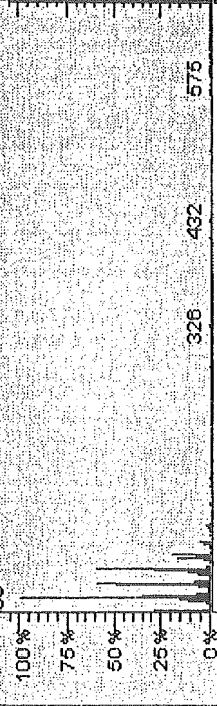
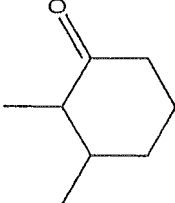
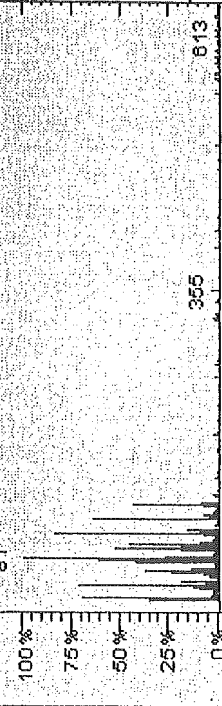
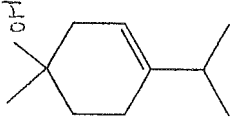
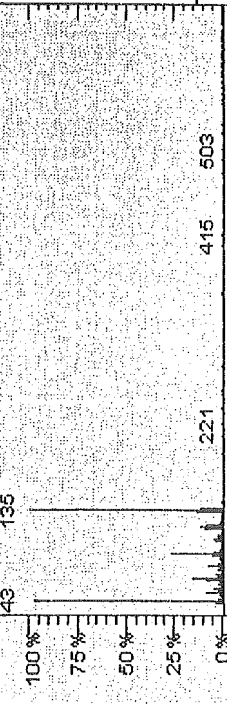
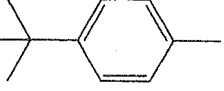

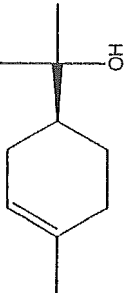



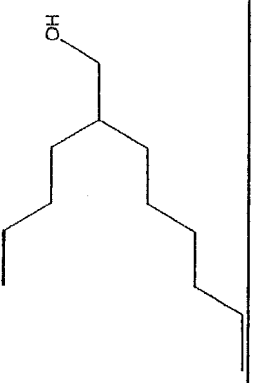

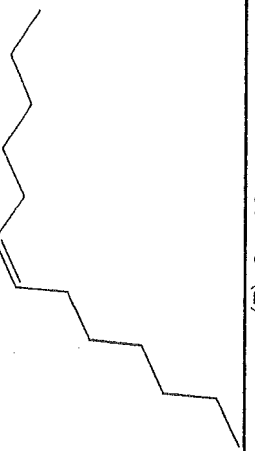

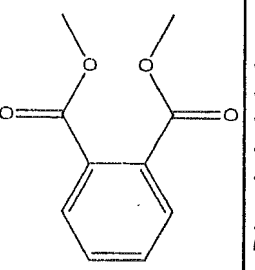
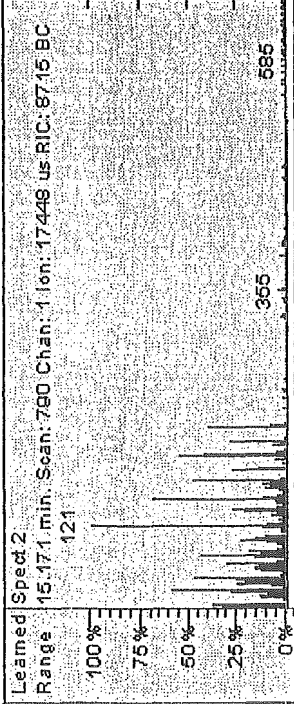
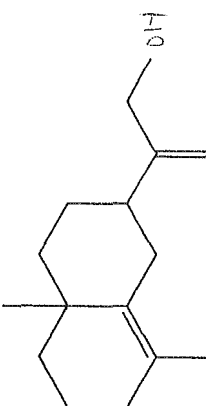
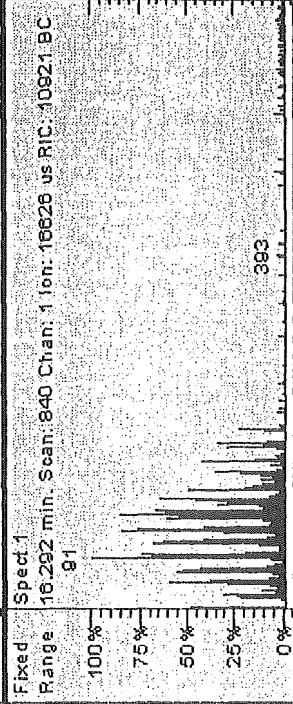
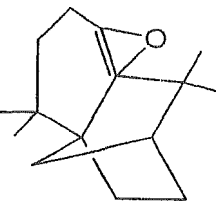
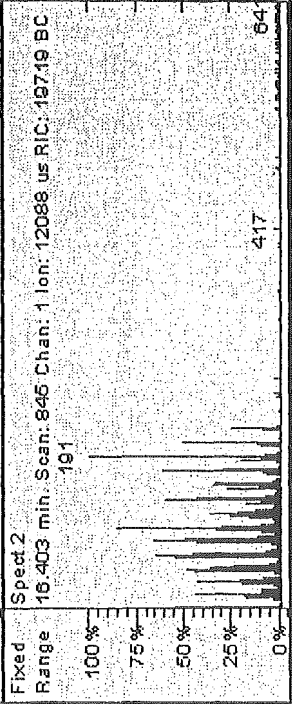
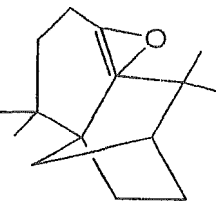
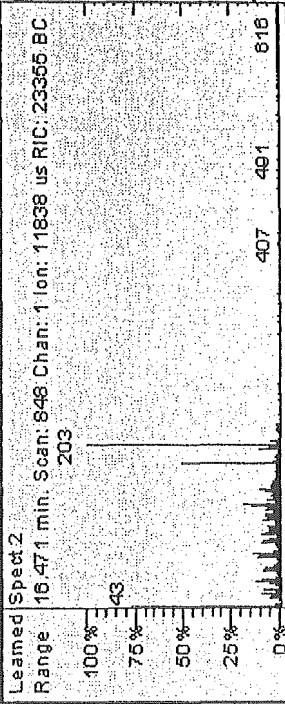


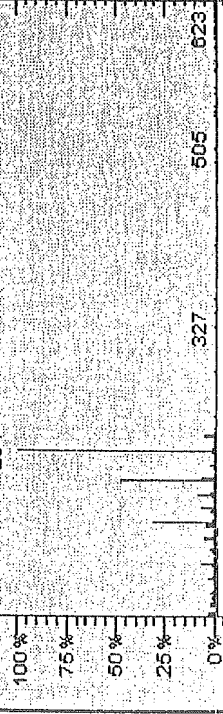
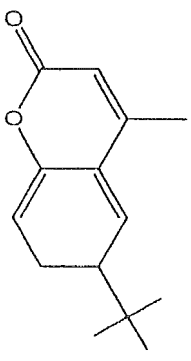

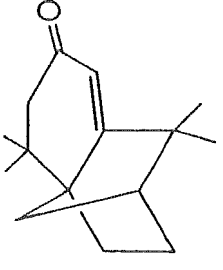

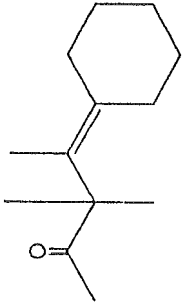
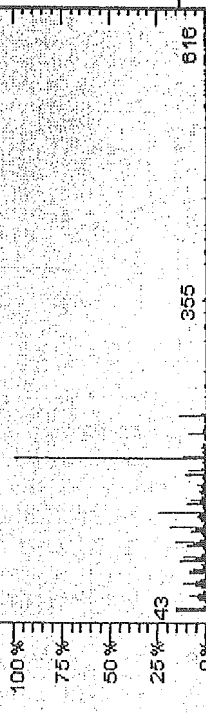
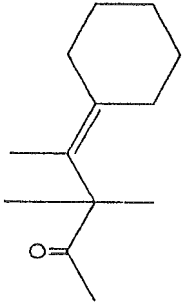
Table.3-10. おわん(No.10)から検出された有機化学物質のマススペクトルと構造式の一覧

No	マススペクトル	フラグメンテーションが一致した化合物の構造式と化合物名	Purity	Fit	信頼度
1	<p>Learned Spect2 Range: 7.502 min., Scan: 442 Chan: 1 Ion: 17522 us RIC: 11979 BC</p>	<p>7-Oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)-</p>	637	859	C
2	<p>Fixed Spect2 Range: 7.654 min., Scan: 440 Chan: 1 Ion: 21394 us RIC: 3928 BC</p>	<p>4-Ethyl-1,2-dimethylbenzene</p>	507	896	D
3	<p>Fixed Spect2 Range: 7.761 min., Scan: 454 Chan: 1 Ion: 18065 us RIC: 6852 BC</p>	<p>1,8-Cineole</p>	560	828	D
4	<p>Fixed Spect2 Range: 7.987 min., Scan: 464 Chan: 1 Ion: 23979 us RIC: 4260 BC</p>	<p>2,2-Dimethyl-cis-3-hexene</p>	438	735	E

5	<p>Fixed Spect 2 Range: 8.184 min. Scan: 473 Chan: 1 Ion: 6862 us RIC: 49803 BC</p> 	 <p>Dimethyl-2,3-cyclohexanone</p>	662	802	C
6	<p>Learned Spect 2 Range: 9.487 min. Scan: 532 Chan: 1 Ion: 17880 us RIC: 7195 BC</p> 	 <p>3-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-</p>	590	816	D
7	<p>Learned Spect 2 Range: 10.263 min. Scan: 567 Chan: 1 Ion: 12646 us RIC: 19281 BC</p> 	 <p>p-cymen-8-ol</p>	708	902	B
8	<p>Learned Spect 2 Range: 10.375 min. Scan: 572 Chan: 1 Ion: 9803 us RIC: 27549 BC</p> 	 <p>alpha-Terpineol</p>	676	853	C

9	<p>Fixed Spect 1 Range 10.732 min. Scan: 588 Chan: 1 Ion: 21038 us RIC: 4327 BC</p> 	 <p>1-Decyne</p>	481	827	E
10	<p>Learned Spect 2 Range 11.176 min. Scan: 608 Chan: 1 Ion: 18884 us RIC: 7890 BC</p> 	 <p>2-Butyl-1-octanol</p>	540	752	D
11	<p>Learned Spect 2 Range 11.442 min. Scan: 620 Chan: 1 Ion: 18453 us RIC: 7271 BC</p> 	 <p>(Z)-6-tridecene</p>	453	836	E
12	<p>Fixed Spect 1 Range 14.197 min. Scan: 748 Chan: 1 Ion: 16341 us RIC: 9672 BC</p> 	 <p>Dimethyl phthalate</p>	767	929	B

13	<p>Learned Spect 2 Range 15.171 min. Scan: 780 Chan: 1 Ion: 17448 us RIC: 8715 BC</p> 	 <p>2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol</p>	560	848	D
14	<p>Fixed Spect 1 Range 16.292 min. Scan: 840 Chan: 1 Ion: 16626 us RIC: 10921 BC</p> 			 <p>4a,7-Methano-4aH-naphth[1,8a-b]oxirene,octahydro-4,8-tetramethyl-</p>	631
15	<p>Learned Spect 2 Range 16.403 min. Scan: 845 Chan: 1 Ion: 12088 us RIC: 19719 BC</p> 	 <p>4a,7-Methano-4aH-naphth[1,8a-b]oxirene,octahydro-4,8-tetramethyl-</p>			
16	<p>Learned Spect 2 Range 16.471 min. Scan: 848 Chan: 1 Ion: 11638 us RIC: 23355 BC</p> 				

17	<p>Learned Spect 2 Range 17.500 min. Scan: 894 Chan: 1 Ion: 45222 us RIC: 85110 BC 201</p> 	 <p>6-tert-Butyl-4-methylcoumarin</p>	703	848	B
18	<p>Fixed Spect 2 Range 17.545 min. Scan: 896 Chan: 1 Ion: 3010 us RIC: 130378 BC 147</p> 	 <p>1,1,5,5-tetramethyl-1,2,3,4,5,6-hexahydro-7H-2,4a-Methanonaphthalen-7-one</p>	821	947	A
19	<p>Fixed Spect 1 Range 17.747 min. Scan: 905 Chan: 1 Ion: 8338 us RIC: 35123 BC 43</p> 	 <p>3,3-dimethyl-4cyclohexylidene-2-pentanone</p>	X	X	X
20	<p>Fixed Spect 2 Range 19.344 min. Scan: 976 Chan: 1 Ion: 14122 us RIC: 16984 BC 193</p> 	 <p>3,3-dimethyl-4cyclohexylidene-2-pentanone</p>	496	760	E

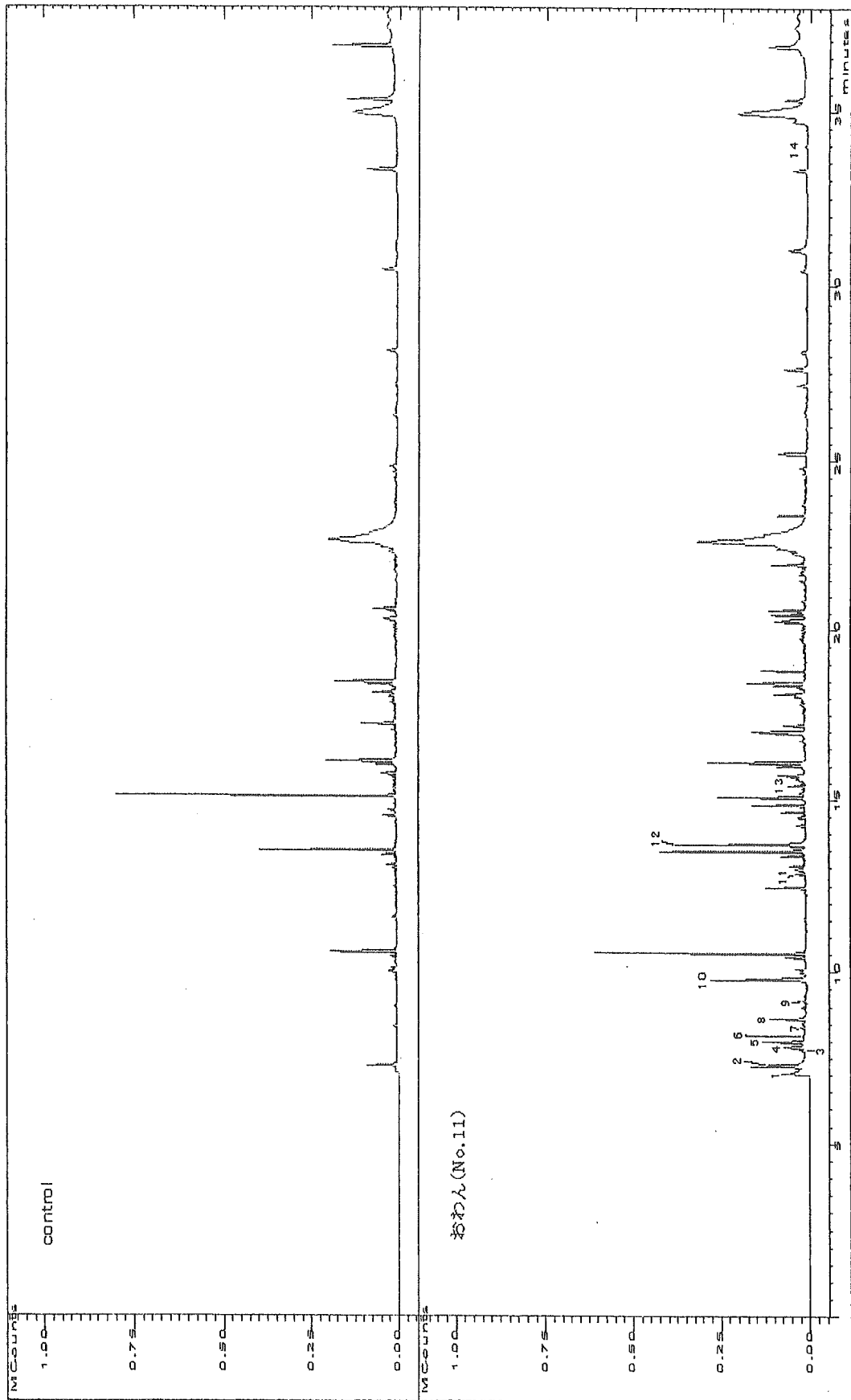
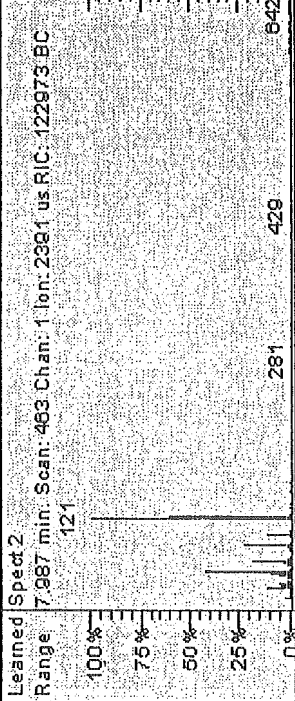
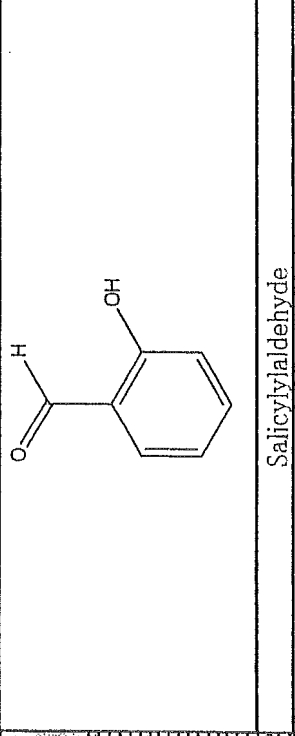
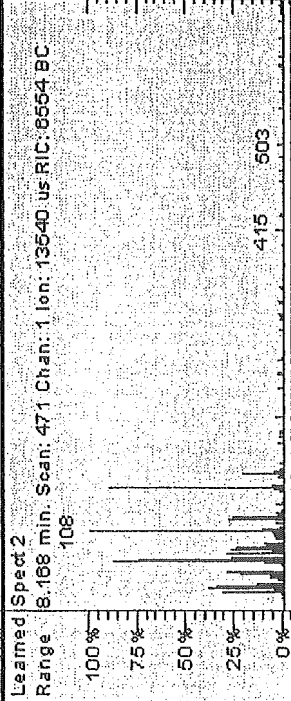
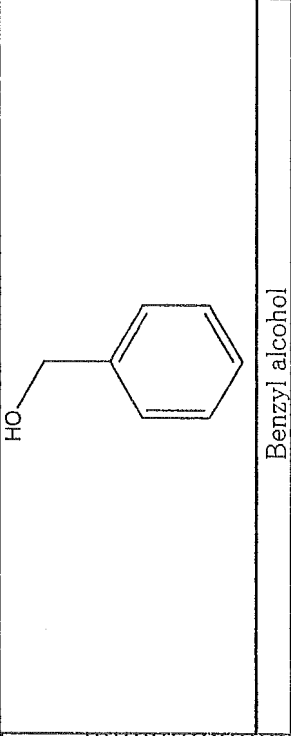
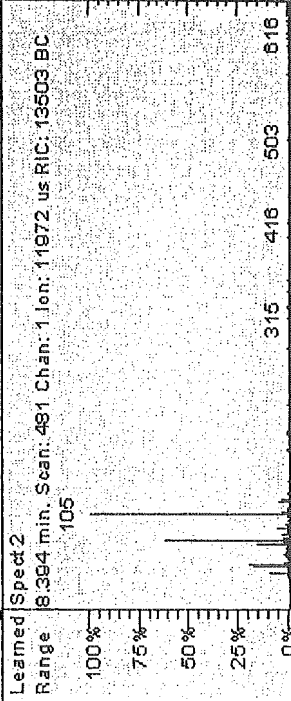
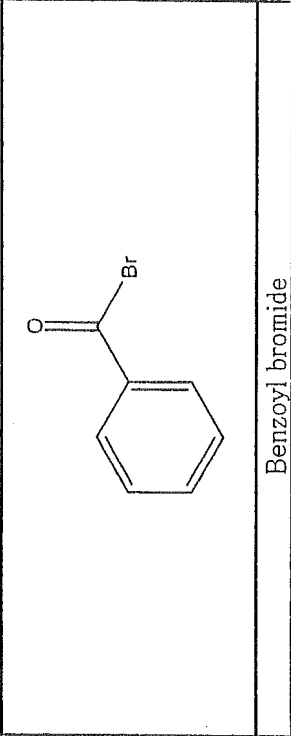
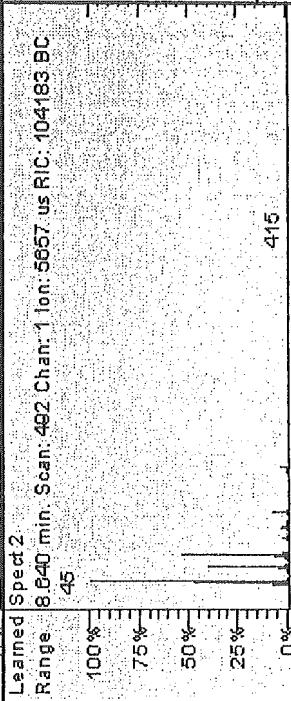
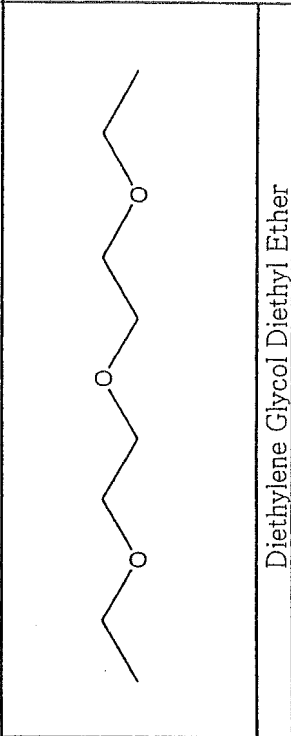
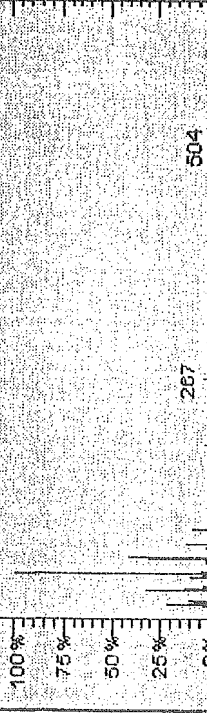
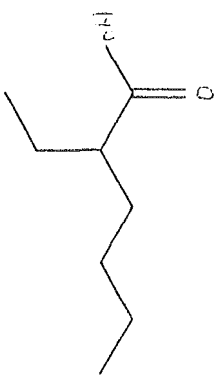
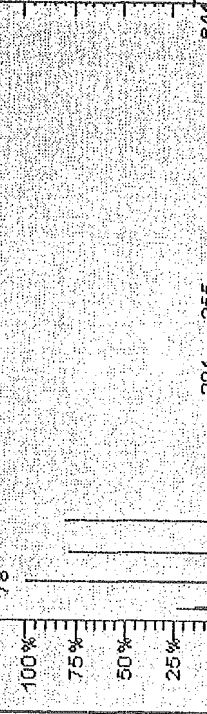
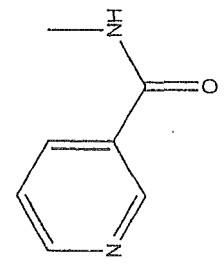

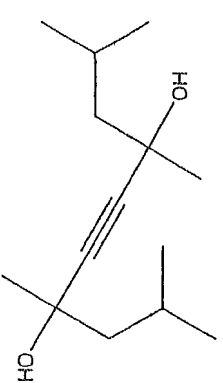
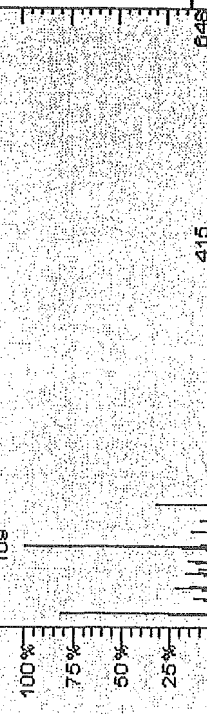
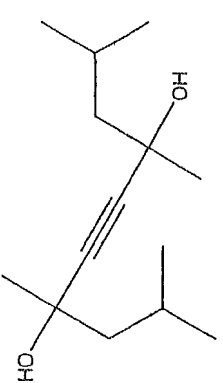


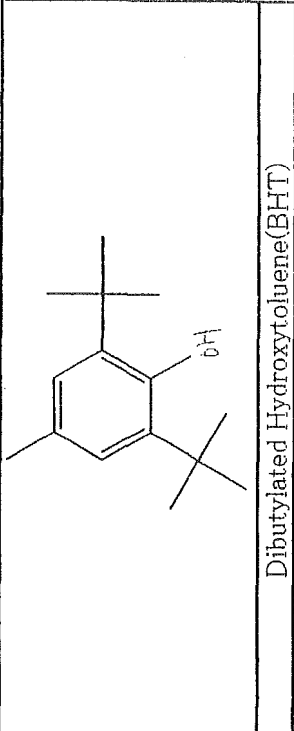
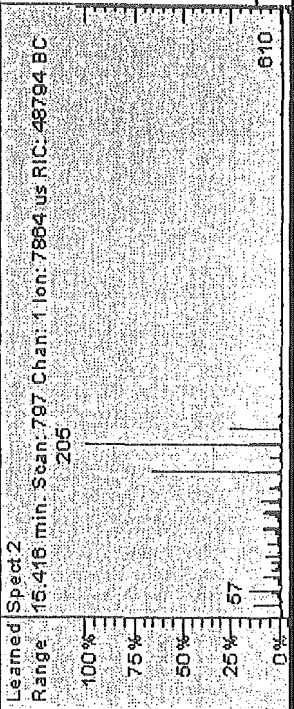
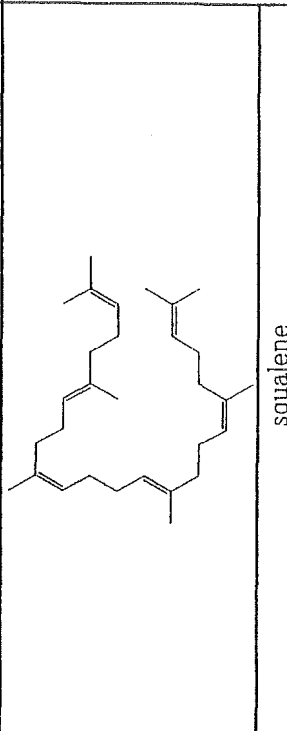
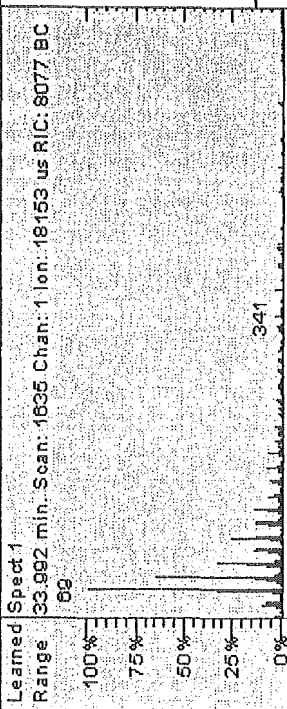
Fig.3-11. おわん(No.11)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

Table.3-11. おわん(No.11)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	フラグメンテーションが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 1 Range: 7.041 min. Scan: 421 Chan: 1 Ion: 3667 us RIC: 66079 BC</p>	 p-Phenolsulfonic Acid	773	878	B
2	<p>Learned Spect 2 Range: 7.308 min. Scan: 433 Chan: 1 Ion: 5059 us RIC: 108557 BC</p>	 propylene glycol monopropyl ether	530	716	D
3	<p>Fixed Spect 2 Range: 7.739 min. Scan: 452 Chan: 1 Ion: 12100 us RIC: 18509 BC</p>	 2-ethylhexyl glycidyl ether	692	819	C
4	<p>Learned Spect 2 Range: 7.830 min. Scan: 456 Chan: 1 Ion: 4115 us RIC: 59677 BC</p>	 Benzyl alcohol	834	927	A

5	<p>Learned Spect2 Range 7.987 min. Scan: 463 Chan: 1 Ion: 2391 us RIC: 122973 BC</p> 	 <p>Salicylaldehyde</p>	816	940	A
6	<p>Learned Spect2 Range 8.188 min. Scan: 471 Chan: 1 Ion: 13540 us RIC: 8554 BC</p> 	 <p>Benzyl alcohol</p>	401	851	E
7	<p>Learned Spect2 Range 8.394 min. Scan: 481 Chan: 1 Ion: 11972 us RIC: 13503 BC</p> 	 <p>Benzoyl bromide</p>	732	936	B
8	<p>Learned Spect2 Range 8.640 min. Scan: 492 Chan: 1 Ion: 5657 us RIC: 104183 BC</p> 	 <p>Diethylene Glycol Diethyl Ether</p>	691	767	C

9	<p>Learned Spect 2 Range: 8.184 min. Scan: 517 Chan: 1 Ion: 13685 us RIC: 12320 BC</p> 	 <p>2-ethylhexanoic acid</p>	562	850	D
10	<p>Fixed Spect 2 Range: 9.785 min. Scan: 544 Chan: 1 Ion: 1188 us RIC: 275563 BC</p> 	 <p>N-Methylnicotinamide</p>	750	842	B
11	<p>Learned Spect 2 Range: 12.837 min. Scan: 682 Chan: 1 Ion: 9082 us RIC: 30281 BC</p> 	 <p>2,4,7,9-Tetramethyl-5-decyn-4,7-diol</p>	702	787	X
12	<p>Fixed Spect 2 Range: 13.696 min. Scan: 720 Chan: 1 Ion: 1235 us RIC: 373008 BC</p> 	 <p>2,4,7,9-Tetramethyl-5-decyn-4,7-diol</p>	702	787	B

13	<p>Learned Spect 2 Range: 16.416 min. Scan: 797 Chan: 1 Ion: 7864 us RIC: 48794 BC</p> 	 <p>Dibutylated Hydroxytoluene(BHT)</p>	697	812	C
14	<p>Learned Spect 1 Range: 33.992 min. Scan: 1635 Chan: 1 Ion: 18153 us RIC: 8077 BC</p> 	 <p>squalene</p>	534	924	D

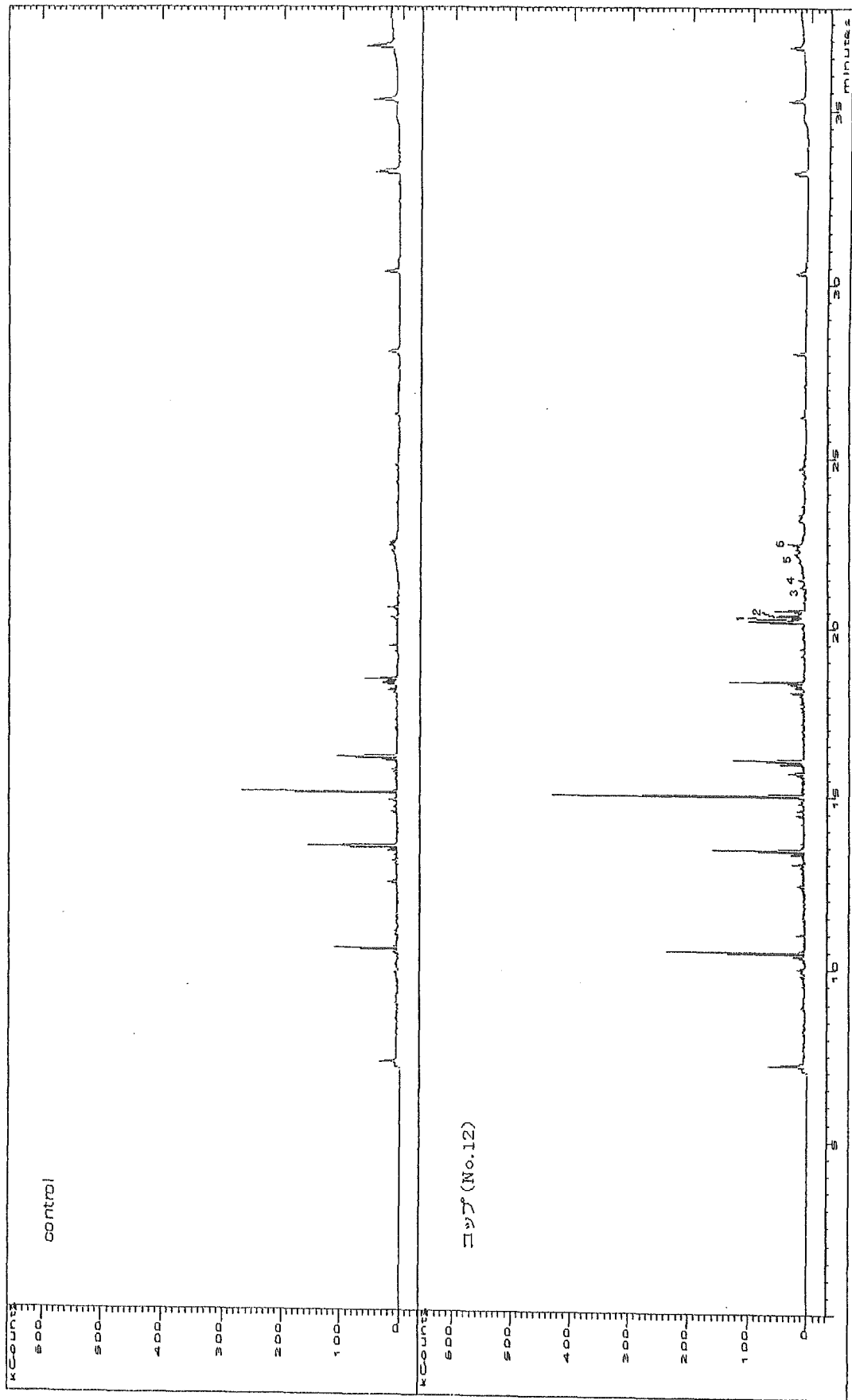
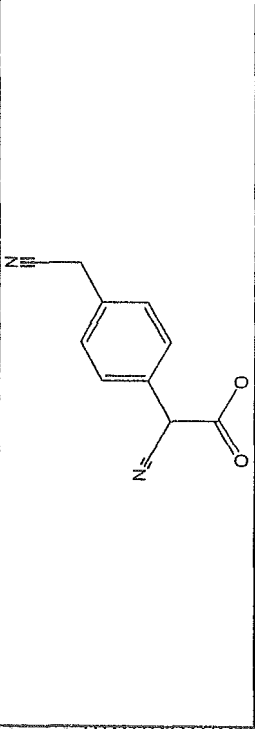
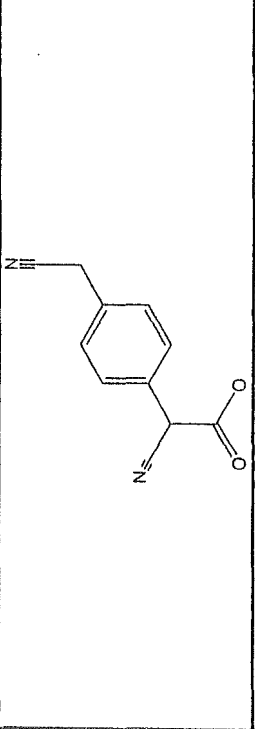
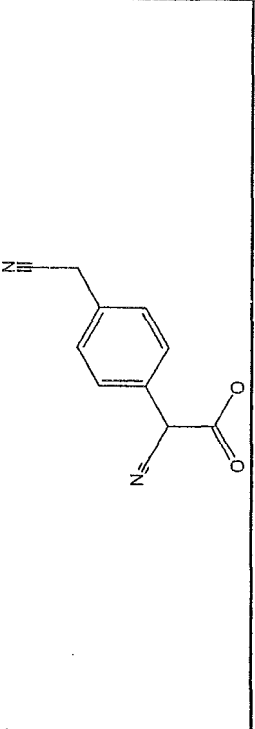

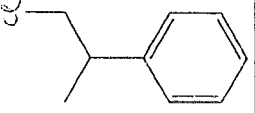
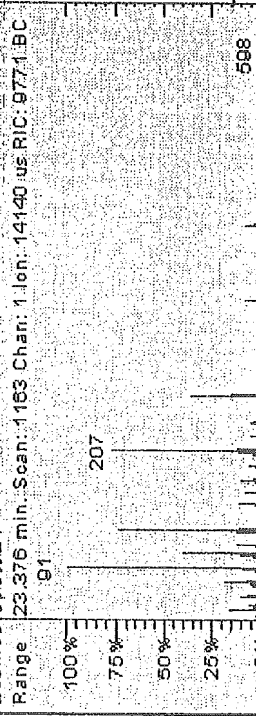
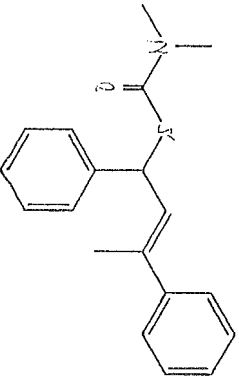


Fig.3-12. コップ (No.12)のトータライオンクロマトグラム(下)とcontrolのトータライオンクロマトグラム(上)

Table.3-12. コップ(No.12)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と構造式の一覧

No	マススペクトル	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	Purity	Fit	信頼度
1	<p>Fixed Spect 2 Range 20.298 min. Scan: 1024 Chan: 1 Ion: 8632 us RIC: 26967 BC</p> <p>Learned Spect 2 Range 20.388 min. Scan: 1028 Chan: 1 Ion: 4125 us RIC: 50528 BC</p>	 <p>α-cyano-4-(cyanomethyl)-ethyl ester</p>	625	834	C
2	<p>Fixed Spect 2 Range 21.246 min. Scan: 1067 Chan: 1 Ion: 13504 us RIC: 9925 BC</p> <p>Learned Spect 2 Range 21.471 min. Scan: 1077 Chan: 1 Ion: 12248 us RIC: 12173 BC</p>	 <p>α-cyano-4-(cyanomethyl)-ethyl ester</p>	598	852	D
3	<p>Fixed Spect 2 Range 21.471 min. Scan: 1077 Chan: 1 Ion: 12248 us RIC: 12173 BC</p>	 <p>5H-Benzocycloheptene,6,7-dihydro-</p>	415	884	E

5	<p>Fixed Spect 2 Range 23.197 min. Scan: 1155 Chan: 1 Ion: 12161 us RIC: 12450 BC</p> 	 <p>Benzene, (2-chloro-1-methylethyl)-</p>	478	831	E
6	<p>Learned Spect 2 Range 23.376 min. Scan: 1163 Chan: 1 Ion: 14140 us RIC: 9771 BC</p> 	 <p>N,N-dimethyl, S-1,3-diphenyl-2-butenyl ester</p>	406	820	E

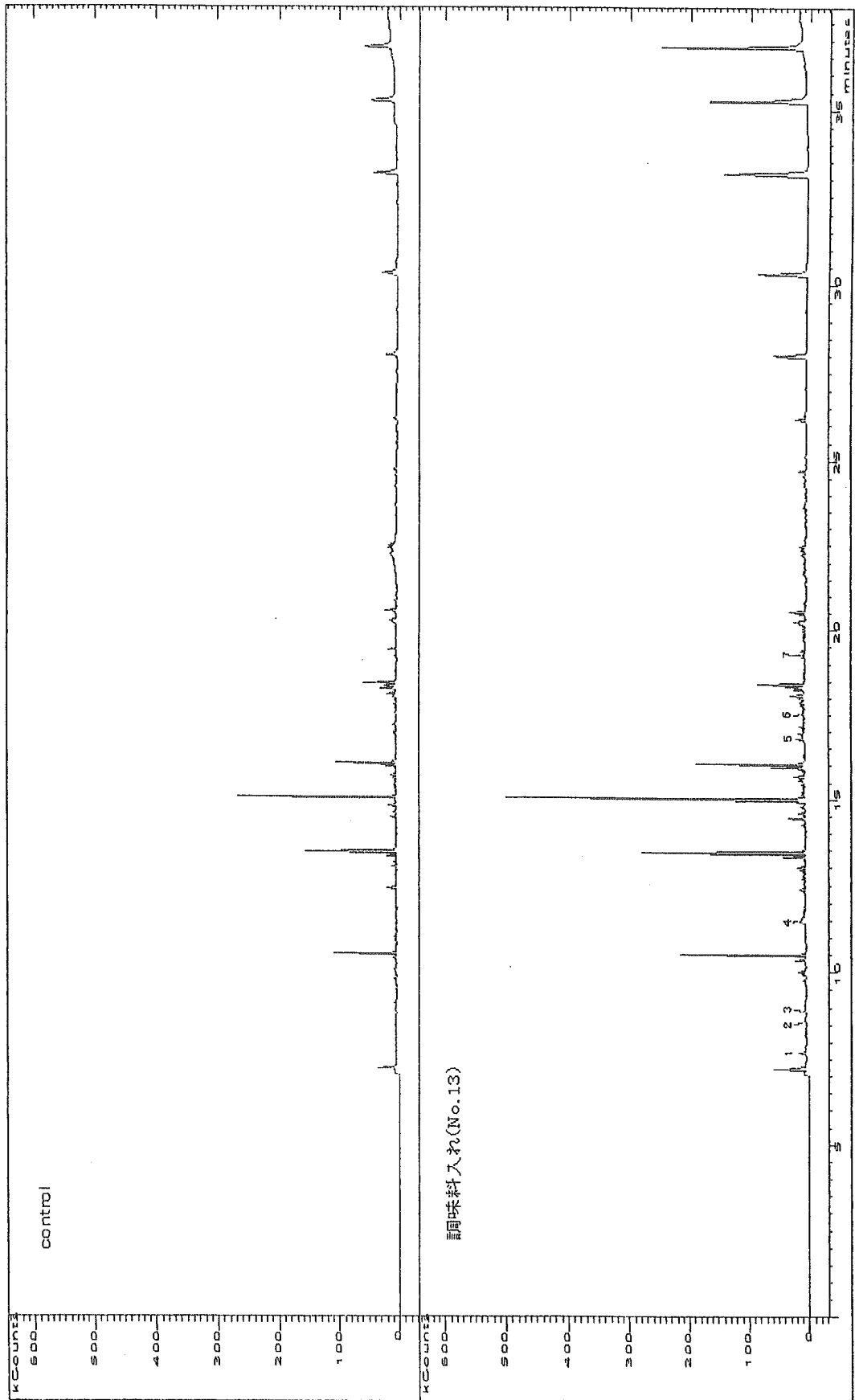
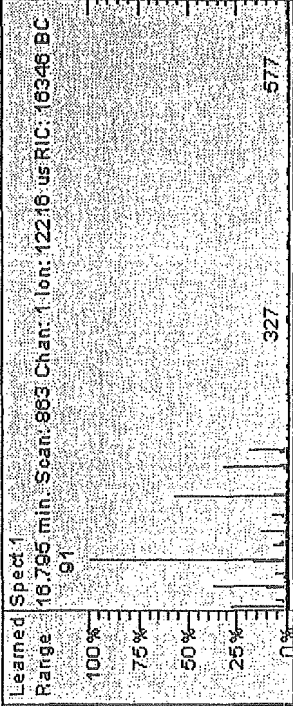
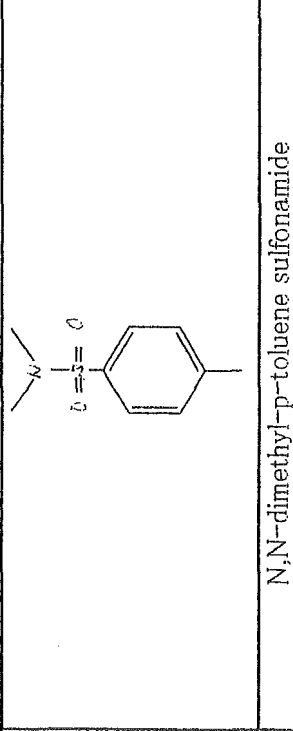
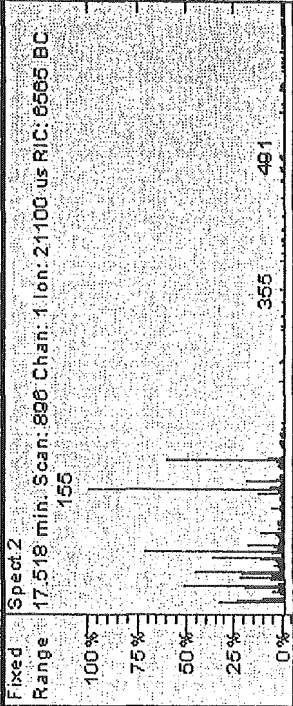
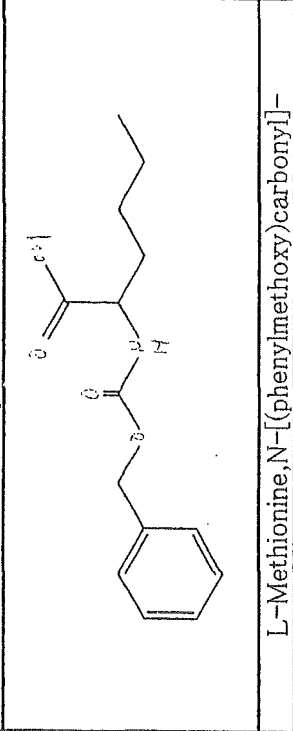
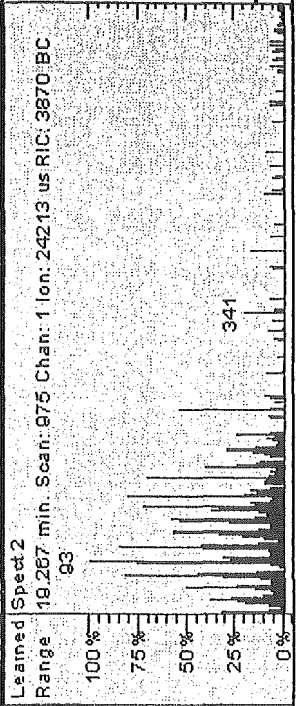
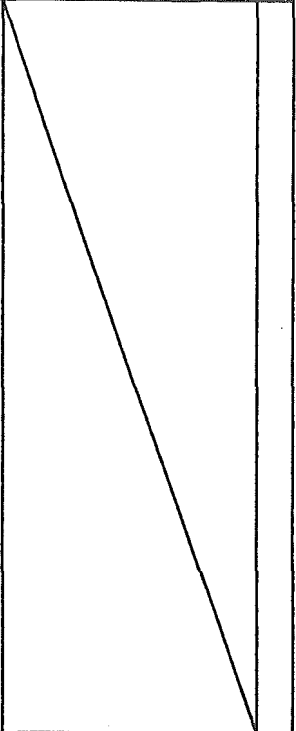


Fig.3-13. 調味料入れ(No.13)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

Table 3-13. 調味料入れ(No.13)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 and compound name	Purity	Fit	信頼度 Reliability
1	<p>Fixed Spect 1 Range: 7.094 min. Scan: 450 Chan: 1 Ion: 19640 us RIC: 12342 BC</p> <p>Learned Spect 2 Range: 8.619 min. Scan: 492 Chan: 1 Ion: 24487 us RIC: 3017 BC</p>	 (Z)-9-methyl-5-Undecene	638	827	C
2	<p>Fixed Spect 1 Range: 8.619 min. Scan: 492 Chan: 1 Ion: 24487 us RIC: 3017 BC</p> <p>Learned Spect 2 Range: 8.669 min. Scan: 508 Chan: 1 Ion: 25000 us RIC: 2714 BC</p>	 Diethylene Glycol Diethyl Ether	347	766	E
3	<p>Fixed Spect 1 Range: 11.465 min. Scan: 621 Chan: 1 Ion: 19823 us RIC: 11070 BC</p> <p>Learned Spect 2 Range: 11.465 min. Scan: 621 Chan: 1 Ion: 19823 us RIC: 11070 BC</p>	 (R)-(-)-(Z)-14-Methyl-8-hexadecan-1-ol	405	794	E
4	<p>Fixed Spect 1 Range: 11.465 min. Scan: 621 Chan: 1 Ion: 19823 us RIC: 11070 BC</p> <p>Learned Spect 2 Range: 11.465 min. Scan: 621 Chan: 1 Ion: 19823 us RIC: 11070 BC</p>	 2-propyl heptanoic acid methyl ester	378	770	E

5	<p>Learned Spect 1 Range 16.796 min. Scan: 863 Chan: 1 Ion: 122.16 us RIC: 16346 BC</p> 	 <p>N,N-dimethyl-p-tolene sulfonamide</p>	657	922	C
6	<p>Fixed Spect 2 Range 17.518 min. Scan: 890 Chan: 1 Ion: 211.00 us RIC: 6665 BC</p> 	 <p>L-Methionine, N-[(phenylmethoxy)carbonyl]-</p>	415	786	E
7	<p>Learned Spect 2 Range 19.267 min. Scan: 975 Chan: 1 Ion: 242.13 us RIC: 3870 BC</p> 				X

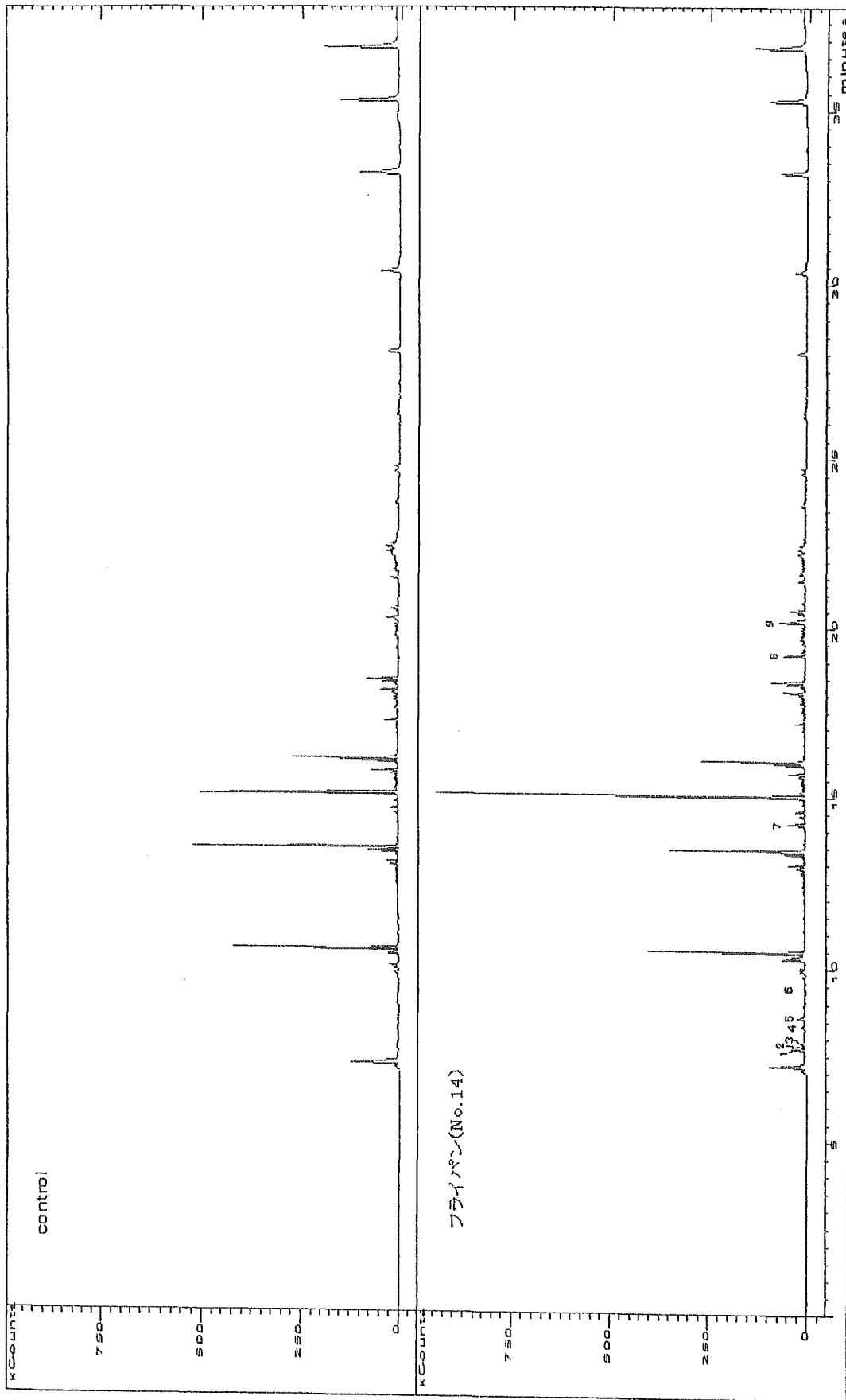

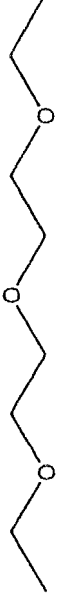



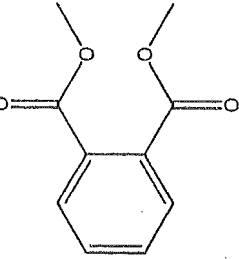

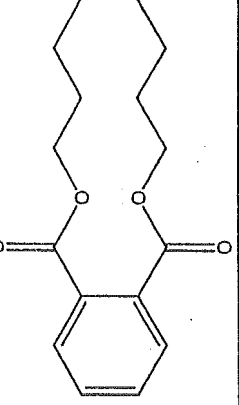
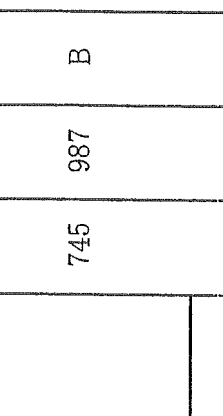
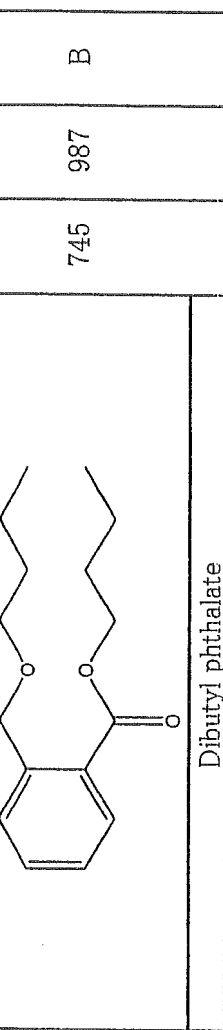


Fig.3-14. フライパン(No.14)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

Table.3-14. フライパン(No.14)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
 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

No	マススペクトル	構造式と化合物名	Purity	Fit	信頼度
1	<p>Fixed Spect 1 Range: 7.692 min. Scan: 460 Chan: 1 Ion: 13683 us RIC: 26235 BC</p> <p>Learned Spect 2 Range: 7.804 min. Scan: 465 Chan: 1 Ion: 23333 us RIC: 5295 BC</p>	 (Z)-9-methyl-5-Undecene	754	828	B
2	<p>Fixed Spect 1 Range: 7.890 min. Scan: 459 Chan: 1 Ion: 22463 us RIC: 10278 BC</p> <p>Learned Spect 2 Range: 8.350 min. Scan: 480 Chan: 1 Ion: 18062 us RIC: 8342 BC</p>	 Benzyl alcohol	649	891	C
3	<p>Fixed Spect 1 Range: 7.890 min. Scan: 459 Chan: 1 Ion: 22463 us RIC: 10278 BC</p> <p>Learned Spect 2 Range: 8.350 min. Scan: 480 Chan: 1 Ion: 18062 us RIC: 8342 BC</p>	 1-Methyl-2-pyrrolidinone	543	845	D
4	<p>Fixed Spect 1 Range: 7.890 min. Scan: 459 Chan: 1 Ion: 22463 us RIC: 10278 BC</p> <p>Learned Spect 2 Range: 8.350 min. Scan: 480 Chan: 1 Ion: 18062 us RIC: 8342 BC</p>	 Benzoyl bromide	770	951	B

5	<p>Learned Spect 2 Range: 8.592 min. Scan: 401 Chan: 1 Ion: 20001 us RIC: 19547 BC</p> 	 <p>Diethylene Glycol Diethyl Ether</p>	657	760	C
6	<p>Learned Spect 2 Range: 9.473 min. Scan: 531 Chan: 1 Ion: 24729 us RIC: 5223 BC</p> 	 <p>Dimethyl Glutarate</p>	693	887	C
7	<p>Learned Spect 2 Range: 14.212 min. Scan: 746 Chan: 1 Ion: 6145 us RIC: 46127 BC</p> 	 <p>Dimethyl phthalate</p>	842	927	A
8	<p>Fixed Spect 2 Range: 19.198 min. Scan: 972 Chan: 1 Ion: 5784 us RIC: 54219 BC</p> 	 <p>Dibutyl phthalate</p>	738	971	B

9	<p>Learned Spect:1 Range: 20.213 min. Scan: 1018 Chan: 1 Ion: 4657 us RIC: 66632 BC</p> 		745	987	B
		Dibutyl phthalate			