

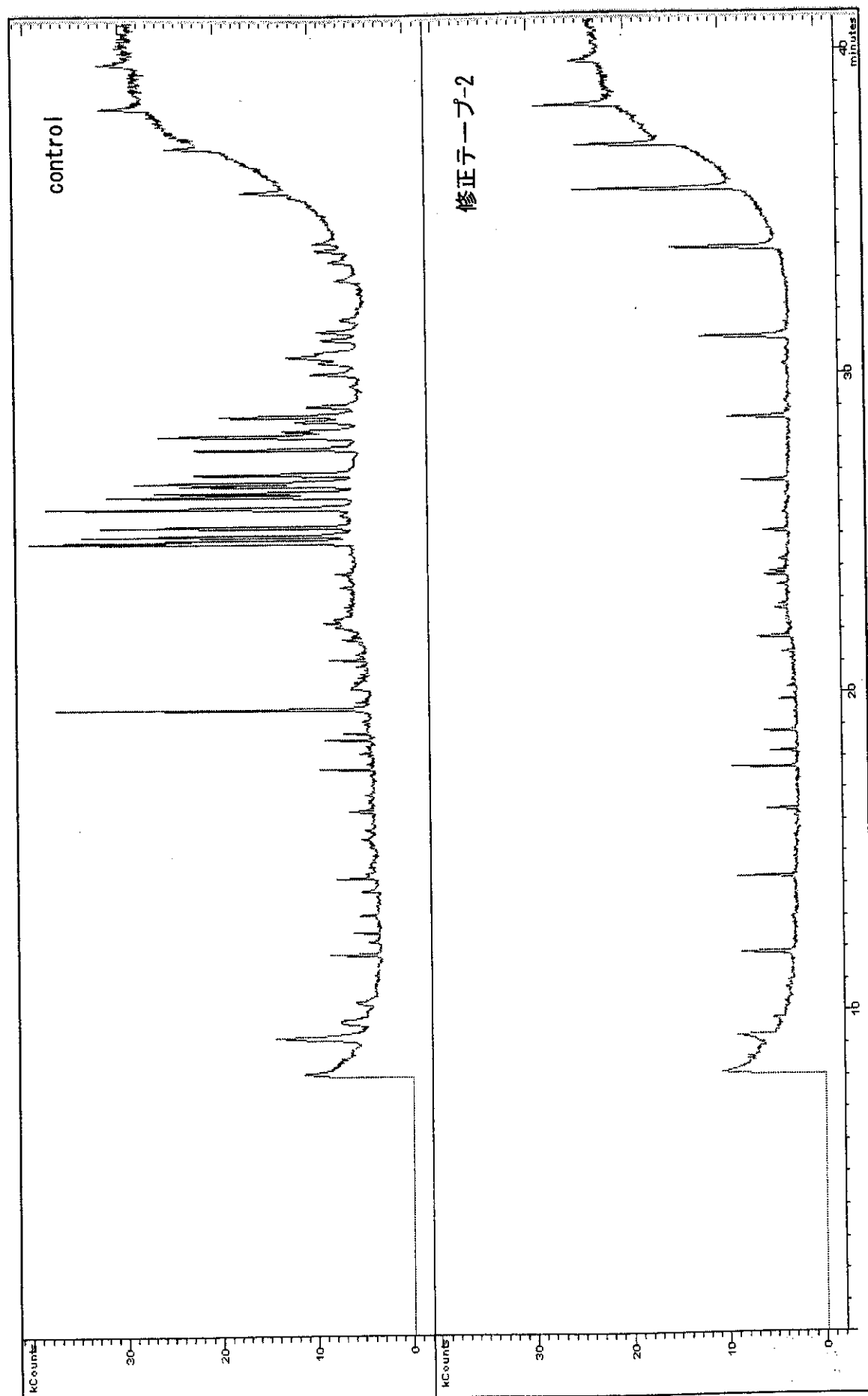
熱湯抽出した修正テープ-1(Sample No.8)から検出された有機化学物質のマススペクトルと構造式

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 14.901 min. Scan: 868 Chan: 1 Ion: 24563 us RIC: 4040 BC	 1,6-Dioxacyclododecane-7,12-dione	47.66
2	Learned Spect 1 Range 15.506 min. Scan: 891 Chan: 1 Ion: 23729 us RIC: 3829 BC	 Diethyl Phthalate	72.79
3	Learned Spect 1 Range 16.036 min. Scan: 920 Chan: 1 Ion: 22721 us RIC: 4004 BC	 Decanamide, n-pentyl-	14.69
4	Learned Spect 1 Range 16.326 min. Scan: 936 Chan: 1 Ion: 23703 us RIC: 4659 BC	 Phenacyl thiocyanate	19.40

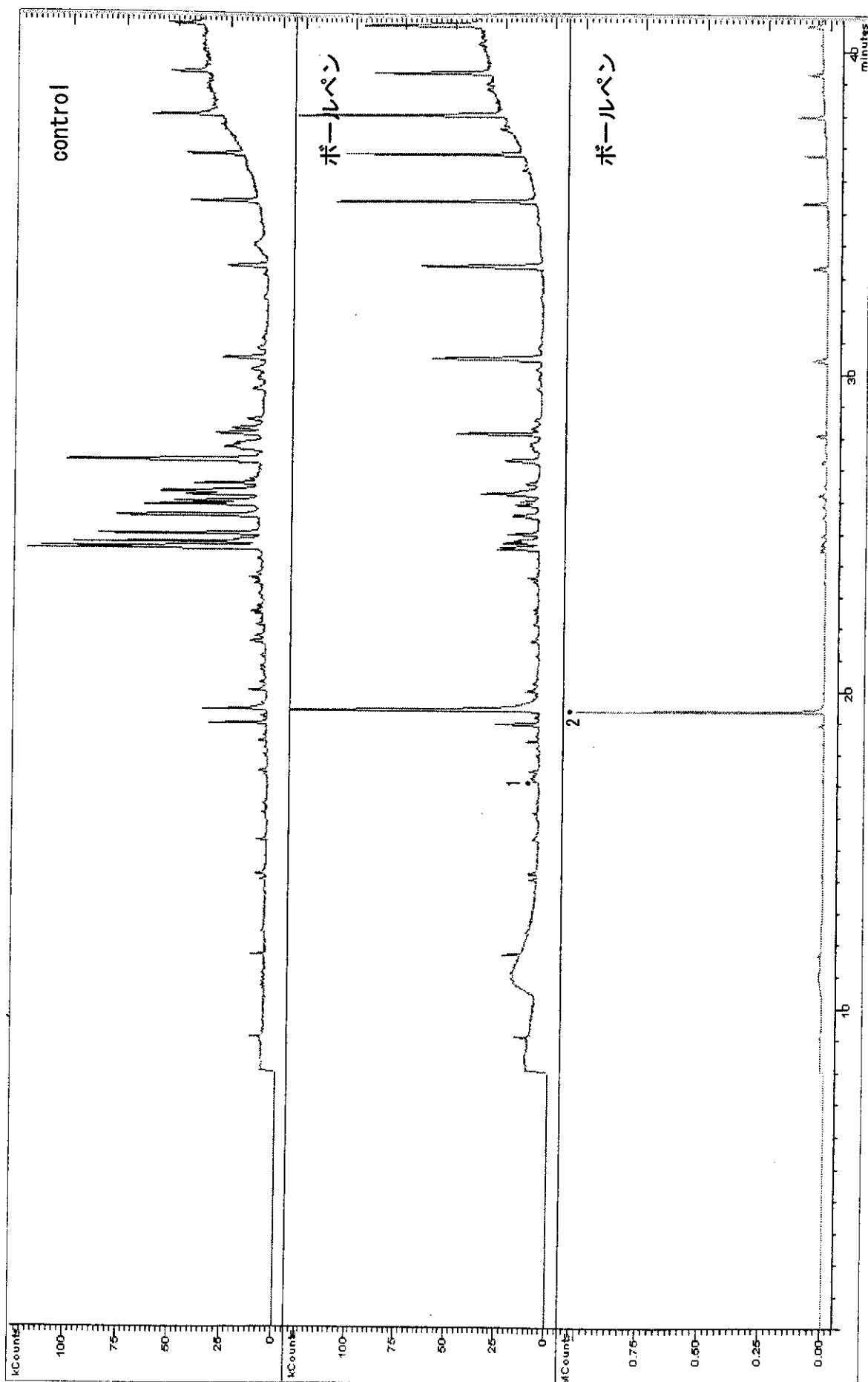
No.	マススペクトル	フラグメンテーションがよく一致した化合物の構造式と化合物名	prb
5	Learned Spect 1 Range 17.061 min. Scan: 976 Chan: 1 Ion: 18402 us RIC: 7220 BC	 Benzene, 1,1'-(2-butene-1,4-diyl)bis-	21.66
6	Learned Spect 1 Range 17.429 min. Scan: 996 Chan: 1 Ion: 21558 us RIC: 4178 BC	 Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, trans-	24.25
7	Learned Spect 1 Range 18.341 min. Scan: 1046 Chan: 1 Ion: 25000 us RIC: 1713 BC	 2-Vinylbenzophenone	19.40
8	Learned Spect 1 Range 18.562 min. Scan: 1058 Chan: 1 Ion: 23865 us RIC: 3367 BC	 Benzamide, N-(2'-iodophenyl)-N-methyl-	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
9	Learned Spect 1 Range 18.856 min. Scan: 1063 Chan: 1 Ion: 16857 us RIC: 10450 BC Mass spectrum for compound 9. The x-axis represents m/z from 0 to 600, and the y-axis represents relative intensity from 0% to 100%. The base peak is at m/z 149. Other significant peaks are labeled at m/z 57, 453, and 564.	Diisobutyl Phthalate	24.62
10	Learned Spect 1 Range 20.086 min. Scan: 1141 Chan: 1 Ion: 24471 us RIC: 3258 BC Mass spectrum for compound 10. The x-axis represents m/z from 0 to 600, and the y-axis represents relative intensity from 0% to 100%. The base peak is at m/z 194. Other significant peaks are labeled at m/z 50, 311, 467, and 644.	2H-1-Benzopyran-2-one, 4-phenyl-	28.57
11	Learned Spect 1 Range 20.825 min. Scan: 1181 Chan: 1 Ion: 21448 us RIC: 7776 BC Mass spectrum for compound 11. The x-axis represents m/z from 0 to 600, and the y-axis represents relative intensity from 0% to 100%. The base peak is at m/z 225. Other significant peaks are labeled at m/z 93, 466, and 605.	Drometrizole	86.47
12	Learned Spect 1 Range 21.667 min. Scan: 1227 Chan: 1 Ion: 17082 us RIC: 10191 BC Mass spectrum for compound 12. The x-axis represents m/z from 0 to 600, and the y-axis represents relative intensity from 0% to 100%. The base peak is at m/z 178. Other significant peaks are labeled at m/z 241, 290, 492, and 642.	2-Ethylhexyl 4-methoxycinnamate	81.60

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
13	Learned Spect 1 Range 24.710 min. Scan: 1392 Chan: 1 Ion: 14044 us RIC: 11760 BC	 Benzoinitrile, m-phenethyl-	10.15
14	Learned Spect 1 Range 26.297 min. Scan: 1477 Chan: 1 Ion: 14736 us RIC: 11465 BC	 Benzene, 1,1'-[2-methyl-2-(phenylthio)cyclopropylidene]bis-	56.54



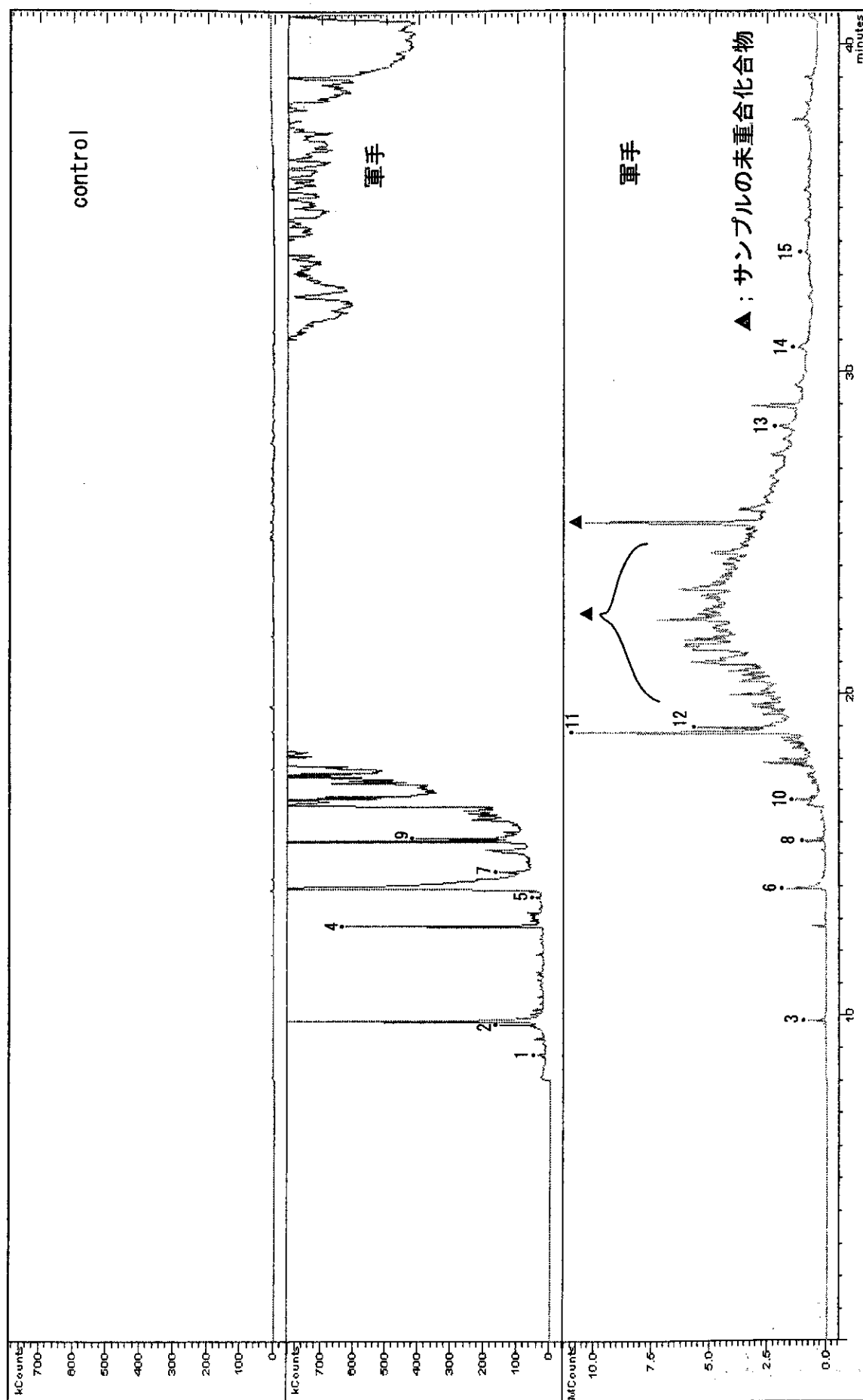
修正テーパー-2 (Sample No. 9) のトータルイオンクロマトグラム (上段はコントロールのクロマトグラム)



ボールペン (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クロマトグラム)

熱湯抽出したボールペン(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 17.107 min. Scan: 966 Chan: 1 Ion: 23056 us RIC: 3484 BC	Diethyl Phthalate	67.97
2	Learned Spect 1 Range 19.350 min. Scan: 1087 Chan: 1 Ion: 319 us RIC: 1016077 B	Dibutyl phthalate	27.73



軍手 (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)

熱湯抽出した軍手(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 9.800 min. Scan: 523 Chan: 1 Ion: 10785 us RIC: 18749 BC	 Hexanoic acid, 2-ethyl-	73.02
2	Learned Spect 1 Range 9.732 min. Scan: 572 Chan: 1 Ion: 4291 us RIC: 118116 BC	 Carbitol acetate	71.07
3	Learned Spect 1 Range 9.849 min. Scan: 578 Chan: 1 Ion: 848 us RIC: 776078 BC	 7-Tetradecene	24.25
4	Learned Spect 1 Range 12.780 min. Scan: 733 Chan: 1 Ion: 843 us RIC: 601109 BC	 1-Heptadecene	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
5	Learned Spect 1 Range 13.675 min. Scan: 780 Chan: 1 Ion: 8253 us RIC: 18884 BC	 Dimethyl phthalate	47.07
6	Learned Spect 1 Range 13.825 min. Scan: 793 Chan: 1 Ion: 288 us RIC: 1882488 BC	 1-Pentadecanol	19.40
7	Learned Spect 1 Range 14.444 min. Scan: 820 Chan: 1 Ion: 3183 us RIC: 71227 BC	 Butylated Hydroxytoluene	24.37
8	Learned Spect 1 Range 15.413 min. Scan: 871 Chan: 1 Ion: 545 us RIC: 841340 BC	 5-Eicosene, (E)-	19.40

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 15.492 min. Scan: 875 Chan: 1 Ion: 1428 us RIC: 323884 BC	 2-Hexyl-1-octanol	21.66
10	Learned Spect 1 Range 15.692 min. Scan: 937 Chan: 1 Ion: 378 us RIC: 1217861 BC	 2-Hexyl-1-octanol	19.40
11	Learned Spect 1 Range 18.784 min. Scan: 1047 Chan: 1 Ion: 57 us RIC: 10539462 BC	 Hexadecane, 1-(ethenylloxy)-	19.40
12	Learned Spect 1 Range 18.953 min. Scan: 1056 Chan: 1 Ion: 87 us RIC: 5277468 BC	 2-Hexyl-1-octanol	19.40

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 28.315 min. Scan: 1555 Chan: 1 Ion: 172 us RIC: 1177510 BC	 Heptyl methyl ethylphosphonate	63.46
14	Learned Spect 1 Range 30.753 min. Scan: 1684 Chan: 1 Ion: 402 us RIC: 521121 BC	 t-Butyl-diphenyl-silanol	24.25
15	Learned Spect 1 Range 33.664 min. Scan: 1837 Chan: 1 Ion: 477 us RIC: 248339 BC	 Cyclohexane,1,3,5-trimethyl-2-octadecyl-	51.72