown	*	-	-	-	-	-	-	-
35	Unknown	*	-	-	-	-	-	-	-
36	β-Eudesmol	-	-	*	*	*	-	-	-
37	Unknown	*	-	-	-	-	-	-	-
38	?Hexadecane	-	-	-	*	-	*	-	-
39	Unknown	*	-	-	-	-	-	-	-
40	Unknown	-	-	*	-	-	-	-	-
41	Unknown	*	-	-	-	-	-	-	-

Table 3.5 (continued)

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
42	Unknown	*	-	-	-	-	-	-	-
43	Unknown	-	-	-	-	-	*	-	-
44	Unknown	*	*	*	-	-	*	-	-
45	Unknown	-	-	-	-	*	-	-	-
46	Unknown	-	*	-	-	-	-	-	-
47	Unknown	-	*	-	-	-	-	-	-
48	Unknown	-	-	*	-	-	-	-	-
49	Unknown	*	*	*	-	-	-	-	-
50	Unknown	-	-	-	-	-	*	-	-
51	(+)-8(15)-Cedren-9-ol	-	-	*	*	-	*	-	-
52	?1-Naphthalenol	*	*	-	-	-	-	-	-
53	Unknown	-	-	*	-	-	-	-	-
54	Unknown	-	-	-	-	*	-	-	-
55	Unknown	-	-	-	*	-	-	-	-
56	?Eremophilene	-	*	-	-	-	-	-	-
57	Alloaroma dendrene	-	-	*	-	-	-	-	-
58	Unknown	*	-	-	-	-	-	-	-
59	Unknown	-	-	*	*	-	-	-	-
60	Unknown	-	*	-	-	-	-	-	-
61	Unknown	*	-	-	-	-	-	-	-
62	Unknown	-	-	*	-	-	-	-	-
63	Unknown	*	-	-	-	-	-	-	-
64	Unknown	*	-	-	-	-	-	-	-
65	Unknown	*	-	-	-	-	-	-	-

Table 3.5 (continued)

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
66	Unknown	-	-	-	*	-	-	-	-
67	Unknown	-	-	-	-	-	*	-	-
68	Unknown	-	-	-	-	*	-	-	-
69	Unknown	*	-	-	-	-	-	-	-
70	Unknown	-	*	-	-	-	-	-	-
71	Unknown	-	-	-	-	-	*	-	-
72	Unknown	-	*	-	-	-	-	-	-
73	?(-)-Prezizanol	-	-	*	-	-	-	-	-
74	Unknown	*	-	-	-	-	-	-	-
75	Unknown	-	*	-	-	-	-	-	-
76	Unknown	-	-	*	-	-	-	-	-
77	Unknown	-	*	-	-	-	-	-	-
78	Unknown	-	-	-	*	-	-	-	-
79	3-Zizanone	-	*	-	-	-	-	-	-
80	Unknown	-	-	-	*	-	-	-	-
81	Unknown	*	-	-	-	-	-	-	-
82	Unknown	-	-	*	-	-	-	-	-
83	Unknown	-	-	-	-	-	*	-	-
84	Unknown	-	-	-	-	*	-	-	-
85	Unknown	*	-	-	-	-	-	-	-
86	Unknown	-	-	*	*	*	-	-	-
87	Unknown	*	*	-	-	-	-	-	-
88	Unknown	*	-	-	-	-	-	-	-
89	?Zierone	-	-	-	*	-	-	-	-
90	Unknown	-	-	*	-	-	-	-	-
91	Unknown	-	-	-	-	-	*	-	-

Table 3.5 (continued)

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
92	Unknown	-	-	-	*	-	-	-	-
93	Unknown	-	-	-	-	-	-	-	*
94	Unknown	-	*	*	-	-	-	-	-
95	Unknown	-	-	-	-	*	-	-	-
96	Unknown	*	-	-	-	-	-	-	-
97	Unknown	-	*	-	-	-	-	-	-
98	Unknown	*	-	-	-	-	-	-	-
99	?7-Acetyl-2-hydroxy-2-methyl-5-isopropylbicycl [4.3.0]nonane	-	-	-	-	-	*	*	-
100	Unknown	-	-	-	-	-	*	-	-
101	Unknown	*	-	-	-	-	-	-	-
102	Unknown	-	*	-	-	-	-	-	-
103	Unknown	-	-	-	-	*	-	-	-
104	?Octadecane	*	-	-	-	-	-	-	-
105	?Aristolone	-	-	-	*	-	-	-	-
106	Unknown	-	-	*	-	-	-	-	-
107	Unknown	-	-	-	-	-	*	-	-
108	Unknown	*	-	-	-	-	-	-	-
109	Nootkatone	-	-	-	-	*	*	-	-
110	Unknown	*	-	-	-	-	-	-	-
111	Unknown	-	-	-	-	-	-	-	*
112	Unknown	-	-	-	-	*	-	-	-
113	Unknown	-	-	-	*	-	-	-	-
114	Unknown	-	-	-	-	-	-	-	*

Table 3.5 (continued)

No.	Structure	Fraction							
		A1	A2	A3	A4	A5	A6	A7	A8
115	Unknown	-	*	-	-	-	-	-	-
116	Unknown	*	-	-	-	-	-	-	-
117	Unknown	-	*	-	-	-	-	-	-
118	β-Nootkatone	-	-	-	-	*	*	-	-
119	Unknown	*	-	-	-	-	-	-	-
120	Khusenic acid	-	-	*	-	-	-	-	-
121	Unknown	-	-	-	-	-	-	*	*
122	Unknown	-	-	-	-	-	-	*	*
123	Unknown	*	-	-	-	-	-	-	-
124	Unknown	-	-	-	-	-	-	-	*
125	Unknown	-	*	-	-	-	-	-	-
126	Unknown	-	-	-	-	-	-	*	*
127	Unknown	*	*	-	-	-	-	*	-
128	Unknown	-	-	*	-	-	-	-	-
129	Unknown	-	-	-	*	-	-	-	-
130	Unknown	-	-	*	-	-	-	-	-
131	?Hexadecanoic acid	*	-	-	-	-	-	-	-
132	Unknown	-	-	-	-	-	-	-	*
133	Unknown	-	-	-	*	-	-	-	-
134	Unknown	-	-	*	-	-	-	-	-
135	Unknown	*	-	*	-	-	-	-	-
136	Unknown	-	*	-	-	-	-	-	-
Total No. of components		56	24	25	15	11	17	5	9

* existence

\- unexistence

From **Fig. 3.6 – 3.14** and **Table 3.4 – 3.5**, it was found that a crude extract of scented vetiver root was able to separate into 8 fractions (A1-A8). Fraction A1 contains a greatest number of components while the less were fractions A3, A2, A6, A4, A5, A8 and A7, respectively. However, a single component can be found in more than one fraction. The possible reason may result from the overlapping of component during the fraction collection. Mass spectrum of each component provided by GC-MS was compared with the Wiley 275 mass spectral library. A total of 136 different compounds can be found of which 33 components could be identified. However, there were lots of components that the identification could not perform due to the effect of overlapping with the other components and also some components were minority having low intensity. Further results indicated that components in fraction A1-A5 mostly were nonpolar hydrocarbons, sesquiterpenes and their derivatives. However, some polar sesquiterpene derivatives were obtained in these fractions. The reason why these polar sesquiterpene derivatives were yielded is due to the greater influent of nonpolar hydrocarbon part than the polar functional group in the molecule. For fraction A6 and A7, the components were rather polar which were eluted by ethyl acetate. Lastly, all additional polar components of both high and low molecular weight were eluted in fraction A8 which was eluted using absolute ethanol as mobile phase.

3.2.2 Separation of fraction A6 using thin layer chromatography (TLC)

Fraction A6 which had been evaluated as having the best aroma character was then subjected to further separation by TLC using silica gel F_{254} as absorbent. Hexane and diethyl ether mixed in the ratio of 1:1 was used as solvent system. Three separated bands (code: B1-B3) were obtained on TLC chromatogram. All of the bands were examined under UV light at λ 365 nm. After that, each band including adsorbent was collected and dissolved in ethanol. All separated fractions were analyzed by GC-FID. The conditions of GC-FID were listed in **Table 2.2**. The GC chromatogram of each fraction was shown in **Fig. 3.15A**, **B**, and **C**, respectively. Each fraction was then subjected to sensory evaluation by 12 judges. The results revealed that more than 80% of the judges agreed that fraction B3 had the best aroma quality among all fractions.

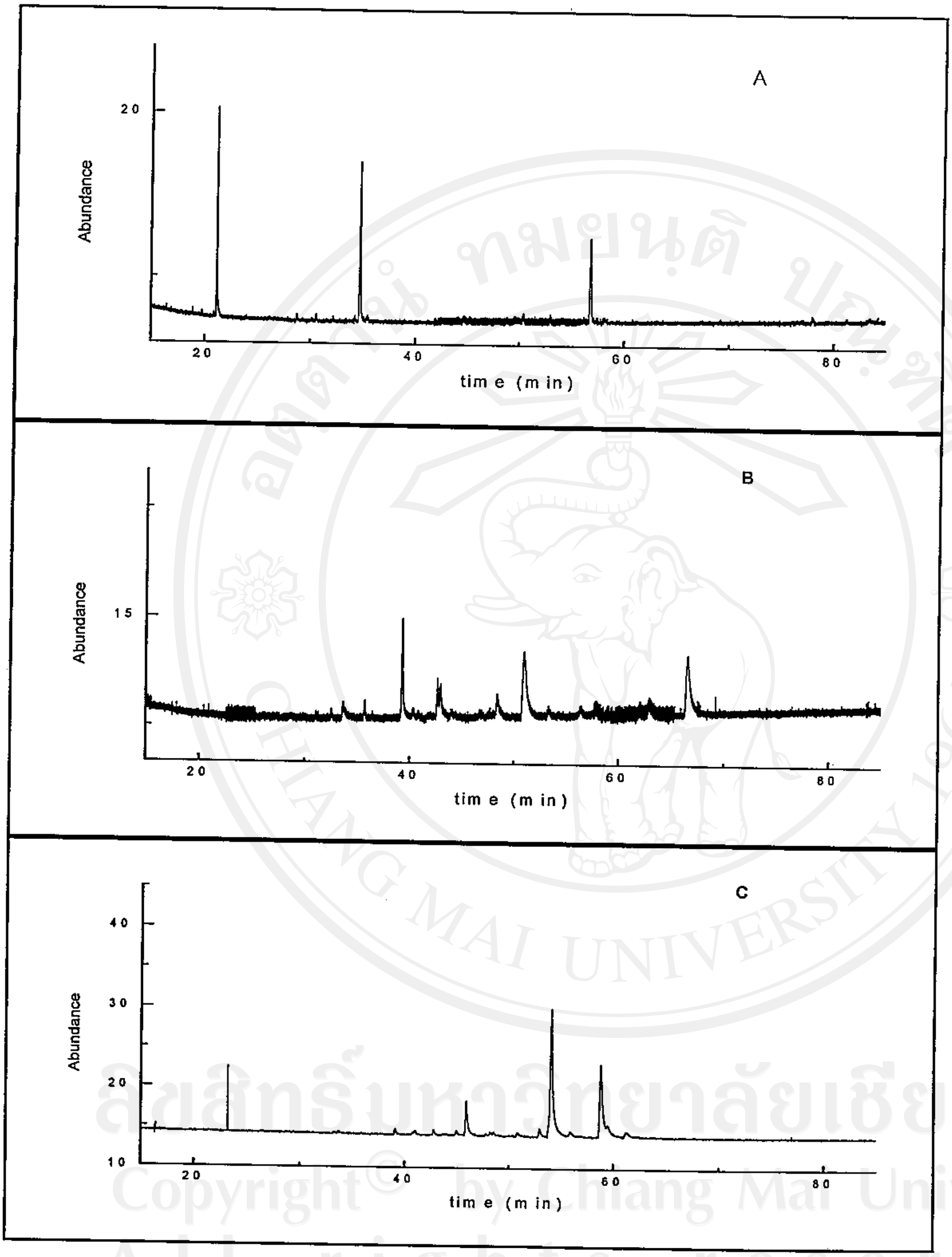


Fig. 3.15 GC-FID chromatograms of each fraction obtained from TLC. A. fraction B1 B. fraction B2 and C. fraction B3.

The obtained results from TLC chromatogram, using UV light at λ 365 nm as the detector, revealed that these separated fractions contained conjugated double bond system. The solvent system used in this experiment provided a good separation because each component was separated into each fraction. Moreover, this separation also includes all components of the fraction A6. The experiment showed that the most dominant components were in the fraction B3 which was the best aroma fraction. Therefore, it could be implied that these components should play important role as aroma components in scent of the vetiver root.

3.2.4 Separation and isolation of the aroma components in fraction B3 by preparative gas chromatography

Fraction B3 which had been evaluated to have the best aroma character was further separated by the use of preparative gas chromatograph. Conditions of preparative gas chromatograph were listed in **item 2.3.2.3**. Twelve separated components (code: C1-C12) were resulted. Each separated component was collected in ethanol after it flowing through an outlet of the preparative gas chromatograph. After evaporation of ethanol, all components were obtained as orange-yellow liquid. The aroma qualities of these components were evaluated using as many descriptions as the judges could think of. It was found that more than 80% of the judges preferred the aroma quality of component C6 while the other components were evaluated as not having aroma quality. The component C6 was then analyzed by GC-MS in order to confirm its purity. GC-MS conditions were shown in **Table 2.1**. The chromatogram and mass spectrum of component C6 were demonstrated in **Fig. 3.16** and **3.17**, respectively.

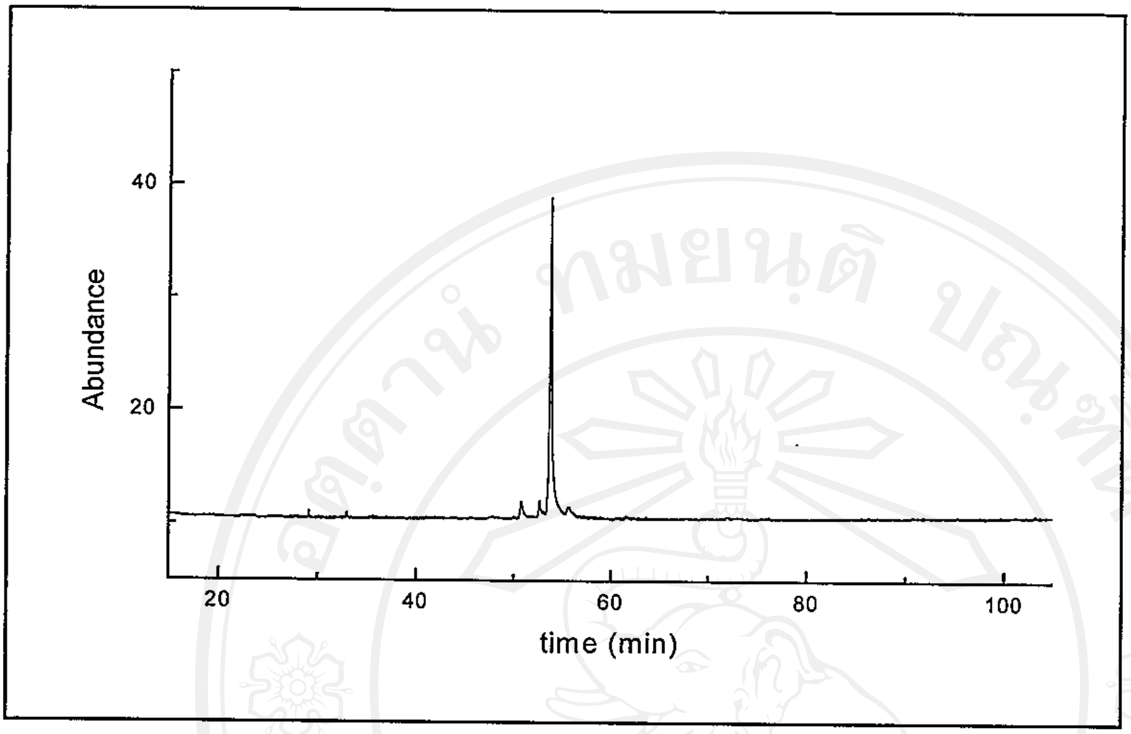


Fig. 3.16 GC-MS chromatogram of component C6 obtained from preparative GC.

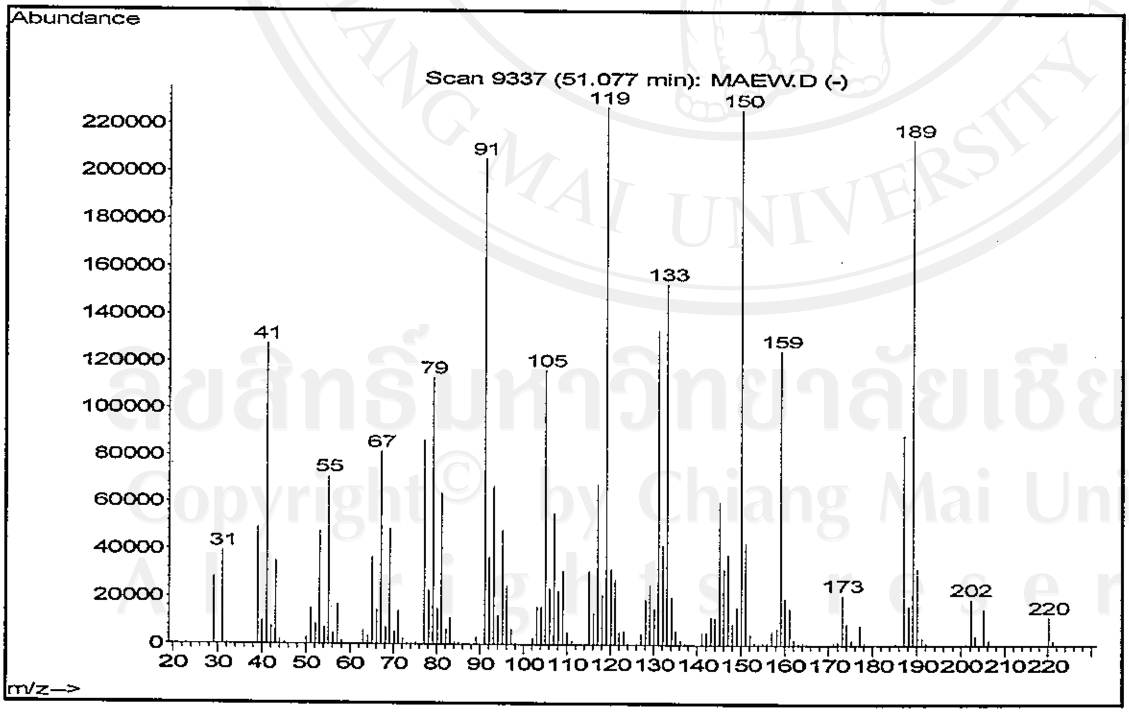


Fig. 3.17 Mass spectrum of component C6 obtained from GC-MS.

In the study, it was found that the aroma component C6 was finally isolated using a high efficiency technique as preparative gas chromatography. The sensory evaluation of this component resulted that its odor was not an odor of scented vetiver root. This compound was then investigated by GC-MS. The mass spectrum obtained was compared with mass spectral library of GC-MS. The obtained results depicted the aroma component C6 was not included in the library which is assumed as unknown compound. It was eluted from GC at retention time 51.077 min. Its mass spectrum showed a molecular ion at m/z 220. This result indicated that the molecular weight of component C6 should be 220. Fragmentation of molecular ion from m/z 220 to 202 showed the lost of mass 18 which equaled to molecular weight of water (H_2O). This fragmentation pathway showed that the component C6 contains a hydroxyl (OH) group. There were other fragmentation pathways for instance m/z 220 fragmented to 205 which showed the lost of methyl group (CH_3). In addition, there were some dominant ions in its mass spectrum such as 91, 105, 119, 150, 159 and 189. Consequently, the conclusion can tentatively be made that component C6 was identified as an alcohol.