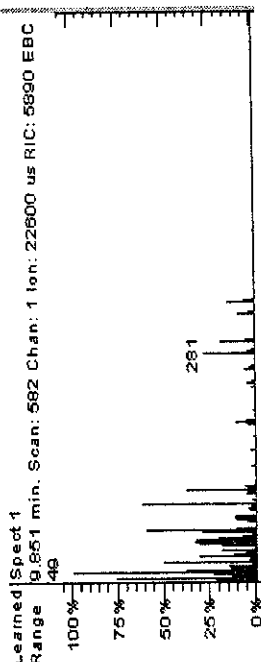
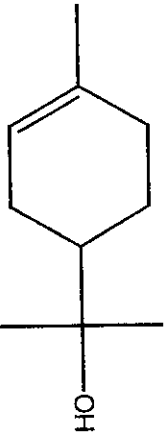
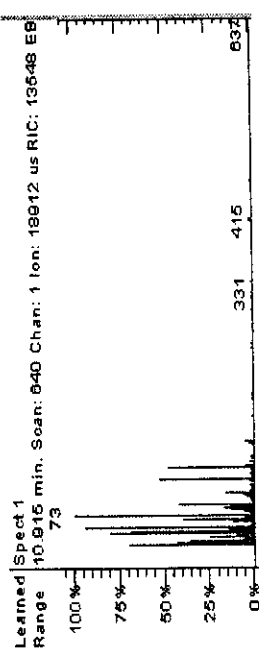
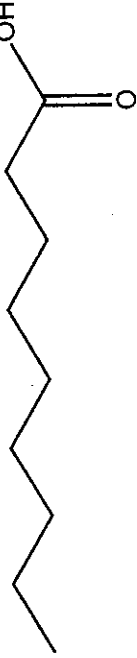
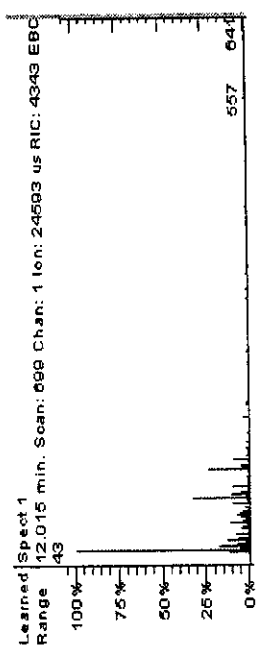
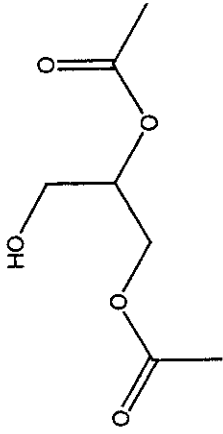
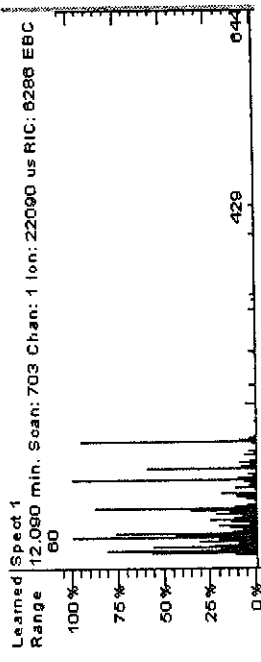
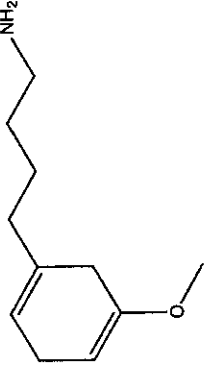
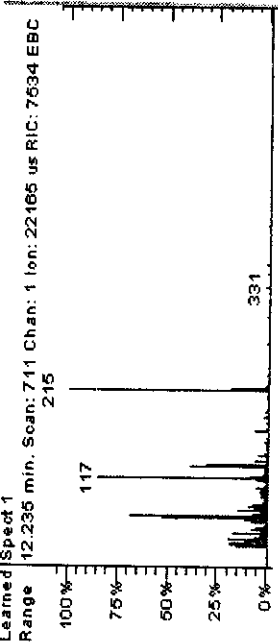
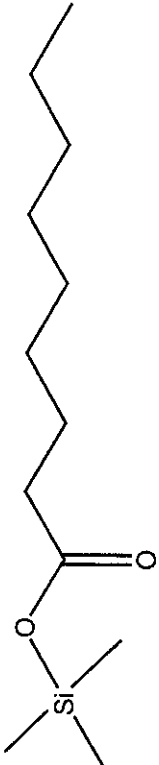
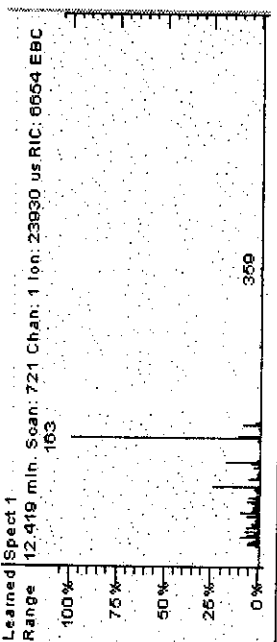
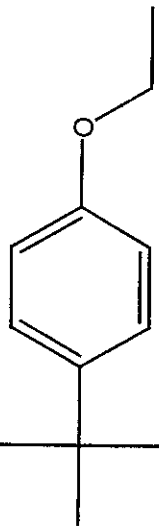
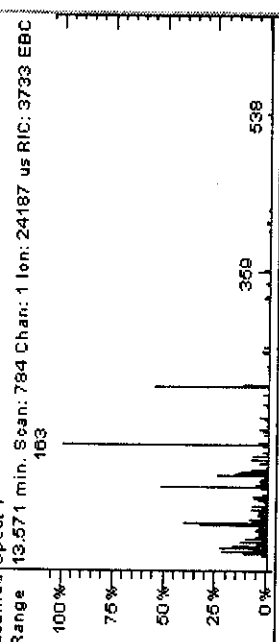
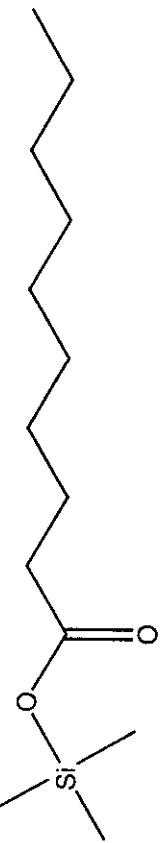
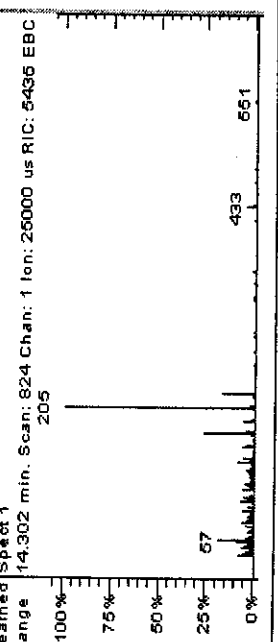
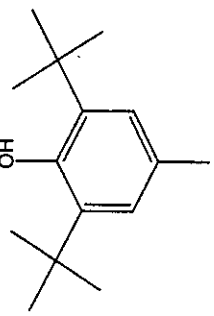
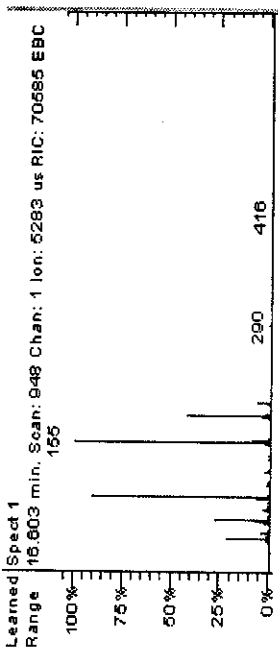
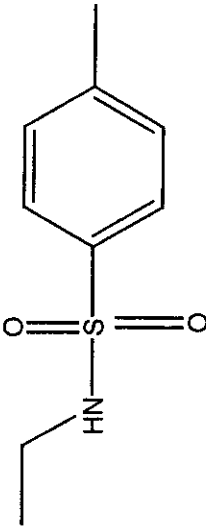
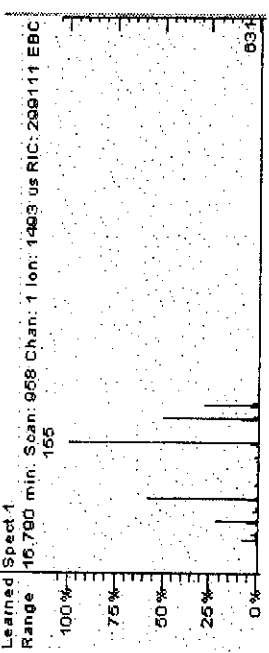
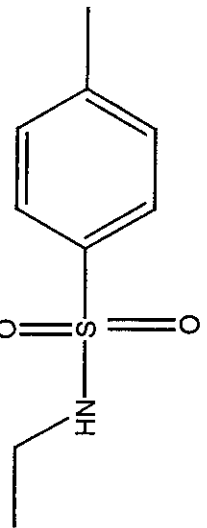
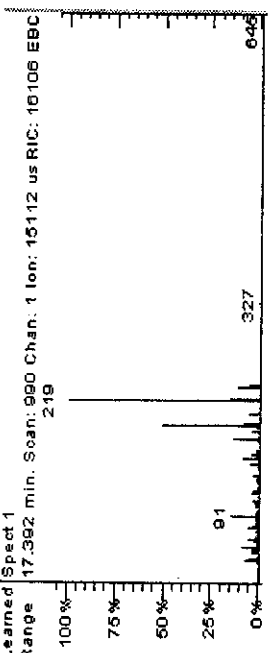
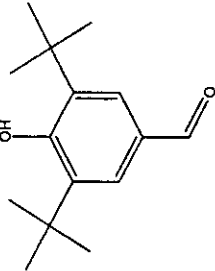
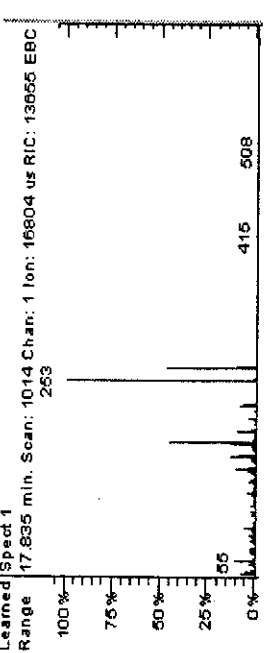
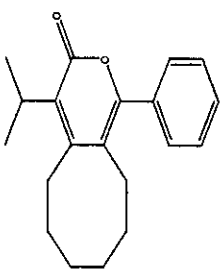


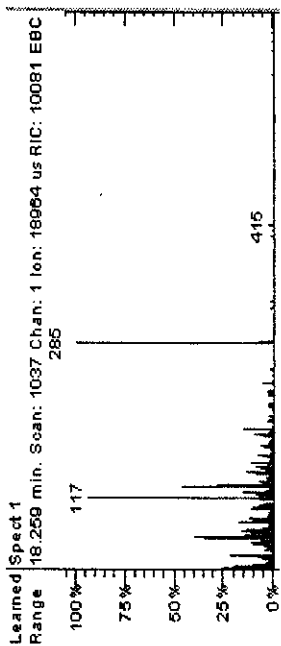
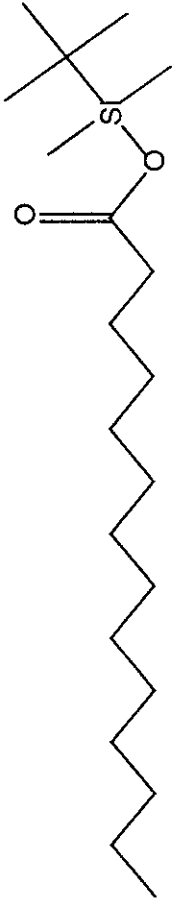
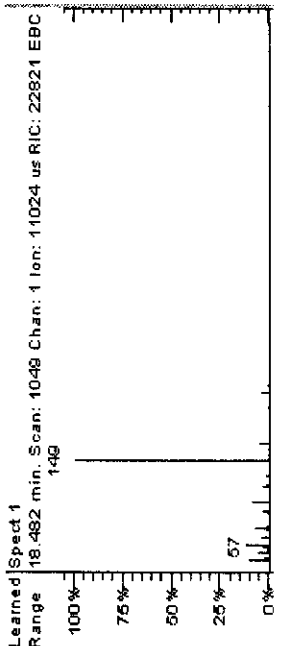
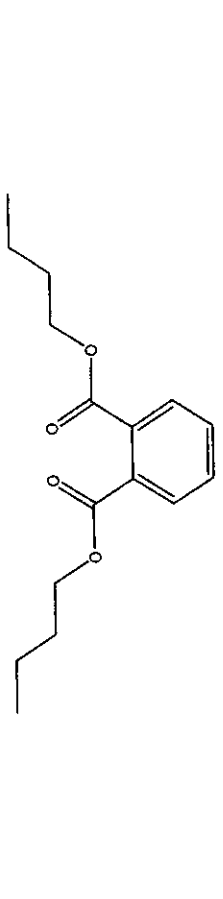
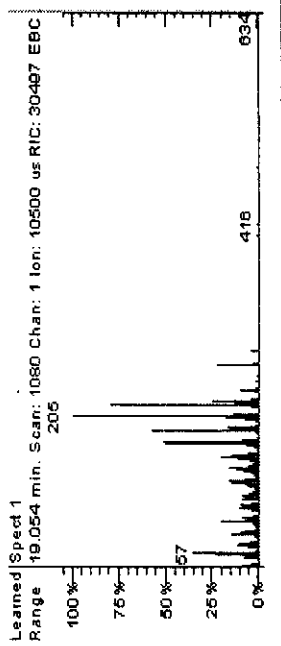
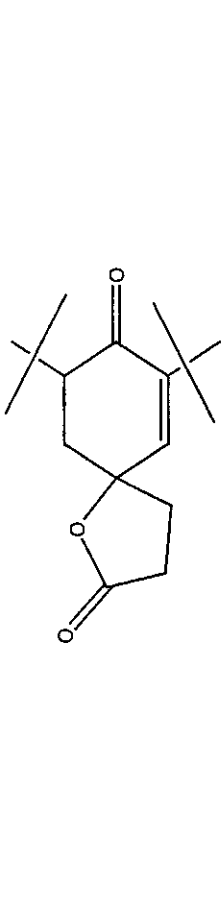
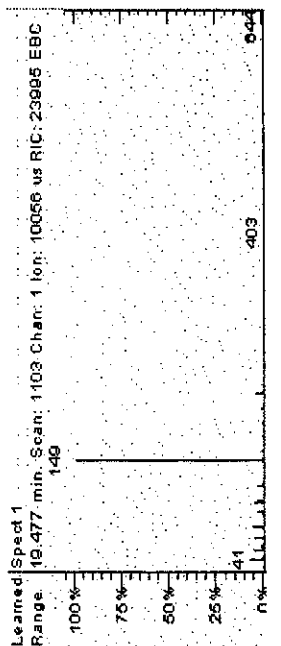
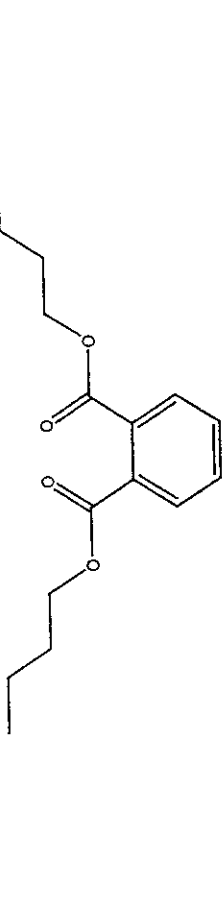
熱湯抽出したふきん(Sample No.11)から検出された有機化学物質のマススペクトルと構造式

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 9.951 min. Scan: 582 Chan: 1 Ion: 22600 us RIC: 5990 EBC 	 α -Terpineol	23.12
2	Learned Spect 1 Range 10.915 min. Scan: 640 Chan: 1 Ion: 19912 us RIC: 13548 EBC 	 Nonanoic acid	50.00
3	Learned Spect 1 Range 12.015 min. Scan: 699 Chan: 1 Ion: 24593 us RIC: 4343 EBC 	 (Hydroxymethyl)ethylene acetate	54.38
4	Learned Spect 1 Range 12.090 min. Scan: 703 Chan: 1 Ion: 22090 us RIC: 6286 EBC 	 4(2,5-Dihydro-3-methoxyphenyl)butylamine	11.84

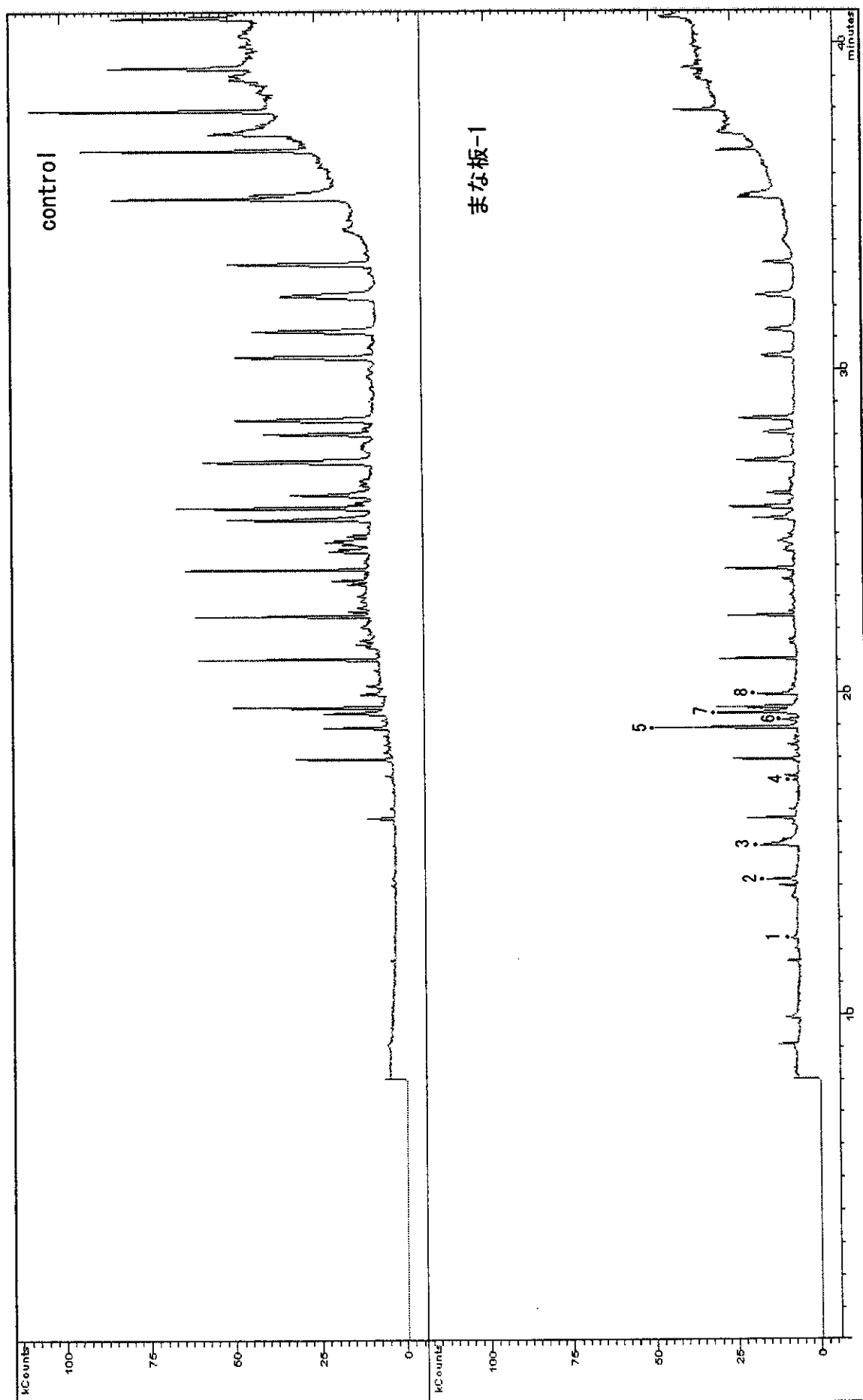
No.	マススペクトル	フラグメーションパターンがよく一致した化合物の構造式と化合物名	prb
5	Learned Spect 1 Range 12.235 min. Scan: 711 Chan: 1 Ion: 22165 us RIC: 7534 EBC 	 Nonanoic acid, trimethylsilyl ester	46.57
6	Learned Spect 1 Range 12.419 min. Scan: 721 Chan: 1 Ion: 23930 us RIC: 6654 EBC 	 Benzene, 1-(1,1-dimethylethyl)-4-ethoxy-	20.29
7	Learned Spect 1 Range 13.571 min. Scan: 784 Chan: 1 Ion: 24187 us RIC: 3733 EBC 	 Decanoic acid, trimethylsilyl ester	24.25
8	Learned Spect 1 Range 14.302 min. Scan: 824 Chan: 1 Ion: 26000 us RIC: 5436 EBC 	 Butylated Hydroxytoluene	48.53

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 15.224 min. Scan: 874 Chan: 1 Ion: 23461 us RIC: 5103 EBC	 Neoisolongifolene, 8-bromo-	38.87
10	Learned Spect 1 Range 15.315 min. Scan: 879 Chan: 1 Ion: 10580 us RIC: 27279 EBC	 Diethyl Phthalate	76.16
11	Learned Spect 1 Range 15.828 min. Scan: 907 Chan: 1 Ion: 22011 us RIC: 5261 EBC	 Benzophenone	37.50
12	Learned Spect 1 Range 16.131 min. Scan: 823 Chan: 1 Ion: 291 us RIC: 966695 EBC	 N-Ethyl-O-toluenesulfonamide	29.48

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: 16.603 min. Scan: 948 Chan: 1 Ion: 5283 us RIC: 70685 EBC 	 N-Ethyl-4-toluenesulfonamide	32.85
14	Learned Spect 1 Range: 16.760 min. Scan: 958 Chan: 1 Ion: 1493 us RIC: 239111 EBC 	 N-Ethyl-4-toluenesulfonamide	56.87
15	Learned Spect 1 Range: 17.392 min. Scan: 990 Chan: 1 Ion: 15112 us RIC: 16106 EBC 	 3,5-di-tert-Butyl-4-hydroxybenzaldehyde	72.86
16	Learned Spect 1 Range: 17.835 min. Scan: 1014 Chan: 1 Ion: 16804 us RIC: 13655 EBC 	 3H-Cycloocta[c]pyran-3-one,5,6,7,8,10-hexahydro-4-isopropyl-1-phenyl	37.87

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
17	Learned Spect 1 Range 18.259 min. Scan: 1037 Chan: 1 Ion: 18064 us RIC: 10081 EBC 	 Tetradecanoic acid, tert-butyl dimethylsilyl ester	20.81
18	Learned Spect 1 Range 18.482 min. Scan: 1048 Chan: 1 Ion: 11024 us RIC: 22821 EBC 	 Dibutyl phthalate	26.92
19	Learned Spect 1 Range 19.054 min. Scan: 1080 Chan: 1 Ion: 10500 us RIC: 30497 EBC 	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	63.46
20	Learned Spect 1 Range 19.477 min. Scan: 1103 Chan: 1 Ion: 10056 us RIC: 23995 EBC 	 Dibutyl phthalate	28.74

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 20.912 min. Scan: 1181 Chan: 1 Ion: 22635 us RIC: 4849 EBC	 3-Hexanamine,3-ethyl-	15.63
22	Learned Spect 1 Range 21.281 min. Scan: 1201 Chan: 1 Ion: 16656 us RIC: 9175 EBC	 Benzene,1,1'-sulfonylbis[2-methyl-	59.71
23	Learned Spect 1 Range 21.821 min. Scan: 1230 Chan: 1 Ion: 21383 us RIC: 6768 EBC	 di-p-Tolyl sulfone	74.04
24	Learned Spect 1 Range 23.417 min. Scan: 1317 Chan: 1 Ion: 22273 us RIC: 6881 EBC	 4a.alpha.,4b.beta.-Gibbane-1.alpha.,10.beta.-dicarboxylic acid,1,4a-dimethyl-8	19.40

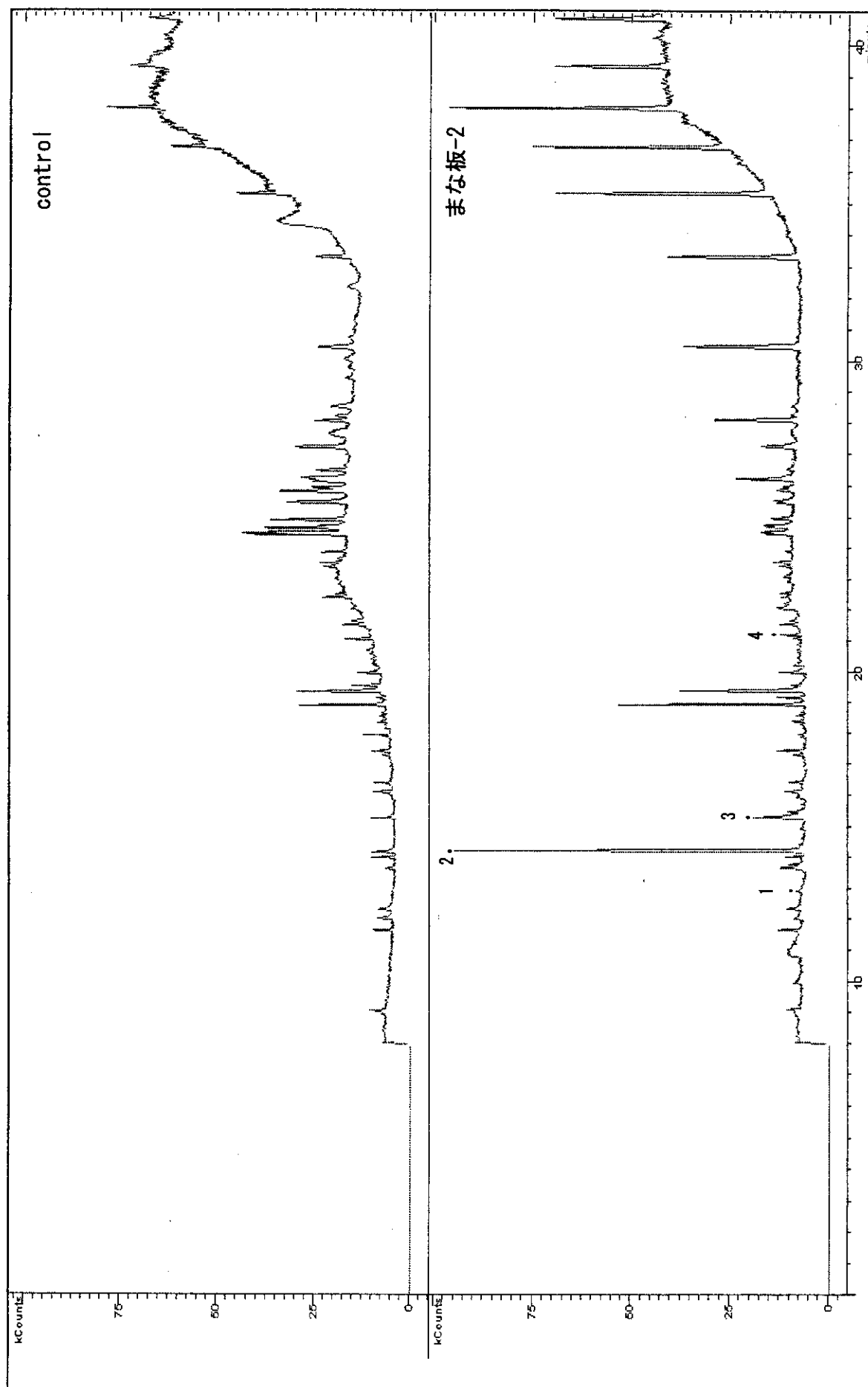


まな板-1 (Sample No. 12) のトータルイオンクロマトグラム(上段はコントロールのクロマトグラム)

Table.2-13. 熱湯抽出したまな板-1(Sample 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

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		 Propanoic acid, 2-methyl-, 3-hydroxy-, 2,4,4-trimethylpentyl ester	24.25
2		 7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-diene-8-one	49.49
3		 Diethyl Phthalate	62.37
4		 3,5-di-tert-Butyl-4-hydroxybenzaldehyde	53.39

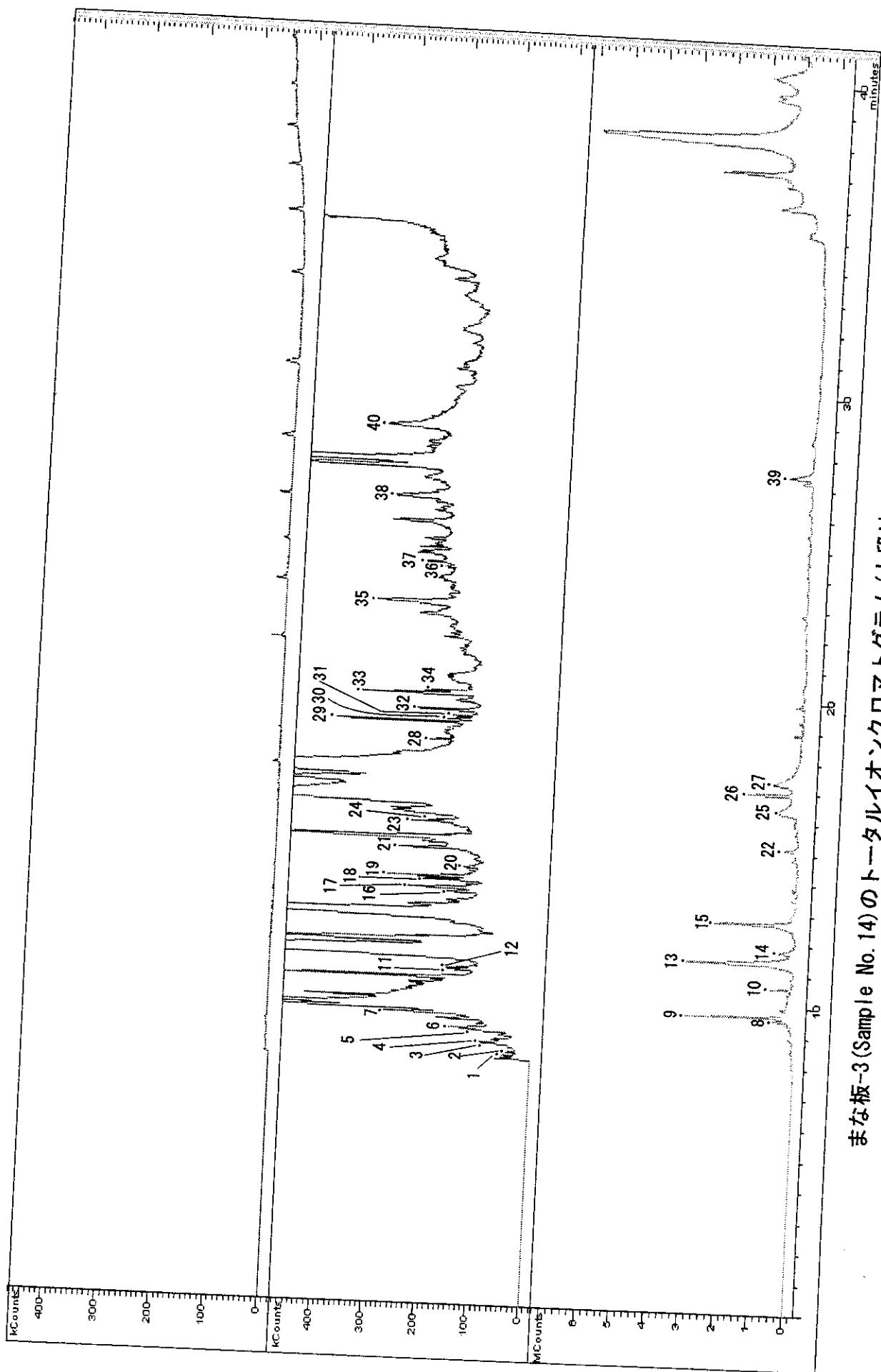
No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
5	Learned Spect 1 Range 18.935 min. Scan: 1070 Chan: 1 Ion: 7703 us RIC: 44229 BC	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	28.57
6	Learned Spect 1 Range 19.160 min. Scan: 1082 Chan: 1 Ion: 20325 us RIC: 5400 BC	 Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	85.86
7	Learned Spect 1 Range 19.392 min. Scan: 1084 Chan: 1 Ion: 10214 us RIC: 25519 BC	 Dibutyl phthalate	29.28
8	Learned Spect 1 Range 19.962 min. Scan: 1125 Chan: 1 Ion: 15702 us RIC: 12969 BC	 Benzo[b]dihydropyran, 6-hydroxy-4,4,5,7,8-pentamethyl-	19.69



まな板-2 (Sample No. 13) 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)

熱湯抽出したまな板-2(Sample 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

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 12.903 min. Scan: 743 Chan: 1 Ion: 23824 us RIC: 2236 BC	5-Isopropenyl-1,2-dimethylcyclohex-2-enol	12.60
2	Learned Spect 1 Range 14.214 min. Scan: 813 Chan: 1 Ion: 4893 us RIC: 89023 BC	Butylated Hydroxytoluene	63.22
3	Learned Spect 1 Range 15.270 min. Scan: 870 Chan: 1 Ion: 15397 us RIC: 13821 BC	Diethyl Phthalate	55.13
4	Learned Spect 1 Range 21.195 min. Scan: 1189 Chan: 1 Ion: 19798 us RIC: 5928 BC	2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane, 1'-ethenyl-	38.87



まな板-3 (Sample No. 14) 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)

熱湯抽出したまな板-3(Sample 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

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 8.137 min. Scan: 488 Chan: 1 Ion: 8873 us RIC: 23678 BC	 2-11-Dodecadiene, 4-acetoxy-	24.25
2	Learned Spect 1 Range 8.250 min. Scan: 494 Chan: 1 Ion: 8368 us RIC: 16592 BC	 Bicyclo[3.1.0]hexane, 6-isopropylidene-	19.40
3	Learned Spect 1 Range 8.520 min. Scan: 508 Chan: 1 Ion: 4264 us RIC: 46788 BC	 Isophorone	24.51
4	Learned Spect 1 Range 8.558 min. Scan: 510 Chan: 1 Ion: 4379 us RIC: 49625 BC	 Hexanoic acid, 2-ethyl-	63.17

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
5	Learned Spect 1 Range 8.918 min. Scan: 529 Chan: 1 Ion: 3344 us RIC: 48563 BC	 1-Hydroxymethyl-2-methyl-1-cyclohexene	11.84
6	Learned Spect 1 Range 8.996 min. Scan: 533 Chan: 1 Ion: 2697 us RIC: 78747 BC	 2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans-	23.18
7	Learned Spect 1 Range 9.442 min. Scan: 556 Chan: 1 Ion: 1466 us RIC: 170270 BC	 (R)-(-)-terpinen-4-ol	15.63
8	Learned Spect 1 Range 9.559 min. Scan: 562 Chan: 1 Ion: 703 us RIC: 493668 BC	 Benzenemethanol, alpha., alpha., 4-trimethyl-	43.59

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
9	Learned Spect 1 Range 9.673 min. Scan: 588 Chan: 1 Ion: 91 us RIC: 3018515 BC	α-Terpineol	19.40
10	Learned Spect 1 Range 10.604 min. Scan: 616 Chan: 1 Ion: 540 us RIC: 594295 BC	3-Cyclohexene-1-one-2-isopropyl-5-methyl-	49.56
11	Learned Spect 1 Range 10.957 min. Scan: 628 Chan: 1 Ion: 2501 us RIC: 53622 BC	2-Cyclohexene-1-one-3-methyl-6-(1-methylethenyl)-, (S)-	38.87
12	Learned Spect 1 Range 10.934 min. Scan: 633 Chan: 1 Ion: 2403 us RIC: 56049 BC	1-Cyclohexene-1-carboxaldehyde, 4(1-methylethyl)-	26.89

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 11.419 min. Scan: 658 Chan: 1 Ion: 98 us RIC: 3075952 BC	 1H-Pyrrole, 1-pentyl-	19.40
14	Learned Spect 1 Range 11.782 min. Scan: 677 Chan: 1 Ion: 748 us RIC: 448769 BC	 4-Terpinenol	24.52
15	Learned Spect 1 Range 12.711 min. Scan: 725 Chan: 1 Ion: 142 us RIC: 2352348 BC	 Vanillin	23.62
16	Learned Spect 1 Range 13.391 min. Scan: 760 Chan: 1 Ion: 2306 us RIC: 85355 BC	 Eugenol	20.35

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 13.510 min. Scan: 766 Chan: 1 Ion: 1543 us RIC: 144700 BC	 Phenol,2-methoxy-4-propyl-	61.11
18	Learned Spect 1 Range 13.766 min. Scan: 779 Chan: 1 Ion: 1768 us RIC: 112110 BC	 4-Hydroxybenzylideneacetone	19.40
19	Learned Spect 1 Range 13.883 min. Scan: 784 Chan: 1 Ion: 1402 us RIC: 184124 BC	 Ethanone,1-(4-hydroxy-3-methoxyphenyl)-	38.87
20	Learned Spect 1 Range 14.166 min. Scan: 801 Chan: 1 Ion: 2978 us RIC: 43347 BC	 2,4-di-tert-butylphenol	22.43

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
21	Learned Spect 1 Range 14.800 min. Scan: 832 Chan: 1 Ion: 1503 us RIC: 123498 BC	 Phenol, 2-ethoxy-5-[1-propenyl]-	14.69
22	Learned Spect 1 Range 15.152 min. Scan: 850 Chan: 1 Ion: 788 us RIC: 393170 BC	 1-Propanone, 3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-	19.40
23	Learned Spect 1 Range 15.886 min. Scan: 877 Chan: 1 Ion: 1380 us RIC: 98953 BC	 Benzophenone	66.56
24	Learned Spect 1 Range 16.743 min. Scan: 880 Chan: 1 Ion: 1980 us RIC: 41624 BC	 Cubenol	24.25

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
25	Learned Spect 1 Range 16.404 min. Scan: 914 Chan: 1 Ion: 547 us RIC: 656737 BC	 Methyl-(2-hydroxy-3-ethoxy-benzyl)ether	60.98
26	Learned Spect 1 Range 16.976 min. Scan: 944 Chan: 1 Ion: 210 us RIC: 1494910 BC	 4-Hydroxy-2-methoxycinnamaldehyde	73.02
27	Learned Spect 1 Range 17.318 min. Scan: 962 Chan: 1 Ion: 380 us RIC: 777686 BC	 Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-	47.66
28	Learned Spect 1 Range 16.359 min. Scan: 1016 Chan: 1 Ion: 1761 us RIC: 50215 BC	 1,2-Benzenedicarboxylic acid, diheptyl ester	12.60

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
29	Learned Spect 1 Range 18.949 min. Scan: 1048 Chan: 1 Ion: 1095 us RIC: 251776 BC	 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	56.03
30	Learned Spect 1 Range 19.047 min. Scan: 1051 Chan: 1 Ion: 1949 us RIC: 51058 BC	 2-(2,5-Dimethoxyphenyl)cyclohex-2-enone	54.64
31	Learned Spect 1 Range 19.169 min. Scan: 1057 Chan: 1 Ion: 2420 us RIC: 47149 BC	 Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	90.81
32	Learned Spect 1 Range 19.302 min. Scan: 1067 Chan: 1 Ion: 1496 us RIC: 117644 BC	 Dibutyl phthalate	28.69