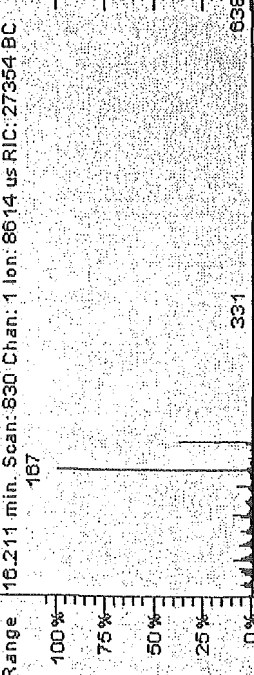
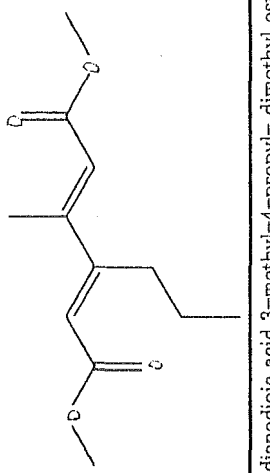
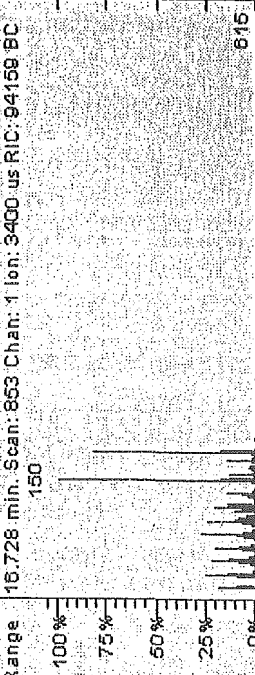
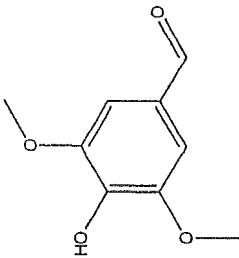
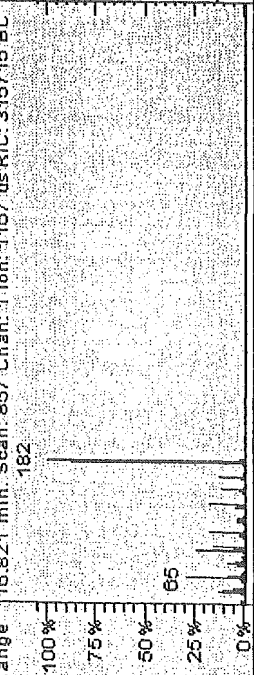
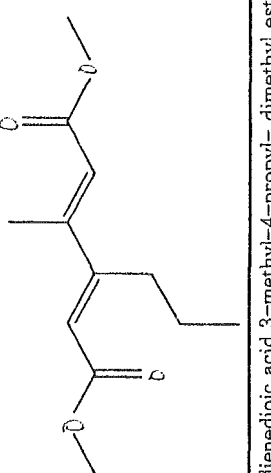
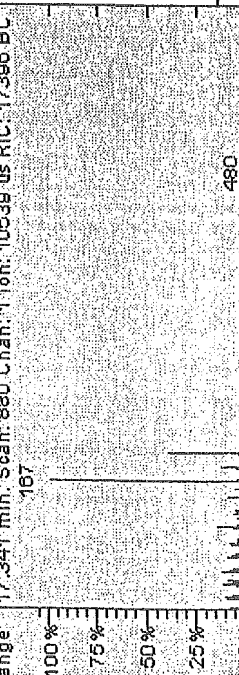
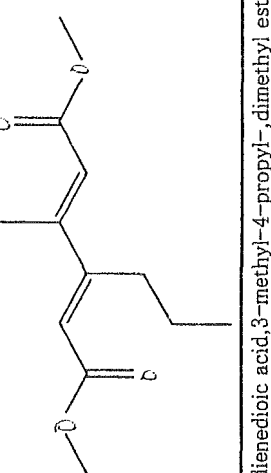
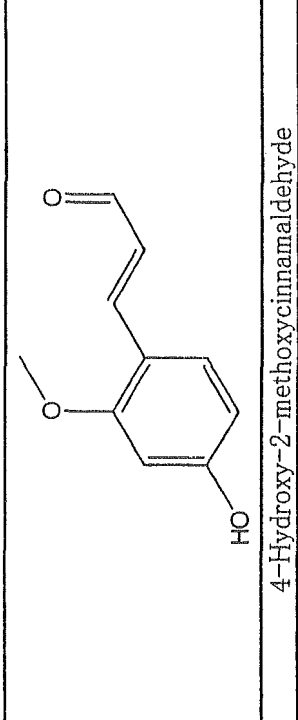
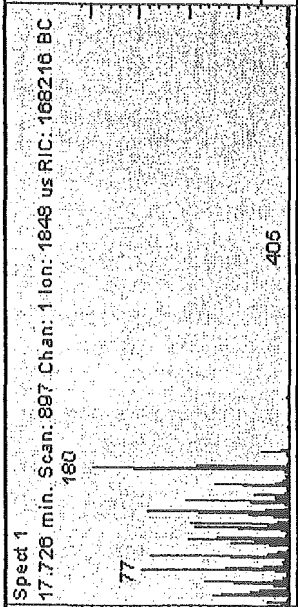
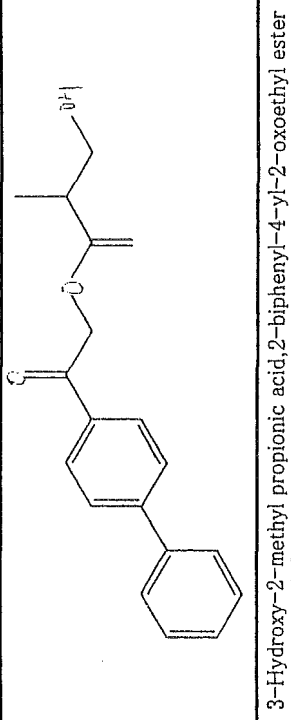
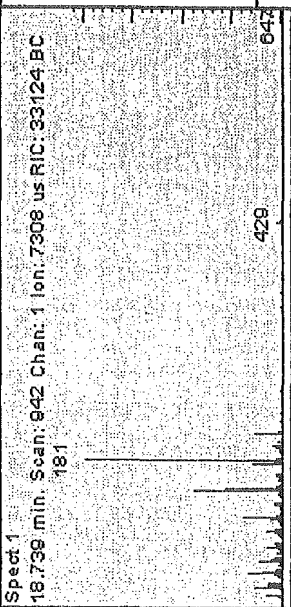
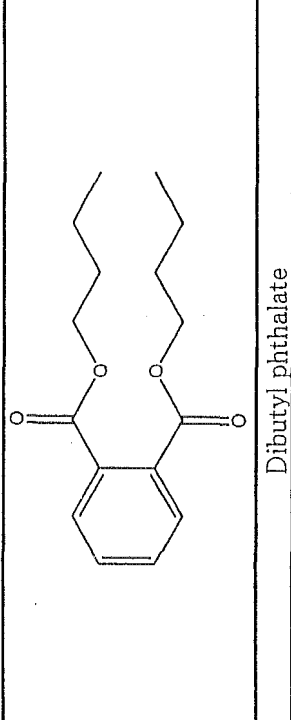
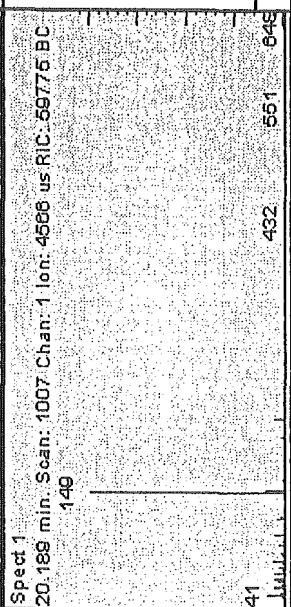
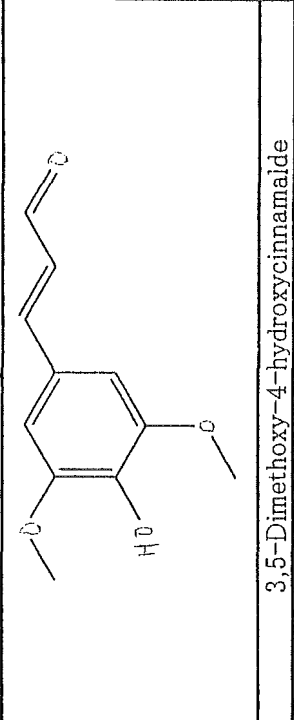
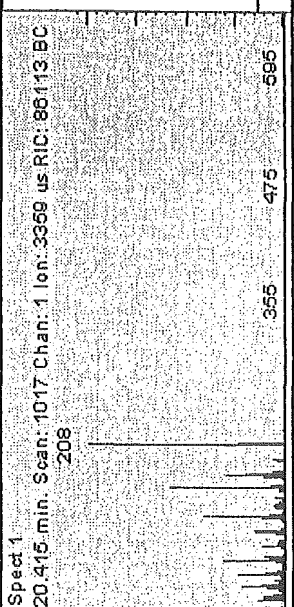
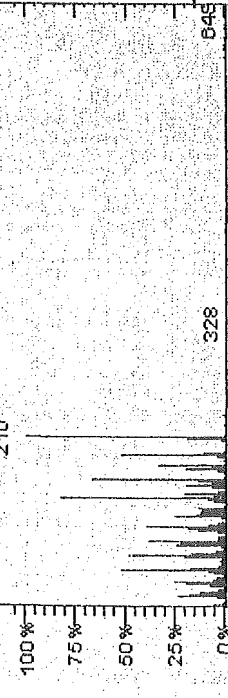
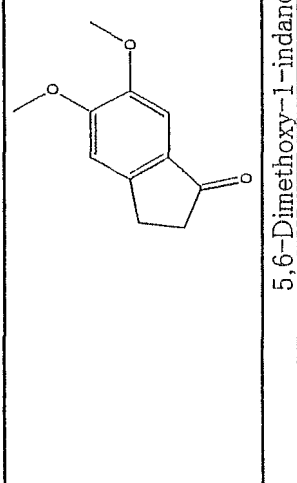
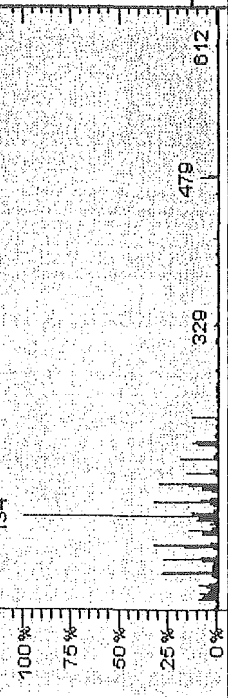
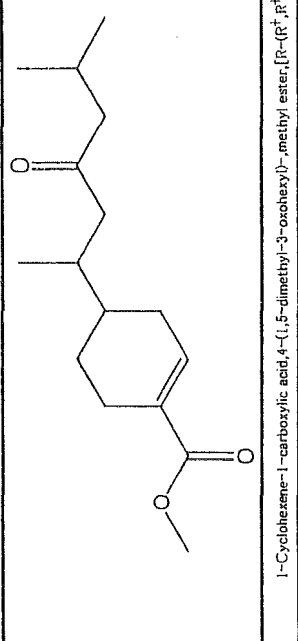
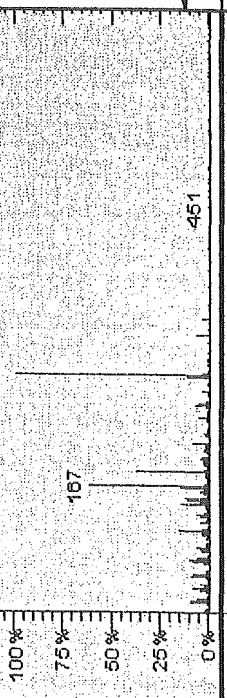
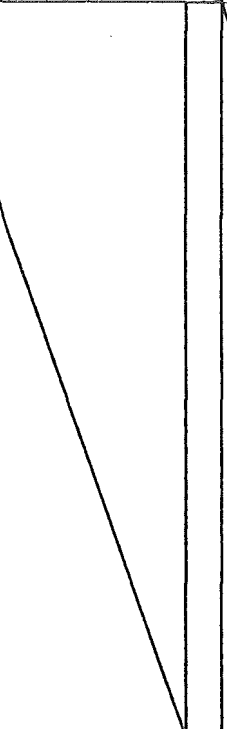
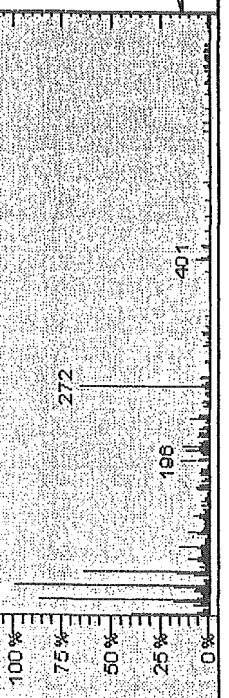
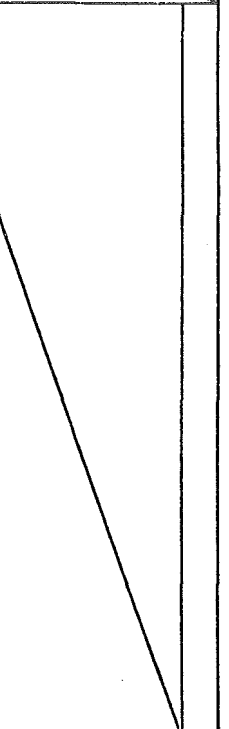
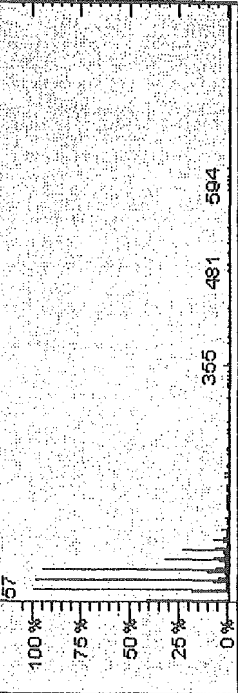
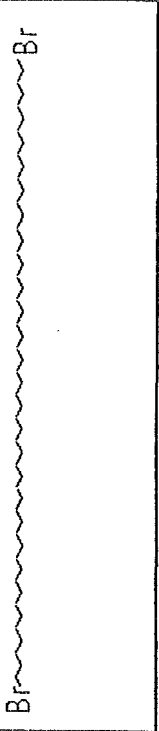


33	<p>Fixed Range</p> <p>Spect 1</p> <p>16.211 min. Scan: 830 Chan: 1 Ion: 8614 us RIC: 27354 BC</p> 	 <p>2,4-Hexadienedioic acid, 3-methyl-4-propyl-, dimethyl ester, (Z,E)-</p>	498	858	E
34	<p>Fixed Range</p> <p>Spect 1</p> <p>16.728 min. Scan: 853 Chan: 1 Ion: 3400 us RIC: 94159 BC</p> 	 <p>4-Hydroxy-3,5-dimethoxybenzaldehyde</p>	844	954	A
35	<p>Learned Range</p> <p>Spect 1</p> <p>16.821 min. Scan: 857 Chan: 1 Ion: 1167 us RIC: 315715 BC</p> 	 <p>2,4-Hexadienedioic acid, 3-methyl-4-propyl-, dimethyl ester, (Z,E)-</p>	431	841	E
36	<p>Learned Range</p> <p>Spect 1</p> <p>17.341 min. Scan: 860 Chan: 1 Ion: 10539 us RIC: 17386 BC</p> 	 <p>4-Hydroxy-3,5-dimethoxybenzaldehyde</p>	431	841	E

<p>37</p>	<p>Learned Spect 1 Range: 17.726 min. Scan: 897 Chan: 1 Ion: 1648 us RIC: 168216 BC</p> 	 <p>4-Hydroxy-2-methoxycinnamaldehyde</p>	<p>521</p> <p>793</p> <p>D</p>
<p>38</p>	<p>Learned Spect 1 Range: 18.736 min. Scan: 942 Chan: 1 Ion: 7308 us RIC: 33124 BC</p> 	 <p>3-Hydroxy-2-methyl propionic acid, 2-biphenyl-4-yl-2-oxoethyl ester</p>	<p>367</p> <p>769</p> <p>E</p>
<p>39</p>	<p>Learned Spect 1 Range: 20.188 min. Scan: 1007 Chan: 1 Ion: 4566 us RIC: 59776 BC</p> 	 <p>Dibutyl phthalate</p>	<p>724</p> <p>950</p> <p>B</p>
<p>40</p>	<p>Learned Spect 1 Range: 20.415 min. Scan: 1017 Chan: 1 Ion: 3359 us RIC: 86113 BC</p> 	 <p>3,5-Dimethoxy-4-hydroxycinnamaldehyde</p>	<p>773</p> <p>947</p> <p>B</p>

41	<p>Learned Spect 1 Range: 20.504 min. Scan: 1021 Chan: 1 Ion: 1609 us RIC: 187918 BC</p> 	 <p>5,6-Dimethoxy-1-indanone</p>	414	764	E
42	<p>Fixed Spect 1 Range: 20.800 min. Scan: 1034 Chan: 1 Ion: 8667 us RIC: 23302 BC</p> 	 <p>1-Cyclohexene-1-carboxylic acid, 4-(1,5-dimethyl-3-oxohexyl)-, methyl ester, [R*, R*]-</p>	385	799	E
43	<p>Learned Spect 2 Range: 27.145 min. Scan: 1320 Chan: 1 Ion: 17713 us RIC: 8498 BC</p> 				X
44	<p>Learned Spect 2 Range: 28.250 min. Scan: 1416 Chan: 1 Ion: 23262 us RIC: 3260 BC</p> 				X

45	<p>Learned Spect 2 Range: 34.708 min. Scan: 1664 Chan: 1 Ion: 17448 us RIC: 9382 BC</p> 	 <p>Tetrapentacotane, 1,54-dibromo-</p>	463	832	E
----	--	---	-----	-----	---

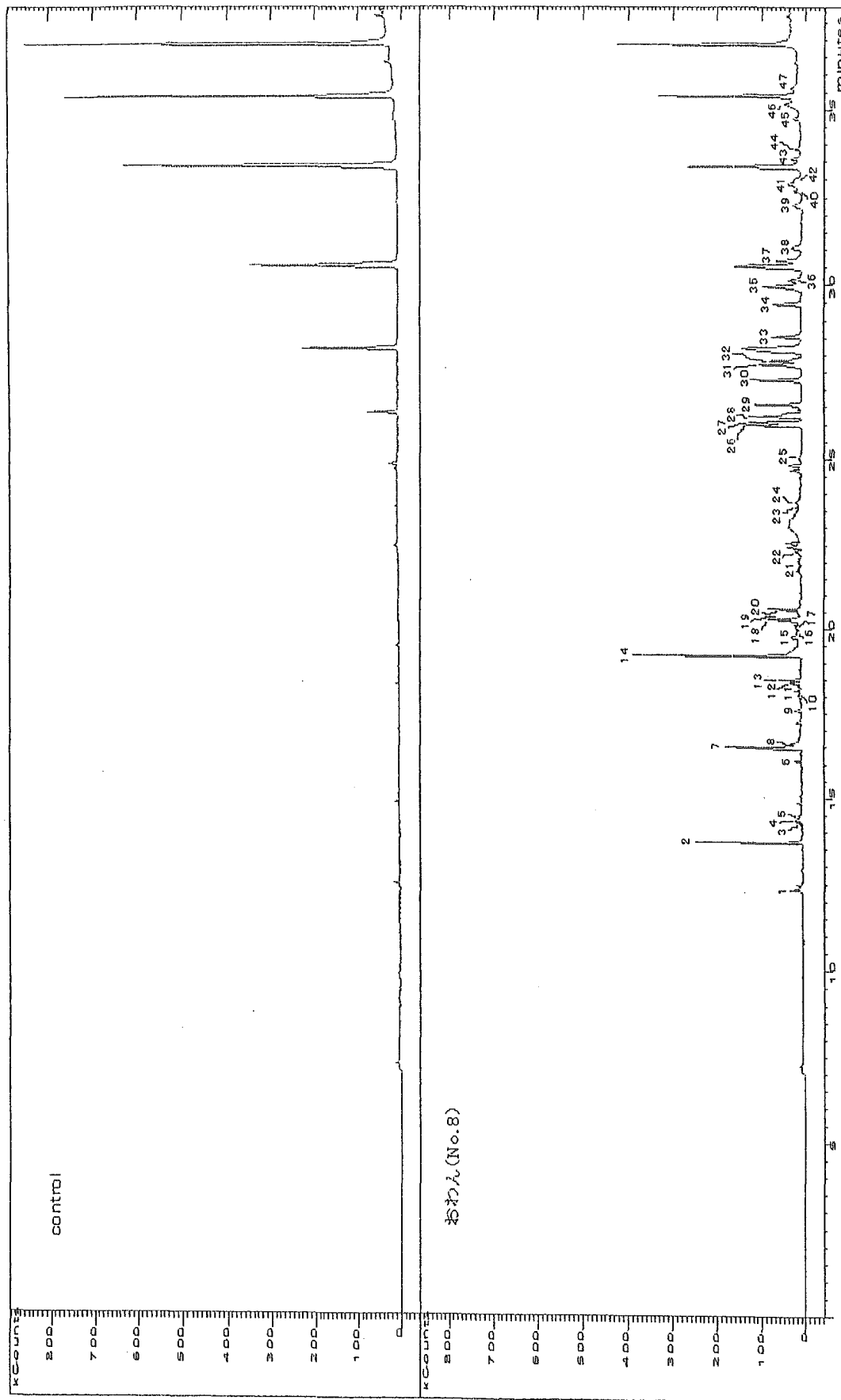
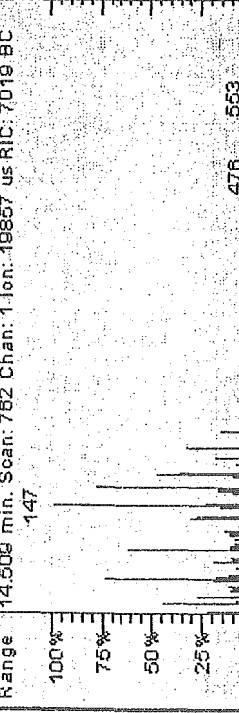
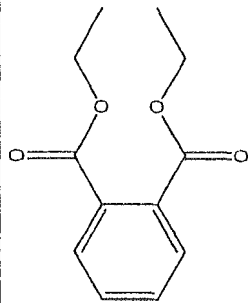

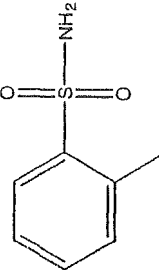
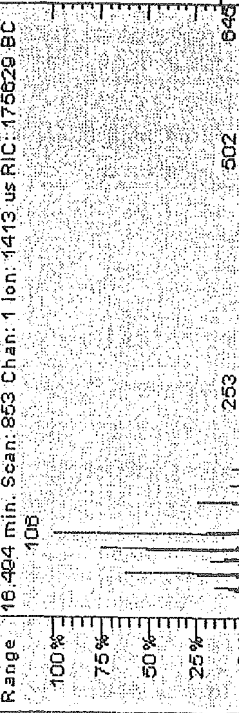
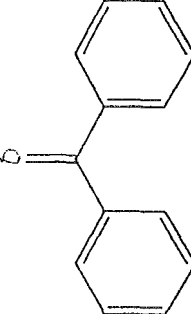

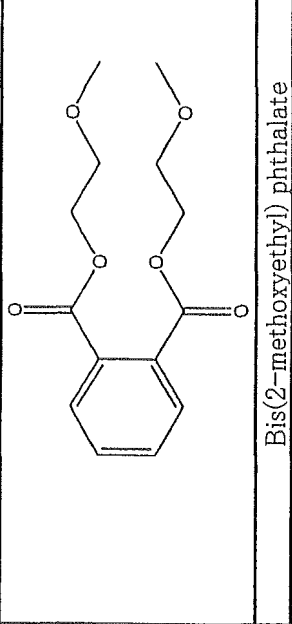
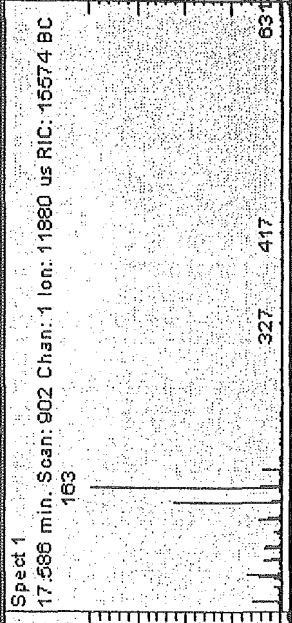
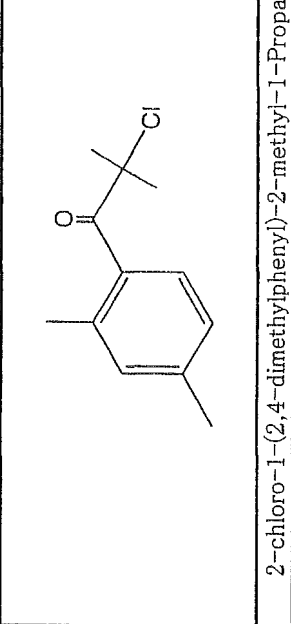
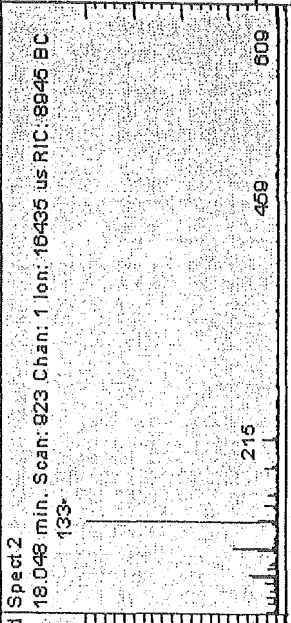
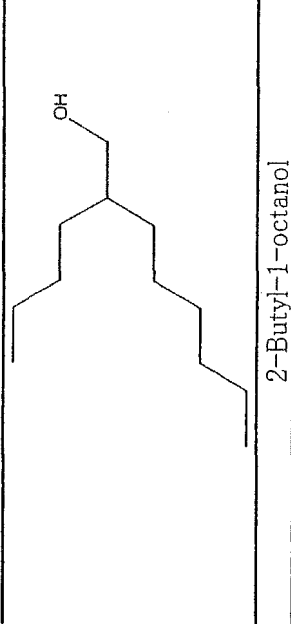
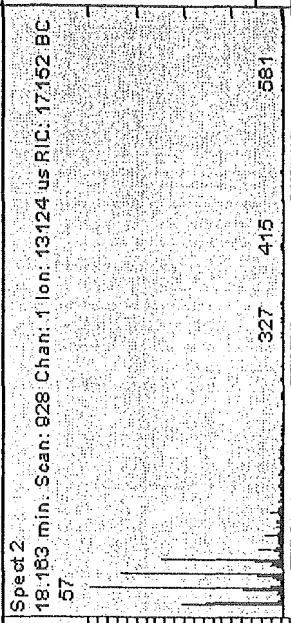
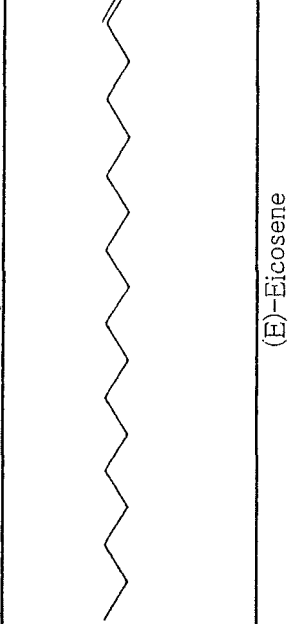
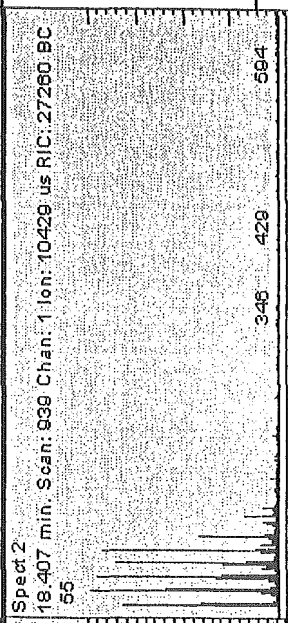


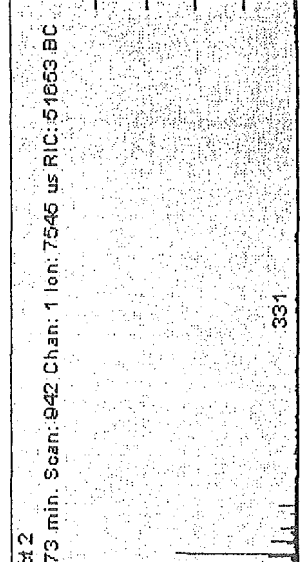
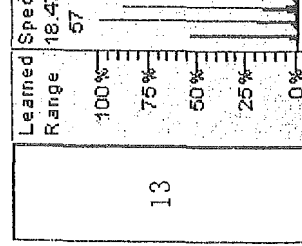
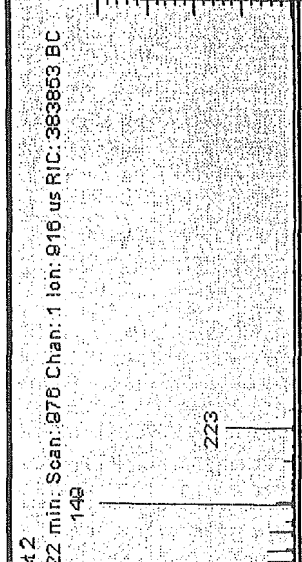
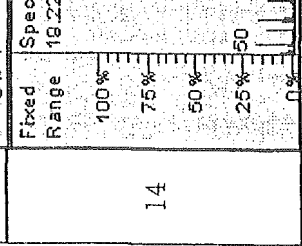
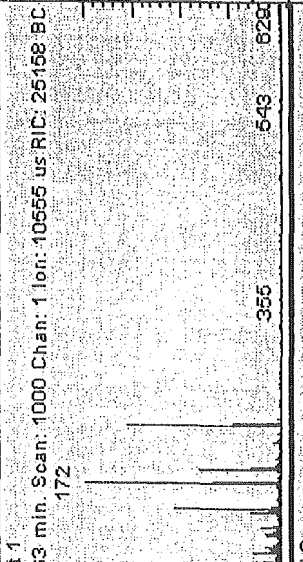
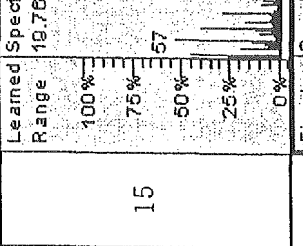
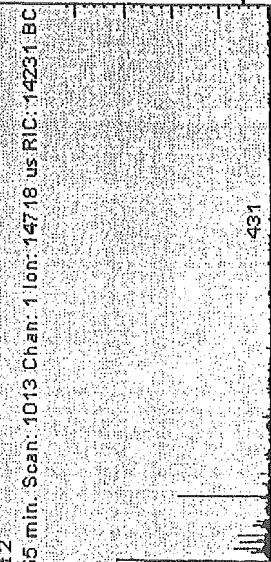
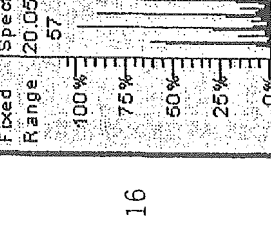


Fig. 3-8. おわん(No.8)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

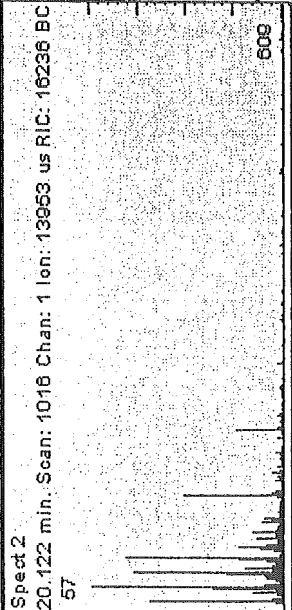
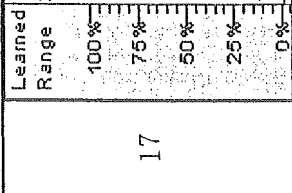
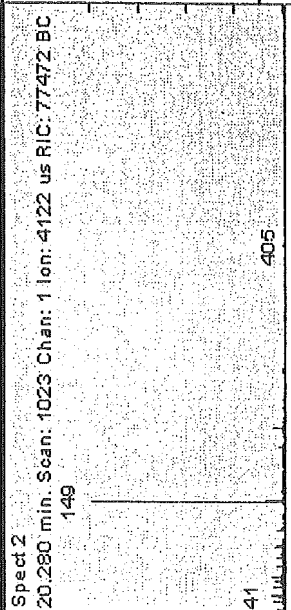
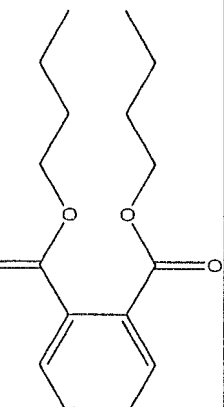
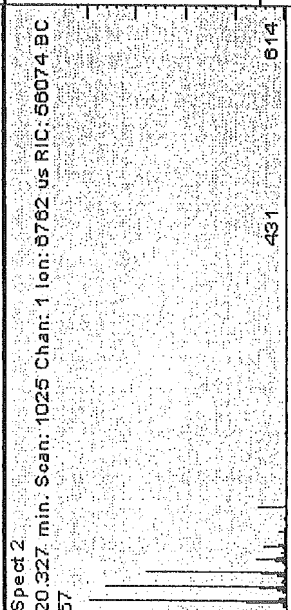
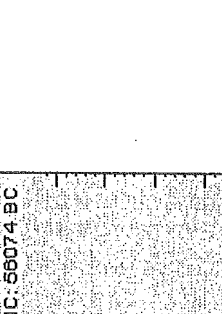
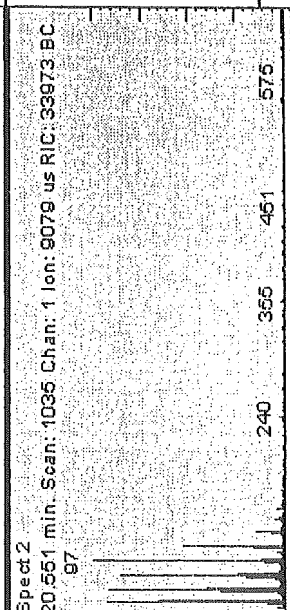

Table.3-8. おわん(No.8)から検出された有機化学物質のマススペクトルと構造式の一覧

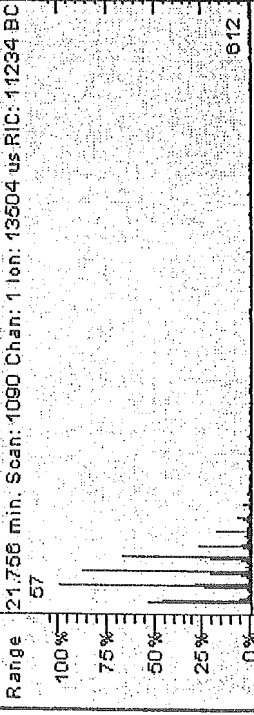
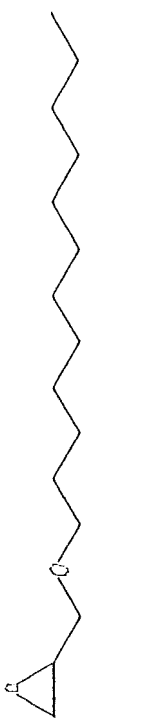
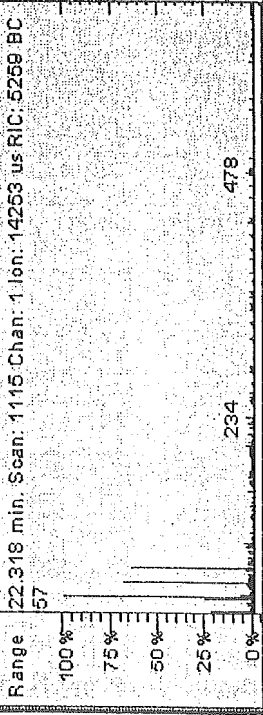
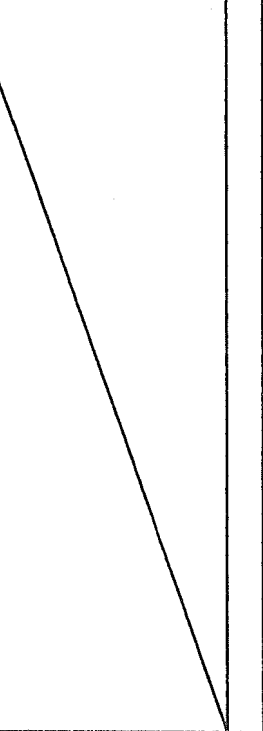
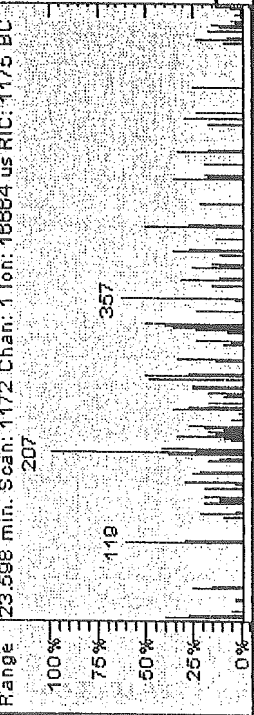
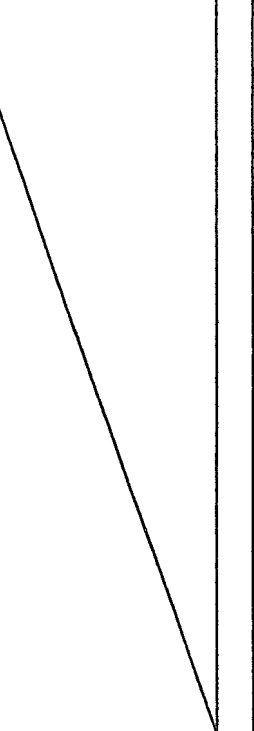
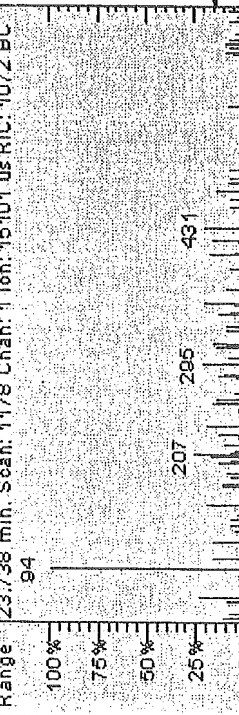
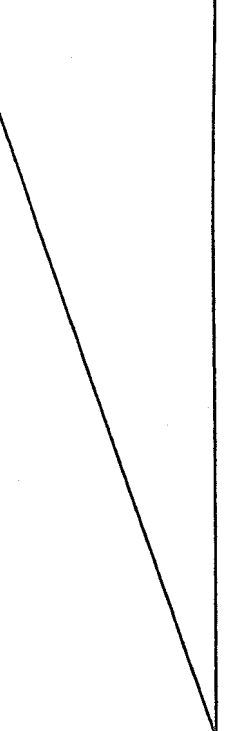
No	マススペクトル Mass Spectrum	フラグメンテーションがよく一致した化合物の構造式と化合物名 Fragmentation pattern consistent with the structure and name of the compound	Purity	Fit	信頼度 Reliability
1	<p>Learned Spect 2 Range 12.332 min. Scan: 663 Chan: 1 Ion: 7536 us RIC: 32760 BC</p> <p>104, 281, 429</p>	 Phthalic anhydride	803	889	A
2	<p>Fixed Spect 2 Range 13.690 min. Scan: 725 Chan: 1 Ion: 8649 us RIC: 41182 BC</p> <p>109, 347, 467, 624</p>	 3-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-2-propenal	596	871	D
3	<p>Fixed Spect 1 Range 14.284 min. Scan: 752 Chan: 1 Ion: 12842 us RIC: 11874 BC</p> <p>163, 77, 345, 475</p>	 Dimethyl phthalate	834	925	A
4	<p>Learned Spect 1 Range 14.350 min. Scan: 755 Chan: 1 Ion: 10757 us RIC: 17664 BC</p> <p>147, 430</p>	 o-Cyanobenzoic acid	785	950	B

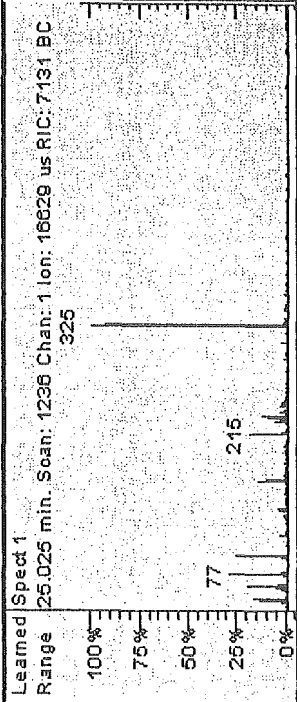
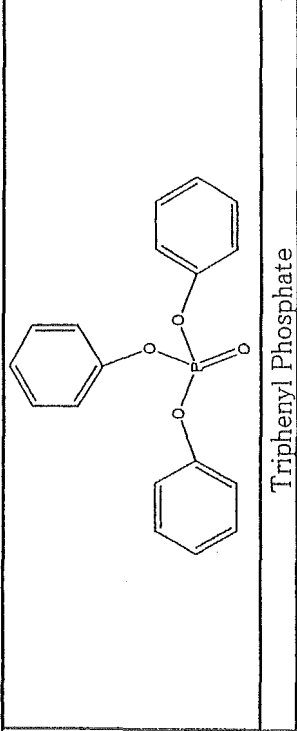
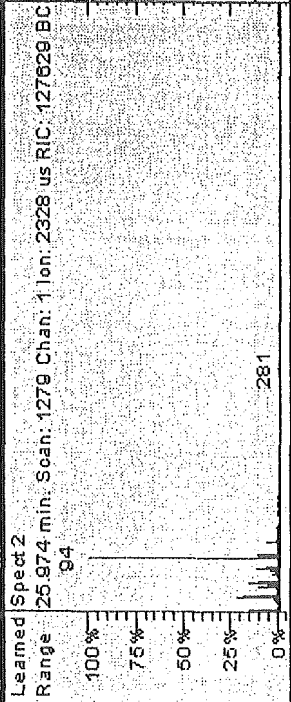
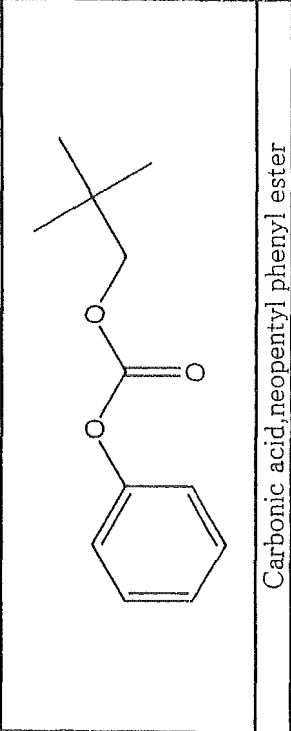
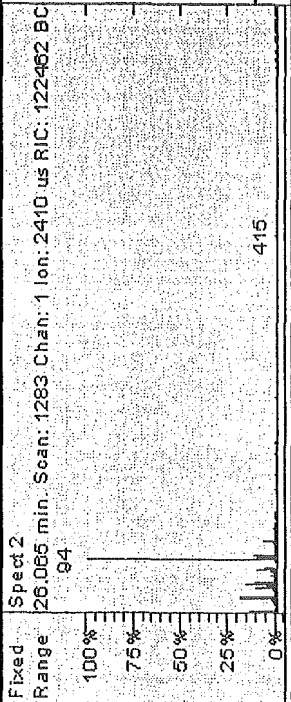
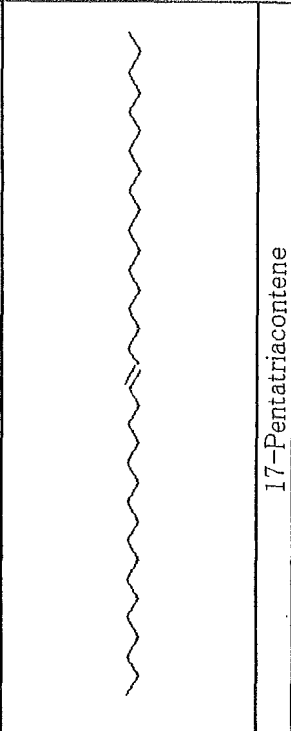
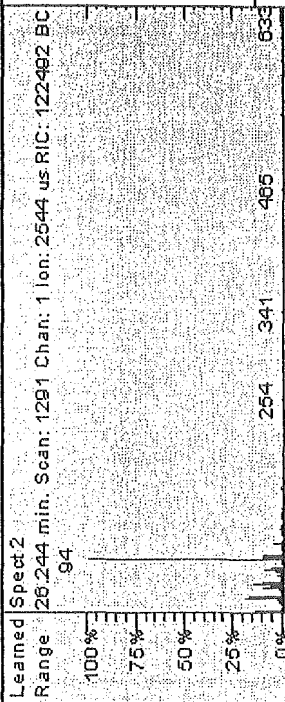
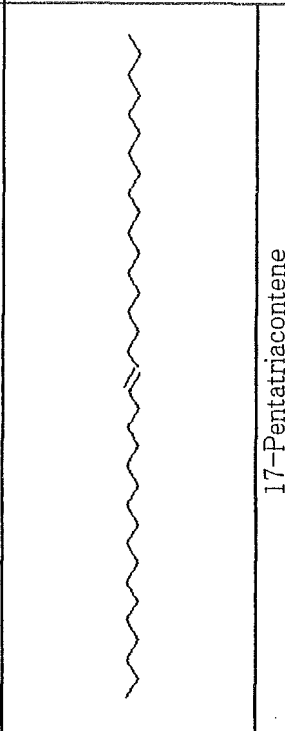
5	<p>Learned Spect 1 Range 14.509 min. Scan: 762 Chan: 1 Ion: 19857 us RIC: 7019 BC</p> 	 <p>Diethyl phthalate</p>	826	960	X
6	<p>Learned Spect 2 Range 16.102 min. Scan: 835 Chan: 1 Ion: 12277 us RIC: 18854 BC</p> 		 <p>o-Toluenesulfonamide</p>	749	867
7	<p>Learned Spect 2 Range 16.484 min. Scan: 853 Chan: 1 Ion: 1413 us RIC: 175629 BC</p> 	 <p>Benzophenone</p>		732	893
8	<p>Learned Spect 2 Range 15.609 min. Scan: 858 Chan: 1 Ion: 5638 us RIC: 36337 BC</p> 				


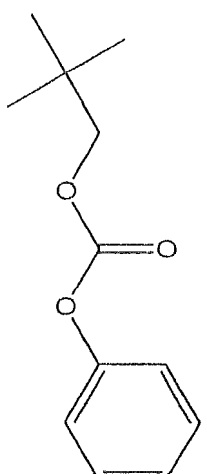
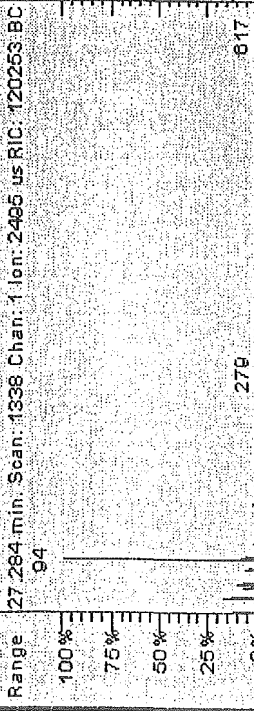
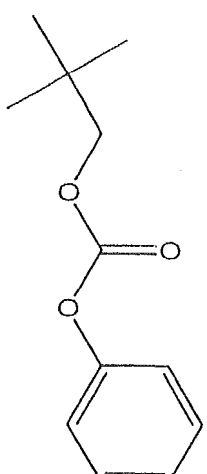
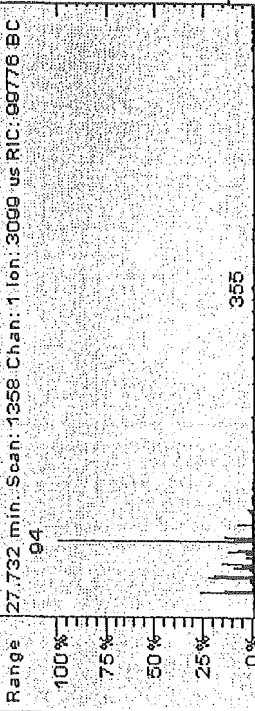

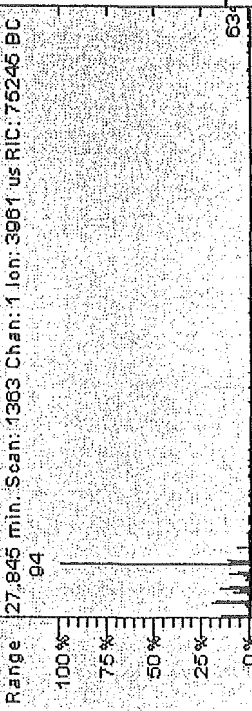

9	<p>Fixed Spect 1 Range: 17.586 min. Scan: 902 Chan: 1 Ion: 11980 us RIC: 15574 BC</p> 	 <p>Bis(2-methoxyethyl) phthalate</p>	745	846	B
10	<p>Learned Spect 2 Range: 18.048 min. Scan: 823 Chan: 1 Ion: 16436 us RIC: 8946 BC</p> 	 <p>2-chloro-1-(2,4-dimethylphenyl)-2-methyl-1-propanone</p>	544	881	D
11	<p>Learned Spect 2 Range: 18.163 min. Scan: 828 Chan: 1 Ion: 13124 us RIC: 17152 BC</p> 	 <p>2-Butyl-1-octanol</p>	548	798	D
12	<p>Fixed Spect 2 Range: 18.407 min. Scan: 939 Chan: 1 Ion: 10429 us RIC: 27260 BC</p> 	 <p>(E)-Eicosene</p>	667	880	C

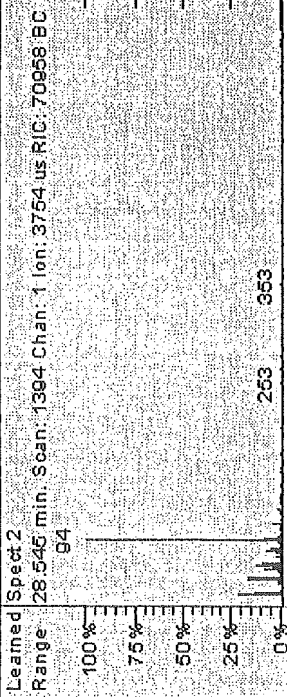
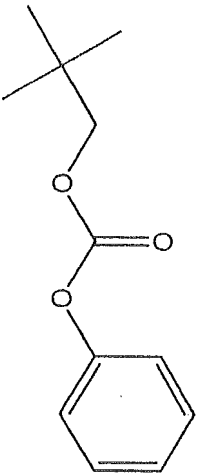
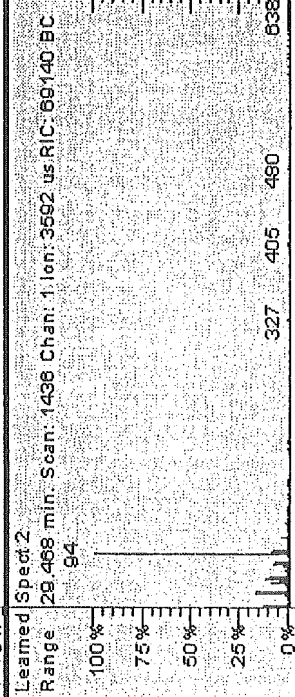
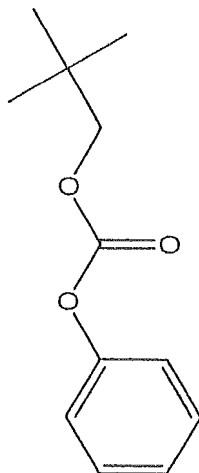
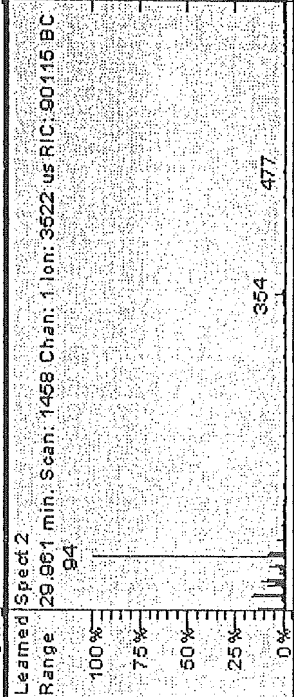
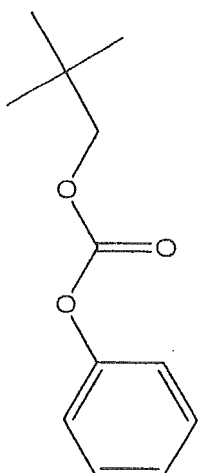
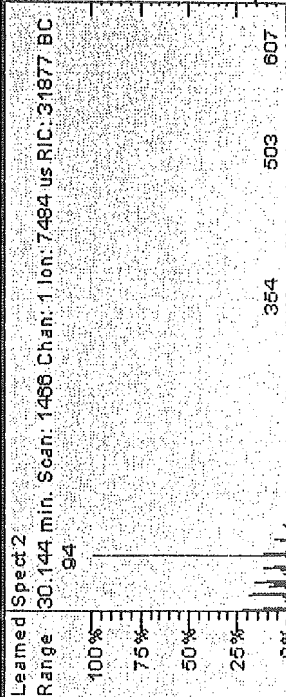

13	<p>Learned Spect 2 Range 18.473 min. Scan: 942 Chan: 1 Ion: 7546 us RIC: 51853 BC</p> 	 <p>4-methyl-1-Undecene</p>	688	840	C
14	<p>Fixed Spect 2 Range 19.222 min. Scan: 876 Chan: 1 Ion: 916 us RIC: 363853 BC</p> 	 <p>Dibutyl phthalate</p>	646	819	C
15	<p>Learned Spect 1 Range 19.763 min. Scan: 1000 Chan: 1 Ion: 10555 us RIC: 26158 BC</p> 	 <p>2,5-Dimethoxy-4-chloroaniline</p>	355	872	E
16	<p>Fixed Spect 2 Range 20.055 min. Scan: 1013 Chan: 1 Ion: 14718 us RIC: 14231 BC</p> 	 <p>2,5-Dimethoxy-4-chloroaniline</p>			X

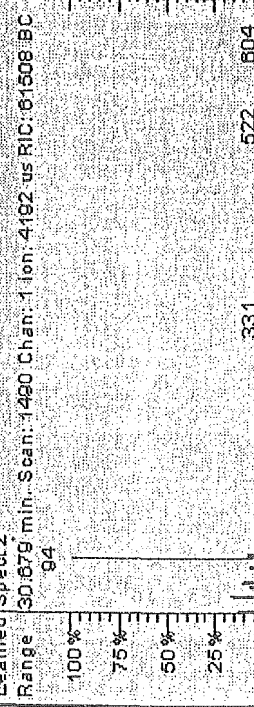
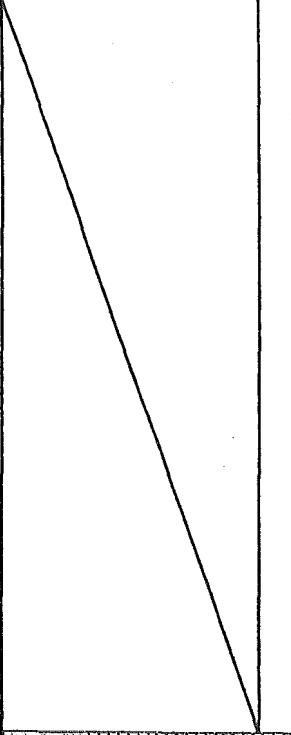
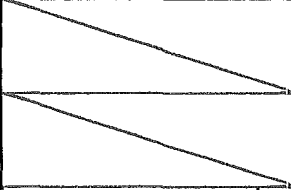

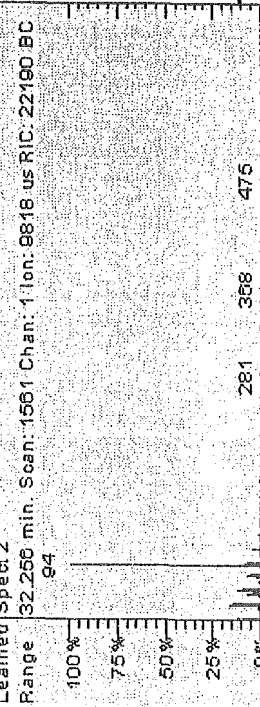
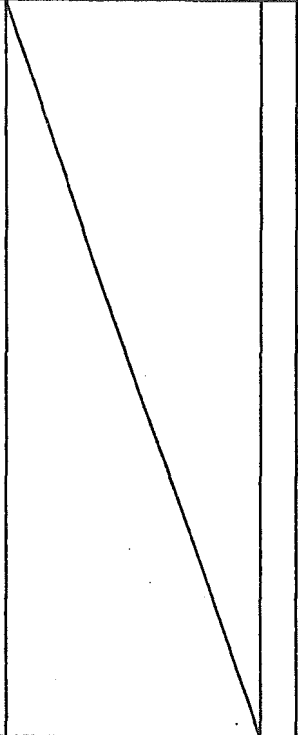
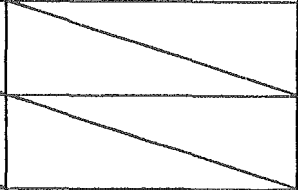
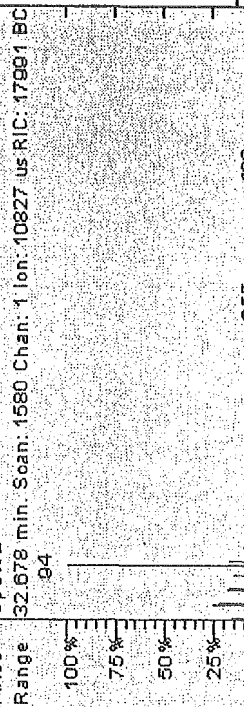
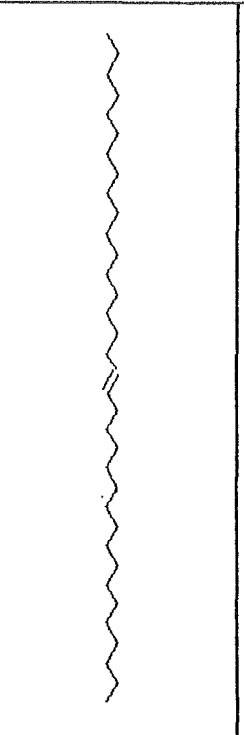
17	<p>Learned Spect 2 Range 20.122 min. Scan: 1016 Chan: 1 Ion: 13953 us RIC: 16236 BC</p> 		X
18	<p>Learned Spect 2 Range 20.280 min. Scan: 1023 Chan: 1 Ion: 4122 us RIC: 77472 BC</p> 	<p>  Dibutyl phthalate </p>	812 966 A
19	<p>Learned Spect 2 Range 20.327 min. Scan: 1025 Chan: 1 Ion: 8762 us RIC: 56074 BC</p> 	<p>  2-Butyl-1-octanol </p>	643 821 C
20	<p>Learned Spect 2 Range 20.561 min. Scan: 1035 Chan: 1 Ion: 9079 us RIC: 33973 BC</p> 	<p>  icosan-1-ol </p>	718 902 B

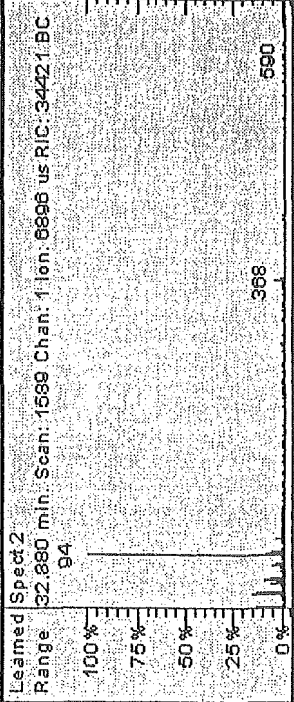
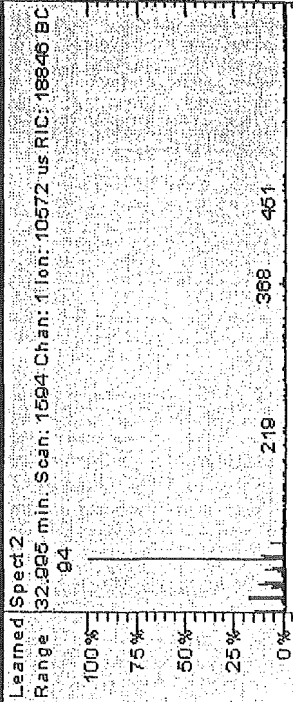
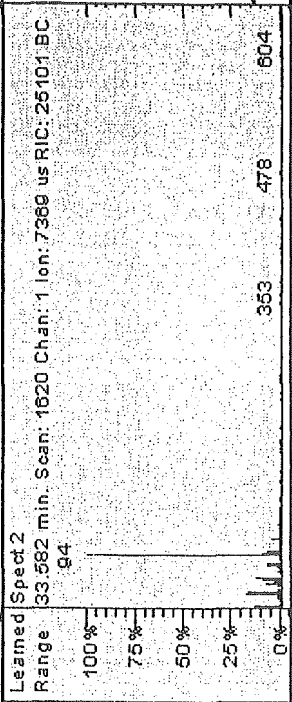
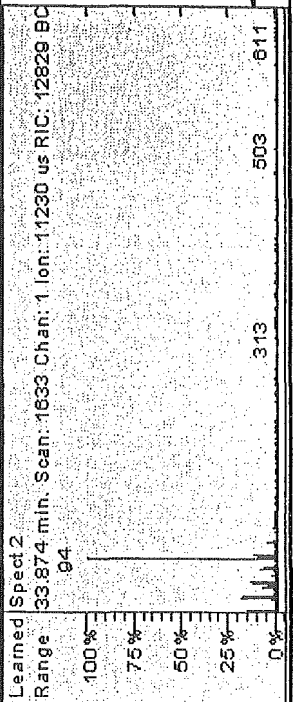
21	<p>Fixed Range Spect 2 21.756 min. Scan: 1090 Chan: 1 Ion: 13504 us RIC: 11234 BC</p> 	 <p>[(dodecyloxy)methyl]oxirane</p>	546	815	D
22	<p>Learned Range Spect 2 22.318 min. Scan: 1115 Chan: 1 Ion: 14253 us RIC: 5259 BC</p> 				X
23	<p>Learned Range Spect 2 23.598 min. Scan: 1172 Chan: 1 Ion: 16664 us RIC: 1175 BC</p> 				X
24	<p>Learned Range Spect 2 23.738 min. Scan: 1178 Chan: 1 Ion: 15101 us RIC: 1072 BC</p> 				X

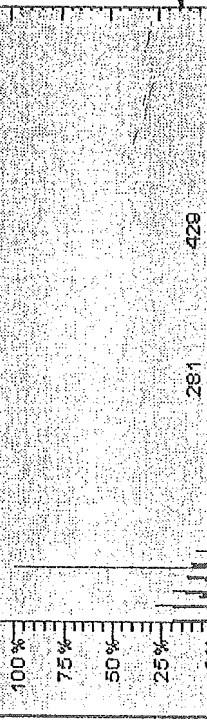
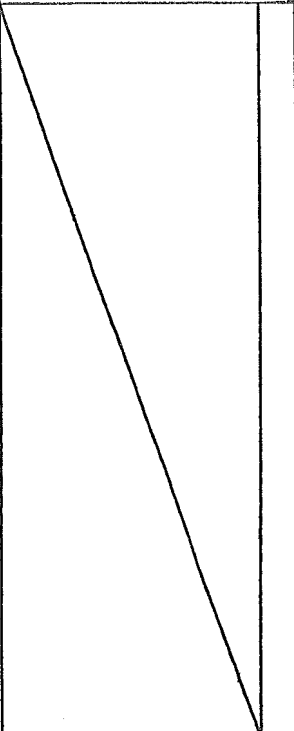
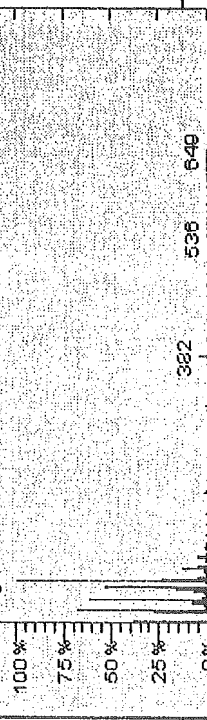
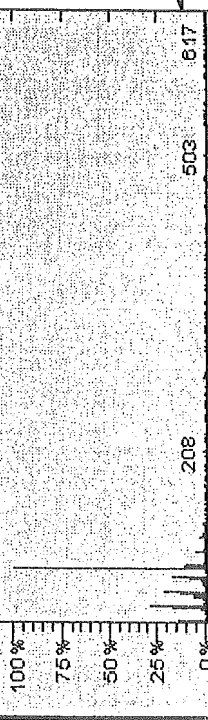
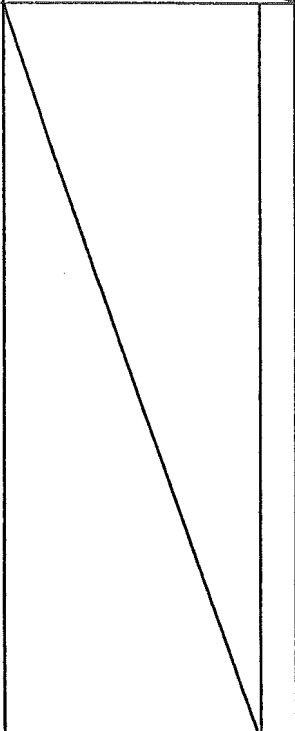
25	<p>Learned Spect 1 Range: 25.025 min. Scan: 1236 Chan: 1 Ion: 16629 us RIC: 7131 BC</p> 	 <p>Triphenyl Phosphate</p>	781	952	B
26	<p>Learned Spect 2 Range: 25.974 min. Scan: 1278 Chan: 1 Ion: 2328 us RIC: 127629 BC</p> 	 <p>Carbonic acid,neopentyl phenyl ester</p>	506	825	D
27	<p>Fixed Spect 2 Range: 26.065 min. Scan: 1283 Chan: 1 Ion: 2410 us RIC: 122462 BC</p> 	 <p>17-Pentatriacontene</p>	431	857	E
28	<p>Learned Spect 2 Range: 26.244 min. Scan: 1291 Chan: 1 Ion: 2544 us RIC: 122462 BC</p> 	 <p>17-Pentatriacontene</p>	409	853	E

29	<p>Fixed Spect 2 Range 26.557 min. Scan: 1305 Chan: 1 Ion: 27.46 us RIC: 110025 BC </p>	 Carboxylic acid, neopentyl phenyl ester	540	823	D
30	<p>Learned Spect 2 Range 27.284 min. Scan: 1338 Chan: 1 Ion: 2465 us RIC: 120263 BC </p>	 Carboxylic acid, neopentyl phenyl ester	559	814	D
31	<p>Learned Spect 1 Range 27.732 min. Scan: 1358 Chan: 1 Ion: 3099 us RIC: 99776 BC </p>	 17-Pentatriacontene	432	852	E
32	<p>Learned Spect 1 Range 27.845 min. Scan: 1363 Chan: 1 Ion: 3061 us RIC: 75246 BC </p>	 17-Pentatriacontene	435	860	E

33	<p>Learned Spect 2 Range: 28.545 min. Scan: 1394 Chan: 1 Ion: 3754 us RIC: 70958 BC</p> 	 <p>Carbonic acid,neopentyl phenyl ester</p>	528	817	D
34	<p>Learned Spect 2 Range: 29.468 min. Scan: 1436 Chan: 1 Ion: 3692 us RIC: 69140 BC</p> 	 <p>Carbonic acid,neopentyl phenyl ester</p>	530	824	D
35	<p>Learned Spect 2 Range: 29.961 min. Scan: 1458 Chan: 1 Ion: 3522 us RIC: 90115 BC</p> 	 <p>Carbonic acid,neopentyl phenyl ester</p>	401	822	E
36	<p>Learned Spect 2 Range: 30.144 min. Scan: 1486 Chan: 1 Ion: 7494 us RIC: 31877 BC</p> 	 <p>icosan-1-ol</p>	392	847	E

37	<p>Learned Spect 2 Range 30.679 min. Scan: 1490 Chan: 1 Ion: 4192 us RIC: 61508 BC</p> 			X
38	<p>Learned Spect 2 Range 31.060 min. Scan: 1507 Chan: 1 Ion: 8891 us RIC: 25200 BC</p> 			
39	<p>Learned Spect 2 Range 32.256 min. Scan: 1561 Chan: 1 Ion: 9818 us RIC: 22190 BC</p> 			X
40	<p>Fixed Spect 2 Range 32.678 min. Scan: 1580 Chan: 1 Ion: 10827 us RIC: 17991 BC</p> 			 <p style="text-align: center;">17-Pentatriacontene</p>

41	<p>Learned Spect 2 Range: 32.880 min. Scan: 1599 Chan: 1 Ion: 6896 us RIC: 34421 BC</p> 			X
42	<p>Learned Spect 2 Range: 32.885 min. Scan: 1594 Chan: 1 Ion: 10572 us RIC: 18646 BC</p> 			X
43	<p>Learned Spect 2 Range: 33.582 min. Scan: 1620 Chan: 1 Ion: 7369 us RIC: 25101 BC</p> 			X
44	<p>Learned Spect 2 Range: 33.874 min. Scan: 1633 Chan: 1 Ion: 11230 us RIC: 12829 BC</p> 			X

45	<p>Learned Spect 2 Range: 34.728 min. Scan: 1671 Chan: 1 Ion: 9697 us RIC: 15764 BC</p> 			X
46	<p>Fixed Spect 2 Range: 35.160 min. Scan: 1690 Chan: 1 Ion: 7135 us RIC: 34867 BC</p> 			
47	<p>Learned Spect 2 Range: 35.611 min. Scan: 1710 Chan: 1 Ion: 10028 us RIC: 16613 BC</p> 			X

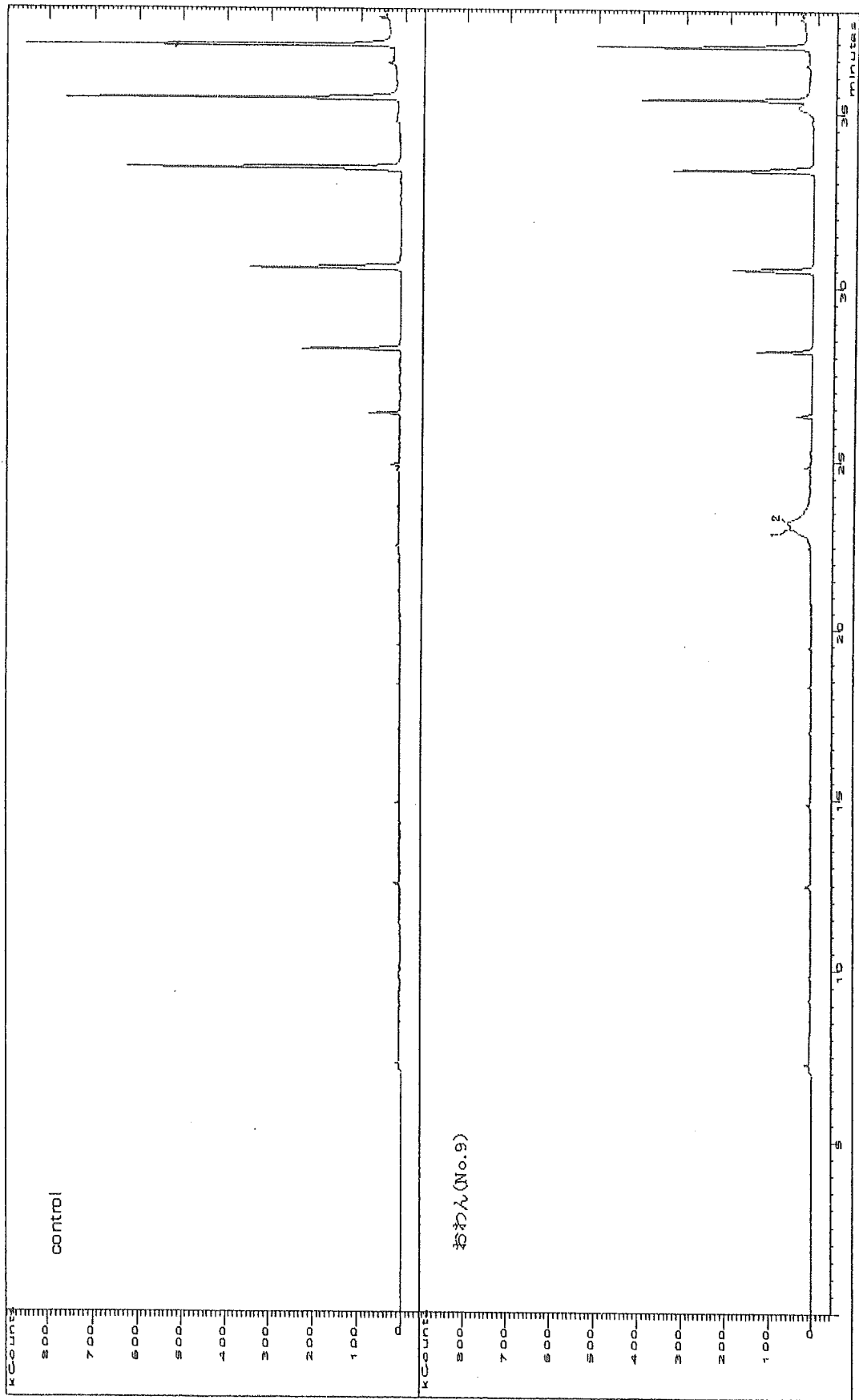


Fig.3-9. おわん (No.9) のトータライオンクロマトグラム (下) と control のトータライオンクロマトグラム (上)

Table.3-9. おわん(No.9)から検出された有機化学物質のマススペクトルと構造式の一覧

No	マススペクトル	フラグメントーションがよく一致した化合物の構造式と化合物名	Purity	Fit	信頼度
1	<p>Learned Spect 2 Range: 23.065 min. Scan: 1140 Chan: 1 Ion: 7756 us RIC: 46757 BC</p>	<p>$C_{54}H_{108}Br_2$</p>	668	828	C
		1,54-dibromo-tertapentacotane			
2	<p>Learned Spect 2 Range: 23.222 min. Scan: 1156 Chan: 1 Ion: 7485 us RIC: 54732 BC</p>		657	816	C
		2-hexyl-1-Decanol			

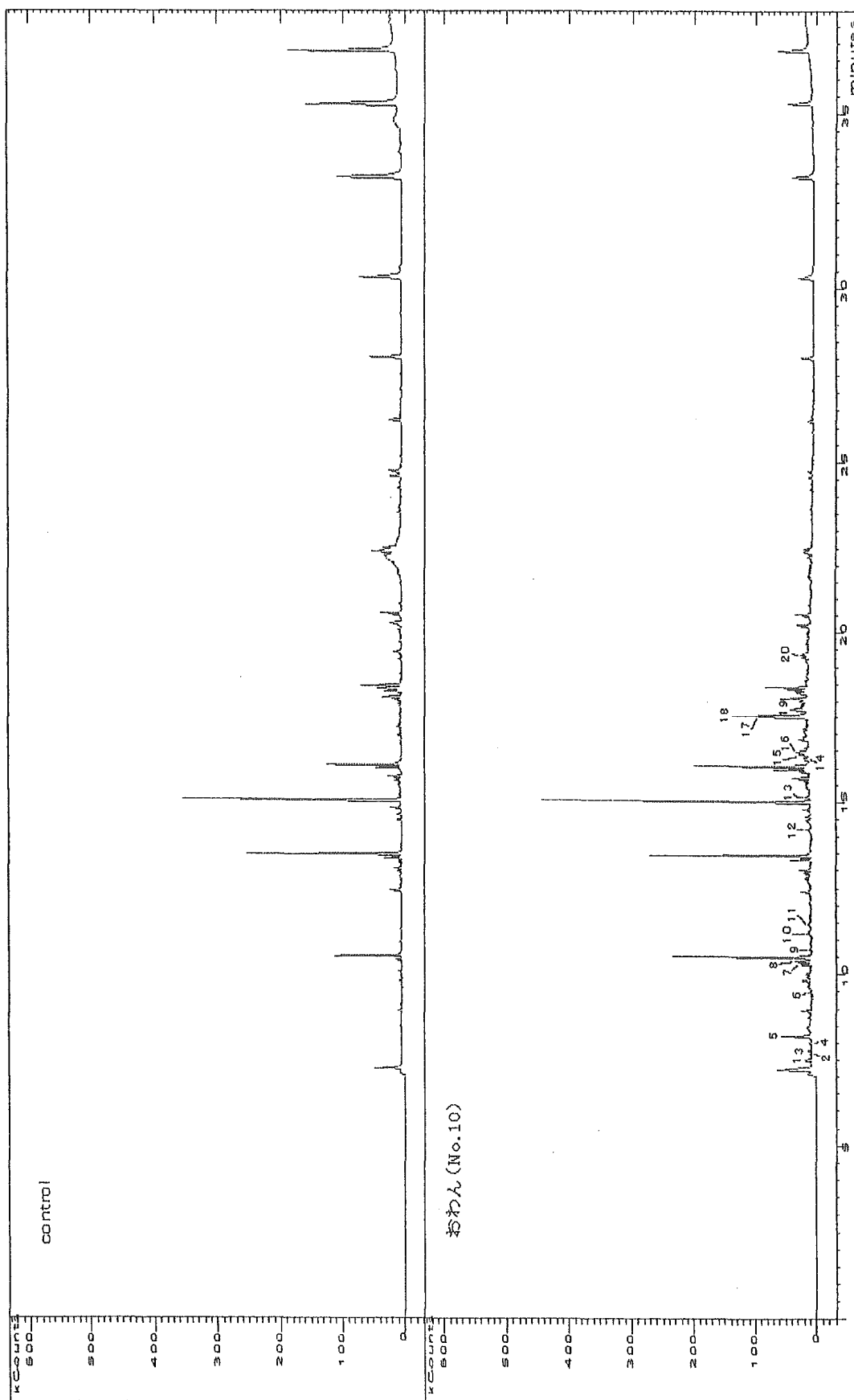


Fig. 3-10. おわん (No.10)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)