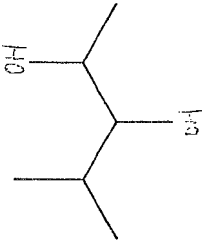
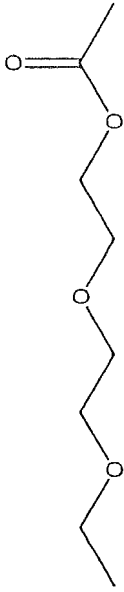
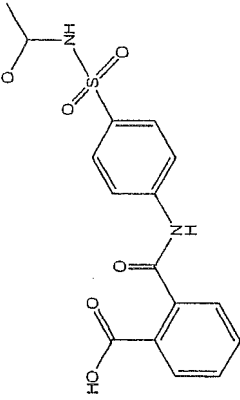
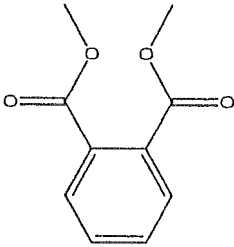
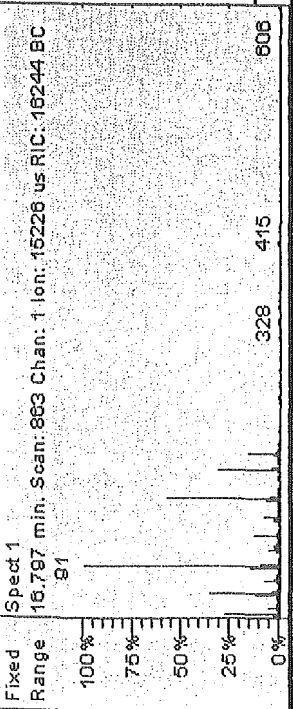
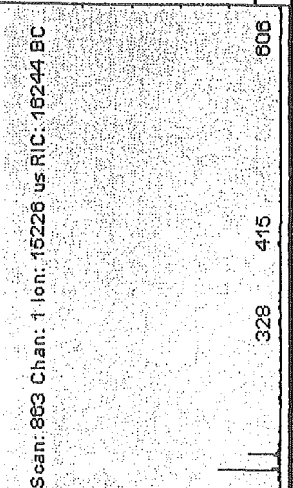


Table.3-2. 耐熱紙コップ(No.1)から検出された有機化学物質のマススペクトルと構造式

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>Learned Spect 1 Range: 8.375 min. Scan: 483 Chan: 1 Ion: 24166 us RIC: 7533 BC</p> <p>Learned Spect 2 Range: 10.256 min. Scan: 558 Chan: 1 Ion: 24786 us RIC: 6669 BC</p>	 <p>(S_r)-or-(r_s)-4-methyl-2,3-pentane diol</p>	603	807	C
2	<p>Learned Spect 1 Range: 12.271 min. Scan: 659 Chan: 1 Ion: 24963 us RIC: 4519 BC</p> <p>Learned Spect 1 Range: 14.201 min. Scan: 746 Chan: 1 Ion: 11003 us RIC: 25887 BC</p>	 <p>Carbitol Acetate</p>	705	857	B
3	<p>Learned Spect 1 Range: 12.271 min. Scan: 659 Chan: 1 Ion: 24963 us RIC: 4519 BC</p> <p>Learned Spect 1 Range: 14.201 min. Scan: 746 Chan: 1 Ion: 11003 us RIC: 25887 BC</p>	 <p>Benzoic acid, 2-[[[4-(acetamino)sulfonyl]phenyl]amino]carbonyl]-</p>	623	864	C
4	<p>Learned Spect 1 Range: 12.271 min. Scan: 659 Chan: 1 Ion: 24963 us RIC: 4519 BC</p> <p>Learned Spect 1 Range: 14.201 min. Scan: 746 Chan: 1 Ion: 11003 us RIC: 25887 BC</p>	 <p>Dimethyl phthalate</p>	884	940	A

5	<p>Fixed Spect 1 Range 16.797 min. Scan: 863 Chan: 1 Ion: 152226 us RIC: 16244 BC</p> 		782	913	B
N-Ethyl-O-toluenesulfonamide					

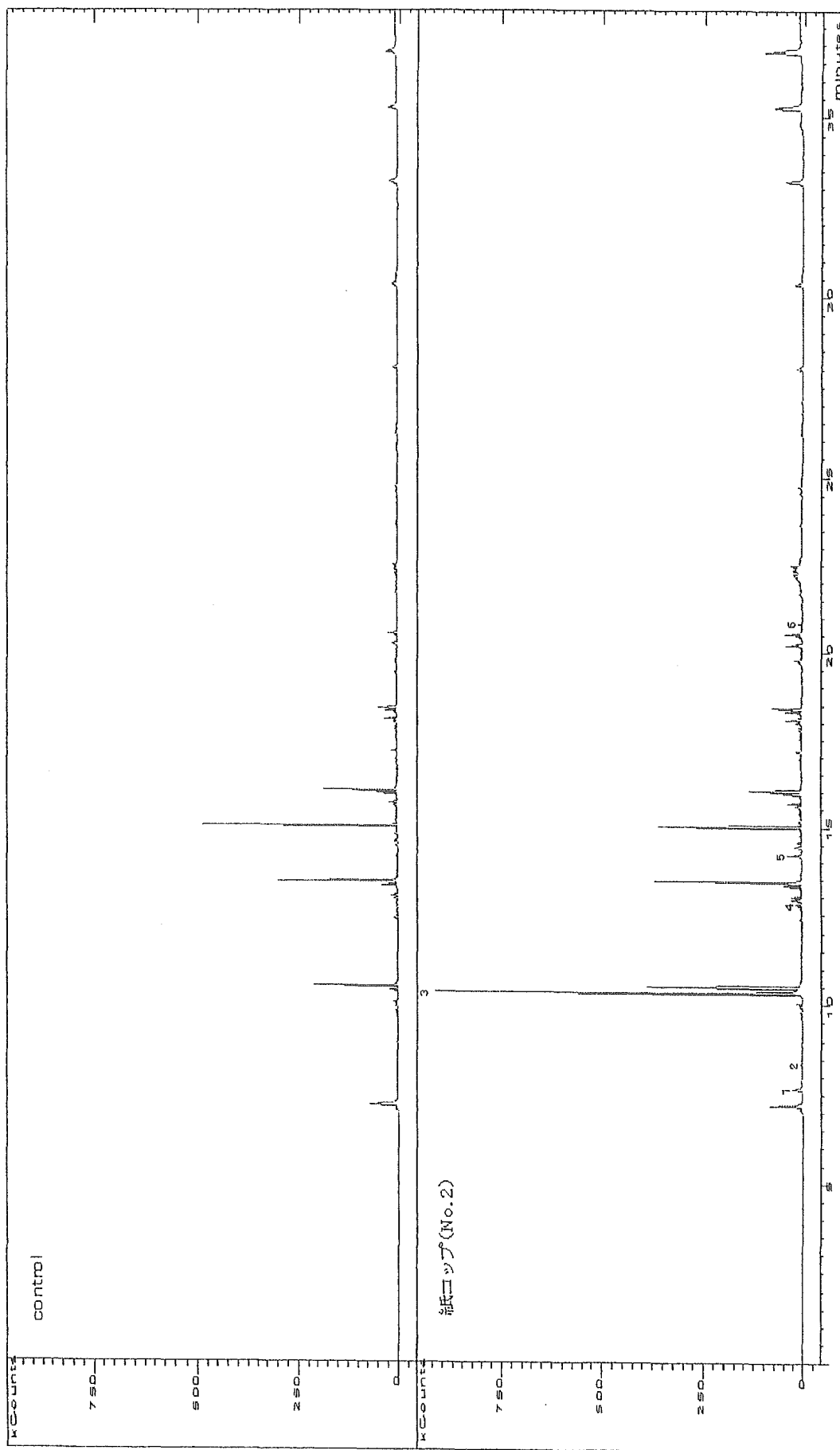
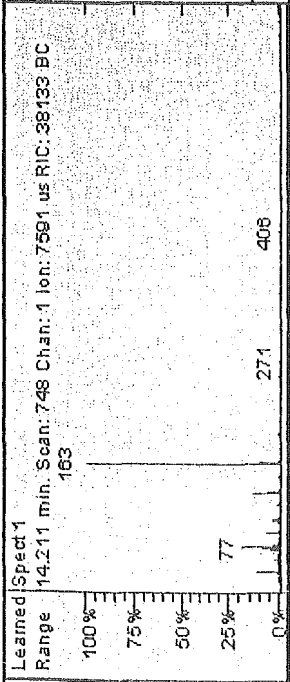
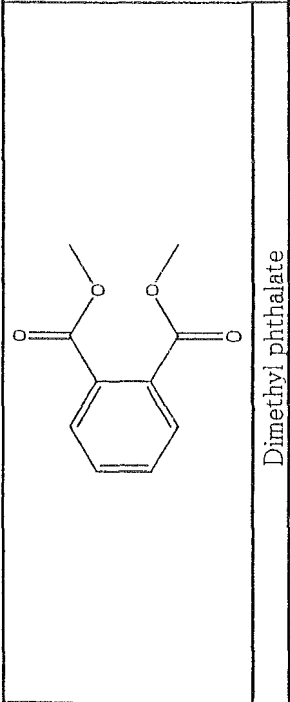
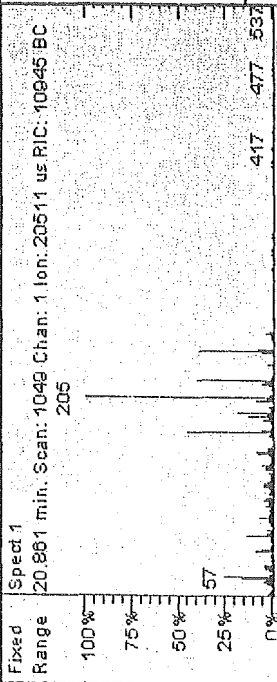
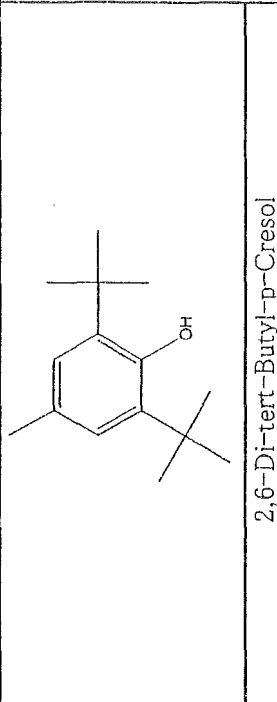


Fig.3-2. 紙コップ(No.2)のトータライオンクロマトグラム(下)とcontrolのトータライオンクロマトグラム(上)

Table.3-3. 紙コップ(No.2)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 Range 7.605 min. Scan: 450 Chan: 1 Ion: 13036 us RIC: 24774 BC</p> <p>69 329 431</p>	<p>2,2'-Azobis(2-methylpropionitrile)</p>	803	881	A
2	<p>Fixed Range 8.371 min. Scan: 482 Chan: 1 Ion: 23680 us RIC: 5304 BC</p> <p>73 205 254 433</p>	<p>meso-2,5-Dimethyl-3,4-hexanediol</p>	567	775	D
3	<p>Fixed Range 10.325 min. Scan: 571 Chan: 1 Ion: 485 us RIC: 914956 BC</p> <p>45 163 614</p>	<p>Diethylene Glycol Di-n-butyl Ether</p>	556	793	D
4	<p>Learned Spect 2 Range 12.802 min. Scan: 684 Chan: 1 Ion: 16659 us RIC: 14598 BC</p> <p>168 253 327</p>				X

5	<p>Learned Spect 1 Range 14.211 min. Scan: 748 Chan: 1 Ion: 7591 us RIC: 38133 BC</p> 	 <p>Dimethyl phthalate</p>	919	939	A
6	<p>Fixed Spect 1 Range 20.861 min. Scan: 1049 Chan: 1 Ion: 20511 us RIC: 10945 BC</p> 	 <p>2,6-Di-tert-Butyl-p-Cresol</p>	548	845	D

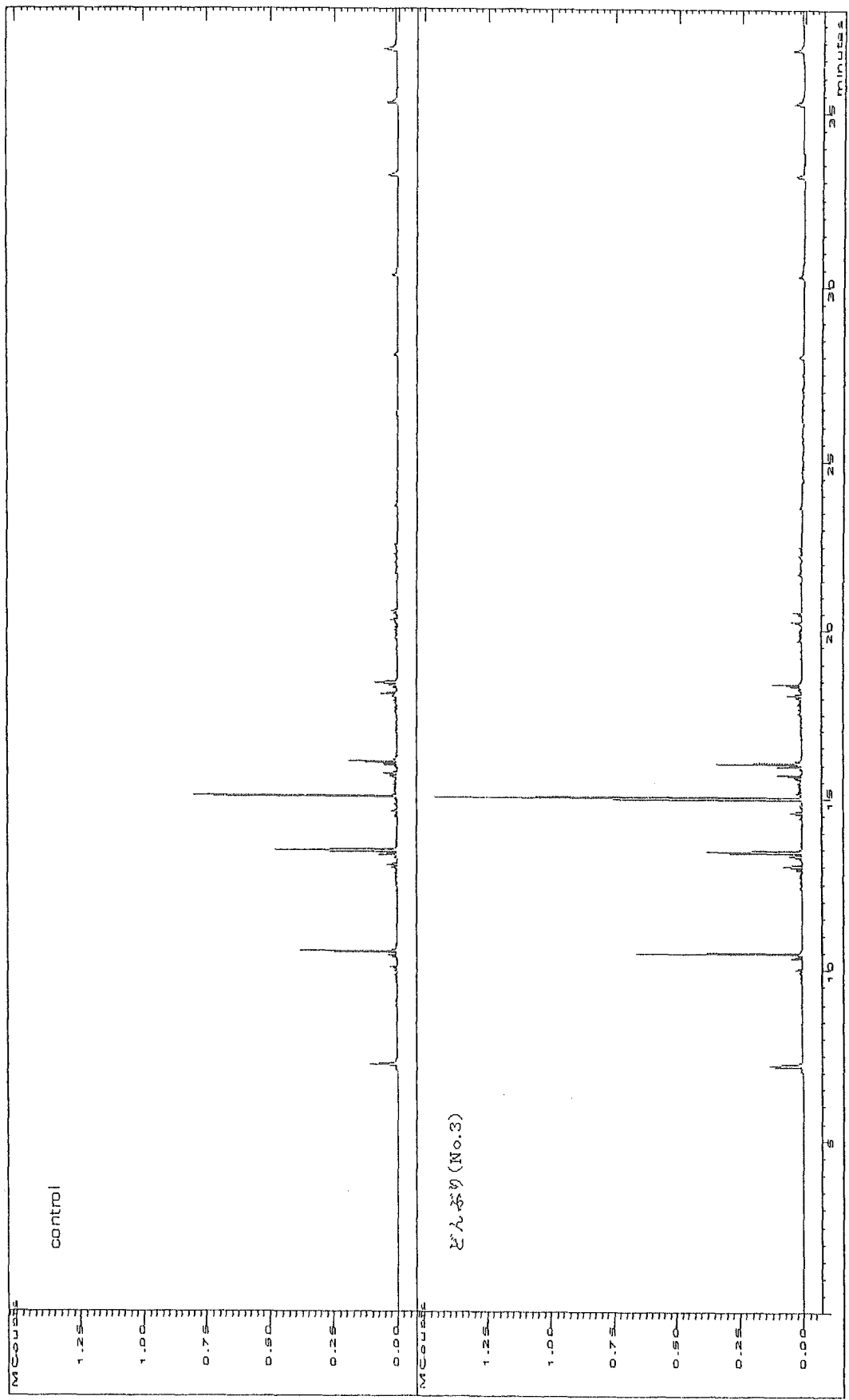


Fig.3-3. どんぶり(No.3)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

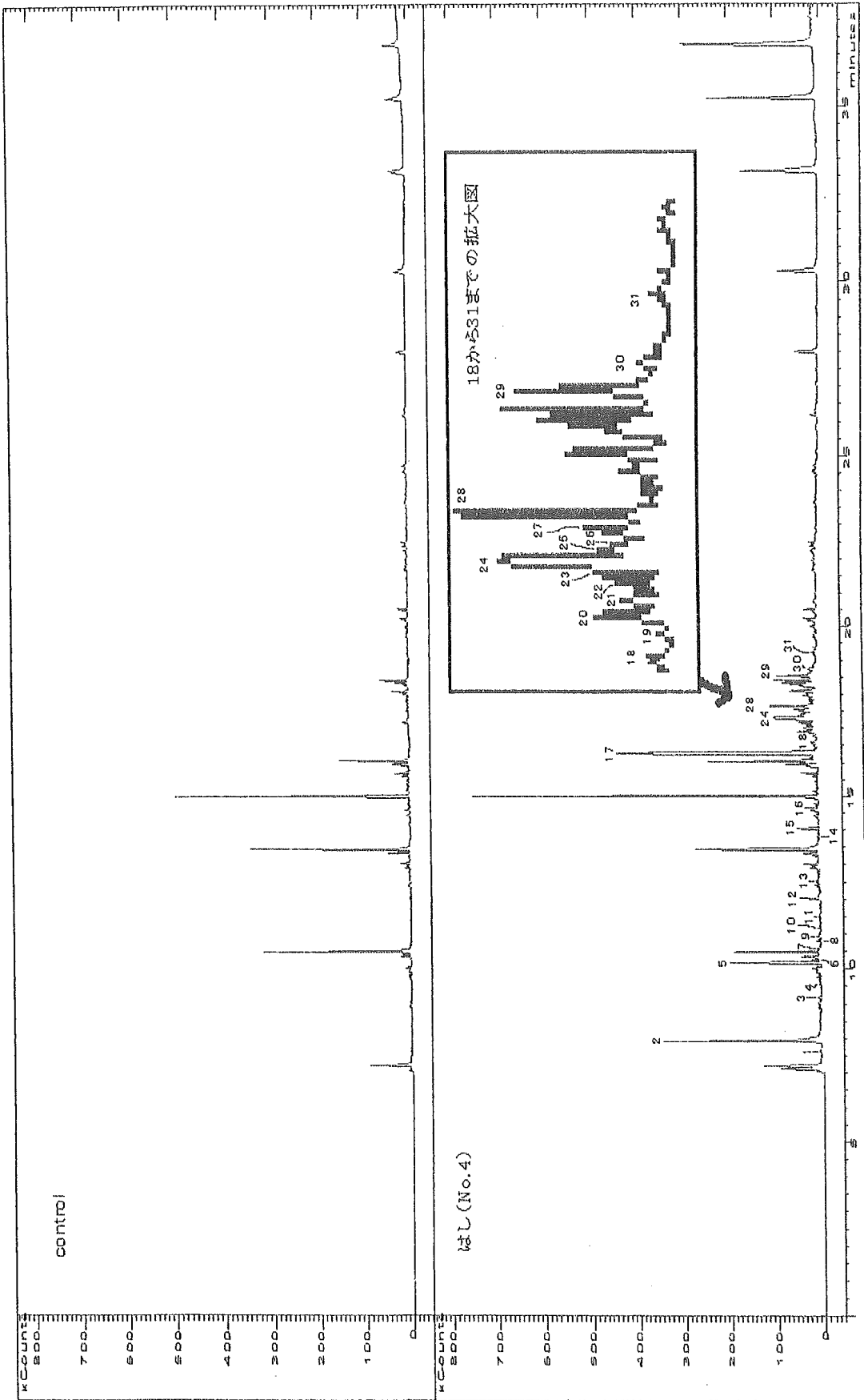
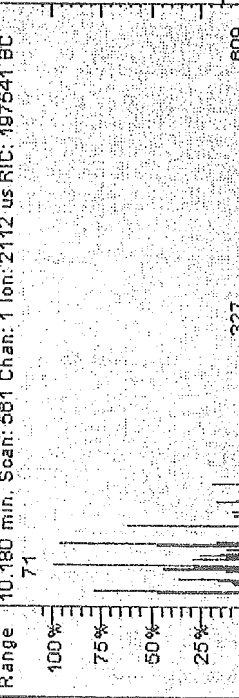
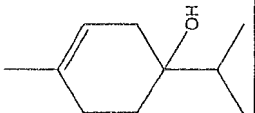
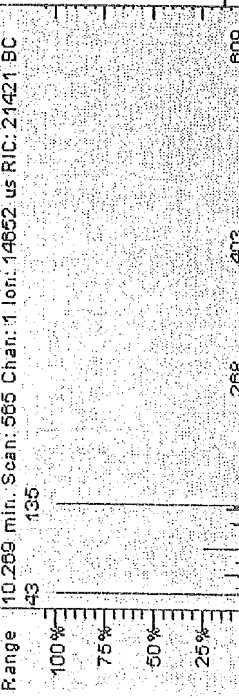
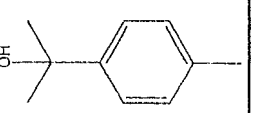
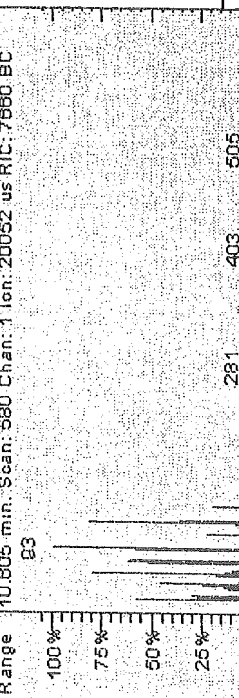
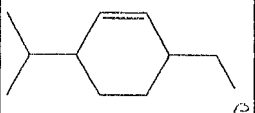
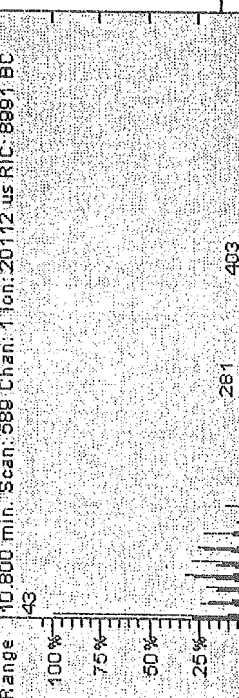
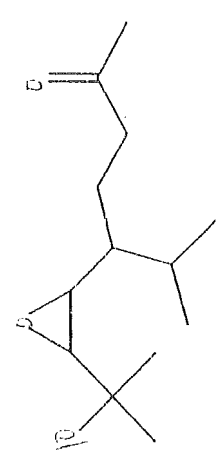
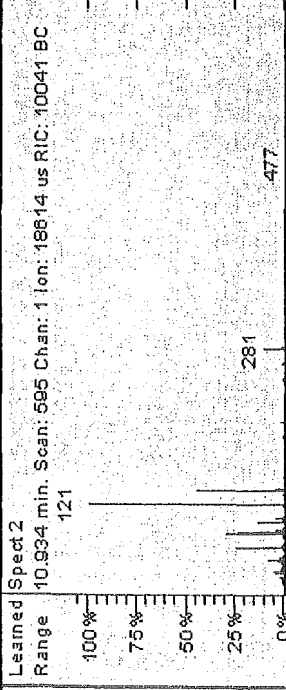
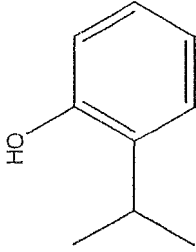
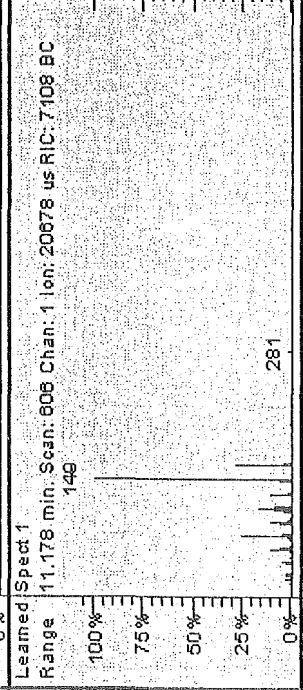
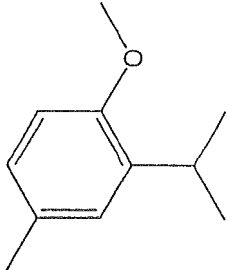
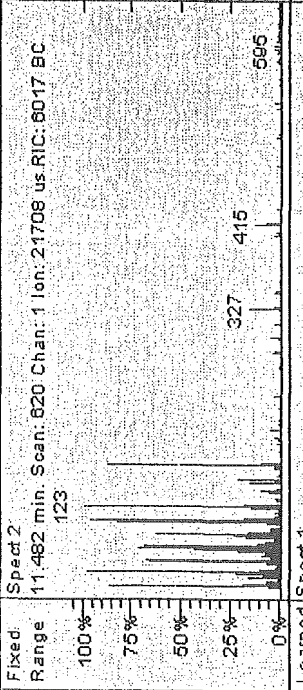
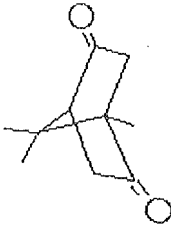
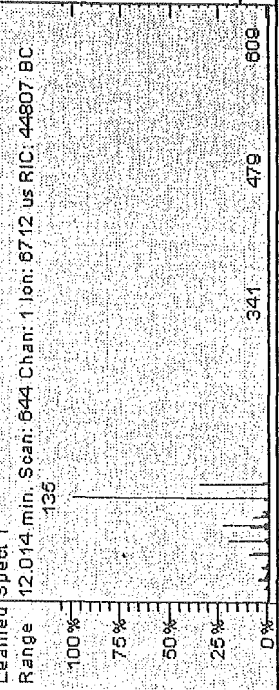
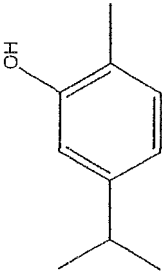


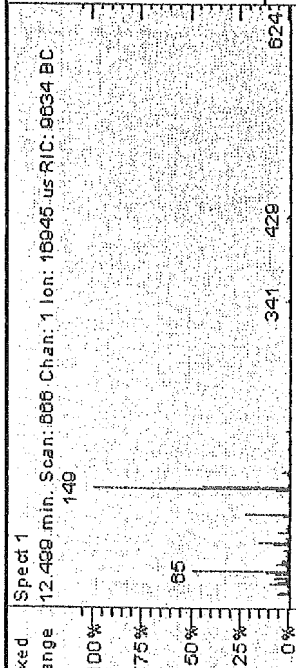
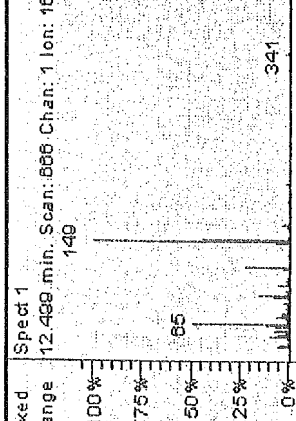
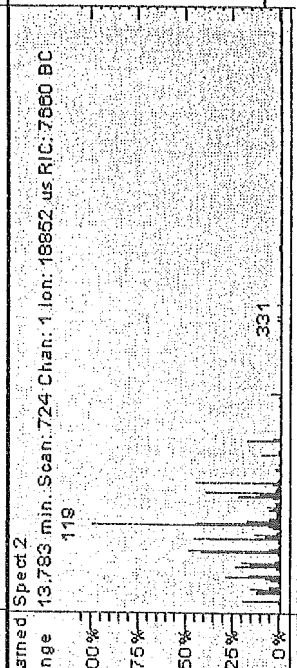
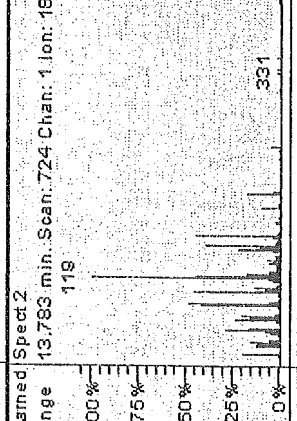
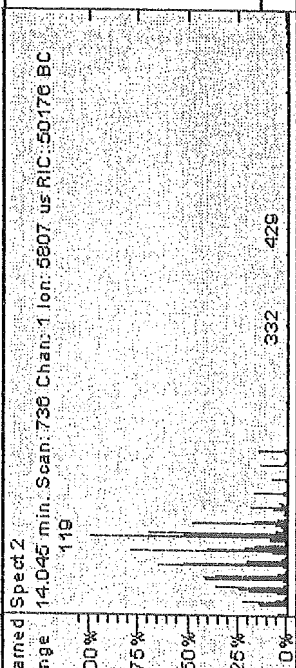
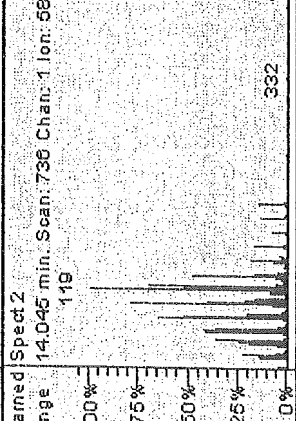
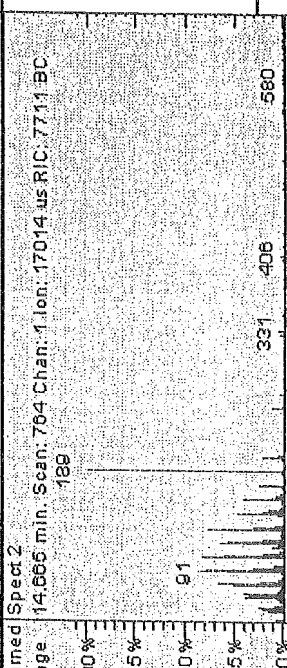
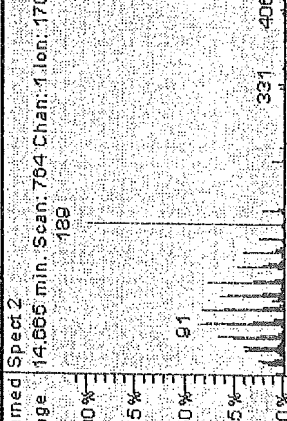
Fig.3-4. はし(No.4)のトータライオンクロマトグラム(下)とcontrolのトータライオンクロマトグラム(上)

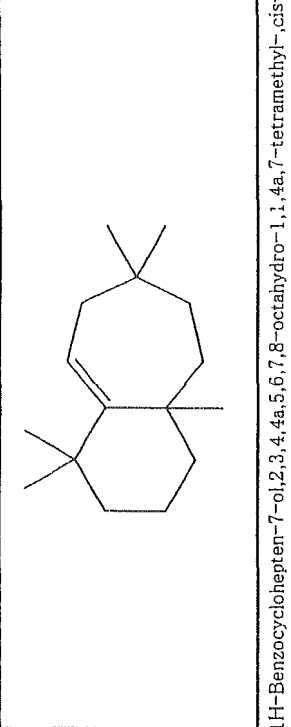
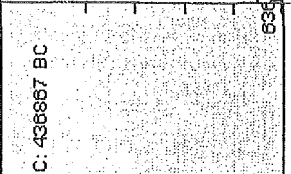
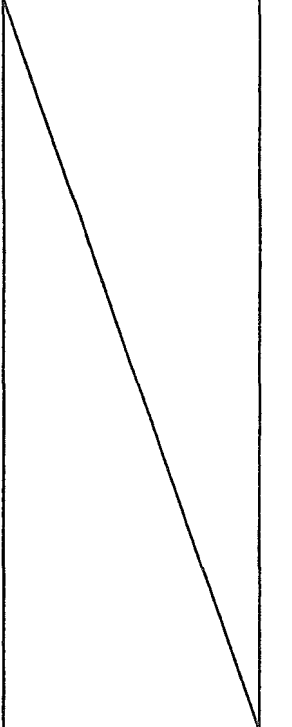
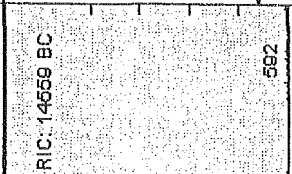

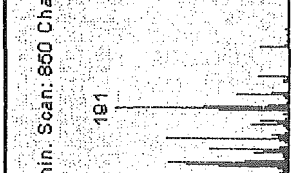
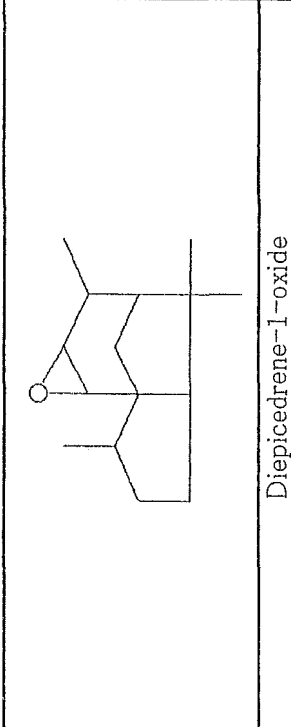
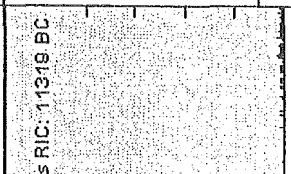
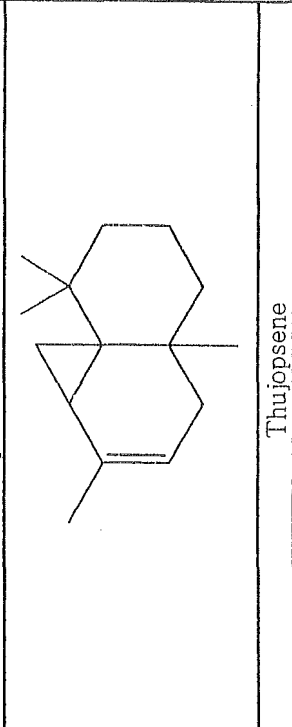
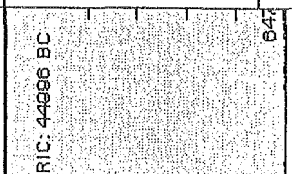
Table.3-4. はし(No.4)から検出された有機化学物質のマススペクトルと構造式の一覧

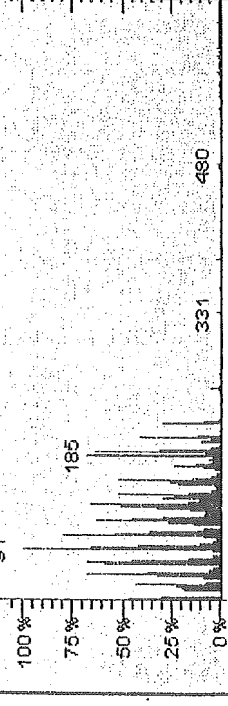
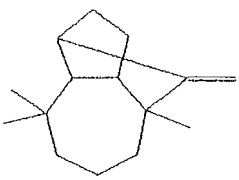
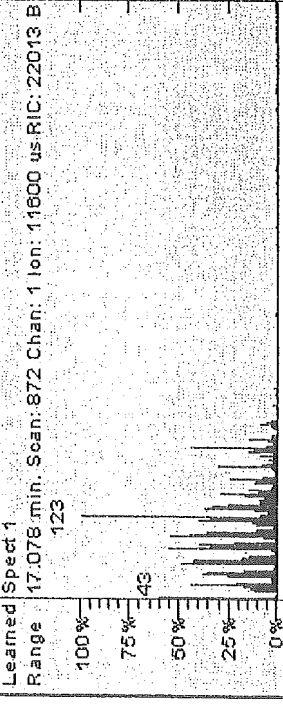
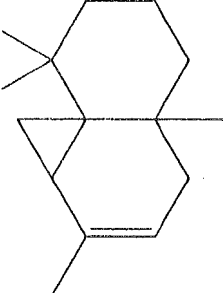
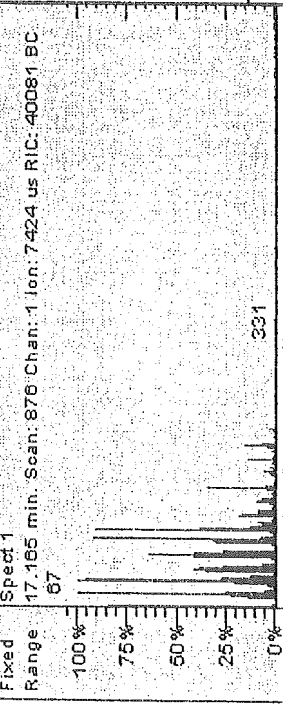
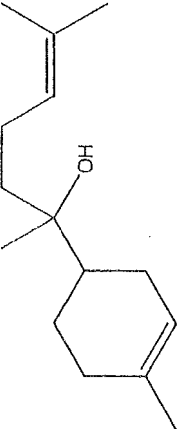
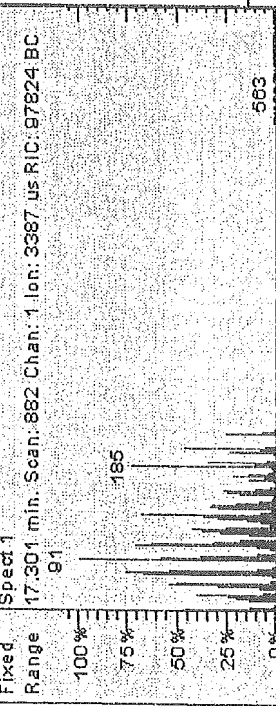
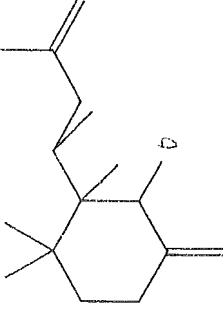
No	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	Purity	Fit	信頼度
1	<p>Learned Spect 2 Range 7.644 min. Scan: 446 Chan: 1 Ion: 22717 us RIC: 4651 BC 119 207 281 429 626</p>	 Cymene	400	804	E
2	<p>Learned Spect 2 Range 7.931 min. Scan: 459 Chan: 1 Ion: 960 us RIC: 344699 BC 121 627</p>	 Salicylaldehyde	801	944	A
3	<p>Spect 2 Range 9.203 min. Scan: 517 Chan: 1 Ion: 19315 us RIC: 8875 BC 95 207 403 627</p>	 Cyclohexene, 1,6-dimethyl-	537	872	D
4	<p>Fixed Spect 1 Range 9.555 min. Scan: 533 Chan: 1 Ion: 22416 us RIC: 5579 BC 78 341 595</p>	 4-Pyridinecarboxamide, N-hydroxy-	519	800	D

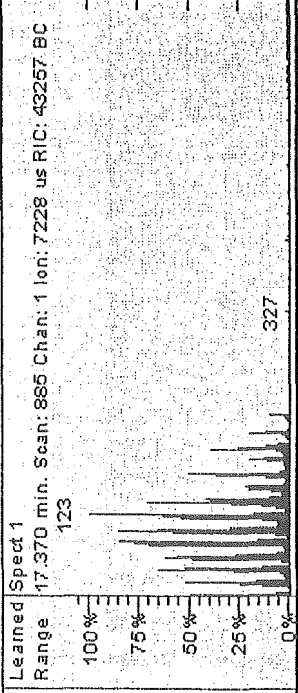
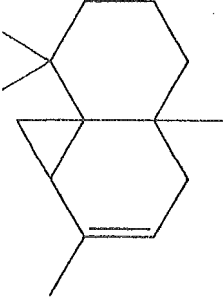
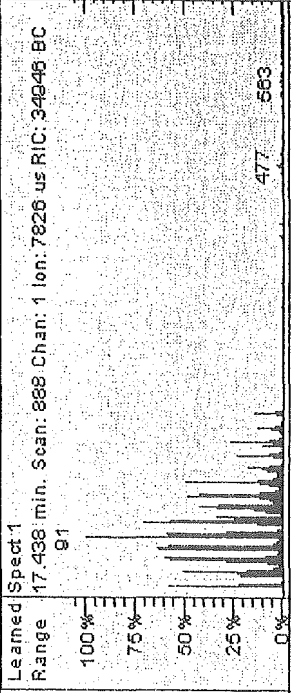
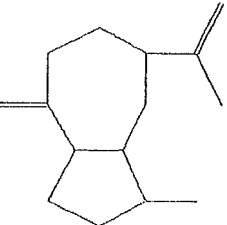
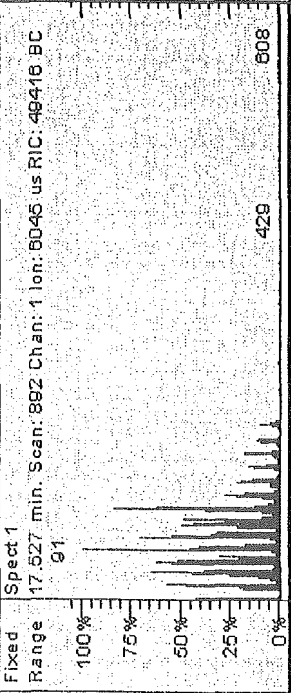
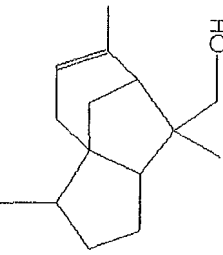
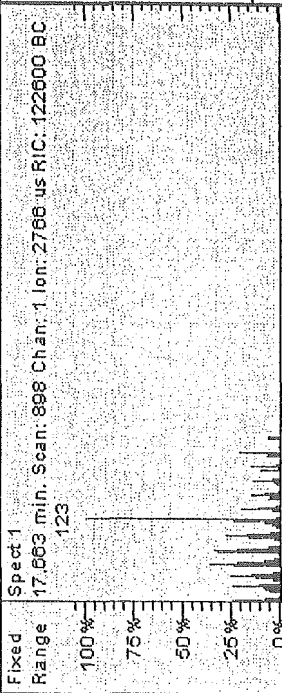
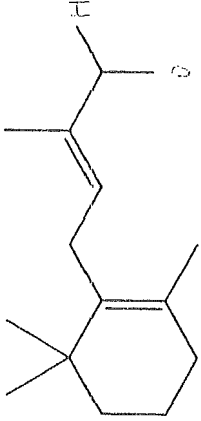
5	<p>Learned Spect 2 Range 10.180 min. Scan: 561 Chan: 1 Ion: 2112 us RIC: 197541 BC</p> 	 <p>terpinen-4-ol</p>	765	885	B
6	<p>Learned Spect 2 Range 10.269 min. Scan: 565 Chan: 1 Ion: 14652 us RIC: 21421 BC</p> 	 <p>p-cymen-8-ol</p>	757	896	B
7	<p>Learned Spect 2 Range 10.805 min. Scan: 580 Chan: 1 Ion: 20052 us RIC: 7660 BC</p> 	 <p>p-Menth-2-en-7-ol,trans-</p>	643	840	C
8	<p>Fixed Spect 2 Range 10.800 min. Scan: 569 Chan: 1 Ion: 20112 us RIC: 6991 BC</p> 	 <p>(E)-5-Isopropyl-6,7-epoxy-8-hydroxy-8-methylnon-2-one</p>	514	708	D

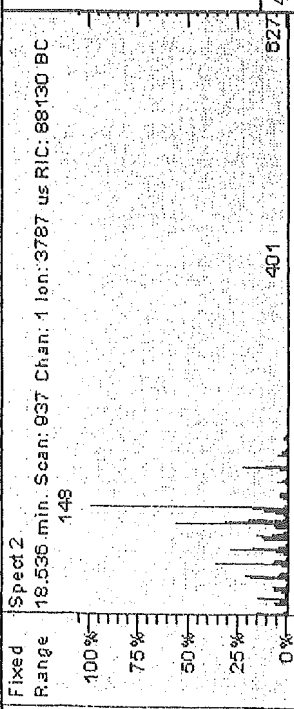
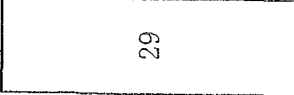
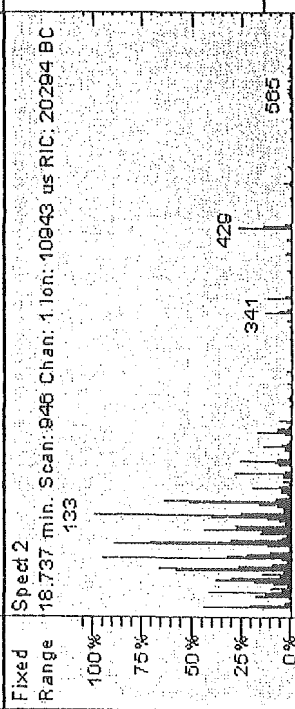
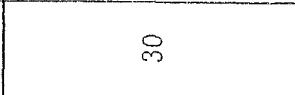
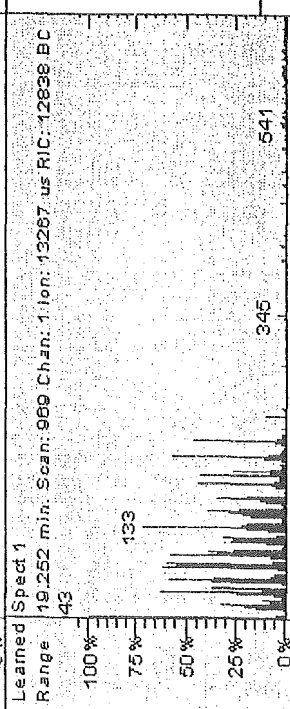
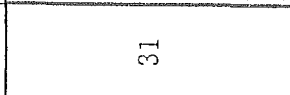
9	<p>Learned Spect 2 Range 10.934 min. Scan: 595 Chan: 1 Ion: 18814 us RIC: 10041 BC</p> 	 <p>2-Isopropylphenol</p>	617	951	C
10	<p>Learned Spect 1 Range 11.178 min. Scan: 606 Chan: 1 Ion: 20678 us RIC: 7108 BC</p> 	 <p>Benzene, 1-methoxy-4-methyl-2-(1-methylethyl)-</p>	772	917	B
11	<p>Fixed Spect 2 Range 11.482 min. Scan: 620 Chan: 1 Ion: 21708 us RIC: 6017 BC</p> 	 <p>Bicyclo[2.2.1]heptane-2,5-dione, 1,7,7-trimethyl-</p>	509	850	D
12	<p>Learned Spect 1 Range 12.014 min. Scan: 644 Chan: 1 Ion: 6712 us RIC: 44807 BC</p> 	 <p>5-isopropyl-2-methylphenol</p>	844	939	A

13	<p>Fixed Spect 1 Range 12.498 min. Scan: 888 Chan: 1 Ion: 15945 us RIC: 9634 BC</p> 	 <p>Heliotropine</p>	554	845	D
14	<p>Learned Spect 2 Range 13.783 min. Scan: 724 Chan: 1 Ion: 19852 us RIC: 7660 BC</p> 	 <p>Di-epi-α-cedrene-1</p>	570	870	D
15	<p>Learned Spect 2 Range 14.045 min. Scan: 736 Chan: 1 Ion: 5607 us RIC: 50176 BC</p> 	 <p>Thujopsene</p>	714	918	B
16	<p>Learned Spect 2 Range 14.665 min. Scan: 764 Chan: 1 Ion: 17014 us RIC: 7711 BC</p> 	 <p>2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalene</p>	618	901	C

17	<p>Learned Spect 1 Range 16.297 min. Scan: 836 Chan: 1 Ion: 908 us RIC: 436887 BC</p> 		720	903	B
18	<p>Learned Spect 1 Range 16.580 min. Scan: 860 Chan: 1 Ion: 14736 us RIC: 14659 BC</p> 				X
19	<p>Learned Spect 1 Range 16.761 min. Scan: 858 Chan: 1 Ion: 13878 us RIC: 11319 BC</p> 		493	833	E
20	<p>Fixed Spect 2 Range 16.887 min. Scan: 864 Chan: 1 Ion: 7120 us RIC: 44886 BC</p> 		539	852	D

21	<p>Fixed Range Spect 2 17.008 min. Scan: 869 Chan: 1 Ion: 8713 us RIC: 31013 BC</p> 	 <p>1,4-Methanocyclodecane, decahydro-4,8-trimethyl-9-methylene-, [1S-(1α,3α,β,4α,8α,β)]-</p>	548	890	D
22	<p>Learned Spect 1 Range 17.078 min. Scan: 872 Chan: 1 Ion: 11600 us RIC: 22013 B</p> 	 <p>Thujopsene</p>	486	778	E
23	<p>Fixed Range Spect 1 17.165 min. Scan: 876 Chan: 1 Ion: 7424 us RIC: 40081 BC</p> 	 <p>(-)-Alpha-bisabolol</p>	676	910	C
24	<p>Fixed Range Spect 1 17.301 min. Scan: 882 Chan: 1 Ion: 3387 us RIC: 97824 BC</p> 	 <p>2,3,3-Trimethyl-2-(3-methylbuta-1,3-dienyl)-6-methylenecyclohexanone</p>	556	851	D

25	<p>Learned Spect 1 Range 17.370 min. Scan: 886 Chan: 1 Ion: 7228 us RIC: 43257 BC</p> 	 <p>Thujopsene</p>	595	806	D
26	<p>Learned Spect 1 Range 17.438 min. Scan: 888 Chan: 1 Ion: 7826 us RIC: 34846 BC</p> 	 <p>Bicyclo[5.3.0]decane, 2-methylene-5-(1-methylvinyl)-8-methyl-</p>	580	872	D
27	<p>Fixed Spect 1 Range 17.527 min. Scan: 892 Chan: 1 Ion: 6046 us RIC: 48418 BC</p> 	 <p>Cedren-13-ol, 8-</p>	538	779	D
28	<p>Fixed Spect 1 Range 17.663 min. Scan: 898 Chan: 1 Ion: 2766 us RIC: 122600 BC</p> 	 <p>2-Butenal, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-</p>	658	851	C

<p>29</p>	<p>Fixed Range</p> <p>Spect 2</p> <p>18.536 min. Scan: 937 Chan: 1 Ion: 3787 us RIC: 68130 BC</p> 	 <p>4-(2,7,7-Trimethylbicyclo[3.2.0]hept-2-en-1-yl)but-3-en-2-one</p>	<p>551</p> <p>772</p> <p>D</p>
<p>30</p>	<p>Fixed Range</p> <p>Spect 2</p> <p>18.737 min. Scan: 946 Chan: 1 Ion: 10943 us RIC: 20294 BC</p> 	 <p>Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1α,4α,7α)]-</p>	<p>471</p> <p>849</p> <p>E</p>
<p>31</p>	<p>Learned Spect 1</p> <p>Range 19.252 min. Scan: 969 Chan: 1 Ion: 13267 us RIC: 12838 BC</p> 	 <p>Acetic acid, 3-hydroxy-6-isopropenyl-4,6a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-2-yl ester</p>	<p>554</p> <p>866</p> <p>D</p>

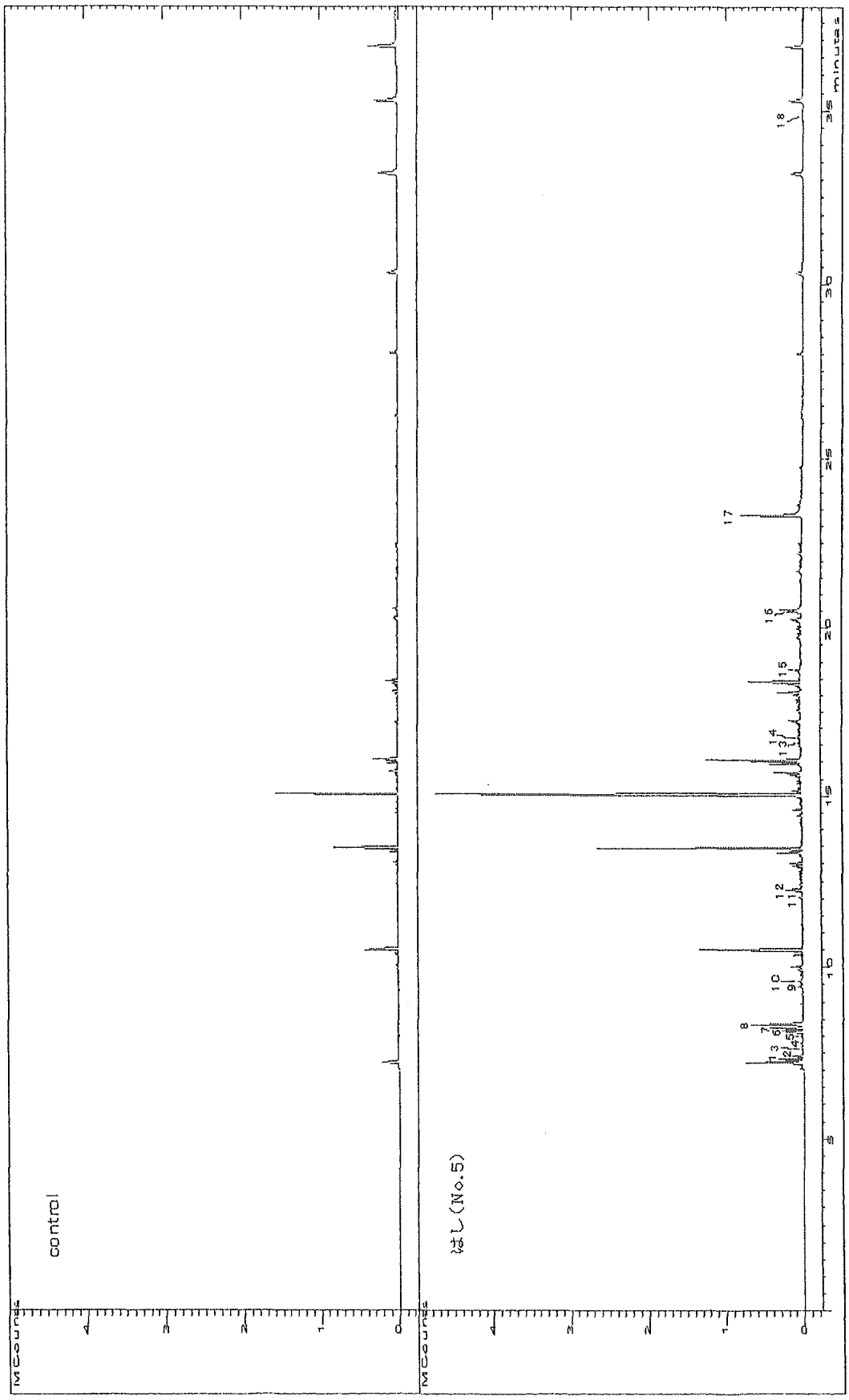
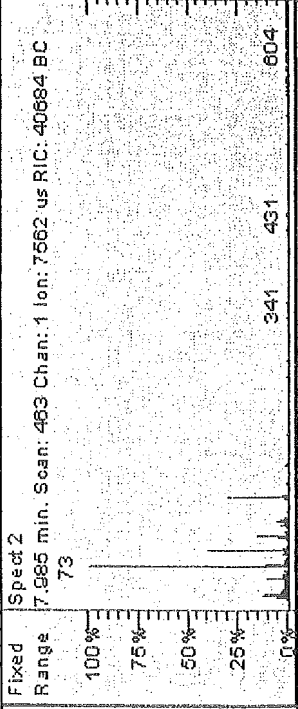
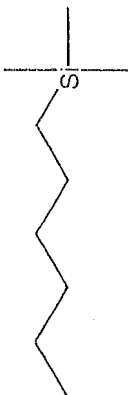
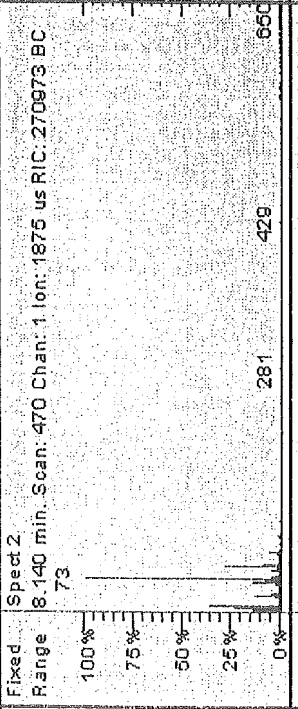
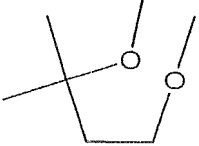
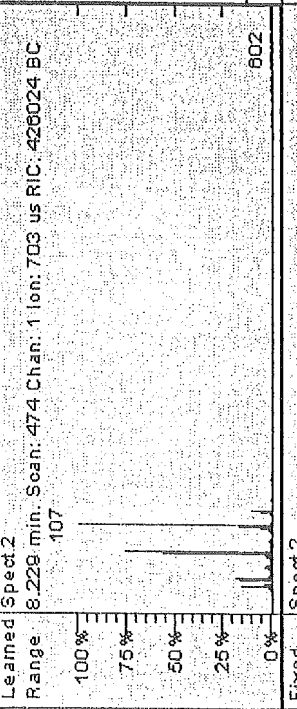
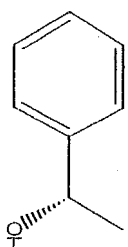
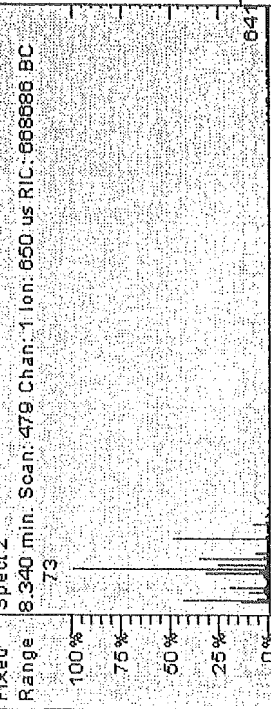
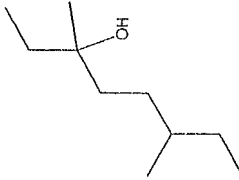
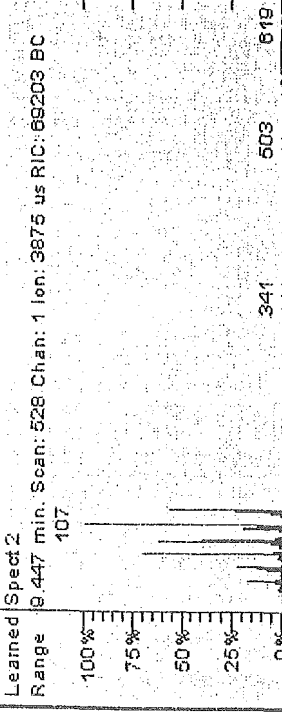
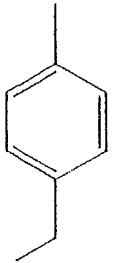
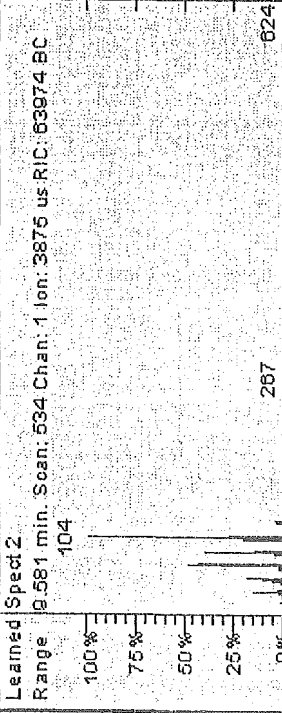
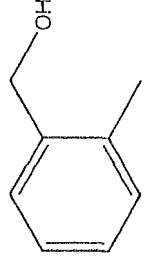
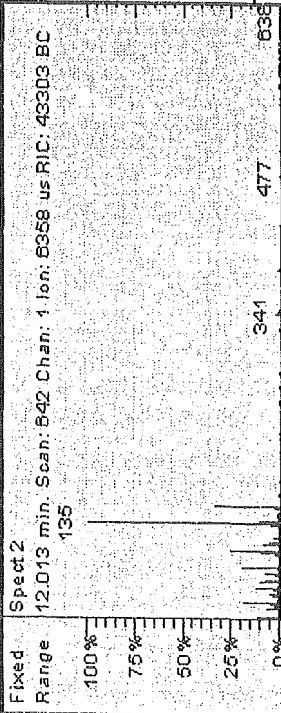
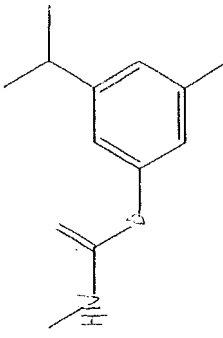
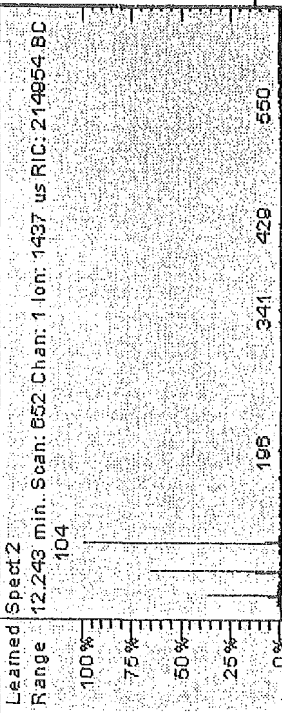
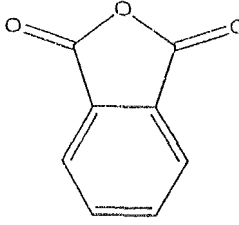


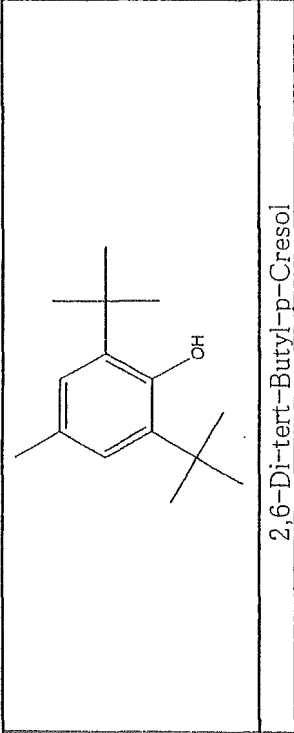
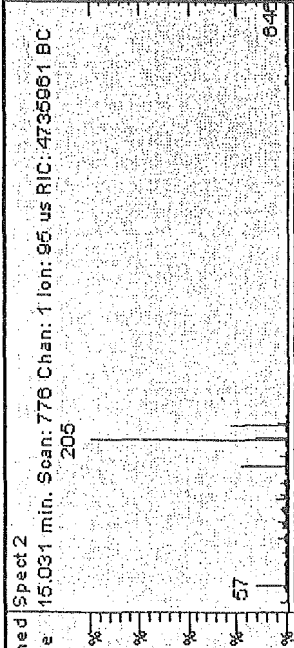
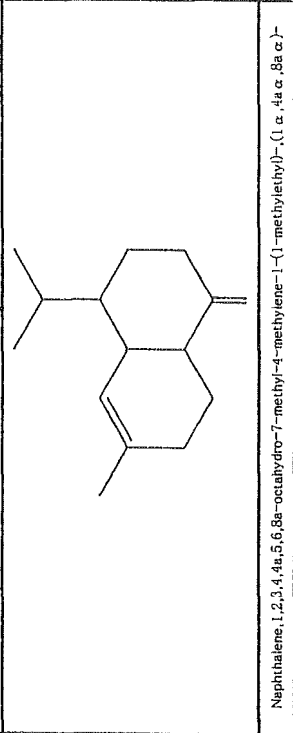
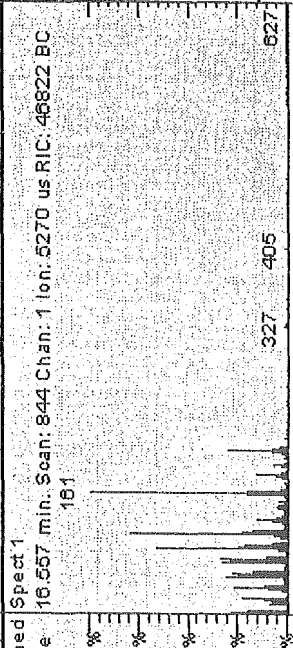
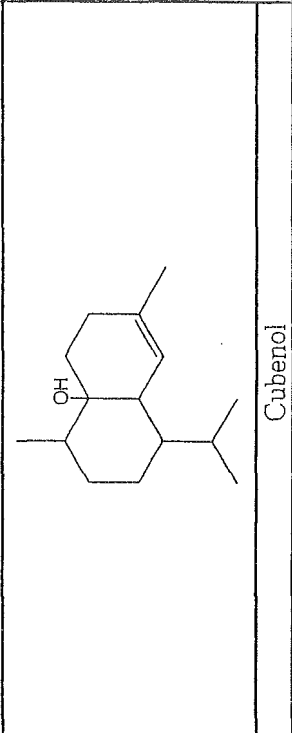
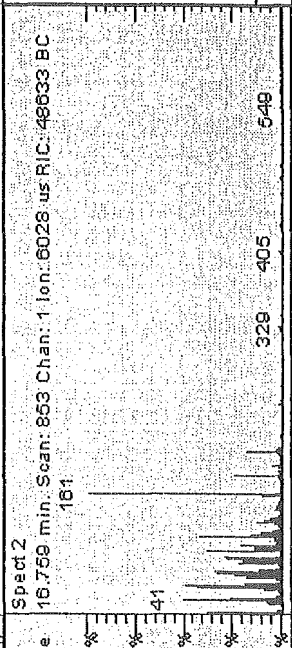
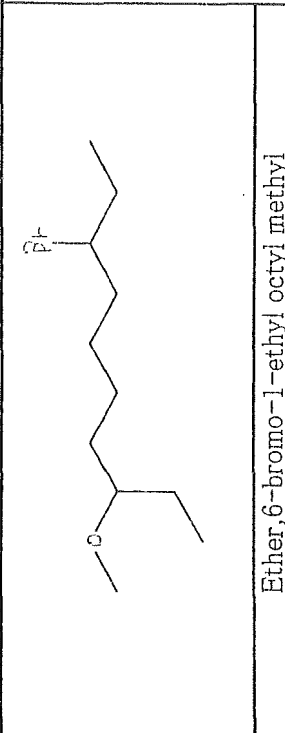
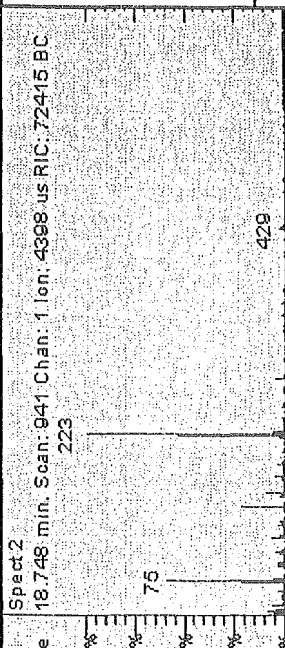
Fig.3-5. はし (No.5)のトータルイオンクロマトグラム(下)とcontrolのトータルイオンクロマトグラム(上)

Table.3-5. はし(No.5)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: 7.334 min. Scan: 434 Chan: 1 Ion: 1981 us RIC: 310449 BC</p> <p>45 281 429 591</p>	<p>6-methoxy-2-methyl-3-hexanone</p>	608	809	C
2	<p>Learned Spect 2 Range: 7.403 min. Scan: 437 Chan: 1 Ion: 3296 us RIC: 133525 BC</p> <p>59 281 639</p>	<p>2-Methyl-2,3-pentanediol</p>	488	813	E
3	<p>Fixed Spect 2 Range: 7.643 min. Scan: 448 Chan: 1 Ion: 15371 us RIC: 18284 BC</p> <p>43 341 429 639</p>	<p>Propane-1,1-diol diacetate</p>	446	892	E
4	<p>Learned Spect 2 Range: 7.779 min. Scan: 454 Chan: 1 Ion: 5356 us RIC: 43434 BC</p> <p>79 341 430 598</p>	<p>Benzyl alcohol</p>	742	922	B

5	<p>Fixed Range 100% 75% 50% 25% 0%</p> <p>Spect 2 7.985 min. Scan: 463 Chan: 1 Ion: 7562 us RIC: 40684 BC</p>  <p>73 341 431 604</p>	 <p>Silane,hexyltrimethyl-</p>	468	814	E
6	<p>Fixed Range 100% 75% 50% 25% 0%</p> <p>Spect 2 8.140 min. Scan: 470 Chan: 1 Ion: 1875 us RIC: 270873 BC</p>  <p>73 281 429 660</p>	 <p>2-Methyl-2,4-dimethoxybutane</p>	662	834	C
7	<p>Learned Spect 2 8.228 min. Scan: 474 Chan: 1 Ion: 703 us RIC: 426024 BC</p>  <p>107 602 73</p>	 <p>alpha-Methylbenzyl alcohol</p>	815	947	A
8	<p>Fixed Range 100% 75% 50% 25% 0%</p> <p>Spect 2 8.340 min. Scan: 479 Chan: 1 Ion: 650 us RIC: 668886 BC</p>  <p>73 64</p>	 <p>3-Octanol, 3,6-dimethyl-</p>	346	795	E

9	<p>Learned Spect 2 Range 9.447 min. Scan: 528 Chan: 1 Ion: 3875 us RIC: 69203 BC</p> 	 <p>4-Methylbenzyl alcohol</p>	778	910	B
10	<p>Learned Spect 2 Range 9.581 min. Scan: 534 Chan: 1 Ion: 3875 us RIC: 69974 BC</p> 	 <p>2-Methylbenzyl alcohol</p>	753	900	C
11	<p>Fixed Spect 2 Range 12.013 min. Scan: 542 Chan: 1 Ion: 6358 us RIC: 43303 BC</p> 	 <p>Promecarb</p>	674	910	D
12	<p>Learned Spect 2 Range 12.243 min. Scan: 652 Chan: 1 Ion: 1437 us RIC: 214954 BC</p> 	 <p>Phthalic anhydride</p>	706	865	B

13	<p>Learned Spect 2 Range 15.031 min. Scan: 776 Chan: 1 Ion: 95 us RIC: 4735961 BC</p> 	 <p>2,6-Di-tert-Butyl-p-Cresol</p>	812	911	A
14	<p>Learned Spect 1 Range 16.557 min. Scan: 844 Chan: 1 Ion: 5270 us RIC: 46822 BC</p> 	 <p>Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-(1.alpha.,4.alpha.,8.alpha.)-</p>	621	865	C
15	<p>Fixed Range Range 16.759 min. Scan: 863 Chan: 1 Ion: 6026 us RIC: 48633 BC</p> 	 <p>Cubenol</p>	591	815	D
16	<p>Fixed Range Range 18.748 min. Scan: 941 Chan: 1 Ion: 4398 us RIC: 72415 BC</p> 	 <p>Ether, 6-bromo-1-ethyl octyl methyl</p>	447	866	E