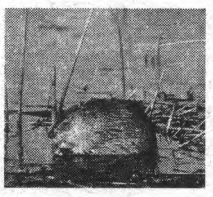
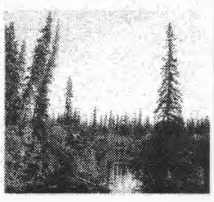
Canada Alberta Northwest Territories

Northern River Basins Study



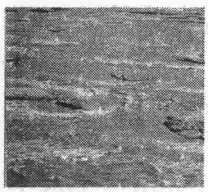



NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 111

BROAD SPECTRUM ANALYSIS OF MUNICIPAL AND INDUSTRIAL EFFLUENTS DISCHARGED INTO THE PEACE, ATHABASCA AND SLAVE RIVER BASINS: REVIEW OF GC-MS DATA, 1989 TO 1994 - VOLUME 3 OF 3






Prepared for the
Northern River Basins Study
under Project 2921-D1

by

C. Ian Johnson
Alberta Environmental Centre

NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 111

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PREFACE:

The Northern River Basins Study was initiated through the "Canada-Alberta-Northwest Territories Agreement Respecting the Peace-Athabasca-Slave River Basin Study, Phase II - Technical Studies" which was signed September 27, 1991. The purpose of the Study is to understand and characterize the cumulative effects of development on the water and aquatic environment of the Study Area by coordinating with existing programs and undertaking appropriate new technical studies.

This publication reports the method and findings of particular work conducted as part of the Northern River Basins Study. As such, the work was governed by a specific terms of reference and is expected to contribute information about the Study Area within the context of the overall study as described by the Study Final Report. This report has been reviewed by the Study Science Advisory Committee in regards to scientific content and has been approved by the Study Board of Directors for public release.

It is explicit in the objectives of the Study to report the results of technical work regularly to the public. This objective is served by distributing project reports to an extensive network of libraries, agencies, organizations and interested individuals and by granting universal permission to reproduce the material.

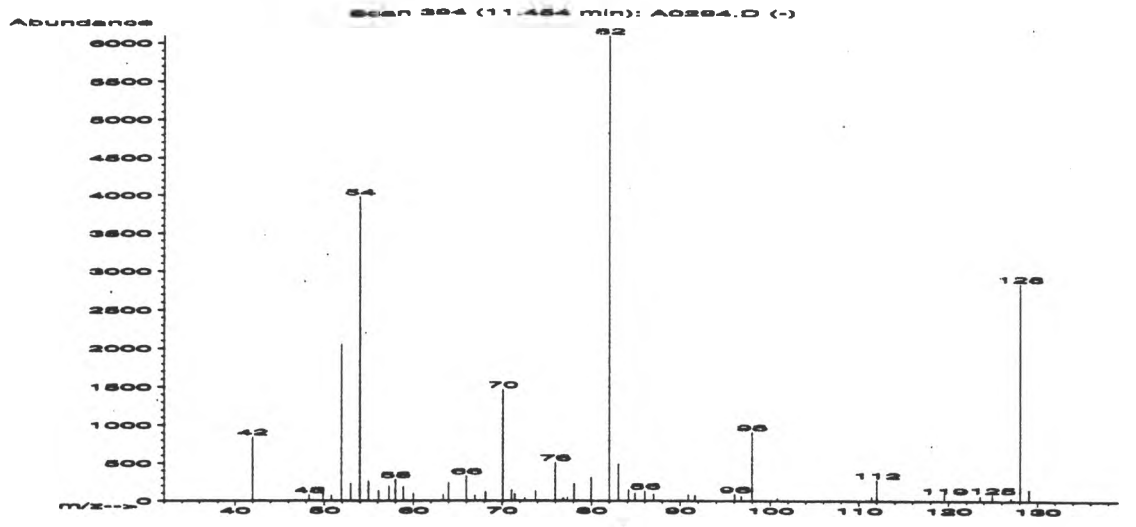
This report contains referenced data obtained from sources external to the Northern River Basins Study. Individuals interested in using external data must obtain permission to do so from the donor agency.

APPENDIX 3

MASS SPECTRAL DATA OF COMPOUNDS IN MUNICIPAL SEWAGE TREATMENT PLANT EFFLUENTS

STP Compounds

Standard 1 Nitrobenzene d5



Scan 394 (11.454 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	843	58.90	184	73.80	132	90.90	81
48.30	79	60.00	99	75.95	505	91.65	74
49.85	175	63.40	86	76.85	37	96.05	88
50.80	71	64.00	238	78.05	228	96.80	60
51.95	2049	66.00	330	79.95	314	97.95	908
52.95	228	66.95	72	82.00	6094	100.80	43
53.95	3976	68.15	121	83.00	488	111.40	53
54.95	259	70.05	1463	84.15	149	112.00	280
56.10	136	71.05	145	84.90	107	119.55	78
57.25	196	71.45	90	86.00	130	123.55	64
58.00	283	72.55	37	87.00	88	124.95	83

Scan 394 (11.454 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	41						
128.05	2854						
129.05	149						

STP Compounds

Scan 394 (11.454 min): A0294.D

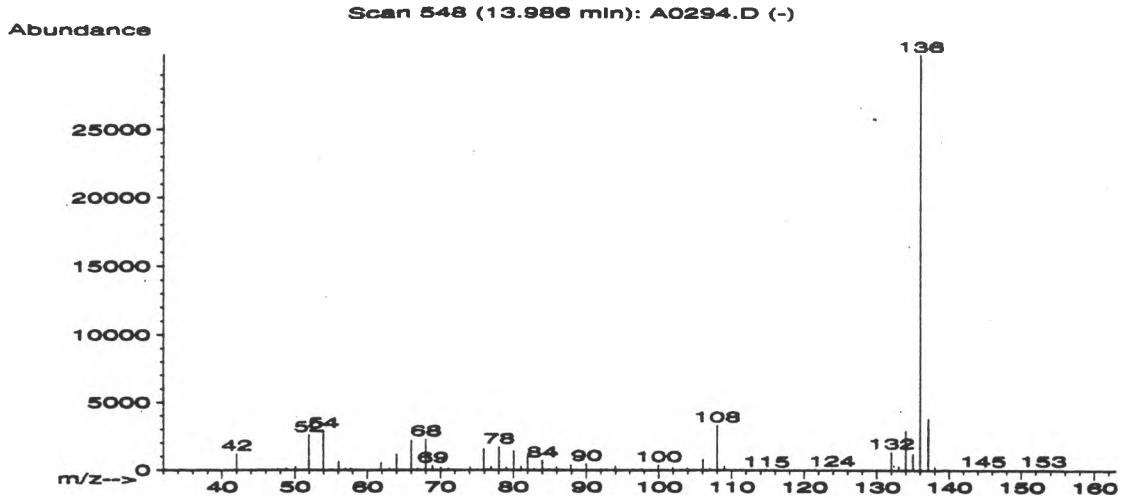
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Cyclopenten-1-one	82	C5H6O	53
2.	Nitrobenzene-d5	123	C6D5NO2	47
3.	1,3-Isobenzofurandione, hexahydro-	154	C8H10O3	36
4.	1H-Pyrazole, 3-methyl-	82	C4H6N2	25
5.	Isoxazole, 3,5-dimethyl-	97	C5H7NO	25
6.	2-Hexyne	82	C6H10	14
7.	1H-Imidazole, 2-methyl-	82	C4H6N2	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	000930-30-3	116755	37	65	1	89	29	28	0	39	9059
2.	*47	000000-00-0	4529	35	61	1	67	39	20	0	41	9854
3.	36	000085-42-7	124143	42	51	2	83	28	12	0	29	9116
4.	*25	001453-58-3	116740	28	62	3	99	55	7	0	33	8752
5.	25	000300-87-8	117634	38	63	2	70	53	7	0	33	8839
6.	*14	000764-35-2	116760	32	56	1	98	66	2	6	39	8780
7.	*12	000693-98-1	116745	28	50	1	68	64	2	0	33	8530

STP Compounds

Standard 2



Scan 548 (13.986 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1212	63.00	146	78.05	1729	92.00	95
47.70	109	64.00	1213	79.05	195	92.75	78
48.80	136	66.00	2202	80.05	1411	93.95	312
50.05	255	66.90	121	81.05	248	96.45	60
51.95	2605	68.00	2303	82.00	1105	97.30	84
53.95	2896	68.95	342	82.90	130	97.80	92
55.05	76	70.05	185	84.00	742	99.95	415
56.05	631	71.10	112	84.90	89	101.95	177
57.00	114	74.05	201	85.95	203	103.30	35
57.75	133	75.95	1558	87.90	373	103.95	134
61.90	553	76.95	264	90.00	482	106.05	830

Scan 548 (13.986 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	109	137.15	3805				
108.00	3312	138.00	252				
109.00	295	144.70	66				
114.75	38	152.95	93				
121.55	39						
123.80	65						
132.00	1379						
133.00	277						
134.00	2906						
135.00	1210						
136.00	30545						

STP Compounds

Scan 548 (13.986 min): A0294.D

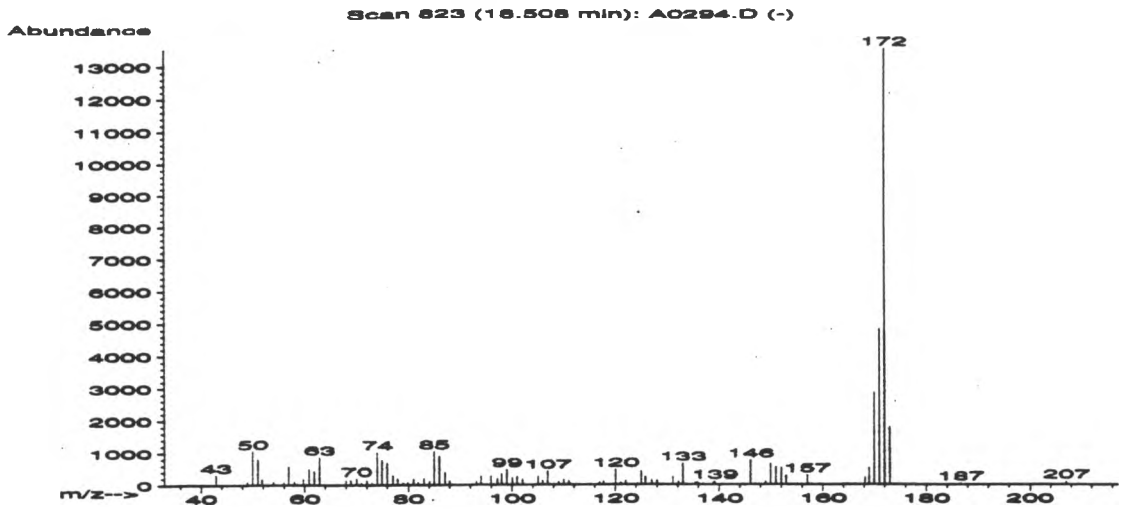
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Naphthalene-d8	128	C10D8	87
2.	Benzamide, 3-amino-	136	C7H8N2O	53
3.	Benzaldehyde, 4-amino-, oxime	136	C7H8N2O	50
4.	Inosine	268	C10H12N4O5	39
5.	2-HYDROXY-3-METHYLBENZALDEHYDE	136	C8H8O2	38
6.	2,1,3-Benzothiadiazole	136	C6H4N2S	36
7.	Pyrazine, tetramethyl-	136	C8H12N2	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000000-00-0	6077	68	25	2	86	8	54	7	58	9917
2.	*53	003544-24-9	7777	38	44	0	84	28	28	5	38	9862
3.	*50	003419-18-9	7780	28	16	1	99	20	25	2	35	9830
4.	39	000058-63-9	62487	36	100	3	98	19	15	0	22	9929
5.	*38	000824-42-0	7825	30	90	2	99	25	14	0	29	7376
6.	*36	000273-13-2	7732	31	58	3	92	28	12	0	29	9842
7.	*36	001124-11-4	121881	28	74	2	92	30	12	0	29	9850

STP Compounds

Standard 3



Scan 823 (18.508 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	312	61.90	417	77.05	287	88.00	122
48.95	87	62.90	856	77.95	187	93.15	97
49.95	1048	68.00	141	79.00	64	94.05	270
50.95	794	68.95	137	79.90	75	95.95	275
51.75	167	70.00	191	81.05	176	97.20	187
53.95	91	70.95	54	81.90	76	97.95	336
55.95	67	72.00	130	83.00	196	98.95	466
56.90	564	73.05	64	84.10	114	100.05	207
58.00	91	74.05	1017	85.00	1039	100.95	257
59.75	180	74.95	770	86.00	891	102.05	163
60.90	481	75.95	696	87.15	380	105.05	265

Scan 823 (18.508 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.95	130	124.20	39	139.15	88	170.95	4839
106.90	418	124.95	410	146.05	757	171.95	13528
109.00	94	125.80	235	148.95	103	172.95	1778
110.00	165	126.95	126	149.95	666	186.65	38
111.00	115	128.05	128	150.95	544	207.00	98
114.95	7	131.05	241	152.05	522		
116.90	78	132.15	91	152.95	275		
117.75	100	133.00	657	157.00	295		
120.05	475	135.40	68	168.15	212		
121.05	59	135.90	72	168.95	509		
122.05	118	138.90	79	169.95	2857		

STP Compounds

Scan 823 (18.508 min): A0294.D

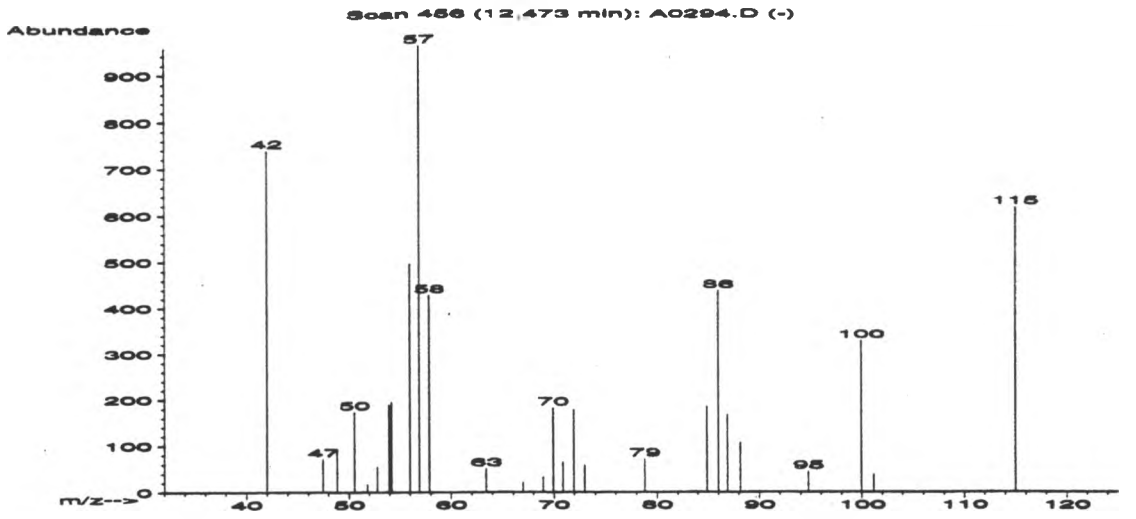
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	96
2.	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	87
3.	4-(2-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	53
4.	4-(4-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	47
5.	2-Propenenitrile, 3-[4-(dimethylamino)ph	172	C11H12N2	37
6.	2-Naphthalenecarboxylic acid	172	C11H8O2	37
7.	1-METHOXY-2-METHYLNAPHTHALENE	172	C12H12O	37
8.	2,2'-BITHIAZOLINE-2	172	C6H8N2S2	36
9.	1-Naphthalenecarboxylic acid	172	C11H8O2	28
10.	2-Naphthalenecarboxylic acid	172	C11H8O2	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000321-60-8	22421	94	6	0	82	12	76	0	96	9809
2.	*87	000324-74-3	22422	74	21	0	84	14	54	0	81	9783
3.	*53	068535-55-7	22263	41	45	1	90	29	28	4	39	9800
4.	*47	023380-78-1	22266	34	87	1	67	37	20	0	39	9366
5.	*37	032444-63-6	22396	28	67	3	99	42	13	0	33	9201
6.	*37	000093-09-4	126214	34	74	2	99	42	13	0	35	9234
7.	*37	000000-00-0	22442	30	55	2	77	43	13	5	34	9197
8.	*36	000000-00-0	21966	30	95	2	99	29	12	0	29	9705
9.	*28	000086-55-5	22387	29	86	3	99	40	8	0	29	9322
10.	*25	000093-09-4	126213	28	79	3	68	43	7	0	29	9197

STP Compounds

Peak 2



Unknown amine
Scan 456 (12.473 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	738	63.40	51	86.90	167		
47.45	71	66.95	22	88.15	106		
48.85	89	68.95	33	94.75	44		
50.55	173	69.95	182	99.95	327		
51.80	17	70.90	65	101.15	38		
52.80	55	71.95	178	115.00	614		
53.95	189	73.00	58				
54.20	195	78.80	71				
56.00	495	83.80	3				
56.90	956	84.90	185				
57.90	428	86.00	436				

STP Compounds

Scan 456 (12.473 min): A0294.D

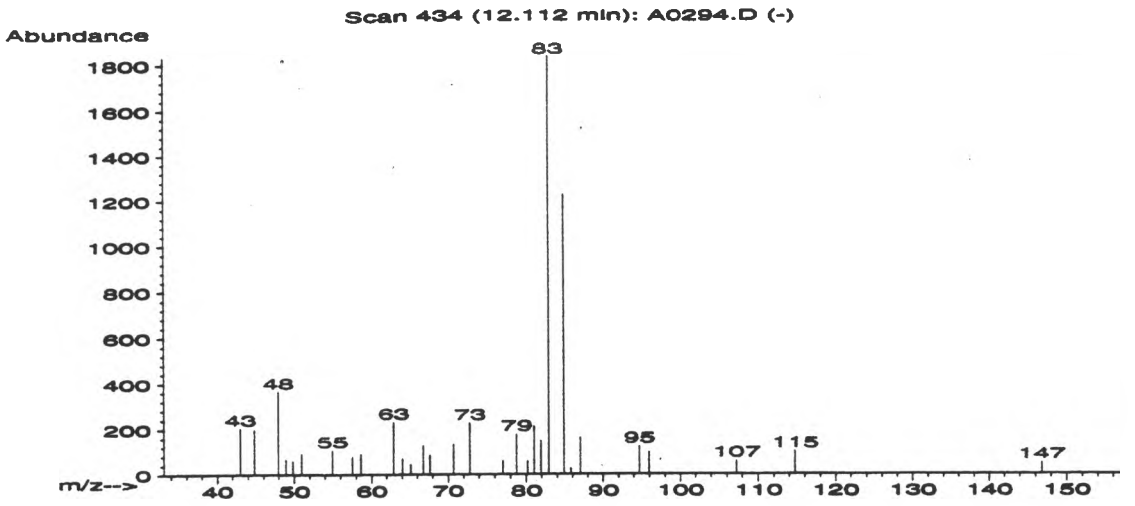
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanamine, N-ethyl-N-[(1-methylethoxy)m	145	C8H19NO	25
2.	3-METHOXY-1,2,4-TRIAZINE (AUTHOR UNSURE	111	C4H5N3O	23
3.	Morpholine, 2,6-dimethyl-	115	C6H13NO	17
4.	Ethanamine, N-(ethoxymethyl)-N-ethyl-	131	C7H17NO	12
5.	1,3-Propanediol, 2,2-bis(hydroxymethyl)-	136	C5H12O4	10
6.	Pentanol, 5-amino-	103	C5H13NO	10
7.	1,3-Propanediol, 2,2-bis(hydroxymethyl)-	136	C5H12O4	10
8.	2H-Pyran, tetrahydro-3-methyl-	100	C6H12O	8
9.	4H-Pyran-4-one, tetrahydro-	100	C5H8O2	8
10.	Oxirane, 2-ethyl-2-methyl-	86	C5H10O	8
11.	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	25	054699-21-7	11028	39	64	1	75	55	7	0	33	7353
2.	23	000000-00-0	2306	34	100	2	78	47	6	0	22	7351
3.*	17	000141-91-3	119409	29	33	1	158	52	3	0	29	7917
4.	12	007352-03-6	6692	33	79	0	54	58	2	0	25	7428
5.	10	000115-77-5	7711	36	75	2	99	61	1	0	22	6478
6.	10	002508-29-4	1539	34	96	1	74	64	1	0	22	6693
7.	10	000115-77-5	121788	34	75	2	99	61	1	0	22	6497
8.*	8	026093-63-0	1222	30	70	1	77	69	1	0	29	6092
9.*	8	029943-42-8	1085	31	64	1	66	67	1	0	29	6317
10.*	8	030095-63-7	90	30	72	1	74	66	1	0	29	6229
11.	7	002461-18-9	53458	37	108	1	71	76	1	0	22	4704

STP Compounds

Peak 1



Scan 434 (12.112 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	204	65.15	44	84.90	1228		
44.80	198	66.75	126	85.80	25		
47.95	365	67.65	85	87.00	161		
48.95	67	70.70	133	94.70	123		
49.85	59	72.80	225	95.95	98		
50.95	92	77.05	60	107.25	59		
54.95	107	78.80	177	114.75	101		
57.50	78	80.20	59	146.80	49		
58.65	91	81.05	209				
62.90	230	81.90	147				
64.05	70	82.90	1831				

STP Compounds

Scan 434 (12.112 min): A0294.D

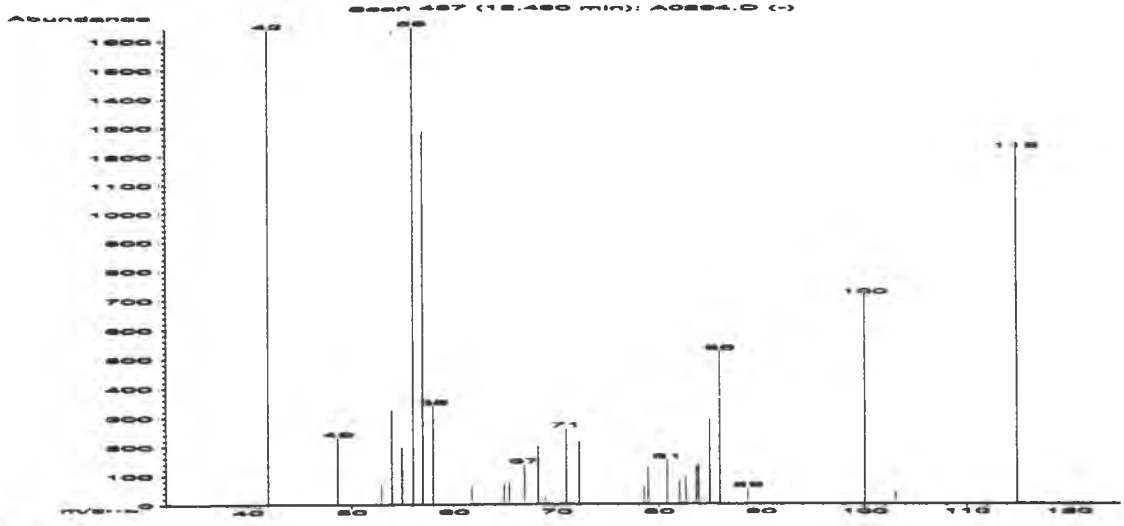
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-BROMO-2,2-DICHLORO-ETHANE	176	C2H3BrCl2	64
2.	Methane, bromodichloro-	162	CHBrCl2	64
3.	Acetyl chloride, dichloro-	146	C2HCl3O	45
4.	Dichloromethyl methyl sulfone	162	C2H4Cl2O2S	45
5.	Hexanoic acid, 2-methyl-3-oxo-, ethyl es	172	C9H16O3	42
6.	Acetic acid, trichloro-	162	C2HCl3O2	38
7.	Chloroform	118	CHCl3	38
8.	Chloroform	118	CHCl3	38
9.	Pyrrolidine, 1-[8-(3-octyloxiranyl)-1-ox	351	C22H41NO2	38
10.	Chloroform	118	CHCl3	38
11.	Acetyl chloride, dichloro-	146	C2HCl3O	36
12.	Ethane, 1,2,2-trichloro-1,1-difluoro-	168	C2HCl3F2	23

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	000000-00-0	23536	59	36	0	84	18	37	3	38	9433
2.	64	000075-27-4	17356	45	43	0	86	18	37	4	41	9912
3.	45	000079-36-7	123056	47	67	2	79	21	19	0	35	9845
4.	45	037557-96-3	17360	47	15	0	98	21	19	12	33	9759
5.	42	029304-40-3	126133	41	53	0	77	28	17	14	35	9815
6.	38	000076-03-9	125014	34	36	1	87	23	14	0	22	9818
7.	38	000067-66-3	119703	39	66	1	92	23	14	0	29	9820
8.	38	000067-66-3	3697	39	66	1	92	23	14	0	29	9820
9.	38	056630-37-6	134973	35	123	1	90	23	14	0	22	9810
10.	38	000067-66-3	119702	39	68	1	85	23	14	0	29	9823
11.	36	000079-36-7	123055	36	75	2	84	26	12	0	21	9828
12.	23	000354-21-2	125678	36	63	0	60	50	6	0	25	9780

STP Compounds

Peak 2; Unidentified Amine



Scan 457 (12.490 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1637	66.90	136	83.90	135		
48.70	229	68.25	198	85.00	291		
52.95	69	68.95	20	86.00	523		
53.95	325	70.95	259	88.75	52		
54.95	197	72.20	216	100.05	716		
56.05	1641	78.55	60	103.05	38		
57.00	1282	78.95	127	115.00	1222		
58.00	338	80.80	150				
61.75	56	82.00	82				
64.90	68	82.65	90				
65.40	76	83.65	132				

STP Compounds

Scan 457 (12.490 min): A0294.D

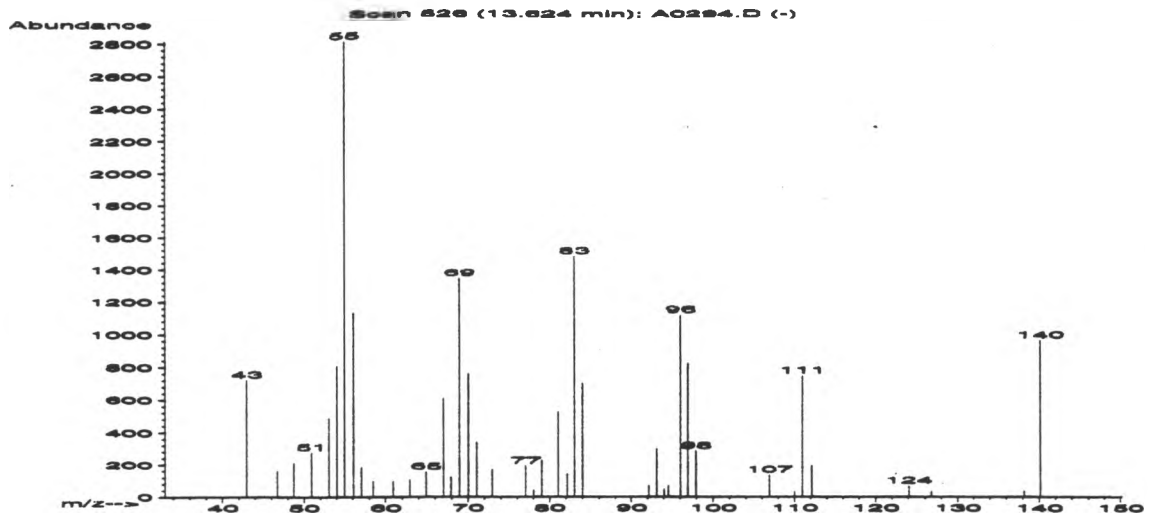
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Propanone, methylhydrazone	86	C4H10N2	38
2.	Hexane	86	C6H14	32
3.	Hexane	86	C6H14	32
4.	Hexane	86	C6H14	32
5.	Ethanol, 2-(diethylamino)-, N-oxide	133	C6H15NO2	28
6.	Hexane	86	C6H14	23
7.	2(3H)-Furanone, dihydro-	86	C4H6O2	16
8.	2H-Pyran-3(4H)-one, dihydro-	100	C5H8O2	12
9.	4H-Pyran-4-one, tetrahydro-	100	C5H8O2	12
10.	2(3H)-Furanone, dihydro-	86	C4H6O2	12
11.	Pentanal, 3-methyl-	100	C6H12O	10
12.	1,6-Hexanediol	118	C6H14O2	10
13.	3,3-Dimethylcyclobutyl methanol	114	C7H14O	8
14.	1,6-Hexanediol	118	C6H14O2	8
15.	1,6-Hexanediol	118	C6H14O2	8
16.	1,2,3-Cyclopentanetriol	118	C5H10O3	7
17.	HEX-1-ENE-5-IMINE	97	C6H11N	7
18.	Oxirane, 2,3-diethyl-	100	C6H12O	7
19.	1,6-Hexanediol	118	C6H14O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	005771-02-8	42	34	59	2	85	48	14	18	38	6626
2.	*32	000110-54-3	117108	29	71	3	223	47	9	0	33	8434
3.	*32	000110-54-3	105	38	51	1	216	47	9	0	35	8399
4.	*32	000110-54-3	117114	29	63	2	208	47	9	0	33	8448
5.	28	016684-49-4	7089	33	89	3	151	37	8	0	22	8043
6.	*23	000110-54-3	117110	29	68	1	181	48	6	0	29	8440
7.	*16	000096-48-0	117002	28	47	0	84	58	3	2	35	7569
8.	*12	023462-75-1	117951	29	36	0	94	65	2	2	35	6320
9.	*12	029943-42-8	1085	31	64	0	67	61	2	0	33	6438
10.	*12	000096-48-0	27	29	68	0	97	63	2	0	33	7624
11.	10	015877-57-3	1132	38	48	0	99	67	1	0	33	6494
12.	10	000629-11-8	119767	43	76	2	92	69	1	0	37	6849
13.	8	075017-17-3	3165	36	58	1	99	70	1	0	22	6297
14.	8	000629-11-8	119765	36	80	3	99	69	1	0	22	6747
15.	8	000629-11-8	3818	35	80	3	107	69	1	0	22	6723
16.	7	056772-27-1	3786	37	76	1	75	80	1	0	21	3644
17.	7	000000-00-0	688	34	71	1	76	77	1	0	22	5779
18.	7	004468-66-0	1202	33	58	3	169	75	1	0	22	3590
19.	7	000629-11-8	119766	41	75	3	100	72	1	0	29	5868

STP Compounds

Peak 3



Scan 526 (13.624 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	720	62.95	107	81.05	525	106.90	136
46.70	160	64.90	155	82.15	141	110.00	33
48.70	211	67.00	609	83.00	1483	111.00	747
50.90	275	67.95	124	84.00	704	112.15	192
53.05	485	68.95	1344	92.15	69	124.05	68
54.05	807	70.05	760	93.15	300	126.80	36
54.95	2812	71.05	338	94.05	46	138.15	37
56.05	1130	72.95	169	94.55	69	140.15	967
57.00	182	77.05	190	96.05	1118		
58.50	95	78.05	41	96.95	823		
60.90	96	79.05	226	97.95	284		

STP Compounds

Scan 526 (13.624 min): A0294.D

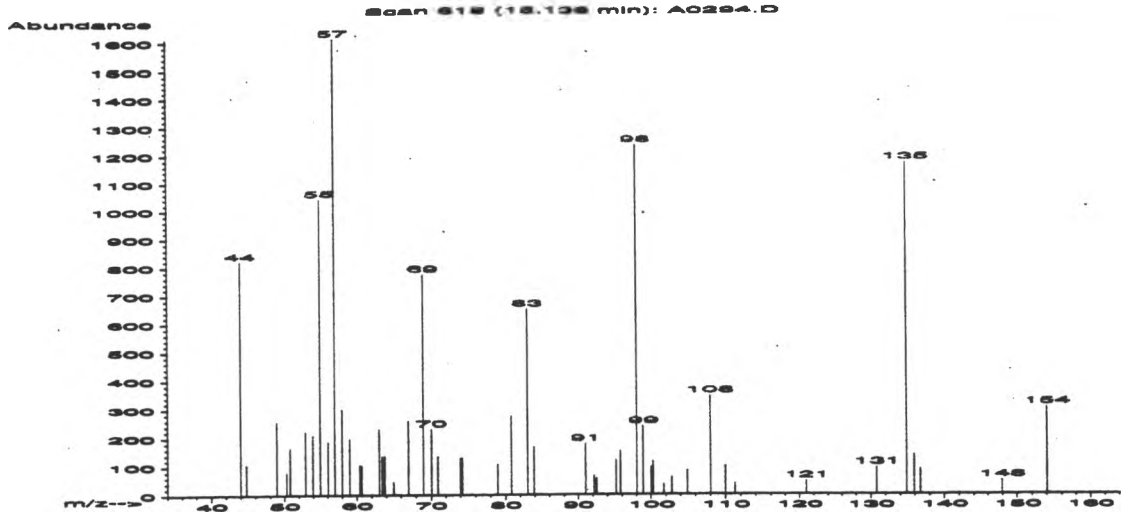
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 2-ethyl-	126	C8H14O	40
2.	Silane, trichloroeicosyl-	414	C20H41Cl3Si	38
3.	Cyclopentane, 1-methyl 3-(2-methylpropyl	140	C10H20	38
4.	Cyclotetradecane	196	C14H28	38
5.	3-Octene, 4-ethyl-	140	C10H20	38
6.	Cyclododecane	168	C12H24	37
7.	1-Dodecene	168	C12H24	37
8.	2-Decene, 7-methyl-, (Z)-	154	C11H22	35
9.	CYCLOPENTANE, 1-ETHYL-2-METHYL-	112	C8H16	35
10.	Cyclopentane, 1-ethyl-2-methyl-, cis-	112	C8H16	35
11.	Phosphonic acid, dioctadecyl ester	587	C36H75O3P	32
12.	2-Octene, 4-ethyl-	140	C10H20	32
13.	Cyclopropane, 1,1,2-trimethyl-3-(2-methy	140	C10H20	27
14.	4-UNDECENE, 6-METHYL-, CIS/TRANS	168	C12H24	27
15.	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	27
16.	2-Heptenal, (E)-	112	C7H12O	27
17.	2-Heptenal, (Z)-	112	C7H12O	25
18.	Cyclopentane, propyl-	112	C8H16	22
19.	5-Decene, (E)-	140	C10H20	22
20.	1-Hexene, 3-methyl-	98	C7H14	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	40	004423-94-3	120601	55	62	3	93	34	16	0	36	5728
2.	38	018733-57-8	99977	57	101	3	120	38	14	0	36	8630
3.	38	029053-04-1	9497	45	61	2	82	38	14	8	37	8529
4.	38	000295-17-0	33202	47	87	2	61	38	14	0	37	8492
5.	*38	053966-51-1	9466	35	74	2	181	48	14	0	39	7252
6.	37	000294-62-2	125808	46	64	1	41	44	13	0	35	8707
7.	37	000112-41-4	125792	48	67	0	52	45	13	14	36	7752
8.	35	074630-23-2	14810	55	36	0	49	54	11	5	40	6618
9.	*35	000930-89-2	2707	37	71	1	55	53	11	0	39	7557
10.	*35	000930-89-2	2706	34	62	1	45	53	11	0	39	7576
11.	32	019047-85-9	112020	43	124	2	42	48	9	0	35	8641
12.	*32	053966-52-2	122506	33	68	3	254	50	9	0	35	8238
13.	*27	041977-43-9	9488	44	52	0	77	56	8	22	40	7585
14.	27	000000-00-0	20709	45	46	1	99	59	8	0	39	6978
15.	*27	062960-76-3	9469	34	67	3	240	56	8	0	39	7720
16.	*27	018829-55-5	2535	33	72	0	49	56	8	0	41	7379
17.	*25	057266-86-1	2534	35	75	1	79	54	7	0	35	7401
18.	*22	002040-96-2	2703	37	61	0	47	64	5	0	41	7107
19.	*22	007433-56-9	9540	38	60	3	254	62	5	0	39	6958
20.	*14	003404-61-3	117786	42	55	0	54	69	2	0	39	5537

STP Compounds

Peak 4 Coeluting conpounds



Scan 618 (15.136 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	820	59.00	196	73.95	130	98.05	1232
44.80	106	60.40	106	74.20	130	98.95	238
48.95	256	60.65	102	78.95	108	100.05	96
50.30	78	63.00	230	80.80	275	100.30	117
50.80	164	63.40	135	83.00	652	101.70	35
52.95	222	63.75	137	83.90	168	102.80	60
53.95	209	65.00	45	91.00	178	104.95	84
54.95	1043	67.00	258	92.15	67	108.00	345
56.05	185	68.95	774	92.50	57	110.00	101
57.00	1611	70.05	229	95.20	122	111.25	39
58.00	300	70.95	135	95.80	152	120.95	46

Scan 618 (15.136 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.80	94						
134.90	1170						
135.90	139						
136.75	89						
147.95	49						
154.05	304						

STP Compounds

Scan 617 (15.120 min): A0294.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzisothiazole	135	C7H5NS	47
2.	Benzothiazole	135	C7H5NS	47
3.	Benzothiazole	135	C7H5NS	47
4.	Adenine	135	C5H5N5	38
5.	Adenine	135	C5H5N5	38
6.	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	37
7.	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	35
8.	1,2-Benzisothiazole	135	C7H5NS	35
9.	Adenine	135	C5H5N5	35
10.	Adenine	135	C5H5N5	35
11.	Adenine	135	C5H5N5	35
12.	Adenine	135	C5H5N5	35
13.	Benzaldehyde, O-methyloxime	135	C8H9NO	27
14.	1,2-Benzisothiazole-3-carboxylic acid	179	C8H5NO2S	25
15.	1H-Pyrazolo[4,3-d]pyrimidin-7-amine	135	C5H5N5	25
16.	Benzothiazole	135	C7H5NS	25
17.	Benzothiazole	135	C7H5NS	25
18.	Benzothiazole	135	C7H5NS	25
19.	N-(1,3-Butadiynyl)morpholine	135	C8H9NO	22
20.	3H-Pyrazolo[3,4-c]pyridin-3-one, 1,2-dih	135	C6H5N3O	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	000272-16-2	121700	48	48	2	67	39	20	0	39	7230
2.	*47	000095-16-9	121694	61	36	2	74	39	20	6	39	7238
3.	*47	000095-16-9	121696	50	50	2	76	39	20	6	39	7228
4.	*38	000073-24-5	121688	37	55	0	56	53	14	10	43	7212
5.	*38	000073-24-5	121685	47	53	0	61	55	14	0	44	7209
6.	*37	000459-22-3	7539	35	75	1	79	44	13	0	35	7068
7.	*35	002380-63-4	7511	33	47	0	79	55	11	0	41	7192
8.	*35	000272-16-2	7531	40	51	1	79	54	11	0	39	7222
9.	*35	000073-24-5	121690	51	44	0	79	55	11	8	41	7185
10.	*35	000073-24-5	121689	46	48	0	68	55	11	6	39	7201
11.	*35	000073-24-5	121686	37	56	0	65	55	11	6	39	7179
12.	*35	000073-24-5	7506	47	48	0	78	55	11	6	39	7194
13.	*27	003376-32-7	7567	33	84	1	77	56	8	0	39	7174
14.	25	040991-34-2	25013	39	59	1	79	54	7	0	33	7230
15.	*25	013877-56-0	7505	43	49	0	69	62	7	0	44	7037
16.	*25	000095-16-9	121699	30	62	0	66	53	7	0	33	7257
17.	*25	000095-16-9	121695	31	37	0	59	53	7	2	35	7189
18.	*25	000095-16-9	121698	31	67	0	57	53	7	0	33	7266
19.	*22	080487-52-1	7545	44	63	2	59	62	5	0	39	6951
20.	*12	053975-70-5	7517	39	60	1	67	64	2	0	35	6893

STP Compounds

Scan 618 (15.136 min): A0294.D

PBM Search of library F:\LIBRARY.L

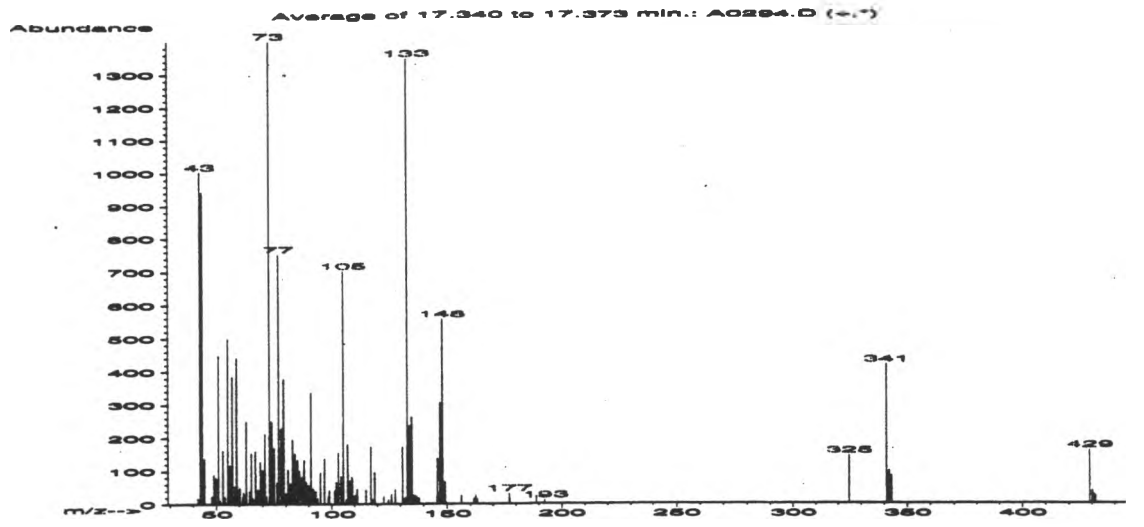
	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 4-(1,1-dimethylethyl)-	154	C10H18O	38
2.	Cyclohexanone, 4-(1,1-dimethylethyl)-	154	C10H18O	35
3.	Cycloheptane	98	C7H14	35
4.	Cycloheptane	98	C7H14	35
5.	4-Hexen-2-one	98	C6H10O	32
6.	3-n-Butylcyclohexanone	154	C10H18O	27
7.	1H-Imidazole-2-methanol	98	C4H6N2O	22
8.	2-Pentenal, 2-methyl-	98	C6H10O	22
9.	2-Pentenal, 2-methyl-	98	C6H10O	22
10.	Benzothiazole	135	C7H5NS	15
11.	2-Pentene, 2,3-dimethyl-	98	C7H14	14
12.	2(3H)-Furanone, dihydro-3-methylene-	98	C5H6O2	14
13.	Adenine	135	C5H5N5	11
14.	Adenine	135	C5H5N5	11
15.	Ethanamine, 1-(2,4-cyclopentadien-1-ylid	135	C9H13N	10
16.	Benzothiazole	135	C7H5NS	10
17.	Adenine	135	C5H5N5	10
18.	Benzothiazole	135	C7H5NS	10
19.	Benzothiazole	135	C7H5NS	10
20.	Benzothiazole	135	C7H5NS	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000098-53-3	124265	43	60	0	91	55	14	0	44	6837
2.	*35	000098-53-3	124264	37	61	0	95	55	11	0	41	6741
3.	*35	000291-64-5	117822	37	82	3	90	53	11	0	39	6697
4.	*35	000291-64-5	945	36	80	3	84	53	11	0	39	6683
5.	*32	025659-22-7	117717	38	58	2	115	47	9	0	35	7594
6.	*27	000936-99-2	14678	39	40	0	83	59	8	0	39	6722
7.	*22	003724-26-3	733	39	65	0	76	61	5	0	39	6472
8.	*22	000623-36-9	117704	36	56	0	119	64	5	0	41	6558
9.	*22	000623-36-9	778	34	53	0	127	62	5	0	41	6570
10.	*15	000095-16-9	121696	67	39	0	65	77	2	20	53	5823
11.	*14	010574-37-5	117802	36	60	3	168	68	2	0	39	5314
12.	*14	000547-65-9	746	33	68	0	73	66	2	0	41	5966
13.	*11	000073-24-5	7506	43	48	0	59	77	2	0	44	5813
14.	*11	000073-24-5	121689	43	47	0	72	77	2	0	44	5824
15.	*10	014469-77-3	7590	37	75	1	52	77	1	0	39	5796
16.	*10	000095-16-9	121699	36	56	0	53	76	1	0	41	5838
17.	*10	000073-24-5	121686	36	51	0	72	77	1	0	41	5809
18.	*10	000095-16-9	121694	36	55	0	59	77	1	0	41	5814
19.	*10	000095-16-9	121698	36	62	0	57	76	1	0	41	5845
20.	*10	000095-16-9	121695	36	26	0	56	72	1	0	41	5807

STP Compounds

STP Compounds

Peak 5



Average of 17.340 to 17.373 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	19	55.00	499	64.50	39	72.95	1400
43.00	1003	55.95	117	65.10	154	74.00	250
43.95	942	56.95	385	65.65	17	75.00	170
44.90	137	57.90	27	65.90	18	76.20	66
48.05	24	58.15	54	66.95	160	77.00	751
48.80	89	58.95	442	67.15	92	78.00	229
49.80	79	59.90	42	68.15	44	79.00	379
50.90	449	60.25	48	69.00	127	80.05	32
51.70	11	61.50	23	70.00	103	80.95	104
52.85	162	61.90	34	71.05	212	82.00	63
53.80	22	63.05	250	71.80	24	82.95	195
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
83.50	26	93.00	38	106.25	14	122.80	24
83.90	152	93.75	17	106.95	181	124.80	13
85.15	133	95.00	97	107.90	69	126.05	29
85.90	100	96.90	138	108.90	80	127.80	44
87.10	81	98.55	22	110.00	26	131.05	173
88.00	134	98.95	42	110.40	26	132.15	20
88.25	18	101.20	42	111.15	45	133.00	1345
88.95	67	102.00	67	115.00	42	133.95	236
89.90	57	102.95	155	117.15	173	135.00	262
90.95	336	104.00	83	117.90	13	136.00	25
92.00	46	105.05	701	118.85	95	136.25	25
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.65	20	162.40	25	429.05	161		
137.00	22	162.90	14	430.15	37		
137.90	18	176.95	31	430.90	27		
145.70	27	177.30	16	431.40	23		
145.95	138	189.00	23				
146.20	30	192.65	12				
147.00	305	324.85	145				
148.00	556	340.95	419				
149.00	66	341.90	76				
156.15	25	342.15	99				
161.50	16	343.05	83				

STP Compounds

Average of 17.340 to 17.373 min.: A0294.D
Converted from RTE data file: >A0294:

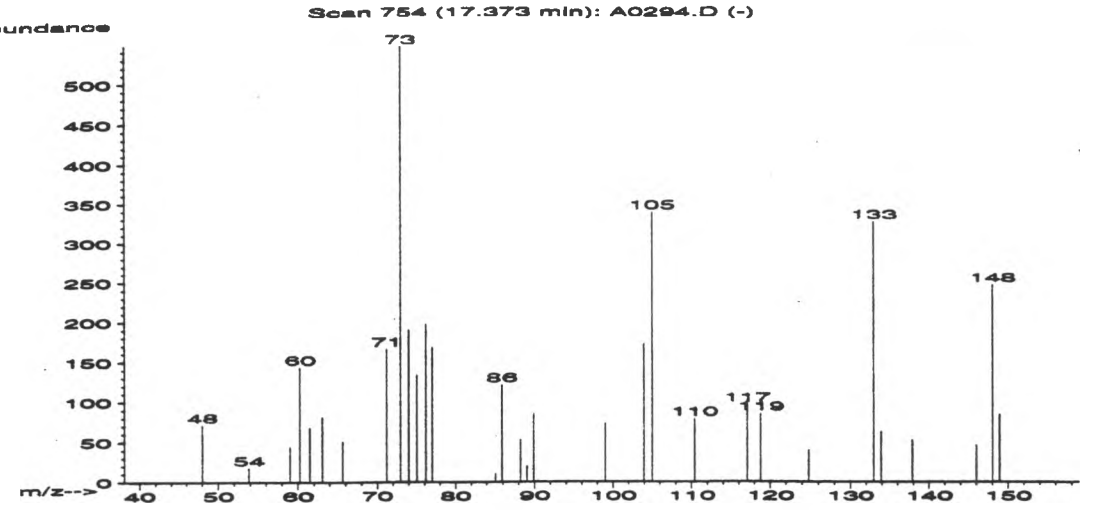
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	55
2.	Ethanone, 1-(2,5-dimethylphenyl)-	148	C10H12O	55
3.	Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	47
4.	Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	46
5.	Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	46
6.	Ethanone, 1-(2,5-dimethylphenyl)-	148	C10H12O	46
7.	Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	46
8.	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	38
9.	Benzene, pentamethyl-	148	C11H16	38
10.	Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	38
11.	Benzene, pentamethyl-	148	C11H16	38
12.	Benzene, pentamethyl-	148	C11H16	38
13.	1-Phenyl-2-buten-1-ol	148	C10H12O	35
14.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	35
15.	Benzene, diethylmethyl-	148	C11H16	35
16.	Benzene, diethylmethyl-	148	C11H16	35
17.	Methanimidamide, N,N-dimethyl-N'-phenyl-	148	C9H12N2	30
18.	6-METHYL-4-INDANOL	148	C10H12O	27
19.	2-PHENYL-2-METHYL-1-D1-AZIRIDINE	133	C9H10DN	25
20.	DIETHYL N-HYDROXYCARBONIMIDATE	133	C5H11NO3	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*55	003637-01-2	123396	81	27	2	77	45	29	25	72	7179
2.	*55	002142-73-6	123395	84	27	1	68	45	29	30	80	7256
3.	*47	003637-01-2	12020	39	16	0	87	38	20	0	39	6509
4.	*46	000089-74-7	12018	59	46	1	66	45	20	12	47	6880
5.	*46	000089-74-7	123394	65	37	1	68	45	20	7	47	6961
6.	*46	002142-73-6	12019	63	44	1	66	45	20	8	47	7173
7.	*46	020944-88-1	12026	69	34	2	81	51	20	30	70	6381
8.	*38	002050-24-0	12119	45	63	1	74	48	14	0	39	6892
9.	*38	000700-12-9	123455	55	41	1	68	50	14	7	40	6606
10.	*38	017851-27-3	12121	48	54	1	64	51	14	6	47	6514
11.	*38	000700-12-9	12123	47	45	1	84	50	14	0	39	6566
12.	*38	000700-12-9	123456	55	38	1	69	50	14	15	42	6548
13.	*35	000000-00-0	12028	51	61	1	46	52	11	0	39	6924
14.	*35	004218-48-8	12115	37	61	2	96	52	11	0	39	6486
15.	*35	025550-13-4	123454	37	61	1	70	51	11	0	39	6529
16.	*35	025550-13-4	12120	36	66	2	83	51	11	0	39	6526
17.	*30	001783-25-1	11981	51	72	2	50	56	9	0	46	5762
18.	*27	020294-32-0	12091	37	65	1	52	58	8	0	39	6833
19.	*25	030691-62-4	7149	51	54	2	65	64	7	0	46	6542
20.	*22	024770-46-5	7085	49	44	0	65	64	5	2	41	8419

STP Compounds

Peak 5a, Unidentified Hydrocarbon (C10H12O



Scan 754 (17.373 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.05	71	76.20	197	110.40	78		
53.85	18	77.00	168	117.10	96		
59.00	44	85.10	11	118.80	85		
60.25	143	85.90	121	124.80	40		
61.50	68	88.25	53	133.00	329		
63.05	81	89.05	20	133.95	63		
65.65	51	89.90	85	137.90	53		
71.20	166	98.95	73	146.00	46		
72.95	548	103.00	1	147.05	1		
74.00	190	103.95	172	148.05	248		
75.05	133	105.00	340	148.95	84		

STP Compounds

Scan 754 (17.373 min): A0294.D

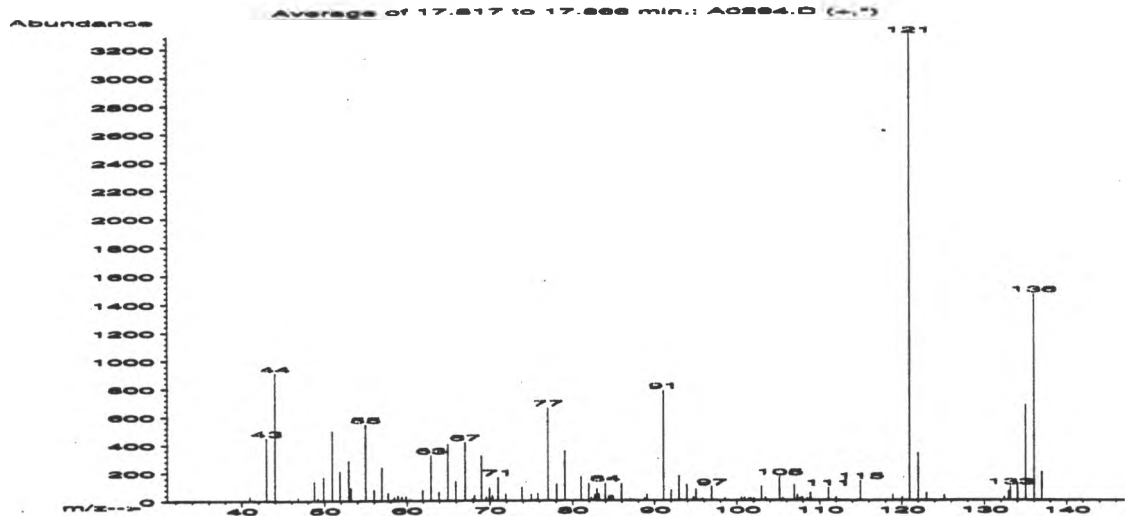
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, (2-methoxy-2-propenyl)-	148	C10H12O	35
2.	ANISOLE, O-ISOPROPENYL-	148	C10H12O	30
3.	Bicyclo[2.2.1]heptane, 7-methylene-2-(1-	148	C11H16	27
4.	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	27
5.	NOPYL ACETATE	208	C13H20O2	23
6.	Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	16
7.	4-CARBOXAMIDONICOTINIC ACID	166	C7H6N2O3	10
8.	Benzene, 1-isocyano-2-methoxy-	133	C8H7NO	10
9.	1H-Indol-4-ol	133	C8H7NO	10
10.	Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	9
11.	Ethanone, 1-(2,5-dimethylphenyl)-	148	C10H12O	9
12.	Silane, diethoxydimethyl-	148	C6H16O2Si	9
13.	2,4,6-Cycloheptatrien-1-one, 4-(1-methyl	148	C10H12O	8
14.	Benzenemethanol, ar-ethenyl-	134	C9H10O	7
15.	1H-Benzotriazole, 1-methyl-	133	C7H7N3	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	026473-60-9	12049	38	77	0	56	53	11	9	38	4594
2.	*30	000000-00-0	12036	34	74	0	56	59	9	2	43	5430
3.	*27	066929-97-3	12140	42	56	0	60	59	8	1	40	5387
4.	*27	000122-03-2	12002	41	58	0	57	59	8	0	39	5433
5.	23	000000-00-0	38581	41	79	1	220	50	6	0	29	5854
6.	*16	020944-88-1	12026	32	72	0	60	59	3	0	33	5431
7.	10	024202-75-3	19166	33	16	0	56	64	1	1	26	3411
8.	*10	020771-60-2	7116	33	85	1	55	69	1	0	35	5129
9.	*10	002380-94-1	7131	32	72	0	59	69	1	0	33	4998
10.	* 9	003637-01-2	123396	39	64	1	96	76	1	1	34	5250
11.	* 9	002142-73-6	123395	35	69	1	90	76	1	12	37	5306
12.	9	000078-62-6	123332	38	69	0	58	79	1	2	35	4657
13.	* 8	013656-81-0	12051	28	79	1	152	66	1	0	29	4431
14.	7	030584-69-1	7395	33	83	1	61	80	1	0	21	4288
15.	* 7	013351-73-0	7106	31	76	1	60	75	1	0	27	4716

STP Compounds

Peak 6



Average of 17.817 to 17.866 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.00	32	55.00	543	62.95	323	70.95	164
43.00	447	56.00	77	63.90	62	71.85	47
44.00	911	56.95	238	65.00	403	73.85	93
46.80	23	57.75	55	65.95	138	74.95	46
48.75	137	58.25	9	67.05	416	75.80	52
49.20	19	58.50	26	67.90	14	77.00	659
49.90	166	58.90	35	68.15	36	78.05	119
50.95	500	59.40	27	69.00	319	79.05	353
51.90	210	59.90	29	69.55	26	81.00	168
52.95	286	60.40	10	69.95	90	81.95	118
53.20	89	61.95	76	70.30	33	82.25	18
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
82.65	38	91.10	780	101.45	13	108.50	15
82.95	82	92.00	74	101.70	14	108.90	56
83.15	43	92.95	174	102.05	15	111.05	90
83.95	124	93.90	111	103.00	100	112.00	24
84.40	30	94.70	24	103.45	20	115.00	139
84.65	35	95.00	80	105.15	167	118.90	41
84.90	30	95.80	15	105.55	14	120.05	24
85.95	118	96.90	95	106.95	111	120.95	3292
87.00	11	98.55	16	107.35	39	122.00	338
88.75	19	100.55	20	107.65	13	123.05	52
89.05	43	100.95	20	107.90	23	125.20	36
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.40	26						
132.90	67						
133.15	98						
134.00	118						
135.00	680						
136.00	1465						
136.95	200						

STP Compounds

Average of 17.817 to 17.866 min.: A0294.D
Converted from RTE data file: >A0294:

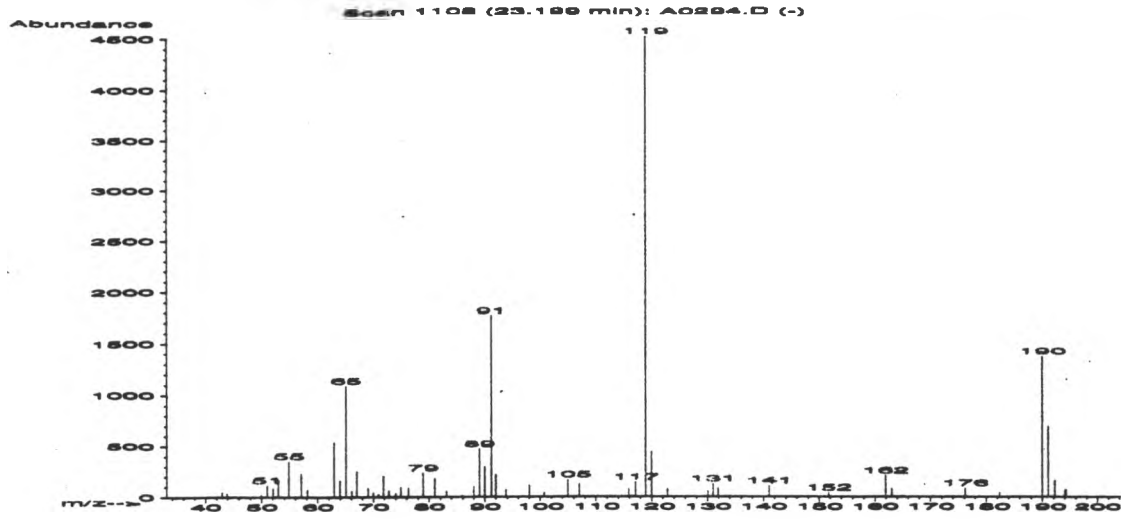
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 3-(1-methylethyl)-	136	C9H12O	89
2.	Phenol, 3,4,5-trimethyl-	136	C9H12O	81
3.	Phenol, 2-ethyl-5-methyl-	136	C9H12O	76
4.	Phenol, 2-ethyl-6-methyl-	136	C9H12O	76
5.	Phenol, 4-ethyl-3-methyl-	136	C9H12O	76
6.	Phenol, 2-ethyl-4-methyl-	136	C9H12O	76
7.	Phenol, 3-ethyl-5-methyl-	136	C9H12O	68
8.	Phenol, 3-(1-methylethyl)-	136	C9H12O	68
9.	Phenol, 4-(1-methylethyl)-	136	C9H12O	62
10.	Phenol, 3-(1-methylethyl)-	136	C9H12O	62
11.	Pyridinium, 1-(acetylamino)-, hydroxide,	136	C7H8N2O	62
12.	Isoterpinolene	136	C10H16	58
13.	Phenol, 2-(1-methylethyl)-	136	C9H12O	58
14.	Benzenemethanol, .alpha.,4-dimethyl-	136	C9H12O	58
15.	1,3-Cyclohexadiene, 1,5,5,6-tetramethyl-	136	C10H16	58
16.	Phenol, 2-(1-methylethyl)-	136	C9H12O	58
17.	Phenol, 2-(1-methylethyl)-	136	C9H12O	58
18.	Phenol, 3-(1-methylethyl)-	136	C9H12O	58
19.	Phenol, 2-(1-methylethyl)-	136	C9H12O	52
20.	Ethanone, 1-(4-hydroxyphenyl)-	136	C8H8O2	52

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*89	000618-45-1	121899	85	13	1	89	25	56	54	90	9465
2.	*81	000527-54-8	121915	78	17	1	95	16	49	10	66	9616
3.	*76	001687-61-2	7902	64	27	1	99	25	45	0	64	9503
4.	*76	001687-64-5	7903	78	18	0	75	25	45	35	81	9504
5.	*76	001123-94-0	121905	74	21	1	81	25	45	26	66	9458
6.	*76	003855-26-3	7901	63	42	3	78	23	45	0	64	9624
7.	*68	000698-71-5	121904	66	28	2	93	23	40	16	56	9513
8.	*68	000618-45-1	121898	68	30	1	90	25	40	4	62	9527
9.	*62	000099-89-8	121901	71	23	1	73	26	36	23	62	9419
10.	*62	000618-45-1	7899	61	36	2	88	26	36	0	56	9537
11.	*62	001468-29-7	7765	60	39	3	93	26	36	0	56	9535
12.	*58	000586-63-0	8112	51	58	2	70	26	32	0	46	9525
13.	*58	000088-69-7	7898	57	36	2	99	26	32	0	49	9470
14.	*58	000536-50-5	7920	52	47	3	83	26	32	0	44	9523
15.	*58	000514-94-3	122003	54	45	2	85	26	32	10	47	9406
16.	*58	000088-69-7	121895	60	33	1	74	26	32	16	47	9411
17.	*58	000088-69-7	121894	62	36	2	79	26	32	12	49	9425
18.	*58	000618-45-1	121897	54	39	2	92	26	32	10	46	9466
19.	*52	000088-69-7	121892	48	50	3	99	34	27	0	46	9492
20.	*52	000099-93-4	121867	53	36	2	92	35	27	0	47	9343

STP Compounds

Peak 7



Scan 1108 (23.199 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	51	63.90	159	76.30	89	98.05	113
43.90	37	65.00	1087	78.95	235	100.70	43
49.95	26	66.15	63	81.05	181	104.95	170
51.00	115	67.00	252	83.10	56	107.00	129
52.05	88	69.00	87	85.90	15	115.90	78
53.00	165	70.00	45	88.00	102	117.15	144
54.80	352	70.95	25	89.00	471	118.95	4503
56.05	4	71.80	206	90.00	294	119.95	445
57.05	228	72.80	61	91.15	1765	122.80	79
58.15	76	74.00	36	92.00	216	130.05	55
62.90	537	74.95	96	93.80	68	130.95	129

Scan 1108 (23.199 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.90	86	194.20	70				
141.00	109						
151.70	42						
161.90	209						
163.00	79						
176.20	84						
182.40	41						
190.00	1373						
191.00	691						
192.15	161						
193.95	68						

STP Compounds

Scan 1108 (23.199 min): A0294.D

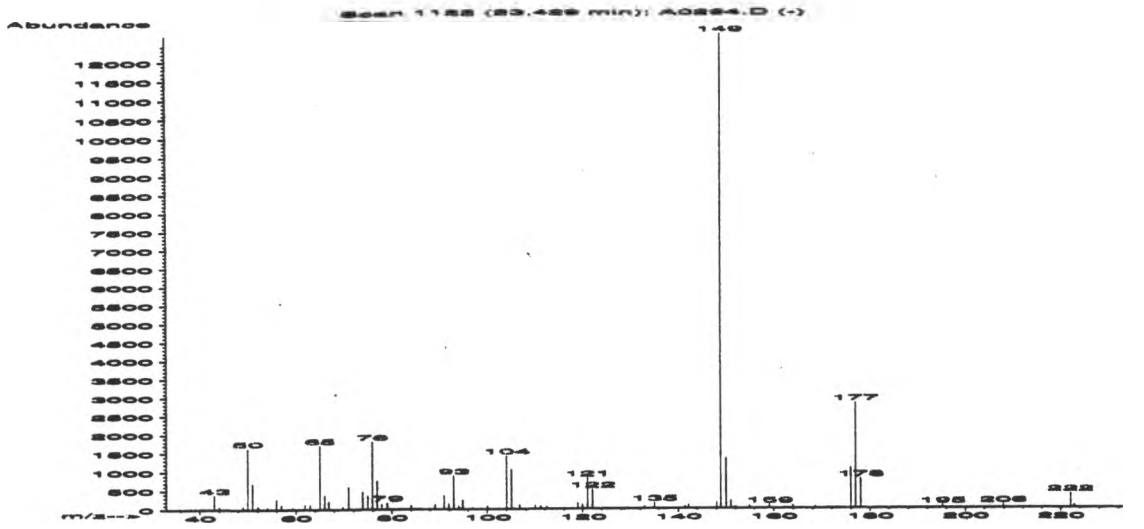
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzamide, N,N-diethyl-3-methyl-	191	C12H17NO	80
2.	Benzamide, N-(1,1-dimethylethyl)-4-methy	191	C12H17NO	80
3.	Benzamide, N-(1,1-dimethylethyl)-3-methy	191	C12H17NO	74
4.	Ethanone, 2-bromo-1-(4-methylphenyl)-	212	C9H9BrO	59
5.	2,4,5-TRIOXO-1-PHENYLIMIDAZOLIDINE	190	C9H6N2O3	58
6.	P-METHYLBENZOYL-FORMIC ACID	164	C9H8O3	53
7.	4-Methylimino-toluene	119	C8H9N	53
8.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	50
9.	Benzoic acid, 4-methyl-, hydrazide	150	C8H10N2O	50
10.	Benzoyl chloride, 2-methyl-	154	C8H7ClO	50
11.	Benzene, (1,1,2-trimethylpropyl)-	162	C12H18	49
12.	2-PHENYL-1-D1-AZIRIDINE	119	C8H8DN	47
13.	Benzonitrile, 3-hydroxy-	119	C7H5NO	47
14.	Benzene, (1,1-dimethylbutyl)-	162	C12H18	47
15.	Benzene, isocyanato-	119	C7H5NO	47
16.	Benzene, isocyanato-	119	C7H5NO	47
17.	Benzoyl chloride, 4-methyl-	154	C8H7ClO	45
18.	Benzene, (1,1-dimethylpropyl)-	148	C11H16	43
19.	Benzonitrile, 3-hydroxy-	119	C7H5NO	43
20.	Benzene, (1,1-dimethylpropyl)-	148	C11H16	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000134-62-3	30397	51	52	0	66	13	48	0	46	9854
2.	*80	042498-32-8	30390	66	41	1	97	14	48	18	47	9555
3.	*74	042498-33-9	30391	59	47	1	89	17	44	0	56	9566
4.	59	000619-41-0	40089	53	53	2	99	25	33	0	39	9457
5.	*58	002211-33-8	29822	34	60	3	99	29	32	22	43	9326
6.	53	000000-00-0	18341	45	40	1	88	28	28	13	41	9408
7.	*53	000000-00-0	3977	40	20	0	83	28	28	12	39	9213
8.	50	000099-75-2	123612	44	48	0	84	34	25	0	39	9437
9.	50	003619-22-5	12558	60	30	0	70	31	25	3	39	9478
10.	50	000933-88-0	14272	47	49	0	86	31	25	16	41	9443
11.	*49	026356-11-6	17838	43	47	2	94	40	23	0	44	9182
12.	*47	030691-60-2	3981	47	51	1	68	40	20	0	40	9174
13.	*47	000873-62-1	119910	37	55	1	99	40	20	0	39	9261
14.	*47	001985-57-5	17833	46	33	1	89	40	20	16	38	9176
15.	*47	000103-71-9	119901	35	56	2	86	40	20	0	39	9291
16.	*47	000103-71-9	119907	35	66	1	73	40	20	0	39	9355
17.	45	000874-60-2	14274	53	37	1	91	25	19	2	37	9466
18.	43	002049-95-8	12107	43	41	0	86	43	18	2	41	9174
19.	*43	000873-62-1	3965	43	49	1	79	43	18	0	40	9173
20.	43	002049-95-8	123443	48	36	0	73	43	18	9	38	9174

STP Compounds

Peak 8



Scan 1122 (23.429 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	381	63.00	115	79.05	169	96.95	41
44.00	63	65.00	1705	84.00	98	100.05	71
48.90	76	66.00	371	84.95	16	104.05	1413
49.95	1637	66.90	204	85.90	23	105.05	1049
50.95	678	69.80	65	87.95	11	106.75	102
52.00	86	71.05	596	89.00	123	110.00	89
54.05	49	73.95	456	91.00	364	111.15	73
55.95	259	75.05	372	91.95	134	112.40	58
56.95	105	75.95	1810	93.00	892	118.95	146
59.25	46	77.00	750	94.05	75	119.95	104
61.90	120	77.90	133	94.80	238	121.05	813

Scan 1122 (23.429 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	509	159.15	79				
132.95	61	164.00	74				
135.00	143	168.55	45				
141.40	45	175.95	1082				
142.15	96	176.95	2823				
148.05	150	178.05	785				
148.95	12680	195.20	69				
150.05	1333	207.90	83				
151.05	196	222.05	379				
152.05	49	222.80	65				
154.95	69						

STP Compounds

Scan 1122 (23.429 min): A0294.D

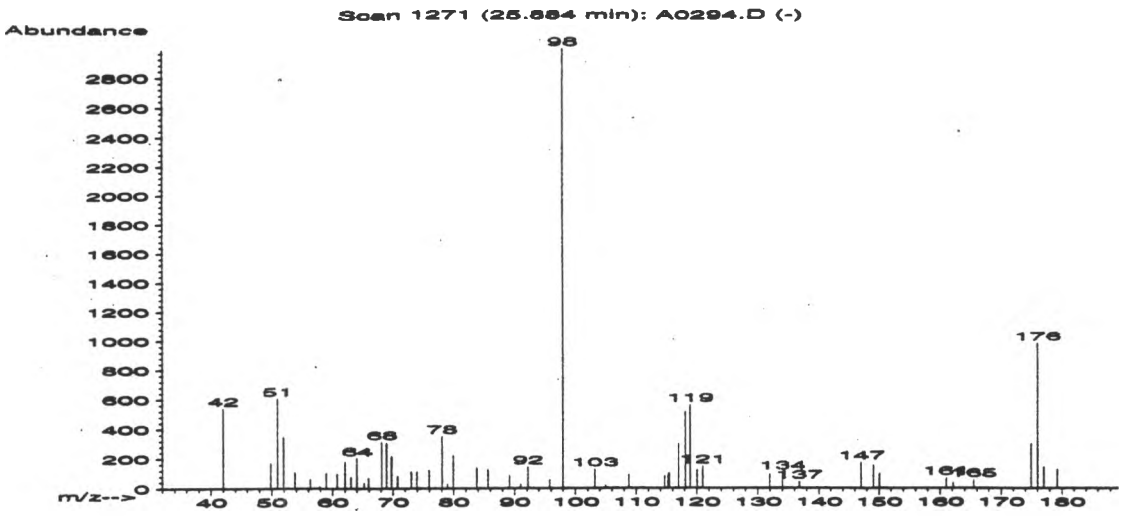
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	96
2.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	94
3.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	93
4.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	93
5.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	91
6.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	90
7.	Phthalic acid, allyl ethyl ester	234	C13H14O4	78
8.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	64
9.	5,6-INDOLEDIOL	149	C8H7NO2	64
10.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	59
11.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	59
12.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	59
13.	2,4-Imidazolidinedione, 1-[[(5-nitro-2-f	238	C8H6N4O5	56
14.	1,2-Benzenedicarboxylic acid, monobutyl	222	C12H14O4	53
15.	M-NITROSTYRENE	149	C8H7NO2	53
16.	1,2-Benzenedicarboxylic acid, di-2-prope	246	C14H14O4	47
17.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	47
18.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	45
19.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	45
20.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	42

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000084-66-2	129815	93	23	0	70	0	76	0	96	9980
2.	*94	000084-66-2	129814	97	22	1	73	0	70	9	90	9932
3.	*93	000084-66-2	129816	85	35	0	63	27	68	0	94	9981
4.	*93	000084-66-2	44597	79	32	0	78	6	66	0	93	9935
5.	91	000084-66-2	129818	94	25	1	74	1	60	0	51	9966
6.	*90	000084-66-2	129819	78	37	1	81	16	59	0	90	9714
7.	78	033672-94-5	49844	66	53	1	78	6	46	0	38	9924
8.	64	000131-16-8	131293	84	25	0	88	21	37	6	45	9694
9.	*64	000000-00-0	12245	54	47	1	89	24	37	0	49	9696
10.	59	000084-74-2	132531	52	55	1	99	22	33	4	38	9672
11.	59	000084-74-2	132527	48	54	3	99	22	33	5	38	9683
12.	59	000084-74-2	132532	49	60	2	69	24	33	3	38	9695
13.	56	000067-20-9	51334	43	78	3	99	14	30	10	37	9942
14.	53	000131-70-4	129812	47	59	0	70	27	28	0	39	9685
15.	*53	000586-39-0	12229	35	68	3	99	27	28	0	41	9667
16.	47	000131-17-9	131091	45	72	3	84	37	20	1	38	9541
17.	47	000084-66-2	129817	57	11	0	64	37	20	15	40	9919
18.	45	000084-74-2	132533	47	56	2	99	21	19	8	33	9666
19.	45	000084-69-5	132539	39	74	1	99	24	19	0	33	9687
20.	42	000605-45-8	131296	67	50	1	85	26	17	4	33	9691

STP Compounds

Peak 9



Scan 1271 (25.884 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	542	64.00	203	79.00	30	108.75	90
49.80	169	65.15	35	79.95	221	114.70	82
50.95	605	65.90	71	83.75	137	115.25	98
51.95	343	68.15	313	85.65	126	115.50	102
53.80	106	68.95	305	89.15	86	117.00	300
56.30	62	69.80	217	90.95	27	118.15	518
57.90	15	70.75	82	92.15	144	118.95	564
59.00	104	72.95	113	95.80	56	120.05	123
60.75	97	73.95	112	97.95	2984	121.00	147
62.00	178	75.95	121	103.20	129	131.90	93
62.95	76	78.05	350	104.95	20	134.00	106

Scan 1271 (25.884 min): A0294.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.75	44						
147.05	174						
149.05	154						
150.05	97						
161.00	70						
162.15	39						
165.50	57						
174.95	302						
176.05	984						
177.05	144						
179.20	126						

STP Compounds

Average of 25.867 to 25.917 min.: A0294.D
Converted from RTE data file: >A0294:

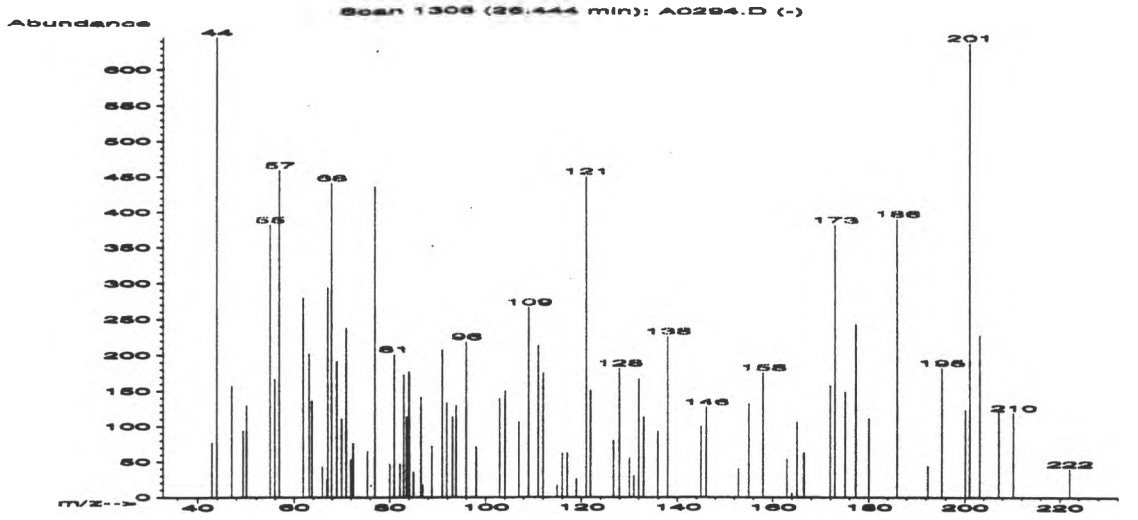
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl	176	C10H12N2O	87
2.	Pyridine, 3-(1-methyl-2-piperidinyl)-, (	176	C11H16N2	80
3.	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl	176	C10H12N2O	80
4.	2-Propenoic acid, 3-(dimethylamino)-, me	129	C6H11NO2	32
5.	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl	176	C10H12N2O	27
6.	N-FORMYLPROLINE METHYL ESTER	157	C7H11NO3	23
7.	2-HEXYL-5-METHYL-(2H)-FURAN-3-ONE	182	C11H18O2	23
8.	Ethene, 1-chloro-1,2-difluoro-	98	C2HClF2	23
9.	Cyclopentanone, 2-(3,3-dimethylbutyl)-3,	196	C13H24O	23
10.	Propanenitrile, 3-(2-methoxy-1-methyleth	143	C7H13NO2	23
11.	16,28-Secosolanid-5-en-3-ol, (3.beta.)-	399	C27H45NO	23
12.	Mepivacaine metabolite	262	C15H22N2O2	23
13.	1-Piperidineethanol	129	C7H15NO	9
14.	1-Piperidinepropanol, .alpha.-cyclopenty	287	C19H29NO	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000486-56-6	126470	65	33	1	85	12	54	0	64	9881
2.	*80	024380-92-5	23907	60	42	2	80	15	48	10	45	9840
3.	*80	000486-56-6	126471	83	22	1	92	12	48	10	46	9847
4.	*32	000999-59-7	6128	35	42	1	68	50	9	9	37	9210
5.	*27	000486-56-6	23792	49	53	3	130	59	8	0	39	9913
6.	23	000000-00-0	15731	33	53	2	69	50	6	0	22	9210
7.	23	000000-00-0	26647	37	50	2	85	50	6	0	25	9210
8.	*23	000359-04-6	708	23	57	2	94	50	6	0	29	9210
9.	23	056247-49-5	33100	34	71	2	77	50	6	0	21	9210
10.	23	035633-52-4	10336	34	57	1	76	50	6	0	20	9210
11.	23	020140-96-9	97730	36	79	3	88	48	6	1	23	9224
12.	23	000000-00-0	60449	33	62	2	87	50	6	0	22	9213
13.	* 9	003040-44-6	6187	32	32	1	47	75	1	0	33	9210
14.	7	000077-39-4	69620	33	71	2	52	75	1	0	22	9210

STP Compounds

Peak 10a Coeluting with nonylphenol, not clean



Scan 1305 (26.444 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	77	66.00	43	80.00	47	91.90	133
43.95	645	66.90	25	80.95	201	93.05	113
47.05	157	67.15	294	82.10	47	93.80	129
49.30	94	67.95	441	82.90	173	95.95	218
50.05	129	69.00	191	83.50	113	98.05	71
54.95	382	70.05	110	84.00	177	102.95	139
55.95	167	70.95	237	84.95	35	104.05	150
56.90	459	71.95	53	86.50	141	106.95	106
61.90	279	72.45	76	86.80	17	109.00	266
63.15	202	75.45	65	88.75	72	111.00	213
63.75	136	76.95	435	90.95	207	112.00	175

Scan 1305 (26.444 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.95	16	133.00	113	166.50	63	203.20	228
116.00	62	135.90	93	171.95	158	207.15	123
117.05	62	138.00	226	172.95	382	210.25	119
119.00	26	144.90	100	175.05	149	222.05	40
121.00	450	146.05	127	177.30	243		
121.90	151	152.90	40	179.95	111		
126.70	80	155.05	132	186.00	391		
127.95	182	158.00	176	192.40	44		
130.05	55	163.00	54	195.20	183		
131.00	30	164.00	5	200.05	123		
132.00	167	165.00	106	201.05	638		

STP Compounds

Scan 1305 (26.444 min): A0294.D

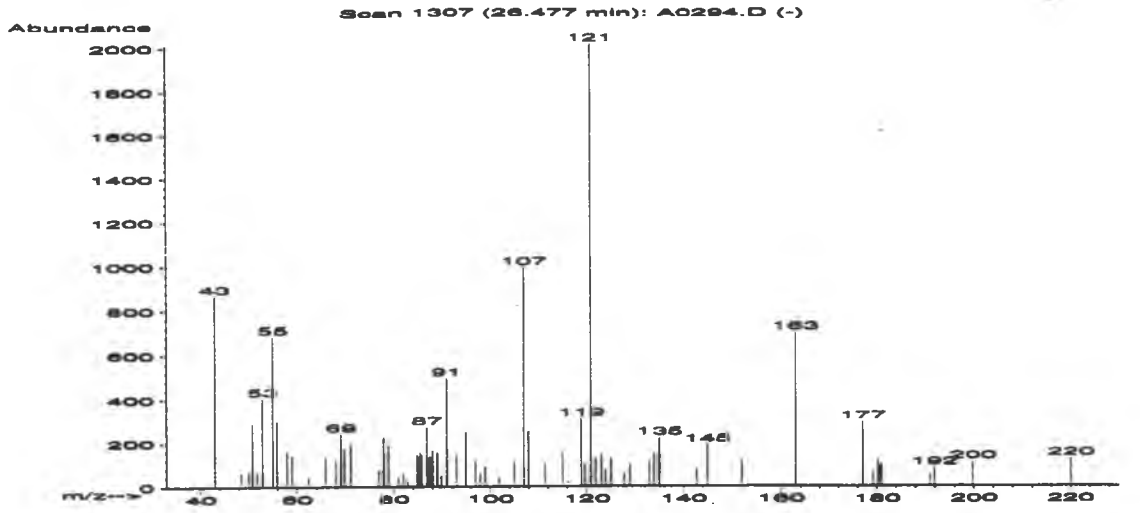
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	50
2.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	46
3.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	43
4.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	42
5.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	35
6.	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N	201	C7H12ClN5	35
7.	2,2,4-TRIMETHYL-5-PHENYL-6-OXA-1-AZABICY	201	C13H15NO	35
8.	Acetamide, 2-(2,4-dichlorophenoxy)-N,N-d	247	C10H11Cl2NO2	25
9.	PROPYL-1-D1 OCTYL ETHER	172	C11H23DO	14
10.	2,5-DIMETHYL-1-[(2-HYDROXYMETHYL)PHENYL]	201	C13H15NO	11
11.	Aluminum, tetraethylbis(.mu.-methylamina	230	C10H28Al2N2	10
12.	1,4-Naphthalenedione, 2-methyl-3-(methyl	201	C12H11NO2	10
13.	2H-Pyran, 2-(ethylthio)tetrahydro-	146	C7H14OS	10
14.	[1]Benzothieno[2,3-d]pyridazine	186	C10H6N2S	9
15.	Silane, trimethyl(nonyloxy)-	216	C12H28OSi	8
16.	1-Amidohexafluoro-1H-azepin	244	C7H2F6N2O	8
17.	Brocresine	217	C7H8BrNO2	8
18.	PROPYL-1-D1 DODECYL ETHER	228	C15H31DO	8
19.	Butane, 1,2-dichloro-	126	C4H8Cl2	8
20.	5,5,5-D3-2-METHYL-4-(D3-METHYL)-1-PENTEN	98	C7H8D6	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	000122-34-9	128441	75	82	1	91	50	25	31	66	9061
2.	*46	000122-34-9	35023	63	95	0	87	54	20	0	64	9121
3.	*43	000122-34-9	128439	74	92	2	93	43	18	3	42	9290
4.	*42	000122-34-9	128442	71	86	1	129	58	17	0	68	9123
5.	*35	000122-34-9	128443	65	79	2	170	66	11	0	64	8589
6.	*35	000122-34-9	128440	76	67	1	146	66	11	0	74	8859
7.	*35	073119-55-8	35183	34	71	0	98	52	11	0	41	6417
8.	25	006333-39-7	55022	45	136	2	122	45	7	0	22	6468
9.	14	029379-40-6	22419	46	71	0	99	68	2	0	39	5911
10.	*11	097690-10-3	35189	56	111	2	98	72	2	0	49	6517
11.	10	023129-28-4	48237	42	65	1	77	70	1	0	33	6392
12.	*10	001694-01-5	35134	36	113	2	90	74	1	0	39	5899
13.	10	016315-51-8	123130	37	72	1	59	64	1	1	22	2736
14.	* 9	000244-92-8	28331	28	89	0	54	80	1	0	33	3365
15.	8	018388-84-6	129458	36	84	1	77	68	1	0	21	5492
16.	8	083925-97-7	53807	36	23	1	76	68	1	0	25	7809
17.	8	000555-65-7	42212	35	150	2	90	68	1	0	20	2402
18.	8	033933-68-5	47813	38	107	1	86	68	1	0	29	5942
19.	8	000616-21-7	120484	35	67	1	95	68	1	6	26	2402
20.	* 8	040316-95-8	919	28	87	3	278	67	1	0	29	2591

STP Compounds

Peak 10b Nonylphenol [1]



Scan 1307 (26.477 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	865	65.90	137	84.90	145	94.95	248
48.45	64	68.00	123	85.15	133	96.95	116
50.00	72	69.05	241	85.50	156	98.00	59
50.80	286	69.80	172	85.75	144	98.95	90
51.80	63	71.05	192	86.90	271	101.80	39
52.95	404	76.95	76	87.50	136	104.95	115
55.05	682	77.95	226	88.00	165	107.00	990
55.95	298	78.95	188	89.00	156	107.90	255
58.00	161	80.95	42	89.90	48	111.40	108
59.00	140	82.00	59	91.00	494	115.00	156
62.40	41	82.90	21	93.00	144	116.10	22

Scan 1307 (26.477 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.95	309	135.00	221	191.90	82		
119.70	100	142.75	79	199.80	110		
120.95	2011	144.95	188	220.05	125		
121.95	131	152.05	120				
123.05	146	163.00	699				
123.95	76	177.05	293				
125.05	129	179.20	66				
127.70	58	180.20	122				
128.95	98	180.70	94				
132.95	112	180.90	99				
133.90	151	191.00	52				

STP Compounds

Scan 1307 (26.477 min): A0294.D

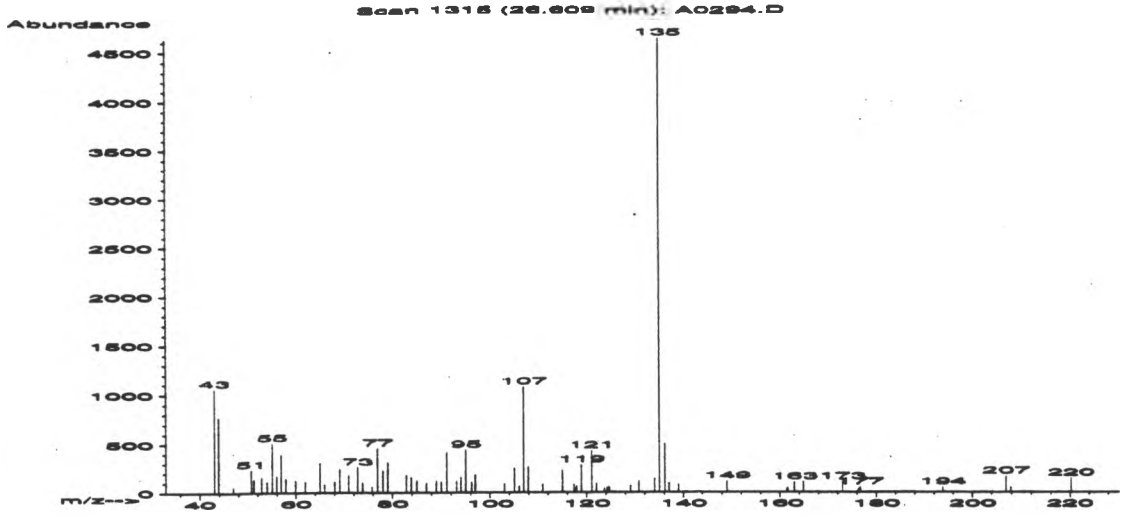
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	9-METHL-10-AZATRICYCLO[5.2.2.0(1,5)]UNDE	163	C11H17N	59
2.	Acetamide, N-methyl-N-(4-methylphenyl)-	163	C10H13NO	35
3.	NONYLPHENOL ISOMER	220	C15H24O	32
4.	(3S,4R,5S,6R)-4,5-Bis(hydroxymethyl)-3,6	170	C10H18O2	25
5.	Methyl pimarate	316	C21H32O2	17
6.	.alpha.-Ionone	192	C13H20O	12
7.	Benzenepropanoic acid, .alpha.-hydroxy-4	210	C11H14O4	12
8.	Methyl pimarate	316	C21H32O2	12
9.	LEDENOXIDE-(I)	220	C15H24O	10
10.	Antalergan	285	C17H23N3O	10
11.	2-Butanone, 4-(4-methoxyphenyl)-	178	C11H14O2	10
12.	Benzeneacetic acid, 4-methoxy-	166	C9H10O3	10
13.	Benzene, 1-(chloromethyl)-4-methoxy-	156	C8H9ClO	10
14.	Phenol, 3-(1-methylethyl)-	136	C9H12O	10
15.	4-Ethyl-3-methylpyridine	121	C8H11N	10
16.	Benzenamine, 2,5-dimethyl-	121	C8H11N	10
17.	1-[5'-((E)-3''-Methyl-1'',3''-butadien-1	220	C14H20O2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000000-00-0	18132	34	33	0	72	22	33	0	41	9463
2.	*35	000612-03-3	18074	36	62	0	74	54	11	0	41	8635
3.	*32	000000-00-0	129726	44	86	2	82	47	9	12	37	9549
4.	25	000000-00-0	21478	48	71	2	72	45	7	0	22	9113
5.	17	003730-56-1	134054	34	103	3	99	54	3	0	22	8630
6.	12	000127-41-3	127728	40	95	2	99	59	2	0	27	8605
7.	12	055301-58-1	39276	39	86	3	77	59	2	0	29	8478
8.	12	003730-56-1	134055	34	109	2	99	56	2	2	24	8599
9.	*10	000000-00-0	44033	47	105	2	55	70	1	0	35	8307
10.	10	000091-84-9	132829	36	90	1	68	62	1	0	22	8251
11.	10	000104-20-1	24706	35	64	1	69	62	1	0	22	8286
12.	10	000104-01-8	125533	33	65	1	68	63	1	0	21	8177
13.	10	000824-94-2	15225	41	30	1	73	63	1	0	22	8177
14.	10	000618-45-1	121899	33	67	1	71	61	1	0	22	8438
15.	*10	076833-16-4	4222	28	84	2	70	62	1	0	27	8340
16.	*10	000095-78-3	4240	29	80	2	97	61	1	0	29	8458
17.	* 9	088354-47-6	43722	53	76	1	28	77	1	0	35	8744

STP Compounds

Peak 11 Nonylphenol isomer [2]



Scan 1315 (26.609 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1056	59.90	123	78.05	231	95.05	442
43.90	773	61.90	107	79.05	312	96.20	104
46.95	56	65.00	306	82.90	180	96.95	181
50.70	238	65.90	81	83.90	157	102.95	89
51.20	132	68.00	111	85.00	121	105.05	252
52.80	156	69.05	246	87.00	96	105.95	65
53.95	114	70.95	175	89.00	123	107.00	1077
55.05	511	72.80	263	90.00	110	107.90	262
55.95	170	73.80	97	91.15	419	110.90	82
56.90	396	75.80	60	93.15	119	115.00	229
57.90	140	76.95	459	94.05	159	117.40	83

Scan 1315 (26.609 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.90	63	136.15	502	193.80	51		
118.95	286	137.00	96	206.90	168		
121.05	431	139.00	78	207.90	49		
122.05	87	149.05	115	220.20	146		
123.70	41	161.40	40				
124.30	48	161.65	45				
124.70	57	163.00	105				
129.05	70	164.90	107				
130.80	114	173.05	108				
134.00	146	176.30	33				
135.00	4633	176.70	52				

STP Compounds

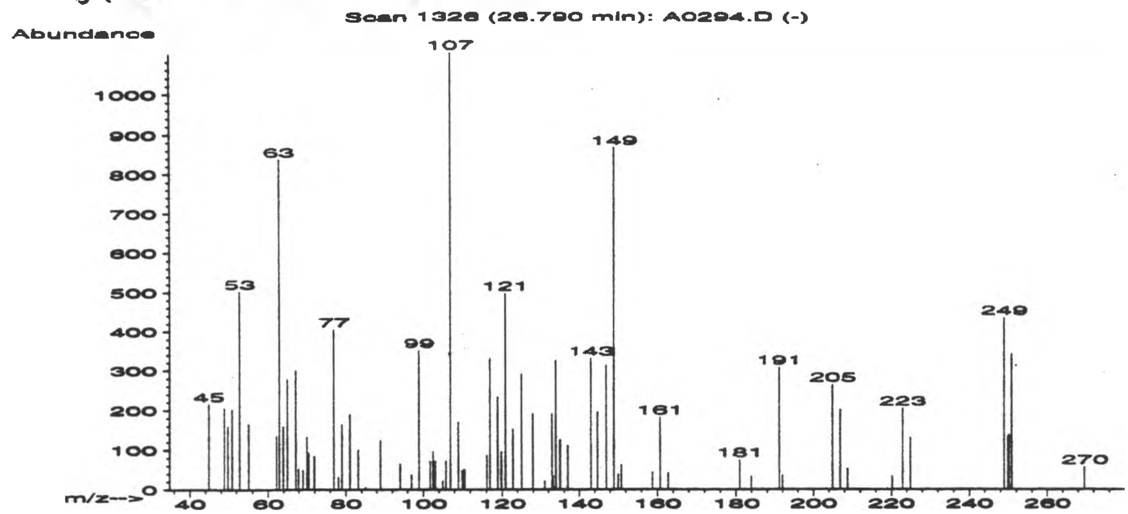
Scan 1315 (26.609 min): A0294.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	72
2.	OCTYL PHENOL ISOMER	206	C14H22O	72
3.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	72
4.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	64
5.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	59
6.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	59
7.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	50
8.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	50
9.	Phenol, 4-nonyl-	220	C15H24O	50
10.	Benzothiazole	135	C7H5NS	47
11.	2H-Imidazo[4,5-b]pyridin-2-one, 1,3-dihy	135	C6H5N3O	45
12.	2-Aziridinone, 1-(1-adamantyl)-3-(1-meth	273	C18H27NO	42
13.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	40
14.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	40
15.	Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl	270	C18H22O2	40
16.	Hexestrol	270	C18H22O2	40
17.	Thiocyanic acid, phenyl ester	135	C7H5NS	38
18.	Benzothiazole	135	C7H5NS	38
19.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	38
20.	3,4-METHYLENEDIOXYBENZYL METHYL KETONE	178	C10H10O3	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000098-54-4	123676	43	44	0	67	15	42	10	41	9913
2.	72	000000-00-0	37565	50	34	0	95	15	42	5	38	9911
3.	72	000585-34-2	123671	41	39	0	76	15	42	10	43	9927
4.	64	000088-18-6	123669	44	25	0	70	18	37	0	39	9886
5.	59	000499-75-2	123691	40	50	3	99	25	33	3	38	9907
6.	59	000499-75-2	123692	40	50	3	99	25	33	3	38	9907
7.	50	000585-34-2	123673	52	39	0	79	18	25	0	35	9918
8.	50	000088-18-6	123665	48	42	2	99	32	25	11	38	9471
9.	*50	000104-40-5	129723	47	71	1	67	20	25	0	35	9765
10.	*47	000095-16-9	121697	36	49	2	99	37	20	0	39	9675
11.	*45	016328-62-4	7518	39	58	1	99	25	19	0	35	9885
12.	42	026905-18-0	64696	42	68	3	70	27	17	13	35	9773
13.	40	000098-54-4	12727	47	43	1	99	35	16	2	35	9937
14.	40	000585-34-2	12726	46	47	1	99	35	16	0	34	9901
15.	40	005635-50-7	63693	60	51	2	99	35	16	0	36	9569
16.	40	000084-16-2	132208	49	67	3	93	33	16	0	35	9172
17.	*38	005285-87-0	7525	35	45	1	94	38	14	6	35	9632
18.	*38	000095-16-9	121696	34	40	2	99	38	14	10	37	9632
19.	*38	015816-45-2	7331	35	49	2	71	38	14	0	35	9634
20.	38	004676-39-5	24601	46	53	2	69	38	14	0	37	9633

Peak [illegible] ; 2 Chloroethyl phosphate



Scan 1326 (26.790 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.80	216	67.90	53	88.90	124	110.00	48
48.80	206	69.00	50	94.00	64	110.50	51
49.80	159	70.05	133	97.00	37	116.15	88
50.85	202	70.45	93	98.95	351	117.00	330
52.80	502	71.95	85	101.80	72	118.90	233
55.05	166	76.95	404	102.55	95	119.80	95
62.15	136	78.05	31	103.05	71	120.95	496
62.90	837	78.95	164	105.00	23	122.80	152
63.90	159	81.00	189	105.80	73	125.05	290
64.95	279	83.15	100	107.00	1099	127.95	190
67.15	300	84.95	5	109.00	170	131.00	22

Scan 1326 (26.790 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.90	190	158.75	44	222.95	203		
133.15	35	160.75	181	224.95	130		
133.90	324	162.75	42	248.95	433		
135.00	125	181.00	75	249.95	134		
137.00	111	183.90	33	250.20	137		
143.00	330	191.15	306	250.95	341		
144.80	196	192.05	36	269.70	56		
147.05	312	204.95	262				
149.00	862	206.90	199				
150.10	38	208.75	52				
150.95	63	220.20	33				

STP Compounds

Scan 1326 (26.790 min): A0294.D

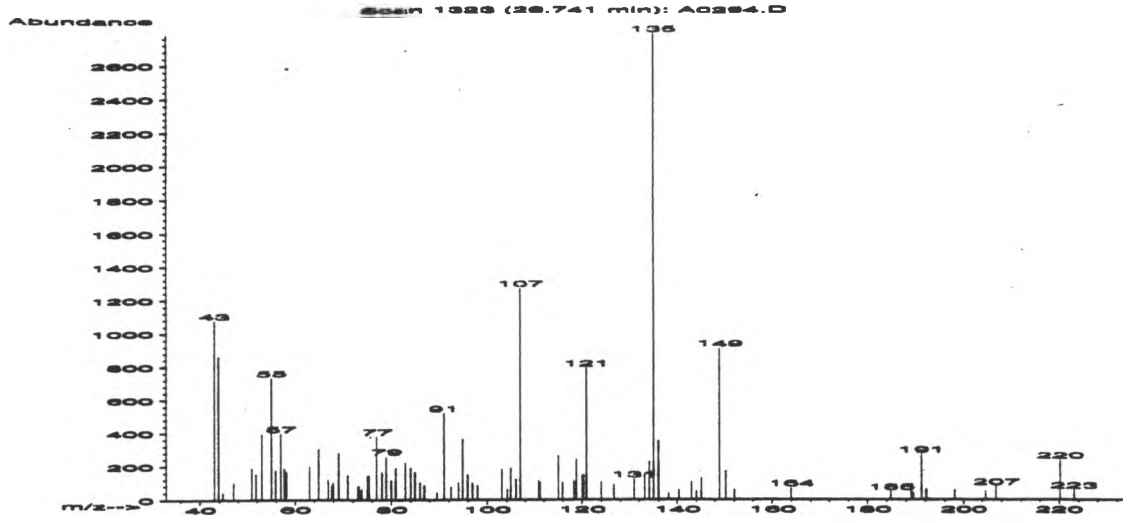
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-chloro-, phosphite (3:1)	268	C6H12Cl3O3P	35
2.	1,3-DIBROMO-1,1-DICHLOROBUTANE	282	C4H6Br2Cl2	32
***	3. Ethanol, 2-chloro-, phosphate (3:1)	284	C6H12Cl3O4P	32
4.	Benzene, [2-(2-chloroethoxy)ethoxy]ethyl	228	C12H17ClO2	32
5.	Benzene, 4-methoxy-1-nitro-2-(trifluorom	221	C8H6F3NO3	20
6.	Azetidine, 1-chloro-	91	C3H6ClN	17
7.	3-BROMO-1,1,1-TRICHLOROBUTANE	238	C4H6BrCl3	12
8.	1,3-BIS(2-CHLOROETHYL)UREA	184	C5H10Cl2N2O	12
9.	1H-Indene, 1-ethylideneoctahydro-7a-meth	164	C12H20	10
10.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	10
11.	2-ACETYLAMINOTOLUENE	149	C9H11NO	10
12.	2,5-Furandione, 3,4-dichlorodihydro-3,4-	196	C6H6Cl2O3	10
13.	Propane, 1,1-dichloro-	112	C3H6Cl2	10
14.	Naphthalene, 1,2,3,4-tetrahydro-5,8-dime	272	C20H32	9
15.	Phenol, 2-(1,1-dimethylethyl)-5-methyl-	164	C11H16O	8
16.	1,3-Benzenedicarboxylic acid	166	C8H6O4	7
17.	Benzenepropanoic acid, .beta.-bromo-	228	C9H9BrO2	7
18.	N-P-TOLYL-BENZENESULFINYL AMIDE	231	C13H13NOS	7
19.	Benzoic acid, 2,5-dichloro-3-hydroxy-6-m	236	C8H6Cl2O4	7
20.	2exo,2endo:3endo,3exo-Bis(epoxymethano)-	154	C8H10O3	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	35	000140-08-9	62438	43	103	0	61	54	11	0	39	4743
2.	32	000000-00-0	67438	50	118	3	92	50	9	0	31	7032
3.	32	000115-96-8	132728	70	94	1	73	49	9	0	37	5873
4.	32	055177-65-6	47520	43	106	1	67	50	9	0	37	7358
5.	20	000344-39-8	44130	33	132	2	65	50	4	0	13	4541
6.	17	032115-53-0	373	35	61	0	70	54	3	1	26	4771
7.	12	000000-00-0	51288	38	98	2	63	58	2	0	28	5877
8.	12	002214-72-4	27143	36	108	3	62	59	2	0	22	5081
9.	10	056362-87-9	18754	36	102	2	78	65	1	0	20	7391
10.	*10	000103-89-9	12284	34	71	2	88	80	1	0	41	7505
11.	*10	000000-00-0	12307	33	73	2	99	80	1	0	39	7500
12.	10	054845-45-3	32539	35	111	1	76	59	1	0	13	4857
13.	10	000078-99-9	118941	35	95	2	76	60	1	0	18	4064
14.	9	055255-58-8	132283	40	90	1	281	80	1	0	33	2698
15.	8	000088-60-8	125359	34	69	1	78	67	1	0	22	5294
16.	7	000121-91-5	125493	33	66	2	73	71	1	1	23	4633
17.	7	015463-91-9	130179	33	106	3	87	80	1	0	22	7489
18.	7	005469-22-7	48699	34	83	0	73	71	1	0	25	5906
19.	7	007600-50-2	50446	36	120	1	50	74	1	0	22	3366
20.	7	076380-09-1	14333	38	76	3	93	80	1	0	28	2698

STP Compounds

Peak 12a Nonylphenol isomer [3]



Scan 1323 (26.741 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1077	58.15	164	75.05	143	86.90	84
43.90	862	63.00	198	75.30	144	89.50	41
44.80	40	64.90	305	76.95	378	91.00	518
47.05	99	66.90	120	78.05	164	92.50	75
50.95	187	67.65	83	78.95	257	94.05	102
51.80	151	67.90	99	79.95	113	94.95	364
53.05	393	69.05	280	80.95	191	95.95	149
55.05	731	70.95	145	82.90	220	96.95	100
55.95	175	73.05	80	84.00	191	97.95	84
57.00	395	73.30	78	84.90	164	103.05	182
57.75	185	73.80	57	86.00	101	104.20	62

Scan 1323 (26.741 min): A0294.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.95	189	120.95	790	144.05	50	198.05	58
106.05	122	124.05	106	145.05	126	204.70	49
107.00	1269	126.70	88	148.95	910	206.90	76
110.90	112	130.95	121	150.20	171	220.20	235
111.15	104	133.15	150	152.05	57	223.05	55
115.00	261	134.15	228	163.90	67		
115.90	100	135.00	2781	184.90	46		
118.25	114	136.00	353	189.00	56		
118.80	243	138.15	37	189.40	39		
120.05	144	140.40	55	191.15	270		
120.30	149	143.00	105	192.15	59		

STP Compounds

Scan 1323 (26.741 min): A0294.D

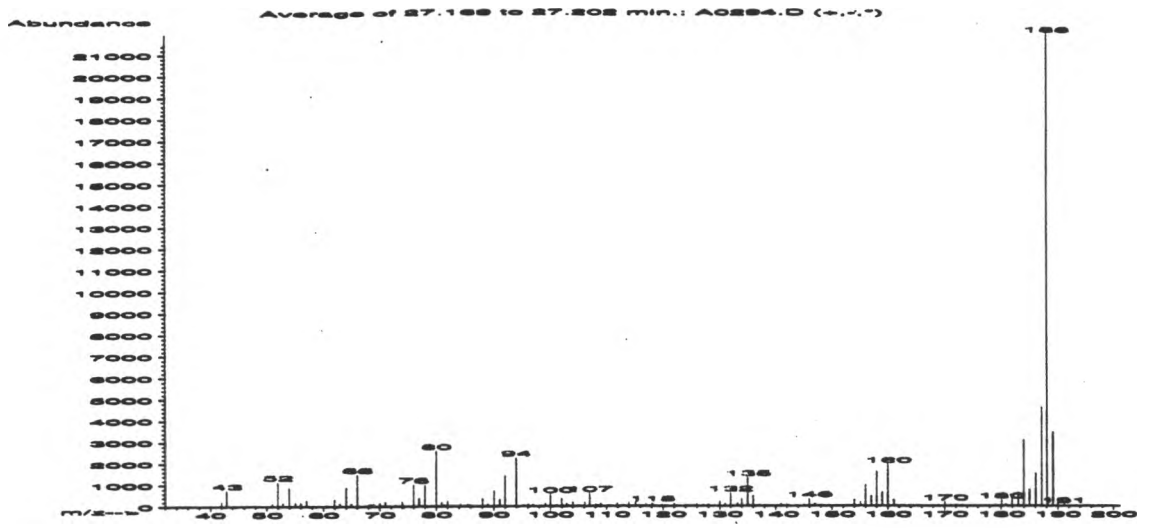
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, nonyl-	220	C15H24O	90
2.	Phenol, 4-nonyl-	220	C15H24O	72
3.	Phenol, 4-nonyl-	220	C15H24O	58
4.	Phenol, 4-nonyl-	220	C15H24O	47
5.	Benzaldehyde, 3-methyl-, oxime	135	C8H9NO	43
6.	Benzaldehyde, 4-methyl-, oxime	135	C8H9NO	43
7.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	38
8.	Thieno[2,3-c]pyridine	135	C7H5NS	38
9.	4-METHYL-4-(P-HYDROXYPHENYL)-2-PENTANONE	192	C12H16O2	38
10.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	38
11.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	35
12.	3,3-DIMETHYL-1-PHENYLAZETIDINE-4-THIONE	191	C11H13NS	35
13.	Phenol, 3-methyl-5-(1-methylethyl)-, met	207	C12H17NO2	35
14.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	35
15.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	35
16.	1H-Indole, 5-fluoro-	135	C8H6FN	35
17.	Adenine	135	C5H5N5	35
18.	Adenine	135	C5H5N5	35
19.	Benzothiazole	135	C7H5NS	35
20.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	025154-52-3	43894	79	49	1	98	18	59	0	84	9563
2.	*72	000104-40-5	129723	66	55	0	83	17	42	8	47	9530
3.	*58	000104-40-5	129724	52	70	0	70	29	32	0	46	9573
4.	*47	000104-40-5	43893	55	74	2	87	38	20	0	40	9560
5.	*43	041977-54-2	7568	34	53	2	80	43	18	1	40	8641
6.	*43	003235-02-7	7571	33	46	2	99	43	18	1	40	8473
7.	*38	000089-83-8	123682	43	43	0	73	52	14	18	47	8662
8.	*38	000272-12-8	7533	43	45	0	79	55	14	0	44	8375
9.	38	000000-00-0	30868	53	39	0	99	47	14	4	41	8948
10.	*38	000089-83-8	123684	43	43	0	73	52	14	18	47	8661
11.	*35	000089-83-8	123679	38	49	0	70	54	11	20	42	8520
12.	*35	096594-26-2	30379	53	52	2	77	52	11	0	40	8338
13.	*35	002631-37-0	128920	34	78	0	80	52	11	0	41	8677
14.	*35	000499-75-2	123689	38	51	1	99	51	11	20	42	8626
15.	*35	000089-83-8	123680	38	47	0	81	54	11	20	42	8482
16.	*35	000399-52-0	7540	33	56	1	97	52	11	7	40	9034
17.	*35	000073-24-5	121690	36	52	0	82	55	11	0	41	8360
18.	*35	000073-24-5	121686	37	51	0	84	55	11	0	41	8376
19.	*35	000095-16-9	121697	35	49	0	89	55	11	0	41	8371
20.	*35	000089-83-8	123681	44	44	0	69	52	11	11	40	8626

STP Compounds

Standard 4



Average of 27.169 to 27.202 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	212	60.40	16	68.95	97	82.00	244
42.95	734	60.70	30	70.00	165	82.95	21
47.70	40	61.95	332	71.00	197	84.25	84
48.70	27	62.95	131	72.70	47	85.05	35
50.95	119	64.00	883	73.95	202	85.50	78
51.95	1130	64.95	117	76.00	1002	85.95	55
52.85	153	66.00	1479	76.95	379	88.05	365
53.95	844	67.05	24	78.00	993	89.00	88
55.00	160	68.00	75	80.00	2571	90.05	722
56.00	159	68.25	52	80.95	158	91.05	334
56.95	272	68.50	56	81.50	54	92.00	1424

Average of 27.169 to 27.202 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.95	2266	105.00	37	113.15	26	125.95	85
95.20	63	106.10	178	113.95	179	126.95	23
96.05	88	106.95	590	115.15	157	127.20	26
96.95	62	108.00	93	116.40	26	128.00	78
99.10	130	108.50	39	117.05	92	130.05	199
100.00	546	108.95	133	118.10	135	131.00	103
101.05	56	110.00	7	118.95	5	131.95	597
101.95	358	110.90	32	119.85	63	133.15	128
102.90	122	111.90	140	122.00	111	133.95	325
103.20	35	112.50	32	124.00	39	135.00	1314
104.00	186	112.90	43	125.20	30	136.00	476

Average of 27.169 to 27.202 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.00	20	155.10	185	171.05	33	185.00	774
139.00	21	156.00	984	171.95	30	186.15	1513
140.95	109	157.05	468	173.05	22	187.15	4633
141.95	65	158.00	1618	176.90	13	188.15	21966
145.05	57	159.00	622	177.95	25	189.15	3479
145.95	326	160.05	1928	179.05	31	190.05	306
147.00	113	161.05	280	180.10	266	191.10	49
148.05	23	162.50	34	180.85	80		
149.80	25	165.15	26	181.95	418		
153.05	17	168.95	32	183.05	635		
154.00	276	170.05	183	184.00	3105		

STP Compounds

Average of 27.169 to 27.202 min.: A0294.D
Converted from RTE data file: >A0294:

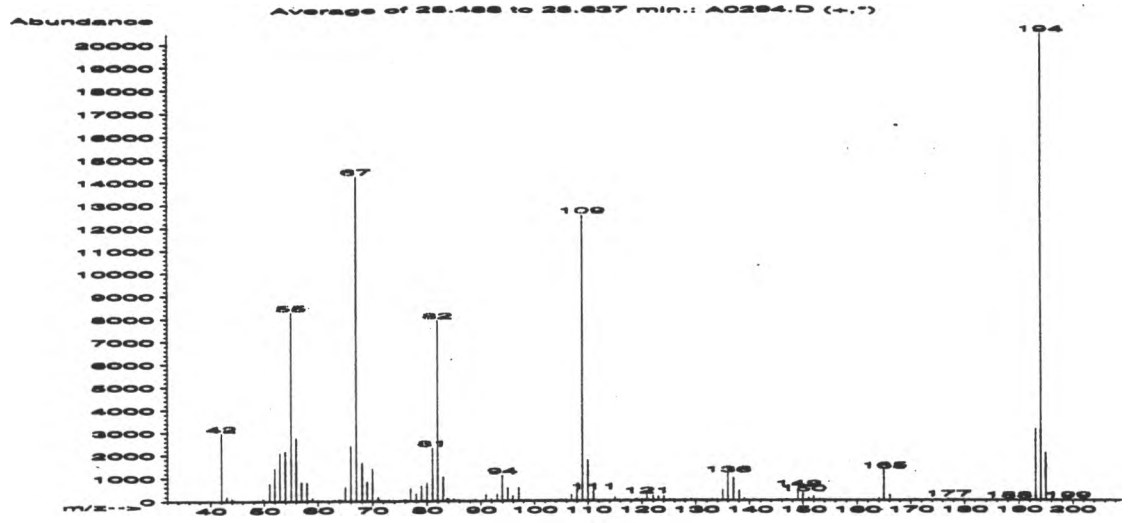
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Anthracene-D10	178	C14D10	93
2.	DECADEUTEROPHENANTHRENE	178	C14D10	87
3.	Acridine-D9	179	C13D9N	64
4.	Acridine-D9	179	C13D9N	64
5.	4,6-DIMETHOXYISOPHTHALONITRILE	188	C10H8N2O2	59
6.	1,2,3,4,6,7,8,9-Octahydrophenazine	188	C12H16N2	53
7.	4-METHYL-2-(4-FLUOROPHENYL)PYRIMIDINE	188	C11H9FN2	50
8.	Di(2,4-dinitrophenoxy)-4,4'-dipyridylium	188	C10H8N2O2	50
9.	4-HYDROXY-6-PHENYL-3-PYRIDAZONE	188	C10H8N2O2	47
10.	Naphthalene, 1,7-dimethoxy-	188	C12H12O2	47
11.	Furfuryl-3-dimethyl-2,5-pyrazine	188	C11H12N2O	47
12.	6-Vinyl-5,7-dimethylphthalide	188	C12H12O2	45
13.	Cyclohexanone, phenylhydrazone	188	C12H16N2	45
14.	5-Oxazolecarboxamide, 2-phenyl-	188	C10H8N2O2	43
15.	[1,2,5]Thiadiazolo[3,4-b]quinoxaline	188	C8H4N4S	43
16.	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimeth	188	C11H12N2O	40
17.	Naphthalene, 2,6-dimethoxy-	188	C12H12O2	38
18.	2,4,7-Trimethylbenzofuran-3-carbaldehyde	188	C12H12O2	38
19.	2-Isopropenyl-5-formyl-2,3-dihydrobenzof	188	C12H12O2	38
20.	Pentacyclo[8.4.0.0(3,7).0(4,14).0(6,11)]	188	C14H20	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000000-00-0	24971	94	13	0	91	6	68	9	93	9849
2.	*87	001517-22-2	24973	75	28	1	99	15	54	22	66	9818
3.	*64	000000-00-0	126726	50	68	3	96	25	37	0	46	9373
4.	*64	000000-00-0	25203	51	68	3	88	21	37	0	46	9556
5.	*59	055937-16-1	29095	33	18	1	99	21	33	11	40	9731
6.	*53	004006-50-2	29327	47	13	0	73	28	28	10	40	9572
7.	*50	076128-67-1	29194	34	76	2	88	31	25	0	39	9721
8.	*50	000000-00-0	29109	33	35	2	87	32	25	0	39	9724
9.	*47	058884-18-7	29107	36	49	2	89	37	20	11	40	9639
10.	*47	005309-18-2	29279	34	87	2	99	37	20	0	39	9570
11.	*47	073570-43-1	29210	34	88	3	99	37	20	0	39	9599
12.	*45	079801-76-6	29272	31	26	2	99	21	19	1	30	9747
13.	*45	000946-82-7	29309	39	87	3	70	25	19	0	33	9776
14.	*43	039819-42-6	29103	33	83	2	75	43	18	0	39	9525
15.	*43	056248-98-7	28958	36	64	3	72	42	18	0	39	9533
16.	*40	000060-80-0	127503	42	38	2	99	31	16	7	36	9720
17.	*38	005486-55-5	29280	39	81	1	87	37	14	0	33	9569
18.	*38	076242-27-8	29267	30	81	3	85	37	14	0	33	9156
19.	*38	085870-17-3	29269	32	41	0	99	36	14	0	33	9558
20.	*38	000000-00-0	29445	29	57	2	96	40	14	1	30	9624

STP Compounds

Peak 13, Caffeine



Average of 28.488 to 28.637 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	2962	52.95	2090	59.95	7	68.95	850
42.95	192	53.70	11	60.65	6	69.45	22
44.00	111	53.95	2168	61.75	8	69.70	16
44.80	17	55.00	8259	62.90	59	69.95	1395
46.20	3	55.95	2750	63.15	8	71.00	164
48.45	8	56.95	812	63.85	59	71.45	6
48.90	23	57.95	788	64.05	53	71.85	27
49.75	112	58.25	12	64.95	611	72.20	6
50.00	44	58.60	24	66.00	2415	72.80	38
51.00	768	58.95	126	67.00	14234	73.00	65
51.95	1422	59.65	6	68.05	1648	73.85	21

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.95	21	83.75	110	91.00	273	99.05	10
75.20	7	84.00	76	92.00	83	100.80	10
75.80	68	85.00	100	93.00	289	101.45	4
76.10	52	85.40	13	93.95	1105	101.80	7
76.95	541	85.75	18	95.00	561	102.95	31
78.00	305	86.05	24	95.95	224	103.20	14
79.00	664	86.95	19	97.00	566	104.20	12
80.00	774	87.95	45	97.80	8	104.55	13
81.00	2321	88.95	62	98.05	12	105.00	50
82.00	7923	89.25	5	98.45	18	105.30	22
83.00	1038	90.15	6	98.75	25	105.55	16

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.80	23	114.00	14	120.90	225	129.45	6
106.05	19	115.00	144	122.00	205	129.80	5
106.25	11	116.75	8	122.20	32	130.20	6
106.95	280	117.05	56	123.00	186	130.55	7
107.75	11	117.65	4	124.00	191	131.15	7
108.00	745	118.45	9	125.05	44	131.50	5
109.00	12516	118.75	48	126.00	12	131.90	22
110.00	1762	119.00	72	127.05	25	132.95	70
111.05	409	119.50	13	127.30	9	133.50	10
112.00	15	120.00	48	128.00	61	133.95	52
112.75	4	120.45	5	129.10	86	135.00	465

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.95	1138	145.55	6	153.30	11	160.40	5
137.00	971	146.30	6	153.70	10	160.90	25
138.05	421	146.70	20	153.95	5	161.15	5
139.00	96	147.00	58	154.20	9	163.00	44
139.90	14	147.95	9	154.45	5	164.05	92

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.90	43	149.05	515	155.05	36	165.00	1309		
141.90	10	150.00	301	155.85	19	166.10	231		
142.40	5	151.10	129	157.00	6	167.00	5		
142.95	18	151.45	16	158.15	7	168.00	6		
144.70	7	152.00	176	158.95	32	168.45	6		
144.95	7	153.00	57	160.15	4	168.95	37		
170.55	4	179.80	8	190.65	4				
171.00	10	181.00	7	191.65	8				
171.80	7	184.15	13	193.10	3122				
172.55	5	184.50	5	194.05	20466				
177.00	72	184.75	6	195.00	2066				
177.55	4	185.10	17	196.05	182				
177.95	20	186.15	6	197.00	19				
178.55	4	186.50	3	197.55	9				
178.95	12	187.00	6	198.05	21				
179.20	4	188.15	17	199.05	6				
179.55	4	188.85	15						

Average of 28.488 to 28.637 min.: A0294.D
Converted from RTE data file: >A0294:

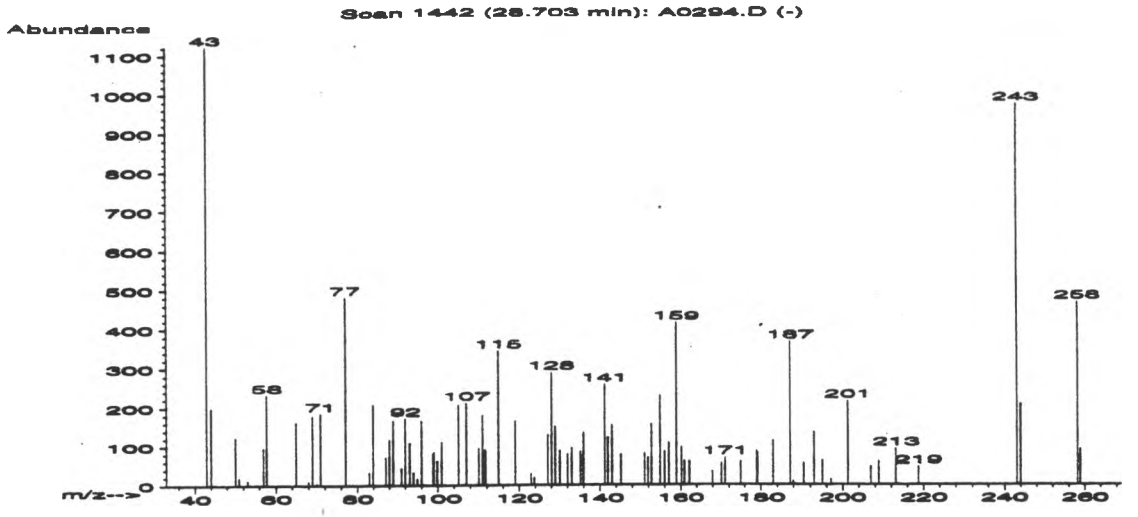
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Caffeine	194	C8H10N4O2	95
2.	Caffeine	194	C8H10N4O2	94
3.	Caffeine	194	C8H10N4O2	94
4.	Caffeine	194	C8H10N4O2	94
5.	Caffeine	194	C8H10N4O2	93
6.	Caffeine	194	C8H10N4O2	89
7.	Caffeine	194	C8H10N4O2	86
8.	Caffeine	194	C8H10N4O2	81
9.	Caffeine	194	C8H10N4O2	76
10.	Caffeine	194	C8H10N4O2	70
11.	Caffeine	194	C8H10N4O2	70
12.	Caffeine	194	C8H10N4O2	58
13.	Pentalene, octahydro-, cis-	110	C8H14	38
14.	Pentalene, octahydro-, cis-	110	C8H14	38
15.	Pentalene, octahydro-, cis-	110	C8H14	38
16.	3-Decyne	138	C10H18	27
17.	Pentalene, octahydro-	110	C8H14	25
18.	Bicyclo[2.2.1]heptane-2-carboxaldehyde,	138	C9H14O	22
19.	Benzo[1,2-c:3,4-c']bis[1,2,5]thiadiazole	194	C6H2N4S2	22
20.	1,4-Hexadiene	82	C6H10	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000058-08-2	127799	114	8	1	91	0	74	0	94	9977
2.	*94	000058-08-2	127797	86	28	0	85	22	70	0	94	9590
3.	*94	000058-08-2	127796	84	27	0	86	23	70	0	94	9434
4.	*94	000058-08-2	127795	93	27	1	90	2	70	35	86	9870
5.	*93	000058-08-2	127793	97	17	2	86	8	66	44	90	9297
6.	*89	000058-08-2	31519	80	34	1	95	22	56	0	90	9480
7.	*86	000058-08-2	127803	80	38	1	76	28	53	0	84	9452
8.	*81	000058-08-2	127794	86	29	0	67	20	49	35	80	9844
9.	*76	000058-08-2	127801	74	51	3	95	22	45	0	81	9676
10.	*70	000058-08-2	127792	73	38	1	95	26	41	0	81	9340
11.	*70	000058-08-2	127800	70	36	2	93	26	41	0	76	9395
12.	*58	000058-08-2	127805	72	42	1	74	34	32	0	53	9348
13.	*38	001755-05-1	2294	64	25	0	59	63	14	0	64	5587
14.	*38	001755-05-1	118910	68	21	0	59	65	14	0	76	5579
15.	*38	001755-05-1	118909	69	23	0	58	63	14	0	76	5582
16.	27	002384-85-2	8718	47	61	2	69	58	8	0	39	6904
17.	*25	000694-72-4	2295	62	24	0	64	63	7	12	47	5591
18.	22	015780-36-6	8658	53	43	2	55	65	5	6	39	6370
19.	*22	000211-16-5	31419	46	63	2	92	63	5	0	40	6995
20.	*14	000592-45-0	116767	36	30	0	55	67	2	0	41	5529

STP Compounds

Peak 14



Scan 1442 (28.703 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1122	70.95	184	94.95	17	114.90	344
44.00	198	77.05	481	95.95	165	119.05	165
50.05	124	82.95	33	98.80	82	123.00	29
50.95	19	83.90	206	99.05	85	123.80	19
53.00	12	87.15	72	99.80	62	127.10	130
56.95	96	88.00	117	100.95	111	128.05	289
57.75	232	89.00	166	105.05	206	128.95	151
64.95	162	91.00	44	107.00	211	130.05	88
67.95	10	92.00	172	110.00	95	132.00	80
68.95	178	93.15	109	111.00	180	133.00	96
70.00	4	94.00	32	111.65	90	135.15	87

Scan 1442 (28.703 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.90	136	159.00	416	187.15	367	243.05	973
141.15	258	160.15	97	188.00	9	244.05	207
142.00	124	161.00	62	190.40	56	258.15	468
143.00	154	162.15	61	192.90	137	258.90	92
145.20	79	167.90	35	195.00	63		
151.05	82	170.05	56	197.15	14		
151.95	71	171.05	70	201.30	215		
152.80	157	174.95	60	206.95	47		
154.95	230	178.95	87	208.90	60		
156.00	87	179.20	82	213.15	93		
157.05	109	182.90	115	218.70	46		

STP Compounds

Scan 1442 (28.703 min): A0294.D

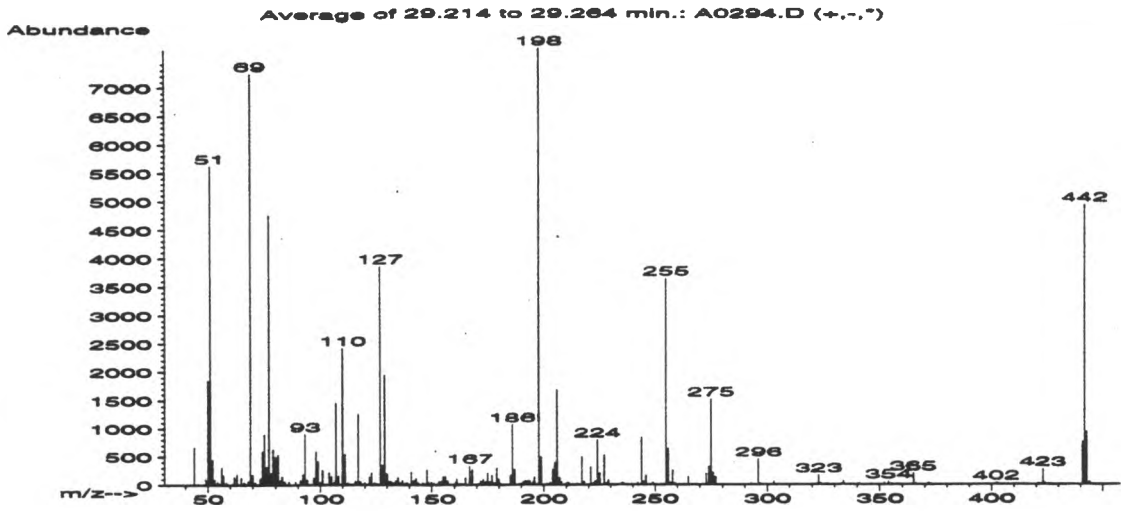
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benz[a]anthracene, 7,12-dihydro-7,12-dim	258	C20H18	80
2.	7-AC-6-ET-1144-ME4-TETRALIN	258	C18H26O	49
3.	Androst-7-ene, (5.alpha.)-	258	C19H30	47
4.	5.alpha.,14.beta.-Androst-7-ene	258	C19H30	47
5.	5.alpha.-Androst-6-ene	258	C19H30	43
6.	5.alpha.-Androst-8(14)-ene	258	C19H30	43
7.	3,3,6,6-TETRAMETHYL-1,2,3,4,5,6,7,8-OCTA	243	C17H25N	25
8.	METHYL ESTER OF O-PHENOXY CARBANILIC ACI	243	C14H13NO3	17
9.	1,2,4-Trimethoxydibenzofuran	258	C15H14O4	14
10.	Furan, 2,3-dihydro-3-[2-methyl-3-(4-nitr	243	C14H13NO3	14
11.	2-AMINOCHRYSENE	243	C18H13N	14
12.	2-METHYL-7-PHENYL-5H-1,3,4-THIADIAZOLO[3	243	C12H9N3OS	12
13.	3,4-O-Isopropyliden-6-O-trityl-D-psicofu	462	C28H30O6	10
14.	Acetamide, N-(4-phenylbicyclo[2.2.2]oct-	243	C16H21NO	10
15.	Maculine	243	C13H9NO4	10
16.	3-AMINOBENZO(C)PHENANTHRENE	243	C18H13N	10
17.	Acetamide, N-acetyl-N-propyl-	143	C7H13NO2	9
18.	Ferrocene, [1-(hydroxyimino)ethyl]-, (Z)	243	C12H13FeNO	8
19.	6-Chrysenamine	243	C18H13N	8
20.	5-AMINOBENZO(C)PHENANTHRENE	243	C18H13N	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	035281-31-3	59144	36	74	0	70	13	48	2	43	7752
2.	*49	000088-29-9	59088	70	71	0	81	41	23	33	58	8138
3.	*47	054411-76-6	59125	36	51	1	69	38	20	0	39	7770
4.	*47	063568-61-6	59124	34	28	1	86	38	20	0	39	7746
5.	*43	084600-52-2	59126	42	38	0	64	43	18	13	38	7778
6.	*43	038863-34-2	59128	35	57	2	86	43	18	0	39	7762
7.	*25	056798-25-5	53766	28	90	0	79	52	7	0	33	7498
8.	*17	000000-00-0	53696	31	131	2	64	53	3	0	29	7984
9.	*14	088256-09-1	131657	33	65	0	45	66	2	0	41	7440
10.	*14	055256-12-7	53688	45	118	2	66	68	2	0	40	7030
11.	*14	000000-00-0	53775	34	112	2	79	68	2	0	39	7038
12.	*12	042484-76-4	53632	32	128	0	86	65	2	0	33	7214
13.	10	085398-08-9	105967	38	80	0	59	67	1	0	33	7275
14.	*10	010207-07-5	53746	31	124	2	70	65	1	0	27	7187
15.	*10	000524-89-0	53656	29	115	0	86	67	1	0	33	7091
16.	*10	000000-00-0	53774	37	99	1	86	68	1	6	35	7159
17.	* 9	001563-84-4	10338	45	64	1	83	79	1	8	37	3951
18.	* 8	032662-57-0	53642	30	108	1	86	68	1	0	29	7031
19.	* 8	002642-98-0	53769	32	108	1	64	68	1	0	29	7032
20.	* 8	000000-00-0	53772	31	116	1	84	68	1	0	29	7038

STP Compounds

Standard 5



Average of 29.214 to 29.264 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	666	58.50	28	71.00	39	82.95	143
49.05	100	61.15	17	73.05	116	83.75	36
49.95	1848	61.90	143	73.95	597	83.95	56
50.95	5616	62.95	189	74.95	902	84.25	24
52.00	441	63.85	3	76.00	315	85.95	48
52.90	89	64.95	121	76.95	4744	88.85	57
54.15	46	66.00	37	78.00	211	91.00	84
55.00	19	66.40	29	78.95	622	92.00	185
56.00	307	67.95	64	79.95	493	93.00	903
56.95	173	68.95	7236	81.00	526	94.05	81
57.75	24	69.95	181	82.00	70	97.00	130

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.90	592	109.95	2416	123.00	213	132.95	33
98.95	416	110.95	532	124.20	33	133.95	80
99.80	31	112.25	33	124.55	21	134.95	134
100.20	42	115.25	34	125.55	20	135.90	32
100.95	262	115.70	65	126.95	3843	136.95	77
102.05	16	116.15	46	127.95	343	138.15	24
103.90	220	116.95	1258	128.95	1939	139.00	33
104.95	146	117.75	11	129.95	190	139.25	26
106.05	43	118.05	55	130.70	16	140.90	220
106.90	1452	119.95	39	131.05	59	141.95	75
108.00	156	121.95	140	131.90	60	142.95	113

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.90	38	154.20	19	165.00	132	177.80	19
145.80	23	154.95	153	166.90	334	178.05	16
146.00	34	156.00	146	168.00	272	179.00	302
146.90	20	157.00	64	170.30	15	179.90	97
147.85	266	157.85	10	171.30	21	180.80	15
148.85	38	160.55	39	171.80	65	185.05	168
150.00	45	161.00	102	172.95	95	186.00	1065
150.95	29	161.90	13	174.05	56	187.00	270
152.70	14	162.40	9	174.95	201	189.15	19
153.05	58	163.00	17	175.95	49	189.65	11
153.95	68	163.90	14	176.90	166	189.90	11

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
190.65	35	197.95	7653	210.65	18	222.55	24
190.90	55	198.95	487	210.90	30	222.90	64
191.95	74	201.30	18	211.15	23	223.20	56
192.75	10	202.80	37	211.90	9	224.00	798
193.05	70	203.05	27	214.15	16	225.00	203

193.90	61	204.00	272	215.00	21	227.00	529				
194.95	26	205.00	399	216.95	497	228.05	17				
195.30	22	206.00	1670	217.75	19	228.45	26				
195.70	72	207.00	117	217.95	53	229.00	82				
196.00	134	207.90	43	221.00	318	234.40	11				
196.95	10	210.25	32	222.20	27	235.15	33				
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.				
235.75	27	256.90	39	295.95	448	364.95	195				
242.15	36	258.00	252	296.80	21	366.15	12				
243.95	838	258.90	19	302.90	55	371.80	32				
244.95	61	264.90	133	322.90	161	402.05	28				
246.00	165	271.80	12	323.80	19	402.95	18				
248.45	9	272.90	197	332.90	12	420.70	10				
248.80	30	273.95	324	333.95	65	420.95	21				
249.05	31	274.95	1505	341.00	15	422.95	272				
252.95	16	275.90	206	351.95	22	423.95	29				
254.95	3624	276.90	137	352.30	18	440.90	754				
255.90	636	292.80	27	353.95	53	441.90	4907				
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.				
442.80	917										
443.95	33										
444.20	34										

Average of 29.214 to 29.264 min.: A0294.D
Converted from RTE data file: >A0294:

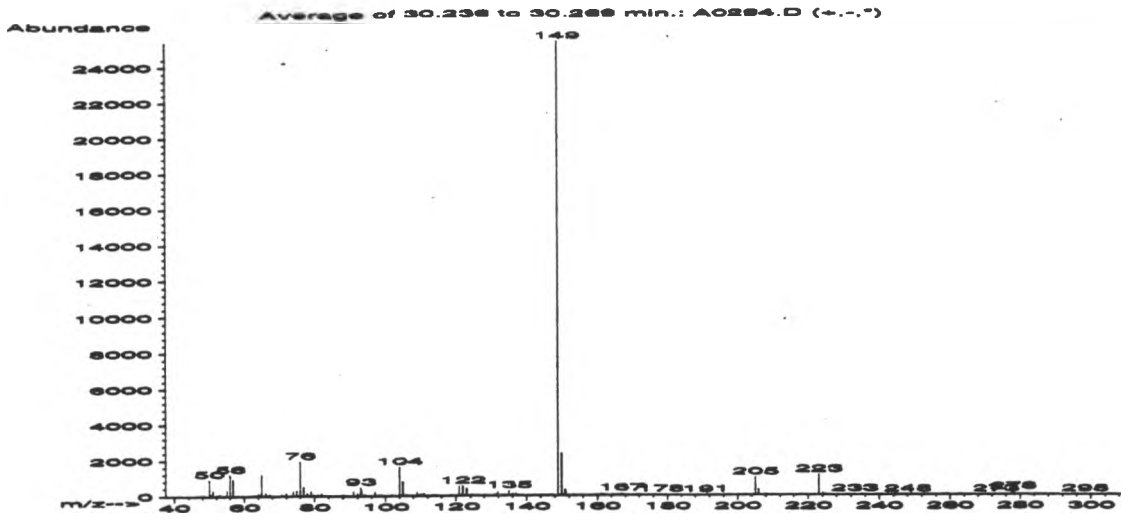
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phosphine, bis(pentafluorophenyl)phenyl-	442	C18H5F10P	94
2.	Phosphine, bis(pentafluorophenyl)phenyl-	442	C18H5F10P	91
3.	Benzene, nitro-	123	C6H5NO2	35
4.	Acetaldehyde, trifluoro-	98	C2HF3O	32
5.	N-BENZENESULFONYLAZETIDIN-3-ONE	211	C9H9NO3S	25
6.	Benzaldehyde, 2-nitroso-	135	C7H5NO2	25
7.	Methyl ester of 4-methoxybenzenebutanoic	208	C12H16O3	25
8.	Benzenamine, N-hydroxy-N-nitroso-, ammon	138	C6H6N2O2	25
9.	Diphenyl Telluride	284	C12H10Te	23
10.	3-(4'-PYRIDINYL)-1-PHENYLPROPENONE	209	C14H11NO	17
11.	Benzene, nitro-	123	C6H5NO2	17
12.	13-(8'-Amino-4'-tosyl-4'-azaoctyl)-12-do	479	C26H45N3O3S	10
13.	7,7-Ethylenedioxy-4a-(2-methoxyethyl)-ci	255	C14H25NO3	10
14.	2-PHENYL-1,3-DITHIANE-5,5-D2	196	C10H10D2S2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	005074-71-5	136554	122	73	0	69	59	70	4	97	8439
2.	*91	005074-71-5	136553	141	61	2	87	15	62	0	91	8289
3.	35	000098-95-3	120296	59	48	2	53	51	11	0	43	3962
4.	*32	000075-90-1	117650	31	55	0	50	50	9	0	33	5781
5.	25	082380-59-4	39797	44	69	2	71	51	7	0	37	3962
6.	*25	029809-25-4	7521	43	61	2	56	51	7	9	30	3962
7.	*25	000000-00-0	38457	35	48	1	54	51	7	0	35	3962
8.	25	000135-20-6	8418	56	35	2	66	51	7	10	37	3962
9.	23	000000-00-0	68234	37	98	1	59	50	6	0	25	4032
10.	17	016208-85-8	39035	33	100	3	61	51	3	0	25	3962
11.	17	000098-95-3	120295	40	61	2	73	51	3	0	27	3962
12.	10	072636-91-0	107395	37	108	1	50	65	1	0	22	4766
13.	10	080595-01-3	58501	33	57	2	99	61	1	0	25	5868
14.	*10	024588-66-7	32741	28	61	3	95	69	1	11	37	5399

STP Compounds

Peak 15



Average of 30.236 to 30.269 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.55	13	56.95	950	72.00	150	87.90	64
48.30	12	57.95	12	74.00	249	88.65	20
48.80	32	60.65	19	74.95	310	90.90	244
49.95	933	61.95	46	75.95	1937	92.00	123
50.55	84	62.90	32	77.00	502	92.95	478
51.00	273	63.20	38	78.00	142	93.15	341
51.95	38	64.05	119	79.10	228	94.05	67
53.00	107	65.00	1186	79.95	49	96.95	207
54.10	43	66.15	148	81.05	73	98.05	40
55.00	327	67.25	78	81.95	134	98.30	37
56.00	1205	70.80	95	86.40	17	98.80	30

Average of 30.236 to 30.269 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	38	113.00	19	124.25	37	136.00	93
101.90	66	113.75	13	124.80	20	137.00	100
104.05	1638	114.00	28	126.20	12	138.00	16
105.00	793	116.15	19	127.85	4	143.50	16
106.05	36	116.50	15	128.30	23	144.70	23
108.00	37	118.15	13	128.70	33	147.00	66
108.95	185	118.80	42	130.70	25	147.45	30
109.40	33	119.95	22	131.15	58	148.95	25358
109.65	35	120.95	528	131.95	213	149.95	2379
110.10	106	121.95	552	133.90	20	150.90	304
111.00	115	123.00	378	135.05	281	153.05	42

Average of 30.236 to 30.269 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
158.40	19	166.15	24	182.25	22	224.10	100
158.75	19	166.95	127	183.00	21	225.05	24
159.00	39	167.40	31	191.00	15	233.00	39
160.00	57	167.75	20	204.20	22	244.05	11
161.15	83	170.05	17	205.05	1009	248.05	13
161.65	18	171.45	41	206.00	291	273.05	12
162.00	24	172.45	14	207.75	25	278.00	161
162.25	26	174.80	20	208.05	42	298.30	11
163.40	17	176.05	22	210.25	29		
164.40	16	178.05	24	218.05	27		
165.15	29	182.00	23	223.05	1145		

STP Compounds

Average of 30.236 to 30.269 min.: A0294.D
Converted from RTE data file: >A0294:

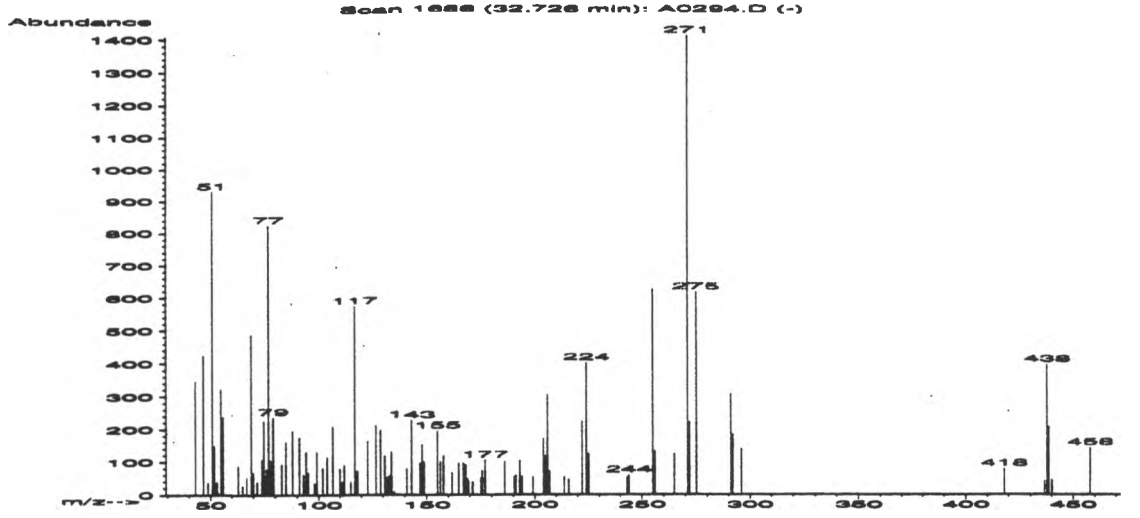
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, butyl 2-me	278	C16H22O4	93
2.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	93
3.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	90
4.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	86
5.	1,2-Benzenedicarboxylic acid, bis(2-meth	282	C14H18O6	86
6.	1,2-Benzenedicarboxylic acid, butyl octy	334	C20H30O4	83
7.	1,2-Benzenedicarboxylic acid, butyl octy	334	C20H30O4	78
8.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	72
9.	1,2-Benzenedicarboxylic acid, butyl 2-et	334	C20H30O4	72
10.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	64
11.	1,2-Benzenedicarboxylic acid, butyl 8-me	362	C22H34O4	64
12.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	64
13.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	64
14.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	64
15.	1,2-Benzenedicarboxylic acid, butyl decy	362	C22H34O4	64
16.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	56
17.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	53
18.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	50
19.	1,2-Benzenedicarboxylic acid, monobutyl	222	C12H14O4	50
20.	CYCLOHEXYL PENTYL PHTHALATE	318	C19H26O4	50

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	017851-53-5	66360	82	22	1	77	6	66	0	93	9993
2.	*93	000084-74-2	132526	84	25	1	88	6	66	44	90	9981
3.	*90	000084-69-5	132535	68	43	2	77	10	59	0	76	9979
4.	86	000084-64-0	75219	74	32	3	99	6	53	0	45	9984
5.	86	000117-82-8	132666	81	21	1	91	6	53	0	47	9992
6.	83	000084-78-6	134557	69	50	3	91	4	50	0	42	9993
7.	78	000084-78-6	84070	61	56	3	97	10	46	0	39	9986
8.	72	000084-74-2	132529	62	38	2	74	12	42	0	43	9980
9.	72	000085-69-8	84071	58	52	3	99	12	42	0	39	9983
10.	64	000084-69-5	132539	54	48	2	85	10	37	6	37	9986
11.	64	000089-18-9	90782	56	60	2	95	10	37	3	37	9961
12.	64	000131-18-0	133655	59	56	2	99	16	37	0	39	9979
13.	64	000131-16-8	131292	43	44	1	88	18	37	2	41	9973
14.	64	000131-16-8	56409	58	44	1	86	16	37	0	43	9973
15.	64	000089-19-0	90781	58	54	2	99	10	37	13	35	9967
16.	56	000084-69-5	66362	55	58	3	93	12	30	0	36	9984
17.	*53	000084-74-2	132527	62	51	1	54	37	28	0	56	9996
18.	50	000605-45-8	131296	59	45	2	78	16	25	0	37	9977
19.	50	000131-70-4	129812	57	38	1	88	16	25	16	37	9980
20.	50	000000-00-0	79548	45	63	1	69	16	25	0	37	9976

STP Compounds

Standard 6



Scan 1686 (32.726 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	346	69.00	486	85.00	160	110.00	79
46.80	424	70.00	66	88.00	195	111.05	37
48.90	36	71.05	2	91.05	174	112.15	89
50.95	931	71.80	38	92.95	61	115.05	38
51.80	149	73.95	108	94.05	129	117.00	573
53.00	38	74.95	224	95.00	66	118.25	71
55.00	321	76.05	77	97.95	34	123.05	163
55.95	237	77.00	823	99.00	129	126.95	210
63.00	87	77.95	104	101.95	80	128.95	197
64.95	26	79.05	236	103.95	113	130.95	117
66.95	52	83.00	92	106.75	206	131.75	50

Scan 1686 (32.726 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.65	54	156.40	100	175.70	72	207.00	70
133.15	56	158.00	118	176.95	105	213.75	53
133.90	130	161.90	66	186.00	101	215.75	45
135.00	8	164.90	96	190.40	54	222.05	223
141.00	79	167.00	96	191.15	58	224.05	400
143.15	227	167.50	69	193.00	104	225.05	123
147.05	95	168.00	90	194.05	54	243.05	53
147.30	92	168.95	47	199.20	52	243.95	59
147.95	151	169.30	37	204.05	170	255.05	626
148.80	100	171.30	37	205.10	116	256.00	131
155.05	195	175.00	51	206.00	302	265.00	123

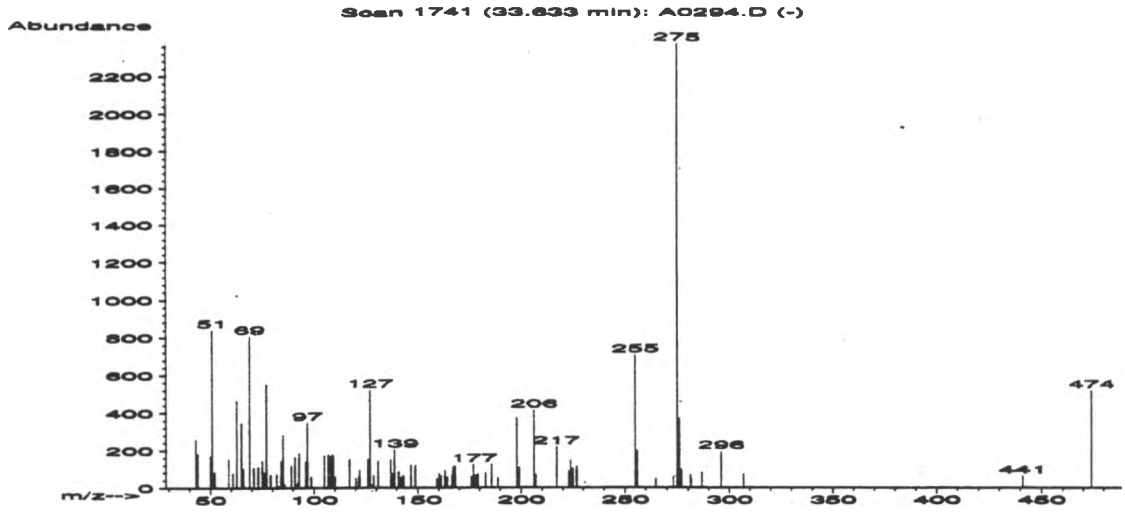
Scan 1686 (32.726 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
270.95	1407	457.90	142				
271.80	220						
274.95	617						
291.00	305						
291.90	183						
295.95	139						
417.95	78						
436.75	40						
438.00	396						
438.75	205						
440.25	43						

STP Compounds

Standard 7



Scan 1741 (33.633 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	257	71.00	107	85.95	17	109.15	177
43.95	180	73.00	112	89.15	117	109.95	56
49.90	169	74.95	144	90.90	166	115.00	7
50.80	839	75.80	81	92.10	25	117.00	152
51.95	82	77.05	552	92.90	184	120.05	50
58.90	157	79.05	69	96.05	139	121.55	62
60.90	79	81.05	1	96.80	347	121.95	92
62.75	468	81.95	72	98.70	57	125.80	153
65.00	348	83.00	9	105.05	171	126.95	521
65.90	100	84.15	145	106.95	177	128.00	14
68.95	807	85.15	282	108.15	170	128.90	63

Scan 1741 (33.633 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.95	143	161.00	64	182.90	79	226.80	113
137.15	150	163.00	91	185.90	126	255.05	706
138.00	73	164.15	54	188.90	51	256.00	196
139.00	203	166.00	10	197.95	375	264.65	47
141.00	84	166.50	66	199.05	107	273.05	57
142.15	53	166.90	112	206.15	415	274.95	2371
143.15	66	168.00	116	206.95	67	275.80	370
146.80	122	175.95	60	217.00	219	276.80	95
148.80	118	177.05	123	222.95	88	281.15	66
159.00	50	178.05	65	223.95	146	281.50	47
160.15	75	179.20	72	225.05	102	286.65	81

Scan 1741 (33.633 min): A0294.D

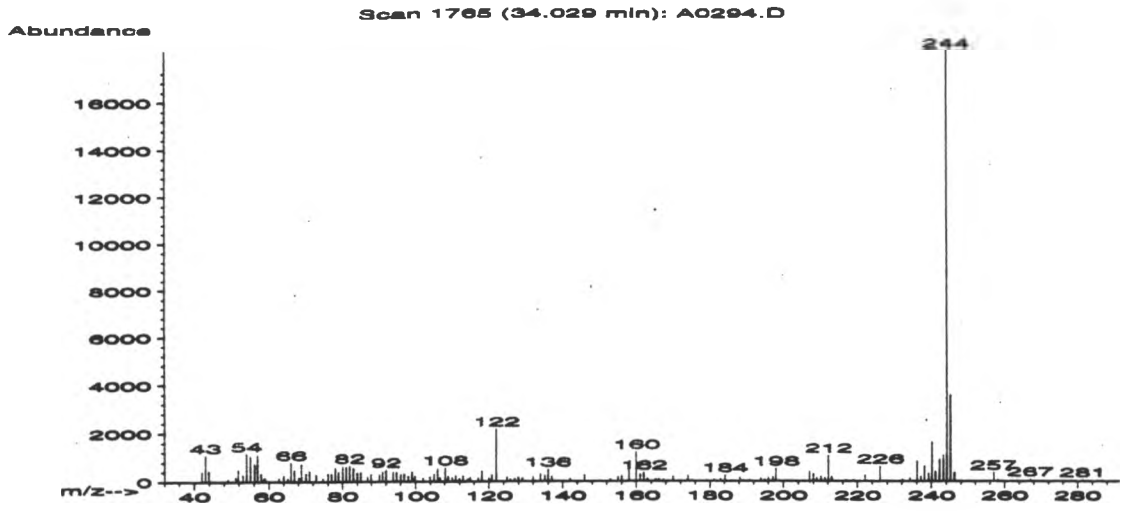
Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
295.95	192						
306.90	72						
441.15	61						
473.95	517						

STP Compounds

STP Compounds

Standard 8



Scan 1765 (34.029 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	410	64.00	253	78.95	194	92.05	307
49.05	104	65.15	127	80.05	629	93.90	219
51.05	199	66.00	661	81.05	185	95.00	40
51.80	428	67.00	478	81.95	419	96.05	275
53.00	32	68.25	187	83.05	110	98.05	117
53.95	1003	70.05	329	84.00	154	99.05	401
56.20	729	72.80	274	85.00	375	99.80	209
57.00	185	74.70	136	86.90	183	102.05	149
58.75	124	76.05	338	87.90	307	103.95	203
59.00	15	76.95	66	90.15	276	105.05	320
62.75	138	78.05	461	90.95	116	106.05	435

Scan 1765 (34.029 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.75	150	122.05	2170	142.00	110	166.00	93
108.15	581	125.00	35	145.95	266	169.95	191
110.05	47	125.80	82	153.05	95	174.05	221
112.05	58	127.00	10	155.05	176	182.90	107
113.00	224	128.00	35	156.00	177	184.15	254
114.25	87	129.05	125	158.00	662	188.25	163
114.90	171	132.00	189	160.00	1099	190.90	68
117.15	139	134.00	291	161.00	278	193.95	127
118.15	443	135.15	225	162.00	360	195.05	66
120.05	147	136.05	362	163.00	97	195.95	140
120.85	129	137.00	181	165.15	108	197.20	171

Scan 1765 (34.029 min): A0294.D

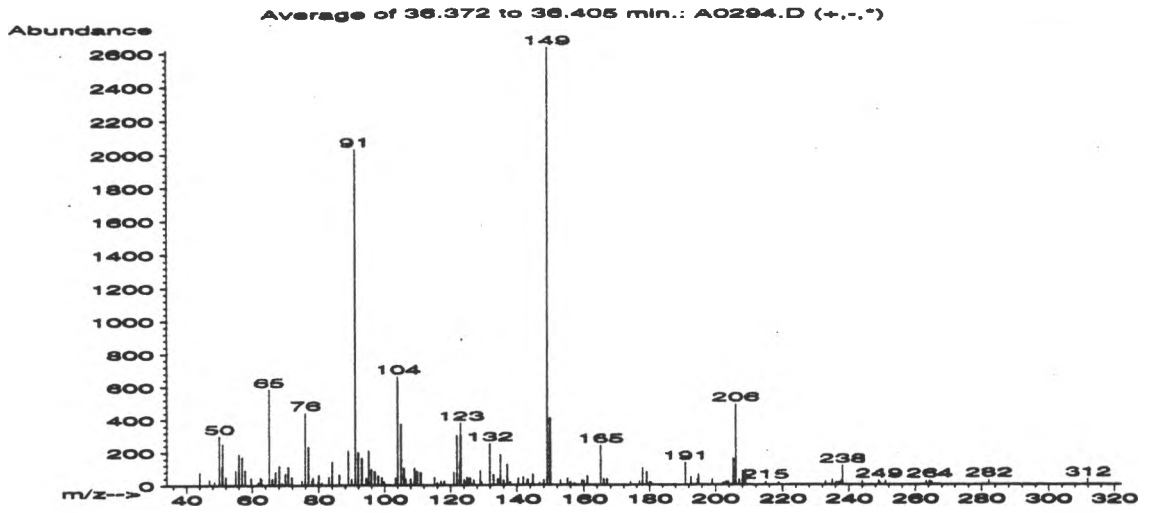
Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
198.05	523	234.10	42	246.20	356		
207.95	153	236.15	819	257.00	356		
209.00	61	237.15	183	258.15	60		
210.15	200	238.15	628	267.00	84		
211.15	129	239.25	324	281.40	69		
212.15	1063	240.15	1634				
213.00	174	241.15	396				
216.90	38	242.15	900				
222.05	251	243.20	1083				
226.20	614	244.20	17886				
232.15	94	245.20	3480				

STP Compounds

STP Compounds

Peak 16



Average of 36.372 to 36.405 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	78	59.65	43	71.90	48	86.15	64
46.90	33	61.75	18	74.95	29	88.95	207
48.55	21	62.40	46	75.95	441	90.00	37
49.90	300	62.75	41	76.95	233	91.00	2024
50.80	115	65.05	583	78.00	27	91.95	201
51.00	251	66.00	38	78.30	44	93.00	164
51.95	50	67.00	81	79.80	18	94.30	42
55.00	92	68.10	118	80.05	62	95.00	210
56.00	190	69.00	11	81.00	13	95.90	95
56.95	171	70.00	71	83.05	50	97.00	84
57.95	92	70.90	113	84.00	142	98.05	57
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.20	44	115.15	49	126.05	12	140.40	40
99.95	20	116.00	15	127.05	29	141.95	48
103.30	44	117.05	25	129.00	86	143.15	31
104.00	661	118.00	26	129.30	17	143.40	31
105.05	373	121.00	80	131.85	252	144.80	66
106.00	103	121.95	303	132.95	63	146.80	12
106.40	34	122.80	136	134.25	36	147.95	31
108.00	39	123.05	380	135.05	184	149.00	2622
109.15	102	124.05	32	136.00	28	149.95	409
110.00	85	124.95	48	137.05	125	152.95	28
111.05	78	125.80	43	137.90	19	155.05	39
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
156.00	17	177.85	102	203.45	19	233.00	22
157.15	12	179.20	77	203.80	17	235.00	31
159.25	28	180.05	16	205.15	162	236.15	16
159.65	22	180.45	13	206.00	488	237.00	15
160.00	25	191.00	135	207.00	30	237.65	26
161.00	57	192.75	49	208.05	84	238.05	115
165.00	241	194.70	32	208.50	40	243.95	21
166.00	37	194.95	63	208.90	92	248.95	25
167.00	37	199.05	33	214.90	20	249.20	15
174.20	19	202.30	16	218.70	13	250.95	23
176.95	24	203.05	19	218.95	13	263.25	21
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
264.25	25						
264.90	16						
282.15	29						
311.90	32						

STP Compounds

Average of 36.372 to 36.405 min.: A0294.D
Converted from RTE data file: >A0294:

PBM Search of library F:\LIBRARY.L

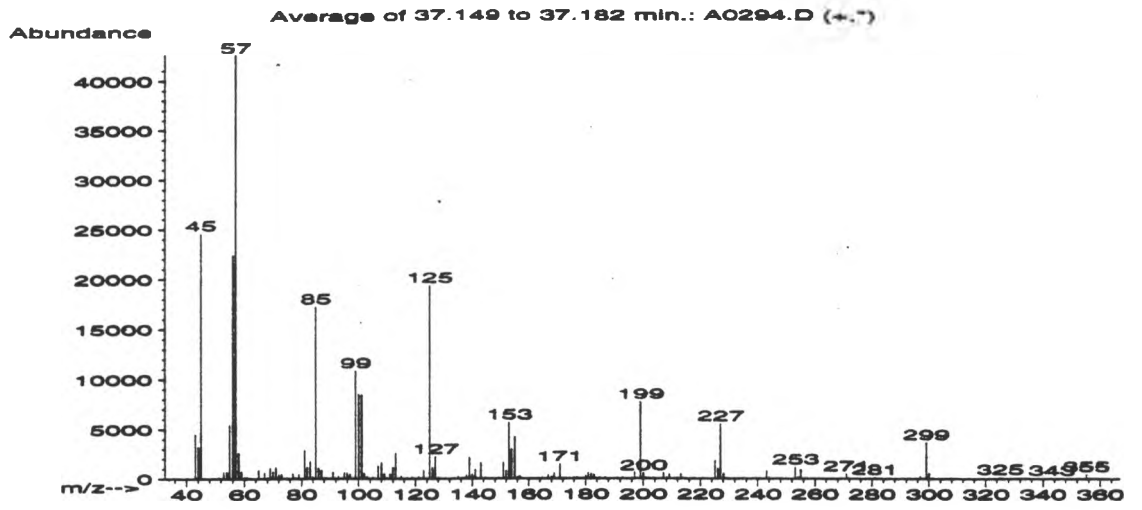
	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	93
2.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	86
3.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	83
4.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	62
5.	Benzenebutanamine	149	C10H15N	50
6.	Benzenamine, 4-butyl-	149	C10H15N	50
7.	PHENYLPROPANAMIDE	149	C9H11NO	49
8.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	47
9.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	47
10.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	47
11.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	45
12.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	43
13.	Tricyclo[4.3.1.1(3,8)]undecane-1-carboxy	208	C13H20O2	43
14.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	40
15.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	38
16.	1,2-Benzenedicarboxylic acid, butyl phen	312	C19H20O4	38
17.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	38
18.	1H-s-Triazolo[1,5-a]pyridin-4-ium, 2-hyd	149	C7H7N3O	38
19.	2-(2-CARBOXYVINYL)PYRIDINE, TRANS	149	C8H7NO2	38
20.	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000085-68-7	77664	112	36	2	95	13	68	0	93	9899
2.	*86	000085-68-7	133825	94	54	2	87	29	53	0	90	9877
3.	83	000085-68-7	133828	98	50	3	69	15	50	0	56	9906
4.	*62	000085-68-7	133824	72	74	1	83	26	36	4	53	9827
5.	*50	013214-66-9	123516	34	14	0	480	33	25	0	41	9558
6.	*50	000104-13-2	123500	34	14	0	480	33	25	0	41	9558
7.	*49	000102-93-2	12324	54	53	2	95	38	23	19	47	9394
8.	47	000084-66-2	129815	55	62	2	80	40	20	9	38	9451
9.	47	000605-45-8	131296	65	51	1	72	37	20	9	38	9444
10.	47	000084-66-2	129818	50	65	2	78	36	20	11	38	9490
11.	45	000085-68-7	133823	62	72	1	99	23	19	14	35	8837
12.	43	000084-74-2	132531	44	65	0	93	44	18	0	39	9402
13.	*43	031083-60-0	38597	36	66	2	99	47	18	14	43	9253
14.	40	000085-68-7	133826	38	31	0	79	33	16	8	37	9641
15.	38	000084-66-2	129819	53	69	3	93	37	14	16	37	9435
16.	38	000085-68-7	133827	44	21	2	68	38	14	0	37	9547
17.	38	000084-66-2	129816	48	68	2	69	40	14	7	35	9458
18.	*38	013980-64-8	12217	33	44	0	82	50	14	10	39	9228
19.	*38	007340-22-9	12247	34	43	2	99	50	14	0	39	8264
20.	*38	000700-87-8	12233	33	73	2	79	50	14	0	39	9239

STP Compounds

Peak 17

1002



Average of 37.149 to 37.182 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4474	54.95	5449	67.00	626	77.00	555
44.00	3220	56.05	22373	68.05	160	77.80	80
44.95	24587	57.00	42637	68.95	1090	78.05	130
48.80	52	58.00	2593	69.95	754	79.00	461
49.70	43	58.95	729	70.95	1174	79.80	43
50.05	82	60.00	166	72.00	408	80.05	78
51.05	170	60.90	153	73.00	463	81.00	2877
51.80	26	61.90	11	73.95	42	81.95	1188
52.05	51	62.80	66	74.70	42	83.00	1756
53.00	690	64.95	890	74.95	91	84.00	202
54.00	707	66.15	41	75.95	42	85.00	17250
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
86.00	1112	93.95	58	105.05	161	117.00	127
87.00	843	94.95	614	105.75	59	119.00	167
87.90	54	95.95	569	106.90	1307	119.70	43
88.15	72	97.00	470	107.95	1615	121.05	238
88.75	73	97.95	67	108.95	526	121.80	64
89.00	127	98.95	10833	110.05	107	122.00	105
89.90	29	100.05	8478	111.00	503	122.95	837
90.15	23	101.05	8414	111.95	1166	123.95	81
90.95	661	102.00	539	113.00	2588	124.95	19344
91.95	99	103.05	191	113.95	89	126.00	1139
92.95	247	104.05	24	114.95	275	127.00	2255
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.95	146	138.95	2109	153.00	5684	166.25	51
129.05	37	139.95	410	153.95	2979	166.95	399
132.90	64	141.00	955	155.00	4211	168.10	218
133.15	77	141.90	32	156.05	203	168.95	582
133.75	26	142.95	1589	156.80	255	170.95	1461
135.00	215	144.00	37	157.15	101	172.95	13
136.00	53	144.80	58	161.00	23	176.00	147
136.95	141	146.70	47	162.90	17	176.95	165
137.25	65	148.85	93	163.15	51	179.00	81
137.65	88	151.00	1663	164.90	153	179.25	81
137.95	365	152.00	800	165.90	48	180.05	296
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
181.00	626	193.00	135	208.15	56	225.05	1811
181.95	482	194.20	27	209.00	431	226.05	1000
183.00	404	194.55	28	210.00	19	227.05	5531
183.65	28	196.00	74	211.00	72	228.10	534
184.90	88	197.00	662	212.00	125	229.10	111

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
186.95	103	199.05	7714	213.05	480	232.90	23
188.15	18	200.05	547	214.00	89	234.00	14
190.20	25	201.00	114	214.90	43	235.05	48
191.15	100	204.45	15	215.15	68	239.00	47
191.40	38	206.95	539	217.00	25	239.65	31
192.40	18	207.90	51	220.80	26	240.25	15
241.15	48	280.95	119	326.05	114		
243.05	811	282.00	29	328.95	13		
244.00	103	282.40	14	341.00	14		
245.20	25	283.00	74	343.00	65		
253.15	1181	296.90	266	355.15	451		
254.20	187	297.80	23	356.25	26		
255.05	924	298.05	25				
256.15	44	299.05	3668				
268.45	11	300.05	549				
269.20	35	325.00	158				
271.05	482	325.80	32				

Average of 37.149 to 37.182 min.: A0294.D
Converted from RTE data file: >A0294:

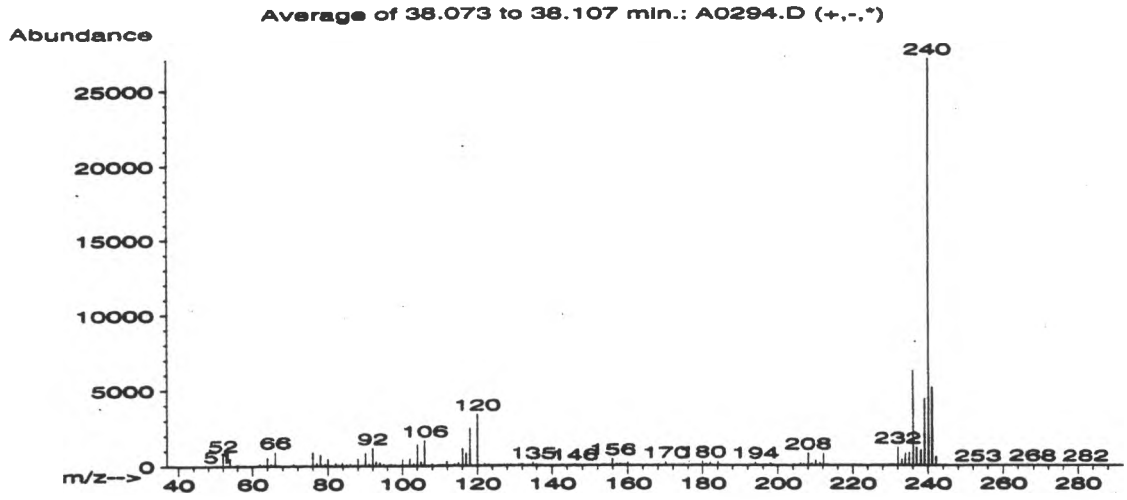
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	72
2.	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	38
3.	BIS(2-BUTOXYETHYL) ETHER	218	C12H26O3	37
4.	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	32
5.	B-D VACUTAINER IMPURITY	398	C18H39O7P	32
6.	2-Propanone, ethylhydrazone	100	C5H12N2	16
7.	Dodecane, 3-methyl-	184	C13H28	10
8.	Undecane, 3,9-dimethyl-	184	C13H28	10
9.	Pentadecane	212	C15H32	10
10.	Hexadecane	226	C16H34	10
11.	Tetracontane, 3,5,24-trimethyl-	605	C43H88	10
12.	2H-Pyran-2-one, tetrahydro-	100	C5H8O2	10
13.	4-(Tetrahydropyran-2-yloxybut-2-ynal	168	C9H12O3	10
14.	Tridecane	184	C13H28	9
15.	Dodecane, 1-iodo-	296	C12H25I	9
16.	Hexadecane, 1-iodo-	352	C16H33I	9
17.	Tridecane	184	C13H28	9
18.	Nonadecane	268	C19H40	9
19.	Pentadecane	212	C15H32	9
20.	Tetradecane	198	C14H30	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000078-51-3	135984	112	48	1	75	20	42	7	45	9514
2.	38	000078-51-3	97400	89	75	1	36	36	14	0	35	9675
3.	37	096077-18-8	42759	39	70	2	99	44	13	8	35	8337
4.	32	000078-51-3	135985	42	97	0	21	48	9	0	33	9676
5.	32	000000-00-0	97401	41	93	0	21	48	9	0	33	9676
6.	*16	007422-99-3	1115	41	30	1	48	58	3	1	36	6441
7.	10	017312-57-1	27733	45	62	2	99	68	1	4	33	6495
8.	10	017301-31-4	27756	41	63	3	99	66	1	0	33	6817
9.	10	000629-62-9	129234	46	62	3	87	77	1	0	39	5309
10.	*10	000544-76-3	130123	35	84	2	99	77	1	0	39	5733
11.	10	055162-61-3	112523	44	124	3	99	66	1	0	37	6653
12.	*10	000542-28-9	1083	33	56	2	84	75	1	0	41	5215
13.	*10	066725-78-8	20211	33	82	3	99	68	1	0	35	6274
14.	9	000629-50-5	127252	38	74	2	68	78	1	0	33	5620
15.	9	004292-19-7	72273	50	76	3	70	76	1	0	31	4982
16.	9	000544-77-4	88383	43	101	3	64	76	1	0	34	4303
17.	9	000629-50-5	127254	45	62	2	99	78	1	0	37	5920
18.	9	000629-92-5	132085	55	62	3	99	80	1	0	36	5252
19.	9	000629-62-9	129232	44	62	2	99	78	1	0	37	5674
20.	9	000629-59-4	128275	39	69	2	99	77	1	0	33	5754

STP Compounds

Standard 9



Average of 38.073 to 38.107 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.95	24	63.95	567	82.05	206	92.00	1177
48.05	13	64.95	133	83.05	16	92.95	287
49.95	37	66.00	954	83.80	187	93.80	90
50.80	51	70.15	12	84.40	32	94.00	193
51.95	749	70.90	128	85.00	81	95.00	118
53.00	41	73.95	37	85.95	139	96.30	97
54.00	484	76.00	914	87.15	42	97.00	116
56.00	104	77.00	201	88.00	495	97.95	43
61.75	68	78.05	723	89.05	75	98.20	71
62.00	125	79.20	136	90.00	872	98.90	48
63.00	56	80.00	446	91.05	125	100.00	429

Average of 38.073 to 38.107 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.70	39	113.15	19	126.05	70	137.65	25
101.00	70	114.00	142	127.20	65	140.00	38
102.00	503	115.00	189	128.05	56	141.00	37
103.00	162	116.05	1151	129.05	79	141.65	12
104.05	1384	117.00	837	131.15	61	142.00	18
105.00	253	118.05	2463	131.90	84	142.95	79
106.00	1664	120.00	3385	132.15	68	144.90	70
107.95	117	122.05	143	135.00	212	145.95	113
110.05	71	122.95	63	135.95	94	146.20	59
111.10	97	123.20	50	137.00	36	147.20	51
111.95	295	124.00	11	137.25	22	150.05	12

Average of 38.073 to 38.107 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
153.95	97	162.75	18	175.05	36	190.95	29
155.05	79	163.00	34	176.95	37	193.05	51
155.95	456	164.95	66	177.30	28	194.00	217
157.00	118	165.90	30	178.30	30	194.80	28
157.90	112	167.00	20	180.00	280	195.05	40
158.15	86	168.00	67	181.00	118	196.10	78
159.10	81	168.55	13	182.05	169	196.70	23
160.00	197	168.95	15	182.75	15	198.00	144
160.90	26	170.05	228	184.10	245	198.30	46
162.15	14	171.95	41	186.40	12	199.05	16
162.40	19	174.00	46	189.00	35	204.10	96

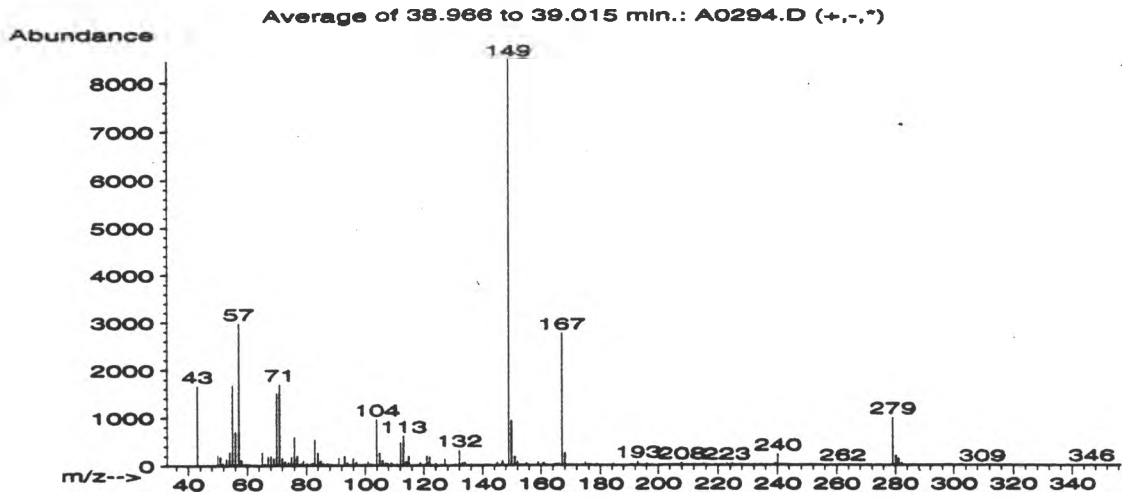
STP Compounds

Average of 38.073 to 38.107 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
206.00	156	220.95	25	235.05	865	266.90	22
207.00	81	222.10	24	236.15	6257	267.80	42
208.05	811	224.95	15	237.10	1183	269.05	19
208.95	38	228.00	84	238.15	1034	271.05	12
209.15	126	229.95	69	239.15	4421	274.70	12
210.10	320	230.20	45	240.15	27058	280.85	30
211.20	180	230.50	19	241.15	5172	281.95	34
212.15	794	231.00	68	242.15	583		
213.15	61	232.05	1205	244.05	24		
219.95	25	233.10	395	253.20	26		
220.45	78	234.05	801	266.00	13		

STP Compounds

Peak 18



Average of 38.966 to 39.015 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1663	58.95	22	71.95	161	80.30	35
46.95	12	59.75	37	72.20	34	81.00	7
49.95	220	60.75	21	72.90	83	81.65	50
50.90	184	62.65	12	74.05	67	82.25	48
51.75	51	65.00	282	75.00	188	82.95	538
53.00	142	65.90	37	76.00	601	84.00	265
54.00	283	67.05	184	77.00	203	85.00	100
55.00	1682	67.95	196	77.95	14	85.90	40
56.00	700	69.00	153	78.20	35	87.15	45
57.00	2979	70.00	1516	79.00	100	87.50	22
57.95	112	71.00	1704	80.00	28	88.75	28

Average of 38.966 to 39.015 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
89.50	13	101.95	34	114.10	85	123.00	9
91.00	158	102.90	8	114.90	201	124.05	47
92.95	193	103.95	958	117.65	17	126.05	20
94.00	64	105.00	258	118.40	16	127.05	141
95.00	14	106.00	113	118.80	63	127.90	12
95.95	152	107.15	55	119.00	13	130.05	16
97.00	73	107.90	38	119.95	15	130.80	22
98.10	17	109.05	60	120.45	19	131.95	321
99.55	10	111.05	29	121.00	200	133.05	62
100.30	23	112.15	481	121.75	71	133.75	16
100.95	79	113.10	617	122.05	181	134.00	73

Average of 38.966 to 39.015 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.00	26	145.95	13	159.00	73	174.95	64
136.40	10	146.75	97	160.75	43	175.80	21
137.05	5	147.00	94	161.00	56	176.30	12
138.65	26	148.95	8443	161.90	18	178.45	18
140.40	8	149.95	936	164.40	27	178.80	31
140.90	20	151.00	182	165.15	41	184.15	14
141.15	21	152.05	83	166.05	28	184.50	37
142.00	13	153.20	9	167.00	2769	190.75	24
144.80	27	153.80	11	168.00	261	191.40	19
145.05	70	154.05	11	170.95	9	192.75	25
145.45	10	155.05	50	173.95	19	193.00	81

STP Compounds

Average of 38.966 to 39.015 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
196.05	35	224.20	19	242.65	10	346.45	16
202.95	11	224.60	35	254.55	17		
205.05	15	224.95	20	262.00	20		
207.00	11	227.30	14	264.40	10		
207.95	48	232.15	14	267.25	11		
211.00	10	234.15	11	268.45	16		
212.40	8	236.15	24	279.05	989		
212.70	18	238.15	9	280.10	199		
215.10	32	239.15	44	280.95	139		
222.90	45	240.10	230	282.10	41		
223.55	11	241.25	11	309.40	12		

Average of 38.966 to 39.015 min.: A0294.D
Converted from RTE data file: >A0294:

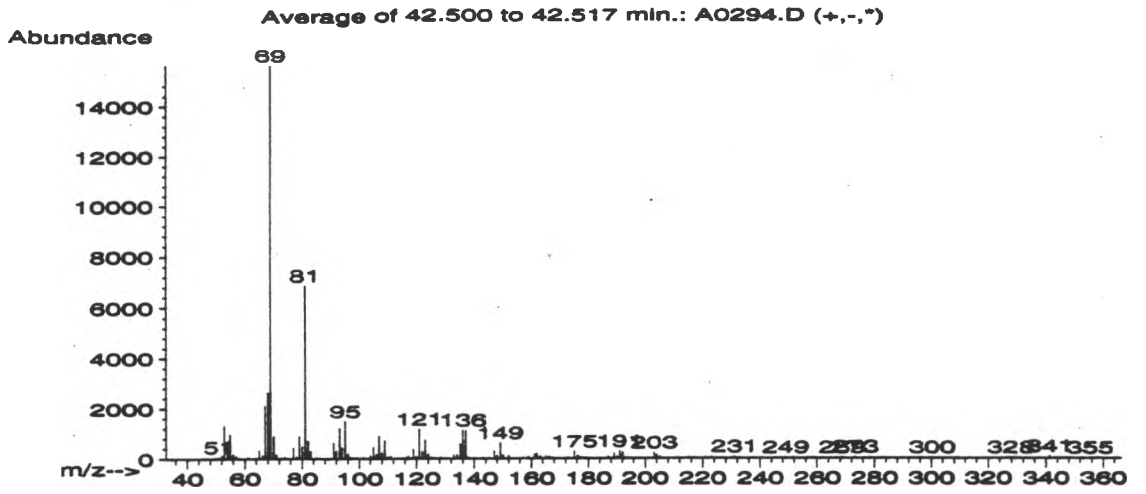
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, 3-nitro-	211	C8H5NO6	87
2.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	80
3.	1,2-Benzenedicarboxylic acid, dioctyl es	390	C24H38O4	64
4.	1,2-Benzenedicarboxylic acid, mono(2-eth	278	C16H22O4	59
5.	1,2-Benzenedicarboxylic acid, dioctyl es	390	C24H38O4	53
6.	1,2-Benzenedicarboxylic acid, dicyclohex	330	C20H26O4	53
7.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	50
8.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	50
9.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	47
10.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	47
11.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	47
12.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	47
13.	CYCLOHEXYL PENTYL PHTHALATE	318	C19H26O4	47
14.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	43
15.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	43
16.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	43
17.	1,2-Benzenedicarboxylic acid, diisooctyl	390	C24H38O4	43
18.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	43
19.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	43
20.	1,2-Benzenedicarboxylic acid, bis(2-meth	282	C14H18O6	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	87	000603-11-2	39769	98	10	1	96	10	54	0	56	9913
2.	80	000117-81-7	135876	78	57	1	76	13	48	0	47	9957
3.	64	000117-84-0	135861	56	86	3	71	20	37	7	41	9876
4.	59	004376-20-9	66373	76	51	3	67	24	33	10	39	9742
5.	53	000117-84-0	135863	44	24	0	85	26	28	0	39	9818
6.	53	000084-61-7	134434	46	83	1	76	30	28	0	39	9753
7.	50	000117-81-7	135873	79	61	0	62	32	25	2	40	9966
8.	50	000131-18-0	133655	54	61	2	99	33	25	0	39	9374
9.	47	000084-66-2	129819	43	63	3	99	36	20	13	41	9278
10.	47	000084-66-2	44597	47	55	2	73	40	20	11	38	9266
11.	47	000084-74-2	132527	46	68	3	86	38	20	0	39	9273
12.	47	000084-69-5	132536	55	47	0	72	40	20	2	41	9347
13.	47	000000-00-0	79548	44	71	3	75	38	20	19	41	9429
14.	43	000131-16-8	131292	45	53	0	76	41	18	0	39	9281
15.	43	000131-16-8	56409	47	55	0	78	41	18	0	39	9259
16.	43	000084-74-2	132529	45	55	2	98	43	18	0	39	9261
17.	43	027554-26-3	135878	81	49	2	65	43	18	5	41	9898
18.	43	000117-81-7	135871	77	55	1	66	41	18	9	39	9900
19.	43	000117-81-7	135874	74	73	2	54	43	18	0	41	9715
20.	43	000117-82-8	132666	61	40	1	85	41	18	0	43	9262

STP Compounds

Peak 19; Squalene



Average of 42.500 to 42.517 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4	64.10	13	77.00	436	93.95	444
49.95	50	64.95	337	78.05	80	95.05	1505
50.95	83	66.10	149	79.05	895	96.00	187
52.00	142	67.00	2110	80.00	474	97.05	62
52.95	1315	68.00	2647	81.05	6879	98.00	41
54.05	233	68.95	15618	82.00	702	99.05	58
55.00	969	70.05	904	83.00	291	100.45	19
56.00	176	71.00	154	85.05	43	101.05	16
56.95	100	72.95	37	91.05	630	101.70	64
61.15	50	73.95	64	92.00	327	102.95	27
63.75	31	74.30	18	93.10	1219	103.95	147

Average of 42.500 to 42.517 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.05	466	117.10	107	127.80	37	143.15	63
106.05	189	117.95	28	128.30	40	145.00	54
107.00	898	118.15	49	128.70	34	147.00	308
108.00	248	119.00	377	128.95	17	148.00	138
109.00	731	120.00	94	132.10	8	149.05	627
110.05	73	121.05	1180	132.90	157	150.00	129
111.05	92	122.00	277	134.00	177	152.00	131
113.05	25	123.00	729	135.05	588	156.90	17
115.00	28	124.00	169	136.05	1146	159.00	93
116.05	46	125.05	52	137.00	1134	161.05	183
116.40	38	125.80	18	138.10	31	162.00	197

Average of 42.500 to 42.517 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.00	35	177.95	22	203.15	231	237.15	32
163.25	100	178.95	15	204.05	131	239.00	11
165.00	89	180.95	10	205.20	64	240.10	21
166.15	86	184.40	25	210.65	35	245.20	29
166.50	23	187.00	94	214.90	46	247.45	29
166.95	20	189.10	200	215.15	40	248.95	38
167.15	31	190.25	72	216.10	25	251.55	20
172.95	20	191.10	303	217.25	31	255.00	9
175.05	281	192.15	231	221.05	58	258.15	40
176.15	121	193.05	25	223.00	74	259.15	27
177.00	52	193.95	44	231.00	84	268.30	28

STP Compounds

Average of 42.500 to 42.517 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
268.70	41	342.30	29				
273.20	62	342.70	29				
282.90	48	345.70	25				
300.20	39	346.95	26				
320.45	19	355.40	30				
326.70	29	355.75	21				
327.80	41						
328.20	22						
328.95	18						
330.90	20						
341.25	96						

Average of 42.500 to 42.517 min.: A0294.D
Converted from RTE data file: >A0294:

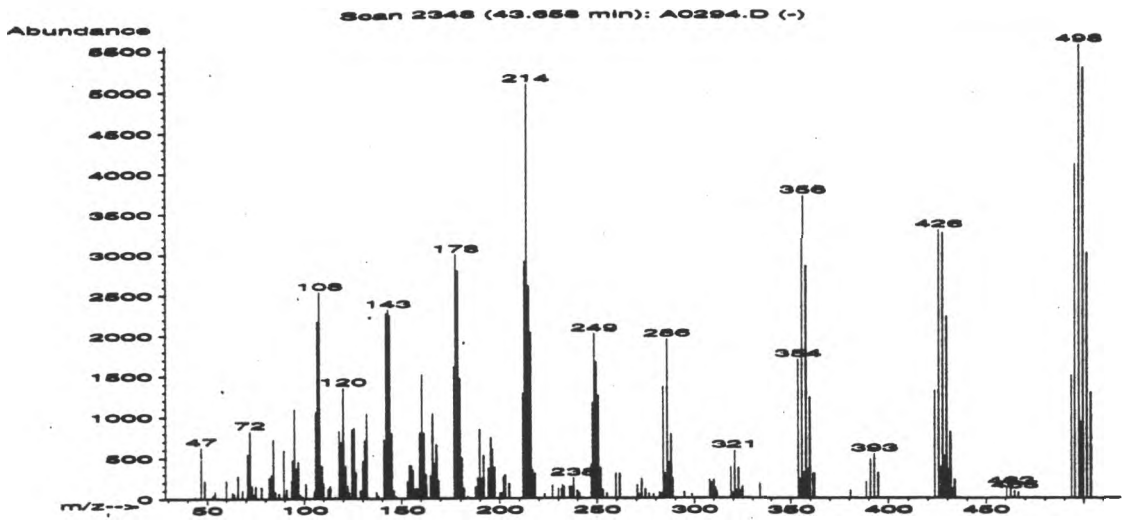
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,6,10,15,19,23-HEXAMETHYL-2,6,10,14,18,	410	C30H50	87
2.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	83
3.	Geranyl acetate	196	C12H20O2	72
4.	11-METHYLSQUALENE	424	C31H52	56
5.	3,7,11-Tridecatrienenitrile, 4,8,12-trim	231	C16H25N	56
6.	trans-Geraniol	154	C10H18O	53
7.	2,6-Octadiene, 4-methyl-	124	C9H16	53
8.	Geraniol formate	182	C11H18O2	53
9.	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	50
10.	Nerol	154	C10H18O	45
11.	Neryl acetate	196	C12H20O2	45
12.	.beta.-Myrcene	136	C10H16	42
13.	Geranyl propionate	210	C13H22O2	42
14.	2,6-OCTADIENE, 2,6-DIMETHYL-	138	C10H18	40
15.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	30
16.	10-DEMETHYLSQUALENE	396	C29H48	25
17.	Lycopersen	547	C40H66	22
18.	cis-Farnesol	222	C15H26O	14
19.	2H-Benzocyclohepten-2-one, 1,4a,5,6,7,8,	178	C12H18O	10
20.	1,5-HEPTADIENE, 2-ETHYL-6-METHYL-	138	C10H18	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	87	000000-00-0	99541	99	33	3	93	9	54	0	51	9986
2.	83	007683-64-9	99537	89	46	2	77	3	50	0	40	9972
3.	72	000105-87-3	128001	46	61	2	99	13	42	13	38	9925
4.	56	063424-36-2	101597	58	73	1	79	15	30	7	35	9844
5.	56	006006-01-5	48808	45	65	3	99	13	30	0	35	9958
6.	53	000106-24-1	124208	56	32	1	74	29	28	0	39	9877
7.	*53	074498-94-5	4878	39	39	0	99	29	28	0	39	9876
8.	53	000105-86-2	127008	44	47	1	74	29	28	23	41	9912
9.	50	018476-57-8	8737	46	27	1	99	33	25	0	39	9845
10.	45	000106-25-2	124194	46	52	2	69	23	19	0	34	9928
11.	45	000141-12-8	127995	45	70	2	75	25	19	0	34	9903
12.	*42	000123-35-3	121977	41	50	2	73	27	17	0	35	9909
13.	42	000105-90-8	129109	45	62	2	88	29	17	0	37	9889
14.	40	002609-23-6	8735	44	43	1	78	33	16	0	35	9877
15.	30	007683-64-9	136175	95	30	0	28	62	9	0	51	9688
16.	25	059681-06-0	97232	63	65	2	56	54	7	1	37	9994
17.	22	000502-62-5	110625	61	56	1	35	62	5	13	39	9812
18.	14	003790-71-4	129869	54	55	0	51	68	2	4	43	9968
19.	10	017429-26-4	24883	44	39	0	11	80	1	0	39	1375
20.	*10	000000-00-0	8744	36	37	0	39	80	1	0	41	9782

STP Compounds

Standard 10



Scan 2348 (43.658 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	18	70.95	543	89.40	590	105.05	92
46.80	626	72.05	826	90.95	112	105.95	1056
48.70	218	73.05	156	93.40	216	106.90	2170
52.95	41	74.00	46	93.95	468	107.90	2532
53.95	81	75.05	145	94.95	1094	109.00	391
59.95	220	78.05	141	95.95	363	109.90	185
63.15	75	81.90	262	96.95	444	112.40	113
63.40	62	82.95	291	97.95	38	112.65	114
64.15	56	84.00	724	99.05	19	113.40	152
65.90	278	84.95	78	100.95	179	115.95	21
68.25	100	87.05	61	104.05	5	117.90	822

Scan 2348 (43.658 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.95	690	131.90	1037	152.95	208	162.80	168
119.95	1350	133.00	3	153.95	403	164.95	283
120.95	392	137.00	79	154.95	399	165.90	1032
121.95	154	138.00	31	155.80	340	166.75	429
122.95	73	140.90	720	157.15	116	167.90	656
124.45	842	142.00	2271	158.00	118	168.95	219
125.45	863	143.00	2311	158.25	113	176.85	1610
126.30	316	143.95	2242	159.25	802	177.80	2990
128.80	93	144.80	795	160.40	1510	178.80	2791
129.95	457	145.85	95	161.40	799	179.80	1460
130.95	710	147.00	23	162.50	295	180.80	496

Scan 2348 (43.658 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
181.90	122	200.20	65	218.00	296	240.90	65
183.95	24	200.95	63	223.05	51	246.95	409
187.75	144	201.95	263	226.95	159	247.80	1167
188.90	248	202.80	287	230.05	119	248.80	2016
189.90	844	204.95	182	231.65	118	249.80	1666
190.95	246	211.90	1288	232.15	162	250.80	1253
191.90	528	212.90	2908	233.00	144	251.95	370
194.30	365	213.90	5055	236.00	143	253.05	102
195.45	746	214.90	2603	236.90	142	255.20	59
196.20	600	215.90	2029	237.90	251	259.65	304
197.30	374	216.75	343	239.95	91	261.75	304

STP Compounds

Scan 2348 (43.658 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
270.55	164	286.90	433	319.70	65	357.75	2840
271.45	49	287.90	781	320.70	583	358.75	352
272.80	238	288.65	242	321.70	94	359.75	1227
274.80	112	294.70	75	322.80	369	361.65	295
276.70	57	298.70	48	323.80	92	361.90	292
278.80	49	307.75	226	324.80	141	380.75	94
281.75	75	308.65	195	333.75	178	388.65	198
282.70	60	309.90	225	353.80	1692	390.75	472
283.75	1363	310.75	121	354.75	240	392.70	538
284.75	304	311.50	78	355.75	3703	394.70	305
285.90	1948	318.80	375	356.90	318	423.70	1309

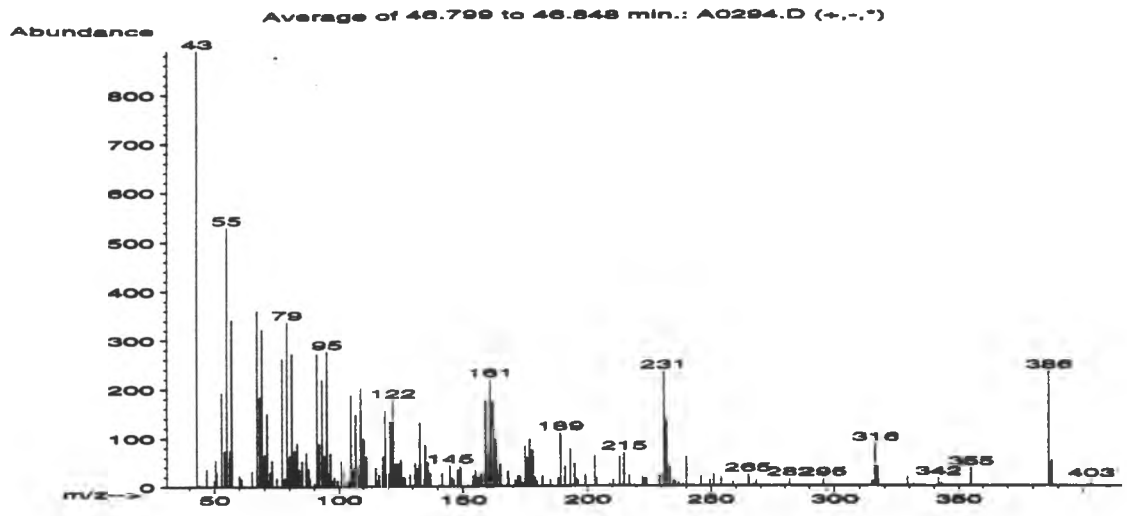
Scan 2348 (43.658 min): A0294.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
425.70	3279	464.65	86				
426.95	378	466.55	69				
427.70	3243	493.70	1494				
428.80	515	495.55	4086				
429.65	2215	497.70	5544				
430.65	339	498.70	923				
431.65	809	499.70	5264				
432.90	113	501.70	2993				
433.75	223	503.70	1285				
460.65	121						
462.65	139						

STP Compounds

Peak 20



Average of 46.799 to 46.848 min.: A0294.D
Converted from RTE data file: >A0294:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	889	56.95	341	72.20	29	85.15	52
44.00	3	60.15	22	73.00	53	86.75	69
46.95	35	60.50	16	74.90	17	87.65	36
49.95	11	60.90	15	77.00	263	88.25	16
50.50	54	65.05	32	78.05	17	90.15	6
50.95	29	67.00	360	79.00	337	91.05	272
52.90	192	68.00	183	80.00	64	92.05	88
54.00	73	68.95	322	81.00	272	93.10	218
54.95	529	69.95	65	81.95	74	93.85	6
56.05	60	71.00	150	83.05	89	94.05	63
56.30	74	71.95	13	83.90	35	95.05	276
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.00	26	106.95	148	118.90	155	129.00	23
96.55	67	107.75	11	120.00	25	131.00	48
96.95	12	108.00	10	121.00	135	131.40	21
98.10	18	108.40	22	122.00	176	131.95	35
99.45	12	109.05	201	123.05	46	133.00	131
101.00	52	110.05	98	124.00	46	133.95	13
101.20	18	111.05	61	124.80	19	135.00	85
101.80	33	115.00	38	125.10	54	136.00	49
103.80	12	115.75	10	125.45	14	136.95	26
105.00	187	116.40	23	125.85	16	140.95	2
106.00	34	117.95	62	126.90	18	141.85	27
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.95	43	157.90	2	170.95	12	182.00	21
145.95	17	159.10	176	171.95	21	185.15	13
146.95	12	160.00	16	173.05	20	188.25	16
147.90	34	160.20	63	173.95	6	189.10	110
149.05	40	161.05	219	175.00	82	190.95	40
154.00	22	162.05	173	175.45	20	193.00	76
154.90	33	163.05	96	175.95	59	194.00	1
155.95	18	163.50	33	176.95	97	194.75	46
156.90	11	164.95	45	178.00	74	195.30	15
157.15	21	168.10	31	178.90	18	195.90	11
157.40	24	168.40	15	179.55	9	199.05	23
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
203.00	62	223.70	16	240.20	60	295.55	14
203.55	16	224.05	15	246.05	20	314.75	10
209.00	4	229.30	22	249.70	12	315.15	10
210.50	13	231.15	235	251.05	23	316.10	82
213.15	60	231.65	25	254.05	18	316.40	87

214.95	69	232.10	136	258.90	9	317.25	38
217.10	21	233.25	38	264.95	23	329.20	18
219.15	2	234.75	10	265.25	16	331.90	3
222.45	18	235.50	9	267.05	3	341.75	16
223.00	11	236.95	7	268.30	11	342.95	5
223.30	13	238.90	4	281.90	14	354.70	16
m/z abund.		m/z abund.		m/z abund.		m/z abund.	
355.00	37						
386.25	235						
387.40	52						
403.30	12						

Average of 46.799 to 46.848 min.: A0294.D
Converted from RTE data file: >A0294:

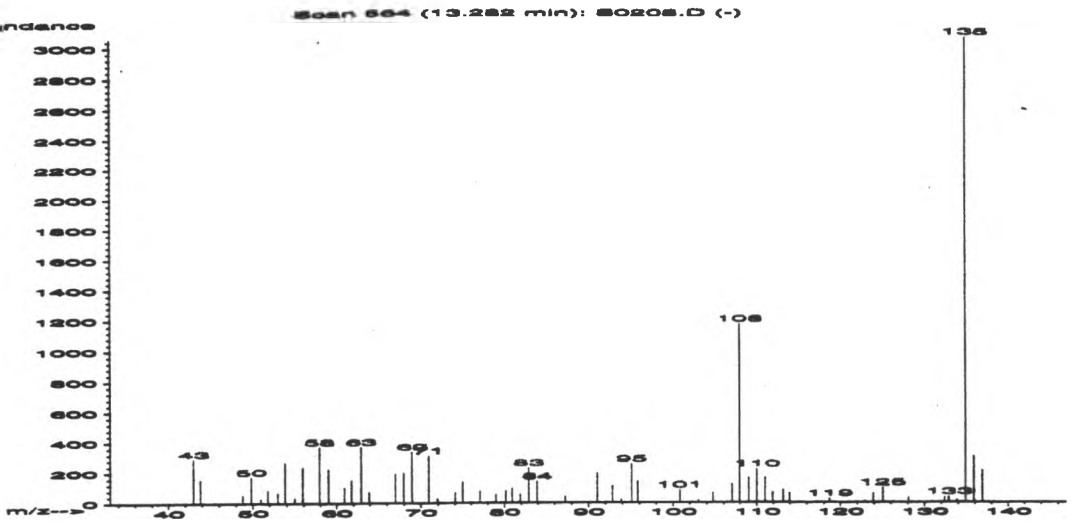
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	B-Homo-A-norcholestan-6-one, (5.alpha.)-	386	C27H46O	18
2.	5.alpha.-Pregnan-3-one, oxime	317	C21H35NO	10
3.	Pregnan-20-one, 5,6-difluoro-3-hydroxy-,	354	C21H32F2O2	10
4.	FURO-EREMOPHIL-9-ONE	232	C15H20O2	10
5.	4a(2H)-Naphthalenecarboxaldehyde, octahy	250	C15H22O3	10
6.	5.alpha.-Pregnane-12,20-dione	316	C21H32O2	9
7.	Pregnane-3,20-dione, (5.alpha.)-	316	C21H32O2	9
8.	Pregnane-3,20-dione, (5.alpha.)-	316	C21H32O2	9
9.	VERIDIFLOROL	222	C15H26O	9
10.	Junipene	204	C15H24	9
11.	Cholest-4-en-3-ol, (3.alpha.)-	386	C27H46O	7
12.	8-Methyl-1,5-dithiaspiro(5,14)eicosan-9-	342	C19H34OS2	7
13.	Pregnane-3,20-dione, (5.beta.)-	316	C21H32O2	7
14.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	7
15.	Tulirinol	306	C17H22O5	7
16.	NEROLIDOL-EPOXYACETATE	296	C17H28O4	7
17.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	6
18.	Pregnenolone	316	C21H32O2	6
19.	(+)-Aromadendrene	204	C15H24	6
20.	12-Nitro-15-hexadecanolide	299	C16H29NO4	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*18	019548-94-8	95490	67	75	3	97	66	3	18	47	6657
2.	10	006845-59-6	79288	43	148	0	65	75	1	0	39	5666
3.	10	056193-66-9	89011	44	138	3	99	63	1	0	22	6700
4.	*10	015404-32-7	49261	37	74	1	23	73	1	0	39	5666
5.	*10	056298-89-6	56528	55	112	3	70	66	1	0	32	6355
6.	9	006022-48-6	79037	61	110	2	94	75	1	0	31	5820
7.	9	000566-65-4	134044	53	126	3	81	75	1	0	36	5416
8.	9	000566-65-4	79032	46	135	3	69	75	1	0	37	5928
9.	* 9	000552-02-3	45053	44	92	3	99	77	1	3	34	6160
10.	9	000475-20-7	128709	53	74	2	42	75	1	0	36	6466
11.	7	000566-90-5	95498	39	141	1	29	72	1	0	24	6834
12.	7	073453-96-0	86041	46	112	3	81	77	1	5	23	5252
13.	* 7	000128-23-4	134041	44	124	2	75	75	1	0	29	7037
14.	7	000057-88-5	135791	35	133	2	50	80	1	0	21	6183
15.	7	072811-84-8	75767	37	38	1	77	77	1	0	21	5350
16.	7	000000-00-0	72435	50	102	2	87	72	1	0	22	6638
17.	* 6	000057-88-5	95482	32	174	3	79	66	1	0	14	6836
18.	6	000145-13-1	134039	36	142	2	90	69	1	0	11	5684
19.	6	000489-39-4	128755	42	83	2	48	80	1	0	17	5517
20.	6	095404-80-1	73511	38	121	2	67	77	1	0	12	5234

STP Compounds

Peak 4a



Scan 564 (13.282 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	291	59.00	224	74.95	135	93.85	20
43.80	154	60.90	103	77.05	78	95.05	256
48.80	55	61.75	151	78.95	58	95.80	141
49.80	173	62.90	371	80.15	81	100.80	83
50.95	29	63.90	72	80.90	98	103.05	17
51.80	86	67.00	192	81.90	54	104.75	65
52.95	67	67.95	197	82.90	229	107.00	121
53.80	268	68.95	337	83.90	141	107.90	1172
54.95	34	70.95	311	87.25	40	109.00	161
55.90	236	71.95	27	91.00	196	110.00	221
57.90	370	74.05	69	92.80	112	111.00	163

Scan 564 (13.282 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.90	67	134.90	3058				
113.15	84	135.90	302				
113.90	62	136.90	210				
118.70	27						
122.95	11						
123.95	59						
125.05	98						
128.05	29						
132.40	35						
132.90	37						
133.85	18						

STP Compounds

Scan 564 (13.282 min): S0208.D

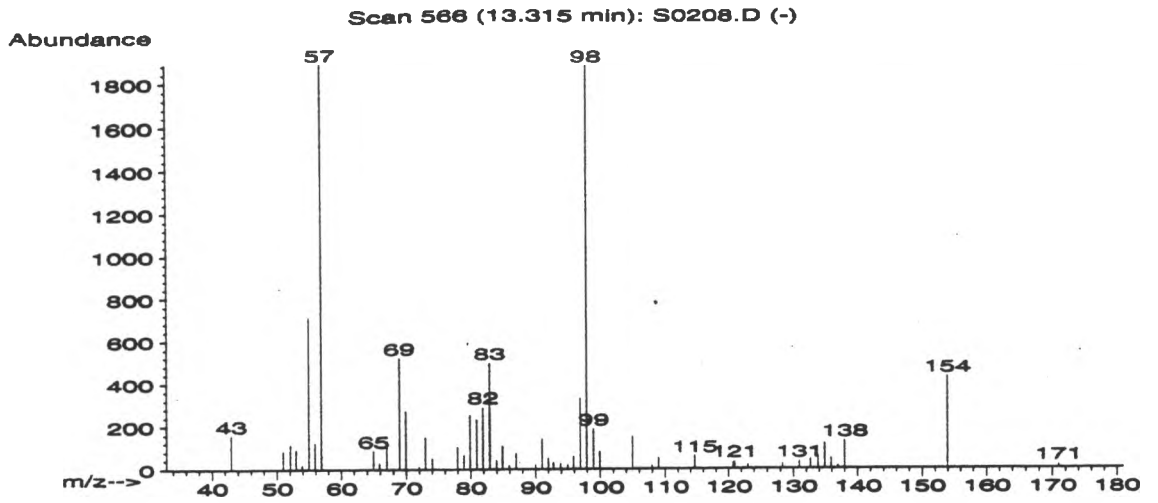
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzothiazole	135	C7H5NS	87
2.	Benzothiazole	135	C7H5NS	83
3.	Benzothiazole	135	C7H5NS	83
4.	Benzothiazole	135	C7H5NS	80
5.	Thieno[3,2-c]pyridine	135	C7H5NS	70
6.	1,2-Benzisothiazole	135	C7H5NS	64
7.	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	64
8.	Thiocyanic acid, phenyl ester	135	C7H5NS	64
9.	1,2-Benzisothiazole-3-carboxylic acid	179	C8H5NO2S	56
10.	Adenine	135	C5H5N5	56
11.	Adenine	135	C5H5N5	56
12.	Adenine	135	C5H5N5	56
13.	Benzothiazole	135	C7H5NS	53
14.	Thieno[2,3-c]pyridine	135	C7H5NS	52
15.	Benzothiazole	135	C7H5NS	52
16.	1,2-Benzisothiazole	135	C7H5NS	52
17.	Pyrazine, 3-ethyl-2,5-dimethyl-	136	C8H12N2	50
18.	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	50
19.	1H-Indole, 5-fluoro-	135	C8H6FN	50
20.	Adenine	135	C5H5N5	50

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000095-16-9	121694	60	35	3	99	10	54	0	51	9948
2.	*83	000095-16-9	121699	59	36	2	85	12	50	0	56	9945
3.	*83	000095-16-9	121698	70	20	1	99	13	50	29	58	9944
4.	*80	000095-16-9	121695	52	14	2	99	13	48	0	46	9942
5.	*70	000272-14-0	7534	69	28	0	70	29	41	0	76	9716
6.	*64	000272-16-2	121700	43	48	3	99	24	37	0	44	9876
7.	*64	002380-63-4	7511	43	31	1	99	18	37	5	38	9855
8.	*64	005285-87-0	7525	37	64	3	99	16	37	0	39	9888
9.	56	040991-34-2	25013	57	37	2	83	12	30	4	37	9876
10.	*56	000073-24-5	121689	37	47	3	99	15	30	10	37	9896
11.	*56	000073-24-5	121687	34	61	2	87	13	30	0	30	9919
12.	*56	000073-24-5	121685	36	67	2	99	13	30	0	35	9926
13.	*53	000095-16-9	121696	37	49	2	78	27	28	0	41	9922
14.	*52	000272-12-8	7533	54	34	1	70	32	27	0	49	9668
15.	*52	000095-16-9	121697	47	38	2	99	32	27	0	44	9618
16.	*52	000272-16-2	7531	49	42	2	75	33	27	0	44	9835
17.	50	013360-65-1	7843	49	43	2	97	16	25	12	33	8457
18.	*50	000459-22-3	7539	55	42	2	99	18	25	7	34	9192
19.	*50	000399-52-0	7540	34	48	1	99	16	25	9	36	9644
20.	*50	000073-24-5	121688	42	42	2	99	20	25	0	35	9877

STP Compounds

Peak 4b



Scan 566 (13.315 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	158	67.95	4	82.95	494	95.90	58
50.95	85	68.95	519	83.95	40	96.95	328
52.05	115	69.95	270	84.90	108	97.95	1868
52.95	90	71.95	12	85.90	17	99.00	186
53.90	20	72.95	148	87.00	73	99.95	82
54.95	710	74.00	50	90.00	21	105.00	150
55.90	122	77.95	104	91.00	140	107.95	15
56.90	1885	78.95	66	92.00	49	109.00	49
65.00	86	79.90	253	92.80	30	114.65	58
65.90	28	80.95	230	93.90	26	120.70	27
67.00	131	81.90	288	95.00	20	120.95	33

Scan 566 (13.315 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.00	16						
128.30	22						
130.90	33						
132.65	45						
133.80	55						
134.90	117						
135.90	46						
136.95	12						
138.00	128						
153.95	425						
170.95	17						

STP Compounds

Scan 566 (13.315 min): S0208.D

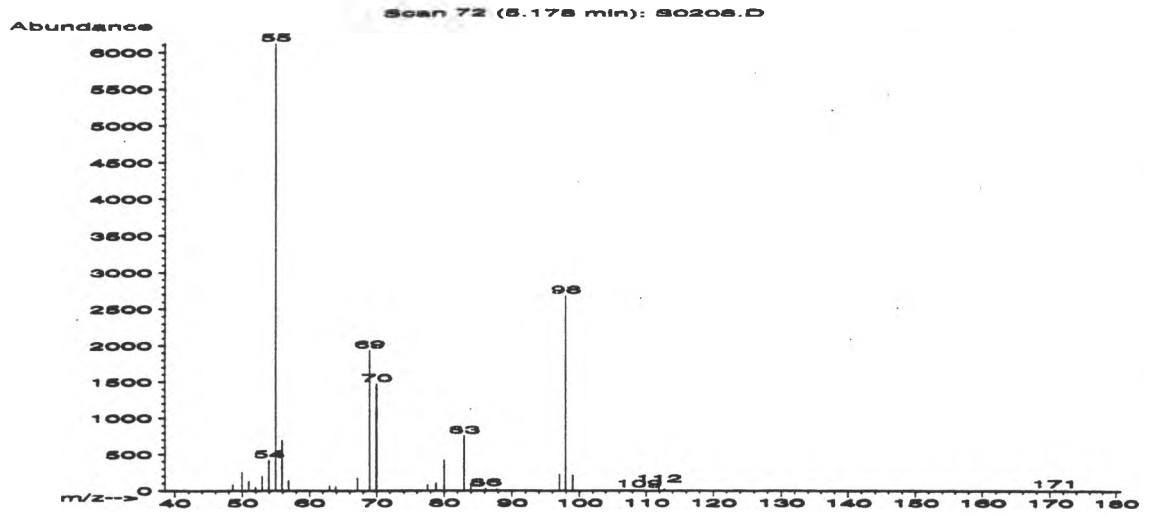
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 4-(1,1-dimethylethyl)-	154	C10H18O	83
2.	Cyclohexanone, 4-(1,1-dimethylethyl)-	154	C10H18O	80
3.	Cyclohexanone, 4-(1,1-dimethylethyl)-	154	C10H18O	59
4.	2-Methyl-3,4-dihydro-2H-pyran	98	C6H10O	53
5.	2-Pentenal, 2-methyl-	98	C6H10O	52
6.	2-Pentenal, 2-methyl-	98	C6H10O	50
7.	Cyclohexylcyclohexanone	180	C12H20O	50
8.	1,3-Dioxolane-2-butanol, 2-butyl-	202	C11H22O3	50
9.	2-Pentenal, 2-methyl-	98	C6H10O	47
10.	2(3H)-Furanone, 5-methyl-	98	C5H6O2	47
11.	1-Oxaspiro[4.5]decane-2,4-dione	168	C9H12O3	43
12.	Cyclohexanone, 2-propyl-	140	C9H16O	40
13.	AMYL CYCLOHEXANONE	168	C11H20O	38
14.	[1,1'-Bicyclohexyl]-2-one	180	C12H20O	37
15.	Furan, 2,5-dihydro-3,4-dimethyl-	98	C6H10O	37
16.	1,3-Dimethylsiletene	98	C5H10Si	32
17.	Piperidine, 1-(2-phenylethyl)-	189	C13H19N	25
18.	2,3,4,5,6-D5-ANILINE	93	C6H2D5N	25
19.	1-Piperidinepropanenitrile	138	C8H14N2	25
20.	3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-	98	C4H6N2O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000098-53-3	124264	61	36	1	93	12	50	0	56	9883
2.	*80	000098-53-3	124265	52	53	2	99	13	48	0	46	9773
3.	*59	000098-53-3	14680	46	52	2	155	24	33	0	40	9398
4.	*53	013039-50-4	884	47	16	1	92	29	28	5	40	9625
5.	*52	000623-36-9	117703	49	44	1	100	35	27	0	46	7076
6.	*50	000623-36-9	117704	37	55	2	141	35	25	0	39	7073
7.	50	000000-00-0	126859	43	19	1	77	35	25	16	38	7040
8.	50	036651-32-8	35532	47	70	0	95	32	25	0	39	7825
9.	*47	000623-36-9	117705	39	39	1	92	40	20	3	38	7088
10.	*47	000591-12-8	117671	49	35	1	99	37	20	0	39	6979
11.	43	022884-78-2	20235	45	37	0	89	41	18	6	41	6958
12.	40	000094-65-5	9389	51	41	2	95	35	16	0	37	7059
13.	38	000000-00-0	20612	44	36	1	76	40	14	0	37	7050
14.	37	000090-42-6	25776	42	44	2	96	41	13	2	31	7013
15.	*37	053720-72-2	880	34	47	1	72	45	13	4	37	6440
16.	*32	084602-65-3	771	34	35	2	82	48	9	0	35	6144
17.	25	000332-14-9	29687	35	52	1	84	51	7	9	31	6757
18.	*25	004165-61-1	442	29	68	1	67	45	7	0	29	6864
19.	*25	003088-41-3	8573	31	54	2	99	45	7	0	29	6814
20.	*25	000108-26-9	735	29	48	2	95	45	7	0	29	6858

STP Compounds

Peak 21 Cyclohexanone



Scan 72 (5.178 min): S0208.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.55	82	67.15	174	97.95	2686		
49.95	255	68.95	1938	99.05	212		
50.95	127	69.95	1474	108.90	15		
51.95	49	77.55	78	111.90	84		
52.95	203	78.80	105	112.75	26		
53.95	425	80.00	425	170.70	18		
54.95	6122	83.00	758				
55.90	699	84.00	95				
56.90	136	86.15	31				
63.00	70	87.75	24				
63.90	59	97.05	224				

STP Compounds

Scan 72 (5.178 min): S0208.D

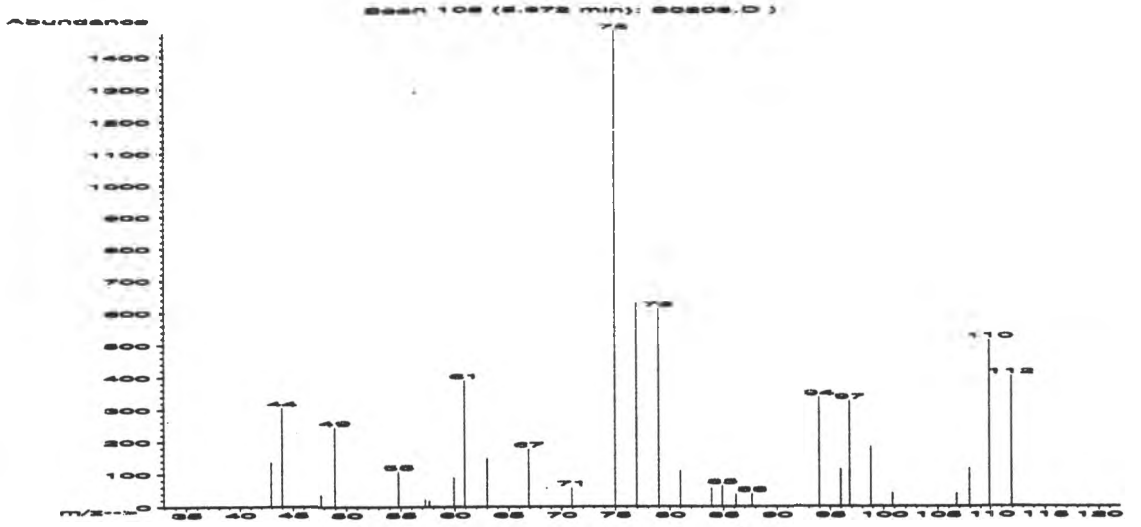
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone	98	C6H10O	91
2.	Cyclohexanone	98	C6H10O	91
3.	Cyclohexanone	98	C6H10O	90
4.	Cyclohexanone	98	C6H10O	86
5.	Cyclohexanone	98	C6H10O	78
6.	Cyclopentanone, 2-methyl-	98	C6H10O	72
7.	Cyclopentanone, 2-methyl-	98	C6H10O	64
8.	Cyclohexanone	98	C6H10O	64
9.	Cyclohexanone	98	C6H10O	64
10.	Cyclohexanone	98	C6H10O	64
11.	Cyclopentanone, 2-methyl-	98	C6H10O	59
12.	2-Pentene, 2,3-dimethyl-	98	C7H14	50
13.	DIETHYLCYANAMIDE	98	C5H10N2	50
14.	3-Penten-2-one, 3-methyl-	98	C6H10O	47
15.	2(3H)-Furanone, 5-methyl-	98	C5H6O2	43
16.	BIS-(2-OXOCYCLOHEXYL PEROXIDE)	226	C12H18O4	39
17.	3-Penten-2-one, 3-methyl-	98	C6H10O	38
18.	2,4-Hexadien-1-ol	98	C6H10O	37
19.	2-Hexene, 3-methyl-, (Z)-	98	C7H14	36
20.	2-Pentene, 3-ethyl-	98	C7H14	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000108-94-1	117749	74	13	0	70	4	62	2	66	9968
2.	*91	000108-94-1	117743	69	20	0	99	4	62	0	76	9967
3.	*90	000108-94-1	117746	65	24	0	78	4	57	14	47	9860
4.	*86	000108-94-1	819	56	40	0	93	6	53	0	49	9921
5.	*78	000108-94-1	117745	49	26	0	95	6	46	1	41	9586
6.	*72	001120-72-5	816	52	43	1	97	20	42	0	46	9022
7.	*64	001120-72-5	117740	43	53	0	63	25	37	0	44	8642
8.	*64	000108-94-1	117748	39	21	0	95	20	37	0	39	9851
9.	*64	000108-94-1	117747	47	58	2	68	18	37	0	40	8383
10.	*64	000108-94-1	117744	51	44	0	59	20	37	2	41	9874
11.	*59	001120-72-5	117739	45	52	1	79	22	33	0	40	9510
12.	*50	010574-37-5	117802	34	58	3	85	31	25	0	41	8055
13.	*50	000617-83-4	760	29	76	2	99	20	25	0	33	9819
14.	*47	000565-62-8	117732	34	54	2	93	37	20	0	41	9621
15.	*43	000591-12-8	117674	35	52	0	51	41	18	0	41	9538
16.	39	000000-00-0	46601	42	72	1	91	20	15	0	29	9934
17.	*38	000565-62-8	798	31	48	2	88	37	14	2	35	9623
18.	*37	000111-28-4	117760	28	68	3	81	43	13	0	33	8986
19.	*36	010574-36-4	907	30	67	2	95	29	12	0	27	9330
20.	*36	000816-79-5	914	32	77	3	111	29	12	0	29	9812

STP Compounds

Peak 22; Trichlorpropane



Scan 102 (5.672 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	136	70.95	57	96.80	323		
43.95	305	74.95	1472	98.80	183		
47.70	37	76.95	630	100.80	40		
48.95	243	78.95	612	106.75	39		
54.80	108	81.00	110	107.90	116		
57.25	22	83.90	55	109.90	513		
57.65	18	84.90	63	111.90	402		
59.90	89	86.15	38				
60.90	386	87.65	39				
63.00	149	93.95	334				
66.90	176	95.95	113				

STP Compounds

Scan 102 (5.672 min): S0208.D

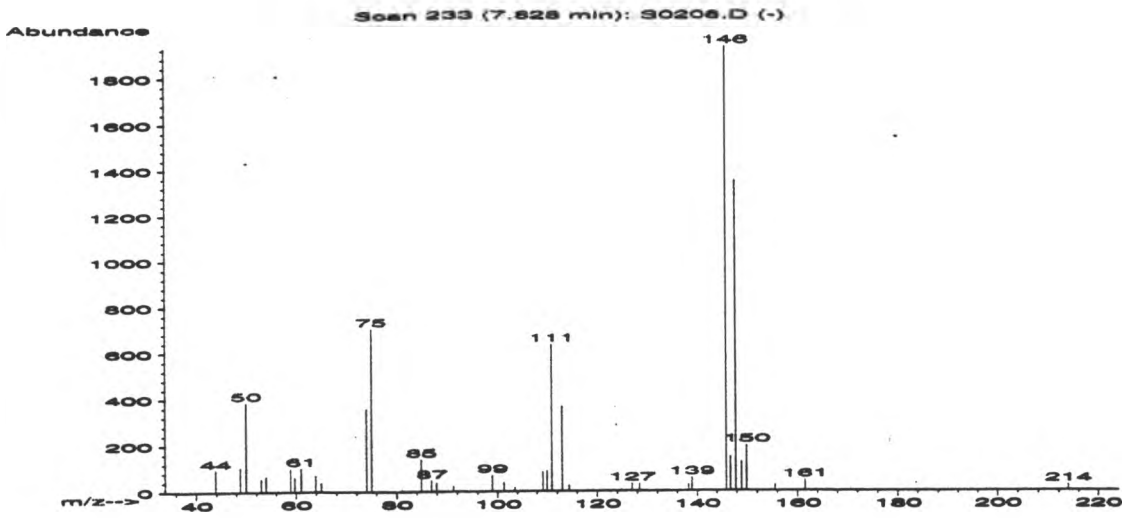
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Propene, 1,3-dichloro-, (Z)-	110	C3H4Cl2	49
2.	1-Propene, 2,3-dichloro-	110	C3H4Cl2	47
3.	1-Propene, 1,2-dichloro-	110	C3H4Cl2	46
4.	Propane, 1,2,3-trichloro-	146	C3H5Cl3	45
5.	Propane, 1,2,3-trichloro-	146	C3H5Cl3	45
6.	1-Propene, 2,3-dichloro-	110	C3H4Cl2	38
7.	1-Propenyl ether of 1-chloropropane	134	C6H11ClO	38
8.	1-Propene, 3,3-dichloro-	110	C3H4Cl2	37
9.	2,2,3-TRICHLOROBUTYRIC ACID	190	C4H5Cl3O2	25
10.	2(3H)-Furanone, 3,3-dichlorodihydro-	154	C4H4Cl2O2	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	010061-01-5	2089	49	52	0	98	39	23	5	44	8845
2.	*47	000078-88-6	2091	40	50	0	99	37	20	11	38	8944
3.	*46	000563-54-2	118810	33	33	0	97	41	20	4	43	8869
4.	45	000096-18-4	123065	51	23	0	99	25	19	7	36	9208
5.	45	000096-18-4	123063	67	37	1	93	21	19	8	35	9075
6.	*38	000078-88-6	118813	33	56	0	99	39	14	9	35	8924
7.	38	000000-00-0	7276	42	10	0	99	39	14	14	35	8826
8.	*37	000563-57-5	2092	34	55	1	95	42	13	11	36	8390
9.	25	005344-55-8	29712	34	65	0	85	44	7	5	26	8868
10.	25	001588-60-9	14164	37	68	0	98	44	7	0	25	8712

STP Compounds

Peak 23



Scan 233 (7.828 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	94	74.95	705	110.95	636	148.95	126
48.80	106	80.95	8	113.00	368	149.95	196
49.95	385	84.90	139	114.40	24	155.50	26
52.95	57	86.95	46	124.85	7	161.50	47
53.95	68	87.90	37	126.95	33	213.90	25
58.90	100	91.25	23	128.45	30		
59.75	60	98.95	71	138.25	28		
61.00	102	101.30	40	138.90	58		
63.85	71	103.45	17	145.95	1928		
65.00	38	109.15	85	146.80	147		
73.95	356	110.00	88	147.80	1349		

STP Compounds

Scan 233 (7.828 min): S0208.D

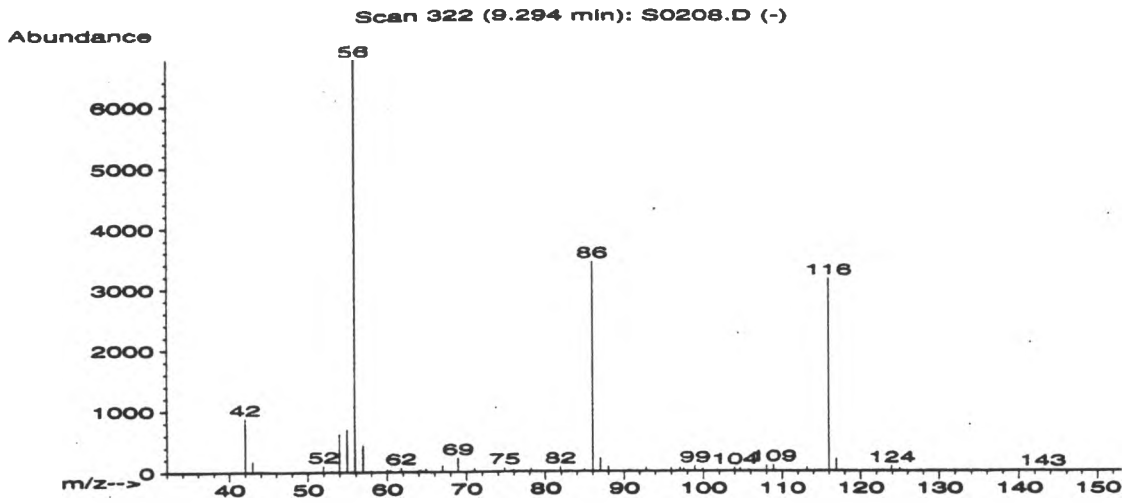
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2-dichloro-	146	C6H4Cl2	94
2.	Benzene, 1,3-dichloro-	146	C6H4Cl2	91
3.	Benzene, 1,3-dichloro-	146	C6H4Cl2	91
4.	Benzene, 1,3-dichloro-	146	C6H4Cl2	91
5.	Benzene, 1,4-dichloro-	146	C6H4Cl2	91
6.	Benzene, 1,4-dichloro-	146	C6H4Cl2	91
7.	Benzene, 1,2-dichloro-	146	C6H4Cl2	91
8.	Benzene, 1,2-dichloro-	146	C6H4Cl2	90
9.	Benzene, 1,3-dichloro-	146	C6H4Cl2	90
10.	Benzene, 1,4-dichloro-	146	C6H4Cl2	87
11.	Benzene, 1,4-dichloro-	146	C6H4Cl2	87
12.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
13.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
14.	Benzene, 1,2-dichloro-	146	C6H4Cl2	81
15.	Benzene, 1,4-dichloro-	146	C6H4Cl2	80
16.	Benzene, 1,3-dichloro-	146	C6H4Cl2	76
17.	(E)-6-Chloro-4-methyl-2-heptene	146	C8H15Cl	50
18.	CIS-DICHLOROMALEONITRILE	146	C4Cl2N2	45
19.	Furan, 3-bromo-	146	C4H3BrO	43
20.	TRANS-DICHLOROFUMARONITRILE	146	C4Cl2N2	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000095-50-1	123077	82	28	0	73	5	70	0	93	9950
2.	*91	000541-73-1	123079	73	36	0	91	5	62	0	81	9942
3.	*91	000541-73-1	123078	82	29	0	93	5	62	20	66	9898
4.	*91	000541-73-1	11153	82	28	0	94	5	62	8	72	9924
5.	*91	000106-46-7	123085	70	41	0	87	5	62	0	76	9959
6.	*91	000106-46-7	123082	81	28	0	92	5	62	16	72	9906
7.	*91	000095-50-1	11151	77	33	0	81	5	62	39	74	9901
8.	*90	000095-50-1	123073	76	34	0	93	7	59	22	68	9890
9.	*90	000541-73-1	123081	63	50	0	82	5	57	8	47	9938
10.	*87	000106-46-7	123084	74	35	1	91	10	54	10	50	9608
11.	*87	000106-46-7	11154	73	34	0	85	14	54	2	66	9845
12.	*87	000095-50-1	123075	73	35	0	90	14	54	2	66	9834
13.	*87	000095-50-1	123074	66	42	0	85	14	54	0	64	9811
14.	*81	000095-50-1	123076	66	34	0	83	16	49	0	64	9835
15.	*80	000106-46-7	123083	67	39	0	86	11	48	1	47	9749
16.	*76	000541-73-1	123080	71	32	1	83	21	45	0	68	9802
17.	*50	092639-31-1	11344	35	78	1	80	19	25	0	35	9340
18.	*45	000000-00-0	11117	38	64	1	85	24	19	0	33	9457
19.	*43	022037-28-1	11119	37	64	0	70	41	18	0	41	8917
20.	*40	000000-00-0	11118	32	61	1	83	32	16	7	34	9522

STP Compounds

Peak 24, nitrosomorpholine



Scan 322 (9.294 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	874	60.00	40	75.95	25	97.55	38
42.95	170	60.40	32	78.20	49	98.95	82
49.80	7	61.75	63	81.90	71	99.95	37
51.95	99	64.00	28	84.95	32	104.00	48
53.00	14	64.25	31	86.00	3444	104.65	42
53.95	621	64.90	49	87.00	209	105.75	23
54.95	695	67.00	98	88.00	68	108.00	85
55.90	6759	68.95	220	90.65	21	108.90	95
56.90	434	69.85	1	92.80	58	113.15	53
57.90	25	71.00	55	95.95	50	116.00	3155
58.95	22	74.80	59	97.05	54	116.95	198

Scan 322 (9.294 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.95	73						
124.95	38						
142.95	16						

STP Compounds

Scan 322 (9.294 min): S0208.D

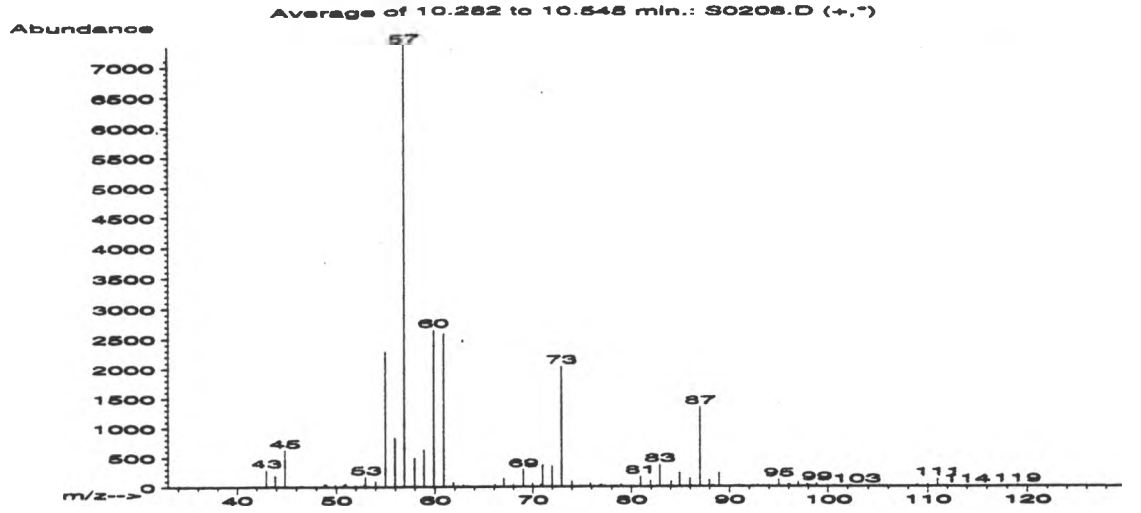
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Morpholine, 4-nitroso-	116	C4H8N2O2	80
2.	Morpholine, 4-nitroso-	116	C4H8N2O2	72
3.	L-Leucine	131	C6H13NO2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000059-89-2	119436	48	37	1	84	15	48	0	46	9905
2.	*72	000059-89-2	119437	37	18	1	81	15	42	11	40	9890
3.	7	000061-90-5	121255	33	42	0	41	75	1	0	25	4250

STP Compounds

Peak 25; unidentified ethoxy compound



Average of 10.282 to 10.545 min.: S0208.D
Converted from RTE data file: >S0208:
Modified:added scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	286	50.20	2	54.00	95	63.25	14
43.85	193	50.45	8	55.00	2279	63.75	2
44.85	623	50.75	39	55.95	828	64.50	5
46.45	2	50.95	54	56.90	7339	64.95	14
46.80	4	51.70	4	57.95	488	65.40	3
47.05	1	52.00	24	58.90	631	65.65	3
47.90	14	52.20	3	59.90	2633	66.10	39
48.80	50	52.45	5	60.90	2576	67.00	145
49.00	43	52.80	42	61.90	80	67.75	8
49.55	3	53.00	167	62.15	4	68.00	36
49.90	37	53.80	2	62.90	32	69.00	287
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.95	61	77.00	33	81.95	106	89.95	3
70.80	38	77.35	8	82.90	369	90.50	1
71.00	363	77.75	4	83.15	8	90.75	3
71.95	346	78.00	15	83.75	5	91.00	22
72.95	2028	78.25	7	84.05	91	91.25	5
74.00	93	78.50	7	84.90	233	92.00	2
74.80	11	78.95	41	85.95	139	92.90	28
75.30	2	79.95	10	87.00	1329	93.30	2
75.85	57	80.25	7	87.95	104	93.95	20
76.20	6	80.95	167	88.30	19	94.20	2
76.80	31	81.70	14	88.95	227	95.00	113
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.45	4	100.80	5	105.10	10	111.75	5
95.90	31	101.20	3	106.35	4	112.10	7
96.10	37	101.90	12	107.05	10	112.40	3
97.00	76	102.15	7	107.65	4	112.70	6
97.20	4	102.55	1	108.00	5	112.90	2
97.90	45	102.85	13	108.40	1	113.15	2
98.10	18	103.25	4	108.95	34	113.40	1
98.45	7	103.55	1	109.40	2	113.65	2
98.85	52	103.80	3	109.75	3	113.95	11
99.90	13	104.05	3	110.00	39	114.25	1
100.50	4	104.75	3	111.00	124	114.90	5
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.15	3						
116.80	3						
117.15	4						
117.45	1						
117.80	1						

118.80	5
119.00	17
119.55	2

Average of 10.282 to 10.545 min.: S0208.D
Converted from RTE data file: >S0208:

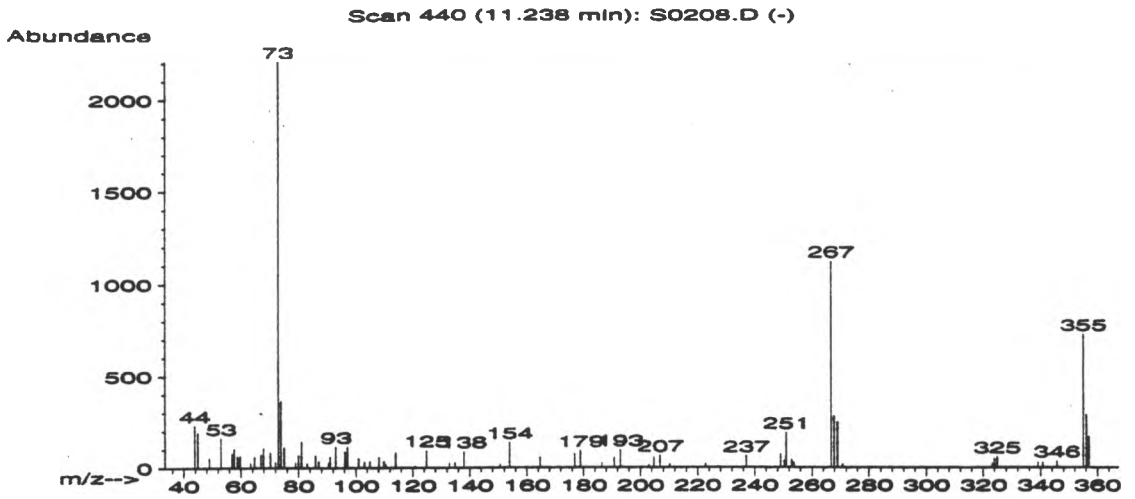
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-butoxy-	118	C6H14O2	27
2.	Oxirane, 2,2'-[oxybis(methylene)]bis-	130	C6H10O3	25
3.	Ethanol, 2-butoxy-	118	C6H14O2	16
4.	Butane, 1-butoxy-2-methyl-	144	C9H20O	12
5.	1-Butene, 4-butoxy-	128	C8H16O	12
6.	Butane, 1,1'-oxybis-	130	C8H18O	12
7.	Propanoic acid, 2,2-dimethyl-, silver(1+	209	C5H10AgO2	12
8.	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	12
9.	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	12
10.	Butane, 1,1'-oxybis-	130	C8H18O	10
11.	Ethanol, 2-butoxy-	118	C6H14O2	10
12.	Ethanol, 2-butoxy-	118	C6H14O2	10
13.	1-Propanol, 2,2-dimethyl-	88	C5H12O	10
14.	2-HEXENE, 5,5-DIMETHYL-	112	C8H16	9
15.	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	9
16.	1-Pentene, 4,4-dimethyl-	98	C7H14	9
17.	1-Octyn-3-ol, 4-ethyl-	154	C10H18O	7
18.	Hexanal, 2-ethyl-	128	C8H16O	7
19.	4-Decene, 2,2-dimethyl-, (Z)-	168	C12H24	7
20.	1-Pentene, 4,4-dimethyl-	98	C7H14	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*27	000111-76-2	3837	36	40	2	96	60	8	18	40	8728
2.	25	002238-07-5	6333	38	44	3	81	54	7	9	31	8911
3.	16	000111-76-2	119786	40	40	2	88	58	3	6	31	8750
4.	12	062238-03-3	10874	39	47	1	99	60	2	0	29	8701
5.	12	034061-76-2	120890	38	34	2	94	65	2	0	33	8679
6.	12	000142-96-1	121220	38	38	0	76	63	2	0	33	8721
7.	12	007324-58-5	38843	48	42	1	95	65	2	0	31	8631
8.	12	000075-98-9	118202	34	30	0	89	60	2	1	26	8636
9.	12	000075-98-9	1357	33	33	0	99	60	2	1	26	8634
10.	10	000142-96-1	121217	28	40	0	77	63	1	1	26	8713
11.	10	000111-76-2	119793	37	42	2	77	63	1	0	25	8694
12.	10	000111-76-2	119788	33	59	2	99	63	1	0	22	8842
13.	10	000075-84-3	263	34	44	1	99	65	1	0	22	8639
14.	9	039761-61-0	2675	41	33	2	91	73	1	0	33	8553
15.	9	039761-61-0	2674	41	33	2	91	73	1	0	33	8553
16.	9	000762-62-9	117800	38	35	3	92	73	1	0	33	8544
17.	7	005877-42-9	124190	34	57	1	96	76	1	0	25	7033
18.	7	000123-05-7	120843	35	50	2	88	71	1	0	25	7004
19.	7	055499-03-1	20733	37	30	2	77	80	1	4	26	8533
20.	7	000762-62-9	922	33	43	2	91	73	1	0	25	8544

STP Compounds

Peak 26; Cyclopentasiloxane, decamethyl



Scan 440 (11.238 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	231	66.95	75	85.90	70	109.90	35
44.90	193	67.95	108	87.05	36	110.40	18
48.95	55	70.30	84	90.40	29	113.90	83
53.05	163	71.95	32	91.00	62	120.85	8
55.80	7	72.95	2209	92.95	115	124.95	94
56.95	81	73.95	365	96.05	89	132.90	24
57.75	106	75.05	113	96.95	114	134.90	29
58.90	63	78.95	28	100.95	53	138.00	90
59.75	66	80.00	70	102.95	32	150.70	19
63.40	27	81.00	142	105.00	36	154.00	138
64.75	62	83.00	23	108.15	57	164.75	58

Scan 440 (11.238 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
176.95	78	248.95	73	324.90	60		
179.00	93	250.30	39	338.95	31		
186.40	24	251.00	192	340.80	28		
190.80	55	252.90	42	345.70	36		
192.95	97	253.65	26	355.00	729		
202.90	18	266.80	1125	356.15	288		
204.75	57	267.80	279	356.90	168		
206.90	67	268.95	248				
210.25	19	270.80	19				
222.70	22	323.20	23				
237.00	63	323.80	50				

STP Compounds

Scan 440 (11.238 min): S0208.D

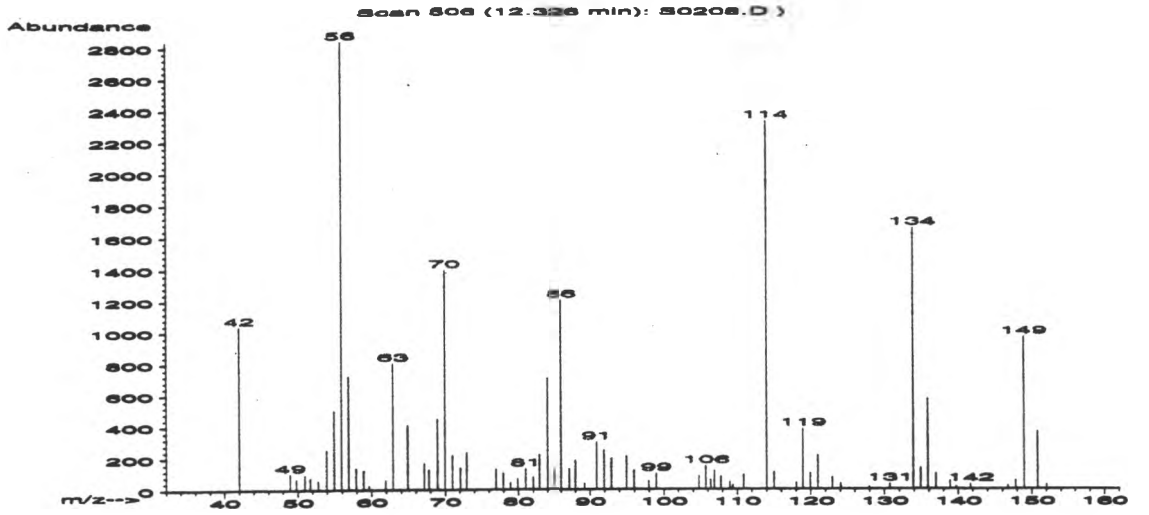
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	91
2.	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	83
3.	(+-)1.BETA.-(2'-HYDROXY-2'-METHOXYCARBON	356	C21H28N2O3	40
4.	Benzoic acid, 2-[(trimethylsilyl)oxy]-,	282	C13H22O3Si2	38
5.	P-HYDROXYPHENYLHYDRACRYLATE 3TMS	398	C18H34O4Si3	38
6.	SYNEPHRINE (TRIMETHYLSILYL DERIVATIVE)	311	C15H29NO2Si2	37
7.	Benzoic acid, 2-[(trimethylsilyl)oxy]-,	282	C13H22O3Si2	28
8.	Benzeneacetic acid, .alpha.,3,4-tris[(tr	472	C20H40O5Si4	25
9.	Benzoic acid, 2,4-bis[(trimethylsilyl)ox	370	C16H30O4Si3	25
10.	1,3-BIS(TRIMETHYLSILYLOXY)-2-TRIMETHYLSI	573	C24H51NO5Si5	25
11.	Benzeneacetic acid, .alpha.,4-bis[(trime	326	C15H26O4Si2	25
12.	1,3,5,7-TETRAETHYLCYCLOTETRASILOXANE	296	C8H24O4Si4	25
13.	Benzaldehyde, 2,5-bis[(trimethylsilyl)ox	282	C13H22O3Si2	25
14.	2,6-DIHYDROXYBENZOIC ACID 3TMS	370	C16H30O4Si3	23
15.	Benzoic acid, 2,5-bis(trimethylsiloxy)-,	370	C16H30O4Si3	23
16.	Benzeneacetic acid, .alpha.,4-bis[(trime	384	C17H32O4Si3	23
17.	4-TRIMETHYLSILYL-9,9-DIMETHYL-9-SILAFLUO	282	C17H22Si2	23
18.	2,6-DIHYDROXYBENZOIC ACID 3TMS	370	C16H30O4Si3	12
19.	Ether, bis(p-tert-butylphenyl)	282	C20H26O	12
20.	OCTOPAMINE-TRITMS	369	C17H35NO2Si3	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	91	000541-02-6	92267	110	37	1	71	5	60	4	52	9949
2.	83	000541-02-6	135460	100	43	1	85	5	50	7	38	9763
3.	*40	065634-79-9	89407	28	35	0	50	34	16	0	33	4829
4.	38	003789-85-3	132654	41	75	2	95	37	14	2	31	9012
5.	38	000000-00-0	97398	45	74	0	42	49	14	0	39	8914
6.	37	000000-00-0	77282	44	87	1	37	41	13	0	35	9008
7.	28	003789-85-3	132652	37	88	3	99	37	8	0	22	9480
8.	25	037148-65-5	106731	38	111	0	69	52	7	0	33	8935
9.	25	010586-16-0	92313	54	87	1	83	52	7	11	33	9004
10.	25	000000-00-0	111594	55	100	3	86	52	7	6	33	8919
11.	25	055334-40-2	134322	36	114	1	52	43	7	0	21	9411
12.	25	016066-10-7	72214	33	92	0	34	44	7	0	25	4482
13.	25	056114-69-3	67552	35	90	0	50	43	7	0	25	5832
14.	23	003782-85-2	135467	36	95	1	34	50	6	0	22	8625
15.	23	003618-20-0	92314	47	95	2	93	50	6	2	23	8591
16.	23	037148-64-4	135719	35	109	1	50	47	6	0	21	9016
17.	23	058263-56-2	67784	34	82	1	35	50	6	0	22	5210
18.	12	003782-85-2	92316	35	94	1	47	58	2	0	21	9045
19.	12	024085-65-2	67892	34	92	0	50	60	2	0	25	4387
20.	12	056145-08-5	135435	37	86	1	49	56	2	0	21	9317

STP Compounds

Peak 27; Unidentified monochloroamine



Scan 506 (12.326 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1037	58.90	125	72.95	239	87.15	135
48.95	102	59.65	25	76.95	131	88.00	187
49.80	68	61.90	63	77.95	106	89.25	40
50.95	95	62.90	804	78.95	45	90.90	303
51.70	77	64.90	408	79.90	68	91.90	252
52.80	58	67.15	169	81.00	134	92.95	198
53.95	255	67.80	130	82.00	80	94.95	213
54.95	503	68.95	450	82.90	224	95.95	123
55.90	2836	69.95	1393	84.00	710	97.95	55
56.90	721	70.95	219	85.00	129	98.95	102
57.90	138	72.05	139	86.00	1207	104.75	89

Scan 506 (12.326 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.75	150	119.95	102	139.75	16		
106.40	62	120.95	214	141.70	33		
106.90	121	122.95	79	146.70	24		
107.75	85	124.05	36	147.80	57		
109.00	48	127.95	17	148.95	969		
109.40	27	130.75	35	150.80	365		
110.90	95	133.90	1655	152.05	29		
114.00	2323	134.90	133				
115.00	110	135.90	577				
118.05	44	137.00	101				
118.95	383	138.90	54				

STP Compounds

Scan 506 (12.326 min): S0208.D

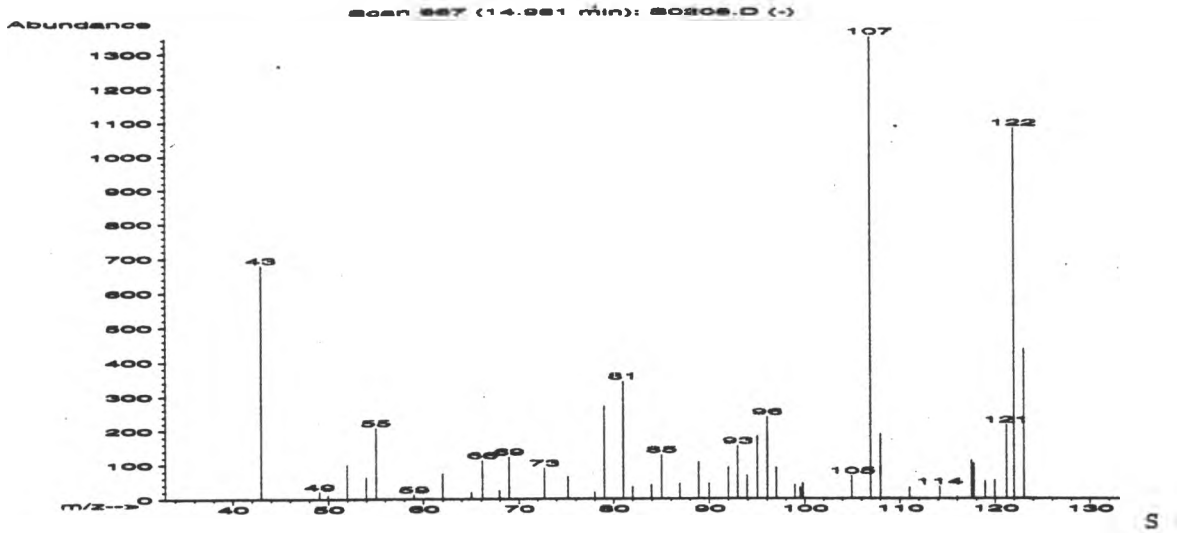
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,4(3H,5H)-Furandione, 3-methyl-	114	C5H6O3	38
2.	2H-Pyran-3(4H)-one, dihydro-6-methyl-	114	C6H10O2	38
3.	2,4(3H,5H)-Furandione, 3-methyl-	114	C5H6O3	25
4.	Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	12
5.	Piperidine, 1-nitroso-	114	C5H10N2O	10
6.	1-Nonanol	144	C9H20O	10
7.	Carbonocyanidothioic amide, dimethyl-	114	C4H6N2S	10
8.	1-Heptene	98	C7H14	10
9.	1-Nonanol	144	C9H20O	10
10.	Cyclopentane, butyl-	126	C9H18	10
11.	Cyclobutane, 1,2-diethyl-	112	C8H16	10
12.	1-Butanamine, N-ethylidene-	99	C6H13N	10
13.	1-Thiacyclohept-2-ene	114	C6H10S	10
14.	Carbonocyanidothioic amide, dimethyl-	114	C4H6N2S	10
15.	Butanal, ethylhydrazone	114	C6H14N2	10
16.	2-Nonenal, (E)-	140	C9H16O	9
17.	1-Pentene, 3,4-dimethyl-	98	C7H14	9
18.	Oxirane, 2-ethyl-2-methyl-	86	C5H10O	9
19.	2H-Pyran, tetrahydro-	86	C5H10O	9
20.	(N-1,3O4-2H3)-3-deazauracil	111	C5H2D3NO2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	001192-51-4	2902	35	53	2	99	54	14	2	43	8004
2.	*38	043152-89-2	119258	39	65	2	89	50	14	0	39	8026
3.	*25	001192-51-4	119200	35	61	1	86	54	7	0	35	8059
4.	12	074663-91-5	14830	41	55	2	67	63	2	10	31	6860
5.	*10	000100-75-4	119204	33	78	2	81	69	1	0	35	6695
6.	10	000143-08-8	122955	39	66	2	69	61	1	11	29	6801
7.	*10	016703-47-2	119198	40	71	2	67	66	1	0	35	5799
8.	10	000592-76-7	117781	42	46	2	74	66	1	6	34	6793
9.	10	000143-08-8	122958	41	61	2	68	63	1	8	29	6897
10.	10	002040-95-1	5448	39	80	3	119	61	1	0	29	6881
11.	10	061141-83-1	119099	45	50	2	99	66	1	1	35	6905
12.	10	006898-74-4	1012	41	42	1	99	70	1	13	34	6399
13.	*10	077566-13-3	119272	28	77	2	81	66	1	0	33	5622
14.	*10	016703-47-2	2883	38	73	2	69	66	1	0	35	5806
15.	*10	051576-30-8	3035	31	89	2	110	61	1	0	29	6193
16.	* 9	018829-56-6	122464	33	77	2	89	77	1	0	35	5523
17.	* 9	007385-78-6	117799	35	52	2	85	77	1	10	32	6771
18.	* 9	030095-63-7	90	31	70	3	70	77	1	3	30	6101
19.	* 9	000142-68-7	117106	29	71	0	63	77	1	0	33	6295
20.	* 9	088278-23-3	2322	32	69	1	81	72	1	0	33	5620

STP Compounds

Peak 28; dimethylphenol + unidentfied compounds



S

can 667 (14.981 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	678	68.95	123	90.00	45	106.95	1344
49.05	21	72.70	89	92.00	92	108.00	188
49.95	11	75.20	64	92.95	154	111.00	32
51.95	99	78.00	19	93.95	66	114.15	35
53.95	63	79.00	271	95.00	184	115.95	5
55.00	207	81.00	343	96.05	238	117.45	111
59.00	12	82.00	35	97.00	90	117.70	102
62.00	73	83.95	41	98.95	40	118.95	51
65.00	20	85.00	128	99.55	33	119.95	53
66.15	112	86.90	44	99.80	45	121.20	215
67.95	24	88.90	107	105.00	66	122.00	1079

Scan 667 (14.981 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	437						

STP Compounds

Scan 667 (14.981 min): S0208.D

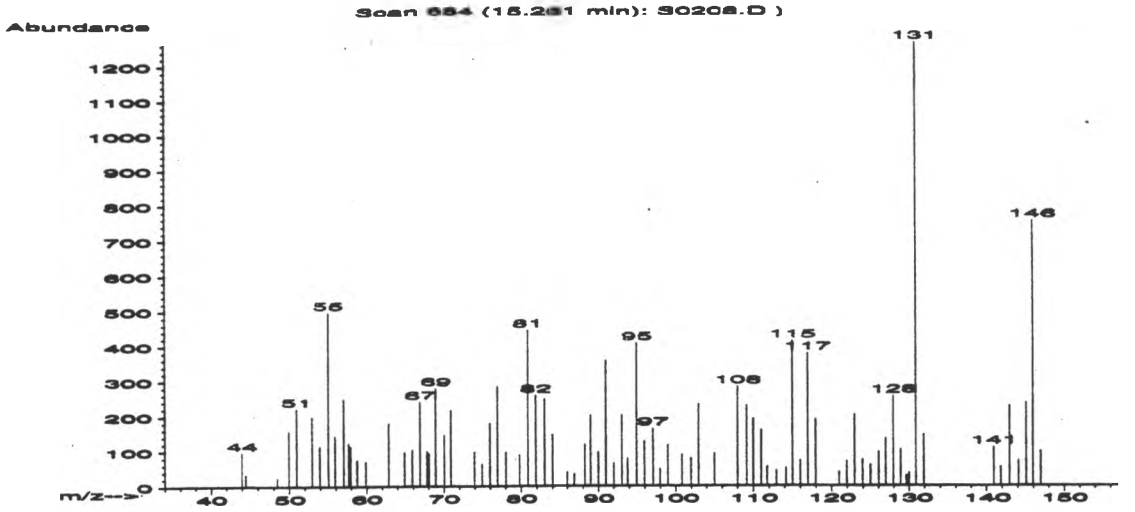
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,3-dimethyl-	122	C8H10O	59
2.	Phenol, 2,4-dimethyl-	122	C8H10O	59
3.	Phenol, 3,4-dimethyl-	122	C8H10O	53
4.	Phenol, 2,5-dimethyl-	122	C8H10O	45
5.	Phenol, 3,4-dimethyl-	122	C8H10O	45
6.	Phenol, 3,4-dimethyl-	122	C8H10O	45
7.	Phenol, 2,3-dimethyl-	122	C8H10O	45
8.	Phenol, 2,6-dimethyl-	122	C8H10O	45
9.	Phenol, 2,3-dimethyl-	122	C8H10O	45
10.	Phenol, 2,6-dimethyl-	122	C8H10O	45
11.	Phenol, 2,3-dimethyl-	122	C8H10O	45
12.	Phenol, 2,6-dimethyl-	122	C8H10O	45
13.	Phenol, 3,4-dimethyl-	122	C8H10O	42
14.	Phenol, 2,4-dimethyl-	122	C8H10O	42
15.	Phenol, 2,6-dimethyl-	122	C8H10O	42
16.	5-Acetylpyrimidine	122	C6H6N2O	40
17.	Benzene, 1-methoxy-4-methyl-	122	C8H10O	38
18.	Benzene, 1-methoxy-2-methyl-	122	C8H10O	37
19.	Benzene, 1-methoxy-2-methyl-	122	C8H10O	37
20.	TRIMETHYLSILYL-BUTADIYNE	122	C7H10Si	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000526-75-0	120209	45	60	2	81	23	33	0	40	9580
2.	*59	000105-67-9	120212	37	63	2	99	23	33	0	39	9460
3.	*53	000095-65-8	120224	35	54	1	99	27	28	11	40	9443
4.	*45	000095-87-4	120215	39	67	2	86	23	19	0	35	9538
5.	*45	000095-65-8	120223	30	61	1	99	25	19	1	30	9443
6.	*45	000095-65-8	4395	42	62	1	99	25	19	0	35	9371
7.	*45	000526-75-0	120210	38	66	2	96	23	19	0	33	9631
8.	*45	000576-26-1	4394	39	69	2	73	25	19	0	35	9477
9.	*45	000526-75-0	120208	39	67	2	87	23	19	0	33	9612
10.	*45	000576-26-1	120219	38	60	3	80	23	19	1	36	9412
11.	*45	000526-75-0	4390	39	68	2	79	23	19	0	35	9587
12.	*45	000576-26-1	120220	39	73	1	82	23	19	0	35	9538
13.	*42	000095-65-8	120225	42	60	1	97	29	17	0	35	9277
14.	*42	000105-67-9	120211	31	66	2	82	27	17	1	30	9251
15.	*42	000576-26-1	120221	32	66	2	83	27	17	9	30	9368
16.	*40	010325-70-9	4313	30	65	2	99	31	16	0	33	9220
17.	*38	000104-93-8	120262	33	63	2	72	48	14	11	40	7746
18.	*37	000578-58-5	120257	28	55	1	68	44	13	1	30	8739
19.	*37	000578-58-5	4414	28	55	1	68	44	13	1	30	8739
20.	*27	000000-00-0	4378	33	60	3	313	58	8	0	41	8494

STP Compounds

Peak 29; Alkylated Indenone ??



Scan 684 (15.261 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	97	57.90	113	70.95	216	86.00	41
44.45	33	58.75	74	73.95	98	86.90	35
48.45	24	59.90	69	74.95	63	88.25	120
49.95	157	62.90	179	75.95	179	89.00	202
50.95	222	64.90	97	76.95	284	90.00	97
52.95	198	65.90	103	78.05	97	91.00	358
53.95	114	66.90	240	79.80	89	92.00	66
55.05	496	67.80	99	80.90	445	93.05	202
55.90	143	68.05	93	81.90	258	93.80	78
57.00	248	68.95	279	83.00	248	94.95	407
57.65	122	70.05	145	84.00	146	95.95	127

Scan 684 (15.261 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.05	164	111.75	54	124.95	60	142.95	229
97.95	49	112.90	43	126.05	97	144.05	72
98.95	117	114.15	52	126.95	136	145.05	237
100.80	90	115.00	415	127.95	257	145.95	755
101.95	79	116.00	73	128.90	104	146.95	99
102.95	233	116.95	380	129.65	30		
105.00	93	117.95	190	130.00	37		
108.00	282	120.95	40	130.90	1265		
109.15	229	121.95	71	131.90	145		
110.00	191	122.95	203	140.95	110		
111.00	159	123.95	76	141.80	54		

STP Compounds

Scan 684 (15.261 min): S0208.D

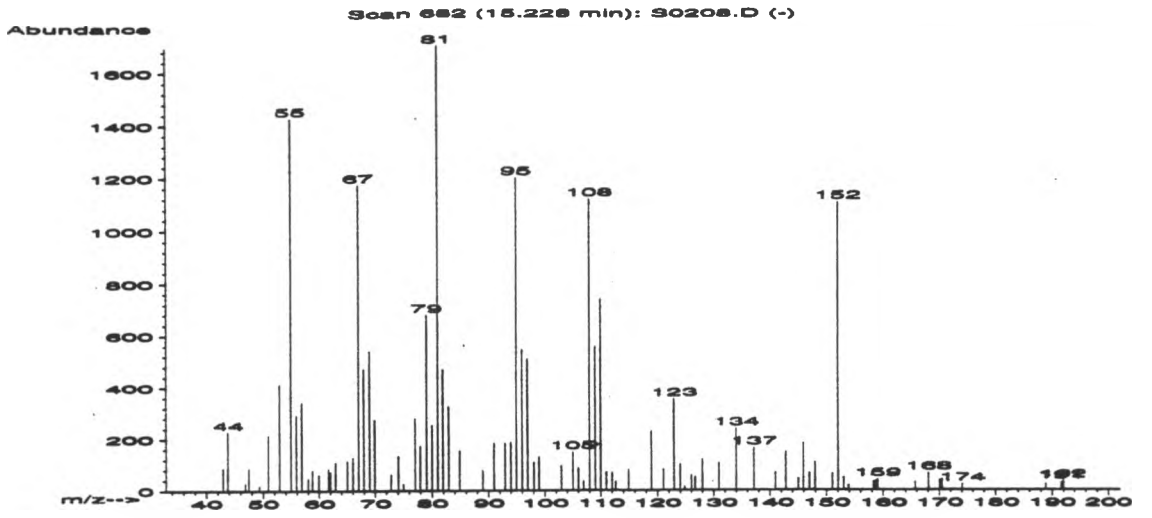
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Inden-1-one, 2,3-dihydro-3-methyl-	146	C10H10O	78
2.	Naphthalene, 1,2,3,4-tetrahydro-5-methyl	146	C11H14	76
3.	2-Methylindanone	146	C10H10O	64
4.	Naphthalene, 1,2,3,4-tetrahydro-6-methyl	146	C11H14	64
5.	2-Propyn-1-ol, 3-p-tolyl-	146	C10H10O	62
6.	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	60
7.	Benzene, ethyl(1-methylethenyl)-	146	C11H14	59
8.	5-Ethylindan	146	C11H14	59
9.	Benzene, (2-methyl-1-methylenepropyl)-	146	C11H14	53
10.	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	49
11.	1H-Indene, 2,3-dihydro-4,7-dimethyl-	146	C11H14	49
12.	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	146	C11H14	49
13.	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	146	C11H14	49
14.	Benzene, (2-methyl-1-butenyl)-	146	C11H14	49
15.	1H-Indene, 2,3-dihydro-1,2-dimethyl-	146	C11H14	47
16.	1H-Benzimidazole, 1-ethyl-	146	C9H10N2	43
17.	Naphth[1,2-b]oxirene, 1a,2,3,7b-tetrahyd	146	C10H10O	25
18.	Naphthalene, 1,2,3,4-tetrahydro-5-methyl	146	C11H14	25
19.	1H-Indole, 1-methyl-	131	C9H9N	25
20.	4-D-QUINAZOLINE	130	C8H5DN2	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	006072-57-7	11461	94	25	1	68	37	46	58	91	9254
2.	*76	002809-64-5	123244	68	57	2	81	25	45	0	68	9349
3.	*64	017496-14-9	11460	48	18	0	85	25	37	0	46	9127
4.	*64	001680-51-9	123251	65	53	2	84	22	37	0	50	9406
5.	*62	016017-24-6	11453	81	32	1	67	29	36	29	56	8980
6.	*60	000769-25-5	11504	64	54	2	71	39	35	0	64	9029
7.	*59	032841-00-2	11503	32	19	0	91	25	33	9	42	8923
8.	*59	052689-24-4	11517	41	17	0	96	25	33	9	42	8189
9.	*53	017498-71-4	11499	67	36	0	78	39	28	34	56	9053
10.	*49	018321-36-3	11502	53	53	1	80	39	23	8	47	8861
11.	*49	006682-71-9	11523	58	45	1	87	36	23	20	49	8998
12.	*49	001559-81-5	123240	52	47	0	88	39	23	19	44	8964
13.	*49	001559-81-5	123239	52	50	0	92	37	23	9	44	8986
14.	*49	056253-64-6	11493	51	55	2	99	37	23	0	46	9249
15.	*47	017057-82-8	11519	57	47	1	90	37	20	7	42	8934
16.	*43	007035-68-9	11429	52	43	0	97	43	18	2	41	8827
17.	*25	002461-34-9	11474	64	49	1	45	62	7	0	50	7275
18.	*25	002809-64-5	123245	48	61	3	168	62	7	0	46	9114
19.	*25	000603-76-9	121267	50	56	1	88	62	7	0	46	7631
20.	*22	013221-69-7	6525	49	35	0	77	62	5	16	41	7626

STP Compounds

Peak 30



Scan 682 (15.228 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	86	58.75	77	72.80	63	89.00	77
43.80	227	59.90	62	74.05	135	91.00	184
46.80	28	61.65	85	74.95	26	92.95	184
47.45	86	62.00	71	77.05	279	93.95	188
49.30	17	62.90	109	77.95	174	94.95	1196
50.95	215	65.00	116	79.05	679	95.95	547
52.95	414	66.00	128	80.00	254	96.95	511
54.95	1425	67.00	1170	81.00	1696	98.05	108
55.90	292	67.95	471	81.90	468	98.95	131
56.90	341	68.95	540	82.90	328	102.95	95
58.00	47	69.95	273	84.90	156	105.00	150

Scan 682 (15.228 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.00	85	122.95	354	145.05	45	165.70	32
106.90	37	124.05	101	145.95	181	168.05	67
108.00	1116	124.85	13	146.95	66	170.05	39
109.00	555	126.05	58	147.95	107	170.45	42
110.00	737	126.70	52	151.05	64	174.05	23
111.00	72	127.95	120	152.05	1101	188.90	23
112.00	69	130.90	106	153.05	49	191.55	31
112.65	34	134.00	238	153.90	18	191.95	36
114.90	81	137.15	164	158.25	34		
118.95	229	140.95	68	158.65	38		
121.05	82	142.80	149	159.00	42		

STP Compounds

Scan 682 (15.228 min): S0208.D

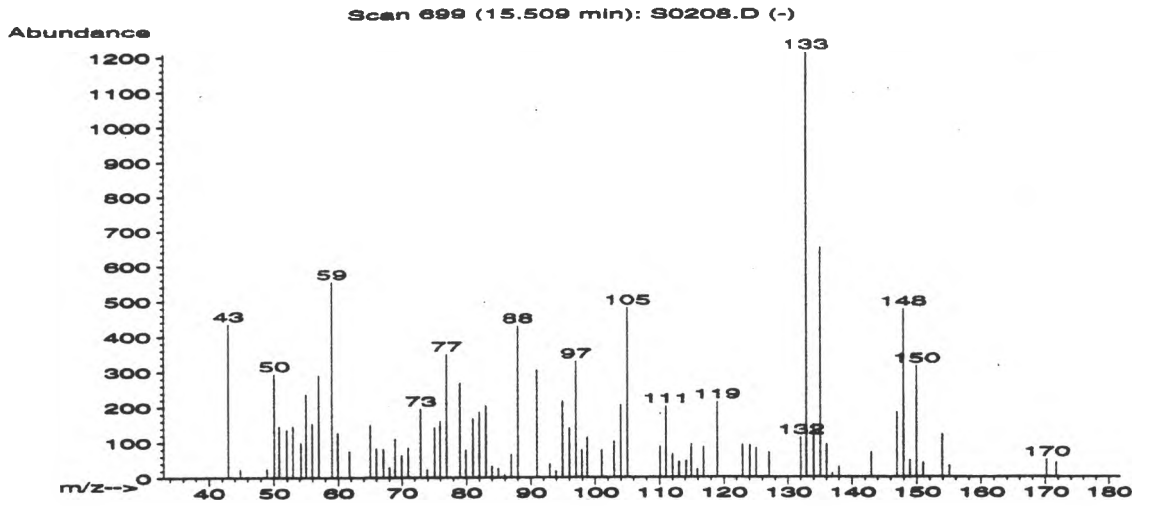
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2(1H)-Naphthalenone, octahydro-, trans-	152	C10H16O	76
2.	BENZOFURANE, HEXAHYDRO-3-METHYLEN-6-METH	152	C10H16O	68
3.	(-)-TRANS-CARANON-(3)	152	C10H16O	60
4.	Camphor	152	C10H16O	53
5.	(-)-TRANS-CARANON-(3)	152	C10H16O	53
6.	2(1H)-Naphthalenone, octahydro-, trans-	152	C10H16O	49
7.	4,7-Methano-1H-inden-1-ol, octahydro-	152	C10H16O	46
8.	(-)-CIS-CARANON-(3)	152	C10H16O	46
9.	Pulegone	152	C10H16O	38
10.	Naphthalene, decahydro-2-methyl-	152	C11H20	38
11.	2-METHYLDECALIN (PROBABLY CIS)	152	C11H20	38
12.	N-HEXYL FURAN	152	C10H16O	30
13.	3,4-Octadiene, 7-methyl-	124	C9H16	30
14.	Phosphine, (1-methylethyl)phenyl-	152	C9H13P	25
15.	CIS-SYN-2-METHYL-DECAHYDRONAPHTHALENE	152	C11H20	25
16.	Naphthalene, decahydro-2-methyl-	152	C11H20	25
17.	4,4,-DIMETHYL-2-(Z-PROP-1-ENYL)-CYCLOPEN	152	C10H16O	25
18.	Cyclohexane, ethylidene-	110	C8H14	25
19.	2-Azetidinone, 1,3,3-trimethyl-4-(1-meth	153	C9H15NO	18
20.	Cyclohexene, 1,2-dimethyl-	110	C8H14	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*76	016021-08-2	124009	71	61	0	77	25	45	0	76	9740
2.	*68	000000-00-0	13756	70	59	2	79	22	40	3	50	9749
3.	*60	004176-04-9	124001	66	32	2	76	38	35	0	64	8750
4.	*53	000076-22-2	124024	67	56	2	71	38	28	25	56	9020
5.	*53	004176-04-9	13728	70	55	2	76	36	28	0	53	8885
6.	*49	016021-08-2	13762	70	63	1	75	41	23	0	53	9714
7.	*46	055255-97-5	13840	56	42	2	68	44	20	0	49	8621
8.	*46	004176-01-6	13727	60	67	2	67	43	20	0	46	8715
9.	*38	000089-82-7	123988	51	68	1	76	54	14	0	44	8183
10.	*38	002958-76-1	124048	60	68	0	69	59	14	0	56	8861
11.	*38	000000-00-0	13880	60	68	0	69	59	14	0	56	8861
12.	*30	000000-00-0	13609	47	45	3	447	59	9	0	44	6985
13.	*30	037050-05-8	4880	50	62	2	118	59	9	0	44	7542
14.	*25	054722-12-2	13542	58	50	1	51	61	7	18	47	6192
15.	*25	000000-00-0	13879	65	59	1	70	61	7	0	47	8647
16.	*25	002958-76-1	124049	65	59	1	70	61	7	0	47	8647
17.	*25	058795-36-1	13630	80	43	1	65	61	7	15	50	7335
18.	*25	001003-64-1	2283	52	53	0	99	62	7	0	46	6974
19.	*18	050483-91-5	14071	51	54	1	113	70	3	0	46	6447
20.	*11	001674-10-8	2279	49	63	0	69	72	2	0	46	7317

STP Compounds

Peak 31; Coeluting compounds, includes t-Butylphenol



Scan 699 (15.509 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	435	59.00	554	73.90	22	85.95	8
44.85	22	59.90	127	75.05	142	86.95	65
48.95	24	61.75	75	75.95	161	88.00	429
50.05	294	65.00	151	76.95	350	91.00	305
50.80	146	66.00	82	79.00	268	93.00	39
51.95	135	67.10	80	79.90	79	93.95	19
52.95	146	68.00	29	81.00	167	94.95	217
54.20	99	68.95	110	82.00	186	96.00	141
55.00	236	69.95	64	83.00	204	97.00	329
55.95	153	71.00	85	84.00	32	97.90	77
56.95	290	72.90	195	84.95	26	98.80	114

Scan 699 (15.509 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.05	77	116.85	86	136.95	11	171.70	42
102.95	103	118.95	214	138.00	30		
103.95	206	122.95	93	143.00	71		
105.00	481	124.05	91	146.95	185		
110.05	87	125.05	83	147.95	477		
111.00	202	127.05	70	148.95	48		
112.00	66	132.00	114	149.95	315		
113.00	44	132.90	1209	150.95	40		
114.15	47	134.00	150	153.90	121		
114.95	95	135.00	653	155.00	32		
115.90	23	136.00	93	170.20	50		

#496

STP Compounds

Scan 699 (15.509 min): S0208.D

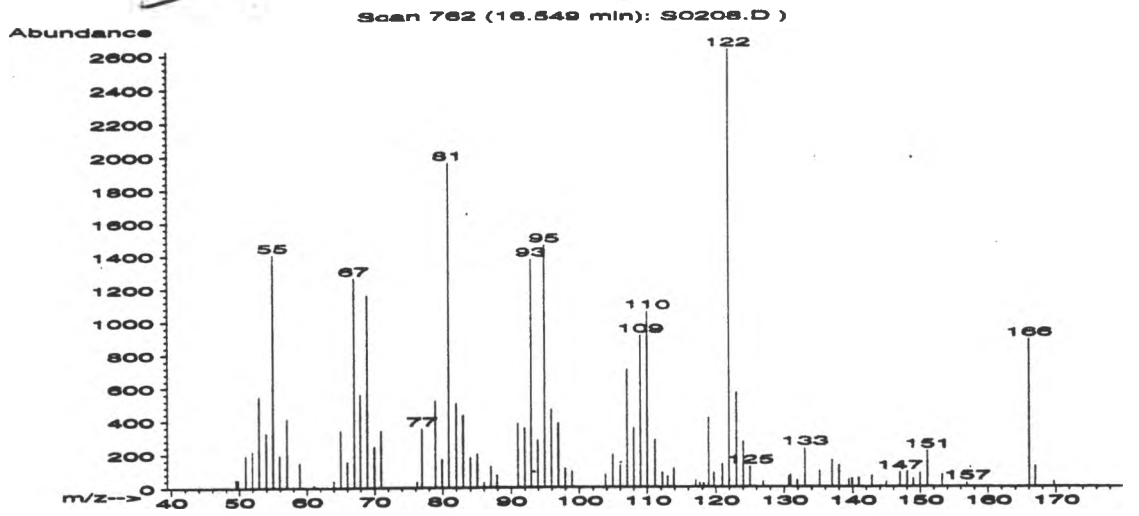
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	49
2.	Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	46
3.	Benzene, (1,1-dimethylethyl)methyl-	148	C11H16	43
4.	Benzene, ethyl-1,2,4-trimethyl-	148	C11H16	43
5.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	42
6.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	42
7.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	38
8.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	30
9.	Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	30
10.	6,7-DIHYDRO-2,5-DIME-5H-CYCLOPENTAPYRAZI	148	C9H12N2	30
11.	Benzene, pentamethyl-	148	C11H16	30
12.	Ethanone, 1-(2,5-dimethylphenyl)-	148	C10H12O	30
13.	Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	30
14.	6-METHYL-4-INDANOL	148	C10H12O	30
15.	2,4-DIMETHYL-5-PYRIMIDINYL METHYL KETONE	150	C8H10N2O	15
16.	[1,2,4]Triazolo[1,5-a]pyridine, 2-methyl	133	C7H7N3	15
17.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	11
18.	Benzenemethanol, 4-(1-methylethyl)-	150	C10H14O	11
19.	5,6,7,8-TETRAHYDROQUINOLINE-6,6-D2	133	C9H9D2N	11
20.	1H-Benzotriazole, 1-methyl-	133	C7H7N3	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	003637-01-2	12020	44	8	0	85	40	23	0	44	7749
2.	*46	004920-99-4	12114	47	26	0	85	45	20	0	44	7746
3.	*43	027138-21-2	12113	55	37	1	99	50	18	0	49	7709
4.	*43	054120-62-6	12122	47	43	0	82	50	18	0	44	7714
5.	*42	004218-48-8	123449	69	28	0	79	57	17	27	70	7689
6.	*42	004218-48-8	12115	64	34	0	85	57	17	0	64	7699
7.	*38	000098-51-1	12112	61	32	1	89	57	14	33	55	7625
8.	*30	000098-51-1	123448	62	37	1	79	57	9	3	47	7685
9.	*30	000089-74-7	123394	45	51	0	72	57	9	0	44	7714
10.	*30	000000-00-0	11992	57	39	0	83	57	9	0	49	7713
11.	*30	000700-12-9	123455	58	39	1	75	57	9	14	47	7671
12.	*30	002142-73-6	12019	54	49	1	71	57	9	0	47	7720
13.	*30	000089-74-7	12018	44	49	0	77	57	9	0	44	7712
14.	*30	020294-32-0	12091	60	48	1	86	57	9	25	46	7621
15.	*15	000000-00-0	12542	58	39	1	50	78	2	0	56	4307
16.	*15	000768-19-4	7102	59	42	1	80	71	2	0	56	7196
17.	*11	000499-75-2	123691	37	43	0	47	78	2	4	43	4417
18.	*11	000536-60-7	123695	56	55	0	50	77	2	0	49	4621
19.	*11	020668-22-8	7164	54	67	1	54	75	2	12	47	6182
20.	*11	013351-73-0	7106	49	59	1	90	71	2	0	46	7182

STP Compounds

Peak 32; ~~Unresolved~~ coeluting compounds 2



Scan 762 (16.549 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.45	51	64.00	43	79.90	170	92.95	1379
49.80	47	65.00	343	80.90	1954	93.95	285
50.95	189	66.00	156	82.00	507	94.95	1464
51.95	217	67.00	1261	83.00	434	95.95	469
52.95	547	67.95	560	84.00	181	96.95	385
53.95	325	68.95	1157	85.00	202	97.95	113
54.95	1405	69.95	244	86.00	29	98.95	95
55.90	191	70.95	341	87.00	125	103.80	74
57.00	411	76.20	37	87.90	74	104.90	196
58.90	149	76.95	354	91.00	383	106.00	130
61.00	16	78.95	523	92.00	357	107.00	711

Scan 762 (16.549 min): S0208.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	352	119.70	86	135.15	95	149.95	82
109.00	914	120.95	140	137.00	160	151.05	215
110.00	1060	121.95	2627	138.00	130	153.25	73
111.15	285	123.05	566	139.40	47	156.90	26
112.15	87	124.05	271	139.90	50	166.05	892
113.00	64	125.05	122	140.90	52	166.95	122
113.90	110	126.95	31	142.80	66	169.70	29
117.05	43	130.65	64	144.95	29		
117.70	26	130.90	71	146.95	86		
118.20	23	131.90	38	148.05	91		
118.95	415	133.00	233	148.95	49		

STP Compounds

Scan 762 (16.549 min): S0208.D

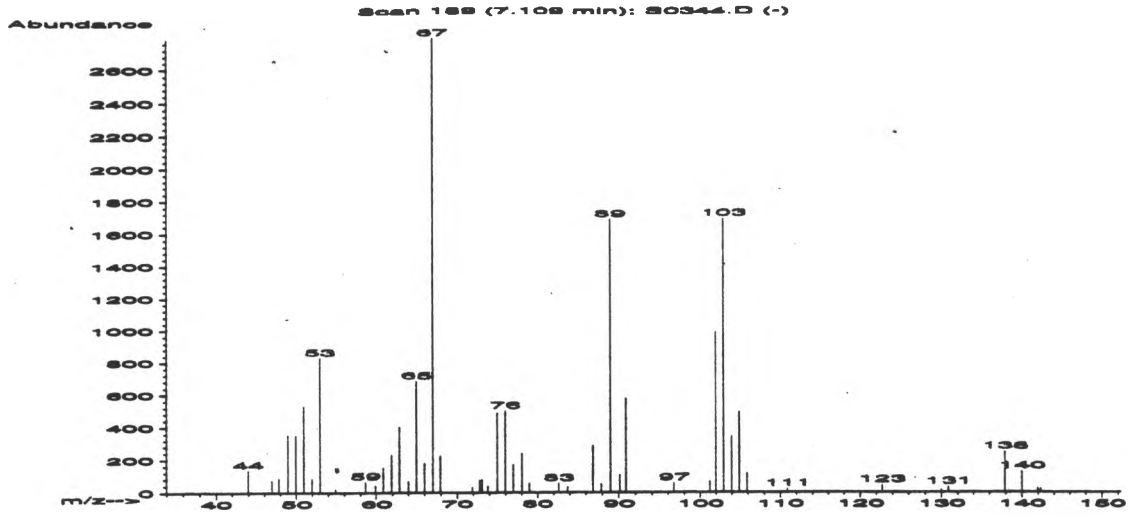
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	TRANS-1,6-DIMETHYLBICYCLO[4.3.0]NONAN-7-	166	C11H18O	46
2.	CIS-10-METHYL-4-KETOPERHYDROAZULENE	166	C11H18O	46
3.	TRANS-10-METHYL-4-KETOPERHYDROAZULENE	166	C11H18O	43
4.	3-Heptyne, 5-methyl-	110	C8H14	30
5.	2-T-BUTYL-3 METHYL-2-CYCLOPENTENDIONE	166	C10H14O2	25
6.	Tricyclo[4.3.1.1(3,8)]undecan-3-ol	166	C11H18O	25
7.	1,4-Hexadiene, 3-ethyl-	110	C8H14	18
8.	2,4-Hexadiene, 3,4-dimethyl-, (E,Z)-	110	C8H14	18
9.	Cyclohexene, 1,2-dimethyl-	110	C8H14	18
10.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	14
11.	cis-4,5-Dimethylcyclopent-2-en-1-one	110	C7H10O	14
12.	1H-Pyrrole, 1-methyl-	81	C5H7N	11
13.	Cyclopropane, trimethylmethylene-	96	C7H12	11
14.	Naphthalene, decahydro-1,5-dimethyl-	166	C12H22	11
15.	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	11
16.	3,5-Octadiene, 4,5-diethyl-, (E,Z)-	166	C12H22	11
17.	Naphthalene, decahydro-2,3-dimethyl-	166	C12H22	11
18.	Ethanol, 2-(dimethylphenoxy)-	166	C10H14O2	11
19.	Cyclohexane, ethylidene-	110	C8H14	11
20.	(-)-TRANS PINANE	138	C10H18	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	062617-82-7	19641	67	8	0	55	44	20	22	47	6173
2.	*46	085318-95-2	19658	54	81	2	57	41	20	0	49	8172
3.	*43	085318-94-1	19659	62	67	2	55	43	18	0	41	7571
4.	*30	061228-09-9	2220	33	50	0	74	60	9	2	43	6341
5.	*25	063160-92-9	19394	48	14	1	65	65	7	0	44	5353
6.	*25	014504-80-4	19697	78	16	0	43	76	7	24	66	4653
7.	*18	002080-89-9	2241	36	57	0	74	66	3	10	43	5488
8.	*18	002417-88-1	2253	47	59	0	55	68	3	0	44	5135
9.	*18	001674-10-8	2279	51	61	0	53	68	3	0	46	6367
10.	*14	000764-13-6	118894	33	61	0	55	68	2	0	41	5215
11.	*14	033765-38-7	2191	36	28	0	55	70	2	0	41	4904
12.	*11	000096-54-8	116733	37	50	1	74	80	2	4	43	4376
13.	*11	034462-28-7	632	50	43	0	54	76	2	0	44	5080
14.	*11	066552-62-3	19758	51	48	0	39	76	2	0	46	6554
15.	*11	000932-66-1	120414	60	35	0	61	73	2	28	49	4896
16.	*11	021293-02-7	19732	46	72	0	53	74	2	0	44	5070
17.	*11	001008-80-6	19760	56	62	1	50	75	2	0	47	5130
18.	*11	054411-20-0	19421	48	40	1	46	75	2	0	46	6336
19.	*11	001003-64-1	118902	48	54	1	101	76	2	0	44	5973
20.	*11	000473-55-2	8827	62	55	1	53	76	2	0	46	4621

STP Compounds

Peak 33



Scan 189 (7.109 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	137	60.90	152	73.80	37	90.15	107
46.95	73	61.90	229	74.95	490	90.90	577
47.80	87	62.90	401	75.95	500	96.70	57
48.95	352	64.00	70	76.95	170	101.20	68
49.95	350	65.00	684	78.05	240	101.95	994
50.95	531	66.00	179	78.95	55	102.95	1694
51.95	82	67.00	2784	82.65	55	103.95	344
52.95	831	67.95	226	83.75	34	104.90	497
54.85	20	71.90	32	86.90	287	105.90	114
58.65	65	72.80	75	87.90	53	110.90	22
59.90	43	73.05	79	89.00	1688	122.70	45

Scan 189 (7.109 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.00	16						
130.90	34						
137.90	249						
140.00	128						
141.95	28						
142.30	21						

STP Compounds

Scan 189 (7.109 min): S0344.D

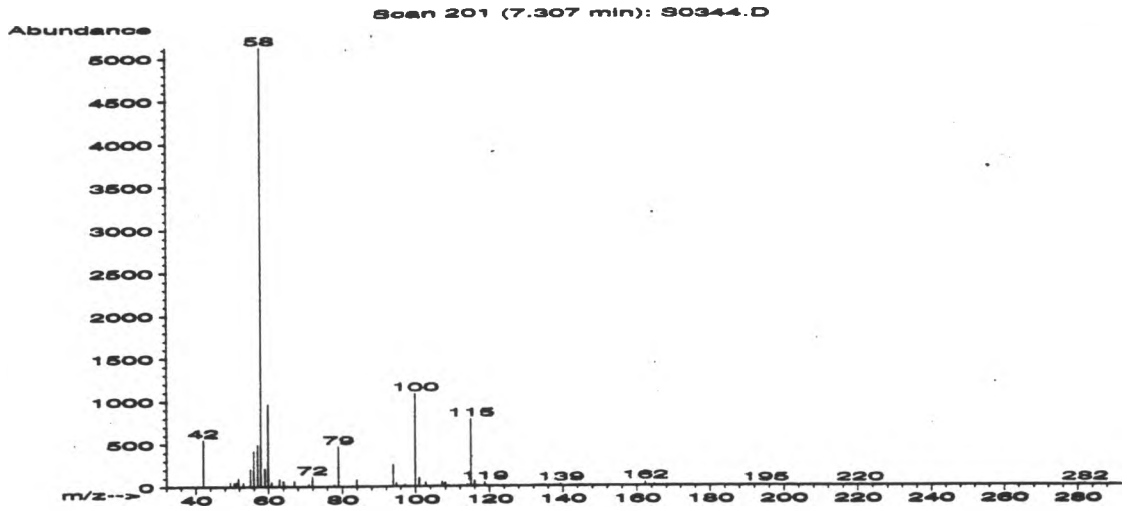
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclopentane, 1,3-dichloro-, cis-	138	C5H8Cl2	50
2.	Cyclopentane, 1,2-dichloro-, trans-	138	C5H8Cl2	45
3.	Cyclopentane, 1,1-dichloro-	138	C5H8Cl2	37
4.	Cyclopentene, 1-chloro-	102	C5H7Cl	32
5.	Cyclopentane, 1,2-dichloro-, cis-	138	C5H8Cl2	25
6.	Silane, methylenebis[methyl-	104	C3H12Si2	12
7.	Benzaldehyde, oxime, (Z)-	121	C7H7NO	10
8.	4,4-DIMETHYL-2-PENTYNAL	110	C7H10O	10
9.	2H-Pyran, 5,6-dihydro-2-methyl-	98	C6H10O	10
10.	Benzene, isocyano-	103	C7H5N	9
11.	Benzonitrile	103	C7H5N	9
12.	2-Cyclopentene-1-undecanoic acid, ethyl	280	C18H32O2	8
13.	6H-1,2,5-Oxadiazine-6-thione, 4,5-dihydr	192	C9H8N2OS	7
14.	2-Butenedioyl dichloride	152	C4H2Cl2O2	7
15.	1-Butyne, 3-chloro-	88	C4H5Cl	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	026688-51-7	8392	64	29	0	83	47	25	0	64	7987
2.	*45	014376-81-9	8391	71	22	0	98	49	19	33	58	7516
3.	37	031038-06-9	122179	48	46	0	91	41	13	1	36	8397
4.	*32	000930-29-0	1352	40	50	2	99	48	9	0	35	7668
5.	*25	031025-65-7	8390	56	28	0	86	63	7	21	46	7103
6.	*12	005654-05-7	1560	44	60	3	60	57	2	2	27	6394
7.	10	000622-32-2	4205	46	45	1	42	75	1	1	38	4479
8.	10	002579-21-7	2159	43	50	1	56	72	1	20	38	7440
9.	10	055230-25-6	889	35	90	2	99	61	1	0	20	7036
10.	* 9	000931-54-4	118398	31	45	2	47	76	1	7	34	4511
11.	* 9	000100-47-0	1541	29	60	0	55	77	1	0	33	4499
12.	8	003552-12-3	67139	35	82	2	80	67	1	0	21	7020
13.	7	033406-07-4	30599	35	57	0	57	77	1	0	25	4472
14.	7	016769-97-4	13215	33	64	1	59	79	1	0	22	4588
15.	6	021020-24-6	179	52	61	1	59	80	1	0	18	4516

STP Compounds

Peak 34



Scan 201 (7.307 min): S0344.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	548	59.90	966	94.80	41	139.40	29
49.55	55	60.90	49	97.05	26	162.25	46
50.55	52	63.00	83	99.95	1084	164.75	15
51.20	56	64.00	64	100.95	103	193.70	17
51.70	104	67.00	67	102.70	45	194.95	17
53.05	48	70.95	36	107.15	58	220.55	17
54.95	213	71.95	115	107.90	43	281.90	21
55.90	420	77.80	22	114.00	21		
57.00	493	78.95	466	115.00	783		
57.90	5125	83.90	82	116.00	64		
59.00	214	93.95	261	118.70	43		

STP Compounds

Scan 201 (7.307 min): S0344.D

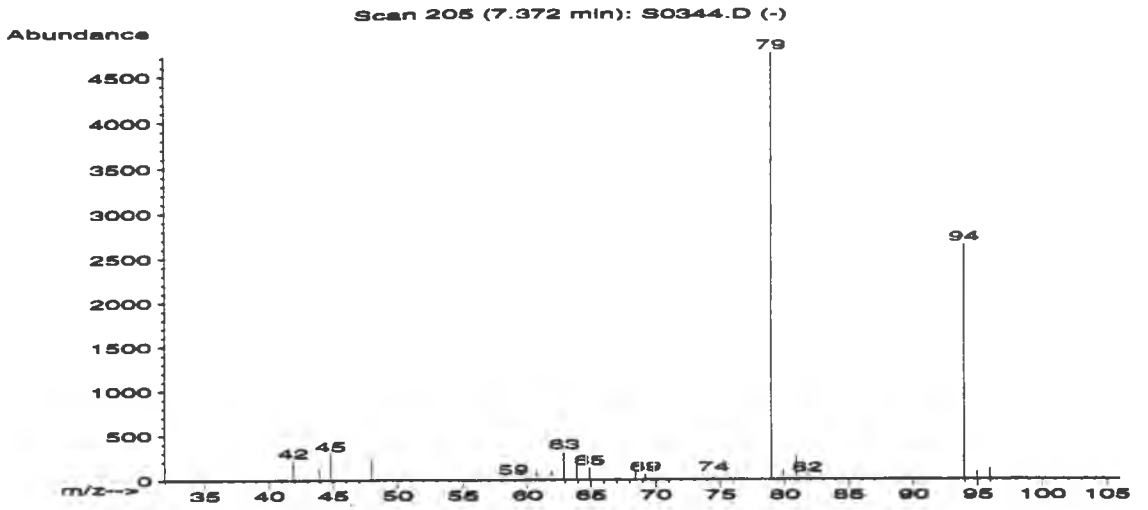
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Propanamine, N-methyl-N-(1-methylethyl	115	C7H17N	42
2.	Piperazine, 1-methyl-	100	C5H12N2	42
3.	Urea, (1,1-dimethylethyl)-	116	C5H12N2O	40
4.	ETHER, ISOPROPENYL ISOPROPYL	100	C6H12O	38
5.	Piperazine, 1-methyl-	100	C5H12N2	36
6.	N-tert-Butylacrylamide	127	C7H13NO	33
7.	Bromo-Benadryl	333	C17H20BrNO	28
8.	Acetamide, N-(2,6-dimethylphenyl)-2-(eth	206	C12H18N2O	28
9.	2-Propanamine, N-methyl-N-(1-methylethyl	115	C7H17N	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	42	010342-97-9	119414	44	40	1	73	26	17	5	30	9386
2.	*42	000109-01-3	1120	32	43	1	94	26	17	3	30	9620
3.	*40	001118-12-3	3384	40	44	2	83	35	16	0	35	9479
4.	*38	000000-00-0	1191	31	54	1	99	24	14	0	29	9519
5.	*36	000109-01-3	117962	31	54	1	78	29	12	0	27	9622
6.	33	000107-58-4	120696	35	46	0	83	35	10	1	26	9474
7.	28	000118-23-0	83727	33	85	1	93	36	8	0	25	9480
8.	28	007728-40-7	37414	35	59	1	73	36	8	0	25	9426
9.	*10	010342-97-9	119415	31	37	0	33	66	1	0	33	9458

STP Compounds

Peak 35



Scan 205 (7.372 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	214	68.45	91				
43.95	149	69.20	61				
44.80	295	74.45	52				
47.95	225	76.90	3				
58.90	27	78.95	4724				
60.75	81	79.90	96				
61.90	92	80.90	244				
62.90	310	81.75	44				
63.90	240	93.95	2622				
64.90	131	94.95	83				
66.95	10	95.95	116				

STP Compounds

Scan 205 (7.372 min): S0344.D

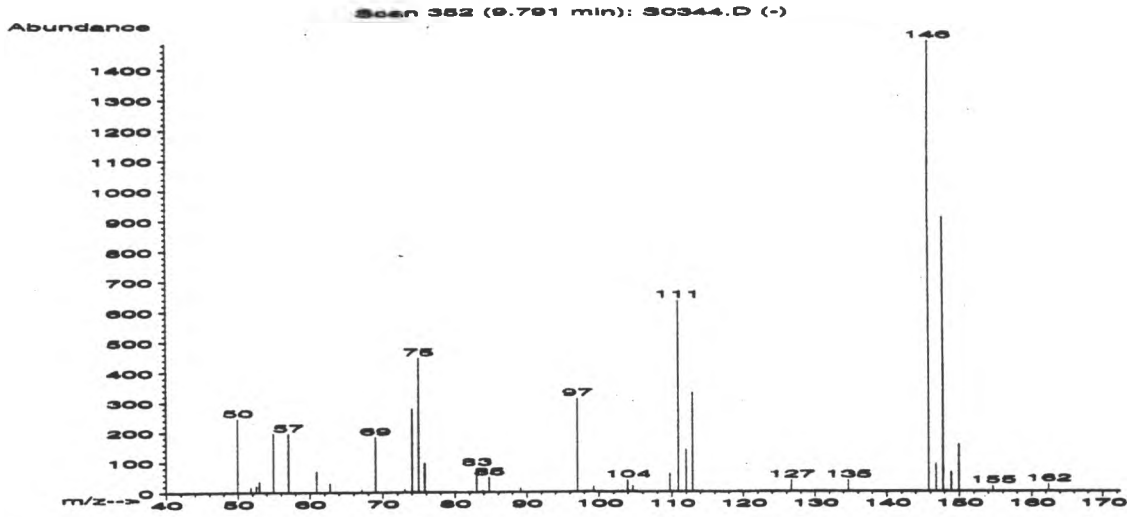
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Methane, sulfonylbis-	94	C2H6O2S	86
2.	Methane, sulfonylbis-	94	C2H6O2S	78
3.	Methane, sulfonylbis-	94	C2H6O2S	78
4.	Methane, sulfonylbis-	94	C2H6O2S	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000067-71-0	452	51	38	0	76	8	53	15	44	9899
2.	*78	000067-71-0	117482	50	39	0	90	6	46	7	40	9976
3.	*78	000067-71-0	117481	47	47	1	94	6	46	0	40	9966
4.	25	000067-71-0	117480	37	57	0	58	45	7	3	26	9956

STP Compounds

Peak 23



Scan 352 (9.791 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.95	245	73.00	9	104.65	19	149.95	157
50.95	1	74.05	277	109.75	59	154.65	18
51.80	17	74.95	446	110.90	635	162.40	23
52.55	21	75.80	95	112.00	140		
52.95	36	83.00	80	112.90	330		
54.95	195	83.85	5	126.70	37		
57.00	195	84.75	49	134.65	37		
60.90	70	89.10	11	145.80	1485		
62.75	29	97.05	311	146.80	91		
67.10	8	99.30	18	147.80	910		
68.95	182	103.95	38	148.95	63		

STP Compounds

Scan 352 (9.791 min): S0344.D

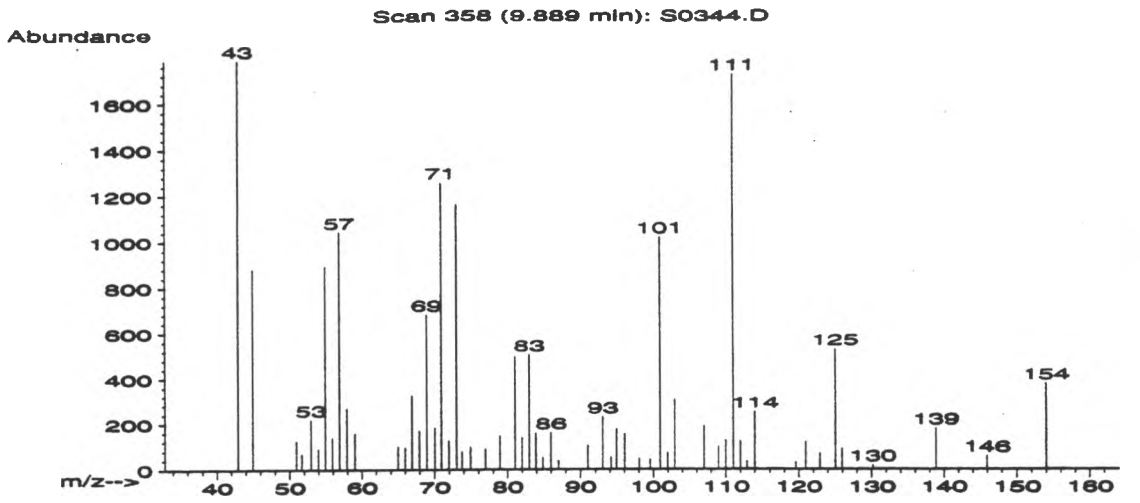
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,3-dichloro-	146	C6H4Cl2	87
2.	Benzene, 1,4-dichloro-	146	C6H4Cl2	87
3.	Benzene, 1,4-dichloro-	146	C6H4Cl2	87
4.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
5.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
6.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
7.	Benzene, 1,3-dichloro-	146	C6H4Cl2	81
8.	Benzene, 1,3-dichloro-	146	C6H4Cl2	74
9.	Benzene, 1,4-dichloro-	146	C6H4Cl2	74
10.	Benzene, 1,4-dichloro-	146	C6H4Cl2	74
11.	Benzene, 1,2-dichloro-	146	C6H4Cl2	74
12.	Benzene, 1,2-dichloro-	146	C6H4Cl2	72
13.	Benzene, 1,4-dichloro-	146	C6H4Cl2	68
14.	Benzene, 1,3-dichloro-	146	C6H4Cl2	64
15.	Benzene, 1,2-dichloro-	146	C6H4Cl2	64
16.	Benzene, 1,3-dichloro-	146	C6H4Cl2	58
17.	(E)-6-Chloro-4-methyl-2-heptene	146	C8H15Cl	53
18.	TRANS-DICHLOROFUMARONITRILE	146	C4Cl2N2	47
19.	CIS-DICHLOROMALEONITRILE	146	C4Cl2N2	47
20.	Peroxide, bis(dichlorobenzoyl)	378	C14H6Cl4O4	42

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000541-73-1	123080	73	29	0	67	15	54	0	81	9793
2.	*87	000106-46-7	123084	78	30	0	89	12	54	31	66	9616
3.	*87	000106-46-7	11154	74	35	0	81	15	54	0	81	9813
4.	*87	000095-50-1	123077	69	42	0	76	15	54	0	76	9832
5.	*87	000095-50-1	123076	72	28	0	78	15	54	0	76	9831
6.	*87	000095-50-1	123073	70	41	1	89	14	54	17	66	9812
7.	*81	000541-73-1	123078	70	40	0	90	16	49	22	66	9786
8.	*74	000541-73-1	11153	69	39	0	86	16	44	2	58	9792
9.	*74	000106-46-7	123083	68	38	0	92	16	44	19	58	9691
10.	*74	000106-46-7	123082	69	38	0	91	16	44	2	58	9778
11.	*74	000095-50-1	123074	59	49	0	78	19	44	0	56	9817
12.	*72	000095-50-1	123075	55	53	1	95	18	42	0	47	9792
13.	*68	000106-46-7	123085	59	50	0	74	25	40	0	56	9823
14.	*64	000541-73-1	123081	57	53	0	83	16	37	5	40	9823
15.	*64	000095-50-1	11151	64	45	0	87	18	37	4	43	9776
16.	*58	000541-73-1	123079	51	55	0	78	26	32	0	46	9792
17.	*53	092639-31-1	11344	33	80	1	92	28	28	0	39	9396
18.	*47	000000-00-0	11118	43	62	1	74	38	20	0	39	9342
19.	*47	000000-00-0	11117	37	52	1	76	38	20	5	40	9295
20.	42	028604-90-2	93875	48	91	0	69	29	17	1	36	9787

STP Compounds

Peak 36; Isocineole



Scan 358 (9.889 min): S0344.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1786	65.00	100	76.95	90	94.20	53
44.95	879	66.00	95	78.95	146	94.95	175
50.95	125	66.90	323	81.00	496	96.05	154
51.70	69	67.95	170	82.00	137	98.05	47
52.95	218	68.95	681	83.00	504	99.55	43
53.95	90	70.05	182	83.90	158	100.95	1021
54.95	892	70.95	1254	84.90	51	101.95	71
55.90	139	71.95	126	86.00	161	102.95	305
56.90	1042	73.05	1159	87.00	37	107.00	190
57.90	266	73.80	78	91.00	104	109.00	98
59.00	157	74.95	98	93.05	228	110.00	124

Scan 358 (9.889 min): S0344.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.00	1721	145.95	59				
112.00	120	154.00	379				
112.90	34						
114.00	251						
119.55	30						
120.95	119						
122.95	68						
125.05	529						
125.95	90						
130.15	18						
138.90	179						

STP Compounds

Scan 358 (9.889 min): S0344.D

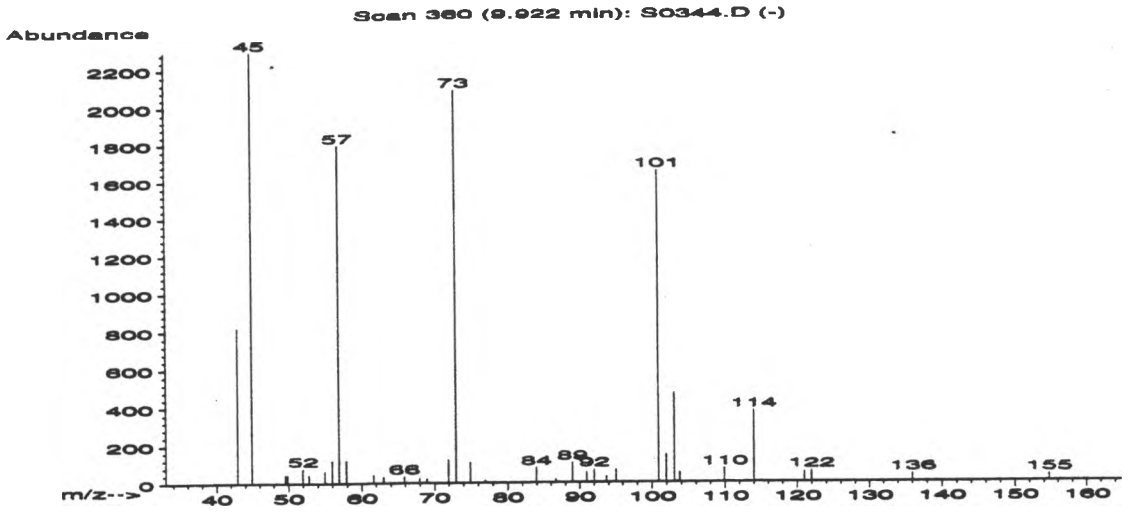
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Isocineole	154	C10H18O	90
2.	Isocineole	154	C10H18O	86
3.	Isocineole	154	C10H18O	60
4.	4-Hepten-3-one, 2,5,6-trimethyl-	154	C10H18O	30
5.	1-METHYLENE-2-TRIMETHYLSILYL-CYCLOPROPAN	126	C7H14Si	27
6.	4(1H)-Pyridinone, 2,3-dihydro-1-methyl-	111	C6H9NO	18
7.	3-Cyclobutene-1,2-dicarboxylic acid, dim	170	C8H10O4	14
8.	Carvomenthone	154	C10H18O	12
9.	(E)-9-((2'S,3'R)-3-HYDROXY-6'-((E)-2''-H	352	C21H36O4	12
10.	2,5-PYRIDINEDIOL	111	C5H5NO2	10
11.	2-Cyclopenten-1-one, 3-amino-2-methyl-	111	C6H9NO	10
12.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
13.	Cyclohexane, methoxy-	114	C7H14O	10
14.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
15.	2-Aminopyrimidin-1-oxide	111	C4H5N3O	10
16.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
17.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
18.	2-Heptanone, 3-propylidene-	154	C10H18O	10
19.	Thiocyanic acid, propyl ester	101	C4H7NS	10
20.	1,3-Dioxane, 4-methyl-	102	C5H10O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000470-67-7	124312	79	27	0	95	37	57	0	93	8433
2.	*86	000470-67-7	124313	80	23	0	99	50	53	0	93	8342
3.	*60	000470-67-7	14755	80	27	0	87	39	35	35	74	8283
4.	*30	016466-21-0	14572	51	47	0	93	57	9	0	46	7754
5.	27	000000-00-0	5279	49	55	3	96	57	8	9	38	7274
6.	*18	035488-00-7	2353	51	47	2	74	69	3	0	44	6777
7.	14	060333-14-4	125900	44	43	2	96	67	2	7	38	6534
8.	*12	000499-70-7	14698	36	67	2	96	64	2	18	37	6659
9.	12	071117-50-5	88544	47	91	1	65	65	2	0	37	6555
10.	*10	000000-00-0	2324	46	43	2	96	71	1	3	38	6505
11.	*10	069687-85-0	2351	33	63	3	254	71	1	0	41	6505
12.	*10	000071-30-7	118915	44	38	1	92	71	1	12	38	6505
13.	*10	000931-56-6	119365	34	52	1	58	80	1	0	39	5211
14.	*10	000071-30-7	2309	34	53	1	75	71	1	11	40	6505
15.	*10	035034-15-2	2307	34	54	2	96	71	1	0	39	6505
16.	*10	000071-30-7	118914	35	48	1	73	71	1	7	40	6505
17.	*10	000071-30-7	118913	33	53	0	96	71	1	0	41	6505
18.	*10	032064-70-3	14568	40	56	0	66	78	1	0	39	6247
19.	*10	004251-16-5	1263	37	61	0	99	80	1	0	41	4547
20.	*10	001120-97-4	118254	49	64	1	72	71	1	0	39	5090

STP Compounds

Peak 37; Unidentified oxy hydrocarbon



S

can 360 (9.922 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	819	63.00	33	91.00	53	120.95	54
44.95	2296	65.85	34	92.00	67	121.95	58
49.55	44	67.95	26	93.70	32	136.00	41
49.80	44	68.95	22	95.05	65	154.75	36
51.95	78	71.95	123	100.95	1653		
52.80	44	72.95	2082	101.95	146		
54.95	63	74.95	109	103.05	472		
55.95	117	76.95	14	103.80	50		
56.90	1794	83.95	77	109.90	73		
57.90	119	86.65	18	113.00	8		
61.65	43	89.00	105	114.00	376		

STP Compounds

Scan 360 (9.922 min): S0344.D

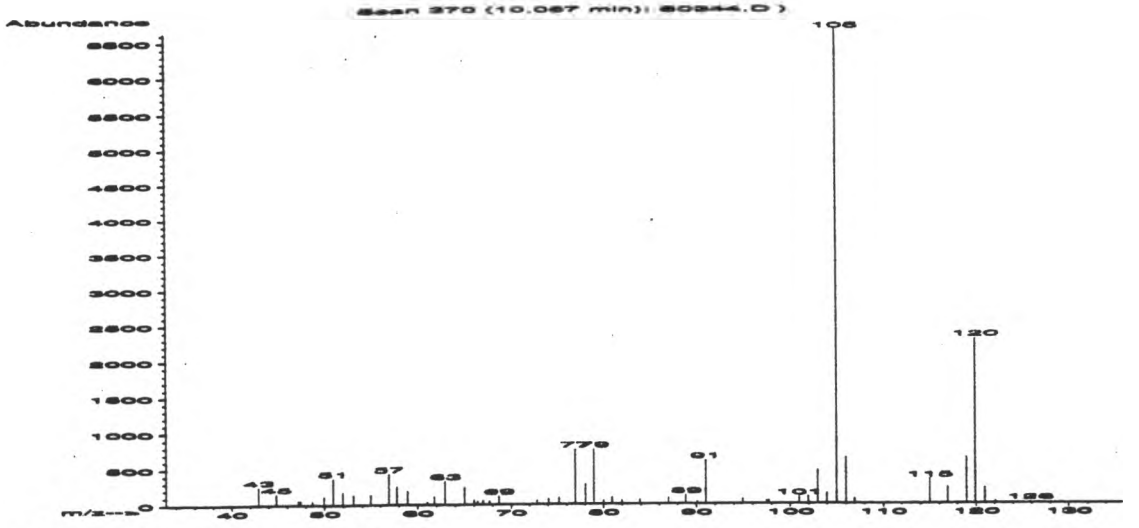
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	5-METHYL-2-OXAZOLIDINONE	101	C4H7NO2	40
2.	Butane, 1,2,4-trimethoxy-	148	C7H16O3	23
3.	Butane, 1-chloro-4-methoxy-	122	C5H11ClO	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*40	001072-70-4	1257	28	62	0	73	32	16	6	35	7727
2.	23	020637-48-3	123351	33	50	0	89	48	6	0	25	6318
3.	*12	017913-18-7	120145	30	44	1	88	61	2	2	35	5745

STP Compounds

Peak 38; Alkylbenzene



Scan 370 (10.087 min): S0344.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	250	57.75	251	72.80	52	88.90	119
44.80	154	58.90	189	74.05	72	90.15	33
47.20	61	61.00	37	75.20	90	91.00	606
47.45	58	61.75	111	76.95	763	94.95	68
48.70	49	62.90	330	78.05	281	97.45	39
49.95	118	65.00	245	78.95	764	97.70	44
50.95	371	66.00	60	80.00	47	100.95	95
51.95	170	66.40	39	80.90	89	101.95	99
53.05	138	67.00	56	82.00	55	102.95	464
54.95	140	67.70	48	83.90	58	103.95	148
56.90	426	68.70	116	87.00	78	105.00	6630

Scan 370 (10.087 min): S0344.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.00	643						
106.90	66						
115.00	340						
116.95	235						
118.95	647						
119.95	2305						
120.95	219						
122.05	31						
125.80	18						

STP Compounds

Scan 370 (10.087 min): S0344.D

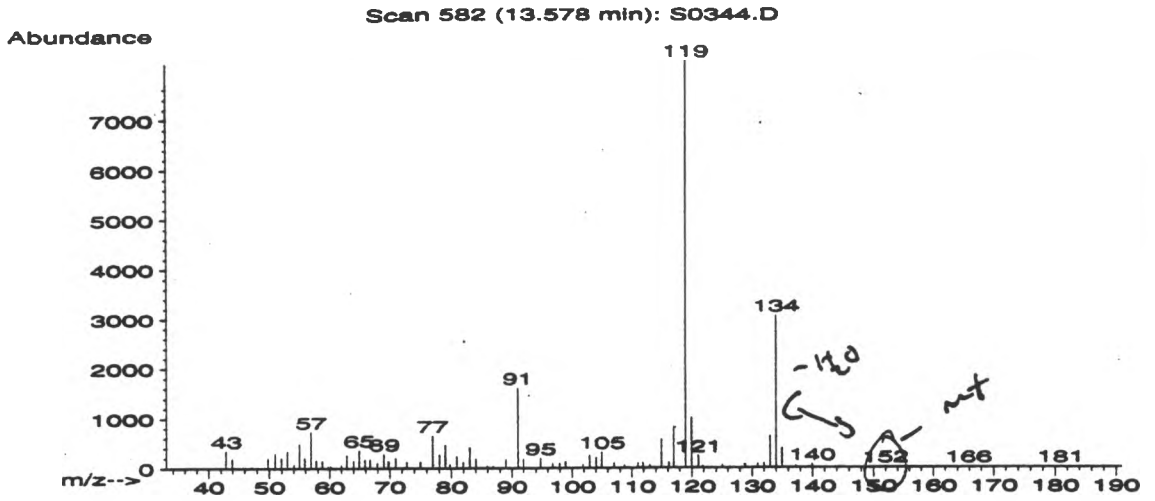
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2,3-trimethyl-	120	C9H12	91
2.	Benzene, 1,3,5-trimethyl-	120	C9H12	91
3.	Benzene, 1,3,5-trimethyl-	120	C9H12	91
4.	Benzene, 1,2,4-trimethyl-	120	C9H12	91
5.	Benzene, 1-ethyl-3-methyl-	120	C9H12	90
6.	Benzene, 1-ethyl-4-methyl-	120	C9H12	90
7.	Benzene, 1-ethyl-2-methyl-	120	C9H12	90
8.	Benzene, 1-ethyl-3-methyl-	120	C9H12	90
9.	Benzene, 1-ethyl-2-methyl-	120	C9H12	90
10.	Benzene, 1-ethyl-4-methyl-	120	C9H12	90
11.	Benzene, 1-ethyl-2-methyl-	120	C9H12	90
12.	Benzene, 1,3,5-trimethyl-	120	C9H12	87
13.	Benzene, 1,2,3-trimethyl-	120	C9H12	87
14.	Benzene, 1,3,5-trimethyl-	120	C9H12	87
15.	Benzene, 1,3,5-trimethyl-	120	C9H12	87
16.	Benzene, 1-ethyl-3-methyl-	120	C9H12	87
17.	Benzene, 1-ethyl-3-methyl-	120	C9H12	87
18.	Benzene, 1,2,4-trimethyl-	120	C9H12	87
19.	Benzene, 1-ethyl-4-methyl-	120	C9H12	87
20.	Benzene, 1,2,4-trimethyl-	120	C9H12	81

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000526-73-8	120024	75	10	0	75	4	62	2	66	9866
2.	*91	000108-67-8	4147	76	10	0	80	4	62	20	66	9732
3.	*91	000108-67-8	120035	81	5	0	72	2	62	23	72	9744
4.	*91	000095-63-6	120028	77	9	0	80	2	62	10	66	9773
5.	*90	000620-14-4	4143	74	11	0	89	9	59	0	81	9964
6.	*90	000622-96-8	4144	72	10	0	92	9	59	0	76	9954
7.	*90	000611-14-3	120012	73	10	0	85	9	59	0	81	9952
8.	*90	000620-14-4	120017	78	12	0	79	7	59	30	72	9951
9.	*90	000611-14-3	4142	72	15	1	89	9	59	6	70	9950
10.	*90	000622-96-8	120021	77	11	0	70	9	59	12	76	9953
11.	*90	000611-14-3	120013	74	10	0	85	9	59	0	81	9963
12.	*87	000108-67-8	120034	73	13	0	70	14	54	27	66	9623
13.	*87	000526-73-8	120023	68	26	1	60	12	54	0	68	9926
14.	*87	000108-67-8	120036	71	15	1	94	12	54	17	66	9672
15.	*87	000108-67-8	120037	77	13	0	51	14	54	0	81	9867
16.	*87	000620-14-4	120016	66	22	1	86	14	54	0	64	9962
17.	*87	000620-14-4	120015	66	22	1	86	14	54	0	64	9962
18.	*87	000095-63-6	120030	77	13	0	66	12	54	0	81	9919
19.	*87	000622-96-8	120018	64	20	1	89	14	54	0	64	9945
20.	*81	000095-63-6	120031	70	18	0	59	17	49	0	76	9827

STP Compounds

Peak 39



Scan 582 (13.578 min): S0344.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	353	57.75	164	69.05	286	83.00	418
43.95	186	58.75	142	69.80	136	84.00	185
47.20	25	59.75	36	70.95	199	85.90	48
49.80	198	60.15	39	72.80	124	86.90	35
50.95	301	62.00	67	74.95	126	89.00	166
51.95	210	62.90	265	76.95	654	91.00	1597
52.95	341	64.00	150	78.05	279	92.00	176
54.05	72	64.90	363	79.05	466	94.80	193
54.95	488	65.90	172	79.80	71	96.80	93
55.90	208	66.75	174	80.90	242	97.95	90
56.90	732	67.95	101	81.90	119	98.95	121

Scan 582 (13.578 min): S0344.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.80	69	116.95	814	134.00	3029		
102.95	253	118.95	8093	135.00	396		
104.05	207	119.95	997	137.25	35		
105.00	316	121.05	237	139.25	20		
107.00	96	121.80	34	139.90	68		
108.75	53	125.05	59	143.70	20		
111.00	92	128.70	65	151.95	18		
111.90	105	128.90	63	165.45	16		
113.00	53	130.90	70	165.80	16		
114.90	567	132.00	92	180.90	16		
116.15	102	133.00	627				

cymenol
elutes between cymene
RT nos KI
1167 – 14.2 min
suggest
cymene-8-ol.

STP Compounds

Scan 582 (13.578 min): S0344.D

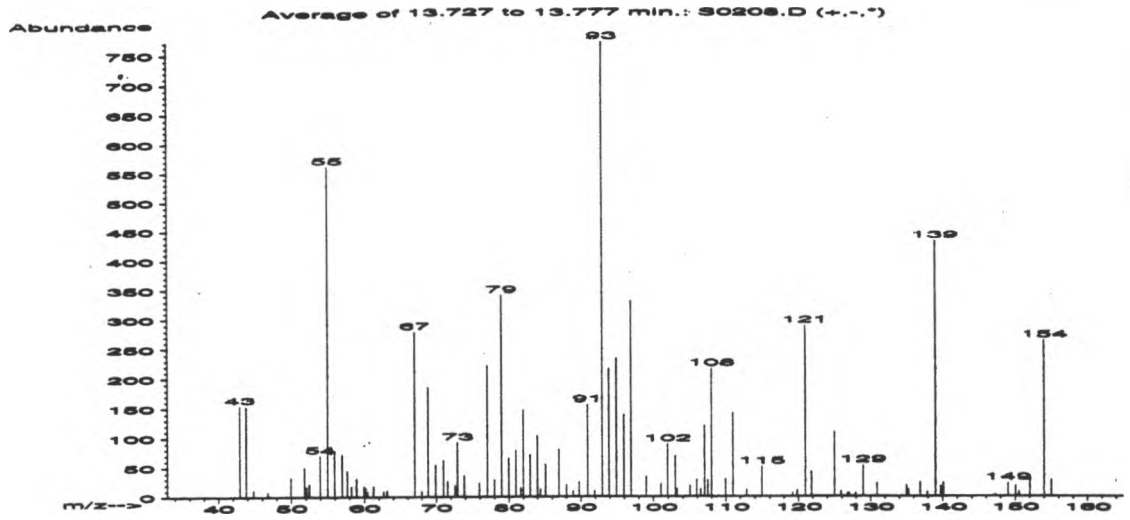
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	93
2.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	93
3.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	93
4.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
5.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	90
6.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	90
7.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	87
8.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	87
9.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	87
10.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	87
11.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	87
12.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	87
13.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	87
14.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	87
15.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	87
16.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	87
17.	Benzene, methyl(1-methylethyl)-	134	C10H14	87
18.	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	87
19.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	87
20.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	83

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000099-87-6	121632	80	10	0	85	13	66	0	93	9935
2.	*93	000535-77-3	121629	78	10	0	77	13	66	50	93	9891
3.	*93	000099-87-6	121635	78	10	0	74	15	66	54	93	9867
4.	*91	000095-93-2	121675	73	17	0	74	5	62	17	66	9842
5.	*90	000095-93-2	121676	73	15	1	69	10	59	33	74	9755
6.	*90	000933-98-2	121653	70	21	1	79	7	59	27	76	9925
7.	*87	000527-53-7	7458	74	17	1	91	11	54	22	66	9862
8.	*87	000934-80-5	121664	62	27	1	89	7	54	0	56	9924
9.	*87	000527-53-7	121672	74	17	1	91	11	54	22	66	9862
10.	*87	000527-84-4	121625	82	5	0	77	15	54	35	81	9883
11.	*87	000535-77-3	121628	76	10	0	83	13	54	43	81	9851
12.	*87	000535-77-3	7446	74	17	1	97	13	54	32	74	9871
13.	*87	000527-84-4	7445	78	12	1	89	15	54	37	80	9848
14.	*87	000099-87-6	121633	73	15	0	70	13	54	39	81	9882
15.	*87	000535-77-3	121627	79	10	0	82	13	54	38	80	9878
16.	*87	000934-74-7	121666	66	21	1	83	13	54	0	64	9939
17.	*87	025155-15-1	121626	74	15	1	79	15	54	33	76	9873
18.	*87	000488-23-3	7457	70	22	1	74	11	54	0	76	9895
19.	*87	000099-87-6	121631	74	16	1	99	15	54	31	74	9850
20.	*83	000527-53-7	121673	64	27	2	86	11	50	10	56	9776

STP Compounds

Peak 40:terpenol



Average of 13.727 to 13.777 min.: S0208.D
Converted from RTE data file: >S0208:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	154	56.95	72	68.00	9	79.00	342
43.85	153	57.70	44	68.90	185	79.95	66
44.80	11	58.25	18	69.90	54	80.95	79
46.80	8	58.95	31	71.00	62	81.65	16
49.95	33	59.90	18	71.55	26	82.00	147
51.80	50	60.15	15	72.55	19	82.95	71
52.05	17	60.40	8	72.90	92	84.00	103
52.45	22	61.25	18	73.85	36	84.40	13
53.95	70	62.65	9	75.90	24	85.10	55
55.00	562	63.15	11	77.00	222	87.00	80
55.95	74	67.00	279	78.00	29	88.00	20

Average of 13.727 to 13.777 min.: S0208.D
Converted from RTE data file: >S0208:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
88.95	10	101.90	89	112.90	12	128.95	53
89.75	25	102.95	69	114.95	51	130.90	23
90.95	156	103.20	13	119.20	7	135.00	19
91.90	10	105.00	19	119.80	11	135.25	12
92.95	772	105.90	29	120.95	289	136.90	24
93.90	217	106.50	13	121.80	42	137.90	8
94.95	234	107.05	120	125.05	109	139.00	434
95.95	139	107.50	28	125.95	9	139.75	18
96.95	331	108.00	216	126.80	6	140.10	24
99.00	34	109.95	30	127.05	6	147.30	4
101.00	22	110.95	141	127.95	6	149.00	23

Average of 13.727 to 13.777 min.: S0208.D
Converted from RTE data file: >S0208:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.05	18						
150.55	8						
152.05	32						
154.00	264						
154.95	28						

STP Compounds

Average of 13.727 to 13.777 min.: S0208.D
Converted from RTE data file: >S0208:

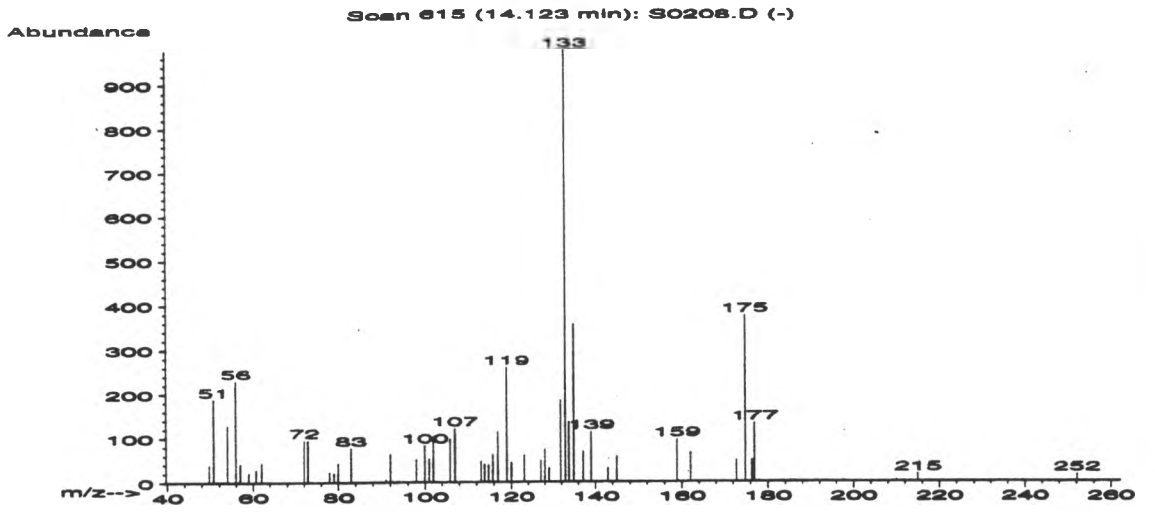
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanemethanol, 4-methylene-	126	C8H14O	38
2.	CHLORO(ETHYL)DIMETHYL-SILANE	122	C4H11ClSi	35
3.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	35
4.	Camphene	136	C10H16	32
5.	Camphene	136	C10H16	25
6.	Bicyclo[3.1.1]heptane, 6,6-dimethyl-3-me	136	C10H16	25
7.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	25
8.	1-PENTENE, 5-(2,2-DIMETHYLCYCLOPROPYL)-2	164	C12H20	25
9.	METHYLESTER OF 5-METHYL-2-METHYLENE-3-HE	154	C9H14O2	22
10.	1,3-Dimethoxy-2-methylcyclohexa-1,4-dien	154	C9H14O2	14
11.	5-METHYL-2-ISOPROPYL-2-HEXENAL	154	C10H18O	14
12.	Silane, chloro(1,1-dimethylethyl)dimethy	150	C6H15ClSi	14
13.	p-Menth-8(10)-en-9-ol, trans-	154	C10H18O	12
14.	2-Cyclohexene-1-thione, 3,6,6-trimethyl-	154	C9H14S	12
15.	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	12
16.	1,4,6-HEPTATRIENE, 3,3,6-TRIMETHYL-	136	C10H16	12
17.	Pyridine, 2-(ethylthio)-	139	C7H9NS	11
18.	2,2-Diethyl-1,3-cyclopentanedione	154	C9H14O2	10
19.	1-(3-Furyl)-4,8-dimethyl-7-hydroxy-1,6-n	310	C17H26O5	10
20.	Cyclofenchene	136	C10H16	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	001004-24-6	5376	43	78	2	93	37	14	0	37	8583
2.	*35	000000-00-0	4300	37	66	2	85	52	11	0	39	7996
3.	35	003779-61-1	121951	54	50	2	86	55	11	3	38	7623
4.	32	000079-92-5	122047	59	51	1	79	46	9	11	33	8174
5.	25	000079-92-5	122052	43	59	2	99	54	7	0	35	8029
6.	25	016022-04-1	8165	47	67	1	59	54	7	17	37	8117
7.	25	003779-61-1	121953	41	66	3	90	54	7	12	34	7711
8.	25	000000-00-0	18718	46	67	2	88	53	7	0	37	7432
9.	*22	072707-71-2	14381	51	9	0	50	61	5	16	41	5765
10.	*14	084247-66-5	14431	41	28	0	43	70	2	1	40	5544
11.	*14	035158-25-9	124185	62	36	2	51	67	2	19	40	4739
12.	*14	018162-48-6	12503	34	57	3	78	66	2	0	41	7322
13.	12	015714-12-2	14719	40	77	0	72	63	2	0	33	7207
14.	*12	038693-71-9	14516	43	79	2	50	64	2	3	33	7546
15.	12	029548-02-5	8069	45	69	1	58	62	2	0	35	7906
16.	12	000000-00-0	8072	45	69	1	58	62	2	0	35	7906
17.	*11	019006-76-9	8905	47	67	0	43	73	2	0	44	4942
18.	*10	062248-57-1	14421	47	62	1	62	74	1	0	39	5283
19.	10	077877-56-6	77009	43	35	0	50	80	1	0	39	4383
20.	10	000488-97-1	8188	45	56	3	185	74	1	1	38	7569

STP Compounds

Peak 41; Chlorinated Amine



Scan 615 (14.123 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.70	39	78.00	23	107.00	121	129.00	31
50.70	188	79.00	20	113.00	47	131.75	185
53.95	128	80.00	43	113.90	40	132.90	977
55.90	230	82.95	77	114.80	39	133.75	135
56.95	41	90.95	7	115.75	62	134.90	357
58.95	21	92.00	63	116.90	113	137.15	69
60.65	29	97.95	51	118.95	260	139.00	113
62.00	44	99.95	83	120.05	44	142.95	31
72.05	95	101.00	53	123.05	61	144.95	57
72.95	94	101.95	102	127.05	49	158.90	96
73.85	2	105.90	97	128.05	74	162.00	66

Scan 615 (14.123 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
172.80	48						
174.80	376						
176.30	49						
176.95	132						
214.95	17						
252.15	16						

STP Compounds

Scan 615 (14.123 min): S0208.D

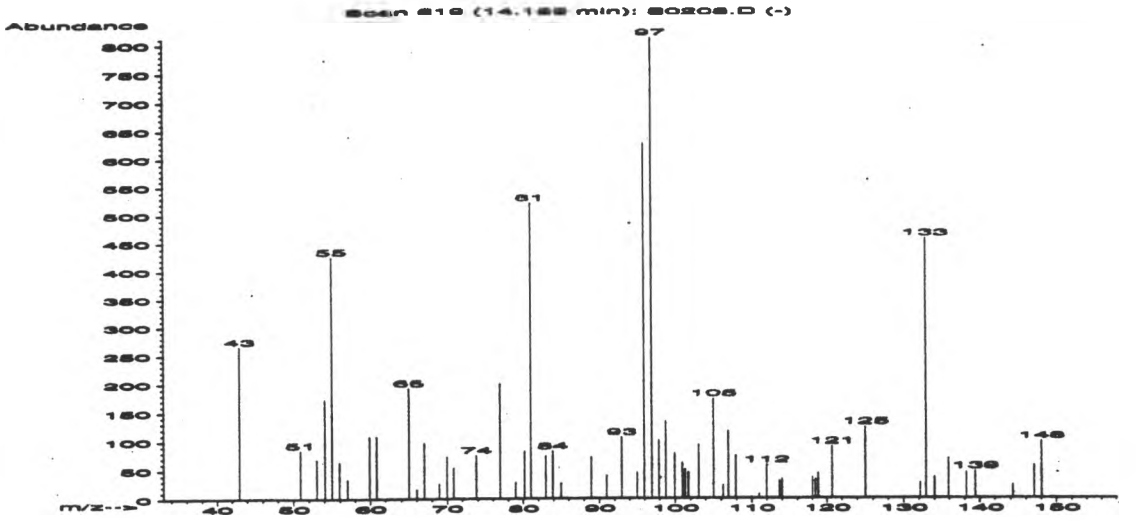
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-ACETAMIDOBENZIMIDAZOLE	175	C9H9N3O	47
2.	Disiloxane, 1,1,3,3-tetramethyl-1,3-bis[	362	C16H34O5Si2	38
3.	1H-1-Silaindene, 2,3-dihydro-1,1-dipropy	218	C14H22Si	38
4.	2-PHENYL-2-METHYL-1-D1-AZIRIDINE	133	C9H10DN	38
5.	Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	37
6.	5,6,7,8-TETRAHYDROQUINOLINE-5-D1	133	C9H10DN	28
7.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	25
8.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	25
9.	Benzene, 1-isocyano-2-methoxy-	133	C8H7NO	25
10.	Benzenepropanoic acid, .beta.,2,4-trimet	206	C13H18O2	23
11.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	23
12.	2-Propanol, (2-cyclohexylphenoxy)-	234	C15H22O2	17
13.	2-BROMO-INDANOL	212	C9H9BrO	17
14.	Benzeneacetic acid, .alpha.,.alpha.,4-tr	206	C13H18O2	17
15.	2H-1-Benzopyran-2-one, 7-methoxy-	176	C10H8O3	17
16.	2-Oxazolidinone, 5-isopropyl-4-phenyl-,	205	C12H15NO2	17
17.	Carbonic acid, methyl ester, ester with	177	C9H7NO3	17
18.	5-(6-Methyl-3-pyridyl)tetrazole	161	C7H7N5	17
19.	6H-1,2,5-Oxadiazine-6-thione, 4,5-dihydr	222	C10H10N2O2S	16
20.	Benzene, 1-isocyano-4-methoxy-	133	C8H7NO	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	060792-56-5	23362	46	37	0	81	38	20	10	39	8954
2.	38	000126-80-7	90620	38	107	1	99	22	14	2	29	9359
3.	38	061141-63-7	42943	38	73	0	66	36	14	15	35	9054
4.	*38	030691-62-4	7149	38	67	0	71	47	14	0	39	8710
5.	37	017851-27-3	12121	42	42	1	90	44	13	9	31	8699
6.	28	020668-21-7	7163	39	79	2	99	40	8	0	28	7322
7.	25	004218-48-8	123449	36	61	1	99	45	7	0	25	8667
8.	25	004218-48-8	12115	36	49	1	99	45	7	1	26	8666
9.	*25	020771-60-2	7116	31	88	0	75	53	7	0	33	8544
10.	23	056298-76-1	37457	36	73	1	99	47	6	4	26	8619
11.	23	004706-90-5	123453	36	53	1	99	50	6	1	23	8598
12.	17	055177-64-5	50006	36	114	1	95	52	3	0	21	8576
13.	17	005400-80-6	40088	37	94	2	99	54	3	0	22	8473
14.	17	032454-24-3	37453	33	62	0	99	53	3	0	25	8431
15.	17	000531-59-9	126468	35	82	1	78	54	3	0	21	8407
16.	17	032461-27-1	36942	34	94	3	99	52	3	0	22	8634
17.	*17	017175-18-7	24159	28	93	1	79	52	3	0	29	8520
18.	17	013599-90-1	17128	35	59	1	87	54	3	1	23	8445
19.	16	033406-09-6	44472	38	90	1	93	56	3	0	33	8409
20.	*16	010349-38-9	7118	30	79	2	99	56	3	0	33	8398

STP Compounds

Peak 42; Unidentified



Scan 619 (14.189 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	266	67.00	97	85.00	26	101.30	50
50.90	84	68.95	26	88.90	72	101.70	45
53.00	68	69.95	73	90.95	40	103.05	93
54.05	172	70.85	53	92.95	106	105.00	173
54.95	425	73.80	75	95.00	45	106.25	23
55.95	63	76.95	201	95.95	627	106.90	117
57.00	33	78.95	28	96.95	811	107.90	74
59.90	108	80.15	82	97.90	101	110.00	2
60.85	108	81.00	521	98.80	134	111.00	7
65.00	192	82.95	74	99.95	78	111.95	58
66.00	16	83.90	82	100.95	61	113.65	30

Scan 619 (14.189 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.00	34	139.40	47				
118.05	37	144.30	23				
118.45	33	147.05	57				
118.80	44	148.05	99				
120.70	90						
125.05	124						
132.15	27						
132.90	458						
134.00	36						
135.90	69						
138.25	45						

STP Compounds

Scan 619 (14.189 min): S0208.D

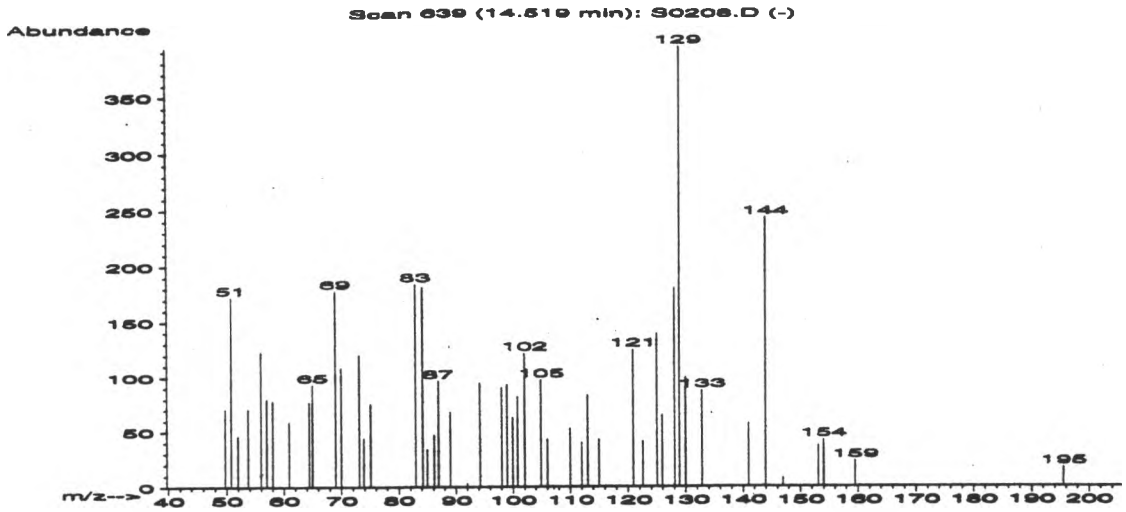
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	TOLUENE-D5	92	C7H3D5	46
2.	1-(2-Methylpropenyl)aziridine	97	C6H11N	43
3.	Cyclohexane, 1-methyl-4-(1-methylethyl)-	140	C10H20	37
4.	2-Azabicyclo[2.2.1]heptane	97	C6H11N	37
5.	Cyclohexane, 1-methyl-4-(1-methylethyl)-	140	C10H20	37
6.	Cyclohexane, 1-methyl-4-(1-methylethyl)-	140	C10H20	37
7.	m-Menthane, (1R,3R)-(+)-	140	C10H20	16
8.	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	14
9.	Cyclohexane, 1,1-dimethyl-	112	C8H16	14
10.	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	14
11.	(Z)-1-(1-Butenyl)aziridine	97	C6H11N	10
12.	(E)-1-(1-Butenyl)aziridine	97	C6H11N	10
13.	Propanedinitrile, (1,2,2-trimethylpropyl	148	C9H12N2	10
14.	1-Pentyne, 3-ethyl-3-methoxy-	126	C8H14O	10
15.	Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	10
16.	Cyclohexane, 1-ethyl-2-methyl-, cis-	126	C9H18	10
17.	Cyclohexane, (bromomethyl)-	176	C7H13Br	10
18.	2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	10
19.	2-Aziridinone, 1-tert-butyl-3-(1-methylc	223	C14H25NO	10
20.	1H-Imidazole, 1-ethyl-	96	C5H8N2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	000000-00-0	413	33	53	0	89	41	20	16	43	8769
2.	*43	080839-93-6	693	40	52	0	99	41	18	3	38	8797
3.	37	006069-98-3	122511	39	53	3	183	41	13	0	33	8699
4.	*37	000279-24-3	699	30	10	0	84	41	13	0	33	8803
5.	37	006069-98-3	9510	41	48	1	92	41	13	6	31	8765
6.	37	006069-98-3	122513	55	26	1	99	41	13	6	37	8820
7.	16	013837-67-7	9508	44	51	2	87	56	3	0	37	8761
8.	*14	053783-91-8	2602	36	58	3	99	70	2	0	41	6987
9.	*14	000590-66-9	2721	33	63	2	68	69	2	0	39	7279
10.	14	053907-59-8	5443	43	47	0	87	70	2	20	41	7057
11.	*10	080839-94-7	691	38	65	1	132	67	1	0	35	7780
12.	*10	080839-92-5	692	42	61	2	144	67	1	0	35	7563
13.	*10	013017-53-3	11967	33	77	2	84	78	1	0	39	4157
14.	10	053941-20-1	5333	44	35	1	91	70	1	0	37	6987
15.	10	006294-39-9	23639	35	49	1	80	69	1	8	36	7253
16.	10	004923-77-7	120635	40	45	2	99	67	1	3	31	7590
17.	10	002550-36-9	23643	40	40	1	99	70	1	9	31	6987
18.	10	023758-27-2	2597	44	57	3	81	70	1	0	37	6987
19.	10	026944-18-3	45341	37	81	2	68	69	1	4	31	7463
20.	*10	007098-07-9	562	29	50	0	77	69	1	0	33	5839

STP Compounds

Peak 43a; dimethylindene??



Scan 639 (14.519 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.70	71	69.95	108	94.20	94	115.00	43
50.80	172	73.05	120	98.05	90	120.95	124
51.95	46	73.85	44	98.95	93	122.55	41
53.70	71	75.05	75	99.95	63	125.05	138
55.95	123	82.95	183	100.80	82	125.95	65
56.95	80	84.15	180	102.05	121	128.05	179
58.00	78	84.95	34	104.90	97	128.90	393
60.90	59	86.15	47	106.00	43	130.00	99
64.40	77	86.95	96	110.00	53	132.85	87
65.00	93	89.00	68	112.00	40	140.95	57
68.95	177	92.00	3	113.00	83	143.95	241

Scan 639 (14.519 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.00	8						
153.05	37						
154.00	42						
159.50	23						
195.55	17						

STP Compounds

Scan 639 (14.519 min): S0208.D

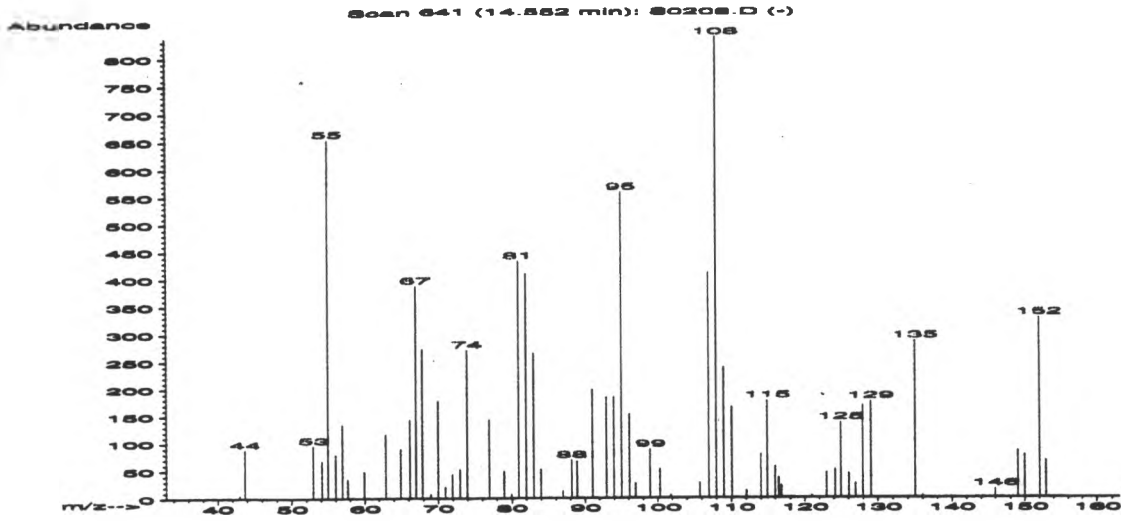
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Indene, 1,1-dimethyl-	144	C11H12	43
2.	Naphthalene, 1,2-dihydro-3-methyl-	144	C11H12	37
3.	Naphthalene, 1,2-dihydro-6-methyl-	144	C11H12	25
4.	1H-Indene, 1,1-dimethyl-	144	C11H12	37
5.	1H-Cyclopropa[b]naphthalene, 1a,2,7,7a-t	144	C11H12	23
6.	2-Quinolinecarboxylic acid	173	C10H7NO2	25
7.	Quinoline	129	C9H7N	27
8.	5-METHYL-2-ETHYLAMINO-2-THIAZOLINE	144	C6H12N2S	10
9.	Isoquinoline	129	C9H7N	16
10.	Quinoline	129	C9H7N	16
11.	Quinoline	129	C9H7N	27
12.	Isoquinoline	129	C9H7N	16
13.	Quinoline	129	C9H7N	16
14.	5-ETHYL-4-HYDRO-3-MERCAPTO-1,2,4-TRIAZOL	129	C4H7N3S	16
15.	4-Piperidinemethanol, 1-methyl-	129	C7H15NO	9
16.	Silane, dichloroethyl-	128	C2H6Cl2Si	17
17.	Citric acid	192	C6H8O7	9
18.	Piperazine, 1,2,4-trimethyl-	128	C7H16N2	10
19.	2(3H)-Furanone, 3-acetyldihydro-	128	C6H8O3	10
20.	Thiazole, 5-ethoxy-	129	C5H7NOS	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	018636-55-0	10896	34	75	0	95	45	18	0	41	8652
2.	*37	002717-44-4	10898	28	83	1	99	45	13	1	30	8629
3.	*25	002717-47-7	10900	28	84	1	84	45	7	0	29	8626
4.	*37	018636-55-0	122998	28	71	0	99	44	13	2	35	8624
5.	*23	006571-72-8	10911	28	84	1	99	46	6	0	29	8540
6.	25	000093-10-7	22597	42	77	0	82	54	7	2	35	7781
7.	*27	000091-22-5	121012	47	54	0	95	60	8	13	38	7639
8.	*10	013578-64-8	10535	46	88	1	55	71	1	0	40	7627
9.	*16	000119-65-3	121014	39	66	1	99	60	3	4	37	7622
10.	*16	000091-22-5	121010	39	66	1	99	60	3	4	37	7610
11.	*27	000091-22-5	121013	47	62	1	99	60	8	1	38	7605
12.	*16	000119-65-3	121015	37	62	1	99	60	3	3	36	7599
13.	*16	000091-22-5	121009	30	82	0	89	60	3	0	33	7576
14.	*16	007271-45-6	120954	31	67	0	89	59	3	4	37	7498
15.	9	020691-89-8	6189	51	59	0	92	80	1	0	35	6439
16.	*17	001789-58-8	5662	32	101	3	177	53	3	0	29	5670
17.	9	000077-92-9	30499	39	99	0	53	78	1	0	33	5287
18.	*10	000120-85-4	5912	44	52	0	44	78	1	10	39	4563
19.	*10	000517-23-7	5732	35	62	2	514	79	1	0	39	4532
20.	*10	025115-63-3	6103	40	71	3	216	68	1	0	35	3652

STP Compounds

Peak43b: terpenoid



Scan 641 (14.552 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	6	66.15	144	79.95	7	95.00	558
43.70	88	67.00	387	80.95	433	96.10	153
52.95	95	67.90	272	82.00	410	96.95	26
54.10	68	69.00	7	83.00	265	98.95	88
54.95	654	70.00	178	84.00	52	100.30	52
56.00	79	70.95	20	86.95	13	101.85	5
56.95	134	71.95	43	88.15	69	105.75	27
57.70	34	73.00	52	88.90	67	107.00	412
59.90	48	73.95	271	91.00	198	108.00	836
62.90	116	77.00	144	92.95	184	109.00	239
64.95	89	78.95	49	93.95	184	110.10	166

Scan 641 (14.552 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.05	13	126.95	26				
114.00	79	127.95	169				
114.90	178	129.05	176				
116.00	57	135.00	287				
116.50	36	136.00	4				
116.85	22	145.95	16				
120.95	4	149.05	85				
123.00	46	150.00	78				
124.20	51	152.05	329				
124.95	138	152.95	67				
126.05	44						

STP Compounds

Scan 641 (14.552 min): S0208.D

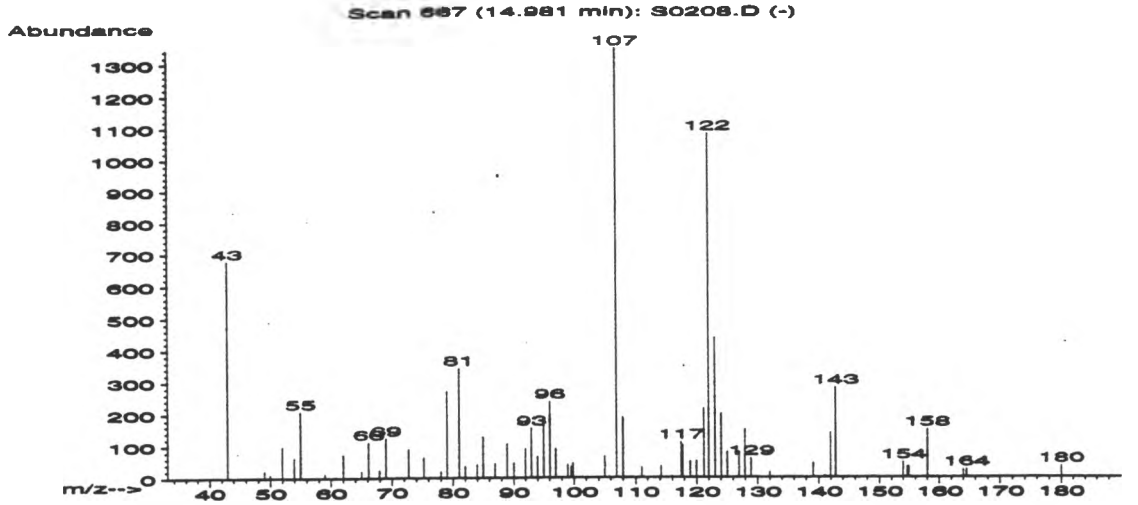
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Pyrimidine, 2-ethoxy-4,6-dimethyl-	152	C8H12N2O	43
2.	Ethanol, 2-(3-methylphenoxy)-	152	C9H12O2	43
3.	Ethanol, 2-(4-methylphenoxy)-	152	C9H12O2	46
4.	Ethanol, 2-(4-methylphenoxy)-	152	C9H12O2	43
5.	Camphor	152	C10H16O	22
6.	Camphor	152	C10H16O	22
7.	Camphor	152	C10H16O	27
8.	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimet	152	C10H16O	14
9.	Pyrimidine, 2,4-dimethyl-	108	C6H8N2	14
10.	Cyclohexanone, 2-methyl-5-(1-methylethen	152	C10H16O	41
11.	Dihydrocarvone	152	C10H16O	41
12.	4,4,-DIMETHYL-2-(Z-PROP-1-ENYL)-CYCLOPEN	152	C10H16O	22
13.	DECADIENAL	152	C10H16O	10
14.	CIS-SYN-2-METHYL-DECAHYDRONAPHTHALENE	152	C11H20	30
15.	Naphthalene, decahydro-2-methyl-	152	C11H20	30
16.	Pulegone	152	C10H16O	11
17.	2-CYANO-4,5,5-TRIMETHYL-1-PYRROLINE 1-OX	152	C8H12N2O	10
18.	(-)-TRANS-CARANON-(3)	152	C10H16O	18
19.	(-)-TRANS-CARANON-(3)	152	C10H16O	11
20.	Pulegone	152	C10H16O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	007781-21-7	13391	49	73	2	94	48	18	0	46	8403
2.	*43	013605-19-1	13466	48	47	2	98	41	18	7	41	8224
3.	*46	015149-10-7	13467	50	46	2	84	45	20	0	46	8154
4.	*43	015149-10-7	123925	48	21	0	78	48	18	0	46	8011
5.	*22	000076-22-2	124022	45	69	2	102	61	5	0	40	7785
6.	*22	000076-22-2	124024	38	74	0	50	62	5	1	40	7718
7.	*27	000076-22-2	124017	55	51	0	66	58	8	5	40	7571
8.	*14	000464-48-2	13786	44	77	3	129	67	2	0	40	7474
9.	*14	014331-54-5	118695	33	82	0	81	69	2	0	41	7342
10.	*41	007764-50-3	13846	68	55	1	58	54	16	19	50	7132
11.	*41	005948-04-9	123991	68	55	1	58	54	16	19	50	7132
12.	*22	058795-36-1	13630	57	59	1	65	64	5	0	40	5737
13.	*10	000000-00-0	13576	43	53	3	264	76	1	0	40	5704
14.	*30	000000-00-0	13879	60	64	2	66	64	9	0	51	5688
15.	*30	002958-76-1	124049	60	64	2	66	64	9	0	51	5688
16.	*11	000089-82-7	123988	49	68	0	51	75	2	0	46	5375
17.	*10	058134-14-8	13381	33	77	0	29	77	1	0	41	5133
18.	*18	004176-04-9	124001	47	39	0	46	70	3	0	44	5054
19.	*11	004176-04-9	13728	69	49	1	51	74	2	14	47	5051
20.	*11	000089-82-7	13693	50	67	0	51	77	2	0	46	4277

STP Compounds

Peak 28; dimethylphenol



Scan 667 (14.981 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	678	68.95	123	90.00	45	106.95	1344
49.05	21	72.70	89	92.00	92	108.00	188
49.95	11	75.20	64	92.95	154	111.00	32
51.95	99	78.00	19	93.95	66	114.15	35
53.95	63	79.00	271	95.00	184	115.95	5
55.00	207	81.00	343	96.05	238	117.45	111
59.00	12	82.00	35	97.00	90	117.70	102
62.00	73	83.95	41	98.95	40	118.95	51
65.00	20	85.00	128	99.55	33	119.95	53
66.15	112	86.90	44	99.80	45	121.20	215
67.95	24	88.90	107	105.00	66	122.00	1079

Scan 667 (14.981 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	437	154.00	48				
124.05	199	154.65	32				
125.05	81	154.90	34				
127.00	81	158.00	149				
127.95	149	164.00	23				
128.95	60	164.50	25				
132.00	16	180.00	35				
139.10	44						
140.95	6						
141.95	139						
142.80	281						

STP Compounds

Scan 667 (14.981 min): S0208.D

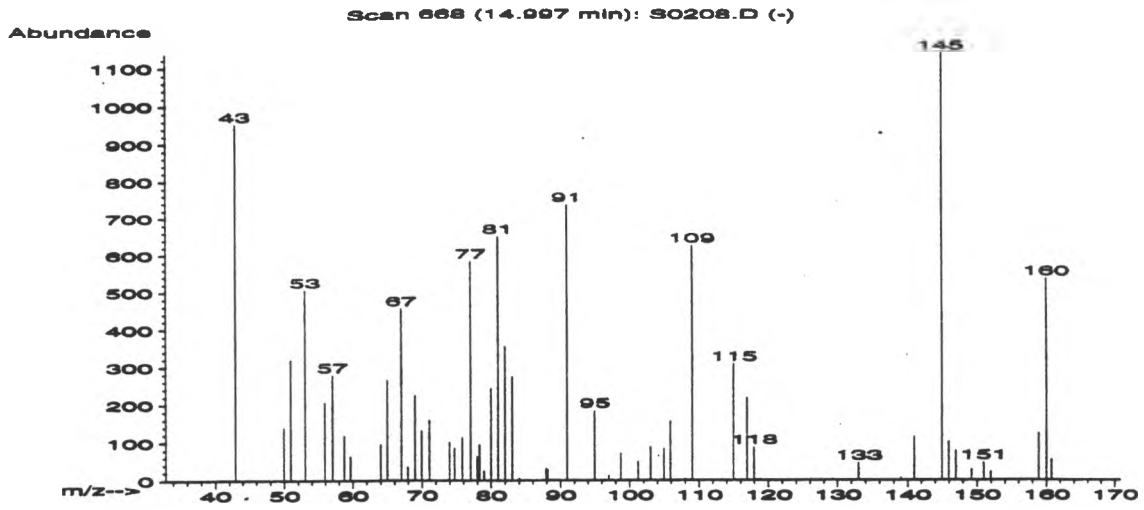
PBM Search of library F:\STP_LIB.L

	Name	MolWt	Formula	Qual
1.	STP Peak 27	122	C8H10O	98

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*98	000000-00-0	45	111	0	0	99	23	79	0	98	9729

STP Compounds

Peak 44; Unidentified hydrocarbon



Scan 668 (14.997 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	952	67.95	35	80.00	243	101.20	50
49.95	139	68.95	225	81.00	650	103.05	88
50.95	319	69.95	132	82.00	355	104.95	84
53.05	505	71.05	160	83.00	276	105.90	156
55.90	205	73.95	101	84.00	6	108.00	3
57.00	278	74.70	86	87.90	31	109.00	625
58.75	118	75.80	114	88.15	28	115.00	307
59.65	63	77.05	583	91.00	736	116.95	218
64.00	95	77.95	63	94.95	184	117.95	87
65.00	265	78.30	94	96.95	12	133.00	45
67.00	456	78.95	25	98.70	71	139.00	6

Scan 668 (14.997 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.95	115						
144.95	1136						
145.95	102						
146.95	78						
149.20	29						
150.95	47						
151.95	22						
158.90	125						
160.00	537						
160.75	54						

STP Compounds

Scan 668 (14.997 min): S0208.D

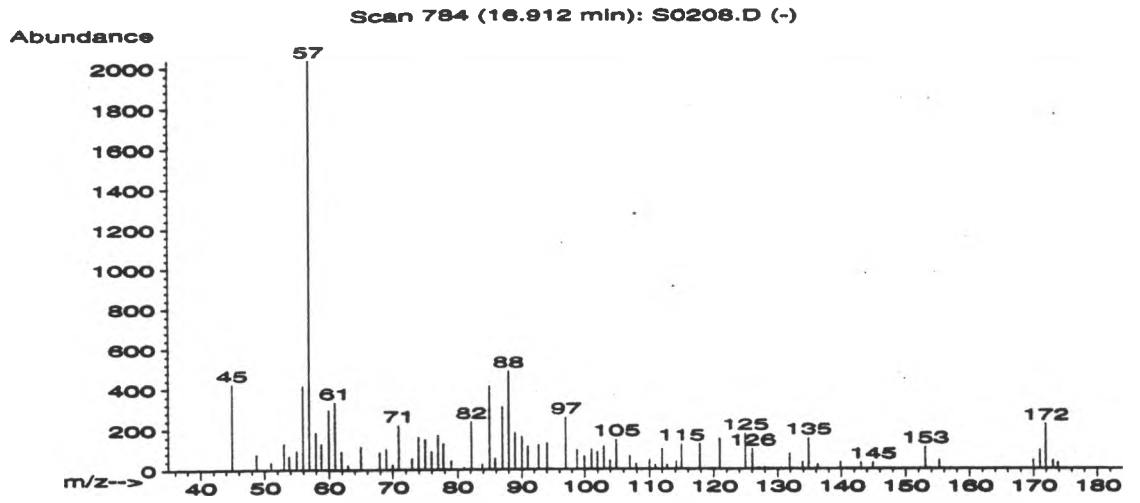
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,4,6-TRIMETHYLINDANE	160	C12H16	78
2.	5-ACETOANTHRANILONITRILE	160	C9H8N2O	53
3.	3-ACETOANTHRANILONITRILE	160	C9H8N2O	53
4.	2-Isopropenyl-2,3-dihydrobenzofuran	160	C11H12O	38
5.	2-Buten-1-ol, 3-methyl-, acetate	128	C7H12O2	27
6.	Pyrido[2,3-d]pyrimidine, 4-methyl-	145	C8H7N3	25
7.	Naphthalene, 1,2,3,4-tetrahydro-5,7-dime	160	C12H16	18
8.	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl	160	C11H12O	18
9.	Naphthalene, 1,2,3,4-tetrahydro-1,4-dime	160	C12H16	14
10.	2,3-Dimethyl-3-phenylbut-1-ene	160	C12H16	11
11.	1H-1,2,4-Triazole, 3-phenyl-	145	C8H7N3	11
12.	6-Quinolinol	145	C9H7NO	10
13.	5,6-DIMETHYL-2H-ISOINDOLE	145	C10H11N	10
14.	4,7-DIMETHYL-2H-ISOINDOLE	145	C10H11N	10
15.	2-PHENYL-1,2,3-TRIAZOLE	145	C8H7N3	10
16.	Quinazoline, 4-methyl-, 3-oxide	160	C9H8N2O	10
17.	Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E	160	C12H16	10
18.	Quinoline, 1-oxide	145	C9H7NO	10
19.	2-METHYLBENZALACETONE	160	C11H12O	10
20.	2-Quinazolinamine	145	C8H7N3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	065001-56-1	17042	38	18	0	69	7	46	3	42	7398
2.	*53	033720-71-7	16788	39	11	0	89	30	28	12	39	7314
3.	*53	000000-00-0	16787	40	11	0	73	30	28	11	38	7320
4.	*38	062452-76-0	16942	38	26	0	57	50	14	6	39	7402
5.	27	001191-16-8	120802	43	55	0	72	56	8	0	39	3966
6.	*25	028732-71-0	11003	37	52	1	76	53	7	9	36	7370
7.	*18	021693-54-9	17056	44	64	0	67	69	3	0	44	7522
8.	*18	026465-81-6	16944	52	52	1	96	69	3	0	46	7437
9.	*14	004175-54-6	17049	45	68	1	99	67	2	0	39	7431
10.	*11	022557-45-5	17004	35	71	0	57	78	2	8	43	7775
11.	*11	003357-42-4	11023	34	63	0	84	80	2	14	43	7305
12.	*10	000580-16-5	11049	36	69	0	68	78	1	0	41	6758
13.	*10	000000-00-0	11087	35	69	0	80	78	1	0	41	6782
14.	*10	000000-00-0	11086	36	71	1	99	78	1	0	39	6776
15.	*10	000000-00-0	11022	35	71	3	99	80	1	10	40	7095
16.	*10	010501-56-1	16795	33	62	0	39	79	1	0	41	3312
17.	*10	054340-86-2	17013	37	67	0	68	72	1	0	41	7481
18.	*10	001613-37-2	123030	35	67	0	84	78	1	0	41	6782
19.	10	016927-82-5	16923	54	53	0	69	71	1	0	39	7420
20.	*10	001687-51-0	11006	29	55	0	72	68	1	10	37	6753

STP Compounds

Peak 45; Unidentified hydrocarbon



Scan 784 (16.912 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	423	60.90	331	75.95	88	88.95	181
48.70	74	61.90	89	77.00	170	90.00	161
51.00	35	62.90	22	77.80	128	91.00	113
53.00	130	65.00	114	79.00	43	92.70	121
53.80	65	67.90	84	81.00	10	94.05	129
54.95	95	68.95	102	82.15	234	97.05	254
55.95	414	70.00	22	83.85	26	98.80	95
56.95	2037	70.95	217	85.00	411	99.95	62
57.95	182	72.95	53	85.85	52	101.05	97
58.80	126	73.95	160	87.00	310	101.95	85
59.95	294	74.95	147	88.00	487	102.95	112

Scan 784 (16.912 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.95	40	120.95	151	144.95	31		
104.90	145	124.95	174	145.85	3		
106.95	62	126.05	98	153.05	107		
107.90	26	127.05	5	155.25	41		
110.00	43	127.95	7	169.95	41		
110.95	19	131.90	73	171.05	93		
112.00	99	133.90	33	171.95	220		
112.75	21	134.85	151	173.05	40		
114.15	37	136.25	21	173.80	28		
115.00	122	139.90	34				
117.85	126	143.05	31				

STP Compounds

Scan 784 (16.912 min): S0208.D

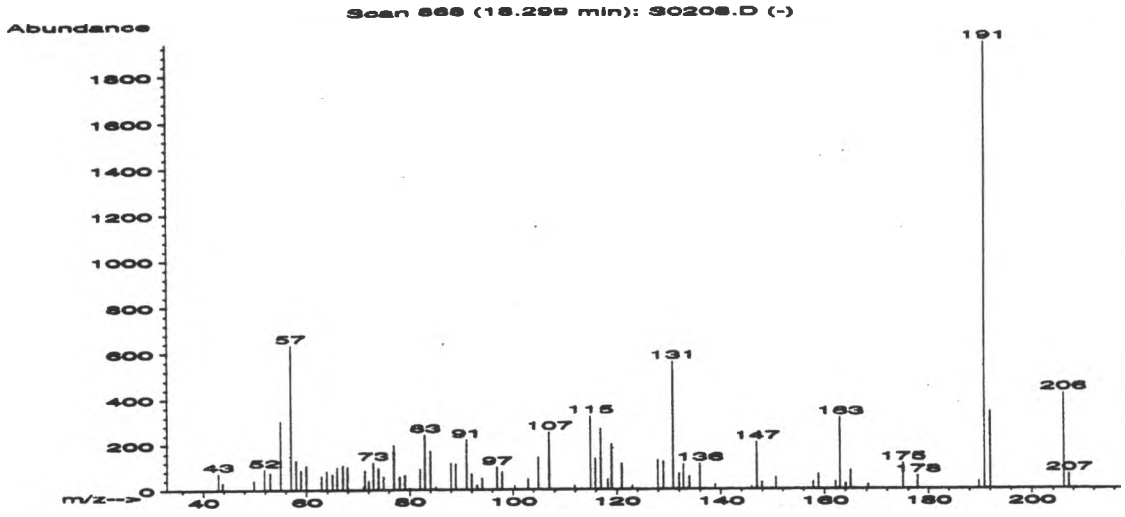
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Dodecane, 2,6,11-trimethyl-	212	C15H32	35
2.	Dodecane	170	C12H26	35
3.	Dodecane	170	C12H26	35
4.	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	25
5.	4-Pentenoic acid, 5-ethoxy-, ethyl ester	172	C9H16O3	22
6.	THIACYCLOHEPTAN-3-OL	132	C6H12OS	22
7.	Butane, 1,1'-oxybis-	130	C8H18O	22
8.	Piperazine, 2-methyl-	100	C5H12N2	22
9.	Cyclohexanol	100	C6H12O	14
10.	2-Hexen-1-ol, (E)-	100	C6H12O	14
11.	7H-1,4-Oxathiepin-7-one, tetrahydro-	132	C5H8O2S	14
12.	2-Hexen-1-ol, (E)-	100	C6H12O	14
13.	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	14
14.	1,4-Oxathian-2-one, 3-methyl-	132	C5H8O2S	14
15.	1,3-Oxathiane, 2-isopropyl-2,6-dimethyl-	174	C9H18OS	10
16.	N-Isovalerylglycine methyl ester	173	C8H15NO3	10
17.	Peroxide, bis(1-methylethyl)	118	C6H14O2	10
18.	Acetic acid, ethoxy-, ethyl ester	132	C6H12O3	10
19.	CIS-2,3-EPOXYOCTANE	128	C8H16O	10
20.	Undecane, 5-methyl-	170	C12H26	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	35	031295-56-4	40639	44	62	3	90	53	11	0	39	9360
2.	*35	000112-40-3	21646	33	60	3	99	55	11	0	41	9329
3.	*35	000112-40-3	126001	33	64	3	89	55	11	0	41	9341
4.	25	018344-37-1	133325	44	80	3	84	53	7	0	35	9369
5.	*22	055162-84-0	22178	38	39	0	20	61	5	0	39	7095
6.	*22	018643-30-6	6850	44	56	0	20	62	5	11	40	2912
7.	22	000142-96-1	6583	43	37	0	70	62	5	0	39	9270
8.	*22	000109-07-9	117960	34	50	1	30	62	5	0	39	6880
9.	*14	000108-93-0	118085	34	62	3	99	70	2	0	39	9153
10.	*14	000928-95-0	118036	34	59	1	94	70	2	0	39	9157
11.	*14	005512-72-1	6785	33	60	0	23	70	2	0	41	2827
12.	14	000928-95-0	118041	43	34	1	91	70	2	18	39	9165
13.	14	002461-18-9	53458	42	74	2	63	68	2	17	38	9316
14.	*14	035562-74-4	6781	51	31	1	18	68	2	20	40	2968
15.	*10	033709-61-4	22935	46	55	1	35	77	1	0	39	2696
16.	*10	056009-37-1	126252	34	68	1	32	74	1	0	39	8949
17.	*10	016642-57-2	3815	40	52	2	82	70	1	0	35	6954
18.	10	000817-95-8	121338	45	65	1	58	68	1	0	37	2973
19.	10	023024-54-6	6032	47	57	0	14	77	1	0	39	2558
20.	*10	001632-70-8	126018	33	66	3	107	70	1	0	35	9110

STP Compounds

Peak 46; 2,6-t-butylphenol



Scan 868 (18.299 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	74	63.90	82	76.95	197	92.00	68
43.75	32	65.00	70	78.05	58	93.00	19
49.80	42	65.90	99	79.05	64	94.00	50
51.80	91	67.00	110	80.00	6	96.95	99
52.95	76	67.95	101	82.00	91	97.95	79
54.95	302	71.00	14	82.95	242	100.30	16
57.00	632	71.30	85	84.00	171	102.95	47
58.00	131	72.05	40	85.05	13	104.95	144
58.90	87	72.95	122	88.00	118	107.00	252
60.00	106	73.95	95	88.90	113	111.90	16
62.90	63	74.95	58	91.00	220	115.00	323

Scan 868 (18.299 min): S0208.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.90	137	134.00	56	164.05	25		
116.95	268	136.00	113	165.00	83		
118.30	45	138.95	21	168.30	19		
119.05	200	145.95	12	175.05	113		
120.95	114	146.95	206	177.90	57		
123.00	17	147.95	31	189.80	34		
127.95	129	150.70	51	190.95	1939		
129.00	123	157.90	34	192.05	338		
130.90	556	158.90	66	206.15	418		
132.00	69	162.15	34	207.15	64		
132.90	109	163.00	312				

STP Compounds

Scan 868 (18.299 min): S0208.D

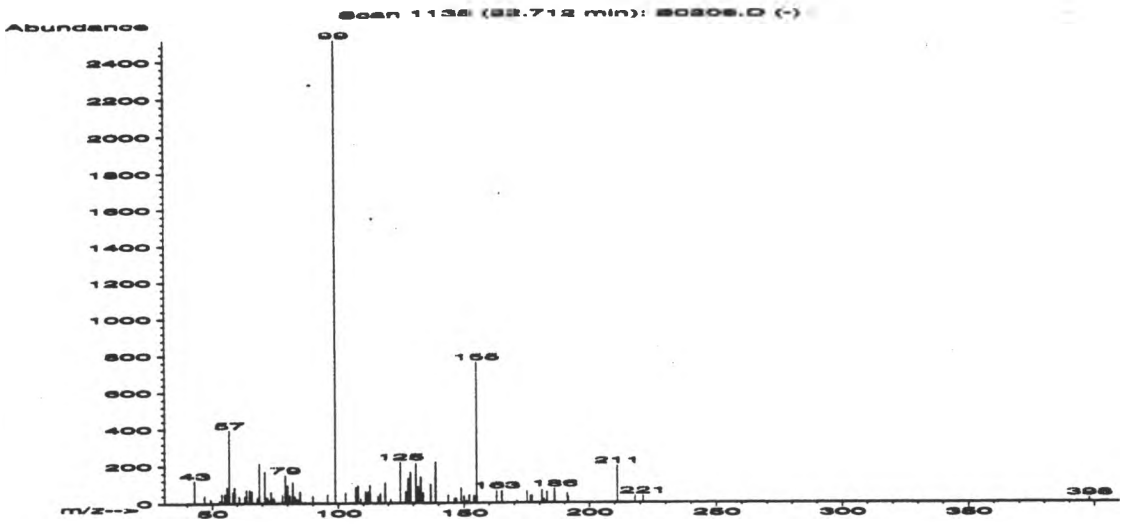
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	76
2.	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	76
3.	METHYL-P-TERT-BUTYL PHENYL ACETATE	206	C13H18O2	74
4.	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	70
5.	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	70
6.	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	68
7.	5-ACETYL-6-METHYLTHIOINDANE	206	C12H14OS	64
8.	Phenol, bis(1,1-dimethylethyl)-	206	C14H22O	58
9.	Oxirane, [[4-(1,1-dimethylethyl)phenoxy]	206	C13H18O2	58
10.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	52
11.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	52
12.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	52
13.	Benzene, 2,4-bis(1,1-dimethylethyl)-1-me	220	C15H24O	50
14.	(E)-4-(2',6',6'-Trimethyl-1'-cyclohexen-	206	C14H22O	49
15.	Oxirane, [[4-(1,1-dimethylethyl)phenoxy]	206	C13H18O2	49
16.	1,3,4,7,7-PENTAMETHYL-2-OXA-BICYCLO(4,4,	206	C14H22O	47
17.	(Z)-4-2',6',6'-Trimethyl-2'-cyclohexen-1	206	C14H22O	47
18.	6-tert-Butyl-2-sec-butyl-phenol	206	C14H22O	47
19.	Phenanthrene, 4,5-dimethyl-	206	C16H14	47
20.	1,2,4-Thiadiazol-5-amine, 3-(phenylmethy	191	C9H9N3S	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*76	000128-39-2	128868	68	45	0	99	21	45	0	76	9720
2.	*76	000128-39-2	128867	68	44	0	99	24	45	0	76	9695
3.	*74	000000-00-0	37452	61	22	1	97	16	44	0	56	9811
4.	*70	000128-39-2	37574	63	52	1	95	28	41	0	64	9642
5.	*70	001138-52-9	37575	75	38	0	99	27	41	42	66	9431
6.	*68	005875-45-6	37573	67	49	0	74	24	40	9	56	9516
7.	*64	062245-83-4	37344	51	26	1	99	20	37	4	39	9439
8.	*58	026746-38-3	37576	59	50	1	99	31	32	0	56	9421
9.	*58	003101-60-8	128852	59	60	1	85	32	32	0	56	9401
10.	*52	000096-76-4	128862	55	52	1	99	32	27	0	49	9374
11.	*52	000096-76-4	128861	49	55	0	99	31	27	0	46	9388
12.	*52	000096-76-4	37572	48	57	0	99	31	27	0	46	9395
13.	50	017177-98-9	129739	55	56	1	99	31	25	21	43	9210
14.	*49	089128-17-6	37622	37	65	2	99	36	23	6	43	9430
15.	*49	003101-60-8	37491	52	66	2	99	37	23	0	46	9252
16.	47	000000-00-0	37704	43	71	0	94	37	20	0	39	9313
17.	*47	093175-79-2	37624	33	70	1	72	37	20	5	40	9407
18.	*47	000000-00-0	37571	37	55	1	66	40	20	0	39	9263
19.	*47	003674-69-9	128902	33	83	1	66	40	20	22	40	8385
20.	*38	017467-27-5	30302	44	54	0	73	50	14	9	39	9140

STP Compounds

Peak 47; Phosporic acid, tributyl ester



Scan 1135 (22.712 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	121	63.00	35	74.45	26	90.00	38
46.95	38	63.75	70	74.75	13	95.85	46
49.30	21	64.95	71	77.90	42	98.95	2514
52.95	15	65.90	63	79.00	149	102.95	55
53.80	51	68.00	28	79.90	94	106.95	83
54.95	48	68.80	215	80.90	38	107.90	92
55.95	87	70.95	168	82.00	110	108.95	22
56.90	394	72.05	30	82.95	33	110.90	62
58.40	59	72.75	14	83.95	20	112.00	58
59.00	82	73.45	59	84.95	61	112.75	95
60.90	36	73.95	12	87.00	5	116.10	36

Scan 1135 (22.712 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.95	51	136.95	98	155.00	763	191.05	51
118.85	109	138.90	219	162.90	65	191.45	32
121.00	19	143.80	41	164.90	62	211.00	199
124.95	221	144.95	1	170.95	12	217.95	35
127.00	61	146.30	25	175.05	61	221.20	35
127.95	132	146.90	25	176.45	35	397.90	22
128.90	167	148.80	77	177.05	37		
131.00	213	150.00	36	180.90	67		
131.95	87	151.00	12	181.90	20		
133.00	138	152.05	42	183.00	58		
133.90	53	154.00	39	186.00	74		

STP Compounds

Scan 1135 (22.712 min): S0208.D

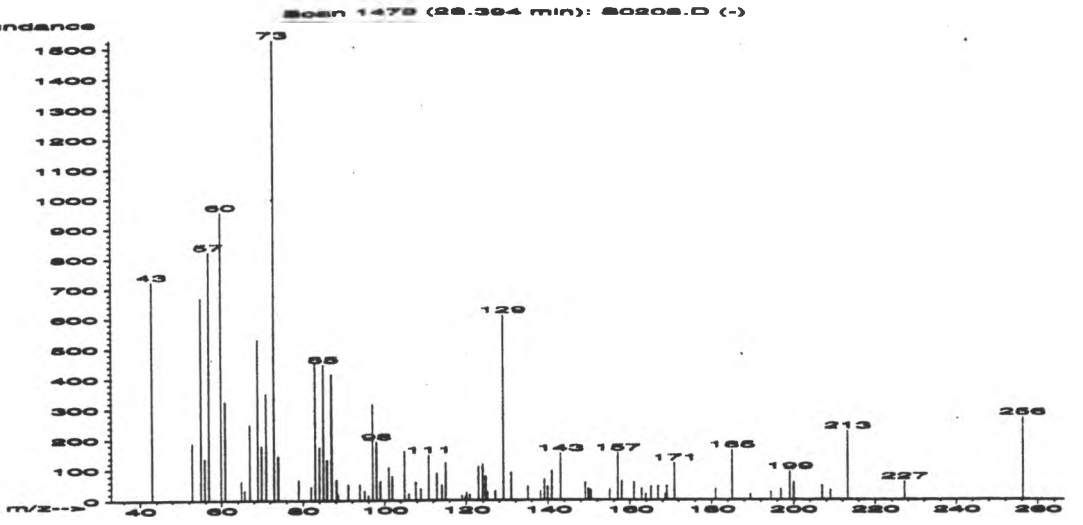
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-HYDROXYCYCLOHEXANECARBOXYLIC ACID	144	C7H12O3	37
2.	Phosphoric acid, tributyl ester	266	C12H27O4P	36
3.	Phosphoric acid, tributyl ester	266	C12H27O4P	35
4.	Hexanethioic acid, S-decyl ester	272	C16H32OS	28
5.	Phosphoric acid, tributyl ester	266	C12H27O4P	25
6.	2,2'-Bioxepane	198	C12H22O2	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*37	001123-28-0	10615	31	44	1	99	41	13	0	33	9431
2.	36	000126-73-8	131963	49	63	1	92	27	12	0	24	9838
3.	35	000126-73-8	131961	49	63	0	54	54	11	9	38	9696
4.	28	002432-81-7	64284	34	84	2	94	40	8	0	21	9469
5.	25	000126-73-8	131964	48	60	0	59	54	7	0	35	9824
6.	25	074793-02-5	33981	35	70	1	94	41	7	0	22	9431

STP Compounds

Peak 48; Hexadecanoic acid



Scan 1479 (28.394 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	724	69.95	178	88.15	67	104.90	160
52.80	189	71.00	351	88.50	19	106.00	21
54.95	670	72.95	1528	91.00	52	107.65	61
55.90	136	73.95	145	93.90	53	108.95	38
56.90	823	78.95	67	95.05	31	110.95	148
59.90	956	81.95	44	96.00	15	112.90	89
60.90	325	83.00	452	97.05	316	114.15	49
64.90	63	84.00	174	97.95	192	115.00	122
65.75	33	85.00	448	98.95	63	119.00	16
67.00	250	85.90	133	101.05	107	119.75	10
68.95	531	87.00	415	101.95	79	120.05	25

Scan 1479 (28.394 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.90	19	139.90	46	162.90	37	196.95	36
122.95	110	140.95	96	163.90	19	199.05	93
123.95	118	143.05	153	165.15	44	200.05	57
124.70	78	149.05	58	166.95	45	207.00	47
125.05	26	149.80	37	168.75	19	209.00	32
127.00	30	150.05	36	169.05	46	213.25	226
129.00	612	150.45	33	170.95	121	227.15	59
130.90	90	155.00	35	181.00	36	256.25	270
135.00	44	156.95	155	185.00	163		
138.15	30	158.00	63	189.50	18		
139.15	68	161.00	58	194.45	26		

STP Compounds

Scan 1479 (28.394 min): S0208.D

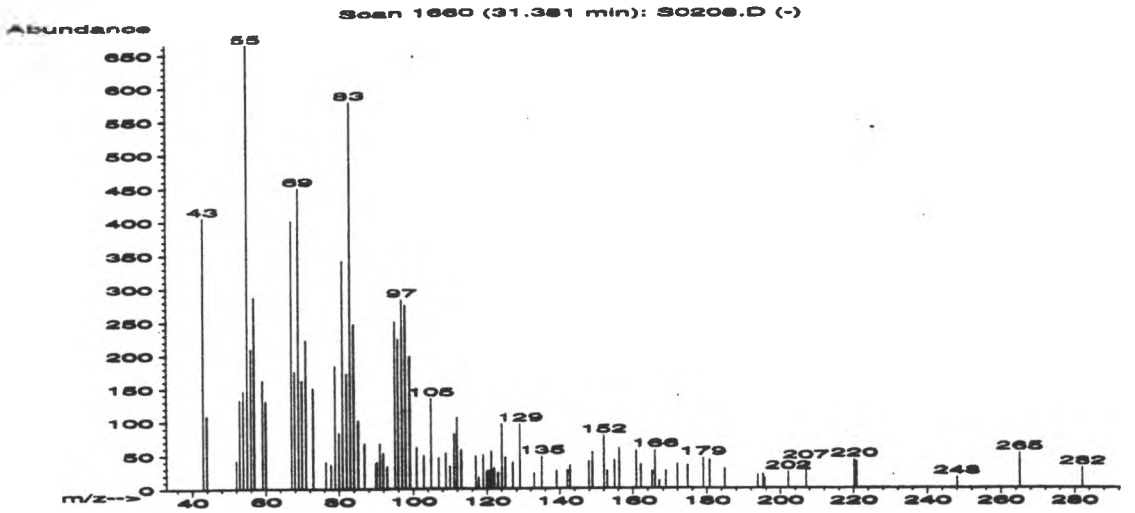
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Hexadecanoic acid	256	C16H32O2	90
2.	Tetradecanoic acid	228	C14H28O2	53
3.	Hexadecanoic acid	256	C16H32O2	53
4.	Decanoic acid	172	C10H20O2	47
5.	Dodecanoic acid	200	C12H24O2	43
6.	Dodecanoic acid	200	C12H24O2	42
7.	Undecanoic acid	186	C11H22O2	38
8.	Decanoic acid	172	C10H20O2	38
9.	Decanoic acid	172	C10H20O2	38
10.	Tetradecanoic acid	228	C14H28O2	35
11.	.beta.-D-Glucopyranose, 4-O-.beta.-D-gal	342	C12H22O11	27
12.	D-Galactose	180	C6H12O6	27
13.	Thiosulfuric acid (H2S2O3), S-(2-aminoet	157	C2H7NO3S2	27
14.	Heptanedioic acid, 4,4-dimethyl-, dimeth	216	C11H20O4	22
15.	3-THIOXO-5-OXO-1,2,4-TRIAZINE	129	C3H3N3OS	22
16.	2,6,6-TRIDEUTERO-4,4-DIMETHYLCYCLOHEXA-2	126	C8H11D3O	14
17.	2-Heptadecanol, acetate	298	C19H38O2	10
18.	Nonanoic acid	158	C9H18O2	10
19.	Octanoic acid, 8-hydroxy-	160	C8H16O3	10
20.	Undecyl acetate	214	C13H26O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000057-10-3	131572	111	44	1	80	9	59	34	81	9646
2.	53	000544-63-8	130227	69	66	0	69	28	28	1	38	9575
3.	*53	000057-10-3	131570	60	81	1	74	36	28	0	56	9589
4.	47	000334-48-5	22282	54	58	0	69	40	20	14	41	8868
5.	*43	000143-07-7	34781	55	70	2	93	42	18	7	38	8615
6.	42	000143-07-7	128387	56	75	2	85	28	17	19	37	9550
7.	38	000112-37-8	127364	58	74	3	117	47	14	0	39	9375
8.	38	000334-48-5	126153	46	70	0	54	50	14	0	39	9253
9.	38	000334-48-5	126150	45	64	0	56	47	14	17	41	9094
10.	35	000544-63-8	130228	43	93	0	57	52	11	0	39	9635
11.	27	005965-66-2	85911	47	86	0	49	59	8	2	41	9104
12.	27	000059-23-4	25298	47	55	1	67	58	8	2	38	8907
13.	27	002937-53-3	15671	46	70	0	34	59	8	0	39	9195
14.	22	054815-28-0	41844	45	73	1	28	64	5	1	38	3587
15.	*22	000626-08-4	6082	42	58	0	97	61	5	0	39	5363
16.	*14	000000-00-0	5368	39	58	3	98	66	2	17	39	8002
17.	10	056599-51-0	73333	52	64	0	32	78	1	3	38	2882
18.	*10	000112-05-0	124678	36	68	3	94	73	1	0	39	8782
19.	10	000764-89-6	16724	44	50	0	48	76	1	23	41	8761
20.	10	001731-81-3	41292	56	2	0	44	80	1	5	40	2169

STP Compounds

Peak 49; Oleic Acid



Scan 1660 (31.381 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	406	67.95	175	83.00	578	97.00	283
43.95	109	69.00	450	84.00	246	97.95	275
52.05	42	69.95	161	85.10	101	99.05	198
52.95	133	70.95	222	86.75	67	100.95	62
53.90	146	72.90	150	89.75	38	102.80	50
54.95	665	76.45	40	90.15	40	104.90	135
56.00	209	77.80	37	90.95	67	106.95	46
56.90	287	78.95	184	91.90	53	108.90	53
59.15	162	80.00	83	92.90	33	110.00	34
60.00	130	81.00	341	95.05	250	111.10	82
67.00	401	82.00	172	95.95	224	111.90	107

Scan 1660 (31.381 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.00	58	127.10	39	155.00	42	180.75	42
116.95	49	129.00	96	156.25	60	184.90	29
117.80	17	132.95	23	160.90	56	193.80	20
118.95	51	135.05	48	162.15	36	195.20	21
119.95	26	139.10	26	165.10	26	195.55	15
120.45	27	141.95	27	165.95	57	202.15	24
121.20	56	142.80	34	167.05	11	207.05	39
121.95	31	147.95	40	168.80	26	220.20	42
123.05	24	148.95	54	171.95	36	220.80	39
124.05	96	152.05	79	174.80	34	248.05	16
125.00	47	152.95	26	179.00	45	265.05	52

Scan 1660 (31.381 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
282.15	30						

STP Compounds

Scan 1660 (31.381 min): S0208.D

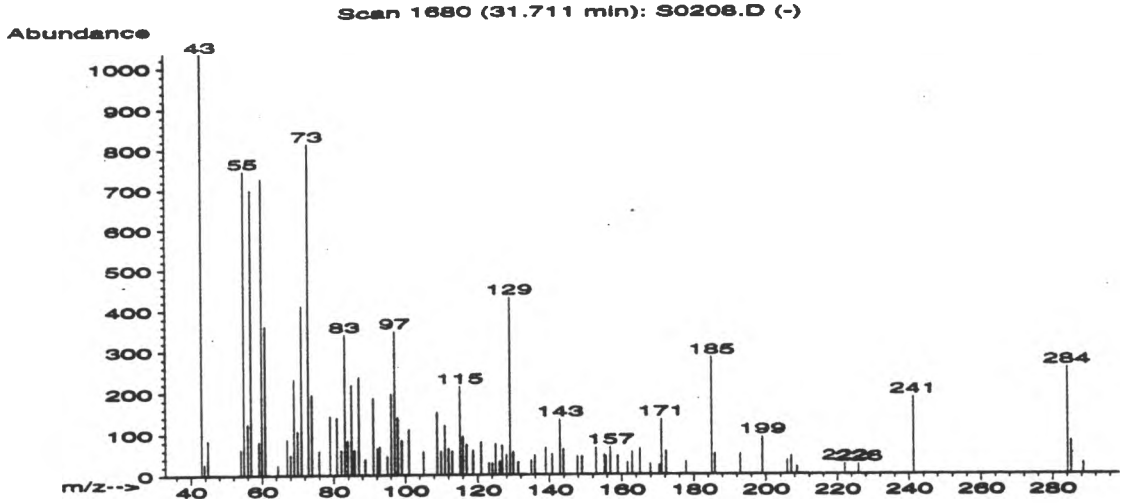
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	9-Azabicyclo[6.1.0]nonane, cis-	125	C8H15N	30
2.	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimet	152	C10H16O	30
3.	2-Hexenal, (E)-	98	C6H10O	30
4.	2-Hexenal	98	C6H10O	27
5.	2,3-Dimethoxy-5-methyl-5-(3-methyl-2-but	220	C14H20O2	22
6.	Cyclohexanamine, N-methyl-N-nitroso-	142	C7H14N2O	18
7.	7-D2-METHYLENECYCLOHEXANE	96	C7H10D2	18
8.	5,7,7-Trimethyl-6,8-dioxabicyclo[3.2.1]o	156	C9H16O2	18
9.	cis stereoisomer of 1-(6-Methyl-2-piperi	155	C9H17NO	14
10.	1-Hexadecanol	242	C16H34O	14
11.	4-OXATRICYCLO(3.2.1.0*2,8)OCTAN-3-ONE	124	C7H8O2	11
12.	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	11
13.	Cyclobuta[1,2:3,4]dicyclooctene, hexadec	220	C16H28	11
14.	CIS-DIHYDROCARVONE	152	C10H16O	11
15.	trans-1,2-Bis(aminomethyl)cyclohexane	142	C8H18N2	10
16.	Nonadecanol	284	C19H40O	10
17.	11,14-Eicosadienoic acid, methyl ester	322	C21H38O2	10
18.	Cyclobutanone, 2-(1,1-dimethylethyl)-	126	C8H14O	10
19.	.alpha.-Thujone	152	C10H16O	10
20.	1,E-8,Z-10-HEXADECATRIENE	220	C16H28	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*30	066387-85-7	5046	63	60	3	80	59	9	0	50	7945
2.	*30	015358-88-0	124028	53	54	1	80	58	9	0	49	8283
3.	*30	006728-26-3	774	50	61	2	157	58	9	0	46	7194
4.	*27	000505-57-7	775	50	50	0	63	57	8	2	41	7287
5.	22	000000-00-0	43755	45	26	0	85	62	5	20	41	6455
6.	*18	005432-28-0	9928	36	67	0	71	67	3	21	43	6872
7.	*18	001560-57-2	650	56	56	0	39	67	3	0	49	8562
8.	*18	016566-96-4	15461	49	53	0	46	69	3	0	46	5636
9.	*14	083285-66-9	15022	37	68	0	42	69	2	0	41	4686
10.	14	036653-82-4	130923	62	87	0	57	67	2	0	43	7749
11.	*11	058790-27-5	4722	44	56	0	38	73	2	0	44	7871
12.	*11	061177-16-0	13884	49	52	2	112	79	2	0	44	4790
13.	*11	061277-45-0	44087	72	75	2	63	72	2	0	47	5857
14.	*11	006909-25-7	13694	45	26	0	48	80	2	0	44	5005
15.	*10	070795-46-9	10122	46	54	2	202	80	1	0	40	4804
16.	10	052783-43-4	68643	55	80	0	38	80	1	9	41	7596
17.	10	002463-02-7	80740	53	79	0	43	79	1	23	41	5768
18.	10	004579-31-1	5340	39	70	0	64	71	1	18	43	7058
19.	*10	000546-80-5	123994	34	49	3	646	80	1	0	41	4956
20.	*10	080625-33-8	44094	45	75	1	42	80	1	0	40	5358

STP Compounds

Peak 50; Stearic Acid



Scan 1680 (31.711 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1036	67.00	87	83.00	340	97.00	348
43.80	27	68.05	49	83.85	83	97.90	139
44.80	84	69.00	232	84.95	218	99.00	84
54.05	63	70.00	106	85.75	60	100.95	110
54.95	746	71.05	411	87.00	237	105.00	56
56.00	124	72.95	813	88.75	38	108.90	153
56.90	699	73.95	194	91.00	187	110.00	58
59.15	81	75.95	58	92.20	65	111.05	120
59.90	727	78.95	142	92.80	68	112.00	64
60.90	362	80.90	139	94.95	46	113.00	58
64.40	24	82.00	60	96.05	196	115.15	214

Scan 1680 (31.711 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.00	93	129.95	55	155.25	47	177.90	30
116.95	73	131.25	31	155.65	43	185.00	283
118.80	59	134.95	35	156.90	66	185.90	50
120.95	80	135.90	47	158.90	45	192.90	50
123.05	28	139.00	65	161.65	29	199.05	90
124.05	28	140.75	50	162.90	55	205.90	34
125.00	75	142.95	134	165.00	62	206.95	44
126.05	32	143.95	62	167.95	25	208.65	19
126.80	71	147.80	43	170.30	23	222.05	25
128.05	49	149.05	44	170.95	134	225.95	23
129.00	430	152.95	64	172.20	56	241.20	186

Scan 1680 (31.711 min): S0208.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
284.15	258						
285.15	81						
288.45	27						

Scan 1680 (31.711 min): S0208.D

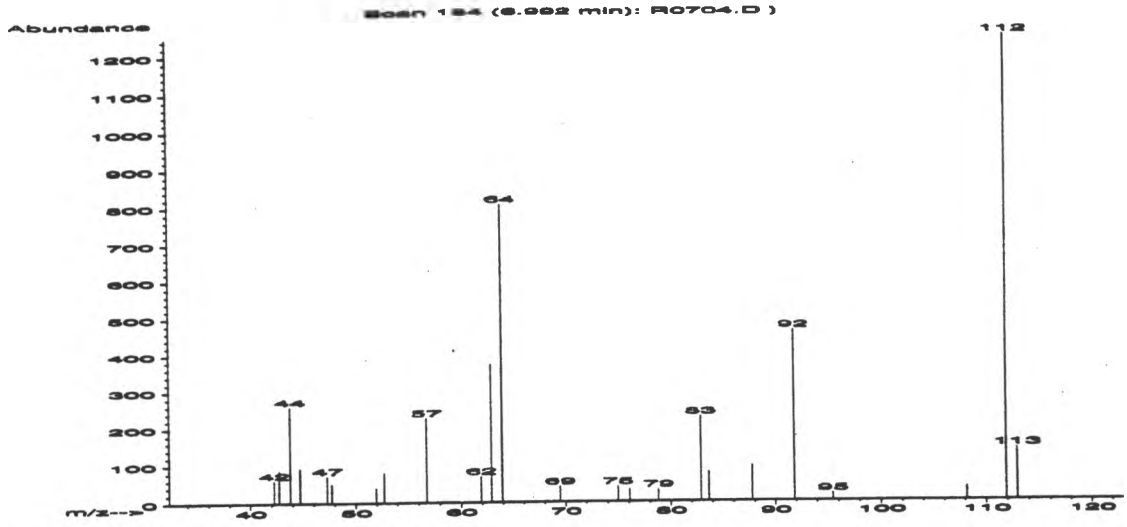
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Octadecanoic acid	284	C18H36O2	96
2.	Octadecanoic acid	284	C18H36O2	94
3.	Octadecanoic acid	284	C18H36O2	93
4.	Octadecanoic acid	284	C18H36O2	64
5.	9-Octadecenoic acid (Z)-	282	C18H34O2	58
6.	Octadecanoic acid	284	C18H36O2	50
7.	Decanoic acid	172	C10H20O2	50
8.	Tridecanoic acid	214	C13H26O2	49
9.	D-Glucose, 4-O-.alpha.-D-glucopyranosyl-	342	C12H22O11	46
10.	Tetradecanoic acid	228	C14H28O2	46
11.	Tetradecanoic acid	228	C14H28O2	46
12.	Decanoic acid	172	C10H20O2	45
13.	1-Tetracosanol	354	C24H50O	18
14.	Undecane	156	C11H24	15
15.	Nonadecane	268	C19H40	11
16.	Undecane	156	C11H24	11
17.	Undecane	156	C11H24	11
18.	Eicosane	282	C20H42	11
19.	Dodecane	170	C12H26	11
20.	4-Octen-3-one	126	C8H14O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000057-11-4	132770	93	70	0	75	19	76	0	96	9772
2.	*94	000057-11-4	132769	115	54	1	82	3	70	46	92	9714
3.	*93	000057-11-4	132776	97	66	0	64	11	68	61	93	9546
4.	*64	000057-11-4	132772	81	83	0	58	34	37	35	74	9645
5.	58	000112-80-1	132678	88	75	1	84	28	32	0	47	9545
6.	*50	000057-11-4	132774	68	92	3	135	50	25	0	76	9647
7.	*50	000334-48-5	126151	68	45	1	90	48	25	0	68	9009
8.	49	000638-53-9	41267	79	65	1	57	38	23	0	43	7599
9.	46	000069-79-4	85910	84	75	1	71	44	20	0	45	8972
10.	46	000544-63-8	130227	81	67	2	118	42	20	0	43	9444
11.	46	000544-63-8	130226	79	67	2	128	42	20	0	43	9410
12.	*45	000334-48-5	126153	61	55	0	57	48	19	0	56	8978
13.	18	000506-51-4	89101	85	79	3	84	69	3	0	47	4061
14.	*15	001120-21-4	124549	59	36	0	67	80	2	0	56	3247
15.	11	000629-92-5	132088	73	54	0	52	75	2	0	45	3370
16.	*11	001120-21-4	15622	55	41	0	77	76	2	0	49	3250
17.	*11	001120-21-4	124547	46	47	0	70	80	2	0	44	3251
18.	11	000112-95-8	132692	73	63	0	65	75	2	0	45	3628
19.	*11	000112-40-3	126002	55	41	0	71	76	2	17	46	3236
20.	*11	014129-48-7	120579	47	50	3	223	80	2	0	44	4963

STP Compounds

Phenol Std; 2-Fluorophenol



Scan 184 (6.992 min): R0704.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.25	60	63.90	802	111.90	1247		
42.75	86	69.45	41	112.90	139		
43.80	259	74.95	40				
44.70	92	76.05	32				
47.30	71	78.80	31				
47.70	49	82.90	228				
51.95	38	83.65	78				
52.70	80	87.75	94				
56.75	227	91.80	462				
61.90	69	95.45	19				
62.90	373	108.15	35				

STP Compounds

Scan 184 (6.992 min): R0704.D

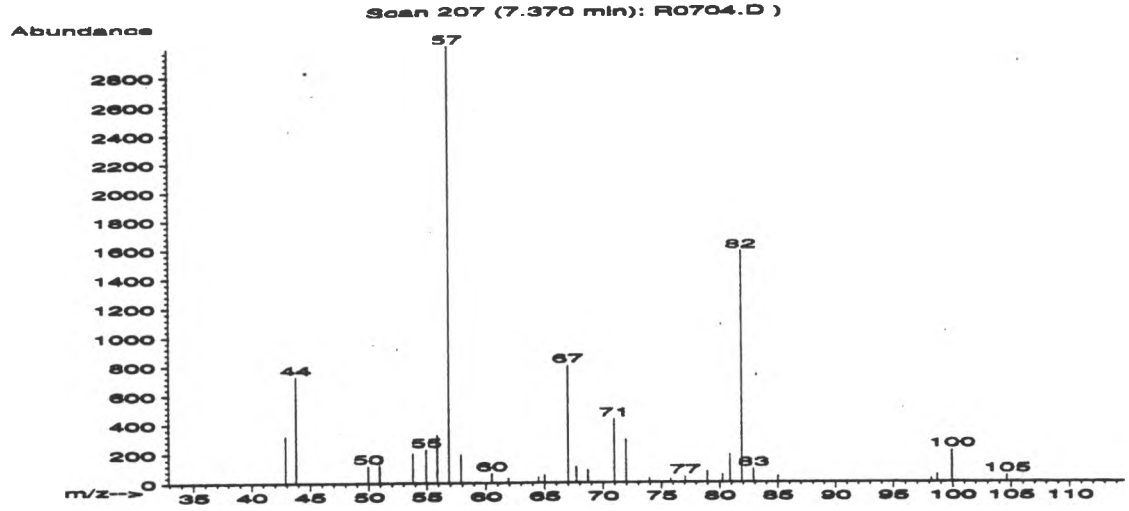
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-fluoro-	112	C6H5FO	87
2.	Benzene, 1-ethoxy-2-fluoro-	140	C8H9FO	64
3.	Phenol, 2-fluoro-	112	C6H5FO	47
4.	1,3-Benzodioxol-2-one	136	C7H4O3	28
5.	2-Thiophenecarboxaldehyde	112	C5H4OS	9
6.	3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimeth	112	C5H8N2O	9
7.	2-Furancarboxylic acid	112	C5H4O3	9
8.	1H-Imidazole-2-methanol, 1-methyl-	112	C5H8N2O	8
9.	1,3-Cyclopentanedione, 2-methyl-	112	C6H8O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000367-12-4	2444	63	29	0	91	10	54	10	56	9746
2.	64	000451-80-9	9165	54	47	1	89	10	37	0	37	9715
3.	47	000367-12-4	118975	51	50	0	52	38	20	5	38	6042
4.	28	002171-74-6	121807	37	67	1	61	38	8	0	22	6133
5.	* 9	000098-03-3	118959	28	57	0	74	72	1	6	35	7706
6.	* 9	006628-22-4	2433	28	65	2	71	72	1	0	33	7707
7.	* 9	000088-14-2	118961	30	67	0	93	72	1	0	33	7700
8.	* 8	017334-08-6	2435	30	95	1	70	66	1	0	29	7844
9.	* 8	000765-69-5	2473	31	68	2	89	69	1	0	29	7846

STP Compounds

Peak 51; Cyclohexanol



Scan 207 (7.370 min): R0704.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	319	64.50	40	80.25	52		
43.80	727	65.00	52	80.90	188		
49.95	117	67.00	801	81.90	1583		
50.95	124	67.70	106	82.90	89		
53.80	200	68.70	86	85.00	44		
54.95	225	70.95	431	98.20	25		
55.90	328	71.95	293	98.70	52		
56.90	2996	73.95	28	99.95	215		
57.90	192	75.80	24	104.65	44		
60.50	64	77.05	40				
61.90	33	78.95	72				

STP Compounds

Scan 207 (7.370 min): R0704.D

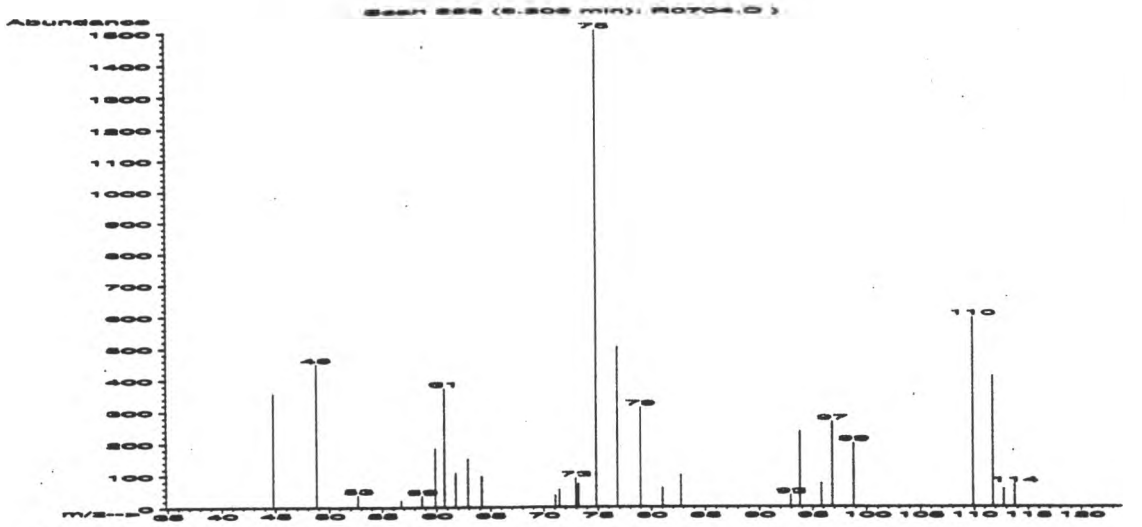
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanol	100	C6H12O	83
2.	Cyclohexanol	100	C6H12O	78
3.	Cyclohexanol	100	C6H12O	74
4.	Cyclohexanol	100	C6H12O	59
5.	2-Hexen-1-ol, (Z)-	100	C6H12O	50
6.	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	50
7.	Cyclohexanol	100	C6H12O	50
8.	Cyclohexanol	100	C6H12O	47
9.	2-Hexen-1-ol, (E)-	100	C6H12O	43
10.	Cyclohexanol	100	C6H12O	42
11.	Cyclohexanol	100	C6H12O	42
12.	Cyclohexanol	100	C6H12O	40
13.	2-Hexen-1-ol, (E)-	100	C6H12O	40
14.	Cyclohexanol	100	C6H12O	39
15.	Nitrous acid, cyclohexyl ester	129	C6H11NO2	39
16.	Cyclohexanol	100	C6H12O	37
17.	Cyclopentanol, 2-methyl-	100	C6H12O	32
18.	2-Hexen-1-ol, (E)-	100	C6H12O	25
19.	2-Hexen-1-ol, (E)-	100	C6H12O	25
20.	2-Hexen-1-ol, (Z)-	100	C6H12O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	83	000108-93-0	118078	60	34	1	81	5	50	0	39	9960
2.	*78	000108-93-0	118075	59	28	1	98	8	46	4	39	9902
3.	74	000108-93-0	1179	60	34	1	88	3	44	0	36	9972
4.	*59	000108-93-0	118081	40	30	0	80	25	33	0	39	9833
5.	50	000928-94-9	1144	51	35	1	72	17	25	10	31	9758
6.	*50	025144-05-2	1177	49	48	1	71	32	25	0	39	9702
7.	*50	000108-93-0	118082	53	42	1	91	17	25	0	35	9979
8.	47	000108-93-0	118083	45	47	0	63	37	20	8	41	9965
9.	*43	000928-95-0	118038	34	49	1	62	41	18	11	40	9511
10.	42	000108-93-0	118077	43	53	2	117	26	17	0	37	9821
11.	42	000108-93-0	118079	45	51	3	84	26	17	0	34	9920
12.	40	000108-93-0	118085	41	51	0	63	35	16	2	37	9971
13.	40	000928-95-0	118037	42	50	1	87	35	16	0	33	9575
14.	39	000108-93-0	118080	40	62	2	77	17	15	0	29	9532
15.	39	005156-40-1	6150	39	57	2	97	19	15	2	29	9960
16.	37	000108-93-0	118076	41	45	0	58	41	13	2	35	9933
17.	*32	024070-77-7	118074	37	62	2	93	46	9	0	35	9641
18.	*25	000928-95-0	118039	28	64	2	127	42	7	0	27	9437
19.	*25	000928-95-0	1145	32	56	0	68	55	7	0	33	9251
20.	25	000928-94-9	118033	36	56	0	62	44	7	0	25	9638

STP Compounds

Peak 22; 1,2,3-Trichloropropanone



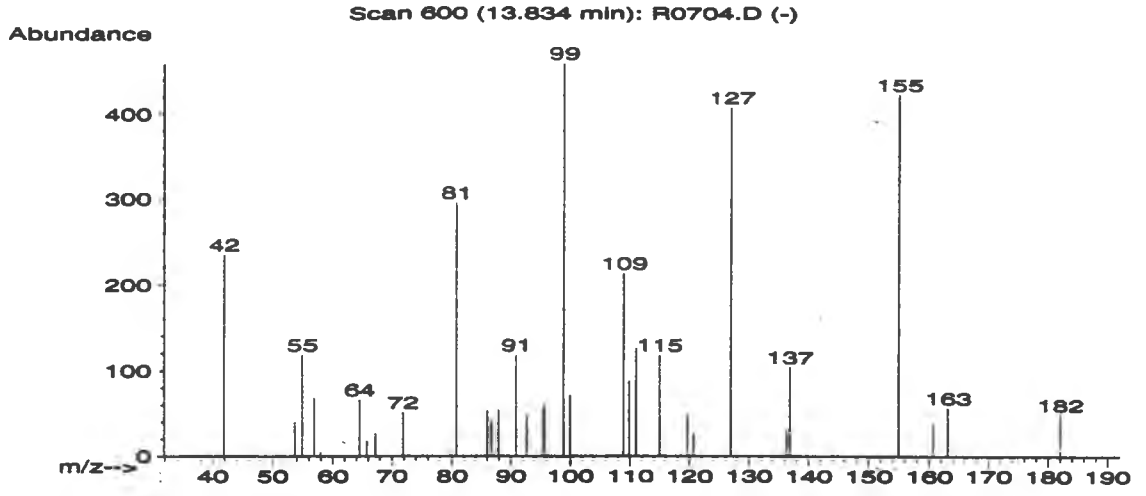
Scan 258 (8.209 min): R0704.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.80	357	71.45	55	96.80	265		
48.80	448	72.95	90	98.80	199		
52.70	37	73.20	73	109.90	596		
56.75	22	74.80	1503	111.75	411		
58.65	34	76.80	503	112.75	55		
59.90	185	78.95	311	113.75	70		
60.75	371	81.00	60				
61.75	107	82.75	100				
62.90	151	92.95	35				
64.15	97	93.80	236				
71.05	36	95.80	74				

STP Compounds

Peak 52; Triethylphospate



Scan 600 (13.834 min): R0704.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	235	86.00	53	111.00	126		
53.70	40	86.75	41	114.95	118		
54.95	118	87.90	54	119.70	48		
56.90	68	90.90	118	120.70	26		
57.90	4	92.70	47	126.95	407		
64.50	66	95.45	55	136.40	30		
65.75	18	95.70	60	136.90	104		
67.25	26	98.90	459	154.90	423		
71.85	51	99.95	71	160.65	38		
79.85	5	108.90	213	163.15	57		
80.75	295	109.90	88	182.00	49		

Scan 600 (13.834 min): R0704.D

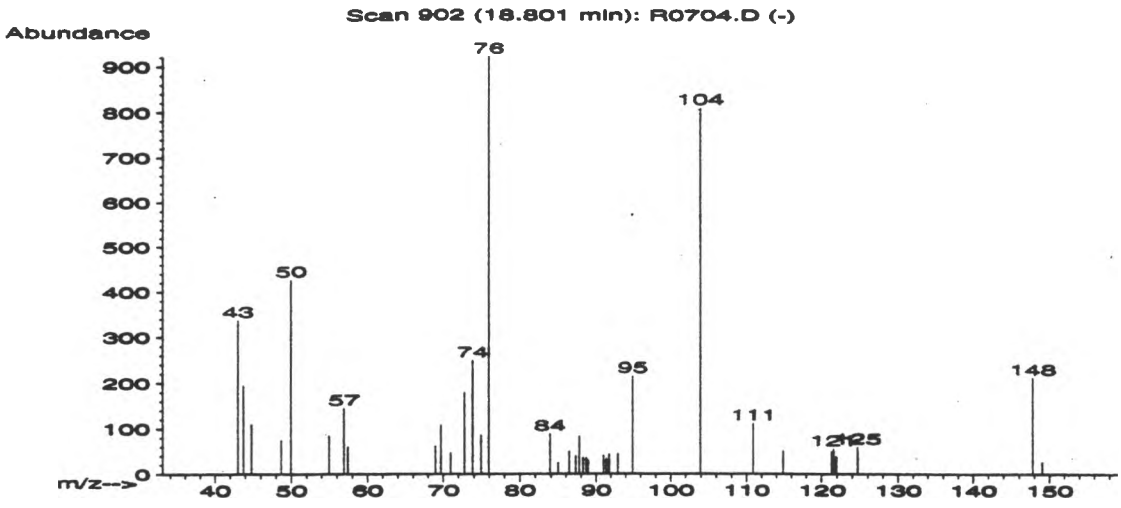
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phosphoric acid, triethyl ester	182	C6H15O4P	64
2.	Phosphoric acid, triethyl ester	182	C6H15O4P	58
3.	Phosphoric acid, triethyl ester	182	C6H15O4P	53
4.	Phosphoric acid, triethyl ester	182	C6H15O4P	50
5.	Phosphoric acid, triethyl ester	182	C6H15O4P	40
6.	Diphosphoric acid, tetraethyl ester	290	C8H20O7P2	38
7.	3-CHLOROFORMANILIDE	155	C7H6ClNO	27
8.	3-Pyridinemethanol, 4,5-dihydroxy-6-meth	155	C7H9NO3	27
9.	CIS DIETHYL ESTER OF 1,2-CYCLOBUTANEDICA	200	C10H16O4	23
10.	Phosphoric acid, triethyl ester	182	C6H15O4P	12
11.	4-AMINO-3-METHYL-5-METHYLAMINO-1,2,4-TRI	127	C4H9N5	10
12.	1,3-Dioxane, 4,6-bis(1-methylethyl)-, tr	172	C10H20O2	9
13.	N-PHENYL,N-DEUTERO-CARBAMIC ACID TRIDEUT	151	C8H5D4NO2	8
14.	1-Methoxy-4-(phenylthio)-1,3-butadiene	192	C11H12OS	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000078-40-0	126950	45	87	0	99	21	37	0	44	9444
2.	*58	000078-40-0	126952	44	41	0	94	27	32	0	44	9218
3.	*53	000078-40-0	26266	35	102	0	99	30	28	0	41	9356
4.	*50	000078-40-0	126954	37	99	0	69	31	25	0	41	9431
5.	40	000078-40-0	126953	38	88	0	99	15	16	4	25	9279
6.	38	000107-49-3	133029	39	107	0	99	23	14	0	25	9346
7.	*27	000139-71-9	14906	33	79	0	92	58	8	0	41	7382
8.	*27	000700-73-2	14922	33	85	1	92	60	8	0	39	6408
9.	23	000000-00-0	34584	33	99	0	92	48	6	0	25	8528
10.	*12	000078-40-0	126955	37	100	2	195	62	2	0	35	9101
11.	*10	065901-89-5	5505	32	71	1	62	65	1	0	29	5791
12.	9	016731-94-5	22352	38	73	0	85	80	1	0	33	5502
13.	* 8	056196-26-0	13089	30	79	1	92	68	1	0	29	5718
14.	8	067700-13-4	30713	38	97	2	71	67	1	0	28	5798

STP Compounds

Peak 53



Scan 902 (18.801 min): R0704.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	337	72.80	179	88.90	30	121.90	38
43.75	195	73.80	249	91.00	41	124.70	59
44.80	109	74.95	85	91.40	33	147.80	213
48.70	74	75.95	921	91.80	43	149.05	26
49.95	426	83.90	88	92.95	45		
54.95	84	84.95	24	94.95	215		
56.90	144	86.40	50	103.90	808		
57.40	59	87.25	39	110.90	111		
68.95	62	87.75	83	114.90	51		
69.70	108	88.25	36	121.30	49		
70.95	46	88.65	35	121.55	55		

STP Compounds

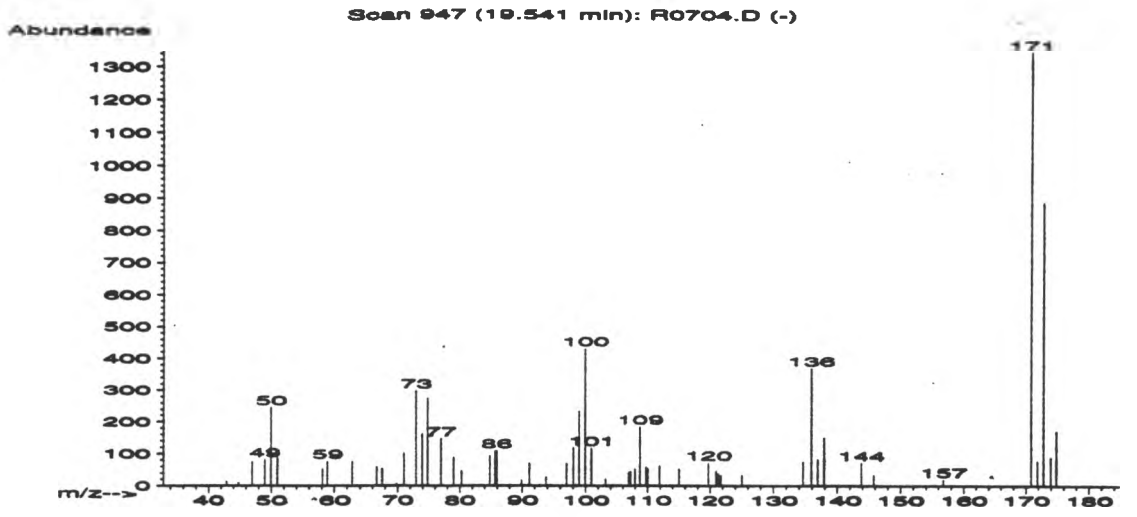
Scan 902 (18.801 min): R0704.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3-Isobenzofurandione	148	C8H4O3	72
2.	1,3-Isobenzofurandione	148	C8H4O3	72
3.	3(2H)-Benzofuranone, 2-methyl-	148	C9H8O2	64
4.	PHTHALIC ACID-D2	166	C8H4D2O4	64
5.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	56
6.	1,2-Benzenedicarboxylic acid	166	C8H6O4	56
7.	1,3-Isobenzofurandione	148	C8H4O3	56
8.	Talsutin	362	C16H14N2O6S	56
9.	1H-Isoindole-1,3(2H)-dione, 2-(hydroxyme	177	C9H7NO3	56
10.	1H-Isoindole-1,3(2H)-dione	147	C8H5NO2	56
11.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	40
12.	1,3-Isobenzofurandione	148	C8H4O3	40
13.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	35
14.	1,2-Benzenedicarboxylic acid	166	C8H6O4	23
15.	1,2-Benzenedicarboxylic acid, monobutyl	222	C12H14O4	17
16.	Phthalaldehydic acid, oxime	165	C8H7NO3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000085-44-9	123355	47	54	1	99	14	42	13	38	9592
2.	72	000085-44-9	123354	47	61	1	87	14	42	13	38	9594
3.	*64	035567-59-0	11946	54	69	1	99	10	37	10	34	8431
4.	64	004123-68-6	19189	54	62	1	99	10	37	0	32	9621
5.	56	004376-18-5	25403	43	77	2	87	14	30	0	35	9460
6.	56	000088-99-3	125486	48	72	1	74	11	30	0	31	9632
7.	56	000085-44-9	11912	51	59	0	86	12	30	3	36	9534
8.	56	000131-69-1	90607	39	101	0	74	12	30	0	33	9655
9.	56	000118-29-6	24166	43	74	1	99	13	30	0	37	9489
10.	56	000085-41-6	123277	51	54	1	99	14	30	2	33	9624
11.	40	004376-18-5	126782	34	76	2	87	14	16	0	21	9435
12.	40	000085-44-9	123353	37	58	1	87	13	16	0	22	9548
13.	35	004376-18-5	126783	47	63	0	64	53	11	0	39	9651
14.	23	000088-99-3	125487	39	70	2	104	47	6	0	28	9620
15.	17	000131-70-4	129810	38	109	1	62	55	3	0	29	9600
16.	10	006383-59-1	18856	33	78	0	82	62	1	0	25	7000

Peak 54



Scan 947 (19.541 min): R0704.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	14	69.85	7	89.90	17	108.00	53
44.80	10	71.05	102	91.15	70	108.75	182
46.95	74	72.95	297	93.80	27	109.75	58
48.95	81	73.90	162	96.95	69	110.00	53
49.95	245	74.80	274	98.05	118	111.90	61
50.95	87	76.95	146	98.95	233	115.00	52
58.15	53	78.95	88	99.95	428	119.70	71
58.90	76	80.25	47	100.95	116	120.95	46
62.75	74	84.85	93	103.20	20	121.30	36
66.65	59	85.65	107	106.95	42	121.70	31
67.55	54	85.90	108	107.25	45	125.05	32

Scan 947 (19.541 min): R0704.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.65	74	174.80	169				
135.90	365						
136.90	81						
137.90	148						
143.80	70						
145.80	33						
156.75	19						
170.80	1346						
171.80	76						
172.80	883						
173.95	88						

STP Compounds

Scan 947 (19.541 min): R0704.D

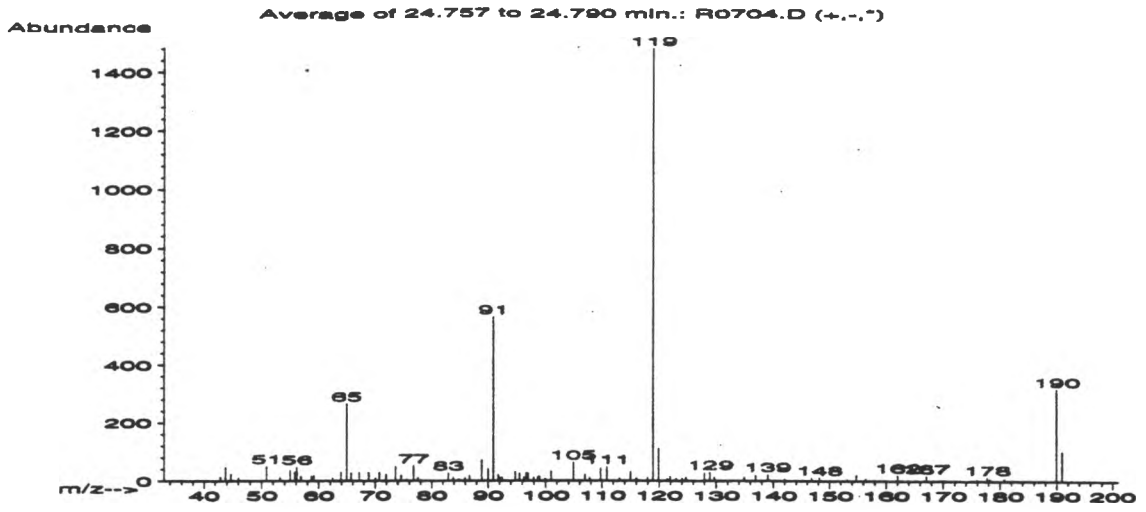
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzonitrile, 2,6-dichloro-	171	C7H3Cl2N	91
2.	Benzonitrile, 2,6-dichloro-	171	C7H3Cl2N	50
3.	2-FLUORO-4,5-DICHLOROTHIAZOLE	171	C3Cl2FNS	47
4.	Thiazolo[5,4-d]pyrimidine, 5-chloro-	171	C5H2ClN3S	25
5.	2-AMINO-3-NITRO-5-CHLOROPYRIDINE	173	C5H4ClN3O2	12
6.	3-AMINOBENZENE SULFONIC ACID	173	C6H7NO3S	10
7.	4-CHLORO-2-NITROPHENOL	173	C6H4ClNO3	10
8.	1,3,5-Triazine, 2,4,6-trimethoxy-	171	C6H9N3O3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	001194-65-6	126040	88	29	1	94	11	62	52	91	9685
2.	*50	001194-65-6	21728	69	48	1	99	33	25	8	41	9630
3.	*47	057314-08-6	21700	50	46	1	87	40	20	6	41	9142
4.	*25	013316-08-0	21705	39	73	1	91	44	7	0	29	9137
5.	*12	000000-00-0	22506	38	75	1	64	64	2	0	33	5682
6.	*10	000000-00-0	22528	35	78	1	51	76	1	0	39	5126
7.	*10	000000-00-0	22519	37	87	2	57	73	1	0	39	5416
8.	*10	000877-89-4	21726	28	104	1	72	62	1	0	29	7606

STP Compounds

Peak 7; N,N-Diethyl-4-methylbenzamide



Average of 24.757 to 24.790 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	15	59.15	18	74.55	19	90.95	566
43.75	48	62.40	12	75.55	6	91.80	21
44.70	25	63.90	30	76.75	52	92.20	11
46.05	12	64.90	265	77.55	12	92.45	13
50.85	50	65.75	27	82.95	27	94.80	31
53.20	14	67.15	30	83.90	12	95.55	26
54.95	36	68.85	29	84.85	7	96.30	14
55.75	30	70.05	11	85.90	12	96.70	28
56.10	48	70.75	29	86.75	18	96.95	27
56.85	16	71.95	23	88.90	71	97.95	13
58.65	17	73.55	49	90.00	42	98.70	15

Average of 24.757 to 24.790 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.95	16	117.95	13	134.90	13	175.95	6
99.95	8	118.95	1483	136.90	19	177.75	14
100.95	34	119.90	112	139.00	23	178.25	7
104.85	65	121.45	7	141.95	7	180.75	8
106.90	21	121.95	16	146.80	12	189.95	318
107.75	11	122.95	8	148.20	12	190.95	101
109.75	44	124.05	8	153.15	5		
110.85	49	124.70	12	154.75	20		
113.15	9	127.95	27	156.40	8		
115.00	31	128.95	30	162.00	20		
116.05	11	129.75	13	167.05	18		

STP Compounds

Average of 24.757 to 24.790 min.: R0704.D
Converted from RTE data file: >R0704:

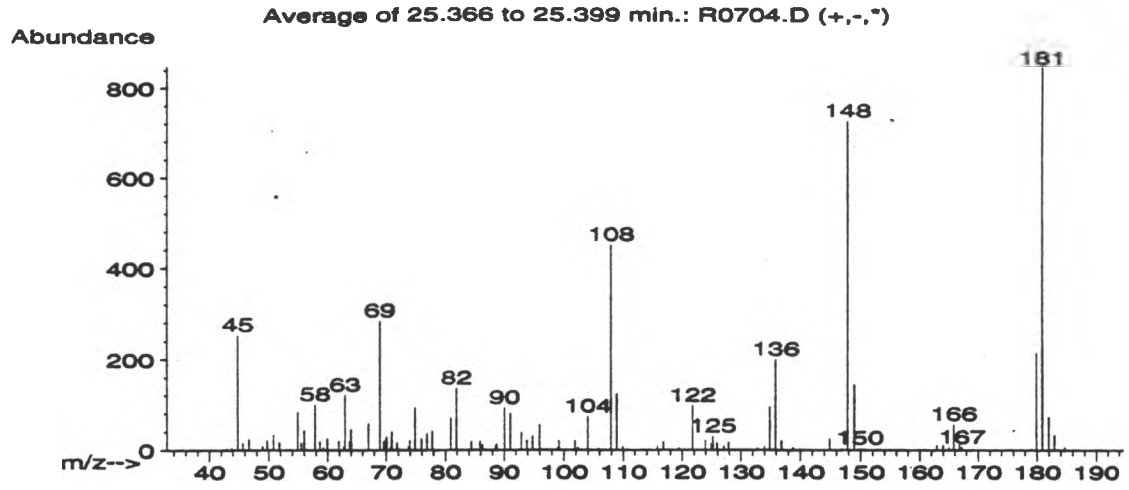
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzamide, N,N-diethyl-3-methyl-	191	C12H17NO	78
2.	Methyl ester of 2-methyl-3-(1-methyl-1-p	425	C26H35NO4	74
3.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	59
4.	ACETOPHENONE, DICHLORO-4'-METHYL-	202	C9H8Cl2O	59
5.	2,4,5-TRIOXO-1-PHENYLIMIDAZOLIDINE	190	C9H6N2O3	59
6.	Benzene, isocyanato-	119	C7H5NO	50
7.	Benzene, isocyanato-	119	C7H5NO	50
8.	Urea, N,N-dimethyl-N'-phenyl-	164	C9H12N2O	50
9.	2,3-DIBROMO-8-PHENYL-P-MENTHANE	372	C16H22Br2	50
10.	N-ISOPROPYL-P-TOLUAMIDE	177	C11H15NO	45
11.	Benzoyl chloride, 4-methyl-	154	C8H7ClO	45
12.	Ethanone, 2-bromo-1-(4-methylphenyl)-	212	C9H9BrO	45
13.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	45
14.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	45
15.	Benzamide, N-(1,1-dimethylethyl)-3-methy	191	C12H17NO	45
16.	Benzoyl chloride, 3-methyl-	154	C8H7ClO	42
17.	ORTHO-D2-BENZYLCYANIDE	117	C8H5D2N	40
18.	Benzene, isocyanato-	119	C7H5NO	40
19.	4-Methylimino-toluene	119	C8H9N	40
20.	4-Isopropenyl-pyridine	119	C8H9N	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	000134-62-3	30397	58	39	2	78	8	46	5	38	9750
2.	74	083991-81-5	101634	39	37	0	75	2	44	0	33	9227
3.	59	000099-75-2	123611	56	32	1	68	25	33	0	39	9695
4.	59	000000-00-0	35303	44	54	1	67	25	33	1	38	9754
5.	*59	002211-33-8	29822	37	57	2	99	22	33	19	40	9215
6.	*50	000103-71-9	119905	34	32	1	91	33	25	11	40	9696
7.	*50	000103-71-9	119901	33	57	2	79	32	25	0	41	9692
8.	50	000101-42-8	18369	43	34	2	95	33	25	12	41	9691
9.	50	000000-00-0	92753	44	61	1	84	35	25	19	41	9499
10.	45	002144-17-4	24290	60	25	1	71	25	19	0	36	9771
11.	45	000874-60-2	14274	57	27	1	76	25	19	2	33	9676
12.	45	000619-41-0	40089	45	60	2	83	25	19	0	31	9777
13.	*45	000140-76-1	119921	38	57	2	81	25	19	0	33	9754
14.	45	000099-75-2	123608	58	19	0	92	25	19	2	35	9665
15.	*45	042498-33-9	30391	42	62	2	75	25	19	0	33	9774
16.	42	001711-06-4	14273	47	38	2	77	28	17	5	34	9665
17.	*40	053897-46-4	119690	31	65	2	73	33	16	0	33	9638
18.	*40	000103-71-9	119906	31	52	1	72	32	16	0	33	9694
19.	*40	000000-00-0	3977	35	22	1	70	34	16	0	35	9447
20.	*40	000000-00-0	3975	30	45	1	83	35	16	1	30	9633

STP Compounds

Peak 55; 2-(Methylthio)-benzothiazole



Average of 25.366 to 25.399 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	3	56.00	43	68.90	284	76.90	37
43.80	5	57.85	100	69.55	18	77.75	42
44.80	253	58.65	19	69.85	21	80.90	70
45.70	15	59.25	6	70.05	28	81.90	137
46.70	24	59.95	25	70.80	8	84.40	19
48.95	9	61.90	20	70.95	40	85.90	20
49.75	22	62.75	9	71.80	16	86.25	11
50.85	33	62.95	121	73.70	7	88.50	9
51.80	17	63.75	19	73.95	21	88.75	14
54.90	84	64.00	45	74.90	94	90.05	93
55.50	16	67.00	59	75.95	25	91.00	80

Average of 25.366 to 25.399 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
92.95	39	108.90	124	127.85	17	149.85	4
93.85	22	109.90	7	130.90	1	150.90	2
94.80	31	115.75	9	132.75	4	162.90	11
95.95	56	116.80	18	134.00	8	164.00	11
98.90	4	119.45	5	134.90	95	165.05	6
99.20	20	121.75	98	135.85	200	165.80	57
101.80	20	123.95	22	136.85	21	166.80	14
102.30	6	124.90	13	138.75	6	167.20	6
103.95	74	125.20	30	144.85	25	179.90	217
105.75	4	125.90	16	147.85	726	180.90	847
107.90	452	127.05	9	148.95	145	181.90	73

Average of 25.366 to 25.399 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
182.90	34						
184.65	7						

STP Compounds

Average of 25.366 to 25.399 min.: R0704.D
Converted from RTE data file: >R0704:

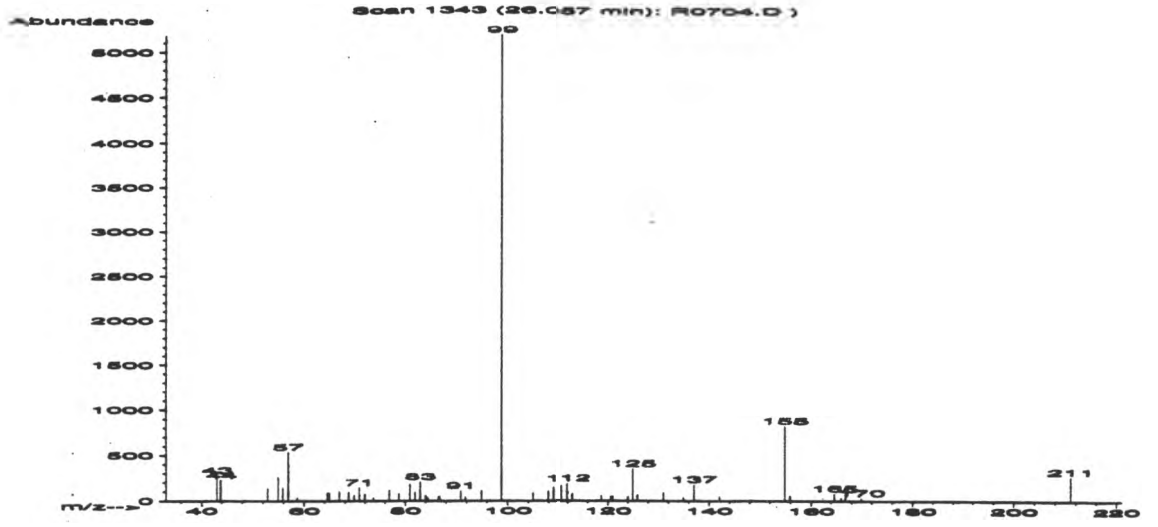
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	87
2.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	72
3.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	40
4.	2(3H)-Benzothiazolethione, 3-methyl-	181	C8H7NS2	28
5.	1-Azabicyclo[2.2.2]oct-2-ene-3-carboxyli	181	C10H15NO2	25
6.	2,1,3-Benzothiadiazole, 4-nitro-	181	C6H3N3O2S	22
7.	5-Cyano-2,6-dimethyl-4-pyrimidineamine	148	C7H8N4	17
8.	5-AMINO-ISO-PHTHALIC ACID	181	C8H7NO4	16
9.	Benzene, 1-ethoxy-2-methyl-	136	C9H12O	11
10.	Pyrazolo[5,1-c][1,2,4]triazine, 3,4-dime	148	C7H8N4	10
11.	.ALPHA.-CAMPHOLENIC ACID METHYL ESTER	182	C11H18O2	9
12.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	9
13.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	9
14.	2-Benzoxazolamine, N-methyl-	148	C8H8N2O	8
15.	3,6-DIMETHYL-5H-ISOTHIAZOLO(5,4-D)PYRIMI	181	C7H7N3OS	7
16.	Benzene, pentafluoro[(pentafluorophenoxy	364	C13H2F10O	7
17.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	7
18.	Benzene, 1-(1,1-dimethylethoxy)-3-methyl	164	C11H16O	7
19.	Pyrazine, 2-methyl-6-propyl-	136	C8H12N2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000615-22-5	126908	69	62	2	88	8	54	0	53	9926
2.	*72	000615-22-5	25993	49	82	2	99	18	42	0	44	9738
3.	40	000615-22-5	126909	61	67	3	115	32	16	0	36	9834
4.	*28	002254-94-6	25992	38	91	3	79	39	8	0	29	9256
5.	*25	006238-32-0	26101	34	112	2	83	53	7	0	30	7842
6.	*22	006583-06-8	126899	33	108	2	79	62	5	0	39	6891
7.	*17	000000-00-0	11870	29	45	1	85	54	3	0	29	6777
8.	*16	000000-00-0	25989	35	80	2	93	58	3	12	35	7519
9.	*11	000614-71-1	121936	51	36	1	39	75	2	0	46	4026
10.	*10	006726-49-4	11874	30	6	0	85	68	1	0	33	5822
11.	9	000000-00-0	127012	46	60	2	47	79	1	0	37	3765
12.	* 9	000622-60-6	7957	36	69	1	53	75	1	0	35	4012
13.	* 9	000621-32-9	121937	35	42	0	38	77	1	6	35	4009
14.	* 8	019776-98-8	11926	28	78	1	85	68	1	0	27	5849
15.	* 7	058648-96-7	25953	32	46	1	70	72	1	0	29	6696
16.	7	038795-53-8	91006	40	96	2	94	71	1	0	29	6727
17.	* 7	000621-32-9	7956	30	77	3	50	75	1	0	29	4015
18.	7	015359-97-4	125365	33	65	2	53	77	1	0	21	3813
19.	7	029444-46-0	7838	40	64	3	53	77	1	0	28	3987

STP Compounds

Peak 56; Tributylphosphate



Scan 1343 (26.057 min): R0704.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	280	69.80	64	86.50	40	112.90	75
43.80	224	70.80	142	86.75	44	118.70	55
52.95	138	71.95	75	90.90	110	120.55	46
54.95	256	73.70	30	91.80	39	120.95	46
55.90	144	76.80	114	94.95	106	123.95	50
56.90	534	78.70	77	98.80	5180	124.95	348
58.65	33	80.90	182	104.90	87	125.80	64
64.50	90	81.90	96	107.90	107	131.00	85
64.90	85	82.90	206	108.90	146	134.90	34
66.90	100	84.00	56	110.75	163	137.00	173
68.70	94	84.40	32	111.90	188	142.05	42

Scan 1343 (26.057 min): R0704.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
154.90	810						
155.90	54						
164.65	78						
165.95	29						
166.80	70						
169.95	30						
211.00	266						

STP Compounds

Scan 1343 (26.057 min): R0704.D

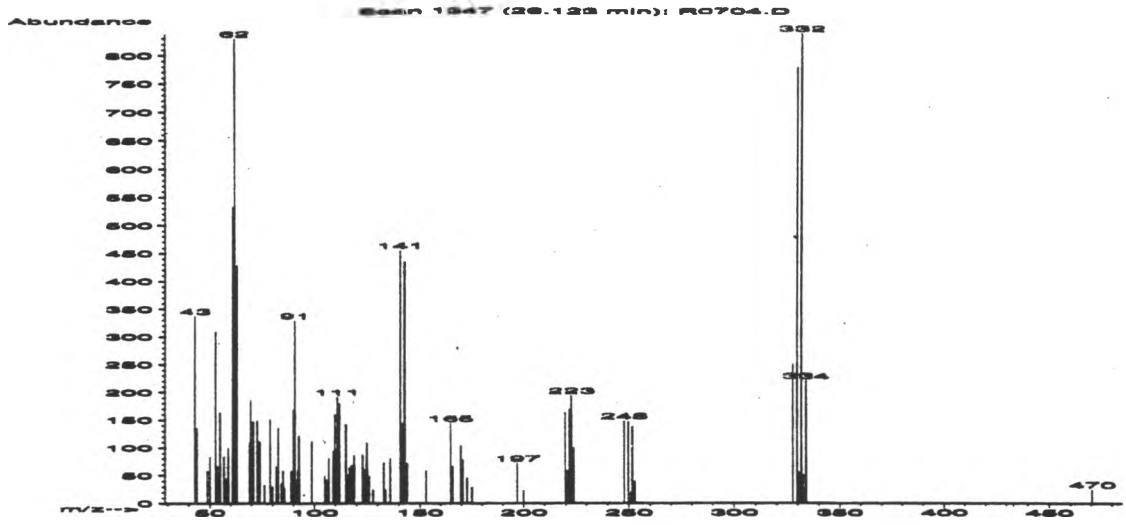
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phosphoric acid, tributyl ester	266	C12H27O4P	78
2.	Phosphoric acid, tributyl ester	266	C12H27O4P	47
3.	Phosphoric acid, diethyl pentyl ester	224	C9H21O4P	42
4.	2-Octen-4-one, 2-methoxy-	156	C9H16O2	40
5.	1-Penten-3-ol, 3-ethyl-2-methyl-	128	C8H16O	36
6.	1',7',7'-TRIMETHYL-SPIRO[BICYCLO[2.2.1]H	210	C12H18O3	28
7.	Phosphoric acid, triethyl ester	182	C6H15O4P	9
8.	Diphosphoric acid, tetraethyl ester	290	C8H20O7P2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	78	000126-73-8	131963	70	37	0	72	6	46	11	38	9930
2.	47	000126-73-8	131964	45	63	0	55	40	20	0	39	9987
3.	42	020195-08-8	45523	38	73	3	71	26	17	0	33	8394
4.	*40	024985-48-6	15390	30	50	0	67	32	16	0	33	9804
5.	36	028832-46-4	5981	33	46	1	99	28	12	1	22	9836
6.	28	000000-00-0	39436	34	54	1	81	36	8	0	25	9785
7.	9	000078-40-0	126950	38	51	0	18	78	1	0	33	8404
8.	7	000107-49-3	133029	36	67	0	16	78	1	0	25	8128

STP Compounds

Standard 13; Tribromophenol



Scan 1347 (26.123 min): R0704.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	337	61.90	829	82.75	136	98.80	111
43.80	135	62.90	428	84.25	35	104.90	49
48.80	58	68.95	109	84.50	35	105.75	42
50.05	83	69.80	185	85.00	58	106.90	81
52.80	309	70.95	147	85.65	27	108.90	94
53.70	66	72.80	148	88.90	58	109.75	160
54.95	163	73.95	111	89.90	168	110.15	74
57.00	84	76.20	33	90.75	328	110.90	191
57.90	44	78.80	151	91.65	41	111.90	179
58.90	100	79.90	30	92.30	60	114.90	142
60.90	532	81.75	66	92.80	121	115.65	51

Scan 1347 (26.123 min): R0704.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.70	63	140.70	454	196.80	72	252.75	39
117.55	68	141.80	143	199.95	23	327.65	249
118.80	86	142.80	434	219.80	163	329.65	776
122.80	87	143.80	71	220.80	59	330.75	56
123.95	60	152.90	58	221.70	169	331.65	837
124.80	109	164.80	144	222.70	194	332.40	50
125.80	47	165.70	66	223.70	100	333.75	220
127.80	24	169.80	104	247.80	148	470.40	25
132.90	73	170.70	78	249.80	147		
133.65	24	172.80	45	251.15	20		
135.90	80	175.20	29	251.75	138		

STP Compounds

Scan 1347 (26.123 min): R0704.D

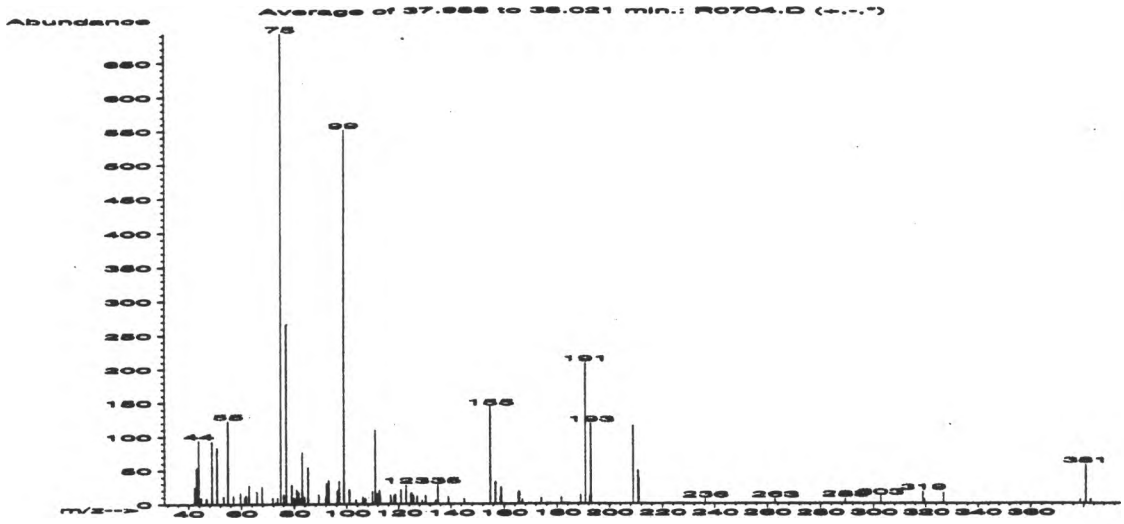
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,4,6-Tribromo-phenol	328	C6H3Br3O	94
2.	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	93
3.	5-Methyl-2,4,6-tribomopyrimidine	328	C5H3Br3N2	90
4.	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	50
5.	Propane, 1-(2,4,6-tribromophenoxy)-2,3-d	526	C9H7Br5O	40
6.	Butane, trichloro-	160	C4H7Cl3	38
7.	Propanoic acid, 2,2-dichloro-	142	C3H4Cl2O2	38
8.	2-(1'-(P-BROMOPHENYL)-1'-HYDROXYMETHYL)-	330	C17H15BrO2	23
9.	Phosphorodithioic acid, O,O-diethyl este	186	C4H11O2PS2	16
10.	BENZENESULFONIC ACID, 2,4,6-TRIBROMO MET	406	C7H5Br3O3S	14
11.	P-METHYLBENZYLDIMETYHYLSULFONIUM PICRATE	395	C19H13N3O7	12
12.	Phosphine, triethyl-	118	C6H15P	12
13.	1-(METHYLTHIO)-2-PROPANOL	106	C4H10OS	12
14.	Butane, 2,3-dichloro-	126	C4H8Cl2	12
15.	.alpha.-(13C-Cyano)-3-cyanotoluene	142	C813CH6N2	10
16.	Sulfur diimide, dimethyl-	90	C2H6N2S	9
17.	4-P-HYDROXYPHENYL-2,2,4-TRIMETHYLSELENAC	332	C18H20OSe	7
18.	3,5-BIS(TRIFLUOROMETHYL) BENZENEBORONATE	332	C14H7BF6O2	7
19.	2,2-DIMETHYL-1,8-DICHLORO-3,6-DIOXAOCTAN	214	C8H16Cl2O2	7
20.	Phenol, 2,3-dichloro-	162	C6H4Cl2O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000000-00-0	82078	91	23	0	85	25	70	48	94	8568
2.	*93	000118-79-6	82077	106	96	3	98	7	68	0	93	9769
3.	*90	064188-81-4	82076	48	23	0	88	0	57	1	47	7262
4.	*50	000118-79-6	134373	84	107	1	80	50	25	52	80	7939
5.	40	035109-60-5	109604	54	137	2	80	33	16	10	37	9540
6.	38	030028-27-4	16549	40	71	0	92	40	14	0	33	5555
7.	38	000075-99-0	122570	46	56	0	98	40	14	15	37	5554
8.	*23	000000-00-0	82801	30	155	2	92	49	6	0	26	7021
9.	16	000298-06-6	127314	39	102	0	98	60	3	0	33	4937
10.	14	000000-00-0	98752	46	114	0	50	68	2	0	39	6377
11.	12	000000-00-0	96928	38	140	3	98	60	2	0	28	4937
12.	12	000554-70-1	119832	34	100	2	98	60	2	0	21	4937
13.	12	000000-00-0	1735	34	58	1	98	58	2	2	23	5205
14.	*12	007581-97-7	5084	35	72	1	106	60	2	0	25	5231
15.	10	000000-00-0	10149	37	158	3	346	65	1	0	21	3657
16.	* 9	013849-02-0	304	30	100	0	63	80	1	0	33	4937
17.	* 7	060032-41-9	83424	29	185	1	105	80	1	0	29	7109
18.	7	073852-85-4	83313	33	106	0	40	77	1	0	25	5453
19.	7	000000-00-0	40990	36	74	1	35	80	1	0	21	2549
20.	7	000576-24-9	125027	42	92	1	51	75	1	0	29	3662

STP Compounds

Peak 57; 2-Propanol, 1,3-Dichloro-, Phospated (3:1)



Average of 37.988 to 38.021 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.15	24	61.25	10	76.95	266	91.80	10
42.95	53	61.75	13	79.05	28	92.20	31
43.80	94	62.90	27	79.90	9	93.05	35
44.80	9	65.75	18	80.90	21	96.25	20
46.85	8	67.70	25	81.50	17	97.05	34
48.80	92	71.80	9	81.85	3	98.85	552
50.80	83	72.95	2	82.15	8	100.95	21
53.30	11	73.70	9	82.95	76	103.55	6
54.95	123	74.85	693	83.75	10	106.15	10
56.90	12	75.95	14	85.20	54	106.90	8
59.65	16	76.20	6	89.25	14	109.80	18

Average of 37.988 to 38.021 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.85	110	124.95	16	158.65	11	208.90	116
111.65	15	125.45	12	158.90	24	210.75	49
112.65	20	126.95	11	165.20	17	211.00	38
112.90	11	128.90	5	165.55	18	236.40	6
116.95	13	130.25	12	166.85	6	262.95	6
117.20	6	134.15	5	173.95	8	289.30	7
118.30	12	134.95	28	181.50	9	302.65	10
118.70	14	139.00	10	188.90	13	318.95	17
120.85	21	145.05	7	190.80	209	319.55	5
122.80	28	154.85	144	192.45	11	326.75	15
124.70	15	156.80	33	192.90	119	378.65	6

Average of 37.988 to 38.021 min.: R0704.D
Converted from RTE data file: >R0704:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
380.90	57						
382.75	6						

STP Compounds

Average of 37.988 to 38.021 min.: R0704.D
Converted from RTE data file: >R0704:

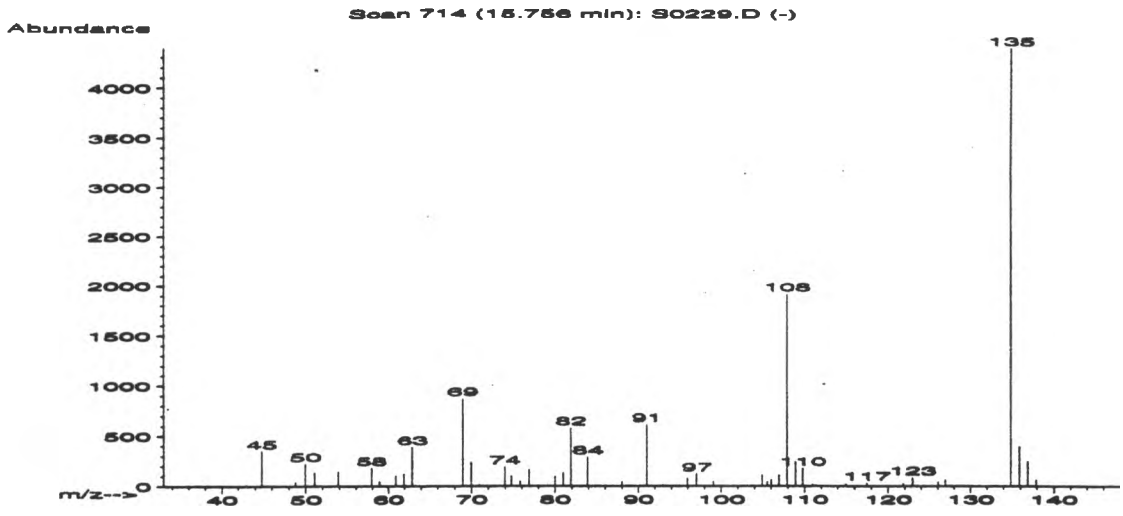
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Propanol, 1,3-dichloro-, phosphate (3:	428	C9H15Cl6O4P	42
2.	1-Propene, 3,3-dichloro-	110	C3H4Cl2	35
3.	1-Propene, 2,3-dichloro-	110	C3H4Cl2	17
4.	1.beta.-Benzoyloxy-5,5-ethylenedioxy-7a.	314	C19H22O4	12
5.	Phosphoric acid, tributyl ester	266	C12H27O4P	10
6.	Ethanethioamide	75	C2H5NS	10
7.	2,4-DIMETHYL-9-OXADODECAN-4-OL	216	C13H28O2	9
8.	Androstan-3-one, cyclic 1,2-ethanediyl a	318	C21H34O2	8
9.	Lupan-3-one, cyclic 1,2-ethanediyl aceta	470	C32H54O2	7
10.	1,1'-BICYCLOHEXYL-1,1'-BIS(TRIMETHYLSILY	342	C18H38O2Si2	7
11.	1,1'-BICYCLOHEXYL-1,1'-DIOL	198	C12H22O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	42	013674-87-8	101923	53	119	2	64	28	17	0	32	9895
2.	*35	000563-57-5	118814	37	40	2	99	54	11	11	40	7586
3.	17	000078-88-6	118813	35	67	2	82	54	3	0	22	7591
4.	12	085573-25-7	78323	34	79	2	67	56	2	0	22	6216
5.	10	000126-73-8	131964	40	68	1	64	64	1	0	29	5835
6.	*10	000062-55-5	116613	29	63	2	83	70	1	0	33	7161
7.	9	000000-00-0	42038	40	93	0	57	71	1	0	33	5613
8.	8	001434-14-6	134135	34	99	2	79	70	1	0	22	5613
9.	7	054498-65-6	106657	38	115	1	60	71	1	0	29	5613
10.	7	019009-71-3	85996	34	56	2	78	71	1	0	25	5613
11.	7	002888-11-1	34005	34	59	2	78	71	1	0	25	5613

STP Compounds

Peak 4a; Benzothiazole



Scan 714 (15.756 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	14	68.95	870	84.95	3	106.90	113
44.80	350	69.95	233	88.00	44	107.90	1917
48.80	43	70.95	18	91.00	612	108.90	241
49.95	223	73.95	190	92.95	14	109.75	179
51.05	132	74.75	101	94.95	8	110.95	19
53.85	142	75.80	50	95.95	77	114.95	23
57.90	180	76.90	164	97.05	120	117.45	30
58.90	44	80.00	98	99.05	47	121.80	26
60.90	103	80.95	133	104.90	110	122.95	84
61.90	124	81.90	580	105.50	43	126.05	41
62.90	388	83.90	290	106.00	65	126.95	60

Scan 714 (15.756 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.90	4391						
135.90	393						
136.90	249						
137.90	66						

STP Compounds

Scan 714 (15.756 min): S0229.D

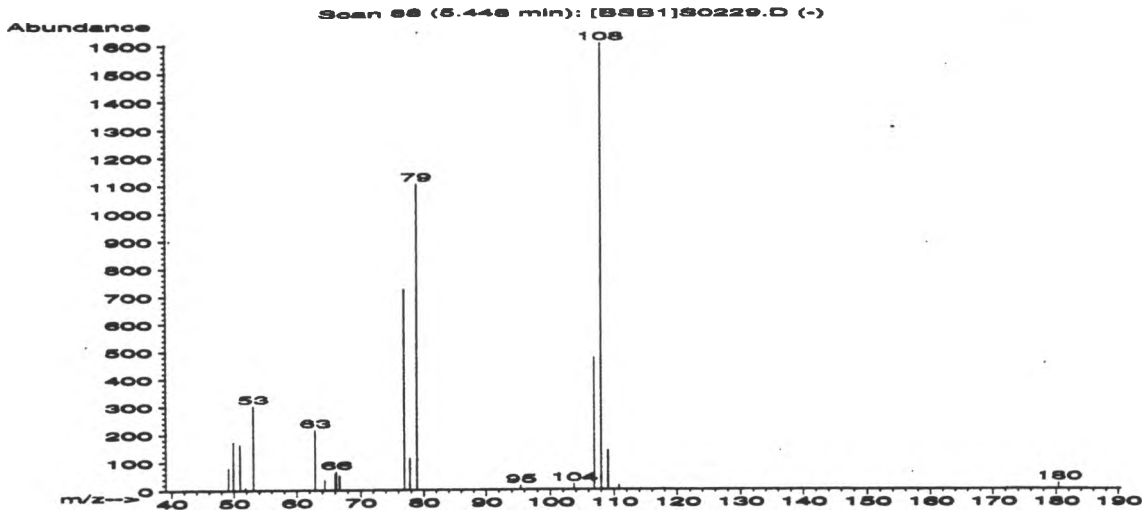
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzothiazole	135	C7H5NS	91
2.	Benzothiazole	135	C7H5NS	91
3.	1,2-Benzisothiazole	135	C7H5NS	90
4.	1,2-Benzisothiazole	135	C7H5NS	87
5.	Benzothiazole	135	C7H5NS	86
6.	1,2-Benzisothiazole-3-carboxylic acid	179	C8H5NO2S	64
7.	Thiocyanic acid, phenyl ester	135	C7H5NS	64
8.	Benzothiazole	135	C7H5NS	64
9.	Benzothiazole	135	C7H5NS	59
10.	Adenine	135	C5H5N5	59
11.	Adenine	135	C5H5N5	59
12.	Adenine	135	C5H5N5	59
13.	4-M-MERCAPTOBENZONITRILE	135	C7H5NS	50
14.	Thieno[3,2-c]pyridine	135	C7H5NS	50
15.	Benzothiazole	135	C7H5NS	50
16.	4-O-MERCAPTOBENZONITRILE	135	C7H5NS	50
17.	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	45
18.	1H-Indole, 5-fluoro-	135	C8H6FN	45
19.	Benzothiazole	135	C7H5NS	40
20.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000095-16-9	121696	75	11	0	98	5	62	0	81	9898
2.	*91	000095-16-9	121694	83	10	1	87	4	62	12	80	9957
3.	*90	000272-16-2	121700	71	21	2	99	10	59	14	70	9838
4.	*87	000272-16-2	7531	65	29	2	87	10	54	10	56	9789
5.	*86	000095-16-9	121695	54	10	1	98	7	53	0	49	9952
6.	64	040991-34-2	25013	59	39	1	93	17	37	0	43	9838
7.	*64	005285-87-0	7525	36	64	3	98	19	37	0	39	9761
8.	*64	000095-16-9	121698	43	58	3	99	16	37	0	39	9880
9.	*59	000095-16-9	121699	55	35	0	67	22	33	11	40	9925
10.	*59	000073-24-5	121689	33	48	2	88	23	33	1	40	9733
11.	*59	000073-24-5	121687	34	61	2	75	23	33	0	39	9809
12.	*59	000073-24-5	7506	33	61	2	99	23	33	0	39	9787
13.	*50	054435-88-0	7528	33	51	1	99	31	25	0	41	9526
14.	*50	000272-14-0	7534	42	54	2	99	19	25	10	33	9539
15.	*50	000095-16-9	121697	36	48	1	93	32	25	0	41	9493
16.	*50	034761-11-0	7527	39	49	2	96	16	25	2	31	9816
17.	*45	000501-00-8	7538	35	63	1	89	22	19	9	35	9780
18.	*45	000399-52-0	7540	38	44	1	92	22	19	2	37	9827
19.	*40	000095-16-9	7530	55	34	1	92	11	16	2	29	9882
20.	*38	015816-45-2	7331	31	54	0	78	37	14	6	35	9177

STP Compounds

Peak 58; alkylfuran



Scan 88 (5.448 min): [BSB1]S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.05	79	77.80	113				
49.90	173	78.95	1102				
50.95	163	95.45	15				
51.85	11	103.70	20				
53.05	302	106.90	476				
62.90	216	108.00	1603				
64.40	36	109.05	140				
66.00	59	110.75	16				
66.25	65	180.40	21				
66.75	50						
76.95	722						

STP Compounds

Scan 88 (5.448 min): [BSB1]S0229.D

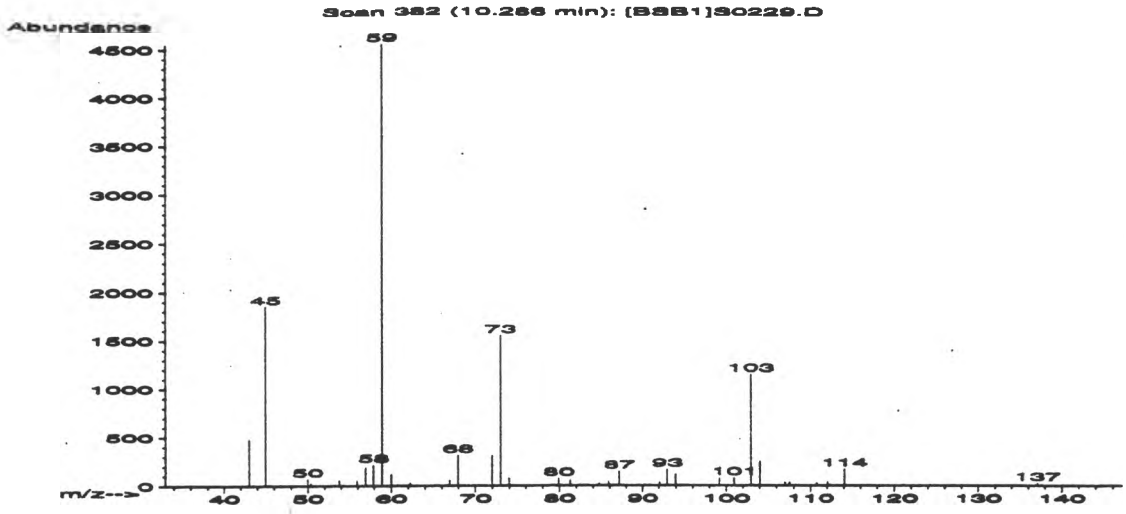
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-(2-PROPENYL)-FURAN	108	C7H8O	78
2.	Phenol, 2-methyl-	108	C7H8O	72
3.	1,2-Cyclooctadiene	108	C8H12	64
4.	1-Formyl-1,3-cyclohexadiene and 1-Formyl	108	C7H8O	64
5.	Phenol, 4-methyl-	108	C7H8O	53
6.	Phenol, 2-methyl-	108	C7H8O	53
7.	Phenol, 2-methyl-	108	C7H8O	53
8.	Benzenemethanol	108	C7H8O	50
9.	3-Octen-5-yne, (E)-	108	C8H12	50
10.	Phenol, 3-methyl-	108	C7H8O	45
11.	Phenol, 2-methyl-	108	C7H8O	45
12.	Phenol, 2-methyl-	108	C7H8O	42
13.	Phenol, 3-methyl-	108	C7H8O	40
14.	2-METHYL-1-HEPTENE-3-YNE	108	C8H12	40
15.	Phenol, 2-methyl-	108	C7H8O	38
16.	2-Pyridinamine, 3-methyl-	108	C6H8N2	37
17.	Phenol, 4-methyl-	108	C7H8O	37
18.	Benzenemethanol	108	C7H8O	37
19.	Benzene, methoxy-	108	C7H8O	37
20.	1,2-Benzenediamine	108	C6H8N2	32

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	000000-00-0	1912	51	41	1	98	10	46	7	40	9871
2.	*72	000095-48-7	118720	53	64	2	84	15	42	13	40	8815
3.	*64	007124-40-5	1979	33	81	2	95	17	37	0	39	9553
4.	*64	001121-54-6	1923	34	22	0	70	16	37	0	41	9591
5.	*53	000106-44-5	118728	35	71	3	133	28	28	0	39	7799
6.	*53	000095-48-7	118717	36	79	2	99	26	28	0	39	9008
7.	*53	000095-48-7	118718	33	96	2	96	26	28	0	39	9009
8.	*50	000100-51-6	118741	40	56	0	75	31	25	6	39	9517
9.	*50	074744-35-7	1934	40	56	0	86	32	25	23	40	8572
10.	*45	000108-39-4	118724	34	69	1	84	23	19	0	35	8959
11.	*45	000095-48-7	118719	37	75	2	98	21	19	0	35	9066
12.	*42	000095-48-7	118715	36	79	2	99	26	17	0	35	8931
13.	*40	000108-39-4	118721	34	74	2	99	32	16	0	35	8798
14.	*40	017669-40-8	1935	36	70	1	87	33	16	15	32	8580
15.	*38	000095-48-7	118716	30	82	2	99	40	14	1	30	8957
16.	*37	001603-40-3	118698	42	58	1	94	44	13	0	35	7856
17.	*37	000106-44-5	118726	29	82	2	119	42	13	6	35	7950
18.	*37	000100-51-6	118742	30	77	2	98	43	13	5	32	9418
19.	*37	000100-66-3	118734	34	81	1	92	41	13	0	35	8799
20.	*32	000095-54-5	1904	29	48	0	86	48	9	6	35	7824

STP Compounds

Peak 59



Scan 382 (10.286 min): [BSB1]S0229.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	480	66.95	57	92.95	165	137.05	26
44.95	1851	67.95	313	93.95	115		
49.95	68	71.95	307	99.20	74		
50.35	24	72.95	1551	100.95	78		
53.80	56	73.95	75	102.95	1150		
55.90	48	79.90	71	104.05	249		
56.95	186	81.25	53	107.00	36		
57.90	215	84.75	21	107.50	34		
58.90	4548	85.90	42	110.75	26		
60.00	117	87.15	147	112.05	37		
62.25	30	92.05	40	114.05	170		

STP Compounds

Scan 382 (10.286 min): [BSB1]S0229.D

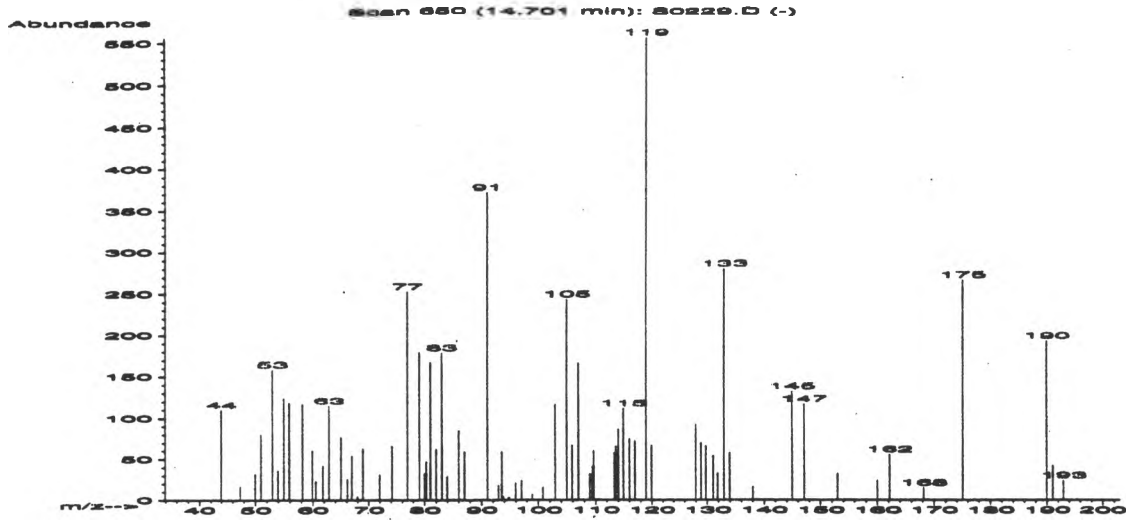
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Propanol, 1-(2-methoxy-1-methylethoxy)	148	C7H16O3	64
2.	DIPROPYLENEGLYCOL METHYL ETHER	148	C7H16O3	64
3.	DIBUTYLENE GLYCOL	162	C8H18O3	45
4.	BIS(1-METHYL-2-HYDROXYETHYL)ETHER	134	C6H14O3	45
5.	2-Propanol, 1,1'-oxybis-	134	C6H14O3	39
6.	Silane, ethyldimethyl-	88	C4H12Si	39
7.	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	38
8.	2-Propanol, 1,1'-[(1-methyl-1,2-ethanedi	192	C9H20O4	33
9.	2-Propanol, 1-[1-methyl-2-(2-propenyloxy	174	C9H18O3	33
10.	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	33

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	020324-32-7	11907	47	42	0	72	19	37	13	41	9910
2.	64	012002-25-4	11908	47	42	0	72	19	37	13	41	9910
3.	45	054305-61-2	17545	39	45	0	75	21	19	0	33	9506
4.	45	000000-00-0	7292	39	45	0	75	21	19	0	33	9506
5.	39	000110-98-5	121515	35	53	1	99	19	15	1	23	9523
6.	39	000758-21-4	251	36	62	3	91	20	15	0	22	9701
7.	38	013588-28-8	11903	39	41	0	75	38	14	2	35	9399
8.	33	001638-16-0	30635	41	53	1	97	32	10	0	29	9322
9.	33	055956-25-7	22959	38	57	2	74	31	10	0	29	9426
10.	33	000106-62-7	7290	37	49	0	73	32	10	0	25	9449

STP Compounds

Peak 60; Unidentified hydrocarbon



Scan 650 (14.701 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	110	61.75	42	80.00	32	93.55	59
47.30	16	62.85	115	80.25	47	93.85	4
49.90	32	65.00	77	81.00	167	95.95	21
50.95	80	66.15	25	82.00	63	97.05	24
52.95	158	66.90	54	83.00	179	98.95	7
53.95	36	67.95	4	83.95	29	100.80	16
54.95	124	68.95	63	85.00	1	102.95	117
55.90	118	71.95	31	86.00	85	105.00	243
58.15	117	74.20	66	87.00	59	105.90	67
59.90	60	76.95	252	91.00	371	107.00	166
60.50	23	79.05	179	92.95	18	108.95	32

Scan 650 (14.701 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.40	41	128.90	70	162.15	56		
109.65	60	129.75	66	168.20	15		
113.25	58	131.10	54	175.05	266		
113.50	66	131.90	33	189.95	193		
114.00	87	133.00	279	191.05	42		
114.90	112	133.95	58	192.95	24		
116.00	75	138.00	16				
116.95	72	144.95	132				
118.95	556	147.05	117				
119.95	67	152.95	32				
127.95	92	160.00	24				

STP Compounds

Scan 650 (14.701 min): S0229.D

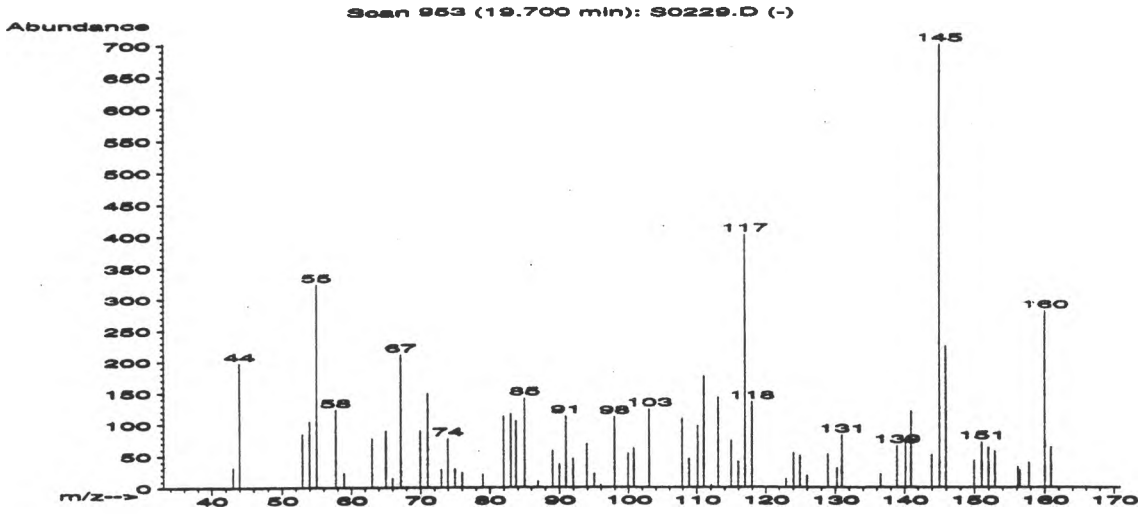
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-1,5-Benzodiazepine, 2,3,4,5-tetrahydr	190	C12H18N2	42
2.	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	27
3.	2-Naphthalenamine, 5,6,7,8-tetrahydro-	147	C10H13N	25
4.	Benzonitrile, 4-ethoxy-	147	C9H9NO	22
5.	Benzene, (1-ethylhexyl)-	190	C14H22	22
6.	5,9,9-Trimethyltricyclo[4.4.0.0(1,5)]dec	190	C13H18O	18
7.	3,7,7-TRIMETHYL-CYCLOHEPTA-1,3,5-TRIENE	134	C10H14	14
8.	1(3H)-Isobenzofuranone, 5-methyl-	148	C9H8O2	14
9.	1,4,4,-Trimethylbicyclo[3.2.0]hept-6-ene	162	C12H18	12
10.	Benzene, 1,3-diethyl-	134	C10H14	12
11.	Benzoxazole	119	C7H5NO	11
12.	2,8-Decadiyne	134	C10H14	10
13.	ORTHO-D2-BENZYLCYANIDE	117	C8H5D2N	10
14.	.ALPHA.-D2-BENZYLCYANIDE	117	C8H5D2N	10
15.	P-MENTHA-1,5,8-TRIENE	134	C10H14	10
16.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	10
17.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	10
18.	1H-Benzotriazole	119	C6H5N3	10
19.	trans-1-(2-Pyrazyl)-1-octene	190	C12H18N2	10
20.	1,3,4-Thiadiazol-2-amine, 5-[(1-methylet	175	C5H9N3S2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*42	040358-38-1	30100	68	55	0	50	58	17	0	76	7916
2.	*27	003277-26-7	121492	34	66	0	67	56	8	0	41	8040
3.	*25	002217-43-8	11727	54	45	0	99	65	7	8	43	6560
4.	*22	025117-74-2	11644	44	64	1	83	65	5	0	39	7388
5.	*22	018335-15-4	30204	45	67	1	107	63	5	3	38	7766
6.	*18	081532-21-0	30182	49	72	0	34	67	3	0	46	8711
7.	*14	000000-00-0	7465	37	57	0	99	70	2	0	41	7316
8.	14	054120-64-8	11954	44	64	0	82	68	2	0	39	7381
9.	12	081532-25-4	17887	62	50	1	69	62	2	0	36	7948
10.	12	000141-93-5	121644	54	61	3	99	65	2	15	37	7366
11.	*11	000273-53-0	3967	34	47	0	99	72	2	10	43	7236
12.	10	004116-93-2	7429	46	73	2	69	67	1	0	34	7821
13.	*10	053897-46-4	119690	34	64	0	99	72	1	0	41	7236
14.	*10	000935-66-0	119689	36	67	1	99	72	1	1	40	7236
15.	10	021195-59-5	7462	44	65	1	84	70	1	0	35	7333
16.	*10	000140-76-1	119921	42	57	0	98	72	1	0	39	7236
17.	*10	000140-76-1	3976	35	65	1	69	72	1	0	39	7236
18.	*10	000095-14-7	3947	35	58	0	99	72	1	0	41	7236
19.	10	083568-44-9	30080	43	84	1	48	66	1	0	35	8186
20.	*10	030062-47-6	23294	28	63	0	37	70	1	10	35	4704

STP Compounds

Peak 61a; Unidentified hydrocarbon



Scan 953 (19.700 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	32	69.95	90	86.90	10	103.05	124
43.95	198	71.05	149	89.00	59	107.90	109
52.90	85	73.00	29	90.00	37	108.90	46
53.95	105	73.95	78	90.95	113	110.15	97
54.95	324	74.95	30	91.95	46	111.00	176
57.75	123	76.00	24	93.90	69	112.10	4
58.95	23	79.00	21	95.00	22	113.05	142
63.00	78	81.95	113	95.95	4	114.95	74
65.00	90	83.00	117	97.95	112	115.95	41
66.00	15	83.75	106	99.95	55	116.95	403
67.15	211	85.00	142	100.80	62	117.95	135

Scan 953 (19.700 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.95	14	143.95	52	160.90	64		
124.05	55	145.05	702				
125.00	50	145.95	225				
125.95	19	149.95	43				
128.95	53	151.05	72				
130.25	31	151.95	63				
130.95	83	152.85	58				
136.50	21	156.15	33				
138.90	66	156.40	27				
140.15	77	157.75	40				
140.95	120	160.00	281				

STP Compounds

Scan 953 (19.700 min): S0229.D

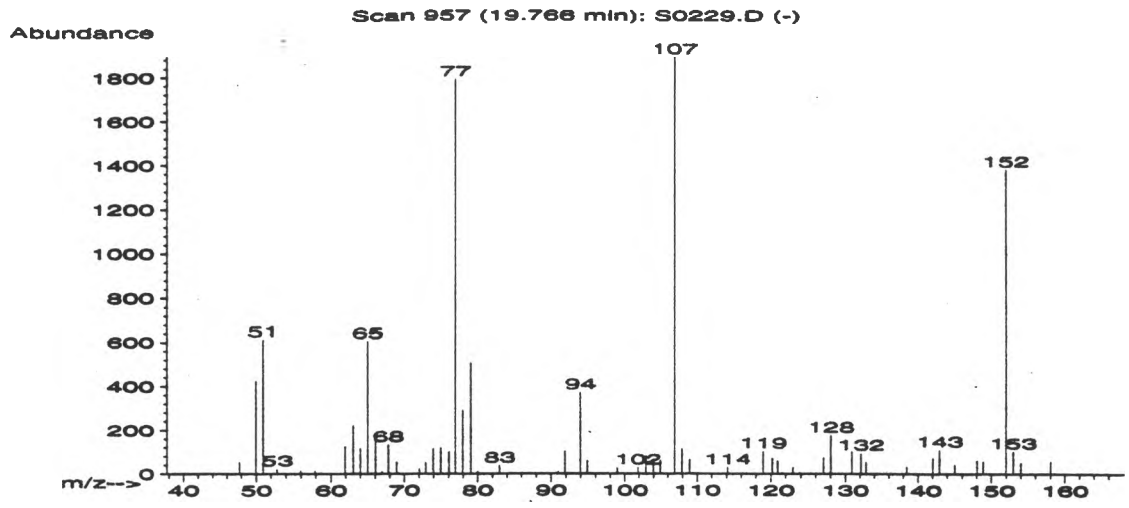
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,4,6-TRIMETHYLINDANE	160	C12H16	78
2.	3-tert-Butyl-4-cyanopyridine	160	C10H12N2	59
3.	4-METHYLBENZALACETONE	160	C11H12O	53
4.	3-METHYLBENZALACETONE	160	C11H12O	50
5.	Benzene, 1-(1,1-dimethylethyl)-4-ethenyl	160	C12H16	47
6.	2H-1-Benzopyran, 2,2-dimethyl-	160	C11H12O	43
7.	Benzene, 1-(1-methylethenyl)-4-(1-methyl	160	C12H16	43
8.	Ethanone, 1-[4-(1-methylethenyl)phenyl]-	160	C11H12O	43
9.	Benzene, (1-methylethenyl)(1-methylethyl	160	C12H16	43
10.	1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	160	C12H16	38
11.	(Z)-2-(1'-PROPENYL)MESITYLENE	160	C12H16	38
12.	Indene, 1,1-dimethyl-1-sila-	160	C10H12Si	38
13.	1H-Benzimidazole, 2-(1-methylethyl)-	160	C10H12N2	38
14.	Benzene, (2,2-dimethyl-1-methylenepropyl	160	C12H16	38
15.	Benzene, 1-(1-methylethenyl)-3-(1-methyl	160	C12H16	38
16.	1H-Indene, 2,3-dihydro-1,1,6-trimethyl-	160	C12H16	38
17.	1H-Indene, 2,3-dihydro-1,4,7-trimethyl-	160	C12H16	38
18.	1H-1,2,4-Triazole, 3-phenyl-	145	C8H7N3	27
19.	1H-Pyrrolo[2,3-b]pyridine, 2-ethyl-	146	C9H10N2	27
20.	1H-Inden-1-one, 2,3-dihydro-4,7-dimethyl	160	C11H12O	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	065001-56-1	17042	30	34	0	99	9	46	9	42	8253
2.	*59	074808-75-6	16889	35	37	0	99	23	33	0	41	9414
3.	*53	003160-38-1	16927	47	71	3	99	27	28	0	40	9372
4.	*50	015753-84-1	16925	46	66	2	89	32	25	0	40	9359
5.	*47	001746-23-2	17025	47	51	0	99	40	20	14	40	8963
6.	*43	002513-25-9	16950	54	32	0	91	49	18	3	43	8015
7.	*43	002388-14-9	17020	36	63	0	93	45	18	0	41	8752
8.	*43	005359-04-6	16931	36	60	2	99	44	18	0	39	8744
9.	*43	027193-71-1	124936	36	63	0	80	47	18	2	43	8727
10.	*38	016204-72-1	17037	42	51	0	99	48	14	16	39	8191
11.	*38	002077-40-9	17016	45	68	2	90	49	14	0	40	8291
12.	*38	058310-24-0	16913	35	58	1	99	47	14	0	41	8503
13.	*38	005851-43-4	16900	37	64	1	99	47	14	0	39	8380
14.	*38	005676-29-9	17015	36	55	0	72	47	14	10	39	8918
15.	*38	001129-29-9	17019	42	57	0	66	47	14	0	39	8811
16.	*38	014276-95-0	17039	29	58	0	99	48	14	19	42	8219
17.	*38	054340-87-3	17040	41	50	0	80	48	14	16	42	8267
18.	*27	003357-42-4	11023	43	64	1	72	60	8	0	40	7942
19.	*27	023612-49-9	11424	36	70	2	82	58	8	0	39	8235
20.	*14	005037-60-5	16945	33	65	0	35	70	2	0	41	5837

STP Compounds

Peak 61b; Phenoxy acetic acid



Scan 957 (19.766 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.70	52	66.95	8	80.00	10	106.90	1895
49.95	423	67.80	134	83.00	37	107.95	114
50.95	612	68.95	52	90.95	10	108.95	64
52.85	21	72.05	23	91.90	103	114.15	29
55.95	14	72.95	51	93.95	372	118.95	102
57.90	15	73.95	116	94.90	59	120.20	72
61.90	125	74.95	119	99.00	24	120.95	58
63.00	222	76.05	101	101.85	27	122.95	28
64.00	116	76.95	1790	102.95	81	126.05	3
65.00	604	77.95	289	103.95	68	127.05	75
66.05	163	79.05	506	104.95	60	128.05	176

Scan 957 (19.766 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.90	103	154.00	50				
132.15	93	158.00	55				
132.85	52						
138.50	30						
142.05	72						
142.95	110						
145.00	41						
148.05	62						
148.90	55						
151.95	1387						
152.95	103						

STP Compounds

Scan 957 (19.766 min): S0229.D

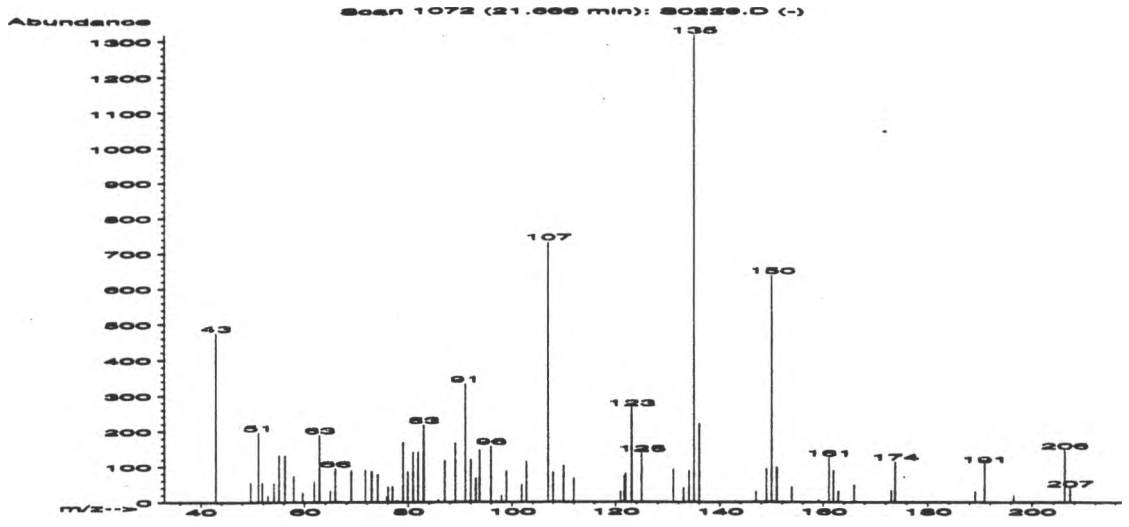
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Acetic acid, phenoxy-	152	C8H8O3	72
2.	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	47
3.	Benzeneacetic acid, .alpha.-hydroxy-	152	C8H8O3	47
4.	Benzene, nitroso-	107	C6H5NO	43
5.	Pyridine, 4-ethyl-	107	C7H9N	38
6.	Pyridine, 4-ethyl-	107	C7H9N	38
7.	Benzeneacetic acid, 3-hydroxy-	152	C8H8O3	38
8.	Pyridine, 4-ethyl-	107	C7H9N	38
9.	Benzene, nitroso-	107	C6H5NO	38
10.	Benzene, nitroso-	107	C6H5NO	38
11.	Benzenamine, 4-methyl-2-nitro-	152	C7H8N2O2	27
12.	Pyridine, 2,3-dimethyl-	107	C7H9N	27
13.	1-Hexen-3-yne, 2-methyl-	94	C7H10	22
14.	Benzaldehyde	106	C7H6O	22
15.	Pyridine, 3-ethyl-	107	C7H9N	22
16.	Pyridine, 4-ethyl-	107	C7H9N	16
17.	Pyridine, 3-ethyl-	107	C7H9N	16
18.	Benzene, 1,1'-oxybis-	170	C12H10O	14
19.	N-Methylmethanesulfenanilide	153	C8H11NS	14
20.	Phenol, 2-chloro-6-methyl-	142	C7H7ClO	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	000122-59-8	13352	50	55	1	70	17	42	0	46	9795
2.	*47	000156-38-7	123893	37	63	1	99	39	20	13	40	8156
3.	*47	000090-64-2	123894	37	75	3	99	37	20	20	40	7071
4.	*43	000586-96-9	118598	58	33	0	74	46	18	16	47	7955
5.	*38	000536-75-4	118609	50	59	2	99	54	14	0	46	6852
6.	*38	000536-75-4	118610	51	64	2	99	51	14	0	46	7374
7.	*38	000621-37-4	13347	34	63	1	99	46	14	0	39	8645
8.	*38	000536-75-4	118608	50	61	2	99	51	14	0	46	7291
9.	*38	000586-96-9	1811	47	39	0	81	46	14	18	39	7771
10.	*38	000586-96-9	118596	48	41	0	74	47	14	2	41	7970
11.	*27	000089-62-3	13300	36	71	2	61	56	8	0	39	7151
12.	*27	000583-61-9	1819	34	78	2	99	60	8	0	39	6704
13.	*22	023056-94-2	484	35	65	2	84	63	5	18	40	5732
14.	22	000100-52-7	118548	43	45	1	75	65	5	20	38	5305
15.	*22	000536-78-7	118607	33	65	2	99	62	5	0	39	7039
16.	*16	000536-75-4	1818	34	74	1	76	60	3	0	35	7271
17.	*16	000536-78-7	118606	36	72	3	99	60	3	0	35	7357
18.	14	000101-84-8	125988	39	52	0	83	67	2	22	43	5842
19.	*14	065605-22-3	14045	35	45	1	69	67	2	18	40	6702
20.	12	000087-64-9	122597	47	59	1	75	63	2	0	37	8042

STP Compounds

Peak 62; .gamma.-Methylionone



Scan 1072 (21.666 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	475	62.90	189	79.00	168	93.80	147
49.55	55	64.95	32	79.90	85	95.95	158
51.05	196	65.90	94	80.90	141	97.00	3
51.80	54	68.95	88	81.90	142	98.00	18
52.95	18	71.70	90	83.00	217	98.95	86
54.05	53	72.95	86	85.80	6	101.95	49
55.05	133	74.05	77	87.00	117	102.80	115
56.15	133	75.80	15	89.00	167	107.00	733
57.90	73	76.05	42	90.95	333	108.00	83
59.65	25	76.95	44	92.00	121	110.00	103
61.90	57	77.85	3	93.00	66	112.00	67

Scan 1072 (21.666 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.05	30	146.95	30	173.80	114		
121.70	75	149.05	93	189.15	30		
121.95	81	150.05	639	190.95	108		
123.05	266	151.05	98	196.55	19		
124.95	138	153.90	42	206.15	146		
131.00	92	159.05	6	207.15	39		
132.95	41	161.15	125				
134.00	88	162.00	89				
135.00	1316	162.95	31				
136.00	221	165.95	49				
142.95	2	173.05	33				

STP Compounds

Scan 1072 (21.666 min): S0229.D

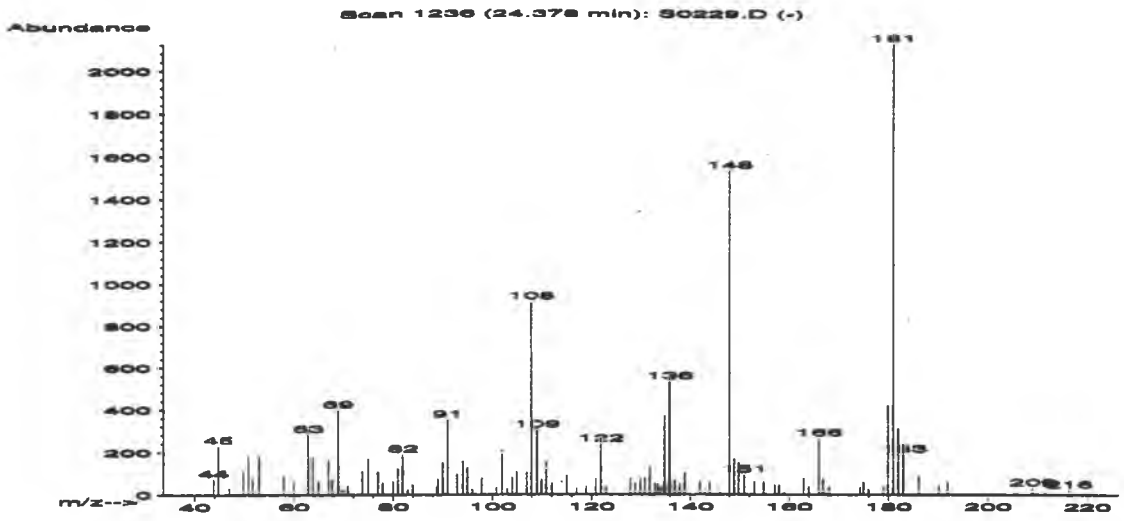
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.GAMMA.-METHYLIONONE	206	C14H22O	81
2.	(Z)-3-METHYL-4-(2',6',6'-TRIMETHYL-CYCLO	206	C14H22O	64
3.	1,3-Dimethylbicyclo[3.3.0]oct-3-en-2-one	150	C10H14O	59
4.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	50
5.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	50
6.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	50
7.	2,5-DIETHYLPHENOL	150	C10H14O	49
8.	(E)-4-(5'-Methyl-2'-furyl)-3-buten-2-one	150	C9H10O2	47
9.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
10.	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	150	C9H10O2	46
11.	Benzene, 1-methoxy-4-(1-methylethyl)-	150	C10H14O	46
12.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
13.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
14.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
15.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	43
16.	Benzene, 2-methoxy-1,3,4-trimethyl-	150	C10H14O	43
17.	2-Cyclohexen-1-one, 3-methyl-6-(1-methyl	150	C10H14O	35
18.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	25
19.	5-Isopropyliden-2,3-dimethyl-2-cyclopent	150	C10H14O	25
20.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*81	000000-00-0	37604	73	25	1	67	16	49	0	74	9705
2.	*64	015789-90-9	37605	56	90	3	70	25	37	0	47	9741
3.	*59	070640-02-7	12804	32	24	0	89	25	33	15	42	8477
4.	*50	000088-18-6	12725	47	49	0	73	31	25	13	40	9602
5.	*50	000499-75-2	123691	35	66	2	99	35	25	1	40	9191
6.	*50	000499-75-2	123690	35	63	2	99	35	25	5	40	9230
7.	*49	000876-20-0	12897	50	52	2	99	39	23	0	46	9081
8.	*47	066434-99-9	12580	36	32	1	99	37	20	1	40	9288
9.	*46	000089-83-8	123682	34	62	1	92	41	20	2	43	8974
10.	*46	001450-72-2	12615	34	58	2	89	41	20	10	43	9228
11.	*46	004132-48-3	12753	54	39	0	84	43	20	16	49	8713
12.	*46	000089-83-8	123684	34	62	1	92	41	20	2	43	8973
13.	*46	000089-83-8	123677	60	33	0	82	43	20	21	47	8735
14.	*46	000089-83-8	123680	47	41	0	82	43	20	21	47	8690
15.	*43	000089-83-8	123681	33	60	0	99	41	18	0	41	8963
16.	*43	021573-36-4	12758	36	62	0	69	47	18	22	43	8125
17.	*35	000491-09-8	12787	35	61	1	42	52	11	11	40	7100
18.	*25	000585-34-2	123672	52	50	2	137	62	7	0	44	9541
19.	*25	042507-33-5	12707	36	20	0	43	61	7	14	43	7163
20.	*25	015816-45-2	7331	37	54	0	92	62	7	10	43	7821

STP Compounds

Peak 55; 2-(Methylthio)-benzothiazole



Scan 1236 (24.378 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	73	63.90	176	79.95	61	92.85	97
44.80	229	65.00	60	80.95	124	94.05	158
47.00	31	67.00	161	81.95	188	94.95	126
49.90	107	67.70	69	82.95	21	95.95	24
50.95	181	68.95	396	83.95	48	97.80	77
51.80	75	69.95	23	86.95	11	100.80	34
53.05	178	70.95	42	88.80	37	101.95	213
55.00	5	73.80	109	89.00	72	103.00	27
57.95	91	75.05	167	90.00	152	104.00	80
60.00	57	76.95	105	91.00	351	104.95	110
62.90	282	77.95	55	91.95	3	107.00	103

Scan 1236 (24.378 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.90	915	122.95	39	136.95	68	153.05	59
109.00	303	128.00	77	137.90	46	154.90	57
109.95	70	128.95	51	138.95	99	157.15	44
110.90	155	130.00	73	141.95	59	158.00	43
112.00	55	130.90	80	142.95	19	159.00	9
115.00	90	131.90	133	143.95	56	162.90	76
116.95	27	132.95	53	146.00	19	163.90	36
117.85	1	133.50	48	147.95	1531	165.95	263
118.95	37	133.95	32	148.95	165	166.80	71
120.90	72	134.90	369	149.85	149	167.95	34
121.95	237	135.90	534	150.95	91	174.30	35

Scan 1236 (24.378 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
174.95	59	209.00	30				
175.95	24	216.30	20				
179.00	38						
179.90	421						
180.90	2122						
182.00	310						
183.00	188						
186.15	90						
189.95	3						
190.20	43						
191.95	58						

Scan 1236 (24.378 min): S0229.D

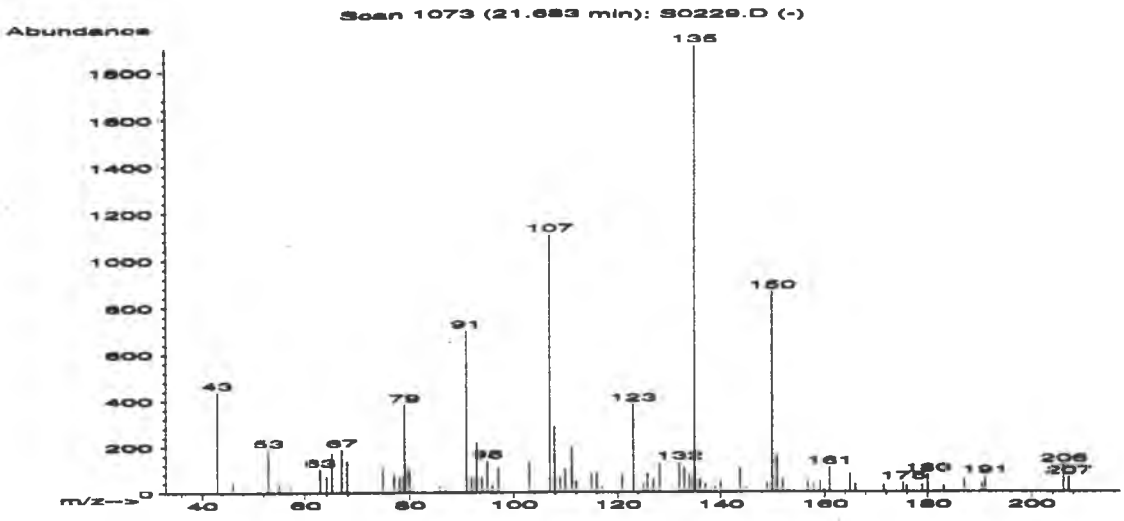
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	94
2.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	93
3.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	93
4.	2(3H)-Benzothiazolethione, 3-methyl-	181	C8H7NS2	59
5.	2,1,3-Benzothiadiazole, 4-nitro-	181	C6H3N3O2S	43
6.	5-AMINO-ISO-PHTHALIC ACID	181	C8H7NO4	38
7.	Benzeneacetic acid, 3-nitro-	181	C8H7NO4	38
8.	Benzenamine, N-(phenylmethylene)-	181	C13H11N	38
9.	Methyl 3-hydroxy-5-methylaminobenzoate	181	C9H11NO3	37
10.	Carbamic acid, (3-methoxyphenyl)-, methy	181	C9H11NO3	27
11.	9H-Carbazole, 9-methyl-	181	C13H11N	27
12.	3-METHYLCARBAZOLE	181	C13H11N	22
13.	Benzenamine, 2-chloro-N-(2-pyridinylmeth	216	C12H9ClN2	22
14.	1-(11'-(PROPEN-2''-YL)TRICYCLO[6.2.1.0(2	357	C22H19N3O2	16
15.	2-Butanone, 3-hydroxy-, (2,4-dinitrophen	268	C10H12N4O5	12
16.	Morpholine, 4-(4-methyl-1-cyclohexen-1-y	181	C11H19NO	12
17.	1,2,3-Benzothiadiazole	136	C6H4N2S	11
18.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	10
19.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	10
20.	cis-7-Methylenebicyclo[3.3.0]octan-2-one	136	C9H12O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000615-22-5	126908	96	35	2	85	2	70	0	93	9967
2.	*93	000615-22-5	25993	94	36	1	92	6	66	0	93	9912
3.	*93	000615-22-5	126909	92	34	1	89	6	66	0	92	9937
4.	*59	002254-94-6	25992	46	84	3	88	22	33	0	39	9668
5.	*43	006583-06-8	126899	49	92	2	81	46	18	0	44	7480
6.	*38	000000-00-0	25989	44	73	1	77	47	14	0	39	8124
7.	*38	001877-73-2	25982	63	38	1	72	53	14	20	47	6380
8.	*38	000538-51-2	126927	34	45	0	75	55	14	8	43	7489
9.	*37	089610-99-1	26027	36	18	1	99	41	13	9	35	7215
10.	*27	051422-77-6	26036	34	67	2	93	59	8	1	40	7659
11.	*27	001484-12-4	26189	47	66	2	82	59	8	0	39	7179
12.	*22	004630-20-0	26187	33	73	2	96	63	5	0	39	6614
13.	*22	026825-33-2	41907	43	56	2	92	63	5	11	40	7350
14.	16	042589-34-4	89611	45	94	2	69	58	3	0	35	7439
15.	12	035015-94-2	132038	45	64	2	99	63	2	12	37	7438
16.	12	005601-45-6	26139	46	58	1	45	62	2	8	37	7854
17.	*11	000273-77-8	121801	53	27	0	32	75	2	18	43	3627
18.	*10	000622-60-6	121941	37	45	1	40	75	1	0	41	3631
19.	*10	000621-32-9	7956	35	46	0	32	75	1	13	39	3617
20.	*10	084642-40-0	8003	36	64	3	96	75	1	0	39	3631

STP Compounds

Peak 62;



Scan 1073 (21.683 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	438	70.05	15	92.95	218	111.95	50
46.05	41	72.85	3	93.95	68	115.00	78
50.90	6	74.80	104	95.00	137	115.95	86
52.90	188	76.95	80	95.95	29	117.00	20
54.95	37	78.00	66	97.05	107	120.90	75
57.10	22	79.00	382	103.05	132	123.05	381
62.75	103	79.90	102	107.00	1103	125.00	33
64.00	70	85.90	26	107.90	286	125.80	82
65.00	174	87.00	21	109.00	65	126.95	58
66.90	189	91.00	697	109.90	101	128.20	125
67.90	138	91.95	63	111.15	198	132.00	129

Scan 1073 (21.683 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.00	110	150.05	858	165.90	36	191.05	68
134.00	73	150.95	157	171.45	32	206.15	115
135.00	1900	152.05	51	171.80	5	207.15	63
136.05	54	152.95	10	174.00	2		
137.00	35	156.75	47	175.30	41		
138.95	24	157.90	25	175.95	26		
140.00	49	159.00	49	178.95	32		
143.80	102	159.90	11	180.00	76		
144.95	19	161.00	107	183.15	27		
146.00	13	163.95	4	187.00	53		
149.05	41	164.90	80	190.45	38		

STP Compounds

Scan 1073 (21.683 min): S0229.D

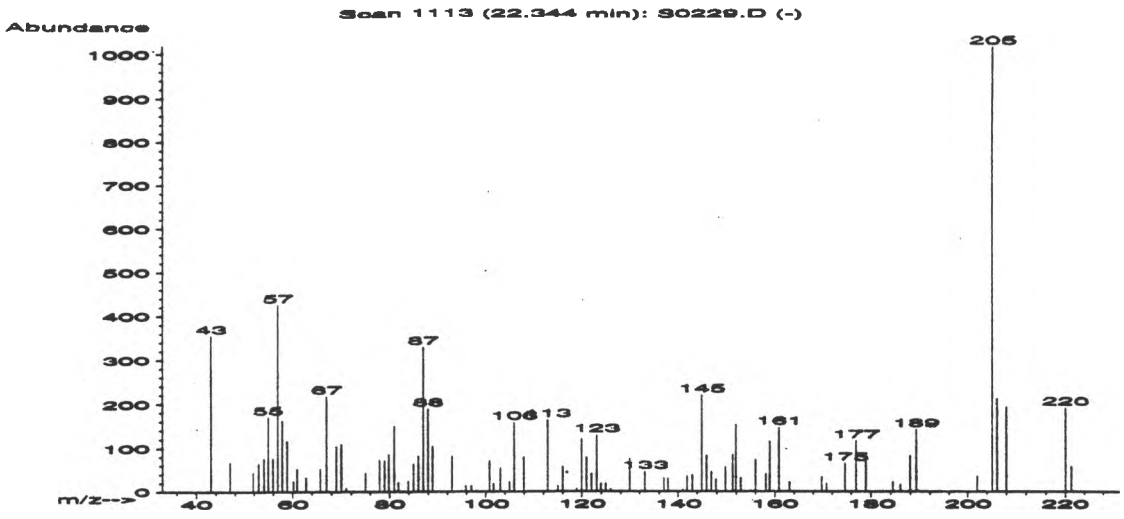
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenemethanol, 4-(1-methylethyl)-	150	C10H14O	58
2.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	58
3.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	53
4.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	53
5.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	53
6.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	47
7.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	47
8.	2,5-DIETHYLPHENOL	150	C10H14O	46
9.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
10.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	46
11.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	43
12.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	43
13.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	43
14.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	43
15.	Phenol, diethyl-	150	C10H14O	38
16.	[3.3.3]Propellane	150	C11H18	30
17.	Adenine	135	C5H5N5	27
18.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	27
19.	Phenol, 4-(2,2,3,3-tetramethylbutyl)-	206	C14H22O	27
20.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	000536-60-7	123697	50	61	1	67	30	32	0	46	9739
2.	*58	000088-18-6	12725	43	51	2	86	29	32	0	44	9630
3.	*53	000088-18-6	123665	44	48	2	99	29	28	4	39	9609
4.	*53	000088-18-6	123670	50	44	2	99	29	28	11	41	9589
5.	*53	000585-34-2	123672	34	68	2	99	29	28	0	39	9530
6.	*47	000499-75-2	123691	36	62	3	96	36	20	13	40	9111
7.	*47	000499-75-2	123692	36	62	3	96	36	20	13	40	9111
8.	*46	000876-20-0	12897	34	55	2	84	45	20	14	43	9045
9.	*46	000089-83-8	123684	48	46	2	99	43	20	0	46	8875
10.	*46	000089-83-8	123682	48	46	2	99	43	20	0	46	8875
11.	*43	000089-83-8	123680	46	46	2	86	45	18	4	43	8600
12.	*43	000089-83-8	123685	43	50	2	99	42	18	0	40	8885
13.	*43	000089-83-8	12728	34	62	3	93	44	18	11	40	8795
14.	*43	000089-83-8	123679	42	53	1	85	45	18	4	39	8743
15.	*38	026967-65-7	12731	34	59	2	99	46	14	0	41	8671
16.	*30	051027-89-5	12967	34	4	0	57	57	9	10	43	5874
17.	*27	000073-24-5	121686	35	52	1	68	60	8	0	39	7927
18.	*27	000140-66-9	128870	35	61	2	99	59	8	0	41	8319
19.	*27	054932-78-4	37578	33	57	2	99	59	8	0	39	8171
20.	*27	000140-66-9	128869	37	67	2	95	58	8	0	39	8350

STP Compounds

Peak 63; 2,6-Bis(1,1-dimethylethyl)-4-methylphenol



Scan 1113 (22.344 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	355	61.00	52	81.00	150	97.95	2
46.95	67	62.75	33	81.90	21	100.80	71
51.80	44	65.75	52	83.90	24	101.70	18
52.90	64	67.00	217	85.00	64	103.05	53
54.05	77	69.00	104	86.00	82	104.95	23
54.95	171	70.05	109	87.00	329	105.90	159
55.95	76	71.00	8	88.00	189	107.90	79
56.95	425	74.95	43	88.90	104	112.90	164
57.90	162	77.90	72	92.95	81	115.00	13
58.90	116	79.00	71	95.85	13	116.00	57
60.25	24	79.90	86	96.95	14	118.95	7

Scan 1113 (22.344 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.95	121	138.95	1	153.00	32	179.00	69
121.00	78	141.00	4	154.95	2	184.40	23
122.00	41	141.90	36	156.00	73	185.95	17
123.05	130	143.00	39	158.15	41	187.90	83
123.95	18	144.95	220	158.95	115	189.15	143
124.95	18	145.95	83	160.90	147	202.00	35
125.95	5	146.90	45	163.05	22	205.15	1019
129.90	76	147.85	29	169.80	34	206.15	213
133.05	46	149.80	57	170.90	19	208.00	194
137.00	32	151.30	85	174.70	65	220.05	192
137.90	30	151.95	154	176.95	117	221.20	57

STP Compounds

Scan 1113 (22.344 min): S0229.D

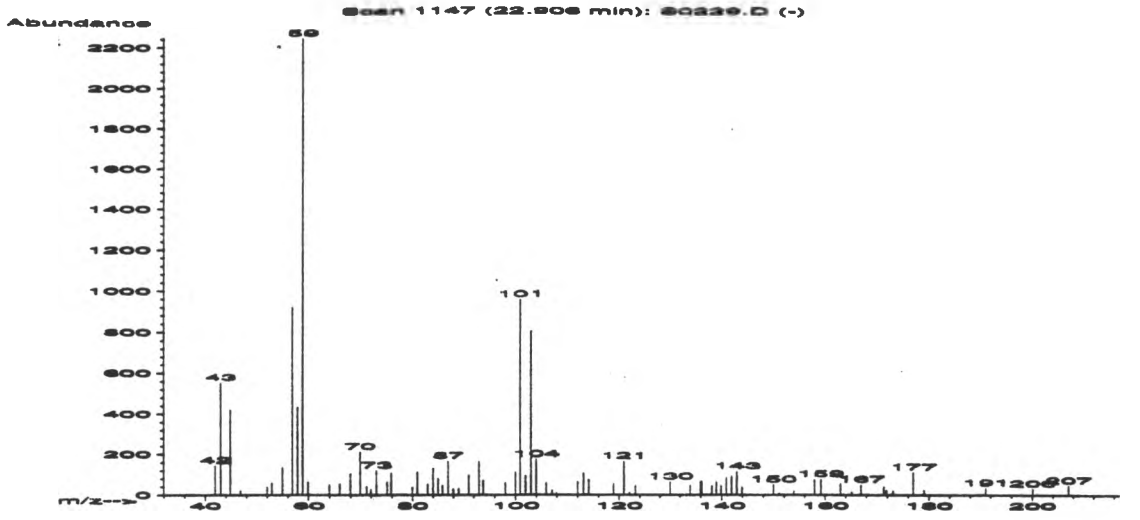
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	58
2.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	58
3.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	53
4.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	53
5.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	49
6.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	49
7.	6-Methyl-2,4-di-tert-butyl-phenol	220	C15H24O	47
8.	Quinoline, 2-phenyl-	205	C15H11N	47
9.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	47
10.	6-Methyl-2,4-di-tert-butyl-phenol	220	C15H24O	46
11.	Bicyclo[4.1.0]hepta-1,3,5-triene-7-carbo	205	C15H11N	43
12.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	43
13.	3-Methyl-4,6-di-tert-butyl-phenol	220	C15H24O	38
14.	5-ETHYL-4-PHENYL-3-MERCAPTO-1,2,4-TRIAZO	205	C10H11N3S	38
15.	7-PHENYLISOQUINOLINE	205	C15H11N	38
16.	3-PHENYLISOQUINOLINE	205	C15H11N	38
17.	Benzeneacetonitrile, .alpha.-(phenylmeth	205	C15H11N	38
18.	9-Phenanthrenecarbonitrile, 9,10-dihydro	205	C15H11N	35
19.	4-PHENYLISOQUINOLINE	205	C15H11N	35
20.	Benzonitrile, 4-(2-phenylethenyl)-, (E)-	205	C15H11N	32

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	000128-37-0	129732	63	55	2	99	26	32	26	47	9196
2.	*58	000128-37-0	43901	59	68	2	94	28	32	12	47	9271
3.	*53	000128-37-0	129735	52	66	1	99	29	28	20	41	9162
4.	*53	000128-37-0	129734	57	60	2	99	26	28	0	39	9227
5.	*49	000128-37-0	129731	44	71	0	87	36	23	0	44	9251
6.	*49	000128-37-0	129738	56	69	2	77	39	23	0	49	9293
7.	*47	000616-55-7	43900	42	68	1	99	40	20	0	39	9115
8.	*47	000612-96-4	37023	35	84	2	90	40	20	5	40	8919
9.	*47	000128-37-0	129733	36	84	1	67	39	20	0	39	9291
10.	*46	000616-55-7	129730	43	23	0	99	41	20	0	44	9067
11.	*43	056666-56-9	37031	37	81	0	85	46	18	18	43	8859
12.	*43	000128-37-0	129736	35	82	1	71	43	18	0	39	9232
13.	*38	000000-00-0	43902	39	26	0	94	46	14	0	39	9016
14.	*38	029448-76-8	128781	34	69	0	95	51	14	16	43	8859
15.	*38	070125-65-4	128795	36	76	0	99	46	14	0	41	8917
16.	*38	037993-76-3	37025	41	75	0	98	46	14	0	39	8911
17.	*38	016610-80-3	37019	36	84	1	99	46	14	0	39	8917
18.	*35	056666-55-8	37032	36	100	2	84	51	11	0	39	8911
19.	*35	019571-30-3	128792	33	77	2	99	51	11	0	41	8859
20.	*32	013041-79-7	37017	42	77	1	99	46	9	0	35	8906

STP Compounds

Peak 64; Unidentified Oxyhydrocarbon



Scan 1147 (22.906 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	145	63.90	51	81.95	2	98.05	61
43.00	553	65.90	56	82.95	55	100.00	113
44.90	421	67.95	105	84.00	132	100.95	959
46.80	21	69.80	212	85.00	82	101.95	96
52.05	40	71.05	42	85.90	48	102.95	807
52.95	61	71.95	28	86.95	167	103.95	177
54.95	135	73.00	119	87.95	31	105.90	59
56.90	920	75.05	66	89.00	32	107.00	24
57.90	434	75.80	108	91.00	99	107.95	10
58.90	2245	79.95	38	92.95	165	112.00	66
59.90	64	80.95	114	93.80	72	113.15	109

Scan 1147 (22.906 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.15	77	139.00	64	163.00	56		
118.95	56	139.90	45	165.10	17		
120.95	168	140.95	87	166.95	51		
122.05	12	141.95	92	171.30	41		
123.15	46	142.95	116	171.80	23		
127.00	4	143.95	39	173.05	20		
130.00	65	149.95	52	176.95	111		
133.90	49	151.00	11	179.00	24		
135.90	67	153.90	22	191.05	35		
136.15	67	157.90	75	200.05	31		
138.15	47	159.15	79	207.00	46		

STP Compounds

Scan 1147 (22.906 min): S0229.D

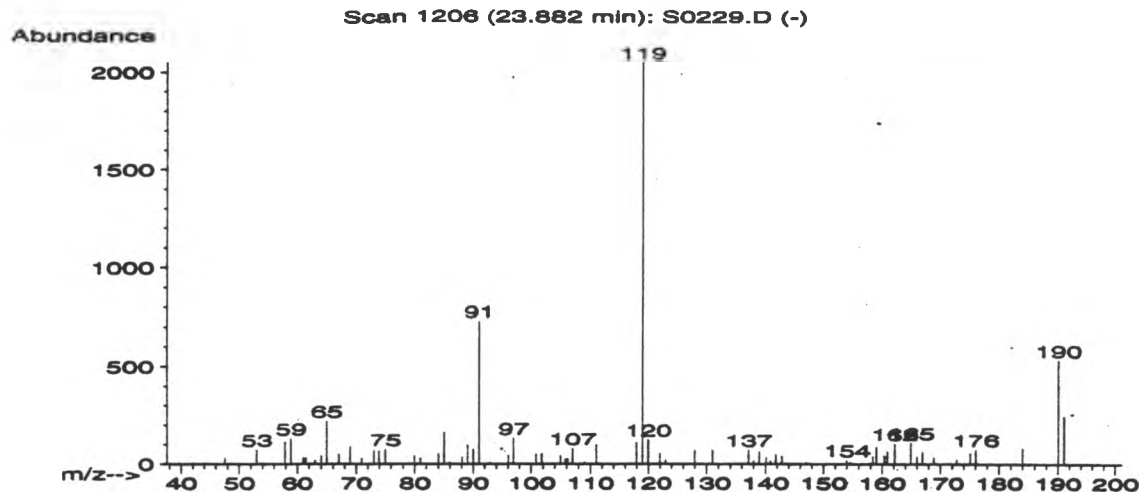
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid, 3-oxo-, 1,1-dimethylethyl	158	C8H14O3	47
2.	2-Propanol, 1-(2-methoxy-1-methylethoxy)	148	C7H16O3	43
3.	DIPROPYLENEGLYCOL METHYL ETHER	148	C7H16O3	43
4.	HEXAETHYLENGLYCOL, DIMETHYLETHER	310	C14H30O7	40
5.	Butanoic acid, 2-hydroxy-	104	C4H8O3	38
6.	2-Propanol, 1-[1-methyl-2-(2-propenyloxy	174	C9H18O3	37
7.	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	37
8.	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	37
9.	Butanoic acid, 4-iodo-, methyl ester	228	C5H9IO2	36
10.	2-Propanol, 1-(isooctyloxy)-2-methyl-	202	C12H26O2	35
11.	Butane, 1-ethoxy-	102	C6H14O	27
12.	Butane, 1-ethoxy-	102	C6H14O	27
13.	Propane, 1-ethoxy-2-methyl-	102	C6H14O	27
14.	Butane, 1-ethoxy-	102	C6H14O	27
15.	Butane, 1-ethoxy-	102	C6H14O	25
16.	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	25
17.	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	25
18.	Silane, hexyl-	116	C6H16Si	23
19.	2-Propanone, 1-cyclohexyl-	140	C9H16O	16
20.	Pentane, 2-methoxy-	102	C6H14O	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	001694-31-1	124667	33	71	2	103	40	20	0	39	9321
2.	43	020324-32-7	11907	47	41	1	72	45	18	9	38	9176
3.	43	012002-25-4	11908	47	41	1	72	45	18	9	38	9176
4.	40	000000-00-0	76911	47	80	3	82	34	16	6	37	9280
5.	*38	000565-70-8	1579	33	75	2	99	46	14	0	39	8736
6.	37	055956-25-7	22959	41	54	1	82	44	13	0	33	9215
7.	37	000143-24-8	129794	52	60	1	69	41	13	0	31	9138
8.	37	000143-24-8	129795	43	69	2	78	44	13	4	35	9047
9.	36	014273-85-9	47292	38	77	1	69	28	12	0	29	9374
10.	35	056282-27-0	35616	48	44	1	78	53	11	17	38	8640
11.	*27	000628-81-9	118353	36	53	0	67	57	8	0	41	8602
12.	*27	000628-81-9	1480	35	60	0	86	57	8	0	41	8579
13.	*27	000627-02-1	1481	36	55	0	82	57	8	0	41	8579
14.	*27	000628-81-9	118352	36	55	0	75	56	8	0	41	8601
15.	*25	000628-81-9	118354	30	56	0	70	54	7	0	33	8710
16.	25	000143-24-8	129793	38	71	1	68	44	7	0	29	9019
17.	25	000143-24-8	129792	40	69	1	75	41	7	0	29	9060
18.	23	001072-14-6	3573	38	51	2	73	49	6	0	29	8724
19.	*16	000103-78-6	9404	29	65	3	79	57	3	0	33	7920
20.	16	006795-88-6	1473	40	37	0	86	56	3	2	35	8633

STP Compounds

Peak 7; N,N-Diethyl-3-methyl benzamide



Scan 1206 (23.882 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.55	31	70.95	31	90.00	77	107.00	79
53.00	73	73.05	71	91.00	729	108.95	8
57.90	113	73.95	66	92.95	5	111.00	98
58.90	131	75.05	75	96.05	45	117.95	110
61.00	34	79.95	42	96.95	132	118.95	2050
61.40	32	81.00	31	98.00	1	119.95	124
63.00	20	84.00	53	100.85	52	121.95	54
64.00	42	85.00	164	101.80	53	123.00	20
64.95	222	85.95	9	104.95	44	127.95	69
67.00	52	88.05	35	105.75	26	131.00	69
68.95	89	89.00	98	106.15	27	137.10	71

Scan 1206 (23.882 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.95	17	159.00	87	184.00	82		
138.90	63	160.40	43	190.05	534		
140.15	33	160.90	65	191.05	246		
140.90	15	162.15	105				
141.80	48	164.95	109				
142.85	40	166.00	38				
147.00	7	166.95	61				
154.00	20	168.80	35				
154.60	8	172.80	24				
158.00	7	175.10	56				
158.40	39	176.05	75				

STP Compounds

Scan 1206 (23.882 min): S0229.D

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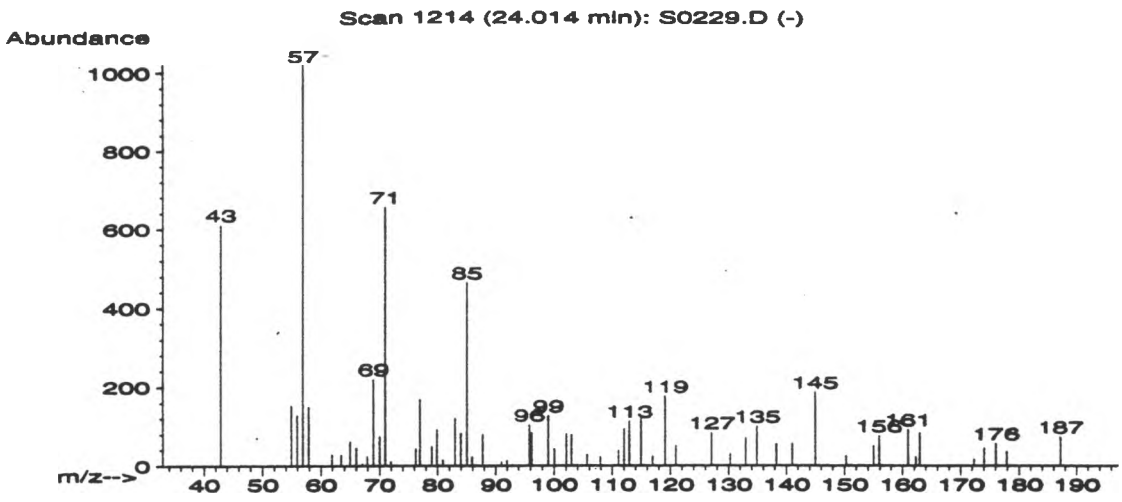
	Name	MolWt	Formula	Qual
1.	Benzamide, N,N-diethyl-3-methyl-	191	C12H17NO	64
2.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	43
3.	Benzene, isocyanato-	119	C7H5NO	43
4.	4-METHYL-1-PENTANOYLBENZENE	176	C12H16O	38
5.	4-Azabenzimidazole	119	C6H5N3	37
6.	ACETOPHENONE, DICHLORO-4'-METHYL-	202	C9H8Cl2O	37
7.	N-ISOPROPYL-P-TOLUAMIDE	177	C11H15NO	25
8.	p-Toluic acid, isobutyl ester	192	C12H16O2	25
9.	Butanedioyl dichloride	154	C4H4Cl2O2	25
10.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	25
11.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000134-62-3	30397	63	37	1	95	17	37	1	40	9809
2.	43	000099-75-2	123608	46	29	1	77	41	18	19	41	9561
3.	*43	000103-71-9	119902	33	67	0	67	41	18	0	41	9560
4.	*38	000000-00-0	23930	28	57	1	73	37	14	0	33	9568
5.	*37	000273-21-2	3958	31	57	2	67	41	13	0	33	9559
6.	37	000000-00-0	35303	38	60	1	67	41	13	0	33	9559
7.	25	002144-17-4	24290	36	59	2	99	41	7	0	20	9570
8.	25	029240-30-0	30808	37	52	1	91	41	7	1	23	9061
9.	25	000543-20-4	14156	33	69	1	99	41	7	0	22	9562
10.	*25	000140-76-1	119921	32	66	2	89	44	7	0	29	9558
11.	8	000099-75-2	123612	35	57	1	64	68	1	0	25	9558

STP Compounds

Peak 65; Alkane



Scan 1214 (24.014 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	611	68.95	219	85.00	464	102.05	81
54.95	152	70.00	75	85.90	22	102.95	78
55.95	128	70.95	655	87.00	2	105.65	28
56.90	1021	71.95	11	87.75	80	107.90	22
57.90	150	76.20	43	91.00	10	111.10	38
61.90	29	76.95	169	91.95	13	112.05	94
63.40	28	79.00	49	92.90	1	112.90	113
64.90	62	79.90	92	95.80	104	114.95	119
66.00	45	80.90	15	96.20	84	116.90	24
67.05	5	82.95	120	99.00	127	119.05	176
67.85	24	83.95	82	100.05	42	120.95	50

Scan 1214 (24.014 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	83	162.25	22				
130.25	30	162.90	84				
132.95	70	172.30	17				
134.90	100	174.05	45				
138.25	54	176.05	57				
141.00	56	177.90	36				
144.95	187	187.15	74				
150.30	25						
154.95	50						
155.90	77						
160.90	92						

STP Compounds

Scan 1214 (24.014 min): S0229.D

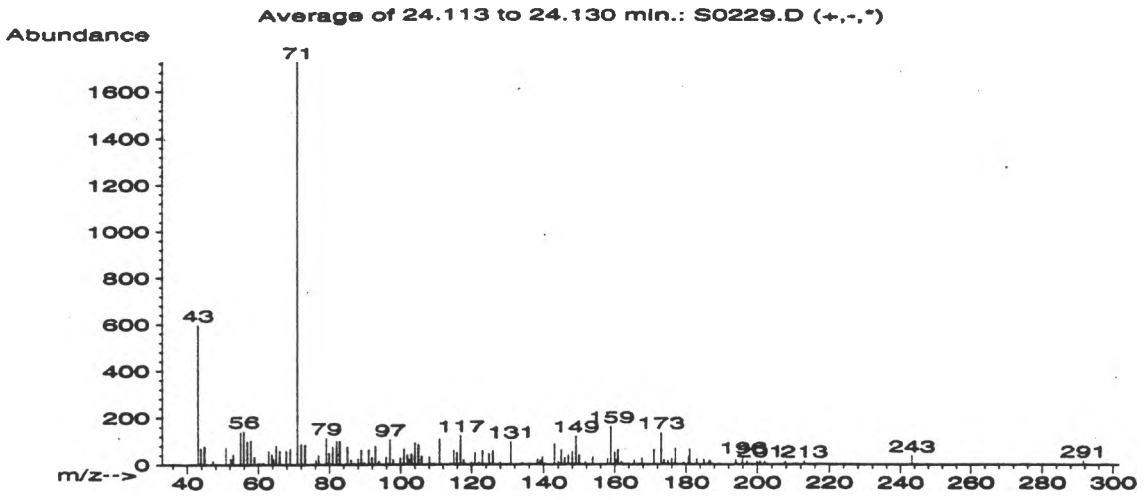
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Undecane	156	C11H24	64
2.	Tricosane	324	C23H48	52
3.	Eicosane, 10-methyl-	296	C21H44	52
4.	Nonacosane	408	C29H60	52
5.	Docosane	310	C22H46	52
6.	Heptacosane	380	C27H56	50
7.	Heptadecane	240	C17H36	50
8.	Octadecane	254	C18H38	50
9.	Hentriacontane	436	C31H64	50
10.	Nonadecane	268	C19H40	50
11.	Hexacosane	366	C26H54	50
12.	Tetracosane	338	C24H50	50
13.	Dodecane, 2-methyl-	184	C13H28	47
14.	Hexadecane	226	C16H34	47
15.	Nonadecane	268	C19H40	47
16.	Pentadecane	212	C15H32	47
17.	Dodecane, 2-methyl-6-propyl-	226	C16H34	47
18.	Decane, 2-methyl-	156	C11H24	43
19.	Decane, 2-methyl-	156	C11H24	43
20.	Hexatriacontane	507	C36H74	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	001120-21-4	124548	65	41	2	99	25	37	14	45	9309
2.	52	000638-67-5	134295	76	59	0	75	35	27	0	45	9329
3.	52	054833-23-7	72672	76	53	0	72	35	27	0	45	9325
4.	52	000630-03-5	99234	75	61	0	85	35	27	0	45	9328
5.	52	000629-97-0	133781	81	62	1	58	33	27	0	43	9356
6.	50	000593-49-7	135672	78	57	1	90	33	25	2	40	9239
7.	50	000629-78-7	130830	47	63	0	60	35	25	7	41	9297
8.	50	000593-45-3	131490	68	52	0	93	33	25	0	42	9358
9.	50	000630-04-6	103144	75	70	1	91	35	25	0	41	9312
10.	50	000629-92-5	132089	57	70	0	56	35	25	19	41	9337
11.	50	000630-01-3	91716	77	53	0	87	35	25	1	40	9322
12.	50	000646-31-1	134673	76	59	1	77	35	25	0	41	9318
13.	47	001560-97-0	127257	56	46	0	79	38	20	23	43	9295
14.	47	000544-76-3	130125	62	54	0	77	38	20	0	43	9310
15.	47	000629-92-5	132085	54	69	3	99	40	20	21	41	9197
16.	47	000629-62-9	129234	56	51	0	73	37	20	14	41	9329
17.	47	055045-08-4	46988	57	48	0	72	38	20	6	41	9322
18.	43	006975-98-0	124552	55	34	0	67	41	18	16	43	9207
19.	43	006975-98-0	124551	55	34	0	67	41	18	16	43	9207
20.	43	000630-06-8	136996	78	79	0	74	48	18	0	47	9315

STP Compounds

Peak 66; Unidentified Hydrocarbon



Average of 24.113 to 24.130 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	598	58.90	34	68.95	69	82.95	100
43.80	70	59.90	6	70.95	1727	85.00	75
44.85	78	60.50	5	72.00	87	86.05	19
47.20	15	60.85	4	73.05	84	86.95	5
50.95	73	61.35	8	74.85	1	88.00	24
52.20	26	62.95	56	76.05	18	88.95	61
52.95	44	63.85	43	76.95	39	89.85	8
55.00	137	64.15	23	79.05	112	91.00	61
55.90	141	65.00	81	79.95	49	91.95	31
56.95	97	66.00	58	80.95	76	92.95	80
57.95	101	67.80	59	82.00	100	93.95	13

Average of 24.113 to 24.130 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.95	32	108.10	32	124.85	44	145.95	29
97.00	106	111.05	110	125.95	57	146.95	41
97.95	20	114.00	5	127.95	8	147.90	2
99.90	29	115.00	60	130.95	96	148.05	55
100.95	66	115.95	50	134.00	6	149.00	119
101.95	39	116.95	122	138.25	23	149.90	39
102.45	20	117.80	17	139.00	16	151.70	9
103.00	44	119.90	9	139.70	32	153.75	32
104.05	92	120.95	49	143.00	87	158.00	24
105.00	84	122.00	9	144.10	11	158.95	160
105.90	34	123.05	59	144.95	62	160.05	49

Average of 24.113 to 24.130 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
160.40	17	176.85	6	194.05	20		
160.95	62	177.05	69	195.95	29		
161.95	11	179.10	5	197.20	14		
163.95	1	179.45	6	199.95	14		
165.45	17	180.75	32	200.80	14		
167.70	27	181.00	65	202.05	10		
171.05	63	183.00	22	207.75	12		
173.00	134	185.00	20	213.00	13		
173.85	20	186.50	15	243.20	37		
174.95	15	186.85	15	291.55	16		
175.95	25	189.15	2				

STP Compounds

Average of 24.113 to 24.130 min.: S0229.D
Converted from RTE data file: >S0229:

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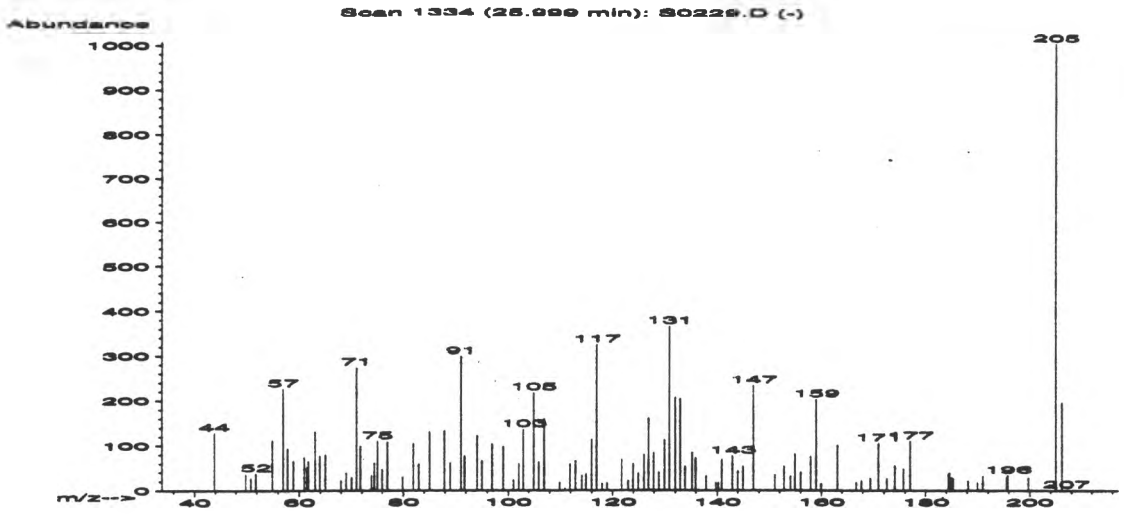
	Name	MolWt	Formula	Qual
1.	Propanoic acid, 2-methyl-, 1-(1,1-dimeth	286	C16H30O4	50
2.	Butyric acid, ester with m-hydroxybenzon	189	C11H11NO2	47
3.	ETHANE-1,1-DIOL DI-N-BUTANOATE	202	C10H18O4	47
4.	TRIMETHYL-2,4,4 HEXENE-1	126	C9H18	47
5.	Propanoic acid, 2-methyl-, 2-(hydroxymet	216	C12H24O3	47
6.	3-Methoxy-1,7-octadiene	140	C9H16O	47
7.	PENTAN-1,3-DIOLDIISOBUTYRATE, 2,2,4-TRIM	286	C16H30O4	40
8.	Morpholine, 3-methyl-2-phenyl-	177	C11H15NO	40
9.	Butanethioic acid, S-butyl ester	160	C8H16OS	40
10.	Decane, 3,3,5-trimethyl-	184	C13H28	38
11.	Pentane, 1,1'-oxybis-	158	C10H22O	38
12.	2-Hepten-3-ol, 4,5-dimethyl-	142	C9H18O	38
13.	Furan, 2-butyltetrahydro-	128	C8H16O	38
14.	Furan, 2-butyltetrahydro-	128	C8H16O	38
15.	PENTAN-1,3-DIOLDIISOBUTYRATE, 2,2,4-TRIM	286	C16H30O4	36
16.	Butanoic acid, 2,3-dihydroxypropyl ester	162	C7H14O4	33
17.	METHYL ESTER OF 5-METHOXY-3-PENTENOIC AC	144	C7H12O3	28
18.	Butane, 1-bromo-2-methyl-	150	C5H11Br	28
19.	Cyclohexane, 1-bromo-2-methoxy-, cis-	192	C7H13BrO	28
20.	Borane, diethyl[1-ethyl-2-(methoxymethyl	196	C12H25BO	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	50	074381-40-1	69174	44	63	1	81	32	25	0	39	9921
2.	47	029052-09-3	29572	44	41	2	82	36	20	12	41	9881
3.	47	025572-25-2	35434	46	43	0	97	36	20	12	41	9881
4.	*47	000000-00-0	5434	33	58	3	98	36	20	0	39	9881
5.	47	074367-32-1	41967	43	54	2	98	36	20	17	38	9881
6.	47	000000-00-0	9365	43	37	2	91	36	20	0	39	9881
7.	40	000000-00-0	69173	40	77	3	81	32	16	0	33	9917
8.	*40	000134-49-6	24274	39	51	3	84	32	16	1	36	9887
9.	*40	002432-52-2	16710	34	42	1	70	32	16	10	32	9835
10.	38	062338-13-0	27790	38	67	2	84	36	14	0	33	9881
11.	*38	000693-65-2	16274	33	59	2	86	36	14	0	35	9881
12.	38	055956-37-1	10200	38	40	1	72	36	14	0	33	9881
13.	38	001004-29-1	120895	35	31	0	99	36	14	5	30	9881
14.	38	001004-29-1	6012	35	31	0	99	36	14	5	30	9881
15.	36	000000-00-0	132866	35	11	1	99	28	12	0	25	9918
16.	33	000557-25-5	17475	35	50	2	88	34	10	0	25	9894
17.	*28	000000-00-0	10583	28	65	2	96	36	8	0	29	9881
18.	*28	010422-35-2	123533	29	66	2	89	36	8	0	27	9881
19.	28	051332-48-0	30537	38	67	2	99	36	8	0	29	9691
20.	28	053670-48-7	33059	35	59	1	89	36	8	0	25	9881

Peak 67; Unidentified Aromatic Amine

STP Compounds



Scan 1334 (25.999 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	129	61.75	65	75.05	110	94.05	123
49.90	36	63.00	132	75.95	47	95.00	66
50.90	27	63.90	76	77.00	108	96.95	104
51.80	38	64.95	80	79.90	30	97.90	1
54.95	112	68.00	22	81.95	105	99.05	98
55.95	1	69.00	39	83.00	59	101.00	23
56.95	226	70.05	29	85.00	131	102.05	60
57.75	93	70.95	274	87.90	134	102.95	137
58.90	66	71.70	99	89.00	62	104.90	219
60.90	74	73.85	33	91.05	299	105.90	64
61.40	52	74.45	61	91.75	77	106.95	160

Scan 1334 (25.999 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.95	18	123.00	21	133.95	54	151.05	34
110.95	5	123.95	60	135.25	85	152.80	54
111.90	59	124.95	38	135.90	73	154.00	32
112.95	66	126.05	80	137.90	32	154.90	82
114.15	33	126.95	161	139.75	18	156.00	41
115.00	36	127.95	84	140.25	18	157.90	76
116.00	114	128.90	40	140.90	69	159.00	204
116.95	325	130.00	114	142.95	77	159.90	15
118.00	15	130.90	367	144.00	43	163.15	101
118.95	16	132.00	208	144.95	54	166.70	18
121.80	68	133.00	205	146.95	235	167.70	22

Scan 1334 (25.999 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
169.45	28	189.95	18				
170.95	106	191.00	32				
172.55	27	195.55	31				
174.05	55	195.80	34				
175.70	48	199.70	29				
177.05	110	205.00	1008				
184.40	37	206.15	197				
184.65	39	207.05	1				
185.00	28						
185.25	27						
188.15	22						

STP Compounds

Scan 1334 (25.999 min): S0229.D

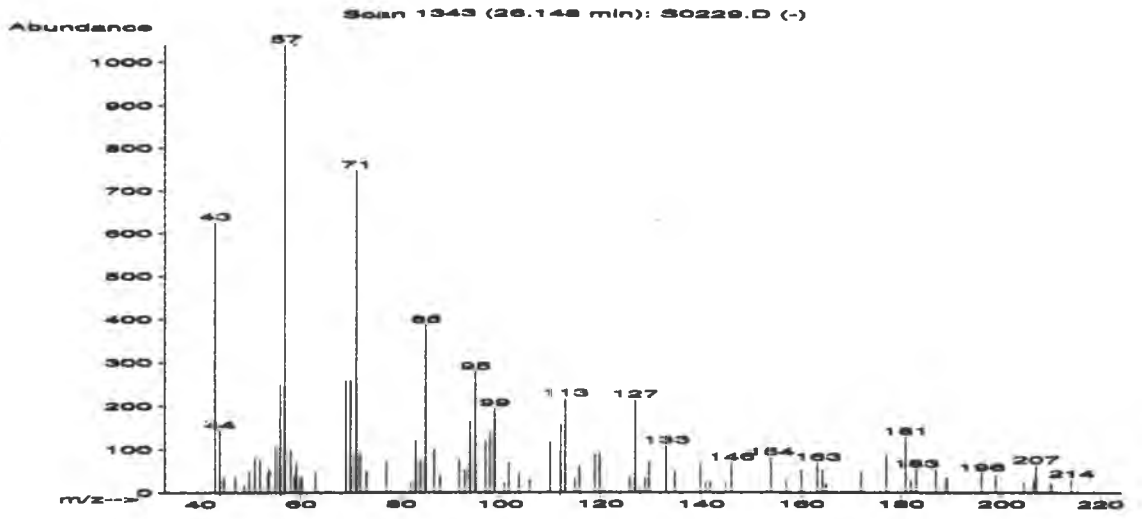
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	4-METHYL-1,2,3,4,5,6-HEXAHYDRO-1,5-METHA	205	C12H16NP	32
2.	7-PHENYLISOQUINOLINE	205	C15H11N	27
3.	5-PHENYLISOQUINOLINE	205	C15H11N	27
4.	Benzonitrile, 3-(2-phenylethenyl)-, (E)-	205	C15H11N	27
5.	2-Phenazinecarbonitrile	205	C13H7N3	27
6.	Benzonitrile, 4-(2-phenylethenyl)-	205	C15H11N	27
7.	2,5-Dimethyl-2-(2-hydroxyphenyl)-3,4-dih	205	C12H15NO2	23
8.	7-PHENYLISOQUINOLINE	205	C15H11N	16
9.	6-PHENYLISOQUINOLINE	205	C15H11N	16
10.	9-Phenanthrenecarbonitrile, 9,10-dihydro	205	C15H11N	16
11.	3-PHENYLISOQUINOLINE	205	C15H11N	16
12.	Benzonitrile, 4-(2-phenylethenyl)-, (E)-	205	C15H11N	16
13.	Phenol, 2,4-bis(1,1-dimethylpropyl)-	234	C16H26O	16
14.	Benzofuran, 2,4,5,6,7,7a-hexahydro-2,4,4	220	C15H24O	12
15.	N,O-PERMETHYL-N-ACETYLGLYCYL TYROSINAMID	349	C18H27N3O4	12
16.	Pyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione	205	C10H11N3O2	12
17.	Benzeneacetonitrile, .alpha.-(phenylmeth	205	C15H11N	9
18.	(E)-2-(Acetoxymethyl)-6-phenyl-4-(tromet	318	C18H26O3Si	7
19.	3-Cyclohexen-1-ol, 5-methylene-6-(1-meth	192	C12H16O2	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*32	052427-87-9	36975	35	82	1	99	48	9	10	35	8736
2.	*27	070125-65-4	128795	40	64	0	76	57	8	5	38	8417
3.	*27	024464-35-5	128793	36	72	1	82	57	8	17	40	8419
4.	*27	014064-35-8	37016	53	69	1	81	57	8	0	40	8417
5.	*27	006479-93-2	36977	43	82	3	92	57	8	0	40	8414
6.	*27	001552-58-5	37018	33	78	3	96	57	8	13	40	8416
7.	*23	086259-60-1	36944	32	35	1	99	48	6	0	29	8921
8.	*16	070125-65-4	37029	32	18	0	97	57	3	2	35	8417
9.	*16	070125-61-0	128794	33	76	2	99	57	3	1	36	8418
10.	*16	056666-55-8	37032	39	97	2	98	57	3	0	35	8413
11.	*16	037993-76-3	37025	41	60	1	87	57	3	4	34	8419
12.	*16	013041-79-7	37017	28	78	2	99	57	3	2	32	8418
13.	16	000120-95-6	130565	38	30	0	85	57	3	0	33	8415
14.	12	069296-94-2	43975	36	91	1	90	57	2	0	21	8417
15.	12	060008-47-1	87776	33	106	0	99	57	2	0	25	8420
16.	*12	016953-81-4	36892	30	81	1	99	57	2	0	29	8408
17.	9	016610-80-3	37019	40	78	0	60	78	1	0	33	8416
18.	7	084681-31-2	79531	34	82	2	58	74	1	0	22	9086
19.	6	054832-23-4	30834	34	66	1	42	79	1	0	18	3792

STP Compounds

Peak 68; Alkane



Scan 1343 (26.148 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	625	55.95	249	71.05	748	91.75	79
43.95	143	56.90	1039	71.80	89	92.95	53
44.80	32	58.00	99	73.05	48	93.95	164
46.95	35	58.80	39	77.00	72	95.05	278
48.80	18	59.15	68	77.95	3	97.05	120
49.80	48	59.90	32	81.95	22	97.95	141
50.90	80	60.15	33	82.95	120	98.95	194
51.95	77	62.95	48	83.95	75	100.90	21
53.45	43	65.10	5	85.00	386	101.80	68
53.70	55	68.95	258	86.75	100	103.80	43
55.00	106	69.95	259	87.90	41	105.95	29

Scan 1343 (26.148 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	117	129.75	71	157.00	30	187.00	53
112.15	157	133.15	108	160.00	53	189.00	34
113.00	216	134.90	48	163.25	69	189.25	33
115.00	32	139.90	67	164.25	51	196.05	46
115.90	62	140.95	20	165.00	19	198.95	39
119.00	88	141.85	25	171.00	3	204.50	22
119.95	92	144.90	21	172.05	47	206.40	30
125.95	36	146.05	69	177.05	88	206.90	63
127.05	213	153.05	6	180.90	129	209.75	21
128.00	11	153.90	81	181.95	28	210.00	19
129.00	33	155.00	1	183.00	54	214.05	30

STP Compounds

Scan 1343 (26.148 min): S0229.D

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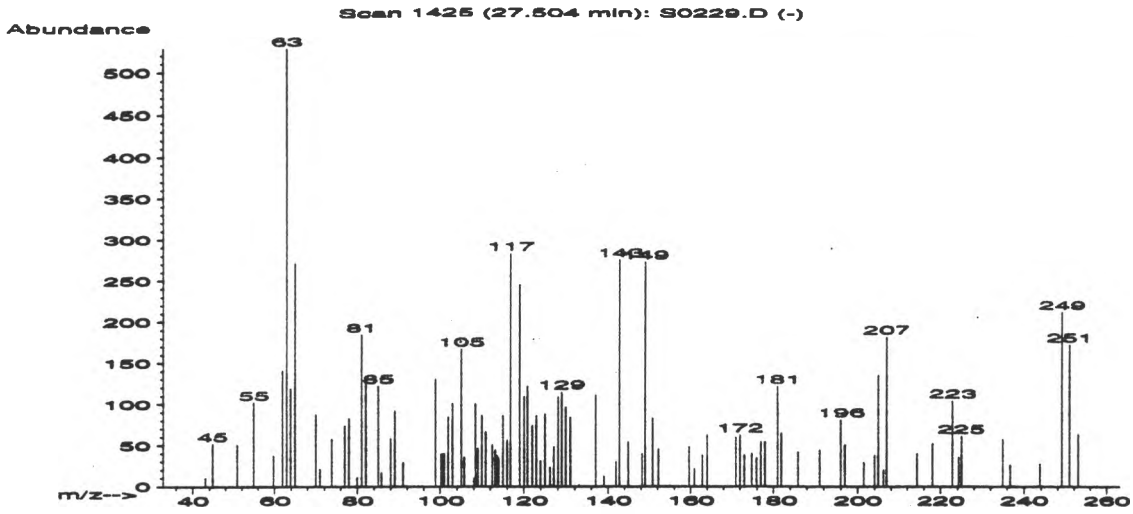
	Name	MolWt	Formula	Qual
1.	3-Octen-2-ol, 2-methyl-, (Z)-	142	C9H18O	43
2.	Decane, 5-ethyl-5-methyl-	184	C13H28	43
3.	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	43
4.	Decane, 2-methyl-	156	C11H24	38
5.	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	35
6.	Tridecane	184	C13H28	35
7.	Octane, 2,6-dimethyl-	142	C10H22	30
8.	Nonane, 3-methyl-	142	C10H22	30
9.	Undecane, 3,5-dimethyl-	184	C13H28	27
10.	DECANE, 2,3,5,8-TETRAMETHYL-	198	C14H30	27
11.	Hexacosane	366	C26H54	27
12.	Dodecane, 2,5-dimethyl-	198	C14H30	27
13.	Nonane, 3-methyl-	142	C10H22	27
14.	Ether, hexyl pentyl	172	C11H24O	22
15.	2-N-HEXYL-1-D1-AZIRIDINE	127	C8H16DN	18
16.	Propanal, 2-propenylhydrazone	112	C6H12N2	14
17.	Decane, 2,6,7-trimethyl-	184	C13H28	14
18.	METHYL ESTER OF SUCCINYLACETONE	172	C8H12O4	11
19.	1,2-Cyclohexanediol, 1-methyl-, trans-	130	C7H14O2	11
20.	Morpholine, 3-methyl-2-phenyl-	177	C11H15NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	018521-07-8	10197	44	60	1	64	45	18	0	40	9237
2.	43	017312-74-2	27768	45	70	1	88	41	18	0	39	9315
3.	43	001921-70-6	132092	79	48	0	73	45	18	10	41	9158
4.	38	006975-98-0	124554	54	46	1	87	48	14	11	40	9088
5.	35	000638-36-8	67906	60	72	1	78	51	11	0	39	9258
6.	35	000629-50-5	127253	47	60	0	62	54	11	4	41	9018
7.	*30	002051-30-1	122741	37	56	0	79	58	9	14	43	8560
8.	*30	005911-04-6	122734	52	42	1	99	58	9	0	46	8458
9.	27	017312-81-1	27752	51	53	0	73	56	8	10	41	8951
10.	27	000000-00-0	34143	53	61	0	67	58	8	15	40	8951
11.	27	000630-01-3	135387	58	79	0	80	58	8	8	39	8933
12.	27	056292-65-0	34140	47	63	2	81	56	8	10	41	9103
13.	*27	005911-04-6	10243	56	37	0	84	58	8	11	40	8408
14.	22	032357-83-8	22420	38	58	0	61	61	5	15	43	8812
15.	*18	030691-57-7	5635	49	61	1	65	67	3	0	44	8618
16.	*14	019031-78-8	2504	34	60	0	55	70	2	0	41	8141
17.	14	062108-25-2	27786	47	51	0	99	67	2	0	39	8595
18.	*11	000000-00-0	126115	48	55	2	75	80	2	0	44	4290
19.	*11	019534-08-8	6491	53	53	1	57	74	2	0	49	7832
20.	*10	000134-49-6	24274	33	61	0	61	74	1	0	41	7832

STP Compounds

Peak 69; 2-Chloroethyl phosphate



Scan 1425 (27.504 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	11	73.80	57	98.85	130	109.90	86
44.80	52	76.95	74	100.20	39	110.90	66
50.85	51	77.95	83	100.55	40	112.40	51
54.95	102	79.90	11	100.95	40	113.15	44
59.75	37	81.00	184	101.95	85	113.50	37
61.90	141	82.00	130	102.95	101	113.90	34
62.90	528	85.00	122	105.00	167	115.00	86
63.90	119	85.80	17	105.75	35	116.00	56
64.95	271	88.00	58	108.00	10	116.80	283
69.90	87	89.00	92	108.40	100	118.95	245
70.95	21	91.00	29	109.00	46	120.05	110

Scan 1425 (27.504 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.95	122	133.00	2	159.65	48	181.00	121
122.00	74	137.00	111	160.95	21	181.90	64
122.95	86	139.00	12	162.90	38	185.90	42
123.95	31	141.95	30	164.00	62	191.00	44
125.00	88	142.80	275	170.95	60	196.05	81
126.20	23	144.95	54	171.95	62	196.95	50
127.05	48	148.20	40	173.00	38	201.45	29
128.05	109	149.00	272	174.80	40	204.00	38
128.90	115	150.80	83	175.95	34	204.90	135
129.90	96	152.20	45	176.95	54	206.15	20
130.95	84	154.90	1	178.00	54	206.90	181

Scan 1425 (27.504 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
214.30	40						
218.05	52						
222.80	104						
224.30	35						
224.95	61						
234.90	57						
236.75	26						
243.70	27						
249.05	212						
250.90	172						
253.00	63						

STP Compounds

Scan 1425 (27.504 min): S0229.D

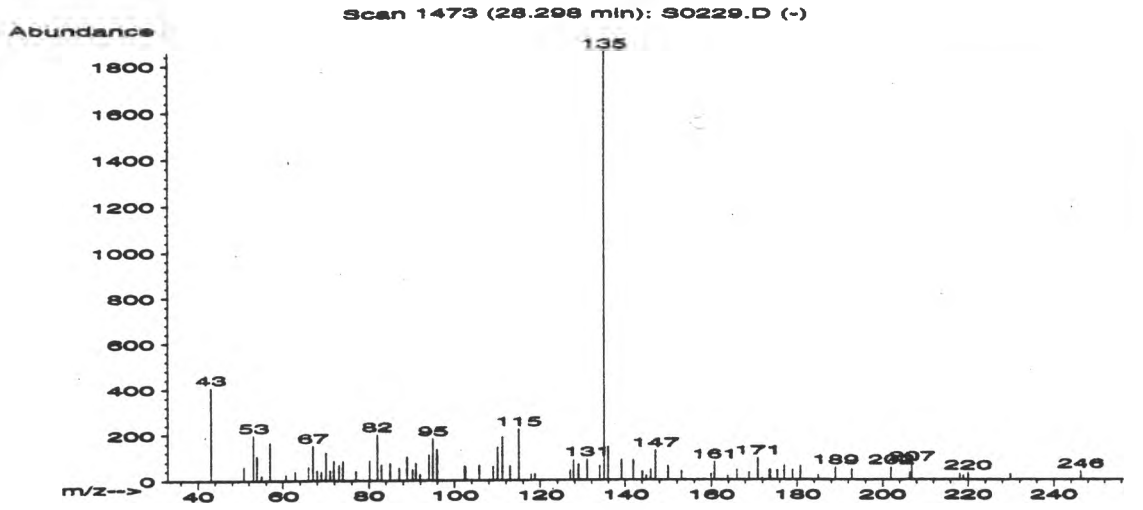
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-chloro-, phosphate (3:1)	284	C6H12Cl3O4P	50
2.	Benzo[b]thiophene, 2-ethyl-5,7-dimethyl-	190	C12H14S	42
3.	Ethanol, 2-chloro-, phosphite (3:1)	268	C6H12Cl3O3P	40
4.	Phenol, 2,3-dichloro-	162	C6H4Cl2O	32
5.	Ethane, 1-(2-chloroethoxy)-2-(o-tolyloxy	214	C11H15ClO2	28
6.	Benzene, [2-(2-chloroethoxy)ethoxy]-	200	C10H13ClO2	28
7.	1,1,3-TRI(2-CHLOROETHOXY)PROPANE	278	C9H17Cl3O3	28
8.	1,3-Dioxonane, 5,5,6,6,7,7,8,8-octafluor	274	C7H6F8O2	27
9.	Propane, 1,2-dichloro-	112	C3H6Cl2	27
10.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	23
11.	Benzene, 1-chloro-2-methoxy-3-nitro-	187	C7H6ClNO3	20
12.	Benzene, 1-azido-4-nitro-	164	C6H4N4O2	14
13.	Propane, 1,2-dichloro-	112	C3H6Cl2	12
14.	3-Butyl-2-(3-butenyl)-cyclohex-2-en-1-on	206	C14H22O	10
15.	1,1-Dimethyl-3,4-methano-3,4-dihydronaph	186	C13H14O	9
16.	Pyrrolidine, 1-(1-cyclohexen-1-yl)-	151	C10H17N	9
17.	Benzeneacetic acid, .alpha.-bromo-, meth	228	C9H9BrO2	8
18.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	7
19.	Benzoic acid, 4-[(dichloroamino)sulfonyl	269	C7H5Cl2NO4S	7
20.	Benzene, 1-methyl-2-nitro-	137	C7H7NO2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	50	000115-96-8	132728	72	92	0	77	35	25	0	42	8314
2.	42	018428-05-2	127617	49	86	2	78	29	17	13	33	7079
3.	40	000140-08-9	62438	48	105	1	99	32	16	0	31	7175
4.	32	000576-24-9	125027	46	92	1	99	49	9	0	35	6353
5.	28	021120-80-9	41102	35	108	3	99	39	8	0	22	6878
6.	28	002243-44-9	34553	33	110	2	78	39	8	0	22	6888
7.	28	000000-00-0	66144	33	126	2	82	36	8	0	21	7344
8.	27	036301-47-0	64725	46	89	0	71	59	8	16	41	6139
9.	*27	000078-87-5	118943	43	75	1	91	56	8	0	39	6549
10.	23	000120-83-2	125030	34	101	3	145	49	6	0	22	6354
11.	20	080866-77-9	28699	38	124	2	91	49	4	0	14	6354
12.	*14	001516-60-5	18179	35	88	0	48	69	2	0	41	6302
13.	*12	000078-87-5	2400	38	78	1	87	56	2	0	29	6501
14.	*10	078601-41-9	37595	33	43	0	36	73	1	0	41	3162
15.	* 9	061463-22-7	28597	29	23	0	42	73	1	2	35	3197
16.	* 9	001125-99-1	123815	29	59	1	39	73	1	0	33	4344
17.	8	003042-81-7	47370	35	117	3	229	69	1	0	21	4809
18.	7	000084-66-2	129815	36	89	3	279	79	1	0	22	3542
19.	7	000080-13-7	63016	37	105	1	35	79	1	0	22	3155
20.	7	000088-72-2	122123	33	72	1	51	78	1	0	25	4623

STP Compounds

Peak 70; Nonylphenol Phenol isomer



Scan 1473 (28.298 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	408	68.00	43	85.00	75	102.55	58
50.80	61	69.00	39	87.10	55	103.00	2
53.05	197	70.05	122	88.90	103	103.95	2
53.95	106	71.00	45	90.25	47	105.75	67
54.95	22	71.80	87	91.00	76	108.95	61
56.95	166	73.05	68	91.95	26	110.00	144
60.75	27	73.95	86	94.05	112	111.15	190
62.80	39	76.95	40	95.00	184	113.00	63
65.00	2	80.15	88	95.95	136	115.00	224
65.95	62	82.00	201	97.05	1	117.95	27
67.00	152	82.95	70	102.30	63	118.90	29

Scan 1473 (28.298 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	45	146.05	48	173.55	44	206.90	69
127.80	88	147.05	130	173.80	45	218.05	28
128.90	70	149.95	61	175.45	42	218.95	18
131.00	91	153.05	40	177.00	63	219.95	31
133.95	64	159.90	27	178.95	45	229.90	24
135.00	1858	160.75	79	180.75	60	246.30	37
135.95	145	163.90	18	185.00	20		
139.15	89	166.05	44	189.00	54		
141.95	88	168.95	33	192.80	47		
144.05	38	170.95	95	202.00	54		
144.95	20	171.95	7	206.40	31		

STP Compounds

Scan 1473 (28.298 min): S0229.D

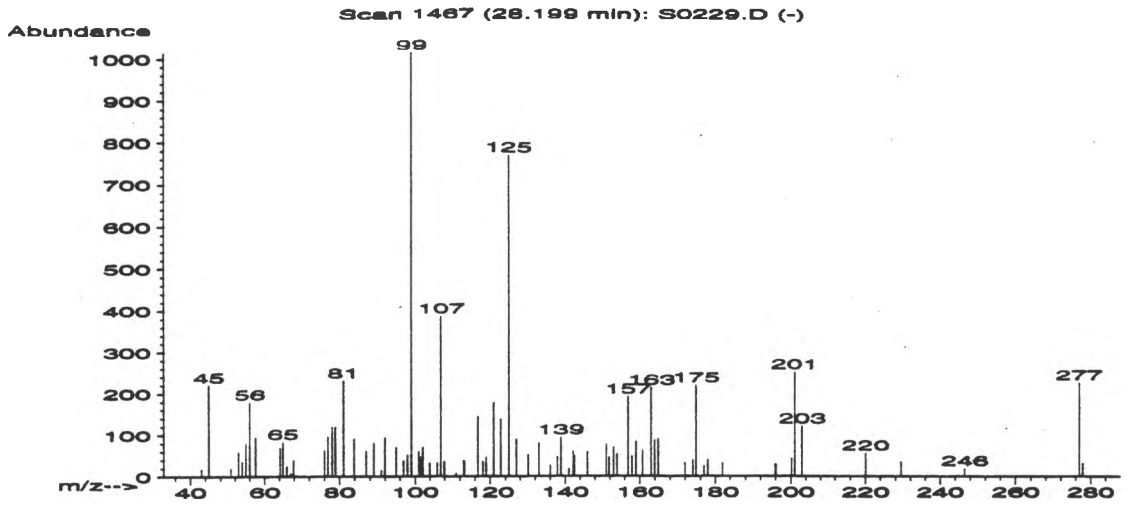
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	OCTYL PHENOL ISOMER	206	C14H22O	50
2.	Adenine	135	C5H5N5	49
3.	Adenine	135	C5H5N5	49
4.	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	47
5.	1H-Indole, 5-fluoro-	135	C8H6FN	47
6.	Adenine	135	C5H5N5	47
7.	Adenine	135	C5H5N5	47
8.	Bicyclo[2.2.1]hept-2-en-7-ol, 7-(4-metho	216	C14H16O2	38
9.	anti-7-Hydroxy-7-anisylnorbornene	216	C14H16O2	38
10.	Pyridine, 4-ethyl-2,6-dimethyl-	135	C9H13N	38
11.	Adenine	135	C5H5N5	38
12.	2-Aziridinone, 1-(1-adamantyl)-3-(1-meth	273	C18H27NO	36
13.	Phenol, 4-(2,2,3,3-tetramethylbutyl)-	206	C14H22O	33
14.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	33
15.	L-Threonine, N-[(1H-purin-6-ylamino)carb	280	C10H12N6O4	28
16.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	28
17.	1,2-Benzisothiazole	135	C7H5NS	28
18.	1,2-Benzisothiazole	135	C7H5NS	28
19.	Benzothiazole	135	C7H5NS	28
20.	Benzothiazole	135	C7H5NS	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	000000-00-0	37565	35	48	1	83	32	25	0	39	9899
2.	*49	000073-24-5	121686	35	31	0	70	36	23	4	43	9866
3.	*49	000073-24-5	7506	52	41	2	87	36	23	0	46	9866
4.	*47	002380-63-4	7511	33	48	1	94	36	20	0	39	9866
5.	*47	000399-52-0	7540	36	55	1	81	36	20	0	39	9866
6.	*47	000073-24-5	121690	37	51	2	92	36	20	0	41	9866
7.	*47	000073-24-5	121689	47	43	1	70	36	20	0	39	9866
8.	38	013143-81-2	129470	47	64	1	83	36	14	0	35	9866
9.	38	000000-00-0	42086	47	61	1	84	36	14	0	37	9866
10.	*38	036917-36-9	7611	33	70	2	74	36	14	0	35	9866
11.	*38	000073-24-5	121687	34	61	2	72	36	14	0	30	9866
12.	36	026905-18-0	64696	34	99	3	74	28	12	0	21	9774
13.	33	054932-78-4	37578	38	50	1	74	34	10	0	29	9894
14.	33	000140-66-9	37577	38	50	1	77	34	10	0	29	9894
15.	28	033422-66-1	66805	39	105	1	68	36	8	0	24	9842
16.	*28	015816-45-2	7331	29	55	2	74	36	8	0	27	9866
17.	*28	000272-16-2	121700	30	59	2	86	36	8	0	29	9866
18.	*28	000272-16-2	7531	30	61	2	84	36	8	0	29	9866
19.	*28	000095-16-9	121698	28	71	2	81	36	8	0	29	9866
20.	*28	000095-16-9	121695	31	31	2	71	36	8	0	29	9866

STP Compounds

Peak 71; Unidentified



Scan 1467 (28.199 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	19	67.00	8	91.90	95	105.95	33
44.95	220	67.80	40	92.95	1	106.95	387
50.90	20	76.05	63	94.95	70	107.90	37
52.95	58	76.95	96	96.95	38	111.00	8
53.95	36	78.05	120	97.95	52	113.00	39
54.95	79	78.95	119	98.95	1014	113.25	36
56.00	179	81.00	231	100.95	61	116.75	145
57.65	94	83.75	91	101.30	47	118.05	36
64.15	69	86.95	61	101.75	19	118.95	46
64.95	83	89.00	81	102.05	71	120.95	179
66.00	24	91.00	15	103.95	32	122.80	139

Scan 1467 (28.199 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.95	769	150.95	77	171.95	32	220.05	56
126.95	90	151.80	46	174.05	40	229.50	35
130.15	52	152.95	71	174.95	220	246.55	19
133.00	81	153.90	54	177.00	24	276.90	227
136.00	27	156.90	192	178.00	40	277.90	31
137.90	47	157.90	48	181.90	33		
138.85	94	158.90	84	195.80	29		
140.95	19	160.75	63	196.05	28		
142.05	60	163.00	214	200.20	43		
142.45	50	163.90	88	201.05	252		
145.95	59	164.90	91	203.00	121		

STP Compounds

Scan 1467 (28.199 min): S0229.D

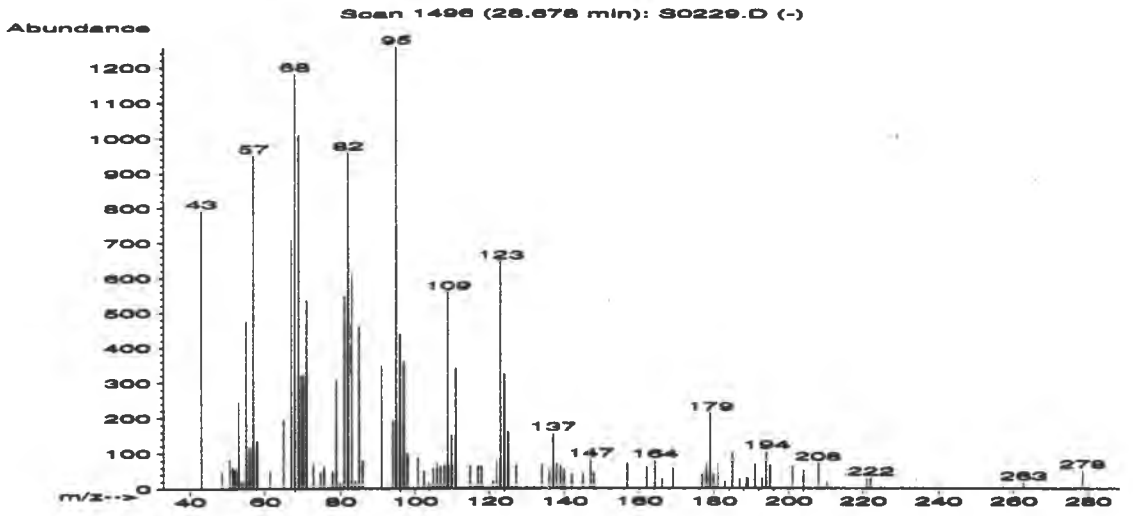
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,3,4,5-TETRAMETHYLCYCLOPENT-2-EN-1-OL	140	C9H16O	12
2.	2,4-Dodecadienoic acid, 11-hydroxy-3,7,1	268	C16H28O3	10
3.	2(1H)-Pyridinethione, 1-methyl-	125	C6H7NS	10
4.	2(1H)-Pyridinethione, 3-methyl-	125	C6H7NS	9
5.	M-TRIDEUTERIOMETHYLANISOLE	122	C8H7D3O	9
6.	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	9
7.	4,5-Isoxazoledione, 3-methyl-, 4-[(3-chl	237	C10H8ClN3O2	8
8.	Silane, dichloroethenylethyl-	154	C4H8Cl2Si	8
9.	2,4-Dimethyl-6-butylphenol	178	C12H18O	7
10.	3-Hexyl-4-methyl-1H-pyrrole-2,5-dione	195	C11H17NO2	7
11.	Pyridine, 2-[(tert-butylthio)methyl]-	181	C10H15NS	7
12.	Benzene, 1-chloro-4-ethyl-	140	C8H9Cl	7
13.	Benzene, 1-chloro-3-ethyl-	140	C8H9Cl	7
14.	Benzene, 1-chloro-2-ethyl-	140	C8H9Cl	7
15.	Benzene, 1-chloro-2-ethyl-	140	C8H9Cl	7
16.	Pyridinium, 3-mercapto-1-methyl-, hydrox	125	C6H7NS	7
17.	2,4,6-Pyrimidinetriamine	125	C4H7N5	7
18.	2,4,6-Pyrimidinetriamine	125	C4H7N5	7
19.	P-TRIDEUTERIOMETHYLANISOLE	122	C8H7D3O	7
20.	2-Butenoic acid, 2-(hydroxymethyl)-, 1a,	376	C20H24O7	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	12	082061-20-9	9432	30	69	2	67	60	2	1	22	6085
2.	10	069687-75-8	62805	38	122	1	75	61	1	0	29	6131
3.*	10	002044-27-1	4966	35	51	0	75	73	1	0	39	5438
4.*	9	018368-66-6	4968	31	61	1	57	73	1	2	35	5438
5.*	9	020369-34-0	4417	26	52	1	54	73	1	6	35	5438
6.*	9	000872-50-4	117840	28	71	0	89	73	1	0	33	7170
7.	8	005707-73-3	51092	35	105	2	67	68	1	0	22	6754
8.	8	010138-21-3	14169	35	70	1	58	70	1	0	21	7015
9.	7	000000-00-0	24812	38	43	1	37	80	1	0	29	3102
10.	7	077586-81-3	32363	39	74	2	75	73	1	0	29	5442
11.	7	018794-45-1	26108	33	64	0	75	73	1	0	25	5438
12.	7	000622-98-0	9148	33	60	1	53	72	1	1	23	5699
13.	7	000620-16-6	9147	36	71	3	64	73	1	0	22	5438
14.	7	000089-96-3	122429	39	60	2	51	73	1	0	29	5438
15.	7	000089-96-3	9146	33	68	3	64	72	1	0	22	5685
16.*	7	036880-58-7	4972	31	65	1	75	73	1	0	29	5438
17.*	7	001004-38-2	120447	32	56	1	52	73	1	0	29	5438
18.*	7	001004-38-2	4940	28	60	2	75	73	1	0	29	5438
19.*	7	014202-49-4	4420	28	49	1	60	73	1	0	29	5438
20.	7	049776-54-7	93609	33	110	1	99	71	1	0	21	7205

STP Compounds

Peak 72; Neophytadien



Scan 1496 (28.678 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	792	57.90	134	76.95	6	93.95	193
48.45	46	61.40	49	78.00	49	94.95	1256
50.55	84	65.00	196	78.95	309	95.95	440
51.30	61	67.00	708	79.95	15	96.95	360
51.55	51	67.95	1183	81.00	549	97.95	99
52.05	54	68.95	1010	82.00	959	100.80	86
52.95	244	69.95	321	83.00	609	102.45	49
53.95	19	71.05	536	83.90	21	103.85	16
54.95	477	72.90	70	85.00	461	104.95	57
55.90	116	74.80	46	85.90	79	106.00	70
56.90	951	75.70	61	91.00	349	106.90	62

Scan 1496 (28.678 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	67	122.95	647	138.00	71	168.95	59
108.90	560	123.95	325	139.00	63	176.85	39
110.00	152	124.95	162	140.00	52	177.90	67
111.05	343	126.00	10	141.95	40	179.00	212
114.90	64	127.05	66	144.95	43	179.90	38
116.15	12	129.90	10	147.05	82	181.00	70
116.95	64	131.00	2	147.95	43	182.90	20
117.95	63	131.95	5	156.90	72	184.90	102
118.90	2	134.00	68	162.00	61	186.95	27
120.95	23	135.90	51	164.15	79	188.75	31
121.95	81	137.00	156	166.05	27	189.15	28

Scan 1496 (28.678 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.05	69	278.40	50				
193.00	29						
194.05	104						
195.05	67						
201.05	65						
204.00	51						
207.90	72						
210.15	17						
221.05	29						
222.05	29						
262.65	16						

STP Compounds

Scan 1496 (28.678 min): S0229.D

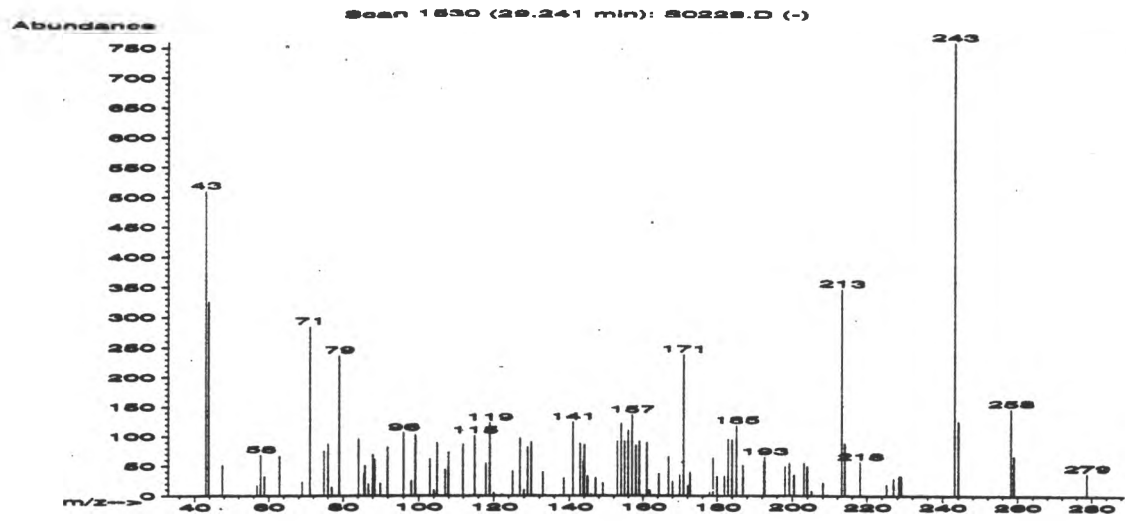
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	NEOPHYTADIENE	278	C20H38	96
2.	NEOPHYTADIENE	278	C20H38	68
3.	Cyclopentane, 1,1'-(1,4-butandiyl)bis-	194	C14H26	47
4.	(+)-2-ENDO,3-ENDO-DIMETHYLBORNANE	166	C12H22	45
5.	3-Eicosyne	278	C20H38	43
6.	1H-Purine-2,6-dione, 7-(2,3-dihydroxypro	254	C10H14N4O4	38
7.	CIS-TETRAHYDROIONONE	196	C13H24O	35
8.	6-Nonen-1-ol, (E)-	142	C9H18O	35
9.	Cyclopropane, 1,1-dimethyl-2-(1-methylet	152	C11H20	35
10.	(4R,5R,9S)-5,9-DIMETHYLSPIRO(3.5)NONAN-1	166	C11H18O	27
11.	Cycloheptane, 1-methyl-4-methylene-	124	C9H16	27
12.	4,8,8-TRIMETHYL-4-ACETYLCYCLOOCTANONE	210	C13H22O2	22
13.	Octadecanal	268	C18H36O	22
14.	3-Nonyne	124	C9H16	22
15.	Naphthalene, 2-(1,1-dimethylethyl)decahy	208	C15H28	18
16.	5-Tetradecen-1-ol, acetate, (Z)-	254	C16H30O2	14
17.	Tridecanal	198	C13H26O	14
18.	Pentadecanal	226	C15H30O	14
19.	1,3-DIMETHYL-6-OXABICYCLO(3.1.0)HEX-3-EN	124	C7H8O2	14
20.	2,4-DIMETHYLCYCLOPENT-4-ENE-1,3-DIONE	124	C7H8O2	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000000-00-0	66586	113	56	0	72	31	76	12	96	8978
2.	68	000000-00-0	132569	104	66	1	94	22	40	0	55	8973
3.	47	002980-70-3	32148	45	71	0	107	40	20	0	39	8371
4.	*45	059599-26-7	19764	71	47	2	99	50	19	0	53	8138
5.	*43	061886-66-6	132567	62	106	2	91	41	18	0	39	8357
6.	38	000479-18-5	57870	55	84	3	99	50	14	6	41	7758
7.	35	060761-23-1	33117	56	20	0	76	54	11	15	40	7195
8.	*35	031502-19-9	10191	53	48	0	75	54	11	1	40	8195
9.	35	056701-50-9	13866	43	64	0	62	55	11	12	41	7385
10.	*27	000000-00-0	19624	38	69	0	46	60	8	5	39	8609
11.	*27	023799-25-9	4920	49	55	0	77	59	8	16	41	6425
12.	*22	058643-96-2	39530	44	101	3	145	62	5	0	40	6395
13.	22	000638-66-4	132074	53	107	0	55	64	5	9	40	7538
14.	*22	020184-89-8	120431	34	69	1	71	65	5	16	40	7868
15.	*18	054934-96-2	38791	57	78	3	99	69	3	0	47	6682
16.	14	035153-13-0	131475	46	28	0	63	70	2	0	39	7633
17.	14	010486-19-8	34068	46	94	0	75	68	2	0	39	7617
18.	14	000000-00-0	130116	56	18	0	75	70	2	1	40	5992
19.	*14	000000-00-0	4719	34	56	1	66	70	2	18	40	5832
20.	*14	000000-00-0	4691	34	66	1	64	68	2	18	40	6420

STP Compounds

Peak 73; Unidentified hydrocarbon



Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	510	77.00	15	98.05	26	120.05	5
43.80	326	78.95	236	99.05	103	122.25	2
47.45	52	84.15	96	102.95	62	125.00	42
56.90	17	85.65	38	104.00	9	126.95	98
57.90	69	85.90	51	104.90	90	127.95	10
58.90	33	86.90	20	107.00	45	128.95	83
62.90	67	88.00	70	107.90	74	129.90	91
68.95	24	88.40	61	111.90	88	133.00	40
71.05	284	90.00	21	114.95	102	138.50	30
74.80	76	91.90	83	117.95	55	140.95	125
75.95	88	96.05	107	118.95	124	142.95	89

Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.80	58	158.00	86	177.90	6	199.20	55
144.05	87	159.00	92	178.90	65	200.45	35
144.95	33	161.00	90	180.00	33	203.00	55
145.85	3	161.85	9	181.90	34	203.90	49
147.05	30	164.25	37	182.90	96	205.00	7
149.00	21	166.80	66	184.00	95	208.00	22
153.00	93	167.95	24	185.15	119	213.15	348
154.00	123	169.95	35	186.90	52	214.00	89
154.95	93	170.95	239	192.45	58	218.20	57
155.90	111	172.15	17	192.70	66	225.20	19
157.00	137	172.70	40	198.05	49	227.00	29

Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
228.50	34						
229.00	33						
243.05	760						
244.10	126						
258.15	148						
258.90	67						
278.65	38						

STP Compounds

Scan 1530 (29.241 min): S0229.D

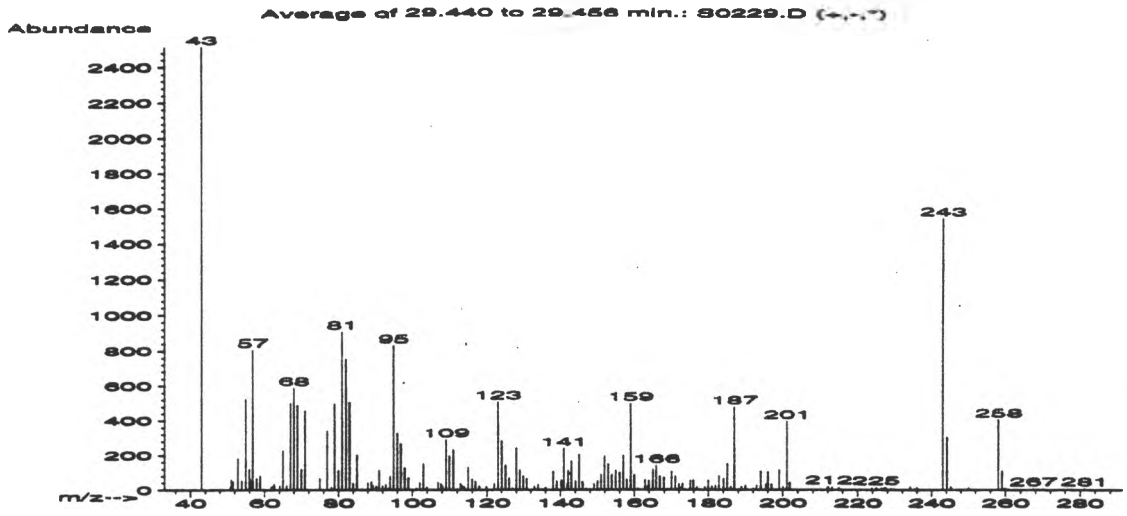
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3,4,6,7,8-HEXAHYDRO-4,6,6,7,8,8-HEXAME	258	C18H26O	83
2.	7-AC-6-ET-1144-ME4-TETRALIN	258	C18H26O	46
3.	6,7,9-Trimethyl-4-azaphenoxathiin	243	C14H13NOS	35
4.	2-Pteridinamine, N,N-dimethyl-4-(trifluo	243	C9H8F3N5	32
5.	BRAVELIN	258	C15H14O4	32
6.	2-AMINOBENZO(C)PHENANTHRENE	243	C18H13N	27
7.	2-METHYL-7-PHENYL-5H-1,3,4-THIADIAZOLO[3	243	C12H9N3OS	25
8.	Acetamide, N-(4-phenylbicyclo[2.2.2]oct-	243	C16H21NO	25
9.	Bis(trimethylsilyl) derivative of (N-1,3	255	C11H18D3NO2Si2	22
10.	3,4DIMETHYL-5-(2,3,4,5,6-PENTAMETHYLPHEN	243	C16H21NO	22
11.	3a,6-Epoxy-3aH-isoindole, 1,2,3,6,7,7a-h	243	C15H17NO2	22
12.	3-AMINOBENZO(C)PHENANTHRENE	243	C18H13N	22
13.	Maculine	243	C13H9NO4	17
14.	2(1H)-Pyridinone, 3-acetyl-4-hydroxy-6-m	243	C14H13NO3	16
15.	1,3-DIMETHYL-(5,10-DIHYDRO)-5-DEAZA-ALLO	243	C13H13N3O2	16
16.	O-(4-TERT-BUTYL-2-CHLOROPHENYL)PHOSPHORO	278	C10H16ClN2OPS	16
17.	3a,6-Epoxy-3aH-isoindole, 1,2,3,6,7,7a-h	243	C15H17NO2	12
18.	Benzene, 1,1',1''-[(cyclohexyloxy)methyl	342	C25H26O	12
19.	2-METHYLSULFONYL-P-METHOXYACETANILIDE	243	C10H13NO4S	12
20.	CHLOROTRIPHENYLMETHANE	278	C19H15Cl	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000000-00-0	59092	68	36	0	76	15	50	18	59	9002
2.	*46	000088-29-9	59088	75	66	0	68	52	20	29	68	8138
3.	*35	083794-95-0	53679	43	81	1	83	54	11	0	40	7974
4.	*32	032706-25-5	53588	35	80	1	90	46	9	7	36	7559
5.	*32	006054-10-0	131656	45	82	2	99	47	9	1	36	8106
6.	*27	000000-00-0	53773	36	104	0	84	60	8	0	41	8273
7.	*25	042484-76-4	53632	48	112	2	89	63	7	0	46	7940
8.	*25	010207-07-5	53746	52	105	3	89	63	7	0	46	7496
9.	*22	088278-27-7	58442	34	104	0	43	64	5	0	41	8090
10.	*22	061314-50-9	53756	43	115	3	88	65	5	0	40	7901
11.	*22	017960-79-1	53720	37	106	2	84	65	5	0	39	7902
12.	*22	000000-00-0	53774	36	106	1	84	61	5	0	39	8232
13.	*17	000524-89-0	53656	30	115	2	99	54	3	0	29	8012
14.	*16	013959-06-3	53686	41	131	2	91	59	3	0	35	8013
15.	*16	000000-00-0	53668	38	122	2	84	58	3	0	33	8477
16.	16	000000-00-0	66159	51	80	2	99	57	3	0	31	8196
17.	*12	071840-23-8	53721	39	113	2	92	65	2	0	35	7902
18.	12	020705-40-2	86233	45	98	3	93	65	2	0	35	7896
19.	*12	064856-19-5	53601	30	126	3	99	59	2	0	29	7897
20.	12	000000-00-0	66532	39	106	0	72	64	2	0	33	7904

STP Compounds

Peak 14; Unidentified Hydrocarbon



Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	510	77.00	15	98.05	26	120.05	5
43.80	326	78.95	236	99.05	103	122.25	2
47.45	52	84.15	96	102.95	62	125.00	42
56.90	17	85.65	38	104.00	9	126.95	98
57.90	69	85.90	51	104.90	90	127.95	10
58.90	33	86.90	20	107.00	45	128.95	83
62.90	67	88.00	70	107.90	74	129.90	91
68.95	24	88.40	61	111.90	88	133.00	40
71.05	284	90.00	21	114.95	102	138.50	30
74.80	76	91.90	83	117.95	55	140.95	125
75.95	88	96.05	107	118.95	124	142.95	89

Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.80	58	158.00	86	177.90	6	199.20	55
144.05	87	159.00	92	178.90	65	200.45	35
144.95	33	161.00	90	180.00	33	203.00	55
145.85	3	161.85	9	181.90	34	203.90	49
147.05	30	164.25	17	182.90	96	205.00	7
149.00	21	166.80	66	184.00	95	208.00	22
153.00	93	167.95	24	185.15	119	213.15	348
154.00	123	169.95	35	186.90	52	214.00	89
154.95	93	170.95	239	192.45	58	218.20	57
155.90	111	172.15	17	192.70	66	225.20	19
157.00	137	172.70	40	198.05	49	227.00	29

Scan 1530 (29.241 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
228.50	34						
229.00	33						
243.05	760						
244.10	126						
258.15	148						
258.90	67						
278.65	38						

STP Compounds

Average of 29.440 to 29.456 min.: S0229.D
Converted from RTE data file: >S0229:

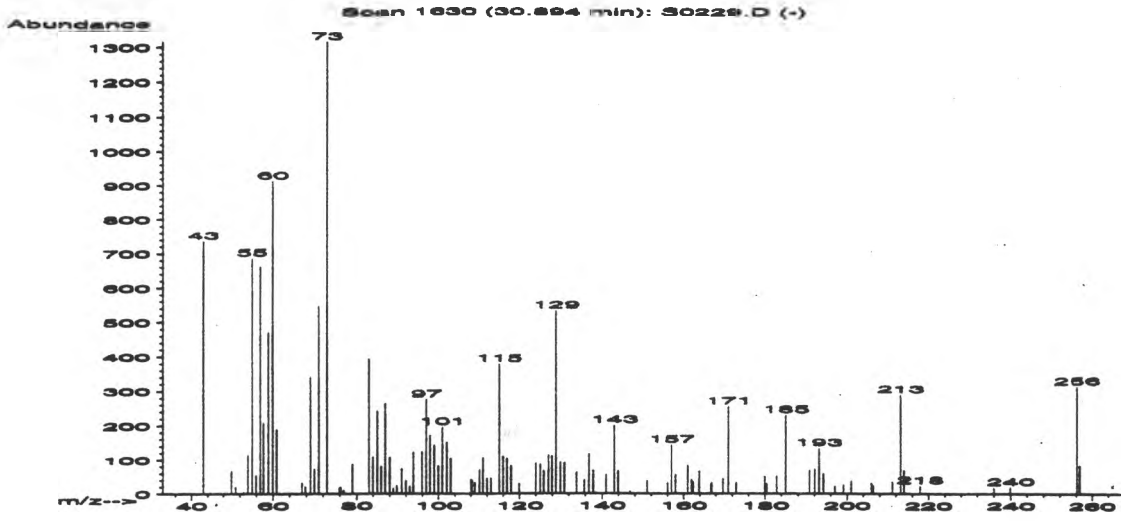
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benz[a]anthracene, 7,12-dihydro-7,12-dim	258	C20H18	72
2.	1,3,4,6,7,8-HEXAHYDRO-4,6,6,7,8,8-HEXAME	258	C18H26O	46
3.	3,3,6,6-TETRAMETHYL-1,2,3,4,5,6,7,8-OCTA	243	C17H25N	43
4.	5.alpha.,14.beta.-Androst-7-ene	258	C19H30	43
5.	7-AC-6-ET-1144-ME4-TETRALIN	258	C18H26O	41
6.	DIHYDROURACIL, O2,O4-BIS(TRIMETHYLSILYL)	258	C10H22N2O2Si2	38
7.	1,1,3,3-TETRAMETHYL-4,6-DIISOPROPYLINDAN	258	C19H30	32
8.	Maculine	243	C13H9NO4	22
9.	Benz[c]acridine, 5-methyl-	243	C18H13N	22
10.	Benz[c]acridine, 5-methyl-	243	C18H13N	22
11.	BRAVELIN	258	C15H14O4	16
12.	Thiazolo[3,2-a]pyridinium, 2,3-dihydro-8	243	C14H13NOS	14
13.	3,4DIMETHYL-5-(2,3,4,5,6-PENTAMETHYLPHEN	243	C16H21NO	12
14.	Furan, 2,3-dihydro-3-[2-methyl-3-(4-nitr	243	C14H13NO3	12
15.	3a,6-Epoxy-3aH-isoindole, 1,2,3,6,7,7a-h	243	C15H17NO2	10
16.	Dihydro-.beta.-ionone	194	C13H22O	10
17.	2-METHYL-7-PHENYL-5H-1,3,4-THIADIAZOLO[3	243	C12H9N3OS	10
18.	11-NOR-8,9.ALPHA.-DRIMANDIOL	226	C14H26O2	9
19.	CIS-TETRAHYDROIONONE	196	C13H24O	9
20.	.beta.-Citronellol	156	C10H20O	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	035281-31-3	59144	37	70	2	42	14	42	0	39	7842
2.	*46	000000-00-0	59092	57	35	1	53	45	20	0	49	7885
3.	*43	056798-25-5	53766	43	54	2	46	45	18	0	39	7949
4.	*43	063568-61-6	59124	33	18	0	43	45	18	0	41	7849
5.	*41	000088-29-9	59088	58	71	0	56	51	16	0	56	8219
6.	*38	000000-00-0	131638	53	96	2	55	53	14	0	47	8062
7.	32	000000-00-0	59119	55	56	1	44	48	9	11	33	8215
8.	*22	000524-89-0	53656	34	86	2	42	65	5	0	39	7712
9.	*22	003519-87-7	53770	35	57	1	52	61	5	1	40	7637
10.	*22	003519-87-7	130978	35	57	1	52	61	5	1	40	7637
11.	*16	006054-10-0	131656	36	59	1	46	60	3	7	36	7860
12.	*14	039137-97-8	53678	45	70	1	51	66	2	15	38	7633
13.	*12	061314-50-9	53756	33	73	2	46	61	2	10	35	8190
14.	*12	055256-12-7	53688	38	125	3	61	63	2	0	35	7646
15.	*10	017960-79-1	53720	35	76	2	57	66	1	1	34	7635
16.	*10	017283-81-7	127876	36	36	0	71	76	1	0	41	4678
17.	*10	042484-76-4	53632	38	117	3	61	66	1	0	33	7636
18.	9	055497-92-2	46837	61	75	2	59	73	1	10	35	4689
19.	9	060761-23-1	128041	75	45	2	93	71	1	9	37	4416
20.	9	000106-22-9	124527	55	57	2	92	73	1	0	36	4724

STP Compounds

Peak 41; Hexadecdanoic Acid



Scan 1630 (30.894 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	736	60.85	190	83.00	393	93.80	124
49.95	67	66.95	32	84.00	110	95.95	125
50.95	20	67.75	21	85.00	242	97.00	276
52.85	6	68.95	341	86.00	81	97.95	172
53.95	114	69.90	74	86.90	265	98.95	143
54.95	686	70.95	546	88.00	108	99.95	82
55.90	54	72.95	1316	88.90	16	100.95	196
56.90	662	75.95	18	89.75	25	102.05	152
57.75	207	76.20	20	91.00	75	103.00	105
58.90	471	76.95	10	92.00	39	108.00	43
59.90	912	79.00	87	92.95	21	108.25	40

Scan 1630 (30.894 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.95	33	123.95	91	137.90	68	162.40	34
110.15	71	125.05	87	140.95	57	163.90	66
111.00	107	125.95	68	142.95	202	166.70	30
112.00	46	127.05	115	143.95	67	166.95	32
113.00	46	127.95	112	146.80	8	169.70	45
115.00	380	128.90	534	150.95	39	171.05	255
116.00	111	130.00	93	156.00	32	172.95	32
116.95	105	130.90	92	157.00	144	179.90	51
117.95	83	133.90	63	158.00	57	180.40	30
119.00	2	135.75	41	161.00	84	182.90	53
119.95	30	136.90	118	162.00	42	185.00	231

Scan 1630 (30.894 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
190.80	69	214.05	69				
192.05	74	217.95	24				
193.05	135	236.00	17				
194.20	60	239.95	19				
197.05	23	256.15	315				
199.05	27	256.90	83				
200.95	38						
206.00	32						
206.40	24						
211.15	36						
213.15	290						

Scan 1630 (30.894 min): S0229.D

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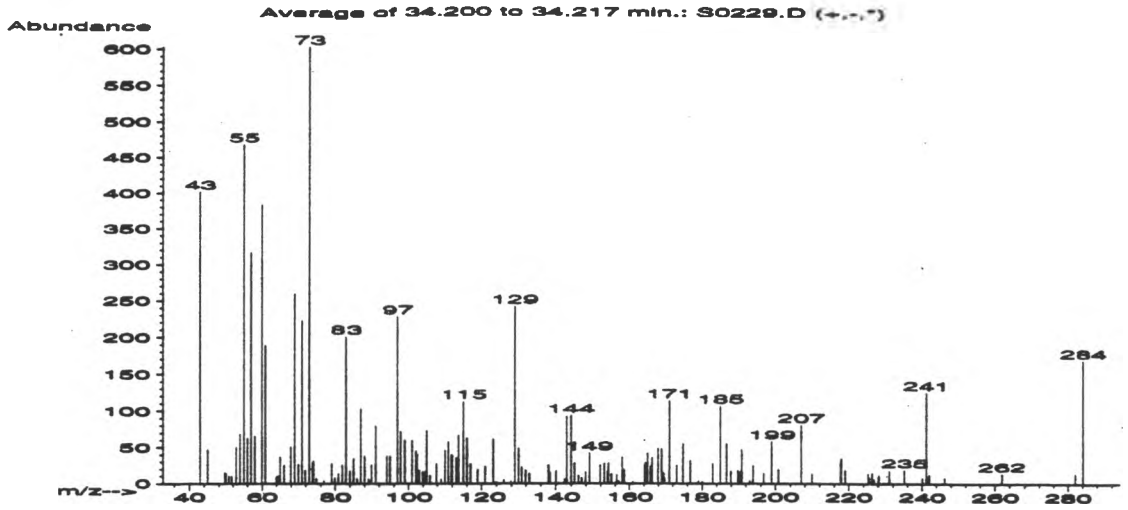
	Name	MolWt	Formula	Qual
1.	Hexadecanoic acid	256	C16H32O2	93
2.	Hexadecanoic acid	256	C16H32O2	91
3.	Hexadecanoic acid	256	C16H32O2	86
4.	Tridecanoic acid	214	C13H26O2	55
5.	Tridecanoic acid	214	C13H26O2	55
6.	Hexadecanoic acid	256	C16H32O2	53
7.	Tridecanoic acid	214	C13H26O2	53
8.	Hexadecanoic acid	256	C16H32O2	50
9.	Pentadecanoic acid	242	C15H30O2	49
10.	Tetradecanoic acid	228	C14H28O2	47
11.	Tetradecanoic acid	228	C14H28O2	38
12.	Decanoic acid	172	C10H20O2	38
13.	Nonanoic acid	158	C9H18O2	38
14.	Tetradecanoic acid	228	C14H28O2	35
15.	.alpha.-D-Glucopyranoside, methyl	194	C7H14O6	30
16.	Hexadecanoic acid	256	C16H32O2	25
17.	Tetradecanoic acid	228	C14H28O2	22
18.	Nonanoic acid	158	C9H18O2	22
19.	Undecanoic acid	186	C11H22O2	22
20.	Butanoic acid, methyl ester	102	C5H10O2	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000057-10-3	131570	120	27	1	91	13	66	40	93	9359
2.	*91	000057-10-3	131575	88	56	2	98	15	62	50	83	8241
3.	*86	000057-10-3	131571	78	77	0	54	50	53	0	93	9487
4.	*55	000638-53-9	129335	81	54	1	67	42	29	32	66	9206
5.	*55	000638-53-9	41267	90	53	0	51	42	29	40	80	6469
6.	*53	000057-10-3	131572	86	74	1	97	26	28	3	40	9374
7.	*53	000638-53-9	129336	75	57	0	70	38	28	27	59	9279
8.	*50	000057-10-3	59026	72	90	0	25	50	25	0	76	6723
9.	49	001002-84-2	130903	85	77	1	62	36	23	0	47	9375
10.	47	000544-63-8	130230	76	66	1	52	40	20	8	39	8954
11.	38	000544-63-8	47715	57	76	0	67	46	14	14	41	9030
12.	38	000334-48-5	126153	60	58	1	71	50	14	0	39	9138
13.	*38	000112-05-0	124681	72	35	1	74	58	14	21	58	8353
14.	35	000544-63-8	130228	68	70	0	82	51	11	0	42	9275
15.	30	000097-30-3	31475	65	41	0	46	57	9	15	43	7256
16.	*25	000057-10-3	131574	47	91	0	43	63	7	0	44	8912
17.	22	000544-63-8	130226	46	96	0	63	62	5	0	39	9205
18.	*22	000112-05-0	124678	58	53	1	73	63	5	15	40	8347
19.	22	000112-37-8	127363	62	64	3	134	61	5	0	39	8603
20.	*18	000623-42-7	118212	36	22	0	45	69	3	14	43	3930

STP Compounds

50

Peak ~~49~~; Stearic Acid



Average of 34.200 to 34.217 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	402	57.95	66	71.90	18	83.95	17
44.95	47	59.95	384	72.95	603	84.95	35
49.70	15	60.95	189	73.80	29	85.90	7
50.05	14	63.90	9	74.05	31	86.90	103
50.80	10	64.35	11	74.90	7	88.00	38
51.65	10	65.00	37	76.95	4	89.10	6
52.90	51	66.00	26	79.00	28	89.95	26
53.95	69	67.90	51	79.90	8	91.05	80
55.00	468	68.95	260	80.90	14	94.05	38
55.95	63	70.00	27	81.95	26	94.95	38
56.95	317	70.95	223	82.95	201	97.00	228
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.90	72	109.00	6	121.00	24	138.15	25
99.05	60	110.05	46	123.05	62	138.50	15
100.95	60	111.00	58	123.85	2	140.05	17
102.00	45	111.75	40	125.95	5	140.95	1
102.30	41	112.00	40	127.90	3	142.30	6
102.90	18	113.05	36	128.90	243	142.85	93
103.90	16	113.75	67	130.00	49	144.00	94
104.20	16	115.05	113	130.90	22	144.95	29
104.95	74	116.00	63	131.90	18	145.95	11
105.90	11	116.95	27	132.90	13	146.90	8
107.65	28	118.95	19	137.90	25	147.90	16
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.95	42	158.50	18	171.00	114	190.30	16
151.80	26	160.95	2	173.05	25	190.80	47
153.00	28	164.15	26	174.85	55	193.00	4
153.90	17	164.40	30	176.80	32	193.90	25
154.15	29	165.00	42	178.95	4	196.80	14
154.95	13	165.80	24	180.00	3	199.00	58
155.95	1	166.25	36	182.90	28	200.80	20
156.40	12	167.95	49	185.00	107	204.95	1
157.00	3	168.85	48	186.70	55	207.00	81
157.90	37	169.45	14	187.90	17	209.95	13
158.15	20	169.70	8	189.80	18	217.70	33

STP Compounds

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
217.95	35	241.95	12				
219.05	18	246.30	8				
225.20	13	261.90	14				
225.55	8	281.90	13				
226.40	14	284.15	170				
226.80	5						
228.10	11						
231.00	17						
235.15	19						
240.05	8						
241.10	125						

Average of 34.200 to 34.217 min.: S0229.D
Converted from RTE data file: >S0229:

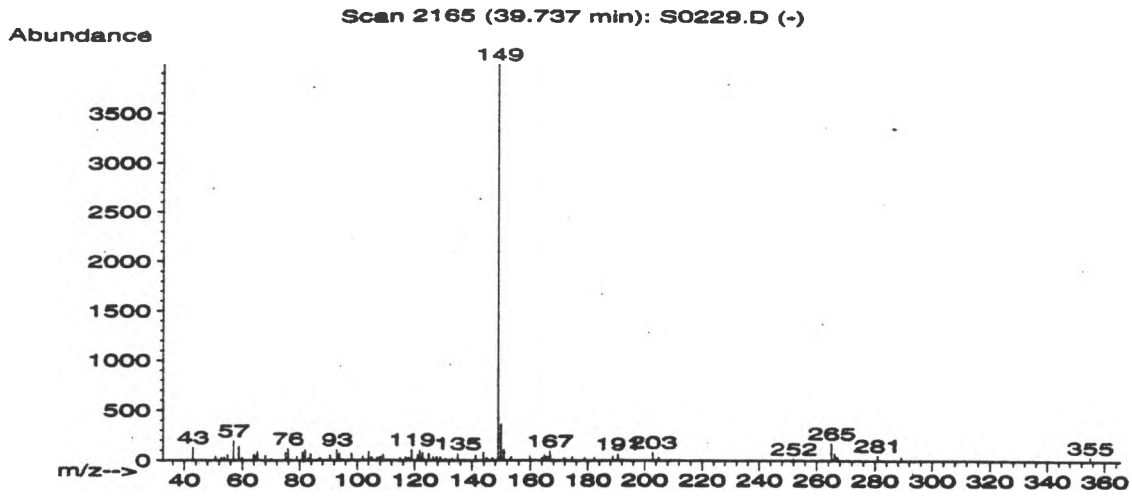
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Octadecanoic acid	284	C18H36O2	90
2.	Tetradecanoic acid	228	C14H28O2	49
3.	Tetradecanoic acid	228	C14H28O2	49
4.	Tetradecanoic acid	228	C14H28O2	46
5.	Pentadecanoic acid	242	C15H30O2	45
6.	Decanoic acid	172	C10H20O2	43
7.	Decanoic acid	172	C10H20O2	38
8.	Tetradecanoic acid	228	C14H28O2	37
9.	Hexadecanoic acid	256	C16H32O2	35
10.	Decanoic acid	172	C10H20O2	35
11.	Decanoic acid	172	C10H20O2	32
12.	9-Octadecenoic acid (Z)-	282	C18H34O2	27
13.	.alpha.-D-Glucopyranoside, O-.alpha.-D-g	504	C18H32O16	25
14.	D-Glucose, 4-O-.beta.-D-galactopyranosyl	342	C12H22O11	25
15.	Dodecanoic acid, silver(1+) salt	307	C12H24AgO2	25
16.	.alpha.-D-Glucopyranoside, .alpha.-D-glu	342	C12H22O11	25
17.	.alpha.-D-Glucopyranoside, .beta.-D-fruc	342	C12H22O11	16
18.	5-Hexenoic acid	114	C6H10O2	14
19.	4,4,6-TRIMETHYLTETRAHYDRO-1,3-THIAZIN-2-	159	C7H13NOS	10
20.	2,6,6-TRIDEUTERO-4,4-DIMETHYLCYCLOHEXA-2	126	C8H11D3O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000057-11-4	132772	99	68	2	73	19	59	63	90	9616
2.	*49	000544-63-8	130226	83	56	1	88	42	23	20	56	9177
3.	*49	000544-63-8	130228	74	65	1	73	42	23	16	50	9238
4.	*46	000544-63-8	130227	77	63	1	79	42	20	15	47	9185
5.	*45	001002-84-2	130903	79	72	1	65	47	19	34	52	9309
6.	43	000334-48-5	126150	71	42	0	76	45	18	3	39	8872
7.	38	000334-48-5	126153	69	49	1	70	47	14	0	38	8945
8.	37	000544-63-8	47715	75	59	2	87	42	13	5	37	9017
9.	35	000057-10-3	131570	57	80	1	82	52	11	16	38	9134
10.	35	000334-48-5	126155	61	62	1	61	52	11	0	39	8784
11.	32	000334-48-5	126152	69	46	1	76	47	9	10	37	8773
12.	27	000112-80-1	132678	71	91	2	65	57	8	0	38	9380
13.	25	000597-12-6	108386	72	92	2	68	52	7	16	37	9045
14.	25	000063-42-3	85907	71	76	3	91	51	7	7	37	9034
15.	25	018268-45-6	76045	56	105	2	69	52	7	15	37	9282
16.	25	000099-20-7	85909	43	105	3	99	55	7	0	37	8959
17.	16	000057-50-1	85908	46	101	2	93	59	3	19	37	8793
18.	*14	001577-22-6	119216	42	53	0	59	70	2	3	38	5812
19.	10	079696-62-1	16385	57	45	0	29	80	1	15	40	4857
20.	*10	000000-00-0	5368	28	67	3	117	79	1	2	39	7582

STP Compounds

Peak 74; Diheptyl Phthalate



Scan 2165 (39.737 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	128	67.95	50	87.25	25	109.00	59
50.80	39	70.00	16	90.50	52	111.10	2
52.75	30	74.95	77	92.95	106	114.95	26
53.80	28	75.95	118	93.80	67	116.95	33
55.00	60	76.95	6	94.95	10	117.95	26
56.95	194	79.00	40	97.95	73	118.95	106
58.75	141	80.95	83	101.95	38	120.95	55
59.90	22	81.90	107	103.95	85	121.80	96
63.90	60	83.00	22	104.95	29	122.80	77
64.50	48	83.75	66	107.00	30	123.05	16
65.15	89	86.75	20	107.95	40	124.95	65

Scan 2165 (39.737 min): S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.45	31	149.95	359	182.40	30	289.20	33
127.70	32	150.95	105	188.90	42	355.00	38
129.00	33	153.40	33	190.70	64		
130.80	18	159.90	41	203.00	80		
133.00	21	164.00	30	205.00	29		
135.00	68	164.90	54	209.00	10		
141.20	51	165.80	37	252.00	18		
143.80	82	166.80	93	265.05	171		
145.05	24	171.80	26	266.20	65		
146.95	25	174.55	36	267.05	34		
148.95	3985	179.00	31	280.90	53		

STP Compounds

Scan 2165 (39.737 min): S0229.D

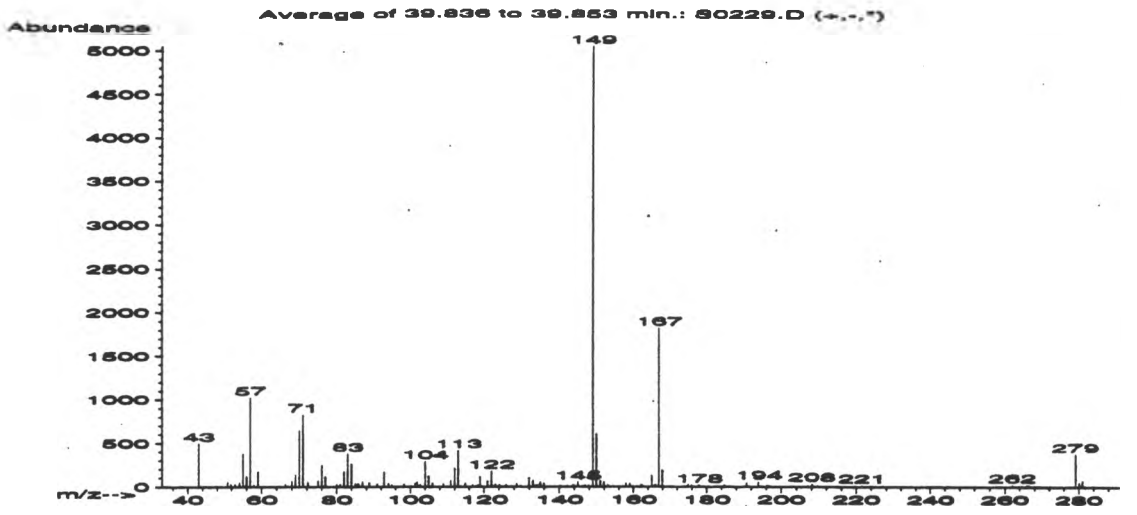
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, diheptyl e	362	C22H34O4	64
2.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	59
3.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	59
4.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	59
5.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	59
6.	1,2-Benzenedicarboxylic acid, butyl decy	362	C22H34O4	50
7.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	50
8.	1,2-Benzenedicarboxylic acid, dicyclohex	330	C20H26O4	50
9.	1,2-Benzenedicarboxylic acid, dicyclohex	330	C20H26O4	45
10.	Phthalic acid, butyl ester, ester with b	336	C18H24O6	45
11.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	45
12.	1,2-Benzenedicarboxylic acid, decyl hexy	390	C24H38O4	45
13.	1,2-Benzenedicarboxylic acid, decyl octy	418	C26H42O4	39
14.	1,2-Benzenedicarboxylic acid, bis(4-meth	334	C20H30O4	38
15.	ETHYL-N-BUTYL PHTHALATE	250	C14H18O4	38
16.	DI-ISOPENTYLPHTHALATE	306	C18H26O4	38
17.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	38
18.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	38
19.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	38
20.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	003648-21-3	90783	49	56	1	75	17	37	10	38	9988
2.	59	000131-18-0	133655	44	56	2	98	21	33	13	38	9979
3.	59	000131-18-0	133652	53	61	2	68	21	33	0	39	9978
4.	59	000084-74-2	132529	43	57	2	68	21	33	0	39	9979
5.	59	000084-74-2	132526	46	60	3	70	21	33	0	39	9979
6.	50	000089-19-0	90781	43	75	3	82	19	25	0	37	9979
7.	50	000605-45-8	131294	46	64	1	68	17	25	0	34	9983
8.	50	000084-61-7	134434	45	83	2	68	17	25	0	37	9980
9.	45	000084-61-7	134437	39	61	3	99	21	19	2	31	9979
10.	45	000085-70-1	134617	38	66	2	69	21	19	4	31	9971
11.	45	000084-64-0	75219	48	57	2	70	21	19	0	31	9979
12.	45	025724-58-7	96181	45	78	2	76	21	19	0	37	9978
13.	39	000119-07-3	100829	41	86	2	92	19	15	0	29	9979
14.	38	000146-50-9	84073	39	84	3	96	21	14	0	27	9979
15.	38	000000-00-0	56408	36	86	3	81	21	14	0	22	9977
16.	38	000000-00-0	75801	37	79	3	68	21	14	0	22	9979
17.	38	000084-69-5	132536	39	68	2	68	21	14	0	28	9978
18.	38	000084-69-5	132535	44	55	3	97	21	14	5	26	9979
19.	38	000084-64-0	133606	33	68	2	74	21	14	0	25	9974
20.	38	000131-16-8	131292	39	59	2	68	21	14	0	29	9979

STP Compounds

Peak 18; Bis(ethylhexyl) Phthalate



Average of 39.836 to 39.853 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	496	67.10	6	82.00	171	94.95	22
50.95	54	68.05	67	82.95	379	98.20	27
51.80	28	68.95	138	84.00	259	100.05	11
52.90	28	70.00	644	85.05	36	101.20	37
54.05	45	70.95	827	85.65	31	101.80	52
55.00	379	72.30	48	85.90	29	102.70	20
55.95	121	75.00	67	86.95	54	104.00	291
56.95	1024	75.95	249	88.90	46	104.95	119
57.90	16	76.95	115	91.00	30	106.00	38
59.00	168	80.00	29	92.85	168	109.00	31
66.25	26	80.95	26	94.05	36	111.00	67

Average of 39.836 to 39.853 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.00	213	127.10	6	143.55	22	159.00	35
113.00	416	128.75	36	143.80	18	161.05	4
114.95	39	129.90	9	144.95	49	162.15	24
116.95	16	131.90	101	146.90	18	162.50	16
118.30	21	133.00	64	147.80	15	165.00	126
118.95	117	133.90	16	148.95	5045	165.80	16
120.95	61	134.15	18	149.95	604	166.05	20
121.95	177	134.95	49	150.95	70	166.95	1826
123.00	24	135.90	40	151.95	50	167.95	186
124.20	19	140.40	18	152.95	21	174.95	26
125.95	20	141.95	14	158.00	40	175.95	17

Average of 39.836 to 39.853 min.: S0229.D
Converted from RTE data file: >S0229:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
177.75	16	209.65	9				
178.00	17	221.55	12				
184.50	13	262.00	19				
184.90	16	264.55	9				
190.45	14	265.80	15				
190.80	48	266.05	14				
193.95	54	266.45	15				
196.30	16	279.05	375				
197.00	5	280.15	46				
207.00	8	281.00	73				
208.15	31						

STP Compounds

Average of 39.836 to 39.853 min.: S0229.D
Converted from RTE data file: >S0229:

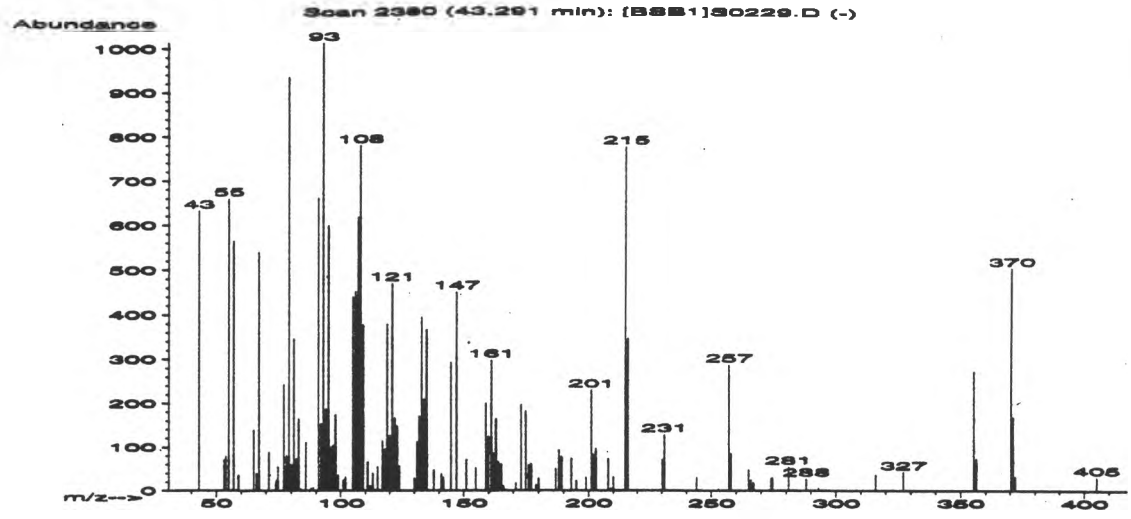
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	78
2.	(1S*,2R*,5R*,7S*)-2,4-Dimethyl-7-ethyl-6	168	C10H16O2	74
3.	1,2-Benzenedicarboxylic acid, 3-nitro-	211	C8H5NO6	72
4.	1,2-Benzenedicarboxylic acid, dicyclohex	330	C20H26O4	72
5.	1,2-Benzenedicarboxylic acid, isodecyl o	418	C26H42O4	53
6.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	50
7.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	50
8.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	50
9.	1,2-Benzenedicarboxylic acid, butyl decy	362	C22H34O4	50
10.	1,2-Benzenedicarboxylic acid, butyl 8-me	362	C22H34O4	50
11.	O-TOLYL ISOTHIOCYANATE	149	C8H7NS	50
12.	1,2-Benzenedicarboxylic acid, bis(2-meth	282	C14H18O6	50
13.	1,2-Benzenedicarboxylic acid, butyl 2-et	334	C20H30O4	50
14.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	47
15.	1,2-Benzenedicarboxylic acid, dioctyl es	390	C24H38O4	43
16.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	40
17.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	40
18.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	40
19.	1,2-Benzenedicarboxylic acid, butyl octy	334	C20H30O4	40
20.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	78	000117-81-7	135876	76	55	0	67	8	46	8	39	9968
2.	*74	091926-28-2	20483	58	30	1	67	17	44	0	51	9893
3.	72	000603-11-2	39769	83	24	0	66	16	42	0	47	9946
4.	72	000084-61-7	134435	54	58	1	71	14	42	16	41	9905
5.	53	001330-96-7	100831	62	61	2	99	28	28	0	39	9491
6.	50	000084-64-0	75219	47	59	2	99	32	25	0	39	9390
7.	50	000131-16-8	56409	54	44	2	87	32	25	5	41	9343
8.	50	000084-66-2	129814	45	50	2	91	32	25	13	38	9346
9.	50	000089-19-0	90781	47	72	2	99	33	25	0	39	9341
10.	50	000089-18-9	90782	59	63	3	80	33	25	3	38	9381
11.	*50	000614-69-7	12248	33	75	1	72	32	25	0	39	9345
12.	50	000117-82-8	132666	50	46	2	94	32	25	3	38	9344
13.	50	000085-69-8	84071	44	66	2	99	33	25	0	39	9345
14.	47	000117-81-7	135870	65	61	2	61	39	20	0	38	9924
15.	43	000117-84-0	96182	74	49	1	43	44	18	0	41	9924
16.	40	000084-69-5	132535	45	68	1	99	32	16	0	37	9398
17.	40	000084-69-5	66362	46	67	1	88	33	16	0	37	9455
18.	40	000084-69-5	132536	45	62	1	88	33	16	0	37	9435
19.	40	000084-78-6	84070	45	72	1	98	32	16	0	37	9349
20.	40	000131-16-8	131292	45	54	2	99	32	16	0	37	9365

STP Compounds

Peak 75; Sterol



Scan 2380 (43.291 min): [BSB1]S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	633	74.05	25	87.95	5	101.15	24
52.95	71	74.70	55	88.95	7	101.95	31
53.80	79	76.95	244	91.00	661	105.00	440
55.00	660	78.00	80	92.00	154	106.00	452
56.90	564	79.05	935	92.95	1013	107.00	617
58.90	35	79.95	60	93.95	187	108.00	780
65.00	140	81.00	346	95.05	598	109.00	377
66.15	40	82.05	73	96.00	100	111.00	65
67.05	540	83.00	164	96.95	104	112.00	11
70.95	89	83.95	4	97.95	174	113.00	40
73.70	19	85.90	111	99.00	35	115.00	54

Scan 2380 (43.291 min): [BSB1]S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.95	114	133.00	395	159.00	200	176.05	59
117.95	96	134.00	209	160.00	124	177.00	61
118.95	379	135.00	367	161.15	298	179.00	13
119.95	126	138.00	48	161.95	86	180.00	28
120.95	470	140.95	38	163.00	164	186.75	50
122.05	166	141.70	30	164.00	65	188.15	93
123.00	147	141.95	23	165.15	60	189.10	78
123.80	56	144.95	293	166.05	10	192.95	73
130.00	29	147.05	451	170.95	18	195.05	23
131.00	112	151.05	71	173.05	196	198.95	30
132.00	170	155.00	52	174.95	182	201.20	230

Scan 2380 (43.291 min): [BSB1]S0229.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
202.00	83	253.00	4	315.95	36		
202.25	78	257.15	287	327.00	43		
203.00	97	258.00	84	355.25	272		
207.90	73	264.95	48	356.25	72		
208.95	5	265.95	24	370.30	504		
210.00	31	266.95	18	371.20	168		
215.05	776	274.05	29	372.05	32		
216.05	346	274.55	30	404.90	31		
230.25	71	281.00	54				
231.00	128	288.05	27				
244.05	30	293.05	6				

STP Compounds

Scan 2380 (43.291 min): [BSB1]S0229.D

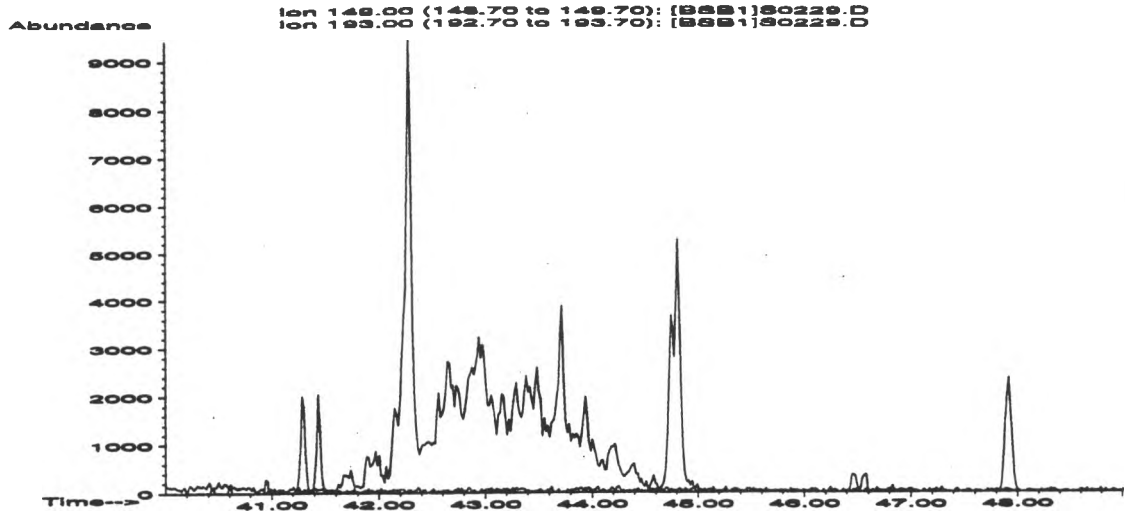
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	6-Heptadecatri-8(Z),11(Z),14(Z)-enyl-2-h	370	C24H34O3	50
2.	Urea, (phenylmethoxy)-	166	C8H10N2O2	22
3.	Borazine, 1,3-dimethyl-	109	C2H10B3N3	22
4.	Cholan-24-oic acid, 3,12-dihydroxy-, (3.	392	C24H40O4	14
5.	Cyclohexene, 3,4-diethenyl-1,6-dimethyl-	162	C12H18	11
6.	Phenol, 3-methyl-	108	C7H8O	11
7.	Benzenemethanol	108	C7H8O	10
8.	METHYL-DIPHENYL PHOSPHINE OXIDE	216	C13H13OP	10
9.	1,2-Butanediol, 1-phenyl-	166	C10H14O2	10
10.	Phenol, 2-methyl-	108	C7H8O	10
11.	1H-Pyrrole, 2,3,5-trimethyl-	109	C7H11N	10
12.	(3S,6R,7E,9S)-4,7-MEGASTIGMADIENE-3,9-DI	210	C13H22O2	10
13.	26,27-Dinorergosta-5,22-dien-3-ol, (3.be	370	C26H42O	10
14.	Phenol, 2-methyl-	108	C7H8O	10
15.	Phenol, o-(o-methoxyphenoxy)-	216	C13H12O3	10
16.	1,2-DIMETHYL-4-METHYLENE-CYCLOPENTENE	108	C8H12	10
17.	2,4,6-OCTATRIENE, ALL-TRANS	108	C8H12	10
18.	Benzenemethanol	108	C7H8O	10
19.	DL-Leucine, N-[(phenylmethoxy)carbonyl]-	265	C14H19NO4	10
20.	Benzenemethanol	108	C7H8O	10

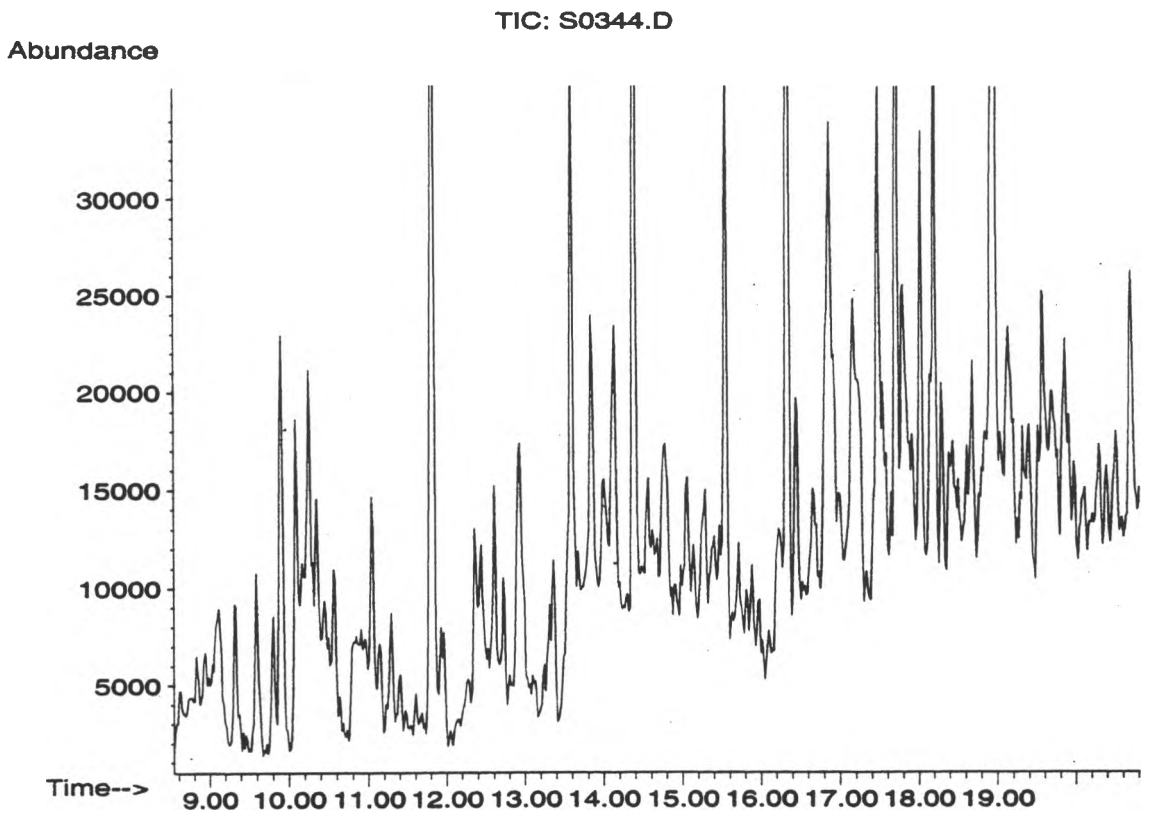
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	083173-24-4	92542	82	121	2	65	47	25	36	72	7823
2.	22	002048-50-2	19210	45	55	2	134	63	5	16	38	6345
3.	*22	023208-28-8	2021	45	79	1	74	63	5	0	39	6347
4.	14	000083-44-3	135913	77	87	2	139	68	2	0	39	6057
5.	*11	061142-14-1	17864	43	56	0	95	77	2	0	44	5260
6.	*11	000108-39-4	118725	46	57	0	55	72	2	0	44	5849
7.	*10	000100-51-6	118738	37	71	1	56	71	1	0	39	5962
8.	*10	002129-89-7	42009	44	85	1	70	76	1	0	39	5050
9.	*10	022607-13-2	19406	36	64	1	76	72	1	0	39	5755
10.	*10	000095-48-7	118720	30	79	2	71	72	1	11	38	5779
11.	*10	002199-41-9	2073	33	62	0	58	79	1	0	41	5000
12.	10	068831-81-2	39512	60	66	0	58	72	1	0	43	5779
13.	*10	052745-87-6	92569	43	160	1	62	80	1	0	39	6274
14.	*10	000095-48-7	1915	35	62	0	72	72	1	0	41	5779
15.	*10	021905-60-2	41994	43	73	0	76	76	1	19	40	4893
16.	*10	000000-00-0	1964	37	67	2	99	79	1	0	39	5042
17.	*10	000000-00-0	1947	43	62	2	96	80	1	0	39	4829
18.	*10	000100-51-6	118744	35	33	1	76	72	1	1	40	5779
19.	*10	003588-60-1	61543	46	97	3	107	72	1	0	39	5716
20.	*10	000100-51-6	118743	35	80	2	92	72	1	0	39	5779

STP Compounds

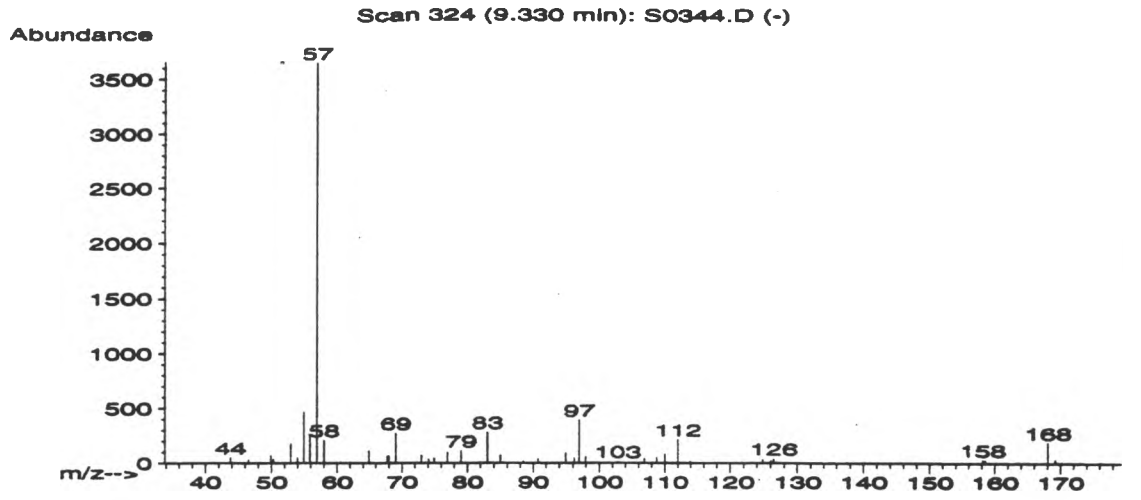
Mixed Nonylphthalates in Grande Prairie effluent 1990. Do not recur.



STP Compounds



Peak 76; C12 Alkene



Scan 324 (9.330 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	50	67.70	66	90.75	38	124.80	32
46.55	29	67.95	66	94.95	96	126.05	25
49.95	68	69.05	275	96.20	45	126.45	42
50.30	35	72.95	71	96.95	395	158.15	34
52.95	180	74.10	37	97.95	58	158.50	26
53.95	46	74.95	46	102.80	17	168.05	193
54.95	469	76.95	101	106.90	41	169.20	34
55.90	256	79.05	112	108.75	53		
56.90	3655	83.00	283	110.00	82		
58.00	210	85.00	71	112.00	217		
64.90	114	88.50	21	113.90	19		

STP Compounds

Scan 324 (9.330 min): S0344.D

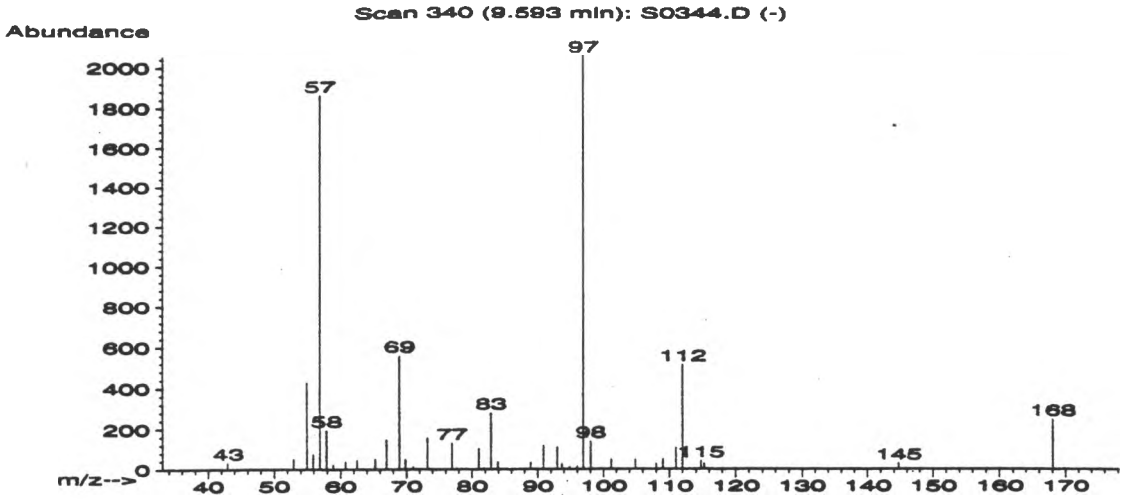
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-Undecene, 6-methyl-, (E)-	168	C12H24	47
2.	1-Hexene, 5,5-dimethyl-	112	C8H16	38
3.	4-Decene, 2,2-dimethyl-, (Z)-	168	C12H24	37
4.	4-Decene, 2,2-dimethyl-, (E)-	168	C12H24	32
5.	4-Hepten-3-one, 5-ethyl-4-methyl-	154	C10H18O	28
6.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	28
7.	2-Undecene, 5-methyl-	168	C12H24	23
8.	1-Propene, 2-methyl-, trimer	168	C12H24	16
9.	Heptane, 2,3,5-trimethyl-	142	C10H22	10
10.	5-Hepten-2-one	112	C7H12O	9
11.	5-Hexen-2-one, 5-methyl-	112	C7H12O	9
12.	5-Hexen-2-one, 5-methyl-	112	C7H12O	9
13.	1-Hexacosanol	382	C26H54O	7
14.	1-Tetracosanol	354	C24H50O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	074630-52-7	20695	35	52	3	99	36	20	0	39	9964
2.	*38	007116-86-1	2666	38	47	1	77	36	14	0	33	9972
3.	37	055499-03-1	20733	41	31	0	99	45	13	0	33	9940
4.	*32	055534-69-5	20734	35	39	1	84	50	9	3	36	9952
5.	28	022319-28-4	124189	33	53	1	68	40	8	0	22	9962
6.	*28	000107-39-1	119085	30	42	1	99	36	8	0	29	9968
7.	*23	056851-34-4	125795	28	65	1	67	50	6	0	27	9912
8.	16	007756-94-7	20739	36	36	0	64	59	3	3	30	9804
9.	10	020278-85-7	10264	34	42	1	99	63	1	0	22	9903
10.	* 9	006714-00-7	2547	29	30	0	42	72	1	0	33	1143
11.	* 9	003240-09-3	119023	29	47	1	66	72	1	0	33	1213
12.	* 9	003240-09-3	2554	29	45	1	63	72	1	0	33	1195
13.	7	000506-52-5	94731	33	71	0	15	72	1	0	25	9701
14.	7	000506-51-4	89101	34	71	0	14	72	1	0	25	9637

STP Compounds

Peak 77; C12 Alkene



Scan 340 (9.593 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	34	68.95	560	92.95	111	112.00	515
52.95	51	69.85	50	93.70	24	114.75	42
54.95	426	71.00	11	94.80	11	115.25	27
55.90	74	73.20	157	96.00	15	144.70	29
56.90	1862	76.95	131	96.95	2054	168.05	249
57.90	194	81.00	105	98.05	139		
58.90	22	81.85	6	101.20	49		
60.75	39	82.90	279	104.90	48		
62.50	45	83.90	36	108.00	27		
65.25	51	88.90	33	109.00	52		
67.00	148	90.90	118	111.00	108		

STP Compounds

Scan 340 (9.593 min): S0344.D

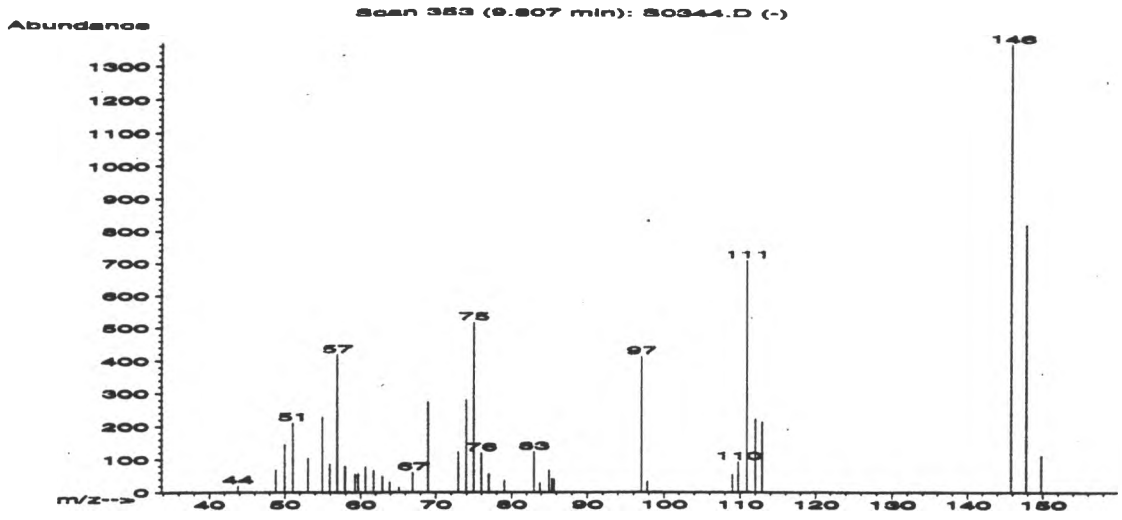
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Thiophene, 2-ethyl-	112	C6H8S	50
2.	Thiophene, 2-ethyl-	112	C6H8S	50
3.	Thiophene, 3-ethyl-	112	C6H8S	50
4.	2-Pentene, 3,4,4-trimethyl-	112	C8H16	50
5.	2-Pentene, 2,3,4-trimethyl-	112	C8H16	50
6.	2-Pentene, 2,4,4-trimethyl-	112	C8H16	42
7.	4,4-Dimethyl-1-hydroxy-2-cyclopentene	112	C7H12O	40
8.	Cyclohexene, 1-(1,1-dimethylethoxy)-3-me	168	C11H20O	40
9.	1H-Pyrazole, 4,5-dihydro-3,4,5-trimethyl	112	C6H12N2	40
10.	2-Pyrazoline, 1,4,5-trimethyl-	112	C6H12N2	40
11.	2-Pentene, 2,4,4-trimethyl-	112	C8H16	40
12.	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	38
13.	Oxazole, 2,4-dimethyl-	97	C5H7NO	38
14.	2-Pentene, 2,3,4-trimethyl-	112	C8H16	33
15.	2-Pentene, 2,4,4-trimethyl-	112	C8H16	33
16.	2-Pentene, 2,4,4-trimethyl-	112	C8H16	33
17.	2-(Propionyl)-6-methyl-2,3-dihydro-4H-py	154	C9H14O2	25
18.	4,4-DIMETHYL-4-SILACYCLOPENTENE	112	C6H12Si	17
19.	1-Hexene, 2-isopentyl-5-methyl-	168	C12H24	16
20.	Thiophene, 2-ethyl-	112	C6H8S	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	000872-55-9	118996	38	42	1	99	32	25	5	38	7392
2.	*50	000872-55-9	2496	33	44	1	99	32	25	7	40	7382
3.	*50	001795-01-3	2497	34	57	1	67	34	25	0	39	7383
4.	*50	000598-96-9	2694	33	61	2	84	34	25	0	39	8700
5.	*50	000565-77-5	119089	39	56	3	83	31	25	0	39	8554
6.	*42	000107-40-4	119092	43	40	1	79	29	17	7	33	8840
7.	*40	068757-99-3	2593	29	38	1	97	34	16	0	33	8567
8.	40	040648-24-6	20632	39	48	2	69	34	16	6	35	7397
9.	*40	022591-95-3	2522	29	53	2	91	34	16	8	35	7419
10.	*40	007423-11-2	2521	33	41	2	82	32	16	2	35	7732
11.	*40	000107-40-4	119094	39	41	1	84	34	16	3	36	8518
12.	*38	054411-01-7	20765	43	42	1	69	38	14	2	37	7304
13.	*38	007208-05-1	673	34	53	1	99	49	14	0	39	7195
14.	*33	000565-77-5	119090	29	38	1	78	31	10	0	29	8662
15.	*33	000107-40-4	119095	29	39	1	84	34	10	0	29	8690
16.	*33	000107-40-4	2693	31	49	1	83	34	10	0	29	8616
17.	25	062255-24-7	14428	34	58	1	71	41	7	0	21	8012
18.	*17	016054-12-9	119016	31	70	2	55	52	3	0	29	7245
19.	*16	033717-92-9	125802	41	54	1	60	58	3	0	35	7319
20.	*14	000872-55-9	118997	37	36	1	19	70	2	0	39	6534

STP Compounds

Peak 23; Dichlorobenzene



Scan 353 (9.807 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	20	60.65	78	76.95	55	110.90	711
48.80	69	61.75	66	79.05	35	112.00	221
49.95	146	62.90	47	83.00	123	112.90	214
51.05	211	63.90	30	83.80	27	145.80	1369
53.05	104	65.15	15	85.00	66	147.80	822
54.95	227	66.95	60	85.40	40	149.80	112
55.90	86	68.95	274	85.65	39		
56.90	418	72.95	123	97.05	413		
57.90	79	73.95	282	97.80	32		
59.25	55	74.95	517	109.00	54		
59.65	55	75.95	119	109.75	93		

STP Compounds

Scan 353 (9.807 min): S0344.D

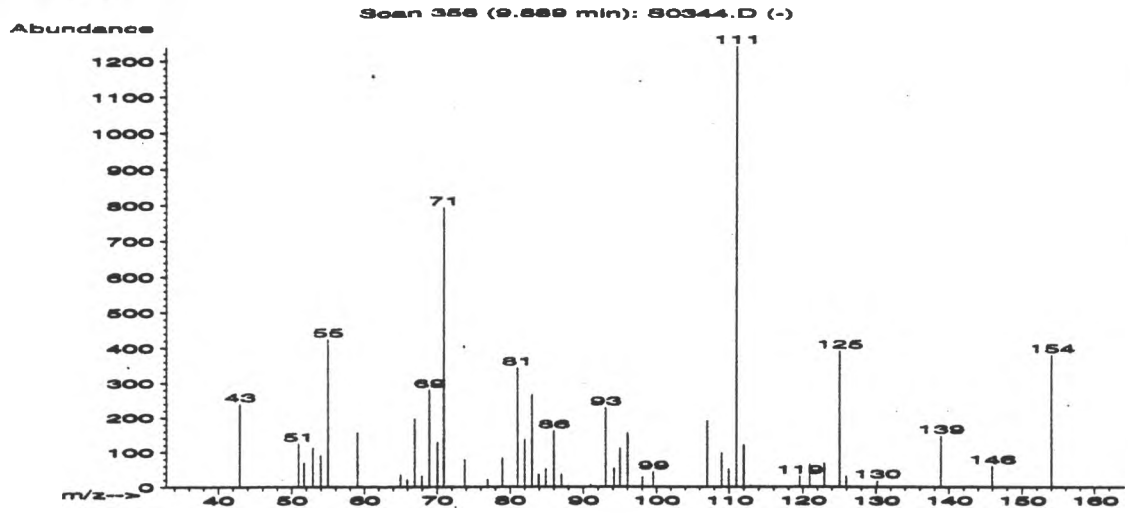
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,3-dichloro-	146	C6H4Cl2	87
2.	Benzene, 1,2-dichloro-	146	C6H4Cl2	87
3.	Benzene, 1,4-dichloro-	146	C6H4Cl2	81
4.	Benzene, 1,2-dichloro-	146	C6H4Cl2	81
5.	Benzene, 1,3-dichloro-	146	C6H4Cl2	74
6.	Benzene, 1,2-dichloro-	146	C6H4Cl2	74
7.	Benzene, 1,2-dichloro-	146	C6H4Cl2	72
8.	Benzene, 1,4-dichloro-	146	C6H4Cl2	64
9.	Benzene, 1,4-dichloro-	146	C6H4Cl2	64
10.	Benzene, 1,3-dichloro-	146	C6H4Cl2	59
11.	Benzene, 1,4-dichloro-	146	C6H4Cl2	58
12.	Benzene, 1,3-dichloro-	146	C6H4Cl2	56
13.	Benzene, 1,3-dichloro-	146	C6H4Cl2	53
14.	Benzene, 1,4-dichloro-	146	C6H4Cl2	50
15.	Benzene, 1,2-dichloro-	146	C6H4Cl2	42
16.	Benzene, 1,2-dichloro-	146	C6H4Cl2	40
17.	(E)-6-Chloro-4-methyl-2-heptene	146	C8H15Cl	38
18.	TRANS-DICHLOROFUMARONITRILE	146	C4Cl2N2	37
19.	1H-Benzimidazole, 2,5-dimethyl-	146	C9H10N2	8
20.	Ethene, 1,2-bis(ethylthio)-	148	C6H12S2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000541-73-1	11153	79	30	1	79	12	54	26	72	9572
2.	*87	000095-50-1	11151	74	43	1	68	12	54	0	81	9674
3.	*81	000106-46-7	11154	77	31	0	69	19	49	20	66	9509
4.	*81	000095-50-1	123077	78	30	0	74	18	49	22	66	9582
5.	*74	000541-73-1	123079	69	39	2	87	20	44	27	62	9471
6.	*74	000095-50-1	123076	70	33	0	84	20	44	15	50	9543
7.	*72	000095-50-1	123073	50	60	1	93	19	42	0	44	9586
8.	*64	000106-46-7	123085	50	61	2	93	21	37	0	46	9538
9.	*64	000106-46-7	123084	57	47	0	69	17	37	4	40	9579
10.	*59	000541-73-1	123080	65	39	0	69	21	33	8	43	9546
11.	*58	000106-46-7	123082	46	59	0	78	29	32	0	44	9543
12.	*56	000541-73-1	123081	52	68	2	88	14	30	0	33	9672
13.	*53	000541-73-1	123078	39	67	0	78	29	28	0	39	9548
14.	*50	000106-46-7	123083	37	63	0	68	33	25	0	41	9402
15.	*42	000095-50-1	123075	39	67	1	79	28	17	0	35	9465
16.	*40	000095-50-1	123074	39	69	1	78	31	16	0	35	9509
17.	*38	092639-31-1	11344	28	85	1	90	21	14	0	27	9062
18.	*37	000000-00-0	11118	39	66	2	73	42	13	0	35	8850
19.	* 8	001792-41-2	11433	28	73	1	99	66	1	0	29	7140
20.	* 7	013105-10-7	11849	31	91	3	60	74	1	0	29	5066

STP Compounds

Peak 32: Unidentified Monoterpene



Scan 358 (9.889 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	240	68.95	279	86.00	161	109.95	51
50.95	125	70.05	128	87.00	37	111.00	1237
51.70	69	70.95	790	91.00	7	112.00	120
52.90	113	73.80	78	93.05	228	112.95	4
53.95	90	76.95	21	94.20	53	119.55	30
54.95	423	78.95	83	95.00	110	120.95	65
59.00	157	81.00	343	96.05	154	122.95	68
65.00	36	82.00	137	98.05	28	125.05	389
65.95	21	83.00	265	99.55	43	125.95	30
66.95	196	83.90	36	107.00	190	130.15	18
67.95	32	84.90	51	109.00	98	138.90	146

Scan 358 (9.889 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
145.95	59						
154.00	379						

STP Compounds

Scan 358 (9.889 min): S0344.D

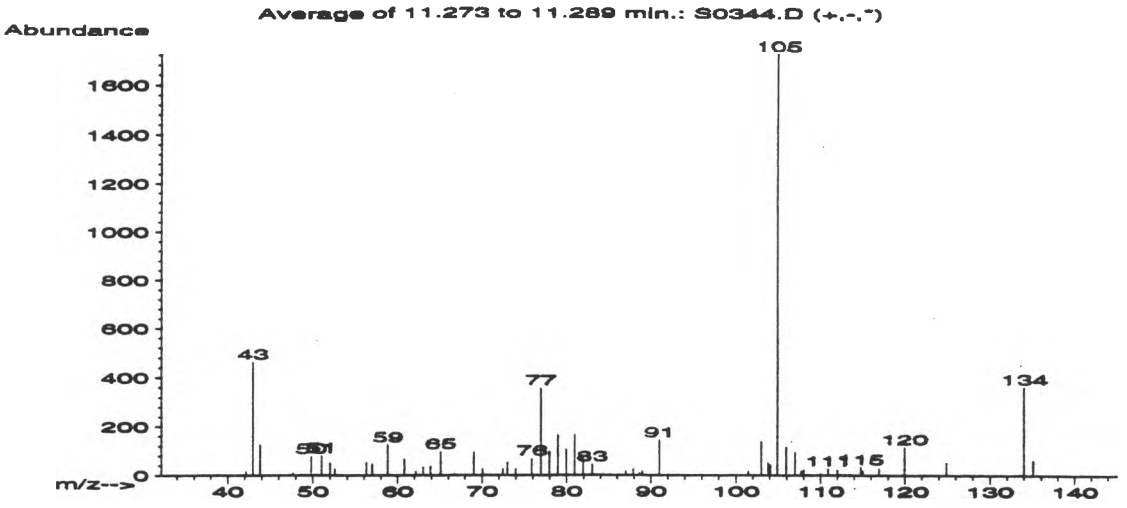
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Carvomenthone	154	C10H18O	47
2.	4-Penten-2-one, 3-methyl-, isopropylhydr	154	C9H18N2	43
3.	3-Cyclohexen-1-ol, 4-methyl-1-(1-methyle	154	C10H18O	43
4.	Valeraldehyde, 2-methylene-, isopropylhy	154	C9H18N2	43
5.	3-Cyclohexen-1-ol, 4-methyl-1-(1-methyle	154	C10H18O	40
6.	3-Cyclohexene-1-methanol, .alpha...alpha	154	C10H18O	38
7.	1-4-Terpineol	154	C10H18O	38
8.	Carvomenthone	154	C10H18O	37
9.	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	35
10.	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	35
11.	4(1H)-Pyrimidinone, 2-amino-	111	C4H5N3O	35
12.	Cyclohexane, 1,4-dimethyl-2-octadecyl-	364	C26H52	35
13.	D-erythro-Pent-1-enitol, 1,5-anhydro-2-d	154	C7H11BO3	32
14.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	27
15.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	27
16.	2,5-PYRIDINEDIOL	111	C5H5NO2	25
17.	Oxazole, trimethyl-	111	C6H9NO	16
18.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	16
19.	2-Aminopyrimidin-1-oxide	111	C4H5N3O	16
20.	Oxazole, trimethyl-	111	C6H9NO	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	000499-70-7	14698	46	63	2	99	39	20	0	39	8193
2.	*43	016713-39-6	14525	36	47	0	94	43	18	17	39	8032
3.	*43	000562-74-3	124239	35	79	3	218	43	18	0	39	7848
4.	*43	033063-80-8	14524	49	45	1	90	41	18	10	39	8257
5.	*40	000562-74-3	124242	54	57	2	77	34	16	3	32	7133
6.	*38	000098-55-5	124248	47	59	2	115	50	14	0	40	8356
7.	*38	020126-76-5	14660	34	75	2	141	47	14	0	39	8518
8.	*37	000499-70-7	124281	37	73	2	99	43	13	0	35	8183
9.	*35	016867-04-2	2319	45	54	2	76	52	11	0	39	7816
10.	*35	003073-66-3	5465	47	51	1	67	52	11	0	39	7809
11.	*35	000108-53-2	2308	42	42	2	99	52	11	5	40	7729
12.	35	055282-02-5	91309	48	79	2	99	55	11	7	38	8031
13.	*32	074793-26-3	14265	33	97	3	99	47	9	0	30	8062
14.	*27	000071-30-7	118913	43	43	1	89	56	8	0	40	7775
15.	*27	000071-30-7	2309	44	41	2	99	56	8	3	38	7798
16.	*25	000000-00-0	2324	40	59	1	83	52	7	0	35	7808
17.	*16	020662-84-4	118924	30	73	3	99	56	3	0	33	7692
18.	*16	000071-30-7	118914	38	42	2	99	56	3	7	36	7727
19.	*16	035034-15-2	2307	39	40	2	84	60	3	1	36	7657
20.	*16	020662-84-4	118925	39	46	2	74	56	3	12	37	7705

STP Compounds

Peak 79; Alkylbenzene



Average of 11.273 to 11.289 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.15	18	60.80	67	73.95	25	88.65	9
42.95	462	62.15	18	75.90	69	89.00	17
43.80	123	63.00	34	76.95	357	91.00	143
47.70	9	63.90	37	77.95	97	101.45	17
49.80	78	65.10	97	78.95	164	103.00	138
51.00	81	66.70	7	79.95	106	103.80	52
52.00	51	69.00	94	80.95	167	104.05	43
52.55	27	69.85	1	81.95	69	104.90	1724
56.25	53	70.05	27	83.00	45	105.95	115
56.95	47	72.45	27	87.00	18	106.95	95
58.80	125	73.00	54	87.90	25	107.75	18

Average of 11.273 to 11.289 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	22	135.05	63				
109.95	8						
110.90	27						
112.00	21						
114.75	34						
115.00	18						
116.95	28						
119.75	4						
119.95	116						
124.90	52						
134.00	363						

STP Compounds

Average of 11.273 to 11.289 min.: S0344.D
Converted from RTE data file: >S0344:

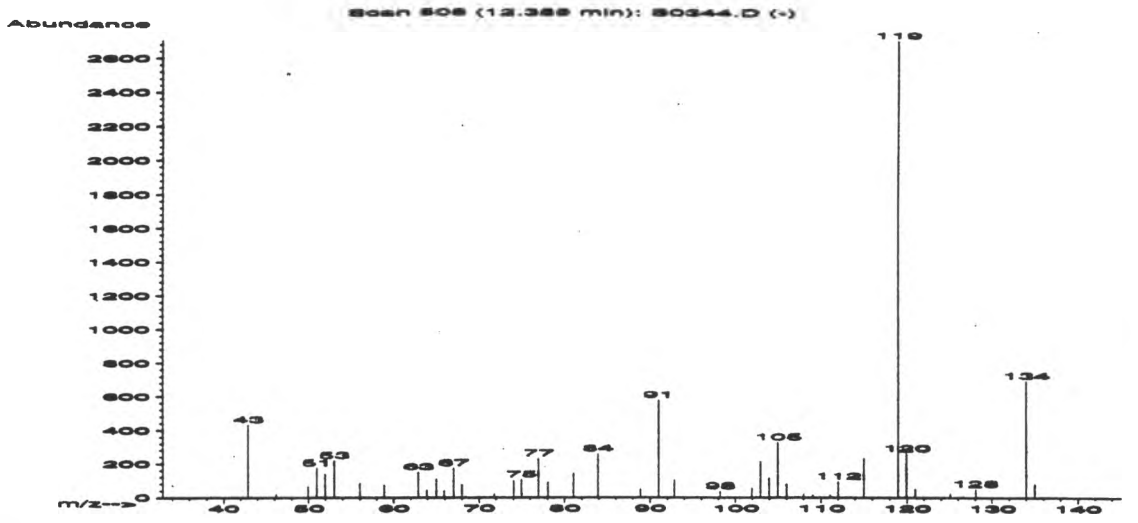
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2-diethyl-	134	C10H14	58
2.	Benzene, (1-methylpropyl)-	134	C10H14	52
3.	Benzene, 1,2-diethyl-	134	C10H14	50
4.	Benzene, 1-methyl-2-propyl-	134	C10H14	49
5.	Benzene, 1,3-diethyl-	134	C10H14	49
6.	Benzene, 1-methyl-2-propyl-	134	C10H14	47
7.	Benzene, 1-methyl-2-propyl-	134	C10H14	46
8.	Benzene, 1-methyl-2-propyl-	134	C10H14	46
9.	Benzene, (1-methylpropyl)-	134	C10H14	46
10.	Benzene, 1-methyl-3-propyl-	134	C10H14	46
11.	Benzene, 1-methyl-2-propyl-	134	C10H14	46
12.	Benzene, 1-methyl-3-propyl-	134	C10H14	46
13.	Benzene, 1-methyl-4-propyl-	134	C10H14	46
14.	DIETHYL BENZENE (PARA?)	134	C10H14	38
15.	Benzene, (1-methylethyl)-	120	C9H12	35
16.	Phenol, o-[(.alpha.-methylbenzyl)sulfony	262	C14H14O3S	27
17.	Benzene, 1,2,4-trimethyl-	120	C9H12	25
18.	Benzene, 1,3,5-trimethyl-	120	C9H12	25
19.	Benzene, (1-methylethyl)-	120	C9H12	22
20.	Benzene, (1-methylethyl)-	120	C9H12	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	000135-01-3	7448	50	35	1	37	30	32	0	46	9791
2.	*52	000135-98-8	121615	49	36	1	98	35	27	0	44	9856
3.	*50	000135-01-3	121642	46	58	2	52	35	25	0	39	9784
4.	*49	001074-17-5	121621	57	26	0	70	37	23	0	49	9856
5.	*49	000141-93-5	121646	49	35	1	41	40	23	0	46	9751
6.	*47	001074-17-5	121618	47	38	1	68	37	20	1	40	9817
7.	*46	001074-17-5	121619	49	33	1	99	45	20	0	46	9830
8.	*46	001074-17-5	7442	49	33	1	99	45	20	0	46	9830
9.	*46	000135-98-8	7441	49	36	1	95	42	20	0	44	9848
10.	*46	001074-43-7	7443	55	31	1	89	42	20	0	49	9831
11.	*46	001074-17-5	121617	51	32	1	89	42	20	0	46	9842
12.	*46	001074-43-7	121622	55	31	1	87	42	20	0	49	9828
13.	*46	001074-55-1	7444	50	33	1	99	42	20	0	44	9837
14.	*38	025340-17-4	121650	35	57	1	51	47	14	0	41	9720
15.	*35	000098-82-8	4141	47	33	0	68	52	11	15	43	9544
16.	27	029634-38-6	60352	43	53	0	72	60	8	0	39	9656
17.	*25	000095-63-6	120031	37	45	0	63	62	7	22	43	8767
18.	*25	000108-67-8	120035	37	44	0	62	62	7	14	43	8586
19.	*22	000098-82-8	120009	41	37	0	65	62	5	10	39	9520
20.	*22	000098-82-8	120007	37	46	1	62	62	5	12	40	9549

STP Compounds

Peak 80; Alkylbenzene



Scan 508 (12.359 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	431	65.90	39	91.00	578	112.00	93
46.20	18	67.00	173	92.80	101	115.00	233
49.95	64	68.00	74	98.20	35	118.95	2706
50.95	174	71.80	18	101.95	55	119.95	260
51.95	137	74.05	99	102.95	211	120.95	50
53.00	218	74.95	104	103.95	112	125.05	21
56.00	83	76.95	231	105.00	327	128.05	50
58.90	72	78.05	89	106.00	76	134.00	698
62.90	150	81.00	143	108.00	19	135.00	78
63.90	44	83.90	260	109.05	13		
65.00	109	88.90	50	111.05	14		

STP Compounds

Scan 508 (12.359 min): S0344.D

PBM Search of library F:\LIBRARY.L

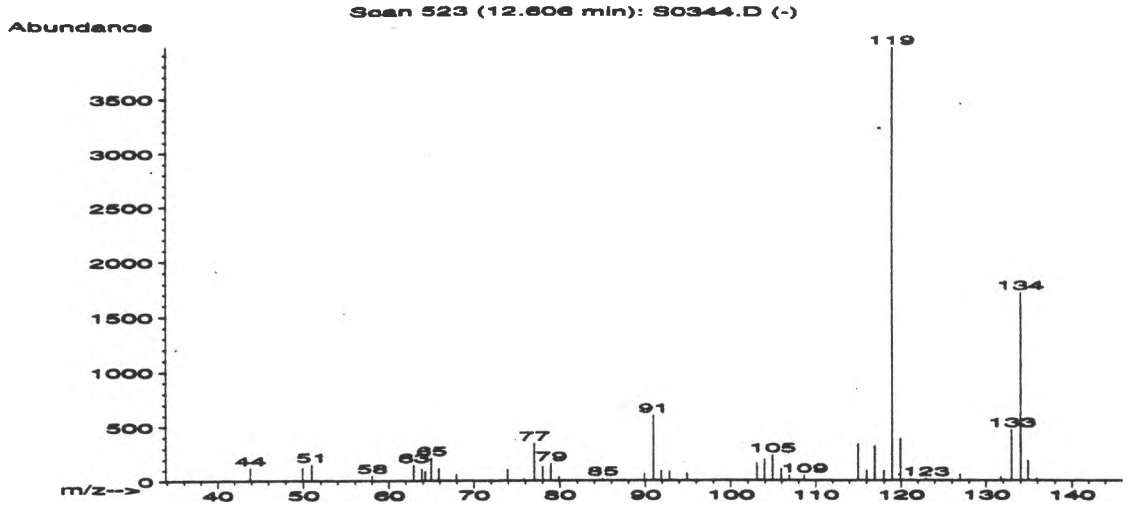
	Name	MolWt	Formula	Qual
1.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	87
2.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	87
3.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	87
4.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	87
5.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	83
6.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	83
7.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	83
8.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	83
9.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	83
10.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	83
11.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	83
12.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	81
13.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	80
14.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	80
15.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	74
16.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	74
17.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	74
18.	Benzene, (1,1-dimethylethyl)-	134	C10H14	74
19.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	72
20.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	72

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000933-98-2	121654	69	20	0	76	11	54	0	76	9947
2.	*87	002870-04-4	121660	68	21	0	94	11	54	21	70	9934
3.	*87	001758-88-9	121657	65	28	0	81	11	54	0	64	9932
4.	*87	000874-41-9	7452	68	21	0	94	11	54	26	70	9916
5.	*83	000934-80-5	121663	65	26	0	89	11	50	12	56	9929
6.	*83	001758-88-9	121658	58	34	0	66	13	50	0	56	9892
7.	*83	001758-88-9	7453	58	34	0	77	11	50	0	56	9924
8.	*83	000874-41-9	121656	62	26	0	94	11	50	14	55	9916
9.	*83	000933-98-2	121651	64	26	0	84	11	50	12	56	9933
10.	*83	000933-98-2	121653	64	26	0	92	11	50	17	56	9922
11.	*83	000934-80-5	121665	70	21	0	94	11	50	2	58	9936
12.	*81	000527-84-4	121625	67	21	0	92	18	49	0	64	9877
13.	*80	000934-80-5	7455	57	34	0	88	11	48	0	49	9937
14.	*80	000934-80-5	121662	57	34	0	88	11	48	0	49	9937
15.	*74	000527-84-4	7445	62	27	0	93	18	44	0	56	9874
16.	*74	000535-77-3	121630	58	34	0	92	18	44	0	56	9880
17.	*74	000099-87-6	121631	62	26	0	93	20	44	0	56	9872
18.	*74	000098-06-6	121609	61	28	1	91	20	44	0	56	9874
19.	*72	000527-84-4	121624	57	35	0	93	18	42	0	49	9874
20.	*72	000933-98-2	7451	53	39	0	75	16	42	0	49	9915

86

STP Compounds

Peak ~~99~~ Cymene



Scan 523 (12.606 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.85	123	75.80	20	103.05	162	119.95	387
49.95	121	77.05	346	103.95	199	122.95	19
50.95	151	78.05	133	104.90	238	126.95	58
58.00	48	79.00	161	105.90	111	131.75	34
62.90	149	79.90	35	106.90	48	133.00	472
63.90	111	84.95	20	108.65	47	134.00	1722
64.25	88	89.90	65	115.00	339	134.90	184
65.00	212	91.00	603	116.00	92	135.90	20
65.90	115	91.90	91	116.95	322		
67.95	60	92.85	86	117.95	92		
73.95	107	94.95	66	118.95	3975		

STP Compounds

Scan 523 (12.606 min): S0344.D

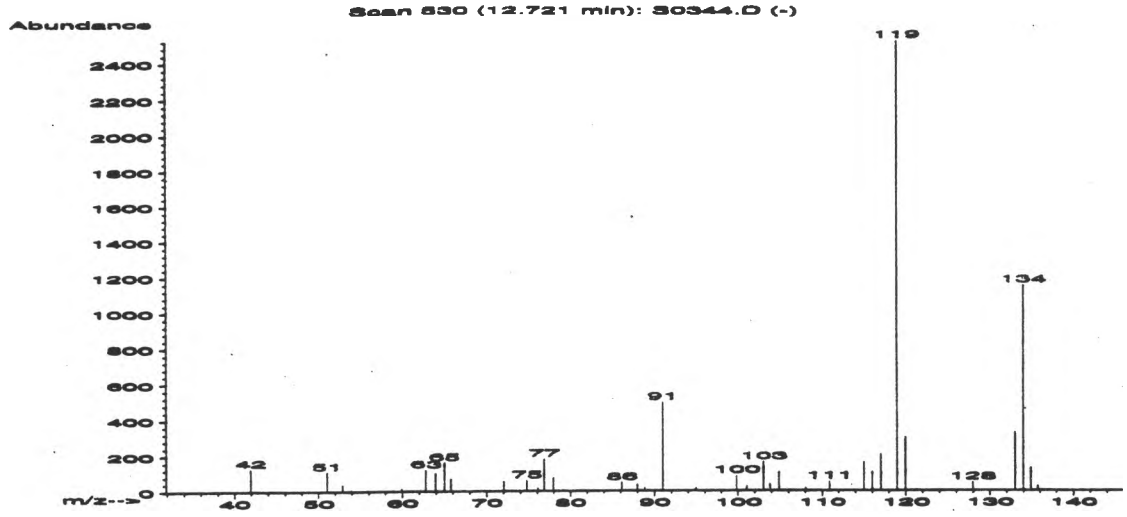
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	94
2.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	94
3.	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	94
4.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	94
5.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	94
6.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	93
7.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	91
8.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
9.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	91
10.	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	91
11.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	91
12.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
13.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	90
14.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	90
15.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	90
16.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	90
17.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	90
18.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	90
19.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	90
20.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	90

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000527-53-7	121672	79	12	0	78	4	70	0	93	9946
2.	*94	000527-53-7	7458	79	12	0	78	4	70	0	93	9946
3.	*94	000488-23-3	7457	82	10	0	82	4	70	0	93	9966
4.	*94	000095-93-2	7459	84	13	1	76	5	70	0	91	9940
5.	*94	000095-93-2	121677	84	13	1	76	5	70	0	91	9941
6.	*93	001758-88-9	7453	81	12	1	88	7	66	0	90	9912
7.	*91	000934-80-5	121664	69	20	1	94	5	62	0	76	9891
8.	*91	000095-93-2	121676	85	5	0	81	4	62	4	80	9874
9.	*91	000933-98-2	121653	69	22	1	94	5	62	0	76	9893
10.	*91	000488-23-3	121669	76	16	0	78	4	62	0	81	9949
11.	*91	000934-74-7	121668	76	16	0	72	5	62	37	76	9923
12.	*91	000095-93-2	121674	82	10	1	96	4	62	16	80	9883
13.	*90	000535-77-3	121630	71	22	0	82	8	59	38	76	9783
14.	*90	002870-04-4	121660	76	15	0	91	7	59	40	81	9841
15.	*90	000933-98-2	121651	71	22	1	90	8	59	40	76	9879
16.	*90	002870-04-4	121659	76	15	0	91	7	59	35	81	9833
17.	*90	000099-87-6	121635	75	14	0	91	10	59	39	81	9800
18.	*90	000535-77-3	121628	70	19	0	86	8	59	34	76	9776
19.	*90	002870-04-4	7454	76	15	0	89	10	59	39	81	9847
20.	*90	000874-41-9	7452	76	15	0	92	7	59	38	81	9856

STP Compounds

Peak 81; Alkylbenzene



Scan 530 (12.721 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	126	72.05	55	101.05	25	119.95	298
51.05	108	74.80	60	103.05	163	127.95	47
52.90	36	76.10	16	103.80	36	133.00	328
53.95	9	76.85	181	104.90	104	134.00	1150
55.85	1	77.95	74	108.05	15	134.90	127
59.00	2	86.15	47	109.05	3	135.75	27
59.90	15	88.00	35	110.90	53		
62.75	120	88.90	16	115.00	159		
63.90	101	91.00	495	116.00	105		
65.00	161	94.95	15	117.05	205		
65.75	70	99.85	84	118.95	2524		

STP Compounds

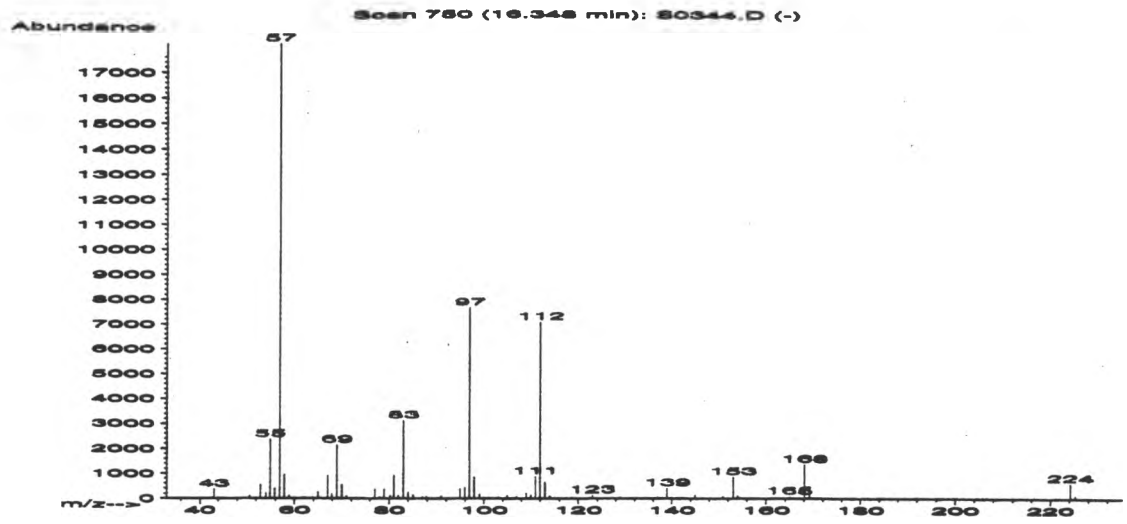
Scan 530 (12.721 min): S0344.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	91
2.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
3.	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	91
4.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	91
5.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
6.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	91
7.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	91
8.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	87
9.	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	87
10.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	87
11.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	87
12.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	87
13.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	87
14.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	87
15.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	87
16.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	87
17.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	87
18.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	87
19.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	86
20.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	86

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000527-53-7	7458	72	22	1	99	4	62	14	70	9960
2.	*91	000095-93-2	121677	67	29	1	70	5	62	0	64	9951
3.	*91	000488-23-3	7457	66	27	1	89	4	62	0	64	9973
4.	*91	000527-53-7	121672	72	22	1	99	4	62	14	70	9960
5.	*91	000095-93-2	7459	67	29	1	70	5	62	0	64	9951
6.	*91	000934-74-7	121668	62	32	1	88	5	60	8	55	9897
7.	*91	000095-93-2	121674	69	28	1	99	4	60	3	59	9914
8.	*87	001758-88-9	121657	60	35	2	99	8	54	0	56	9868
9.	*87	000488-23-3	121671	64	25	0	73	7	54	9	53	9918
10.	*87	001758-88-9	121658	60	34	3	99	8	54	0	56	9921
11.	*87	000933-98-2	7451	60	35	2	99	8	54	0	56	9880
12.	*87	000934-80-5	121661	61	32	1	92	7	54	6	55	9893
13.	*87	001758-88-9	7453	60	34	2	99	8	54	0	56	9886
14.	*87	002870-04-4	7454	61	30	2	90	10	54	11	55	9816
15.	*87	000095-93-2	121676	59	31	0	68	7	54	0	56	9901
16.	*87	000527-53-7	121673	59	34	0	70	7	54	0	56	9914
17.	*87	000095-93-2	121675	60	37	1	77	7	54	0	56	9932
18.	*87	000934-74-7	7456	60	36	2	99	7	54	0	56	9934
19.	*86	000934-74-7	121667	56	39	1	92	8	53	3	49	9910
20.	*86	002870-04-4	121660	55	35	1	92	10	53	10	49	9803

Peak 82; Unidentified Alkene



Scan 750 (16.348 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	366	58.90	114	77.00	366	88.95	20
49.30	22	59.95	18	77.95	66	91.00	88
49.95	5	61.65	27	78.95	362	94.95	387
50.70	116	63.90	48	80.25	120	95.95	437
51.95	44	65.00	257	81.00	929	96.95	7656
52.95	549	67.00	908	81.95	120	97.95	876
54.05	220	67.95	179	83.00	3121	99.05	172
54.95	2367	68.95	2143	84.00	253	99.95	42
55.90	404	69.95	543	85.00	147	100.95	43
56.90	18107	70.90	102	87.00	75	103.05	59
57.90	949	72.95	33	87.90	84	104.95	128

Scan 750 (16.348 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	93	127.30	17	152.05	34		
109.00	207	128.90	51	153.05	859		
110.00	153	132.90	15	154.00	106		
111.00	890	134.95	4	164.90	83		
112.00	7074	136.90	67	168.05	1352		
113.00	642	137.95	24	169.05	205		
114.00	112	139.00	408	224.20	600		
118.70	60	140.00	47	225.20	107		
122.30	30	140.95	31				
122.95	141	144.95	137				
125.05	18	150.95	90				

STP Compounds

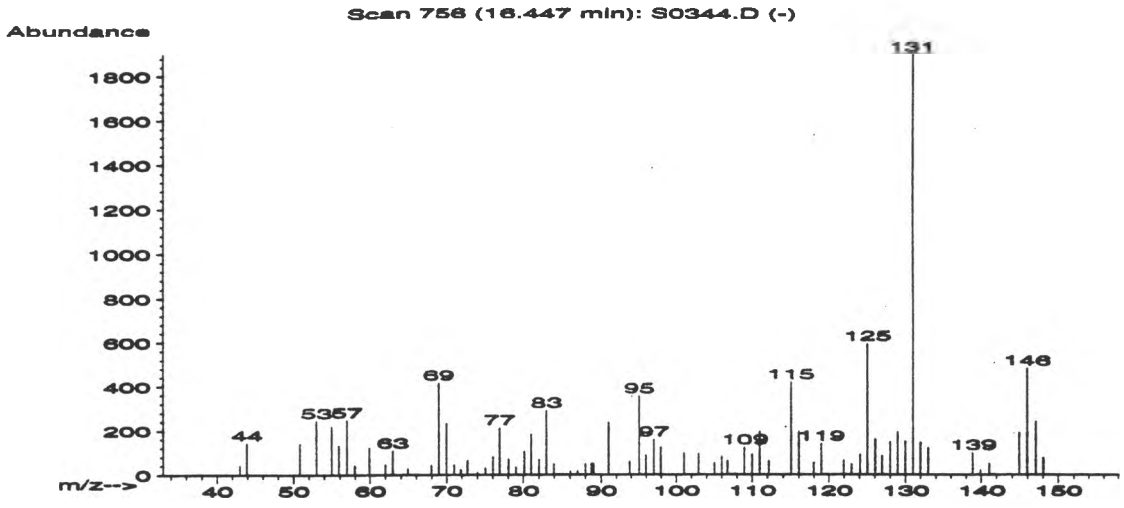
Scan 750 (16.348 min): S0344.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Propene, 2-methyl-, trimer	168	C12H24	49
2.	1-Propene, 2-methyl-, tetramer	224	C16H32	43
3.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	32
4.	3,3,7,7-Tetramethyl-1,5-diazabicyclo[3.3	168	C10H20N2	25
5.	2-Undecene, 5-methyl-	168	C12H24	16
6.	6-Undecen-3-one, 5-butyl-2,2-dimethyl-,	252	C17H32O	16
7.	6-Tridecene, 2,2,4,10,12,12-hexamethyl-7	392	C28H56	8
8.	1-Octadecanol	270	C18H38O	8
9.	1-Octanol, 5,7,7-trimethyl-2-(1,3,3-trim	270	C18H38O	8
10.	1-Pentene, 4,4-dimethyl-	98	C7H14	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	007756-94-7	20739	54	26	2	99	36	23	0	49	9496
2.	43	015220-85-6	46067	43	58	1	65	43	18	1	38	9374
3.	*32	000107-39-1	2689	41	47	3	95	47	9	6	31	9599
4.	25	002940-98-9	125769	34	66	1	70	40	7	0	13	9176
5.	*16	056851-34-4	125795	29	68	3	99	60	3	0	33	9021
6.	16	055976-05-1	57547	39	80	0	70	58	3	0	33	9313
7.	8	055255-73-7	96609	34	90	2	54	69	1	0	22	9322
8.	8	000112-92-5	132222	36	78	0	13	69	1	0	25	8209
9.	8	036400-98-3	63741	36	79	2	91	67	1	0	21	8916
10.	7	000762-62-9	117800	34	39	1	99	76	1	0	22	8653

Peak 29; Unidentified C11H14



Scan 756 (16.447 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	41	62.90	107	76.90	213	88.75	50
43.90	143	64.85	27	78.05	70	89.00	47
50.80	139	67.95	42	79.00	34	91.00	238
52.95	243	68.95	415	80.15	105	93.80	58
53.90	1	69.95	233	81.00	184	95.05	354
54.95	218	70.95	43	82.00	67	95.95	87
55.90	133	71.85	22	83.00	290	97.00	159
56.95	246	72.70	63	83.95	46	97.95	124
57.95	42	74.00	10	86.05	16	101.05	97
59.90	122	75.05	30	86.95	16	102.95	95
62.00	45	76.05	81	88.00	47	105.00	54

Scan 756 (16.447 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.00	81	121.95	63	133.00	120		
106.75	61	122.95	46	138.90	99		
107.80	5	124.05	91	139.90	19		
109.00	122	125.05	592	141.05	50		
110.00	92	126.05	160	144.95	191		
111.00	195	126.95	85	145.95	483		
112.15	59	128.00	148	147.05	241		
115.00	418	129.00	194	148.05	75		
116.00	195	130.00	150				
117.95	54	131.00	1900				
119.00	140	132.00	144				

STP Compounds

Scan 756 (16.447 min): S0344.D

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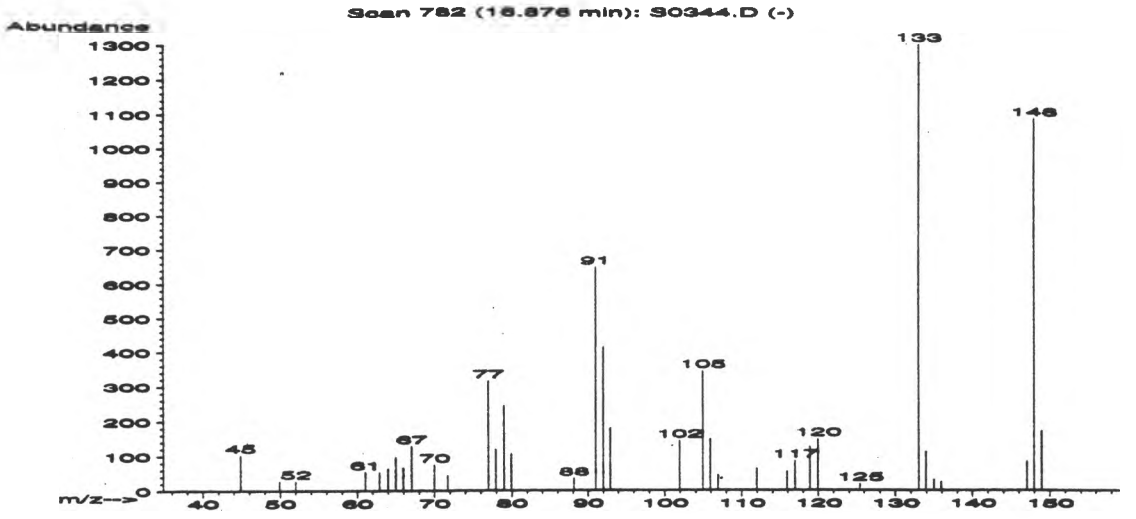
	Name	MolWt	Formula	Qual
1.	1H-Indene, 2,3-dihydro-4,7-dimethyl-	146	C11H14	70
2.	Benzene, (2-methyl-1-butenyl)-	146	C11H14	62
3.	1H-Indene, 2,3-dihydro-4,7-dimethyl-	146	C11H14	58
4.	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	146	C11H14	52
5.	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	146	C11H14	52
6.	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	146	C11H14	52
7.	1H-Indene, 2,3-dihydro-1,6-dimethyl-	146	C11H14	52
8.	1H-Indene, 2,3-dihydro-1,1-dimethyl-	146	C11H14	50
9.	1H-Indene, 2,3-dihydro-1,2-dimethyl-	146	C11H14	43
10.	Naphthalene, 1,2,3,4-tetrahydro-5-methyl	146	C11H14	43
11.	Indan, 5,6-dimethyl-	146	C11H14	38
12.	1H-Indene, 2,3-dihydro-4,6-dimethyl-	146	C11H14	38
13.	Benzene, (3-methyl-2-butenyl)-	146	C11H14	38
14.	1H-Indene, 2,3-dihydro-1,3-dimethyl-	146	C11H14	38
15.	4-D-QUINAZOLINE	130	C8H5DN2	38
16.	1H-Indene, 2,3-dihydro-4,7-dimethyl-	146	C11H14	38
17.	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	35
18.	1H-Indene, 2,3-dihydro-4,6-dimethyl-	146	C11H14	35
19.	2-Oxazolidinethione, 4,4-dimethyl-	131	C5H9NOS	35
20.	Naphthalene, 1,2,3,4-tetrahydro-5-methyl	146	C11H14	30

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*70	006682-71-9	123238	74	22	0	68	28	41	22	66	9227
2.	*62	056253-64-6	11493	65	35	0	67	27	36	25	53	9065
3.	*58	006682-71-9	123237	58	41	0	66	31	32	0	56	9337
4.	*52	001559-81-5	123240	54	44	1	66	35	27	0	49	9340
5.	*52	001559-81-5	123239	48	53	1	66	35	27	0	46	9358
6.	*52	001559-81-5	11525	55	46	1	66	32	27	0	49	9359
7.	*52	017059-48-2	11521	55	39	0	66	33	27	0	49	9359
8.	*50	004912-92-9	11518	35	57	1	99	33	25	5	40	9241
9.	*43	017057-82-8	11519	53	48	0	66	48	18	0	49	9385
10.	*43	002809-64-5	123245	51	52	1	66	48	18	0	46	9357
11.	*38	001075-22-5	11524	48	53	0	57	53	14	0	46	9282
12.	*38	001685-82-1	123236	54	46	0	54	53	14	0	49	9290
13.	*38	004489-84-3	11494	49	53	0	51	53	14	0	46	9180
14.	*38	004175-53-5	11520	45	50	0	63	53	14	0	44	9364
15.	*38	013221-69-7	6525	50	48	0	94	55	14	0	46	8807
16.	*38	006682-71-9	11523	54	45	0	63	53	14	0	49	9288
17.	*35	018321-36-3	11502	33	65	0	55	55	11	0	41	9339
18.	*35	001685-82-1	11522	41	57	0	57	53	11	0	39	9320
19.	*35	054013-55-7	6640	38	43	0	94	55	11	19	40	8792
20.	*30	002809-64-5	123244	56	48	1	34	60	9	0	49	8740

STP Compounds

Peak 83; Alkyl benzene



Scan 782 (16.876 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.85	103	76.95	317	106.90	45	147.05	85
49.90	27	77.95	118	111.95	63	147.95	1088
52.00	28	79.00	244	115.90	55	148.95	172
61.05	54	79.90	106	116.95	86		
62.90	53	88.15	35	118.90	126		
64.00	63	91.00	649	119.95	148		
65.00	97	92.00	413	125.45	19		
65.95	67	92.95	180	133.00	1301		
67.00	128	101.95	143	133.95	111		
70.00	75	104.95	345	135.00	31		
71.70	45	105.90	148	135.90	25		

STP Compounds

Scan 782 (16.876 min): S0344.D

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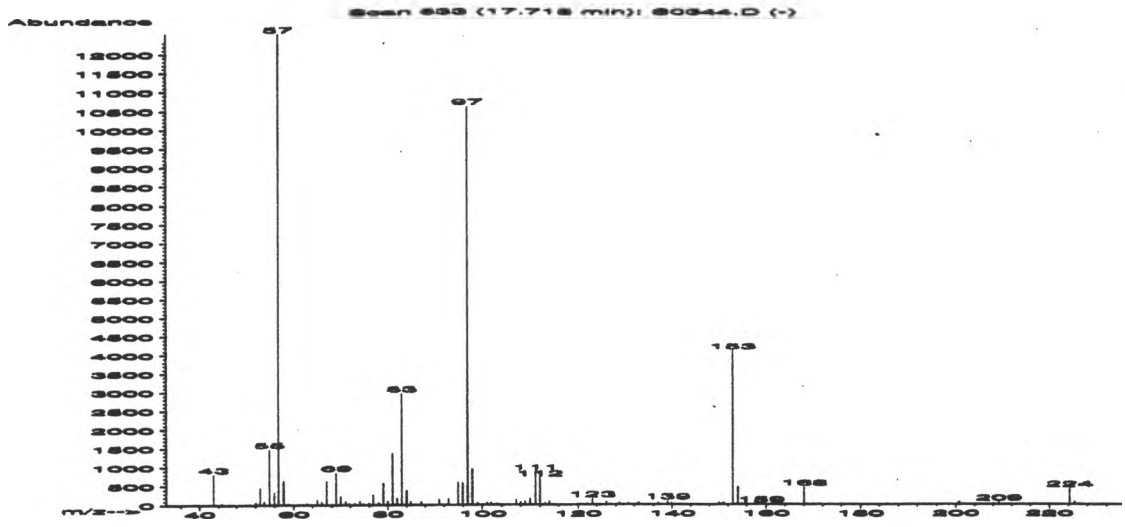
	Name	MolWt	Formula	Qual
1.	Phenol, p-(2-methylallyl)-	148	C10H12O	83
2.	Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	68
3.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	64
4.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	59
5.	2H-1-Benzopyran, 3,4-dihydro-2-methyl-	148	C10H12O	59
6.	Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	59
7.	6-METHYL-4-INDANOL	148	C10H12O	59
8.	6-Methylspiro[4.4]nona-2,6-dien-1-one	148	C10H12O	59
9.	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	58
10.	1,4-DIMETHYL-3,4-DIHYDRO-PYRROLO(1,2-A)P	148	C9H12N2	53
11.	Benzene, 1-(1,1-dimethylethyl)-3-methyl-	148	C11H16	53
12.	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	53
13.	Benzene, pentamethyl-	148	C11H16	50
14.	2,5-DIMETHYL-3-TRANS-PROPENYLPYRAZINE	148	C9H12N2	47
15.	Benzofuran, 5-methoxy-	148	C9H8O2	47
16.	Benzene, diethylmethyl-	148	C11H16	40
17.	2-Butanone, 3-phenyl-	148	C10H12O	38
18.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	38
19.	2-Butanone, 4-phenyl-	148	C10H12O	38
20.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	033641-78-0	12027	61	50	1	83	14	50	0	56	9662
2.	*68	000089-74-7	123394	63	33	0	79	21	40	20	53	8999
3.	*64	004218-48-8	12115	47	45	0	68	25	37	20	47	8702
4.	*59	000098-51-1	12112	42	54	2	99	25	33	17	39	8473
5.	*59	013030-26-7	12060	49	64	1	75	21	33	0	39	9521
6.	*59	020944-88-1	12026	46	58	1	68	25	33	4	39	9446
7.	*59	020294-32-0	12091	36	71	2	99	25	33	0	39	9460
8.	*59	089950-43-6	12058	56	31	0	69	25	33	5	40	9415
9.	*58	002050-24-0	12119	54	45	1	71	26	32	27	49	7656
10.	*53	064608-68-0	11989	44	74	3	87	29	28	10	39	9249
11.	*53	001075-38-3	12111	33	61	1	67	30	28	15	40	8550
12.	*53	000122-03-2	12002	48	52	1	83	27	28	4	39	9058
13.	*50	000700-12-9	123455	44	54	2	99	31	25	16	43	9181
14.	*47	000000-00-0	11975	44	68	2	86	37	20	0	40	9268
15.	*47	013391-28-1	11952	36	70	2	61	39	20	0	39	9280
16.	*40	025550-13-4	12120	40	59	1	79	32	16	10	37	8357
17.	*38	000769-59-5	12024	48	59	1	66	53	14	0	46	6766
18.	*38	004706-90-5	123452	33	58	3	264	50	14	0	41	8587
19.	*38	002550-26-7	12025	43	67	2	88	50	14	0	40	6602
20.	35	000098-51-1	123447	42	52	0	71	53	11	21	43	8189

STP Compounds

Peak 84; Branched Alkene



Scan 833 (17.718 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	798	57.90	626	72.95	56	84.05	372
44.80	51	58.95	24	74.05	109	84.95	86
46.45	28	62.85	41	74.80	28	86.00	24
49.95	30	65.00	141	75.95	53	87.15	88
50.80	18	66.00	87	76.90	266	91.00	147
52.05	83	67.00	627	78.05	73	93.00	168
52.95	444	67.95	23	79.05	577	93.75	5
53.85	93	68.95	844	80.00	105	94.95	593
54.95	1464	70.00	223	81.00	1355	95.95	574
56.00	326	71.00	98	81.95	177	96.95	10583
56.90	12545	71.80	45	83.00	2953	97.95	940

Scan 833 (17.718 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.00	57	114.00	97	139.00	87	177.90	20
101.05	63	114.90	21	139.90	46	208.15	26
101.80	59	120.20	21	142.05	27	209.25	48
102.95	35	120.70	23	150.05	61	224.20	406
107.00	142	121.95	37	150.80	49	225.20	74
108.00	80	123.00	151	151.05	50		
108.95	98	126.05	84	153.05	4090		
109.95	176	128.85	52	154.15	458		
111.05	859	130.75	42	154.95	19		
112.00	699	132.90	62	158.95	6		
113.10	54	137.00	59	168.05	442		

STP Compounds

Scan 833 (17.718 min): S0344.D

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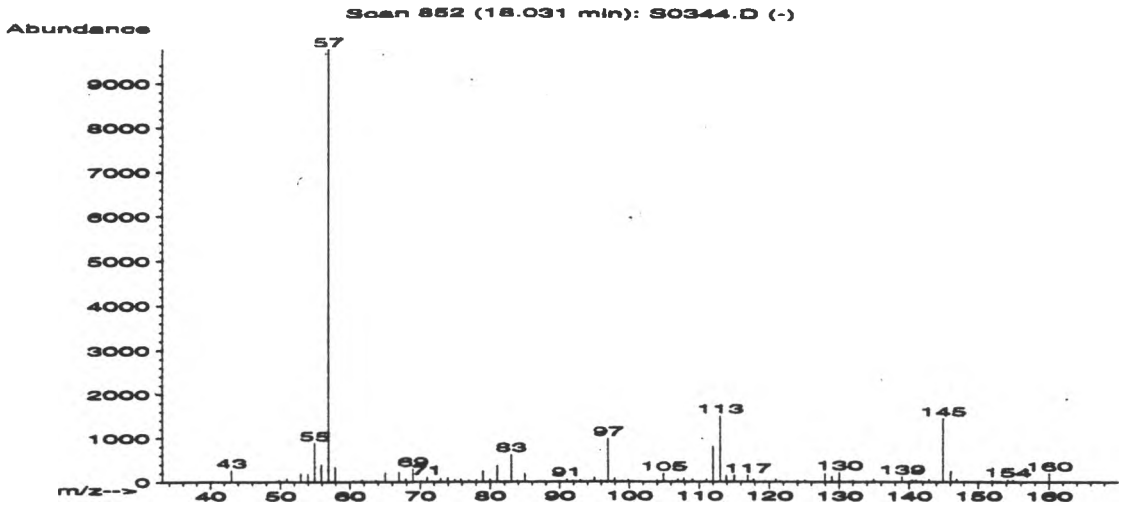
	Name	MolWt	Formula	Qual
1.	Cyclohexane, 1,2-dimethyl-3-pentyl-4-pro	224	C16H32	58
2.	1-Propene, 2-methyl-, trimer	168	C12H24	45
3.	Thiophene, 3-ethyl-	112	C6H8S	43
4.	Thiophene, 2-ethyl-	112	C6H8S	43
5.	Thiophene, 2-ethyl-	112	C6H8S	43
6.	Thiophene, 2-hexyl-	168	C10H16S	43
7.	Cyclohexane, 1,1-dimethyl-	112	C8H16	43
8.	3-ETHYL-4-METHYL-2-PYRAZOLINE	112	C6H12N2	40
9.	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	38
10.	Cycloheptane, bromo-	176	C7H13Br	38
11.	Furan, 2,3-dihydro-4-(1-methylpropyl)-,	126	C8H14O	37
12.	Carbonic acid, dithio-, S-methyl O-(2-me	204	C9H16OS2	32
13.	Thiophene, 2-hexyl-	168	C10H16S	32
14.	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	32
15.	Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	32
16.	Thiophene, 3-ethyl-	112	C6H8S	23
17.	4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	23
18.	Furan, 2,5-dihydro-2,2,4-trimethyl-	112	C7H12O	23
19.	Cyclohexane, 1-bromo-3-methyl-	176	C7H13Br	23
20.	5-Nonen-4-one	140	C9H16O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	062376-17-4	46075	48	91	3	71	29	32	0	44	6232
2.	45	007756-94-7	20739	51	34	2	92	23	19	3	36	8905
3.	*43	001795-01-3	118998	38	36	1	59	44	18	14	42	5882
4.	*43	000872-55-9	2496	44	31	3	74	44	18	18	40	5892
5.	*43	000872-55-9	118996	39	36	3	73	44	18	13	42	5913
6.	*43	018794-77-9	125766	34	45	2	76	46	18	23	43	6100
7.	*43	000590-66-9	2721	37	43	2	58	44	18	10	39	7030
8.	40	054490-63-0	2518	41	54	2	58	34	16	9	31	5532
9.	*38	053783-91-8	2602	36	55	2	79	40	14	5	32	6386
10.	38	002404-35-5	23642	44	31	1	76	49	14	9	38	6159
11.	37	034379-54-9	5350	41	44	0	58	44	13	0	33	6210
12.	32	015288-13-8	36213	49	45	1	65	49	9	10	31	6158
13.	*32	018794-77-9	125767	35	43	1	60	46	9	16	37	6074
14.	32	006294-40-2	23641	38	43	2	74	49	9	0	33	6159
15.	32	006294-39-9	23639	40	35	0	74	46	9	6	35	6273
16.	23	001795-01-3	2497	30	46	2	83	47	6	6	28	5938
17.	*23	043183-55-7	667	28	52	1	84	47	6	0	29	6178
18.	23	023230-79-7	2621	33	53	0	68	47	6	0	25	6224
19.	23	013905-48-1	23640	33	47	3	76	49	6	0	25	6159
20.	* 8	032064-77-0	9333	31	46	1	52	68	1	0	29	6204

Peak 85; Unidentified Branched Alkene



Scan 852 (18.031 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	267	62.90	17	73.95	102	85.00	186
49.85	40	63.65	44	74.95	55	91.00	60
50.95	77	63.90	16	75.85	63	91.90	27
52.95	183	65.00	166	76.95	44	92.95	42
53.95	171	66.00	9	78.05	57	94.95	102
54.95	875	67.00	223	78.95	248	95.95	24
55.90	400	67.90	66	80.00	62	96.95	988
56.90	9782	68.95	295	81.00	372	97.95	81
57.90	334	70.05	14	82.00	15	98.95	22
60.50	23	71.00	106	83.00	624	99.90	56
61.75	46	72.95	74	83.90	31	103.95	31

Scan 852 (18.031 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.90	194	120.95	66	140.20	24	154.15	60
107.00	61	124.05	35	140.50	51	154.90	44
107.80	88	125.05	39	141.05	41	160.00	200
109.00	63	126.05	1	141.80	17		
111.00	62	127.95	190	142.95	64		
112.00	807	128.95	131	144.95	1448		
113.00	1505	130.00	215	146.05	240		
113.90	141	132.00	44	146.95	65		
115.00	153	133.90	19	148.05	17		
116.95	151	134.90	64	152.00	36		
117.80	66	139.00	122	153.05	8		

STP Compounds

Scan 852 (18.031 min): S0344.D

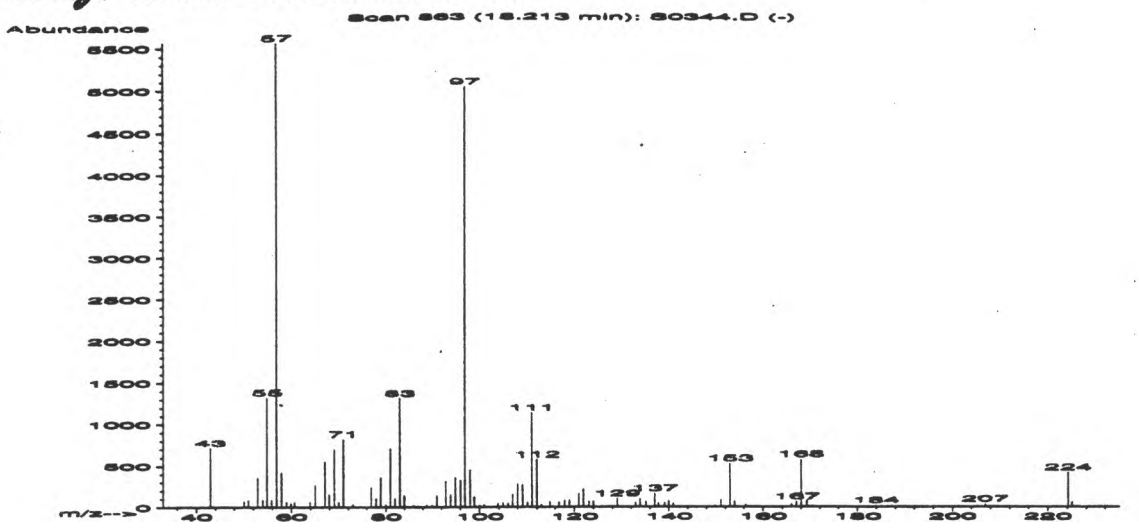
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Propene, 2-methyl-, tetramer	224	C16H32	35
2.	3-Hexanethiol, 3-ethyl-	146	C8H18S	33
3.	2-HEXENE, 5,5-DIMETHYL-	112	C8H16	32
4.	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	32
5.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	32
6.	Nonane, 3-methyl-	142	C10H22	25
7.	Octane, 2,6-dimethyl-	142	C10H22	25
8.	2-Propanamine, N,N'-1,2-ethanediylideneb	168	C10H20N2	23
9.	Undecane, 6,6-dimethyl-	184	C13H28	12
10.	QUINUCLIDINE-3,3-D2	111	C7H11D2N	10
11.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	35	015220-85-6	46067	54	31	1	74	55	11	16	43	9700
2.	33	055956-00-8	11388	31	51	2	99	33	10	0	29	9855
3.	*32	039761-61-0	2675	33	40	2	77	48	9	2	37	9783
4.	*32	039761-61-0	2674	33	40	2	77	48	9	2	37	9783
5.	*32	000107-39-1	119085	34	38	1	79	48	9	8	37	9770
6.	25	005911-04-6	10243	34	60	2	75	44	7	0	22	9829
7.	25	002051-30-1	122741	35	56	2	85	44	7	0	22	9833
8.	23	030834-74-3	20560	34	42	1	77	48	6	1	23	9771
9.	12	017312-76-4	27765	39	58	2	64	59	2	0	29	9812
10.	*10	033259-51-7	2381	29	48	1	43	62	1	0	29	5168
11.	* 8	000107-39-1	119086	29	40	2	33	70	1	0	29	9696

STP Compounds

Peak 86; Unidentified Alkene, Branched



Scan 863 (18.213 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	715	60.65	59	76.95	240	90.00	20
50.05	65	62.80	6	77.95	103	91.00	138
50.95	82	63.90	63	78.95	363	92.95	315
52.95	352	65.00	262	80.00	26	93.95	150
54.05	86	67.00	552	80.95	705	94.95	361
54.95	1317	67.90	150	82.00	102	96.05	326
55.90	84	69.00	696	83.00	1311	96.95	5030
56.90	5563	69.95	58	84.00	141	98.05	449
57.90	416	70.95	818	86.00	21	98.95	118
58.95	59	72.95	30	87.00	14	100.05	19
59.90	42	74.95	2	88.80	24	100.95	29

Scan 863 (18.213 min): S0344.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.80	44	116.80	58	137.00	167	167.05	66
104.90	52	117.95	80	137.75	41	168.05	577
105.90	41	118.95	82	139.10	50	169.20	80
106.90	151	120.95	163	140.00	69	183.90	20
108.00	277	121.95	216	140.90	40	206.90	34
109.00	269	123.05	65	149.80	17	224.20	416
110.00	54	123.95	70	151.05	87	225.05	54
111.00	1139	129.00	103	153.05	526		
112.10	578	132.95	51	153.95	67		
113.00	29	133.90	95	156.40	29		
114.90	58	135.10	62	165.95	36		

STP Compounds

Scan 863 (18.213 min): S0344.D

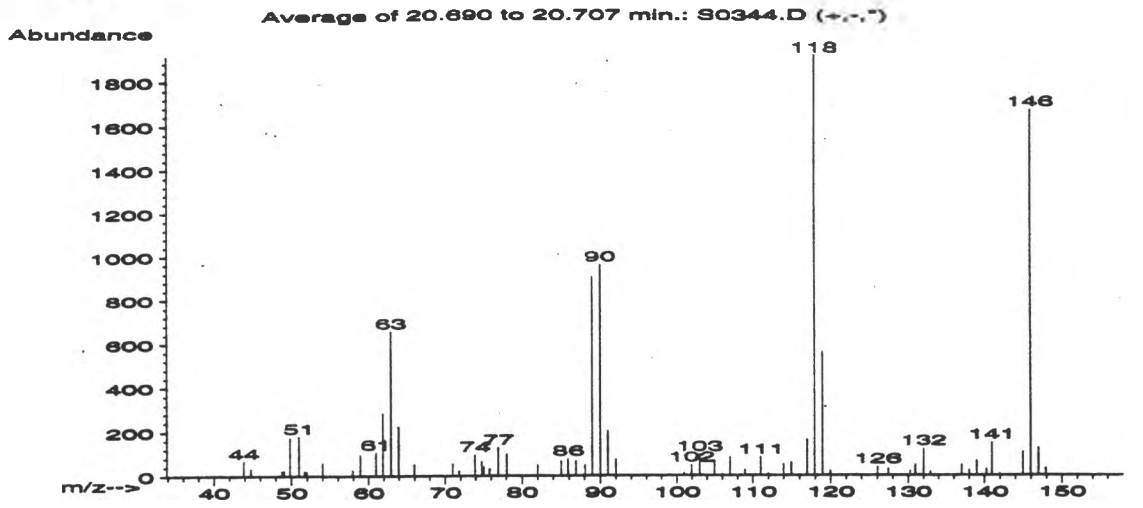
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Pyrazole-1-carboxaldehyde, 4-ethyl-4,	168	C9H16N2O	46
2.	1-Propene, 2-methyl-, tetramer	224	C16H32	40
3.	Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	38
4.	Cyclohexane, 1,1-dimethyl-	112	C8H16	38
5.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	38
6.	2-Acetyl-cis-indazolidin-3-one	182	C9H14N2O2	38
7.	1-METHYL-4-N-PENTYLCYCLOHEXANE (CIS+TRAN	168	C12H24	38
8.	Cyclohexane, 1-(cyclohexylmethyl)-2-meth	194	C14H26	37
9.	Cyclohexane, 1-(cyclohexylmethyl)-2-meth	194	C14H26	37
10.	5-Nonen-4-one	140	C9H16O	35
11.	Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	35
12.	Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	35
13.	Cycloheptane, bromo-	176	C7H13Br	27
14.	m-Menthane, (1S,3R)-(+)-	140	C10H20	25
15.	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	25
16.	Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	25
17.	2,4-(D2)MENTH-2-ENE	138	C10H16D2	17
18.	6-Tridecene, 2,2,4,10,12,12-hexamethyl-7	392	C28H56	14
19.	1,1-Di(1,1-dimethylethyl)cyclopropane	154	C11H22	12
20.	1-Pentene, 2,4,4-trimethyl-	112	C8H16	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	054411-09-5	20257	48	38	0	69	45	20	20	44	6530
2.	40	015220-85-6	46067	57	54	1	96	32	16	3	34	8680
3.	*38	054411-02-8	20766	44	41	2	75	48	14	4	39	6606
4.	*38	000590-66-9	2721	41	36	2	63	50	14	11	40	7340
5.	*38	000107-39-1	2689	41	42	3	79	37	14	9	36	8710
6.	38	056700-60-8	26444	38	49	2	87	40	14	11	35	6666
7.	*38	000000-00-0	20767	45	41	2	68	47	14	4	39	6638
8.	37	054823-94-8	32154	60	41	2	71	41	13	4	35	6723
9.	37	054824-04-3	32153	60	40	2	81	43	13	0	35	6689
10.	*35	032064-77-0	9333	35	43	2	90	52	11	0	39	6528
11.	*35	004413-21-2	125607	47	48	2	64	54	11	0	39	6475
12.	35	006294-39-9	23639	46	34	0	62	54	11	8	41	6578
13.	27	002404-35-5	23642	44	38	2	76	56	8	14	41	6466
14.	25	013837-66-6	9509	44	52	3	66	54	7	0	37	6577
15.	*25	053783-91-8	2602	33	62	3	90	45	7	7	29	6700
16.	25	004413-21-2	19749	44	54	2	74	54	7	0	31	6475
17.	17	005256-68-8	8797	41	46	2	62	54	3	7	29	6645
18.	14	055255-73-7	96609	43	82	0	75	68	2	0	39	7986
19.	12	080816-10-0	124361	39	65	3	83	64	2	13	34	7999
20.	*10	000107-39-1	119084	33	52	0	98	78	1	0	41	7784

STP Compounds

Peak [redacted]: Benzopyran-2-one



Average of 20.690 to 20.707 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.85	68	60.95	106	76.95	128	98.95	2
44.80	33	61.90	283	78.05	99	101.00	11
48.80	22	62.95	657	82.00	48	101.95	48
49.05	24	63.95	223	85.00	67	103.00	96
49.85	171	65.95	52	85.90	77	104.95	66
50.95	179	70.95	55	86.90	68	106.00	7
51.70	22	71.80	24	88.05	48	107.00	83
51.95	19	73.90	96	89.00	907	109.00	25
54.00	59	74.80	65	90.00	964	111.05	84
57.90	26	75.05	39	90.95	204	112.00	9
58.90	96	75.80	32	92.00	73	114.00	51

Average of 20.690 to 20.707 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.00	59	137.00	47				
116.95	163	138.00	25				
117.95	1912	139.00	66				
118.95	558	140.25	29				
119.95	20	140.95	150				
126.05	39	141.95	7				
127.45	30	144.95	107				
130.25	21	145.95	1670				
130.90	48	146.95	123				
132.00	121	147.95	33				
132.95	16						

STP Compounds

Average of 20.690 to 20.707 min.: S0344.D
Converted from RTE data file: >S0344:

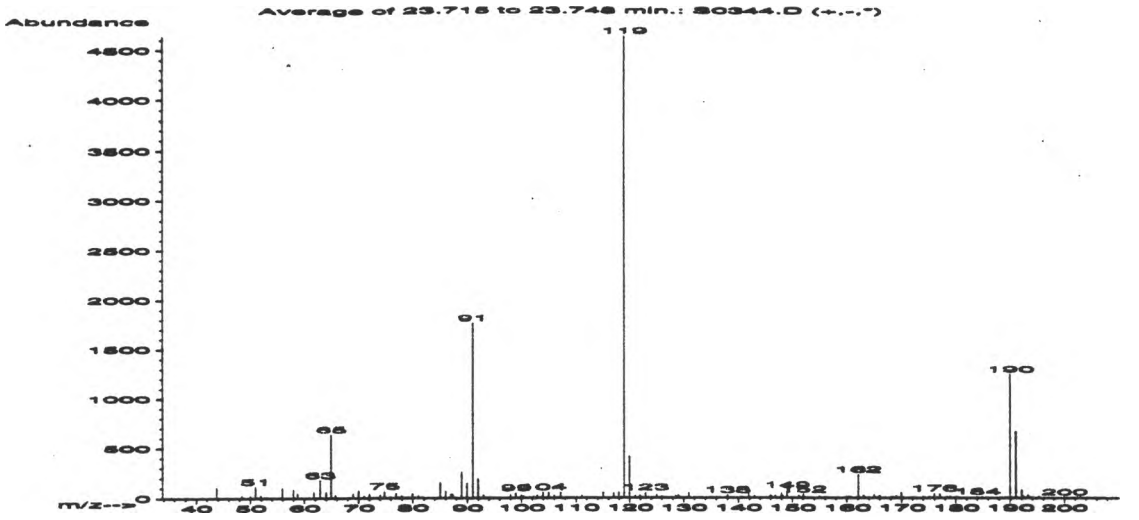
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2H-1-Benzopyran-2-one	146	C9H6O2	94
2.	2H-1-Benzopyran-2-one	146	C9H6O2	94
3.	2H-1-Benzopyran-2-one	146	C9H6O2	93
4.	2H-1-Benzopyran-2-one	146	C9H6O2	93
5.	2H-1-Benzopyran-2-one	146	C9H6O2	91
6.	2H-1-Benzopyran-2-one	146	C9H6O2	90
7.	2H-1-Benzopyran-2-one	146	C9H6O2	90
8.	2H-1-Benzopyran-2-one	146	C9H6O2	81
9.	Benzofuran	118	C8H6O	70
10.	Benzofuran	118	C8H6O	70
11.	Benzofuran	118	C8H6O	70
12.	Benzofuran	118	C8H6O	62
13.	Benzofuran	118	C8H6O	58
14.	1H-Benzimidazole-2-carboxaldehyde	146	C8H6N2O	58
15.	1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	50
16.	4-PHENYLOXAZOLE-2-D	145	C9H6DNO	49
17.	Phthalazin-1-one	146	C8H6N2O	38
18.	1H-Indazole	118	C7H6N2	35
19.	7-CYANO,7-DEUTERO-CYCLOHEPTATRIENE	117	C8H6DN	35
20.	Benzonitrile, 2-amino-	118	C7H6N2	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000091-64-5	123197	81	32	1	99	5	70	0	90	9883
2.	*94	000091-64-5	123196	85	32	1	73	5	70	0	91	9863
3.	*93	000091-64-5	11406	83	35	1	81	7	66	0	87	9887
4.	*93	000091-64-5	123195	84	27	2	99	10	66	58	90	9535
5.	*91	000091-64-5	123199	70	39	2	99	5	62	0	68	9854
6.	*90	000091-64-5	123194	76	39	3	99	7	59	47	74	9778
7.	*90	000091-64-5	123193	89	22	1	99	8	59	31	70	9767
8.	*81	000091-64-5	123201	76	33	0	69	20	49	0	81	9852
9.	*70	000271-89-6	119849	68	35	1	92	30	41	0	76	8147
10.	*70	000271-89-6	3894	67	32	0	99	29	41	0	64	8143
11.	*70	000271-89-6	119848	84	20	1	90	29	41	31	70	8113
12.	*62	000271-89-6	119850	68	37	2	97	30	36	36	58	7934
13.	*58	000271-89-6	119851	52	48	2	94	30	32	8	47	7480
14.	*58	003314-30-5	11320	55	64	3	70	29	32	0	47	9111
15.	*50	000529-34-0	123224	46	56	2	99	35	25	0	39	9388
16.	*49	054020-54-1	11035	44	62	0	58	37	23	0	44	9230
17.	*38	000119-39-1	11332	44	60	1	65	48	14	0	40	8099
18.	*35	000271-44-3	3886	43	57	1	73	54	11	0	40	7191
19.	*35	026902-50-1	3691	36	74	3	99	51	11	0	39	7752
20.	*18	001885-29-6	119835	43	43	1	83	68	3	0	44	6943

STP Compounds

Peak 7



Average of 23.715 to 23.748 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.80	101	61.75	61	75.95	8	89.95	146
48.45	25	62.90	176	76.95	44	91.00	1765
48.75	4	64.00	61	77.95	18	91.95	192
49.95	25	64.95	635	79.95	41	92.95	23
50.90	112	65.75	25	81.00	18	97.95	34
51.90	23	68.95	42	85.00	152	98.95	50
53.90	6	70.00	71	86.00	66	99.95	25
55.95	99	71.00	19	86.95	39	100.20	14
57.95	84	71.95	37	87.25	33	100.45	12
58.75	44	73.95	29	87.80	1	101.80	2
60.90	12	74.80	65	88.95	259	102.20	12

Average of 23.715 to 23.748 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.95	27	119.95	412	138.00	27	149.00	75
103.95	56	121.00	20	140.50	12	151.20	23
105.00	55	121.95	22	141.00	3	152.05	34
106.00	23	122.95	55	141.85	39	155.00	16
107.15	52	125.00	29	142.95	17	156.00	8
111.05	24	126.05	14	144.95	2	160.00	19
115.00	58	128.55	20	145.85	19	160.40	13
115.95	3	129.00	23	146.05	24	160.75	8
116.95	51	130.95	50	146.90	22	162.05	232
117.95	56	132.95	5	147.95	49	163.00	21
118.95	4634	136.05	9	148.20	21	165.00	28

Average of 23.715 to 23.748 min.: S0344.D
Converted from RTE data file: >S0344:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
165.80	10	179.00	14				
166.00	22	180.00	12				
168.05	11	184.00	12				
168.45	7	184.90	11				
169.05	16	185.90	6				
169.90	52	190.00	1247				
174.05	14	191.00	667				
175.10	10	192.05	80				
175.95	45	193.20	26				
177.00	37	195.20	14				
178.40	13	199.95	6				

STP Compounds

Average of 23.715 to 23.748 min.: S0344.D
Converted from RTE data file: >S0344:

PBM Search of library F:\LIBRARY.L

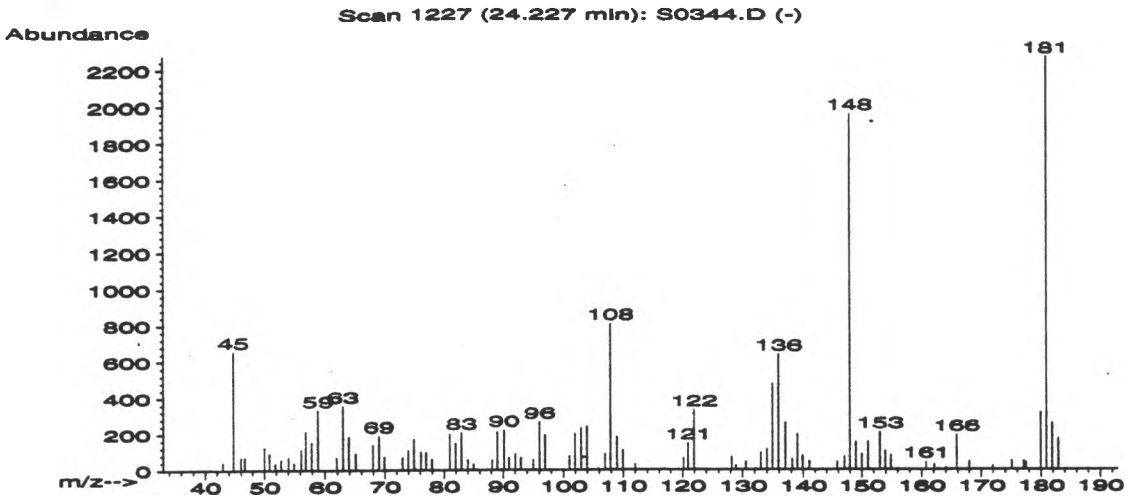
	Name	MolWt	Formula	Qual
1.	Benzamide, N,N-diethyl-3-methyl-	191	C12H17NO	95
2.	Benzamide, N-(1,1-dimethylethyl)-4-methy	191	C12H17NO	64
3.	2,4,5-TRIOXO-1-PHENYLIMIDAZOLIDINE	190	C9H6N2O3	64
4.	N-ISOPROPYL-P-TOLUAMIDE	177	C11H15NO	59
5.	4-Methylimino-toluene	119	C8H9N	53
6.	Ethanone, 2-bromo-1-(4-methylphenyl)-	212	C9H9BrO	50
7.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	50
8.	Benzene, isocyanato-	119	C7H5NO	50
9.	Benzene, isocyanato-	119	C7H5NO	50
10.	Benzene, isocyanato-	119	C7H5NO	50
11.	1H-Benzotriazole	119	C6H5N3	50
12.	1H-Benzotriazole	119	C6H5N3	50
13.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	50
14.	Benzene, isocyanato-	119	C7H5NO	50
15.	Azocine, 2-methoxy-3,5,6,8-tetramethyl-	191	C12H17NO	45
16.	p-Toluic acid, isobutyl ester	192	C12H16O2	42
17.	Benzoyl chloride, 4-methyl-	154	C8H7ClO	42
18.	ACETOPHENONE, DICHLORO-4'-METHYL-	202	C9H8Cl2O	42
19.	Benzoic acid, 4-methyl-, methyl ester	150	C9H10O2	40
20.	Ethanone, 1-(methylphenyl)-	134	C9H10O	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000134-62-3	30397	97	5	1	85	1	72	17	93	9881
2.	*64	042498-32-8	30390	61	40	1	69	22	37	9	49	9685
3.	*64	002211-33-8	29822	46	46	3	75	20	37	7	40	9427
4.	59	002144-17-4	24290	60	34	3	81	24	33	0	39	9610
5.	*53	000000-00-0	3977	43	16	0	71	27	28	15	40	9406
6.	50	000619-41-0	40089	54	45	2	75	31	25	1	38	9604
7.	*50	000140-76-1	119921	37	53	3	96	31	25	5	40	9604
8.	*50	000103-71-9	119906	33	33	1	99	31	25	13	40	9588
9.	*50	000103-71-9	119905	37	29	1	99	31	25	5	40	9593
10.	*50	000103-71-9	119907	40	32	2	92	31	25	9	38	9520
11.	*50	000095-14-7	119895	37	32	2	95	31	25	12	39	9008
12.	*50	000095-14-7	119894	33	35	3	99	31	25	10	39	9346
13.	50	000099-75-2	123608	46	33	2	99	32	25	0	39	9525
14.	*50	000103-71-9	119902	39	34	2	86	31	25	15	38	9553
15.	*45	027153-51-1	30399	35	87	1	73	24	19	0	35	9601
16.	42	029240-30-0	30808	66	24	1	78	27	17	2	37	9549
17.	42	000874-60-2	14274	58	26	3	89	27	17	2	37	9506
18.	42	000000-00-0	35303	69	28	2	84	27	17	1	37	9594
19.	40	000099-75-2	123612	49	32	2	96	34	16	2	36	9585
20.	35	026444-19-9	121574	54	36	0	51	55	11	0	39	9338

STP Compounds

5

Peak 5; 2-(Methylthio)-benzothiazole



Scan 1227 (24.227 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	42	56.90	212	73.00	68	88.15	55
44.80	657	57.90	152	73.95	107	89.00	211
46.05	69	58.90	332	74.95	172	90.15	221
46.70	68	61.90	69	76.10	100	90.95	67
49.95	123	62.90	354	77.00	97	92.05	89
50.85	92	63.90	184	77.95	60	92.95	67
51.80	34	65.00	91	81.00	200	95.00	57
52.80	58	66.95	2	81.95	149	96.05	266
54.05	71	67.95	138	82.95	207	96.95	194
54.95	38	68.95	189	84.00	57	101.00	75
56.15	113	69.90	73	85.00	32	101.95	202

Scan 1227 (24.227 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.95	231	121.95	331	139.00	196	154.90	79
103.95	240	128.20	70	139.90	77	160.75	42
105.90	8	128.90	22	141.00	45	162.15	28
106.95	88	130.50	46	145.80	43	164.00	11
107.90	811	132.10	9	147.05	70	165.85	193
109.00	183	132.95	95	147.95	1959	167.95	46
109.95	107	134.00	113	149.00	152	171.95	19
112.00	29	134.90	476	150.00	87	175.05	48
116.95	6	135.90	639	151.05	154	177.05	47
120.20	65	137.00	260	153.05	209	177.45	41
120.95	146	138.15	58	153.95	103	179.95	318

Scan 1227 (24.227 min): S0344.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
180.90	2275						
181.90	259						
182.90	174						

STP Compounds

Scan 1227 (24.227 min): S0344.D

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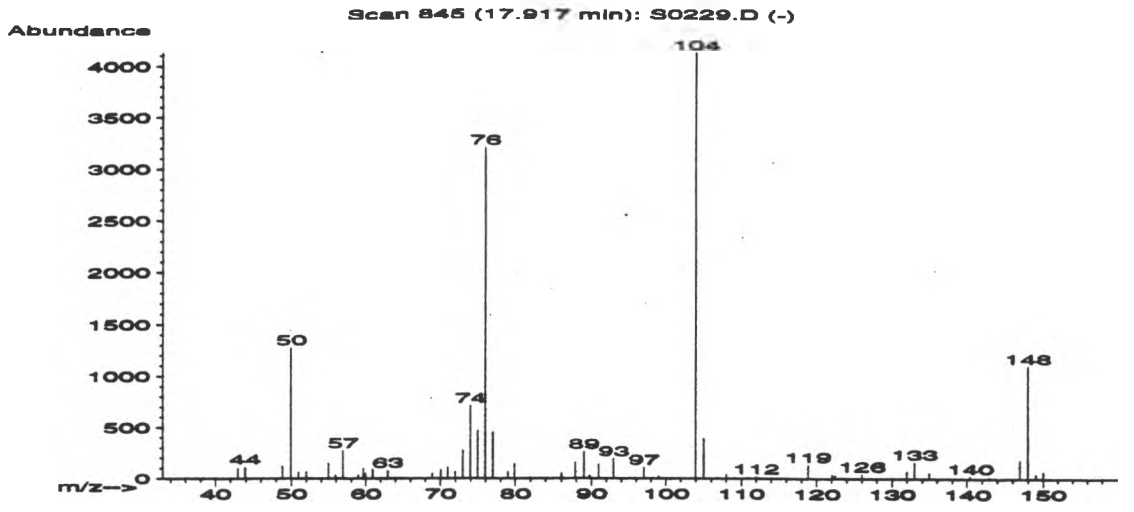
	Name	MolWt	Formula	Qual
1.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	80
2.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	74
3.	5-AMINO-ISO-PHTHALIC ACID	181	C8H7NO4	38
4.	1-Azabicyclo[2.2.2]oct-2-ene-3-carboxyli	181	C10H15NO2	35
5.	1H-Purin-2-amine, 6-(methylthio)-	181	C6H7N5S	35
6.	4-METHYLCARBAZOLE	181	C13H11N	30
7.	2-METHYL-1,2-BENZISOTHIAZOLINE-3-THIONE	181	C8H7NS2	30
8.	1-METHYLCARBAZOLE	181	C13H11N	25
9.	4'-NITRO-PHENYLACETIC ACID	181	C8H7NO4	25
10.	9H-Carbazole, 9-methyl-	181	C13H11N	25
11.	1-METHYLCARBAZOLE	181	C13H11N	25
12.	9H-Carbazole, 2-methyl-	181	C13H11N	25
13.	9H-Carbazole, 2-methyl-	181	C13H11N	22
14.	9H-Fluoren-2-amine	181	C13H11N	22
15.	VANADIUM, BIS(CYCLOPENTADIENYL)-	181	C10H10V	22
16.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	22
17.	4-METHYLCARBAZOLE	181	C13H11N	18
18.	Thiazolo[3,2-a]pyridinium, 2,3-dihydro-8	181	C9H11NOS	16
19.	3-METHYLCARBAZOLE	181	C13H11N	14
20.	3H-1,2-Dithiole-3-thione, 5-methyl-	148	C4H4S3	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000615-22-5	126909	65	65	2	87	14	48	4	45	9807
2.	*74	000615-22-5	126908	84	46	1	80	18	44	0	62	9888
3.	*38	000000-00-0	25989	49	67	1	71	53	14	0	46	7707
4.	*35	006238-32-0	26101	34	73	0	69	55	11	15	39	7564
5.	*35	001198-47-6	25939	44	78	3	67	52	11	0	40	7625
6.	*30	003770-48-7	126940	60	48	1	85	62	9	0	51	6044
7.	*30	000000-00-0	25994	52	67	2	99	58	9	0	44	7300
8.	*25	006510-65-2	126933	54	54	1	86	64	7	0	47	6018
9.	*25	000104-03-0	25983	39	60	2	98	55	7	7	37	7365
10.	*25	001484-12-4	26189	48	65	2	82	65	7	0	44	6612
11.	*25	006510-65-2	26185	45	64	2	84	64	7	0	44	6245
12.	*25	003652-91-3	126938	55	53	1	86	62	7	0	47	5957
13.	*22	003652-91-3	126935	34	72	2	80	64	5	0	41	6233
14.	*22	000153-78-6	26191	48	61	1	74	62	5	0	39	5882
15.	*22	001277-47-0	126915	38	63	0	81	65	5	0	39	7026
16.	22	000615-22-5	25993	44	63	0	48	61	5	0	39	9749
17.	*18	003770-48-7	26188	53	55	3	99	66	3	0	49	6185
18.	*16	023933-08-6	26008	41	75	3	75	59	3	0	35	7086
19.	*14	004630-20-0	26187	46	60	2	99	68	2	0	40	6060
20.	*14	003354-40-3	11753	34	64	2	73	70	2	11	40	5990

STP Compounds

53

Peak ~~86~~; 1,3-Isobenzofurandione



Scan 845 (17.917 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	102	59.95	50	75.95	3203	96.00	3
43.90	114	60.95	92	77.00	453	97.00	107
48.80	124	62.95	79	79.00	69	99.00	26
49.95	1273	65.90	2	79.90	145	103.95	4128
50.95	62	68.95	50	81.95	9	105.00	393
52.00	66	70.05	88	86.00	54	106.95	10
54.95	151	70.95	111	87.85	156	108.00	46
55.90	34	71.95	66	89.00	265	109.00	1
56.90	272	72.95	275	89.75	31	110.95	13
58.95	37	73.95	712	90.95	140	111.95	20
59.65	101	74.95	468	92.95	191	118.85	135

Scan 845 (17.917 min): S0229.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	43	150.00	69				
122.45	33						
126.00	45						
131.95	72						
132.95	163						
134.95	57						
140.40	26						
142.95	10						
146.90	185						
147.95	1104						
149.00	45						

STP Compounds

Scan 845 (17.917 min): S0229.D

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	Name	MolWt	Formula	Qual
1.	1,3-Isobenzofurandione	148	C8H4O3	91
2.	1,3-Isobenzofurandione	148	C8H4O3	83
3.	1H-Indene-1,3(2H)-dione, 2,2-dihydroxy-	178	C9H6O4	78
4.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	78
5.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	78
6.	Talsutin	362	C16H14N2O6S	78
7.	1,2-Benzenedicarboxylic acid	166	C8H6O4	78
8.	1,3-Isobenzofurandione	148	C8H4O3	78
9.	1,2-Benzenedicarboxylic acid, monomethyl	180	C9H8O4	74
10.	1,2-Benzenedicarboxylic acid	166	C8H6O4	74
11.	PHTHALIC ACID-D2	166	C8H4D2O4	72
12.	1H-Indene-1,2,3-trione	160	C9H4O3	64
13.	1H-Indene-1,3(2H)-dione, 2,2-dihydroxy-	178	C9H6O4	64
14.	1,2-Benzenedicarboxylic acid, monobutyl	222	C12H14O4	64
15.	1,2-Benzenedicarboxylic acid	166	C8H6O4	64
16.	1H-Isoindole-1,3(2H)-dione, 2-(hydroxyme	177	C9H7NO3	64
17.	1,3-Isobenzofurandione	148	C8H4O3	64
18.	1,3-Isobenzofurandione	148	C8H4O3	64
19.	Monoallyl phthalate	206	C11H10O4	64
20.	1H-Isoindole-1,3(2H)-dione	147	C8H5NO2	56

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000085-44-9	11912	72	27	2	99	4	60	12	58	9917
2.	*83	000085-44-9	123353	51	36	1	89	4	50	7	41	9826
3.	78	000485-47-2	126574	53	43	2	82	8	46	9	40	9694
4.	78	004376-18-5	126782	45	53	3	96	6	46	16	38	9883
5.	78	004376-18-5	25403	51	53	2	76	8	46	9	38	9879
6.	78	000131-69-1	90607	76	63	1	71	6	46	0	40	9875
7.	78	000088-99-3	125488	43	11	0	85	7	46	0	39	9642
8.	*78	000085-44-9	123356	62	31	2	99	8	46	0	38	9870
9.	74	004376-18-5	126783	80	25	1	80	4	44	14	37	9790
10.	74	000088-99-3	125487	73	25	1	98	4	44	19	37	9738
11.	72	004123-68-6	19189	60	48	0	56	15	42	11	38	9381
12.	64	000938-24-9	124881	61	32	1	86	8	37	6	33	9718
13.	64	000485-47-2	24518	54	49	0	63	19	37	5	40	9546
14.	64	000131-70-4	129810	69	40	2	99	6	37	14	36	9661
15.	64	000088-99-3	19188	64	33	2	99	6	37	20	37	9887
16.	64	000118-29-6	24166	58	58	0	69	18	37	0	43	8141
17.	64	000085-44-9	123355	48	45	0	62	20	37	9	38	9728
18.	64	000085-44-9	123354	56	42	1	97	6	37	15	37	9723
19.	64	000000-00-0	37263	41	27	0	66	6	37	0	33	9881
20.	56	000085-41-6	123276	40	75	0	78	12	30	0	33	8658

APPENDIX 4

WELDWOOD BLEACHED KRAFT MILL IN HINTON

Weldwood Bleached Kraft Mill In Hinton

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-May-89	15-Feb-90	8-Feb-91	13-Jun-91	19-Sep-91
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd	nd	nd
Cpnd2	Methylcyclohexane	0.78	0.49	0.31	2.75	nd
Cpnd3	2-Heptanone (91)	nd	0.24	nd	nd	0.66
Cpnd4	Dimethylcyclohexane	nd	nd	0.24	nd	nd
Cpnd5	$C_7H_{12}O$	0.74	0.37	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	nd	0.14	nd	nd
Cpnd7	Methylcyclopentenone	6.83	0.29	1.64	4.12	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	0.62	nd	0.24	0.37	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	1.52	0.90	nd	nd
Cpnd10	Diethylcyclopentenone	6.25	0.61	2.26	4.86	nd
Cpnd11	Methylcyclopentenone	3.37	0.30	nd	nd	nd
Cpnd12	Dimethyltrisulphide	7.02	0.34	6.33	3.73	nd
Cpnd13	Diethylcyclopentenone	2.66	0.31	1.71	1.51	nd
Cpnd14	α-Thujene (91)	3.43	6.61	5.53	7.77	nd
Cpnd15	Monoterpene [1]	3.43	8.01	nd	nd	nd
Cpnd16	Unidentified	nd	nd	nd	nd	nd
Cpnd17	α-Terpinene (96)	1.04	1.07	3.02	7.64	nd
Cpnd18	Cymene (not para) (91)	3.44	5.08	4.01	6.56	nd
Cpnd19	{Guaiacol 80}	0.55	nd	0.36	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	nd	1.11	0.33	0.53	nd
Cpnd21	Sabinene (90)	2.76	1.70	4.53	4.22	nd
Cpnd22	Unidentified	1.34	0.32	0.72	1.11	nd
Cpnd23	Dimethylcyclopentenone	nd	0.75	nd	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	3.61	0.35	1.20	1.81	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	2.08	0.55	0.40	0.62	nd
Cpnd26	{Guaiacol 76}	18.90	3.01	1.91	3.44	nd
Cpnd27	1-phenylethanone (94)	3.16	1.71	1.28	1.41	nd
Cpnd28	Monoterpene	nd	nd	0.26	0.57	nd
Cpnd29	1-(2-thienyl)ethanone (86)	8.46	nd	3.77	2.15	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	0.78	2.77	0.41	1.09	nd
Cpnd31	1-(2-thienyl)ethanone	16.48	0.73	7.04	4.49	nd
Cpnd32	Fenchone (83)	7.99	nd	6.92	5.31	nd
Cpnd33	Thioanisole	10.03	nd	6.15	7.00	nd
Cpnd34	Unidentified Hydrocarbon	1.19	nd	0.48	0.48	nd
Cpnd35	Unidentified (contains sulphur)	nd	139.05	0.41	0.65	nd
Cpnd36	Unidentified (contains sulphur)	1.11	0.20	0.37	0.60	0.89
Cpnd37	Hydrocarbon (see binder)	0.98	9.22	0.55	nd	nd
Cpnd38	{Methylguaiacol 80}	3.19	0.51	3.21	3.85	0.89
Cpnd39	Dichloromethyl methyl sulphone	82.48	12.21	49.43	58.89	5.48
Cpnd40	Methyl (methylthio)methyl disulphide	0.99	0.42	nd	0.36	nd
Cpnd41	Terpenone	1.65	1.23	nd	1.24	nd
Cpnd42	Unidentified hydrocarbon	nd	0.34	0.40	0.26	nd
Cpnd43	{Veratrole 96}	5.52	0.89	0.36	0.47	nd
Cpnd44	C7H8O3 (based on MI)	0.99	1.47	0.54	nd	nd
Cpnd45	Camphor (96)	0.57	2.72	0.50	0.38	nd
Cpnd46	Unidentified	2.17	0.45	1.10	0.62	nd
Cpnd47	Alkylated cyclopentenone	1.71	0.27	0.73	1.26	nd

Weldwood Bleached Kraft Mill In Hinton Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	11-May-89	15-Feb-90	8-Feb-91	13-Jun-91	19-Sep-91
Cpnd48	Unidentified	nd	1.47	0.63	nd	nd
Cpnd49	Unidentified	nd	0.40	0.33	0.45	nd
Cpnd50	Unidentified	nd	1.28	0.55	nd	nd
Cpnd51	1-Phenylpropanone (90)	4.13	0.68	2.78	4.08	0.52
Cpnd52	Monoterpene(s)	0.72	1.44	nd	nd	nd
Cpnd53	Unidentified	nd	nd	0.26	0.63	nd
Cpnd54	Dichlorophenol	nd	nd	0.70	0.41	nd
Cpnd55	Methylphenolsulphonyl	nd	0.61	3.27	3.34	nd
Cpnd56	2-(2-Thienyl)propanal	nd	9.66	3.67	1.23	nd
Cpnd57	t-Butylthiophene	nd	0.44	3.29	3.42	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	0.46	3.29	3.39	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	1.06	0.77	0.48	0.44	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	26.63	3.32	10.77	4.28	0.43
Cpnd61	Coeluting Monoterpenes	3.06	7.12	0.39	1.77	nd
Cpnd62	4-Methylthiophenol	1.57	0.44	1.00	0.73	nd
Cpnd63	Coeluting monoterpenes	0.56	2.13	0.83	0.81	nd
Cpnd64	Dimethyltetrasulphide	nd	0.15	nd	nd	nd
Cpnd65	Monoterpenone	3.42	0.53	0.95	2.64	1.67
Cpnd66	Contains dichloromethyl	3.18	0.60	3.51	3.43	0.71
Cpnd67	Contains Sulphur S4	nd	nd	0.16	0.50	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	3.19	0.45	2.94	6.82	nd
Cpnd69	not identified	1.10	0.42	0.51	0.75	0.55
Cpnd70	Coeluting Compounds; 1 is monoterpene.	1.33	1.61	3.34	0.97	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	1.65	2.13	2.42	nd
Cpnd72	Monoterpene	nd	nd	0.39	0.23	nd
Cpnd73	Unidentified	1.05	nd	0.27	0.67	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	1.64	nd	3.41	2.28	0.56
Cpnd75	Syringol (94)	nd	nd	nd	nd	nd
Cpnd76	Chloroterpene	nd	0.54	nd	nd	nd
Cpnd77	Monoterpene	1.31	2.31	0.46	0.44	nd
Cpnd78	Trichlorophenol	1.46	nd	1.11	1.73	nd
Cpnd79	Alkylnaphthalene	1.66	0.54	4.30	3.92	nd
Cpnd80	Vanillin (74)	4.23	0.59	3.22	1.96	1.00
Cpnd81	Junipene (83)	0.96	0.29	0.33	0.19	nd
Cpnd82	Alkylbenzene	1.70	2.22	1.62	1.84	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	0.23	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd	nd
Cpnd85	Monoterpene	1.50	1.71	0.39	0.85	nd
Cpnd86	Coeluting compounds Terpenoid	2.67	2.27	0.50	0.98	nd
Cpnd87	Monoterpene	nd	1.25	0.32	0.30	nd
Cpnd88	Chloromonoterpene	nd	1.30	0.22	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	4.24	nd	0.82	0.67	nd
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	0.56	nd
Cpnd91	Dichloroguaiacol	nd	nd	1.09	1.18	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-May-89	15-Feb-90	8-Feb-91	13-Jun-91	19-Sep-91
Cpnd92	Acetovanillone	2.83	197.25	0.60	0.88	nd
Cpnd93	Alkylthiophene	1.41	7.48	0.67	1.85	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	5.54	3.43	0.98	0.59	nd
Cpnd96	δ-Cadinene (64)	6.71	7.01	0.73	0.62	nd
Cpnd97	Sesquiterpene (204), not Peak 116	2.59	2.08	0.33	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	6.65	4.30	0.91	0.73	nd
Cpnd100	Sesquiterpene	6.26	nd	0.83	0.62	nd
Cpnd101	Unknown (terpenoid)	1.97	nd	0.52	1.62	0.89
Cpnd102	Dichloro, methyl loss,terpenoid	2.36	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	1.62	nd	1.95	1.64	0.86
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	1.11	nd	1.09	1.27	1.68
Cpnd106	Chlorovanillone	1.62	nd	7.01	5.01	1.67
Cpnd107	Dichloro, terpenoid	2.36	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	2.53	nd	0.29	0.35	0.62
Cpnd109	Trichloroguaiacol	3.59	nd	3.44	5.55	0.71
Cpnd110	Terpenoid	nd	5.94	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	0.21	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	0.49	0.85	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	2.05	nd	3.44	0.36	3.31
Cpnd116	Nonylphenol Isomer [2]	8.63	3.11	9.31	2.18	15.93
Cpnd117	Nonylphenol Isomer [3]	8.66	3.86	18.36	2.47	6.81
Cpnd118	Nonylphenol Isomer [4]	3.29	nd	4.84	0.79	4.04
Cpnd119	Nonylphenol Isomer [5]	4.55	4.29	18.38	2.18	5.94
Cpnd120	Nonylphenol Isomer [6]	3.01	nd	4.98	0.90	4.65
Cpnd121	Nonylphenol Isomer [7]	5.73	6.39	8.02	14.52	9.45
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	3.47	1.73	6.61	7.51	4.32
Cpnd123	Nonylphenol Isomer [8]	1.71	1.49	4.96	2.62	5.44
Cpnd124	Nonylphenol Isomer [9]	3.31	nd	3.64	4.03	7.14
Cpnd125	Nonylphenol Isomer [10]	2.96	5.69	8.05	14.55	18.96
Cpnd126	Nonylphenol Isomer [11]	7.28	6.91	8.97	6.22	18.08
Cpnd127	Nonylphenol Isomer [12]	3.99	1.31	8.15	4.08	8.65
Cpnd128	Diterpenoid (nor)	nd	nd	0.55	0.63	nd
Cpnd129	Diterpene	1.51	nd	0.88	1.41	nd
Cpnd130	Diterpene	5.14	0.90	2.09	3.20	1.09
Cpnd131	Diterpene	6.07	4.61	2.08	2.98	2.17
Cpnd132	Diterpene	3.99	2.73	0.76	3.12	0.99
Cpnd133	Sandaracopimaradiene	49.59	13.31	16.48	38.15	14.06
Cpnd134	Diterpene	17.83	5.05	6.80	11.48	4.06
Cpnd135	Diterpene	9.41	11.55	2.19	2.58	0.78
Cpnd136	Diterpene	2.26	4.60	0.49	0.43	0.44

Weldwood Bleached Kraft Mill In Hinton Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	11-May-89	15-Feb-90	8-Feb-91	13-Jun-91	19-Sep-91
Cpnd137	Diterpene	3.99	1.25	2.68	3.31	0.67
Cpnd138	Diterpene	2.46	4.56	0.36	nd	nd
Cpnd139	Diterpene	nd	1.17	0.42	nd	nd
Cpnd140	Diterpene	2.74	0.63	1.54	2.45	0.72
Cpnd141	8,12.Xi.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	0.50	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	1.45	nd	nd	nd
Cpnd144	Pimarinal	1.61	3.41	0.50	1.35	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	1.57	3.26	0.56	1.29	nd
Cpnd147	Diterpene	nd	6.63	0.75	0.69	nd
Cpnd148	Diterpene	nd	nd	0.46	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	nd	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-91	29-Jan-92	14-May-92	6-Aug-92	8-Dec-92
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd	nd	nd
Cpnd2	Methylcyclohexane	2.80	nd	nd	2.69	1.57
Cpnd3	2-Heptanone (91)	nd	nd	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	nd	nd	nd
Cpnd5	$C_7H_{12}O$	nd	nd	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	0.22	nd	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd	nd	nd	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	0.22	nd	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	nd	0.29	nd	nd
Cpnd10	Diethylcyclopentenone	1.27	3.60	0.83	1.60	2.03
Cpnd11	Methylcyclopentenone	nd	2.37	nd	nd	nd
Cpnd12	Dimethyltrisulphide	4.31	3.52	0.72	0.76	nd
Cpnd13	Diethylcyclopentenone	nd	1.91	0.26	nd	nd
Cpnd14	α-Thujene (91)	nd	nd	2.72	0.98	0.88
Cpnd15	Monoterpene [1]	nd	nd	nd	nd	nd
Cpnd16	Unidentified	nd	nd	nd	nd	nd
Cpnd17	α-Terpinene (96)	nd	1.54	1.33	1.38	nd
Cpnd18	Cymene (not para) (91)	0.71	3.93	1.95	nd	nd
Cpnd19	{Guaiacol 80}	nd	0.34	nd	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	2.37	nd	nd	nd	nd
Cpnd21	Sabinene (90)	1.42	6.27	2.45	0.62	0.89
Cpnd22	Unidentified	0.46	1.60	0.36	nd	nd
Cpnd23	Dimethylcyclopentenone	nd	2.44	nd	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	0.87	1.70	0.32	1.03	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd	1.49	nd	nd	nd
Cpnd26	{Guaiacol 76}	nd	14.79	nd	nd	nd
Cpnd27	1-phenylethanone (94)	nd	5.27	0.21	nd	nd
Cpnd28	Monoterpene	nd	0.87	nd	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd	nd	nd	nd	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	4.02	nd	nd	nd
Cpnd31	1-(2-thienyl)ethanone	nd	7.72	nd	2.46	1.47
Cpnd32	Fenchone (83)	0.48	0.66	nd	nd	nd
Cpnd33	Thioanisole	nd	8.03	nd	nd	nd
Cpnd34	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cpnd35	Unidentified (contains sulphur)	nd	5.45	nd	nd	nd
Cpnd36	Unidentified (contains sulphur)	nd	nd	nd	nd	nd
Cpnd37	Hydrocarbon (see binder)	nd	0.52	nd	nd	nd
Cpnd38	{Methylguaiacol 80}	3.62	3.86	0.99	2.46	2.52
Cpnd39	Dichloromethyl methyl sulphone	23.79	85.66	12.43	25.82	30.45
Cpnd40	Methyl (methylthio)methyl disulphide	nd	0.46	nd	nd	nd
Cpnd41	Terpenone	nd	1.58	nd	nd	nd
Cpnd42	Unidentified hydrocarbon	nd	0.49	nd	nd	nd
Cpnd43	{Veratrole 96}	nd	1.84	nd	nd	nd
Cpnd44	C7H8O3 (based on MI)	nd	0.47	nd	nd	nd
Cpnd45	Camphor (96)	0.59	2.00	0.35	nd	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-91	29-Jan-92	14-May-92	6-Aug-92	8-Dec-92
Cpnd46	Unidentified	0.73	0.78	0.42	nd	nd
Cpnd47	Alkylated cyclopentenone	nd	1.02	nd	nd	nd
Cpnd48	Unidentified	nd	0.45	nd	nd	nd
Cpnd49	Unidentified	0.33	1.08	nd	nd	nd
Cpnd50	Unidentified	nd	0.44	nd	nd	nd
Cpnd51	1-Phenylpropanone (90)	nd	3.65	0.75	nd	2.61
Cpnd52	Monoterpene(s)	nd	0.57	nd	nd	nd
Cpnd53	Unidentified	0.46	nd	nd	nd	nd
Cpnd54	Dichlorophenol	nd	0.52	nd	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	3.66	nd	nd	nd
Cpnd56	2-(2-Thienyl)propanal	nd	2.97	nd	nd	nd
Cpnd57	t-Butylthiophene	nd	3.58	nd	nd	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	3.57	nd	nd	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd	0.35	nd	nd	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	0.62	24.56	nd	nd	nd
Cpnd61	Coeluting Monoterpenes	2.03	2.06	nd	nd	nd
Cpnd62	4-Methylthiophenol	nd	0.70	nd	nd	1.93
Cpnd63	Coeluting monoterpenes	nd	0.61	nd	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd	nd	nd	nd
Cpnd65	Monoterpenone	2.14	5.41	1.03	2.20	2.94
Cpnd66	Contains dichloromethyl	nd	4.73	0.68	2.11	1.90
Cpnd67	Contains Sulphur S4	0.39	0.50	nd	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	nd	3.06	1.19	3.44	nd
Cpnd69	not identified	1.40	2.25	nd	nd	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd	0.29	nd	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	0.57	nd	nd	nd
Cpnd72	Monoterpene	0.37	nd	nd	nd	nd
Cpnd73	Unidentified	nd	0.35	nd	nd	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	1.70	0.42	0.72	1.23	1.35
Cpnd75	Syringol (94)	nd	nd	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd	nd	nd
Cpnd77	Monoterpene	0.78	1.44	nd	nd	nd
Cpnd78	Trichlorophenol	nd	1.33	nd	nd	nd
Cpnd79	Alkylnaphthalene	nd	2.83	0.58	nd	nd
Cpnd80	Vanillin (74)	1.55	1.55	0.56	1.35	nd
Cpnd81	Junipene (83)	0.45	nd	nd	nd	nd
Cpnd82	Alkylbenzene	0.62	1.36	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd	nd
Cpnd85	Monoterpene	1.07	2.18	nd	nd	nd
Cpnd86	Coeluting compounds Terpenoid	1.08	1.62	nd	nd	nd
Cpnd87	Monoterpene	nd	0.94	nd	nd	nd
Cpnd88	Chloromonoterpene	nd	nd	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	10.93	nd	nd	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-91	29-Jan-92	14-May-92	6-Aug-92	8-Dec-92
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	nd	nd
Cpnd91	Dichloroguaiacol	nd	0.97	nd	nd	nd
Cpnd92	Acetovanillone	nd	nd	nd	nd	nd
Cpnd93	Alkylthiophene	7.49	1.00	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	0.89	nd	nd	nd
Cpnd96	δ-Cadinene (64)	nd	0.88	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	1.39	nd	nd	nd
Cpnd100	Sesquiterpene	nd	0.92	nd	nd	nd
Cpnd101	Unknown (terpenoid)	1.28	2.44	nd	nd	nd
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	1.71	2.49	nd	nd	nd
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd	2.90	nd	nd	nd
Cpnd106	Chlorovanillone	nd	3.44	nd	4.59	nd
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	1.07	1.23	nd	nd	nd
Cpnd109	Trichloroguaiacol	nd	8.85	nd	2.82	2.80
Cpnd110	Terpenoid	nd	nd	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	1.17	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	9.10	4.50	6.29	4.77	nd
Cpnd116	Nonylphenol Isomer [2]	34.55	14.97	3.44	20.71	3.07
Cpnd117	Nonylphenol Isomer [3]	13.89	5.89	23.16	9.00	2.57
Cpnd118	Nonylphenol Isomer [4]	13.66	3.49	12.57	4.90	0.99
Cpnd119	Nonylphenol Isomer [5]	8.18	5.19	23.16	6.17	2.96
Cpnd120	Nonylphenol Isomer [6]	25.45	3.31	4.28	3.82	3.57
Cpnd121	Nonylphenol Isomer [7]	21.37	7.99	12.17	8.36	4.18
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	3.15	5.84	1.66	nd	2.54
Cpnd123	Nonylphenol Isomer [8]	24.36	3.44	13.06	4.89	nd
Cpnd124	Nonylphenol Isomer [9]	16.14	6.23	5.70	9.30	3.58
Cpnd125	Nonylphenol Isomer [10]	45.99	16.95	10.00	18.80	8.64
Cpnd126	Nonylphenol Isomer [11]	56.67	16.99	11.44	25.24	8.64
Cpnd127	Nonylphenol Isomer [12]	22.74	7.87	nd	8.94	3.61
Cpnd128	Diterpenoid (nor)	1.10	nd	nd	nd	nd
Cpnd129	Diterpene	1.30	0.56	nd	nd	nd
Cpnd130	Diterpene	3.88	2.95	1.48	nd	nd
Cpnd131	Diterpene	4.97	3.26	1.20	0.89	nd
Cpnd132	Diterpene	1.92	2.06	0.77	2.01	nd
Cpnd133	Sandaracopimaradiene	34.28	28.38	12.93	10.89	11.00
Cpnd134	Diterpene	11.94	11.40	4.71	3.65	4.64

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-91	29-Jan-92	14-May-92	6-Aug-92	8-Dec-92
Cpnd135	Diterpene	1.08	0.91	0.63	0.79	nd
Cpnd136	Diterpene	1.14	nd	nd	nd	nd
Cpnd137	Diterpene	2.57	1.60	0.54	1.14	nd
Cpnd138	Diterpene	1.15	nd	0.37	nd	nd
Cpnd139	Diterpene	nd	nd	nd	nd	nd
Cpnd140	Diterpene	3.14	1.92	0.69	nd	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd	nd	nd	nd
Cpnd144	Pimarinal	nd	nd	nd	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	nd	nd	0.43	nd	nd
Cpnd147	Diterpene	nd	nd	1.81	nd	nd
Cpnd148	Diterpene	nd	nd	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	nd	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Jun-93	12-Aug-93	25-Nov-93	1-Oct-94
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd	nd
Cpnd2	Methylcyclohexane	nd	nd	nd	nd
Cpnd3	2-Heptanone (91)	nd	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	2.17	1.77
Cpnd5	$C_7H_{12}O$	nd	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	nd	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd	1.85	0.72
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	nd	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	nd	nd	nd
Cpnd10	Diethylcyclopentenone	nd	nd	2.32	1.02
Cpnd11	Methylcyclopentenone	nd	nd	nd	nd
Cpnd12	Dimethyltrisulphide	nd	nd	nd	nd
Cpnd13	Diethylcyclopentenone	1.81	nd	0.96	0.75
Cpnd14	α-Thujene (91)	nd	nd	nd	nd
Cpnd15	Monoterpene [1]	nd	nd	nd	nd
Cpnd16	Unidentified	nd	nd	nd	nd
Cpnd17	α-Terpinene (96)	nd	nd	nd	nd
Cpnd18	Cymene (not para) (91)	nd	nd	nd	nd
Cpnd19	{Guaiacol 80}	nd	nd	nd	0.07
Cpnd20	1,2-bis(methylthio)ethane	nd	nd	nd	nd
Cpnd21	Sabinene (90)	nd	nd	nd	0.10
Cpnd22	Unidentified	nd	nd	0.83	0.20
Cpnd23	Dimethylcyclopentenone	nd	nd	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	nd	nd	1.19	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd	nd	nd	nd
Cpnd26	{Guaiacol 76}	nd	nd	nd	nd
Cpnd27	1-phenylethanone (94)	nd	nd	nd	nd
Cpnd28	Monoterpene	nd	nd	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd	nd	1.05	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	nd	nd
Cpnd31	1-(2-thienyl)ethanone	1.10	nd	1.04	nd
Cpnd32	Fenchone (83)	nd	nd	nd	nd
Cpnd33	Thioanisole	nd	nd	nd	nd
Cpnd34	Unidentified Hydrocarbon	nd	nd	nd	0.31
Cpnd35	Unidentified (contains sulphur)	nd	nd	nd	nd
Cpnd36	Unidentified (contains sulphur)	nd	2.94	3.03	nd
Cpnd37	Hydrocarbon (see binder)	nd	nd	nd	nd
Cpnd38	{Methylguaiacol 80}	2.48	nd	3.08	1.28
Cpnd39	Dichloromethyl methyl sulphone	25.33	20.91	23.98	5.99
Cpnd40	Methyl (methylthio)methyl disulphide	nd	nd	nd	nd
Cpnd41	Terpenone	nd	nd	0.46	nd
Cpnd42	Unidentified hydrocarbon	nd	nd	0.73	nd
Cpnd43	{Veratrole 96}	nd	nd	nd	nd
Cpnd44	C7H8O3 (based on MI)	nd	nd	nd	0.13
Cpnd45	Camphor (96)	nd	1.05	0.68	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Jun-93	12-Aug-93	25-Nov-93	1-Oct-94
Cpnd46	Unidentified	nd	nd	0.63	0.08
Cpnd47	Alkylated cyclopentenone	nd	nd	nd	0.11
Cpnd48	Unidentified	nd	nd	nd	0.10
Cpnd49	Unidentified	nd	nd	nd	0.11
Cpnd50	Unidentified	nd	nd	nd	nd
Cpnd51	1-Phenylpropanone (90)	nd	1.21	1.95	nd
Cpnd52	Monoterpene(s)	nd	nd	nd	nd
Cpnd53	Unidentified	nd	0.99	nd	nd
Cpnd54	Dichlorophenol	nd	nd	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	1.16	nd	nd
Cpnd56	2-(2-Thienyl)propanal	nd	nd	nd	nd
Cpnd57	t-Butylthiophene	nd	1.16	nd	0.10
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	1.01	nd	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	nd	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	nd	nd	nd	nd
Cpnd61	Coeluting Monoterpenes	nd	nd	nd	nd
Cpnd62	4-Methylthiophenol	nd	nd	1.71	nd
Cpnd63	Coeluting monoterpenes	nd	nd	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd	nd	nd
Cpnd65	Monoterpenone	2.40	2.15	4.62	2.07
Cpnd66	Contains dichloromethyl	1.77	1.11	1.52	nd
Cpnd67	Contains Sulphur S4	nd	nd	0.76	0.60
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	nd	2.43	4.88	0.52
Cpnd69	not identified	nd	nd	nd	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd	nd	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	nd	nd	nd
Cpnd72	Monoterpene	nd	nd	nd	nd
Cpnd73	Unidentified	nd	nd	nd	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	1.85	1.87	2.49	nd
Cpnd75	Syringol (94)	nd	nd	nd	nd
Cpnd76	Chloroterpene	1.25	nd	nd	nd
Cpnd77	Monoterpene	nd	1.18	0.97	0.20
Cpnd78	Trichlorophenol	nd	nd	nd	nd
Cpnd79	Alkylnaphthalene	3.37	2.38	3.56	nd
Cpnd80	Vanillin (74)	nd	nd	2.55	nd
Cpnd81	Junipene (83)	nd	nd	nd	nd
Cpnd82	Alkylbenzene	nd	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd
Cpnd85	Monoterpene	nd	nd	0.82	0.41
Cpnd86	Coeluting compounds Terpenoid	nd	nd	nd	0.02
Cpnd87	Monoterpene	nd	nd	nd	nd
Cpnd88	Chloromonoterpene	nd	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	nd	nd	nd

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Jun-93	12-Aug-93	25-Nov-93	1-Oct-94
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	0.20
Cpnd91	Dichloroguaiacol	nd	nd	nd	nd
Cpnd92	Acetovanillone	nd	nd	nd	nd
Cpnd93	Alkylthiophene	nd	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	nd	nd	nd
Cpnd96	δ-Cadinene (64)	nd	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	nd	nd	0.10
Cpnd100	Sesquiterpene	nd	nd	nd	nd
Cpnd101	Unknown (terpenoid)	nd	nd	nd	nd
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	nd	1.63	1.58	0.76
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd	1.55	nd	nd
Cpnd106	Chlorovanillone	0.72	nd	1.60	nd
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	nd	nd	nd	nd
Cpnd109	Trichloroguaiacol	1.59	nd	nd	nd
Cpnd110	Terpenoid	nd	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	2.38	2.94	1.46	nd
Cpnd116	Nonylphenol Isomer [2]	4.46	8.98	2.69	nd
Cpnd117	Nonylphenol Isomer [3]	1.87	4.52	2.74	nd
Cpnd118	Nonylphenol Isomer [4]	2.63	5.34	1.86	nd
Cpnd119	Nonylphenol Isomer [5]	2.26	3.50	2.97	nd
Cpnd120	Nonylphenol Isomer [6]	2.59	3.15	1.86	nd
Cpnd121	Nonylphenol Isomer [7]	2.94	6.68	3.41	nd
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	1.39	5.56	2.74	nd
Cpnd123	Nonylphenol Isomer [8]	0.63	2.64	3.22	nd
Cpnd124	Nonylphenol Isomer [9]	2.55	4.70	2.78	nd
Cpnd125	Nonylphenol Isomer [10]	5.11	9.78	6.95	nd
Cpnd126	Nonylphenol Isomer [11]	5.84	9.76	7.00	nd
Cpnd127	Nonylphenol Isomer [12]	2.48	5.86	2.81	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd	0.16
Cpnd129	Diterpene	nd	nd	nd	nd
Cpnd130	Diterpene	nd	1.04	0.74	0.34
Cpnd131	Diterpene	nd	nd	1.11	0.62
Cpnd132	Diterpene	nd	nd	nd	0.12
Cpnd133	Sandaracopimaradiene	11.08	12.41	11.96	5.50
Cpnd134	Diterpene	4.24	5.28	4.03	1.47

Weldwood Bleached Kraft Mill In Hinton Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Jun-93	12-Aug-93	25-Nov-93	1-Oct-94
Cpnd135	Diterpene	nd	1.03	0.72	0.13
Cpnd136	Diterpene	nd	nd	nd	nd
Cpnd137	Diterpene	nd	1.05	0.69	0.56
Cpnd138	Diterpene	nd	nd	nd	nd
Cpnd139	Diterpene	nd	nd	nd	nd
Cpnd140	Diterpene	nd	nd	0.58	0.16
Cpnd141	8,12.Xl.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd	nd	nd
Cpnd144	Pimarinal	nd	nd	nd	0.47
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd
Cpnd146	Diterpene	nd	nd	nd	0.27
Cpnd147	Diterpene	nd	nd	nd	nd
Cpnd148	Diterpene	nd	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	nd

APPENDIX 5

PROCTER AND GAMBLE/WEYERHAUSER KRAFT PULP MILL

Procter and Gamble/Weyerhauser Kraft Pulp Mill

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	3-Oct-89	28-Feb-90	27-Feb-91	3-Jul-91
Cpnd1	Dimethylsulphoxide (86)	nd	2.13	1.03	nd	nd
Cpnd2	Methylcyclohexane	1.28	0.58	0.89	1.22	3.26
Cpnd3	2-Heptanone (91)	2.54	0.53	0.37	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	nd	0.47	0.44
Cpnd5	$C_7H_{12}O$	4.45	0.93	2.45	nd	nd
Cpnd6	$C_4H_6S_2$	1.73	2.07	0.94	1.39	0.81
Cpnd7	Methylcyclopentenone	27.27	7.73	10.42	2.25	15.42
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	2.29	0.92	1.18	0.31	1.48
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	1.79	0.96	14.02	21.95	12.64
Cpnd10	Diethylcyclopentenone	23.01	28.20	25.29	19.23	10.39
Cpnd11	Methylcyclopentenone	10.72	1.63	4.52	1.53	6.09
Cpnd12	Dimethyltrisulphide	24.70	10.74	16.13	16.74	4.78
Cpnd13	Diethylcyclopentenone	9.05	15.99	13.14	9.28	6.03
Cpnd14	α-Thujene (91)	19.77	2.78	5.69	11.02	3.44
Cpnd15	Monoterpene [1]	nd	2.37	1.25	0.58	0.24
Cpnd16	Unidentified	2.62	0.63	nd	0.80	0.18
Cpnd17	α-Terpinene (96)	6.15	0.71	1.69	7.78	1.05
Cpnd18	Cymene (not para) (91)	22.37	4.64	5.89	13.86	5.89
Cpnd19	{Guaiacol 80}	2.39	2.86	4.37	2.88	1.00
Cpnd20	1,2-bis(methylthio)ethane	9.27	14.86	10.68	9.02	4.00
Cpnd21	Sabinene (90)	26.63	3.56	3.44	5.70	3.21
Cpnd22	Unidentified	6.19	7.83	8.51	5.45	2.04
Cpnd23	Dimethylcyclopentenone	19.03	2.92	2.71	2.85	0.48
Cpnd24	Bis-(chloromethyl)-sulphonyl	6.99	10.67	5.84	5.56	5.45
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	21.23	12.85	6.09	2.49	9.06
Cpnd26	{Guaiacol 76}	66.20	4.41	46.51	41.46	9.90
Cpnd27	1-phenylethanone (94)	5.12	1.92	6.96	5.04	2.53
Cpnd28	Monoterpene	1.45	nd	1.14	1.28	0.38
Cpnd29	1-(2-thienyl)ethanone (86)	26.99	17.30	33.53	8.06	17.74
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	7.11	1.12	1.60	2.36	1.47
Cpnd31	1-(2-thienyl)ethanone	64.23	44.94	71.04	19.04	53.87
Cpnd32	Fenchone (83)	43.79	5.34	36.87	4.40	3.47
Cpnd33	Thioanisole	50.35	3.22	34.83	3.08	3.28
Cpnd34	Unidentified Hydrocarbon	6.70	3.47	2.45	1.54	1.18
Cpnd35	Unidentified (contains sulphur)	1.94	1.65	2.01	1.94	1.29
Cpnd36	Unidentified (contains sulphur)	5.17	2.44	5.04	2.94	1.88
Cpnd37	Hydrocarbon (see binder)	7.17	4.72	4.01	2.39	2.42
Cpnd38	{Methylguaiacol 80}	10.88	13.87	16.10	10.71	4.42
Cpnd39	Dichloromethyl methyl sulphone	131.24	176.57	125.68	118.93	55.37
Cpnd40	Methyl (methylthio)methyl disulphide	0.97	1.25	0.98	0.93	1.96
Cpnd41	Terpenone	1.46	0.82	0.54	0.40	0.40
Cpnd42	Unidentified hydrocarbon	1.88	4.18	1.17	1.66	0.60
Cpnd43	{Veratrole 96}	17.89	1.22	2.21	3.50	0.36
Cpnd44	C7H8O3 (based on MI)	7.27	4.22	4.38	1.38	2.09
Cpnd45	Camphor (96)	25.51	3.21	2.50	3.02	0.84
Cpnd46	Unidentified	14.55	13.74	16.39	6.54	8.17

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	3-Oct-89	28-Feb-90	27-Feb-91	3-Jul-91
Cpnd47	Alkylated cyclopentenone	6.07	2.60	5.06	3.97	2.27
Cpnd48	Unidentified	7.33	4.30	4.89	2.41	3.42
Cpnd49	Unidentified	1.53	1.10	1.68	1.05	0.66
Cpnd50	Unidentified	2.41	3.42	0.71	1.95	1.23
Cpnd51	1-Phenylpropanone (90)	7.24	6.57	5.28	8.21	4.84
Cpnd52	Monoterpene(s)	3.51	0.52	2.69	4.92	3.97
Cpnd53	Unidentified	1.28	1.04	1.40	1.88	0.74
Cpnd54	Dichlorophenol	3.00	2.16	4.39	2.39	1.11
Cpnd55	Methylphenolsulphonyl	12.47	9.70	8.00	6.64	6.26
Cpnd56	2-(2-Thienyl)propanal	42.65	65.28	48.03	17.33	35.34
Cpnd57	t-Butylthiophene	12.57	9.67	14.61	6.66	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	12.80	9.72	14.71	6.73	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	0.72	1.16	1.80	0.68	0.09
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	58.80	0.91	2.17	nd	0.55
Cpnd61	Coeluting Monoterpenes	0.95	1.33	2.05	2.42	0.52
Cpnd62	4-Methylthiophenol	4.90	4.16	4.93	2.09	2.74
Cpnd63	Coeluting monoterpenes	2.26	1.70	2.07	1.47	0.96
Cpnd64	Dimethyltetrasulphide	4.98	nd	4.17	1.27	0.28
Cpnd65	Monoterpenone	13.16	6.52	14.15	7.32	2.16
Cpnd66	Contains dichloromethyl	3.96	3.18	3.55	1.27	1.55
Cpnd67	Contains Sulphur S4	nd	nd	nd	0.66	0.20
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	0.90	6.11	8.06	4.03	9.43
Cpnd69	not identified	8.92	0.53	0.76	0.83	0.69
Cpnd70	Coeluting Compounds; 1 is monoterpene.	10.21	0.72	6.87	23.78	1.16
Cpnd71	methyl(1-methylethyl)phenol (62)	1.20	1.94	4.29	3.72	3.30
Cpnd72	Monoterpene	2.00	0.43	0.48	1.09	0.37
Cpnd73	Unidentified	1.47	0.88	4.04	4.28	3.14
Cpnd74	Mulitple Compounds (Monoterpenes)	1.31	1.97	5.05	4.59	2.43
Cpnd75	Syringol (94)	nd	nd	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd	nd	2.49
Cpnd77	Monoterpene	0.75	0.84	3.19	8.74	4.26
Cpnd78	Trichlorophenol	7.00	2.49	11.37	3.50	1.56
Cpnd79	Alkylnaphthalene	2.53	0.57	0.60	8.15	5.59
Cpnd80	Vanillin (74)	2.40	0.70	0.51	1.47	2.79
Cpnd81	Junipene (83)	4.21	0.59	3.10	0.48	0.29
Cpnd82	Alkylbenzene	16.48	5.44	9.97	13.58	5.39
Cpnd83	Dimethoxybenzoic acid (25)	1.55	nd	0.66	1.42	0.49
Cpnd84	Chlorinated monoterpene ??	nd	nd	0.80	2.73	0.50
Cpnd85	Monoterpene	2.07	4.94	3.44	2.05	0.63
Cpnd86	Coeluting compounds Terpenoid	2.00	2.28	12.15	8.58	2.61
Cpnd87	Monoterpene	0.79	1.95	6.77	4.62	0.92
Cpnd88	Chloromonoterpene	0.86	nd	nd	0.65	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	4.21	2.76	1.83	5.26	4.95
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	1.83	2.84	3.54

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	3-Oct-89	28-Feb-90	27-Feb-91	3-Jul-91
Cpnd91	Dichloroguaiacol	1.26	1.50	2.12	1.88	1.24
Cpnd92	Acetovanillone	2.74	nd	2.27	0.94	0.57
Cpnd93	Alkylthiophene	12.23	12.70	11.48	10.80	6.09
Cpnd94	Trichloroveratrole	nd	nd	nd	1.15	nd
Cpnd95	(+)-Aromadendrene (78)	2.08	nd	3.56	0.45	0.52
Cpnd96	δ-Cadinene (64)	2.40	nd	7.81	0.77	0.62
Cpnd97	Sesquiterpene (204), not Peak 116	1.00	nd	3.43	0.37	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	0.40	nd
Cpnd99	Sesquiterpene mw 202	1.64	nd	4.61	1.53	0.72
Cpnd100	Sesquiterpene	2.43	nd	3.40	0.92	0.52
Cpnd101	Unknown (terpenoid)	2.52	1.53	3.31	2.05	0.84
Cpnd102	Dichloro, methyl loss,terpenoid	1.99	2.20	5.86	1.43	0.95
Cpnd103	Sesquiterpene C14H24O	3.63	6.75	7.26	4.52	2.31
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	0.89	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	3.67	1.84	4.51	0.40	nd
Cpnd106	Chlorovanillone	4.82	4.32	3.58	8.81	8.77
Cpnd107	Dichloro, terpenoid	1.99	2.44	1.18	0.43	0.95
Cpnd108	Unidentified chlorinated hydrocarbon	3.37	7.09	12.24	18.81	12.56
Cpnd109	Trichloroguaiacol	1.18	nd	4.68	1.83	nd
Cpnd110	Terpenoid	nd	nd	1.01	9.77	0.72
Cpnd111	coeluting compounds	nd	nd	nd	1.12	0.67
Cpnd112	Unidentified hydrocarbons	3.70	1.81	3.83	7.54	1.83
Cpnd113	Trichlorinated terpene	nd	nd	nd	2.44	0.67
Cpnd114	Unidentified, contains S	nd	nd	nd	3.51	nd
Cpnd115	Nonylphenol Isomer [1]	0.76	nd	1.83	nd	nd
Cpnd116	Nonylphenol Isomer [2]	2.76	nd	0.42	nd	1.48
Cpnd117	Nonylphenol Isomer [3]	4.49	nd	1.91	nd	nd
Cpnd118	Nonylphenol Isomer [4]	nd	nd	nd	nd	nd
Cpnd119	Nonylphenol Isomer [5]	4.44	nd	2.28	nd	nd
Cpnd120	Nonylphenol Isomer [6]	nd	nd	nd	nd	nd
Cpnd121	Nonylphenol Isomer [7]	3.49	nd	2.41	nd	nd
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	11.88	5.26	8.87	9.50	1.00
Cpnd123	Nonylphenol Isomer [8]	0.80	nd	1.69	nd	nd
Cpnd124	Nonylphenol Isomer [9]	nd	nd	nd	nd	nd
Cpnd125	Nonylphenol Isomer [10]	3.64	nd	2.12	nd	nd
Cpnd126	Nonylphenol Isomer [11]	3.32	nd	2.16	nd	nd
Cpnd127	Nonylphenol Isomer [12]	nd	nd	nd	nd	nd
Cpnd128	Diterpenoid (nor)	0.70	nd	nd	nd	nd
Cpnd129	Diterpene	1.54	nd	0.80	nd	nd
Cpnd130	Diterpene	3.30	nd	1.33	1.11	0.30
Cpnd131	Diterpene	2.47	nd	1.79	0.93	0.89
Cpnd132	Diterpene	2.63	2.92	1.27	0.56	nd
Cpnd133	Sandaracopimaradiene	45.25	6.29	13.54	4.32	4.32
Cpnd134	Diterpene	21.52	4.02	7.13	2.73	1.24
Cpnd135	Diterpene	8.50	1.23	1.92	0.90	0.66

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	3-Oct-89	28-Feb-90	27-Feb-91	3-Jul-91
Cpnd136	Diterpene	6.22	nd	1.81	0.55	nd
Cpnd137	Diterpene	6.92	nd	2.72	1.08	0.46
Cpnd138	Diterpene	22.61	nd	nd	0.35	nd
Cpnd139	Diterpene	1.42	nd	nd	0.86	nd
Cpnd140	Diterpene	4.86	nd	1.69	0.55	nd
Cpnd141	8,12.Xl.-Epoxylabd-14-en-13.XCl.-ol unide	5.26	nd	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	10.97	nd	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	41.01	nd	nd	nd	nd
Cpnd144	Pimarinal	9.04	nd	nd	0.71	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	9.22	nd	0.99	0.47	nd
Cpnd147	Diterpene	nd	nd	nd	nd	nd
Cpnd148	Diterpene	1.61	nd	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	1.82	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	11-Sep-91	6-Nov-91	12-Mar-92	16-Mar-92	11-Jun-92
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd	nd	nd
Cpnd2	Methylcyclohexane	nd	2.27	nd	nd	0.31
Cpnd3	2-Heptanone (91)	0.60	0.68	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	nd	nd	nd
Cpnd5	$C_7H_{12}O$	nd	nd	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	1.18	nd	nd	0.50
Cpnd7	Methylcyclopentenone	nd	0.46	1.04	1.31	1.03
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	3.19	0.71	17.11	19.44	0.25
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	1.34	2.38	nd	2.93	1.28
Cpnd10	Diethylcyclopentenone	1.32	0.35	0.68	0.71	7.83
Cpnd11	Methylcyclopentenone	nd	1.16	0.75	0.45	0.38
Cpnd12	Dimethyltrisulphide	nd	16.38	1.17	15.82	10.40
Cpnd13	Diethylcyclopentenone	0.87	7.85	0.71	0.74	5.04
Cpnd14	α-Thujene (91)	nd	0.37	nd	4.84	2.08
Cpnd15	Monoterpene [1]	nd	0.52	nd	4.73	1.22
Cpnd16	Unidentified	0.33	0.90	nd	2.68	1.15
Cpnd17	α-Terpinene (96)	nd	1.38	6.22	0.52	1.15
Cpnd18	Cymene (not para) (91)	nd	0.32	11.64	12.15	3.84
Cpnd19	{Guaiacol 80}	0.36	2.55	nd	nd	0.37
Cpnd20	1,2-bis(methylthio)ethane	1.21	10.97	nd	6.62	4.64
Cpnd21	Sabinene (90)	nd	8.19	7.10	9.45	2.80
Cpnd22	Unidentified	0.76	3.93	5.13	5.67	2.14
Cpnd23	Dimethylcyclopentenone	nd	12.18	1.08	nd	1.82
Cpnd24	Bis-(chloromethyl)-sulphonyl	0.68	2.43	2.63	2.41	2.66
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	0.38	8.35	8.81	5.97	2.80
Cpnd26	{Guaiacol 76}	0.32	25.10	3.50	1.82	0.63
Cpnd27	1-phenylethanone (94)	nd	4.70	2.31	1.61	nd
Cpnd28	Monoterpene	nd	0.73	0.89	0.85	0.63
Cpnd29	1-(2-thienyl)ethanone (86)	0.55	nd	nd	13.22	3.55
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	nd	1.38	0.67
Cpnd31	1-(2-thienyl)ethanone	0.55	14.59	21.52	11.29	3.55
Cpnd32	Fenchone (83)	nd	nd	4.82	2.73	2.89
Cpnd33	Thioanisole	0.32	5.95	0.53	0.67	3.24
Cpnd34	Unidentified Hydrocarbon	0.50	3.19	2.29	1.80	1.50
Cpnd35	Unidentified (contains sulphur)	nd	4.93	0.69	0.72	nd
Cpnd36	Unidentified (contains sulphur)	nd	3.60	7.68	7.36	0.76
Cpnd37	Hydrocarbon (see binder)	0.56	1.98	nd	2.56	2.30
Cpnd38	{Methylguaiacol 80}	1.74	3.60	7.68	7.72	5.70
Cpnd39	Dichloromethyl methyl sulphone	12.32	51.26	79.48	80.63	37.38
Cpnd40	Methyl (methylthio)methyl disulphide	0.37	0.42	nd	0.41	1.59
Cpnd41	Terpenone	0.39	1.06	nd	nd	0.99
Cpnd42	Unidentified hydrocarbon	0.35	0.69	1.60	2.09	0.91
Cpnd43	{Veratrole 96}	0.39	0.58	3.03	1.29	0.60
Cpnd44	C7H8O3 (based on MI)	0.37	3.52	2.74	1.79	1.35
Cpnd45	Camphor (96)	0.49	2.14	4.06	2.92	2.36

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-Sep-91	6-Nov-91	12-Mar-92	16-Mar-92	11-Jun-92
Cpnd46	Unidentified	0.71	9.99	12.38	8.59	4.72
Cpnd47	Alkylated cyclopentenone	0.39	0.58	0.14	0.93	0.39
Cpnd48	Unidentified	0.37	3.65	3.08	1.79	0.85
Cpnd49	Unidentified	0.62	0.64	0.59	0.77	0.61
Cpnd50	Unidentified	1.68	2.62	3.00	nd	0.86
Cpnd51	1-Phenylpropanone (90)	1.20	3.84	6.73	5.52	1.97
Cpnd52	Monoterpene(s)	0.70	2.64	1.44	1.62	1.11
Cpnd53	Unidentified	nd	1.60	1.45	0.40	0.22
Cpnd54	Dichlorophenol	nd	nd	0.83	0.88	1.12
Cpnd55	Methylphenolsulphonyl	0.70	6.45	6.22	6.06	2.16
Cpnd56	2-(2-Thienyl)propanal	4.55	29.07	15.57	11.06	14.61
Cpnd57	t-Butylthiophene	0.70	6.48	6.20	6.10	2.13
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	0.70	6.47	6.24	6.10	2.16
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	0.66	1.01	nd	nd	3.34
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	0.47	nd	0.40	0.53	1.00
Cpnd61	Coeluting Monoterpenes	0.88	0.63	0.94	0.86	1.38
Cpnd62	4-Methylthiophenol	0.39	3.02	1.47	1.77	1.13
Cpnd63	Coeluting monoterpenes	nd	0.67	nd	0.57	1.24
Cpnd64	Dimethyltetrasulphide	nd	1.81	0.47	0.80	nd
Cpnd65	Monoterpenone	1.91	7.18	8.74	8.49	5.30
Cpnd66	Contains dichloromethyl	nd	0.92	2.27	2.98	nd
Cpnd67	Contains Sulphur S4	nd	nd	nd	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	1.25	2.71	7.04	7.19	4.72
Cpnd69	not identified	0.51	2.37	0.77	0.57	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	0.64	3.87	2.45	1.05	0.67
Cpnd71	methyl(1-methylethyl)phenol (62)	0.63	3.73	1.42	1.02	0.01
Cpnd72	Monoterpene	nd	0.49	nd	nd	nd
Cpnd73	Unidentified	0.79	1.01	0.53	0.88	0.59
Cpnd74	Mulitple Compounds (Monoterpenes)	0.57	1.30	3.02	3.40	2.39
Cpnd75	Syringol (94)	nd	0.43	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd	0.38	nd
Cpnd77	Monoterpene	0.56	0.45	1.15	1.25	0.40
Cpnd78	Trichlorophenol	0.63	1.10	1.06	1.11	1.12
Cpnd79	Alkylnaphthalene	nd	3.73	5.16	5.68	3.87
Cpnd80	Vanillin (74)	0.64	1.36	2.84	4.48	2.04
Cpnd81	Junipene (83)	nd	0.37	0.34	0.46	nd
Cpnd82	Alkylbenzene	0.25	0.84	6.76	28.00	10.79
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	2.12	1.39
Cpnd84	Chlorinated monoterpene ??	nd	0.47	nd	0.33	nd
Cpnd85	Monoterpene	0.43	1.96	2.34	2.58	1.39
Cpnd86	Coeluting compounds Terpenoid	0.75	2.06	4.84	2.30	nd
Cpnd87	Monoterpene	0.52	1.36	2.77	2.39	1.30
Cpnd88	Chloromonoterpene	nd	nd	1.13	0.66	0.48
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	2.35	5.13	4.84	0.43

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-Sep-91	6-Nov-91	12-Mar-92	16-Mar-92	11-Jun-92
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	nd	0.92
Cpnd91	Dichloroguaiacol	0.56	nd	2.83	2.04	1.46
Cpnd92	Acetovanillone	nd	nd	2.90	1.94	0.58
Cpnd93	Alkylthiophene	1.10	2.23	9.57	34.38	14.50
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	0.61	0.82	0.76	nd
Cpnd96	δ-Cadinene (64)	nd	1.05	0.79	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	0.43	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	1.31	1.99	2.97	nd
Cpnd100	Sesquiterpene	nd	1.05	1.46	1.95	nd
Cpnd101	Unknown (terpenoid)	nd	2.77	2.00	1.63	0.18
Cpnd102	Dichloro, methyl loss,terpenoid	0.47	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	0.82	3.08	4.72	4.02	2.36
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd	nd	nd	0.89	0.66
Cpnd106	Chlorovanillone	7.46	2.64	16.06	26.09	9.71
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	4.59	8.13	6.29	4.81	2.84
Cpnd109	Trichloroguaiacol	nd	nd	3.35	1.20	1.58
Cpnd110	Terpenoid	nd	1.50	1.15	1.67	1.44
Cpnd111	coeluting compounds	nd	nd	3.12	1.31	0.62
Cpnd112	Unidentified hydrocarbons	nd	1.88	4.47	6.61	1.82
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	1.71	0.25	0.63
Cpnd115	Nonylphenol Isomer [1]	nd	nd	nd	0.69	0.57
Cpnd116	Nonylphenol Isomer [2]	0.41	1.02	1.39	2.64	0.78
Cpnd117	Nonylphenol Isomer [3]	nd	1.04	1.37	2.59	0.61
Cpnd118	Nonylphenol Isomer [4]	nd	nd	2.78	0.63	0.36
Cpnd119	Nonylphenol Isomer [5]	nd	3.04	1.30	2.70	0.74
Cpnd120	Nonylphenol Isomer [6]	nd	nd	2.75	0.66	0.45
Cpnd121	Nonylphenol Isomer [7]	nd	1.32	1.39	1.15	0.87
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	1.85	4.14	10.02	11.38	4.49
Cpnd123	Nonylphenol Isomer [8]	nd	nd	1.44	1.50	0.54
Cpnd124	Nonylphenol Isomer [9]	nd	nd	1.38	0.66	nd
Cpnd125	Nonylphenol Isomer [10]	0.76	0.46	2.65	2.16	0.61
Cpnd126	Nonylphenol Isomer [11]	nd	0.44	2.58	2.16	1.58
Cpnd127	Nonylphenol Isomer [12]	nd	nd	1.32	0.93	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd	nd	nd
Cpnd129	Diterpene	nd	nd	nd	nd	nd
Cpnd130	Diterpene	nd	0.67	1.82	1.20	nd
Cpnd131	Diterpene	nd	1.38	1.31	0.88	nd
Cpnd132	Diterpene	nd	1.34	2.54	2.18	nd
Cpnd133	Sandaracopimaradiene	1.21	7.83	9.12	12.86	1.37
Cpnd134	Diterpene	0.59	3.31	4.32	6.34	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-Sep-91	6-Nov-91	12-Mar-92	16-Mar-92	11-Jun-92
Cpnd135	Diterpene	nd	0.74	0.90	1.27	nd
Cpnd136	Diterpene	nd	0.78	1.88	0.70	nd
Cpnd137	Diterpene	1.25	1.35	0.95	1.89	nd
Cpnd138	Diterpene	nd	0.88	2.02	2.38	nd
Cpnd139	Diterpene	nd	nd	1.97	0.53	1.61
Cpnd140	Diterpene	nd	0.93	0.74	1.22	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd	0.42	1.10
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	1.96	0.99	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	0.13	nd	1.32	nd
Cpnd144	Pimarinal	nd	1.78	1.52	2.18	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	nd	1.64	1.91	2.98	nd
Cpnd147	Diterpene	nd	nd	5.78	nd	0.47
Cpnd148	Diterpene	nd	nd	2.61	nd	0.50
Cpnd149	Coeluting compounds	nd	nd	nd	1.09	0.61

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Sep-92	4-Nov-92	25-Mar-93	19-May-93	8-Sep-93
Cpnd1	Dimethylsulphoxide (86)	nd	0.63	nd	nd	nd
Cpnd2	Methylcyclohexane	0.66	3.58	nd	nd	nd
Cpnd3	2-Heptanone (91)	nd	nd	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	nd	nd	nd
Cpnd5	$C_7H_{12}O$	nd	nd	nd	nd	nd
Cpnd6	$C_4H_6S_2$	0.69	nd	nd	nd	nd
Cpnd7	Methylcyclopentenone	1.12	nd	nd	nd	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	0.67	nd	nd	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	2.08	12.06	0.38	nd	nd
Cpnd10	Diethylcyclopentenone	0.66	11.43	12.32	nd	nd
Cpnd11	Methylcyclopentenone	nd	nd	0.96	nd	nd
Cpnd12	Dimethyltrisulphide	19.42	4.01	6.16	1.69	nd
Cpnd13	Diethylcyclopentenone	9.05	5.93	6.01	2.15	nd
Cpnd14	α-Thujene (91)	2.72	3.46	nd	nd	nd
Cpnd15	Monoterpene [1]	1.40	2.24	nd	nd	nd
Cpnd16	Unidentified	nd	nd	1.68	nd	nd
Cpnd17	α-Terpinene (96)	1.46	2.06	nd	nd	nd
Cpnd18	Cymene (not para) (91)	4.11	1.68	nd	nd	nd
Cpnd19	{Guaiacol 80}	1.71	1.08	1.71	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	4.61	nd	5.64	nd	0.98
Cpnd21	Sabinene (90)	4.74	2.87	nd	nd	nd
Cpnd22	Unidentified	2.74	3.15	3.23	nd	0.67
Cpnd23	Dimethylcyclopentenone	1.23	nd	1.77	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	3.33	3.04	nd	nd	2.37
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	3.60	nd	nd	nd	1.60
Cpnd26	{Guaiacol 76}	nd	nd	1.60	nd	nd
Cpnd27	1-phenylethanone (94)	1.88	nd	nd	nd	nd
Cpnd28	Monoterpene	nd	nd	nd	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	3.17	1.37	5.41	nd	3.15
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	nd	nd	nd
Cpnd31	1-(2-thienyl)ethanone	8.70	1.48	5.41	nd	3.24
Cpnd32	Fenchone (83)	nd	nd	nd	nd	nd
Cpnd33	Thioanisole	1.57	nd	nd	nd	nd
Cpnd34	Unidentified Hydrocarbon	2.30	nd	nd	nd	1.32
Cpnd35	Unidentified (contains sulphur)	nd	nd	nd	nd	nd
Cpnd36	Unidentified (contains sulphur)	8.77	6.99	1.14	nd	3.19
Cpnd37	Hydrocarbon (see binder)	2.60	nd	nd	nd	1.59
Cpnd38	{Methylguaiacol 80}	8.25	7.10	1.14	3.85	3.20
Cpnd39	Dichloromethyl methyl sulphone	50.63	49.33	38.81	24.87	37.07
Cpnd40	Methyl (methylthio)methyl disulphide	nd	nd	nd	nd	nd
Cpnd41	Terpenone	nd	nd	nd	nd	nd
Cpnd42	Unidentified hydrocarbon	2.31	1.14	nd	nd	36.97
Cpnd43	{Veratrole 96}	nd	nd	nd	nd	1.48
Cpnd44	C7H8O3 (based on MI)	2.15	nd	nd	nd	nd
Cpnd45	Camphor (96)	2.52	2.60	2.11	nd	1.72

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Sep-92	4-Nov-92	25-Mar-93	19-May-93	8-Sep-93
Cpnd46	Unidentified	4.38	2.24	4.14	nd	2.42
Cpnd47	Alkylated cyclopentenone	nd	nd	nd	nd	1.10
Cpnd48	Unidentified	2.69	nd	nd	nd	nd
Cpnd49	Unidentified	nd	nd	nd	nd	1.16
Cpnd50	Unidentified	1.33	nd	nd	nd	0.69
Cpnd51	1-Phenylpropanone (90)	2.94	3.89	3.04	nd	nd
Cpnd52	Monoterpene(s)	nd	nd	1.95	nd	0.92
Cpnd53	Unidentified	nd	nd	nd	nd	1.44
Cpnd54	Dichlorophenol	nd	nd	nd	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	nd	4.53	nd	2.21
Cpnd56	2-(2-Thienyl)propanal	13.13	2.48	1.43	nd	0.93
Cpnd57	t-Butylthiophene	2.68	nd	4.46	nd	2.10
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	2.67	2.18	4.52	nd	2.21
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	2.49	1.31	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	0.90	nd	nd	nd	nd
Cpnd61	Coeluting Monoterpenes	2.26	nd	nd	nd	nd
Cpnd62	4-Methylthiophenol	1.77	1.83	4.52	nd	2.12
Cpnd63	Coeluting monoterpenes	nd	nd	nd	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd	nd	nd	nd
Cpnd65	Monoterpenone	2.55	4.27	6.42	nd	1.55
Cpnd66	Contains dichloromethyl	nd	nd	nd	nd	nd
Cpnd67	Contains Sulphur S4	nd	nd	nd	nd	0.74
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	3.13	nd	1.13	nd	nd
Cpnd69	not identified	nd	nd	nd	nd	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	3.21	nd	nd	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	2.82	nd	nd	nd	nd
Cpnd72	Monoterpene	nd	nd	nd	nd	nd
Cpnd73	Unidentified	nd	nd	nd	nd	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	2.04	2.51	3.45	1.77	2.70
Cpnd75	Syringol (94)	nd	nd	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd	1.20	nd
Cpnd77	Monoterpene	1.75	nd	nd	nd	1.26
Cpnd78	Trichlorophenol	nd	nd	nd	nd	nd
Cpnd79	Alkylnaphthalene	4.76	1.87	3.57	nd	nd
Cpnd80	Vanillin (74)	3.81	nd	nd	nd	3.39
Cpnd81	Junipene (83)	nd	nd	nd	nd	nd
Cpnd82	Alkylbenzene	1.73	nd	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd	nd
Cpnd85	Monoterpene	2.27	nd	nd	nd	0.97
Cpnd86	Coeluting compounds Terpenoid	nd	nd	nd	nd	nd
Cpnd87	Monoterpene	nd	nd	nd	nd	nd
Cpnd88	Chloromonoterpene	nd	nd	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	nd	nd	nd	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Sep-92	4-Nov-92	25-Mar-93	19-May-93	8-Sep-93
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	nd	nd
Cpnd91	Dichloroguaiacol	nd	nd	nd	nd	nd
Cpnd92	Acetovanillone	1.18	nd	nd	nd	nd
Cpnd93	Alkylthiophene	0.99	nd	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	nd	nd	nd	nd
Cpnd96	δ-Cadinene (64)	nd	nd	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	nd	nd	nd	nd
Cpnd100	Sesquiterpene	nd	nd	nd	nd	nd
Cpnd101	Unknown (terpenoid)	nd	nd	3.45	nd	2.35
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	2.92	nd	4.24	2.35	2.87
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	4.05	nd	nd	nd	nd
Cpnd106	Chlorovanillone	5.31	nd	nd	nd	5.05
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	2.14	nd	nd	nd	nd
Cpnd109	Trichloroguaiacol	nd	nd	nd	nd	nd
Cpnd110	Terpenoid	nd	nd	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	nd	nd	nd	nd	nd
Cpnd116	Nonylphenol Isomer [2]	1.51	nd	nd	nd	2.22
Cpnd117	Nonylphenol Isomer [3]	2.52	nd	nd	nd	1.97
Cpnd118	Nonylphenol Isomer [4]	nd	nd	nd	nd	nd
Cpnd119	Nonylphenol Isomer [5]	nd	nd	nd	nd	2.13
Cpnd120	Nonylphenol Isomer [6]	nd	nd	nd	nd	nd
Cpnd121	Nonylphenol Isomer [7]	2.02	nd	nd	nd	1.51
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	4.25	5.10	10.85	5.01	5.63
Cpnd123	Nonylphenol Isomer [8]	nd	nd	nd	nd	nd
Cpnd124	Nonylphenol Isomer [9]	nd	nd	nd	nd	nd
Cpnd125	Nonylphenol Isomer [10]	nd	nd	nd	nd	1.46
Cpnd126	Nonylphenol Isomer [11]	nd	nd	nd	nd	1.42
Cpnd127	Nonylphenol Isomer [12]	nd	nd	nd	nd	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd	nd	nd
Cpnd129	Diterpene	nd	nd	nd	nd	nd
Cpnd130	Diterpene	nd	nd	nd	nd	nd
Cpnd131	Diterpene	nd	nd	nd	nd	nd
Cpnd132	Diterpene	nd	nd	nd	nd	0.83
Cpnd133	Sandaracopimaradiene	5.63	nd	nd	nd	nd
Cpnd134	Diterpene	1.90	nd	nd	nd	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Sep-92	4-Nov-92	25-Mar-93	19-May-93	8-Sep-93
Cpnd135	Diterpene	nd	nd	nd	nd	nd
Cpnd136	Diterpene	nd	nd	nd	nd	nd
Cpnd137	Diterpene	nd	nd	nd	nd	nd
Cpnd138	Diterpene	nd	nd	nd	nd	nd
Cpnd139	Diterpene	nd	nd	nd	nd	nd
Cpnd140	Diterpene	nd	nd	nd	nd	nd
Cpnd141	8,12.Xl.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd	nd	nd	nd
Cpnd144	Pimarinal	nd	nd	nd	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	nd	nd	nd	nd	nd
Cpnd147	Diterpene	nd	nd	nd	2.96	nd
Cpnd148	Diterpene	nd	nd	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	nd	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Concentrations in µg/L

Date Sampled	Compound Name, Formula or Description	3-Feb-94
Cpnd1	Dimethylsulphoxide (86)	nd
Cpnd2	Methylcyclohexane	2.93
Cpnd3	2-Heptanone (91)	nd
Cpnd4	Dimethylcyclohexane	nd
Cpnd5	$C_7H_{12}O$	nd
Cpnd6	$C_4H_6S_2$	nd
Cpnd7	Methylcyclopentenone	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd
Cpnd10	Diethylcyclopentenone	1.13
Cpnd11	Methylcyclopentenone	nd
Cpnd12	Dimethyltrisulphide	nd
Cpnd13	Diethylcyclopentenone	nd
Cpnd14	α-Thujene (91)	nd
Cpnd15	Monoterpene [1]	nd
Cpnd16	Unidentified	nd
Cpnd17	α-Terpinene (96)	nd
Cpnd18	Cymene (not para) (91)	nd
Cpnd19	{Guaiacol 80}	nd
Cpnd20	1,2-bis(methylthio)ethane	nd
Cpnd21	Sabinene (90)	nd
Cpnd22	Unidentified	nd
Cpnd23	Dimethylcyclopentenone	1.98
Cpnd24	Bis-(chloromethyl)-sulphonyl	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd
Cpnd26	{Guaiacol 76}	nd
Cpnd27	1-phenylethanone (94)	nd
Cpnd28	Monoterpene	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd
Cpnd31	1-(2-thienyl)ethanone	nd
Cpnd32	Fenchone (83)	nd
Cpnd33	Thioanisole	nd
Cpnd34	Unidentified Hydrocarbon	nd
Cpnd35	Unidentified (contains sulphur)	nd
Cpnd36	Unidentified (contains sulphur)	1.37
Cpnd37	Hydrocarbon (see binder)	nd
Cpnd38	{Methylguaiacol 80}	nd
Cpnd39	Dichloromethyl methyl sulphone	55.96
Cpnd40	Methyl (methylthio)methyl disulphide	nd
Cpnd41	Terpenone	nd
Cpnd42	Unidentified hydrocarbon	nd
Cpnd43	{Veratrole 96}	nd
Cpnd44	C7H8O3 (based on MI)	nd
Cpnd45	Camphor (96)	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Concentrations in µg/L

Date Sampled	Compound Name, Formula or Description	3-Feb-94
Cpnd46	Unidentified	nd
Cpnd47	Alkylated cyclopentenone	nd
Cpnd48	Unidentified	nd
Cpnd49	Unidentified	nd
Cpnd50	Unidentified	nd
Cpnd51	1-Phenylpropanone (90)	nd
Cpnd52	Monoterpene(s)	nd
Cpnd53	Unidentified	nd
Cpnd54	Dichlorophenol	nd
Cpnd55	Methylphenolsulphonyl	nd
Cpnd56	2-(2-Thienyl)propanal	nd
Cpnd57	t-Butylthiophene	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	nd
Cpnd61	Coeluting Monoterpenes	nd
Cpnd62	4-Methylthiophenol	nd
Cpnd63	Coeluting monoterpenes	nd
Cpnd64	Dimethyltetrasulphide	nd
Cpnd65	Monoterpenone	nd
Cpnd66	Contains dichloromethyl	nd
Cpnd67	Contains Sulphur S4	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	nd
Cpnd69	not identified	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd
Cpnd72	Monoterpene	nd
Cpnd73	Unidentified	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	3.66
Cpnd75	Syringol (94)	nd
Cpnd76	Chloroterpene	nd
Cpnd77	Monoterpene	nd
Cpnd78	Trichlorophenol	nd
Cpnd79	Alkylnaphthalene	nd
Cpnd80	Vanillin (74)	3.52
Cpnd81	Junipene (83)	nd
Cpnd82	Alkylbenzene	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd
Cpnd84	Chlorinated monoterpene ??	nd
Cpnd85	Monoterpene	nd
Cpnd86	Coeluting compounds Terpenoid	nd
Cpnd87	Monoterpene	nd
Cpnd88	Chloromonoterpene	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Concentrations in µg/L

Date Sampled	Compound Name, Formula or Description	3-Feb-94
Cpnd90	Dichloro- Methyl terpenoid	nd
Cpnd91	Dichloroguaiacol	nd
Cpnd92	Acetovanillone	nd
Cpnd93	Alkylthiophene	nd
Cpnd94	Trichloroveratrole	nd
Cpnd95	(+)-Aromadendrene (78)	nd
Cpnd96	δ-Cadinene (64)	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd
Cpnd99	Sesquiterpene mw 202	nd
Cpnd100	Sesquiterpene	nd
Cpnd101	Unknown (terpenoid)	3.21
Cpnd102	Dichloro, methyl loss,terpenoid	nd
Cpnd103	Sesquiterpene C14H24O	2.81
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd
Cpnd106	Chlorovanillone	4.33
Cpnd107	Dichloro, terpenoid	nd
Cpnd108	Unidentified chlorinated hydrocarbon	nd
Cpnd109	Trichloroguaiacol	nd
Cpnd110	Terpenoid	nd
Cpnd111	coeluting compounds	nd
Cpnd112	Unidentified hydrocarbons	nd
Cpnd113	Trichlorinated terpene	nd
Cpnd114	Unidentified, contains S	nd
Cpnd115	Nonylphenol Isomer [1]	nd
Cpnd116	Nonylphenol Isomer [2]	2.90
Cpnd117	Nonylphenol Isomer [3]	3.63
Cpnd118	Nonylphenol Isomer [4]	nd
Cpnd119	Nonylphenol Isomer [5]	3.28
Cpnd120	Nonylphenol Isomer [6]	nd
Cpnd121	Nonylphenol Isomer [7]	1.56
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	nd
Cpnd123	Nonylphenol Isomer [8]	nd
Cpnd124	Nonylphenol Isomer [9]	nd
Cpnd125	Nonylphenol Isomer [10]	1.49
Cpnd126	Nonylphenol Isomer [11]	1.51
Cpnd127	Nonylphenol Isomer [12]	nd
Cpnd128	Diterpenoid (nor)	nd
Cpnd129	Diterpene	nd
Cpnd130	Diterpene	nd
Cpnd131	Diterpene	nd
Cpnd132	Diterpene	nd
Cpnd133	Sandaracopimaradiene	1.82
Cpnd134	Diterpene	nd

Procter and Gamble/Weyerhauser Kraft Pulp Mill Continued

Concentrations in µg/L

Date Sampled	Compound Name, Formula or Description	3-Feb-94
Cpnd135	Diterpene	nd
Cpnd136	Diterpene	nd
Cpnd137	Diterpene	nd
Cpnd138	Diterpene	nd
Cpnd139	Diterpene	nd
Cpnd140	Diterpene	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCI.-ol unide	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd
Cpnd144	Pimarinal	nd
Cpnd145	4-Androsten-3-one (22)	nd
Cpnd146	Diterpene	nd
Cpnd147	Diterpene	nd
Cpnd148	Diterpene	nd
Cpnd149	Coeluting compounds	nd

APPENDIX 6

DAISHOWA KRAFT PULP MILL IN PEACE RIVER

Daishowa Kraft Pulp Mill in Peace River

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Oct-90	12-Mar-91	20-Jun-91	12-Sep-91	3-Dec-91
Cpnd1	Dimethylsulphoxide (86)	nd	nd	1.57	nd	nd
Cpnd2	Methylcyclohexane	nd	nd	2.85	nd	1.97
Cpnd3	2-Heptanone (91)	nd	nd	1.70	1.27	1.15
Cpnd4	Dimethylcyclohexane	nd	nd	nd	nd	nd
Cpnd5	$C_7H_{12}O$	nd	nd	0.45	nd	1.81
Cpnd6	$C_4H_6S_2$	nd	nd	nd	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd	1.96	nd	8.38
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	nd	1.32	nd	0.34
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	4.38	2.53	nd	nd	1.08
Cpnd10	Diethylcyclopentenone	nd	nd	2.28	nd	nd
Cpnd11	Methylcyclopentenone	nd	nd	0.59	nd	0.74
Cpnd12	Dimethyltrisulphide	nd	nd	3.72	nd	0.81
Cpnd13	Diethylcyclopentenone	nd	nd	0.59	nd	3.10
Cpnd14	α-Thujene (91)	1.49	nd	0.40	nd	nd
Cpnd15	Monoterpene [1]	nd	nd	nd	nd	nd
Cpnd16	Unidentified	nd	nd	nd	0.55	1.65
Cpnd17	α-Terpinene (96)	nd	nd	nd	nd	nd
Cpnd18	Cymene (not para) (91)	nd	nd	nd	nd	nd
Cpnd19	{Guaiacol 80}	nd	nd	0.34	0.92	1.15
Cpnd20	1,2-bis(methylthio)ethane	nd	nd	0.34	nd	nd
Cpnd21	Sabinene (90)	nd	nd	0.52	nd	nd
Cpnd22	Unidentified	nd	nd	0.61	nd	3.26
Cpnd23	Dimethylcyclopentenone	nd	nd	5.51	nd	18.52
Cpnd24	Bis-(chloromethyl)-sulphonyl	1.10	0.72	1.58	nd	0.15
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd	nd	1.53	nd	nd
Cpnd26	{Guaiacol 76}	1.49	nd	9.28	1.41	24.29
Cpnd27	1-phenylethanone (94)	nd	nd	3.21	nd	2.18
Cpnd28	Monoterpene	nd	0.28	0.44	nd	0.71
Cpnd29	1-(2-thienyl)ethanone (86)	nd	nd	2.07	nd	4.25
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	0.33	nd	nd
Cpnd31	1-(2-thienyl)ethanone	nd	nd	5.10	nd	3.72
Cpnd32	Fenchone (83)	16.49	nd	14.37	nd	90.48
Cpnd33	Thioanisole	9.53	nd	27.73	nd	101.03
Cpnd34	Unidentified Hydrocarbon	5.06	0.29	0.91	nd	2.78
Cpnd35	Unidentified (contains sulphur)	nd	nd	0.75	nd	nd
Cpnd36	Unidentified (contains sulphur)	nd	nd	0.36	0.35	1.70
Cpnd37	Hydrocarbon (see binder)	nd	nd	0.79	nd	2.12
Cpnd38	{Methylguaiacol 80}	nd	1.04	1.90	0.35	1.67
Cpnd39	Dichloromethyl methyl sulphone	44.32	43.55	44.87	9.12	45.34
Cpnd40	Methyl (methylthio)methyl disulphide	nd	nd	0.91	nd	nd
Cpnd41	Terpenone	nd	nd	0.31	nd	9.62
Cpnd42	Unidentified hydrocarbon	nd	nd	0.63	nd	1.65
Cpnd43	{Veratrole 96}	1.35	nd	2.26	0.63	10.22
Cpnd44	C7H8O3 (based on MI)	nd	nd	1.20	nd	4.36
Cpnd45	Camphor (96)	0.51	nd	0.90	nd	27.09
Cpnd46	Unidentified	nd	nd	0.54	nd	2.47

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Oct-90	12-Mar-91	20-Jun-91	12-Sep-91	3-Dec-91
Cpnd47	Alkylated cyclopentenone	nd	nd	0.99	0.65	2.86
Cpnd48	Unidentified	nd	nd	1.28	nd	4.44
Cpnd49	Unidentified	nd	nd	0.99	nd	0.79
Cpnd50	Unidentified	nd	nd	1.20	nd	1.17
Cpnd51	1-Phenylpropanone (90)	nd	nd	0.37	nd	1.08
Cpnd52	Monoterpene(s)	nd	nd	0.50	nd	0.78
Cpnd53	Unidentified	nd	nd	0.52	nd	nd
Cpnd54	Dichlorophenol	nd	nd	0.47	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	nd	2.08	nd	nd
Cpnd56	2-(2-Thienyl)propanal	nd	nd	1.86	nd	nd
Cpnd57	t-Butylthiophene	nd	nd	nd	nd	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	nd	nd	5.17
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	0.58	nd	0.70	nd	1.70
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	0.70	nd	1.94	nd	15.69
Cpnd61	Coeluting Monoterpenes	1.31	nd	1.35	nd	8.67
Cpnd62	4-Methylthiophenol	nd	nd	0.44	nd	1.14
Cpnd63	Coeluting monoterpenes	nd	nd	nd	nd	6.51
Cpnd64	Dimethyltetrasulphide	nd	nd	nd	nd	nd
Cpnd65	Monoterpenone	1.21	nd	1.44	nd	9.92
Cpnd66	Contains dichloromethyl	1.27	0.97	2.96	1.06	1.86
Cpnd67	Contains Sulphur S4	nd	nd	nd	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	1.36	nd	2.68	nd	0.61
Cpnd69	not identified	0.73	nd	3.78	0.94	2.42
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd	nd	0.30	nd	1.87
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	nd	0.53	nd	nd
Cpnd72	Monoterpene	nd	nd	nd	nd	nd
Cpnd73	Unidentified	nd	nd	nd	nd	4.30
Cpnd74	Mulitple Compounds (Monoterpenes)	0.54	1.09	1.94	nd	1.40
Cpnd75	Syringol (94)	nd	nd	12.83	nd	nd
Cpnd76	Chloroterpene	nd	nd	3.64	nd	nd
Cpnd77	Monoterpene	nd	0.68	nd	nd	0.30
Cpnd78	Trichlorophenol	nd	nd	nd	nd	1.66
Cpnd79	Alkylnaphthalene	0.94	1.08	1.88	nd	nd
Cpnd80	Vanillin (74)	nd	0.63	1.49	nd	nd
Cpnd81	Junipene (83)	nd	nd	0.32	nd	1.23
Cpnd82	Alkylbenzene	nd	0.38	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd	nd
Cpnd85	Monoterpene	nd	nd	nd	nd	1.60
Cpnd86	Coeluting compounds Terpenoid	nd	0.25	nd	nd	1.70
Cpnd87	Monoterpene	nd	nd	0.76	nd	1.77
Cpnd88	Chloromonoterpene	nd	nd	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	nd	1.96	nd	nd
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd	nd	nd
Cpnd91	Dichloroguaiacol	nd	nd	1.85	1.02	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Oct-90	12-Mar-91	20-Jun-91	12-Sep-91	3-Dec-91
Cpnd92	Acetovanillone	nd	nd	nd	nd	nd
Cpnd93	Alkylthiophene	nd	nd	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	nd	nd	nd	nd
Cpnd96	δ-Cadinene (64)	nd	nd	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	nd	nd	nd	nd
Cpnd100	Sesquiterpene	nd	nd	nd	nd	nd
Cpnd101	Unknown (terpenoid)	nd	nd	nd	0.60	2.04
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	nd	0.41	0.60	nd	1.11
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	1.45	nd	2.24	0.59	4.74
Cpnd106	Chlorovanillone	nd	0.69	1.34	nd	nd
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	nd	nd	nd	nd	nd
Cpnd109	Trichloroguaiacol	nd	nd	nd	nd	2.58
Cpnd110	Terpenoid	nd	nd	0.45	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	nd	nd	nd	nd	0.16
Cpnd116	Nonylphenol Isomer [2]	nd	nd	nd	nd	3.03
Cpnd117	Nonylphenol Isomer [3]	nd	nd	0.96	nd	5.10
Cpnd118	Nonylphenol Isomer [4]	nd	nd	nd	nd	1.35
Cpnd119	Nonylphenol Isomer [5]	nd	nd	0.82	nd	5.08
Cpnd120	Nonylphenol Isomer [6]	nd	nd	nd	nd	1.21
Cpnd121	Nonylphenol Isomer [7]	nd	nd	0.80	nd	3.25
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	49.25	nd	1.52	nd	4.94
Cpnd123	Nonylphenol Isomer [8]	nd	nd	nd	nd	nd
Cpnd124	Nonylphenol Isomer [9]	nd	nd	nd	nd	2.00
Cpnd125	Nonylphenol Isomer [10]	nd	nd	0.81	nd	3.23
Cpnd126	Nonylphenol Isomer [11]	nd	nd	0.76	nd	4.07
Cpnd127	Nonylphenol Isomer [12]	nd	nd	nd	nd	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd	nd	nd
Cpnd129	Diterpene	nd	nd	nd	nd	nd
Cpnd130	Diterpene	nd	0.98	nd	nd	nd
Cpnd131	Diterpene	nd	nd	nd	nd	0.77
Cpnd132	Diterpene	nd	0.40	nd	nd	0.72
Cpnd133	Sandaracopimaradiene	nd	0.41	1.54	nd	0.86
Cpnd134	Diterpene	nd	0.34	1.01	nd	3.39
Cpnd135	Diterpene	nd	nd	0.75	nd	0.72
Cpnd136	Diterpene	nd	nd	0.68	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 24-Oct-90	12-Mar-91	20-Jun-91	12-Sep-91	3-Dec-91
Cpnd137	Diterpene	nd	1.61	0.67	nd	1.11
Cpnd138	Diterpene	nd	nd	0.52	nd	16.49
Cpnd139	Diterpene	nd	nd	0.54	nd	3.41
Cpnd140	Diterpene	nd	nd	nd	nd	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCI.-ol unide	nd	nd	1.18	nd	54.07
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	0.51	nd	51.27
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd	0.67	nd	63.00
Cpnd144	Pimarinal	nd	nd	nd	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	4.63
Cpnd146	Diterpene	nd	nd	nd	nd	1.17
Cpnd147	Diterpene	nd	nd	0.60	nd	6.59
Cpnd148	Diterpene	nd	nd	nd	nd	2.34
Cpnd149	Coeluting compounds	nd	nd	nd	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	25-Mar-92	9-Jun-92	3-Sep-92	17-Nov-92	9-Sep-93
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd	nd	nd
Cpnd2	Methylcyclohexane	nd	2.41	2.73	1.72	nd
Cpnd3	2-Heptanone (91)	nd	nd	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	nd	nd	nd	nd
Cpnd5	$C_7H_{12}O$	nd	nd	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	nd	nd	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd	nd	nd	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	nd	nd	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	nd	4.07	1.36	nd
Cpnd10	Diethylcyclopentenone	3.92	1.81	nd	nd	nd
Cpnd11	Methylcyclopentenone	1.57	0.23	nd	nd	nd
Cpnd12	Dimethyltrisulphide	0.84	nd	nd	nd	nd
Cpnd13	Diethylcyclopentenone	2.40	1.10	nd	nd	nd
Cpnd14	α-Thujene (91)	nd	nd	nd	nd	nd
Cpnd15	Monoterpene [1]	nd	nd	nd	nd	nd
Cpnd16	Unidentified	0.83	0.28	nd	nd	nd
Cpnd17	α-Terpinene (96)	nd	nd	nd	nd	nd
Cpnd18	Cymene (not para) (91)	nd	nd	nd	nd	nd
Cpnd19	{Guaiacol 80}	nd	nd	nd	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	4.19	nd	nd	nd	nd
Cpnd21	Sabinene (90)	nd	nd	nd	nd	nd
Cpnd22	Unidentified	1.29	nd	nd	nd	nd
Cpnd23	Dimethylcyclopentenone	nd	nd	nd	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	2.54	1.73	nd	0.99	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	2.84	nd	nd	nd	nd
Cpnd26	{Guaiacol 76}	20.34	9.41	3.70	0.49	nd
Cpnd27	1-phenylethanone (94)	2.41	0.64	nd	nd	nd
Cpnd28	Monoterpene	0.43	nd	nd	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd	0.52	nd	nd	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	nd	nd	nd
Cpnd31	1-(2-thienyl)ethanone	16.64	nd	nd	nd	nd
Cpnd32	Fenchone (83)	nd	nd	nd	nd	nd
Cpnd33	Thioanisole	nd	35.26	nd	nd	nd
Cpnd34	Unidentified Hydrocarbon	1.37	0.86	nd	nd	nd
Cpnd35	Unidentified (contains sulphur)	nd	nd	nd	nd	nd
Cpnd36	Unidentified (contains sulphur)	3.49	nd	nd	nd	nd
Cpnd37	Hydrocarbon (see binder)	1.41	nd	nd	nd	nd
Cpnd38	{Methylguaiacol 80}	0.29	nd	nd	nd	nd
Cpnd39	Dichloromethyl methyl sulphone	55.85	38.14	46.08	27.93	48.27
Cpnd40	Methyl (methylthio)methyl disulphide	0.30	nd	nd	nd	nd
Cpnd41	Terpenone	1.69	nd	nd	nd	nd
Cpnd42	Unidentified hydrocarbon	0.32	nd	nd	nd	nd
Cpnd43	{Veratrole 96}	0.32	2.76	nd	nd	nd
Cpnd44	C7H8O3 (based on MI)	0.64	nd	nd	nd	nd
Cpnd45	Camphor (96)	2.39	nd	nd	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 25-Mar-92	9-Jun-92	3-Sep-92	17-Nov-92	9-Sep-93
Cpnd46	Unidentified	2.65	nd	nd	nd	nd
Cpnd47	Alkylated cyclopentenone	1.33	0.70	nd	nd	nd
Cpnd48	Unidentified	0.64	nd	nd	nd	nd
Cpnd49	Unidentified	0.35	nd	nd	nd	nd
Cpnd50	Unidentified	0.30	nd	nd	nd	nd
Cpnd51	1-Phenylpropanone (90)	1.29	nd	nd	nd	nd
Cpnd52	Monoterpene(s)	0.86	nd	nd	nd	nd
Cpnd53	Unidentified	0.48	nd	nd	nd	nd
Cpnd54	Dichlorophenol	nd	0.40	nd	nd	nd
Cpnd55	Methylphenolsulphonyl	6.30	1.57	nd	nd	nd
Cpnd56	2-(2-Thienyl)propanal	16.69	nd	nd	nd	nd
Cpnd57	t-Butylthiophene	nd	nd	nd	nd	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	nd	nd	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	0.58	0.75	nd	nd	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	0.27	nd	nd	nd	nd
Cpnd61	Coeluting Monoterpenes	0.95	nd	nd	nd	nd
Cpnd62	4-Methylthiophenol	1.77	nd	nd	nd	nd
Cpnd63	Coeluting monoterpenes	nd	0.55	nd	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd	nd	nd	nd
Cpnd65	Monoterpenone	5.29	1.38	nd	nd	nd
Cpnd66	Contains dichloromethyl	4.14	2.77	3.86	2.44	5.19
Cpnd67	Contains Sulphur S4	nd	0.55	nd	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	9.13	nd	nd	nd	nd
Cpnd69	not identified	5.34	nd	4.68	0.90	1.65
Cpnd70	Coeluting Compounds; 1 is monoterpene.	1.09	0.81	nd	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	1.08	nd	nd	nd	nd
Cpnd72	Monoterpene	nd	nd	nd	nd	nd
Cpnd73	Unidentified	0.87	nd	nd	nd	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	1.45	0.36	nd	nd	nd
Cpnd75	Syringol (94)	0.66	nd	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd	nd	nd
Cpnd77	Monoterpene	nd	nd	nd	nd	nd
Cpnd78	Trichlorophenol	0.08	1.99	nd	nd	nd
Cpnd79	Alkylnaphthalene	7.07	nd	nd	nd	nd
Cpnd80	Vanillin (74)	1.29	nd	nd	nd	nd
Cpnd81	Junipene (83)	nd	nd	nd	nd	nd
Cpnd82	Alkylbenzene	1.01	nd	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd	nd	nd
Cpnd85	Monoterpene	1.20	nd	nd	nd	nd
Cpnd86	Coeluting compounds Terpenoid	1.18	nd	nd	nd	nd
Cpnd87	Monoterpene	3.23	nd	nd	nd	nd
Cpnd88	Chloromonoterpene	nd	nd	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	6.51	nd	nd	nd	nd
Cpnd90	Dichloro- Methyl terpenoid	2.17	1.90	nd	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 25-Mar-92	9-Jun-92	3-Sep-92	17-Nov-92	9-Sep-93
Cpnd91	Dichloroguaiacol	1.04	3.88	nd	1.34	nd
Cpnd92	Acetovanillone	1.72	nd	nd	nd	nd
Cpnd93	Alkylthiophene	nd	nd	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	0.61	nd	nd	nd	nd
Cpnd96	δ-Cadinene (64)	0.81	nd	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	0.42	nd	nd	nd	nd
Cpnd100	Sesquiterpene	0.47	nd	nd	nd	nd
Cpnd101	Unknown (terpenoid)	0.82	nd	nd	nd	nd
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	1.05	1.36	nd	nd	nd
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	2.00	1.15	nd	nd	nd
Cpnd106	Chlorovanillone	1.35	1.23	nd	nd	nd
Cpnd107	Dichloro, terpenoid	nd	nd	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	0.74	nd	nd	nd	nd
Cpnd109	Trichloroguaiacol	nd	0.59	nd	nd	nd
Cpnd110	Terpenoid	nd	nd	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	4.09	0.76	nd	nd	nd
Cpnd116	Nonylphenol Isomer [2]	nd	nd	nd	nd	nd
Cpnd117	Nonylphenol Isomer [3]	1.08	nd	nd	nd	nd
Cpnd118	Nonylphenol Isomer [4]	4.39	nd	nd	nd	nd
Cpnd119	Nonylphenol Isomer [5]	nd	nd	nd	nd	nd
Cpnd120	Nonylphenol Isomer [6]	4.52	nd	nd	nd	nd
Cpnd121	Nonylphenol Isomer [7]	nd	nd	nd	nd	nd
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	1.91	1.47	nd	nd	nd
Cpnd123	Nonylphenol Isomer [8]	5.63	nd	nd	nd	nd
Cpnd124	Nonylphenol Isomer [9]	4.42	nd	nd	nd	nd
Cpnd125	Nonylphenol Isomer [10]	4.22	0.82	nd	nd	nd
Cpnd126	Nonylphenol Isomer [11]	4.39	nd	nd	nd	nd
Cpnd127	Nonylphenol Isomer [12]	3.96	nd	nd	nd	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd	nd	nd
Cpnd129	Diterpene	nd	nd	nd	nd	nd
Cpnd130	Diterpene	nd	nd	nd	nd	nd
Cpnd131	Diterpene	nd	nd	nd	nd	nd
Cpnd132	Diterpene	nd	nd	nd	nd	nd
Cpnd133	Sandaracopimaradiene	1.21	1.02	nd	nd	nd
Cpnd134	Diterpene	1.83	0.69	nd	nd	nd
Cpnd135	Diterpene	0.60	0.75	nd	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 25-Mar-92	9-Jun-92	3-Sep-92	17-Nov-92	9-Sep-93
Cpnd136	Diterpene	nd	nd	nd	nd	nd
Cpnd137	Diterpene	0.73	0.67	nd	nd	nd
Cpnd138	Diterpene	0.60	nd	nd	nd	nd
Cpnd139	Diterpene	nd	nd	nd	nd	nd
Cpnd140	Diterpene	nd	nd	nd	nd	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	2.77	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	0.35	1.69	nd	nd	nd
Cpnd144	Pimarinal	nd	nd	nd	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd	nd	nd
Cpnd146	Diterpene	nd	0.57	nd	nd	nd
Cpnd147	Diterpene	nd	nd	nd	nd	nd
Cpnd148	Diterpene	0.78	nd	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 28-Oct-93	2-Feb-94
Cpnd1	Dimethylsulphoxide (86)	nd	nd
Cpnd2	Methylcyclohexane	nd	nd
Cpnd3	2-Heptanone (91)	nd	nd
Cpnd4	Dimethylcyclohexane	2.00	2.19
Cpnd5	$C_7H_{12}O$	nd	nd
Cpnd6	$C_4H_6S_2$	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	1.40
Cpnd10	Diethylcyclopentenone	nd	1.00
Cpnd11	Methylcyclopentenone	nd	nd
Cpnd12	Dimethyltrisulphide	nd	nd
Cpnd13	Diethylcyclopentenone	nd	nd
Cpnd14	α-Thujene (91)	nd	nd
Cpnd15	Monoterpene [1]	nd	nd
Cpnd16	Unidentified	nd	nd
Cpnd17	α-Terpinene (96)	nd	nd
Cpnd18	Cymene (not para) (91)	nd	nd
Cpnd19	{Guaiacol 80}	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	nd	nd
Cpnd21	Sabinene (90)	nd	nd
Cpnd22	Unidentified	nd	nd
Cpnd23	Dimethylcyclopentenone	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	1.21	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd	nd
Cpnd26	{Guaiacol 76}	nd	5.99
Cpnd27	1-phenylethanone (94)	nd	0.89
Cpnd28	Monoterpene	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd	2.15
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd
Cpnd31	1-(2-thienyl)ethanone	nd	4.70
Cpnd32	Fenchone (83)	nd	nd
Cpnd33	Thioanisole	nd	nd
Cpnd34	Unidentified Hydrocarbon	nd	nd
Cpnd35	Unidentified (contains sulphur)	nd	nd
Cpnd36	Unidentified (contains sulphur)	nd	1.35
Cpnd37	Hydrocarbon (see binder)	nd	nd
Cpnd38	{Methylguaiacol 80}	0.97	nd
Cpnd39	Dichloromethyl methyl sulphone	51.20	43.11
Cpnd40	Methyl (methylthio)methyl disulphide	nd	nd
Cpnd41	Terpenone	nd	nd
Cpnd42	Unidentified hydrocarbon	nd	nd
Cpnd43	{Veratrole 96}	nd	1.45
Cpnd44	C7H8O3 (based on MI)	nd	nd
Cpnd45	Camphor (96)	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 28-Oct-93	2-Feb-94
Cpnd46	Unidentified	nd	nd
Cpnd47	Alkylated cyclopentenone	1.13	nd
Cpnd48	Unidentified	nd	nd
Cpnd49	Unidentified	nd	nd
Cpnd50	Unidentified	nd	nd
Cpnd51	1-Phenylpropanone (90)	nd	nd
Cpnd52	Monoterpene(s)	nd	nd
Cpnd53	Unidentified	nd	nd
Cpnd54	Dichlorophenol	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	1.61
Cpnd56	2-(2-Thienyl)propanal	nd	nd
Cpnd57	t-Butylthiophene	nd	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	nd	nd
Cpnd61	Coeluting Monoterpenes	nd	nd
Cpnd62	4-Methylthiophenol	nd	nd
Cpnd63	Coeluting monoterpenes	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd
Cpnd65	Monoterpenone	nd	1.28
Cpnd66	Contains dichloromethyl	3.78	2.39
Cpnd67	Contains Sulphur S4	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	nd	nd
Cpnd69	not identified	0.75	1.87
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	nd
Cpnd72	Monoterpene	nd	nd
Cpnd73	Unidentified	nd	1.24
Cpnd74	Mulitple Compounds (Monoterpenes)	nd	nd
Cpnd75	Syringol (94)	nd	nd
Cpnd76	Chloroterpene	nd	nd
Cpnd77	Monoterpene	nd	nd
Cpnd78	Trichlorophenol	nd	nd
Cpnd79	Alkylnaphthalene	nd	nd
Cpnd80	Vanillin (74)	nd	nd
Cpnd81	Junipene (83)	nd	nd
Cpnd82	Alkylbenzene	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd
Cpnd85	Monoterpene	nd	nd
Cpnd86	Coeluting compounds Terpenoid	nd	nd
Cpnd87	Monoterpene	nd	nd
Cpnd88	Chloromonoterpene	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 28-Oct-93	2-Feb-94
Cpnd90	Dichloro- Methyl terpenoid	nd	nd
Cpnd91	Dichloroguaiacol	nd	nd
Cpnd92	Acetovanillone	nd	nd
Cpnd93	Alkylthiophene	nd	nd
Cpnd94	Trichloroveratrole	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	nd
Cpnd96	δ-Cadinene (64)	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	nd
Cpnd100	Sesquiterpene	nd	nd
Cpnd101	Unknown (terpenoid)	nd	nd
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd
Cpnd103	Sesquiterpene C14H24O	nd	nd
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd	nd
Cpnd106	Chlorovanillone	1.37	nd
Cpnd107	Dichloro, terpenoid	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	nd	nd
Cpnd109	Trichloroguaiacol	1.79	nd
Cpnd110	Terpenoid	nd	nd
Cpnd111	coeluting compounds	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd
Cpnd114	Unidentified, contains S	nd	nd
Cpnd115	Nonylphenol Isomer [1]	nd	nd
Cpnd116	Nonylphenol Isomer [2]	nd	nd
Cpnd117	Nonylphenol Isomer [3]	nd	nd
Cpnd118	Nonylphenol Isomer [4]	nd	nd
Cpnd119	Nonylphenol Isomer [5]	nd	nd
Cpnd120	Nonylphenol Isomer [6]	nd	nd
Cpnd121	Nonylphenol Isomer [7]	nd	nd
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	nd	nd
Cpnd123	Nonylphenol Isomer [8]	nd	nd
Cpnd124	Nonylphenol Isomer [9]	nd	nd
Cpnd125	Nonylphenol Isomer [10]	nd	nd
Cpnd126	Nonylphenol Isomer [11]	nd	nd
Cpnd127	Nonylphenol Isomer [12]	nd	nd
Cpnd128	Diterpenoid (nor)	nd	nd
Cpnd129	Diterpene	nd	nd
Cpnd130	Diterpene	nd	nd
Cpnd131	Diterpene	nd	nd
Cpnd132	Diterpene	nd	nd
Cpnd133	Sandaracopimaradiene	nd	nd
Cpnd134	Diterpene	nd	nd
Cpnd135	Diterpene	nd	nd

Daishowa Kraft Pulp Mill in Peace River Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 28-Oct-93	2-Feb-94
Cpnd136	Diterpene	nd	nd
Cpnd137	Diterpene	nd	nd
Cpnd138	Diterpene	nd	nd
Cpnd139	Diterpene	nd	nd
Cpnd140	Diterpene	nd	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCI.-ol unide	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd
Cpnd144	Pimarinal	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd
Cpnd146	Diterpene	nd	nd
Cpnd147	Diterpene	nd	nd
Cpnd148	Diterpene	nd	nd
Cpnd149	Coeluting compounds	nd	nd

APPENDIX 7

ALBERTA PACIFIC KRAFT PULP MILL IN GRASSLANDS

Alberta Pacific Kraft Pulp Mill in Grasslands

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 12-May-93	6-Oct-93	8-Feb-94
Cpnd1	Dimethylsulphoxide (86)	nd	nd	nd
Cpnd2	Methylcyclohexane	nd	nd	nd
Cpnd3	2-Heptanone (91)	nd	nd	nd
Cpnd4	Dimethylcyclohexane	nd	4.15	5.56
Cpnd5	$C_7H_{12}O$	nd	nd	nd
Cpnd6	$C_4H_6S_2$	nd	nd	nd
Cpnd7	Methylcyclopentenone	nd	nd	nd
Cpnd8	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	nd	nd	nd
Cpnd9	Methane, sulphonylbis- $C_2H_6O_2S$	nd	nd	nd
Cpnd10	Diethylcyclopentenone	nd	nd	nd
Cpnd11	Methylcyclopentenone	nd	nd	nd
Cpnd12	Dimethyltrisulphide	nd	nd	nd
Cpnd13	Diethylcyclopentenone	nd	nd	nd
Cpnd14	α-Thujene (91)	nd	nd	nd
Cpnd15	Monoterpene [1]	nd	nd	nd
Cpnd16	Unidentified	nd	nd	nd
Cpnd17	α-Terpinene (96)	nd	nd	nd
Cpnd18	Cymene (not para) (91)	nd	nd	nd
Cpnd19	{Guaiacol 80}	nd	nd	nd
Cpnd20	1,2-bis(methylthio)ethane	nd	nd	nd
Cpnd21	Sabinene (90)	nd	nd	nd
Cpnd22	Unidentified	nd	nd	nd
Cpnd23	Dimethylcyclopentenone	nd	nd	nd
Cpnd24	Bis-(chloromethyl)-sulphonyl	nd	nd	nd
Cpnd25	3,5-Dimethylcyclopentane-1,2-dione (64)	nd	nd	nd
Cpnd26	{Guaiacol 76}	nd	nd	nd
Cpnd27	1-phenylethanone (94)	nd	nd	nd
Cpnd28	Monoterpene	nd	nd	nd
Cpnd29	1-(2-thienyl)ethanone (86)	nd	nd	nd
Cpnd30	1-methyl-4-(1-methylethenyl)benzene (92)	nd	nd	nd
Cpnd31	1-(2-thienyl)ethanone	nd	nd	nd
Cpnd32	Fenchone (83)	nd	nd	nd
Cpnd33	Thioanisole	nd	nd	nd
Cpnd34	Unidentified Hydrocarbon	nd	nd	nd
Cpnd35	Unidentified (contains sulphur)	nd	nd	nd
Cpnd36	Unidentified (contains sulphur)	nd	nd	nd
Cpnd37	Hydrocarbon (see binder)	nd	nd	nd
Cpnd38	{Methylguaiacol 80}	nd	nd	nd
Cpnd39	Dichloromethyl methyl sulphone	nd	38.44	30.25
Cpnd40	Methyl (methylthio)methyl disulphide	nd	nd	nd
Cpnd41	Terpenone	nd	nd	nd

Alberta Pacific Kraft Pulp Mill in Grasslands Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 12-May-93	6-Oct-93	8-Feb-94
Cpnd42	Unidentified hydrocarbon	nd	nd	nd
Cpnd43	{Veratrole 96}	nd	nd	nd
Cpnd44	C7H8O3 (based on MI)	nd	nd	nd
Cpnd45	Camphor (96)	nd	nd	nd
Cpnd46	Unidentified	nd	nd	nd
Cpnd47	Alkylated cyclopentenone	nd	nd	nd
Cpnd48	Unidentified	nd	nd	nd
Cpnd49	Unidentified	nd	nd	nd
Cpnd50	Unidentified	nd	nd	nd
Cpnd51	1-Phenylpropanone (90)	nd	nd	nd
Cpnd52	Monoterpene(s)	nd	nd	nd
Cpnd53	Unidentified	nd	nd	nd
Cpnd54	Dichlorophenol	nd	nd	nd
Cpnd55	Methylphenolsulphonyl	nd	nd	nd
Cpnd56	2-(2-Thienyl)propanal	nd	nd	nd
Cpnd57	t-Butylthiophene	nd	nd	nd
Cpnd58	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	nd
Cpnd59	Coeluting Monoterpene and alkylcyclohexenone	nd	nd	nd
Cpnd60	Benzenemethanol, 4-(1-methylethyl) (59)	nd	nd	nd
Cpnd61	Coeluting Monoterpenes	nd	nd	nd
Cpnd62	4-Methylthiophenol	nd	nd	nd
Cpnd63	Coeluting monoterpenes	nd	nd	nd
Cpnd64	Dimethyltetrasulphide	nd	nd	nd
Cpnd65	Monoterpenone	nd	nd	nd
Cpnd66	Contains dichloromethyl	nd	nd	nd
Cpnd67	Contains Sulphur S4	nd	nd	nd
Cpnd68	3-methyl-2-thiophenecarboxylic acid (53)	nd	nd	nd
Cpnd69	not identified	nd	nd	nd
Cpnd70	Coeluting Compounds; 1 is monoterpene.	nd	nd	nd
Cpnd71	methyl(1-methylethyl)phenol (62)	nd	nd	nd
Cpnd72	Monoterpene	nd	nd	nd
Cpnd73	Unidentified	nd	nd	nd
Cpnd74	Mulitple Compounds (Monoterpenes)	nd	nd	nd
Cpnd75	Syringol (94)	nd	nd	nd
Cpnd76	Chloroterpene	nd	nd	nd
Cpnd77	Monoterpene	nd	nd	nd
Cpnd78	Trichlorophenol	nd	nd	nd
Cpnd79	Alkylnaphthalene	nd	nd	nd
Cpnd80	Vanillin (74)	nd	nd	nd
Cpnd81	Junipene (83)	nd	nd	nd

Alberta Pacific Kraft Pulp Mill in Grasslands Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 12-May-93	6-Oct-93	8-Feb-94
Cpnd82	Alkylbenzene	nd	nd	nd
Cpnd83	Dimethoxybenzoic acid (25)	nd	nd	nd
Cpnd84	Chlorinated monoterpene ??	nd	nd	nd
Cpnd85	Monoterpene	nd	nd	nd
Cpnd86	Coeluting compounds Terpenoid	nd	nd	nd
Cpnd87	Monoterpene	nd	nd	nd
Cpnd88	Chloromonoterpene	nd	nd	nd
Cpnd89	Methoxy-2-ethoxyethyl-1-furan (53)	nd	nd	nd
Cpnd90	Dichloro- Methyl terpenoid	nd	nd	nd
Cpnd91	Dichloroguaiacol	nd	nd	nd
Cpnd92	Acetovanillone	nd	nd	nd
Cpnd93	Alkylthiophene	nd	nd	nd
Cpnd94	Trichloroveratrole	nd	nd	nd
Cpnd95	(+)-Aromadendrene (78)	nd	nd	nd
Cpnd96	δ-Cadinene (64)	nd	nd	nd
Cpnd97	Sesquiterpene (204), not Peak 116	nd	nd	nd
Cpnd98	Dichloro compounds 221,223,225 no MI.	nd	nd	nd
Cpnd99	Sesquiterpene mw 202	nd	nd	nd
Cpnd100	Sesquiterpene	nd	nd	nd
Cpnd101	Unknown (terpenoid)	nd	nd	nd
Cpnd102	Dichloro, methyl loss,terpenoid	nd	nd	nd
Cpnd103	Sesquiterpene C14H24O	nd	nd	nd
Cpnd104	dichloro compounds 221,223,225 no MI., terpenoid	nd	nd	nd
Cpnd105	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	nd	nd	nd
Cpnd106	Chlorovanillone	nd	nd	nd
Cpnd107	Dichloro, terpenoid	nd	nd	nd
Cpnd108	Unidentified chlorinated hydrocarbon	nd	nd	nd
Cpnd109	Trichloroguaiacol	nd	nd	nd
Cpnd110	Terpenoid	nd	nd	nd
Cpnd111	coeluting compounds	nd	nd	nd
Cpnd112	Unidentified hydrocarbons	nd	nd	nd
Cpnd113	Trichlorinated terpene	nd	nd	nd
Cpnd114	Unidentified, contains S	nd	nd	nd
Cpnd115	Nonylphenol Isomer [1]	nd	nd	nd
Cpnd116	Nonylphenol Isomer [2]	nd	nd	nd
Cpnd117	Nonylphenol Isomer [3]	nd	nd	nd
Cpnd118	Nonylphenol Isomer [4]	nd	nd	nd
Cpnd119	Nonylphenol Isomer [5]	nd	nd	nd
Cpnd120	Nonylphenol Isomer [6]	nd	nd	nd
Cpnd121	Nonylphenol Isomer [7]	nd	nd	nd

Alberta Pacific Kraft Pulp Mill in Grasslands Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 12-May-93	6-Oct-93	8-Feb-94
Cpnd122	3,4,5-Trimethoxybenzaldehyde (50)	nd	nd	nd
Cpnd123	Nonylphenol Isomer [8]	nd	nd	nd
Cpnd124	Nonylphenol Isomer [9]	nd	nd	nd
Cpnd125	Nonylphenol Isomer [10]	nd	nd	nd
Cpnd126	Nonylphenol Isomer [11]	nd	nd	nd
Cpnd127	Nonylphenol Isomer [12]	nd	nd	nd
Cpnd128	Diterpenoid (nor)	nd	nd	nd
Cpnd129	Diterpene	nd	nd	nd
Cpnd130	Diterpene	nd	nd	nd
Cpnd131	Diterpene	nd	nd	nd
Cpnd132	Diterpene	2.01	nd	nd
Cpnd133	Sandaracopimaradiene	nd	nd	nd
Cpnd134	Diterpene	nd	nd	nd
Cpnd135	Diterpene	nd	nd	nd
Cpnd136	Diterpene	nd	nd	nd
Cpnd137	Diterpene	nd	1.87	nd
Cpnd138	Diterpene	nd	nd	nd
Cpnd139	Diterpene	nd	nd	nd
Cpnd140	Diterpene	nd	nd	nd
Cpnd141	8,12.XI.-Epoxylabd-14-en-13.XCl.-ol unide	nd	nd	nd
Cpnd142	(11E,13Z)-11813-Labdadien-8-ol (59)	nd	nd	nd
Cpnd143	(11E,13Z)-11813-Labdadien-8-ol (55)	nd	nd	nd
Cpnd144	Pimarinal	nd	nd	nd
Cpnd145	4-Androsten-3-one (22)	nd	nd	nd
Cpnd146	Diterpene	nd	nd	nd
Cpnd147	Diterpene	nd	nd	nd
Cpnd148	Diterpene	nd	nd	nd
Cpnd149	Coeluting compounds	nd	nd	nd

APPENDIX 8

MILLAR WESTERN CTMP MILL IN WHITECOURT

Millar Western CTMP Mill in Whitecourt

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	21-Feb-90	13-Feb-91	29-May-91	31-Jul-91
Cmpd 001	Hexanal	nd	4.9	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	103.0	9.3	nd	3.8
Cmpd 003	2-Methylbutanoic Acid	nd	65.2	5.1	nd	nd
Cmpd 004	Pentanoic Acid	nd	32.1	12.5	nd	3.9
Cmpd 005	Cyclohexanone	nd	5.7	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	5.8	2.2	nd	9.6
Cmpd 007	Benzaldehyde	nd	9.0	6.0	nd	8.9
Cmpd 008	Monoterpene (Sabinene)	nd	7.9	2.2	nd	9.9
Cmpd 009	Hexanoic Acid	nd	25.1	19.0	nd	23.0
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	24.5	13.0	nd	36.4
Cmpd 012	Monoterpene (α-Terpinene)	nd	17.9	5.5	nd	17.9
Cmpd 013	Monoterpene (*p*-Cymene)	nd	9.7	17.8	nd	40.9
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	nd	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	67.8	21.8	nd	64.7
Cmpd 016	Monoterpene (γ-Terpinene)	nd	25.8	6.9	nd	20.3
Cmpd 017	Monoterpene	nd	2.6	nd	nd	3.5
Cmpd 018	4-Methylphenol	nd	5.9	nd	nd	nd
Cmpd 019	Monoterpene	nd	2.5	5.7	nd	11.7
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	28.0	nd	nd	nd
Cmpd 021	Unidentified Amine	6.6	nd	6.8	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	4.2	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	8.4	3.0	nd	11.6
Cmpd 025	Unidentified Hydrocarbon	nd	2.7	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	2.7	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	8.5	3.1	nd	8.4
Cmpd 028	Octanoic Acid	nd	8.8	nd	nd	6.3
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	nd	nd	nd
Cmpd 030	Monoterpene	nd	3.6	2.0	nd	7.8
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	2.3	3.3	nd	5.0
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	10.4	nd	nd	nd
Cmpd 035	Benzothiazole	12.5	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	127.5	1.8	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	6.0	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 040	Indole	nd	12.5	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	21-Feb-90	13-Feb-91	29-May-91	31-Jul-91
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	8.6	2.7	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	4.8	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 051	Vanillin	nd	48.9	17.4	nd	17.2
Cmpd 052	Unidentified Amine	nd	nd	13.9	nd	18.6
Cmpd 053	Pentadecane	nd	58.0	6.9	nd	nd
Cmpd 054	Acetovanillone	nd	nd	5.4	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	72.8	nd	32.9	nd	6.2
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	12.6	17.8	nd	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	57.2	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	14.7	7.8	54.3	nd	203.2
Cmpd 067	Unidentified	nd	nd	nd	nd	70.6
Cmpd 068	Unidentified Hydrocarbon	nd	7.1	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd	23.6
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	22.5	5.2	nd	nd
Cmpd 072	Heptadecene	nd	nd	2.3	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	11.4	nd	18.8
Cmpd 074	Heptacecane	16.2	520.2	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	4.2	nd	1.9	nd
Cmpd 076	Monoterpene	nd	2.9	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	9.0	nd	15.0
Cmpd 078	Sesquiterpene	nd	nd	nd	nd	39.7
Cmpd 079	Syringone	nd	nd	5.1	nd	11.0
Cmpd 080	Methylheptadecane	nd	26.8	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	26.5	nd	nd	4.5
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd	nd
Cmpd 083	OXYhydrocarbon	nd	nd	2.5	nd	6.2

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 8-Jun-89	21-Feb-90	13-Feb-91	29-May-91	31-Jul-91
Cmpd 084	Diterpene	nd	4.7	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd	55.4
Cmpd 086	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	nd	11.1	37.5	40.9	17.7
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	64.1	nd	nd	10.3
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	7.4	2.1	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	4.7	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	19.0
Cmpd 104	Diterpene	nd	nd	10.6	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	nd	15.9	150.1	11.3	71.4
Cmpd 106	Diterpene	nd	nd	nd	nd	nd
Cmpd 107	Squalene	nd	10.5	31.0	2.4	76.0
Cmpd 108	Triterpene	nd	nd	21.9	nd	13.4
Cmpd 109	Triterpene	nd	nd	3.9	nd	6.8
Cmpd 110	Triterpene	nd	nd	6.8	nd	11.5
Cmpd 111	Triterpene	nd	nd	20.9	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd	44.6
Cmpd 114	Triterpene	nd	nd	6.3	nd	nd
Cmpd 115	Triterpene	nd	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	18.8	nd	nd
Cmpd 118	Triterpene	nd	nd	nd	nd	nd
Cmpd 119	Triterpene	nd	nd	61.9	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

		Concentrations in µg/L				
CTMP Number	Compound Name, Formula or Description	19-Nov-91	4-Feb-92	21-May-92	13-Aug-92	28-Oct-92
Cmpd 001	Hexanal	nd	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	nd	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	nd	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	nd	10.8	nd	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	13.1	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	2.7	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	nd	nd	nd	nd
Cmpd 019	Monoterpene	nd	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	nd	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	nd	nd	nd
Cmpd 030	Monoterpene	nd	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	nd	nd	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 040	Indole	nd	nd	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 19-Nov-91	4-Feb-92	21-May-92	13-Aug-92	28-Oct-92
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 051	Vanillin	nd	17.1	nd	nd	nd
Cmpd 052	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 053	Pentadecane	nd	nd	nd	nd	nd
Cmpd 054	Acetovanillone	nd	nd	nd	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	122.3	49.5	nd	99.4	nd
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	nd	nd	nd	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	nd	67.7	45.6	10.6	76.8
Cmpd 067	Unidentified	nd	33.6	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 069	Unidentified	25.6	23.3	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	9.7	nd	nd	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd	24.6
Cmpd 075	Cyclododecane of Dodecene	nd	nd	nd	nd	nd
Cmpd 076	Monoterpene	nd	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	31.0	23.2	nd	nd	nd
Cmpd 079	Syringone	nd	nd	nd	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	18.6	nd	nd	49.4
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

		Concentrations in µg/L				
CTMP Number	Compound Name, Formula or Description	19-Nov-91	4-Feb-92	21-May-92	13-Aug-92	28-Oct-92
Cmpd 083	OXYhydrocarbon	nd	nd	nd	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	14.7	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	80.2	27.7	48.9	nd	nd
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	204.5	62.9	11.2	40.5	nd
Cmpd 106	Diterpene	nd	nd	nd	nd	nd
Cmpd 107	Squalene	6.7	12.1	nd	nd	31.3
Cmpd 108	Triterpene	nd	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	nd	nd	nd
Cmpd 111	Triterpene	nd	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd	nd
Cmpd 114	Triterpene	62.6	nd	nd	nd	nd
Cmpd 115	Triterpene	112.6	nd	nd	nd	nd
Cmpd 116	Triterpene	102.0	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd	nd
Cmpd 118	Triterpene	394.6	nd	nd	nd	nd
Cmpd 119	Triterpene	48.5	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 17-Feb-93	3-Mar-93	19-Sep-93	15-Feb-94
Cmpd 001	Hexanal	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	nd	nd	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	7.8
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	10.0
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	nd	nd	nd
Cmpd 019	Monoterpene	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	nd	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	nd	nd
Cmpd 030	Monoterpene	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	nd	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd
Cmpd 040	Indole	nd	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 17-Feb-93	3-Mar-93	19-Sep-93	15-Feb-94
Cmpd 042	Monoterpene	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 051	Vanillin	nd	nd	nd	nd
Cmpd 052	Unidentified Amine	nd	11.0	nd	nd
Cmpd 053	Pentadecane	nd	nd	nd	15.1
Cmpd 054	Acetovanillone	nd	nd	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	nd	nd	nd	nd
Cmpd 057	Unidentified	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	nd	nd	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	nd	nd	nd	nd
Cmpd 067	Unidentified	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	nd	nd	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	nd	nd	nd
Cmpd 076	Monoterpene	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd
Cmpd 079	Syringone	nd	nd	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	nd	nd	nd
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd

Millar Western CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 17-Feb-93	3-Mar-93	19-Sep-93	15-Feb-94
Cmpd 083	OXYhydrocarbon	nd	nd	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	nd	39.2	37.0	nd
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	20.7
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	nd	12.6	85.5	nd
Cmpd 106	Diterpene	nd	nd	nd	nd
Cmpd 107	Squalene	nd	nd	nd	15.0
Cmpd 108	Triterpene	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	nd	nd
Cmpd 111	Triterpene	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	21.6
Cmpd 114	Triterpene	nd	nd	nd	nd
Cmpd 115	Triterpene	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd
Cmpd 118	Triterpene	nd	nd	nd	nd
Cmpd 119	Triterpene	nd	nd	nd	nd

APPENDIX 9

ALBERTA NEWSPRINT COMPANY CTMP MILL IN WHITECOURT

Alberta Newsprint Company CTMP Mill in Whitecourt

		Concentrations in µg/L				
CTMP Number	Compound Name, Formula or Description	13-Feb-91	30-May-91	19-Nov-91	3-Feb-92	21--may-92
Cmpd 001	Hexanal	nd	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	1.2	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	1.3	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	6.3	18.4	14.9	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	nd	nd	nd	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	3.0	3.3	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	5.7	6.1	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	nd	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	2.4	5.6	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	nd	nd	nd	nd
Cmpd 019	Monoterpene	1.1	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	6.1	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	8.7	nd	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	39.0	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	nd	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	nd	nd	nd
Cmpd 030	Monoterpene	1.7	3.3	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 035	Benzothiazole	10.0	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	nd	nd	nd	nd
Cmpd 037	OXY Hydrocarbon	134.6	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 040	Indole	nd	nd	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 13-Feb-91	30-May-91	19-Nov-91	3-Feb-92	21--may-92
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	257.5	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	109.4	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 051	Vanillin	17.9	191.3	105.7	nd	12.5
Cmpd 052	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 053	Pentadecane	4.3	nd	nd	nd	nd
Cmpd 054	Acetovanillone	nd	nd	nd	nd	nd
Cmpd 055	Monterpene	11.5	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	nd	nd	nd	nd	nd
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	nd	nd	nd	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	11.6	18.1	nd	nd	nd
Cmpd 067	Unidentified	nd	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	15.3	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	nd	nd	nd	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	2.3	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	nd	nd	nd	nd
Cmpd 076	Monoterpene	nd	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 079	Syringone	nd	nd	nd	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 13-Feb-91	30-May-91	19-Nov-91	3-Feb-92	21--may-92
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd	nd
Cmpd 083	OXYhydrocarbon	nd	nd	nd	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	36.5	9.6	29.9	nd	40.3
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	1056.3	7.5	80.0	nd	10.8
Cmpd 106	Diterpene	nd	nd	nd	nd	nd
Cmpd 107	Squalene	2.3	6.2	36.8	nd	nd
Cmpd 108	Triterpene	nd	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	nd	nd	nd
Cmpd 111	Triterpene	nd	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd	nd
Cmpd 114	Triterpene	nd	nd	nd	nd	nd
Cmpd 115	Triterpene	nd	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd	nd
Cmpd 118	Triterpene	nd	nd	nd	nd	nd
Cmpd 119	Triterpene	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

		Concentrations in µg/L				
CTMP Number	Compound Name, Formula or Description	13-Aug-92	4-Nov-92	16-Feb-93	3-Jun-93	22-Sep-93
Cmpd 001	Hexanal	nd	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	nd	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	10.5	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	nd	nd	nd	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	nd	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	nd	nd	nd	nd
Cmpd 019	Monoterpene	nd	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	57.1	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	nd	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	33.5	nd	nd	nd
Cmpd 030	Monoterpene	nd	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	nd	nd	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	51.9	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 040	Indole	nd	nd	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

		Concentrations in µg/L				
CTMP Number	Compound Name, Formula or Description	13-Aug-92	4-Nov-92	16-Feb-93	3-Jun-93	22-Sep-93
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 051	Vanillin	33.9	25.1	nd	nd	nd
Cmpd 052	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 053	Pentadecane	nd	nd	nd	nd	nd
Cmpd 054	Acetovanillone	nd	nd	nd	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	nd	nd	nd	nd	nd
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	nd	nd	nd	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 067	Unidentified	nd	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	nd	nd	nd	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	nd	nd	nd	nd
Cmpd 076	Monoterpene	11.5	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 079	Syringone	nd	nd	nd	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 13-Aug-92	4-Nov-92	16-Feb-93	3-Jun-93	22-Sep-93
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd	nd
Cmpd 083	OXYhydrocarbon	nd	nd	nd	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	14.8	nd	42.6	39.3	28.6
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	23.3	nd	nd	13.5	8.3
Cmpd 106	Diterpene	nd	nd	nd	nd	nd
Cmpd 107	Squalene	nd	nd	nd	nd	nd
Cmpd 108	Triterpene	nd	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	nd	nd	nd
Cmpd 111	Triterpene	nd	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd	nd
Cmpd 114	Triterpene	nd	nd	nd	nd	nd
Cmpd 115	Triterpene	nd	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd	nd
Cmpd 118	Triterpene	nd	nd	nd	nd	nd
Cmpd 119	Triterpene	nd	nd	nd	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-93	22-Sep-93
Cmpd 001	Hexanal	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd
Cmpd 005	Cyclohexanone	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd
Cmpd 007	Benzaldehyde	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd
Cmpd 009	Hexanoic Acid	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd
Cmpd 017	Monoterpene	nd	nd
Cmpd 018	4-Methylphenol	nd	nd
Cmpd 019	Monoterpene	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd
Cmpd 021	Unidentified Amine	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	nd
Cmpd 023	Monoterpene	nd	nd
Cmpd 024	Monoterpene	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd
Cmpd 026	Alkylbenzene	nd	nd
Cmpd 027	Benzoic Acid	nd	nd
Cmpd 028	Octanoic Acid	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd
Cmpd 030	Monoterpene	nd	nd
Cmpd 031	Terpinol	nd	nd
Cmpd 032	Monoterpene	nd	nd
Cmpd 033	Monoterpene	nd	nd
Cmpd 034	Hydrocarbon	nd	nd
Cmpd 035	Benzothiazole	12.6	nd
Cmpd 036	Benzeneacetic Acid	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd
Cmpd 038	Hydrocarbon	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd
Cmpd 040	Indole	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-93	22-Sep-93
Cmpd 042	Monoterpene	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd
Cmpd 044	Monoterpene	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd
Cmpd 046	Decanoic Acid	nd	nd
Cmpd 047	Sesquiterpene	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd
Cmpd 051	Vanillin	10.5	nd
Cmpd 052	Unidentified Amine	nd	nd
Cmpd 053	Pentadecane	nd	nd
Cmpd 054	Acetovanillone	nd	nd
Cmpd 055	Monterpene	nd	nd
Cmpd 056	Monoterpene Acetate ??	nd	nd
Cmpd 057	Unidentified	nd	nd
Cmpd 058	Unidentified	nd	nd
Cmpd 059	Monoterpene	nd	nd
Cmpd 060	Syringaldehyde	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd
Cmpd 062	Hexadecane	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	11.6	nd
Cmpd 065	Diphenylamine	nd	nd
Cmpd 066	Sesquiterpene	nd	nd
Cmpd 067	Unidentified	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd
Cmpd 069	Unidentified	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd
Cmpd 071	Heptadecene	nd	nd
Cmpd 072	Heptadecene	nd	nd
Cmpd 073	Sesquiterpene	nd	nd
Cmpd 074	Heptacecane	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	nd
Cmpd 076	Monoterpene	nd	nd
Cmpd 077	Sequiterpene	nd	nd
Cmpd 078	Sesquiterpene	nd	nd
Cmpd 079	Syringone	nd	nd
Cmpd 080	Methylheptadecane	nd	nd
Cmpd 081	Hydrocarbon	nd	nd

Alberta Newsprint Company CTMP Mill in Whitecourt Continued

CTMP Number	Compound Name, Formula or Description	Concentrations in µg/L 4-Nov-93	22-Sep-93
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd
Cmpd 083	OXYhydrocarbon	nd	nd
Cmpd 084	Diterpene	nd	nd
Cmpd 085	Sesquiterpene	nd	nd
Cmpd 086	Sesquiterpene	nd	nd
Cmpd 087	Unidentified	nd	nd
Cmpd 088	Dibutylphthalate	38.1	11.5
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd
Cmpd 092	Sesquiterpene	nd	nd
Cmpd 093	Sesquiterpene	nd	nd
Cmpd 094	Diterpene	nd	nd
Cmpd 095	Sulphur S8	nd	nd
Cmpd 096	Sesquiterpene	nd	nd
Cmpd 097	Diterpene	nd	nd
Cmpd 098	Linoleic Acid	nd	nd
Cmpd 099	Unidentified	nd	nd
Cmpd 100	Unidentified	nd	nd
Cmpd 101	Unidentified	nd	nd
Cmpd 102	Unidentified	nd	nd
Cmpd 103	Diterpene	nd	nd
Cmpd 104	Diterpene	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	10.8	nd
Cmpd 106	Diterpene	nd	nd
Cmpd 107	Squalene	12.5	nd
Cmpd 108	Triterpene	nd	nd
Cmpd 109	Triterpene	nd	nd
Cmpd 110	Triterpene	nd	nd
Cmpd 111	Triterpene	nd	nd
Cmpd 112	Sterol	nd	nd
Cmpd 113	Triterpene	nd	nd
Cmpd 114	Triterpene	nd	nd
Cmpd 115	Triterpene	nd	nd
Cmpd 116	Triterpene	nd	nd
Cmpd 117	Triterpene	nd	nd
Cmpd 118	Triterpene	nd	nd
Cmpd 119	Triterpene	nd	nd

APPENDIX 10

SLAVE LAKE PULP CTMP MILL IN SLAVE LAKE

Slave Lake Pulp CTMP Mill in Slave Lake

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 21-Feb-91	20-Jun-91	23-Jul-91	15-Aug-91	6-Nov-91
Cmpd 001	Hexanal	nd	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	0	70	25	42	159
Cmpd 003	2-Methylbutanoic Acid	4	64	15	23	10
Cmpd 004	Pentanoic Acid	6	186	4	42	34
Cmpd 005	Cyclohexanone	nd	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	nd	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	26	27	18	50	10
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	173	24	13	13	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	63	nd	9	nd	9
Cmpd 019	Monoterpene	nd	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	9	72	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	4	nd	8	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd	nd
Cmpd 024	Monoterpene	8	nd	nd	5	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	26	14	nd
Cmpd 028	Octanoic Acid	11	22	nd	4	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	10	6	8
Cmpd 030	Monoterpene	nd	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	9	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	109	24	nd
Cmpd 036	Benzeneacetic Acid	565	357	52	72	992
Cmpd 037	OXY Hydrocarbon	6	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	37	nd
Cmpd 040	Indole	315	76	nd	31	407
Cmpd 041	Methylnaphthalene	nd	nd	48	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 21-Feb-91	20-Jun-91	23-Jul-91	15-Aug-91	6-Nov-91
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	32	15	57	nd
Cmpd 044	Monoterpene	1	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	4	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	8	nd	nd	nd
Cmpd 051	Vanillin	11	11	6	15	nd
Cmpd 052	Unidentified Amine	22	22	26	44	nd
Cmpd 053	Pentadecane	8	nd	nd	nd	nd
Cmpd 054	Acetovanillone	13	32	15	40	nd
Cmpd 055	Monterpene	nd	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	8	428	257	173	nd
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	6	5	nd	nd
Cmpd 059	Monoterpene	52	9	nd	16	89
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd	nd
Cmpd 062	Hexadecane	4	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	62	25	nd
Cmpd 065	Diphenylamine	nd	nd	46	42	nd
Cmpd 066	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 067	Unidentified	nd	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	nd	8	7	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	13	nd
Cmpd 074	Heptacecane	8	nd	nd	20	nd
Cmpd 075	Cyclododecane of Dodecene	18	nd	nd	12	nd
Cmpd 076	Monoterpene	5	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 079	Syringone	40	163	47	140	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	nd	nd	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 21-Feb-91	20-Jun-91	23-Jul-91	15-Aug-91	6-Nov-91
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	961	257	nd
Cmpd 083	OXYhydrocarbon	19	nd	nd	156	nd
Cmpd 084	Diterpene	nd	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	29	nd
Cmpd 086	Sesquiterpene	nd	9	nd	nd	nd
Cmpd 087	Unidentified	8	62	nd	nd	nd
Cmpd 088	Dibutylphthalate	25	100	372	448	nd
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	100	53	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	9	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd	120
Cmpd 096	Sesquiterpene	2	186	74	16	nd
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	11	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	15	13	15	nd
Cmpd 102	Unidentified	nd	168	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	nd
Cmpd 104	Diterpene	5	10	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	15	18	21	35	21
Cmpd 106	Diterpene	nd	25	nd	nd	nd
Cmpd 107	Squalene	3	7	6	278	17
Cmpd 108	Triterpene	nd	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd	nd
Cmpd 110	Triterpene	10	nd	nd	12	nd
Cmpd 111	Triterpene	10	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd	nd
Cmpd 114	Triterpene	nd	nd	nd	nd	19
Cmpd 115	Triterpene	nd	nd	nd	nd	21
Cmpd 116	Triterpene	nd	nd	nd	nd	19
Cmpd 117	Triterpene	5	nd	nd	32	nd
Cmpd 118	Triterpene	nd	nd	nd	67	103
Cmpd 119	Triterpene	33	nd	nd	130	12

Slave Lake Pulp CTMP Mill in Slave Lake Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	11-Feb-92	9-Mar-92	13-Mar-92	29-Apr-92	9-Mar-92
Cmpd 001	Hexanal	nd	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	nd	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	nd	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	7	25	47	6	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	25	26	20	10	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	124	29	nd	nd
Cmpd 019	Monoterpene	nd	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	nd	nd	25	5	nd
Cmpd 022	C8 Acid (C8H16O2)	33	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	nd	nd
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	7	9	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	27	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	3	nd	nd	nd	nd
Cmpd 030	Monoterpene	nd	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	nd	nd
Cmpd 034	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	nd	13	nd
Cmpd 036	Benzeneacetic Acid	nd	91	765	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd	13	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd	nd
Cmpd 040	Indole	nd	302	1322	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	4	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 11-Feb-92	9-Mar-92	13-Mar-92	29-Apr-92	9-Mar-92
Cmpd 042	Monoterpene	nd	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	2983	2079	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 051	Vanillin	nd	9	24	5	nd
Cmpd 052	Unidentified Amine	9	37	47	nd	nd
Cmpd 053	Pentadecane	nd	12	nd	nd	nd
Cmpd 054	Acetovanillone	nd	nd	29	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	25	nd	nd	nd	407
Cmpd 057	Unidentified	nd	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd	nd
Cmpd 059	Monoterpene	23	nd	nd	26	nd
Cmpd 060	Syringaldehyde	nd	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	25	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	11	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	18	nd	nd	nd
Cmpd 065	Diphenylamine	nd	19	22	nd	nd
Cmpd 066	Sesquiterpene	nd	nd	nd	6	nd
Cmpd 067	Unidentified	nd	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd	nd
Cmpd 071	Heptadecene	18	28	10	9	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	36	363	nd	nd
Cmpd 076	Monoterpene	nd	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 079	Syringone	nd	71	120	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd	nd
Cmpd 081	Hydrocarbon	nd	nd	14	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

		Concentrations in µg/L				
Date Sampled	Compound Name, Formula or Description	11-Feb-92	9-Mar-92	13-Mar-92	29-Apr-92	9-Mar-92
Cmpd 082	N-Butyl-benzenesulphonamide	nd	398	130	360	nd
Cmpd 083	OXYhydrocarbon	nd	nd	1980	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	28	13	nd	nd
Cmpd 088	Dibutylphthalate	485	161	559	598	nd
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	32	9	nd	nd
Cmpd 096	Sesquiterpene	58	nd	nd	nd	95
Cmpd 097	Diterpene	nd	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd	nd
Cmpd 101	Unidentified	15	nd	nd	nd	nd
Cmpd 102	Unidentified	17	nd	nd	10	nd
Cmpd 103	Diterpene	nd	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	18	28	26	85	nd
Cmpd 106	Diterpene	nd	nd	nd	nd	nd
Cmpd 107	Squalene	nd	150	26	9	nd
Cmpd 108	Triterpene	nd	32	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	16	nd	nd
Cmpd 111	Triterpene	nd	42	27	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	40	27	nd	nd
Cmpd 114	Triterpene	nd	54	104	nd	nd
Cmpd 115	Triterpene	nd	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd	nd
Cmpd 118	Triterpene	nd	155	78	nd	nd
Cmpd 119	Triterpene	nd	22	76	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Nov-92	10-Jun-93	18-Aug-93	28-Oct-93
Cmpd 001	Hexanal	nd	nd	nd	nd
Cmpd 002	3-Methylbutanoic Acid	nd	nd	nd	nd
Cmpd 003	2-Methylbutanoic Acid	nd	nd	nd	nd
Cmpd 004	Pentanoic Acid	nd	nd	nd	nd
Cmpd 005	Cyclohexanone	nd	nd	nd	nd
Cmpd 006	Monoterpene (α-Thujene)	nd	nd	nd	nd
Cmpd 007	Benzaldehyde	nd	nd	nd	nd
Cmpd 008	Monoterpene (Sabinene)	nd	nd	nd	nd
Cmpd 009	Hexanoic Acid	nd	nd	nd	nd
Cmpd 010	1-(Methylethenyl)-benzene	nd	nd	nd	nd
Cmpd 011	Monoterpene (α-Phellandrene)	nd	nd	nd	nd
Cmpd 012	Monoterpene (α-Terpinene)	nd	nd	nd	nd
Cmpd 013	Monoterpene (*p*-Cymene)	nd	nd	nd	nd
Cmpd 014	2,2'-Azobis[2-methylpropanenitrile]	7	nd	nd	nd
Cmpd 015	Monoterpene (β-Thujene)	nd	nd	nd	nd
Cmpd 016	Monoterpene (γ-Terpinene)	nd	nd	nd	nd
Cmpd 017	Monoterpene	nd	nd	nd	nd
Cmpd 018	4-Methylphenol	nd	nd	nd	nd
Cmpd 019	Monoterpene	nd	nd	nd	nd
Cmpd 020	a,a-Dimethylbenzenemethanol	nd	nd	nd	nd
Cmpd 021	Unidentified Amine	nd	nd	nd	nd
Cmpd 022	C8 Acid (C8H16O2)	nd	nd	nd	nd
Cmpd 023	Monoterpene	nd	nd	nd	nd
Cmpd 024	Monoterpene	nd	nd	nd	8
Cmpd 025	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 026	Alkylbenzene	nd	nd	nd	nd
Cmpd 027	Benzoic Acid	nd	nd	nd	nd
Cmpd 028	Octanoic Acid	nd	nd	nd	nd
Cmpd 029	4-(1-methylethyl)-benzenemethanol	nd	nd	nd	nd
Cmpd 030	Monoterpene	nd	nd	nd	nd
Cmpd 031	Terpinol	nd	nd	nd	nd
Cmpd 032	Monoterpene	nd	nd	nd	nd
Cmpd 033	Monoterpene	nd	nd	nd	71
Cmpd 034	Hydrocarbon	nd	nd	nd	nd
Cmpd 035	Benzothiazole	nd	nd	nd	nd
Cmpd 036	Benzeneacetic Acid	nd	nd	nd	nd
Cmpd 037	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 038	Hydrocarbon	nd	nd	nd	nd
Cmpd 039	Methylnaphthalene	nd	nd	nd	nd
Cmpd 040	Indole	nd	nd	nd	nd
Cmpd 041	Methylnaphthalene	nd	nd	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Nov-92	10-Jun-93	18-Aug-93	28-Oct-93
Cmpd 042	Monoterpene	nd	nd	nd	nd
Cmpd 043	Alkyl Phenol	nd	nd	nd	nd
Cmpd 044	Monoterpene	nd	nd	nd	nd
Cmpd 045	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 046	Decanoic Acid	nd	nd	nd	nd
Cmpd 047	Sesquiterpene	nd	nd	nd	nd
Cmpd 048	Oxyhydrocarbon	nd	nd	nd	nd
Cmpd 049	OXY Hydrocarbon	nd	nd	nd	nd
Cmpd 050	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 051	Vanillin	nd	nd	nd	nd
Cmpd 052	Unidentified Amine	nd	17	nd	nd
Cmpd 053	Pentadecane	nd	nd	nd	nd
Cmpd 054	Acetovanillone	nd	nd	nd	nd
Cmpd 055	Monterpene	nd	nd	nd	nd
Cmpd 056	Monoterpene Acetate ??	nd	nd	nd	179
Cmpd 057	Unidentified	nd	nd	nd	nd
Cmpd 058	Unidentified	nd	nd	nd	nd
Cmpd 059	Monoterpene	nd	18	nd	13
Cmpd 060	Syringaldehyde	nd	nd	nd	nd
Cmpd 061	Monoterpene Acid	nd	nd	nd	nd
Cmpd 062	Hexadecane	nd	nd	nd	nd
Cmpd 063	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 064	2-(Methylthio)-benzothiazole	nd	nd	nd	nd
Cmpd 065	Diphenylamine	nd	nd	nd	nd
Cmpd 066	Sesquiterpene	nd	nd	nd	nd
Cmpd 067	Unidentified	nd	nd	nd	nd
Cmpd 068	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 069	Unidentified	nd	nd	nd	nd
Cmpd 070	1,3,5-tri-2-popenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	nd	nd	nd	nd
Cmpd 071	Heptadecene	nd	nd	nd	nd
Cmpd 072	Heptadecene	nd	nd	nd	nd
Cmpd 073	Sesquiterpene	nd	nd	nd	nd
Cmpd 074	Heptacecane	nd	nd	nd	nd
Cmpd 075	Cyclododecane of Dodecene	nd	nd	nd	nd
Cmpd 076	Monoterpene	nd	nd	nd	nd
Cmpd 077	Sequiterpene	nd	nd	nd	nd
Cmpd 078	Sesquiterpene	nd	nd	nd	nd
Cmpd 079	Syringone	nd	nd	nd	nd
Cmpd 080	Methylheptadecane	nd	nd	nd	nd

Slave Lake Pulp CTMP Mill in Slave Lake Continued

Date Sampled	Compound Name, Formula or Description	Concentrations in µg/L 17-Nov-92	10-Jun-93	18-Aug-93	28-Oct-93
Cmpd 081	Hydrocarbon	nd	nd	nd	nd
Cmpd 082	N-Butyl-benzenesulphonamide	nd	nd	nd	nd
Cmpd 083	OXYhydrocarbon	nd	nd	nd	nd
Cmpd 084	Diterpene	nd	nd	nd	nd
Cmpd 085	Sesquiterpene	nd	nd	nd	nd
Cmpd 086	Sesquiterpene	nd	nd	nd	nd
Cmpd 087	Unidentified	nd	nd	nd	nd
Cmpd 088	Dibutylphthalate	nd	nd	34	nd
Cmpd 089	Diterpene (Sandaracopimaradiene)	nd	nd	nd	nd
Cmpd 090	N-Phenylbenzamide	nd	nd	nd	nd
Cmpd 091	Hexadecanoic Acid	nd	nd	nd	nd
Cmpd 092	Sesquiterpene	nd	nd	nd	nd
Cmpd 093	Sesquiterpene	nd	nd	nd	nd
Cmpd 094	Diterpene	nd	nd	nd	nd
Cmpd 095	Sulphur S8	nd	nd	nd	nd
Cmpd 096	Sesquiterpene	nd	nd	nd	nd
Cmpd 097	Diterpene	nd	nd	nd	nd
Cmpd 098	Linoleic Acid	nd	nd	nd	nd
Cmpd 099	Unidentified	nd	nd	nd	nd
Cmpd 100	Unidentified	nd	nd	nd	nd
Cmpd 101	Unidentified	nd	nd	nd	nd
Cmpd 102	Unidentified	nd	nd	nd	nd
Cmpd 103	Diterpene	nd	nd	nd	nd
Cmpd 104	Diterpene	nd	nd	nd	nd
Cmpd 105	Bis(2-ethylhexyl)phthalate	nd	15	240	31
Cmpd 106	Diterpene	nd	nd	nd	nd
Cmpd 107	Squalene	nd	nd	12	25
Cmpd 108	Triterpene	nd	nd	nd	nd
Cmpd 109	Triterpene	nd	nd	nd	nd
Cmpd 110	Triterpene	nd	nd	nd	nd
Cmpd 111	Triterpene	nd	nd	nd	nd
Cmpd 112	Sterol	nd	nd	nd	nd
Cmpd 113	Triterpene	nd	nd	nd	nd
Cmpd 114	Triterpene	nd	nd	nd	25
Cmpd 115	Triterpene	nd	nd	nd	nd
Cmpd 116	Triterpene	nd	nd	nd	nd
Cmpd 117	Triterpene	nd	nd	nd	nd
Cmpd 118	Triterpene	nd	nd	nd	34
Cmpd 119	Triterpene	nd	nd	nd	nd

APPENDIX 11

SEWAGE TREATMENT PLANT EFFLUENTS

Grande Prairie Municipal STP Effluent

	Compoud Name, Formula or Description	Concentrations in µg/L 10-Mar-89	28-Feb-90	27-Feb-91	12-Mar-92
Cmpd 01	Alkylfuran	nd	0.2	nd	nd
Cmpd 02	Cyclohexanol	0.7	nd	nd	nd
Cmpd 03	Dichlorinated Hydrocarbon	nd	nd	nd	nd
Cmpd 04	C7 Amine (Tertiary	nd	nd	nd	nd
Cmpd 05	Sulphonylbismethane	nd	nd	nd	nd
Cmpd 06	Cyclohexanone	0.6	0.4	nd	nd
Cmpd 07	Trichloropropane	0.2	0.1	nd	nd
Cmpd 08	Alkene (C12)	nd	0.2	nd	nd
Cmpd 09	Alkene (C12)	nd	nd	nd	nd
Cmpd 10	Isocineole	nd	nd	nd	nd
Cmpd 11	OXY Hydrocarbon	nd	0.4	2.0	0.7
Cmpd 12	Dichlorobenzene	nd	0.1	nd	nd
Cmpd 13	Alkyl Benzene	nd	nd	nd	nd
Cmpd 14	OXY Hydrocarbon	nd	0.5	nd	nd
Cmpd 15	Alkylbenzene	nd	0.2	nd	nd
Cmpd 16	Nitrosomorpholine	nd	3.2	nd	nd
Cmpd 17	Alkylbenzene	nd	nd	nd	nd
Cmpd 18	1,1-Dichlorodimethylsulphone	0.3	0.2	nd	nd
Cmpd 19	Alkylbenzene	nd	nd	nd	nd
Cmpd 20	Unidentified Alkoxy compound	nd	nd	nd	nd
Cmpd 21	Alkylbenzene	nd	nd	nd	nd
Cmpd 22	Triethylphosphate	nd	0.1	1.8	nd
Cmpd 23	Unidentified Amine (Morpholine ??)	nd	0.3	nd	nd
Cmpd 24	Decamethylcyclopentasiloxane	nd	nd	nd	nd
Cmpd 25	Cymene	nd	nd	nd	nd
Cmpd 26	*2-Ethylcyclohexanone*	nd	nd	nd	nd
Cmpd 27	Unidentified Monochloroamine	nd	0.1	nd	nd
Cmpd 28	Unidentified Hydrocarbon	nd	0.1	nd	nd
Cmpd 29	*t-Butylcyclohexanone*	nd	0.2	nd	nd
Cmpd 30	1,2-Benzothiazole	0.4	0.6	1.4	nd
Cmpd 31	Terpenol	nd	0.1	nd	nd
Cmpd 32	Chlorinated Amine	nd	nd	nd	nd
Cmpd 33	Unidentified Alkene	nd	nd	nd	nd
Cmpd 34	Unidentified	nd	nd	nd	nd
Cmpd 35	Alkyl Indene ??	nd	nd	nd	nd
Cmpd 36	Terpene	nd	nd	nd	nd

Grande Prairie Municipal STP Effluent Continued

	Compoud Name, Formula or Description	Concentrations in µg/L 10-Mar-89	28-Feb-90	27-Feb-91	12-Mar-92
Cmpd 37	Alkylbenzene	nd	nd	nd	nd
Cmpd 38	Alkyl Indanone	nd	nd	nd	nd
Cmpd 39	Dimethyl Phenol	nd	0.1	nd	nd
Cmpd 40	Alkyl Indan ??	nd	nd	nd	nd
Cmpd 41	Monoterpene	nd	nd	nd	nd
Cmpd 42	Branched Alkene	nd	nd	nd	nd
Cmpd 43	Unidentified Chlorinated Compound	nd	nd	nd	nd
Cmpd 44	Unidentified	nd	nd	nd	nd
Cmpd 45	Propenyl Anisole	nd	0.2	nd	nd
Cmpd 46	1,3-Isobenzofurandione	0.3	0.6	nd	nd
Cmpd 47	Branched Alkene	nd	0.1	nd	nd
Cmpd 48	Branched Alkene	nd	nd	nd	nd
Cmpd 49	3-Isopropylphenol	nd	nd	nd	nd
Cmpd 50	Dichlorobenzonitrile	0.5	0.1	nd	nd
Cmpd 51	Unidentified Hydrocarbon	nd	nd	nd	nd
Cmpd 52	Branched Alkane	nd	nd	nd	nd
Cmpd 53	Alkyl Indan	nd	0.2	nd	nd
Cmpd 54	Phenoxyacetic Acid	nd	0.4	nd	nd
Cmpd 55	2,6-t-Butylphenol	nd	0.3	nd	nd
Cmpd 56	Benzopyran-2-one	nd	0.1	nd	nd
Cmpd 57	Dibutyl phthalate	nd	nd	nd	nd
Cmpd 58	g-Methylionone	nd	0.5	nd	nd
Cmpd 59	Unidentified Oxy Hydrocarbon	0.3	0.3	nd	nd
Cmpd 60	2,6-Bis(1,1-dimethylethyl)-4-methylphenol	nd	0.3	nd	nd
Cmpd 61	N,N-Diethyl-3-methyl Benzamide	1.1	0.6	1.3	1.6
Cmpd 62	Alkane	nd	0.3	nd	nd
Cmpd 63	Diethylphthalate	0.4	nd	nd	nd
Cmpd 64	Unidentified Oxy Hydrocarbon	0.5	0.5	0.9	2.2
Cmpd 65	2-(Methylthio)benzothiazole	0.7	0.6	0.8	nd
Cmpd 66	Tributylphosphate	3.2	14.2	20.9	2.6
Cmpd 67	Unidentified Amine	nd	0.4	nd	nd
Cmpd 68	Alkane	nd	0.3	nd	nd
Cmpd 69	Unidentified	nd	nd	nd	nd
Cmpd 70	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	nd	nd	nd	nd
Cmpd 71	Nonyl Phenol Isomer	nd	0.7	2.2	6.2
Cmpd 72	Nonyl Phenol Isomer	nd	1.2	2.0	5.3

Grande Prairie Municipal STP Effluent Continued

	Compoud Name, Formula or Description	Concentrations in µg/L 10-Mar-89	28-Feb-90	27-Feb-91	12-Mar-92
Cmpd 73	Nonyl Phenol Isomer	nd	0.7	nd	3.8
Cmpd 74	2-Chloroethylphosphate	nd	nd	nd	nd
Cmpd 75	Unidentified	nd	0.3	nd	nd
Cmpd 76	Nonylphenol Isomer	nd	0.9	2.5	9.6
Cmpd 77	Neophytadiene	nd	0.2	nd	nd
Cmpd 78	Unidentified	nd	0.4	nd	nd
Cmpd 79	Caffeine	0.4	2.3	7.4	8.0
Cmpd 80	Unidentified Diterpene	nd	0.5	0.9	nd
Cmpd 81	Hexadecanoic Acid	nd	0.3	nd	nd
Cmpd 91	Unidentified Sterol	nd	nd	nd	nd
Cmpd 82	Oleic Acid	nd	nd	nd	nd
Cmpd 83	Stearic Acid	nd	nd	nd	nd
Cmpd 84	1,3-Dichloro-iso-propylphosphate	nd	nd	nd	nd
Cmpd 85	Butylphenyl phthalate	nd	nd	nd	nd
Cmpd 86	2-Butoxyethyl phosphate	0.6	2.0	3.5	6.6
Cmpd 87	Diheptyphosphate	nd	1.3	nd	nd
Cmpd 88	Bis(ethylhexyl)phthalate	1.1	1.6	1.8	5.3
Cmpd 89	Sterol	nd	0.1	nd	nd
Cmpd 90	Squalene	nd	0.3	nd	5.1
Cmpd 91	Unidentified Sterol	nd	nd	nd	nd

Whitecourt Municipal STP Effluent

STP Number	Compoud Name, Formula or Description	Concentrations in µg/L				
		20-Feb-90	12-Feb-91	5-Feb-92	17-Feb-93	15-Feb-94
Cmpd 01	Alkylfuran	nd	nd	nd	nd	nd
Cmpd 02	Cyclohexanol	nd	nd	nd	nd	nd
Cmpd 03	Dichlorinated Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 04	C7 Amine (Tertiary	nd	nd	nd	nd	nd
Cmpd 05	Sulphonylbismethane	nd	nd	nd	nd	nd
Cmpd 06	Cyclohexanone	0.3	nd	nd	nd	nd
Cmpd 07	Trichloropropane	0.0	nd	nd	nd	nd
Cmpd 08	Alkene (C12)	nd	nd	nd	nd	nd
Cmpd 09	Alkene (C12)	nd	nd	nd	nd	nd
Cmpd 10	Isocineole	nd	nd	nd	nd	nd
Cmpd 11	OXY Hydrocarbon	0.1	nd	nd	nd	nd
Cmpd 12	Dichlorobenzene	0.3	0.9	nd	nd	nd
Cmpd 13	Alkyl Benzene	nd	nd	nd	nd	nd
Cmpd 14	OXY Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 15	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 16	Nitrosomorpholine	0.5	nd	nd	nd	nd
Cmpd 17	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 18	1,1-Dichlorodimethylsulphone	0.5	1.3	nd	nd	nd
Cmpd 19	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 20	Unidentified Alkoxy compound	2.0	nd	nd	nd	nd
Cmpd 21	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 22	Triethylphosphate	nd	nd	nd	nd	nd
Cmpd 23	Unidentified Amine (Morpholine ??)	0.8	nd	0.7	nd	nd
Cmpd 24	Decamethylcyclopentasiloxane	0.1	0.7	nd	nd	nd
Cmpd 25	Cymene	nd	nd	nd	nd	nd
Cmpd 26	*2-Ethylcyclohexanone*	nd	nd	nd	nd	nd
Cmpd 27	Unidentified Monochloroamine	0.2	nd	nd	nd	nd
Cmpd 28	Unidentified Hydrocarbon	0.2	nd	nd	nd	nd
Cmpd 29	*t-Butylcyclohexanone*	0.3	nd	nd	nd	nd
Cmpd 30	1,2-Benzothiazole	0.7	2.2	1.4	nd	nd
Cmpd 31	Terpenol	0.1	nd	nd	nd	nd
Cmpd 32	Chlorinated Amine	0.2	nd	nd	nd	nd
Cmpd 33	Unidentified Alkene	nd	nd	nd	nd	nd
Cmpd 34	Unidentified	0.2	nd	nd	nd	nd
Cmpd 35	Alkyl Indene ??	0.1	nd	nd	nd	nd
Cmpd 36	Terpene	0.1	nd	nd	nd	nd

Whitecourt Municipal STP Effluent Continued

STP Number	Compoud Name, Formula or Description	Concentrations in µg/L 20-Feb-90	12-Feb-91	5-Feb-92	17-Feb-93	15-Feb-94
Cmpd 37	Alkylbenzene	nd	nd	nd	nd	nd
Cmpd 38	Alkyl Indanone	0.2	nd	nd	nd	nd
Cmpd 39	Dimethyl Phenol	0.3	0.5	nd	nd	nd
Cmpd 40	Alkyl Indan ??	0.1	nd	nd	nd	nd
Cmpd 41	Monoterpene	0.1	nd	nd	nd	nd
Cmpd 42	Branched Alkene	0.1	nd	nd	nd	nd
Cmpd 43	Unidentified Chlorinated Compound	0.1	nd	nd	nd	nd
Cmpd 44	Unidentified	nd	nd	nd	nd	nd
Cmpd 45	Propenyl Anisole	0.1	nd	nd	nd	nd
Cmpd 46	1,3-Isobenzofurandione	0.1	nd	nd	nd	nd
Cmpd 47	Branched Alkene	nd	nd	nd	nd	nd
Cmpd 48	Branched Alkene	nd	nd	nd	nd	nd
Cmpd 49	3-Isopropylphenol	nd	nd	nd	nd	nd
Cmpd 50	Dichlorobenzonitrile	nd	nd	nd	nd	nd
Cmpd 51	Unidentified Hydrocarbon	0.3	0.8	nd	nd	nd
Cmpd 52	Branched Alkane	nd	nd	nd	nd	nd
Cmpd 53	Alkyl Indan	nd	nd	nd	nd	nd
Cmpd 54	Phenoxyacetic Acid	nd	nd	1.2	nd	nd
Cmpd 55	2,6-t-Butylphenol	0.8	nd	nd	nd	nd
Cmpd 56	Benzopyran-2-one	0.7	nd	nd	nd	nd
Cmpd 57	Dibutyl phthalate	0.2	nd	nd	nd	nd
Cmpd 58	g-Methylionone	0.5	nd	nd	nd	nd
Cmpd 59	Unidentified Oxy Hydrocarbon	nd	nd	nd	nd	nd
Cmpd 60	2,6-Bis(1,1-dimethylethyl)-4-methylphenol	nd	0.3	nd	nd	nd
Cmpd 61	N,N-Diethyl-3-methyl Benzamide	0.4	1.2	1.7	nd	nd
Cmpd 62	Alkane	0.3	0.6	nd	nd	nd
Cmpd 63	Diethylphthalate	nd	nd	nd	nd	nd
Cmpd 64	Unidentified Oxy Hydrocarbon	nd	0.6	1.1	nd	nd
Cmpd 65	2-(Methylthio)benzothiazole	nd	nd	nd	nd	nd
Cmpd 66	Tributylphosphate	1.4	2.8	nd	nd	nd
Cmpd 67	Unidentified Amine	nd	nd	nd	nd	nd
Cmpd 68	Alkane	0.3	1.4	nd	nd	nd
Cmpd 69	Unidentified	nd	nd	nd	nd	nd
Cmpd 70	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	nd	nd	nd	nd	nd
Cmpd 71	Nonyl Phenol Isomer	nd	nd	nd	nd	nd
Cmpd 72	Nonyl Phenol Isomer	nd	1.3	nd	nd	nd

Whitecourt Municipal STP Effluent Continued

STP Number	Compoud Name, Formula or Description	Concentrations in µg/L 20-Feb-90	12-Feb-91	5-Feb-92	17-Feb-93	15-Feb-94
Cmpd 73	Nonyl Phenol Isomer	nd	2.0	nd	nd	nd
Cmpd 74	2-Chloroethylphosphate	nd	0.5	nd	nd	nd
Cmpd 75	Unidentified	nd	nd	nd	nd	nd
Cmpd 76	Nonylphenol Isomer	nd	1.0	nd	nd	nd
Cmpd 77	Neophytadiene	nd	nd	nd	nd	nd
Cmpd 78	Unidentified	0.5	1.9	nd	nd	nd
Cmpd 79	Caffeine	nd	nd	nd	nd	nd
Cmpd 80	Unidentified Diterpene	0.5	1.9	nd	nd	nd
Cmpd 81	Hexadecanoic Acid	0.5	0.8	14.2	nd	11.6
Cmpd 82	Oleic Acid	0.3	1.8	nd	nd	nd
Cmpd 83	Stearic Acid	0.3	nd	1.5	nd	5.2
Cmpd 84	1,3-Dichloro-iso-propylphosphate	nd	nd	nd	nd	nd
Cmpd 85	Butylphenyl phthalate	nd	0.6	1.4	nd	nd
Cmpd 86	2-Butoxyethyl phosphate	1.0	0.8	nd	2.5	nd
Cmpd 87	Diheptyphosphate	nd	nd	nd	nd	nd
Cmpd 88	Bis(ethylhexyl)phthalate	2.4	10.9	7.3	5.5	3.3
Cmpd 89	Sterol	nd	nd	nd	nd	nd
Cmpd 90	Squalene	0.2	3.1	3.5	4.1	nd
Cmpd 91	Unidentified Sterol	nd	nd	nd	nd	nd

Fort McMurray Municipal STP Effluent

STP Number	Compoud Name, Formula or Description	(Concentrations in ug/L) 14-Mar-90	6-Mar-91	26-Feb-92
Cmpd 01	Alkylfuran	nd	nd	nd
Cmpd 02	Cyclohexanol	nd	nd	nd
Cmpd 03	Dichlorinated Hydrocarbon	0.2	nd	nd
Cmpd 04	C7 Amine (Tertiary	0.1	nd	nd
Cmpd 05	Sulphonylbismethane	0.6	nd	nd
Cmpd 06	Cyclohexanone	0.1	nd	nd
Cmpd 07	Trichloropropane	nd	nd	nd
Cmpd 08	Alkene (C12)	0.7	nd	nd
Cmpd 09	Alkene (C12)	0.3	nd	nd
Cmpd 10	Isocineole	nd	nd	nd
Cmpd 11	OXY Hydrocarbon	0.3	1.0	1.4
Cmpd 12	Dichlorobenzene	0.2	0.7	nd
Cmpd 13	Alkyl Benzene	0.9	1.3	nd
Cmpd 14	OXY Hydrocarbon	0.9	nd	nd
Cmpd 15	Alkylbenzene	0.3	0.9	nd
Cmpd 16	Nitrosomorpholine	nd	nd	nd
Cmpd 17	Alkylbenzene	0.3	nd	nd
Cmpd 18	1,1-Dichlorodimethylsulphone	0.6	1.0	1.2
Cmpd 19	Alkylbenzene	0.5	0.4	nd
Cmpd 20	Unidentified Alkoxy compound	0.1	0.8	nd
Cmpd 21	Alkylbenzene	0.4	1.0	nd
Cmpd 22	Triethylphosphate	nd	nd	nd
Cmpd 23	Unidentified Amine (Morpholine ??)	nd	0.9	nd
Cmpd 24	Decamethylcyclopentasiloxane	nd	nd	nd
Cmpd 25	Cymene	1.6	1.5	nd
Cmpd 26	*2-Ethylcyclohexanone*	nd	nd	nd
Cmpd 27	Unidentified Monochloroamine	nd	nd	nd
Cmpd 28	Unidentified Hydrocarbon	nd	nd	nd
Cmpd 29	*t-Butylcyclohexanone*	0.7	1.0	0.8
Cmpd 30	1,2-Benzothiazole	0.6	1.1	1.7
Cmpd 31	Terpenol	nd	nd	nd
Cmpd 32	Chlorinated Amine	nd	nd	nd
Cmpd 33	Unidentified Alkene	0.8	nd	nd
Cmpd 34	Unidentified	nd	nd	nd
Cmpd 35	Alkyl Indene ??	nd	nd	nd
Cmpd 36	Terpene	nd	nd	nd

Fort McMurray Municipal STP Effluent Continued

STP Number	Compoud Name, Formula or Description	(Concentrations in ug/L) 14-Mar-90	6-Mar-91	26-Feb-92
Cmpd 37	Alkylbenzene	0.3	nd	nd
Cmpd 38	Alkyl Indanone	0.3	nd	nd
Cmpd 39	Dimethyl Phenol	0.1	nd	nd
Cmpd 40	Alkyl Indan ??	nd	nd	nd
Cmpd 41	Monoterpene	nd	nd	nd
Cmpd 42	Branched Alkene	1.5	nd	nd
Cmpd 43	Unidentified Chlorinated Compound	nd	nd	nd
Cmpd 44	Unidentified	nd	0.4	nd
Cmpd 45	Propenyl Anisole	nd	nd	nd
Cmpd 46	1,3-Isobenzofurandione	0.7	nd	nd
Cmpd 47	Branched Alkene	0.3	nd	nd
Cmpd 48	Branched Alkene	0.8	nd	nd
Cmpd 49	3-Isopropylphenol	nd	nd	nd
Cmpd 50	Dichlorobenzonitrile	nd	nd	nd
Cmpd 51	Unidentified Hydrocarbon	nd	nd	nd
Cmpd 52	Branched Alkane	nd	nd	nd
Cmpd 53	Alkyl Indan	0.5	0.8	nd
Cmpd 54	Phenoxyacetic Acid	nd	nd	nd
Cmpd 55	2,6-t-Butylphenol	nd	nd	nd
Cmpd 56	Benzopyran-2-one	0.7	0.7	nd
Cmpd 57	Dibutyl phthalate	nd	nd	nd
Cmpd 58	g-Methylionone	0.3	0.7	1.6
Cmpd 59	Unidentified Oxy Hydrocarbon	nd	nd	nd
Cmpd 60	2,6-Bis(1,1-dimethylethyl)-4-methylphenol	nd	nd	nd
Cmpd 61	N,N-Diethyl-3-methyl Benzamide	1.7	2.4	8.6
Cmpd 62	Alkane	nd	nd	nd
Cmpd 63	Diethylphthalate	0.2	1.9	3.4
Cmpd 64	Unidentified Oxy Hydrocarbon	0.3	0.7	4.1
Cmpd 65	2-(Methylthio)benzothiazole	0.7	0.7	nd
Cmpd 66	Tributylphosphate	0.7	0.8	nd
Cmpd 67	Unidentified Amine	0.2	nd	1.6
Cmpd 68	Alkane	0.4	nd	nd
Cmpd 69	Unidentified	0.3	1.1	1.2
Cmpd 70	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	nd	nd	nd
Cmpd 71	Nonyl Phenol Isomer	nd	nd	nd
Cmpd 72	Nonyl Phenol Isomer	0.5	nd	3.7

Fort McMurray Municipal STP Effluent Continued

STP Number	Compoud Name, Formula or Description	(Concentrations in ug/L) 14-Mar-90	6-Mar-91	26-Feb-92
Cmpd 73	Nonyl Phenol Isomer	0.3	nd	1.5
Cmpd 74	2-Chloroethylphosphate	nd	nd	nd
Cmpd 75	Unidentified	nd	nd	nd
Cmpd 76	Nonylphenol Isomer	nd	nd	2.8
Cmpd 77	Neophytadiene	nd	nd	nd
Cmpd 78	Unidentified	0.4	0.9	1.6
Cmpd 79	Caffeine	11.5	47.5	24.3
Cmpd 80	Unidentified Diterpene	0.4	0.9	1.3
Cmpd 81	Hexadecanoic Acid	0.3	nd	nd
Cmpd 82	Oleic Acid	nd	nd	nd
Cmpd 83	Stearic Acid	0.2	nd	nd
Cmpd 84	1,3-Dichloro-iso-propylphosphate	nd	nd	nd
Cmpd 85	Butylphenyl phthalate	nd	nd	nd
Cmpd 86	2-Butoxyethyl phosphate	3.4	13.9	33.9
Cmpd 87	Diheptyphosphate	0.4	nd	nd
Cmpd 88	Bis(ethylhexyl)phthalate	2.1	12.0	1.6
Cmpd 89	Sterol	nd	nd	nd
Cmpd 90	Squalene	1.1	4.7	21.3
Cmpd 91	Unidentified Sterol	nd	nd	nd

Athabasca Municipal STP Effluent

	Compoud Name, Formula or Description	(Concentrations in ug/L) 25-Feb-91	18-Feb-92
Cmpd 01	Alkylfuran	nd	nd
Cmpd 02	Cyclohexanol	nd	nd
Cmpd 03	Dichlorinated Hydrocarbon	nd	nd
Cmpd 04	C7 Amine (Tertiary	nd	nd
Cmpd 05	Sulphonylbismethane	nd	nd
Cmpd 06	Cyclohexanone	nd	nd
Cmpd 07	Trichloropropane	nd	nd
Cmpd 08	Alkene (C12)	nd	nd
Cmpd 09	Alkene (C12)	nd	nd
Cmpd 10	Isocineole	nd	nd
Cmpd 11	OXY Hydrocarbon	0.2	0.8
Cmpd 12	Dichlorobenzene	0.3	nd
Cmpd 13	Alkyl Benzene	0.3	5.4
Cmpd 14	OXY Hydrocarbon	nd	nd
Cmpd 15	Alkylbenzene	0.2	1.6
Cmpd 16	Nitrosomorpholine	nd	nd
Cmpd 17	Alkylbenzene	nd	nd
Cmpd 18	1,1-Dichlorodimethylsulphone	1.0	2.0
Cmpd 19	Alkylbenzene	nd	2.2
Cmpd 20	Unidentified Alkoxy compound	nd	nd
Cmpd 21	Alkylbenzene	nd	nd
Cmpd 22	Triethylphosphate	nd	nd
Cmpd 23	Unidentified Amine (Morpholine ??)	0.6	1.0
Cmpd 24	Decamethylcyclopentasiloxane	nd	nd
Cmpd 25	Cymene	0.3	4.1
Cmpd 26	*2-Ethylcyclohexanone*	0.4	nd
Cmpd 27	Unidentified Monochloroamine	nd	nd
Cmpd 28	Unidentified Hydrocarbon	nd	nd
Cmpd 29	*t-Butylcyclohexanone*	0.5	nd
Cmpd 30	1,2-Benzothiazole	0.6	0.8
Cmpd 31	Terpenol	nd	nd
Cmpd 32	Chlorinated Amine	nd	nd
Cmpd 33	Unidentified Alkene	nd	nd
Cmpd 34	Unidentified	nd	nd
Cmpd 35	Alkyl Indene ??	nd	nd
Cmpd 36	Terpene	nd	nd

Athabasca Municipal STP Effluent Continued

	Compoud Name, Formula or Description	(Concentrations in ug/L) 25-Feb-91	18-Feb-92
Cmpd 37	Alkylbenzene	0.3	nd
Cmpd 38	Alkyl Indanone	0.2	nd
Cmpd 39	Dimethyl Phenol	nd	nd
Cmpd 40	Alkyl Indan ??	nd	nd
Cmpd 41	Monoterpene	nd	nd
Cmpd 42	Branched Alkene	nd	nd
Cmpd 43	Unidentified Chlorinated Compound	0.7	nd
Cmpd 44	Unidentified	0.2	nd
Cmpd 45	Propenyl Anisole	nd	nd
Cmpd 46	1,3-Isobenzofurandione	nd	nd
Cmpd 47	Branched Alkene	nd	nd
Cmpd 48	Branched Alkene	nd	nd
Cmpd 49	3-Isopropylphenol	2.9	2.7
Cmpd 50	Dichlorobenzonitrile	nd	nd
Cmpd 51	Unidentified Hydrocarbon	0.3	nd
Cmpd 52	Branched Alkane	nd	nd
Cmpd 53	Alkyl Indan	nd	nd
Cmpd 54	Phenoxyacetic Acid	nd	nd
Cmpd 55	2,6-t-Butylphenol	nd	nd
Cmpd 56	Benzopyran-2-one	nd	nd
Cmpd 57	Dibutyl phthalate	nd	nd
Cmpd 58	g-Methylionone	0.5	nd
Cmpd 59	Unidentified Oxy Hydrocarbon	nd	nd
Cmpd 60	2,6-Bis(1,1-dimethylethyl)-4-methylphenol	nd	nd
Cmpd 61	N,N-Diethyl-3-methyl Benzamide	2.5	5.5
Cmpd 62	Alkane	0.2	nd
Cmpd 63	Diethylphthalate	6.7	nd
Cmpd 64	Unidentified Oxy Hydrocarbon	0.7	1.1
Cmpd 65	2-(Methylthio)benzothiazole	0.3	nd
Cmpd 66	Tributylphosphate	0.6	nd
Cmpd 67	Unidentified Amine	0.6	1.3
Cmpd 68	Alkane	nd	nd
Cmpd 69	Unidentified	2.1	2.0
Cmpd 70	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	0.4	nd
Cmpd 71	Nonyl Phenol Isomer	1.9	2.5
Cmpd 72	Nonyl Phenol Isomer	4.6	3.1

Athabasca Municipal STP Effluent Continued

	Compoud Name, Formula or Description	(Concentrations in ug/L) 25-Feb-91	18-Feb-92
Cmpd 73	Nonyl Phenol Isomer	2.9	2.6
Cmpd 74	2-Chloroethylphosphate	0.3	nd
Cmpd 75	Unidentified	0.4	nd
Cmpd 76	Nonylphenol Isomer	3.9	7.3
Cmpd 77	Neophytadiene	nd	nd
Cmpd 78	Unidentified	0.5	nd
Cmpd 79	Caffeine	44.0	9.4
Cmpd 80	Unidentified Diterpene	0.6	nd
Cmpd 81	Hexadecanoic Acid	nd	2.4
Cmpd 82	Oleic Acid	nd	nd
Cmpd 83	Stearic Acid	nd	1.5
Cmpd 84	1,3-Dichloro-iso-propylphosphate	nd	nd
Cmpd 85	Butylphenyl phthalate	1.9	nd
Cmpd 86	2-Butoxyethyl phosphate	13.8	38.3
Cmpd 87	Diheptyphosphate	nd	nd
Cmpd 88	Bis(ethylhexyl)phthalate	6.6	1.1
Cmpd 89	Sterol	nd	nd
Cmpd 90	Squalene	4.4	13.9
Cmpd 91	Unidentified Sterol	nd	nd