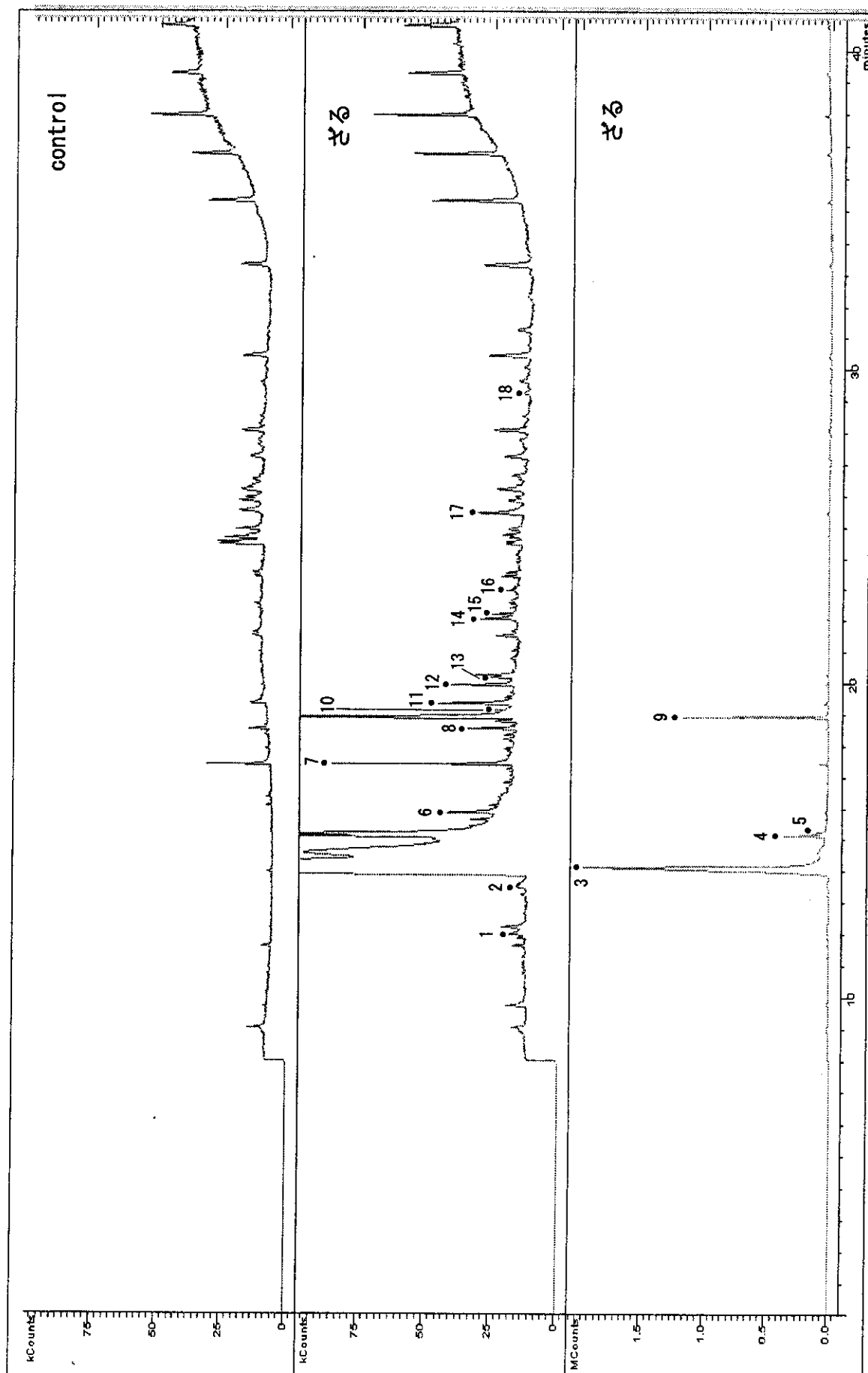


No.	マススペクトル	フラグメーションパターンがよく一致した化合物の構造式と化合物名	prb
13	Learned Spect 1 Range 17.442 min. Scan: 981 Chan: 1 Ion: 15087 us RIC: 12084 BC	 <chem>CC(C)(C)c1cc(C=O)cc(C(C)(C)C)c1O</chem> 3,5-di-tert-Butyl-4-hydroxybenzaldehyde	36.67
14	Learned Spect 1 Range 18.520 min. Scan: 1038 Chan: 1 Ion: 16488 us RIC: 9338 BC	 <chem>CCCCOC(=O)c1ccccc1C(=O)OCCCC</chem> Dibutyl phthalate	21.77
15	Learned Spect 1 Range 19.092 min. Scan: 1068 Chan: 1 Ion: 981 us RIC: 494251 BC	 <chem>CC1(C)C(=O)OCC2(C)C=CC(=O)C21</chem> 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	61.29
16	Learned Spect 1 Range 19.321 min. Scan: 1080 Chan: 1 Ion: 12396 us RIC: 21070 BC	 <chem>CCOC(=O)CCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1</chem> Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	94.10

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	prb
17	Learned Spect 1 Range 19.516 min. Scan: 1090 Chan: 1 Ion: 3004 us RIC: 117525 BC	1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester	22.18
18	Learned Spect 1 Range 19.590 min. Scan: 1094 Chan: 1 Ion: 4046 us RIC: 99891 BC	Oleamide	63.30
19	Learned Spect 1 Range 20.126 min. Scan: 1122 Chan: 1 Ion: 10632 us RIC: 22605 BC	Butylated Hydroxytoluene	6.24
20	Learned Spect 1 Range 21.464 min. Scan: 1192 Chan: 1 Ion: 6564 us RIC: 45698 BC	Oleamide	68.06

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	prb
21	Learned Spect 1 Range 23.306 min. Scan: 1202 Chan: 1 Ion: 3894 us RIC: 86022 BC 94 238	Oleamide	68.61
22	Learned Spect 1 Range 25.794 min. Scan: 1420 Chan: 1 Ion: 10864 us RIC: 15460 BC 94 313 387 555 646	Decyloxybenzene	19.40
23	Learned Spect 1 Range 26.575 min. Scan: 1461 Chan: 1 Ion: 10702 us RIC: 12213 BC 94 281 359 646	Dodecanoic acid, phenyl ester	19.40
24	Learned Spect 1 Range 28.090 min. Scan: 1540 Chan: 1 Ion: 3391 us RIC: 114845 BC 131 343 601	Octadecanoic acid, 2,3-bis(trimethylsilyl)oxypropyl ester	43.59



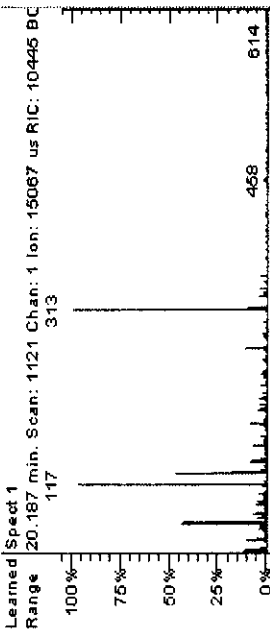
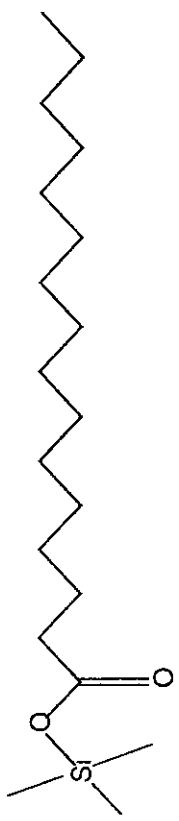
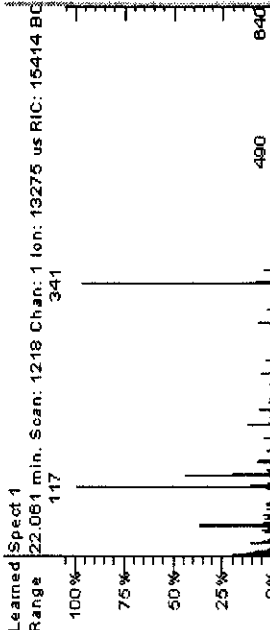
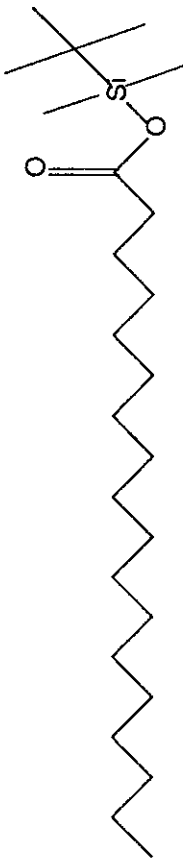
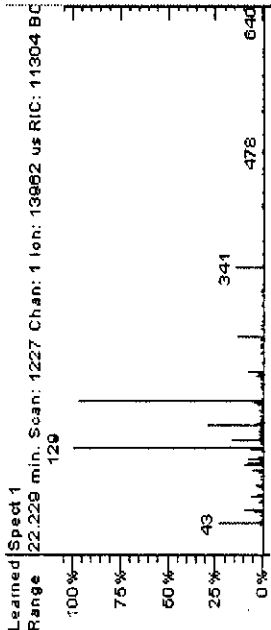
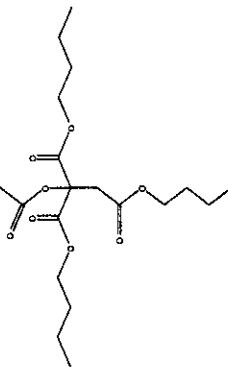
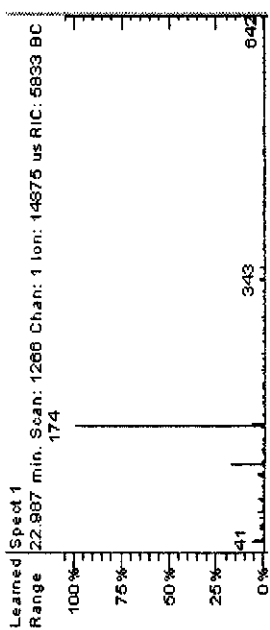
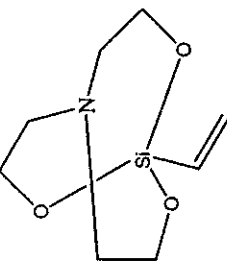
ざる (Sample No. 7) のトータルイオンクロマトグラム (上段はコントロールのトータルイオンクロマトグラム)

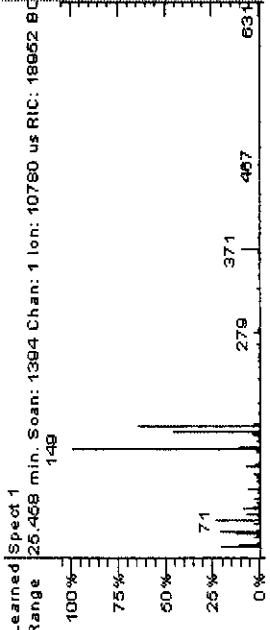
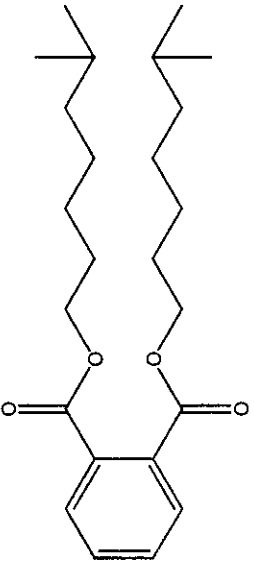
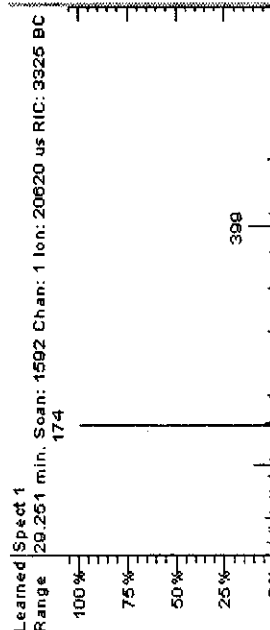
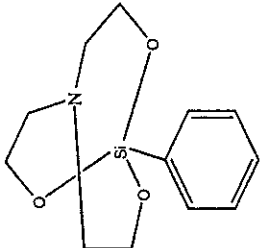
熱湯抽出したざる(Sample No.7)から検出された有機化学物質のマススペクトルと構造式

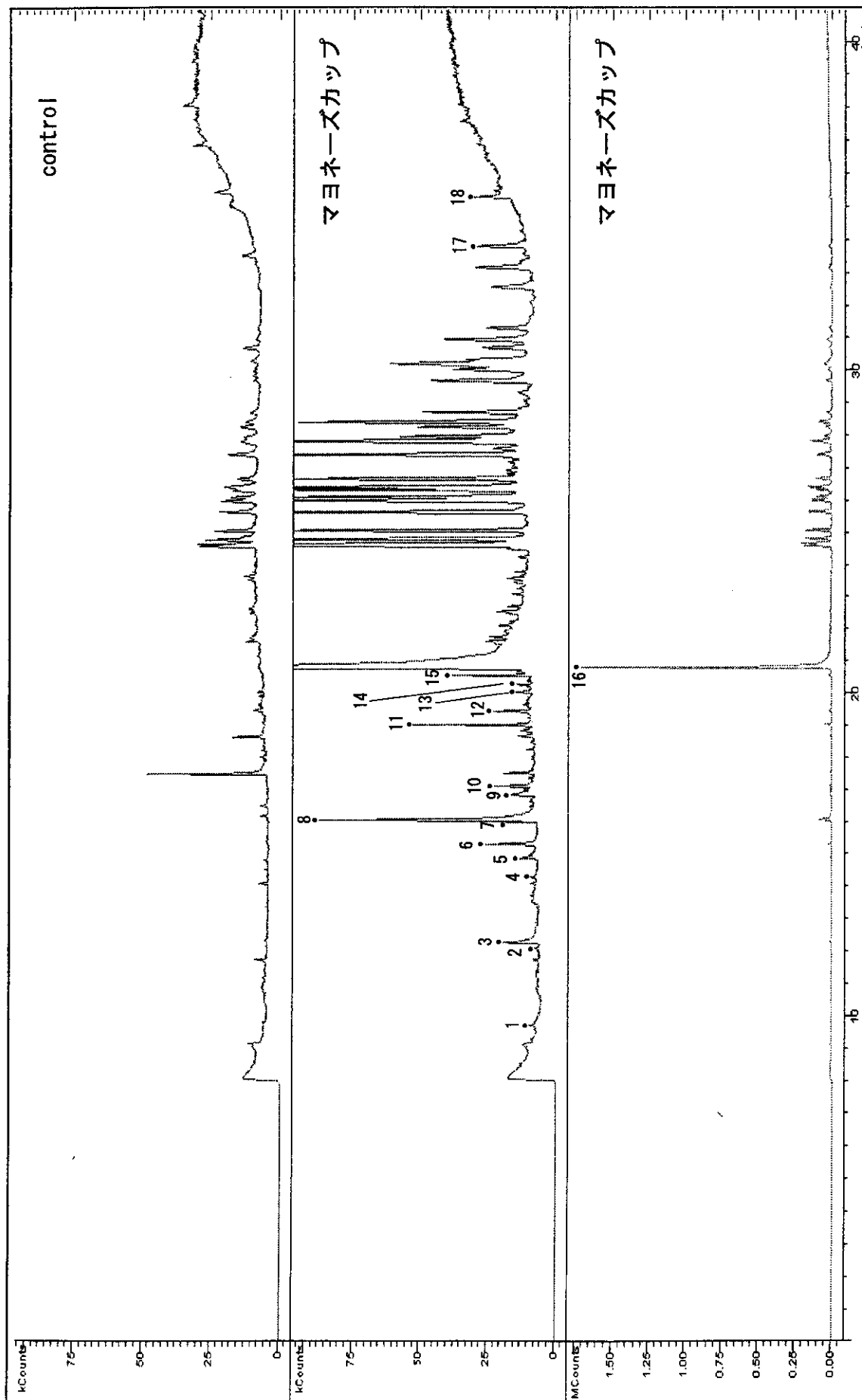
Peak No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
1	Learned Spect 1 Range 12.012 min. Scan: 893 Chan: 1 Ion: 18189 us RIC: 8809 BC	 3-(3-Methoxyphenyl)propan-1-ol	15.63
2	Learned Spect 1 Range 13.512 min. Scan: 772 Chan: 1 Ion: 10822 us RIC: 4439 BC	 Dimethyl phthalate	41.87
3	Learned Spect 1 Range 14.144 min. Scan: 805 Chan: 1 Ion: 188 us RIC: 1959319 BC	 p-tert-butylbenzoic acid	68.55
4	Learned Spect 1 Range 16.146 min. Scan: 857 Chan: 1 Ion: 1582 us RIC: 353210 BC	 1,3-Benzenedicarboxylic acid, 5-(1,1-dimethylethyl)-, dimethyl ester	30.33

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	prb
5	Learned Spect 1 Range 15.200 min. Scan: 860 Chan: 1 Ion: 3048 us RIC: 121534 BC	 Diethyl Phthalate.cdx <chem>CCOC(=O)c1ccccc1C(=O)OCC</chem>	55.96
6	Learned Spect 1 Range 15.884 min. Scan: 895 Chan: 1 Ion: 7623 us RIC: 23107 BC	 Tributyl phosphate <chem>CCOP(=O)(OCC)OCC</chem>	68.30
7	Learned Spect 1 Range 17.427 min. Scan: 977 Chan: 1 Ion: 4935 us RIC: 70040 BC	 Phenol, 2-(1,1-dimethylethyl)-4-(1-methyl-1-phenylethyl)- <chem>CC(C)(C)c1cc(O)ccc1C(C)c2ccccc2</chem>	19.40
8	Learned Spect 1 Range 18.566 min. Scan: 1036 Chan: 1 Ion: 11911 us RIC: 20463 BC	 Borazine, 2,4,6-triphenyl-1,3,5-tripropyl- <chem>CCCN1B(C2=CC=CC=C2)N(C3=CC=CC=C3)B(C4=CC=CC=C4)N1CC3</chem>	47.66

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	prb
9	Learned Spect 1 Range 16.929 min. Scan: 1055 Chan: 1 Ion: 376 us RIC: 1173767 BC	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	55.55
10	Learned Spect 1 Range 19.156 min. Scan: 1087 Chan: 1 Ion: 14382 us RIC: 8363 BC	 Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	67.17
11	Learned Spect 1 Range 19.365 min. Scan: 1078 Chan: 1 Ion: 7552 us RIC: 30667 BC	 Dibutyl phthalate	33.87
12	Learned Spect 1 Range 19.955 min. Scan: 1109 Chan: 1 Ion: 9075 us RIC: 25055 BC	 Butylated Hydroxytoluene	11.84

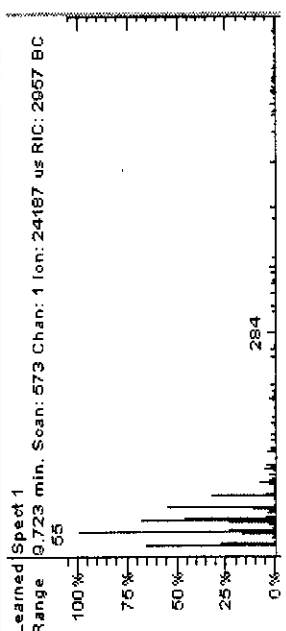
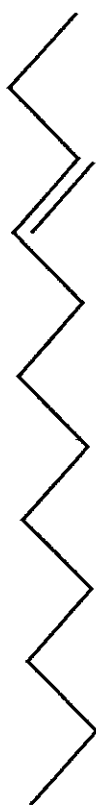
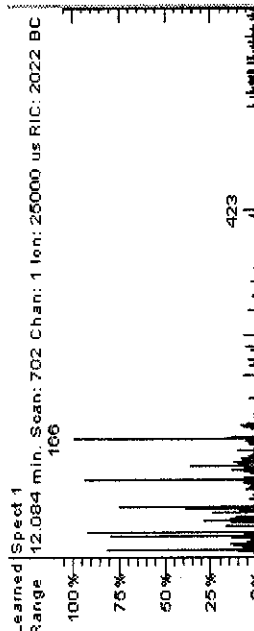
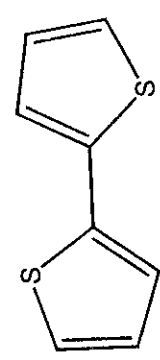
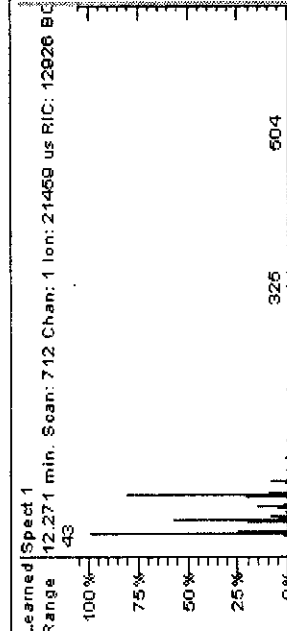
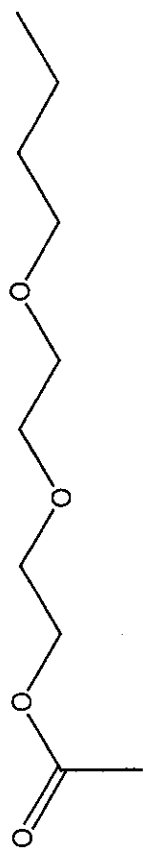
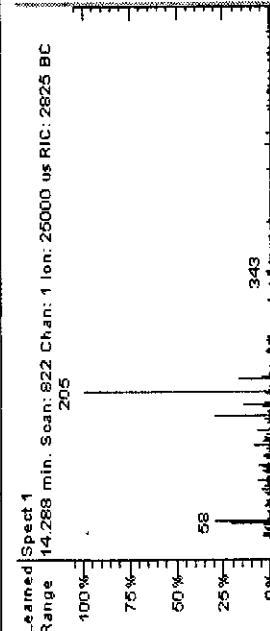
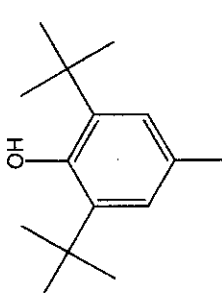
No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
13	Learned Spect 1 Range 20.187 min. Scan: 1121 Chan: 1 Ion: 15067 us RIC: 10445 BC 	 Hexadecanoic acid, trimethylsilyl ester	69.81
14	Learned Spect 1 Range 22.061 min. Scan: 1218 Chan: 1 Ion: 13275 us RIC: 15414 BC 	 Octadecanoic acid, tert-butyl dimethylsilyl ester	56.12
15	Learned Spect 1 Range 22.229 min. Scan: 1227 Chan: 1 Ion: 13952 us RIC: 11304 BC 	 Tributyl acetylacrylate	20.42
16	Learned Spect 1 Range 22.987 min. Scan: 1266 Chan: 1 Ion: 14375 us RIC: 5933 BC 	 2,8,9-Trioxa-5-aza-1-silabicyclo[3,3,3]undecane, 1-ethenyl	19.40

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	prb
17	Learned Spect 1 Range 25.458 min. Scan: 1394 Chan: 1 Ion: 10780 us RIC: 19052 BC 	 1,2-Benzenedicarboxylic acid diisooctyl ester	49.42
18	Learned Spect 1 Range 20.251 min. Scan: 1592 Chan: 1 Ion: 20620 us RIC: 3325 BC 	 Phenylsilatrane	24.25

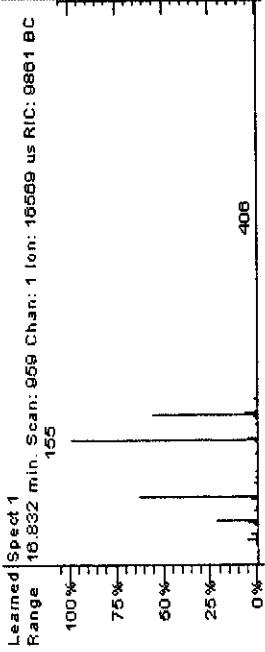
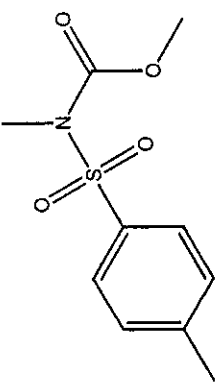
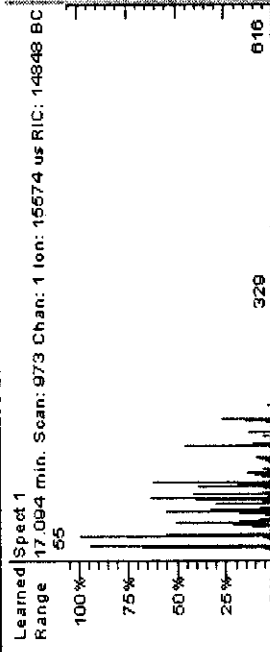
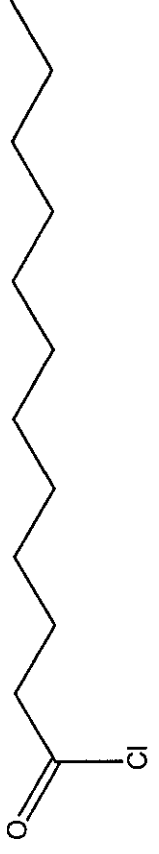
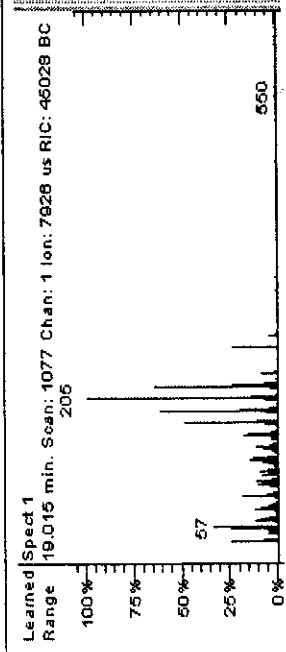
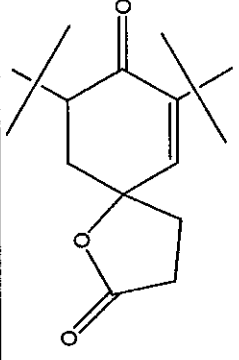
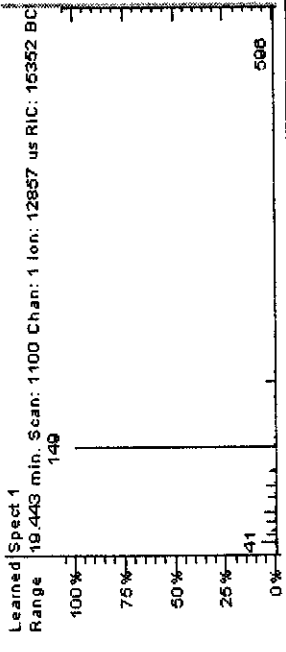
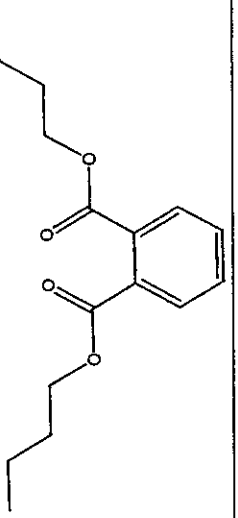


マヨネーズカップ (Sample No. 8) のトータルイオンクロマトグラム (上段はコントロールのクロマトグラム)

熱湯抽出したマヨネーズカップ (Sample 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

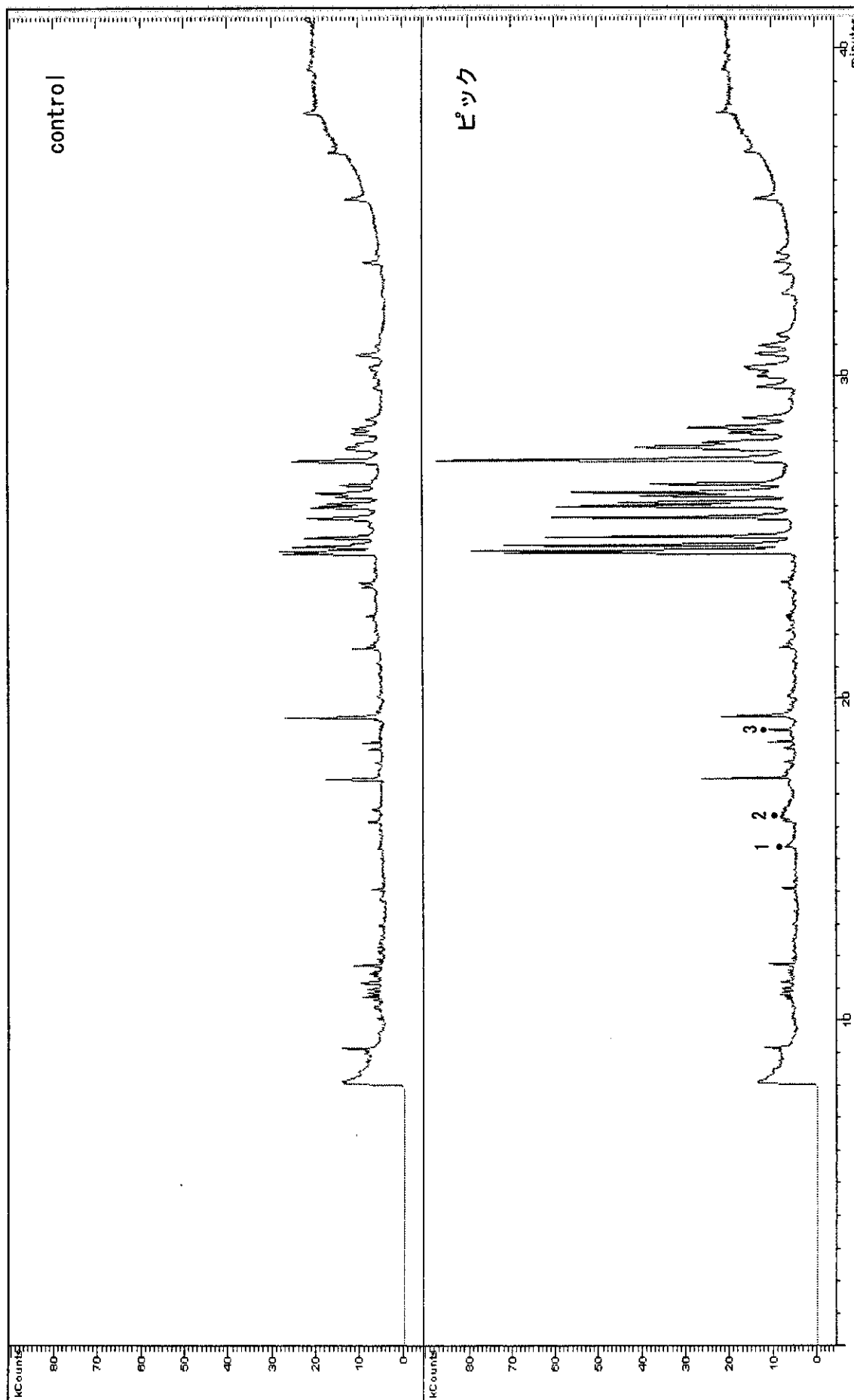
Peak No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
1	Learned Spect 1 Range 9.723 min. Scan: 573 Chan: 1 Ion: 24187 us RIC: 2857 BC 	 3-Dodecene, (E)-	19.40
2	Learned Spect 1 Range 12.084 min. Scan: 702 Chan: 1 Ion: 25000 us RIC: 2022 BC 	 2,2'-Bithiophene	24.25
3	Learned Spect 1 Range 12.271 min. Scan: 712 Chan: 1 Ion: 21459 us RIC: 12926 BC 	 Butyl Carbitol Acetate	85.11
4	Learned Spect 1 Range 14.288 min. Scan: 822 Chan: 1 Ion: 25000 us RIC: 2825 BC 	 Butylated Hydroxytoluen	28.57

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	prb
5	Learned Spect 1 Range 14.861 min. Scan: 853 Chan: 1 Ion: 22481 us RIC: 8834 BC	 Lauric acid	20.81
6	Learned Spect 1 Range 15.304 min. Scan: 877 Chan: 1 Ion: 13872 us RIC: 18670 BC	 Diethyl Phthalate	82.27
7	Learned Spect 1 Range 15.998 min. Scan: 915 Chan: 1 Ion: 18898 us RIC: 11808 BC	 Dodecanoic acid, tert-butyltrimethylsilyl ester	72.68
8	Learned Spect 1 Range 16.068 min. Scan: 918 Chan: 1 Ion: 4068 us RIC: 82134 BC	 N-Ethyl-O-toluenesulfonamide	49.31

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	prb
9	Learned Spect 1 Range 10.832 min. Scan: 959 Chan: 1 Ion: 16569 us RIC: 9861 BC 	 Carbamic acid, methyl[(4-methylphenyl)sulfonyl]-, methyl ester	28.90
10	Learned Spect 1 Range 17.094 min. Scan: 973 Chan: 1 Ion: 15674 us RIC: 14948 BC 	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	47.66
11	Learned Spect 1 Range 19.015 min. Scan: 1077 Chan: 1 Ion: 7928 us RIC: 46028 BC 	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	50.00
12	Learned Spect 1 Range 19.443 min. Scan: 1100 Chan: 1 Ion: 12857 us RIC: 16352 BC 	 Dibutyl phthalate	44.67

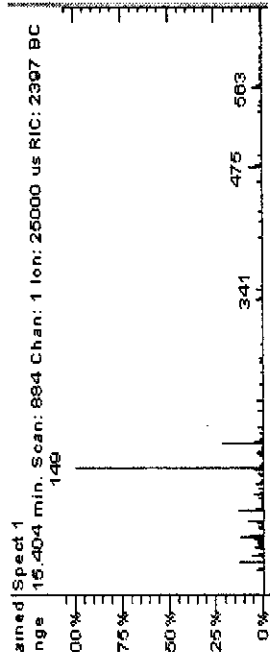
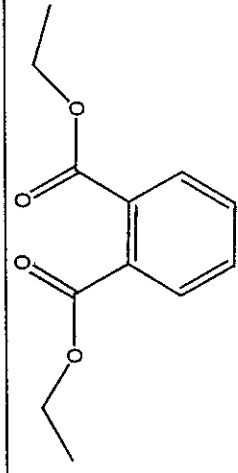
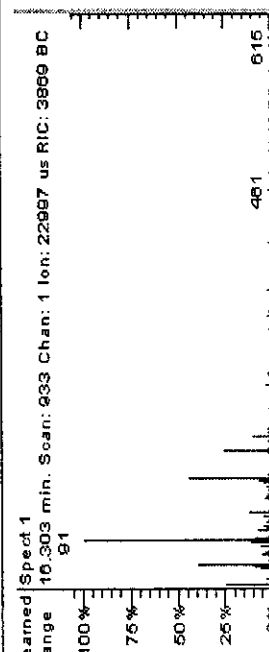
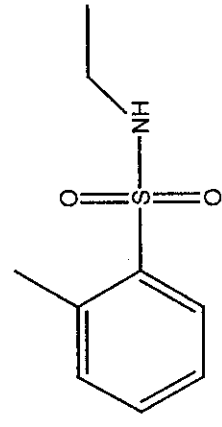
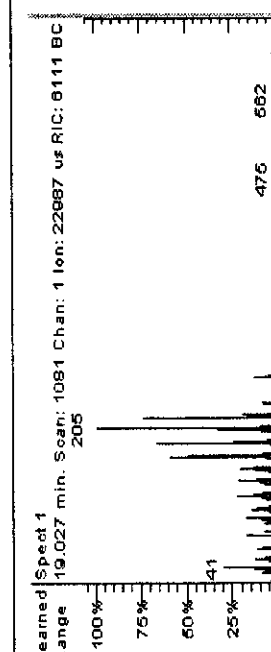
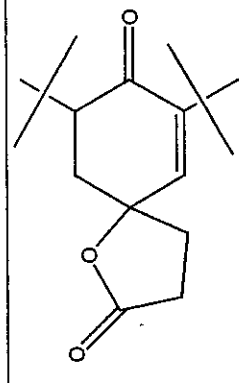
No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
13	Learned Spect 1 Range 20.036 min. Scan: 1132 Chan: 1 Ion: 21345 us RIC: 6481 BC	Butylated Hydroxytoluene	10.15
14	Learned Spect 1 Range 20.281 min. Scan: 1145 Chan: 1 Ion: 10835 us RIC: 6287 BC	Hexadecanoic acid, trimethylsilyl ester	50.91
15	Learned Spect 1 Range 20.558 min. Scan: 1180 Chan: 1 Ion: 10295 us RIC: 29878 BC	Lauric acid, 2,3-bis(trimethylsiloxy)propyl ester	53.23
16	Learned Spect 1 Range 20.785 min. Scan: 1172 Chan: 1 Ion: 229 us RIC: 1707801 BC	Lauroyl chloride	15.63

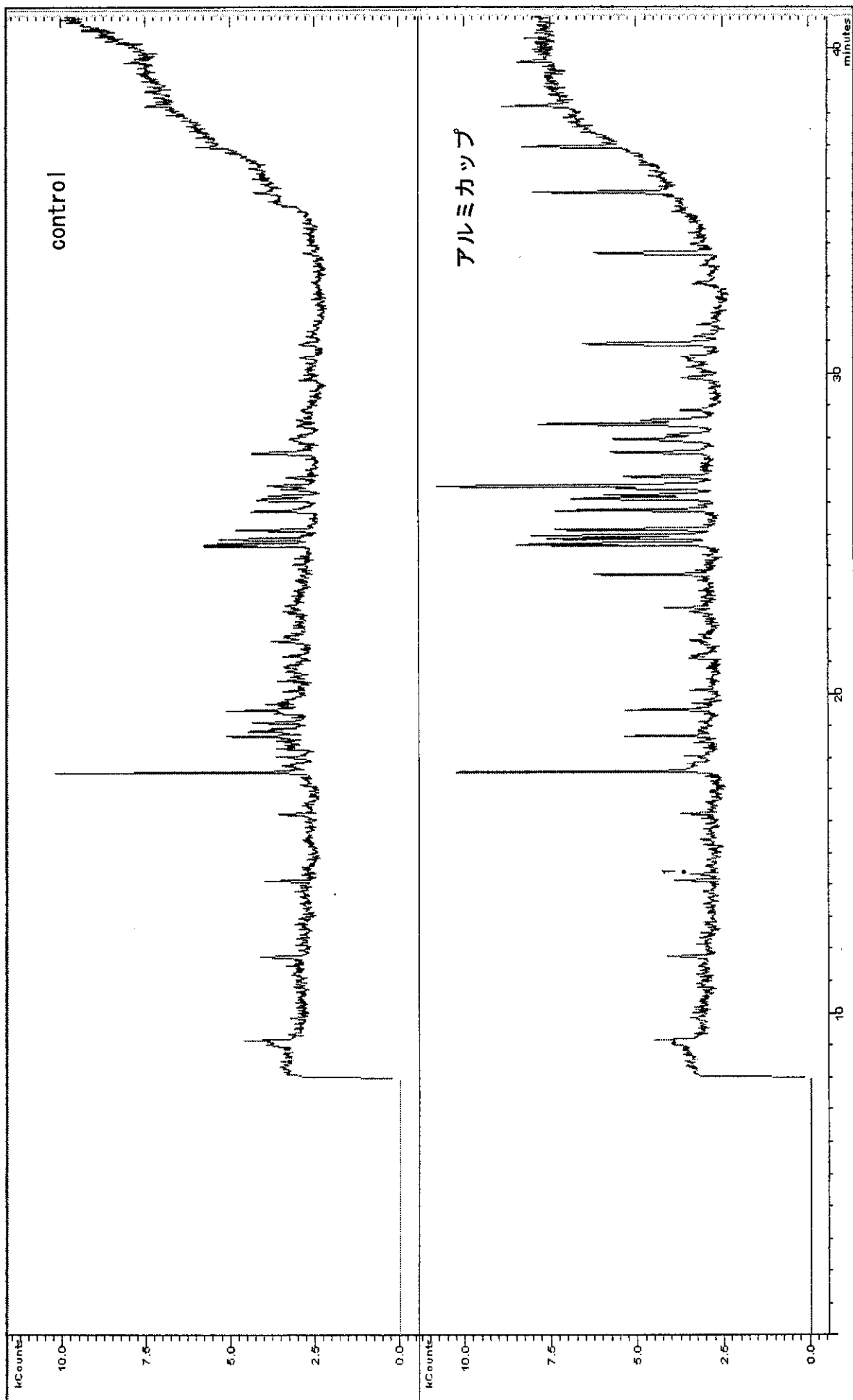
No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
17	Learned Spect 1 Range 33.804 min. Scan: 1865 Chan: 1 Ion: 8865 us RIC: 10754 BC	Phenyl 3-deoxy-α-D-ribo-hexoside	45.59
18	Learned Spect 1 Range 35.279 min. Scan: 1932 Chan: 1 Ion: 10983 us RIC: 14032 BC	Decyloxybenzene	19.40



ピック (Sample No. 9) のトータルイオンクロマトグラム (上段はコントロールのクロマトグラム)

熱湯抽出したピーク (Sample 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

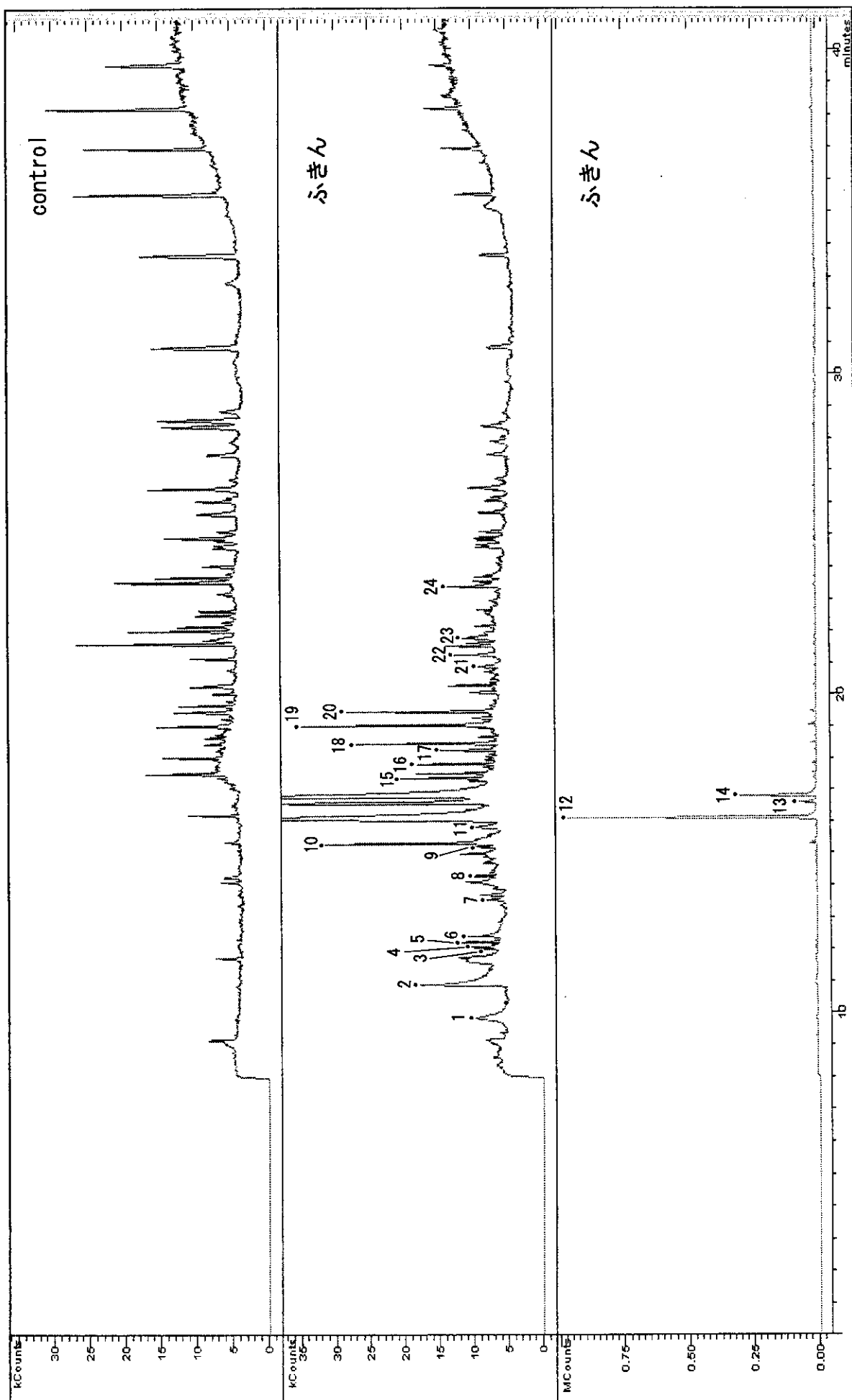
Peak No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
1	Learned Spect 1 Range 15.404 min. Scan: 894 Chan: 1 Ion: 25000 us RIC: 2397 BC 	 Diethyl Phthalate	38.87
2	Learned Spect 1 Range 16.303 min. Scan: 933 Chan: 1 Ion: 22987 us RIC: 3899 BC 	 N-Ethyl-O-toluenesulfonamide	28.76
3	Learned Spect 1 Range 19.027 min. Scan: 1081 Chan: 1 Ion: 22987 us RIC: 8111 BC 	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	34.93



アルミカップ (Sample No. 10) のトータルイオンクロマトグラム (上段はコントロールのトータルイオンクロマトグラム)

熱湯抽出したアルミカップ(Sample 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

Peak 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	prb
1	Learned Spect 1 Range 14.315 min. Scan: 827 Chan: 1 Ion: 25000 us RIC: 1079 BC Mass spectrum showing relative intensity (%) on the y-axis (0% to 100%) and m/z on the x-axis (0 to 600). The base peak is at m/z 205. Other significant peaks are labeled at m/z 57, 405, and 562.	Butylated Hydroxytoluene	32.53



ふきん (Sample No. 11) のトータルイオンクロマトグラム (上段はコントロールのクロマトグラム)