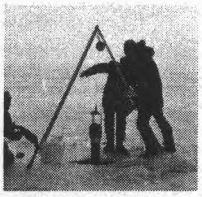
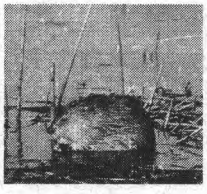
Canada Alberta Northwest Territories

Northern River Basins Study



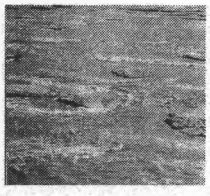


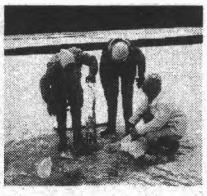





NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 111

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 2 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

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 2 OF 3

Published by the
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Edmonton, Alberta
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CANADIAN CATALOGUING IN PUBLICATION DATA

Johnson, C. Ian

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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.

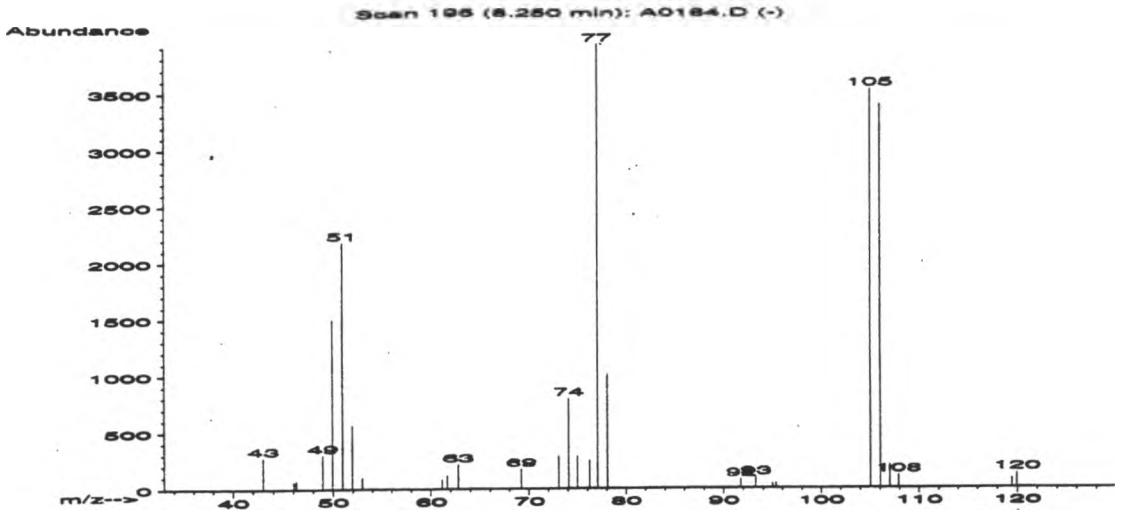
It is explicit in the objectives of the Study to report the results of technical work regularly to the public. This objective is served by distributing project reports to an extensive network of libraries, agencies, organizations and interested individuals and by granting universal permission to reproduce 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 2
MASS SPECTRAL DATA OF COMPOUNDS IN CHEMI-THERMOMECHANICAL PULP MILL EFFLUENTS

CTMP Compounds

Peak 1; Benzaldehyde



Scan 195 (8.250 min): A0184.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	278	69.20	171	105.05	3507		
46.05	64	73.05	283	106.05	3373		
46.30	72	74.05	792	107.00	197		
48.95	300	74.95	282	107.90	111		
49.95	1495	76.20	247	119.45	81		
50.95	2180	77.05	3902	119.95	127		
51.95	568	78.05	1008				
52.95	99	91.75	76				
61.15	85	93.25	89				
61.65	117	94.95	39				
62.75	212	95.30	41				

CTMP Compounds

Scan 195 (8.250 min): A0184.D

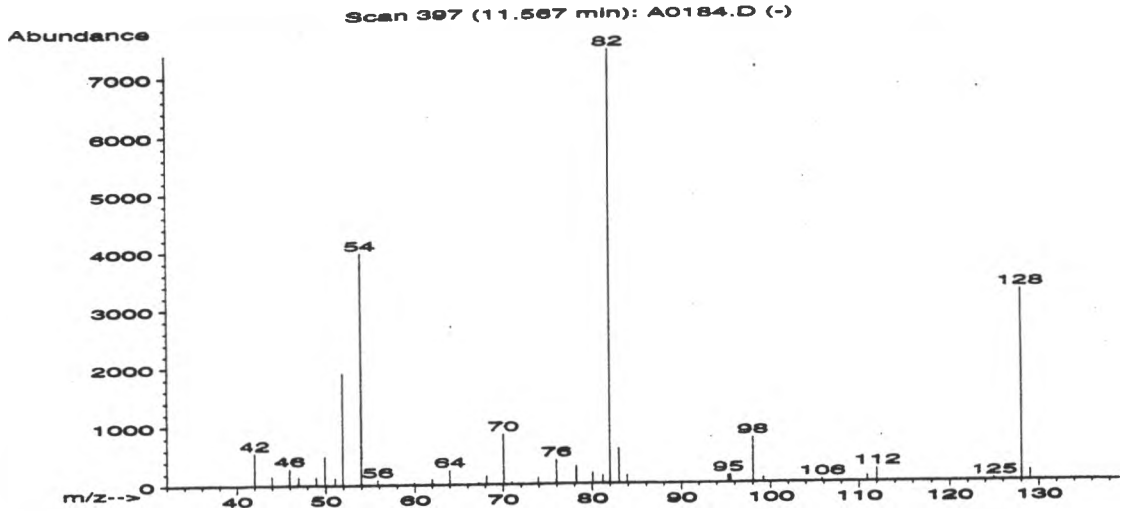
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde	106	C7H6O	94
2.	Benzaldehyde	106	C7H6O	91
3.	Benzaldehyde	106	C7H6O	91
4.	Benzaldehyde	106	C7H6O	91
5.	Benzaldehyde	106	C7H6O	91
6.	Benzaldehyde	106	C7H6O	90
7.	Benzaldehyde	106	C7H6O	87
8.	Benzoyl bromide	184	C7H5BrO	59
9.	Benzaldehyde	106	C7H6O	46
10.	Benzoyl chloride	140	C7H5ClO	45
11.	Benzoyl chloride	140	C7H5ClO	45
12.	Pyridine, 2-ethenyl-	105	C7H7N	43
13.	Benzoyl chloride	140	C7H5ClO	42
14.	Benzaldehyde	106	C7H6O	38
15.	Pyridine, 4-ethenyl-	105	C7H7N	37
16.	Benzenecarbothioic acid	138	C7H6OS	27
17.	Benzenamine, N-hydroxy-N-nitroso-, ammon	138	C6H6N2O2	10
18.	1,3-Dithiolane	106	C3H6S2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000100-52-7	118552	81	24	1	96	4	70	0	90	9968
2.	*91	000100-52-7	118551	74	30	1	87	5	62	0	74	9950
3.	*91	000100-52-7	118545	76	30	1	94	4	62	0	81	9966
4.	*91	000100-52-7	118547	74	42	1	85	4	62	0	81	9964
5.	*91	000100-52-7	118546	75	30	1	99	4	60	3	59	9906
6.	*90	000100-52-7	1777	68	35	1	94	8	59	31	70	9812
7.	*87	000100-52-7	118548	73	29	0	82	8	54	20	59	8791
8.	59	000618-32-6	27174	55	50	0	88	25	33	19	40	8169
9.	*46	000100-52-7	118553	55	47	2	86	45	20	0	49	9541
10.	45	000098-88-4	122405	58	40	0	88	25	19	14	35	8169
11.	45	000098-88-4	122403	50	48	0	90	25	19	7	36	8688
12.	*43	000100-69-6	118501	43	70	1	89	42	18	0	39	6816
13.	42	000098-88-4	122406	50	44	1	89	26	17	0	35	8847
14.	*38	000100-52-7	118549	40	50	0	90	50	14	5	38	9362
15.	*37	000100-43-6	1702	29	80	2	89	42	13	4	34	7428
16.	27	000098-91-9	8428	47	50	0	70	58	8	0	39	8929
17.	10	000135-20-6	8418	42	42	0	91	63	1	2	29	6328
18.	* 7	004829-04-3	1717	29	81	2	62	74	1	0	29	5576

CTMP Compounds

Standard 1; Nitrobenzene d5



Scan 397 (11.567 min): A0184.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	555	62.00	96	82.00	7390	128.05	3263
43.95	163	64.00	247	83.00	599	129.05	173
45.95	285	67.25	41	83.90	137		
46.95	137	68.15	143	95.30	133		
48.95	136	70.05	856	95.55	129		
49.95	491	70.95	35	98.05	765		
51.05	126	73.95	110	99.20	80		
51.95	1913	75.95	412	105.80	48		
53.95	3967	78.20	300	110.90	100		
55.80	86	80.05	184	112.00	219		
59.95	37	81.20	131	124.95	39		

CTMP Compounds

Scan 397 (11.567 min): A0184.D

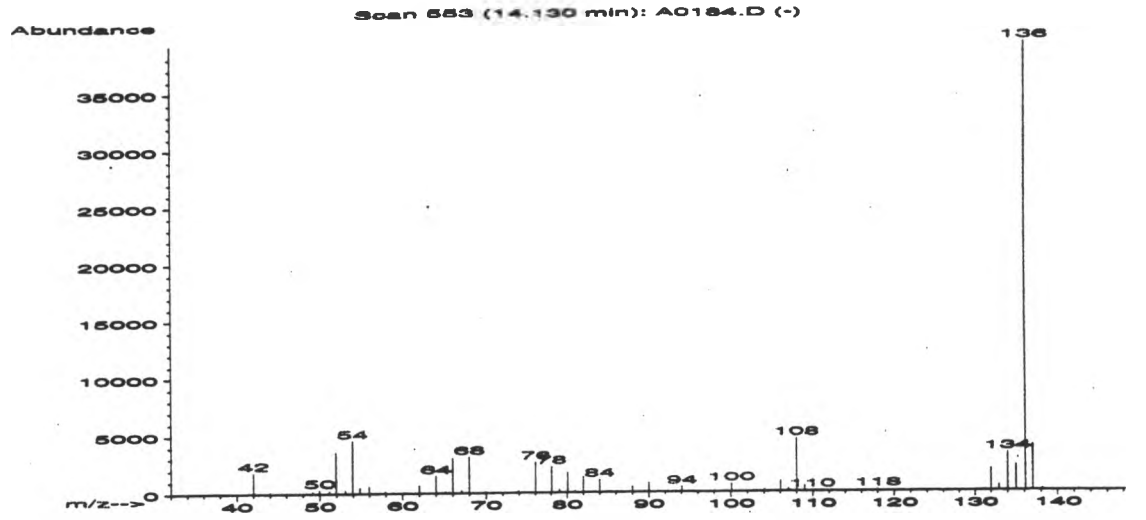
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Nitrobenzene-d5	123	C6D5NO2	53
2.	Nitrobenzene-d5	123	C6D5NO2	53
3.	1H-Imidazole, 4-methyl-	82	C4H6N2	25
4.	1H-Pyrazole, 3-methyl-	82	C4H6N2	17
5.	2-Cyclopenten-1-one	82	C5H6O	12
6.	5,6-DIHYDRO-4-METHYL-2H-PYRAN-2-ONE	112	C6H8O2	10
7.	1,3-DIMETHYL-5-(2,3-BIS(PERDEUTERIOTRIME	444	C20H22D18N2O5Si2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	000000-00-0	120299	51	42	1	86	30	28	10	39	9350
2.	*53	000000-00-0	4529	56	39	1	80	30	28	1	40	9939
3.	*25	000822-36-6	116748	31	54	2	77	54	7	5	32	9118
4.	*17	001453-58-3	116740	31	59	2	99	54	3	0	29	9072
5.	*12	000930-30-3	116755	30	73	3	99	56	2	0	27	9190
6.	*10	002381-87-5	2484	24	51	0	77	63	1	1	26	9005
7.	10	055401-60-0	103965	41	79	3	98	67	1	0	33	7962

CTMP Compounds

Standard 2; Naphthalene d8



Scan 553 (14.130 min): A0184.D

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m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1816	62.00	692	80.05	1739	103.05	57
44.00	156	64.00	1492	80.95	153	104.05	208
49.20	178	65.15	150	82.00	1353	106.05	915
49.95	319	66.00	3049	84.00	1081	107.00	237
51.10	236	67.05	241	86.00	26	108.00	4589
51.95	3603	68.00	3120	88.00	452	109.00	496
53.05	320	69.95	95	90.00	797	109.90	61
53.95	4590	73.95	194	94.05	431	115.50	42
54.80	502	76.05	2653	98.05	128	118.00	143
55.95	615	78.05	2242	99.30	39	131.15	120
57.90	184	79.05	256	100.05	692	132.00	1914

Scan 553 (14.130 min): A0184.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.00	484						
134.00	3309						
135.00	2206						
136.15	39176						
137.00	3980						
138.15	215						

CTMP Compounds

Scan 553 (14.130 min): A0184.D

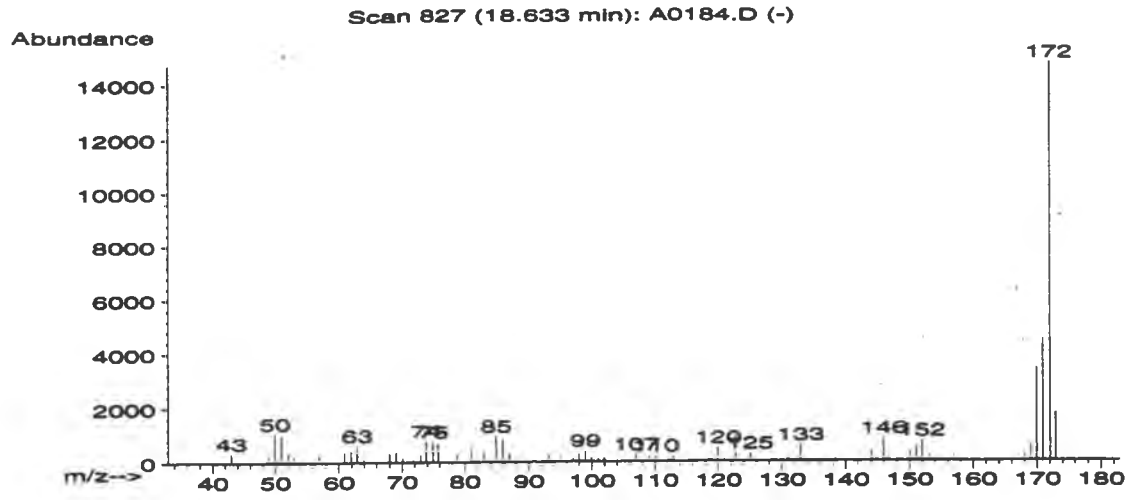
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Naphthalene-d8	128	C10D8	90
2.	Benzamide, 3-amino-	136	C7H8N2O	64
3.	2,5-Cyclohexadiene-1,4-dione, 2,3-dimeth	136	C8H8O2	59
4.	2,1,3-Benzothiadiazole	136	C6H4N2S	59
5.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	59
6.	Pyrazine, tetramethyl-	136	C8H12N2	42
7.	Inosine	268	C10H12N4O5	40
8.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	39
9.	3-DEUTERIO-1,2-BENZISOTHIAZOLE	135	C7H4DNS	38
10.	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	137	C9H15N	38
11.	2-HYDROXY-3-METHYLBENZALDEHYDE	136	C8H8O2	38
12.	Benzaldehyde, 3-methoxy-	136	C8H8O2	38
13.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000000-00-0	6077	77	13	1	67	9	59	30	66	9926
2.	*64	003544-24-9	7777	33	49	0	78	25	37	14	43	9847
3.	*59	000526-86-3	7809	38	42	2	87	25	33	21	38	9648
4.	*59	000273-13-2	7732	37	52	2	80	22	33	0	39	9845
5.	*59	000068-94-0	121783	34	41	3	99	22	33	6	39	9887
6.	*42	001124-11-4	121881	33	44	2	87	27	17	11	36	9842
7.	40	000058-63-9	62487	42	94	3	87	12	16	0	29	9927
8.	*39	000068-94-0	121782	29	51	3	99	20	15	0	29	9870
9.	*38	040991-32-0	7532	32	57	2	99	24	14	0	29	9837
10.	38	007148-07-4	8325	35	67	3	99	25	14	0	22	9583
11.	*38	000824-42-0	7825	30	90	1	99	22	14	0	29	7482
12.	*38	000591-31-1	121853	28	95	2	81	22	14	0	29	7825
13.	*38	000068-94-0	121781	29	52	2	84	24	14	0	29	9856

CTMP Compounds

Standard 2; 2-Fluorobiphenyl



Scan 827 (18.633 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	331	63.90	95	78.80	229	93.15	229
48.95	248	66.95	31	80.05	48	95.05	179
49.95	1065	68.00	315	81.05	521	97.05	118
50.95	967	69.05	345	81.80	19	97.95	282
52.05	335	70.10	150	83.00	352	98.95	390
52.95	188	70.90	39	84.90	944	99.95	134
56.90	253	71.80	85	85.90	844	101.05	103
59.90	29	72.95	271	86.90	285	101.95	135
60.90	360	73.80	778	87.90	128	107.00	247
61.90	402	74.95	737	89.15	89	108.00	91
62.90	607	75.80	639	91.00	71	109.00	185

Scan 827 (18.633 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.15	187	130.95	152	153.05	178		
112.25	76	132.90	583	156.90	196		
112.65	148	134.90	40	168.00	249		
112.90	147	138.40	46	168.95	554		
118.40	67	144.05	363	169.95	3416		
118.70	47	144.95	165	170.95	4482		
119.05	40	145.95	818	172.05	14720		
119.95	484	146.80	152	172.95	1760		
121.00	44	150.05	325				
122.80	286	151.05	484				
125.05	272	151.95	727				

CTMP Compounds

Scan 827 (18.633 min): A0184.D

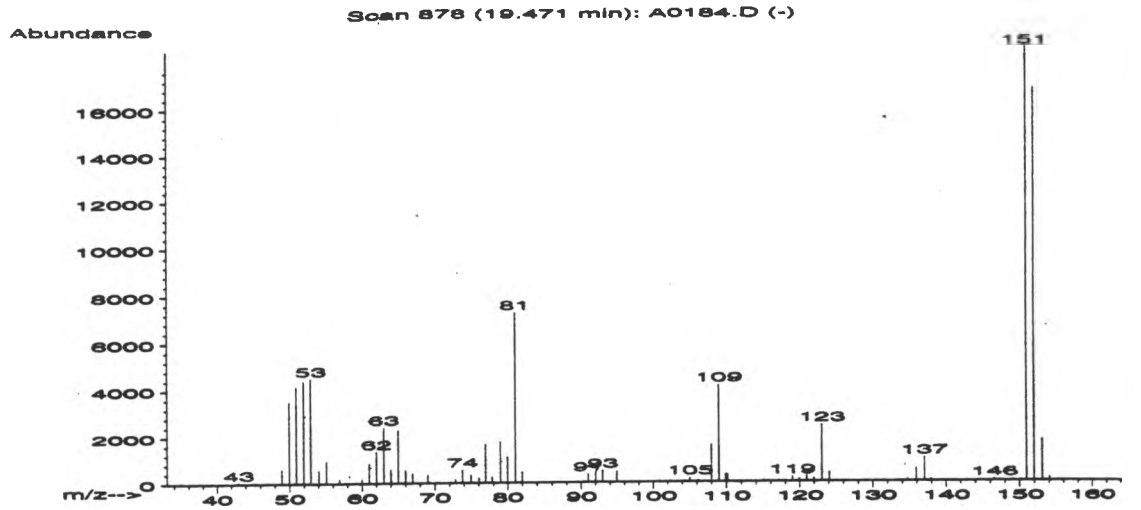
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	96
2.	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	93
3.	2-Naphthalenecarboxylic acid	172	C11H8O2	47
4.	4-(2-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	38
5.	2-Naphthalenecarboxylic acid	172	C11H8O2	38
6.	2-Naphthalenecarboxylic acid	172	C11H8O2	38
7.	1-METHOXY-2-METHYLNAPHTHALENE	172	C12H12O	38
8.	1-Naphthalenecarboxylic acid	172	C11H8O2	28
9.	1-Naphthalenecarboxylic acid	172	C11H8O2	28
10.	1-Naphthalenecarboxylic acid	172	C11H8O2	28
11.	1-Naphthalenecarboxylic acid	172	C11H8O2	28
12.	4-(4-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000321-60-8	22421	93	6	0	68	12	76	0	96	9758
2.	*93	000324-74-3	22422	97	0	0	69	12	68	3	93	9759
3.	*47	000093-09-4	126215	34	78	2	93	40	20	0	39	9296
4.	*38	068535-55-7	22263	33	63	3	99	39	14	0	35	9727
5.	*38	000093-09-4	126214	39	69	1	90	39	14	0	33	9328
6.	*38	000093-09-4	126213	39	70	2	95	40	14	0	35	9296
7.	*38	000000-00-0	22442	29	53	1	73	37	14	6	35	9315
8.	*28	000086-55-5	126211	28	82	1	88	39	8	0	29	9395
9.	*28	000086-55-5	126210	28	82	1	88	39	8	0	29	9395
10.	*28	000086-55-5	126209	29	83	2	95	39	8	0	29	9379
11.	*28	000086-55-5	22387	29	86	2	95	37	8	0	29	9404
12.	*28	023380-78-1	22266	29	93	2	86	37	8	0	29	9429

CTMP Compounds

Peak 2; Vanillin



Scan 878 (19.471 min): A0184.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	79	62.00	1365	76.95	1681	106.05	51
48.95	631	63.00	2414	77.80	254	106.25	56
49.95	3525	64.00	579	78.95	1787	108.00	1601
50.95	4159	65.00	2308	79.95	1119	109.00	4169
51.95	4382	66.00	555	81.05	7281	109.90	341
52.95	4508	67.00	402	82.00	467	110.15	322
54.05	582	69.05	352	91.00	362	115.00	63
55.05	958	72.80	174	92.00	437	118.95	212
56.90	188	73.80	564	93.00	503	119.95	118
60.00	200	74.95	347	94.95	472	120.95	353
61.00	855	76.05	210	105.05	183	122.00	148

Scan 878 (19.471 min): A0184.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	2464	153.05	1807				
124.05	409	154.05	163				
134.75	103						
135.90	561						
137.00	1042						
137.90	94						
146.55	81						
149.05	65						
150.05	63						
150.95	18536						
151.95	16776						

CTMP Compounds

Scan 878 (19.471 min): A0184.D

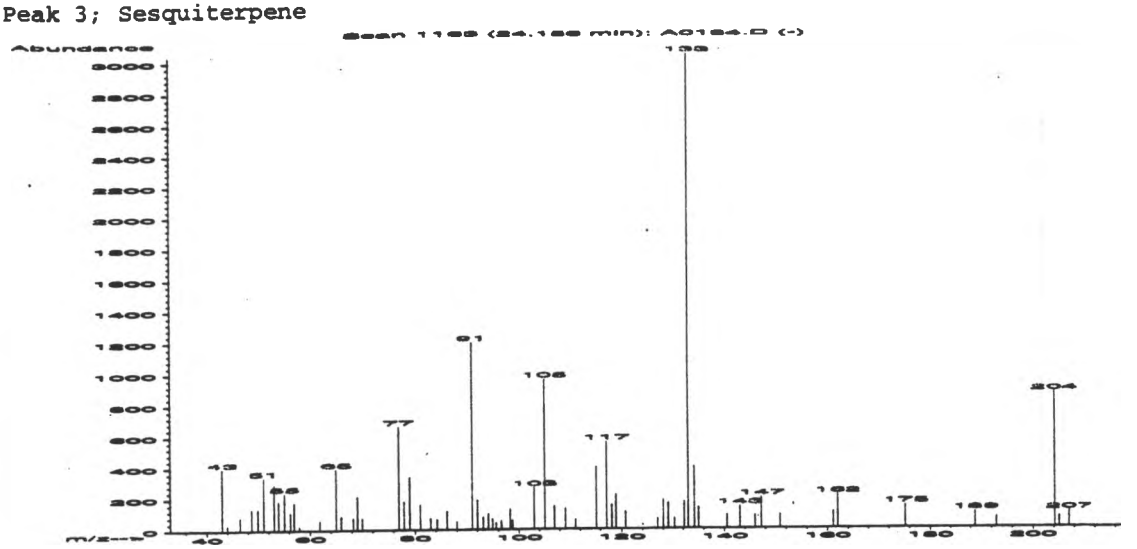
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	97
2.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	96
3.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	96
4.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	95
5.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	95
6.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	89
7.	2-METHOXY-4,5,6-TRIMETHYLPYRIMIDINE	152	C8H12N2O	59
8.	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	52
9.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	50
10.	Benzaldehyde, 3-(chloroacetoxy)-4-methox	228	C10H9ClO4	50
11.	Benzenamine, 2-methyl-5-nitro-	152	C7H8N2O2	47
12.	Thiazolo[5,4-d]pyrimidine, 5-methyl-	151	C6H5N3S	46
13.	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	46
14.	Benzaldehyde, 2,4-dihydroxy-6-methyl-	152	C8H8O3	43
15.	2-AMINO-3-HYDROXY-ACETOPHENONE	151	C8H9NO2	43
16.	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10	152	C9H16N2	43
17.	Benzaldehyde, 4-(methylthio)-	152	C8H8OS	38
18.	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	35
19.	1H-Inden-1-one, octahydro-7a-methyl-, ci	152	C10H16O	35
20.	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	30

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*97	000121-33-5	123902	105	5	1	75	1	78	19	95	9887
2.	*96	000121-33-5	123898	99	25	0	69	3	76	0	96	9952
3.	*96	000121-33-5	13356	111	0	0	77	1	76	14	95	9962
4.	*95	000121-33-5	123901	100	12	0	77	1	74	0	94	9943
5.	*95	000121-33-5	123900	97	15	0	73	4	72	12	93	9901
6.	*89	000121-33-5	123903	94	12	0	77	22	56	39	83	9925
7.	*59	065641-61-4	123916	43	79	3	90	22	33	0	40	9227
8.	*52	000621-59-0	13355	53	50	1	96	34	27	0	49	9760
9.	*50	000121-33-5	123899	68	27	0	66	50	25	27	66	9361
10.	50	066267-38-7	47410	58	66	2	90	33	25	0	43	9773
11.	*47	000099-55-8	123857	33	94	3	67	39	20	0	39	6911
12.	*46	013554-89-7	13010	35	39	0	99	44	20	14	43	6285
13.	*46	000673-22-3	13357	49	47	3	97	43	20	0	46	9444
14.	*43	000487-69-4	13353	44	44	2	84	47	18	0	44	9360
15.	*43	004502-10-7	13112	43	64	2	71	42	18	0	39	7887
16.	*43	006674-22-2	123940	39	22	0	70	45	18	11	40	9088
17.	*38	003446-89-7	13330	49	56	2	63	54	14	0	46	9602
18.	*35	000621-59-0	123897	37	56	1	88	53	11	5	40	9541
19.	*35	013025-91-7	124002	33	69	2	61	53	11	0	41	5112
20.	*30	000148-53-8	13354	36	59	2	80	59	9	14	43	8632

CTMP Compounds

Peak 3; Sesquiterpene



Scan 1163 (24.156 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	394	57.95	24	83.05	74	98.30	130
44.00	31	61.90	62	84.25	67	98.70	58
46.45	85	65.00	390	86.15	119	103.05	267
48.70	134	66.00	90	88.00	54	105.05	962
49.95	135	68.25	76	91.00	1198	106.95	150
51.05	337	69.05	215	92.00	188	109.15	133
53.05	292	70.00	74	93.05	81	111.15	63
53.95	185	76.95	661	94.05	100	115.15	400
55.05	236	77.95	183	94.85	69	117.15	561
56.20	113	79.05	338	95.55	44	118.15	156
56.90	177	81.05	162	96.55	56	118.95	219

Scan 1163 (24.156 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.80	109	145.95	85				
126.95	66	147.20	198				
128.05	184	150.80	87				
129.05	165	161.15	106				
130.30	66	162.00	214				
132.15	174	175.20	145				
133.00	3037	188.90	101				
134.15	398	193.00	67				
135.00	134	204.20	864				
140.50	90	205.05	68				
143.00	143	207.00	100				

CTMP Compounds

Scan 1163 (24.156 min): A0184.D

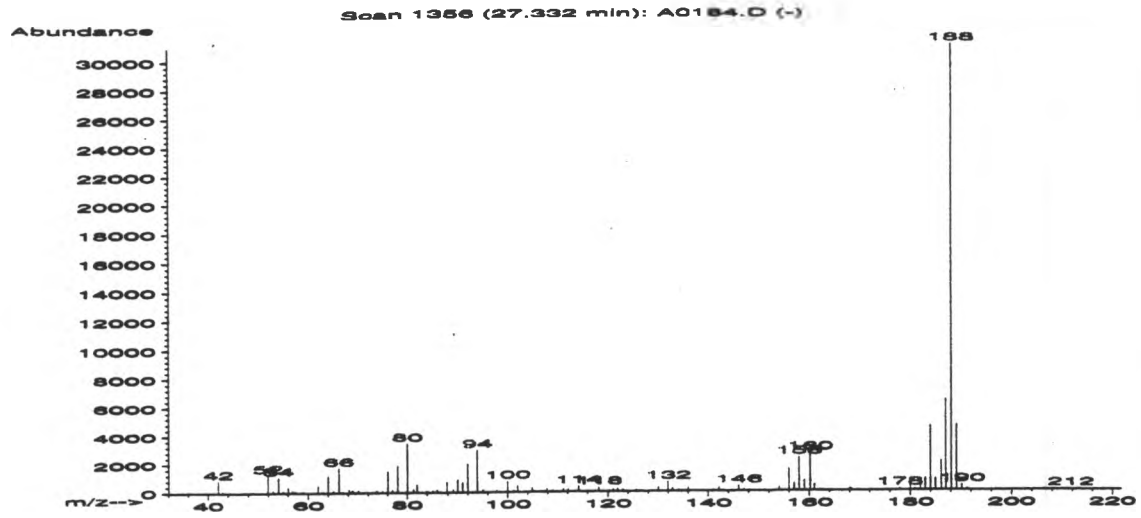
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Indol-5-ol	133	C8H7NO	59
2.	1H-Benzotriazole, 1-methyl-	133	C7H7N3	47
3.	1H-Benzimidazol-2-amine	133	C7H7N3	47
4.	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	46
5.	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	46
6.	1H-Benzimidazol-2-amine	133	C7H7N3	43
7.	3-AMINOINDAZOLE	133	C7H7N3	43
8.	[1,2,4]Triazolo[1,5-a]pyridine, 2-methyl	133	C7H7N3	43
9.	3-METHYL-1,2,4-BENZOXAZINONE	161	C9H7NO2	43
10.	Benzoxazole, 2-methyl-	133	C8H7NO	43
11.	1-Propanone, 3-cyclopentyl-1-(2,4-dimeth	230	C16H22O	42
12.	1H-Indol-4-ol	133	C8H7NO	42
13.	Benzoic acid, 3,4-dimethyl-, methyl este	164	C10H12O2	40
14.	1-PHENYLCYCLOPENTANOL-1	162	C11H14O	40
15.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	40
16.	Carbamic acid, acetylthio-, O-methyl est	133	C4H7NO2S	38
17.	1-Propanone, 2-chloro-1-(2,5-dimethylphe	210	C12H15ClO	38
18.	1,2-Benzisoxazole, 3-methyl-	133	C8H7NO	38
19.	1H-Indol-5-ol	133	C8H7NO	38
20.	Benzenamine, 2-(1-methylethenyl)-	133	C9H11N	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	001953-54-4	121469	47	44	2	93	25	33	0	39	9483
2.	*47	013351-73-0	7106	39	48	0	99	36	20	9	38	8804
3.	*47	000934-32-7	121459	34	59	0	85	36	20	0	41	9349
4.	*46	062108-16-1	7157	35	41	0	99	45	20	8	43	9432
5.	*46	000059-48-3	121467	37	45	0	95	43	20	4	43	9465
6.	*43	000934-32-7	121458	33	58	0	75	44	18	0	41	9284
7.	*43	000874-05-5	7110	35	72	2	92	41	18	0	39	9398
8.	*43	000768-19-4	7102	48	41	1	69	42	18	10	39	9279
9.	*43	007653-60-3	17201	44	39	0	91	41	18	19	40	7485
10.	*43	000095-21-6	7127	37	54	1	88	44	18	0	41	9154
11.	42	055191-11-2	48547	42	61	0	99	27	17	6	35	9356
12.	*42	002380-94-1	7131	36	70	2	90	27	17	0	30	9488
13.	40	038404-42-1	18505	35	51	0	69	33	16	5	30	9459
14.	40	010487-96-4	17816	44	55	2	98	34	16	0	35	9083
15.	40	004706-90-5	123453	45	55	1	99	31	16	4	37	9262
16.	*38	016696-87-0	121437	35	70	1	77	50	14	0	39	8877
17.	38	054965-52-5	39357	41	62	1	99	38	14	4	33	9430
18.	*38	004825-75-6	7126	48	39	0	75	50	14	2	41	8872
19.	*38	001953-54-4	7129	38	59	1	93	38	14	0	33	9390
20.	*38	052562-19-3	7134	35	81	3	99	50	14	0	39	8559

CTMP Compounds

Standard 4



Scan 1356 (27.332 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	851	58.90	93	73.80	120	86.00	176
43.00	102	62.00	472	75.05	82	87.90	725
48.95	87	63.05	114	76.05	1493	89.15	189
51.95	1252	64.00	1193	77.05	164	90.00	871
52.95	140	65.05	135	78.05	1857	91.00	667
54.05	1079	66.15	1728	80.05	3454	92.00	1996
55.00	92	66.90	32	81.30	221	93.95	2975
56.05	369	68.15	205	82.00	526	95.00	162
56.90	102	68.90	183	83.00	41	97.80	115
57.40	70	70.05	148	83.90	92	99.95	761
57.75	35	72.80	59	85.15	127	101.20	84

Scan 1356 (27.332 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.95	430	120.20	49	141.00	85	162.15	98
102.95	1	121.05	146	142.15	229	168.00	135
104.95	268	121.95	173	146.05	357	168.25	136
107.90	198	122.95	118	147.05	112	177.95	121
109.05	83	125.70	104	154.05	236	179.00	5
110.05	34	130.05	260	156.00	1539	180.05	477
111.15	161	132.00	650	157.00	485	180.90	108
112.15	166	132.90	198	158.00	2340	182.00	345
114.15	378	134.15	91	159.00	703	183.00	839
115.90	59	135.00	19	160.15	2675	184.00	4521
118.25	276	136.00	247	161.00	416	185.00	823

Scan 1356 (27.332 min): A0184.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
186.15	2093						
187.00	6358						
188.15	30936						
189.15	4574						
190.15	344						
191.15	113						
211.75	37						

CTMP Compounds

Scan 1356 (27.332 min): A0184.D

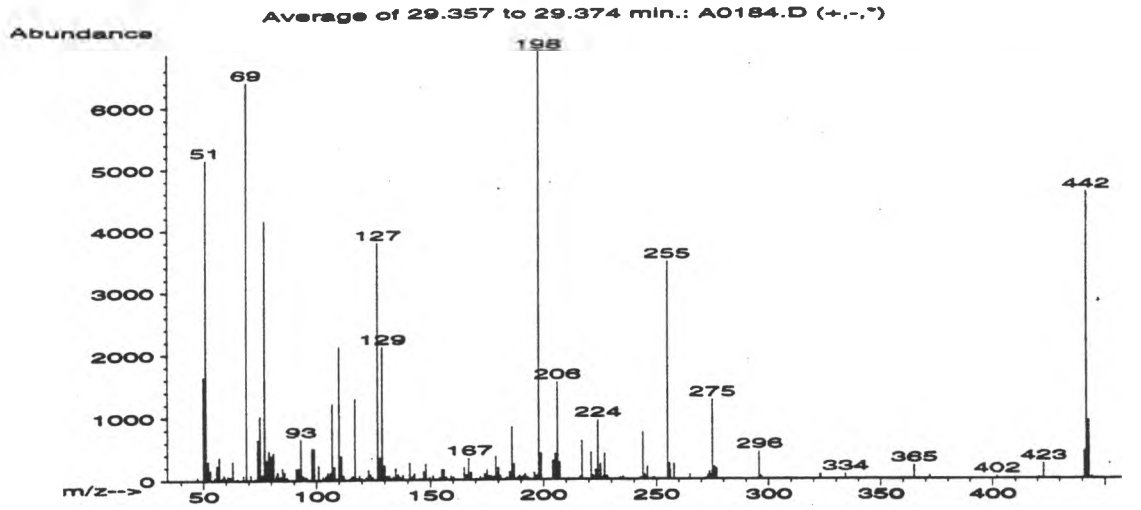
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Anthracene-D10	178	C14D10	89
2.	DECADEUTEROPHENANTHRENE	178	C14D10	87
3.	Acridine-D9	179	C13D9N	64
4.	Di(2,4-dinitrophenoxy)-4,4'-dipyridylium	188	C10H8N2O2	64
5.	1,2,3,4,6,7,8,9-Octahydrophenazine	188	C12H16N2	53
6.	Cyclohexanone, phenylhydrazone	188	C12H16N2	52
7.	4,6-DIMETHOXYISOPHTHALONITRILE	188	C10H8N2O2	50
8.	6-Vinyl-5,7-dimethylphthalide	188	C12H12O2	50
9.	Naphthalene, 1,5-dimethoxy-	188	C12H12O2	47
10.	1-(P-TOLYL)-3-METHYL-PYRAZOL-5-ONE	188	C11H12N2O	46
11.	Acridine-D9	179	C13D9N	42
12.	1-PHENYL-4,5-DIMETHYL-4-IMIDAZOLIN-2-ONE	188	C11H12N2O	40
13.	Benzene, 1-(1-cyclohexen-1-yl)-4-methoxy	188	C13H16O	40
14.	Naphthalene, 1,7-dimethoxy-	188	C12H12O2	40
15.	2,6-Dioxo-1,2,3,5,6,7-hexahydrobenzo[1,2	188	C10H8N2O2	40
16.	4-HYDROXY-6-PHENYL-3-PYRIDAZONE	188	C10H8N2O2	38
17.	4-METHYL-2-(3-FLUOROPHENYL)PYRIMIDINE	188	C11H9FN2	38
18.	2-Isopropenyl-5-formyl-2,3-dihydrobenzof	188	C12H12O2	38
19.	2,6-Diallyl-4-methyl-phenol	188	C13H16O	38
20.	6-Hydroxy-2-naphthalenecarboxylic acid	188	C11H8O3	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	TiIt	R_IV	XCORR
1.	*89	000000-00-0	24971	79	30	1	70	21	56	0	84	9842
2.	*87	001517-22-2	24973	69	32	0	75	10	54	23	58	9815
3.	*64	000000-00-0	126726	50	68	3	89	25	37	0	46	9371
4.	*64	000000-00-0	29109	37	30	1	68	17	37	0	39	9707
5.	*53	004006-50-2	29327	46	13	0	74	28	28	1	40	9553
6.	*52	000946-82-7	29309	37	52	1	77	31	27	8	43	9754
7.	*50	055937-16-1	29095	30	21	1	97	19	25	1	30	9727
8.	*50	079801-76-6	29272	31	54	0	88	19	25	0	33	9732
9.	*47	010075-63-5	29278	34	81	1	80	37	20	0	39	9559
10.	*46	035496-19-6	29202	37	34	1	84	43	20	2	43	9537
11.	*42	000000-00-0	25203	37	82	3	90	28	17	0	35	9546
12.	*40	041647-53-4	29205	28	58	0	70	31	16	6	35	9712
13.	*40	020758-60-5	29353	31	56	1	94	32	16	7	30	9274
14.	*40	005309-18-2	29279	40	80	1	80	34	16	0	35	9586
15.	*40	000000-00-0	29122	32	29	2	97	35	16	1	34	9389
16.	*38	058884-18-7	29107	28	54	2	99	37	14	1	30	9631
17.	*38	076128-66-0	29193	28	52	2	80	40	14	2	35	9697
18.	*38	085870-17-3	29269	28	45	0	87	36	14	0	33	9553
19.	*38	000000-00-0	29331	28	76	0	90	36	14	0	33	9550
20.	*38	000000-00-0	29187	28	27	0	74	37	14	6	35	9567

CTMP Compounds

Standard 5



Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.20	47	59.50	34	75.00	1025	84.00	51
49.95	1642	60.90	61	75.95	89	85.00	185
50.95	5150	61.90	58	77.00	4156	85.90	126
52.00	294	62.85	303	78.00	316	87.00	42
52.95	155	65.00	33	79.05	460	91.05	182
54.95	43	67.75	80	80.00	387	92.00	186
55.90	233	68.95	6402	81.00	435	93.00	651
56.90	366	70.00	8	82.20	50	94.05	66
58.05	26	71.05	81	82.40	74	95.25	45
58.40	40	72.80	27	82.95	126	95.95	28
59.15	85	74.00	648	83.80	30	97.95	510

Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.95	502	112.00	67	123.80	81	134.95	184
100.95	228	114.95	25	124.90	47	135.95	84
103.00	53	115.75	58	127.00	3787	136.75	41
104.05	63	116.00	56	128.05	352	137.95	71
105.00	116	117.00	1290	129.00	2119	140.95	277
106.05	121	117.90	26	129.95	230	142.00	48
106.95	1220	118.95	69	130.95	60	142.90	99
108.00	215	120.05	20	132.00	61	145.45	25
108.95	24	121.85	18	132.70	17	146.95	134
110.00	2123	122.05	36	133.90	45	147.95	253
111.00	387	122.95	160	134.20	32	148.95	1

Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
149.80	34	166.25	37	178.05	46	190.15	30
151.20	67	167.00	343	178.90	371	190.50	29
153.70	23	168.15	112	180.05	192	190.95	23
154.05	36	170.30	21	180.90	62	191.15	56
155.10	166	171.95	46	183.75	42	191.95	87
156.00	161	172.95	14	184.95	126	193.00	37
156.90	39	173.95	94	185.95	848	195.95	110
159.05	63	174.95	161	187.05	249	196.95	66
160.25	40	175.95	57	188.50	24	197.95	6866
164.95	197	176.70	28	189.15	46	198.95	423
166.00	77	177.05	52	189.40	65	204.05	302

CTMP Compounds

Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
205.00	412	225.05	247	248.45	24	273.95	82
206.05	1557	226.20	40	249.05	26	274.95	1271
207.05	273	227.00	415	255.00	3486	276.00	202
211.00	21	227.95	55	255.90	247	276.75	170
215.90	36	228.30	36	256.15	155	295.85	442
216.25	47	234.05	35	257.85	243	296.80	46
217.00	618	235.15	46	264.90	80	322.80	74
221.00	432	242.95	34	271.55	21	323.05	76
221.80	64	244.00	752	272.70	43	334.10	83
222.95	154	244.90	76	272.95	70	364.90	220
224.00	953	246.00	200	273.70	132	371.95	56

Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
401.95	42						
420.80	24						
422.80	244						
440.90	449						
441.80	4608						
442.80	937						
444.20	31						

Average of 29.357 to 29.374 min.: A0184.D
Converted from RTE data file: >A0184:

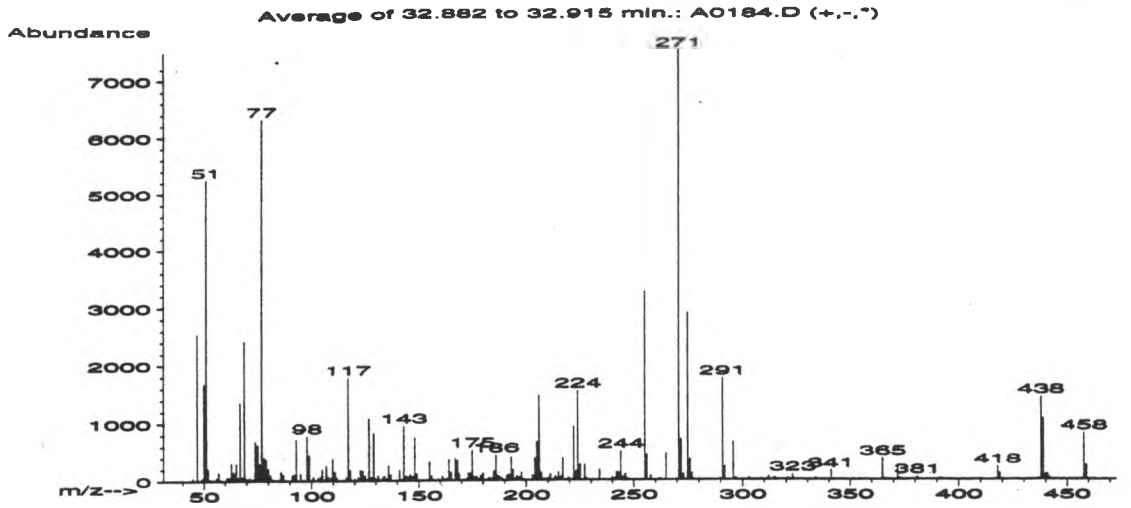
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phosphine, bis(pentafluorophenyl)phenyl-	442	C18H5F10P	95
2.	Phosphine, bis(pentafluorophenyl)phenyl-	442	C18H5F10P	84
3.	Benzenamine, N-hydroxy-N-nitroso-, ammon	138	C6H6N2O2	38
4.	4,4',5,5',6,6'-Hexamethoxyindigo	442	C22H22N2O8	32
5.	Benzene, nitro-	123	C6H5NO2	32
6.	2-PROPARGYL-4,5-DIPHENYL-1,2,4-TRIAZOL-3	275	C17H13N3O	23
7.	Diphenyl Telluride	284	C12H10Te	23
8.	13-(8'-Amino-4'-tosyl-4'-azaoctyl)-12-do	479	C26H45N3O3S	10
9.	2-PHENYL-1,3-DITHIANE-5,5-D2	196	C10H10D2S2	10
10.	Methylester of 9-Oxotricyclo[4.4.0.0(3,7	206	C12H14O3	9
11.	BIS(TRIFLUOROMETHYL)THIONE S-OXIDE	198	C3F6OS	7
12.	METHYLDIBENZOTHIOPHENE	198	C13H10S	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	005074-71-5	136554	156	41	1	83	12	72	1	95	8516
2.	*84	005074-71-5	136553	139	61	1	70	59	51	27	95	8372
3.	38	000135-20-6	8418	56	35	1	52	50	14	15	39	3997
4.	*32	080981-90-4	103681	28	8	0	52	50	9	0	33	3645
5.	*32	000098-95-3	120296	57	41	1	52	50	9	7	34	3997
6.	*23	065091-81-8	65359	28	119	3	160	48	6	0	29	4485
7.	23	000000-00-0	68234	37	99	1	71	49	6	0	25	4063
8.	10	072636-91-0	107395	37	108	1	55	62	1	0	22	5016
9.	*10	024588-66-7	32741	33	75	3	87	66	1	0	35	5329
10.	* 9	000000-00-0	37399	36	37	1	50	75	1	6	32	3170
11.	* 7	087108-79-0	33441	30	112	2	99	75	1	0	27	7248
12.	* 7	030995-64-3	34047	31	83	2	84	75	1	0	26	5329

CTMP Compounds

Standard 6



Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.80	55	57.80	14	68.15	70	79.00	366
46.85	2544	60.90	70	68.95	2419	80.00	204
48.80	19	61.75	23	69.80	34	81.05	93
49.00	38	62.00	63	71.30	49	81.85	25
49.95	1677	62.95	314	71.95	19	85.75	38
50.95	5246	64.00	156	73.05	29	86.00	152
52.00	218	64.95	8	74.00	682	86.90	103
52.90	19	65.15	299	75.00	626	91.05	96
56.00	55	65.95	51	76.00	296	91.95	115
56.20	38	67.00	1358	77.05	6313	93.00	715
56.95	148	67.95	33	78.00	409	95.00	128

Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.90	9	107.95	69	122.05	22	131.90	17
97.95	778	109.05	47	122.95	188	133.15	56
99.00	449	109.95	390	123.95	176	134.00	88
100.05	18	110.95	157	125.00	88	135.00	37
100.95	66	111.90	54	126.05	31	135.95	260
102.55	12	116.15	59	127.00	1086	137.00	105
103.00	45	117.00	1775	127.95	66	138.75	15
104.00	63	118.00	181	129.00	828	139.15	9
105.00	199	120.05	29	129.95	42	141.00	181
106.05	30	120.45	18	131.05	87	142.00	17
106.95	270	121.70	57	131.65	5	143.00	947

Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.95	79	155.80	35	167.00	385	177.70	23
144.95	66	155.95	88	168.00	354	178.95	80
145.90	109	157.00	16	168.85	113	180.00	129
146.95	73	159.00	28	170.95	17	182.65	45
147.95	742	160.90	76	172.30	36	183.05	20
148.90	113	161.15	54	172.80	31	183.90	39
151.05	13	162.00	20	173.05	125	184.95	158
151.90	4	163.10	36	173.95	128	185.25	24
153.00	15	164.00	369	174.95	528	185.95	435
153.95	22	164.65	54	175.85	65	186.90	79
154.95	331	165.10	144	177.05	71	187.15	65

Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
188.00	48	196.05	76	209.15	20	216.95	385
188.40	13	197.10	56	210.15	25	219.20	30
188.75	27	198.00	137	210.50	36	219.55	38
189.15	18	198.95	14	210.75	39	219.80	29
191.00	87	202.90	89	211.05	109	220.80	21
192.00	109	204.00	386	213.00	33	221.95	930
193.10	403	205.00	670	213.40	66	223.00	152
194.00	176	205.95	1468	213.75	40	224.00	1543
195.20	38	206.95	126	215.00	140	225.00	275
195.55	32	208.00	18	215.65	32	227.05	269
195.80	48	208.75	19	216.15	65	227.80	35

Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
232.90	18	245.05	52	261.75	22	280.90	15
234.00	181	245.55	39	262.75	19	289.75	26
236.15	21	246.00	105	264.90	471	290.90	1747
239.90	52	246.80	18	269.80	14	292.00	231
241.00	26	247.20	16	270.85	7493	295.90	663
241.40	39	253.75	6	271.85	714	296.80	34
241.90	147	255.00	3269	272.95	105	302.80	19
242.25	36	255.85	444	274.95	2891	303.05	49
242.65	39	257.65	78	276.00	365	311.25	13
242.95	134	257.90	73	276.80	114	311.95	62
244.00	505	261.50	21	277.45	16	314.65	29
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
314.90	34	365.90	16	438.00	1427		
320.70	32	371.90	263	438.90	1054		
320.95	23	372.80	25	440.05	99		
323.00	92	380.90	48	440.45	97		
323.55	31	389.00	15	440.75	91		
330.90	16	391.50	31	441.00	87		
333.90	37	416.75	11	441.90	34		
341.05	158	417.90	229	456.75	18		
351.95	22	418.80	107	457.90	807		
354.05	23	420.70	15	458.15	208		
364.90	367	436.75	27	458.95	256		

Average of 32.882 to 32.915 min.: A0184.D
Converted from RTE data file: >A0184:

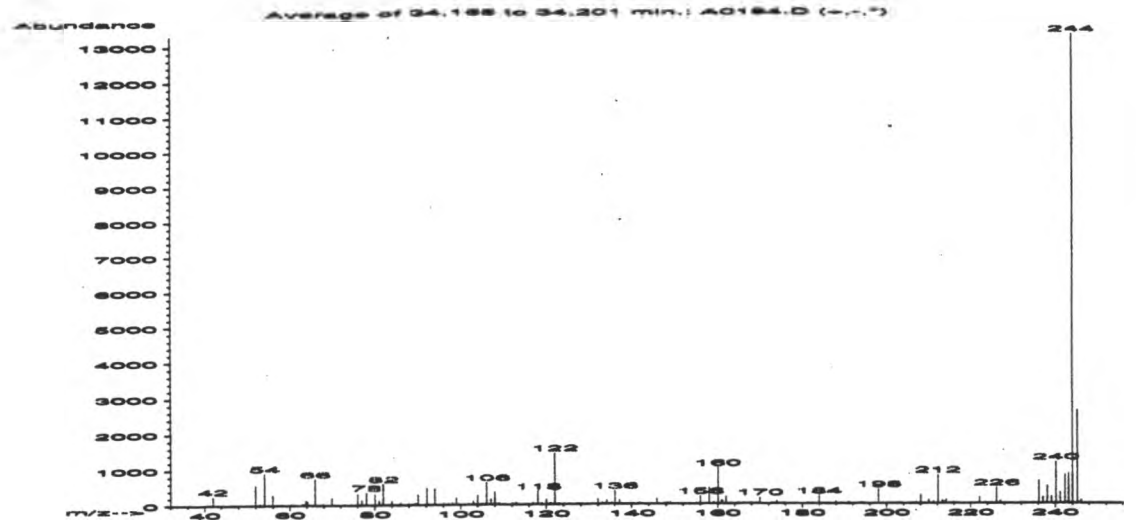
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenamine, N-[(pentafluorophenyl)methy	271	C13H6F5N	35
2.	Isoxazole, 4-iodo-3-phenyl-	271	C9H6INO	22
3.	PHENOXYPENTAFLUOROPROPENE	224	C9H5F5O	14
4.	Methanone, [3-(1-methylethyl)phenyl]phen	224	C16H16O	10
5.	4-BROMO-2-(METHYLTHIO)SPIRO(3H-INDOLE-3,	269	C10H8BrNOS	8
6.	Benzaldehyde, 4-methoxy-, (4-nitrophenyl	271	C14H13N3O3	8
7.	(Cyclopentadienyl)(p-tolylcyclopentadien	271	C17H16V	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	002341-86-8	63843	34	104	2	91	51	11	0	41	8716
2.	*22	023253-50-1	63806	49	91	3	81	64	5	2	41	8519
3.	*14	000000-00-0	45499	51	62	2	84	70	2	11	39	5203
4.	*10	032388-73-1	46042	34	75	3	74	70	1	9	36	5770
5.	8	000000-00-0	63028	36	149	2	73	69	1	0	22	7020
6.	* 8	005880-63-7	132240	32	131	2	69	69	1	0	27	8459
7.	* 7	064406-46-8	63923	32	54	2	75	75	1	0	27	6700

CTMP Compounds

Standard 7;



Average of 34.168 to 34.201 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	260	60.65	20	73.05	30	88.80	14
46.30	18	60.90	17	76.00	324	89.15	32
50.85	10	63.00	53	77.00	147	89.50	45
51.95	566	63.25	40	78.05	350	90.05	296
53.00	50	63.75	147	80.05	310	92.10	470
54.05	912	64.15	111	81.05	119	94.00	452
55.00	28	64.80	5	82.00	602	96.00	48
56.00	300	65.00	9	83.05	2	97.20	33
57.00	23	65.95	742	83.95	122	97.85	34
57.90	32	67.90	42	86.05	59	98.20	52
60.20	41	69.95	215	88.00	44	99.00	197

Average of 34.168 to 34.201 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.95	36	111.90	43	123.00	38	138.45	7
101.95	43	112.25	26	123.95	23	141.95	60
102.95	113	112.90	70	124.55	16	144.00	4
104.00	269	113.15	28	125.20	24	145.00	10
105.00	41	116.95	59	127.35	23	145.90	154
106.10	627	118.10	367	132.00	148	147.85	43
107.10	161	118.95	52	133.05	54	148.30	29
107.95	354	120.05	151	134.10	112	149.00	62
109.00	45	120.85	27	135.25	39	150.80	15
110.00	7	121.05	49	136.05	378	151.90	2
111.10	7	122.05	1454	137.10	112	155.05	28

Average of 34.168 to 34.201 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
156.00	221	166.25	9	183.95	224	195.50	7
158.00	460	168.00	38	185.25	23	197.00	17
159.10	62	168.95	20	186.40	13	198.10	409
160.05	1013	169.95	175	187.95	64	199.05	26
160.95	91	171.20	18	189.10	15	200.70	21
161.15	83	173.00	9	191.05	48	202.20	24
162.00	203	173.95	91	193.55	23	203.05	28
163.00	27	174.20	36	193.95	27	207.00	51
164.00	21	178.00	13	194.20	43	208.05	244
164.95	27	181.40	12	194.80	20	209.05	10
166.00	29	183.00	3	195.05	18	210.00	105

CTMP Compounds

Average of 34.168 to 34.201 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
211.10	61	227.05	72	242.25	812		
212.15	810	231.90	23	243.10	853		
213.25	91	232.25	22	244.05	13285		
213.65	39	233.05	11	245.20	2615		
214.10	104	234.90	18	246.05	99		
214.75	12	236.15	639				
215.15	13	237.10	182				
216.00	39	238.10	493				
222.10	182	239.10	196				
223.55	18	240.15	1162				
226.15	440	241.15	315				

Average of 34.168 to 34.201 min.: A0184.D
Converted from RTE data file: >A0184:

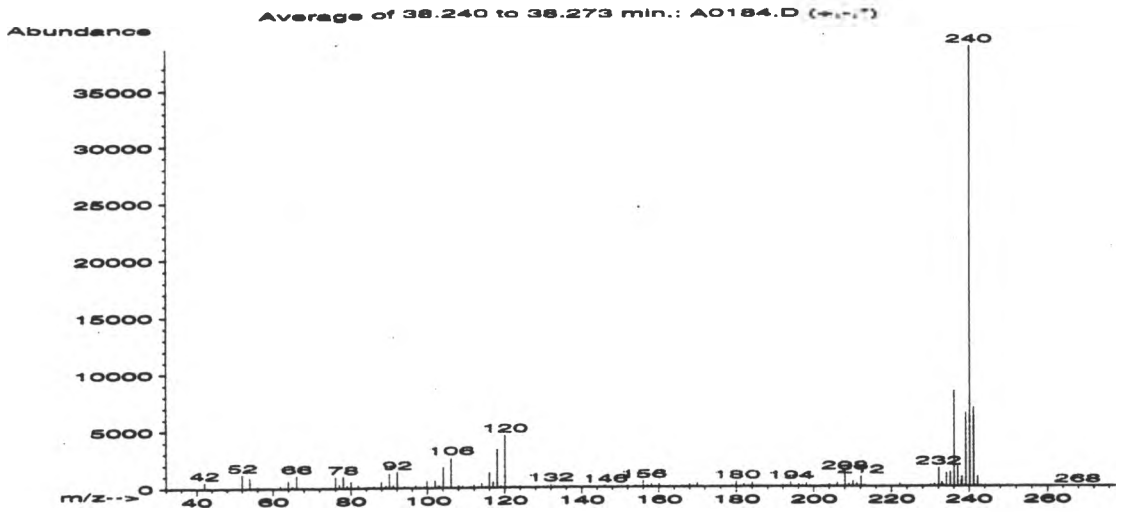
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimet	244	C14H16N2O2	53
2.	Ferrocene, (3-hydroxypropyl)-	244	C13H16FeO	50
3.	9H-Xanthen-9-one, 1,3,8-trihydroxy-	244	C13H8O5	42
4.	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimet	244	C14H16N2O2	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	000119-90-4	54095	34	106	2	73	28	28	0	39	9897
2.	*50	012093-88-8	54017	36	91	2	96	17	25	0	35	9903
3.	*42	006052-93-3	53986	28	89	2	99	26	17	0	33	9851
4.	*36	000119-90-4	131022	39	103	3	70	29	12	0	29	9881

CTMP Compounds

Standard 8: Benzo[a]anthracene d12



Average of 38.240 to 38.273 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	546	64.95	130	75.05	37	84.75	47
50.70	27	65.15	47	76.00	970	85.00	20
51.95	1209	66.05	1082	77.05	288	85.30	44
54.00	887	66.95	49	78.00	998	86.05	174
55.00	7	67.90	9	79.00	226	87.00	66
55.95	115	68.95	18	80.05	558	87.95	558
56.95	17	70.05	36	81.00	47	88.80	17
57.90	20	70.40	12	81.95	240	89.10	184
61.90	205	73.00	22	83.65	86	90.00	1265
62.95	34	73.80	63	84.00	1	91.05	207
63.90	685	74.80	32	84.50	43	92.10	1410

Average of 38.240 to 38.273 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.95	133	104.05	1810	117.00	483	129.20	17
94.80	50	104.95	81	118.05	3359	129.95	42
95.95	30	106.05	2639	119.00	133	131.05	25
96.95	204	108.05	177	120.05	4591	132.00	268
97.55	44	108.95	133	122.00	77	133.00	70
97.95	19	111.00	36	122.20	26	133.95	35
99.20	65	112.00	247	122.85	87	135.40	36
99.95	574	113.10	68	124.05	107	135.75	34
101.05	60	114.00	380	125.90	9	136.90	39
102.00	636	115.05	97	127.05	3	137.50	28
103.00	182	116.00	1348	127.95	1	137.90	68

Average of 38.240 to 38.273 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.30	6	147.45	23	159.25	34	168.95	107
140.85	30	147.85	3	160.10	277	170.00	373
141.20	18	149.05	46	160.95	8	171.05	72
141.50	32	150.95	7	161.15	33	174.05	69
142.15	95	151.95	101	162.00	24	175.00	28
143.05	35	153.95	58	162.95	80	175.70	17
143.50	20	154.20	85	164.40	18	176.30	26
143.85	51	155.05	26	165.00	2	176.70	29
144.45	22	156.00	520	165.95	90	177.00	37
144.95	39	157.05	142	166.15	53	177.95	29
146.05	135	158.05	279	168.00	232	178.80	14

CTMP Compounds

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
179.00	123	192.05	125	203.25	46	217.65	19		
180.05	452	193.05	66	204.05	150	217.90	15		
180.95	57	194.05	397	204.95	55	220.00	47		
181.95	223	195.05	56	206.05	302	222.15	230		
182.90	67	196.10	194	207.00	49	227.80	47		
184.05	319	197.05	78	208.05	1243	228.05	46		
184.95	81	198.10	266	209.05	224	230.05	160		
185.65	20	199.00	69	210.05	498	231.05	225		
186.00	26	200.15	15	211.10	253	232.10	1623		
188.25	37	201.20	26	212.15	903	232.95	319		
191.00	34	201.95	41	213.10	117	233.15	163		
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.		
234.15	1176	244.20	21						
235.10	1256	267.65	12						
236.15	8410								
237.15	1738								
238.00	468								
238.20	831								
239.15	6450								
240.15	38682								
241.15	6924								
242.15	836								
243.25	37								

Average of 38.240 to 38.273 min.: A0184.D
Converted from RTE data file: >A0184:

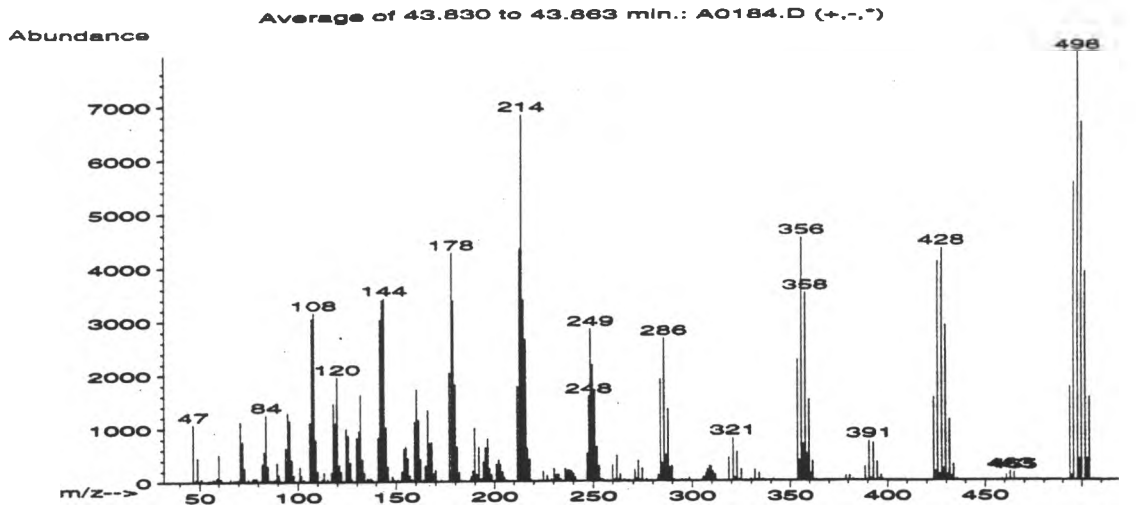
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzo[b]selenophene-3-carboxylic acid, 2	240	C10H8O2Se	59
2.	[1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-	240	C16H20N2	59
3.	Iron, (.eta.5-2,4-cyclopentadien-1-yl)[(	240	C14H16Fe	59
4.	9,10-Anthracenedione, 1,8-dihydroxy-	240	C14H8O4	53
5.	2-Propen-1-one, 1-(2-hydroxyphenyl)-3-(4	240	C15H12O3	42
6.	(+-)-Costaclavine	240	C16H20N2	40
7.	Benzene, 1,1'-(1,2-ethenediyl)bis[4-meth	240	C16H16O2	40
8.	Benzaldehyde, 2-hydroxy-, [(2-hydroxyphe	240	C14H12N2O2	40
9.	N-PHENYL(F)(3,5)PYRAZOLOPHANE	240	C16H20N2	38
10.	[1]Benzothieno[3,2-b][1]benzothiophene	240	C14H8S2	36
11.	4H-Naphtho[1,2-b]pyran-4-one, 5-methoxy-	240	C15H12O3	36
12.	1H-Naphtho[2,1-b]pyran-1-one, 6-methoxy-	240	C15H12O3	33
13.	1,9-(1'-ETHYLIDENEETHYLENE)DIAMANTANE	240	C18H24	28
14.	s-Triazolo[1,5-a]pyridine, 6-nitro-2-phe	240	C12H8N4O2	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	026526-42-1	52305	34	146	3	99	22	33	0	39	7920
2.	*59	054827-17-7	52756	52	59	3	93	25	33	4	39	9379
3.	*59	033039-67-7	52557	34	77	3	94	25	33	14	40	9765
4.	*53	000117-10-2	130798	34	96	1	88	28	28	0	39	9697
5.	*42	013323-66-5	52609	37	69	2	85	30	17	5	32	8628
6.	*40	074644-95-4	52753	29	34	0	90	32	16	6	35	9628
7.	*40	004705-34-4	52693	30	79	0	79	32	16	0	33	9624
8.	*40	000959-36-4	52526	43	56	1	88	32	16	4	37	9658
9.	*38	037072-11-0	52743	28	104	0	94	38	14	0	33	9563
10.	*36	000248-70-4	52514	32	79	2	69	28	12	0	29	9662
11.	*36	032454-43-6	52625	32	136	2	89	28	12	0	27	9431
12.	*33	005891-93-0	52628	28	70	2	75	32	10	0	27	9623
13.	*28	059297-01-7	52800	29	78	2	86	38	8	0	27	9561
14.	*28	031040-17-2	52374	29	63	1	97	38	8	1	28	9560

CTMP Compounds

Standard 9; Decachlorobiphenyl



Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.80	1076	58.15	24	74.90	40	86.90	18
47.95	35	58.95	88	77.20	66	88.00	34
48.90	455	59.90	520	78.00	66	89.10	64
49.95	22	61.00	61	79.05	66	89.40	359
50.55	25	65.90	50	79.85	14	90.25	133
50.85	60	67.90	31	80.10	16	90.65	65
54.15	11	69.00	28	81.85	340	93.80	640
55.00	26	69.95	35	82.95	566	94.95	1294
55.80	20	70.90	1127	83.95	1253	95.90	1140
57.15	53	71.95	752	84.90	297	96.90	412
57.90	23	73.00	257	86.00	26	97.85	119

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.95	284	113.30	175	126.50	362	137.40	42
101.70	122	115.00	47	127.45	38	138.00	35
103.05	37	116.95	183	129.95	822	140.90	832
105.95	1106	117.95	1459	130.95	944	141.90	3025
106.90	3046	118.95	1095	131.90	1626	142.90	3398
107.90	3147	119.85	1955	132.95	422	143.95	3423
108.90	779	120.85	95	133.95	172	144.90	1016
109.85	194	121.00	315	135.50	47	145.85	279
112.00	31	121.85	187	135.75	53	147.95	18
112.25	49	124.50	994	136.65	41	148.20	98
112.50	25	125.45	860	137.05	70	148.50	58

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
149.55	19	161.35	1147	172.80	33	187.75	49
151.05	40	162.40	417	173.05	27	188.00	89
152.80	80	163.90	18	176.90	2038	188.85	202
153.00	192	164.15	30	177.95	4260	189.90	999
153.95	613	164.90	304	178.90	3383	190.95	131
154.90	653	165.90	1333	179.90	1810	192.00	644
156.00	434	166.90	723	180.85	649	193.00	39
156.95	110	167.95	741	181.90	172	193.70	47
158.00	45	168.70	100	183.00	19	194.30	368
159.40	1113	169.00	149	185.00	18	195.40	629
160.40	1724	169.90	209	186.95	2	196.45	799

CTMP Compounds

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
197.25	244	211.85	1773	227.20	38	236.95	208
197.55	133	212.90	4329	228.80	32	237.40	71
198.50	117	213.90	6791	229.05	27	237.70	197
200.05	11	214.90	3398	230.35	237	238.00	185
200.95	321	215.95	2652	231.25	49	238.95	194
202.05	405	216.80	617	231.45	119	239.40	70
202.95	313	217.90	409	232.45	125	239.65	73
203.80	66	218.55	27	232.65	18	239.95	140
204.00	177	224.85	181	233.25	22	240.95	73
204.80	71	225.95	10	233.50	38	246.85	524
205.90	20	226.80	105	235.80	249	247.85	1586

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
248.80	2850	263.70	126	276.55	25	290.75	27
249.80	2178	265.40	20	276.80	40	294.80	32
250.75	1686	265.90	28	282.40	41	296.80	28
251.85	642	267.80	17	282.75	123	298.50	61
252.95	284	268.80	2	283.80	1908	305.50	54
253.95	35	270.75	214	284.75	345	305.80	89
254.95	29	271.60	52	285.75	2666	306.85	153
259.80	302	271.95	24	286.75	488	307.70	226
261.15	39	272.70	386	287.80	1334	307.90	129
261.85	476	273.80	26	288.85	251	308.95	281
262.75	25	274.65	240	289.85	282	309.80	273

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

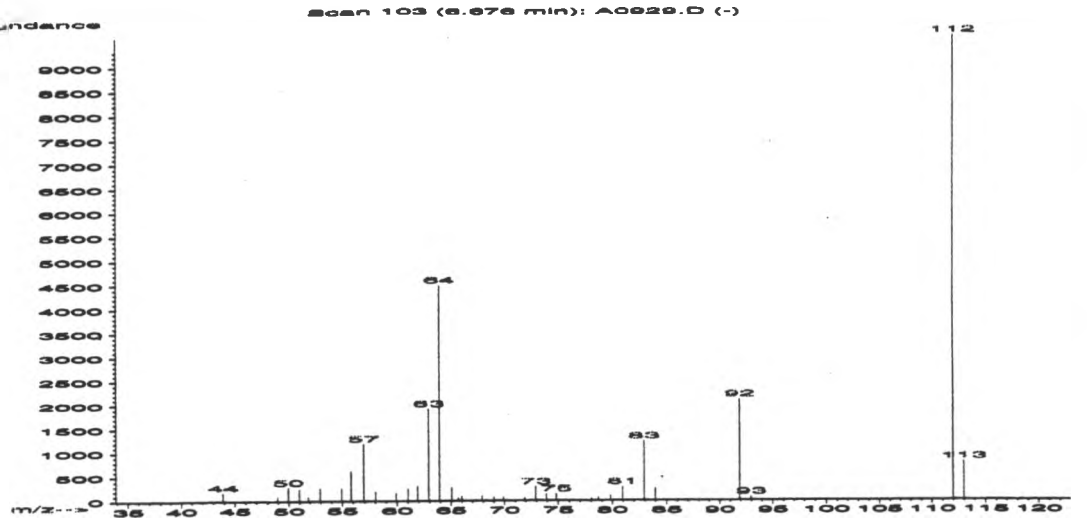
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
310.80	175	331.75	207	358.70	498	388.70	268
311.80	123	333.15	19	359.70	1511	388.90	71
318.70	434	333.90	154	360.75	140	390.75	740
320.75	802	335.75	23	361.00	87	391.75	46
321.85	68	341.25	23	361.65	360	392.75	700
322.75	545	341.50	22	362.65	13	394.75	348
323.95	25	353.75	2252	363.65	17	395.70	25
324.90	222	354.75	387	378.75	94	396.20	32
329.55	33	355.75	4516	380.50	16	396.45	33
329.80	39	356.75	685	380.85	97	396.75	95
330.95	8	357.75	3500	382.65	31	397.20	30

Average of 43.830 to 43.863 min.: A0184.D
Converted from RTE data file: >A0184:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
405.15	20	433.65	304	495.60	5525		
423.65	1550	435.50	31	497.70	7934		
424.70	175	458.65	27	498.70	396		
425.70	4078	460.70	107	499.60	6642		
426.70	121	462.50	27	501.65	3883		
427.70	4318	462.75	167	502.70	400		
428.80	231	464.65	153	503.70	1536		
429.70	2898	466.50	21				
430.90	120	492.70	14				
431.65	1140	493.55	1741				
432.65	78	494.55	98				

CTMP Compounds

Standard 10



Scan 103 (6.676 min): A0929.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	171	61.00	253	72.90	285	111.95	9600
48.95	89	61.90	308	73.90	130	112.95	793
49.95	276	62.90	1914	74.80	138		
50.95	247	63.90	4488	78.05	50		
51.80	85	65.05	276	78.70	70		
52.95	255	65.65	60	79.80	102		
54.95	267	66.00	83	80.95	282		
55.80	611	67.90	100	82.95	1227		
56.95	1180	69.00	76	83.95	242		
58.05	188	69.90	65	91.90	2104		
59.90	157	71.90	57	92.95	70		

CTMP Compounds

Scan 103 (6.676 min): A0929.D

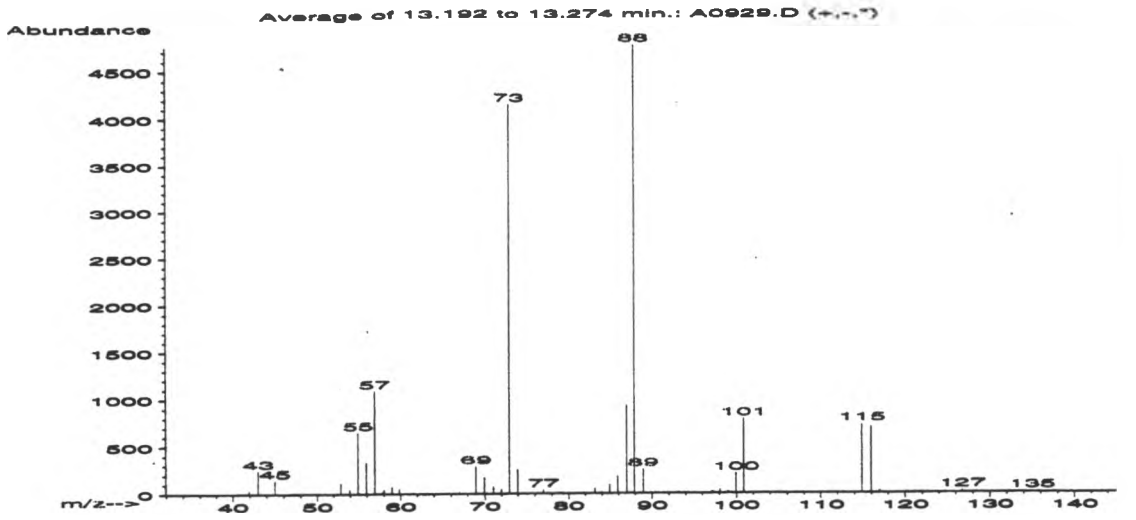
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-fluoro-	112	C6H5FO	91
2.	Phenol, 4-fluoro-	112	C6H5FO	22
3.	Phenol, 4-fluoro-	112	C6H5FO	12
4.	1-D3-METHYL-2-PYRIDONE	109	C6H4D3NO	8
5.	Pyrazine, 1,4-dioxide	112	C4H4N2O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000367-12-4	2444	75	16	0	87	4	62	27	66	9667
2.	*22	000371-41-5	2446	38	54	2	74	64	5	4	39	9094
3.	*12	000371-41-5	118976	39	60	1	70	64	2	0	35	9072
4.	* 8	053808-90-5	2044	28	68	2	99	66	1	0	27	8106
5.	* 7	002423-84-9	2410	28	52	2	73	72	1	0	29	8637

CTMP Compounds

CTMP Peak 4; C8 organic acid



Average of 13.192 to 13.274 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	35	58.95	72	77.00	37	88.95	255
42.95	243	59.85	47	78.75	3	93.00	11
44.95	144	65.40	7	78.95	9	93.25	10
49.70	6	65.75	7	80.95	4	95.00	4
52.85	115	67.00	18	81.80	10	97.15	22
53.90	44	68.95	288	83.10	56	97.40	14
54.95	644	69.95	168	83.85	12	98.05	36
55.95	332	71.00	70	84.90	93	99.00	24
56.95	1080	71.95	40	85.90	178	99.95	210
57.80	16	72.95	4127	86.95	927	100.90	784
58.00	39	73.95	254	87.90	4750	114.90	724

Average of 13.192 to 13.274 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.95	695						
116.95	24						
126.75	22						
127.00	2						
134.95	9						

CTMP Compounds

Average of 13.192 to 13.274 min.: A0929.D
Converted from RTE data file: >A0929:

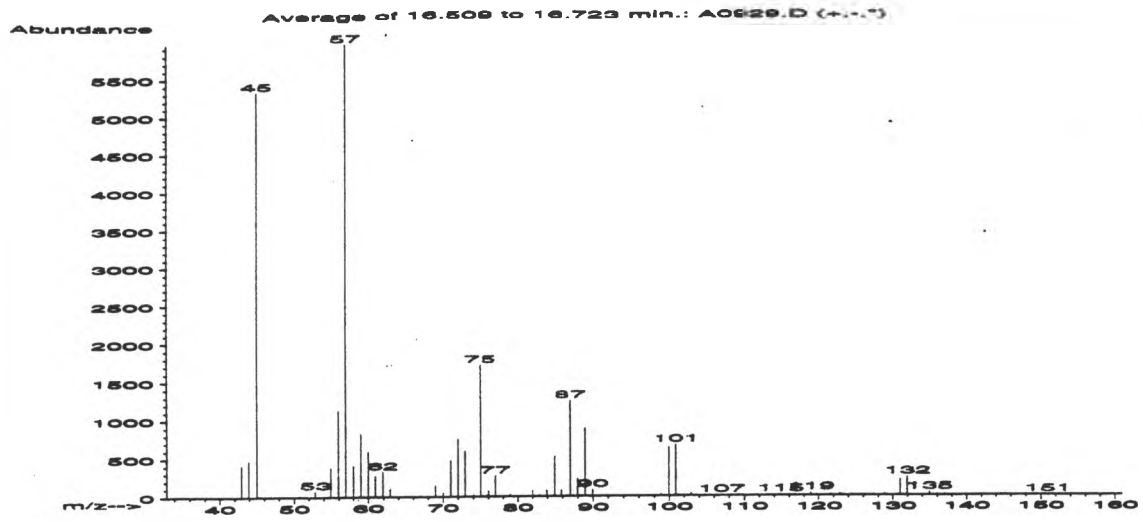
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Hexanoic acid, 2-ethyl-	144	C8H16O2	78
2.	Hexanoic acid, 2-ethyl-	144	C8H16O2	64
3.	Heptanoic acid, 2-ethyl-	158	C9H18O2	59
4.	Hexanoic acid, 2-ethyl-	144	C8H16O2	50
5.	Butanoic acid, 2-ethyl-, 1,2,3-propanetr	386	C21H38O6	50
6.	Pentanoic acid, 2-methyl-, methyl ester	130	C7H14O2	38
7.	Pentanoic acid, 2-methyl-, methyl ester	130	C7H14O2	28
8.	Pentanoic acid, 2-methyl-, methyl ester	130	C7H14O2	28
9.	Urea, N,N'-dimethyl-	88	C3H8N2O	23
10.	Butane, 2-methoxy-2-methyl-	102	C6H14O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	78	000149-57-5	122873	56	15	1	96	10	46	2	41	9953
2.	64	000149-57-5	122874	68	24	1	72	10	37	6	37	9951
3.	59	003274-29-1	16096	47	45	2	67	25	33	6	41	9775
4.	50	000149-57-5	10654	50	34	1	39	31	25	18	38	9855
5.	50	056554-54-2	95359	44	78	3	.99	32	25	20	41	9719
6.	38	002177-77-7	121079	38	56	2	99	38	14	0	33	7621
7.	28	002177-77-7	121080	37	57	2	97	37	8	0	25	7651
8.	28	002177-77-7	121081	33	66	1	69	38	8	0	25	7706
9.	*23	000096-31-1	117163	29	61	1	117	49	6	0	29	7318
10.	7	000994-05-8	118350	35	50	2	64	76	1	0	22	6605

CTMP Compounds

CTMP Peak 5



Average of 16.509 to 16.723 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	414	60.00	589	74.00	21	87.00	1250
43.90	476	60.90	274	74.95	1719	87.95	231
45.00	5329	61.90	325	75.80	17	88.95	892
50.80	13	62.90	103	76.00	72	89.95	85
52.85	76	64.90	3	76.90	273	95.00	1
53.95	1	66.95	5	78.95	29	98.95	28
54.90	388	68.95	146	82.00	72	99.95	637
55.95	1133	70.00	50	82.90	19	100.90	671
56.95	5955	71.00	480	83.90	75	101.95	15
58.00	407	72.00	757	84.95	526	102.90	36
59.00	829	72.95	600	85.85	83	104.70	3

Average of 16.509 to 16.723 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.05	4	131.95	242				
106.95	10	132.70	5				
107.85	5	134.95	39				
108.90	3	135.30	3				
109.45	3	136.00	16				
114.85	14	137.00	12				
116.90	7	150.95	1				
118.95	39						
122.90	20						
128.85	23						
131.00	207						

CTMP Compounds

Average of 16.509 to 16.723 min.: A0929.D
Converted from RTE data file: >A0929:

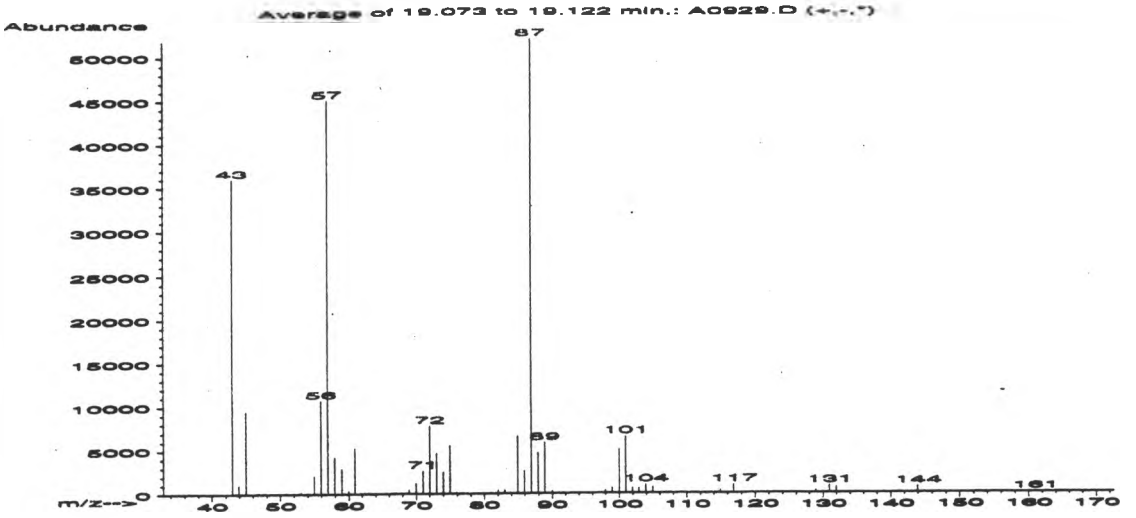
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	90
2.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	90
3.	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	86
4.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	86
5.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	83
6.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	78
7.	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	72
8.	Ethanol, 2-[2-(2-ethoxyethoxy)ethoxy]-	178	C8H18O4	47
9.	Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	45
10.	Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	42
11.	15-CROWN-5	220	C10H20O5	40
12.	ERYTHRITE-TETRAMETHYL ETHER	178	C8H18O4	40
13.	Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	32
14.	4-(2-(HYDROXYETHOXY)ETHOXY)BUTYL 2,4,5-T	414	C16H21Cl3O6	32
15.	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	32
16.	Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]	218	C12H26O3	32
17.	Ethanol, 2,2'-[oxybis(2,1-ethanediyloxy)	194	C8H18O5	32
18.	2-Butanol	74	C4H10O	32
19.	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	25
20.	3-Penten-2-ol	86	C5H10O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	90	000112-34-5	125085	100	5	0	83	5	57	7	49	9695
2.	90	000112-34-5	17547	96	13	1	84	5	57	8	43	9717
3.	86	054446-78-5	17558	75	27	0	86	10	53	0	45	9862
4.	86	000112-34-5	125081	75	27	0	86	10	53	0	45	9862
5.	83	000112-34-5	125084	80	18	0	99	5	50	4	40	9465
6.	78	000112-34-5	125082	60	39	2	120	7	46	0	39	9848
7.	72	000112-34-5	125083	60	38	0	99	13	42	0	43	9849
8.	47	000112-50-5	126559	44	52	2	60	38	20	0	39	9212
9.	45	000143-22-6	37244	49	74	2	89	21	19	8	37	9674
10.	42	000143-22-6	128828	46	68	1	89	26	17	0	35	9605
11.	40	033100-27-5	43495	39	74	3	63	32	16	12	34	9269
12.	40	003011-85-6	126562	40	59	3	89	31	16	2	31	9221
13.	32	000143-22-6	128826	51	66	1	53	47	9	0	31	9718
14.	32	000000-00-0	99947	48	67	1	64	50	9	0	35	9767
15.	32	053907-92-9	121060	44	55	3	69	47	9	0	37	8181
16.	32	000112-73-2	42758	47	72	1	67	50	9	6	32	8235
17.	32	000112-60-7	31536	38	51	2	88	47	9	0	33	9161
18.	*32	000078-92-2	116568	30	51	0	63	50	9	0	33	8948
19.	25	001559-34-8	56322	38	84	2	52	55	7	0	33	9370
20.	*25	001569-50-2	66	31	68	0	61	51	7	0	33	8942

CTMP Compounds

Peak 6



Average of 19.073 to 19.122 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	36021	57.95	4208	71.00	2670	83.90	107
43.90	1029	58.95	2930	72.00	7780	84.95	6659
44.95	9453	59.95	333	73.00	4687	85.95	2622
49.90	38	60.90	5233	74.00	2511	86.95	51830
50.80	123	61.90	98	74.95	5585	87.90	4701
52.80	121	62.40	36	75.90	170	88.90	5875
53.00	180	62.95	106	76.95	134	90.00	266
53.95	136	66.95	109	78.80	7	90.95	65
54.95	2119	67.90	17	81.00	80	96.00	3
55.95	10697	68.95	507	82.00	423	96.90	22
56.95	44981	69.95	1192	83.00	444	97.95	335

Average of 19.073 to 19.122 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.95	645	114.90	376	147.00	130		
100.00	5086	115.90	18	148.95	51		
100.95	6561	116.90	1008	160.80	34		
101.95	634	117.95	57	161.00	63		
102.90	606	128.95	359	161.95	14		
103.90	1054	130.00	48	162.55	9		
104.95	728	130.95	859				
106.70	22	131.95	669				
106.95	41	132.85	39				
108.95	13	143.95	738				
112.80	20	144.95	87				

CTMP Compounds

Average of 19.073 to 19.122 min.: A0929.D
Converted from RTE data file: >A0929:

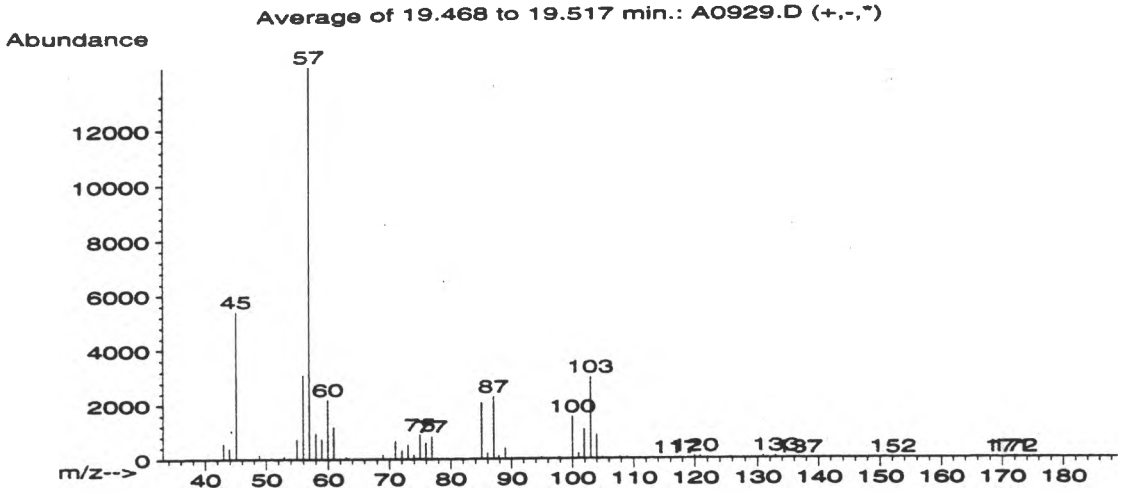
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-(2-butoxyethoxy)-, acetate	204	C10H20O4	91
2.	3,4-DI-O-METHYL-L-ARABINOPYRANOSE	178	C7H14O5	45
3.	Ethanol, 2-(2-butoxyethoxy)-, acetate	204	C10H20O4	43
4.	Acetamide, N-ethyl-	87	C4H9NO	43
5.	.alpha.-D-Xylofuranoside, methyl 3-O-met	178	C7H14O5	42
6.	Ethane, isothiocyanato-	87	C3H5NS	38
7.	MONOETHYL ESTER OF MALONIC ACID	132	C5H8O4	37
8.	Ethanol, 2,2'-[1,2-ethanediylbis(oxy)]bi	234	C10H18O6	32
9.	1,3-Dioxolane, 2-butyl-2-methyl-	144	C8H16O2	28
10.	Cyclobutene, 3,4-dichloro-	122	C4H4Cl2	28
11.	1,3-Butadiene, 1,4-dichloro-	122	C4H4Cl2	28
12.	1,3-Dioxolane, 2-methyl-2-pentyl-	158	C9H18O2	25
13.	Thiophane, propyl-	130	C7H14S	25
14.	4-Heptanol, 4-methyl-	130	C8H18O	25
15.	1,3-Dioxolane, 2-(3-methoxypropyl)-2-met	160	C8H16O3	23
16.	1,3-Dioxane, 2-pentadecyl-	298	C19H38O2	23
17.	Butyl glycol acetate	160	C8H16O3	17
18.	2-N-BUTOXYETHYL GLYCIDYL ETHER	174	C9H18O3	10
19.	Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]	218	C12H26O3	10
20.	Propanoic acid, ethyl ester	102	C5H10O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	91	000124-17-4	36294	98	26	2	98	0	60	0	51	9994
2.	45	086049-20-9	24446	45	58	3	99	25	19	0	37	7553
3.	43	000124-17-4	128610	65	46	1	75	44	18	0	38	9750
4.	*43	000625-50-3	130	33	59	1	107	44	18	0	41	7445
5.	42	034338-86-8	24439	50	55	3	99	27	17	5	33	7558
6.	*38	000542-85-8	117133	32	41	2	99	38	14	1	30	7373
7.	*37	000000-00-0	6795	35	67	1	75	44	13	0	35	7400
8.	32	000111-21-7	49711	39	50	1	93	47	9	13	35	7400
9.	28	014447-27-9	10712	37	54	1	99	38	8	0	25	8002
10.	28	041326-64-1	120118	34	78	1	87	36	8	0	22	7375
11.	28	002984-42-1	4274	34	77	1	86	36	8	0	22	7387
12.	25	004352-95-8	16151	33	41	1	99	44	7	2	23	7438
13.	25	001551-34-4	6505	40	62	2	76	41	7	0	29	7458
14.	25	000598-01-6	121189	34	48	1	99	45	7	2	23	7735
15.	23	054751-80-3	16756	31	50	2	92	48	6	1	23	7421
16.	23	017352-27-1	133420	35	76	3	93	47	6	0	22	7719
17.	17	000112-07-2	16742	40	55	2	100	52	3	0	28	8468
18.	10	013483-47-1	22960	52	41	1	64	66	1	0	35	7361
19.	10	000112-73-2	42758	47	60	0	27	73	1	0	39	7851
20.	*10	000105-37-3	118220	37	52	1	66	76	1	0	39	6625

CTMP Compounds

Peak 7



Average of 19.468 to 19.517 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	565	56.95	14235	70.95	647	85.95	215
43.90	380	58.00	951	72.00	316	87.00	2296
45.00	5410	58.95	744	73.00	527	87.85	125
48.05	9	59.95	2182	73.95	152	88.95	392
48.85	155	60.90	1176	74.95	894	89.95	41
49.80	19	61.90	15	75.90	587	90.90	13
50.85	48	62.90	80	76.95	827	94.95	71
52.90	105	63.40	14	77.90	20	97.90	69
53.85	35	67.75	11	80.95	12	100.00	1548
54.95	730	68.95	151	83.90	34	101.00	206
55.95	3092	70.10	44	85.00	2061	101.90	1083

Average of 19.468 to 19.517 min.: A0929.D
Converted from RTE data file: >A0929:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.95	2984	125.70	4				
103.95	859	125.90	11				
104.95	51	130.90	79				
106.90	4	132.95	91				
108.90	46	134.95	27				
111.00	3	136.80	12				
116.90	21	152.05	10				
117.40	19	170.90	13				
119.95	94	171.75	17				
120.85	73	171.95	24				
122.00	17	179.00	9				

CTMP Compounds

Average of 19.468 to 19.517 min.: A0929.D
Converted from RTE data file: >A0929:

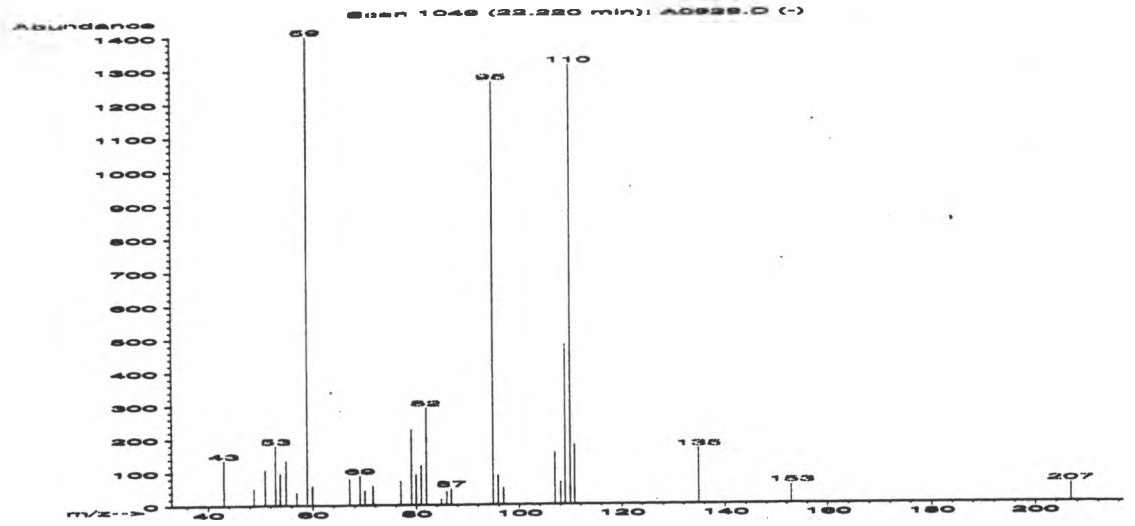
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid, 4-butoxy-	160	C8H16O3	36
2.	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	32
3.	Ethanol, 2-butoxy-	118	C6H14O2	32
4.	Ethanol, 2-butoxy-	118	C6H14O2	32
5.	Propene, 3-tert-butoxy-2-(methoxymethyl)	158	C9H18O2	32
6.	Ethanol, 2-butoxy-	118	C6H14O2	27
7.	Orthoformic acid, tri-sec-butyl ester	232	C13H28O3	27
8.	Ethanol, 2-butoxy-	118	C6H14O2	25
9.	Ethanol, 2-butoxy-	118	C6H14O2	25
10.	Ethanol, 2-butoxy-	118	C6H14O2	25
11.	L-Threonine	119	C4H9NO3	23
12.	6,8-DIOXABICYCLO(3.2.21)OCTAN-4L-OL-O-D1	130	C6H9DO3	17
13.	Butane, 1,1'-oxybis-	130	C8H18O	16
14.	Butane, 1,1'-oxybis-	130	C8H18O	16
15.	6,8-DIOXABICYCLO(3.2.1)OCTAN-4.BETA.-OL-	130	C6H9DO3	12
16.	Butanoic acid, 3-methyl-, 2-methylpropyl	158	C9H18O2	12
17.	Propanoic acid, 2-methylpropyl ester	130	C7H14O2	12
18.	1-Butene, 4-butoxy-	128	C8H16O	10
19.	Propionaldehyde, ethylhydrazone	100	C5H12N2	9
20.	Butane, 1,1'-oxybis-	130	C8H18O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	36	055724-73-7	16725	40	71	2	72	28	12	0	28	8463
2.	32	013343-98-1	6932	50	42	2	85	46	9	2	33	9513
3.	32	000111-76-2	119792	45	42	1	70	48	9	0	35	9550
4.	32	000111-76-2	119788	48	43	1	73	50	9	0	31	9531
5.	32	023230-86-6	16144	39	54	2	93	50	9	10	31	9540
6.	27	000111-76-2	119793	40	33	2	95	57	8	4	43	9520
7.	27	016754-48-6	49145	45	51	0	65	57	8	12	41	9162
8.	25	000111-76-2	119789	47	42	1	71	53	7	0	37	9558
9.	25	000111-76-2	119786	51	32	1	82	51	7	1	36	9554
10.	25	000111-76-2	3837	51	28	0	78	55	7	1	36	9526
11.	23	000072-19-5	119886	40	58	1	99	48	6	0	29	9494
12.	*17	000000-00-0	6354	32	74	1	58	55	3	0	29	4150
13.	16	000142-96-1	121217	46	24	0	99	59	3	1	34	9049
14.	16	000142-96-1	6583	48	24	0	81	59	3	7	36	9085
15.	*12	000000-00-0	6351	29	58	0	45	61	2	0	33	4203
16.	12	000589-59-3	124708	40	59	3	99	59	2	0	29	7942
17.	12	000540-42-1	121123	40	32	0	72	65	2	0	33	8947
18.	10	034061-76-2	120890	34	33	2	90	65	1	1	26	9037
19.	* 9	007422-92-6	1113	30	39	0	15	80	1	0	33	2034
20.	8	000142-96-1	121219	38	30	0	85	69	1	7	29	9033

CTMP Compounds

Peak 8



Scan 1049 (22.220 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	136	69.90	44	95.90	89		
48.75	51	71.50	58	96.90	51		
50.95	107	76.95	73	106.95	157		
52.95	179	79.05	227	108.05	68		
53.80	96	79.95	91	108.95	481		
54.95	134	80.95	118	109.95	1311		
56.95	39	81.95	292	110.80	180		
58.95	1402	84.85	18	134.95	168		
59.95	58	85.90	41	152.90	57		
67.00	78	86.80	49	206.75	57		
69.00	89	94.90	1260				

CTMP Compounds

Scan 1049 (22.220 min): A0929.D

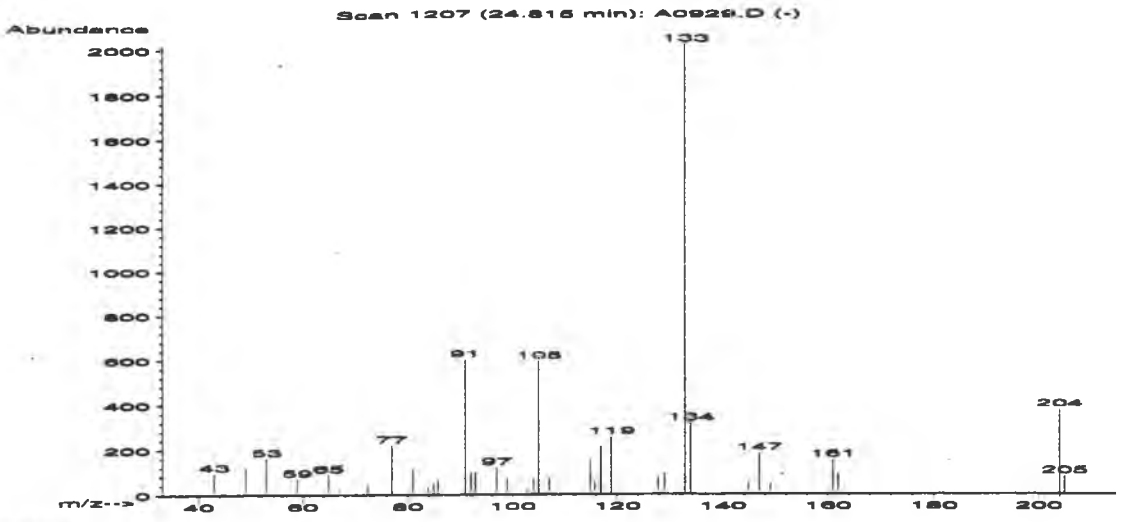
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	8-HYDROXYCARVOTANACETONE	168	C10H16O2	74
2.	1,2-CIS-1,5-TRANS-2,5-DIHYDROXY-4-METHYL	186	C10H18O3	56
3.	Cyclobutene, 1,2,3,4-tetramethyl-, trans	110	C8H14	50
4.	2-HEXANOYL FURAN	166	C10H14O2	38
5.	MENTHENE ISOMER B	138	C10H18	37
6.	2-Cyclohexen-1-one, 6-methyl-3-(1-methyl	152	C10H16O	37
7.	2-PENTANOYLFURAN	152	C9H12O2	32
8.	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-,	170	C9H14O3	25
9.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	16
10.	Iridomyrmecin	168	C10H16O2	16
11.	1,2-Benzenediol	110	C6H6O2	14
12.	2-(1'-OCTANONE-8-CARBOXYLIC ACID FURAN	224	C12H16O4	12
13.	1,3-Benzenediol	110	C6H6O2	12
14.	1,3-Benzenediol	110	C6H6O2	12
15.	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	10
16.	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	10
17.	Butanal, oxime	87	C4H9NO	10
18.	Butanamide	87	C4H9NO	9
19.	4(1H)-Pyrimidinone, 2-methyl-	110	C5H6N2O	8
20.	1,2-Benzenediol	110	C6H6O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	74	007712-46-1	20525	73	31	1	79	3	44	9	37	9047
2.	56	087096-70-6	28412	43	83	3	89	15	30	0	31	9768
3.*	50	003200-65-5	2266	31	17	0	79	19	25	0	33	7697
4.	38	000000-00-0	125558	45	21	0	93	46	14	0	39	7536
5.	37	029350-67-2	122308	48	46	1	70	43	13	0	31	7879
6.	37	000499-74-1	13661	46	48	1	93	43	13	0	37	7736
7.	32	000000-00-0	123920	41	24	0	92	46	9	2	35	7652
8.	25	014919-56-3	21259	40	46	2	93	42	7	8	29	7736
9.	16	001072-91-9	2139	46	51	2	111	59	3	15	37	7440
10.	16	000485-43-8	20454	44	65	2	65	60	3	0	37	6261
11.*	14	000120-80-9	118832	37	56	0	77	68	2	0	41	5698
12.	12	000000-00-0	45650	33	67	0	64	58	2	1	26	7614
13.*	12	000108-46-3	118835	33	53	1	93	64	2	2	37	5778
14.*	12	000108-46-3	2130	36	49	1	93	64	2	8	37	5769
15.*	10	003524-87-6	118822	29	45	1	65	67	1	0	33	5648
16.*	10	003524-87-6	2115	32	60	1	64	67	1	0	33	5669
17.*	10	000110-69-0	134	34	60	0	85	75	1	0	41	5882
18.*	9	000541-35-5	117137	28	55	2	97	75	1	0	33	5882
19.*	8	019875-04-8	2114	31	65	1	77	66	1	0	29	5912
20.*	8	000120-80-9	118830	28	68	1	88	67	1	0	29	5673

CTMP Compounds

Peak 3; Unidentified Sesquiterpene



Scan 1207 (24.815 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	95	84.95	49	114.90	150	160.95	151
48.95	121	85.80	64	115.75	58	161.95	88
52.95	162	90.90	602	116.90	212	204.00	378
54.95	5	92.00	101	118.90	256	204.90	79
58.95	70	92.90	100	127.80	76		
64.90	89	96.95	120	129.05	94		
67.00	20	99.00	71	132.95	2018		
72.40	45	102.75	22	133.95	317		
76.95	218	103.95	69	144.90	52		
80.95	113	104.95	595	146.90	182		
83.80	33	107.00	73	149.00	49		

CTMP Compounds

Scan 1207 (24.815 min): A0929.D

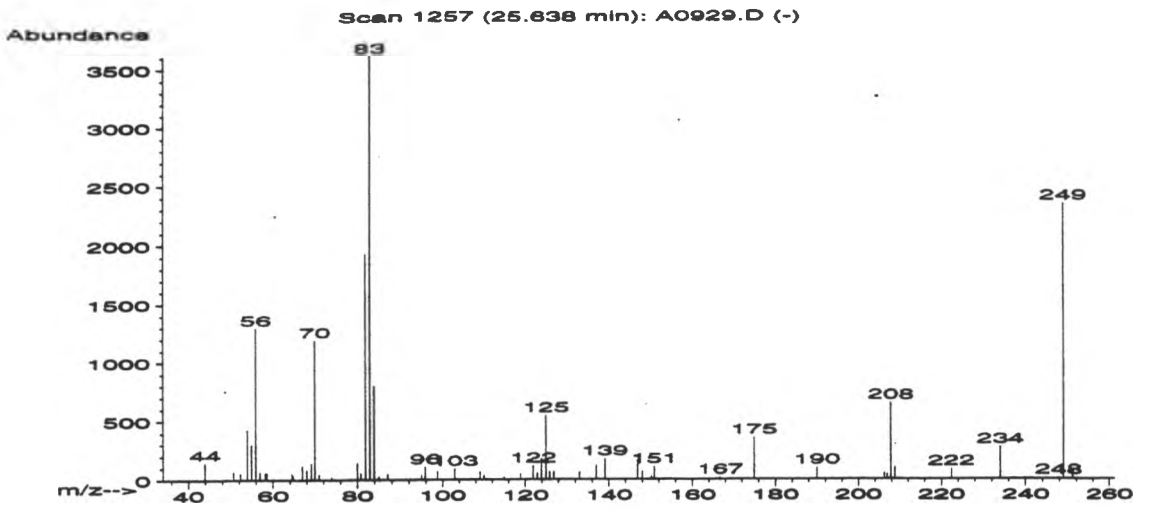
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 2,4-dimethyl-1-(1-methylpropyl)	162	C12H18	53
2.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	53
3.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	53
4.	1H-Benzimidazol-2-amine	133	C7H7N3	52
5.	Silane, diethoxymethyl[3-(oxiranylmethox	248	C11H24O4Si	45
6.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	45
7.	2-Oxazolidinone, 5-isopropyl-4-phenyl-,	205	C12H15NO2	38
8.	1-Propanone, 2-chloro-1-(2,5-dimethylphe	210	C12H15ClO	38
9.	1-Butyl-2,4,6-trimethylbenzene	176	C13H20	36
10.	1-(2,6-Dimethylphenyl)-2-buten-1-ol	176	C12H16O	36
11.	Benzene, ethyl-1,2,4-trimethyl-	148	C11H16	36
12.	Benzene, (1,1-dimethylethyl)methyl-	148	C11H16	36
13.	Benzoic acid, 4-ethyl-, methyl ester	164	C10H12O2	33
14.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	33
15.	[1,2,4]Triazolo[1,5-a]pyridine, 2-methyl	133	C7H7N3	33
16.	2-PHENYL-2-METHYL-1-D1-AZIRIDINE	133	C9H10DN	30
17.	Benzene, (1-chloroethyl)dimethyl-	168	C10H13Cl	28
18.	1-Propanone, 3-cyclopentyl-1-(2,4-dimeth	230	C16H22O	28
19.	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	28
20.	2-Oxazolidinone, 5-isopropyl-4-phenyl-,	205	C12H15NO2	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	001483-60-9	17844	46	41	0	98	28	28	18	40	9343
2.	53	000098-51-1	123445	45	32	0	73	27	28	19	41	9656
3.	53	000098-51-1	12112	38	50	1	75	27	28	10	39	9699
4.	*52	000934-32-7	121459	34	49	0	99	33	27	2	43	9650
5.	45	002897-60-1	55351	51	98	2	69	21	19	0	31	9522
6.	45	004706-90-5	123453	38	61	2	99	25	19	10	31	9676
7.	*38	032461-27-1	36942	42	85	1	77	36	14	0	33	9093
8.	38	054965-52-5	39357	42	69	1	99	21	14	0	29	9752
9.	36	084651-10-5	24036	40	29	0	99	30	12	0	25	9511
10.	36	080445-61-0	23944	41	66	2	89	28	12	0	29	9631
11.	36	054120-62-6	12122	40	50	1	96	26	12	0	29	9536
12.	36	027138-21-2	12113	34	55	1	66	29	12	0	22	9681
13.	33	007364-20-7	18507	34	55	1	80	33	10	1	23	9631
14.	33	004706-90-5	12118	37	53	1	99	31	10	0	25	9560
15.	*33	000768-19-4	7102	28	73	1	73	31	10	0	26	9626
16.	*30	030691-62-4	7149	46	59	0	56	57	9	0	44	9396
17.	28	054411-21-1	20290	35	63	0	72	36	8	0	25	9540
18.	28	055191-11-2	48547	38	76	2	93	37	8	0	29	9599
19.	28	004218-48-8	123449	38	54	2	95	39	8	0	29	9679
20.	*12	032461-27-1	128786	30	81	0	30	62	2	0	33	9149

CTMP Compounds

Peak 9; 1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione



Scan 1257 (25.638 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	144	64.80	33	83.95	801	118.90	49
48.90	10	66.90	119	85.00	25	121.90	118
50.70	69	68.00	81	87.05	47	122.90	53
52.30	56	69.10	141	95.00	39	123.90	178
53.95	426	69.90	1195	95.90	110	125.00	549
54.95	298	70.90	44	98.80	68	125.90	67
55.95	1302	73.90	23	102.95	92	126.90	66
56.95	65	80.05	144	106.75	2	132.95	62
58.20	58	80.90	56	109.00	65	136.95	119
58.55	58	81.95	1929	110.00	35	139.05	178
64.50	55	82.95	3613	114.90	22	146.90	165

Scan 1257 (25.638 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.00	68	234.00	276				
150.15	27	247.75	11				
150.90	110	248.90	2351				
166.70	18	251.05	46				
174.90	356	251.25	67				
189.95	102						
206.25	51						
206.95	41						
207.80	655						
208.80	99						
222.40	88						

CTMP Compounds

Scan 1257 (25.638 min): A0929.D

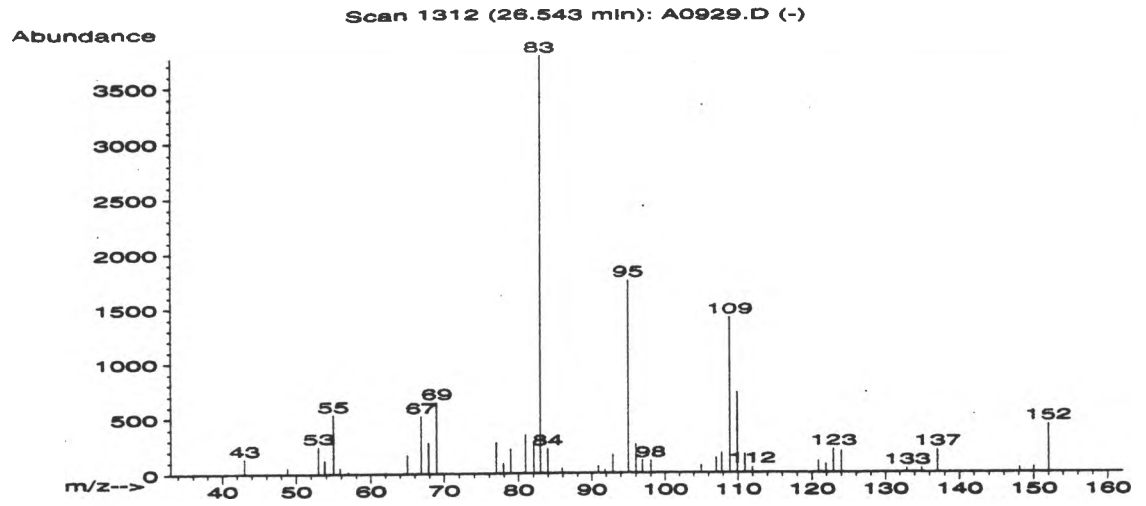
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1	249	C12H15N3O3	72
2.	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1	249	C12H15N3O3	59
3.	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1	249	C12H15N3O3	52
4.	2L,4D-DIHYDROXYEICOSANE	314	C20H42O2	25
5.	Cyclohexane, 2-propenyl-	124	C9H16	23
6.	1-Octadecanol	270	C18H38O	23
7.	Hemiloline	125	C7H11NO	14
8.	TRIS(ALLYLOXY)-S-TRIAZINE	249	C12H15N3O3	12
9.	1H-Pyrazole, 4,5-dihydro-1,5-dimethyl-	98	C5H10N2	12
10.	9-Azabicyclo[6.1.0]nonane, cis-	125	C8H15N	12
11.	Dodecane 3-cyclohexyl-, 3-cyclohexyl-	252	C18H36	10
12.	2-Cyclohexen-1-one, 3,5,5-trimethyl-	138	C9H14O	8
13.	Heptadecanenitrile	251	C17H33N	7
14.	2H-Pyran-2-one, 5,6-dihydro-4,6,6-trimet	140	C8H12O2	7
15.	2,2-d2-3-Cyclohexen-1-ol	98	C6H8D2O	7
16.	5-Undecene, 8-methyl-, (E)-	168	C12H24	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	001025-15-6	131231	55	20	0	72	17	42	0	49	9615
2.	59	001025-15-6	131230	77	69	0	57	23	33	4	42	9862
3.	*52	001025-15-6	55945	54	92	1	58	35	27	0	49	9657
4.	25	000000-00-0	78411	35	135	2	132	41	7	0	22	8243
5.	*23	002114-42-3	4917	28	68	2	72	50	6	0	27	7957
6.	23	000112-92-5	132220	36	113	1	126	43	6	0	18	8319
7.	*14	029079-42-3	5023	40	22	0	53	70	2	0	39	4697
8.	12	000000-00-0	55942	38	88	2	101	58	2	0	28	7378
9.	12	005775-96-2	765	34	56	0	71	58	2	0	25	7424
10.	12	066387-85-7	5046	33	77	2	53	60	2	2	23	6476
11.	10	013151-83-2	131395	33	96	1	60	62	1	3	23	7849
12.	8	000078-59-1	122271	33	62	2	53	68	1	0	22	7315
13.	* 7	005399-02-0	56959	28	129	3	172	72	1	0	29	6794
14.	7	006970-56-5	9216	37	47	0	53	77	1	0	25	4640
15.	7	082299-78-3	864	33	44	1	37	76	1	0	21	4433
16.	7	039546-85-5	20723	33	63	1	83	76	1	0	21	3712

CTMP Compounds

Peak 10



Scan 1312 (26.543 min): A0929.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	134	76.95	280	95.00	1752	120.90	108
48.80	55	77.95	89	96.00	261	121.90	77
52.95	244	78.95	221	96.90	115	122.90	212
53.80	122	80.95	345	98.00	110	124.00	196
54.95	529	82.05	290	105.00	66	132.95	38
55.85	54	82.95	3761	107.05	134	134.95	37
56.95	15	83.95	222	107.80	181	137.05	205
65.00	166	85.90	44	108.95	1414	148.15	41
66.90	516	90.90	59	109.95	722	150.00	52
67.90	275	91.80	29	110.95	167	152.00	437
69.00	640	92.90	164	111.95	52		

CTMP Compounds

Scan 1312 (26.543 min): A0929.D

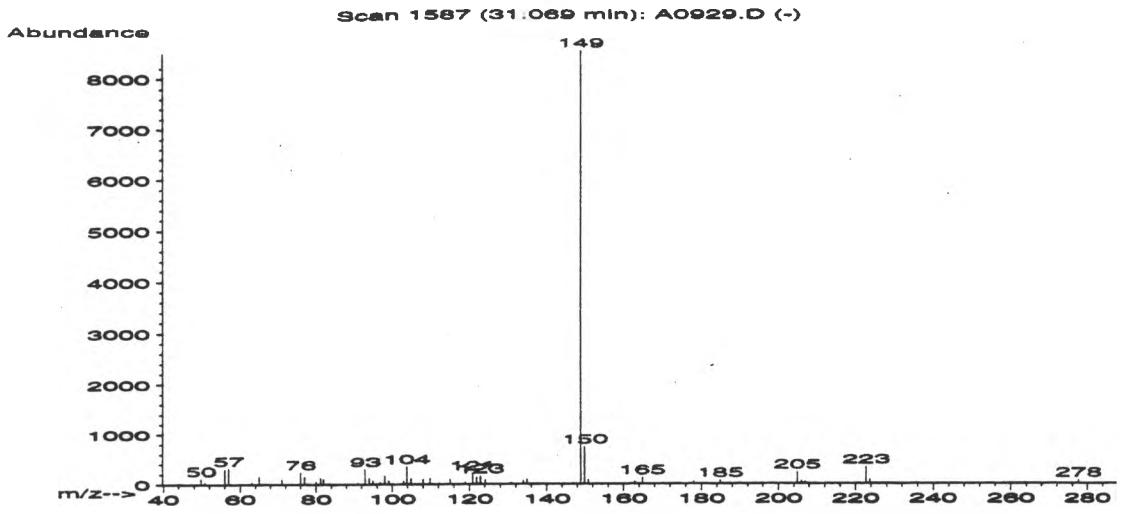
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Bicyclo[3.1.1]heptan-2-one, 3,6,6-trimet	152	C10H16O	87
2.	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimet	152	C10H16O	37
3.	1H-1,2,4-Triazole, 3-propyl-	111	C5H9N3	32
4.	Cyclohexane, eicosyl-	364	C26H52	25
5.	1H-1,2,4-Triazole, 3-(1-methylethyl)-	111	C5H9N3	23
6.	1(2H)-Pyrazineacetonitrile, 5-amino-3,6-	151	C6H9N5	17
7.	Cyclohexane, eicosyl-	364	C26H52	17
8.	MENTHYL ESTER OF 1-METHYL-SPIRO[2.3]HEXA	278	C18H30O2	16
9.	2-Pyrazoline, 1-allyl-	110	C6H10N2	12
10.	2,6-Nonadien-4-one, 9-(3-furanyl)-2,6-di	232	C15H20O2	12
11.	Cyclohexane, ethyl-	112	C8H16	12
12.	5-OXO-7-METHYL-6-OCTENENITRILE	151	C9H13NO	12
13.	d-Isothujone	152	C10H16O	10
14.	Cyclohexane, 2-propenyl-	124	C9H16	10
15.	Cyclohexanecarbonyl chloride	146	C7H11ClO	9
16.	6-Octenoic acid, 3,7-dimethyl-, methyl e	184	C11H20O2	8
17.	Cyclopentanepropanoic acid	142	C8H14O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	016022-08-5	13804	72	36	2	82	7	54	11	52	9892
2.	*37	000547-60-4	13806	33	66	2	79	44	13	0	35	9151
3.	*32	019932-60-6	2329	30	54	2	88	46	9	0	33	8512
4.	25	004443-55-4	135347	43	98	3	99	55	7	0	37	8443
5.	23	023161-10-6	2330	34	42	1	99	47	6	0	22	8535
6.	17	035975-34-9	13013	34	38	0	66	55	3	1	26	8413
7.	17	004443-55-4	91307	34	96	3	99	55	3	0	22	8440
8.	16	000000-00-0	66510	45	89	2	51	56	3	0	35	9189
9.	*12	019804-38-7	2140	29	55	1	64	65	2	2	30	8765
10.	12	053098-76-3	49216	32	53	0	72	56	2	1	26	8524
11.	12	001678-91-7	119107	36	60	2	85	57	2	0	25	8406
12.	12	000000-00-0	13133	41	31	1	98	56	2	0	29	8396
13.	*10	000471-15-8	13717	29	92	3	86	64	1	0	26	4819
14.	*10	002114-42-3	4917	35	61	2	64	75	1	0	39	8478
15.	9	002719-27-9	11234	39	40	1	63	76	1	2	31	8413
16.	8	002270-60-2	27517	33	87	1	65	69	1	0	20	4942
17.	7	000140-77-2	10048	35	64	0	65	78	1	0	25	8535

CTMP Compounds

Peak 11



Scan 1587 (31.069 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.80	116	81.95	105	102.95	67	125.00	1
50.80	38	82.95	16	103.80	352	130.80	38
55.95	299	83.95	16	104.95	113	132.95	2
57.00	322	90.95	29	108.05	95	133.95	71
63.15	48	92.90	302	109.80	123	134.90	99
65.00	159	94.00	123	115.00	99	136.80	2
71.00	95	94.95	72	118.95	36	146.90	27
75.95	239	95.95	7	120.90	220	148.90	8494
76.95	153	96.80	42	121.90	138	149.90	749
79.95	57	98.00	165	122.90	159	150.90	84
81.20	129	99.15	74	124.15	82	162.80	54

Scan 1587 (31.069 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
164.80	126						
178.00	53						
184.80	72						
204.90	232						
206.00	52						
206.95	39						
222.75	335						
223.75	76						
277.65	66						

CTMP Compounds

Scan 1587 (31.069 min): A0929.D

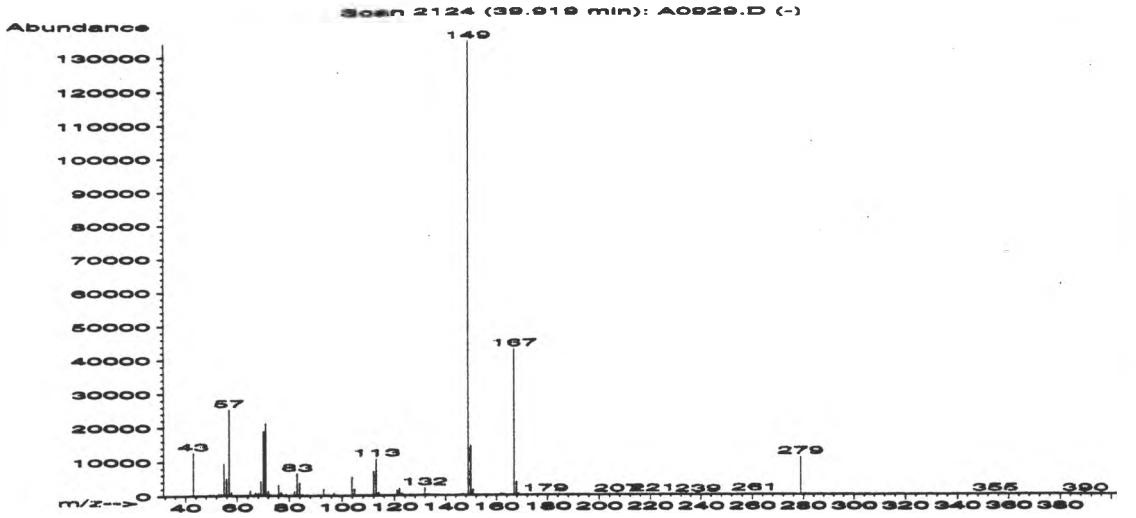
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	93
2.	1,2-Benzenedicarboxylic acid, butyl 2-et	334	C20H30O4	78
3.	1,2-Benzenedicarboxylic acid, bis(2-meth	282	C14H18O6	78
4.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	72
5.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	64
6.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	64
7.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	64
8.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	64
9.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	64
10.	1,2-Benzenedicarboxylic acid, butyl octy	334	C20H30O4	64
11.	1,2-Benzenedicarboxylic acid, butyl 2-me	278	C16H22O4	60
12.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	56
13.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	56
14.	1,2-Benzenedicarboxylic acid, butyl cycl	304	C18H24O4	56
15.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	56
16.	1,2-Benzenedicarboxylic acid, diheptyl e	362	C22H34O4	50
17.	1,2-Benzenedicarboxylic acid, butyl decy	362	C22H34O4	50
18.	1,2-Benzenedicarboxylic acid, dibutyl es	278	C16H22O4	49
19.	1,2-Benzenedicarboxylic acid, bis(2-meth	278	C16H22O4	49
20.	Phthalic acid, butyl ester, ester with b	336	C18H24O6	47

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000084-74-2	132526	78	28	1	70	6	66	0	90	9993
2.	78	000085-69-8	84071	76	26	1	90	6	46	2	40	9992
3.	78	000117-82-8	132666	71	30	1	77	9	46	0	38	9995
4.	72	000084-69-5	66362	56	50	1	80	11	42	16	38	9987
5.	64	000084-74-2	132531	68	33	1	73	9	37	1	36	9993
6.	64	000131-18-0	75798	45	76	1	70	18	37	0	39	9984
7.	64	000131-18-0	133653	43	65	2	80	18	37	0	39	9983
8.	64	000131-16-8	131292	45	53	1	68	18	37	0	39	9985
9.	64	000131-16-8	56409	54	48	1	66	18	37	0	39	9985
10.	64	000084-78-6	134557	66	43	1	77	6	37	1	37	9996
11.	*60	017851-53-5	66360	68	36	0	53	40	35	0	76	9995
12.	56	000084-74-2	132529	64	30	1	78	11	30	0	37	9991
13.	56	000084-64-0	133606	44	57	1	68	15	30	0	35	9988
14.	56	000084-64-0	75219	58	40	1	81	11	30	1	36	9996
15.	56	000084-74-2	66361	43	62	3	84	11	30	0	35	9996
16.	50	003648-21-3	90783	47	67	1	90	18	25	0	37	9984
17.	50	000089-19-0	90781	47	71	2	90	20	25	0	37	9980
18.	*49	000084-74-2	132533	55	39	0	42	40	23	0	49	9989
19.	*49	000084-69-5	132535	61	49	1	58	45	23	0	51	9979
20.	47	000085-70-1	134617	58	31	0	44	40	20	0	43	9985

CTMP Compounds

Peak 12



Scan 2124 (39.919 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	12673	58.95	118	73.00	319	83.95	3847
48.05	70	62.90	120	74.00	107	84.95	459
48.80	97	64.00	116	74.95	348	85.85	31
49.80	542	65.00	1594	75.95	3193	87.05	131
50.95	416	66.00	195	76.95	1097	87.90	66
52.95	830	67.00	975	77.80	152	91.00	276
53.95	611	68.00	818	78.80	414	92.00	117
54.95	9459	69.00	4284	79.95	47	93.00	2004
55.95	5011	70.00	18976	80.90	270	93.90	147
56.95	25376	71.00	21253	81.95	1313	94.95	160
57.95	1150	72.00	1394	82.95	6565	96.00	181

Scan 2124 (39.919 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.00	825	112.05	7088	126.90	86	148.90	134025
98.00	149	113.05	10772	128.95	36	149.90	14589
99.00	53	114.05	907	130.85	21	150.90	1651
102.85	68	114.95	73	131.80	2247	152.00	149
103.95	5399	115.75	63	132.90	353	153.00	68
104.95	1960	117.90	74	133.95	123	158.80	67
105.95	237	119.75	100	134.95	86	159.95	82
106.95	70	120.90	1556	137.05	84	160.80	126
107.95	92	121.90	2031	137.95	60	161.95	641
109.95	153	122.90	603	144.90	116	162.95	438
110.95	267	123.95	61	146.90	371	163.80	103

Scan 2124 (39.919 min): A0929.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
164.95	94	185.05	74	260.90	273		
166.95	43172	190.90	33	261.80	161		
167.90	3939	191.95	86	266.95	60		
168.75	504	192.45	51	278.90	11017		
170.75	52	206.95	90	280.85	334		
171.00	53	212.80	43	282.15	93		
175.75	60	221.05	201	354.70	95		
176.90	40	235.70	64	354.90	94		
178.00	53	238.80	62	356.25	60		
179.00	193	239.95	32	389.75	63		
180.00	189	252.75	36	390.25	48		

CTMP Compounds

Scan 2124 (39.919 min): A0929.D

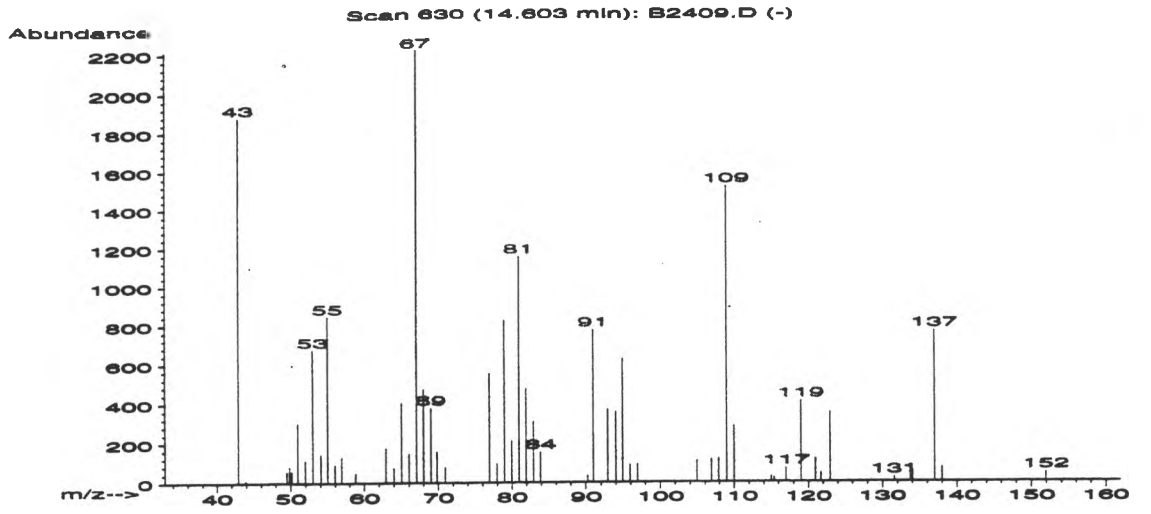
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	90
2.	1,2-Benzenedicarboxylic acid, 3-nitro-	211	C8H5NO6	87
3.	1,2-Benzenedicarboxylic acid, mono(2-eth	278	C16H22O4	72
4.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	58
5.	1,2-Benzenedicarboxylic acid, dioctyl es	390	C24H38O4	56
6.	1,2-Benzenedicarboxylic acid, diisooctyl	390	C24H38O4	52
7.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	52
8.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	52
9.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	52
10.	1,2-Benzenedicarboxylic acid, dioctyl es	390	C24H38O4	52
11.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	50
12.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	50
13.	1,2-Benzenedicarboxylic acid, diheptyl e	362	C22H34O4	50
14.	1,2-Benzenedicarboxylic acid, decyl hexy	390	C24H38O4	50
15.	1,2-Benzenedicarboxylic acid, butyl decy	362	C22H34O4	47
16.	1,2-Benzenedicarboxylic acid, bis(4-meth	334	C20H30O4	47
17.	(1S*,2R*,5R*,7S*)-2,4-Dimethyl-7-ethyl-6	168	C10H16O2	46
18.	1,2-Benzenedicarboxylic acid, dipentyl e	306	C18H26O4	42
19.	1,2-Benzenedicarboxylic acid, bis(2-ethy	390	C24H38O4	40
20.	1,2-Benzenedicarboxylic acid, diisooctyl	390	C24H38O4	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	90	000117-81-7	135870	83	43	2	66	3	57	0	47	9877
2.	87	000603-11-2	39769	98	9	0	68	9	54	0	56	9804
3.	72	004376-20-9	66373	75	46	3	85	12	42	15	39	9755
4.	58	000117-81-7	135876	95	40	0	59	31	32	0	51	9914
5.	56	000117-84-0	135861	53	84	3	70	12	30	17	37	9598
6.	52	027554-26-3	96185	115	26	0	55	31	27	12	50	9693
7.	52	000117-81-7	135873	85	31	1	48	31	27	0	47	9789
8.	52	000117-81-7	135874	80	67	3	52	34	27	0	43	9705
9.	52	000117-81-7	135866	115	26	0	55	31	27	12	50	9693
10.	52	000117-84-0	96182	83	40	1	39	31	27	0	47	9596
11.	50	000131-18-0	133653	45	56	2	91	34	25	12	41	9276
12.	50	000117-81-7	135868	63	55	1	40	34	25	0	38	9759
13.	50	003648-21-3	90783	61	53	1	91	31	25	0	43	9317
14.	50	025724-58-7	96181	44	80	3	94	34	25	0	39	9321
15.	47	000089-19-0	90781	44	74	2	91	37	20	0	39	9217
16.	47	000146-50-9	84073	58	64	1	68	37	20	0	39	9288
17.	*46	091926-28-2	20483	37	33	0	45	43	20	4	43	9848
18.	42	000131-18-0	133652	44	71	1	74	26	17	0	37	9418
19.	40	000117-81-7	135871	64	47	2	48	34	16	0	36	9831
20.	38	027554-26-3	135878	55	49	1	48	37	14	1	37	9847

CTMP Compounds

Peak 13



Scan 630 (14.603 min): B2409.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1879	56.90	131	76.95	552	94.00	357
43.90	11	58.75	48	77.95	96	94.95	628
49.45	56	62.90	176	78.95	827	95.95	88
49.80	83	64.00	75	79.95	211	96.95	93
50.10	58	65.00	402	80.95	1158	104.95	109
50.95	302	66.00	147	81.90	476	106.90	116
51.95	115	67.00	2213	82.90	310	107.90	122
52.95	675	68.00	470	83.90	155	109.00	1522
54.05	144	69.00	376	90.25	34	110.00	285
54.95	845	69.80	157	91.00	775	115.00	27
55.95	91	70.95	75	92.90	369	115.40	21

Scan 630 (14.603 min): B2409.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.00	70						
119.00	409						
120.95	117						
121.70	46						
122.95	353						
131.55	22						
133.75	56						
134.00	55						
137.00	770						
138.00	70						
151.95	46						

CTMP Compounds

Scan 630 (14.603 min): B2409.D

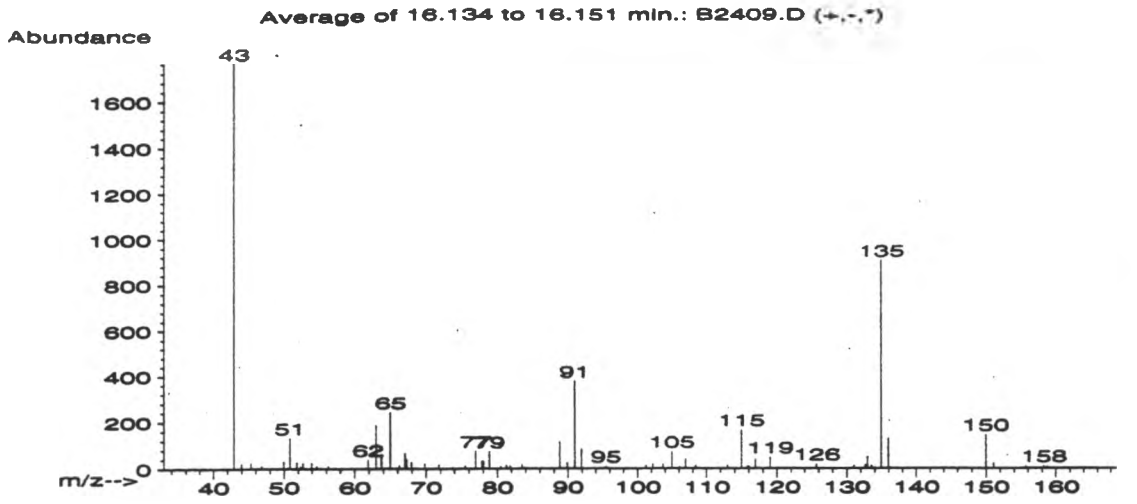
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(1,4-dimethyl-3-cyclohexen-1	152	C10H16O	59
2.	Cyclopropane, hexyl(1-methylethylidene)-	166	C12H22	53
3.	Cyclohexane, decylidene-	222	C16H30	50
4.	1,E-8,Z-10-HEXADECATRIENE	220	C16H28	47
5.	cis-1-(hexahydro-3a(1H)-pentalenyl)ethan	152	C10H16O	47
6.	5,7-Dodecadiene, (Z,Z)-	166	C12H22	47
7.	Cyclooctene, 3-(2-propenyl)-	150	C11H18	47
8.	1-(1,3-BUTADIENE-2-YL)-CYCLOPENTANOL	138	C9H14O	38
9.	3-Hexadecyne	222	C16H30	38
10.	6,6-Dimethyl-2,3-diazabicyclo[3.1.0]hex-	110	C6H10N2	38
11.	3-Octyne	110	C8H14	38
12.	4-Octyne	110	C8H14	35
13.	Bicyclo[2.2.1]heptane-2-carboxaldehyde,	138	C9H14O	35
14.	2-Methylene-6-methyl-5,7-octadien-3-ol	152	C10H16O	27
15.	Cyclopentene, 1-methyl-	82	C6H10	27
16.	CYCLOPROPENE, 3,3-DIETHYL-	96	C7H12	27
17.	1,5,7-Octatrien-3-ol, 2,6-dimethyl-	152	C10H16O	25
18.	.delta.-Fenchane	138	C10H18	22
19.	Cyclopentane, 1,2-dichloro-, trans-	138	C5H8Cl2	22
20.	4-Octyne	110	C8H14	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	043219-68-7	123977	44	58	1	94	25	33	18	38	9060
2.	53	056701-46-3	19736	43	74	2	77	30	28	18	38	8920
3.	50	062338-40-3	45109	59	72	1	77	33	25	0	39	9166
4.	47	080625-33-8	44094	62	82	3	82	39	20	0	39	8305
5.	*47	065682-11-3	13736	40	34	0	87	39	20	7	40	9085
6.	47	006108-62-9	19717	44	63	2	81	36	20	10	38	8352
7.	47	061141-59-1	12927	47	42	1	97	36	20	8	41	8988
8.	*38	000000-00-0	8613	54	65	0	38	54	14	0	49	8501
9.	38	061886-62-2	45098	45	71	1	38	48	14	7	38	8947
10.	*38	068914-93-2	2146	56	54	1	99	47	14	0	40	7637
11.	*38	015232-76-5	118878	45	51	1	74	46	14	14	38	6975
12.	*35	001942-45-6	118883	48	53	0	68	51	11	13	41	7531
13.	*35	015780-36-6	8658	35	63	1	68	52	11	0	39	8826
14.	*27	000000-00-0	13595	49	82	2	61	60	8	0	39	8825
15.	*27	000693-89-0	116781	34	48	0	99	56	8	0	41	7554
16.	27	000000-00-0	629	45	47	1	99	59	8	9	38	7458
17.	*25	029414-56-0	13592	49	83	3	57	65	7	0	46	8574
18.	*22	006248-88-0	8823	59	48	0	50	61	5	24	41	6871
19.	*22	014376-81-9	8391	34	53	0	99	65	5	0	41	7387
20.	*14	001942-45-6	2219	45	57	0	65	69	2	12	40	7273

CTMP Compounds

Peak 14; 4-(1-Methylethyl)-benzenemethanol



Average of 16.134 to 16.151 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1764	56.30	12	71.80	19	83.90	6
43.95	22	57.30	5	73.70	7	85.40	4
45.30	25	61.90	38	75.50	15	88.85	115
46.80	11	63.00	188	76.95	76	89.90	24
49.95	31	63.75	60	77.80	32	90.95	379
50.80	132	65.00	243	78.05	33	91.90	83
51.85	28	66.20	14	78.85	73	95.45	10
52.40	10	67.00	67	80.45	12	101.20	14
52.70	26	67.25	40	81.30	16	102.20	20
53.95	25	67.90	28	81.80	11	103.70	18
54.70	11	69.80	21	83.50	18	104.95	74

Average of 16.134 to 16.151 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.05	8	132.65	16				
106.95	39	132.95	50				
108.40	13	133.50	11				
113.00	14	134.95	901				
114.95	166	135.95	130				
115.75	10	149.95	145				
116.00	10	151.05	22				
116.90	40	155.70	9				
119.05	48	158.25	10				
125.70	19	158.75	7				
131.05	13						

CTMP Compounds

Average of 16.134 to 16.151 min.: B2409.D
Converted from RTE data file: >B2409:

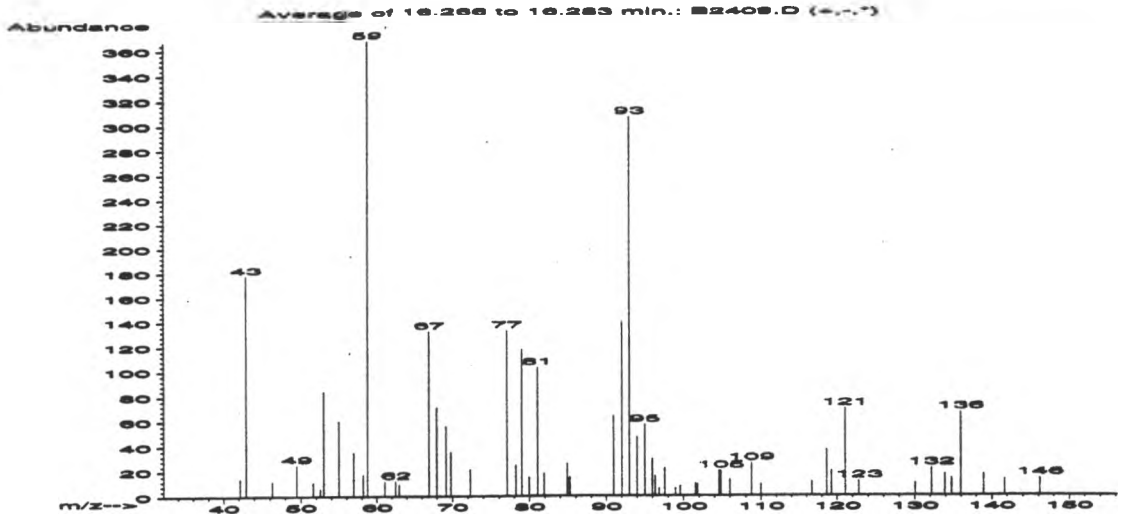
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenemethanol, 4-(1-methylethyl)-	150	C10H14O	58
2.	Methyl 1-(p-tolyl)ethyl ether	150	C10H14O	53
3.	Benzaldehyde, 4-methyl-, oxime, (Z)-	135	C8H9NO	50
4.	N-(1,3-Butadiynyl)morpholine	135	C8H9NO	43
5.	Benzenemethanol, .alpha.,.alpha.,4-trime	150	C10H14O	42
6.	Benzenemethanol, .alpha.,.alpha.,4-trime	150	C10H14O	42
7.	PROPYLIDENMALONONITRILE, 2-METHOXY-2-MET	150	C8H10N2O	38
8.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	37
9.	Silane, trichloromethyl-	148	CH3Cl3Si	37
10.	4-Picolinium, 1-acetamido-, hydroxide, i	150	C8H10N2O	32
11.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	32
12.	Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	32
13.	Silane, trimethylphenyl-	150	C9H14Si	27
14.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	27
15.	Silane, trimethylphenyl-	150	C9H14Si	25
16.	2-D3-METHYL-2H-CYCLOPENTA(D)PYRIDAZINE	132	C8H5D3N2	25
17.	Benzene, 1-cyclopropyl-2-nitro-	163	C9H9NO2	25
18.	2,1-Benzisoxazol-3(1H)-one	135	C7H5NO2	23
19.	ACETOPHENONE, 2'-METHOXY-	150	C9H10O2	17
20.	Benzothiazole	135	C7H5NS	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	000536-60-7	12736	46	36	0	84	26	32	0	44	9881
2.	*53	021573-35-3	12760	33	20	0	41	28	28	0	41	4542
3.	*50	003717-16-6	7569	36	68	2	34	34	25	0	39	4113
4.	*43	080487-52-1	7545	35	55	2	41	43	18	0	39	4721
5.	42	001197-01-9	123699	48	42	3	98	28	17	1	36	9833
6.	42	001197-01-9	123698	44	45	2	80	26	17	2	33	9784
7.	*38	000000-00-0	12537	33	70	2	51	47	14	0	39	4620
8.	*37	015816-45-2	7331	28	50	1	49	44	13	1	30	4527
9.	*37	000075-79-6	11736	29	80	0	51	41	13	0	33	3650
10.	*32	007584-29-4	12544	33	50	1	34	50	9	0	30	4656
11.	*32	000089-83-8	123683	34	45	2	37	50	9	0	35	4659
12.	32	004565-32-6	7830	38	48	0	38	50	9	0	33	3727
13.	*27	000768-32-1	123658	55	22	0	50	56	8	4	39	4541
14.	*27	000098-54-4	123676	34	43	1	35	56	8	0	39	4538
15.	*25	000768-32-1	12691	31	29	0	40	54	7	0	33	5057
16.	*25	024340-85-0	6967	39	41	2	37	45	7	0	29	4622
17.	25	010292-65-6	18028	44	57	1	16	54	7	0	37	4512
18.	*23	031499-90-8	7524	32	51	2	35	50	6	0	27	4590
19.	*17	000000-00-0	12617	31	34	0	36	54	3	5	25	4556
20.	*17	000095-16-9	7530	28	55	1	41	52	3	0	29	4577

CTMP Compounds

Peak 15; Terpinol



Average of 16.266 to 16.283 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.15	14	61.05	12	79.95	15	96.35	16
42.95	178	62.50	12	81.05	103	96.85	6
46.30	12	63.00	9	81.90	18	97.55	22
49.45	25	66.95	132	84.90	26	98.95	6
51.60	11	67.95	71	85.25	15	99.55	8
52.55	6	69.15	56	90.95	64	101.55	10
53.00	84	69.80	35	92.05	140	101.80	9
54.95	60	72.30	21	93.00	306	104.55	20
56.90	35	77.05	133	94.00	47	104.80	20
58.15	17	78.20	25	95.00	57	105.95	13
58.75	367	79.00	118	95.95	30	108.75	26

Average of 16.266 to 16.283 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	9	138.90	17				
116.65	11	141.65	13				
118.65	37	146.20	14				
119.25	20						
121.05	70						
122.80	12						
130.05	10						
132.15	22						
133.90	17						
134.75	14						
135.95	67						

CTMP Compounds

Average of 16.266 to 16.283 min.: B2409.D
Converted from RTE data file: >B2409:

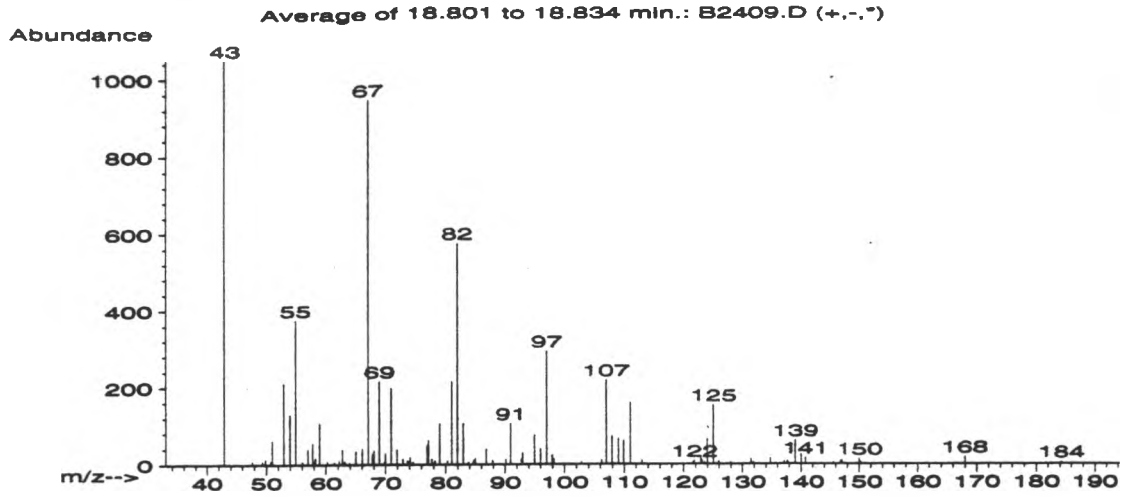
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	l-.alpha.-Terpineol	154	C10H18O	59
2.	l-Phellandrene	136	C10H16	43
3.	.ALPHA.-PINENE, (-)-	136	C10H16	41
4.	l-Phellandrene	136	C10H16	38
5.	(-)-TRANS-2-CARENE	136	C10H16	38
6.	THUJENE	136	C10H16	38
7.	Bicyclo[3.1.0]hexane, 4-methyl-1-(1-meth	136	C10H16	38
8.	Cyclohexene, 1-methyl-5-(1-methylethenyl	136	C10H16	38
9.	l-Phellandrene	136	C10H16	38
10.	Tricyclene	136	C10H16	38
11.	(-)-CIS-2-CARENE	136	C10H16	38
12.	l-Phellandrene	136	C10H16	35
13.	l-Phellandrene	136	C10H16	35
14.	.DELTA.3-Carene	136	C10H16	35
15.	.DELTA.3-Carene	136	C10H16	35
16.	Camphene	136	C10H16	30
17.	l-Phellandrene	136	C10H16	30
18.	Camphene	136	C10H16	30
19.	.beta.-Thujene	136	C10H16	30
20.	Camphene	136	C10H16	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	010482-56-1	124255	58	64	2	90	24	33	0	39	9326
2.	*43	000099-83-2	121994	46	49	0	59	50	18	0	44	6783
3.	*41	000080-56-8	122070	63	39	1	66	54	16	25	53	6609
4.	*38	000099-83-2	121996	44	25	1	83	47	14	0	40	6654
5.	*38	005208-50-4	8169	48	51	0	70	53	14	0	46	6693
6.	38	002867-05-2	8156	46	44	1	83	49	14	2	41	6606
7.	38	058037-87-9	8157	46	44	1	83	49	14	2	41	6606
8.	*38	001461-27-4	8106	48	66	2	77	48	14	0	39	6766
9.	*38	000099-83-2	121991	36	56	2	80	53	14	4	43	6640
10.	*38	000508-32-7	122098	58	41	1	78	57	14	20	55	6581
11.	*38	005208-49-1	122085	50	48	0	78	50	14	8	41	6690
12.	*35	000099-83-2	8088	39	51	1	83	53	11	0	39	6646
13.	*35	000099-83-2	121989	34	54	1	83	54	11	1	40	6603
14.	*35	013466-78-9	122090	35	66	2	83	54	11	11	40	6600
15.	*35	013466-78-9	122095	52	49	1	83	53	11	1	40	6634
16.	*30	000079-92-5	122049	64	50	1	60	56	9	24	45	6530
17.	*30	000099-83-2	121992	36	58	0	60	59	9	8	43	6555
18.	*30	000079-92-5	122050	49	66	2	69	56	9	0	46	6517
19.	*30	028634-89-1	8155	58	43	1	66	60	9	18	47	6326
20.	27	000079-92-5	122051	56	55	1	63	57	8	4	39	6540

CTMP Compounds

Peak 16; Unidentified hydrocarbon



Average of 18.801 to 18.834 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1050	57.80	56	67.00	944	74.60	6
47.70	8	58.25	17	67.75	27	76.90	49
49.30	8	58.95	107	68.00	36	77.15	62
49.80	13	60.20	7	68.95	216	77.75	14
50.70	9	61.40	6	69.80	8	78.20	9
50.95	62	62.15	10	70.00	28	79.00	106
52.95	210	62.70	38	70.95	198	80.30	9
53.95	130	63.15	8	71.95	38	81.00	215
54.90	375	63.90	5	72.95	15	81.95	574
56.05	7	64.95	35	73.70	11	82.90	106
56.95	41	66.05	42	74.15	18	83.80	6

Average of 18.801 to 18.834 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
84.65	11	97.95	23	121.80	8	137.15	7
84.95	16	98.20	14	122.85	18	137.70	8
86.80	39	102.80	7	123.10	11	139.00	61
87.90	10	106.20	11	123.50	5	140.00	25
90.15	13	106.95	218	123.95	64	140.75	16
90.95	106	107.95	73	125.00	153	145.55	4
92.75	13	109.00	66	125.95	9	146.80	8
93.00	30	109.85	61	127.95	5	147.05	8
95.00	76	111.00	160	131.45	12	150.05	13
96.00	40	113.00	10	131.90	5	150.30	4
97.00	294	121.55	6	134.75	15	168.00	18

Average of 18.801 to 18.834 min.: B2409.D
Converted from RTE data file: >B2409:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
184.25	5						

CTMP Compounds

Average of 18.801 to 18.834 min.: B2409.D
Converted from RTE data file: >B2409:

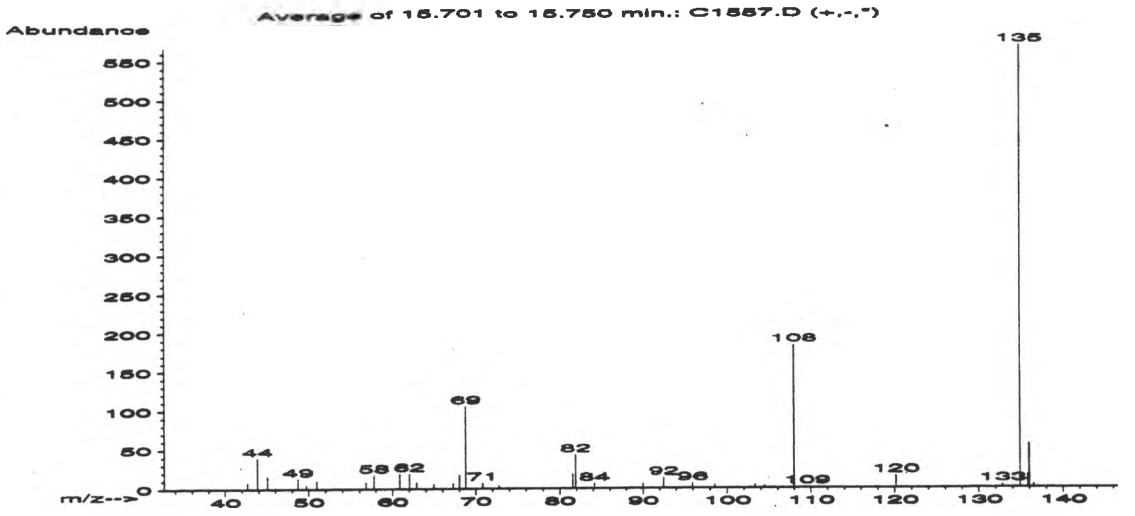
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-Octyne, 7-methyl-	124	C9H16	52
2.	3-Hexyne	82	C6H10	47
3.	Cyclopentene, 1-methyl-	82	C6H10	47
4.	3-Octyne, 2-methyl-	124	C9H16	47
5.	Cyclopentane, methylene-	82	C6H10	46
6.	Cyclopropene, 1-butyl-2-ethyl-	124	C9H16	46
7.	Cyclopentene, 1-(2-methylbutyl)-	138	C10H18	43
8.	Cyclopropane, (1-methylethenyl)-	82	C6H10	43
9.	Cyclopentene, 3-methyl-	82	C6H10	43
10.	(1R*,6S*,7R*)-Bicyclo[4.2.0]octan-7-ol	126	C8H14O	43
11.	1,4-Hexadiene	82	C6H10	43
12.	Cyclopropane, 1-methyl-2-(1-methylethyl)	138	C10H18	40
13.	4-Nonyne	124	C9H16	38
14.	Cyclohexene	82	C6H10	38
15.	6,6-DIMETHYL-SPIRO[2.3]HEXAN-4-ONE	124	C8H12O	38
16.	1,6-Octadiene, 2,7-dimethyl-	138	C10H18	35
17.	3-Hexyne	82	C6H10	27
18.	1,3,7-Octatriene	108	C8H12	22
19.	2-Cyclohexen-1-one, 4,4-dimethyl-	124	C8H12O	12
20.	8-Azabicyclo[3.2.1]octan-3-one, 8-methyl	139	C8H13NO	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*52	037050-06-9	4876	52	46	2	89	34	27	0	44	9197
2.	*47	000928-49-4	116764	46	53	2	70	36	20	0	40	9220
3.	*47	000693-89-0	116782	37	25	0	73	40	20	0	41	9245
4.	*47	055402-15-8	120437	44	50	2	76	38	20	10	38	9279
5.	*46	001528-30-9	116784	43	33	0	81	44	20	14	47	8891
6.	*46	050915-91-8	4898	54	44	2	89	43	20	0	49	9074
7.	43	053366-53-3	8763	46	40	2	66	45	18	10	38	9107
8.	*43	004663-22-3	116778	41	33	1	88	43	18	13	38	8788
9.	*43	001120-62-3	116783	32	40	1	85	44	18	9	42	8736
10.	*43	027655-77-2	5393	33	26	2	79	45	18	0	39	9106
11.	*43	000592-45-0	116766	51	33	1	84	43	18	14	39	9179
12.	40	024524-52-5	8760	43	67	3	89	32	16	0	37	9245
13.	*38	020184-91-2	4865	44	53	2	64	50	14	0	39	8432
14.	*38	000110-83-8	116789	37	62	2	66	36	14	0	35	9197
15.	*38	000000-00-0	4817	35	65	2	72	38	14	13	35	8741
16.	*35	040195-09-3	8728	40	57	3	130	54	11	0	39	8284
17.	*27	000928-49-4	116762	33	52	1	58	59	8	11	40	9008
18.	*22	001002-35-3	118750	35	43	2	80	62	5	5	40	7871
19.	12	001073-13-8	120411	47	67	2	51	61	2	0	35	7664
20.	*11	000532-24-1	8950	34	43	0	43	76	2	14	43	5072

CTMP Compounds

Peak 17; Benzothiazole



Average of 15.701 to 15.750 min.: C1557.D
Converted from RTE data file: >C1557:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.65	8	64.95	6	95.95	6	136.50	4
43.85	39	67.25	7	98.55	4		
45.05	16	68.00	17	103.30	4		
48.70	13	68.80	105	104.45	3		
49.70	5	70.80	7	107.95	183		
50.95	10	72.75	4	109.50	1		
56.80	9	81.55	18	120.15	15		
57.75	17	81.90	43	132.80	4		
60.90	19	84.15	6	134.90	567		
62.05	19	90.00	6	135.80	16		
62.90	8	92.50	13	135.95	56		

CTMP Compounds

Average of 15.701 to 15.750 min.: C1557.D
Converted from RTE data file: >C1557:

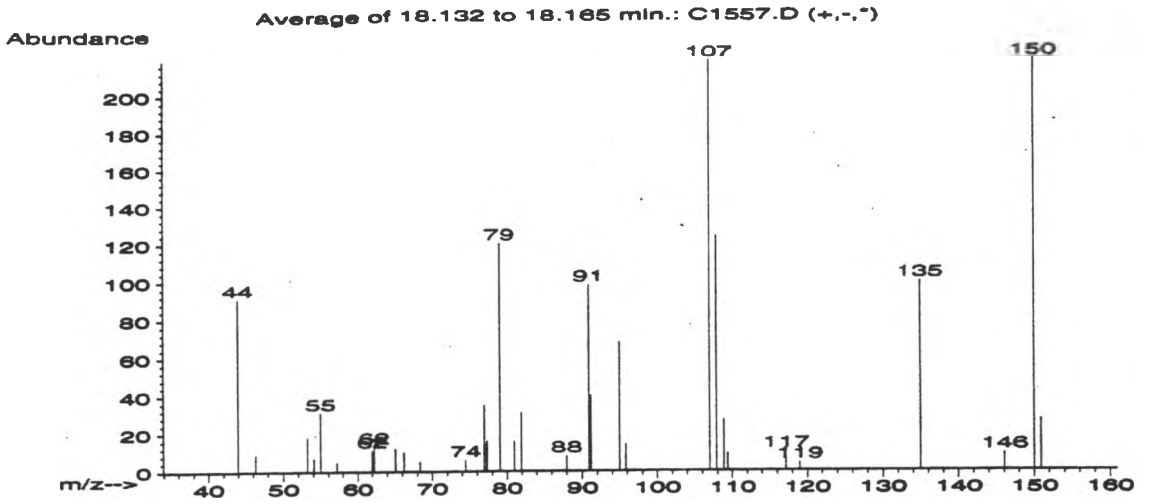
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzisothiazole	135	C7H5NS	80
2.	Thiocyanic acid, phenyl ester	135	C7H5NS	72
3.	1,2-Benzisothiazole	135	C7H5NS	72
4.	Benzothiazole	135	C7H5NS	72
5.	Benzothiazole	135	C7H5NS	72
6.	4-0-MERCAPTOBENZONITRILE	135	C7H5NS	64
7.	1,2-Benzisothiazole-3-carboxylic acid	179	C8H5NO2S	56
8.	Thieno[3,2-c]pyridine	135	C7H5NS	56
9.	Benzothiazole	135	C7H5NS	50
10.	Adenine	135	C5H5N5	50
11.	Adenine	135	C5H5N5	50
12.	Adenine	135	C5H5N5	50
13.	Adenine	135	C5H5N5	50
14.	2(3H)-Benzothiazolethione	167	C7H5NS2	43
15.	Adenine	135	C5H5N5	39
16.	Adenine	135	C5H5N5	39
17.	Adenine	135	C5H5N5	39
18.	Thieno[2,3-c]pyridine	135	C7H5NS	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000272-16-2	121700	35	55	2	99	11	48	4	43	9958
2.	*72	005285-87-0	7525	36	65	2	99	14	42	0	41	9833
3.	*72	000272-16-2	7531	33	58	2	95	11	42	0	41	9933
4.	*72	000095-16-9	121696	41	47	3	99	11	42	0	39	9972
5.	*72	000095-16-9	121694	40	48	2	78	11	42	0	39	9977
6.	*64	034761-11-0	7527	35	69	1	86	16	37	0	39	9609
7.	56	040991-34-2	25013	41	59	2	99	11	30	0	33	9958
8.	*56	000272-14-0	7534	30	62	2	99	11	30	1	30	9842
9.	*50	000095-16-9	121695	30	32	2	68	16	25	0	33	9818
10.	*50	000073-24-5	121690	28	48	2	99	16	25	6	35	9785
11.	*50	000073-24-5	121688	29	44	1	88	16	25	2	35	9831
12.	*50	000073-24-5	121687	29	66	1	73	16	25	0	33	9781
13.	*50	000073-24-5	121686	28	50	1	99	16	25	2	35	9782
14.	43	000149-30-4	125646	36	42	1	75	9	18	0	25	9972
15.	*39	000073-24-5	121689	28	63	1	99	16	15	0	29	9824
16.	*39	000073-24-5	121685	29	73	1	84	16	15	0	29	9834
17.	*39	000073-24-5	7506	28	65	1	89	16	15	0	29	9827
18.	*38	000272-12-8	7533	32	56	2	79	22	14	0	29	9763

CTMP Compounds

Peak 18



Average of 18.132 to 18.165 min.: C1557.D
Converted from RTE data file: >C1557:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	91	74.45	6	107.00	218		
46.30	9	76.95	35	107.90	124		
53.20	18	77.30	16	108.90	27		
54.05	7	79.00	120	109.40	9		
54.95	31	81.00	16	117.15	10		
57.20	5	81.95	31	119.00	4		
62.00	11	88.00	8	134.95	100		
62.25	13	90.90	98	146.05	9		
65.10	12	91.15	40	150.00	219		
66.20	10	95.00	68	150.90	27		
68.35	5	95.80	14				

CTMP Compounds

Average of 18.132 to 18.165 min.: C1557.D
Converted from RTE data file: >C1557:

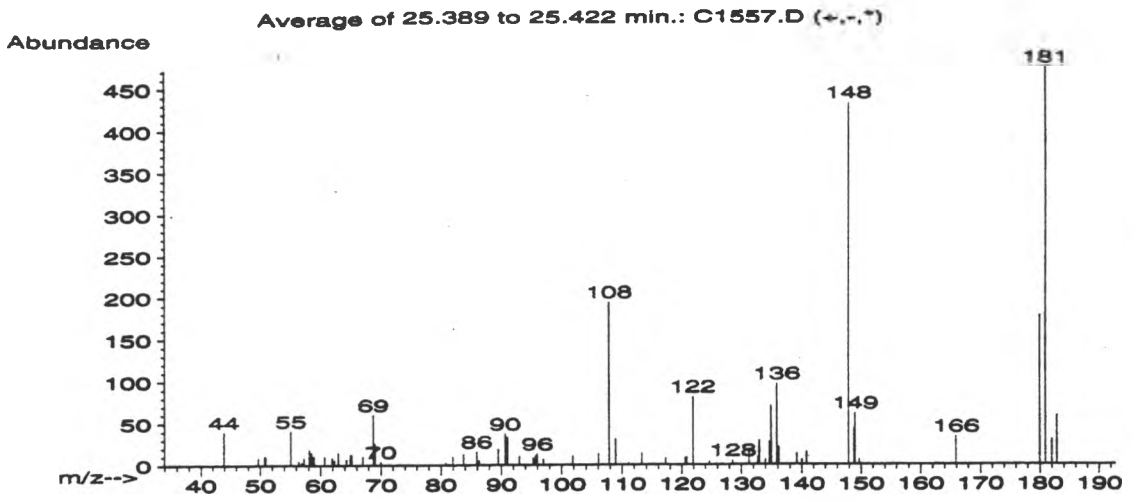
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	(+)-.alpha.-methylene-.alpha.-fenchocamp	150	C10H14O	72
2.	(+)-6-OXOCAMPHENE	150	C10H14O	64
3.	[3.3.3]Propellane	150	C11H18	58
4.	5-Isopropenyl-2,3-dimethyl-2-cyclopenten	150	C10H14O	58
5.	(+)-Car-2-en-4-one	150	C10H14O	52
6.	1,7-exo-Trimethylenebicyclo[3.2.1]octane	150	C11H18	52
7.	exo-2-Methyl-4-homobrendane	150	C11H18	50
8.	2,4-Cycloheptadien-1-one, 2,6,6-trimethy	150	C10H14O	50
9.	2,4-Cycloheptadien-1-one, 2,6,6-trimethy	150	C10H14O	50
10.	5-Isopropyliden-2,3-dimethyl-2-cyclopent	150	C10H14O	47
11.	ALLYLHYDROQUINONE	150	C9H10O2	38
12.	3-ACETAMIDOMETHYLPYRIDINE	150	C8H10N2O	38
13.	Tricyclo[4.3.1.1(3,8)]undecane	150	C11H18	38
14.	2-Cyclohexen-1-one, 3-methyl-6-(1-methyl	150	C10H14O	38
15.	2,5-Cyclohexadien-1-one, 4-ethyl-3,4-dim	150	C10H14O	37
16.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	35
17.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	35
18.	4-Homoisotwistane	150	C11H18	27
19.	2-Cyclopenten-1-one, 2-(2-pentenyl)-, (Z	150	C10H14O	25
20.	2-Cyclopenten-1-one, 2-(2-pentenyl)-, (Z	150	C10H14O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	074033-53-7	12840	46	43	1	76	15	42	1	40	9335
2.	*64	055659-42-2	12838	36	37	0	99	19	37	0	41	8252
3.	*58	051027-89-5	123745	52	65	0	91	27	32	15	44	8851
4.	*58	089950-37-8	12705	53	51	1	99	30	32	0	49	9000
5.	*52	000000-00-0	12815	33	53	0	70	34	27	10	43	9076
6.	*52	055954-92-2	12952	56	78	1	91	32	27	0	47	9462
7.	*50	066140-53-2	12969	48	61	0	86	35	25	16	41	7670
8.	*50	000503-93-5	123729	43	41	0	99	35	25	13	38	8658
9.	*50	000503-93-5	12794	46	65	0	99	31	25	9	38	8794
10.	*47	042507-33-5	12707	43	34	1	99	36	20	0	39	8849
11.	*38	005721-21-1	12620	33	44	0	77	46	14	0	41	8022
12.	*38	022977-34-0	12547	35	49	0	82	47	14	0	41	8355
13.	*38	000281-46-9	12961	33	86	0	80	52	14	2	43	8683
14.	*38	000491-09-8	123726	44	64	1	99	37	14	0	35	9247
15.	*37	017429-35-5	12775	34	85	2	99	45	13	6	35	8106
16.	*35	000080-57-9	12854	33	96	3	144	55	11	0	39	9026
17.	*35	000585-34-2	12726	35	61	3	213	51	11	0	39	5908
18.	*27	043000-53-9	12962	33	83	2	97	60	8	0	41	7733
19.	*25	041031-88-3	123660	35	63	1	98	52	7	0	35	7554
20.	*25	041031-88-3	12703	35	63	1	98	52	7	0	35	7554

CTMP Compounds

Peak 19; 2-(Methylthio)-benzothiazole



Average of 25.389 to 25.422 min.: C1557.D
Converted from RTE data file: >C1557:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	40	60.65	11	80.80	3	95.95	13
49.70	9	61.90	9	81.95	10	96.95	7
50.70	11	62.25	6	83.75	13	101.80	11
50.95	10	62.90	15	85.90	16	106.05	13
55.05	41	64.25	7	86.25	5	107.85	193
56.35	5	64.90	13	89.50	19	108.90	31
56.85	3	65.15	12	90.60	37	111.00	2
57.20	9	67.00	10	91.00	33	113.25	14
58.15	19	68.75	60	93.00	10	117.25	8
58.50	15	69.00	26	95.30	8	120.55	8
58.90	11	69.95	4	95.70	11	120.80	9

Average of 25.389 to 25.422 min.: C1557.D
Converted from RTE data file: >C1557:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.85	81	139.15	13	182.80	58		
124.70	4	140.00	6				
128.55	5	140.75	15				
131.30	16	147.90	429				
132.70	9	148.80	43				
132.95	29	149.00	61				
134.00	6	149.70	6				
134.65	27	165.90	33				
134.90	70	179.95	176				
135.85	96	180.90	472				
136.15	21	181.95	30				

CTMP Compounds

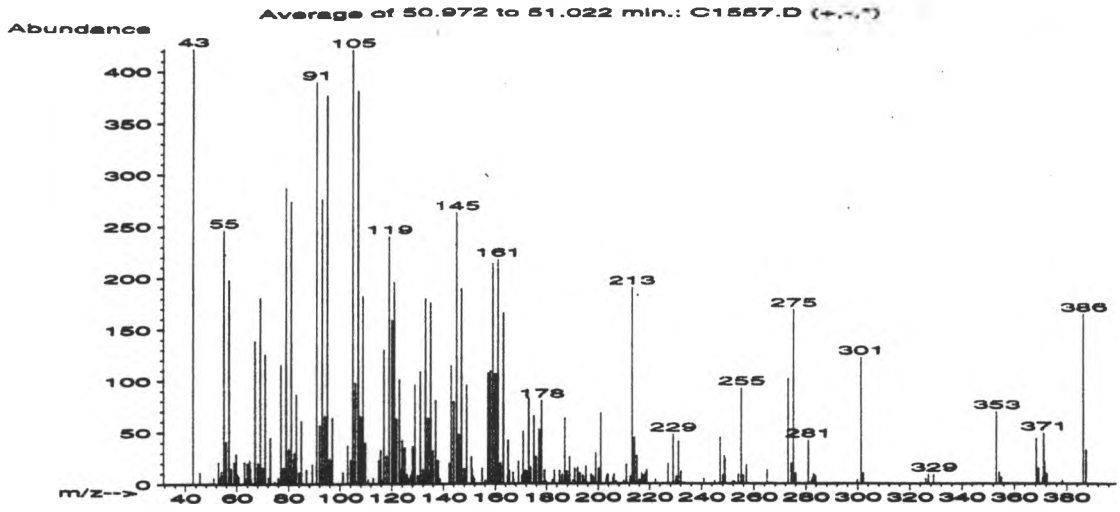
Average of 25.389 to 25.422 min.: C1557.D
Converted from RTE data file: >C1557:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	91
2.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	91
3.	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	91
4.	2(3H)-Benzothiazolethione, 3-methyl-	181	C8H7NS2	38
5.	Benzene, 1-ethoxy-2-methyl-	136	C9H12O	11
6.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	10
7.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	10
8.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	10
9.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	10
10.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	10
11.	[1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-di	148	C7H8N4	9
12.	Benzene, 1-ethoxy-4-methyl-	136	C9H12O	9
13.	Benzene, 1-ethoxy-2-methyl-	136	C9H12O	9
14.	2(3H)-Benzoxazolimine, 3-methyl-	148	C8H8N2O	8
15.	9H-Carbazole, 9-methyl-	181	C13H11N	7
16.	9H-Carbazole, 2-methyl-	181	C13H11N	7
17.	9H-Carbazole, 2-methyl-	181	C13H11N	7
18.	VANADIUM, BIS(CYCLOPENTADIENYL)-	181	C10H10V	7
19.	2-METHYL-5,6,7,8-TETRAHYDROCHINOXALIN	148	C9H12N2	7
20.	3-Ethenyl-4-methylcyclohex-2-en-1-one	136	C9H12O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000615-22-5	126909	74	57	2	93	4	60	10	50	9818
2.	*91	000615-22-5	126908	68	56	3	99	4	60	3	50	9886
3.	*91	000615-22-5	25993	68	60	2	88	4	60	14	53	9735
4.	*38	002254-94-6	25992	38	92	2	87	39	14	0	35	9276
5.	*11	000614-71-1	7955	47	45	0	40	80	2	0	44	3124
6.	*10	000622-60-6	121942	33	48	0	40	80	1	0	41	3122
7.	*10	000622-60-6	121939	38	56	0	40	80	1	0	39	3123
8.	*10	000622-60-6	7957	36	54	0	40	80	1	0	41	3103
9.	*10	000621-32-9	121938	34	45	0	40	80	1	0	41	3119
10.	*10	000621-32-9	121937	42	48	0	40	80	1	0	39	3121
11.	* 9	007681-99-4	11885	28	61	2	62	72	1	0	33	6059
12.	* 9	000622-60-6	121941	32	50	0	40	80	1	0	33	3130
13.	* 9	000614-71-1	121936	32	55	0	40	80	1	0	33	3124
14.	* 8	018034-93-0	11927	31	89	1	66	67	1	0	23	6102
15.	* 7	001484-12-4	26189	28	85	2	72	72	1	0	23	6934
16.	* 7	003652-91-3	126936	31	79	1	71	73	1	0	26	6728
17.	* 7	003652-91-3	126934	31	79	1	71	73	1	0	26	6728
18.	* 7	001277-47-0	126915	30	71	1	93	72	1	0	27	6572
19.	* 7	038917-65-6	11990	28	76	1	67	72	1	0	29	6067
20.	* 7	000000-00-0	7967	28	72	2	28	80	1	0	29	3088

Peak 20; Sterol - PBM + (3.beta.)-Cholest-5-en-ol



Average of 50.972 to 51.022 min.: C1557.D
Converted from RTE data file: >C1557:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	422	58.95	21	66.95	139	78.05	16
45.70	11	59.75	29	68.00	20	78.95	287
51.05	6	60.15	9	69.00	181	79.90	34
52.90	21	60.75	7	69.95	16	80.95	274
53.20	5	62.90	21	70.95	126	81.95	24
53.70	7	63.40	5	72.20	6	82.20	30
54.00	12	64.00	20	72.90	45	82.95	87
54.95	246	64.70	4	74.80	2	84.00	11
55.90	41	64.95	23	75.95	6	84.95	61
56.95	198	65.15	15	77.00	116	86.95	14
57.90	15	65.40	4	77.70	15	89.15	19

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
90.95	389	105.95	98	117.95	27	126.80	5
92.05	57	107.00	380	119.00	240	127.25	8
93.00	276	107.90	65	120.05	159	127.80	12
93.95	66	108.95	182	120.95	196	128.00	36
95.00	376	109.95	40	121.80	63	128.95	96
95.95	24	111.05	4	123.00	101	130.00	8
96.95	64	113.05	6	123.55	13	131.00	109
101.05	11	114.95	23	124.00	42	131.95	14
102.90	37	115.75	33	125.00	35	133.00	180
104.00	23	116.00	5	125.95	9	133.75	16
104.95	420	117.00	130	126.30	2	134.00	64

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.95	176	146.95	190	158.00	110	167.15	4
135.90	32	147.95	15	159.00	214	169.00	22
137.00	81	148.20	13	160.00	107	170.40	8
138.00	23	148.95	96	160.95	218	170.95	51
138.60	5	150.80	26	161.75	8	171.80	13
142.25	20	151.05	15	162.00	20	172.20	12
143.00	115	151.45	7	163.05	166	173.00	83
144.00	80	151.90	5	164.65	7	173.80	16
145.00	263	154.85	15	164.95	42	175.00	66
145.90	48	156.15	3	165.40	13	175.90	26
146.25	28	157.05	108	166.90	11	177.00	53

CTMP Compounds

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
178.00	81	188.95	26	197.55	5	209.95	3
178.95	2	190.10	3	197.95	7	210.90	19
179.20	13	190.55	3	199.00	30	212.40	7
179.80	2	190.95	15	200.05	15	213.10	191
182.20	4	192.00	16	201.00	69	213.95	45
182.95	13	192.65	10	203.05	4	215.05	27
185.00	13	193.00	10	203.30	8	215.95	4
186.00	9	194.10	8	203.70	9	216.90	10
187.05	64	195.00	4	205.70	6	217.50	8
187.90	12	195.25	17	206.05	9	217.90	5
188.25	7	197.20	9	206.95	2	218.40	10
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
218.90	13	247.05	45	265.00	13	299.70	4
222.20	4	248.05	8	273.00	102	301.20	123
227.00	20	248.30	8	274.20	20	302.05	10
229.05	48	248.70	27	275.10	169	326.05	5
230.05	3	248.95	24	276.05	10	327.10	9
230.30	7	251.85	2	280.90	42	329.20	9
231.15	41	252.50	2	281.90	2	353.20	70
232.10	12	253.95	9	282.30	5	354.20	11
233.15	1	255.15	93	282.80	9	355.05	6
240.90	5	255.95	8	283.30	7	368.25	44
245.00	3	257.15	18	283.55	7	369.15	15
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
370.75	6						
371.20	49						
371.40	21						
371.90	10						
372.25	9						
378.20	3						
386.35	165						
387.40	33						

CTMP Compounds

Average of 50.972 to 51.022 min.: C1557.D
Converted from RTE data file: >C1557:

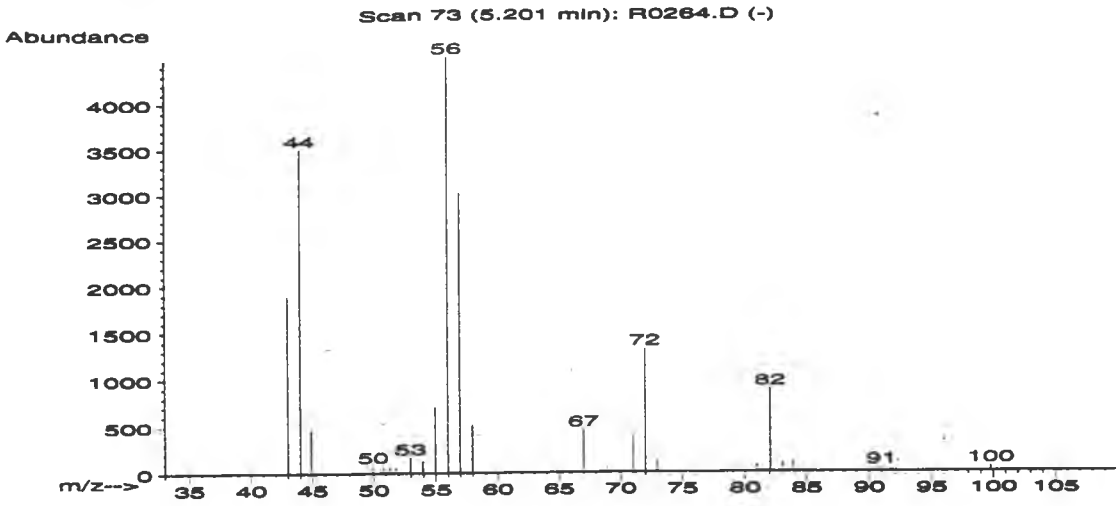
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	83
2.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	70
3.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	60
4.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	30
5.	Cholest-5-en-3-ol (3.beta.)-	386	C27H46O	30
6.	Cholestane, 4,5-epoxy-, (4.alpha.,5.alph	386	C27H46O	25
7.	(4R,6R,7R,9S)-4,7-Epoxy-5(11)-megastigme	210	C13H22O2	12
8.	CHLORODIMETHYLVINYL-SILANE	120	C4H9ClSi	11
9.	Cholesta-3,5-diene	368	C27H44	11
10.	3.ALPHA.,5-CYCLO-6.BETA.-METHOXYPREGNANE	330	C22H34O2	10
11.	(-)-Nerolidol	222	C15H26O	10
12.	Nerolidol	222	C15H26O	10
13.	.delta.-Guaiene	204	C15H24	10
14.	1H-Pyrrolo[2,1-c][1,4]oxazin-1-one, 3,4-	213	C13H11NO2	10
15.	N-(P-TOLYL)-ACRYLIC ACID AMIDE	161	C10H11NO	10
16.	VULGAROL A	220	C15H24O	10
17.	Borinic acid, diethyl-, 1-ethynylcyclohe	192	C12H21BO	10
18.	Ethanone, 2-(2-methylpropoxy)-1,2-diphen	268	C18H20O2	9
19.	Cholest-5-en-3.beta.-yl A-homo-4-oxachol	771	C54H90O2	9
20.	Junipene	204	C15H24	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000057-88-5	135788	106	124	3	87	15	50	0	52	9574
2.	*70	000057-88-5	135793	99	134	2	61	45	41	0	84	9489
3.	*60	000057-88-5	135791	121	99	3	87	36	35	37	66	8830
4.	*30	000057-88-5	135794	83	119	3	87	59	9	16	45	7671
5.	*30	000057-88-5	95482	50	158	2	87	56	9	0	46	9786
6.	*25	006079-19-2	95492	65	118	3	153	63	7	0	44	7482
7.	12	072505-41-0	39575	58	90	2	71	63	2	0	36	7381
8.	*11	000000-00-0	4047	48	54	2	253	79	2	0	44	5900
9.	*11	000747-90-0	135429	69	135	2	64	72	2	12	47	8789
10.	10	032249-55-1	83054	51	71	1	99	66	1	14	36	4704
11.	*10	017430-12-5	44949	33	63	3	223	72	1	0	39	5989
12.	*10	007212-44-4	129867	34	63	3	223	72	1	0	39	5989
13.	10	003691-11-0	128700	43	115	2	90	70	1	1	35	7265
14.	*10	035566-71-3	40840	58	69	2	90	72	1	9	40	5615
15.	*10	000000-00-0	17242	38	54	0	66	72	1	0	39	6040
16.	10	011056-03-4	44015	57	103	1	67	79	1	1	38	5573
17.	10	055848-34-5	30957	58	56	0	90	79	1	6	39	5634
18.	9	022499-12-3	62896	43	82	2	82	72	1	0	37	5722
19.	9	077551-24-7	114951	58	131	1	59	76	1	9	35	8165
20.	9	000475-20-7	128709	65	86	3	118	72	1	0	36	7557

CTMP Compounds

Peak 21; Hexanal



Scan 73 (5.201 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1893	56.95	3014	91.00	38		
44.00	3503	57.95	506	98.85	4		
44.90	461	67.00	453	99.80	51		
49.95	77	68.90	56				
50.80	67	71.00	380				
51.30	59	72.00	1319				
51.80	58	72.95	117				
52.95	164	80.95	76				
53.95	127	82.05	881				
54.95	709	83.05	93				
55.95	4482	83.90	110				

CTMP Compounds

Scan 73 (5.201 min): R0264.D

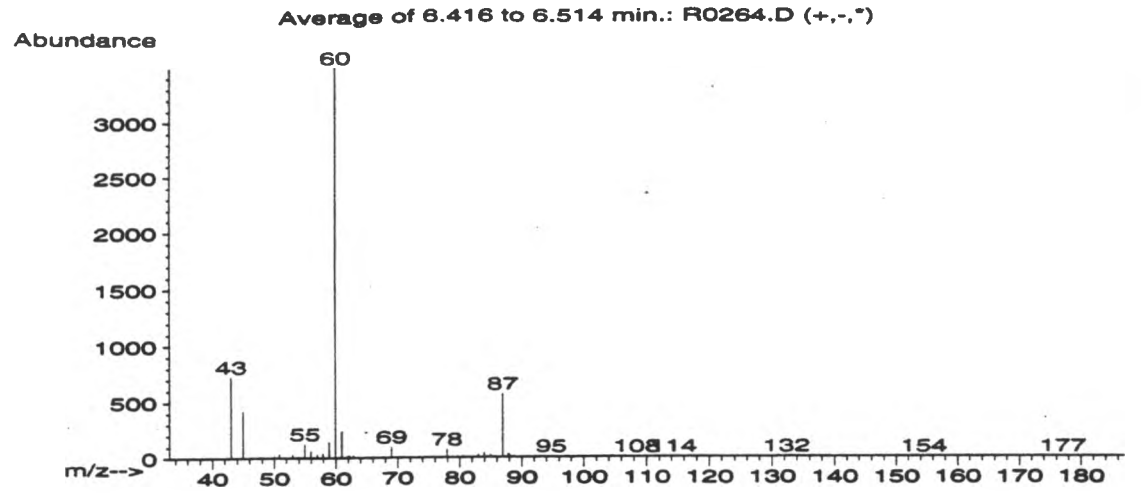
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Hexanal	100	C6H12O	50
2.	Hexanal	100	C6H12O	49
3.	Hexanal	100	C6H12O	49
4.	Hexanal	100	C6H12O	47
5.	Hexanal	100	C6H12O	42
6.	Ethene, ethoxy-	72	C4H8O	38
7.	Hexanal	100	C6H12O	37
8.	Urea, 2-propenyl-	100	C4H8N2O	36
9.	Ethene, ethoxy-	72	C4H8O	35
10.	Hexanal	100	C6H12O	25
11.	Propanamide, 2-methyl-	87	C4H9NO	12
12.	2-Propen-1-ol, 2-methyl-	72	C4H8O	10
13.	2-Hexen-1-ol, (E)-	100	C6H12O	9
14.	1-Hexen-3-ol	100	C6H12O	9
15.	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	000066-25-1	117976	44	50	0	56	35	25	20	40	9279
2.	*49	000066-25-1	117974	49	57	2	103	37	23	0	44	9816
3.	*49	000066-25-1	117973	52	50	2	105	37	23	0	46	9642
4.	47	000066-25-1	117978	42	57	1	64	38	20	7	39	9826
5.	*42	000066-25-1	117979	35	57	1	73	29	17	13	37	8789
6.	*38	000109-92-2	116429	34	36	0	58	54	14	2	43	5699
7.	37	000066-25-1	117977	43	51	1	65	42	13	0	37	9660
8.	*36	000557-11-9	1047	29	77	1	73	29	12	0	27	9561
9.	*35	000109-92-2	116428	35	53	0	52	54	11	0	41	5668
10.	25	000066-25-1	117975	33	71	3	121	42	7	0	22	9480
11.	12	000563-83-7	117138	33	62	0	70	57	2	0	25	5630
12.	*10	000513-42-8	116425	33	62	1	51	79	1	0	39	5563
13.	* 9	000928-95-0	118036	28	63	1	60	73	1	0	33	6758
14.	* 9	004798-44-1	118060	35	47	1	168	78	1	0	35	5108
15.	8	025144-05-2	1177	41	56	2	51	69	1	0	27	7565

CTMP Compounds

Peak 22; 3-Methylbutanoic Acid



Average of 6.416 to 6.514 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	723	57.00	29	69.00	96	82.95	23
44.95	419	57.95	39	69.75	5	83.95	40
47.80	4	58.95	143	70.50	8	84.95	21
49.95	17	59.90	3490	71.00	6	86.95	566
50.85	35	60.95	238	75.90	6	87.90	30
53.00	30	61.90	15	76.95	6	88.15	12
53.55	5	62.15	15	77.90	72	88.40	2
53.80	6	62.85	18	78.95	4	88.75	8
54.00	11	64.75	2	79.70	5	91.90	2
54.95	125	67.00	3	80.20	3	92.65	5
55.95	65	67.75	9	80.65	14	94.75	6

Average of 6.416 to 6.514 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.05	3						
104.45	3						
104.95	2						
108.45	3						
114.25	3						
131.05	3						
132.30	4						
154.45	2						
177.05	2						

CTMP Compounds

Average of 6.416 to 6.514 min.: R0264.D
Converted from RTE data file: >R0264:

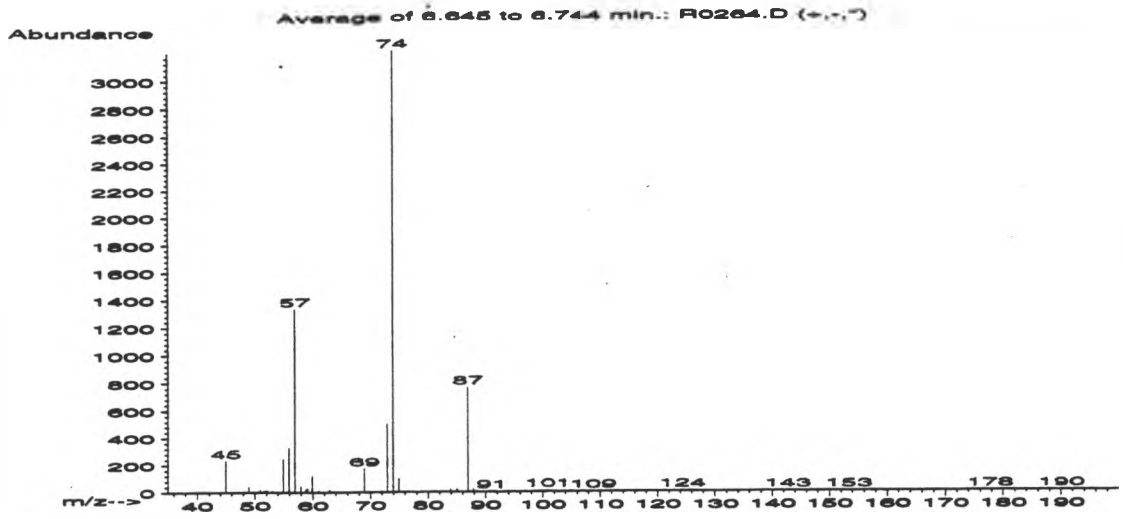
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid, 3-methyl-	102	C5H10O2	64
2.	Hexanoic acid	116	C6H12O2	39

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	000503-74-2	118199	40	39	1	96	8	37	10	31	9977
2.	39	000142-62-1	119466	33	51	3	68	16	15	0	25	9940

CTMP Compounds

Peak 23; 2-Methylbutanoic Acid



Average of 6.645 to 6.744 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	233	57.95	42	67.90	5	78.95	2
48.95	42	58.80	19	68.95	173	80.70	3
50.90	18	59.05	29	69.90	2	81.20	4
51.45	5	59.90	118	70.50	2	81.45	3
51.80	11	61.10	12	71.00	5	81.95	3
52.05	7	62.90	18	71.90	7	83.20	2
52.25	7	63.50	5	72.95	502	83.90	22
52.95	10	64.15	4	73.95	3199	85.00	23
54.95	242	65.65	2	74.95	99	86.95	763
55.95	325	66.90	1	76.70	6	87.90	21
56.95	1331	67.25	4	77.95	1	88.75	1

Average of 6.645 to 6.744 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
90.65	6	187.80	2				
91.05	6	190.00	3				
99.80	5						
100.90	11						
107.05	3						
108.80	3						
111.65	2						
124.30	7						
142.65	3						
153.30	3						
177.70	3						

CTMP Compounds

Average of 6.645 to 6.744 min.: R0264.D
Converted from RTE data file: >R0264:

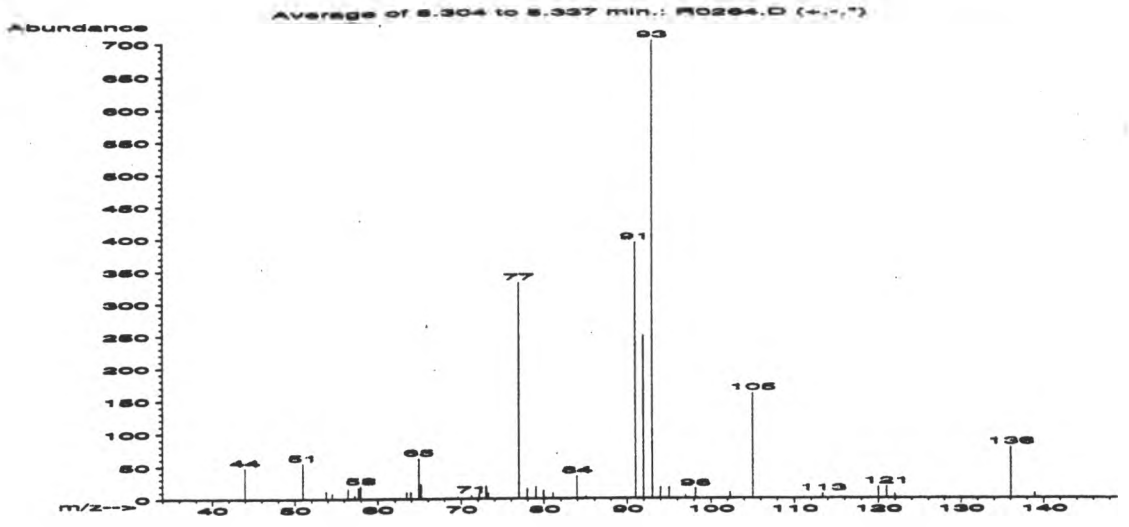
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid, 2-methyl-	102	C5H10O2	78
2.	Butanoic acid, 2-methyl-	102	C5H10O2	43
3.	Hexanoic acid, 2-methyl-	130	C7H14O2	39
4.	Pentanoic acid, methyl ester	116	C6H12O2	39
5.	Pentanoic acid, methyl ester	116	C6H12O2	39

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	78	000116-53-0	1355	57	24	1	84	8	46	13	41	9827
2.	43	000116-53-0	118198	46	32	1	78	10	18	1	23	9611
3.	39	004536-23-6	121067	39	44	1	66	16	15	0	29	9619
4.	39	000624-24-8	119478	34	67	0	85	18	15	0	25	9556
5.	39	000624-24-8	119475	33	62	1	76	18	15	0	22	9670

CTMP Compounds

Peak 24; Monoterpene



Average of 8.304 to 8.337 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	48	65.15	22	83.90	35	113.40	7
50.95	54	69.60	3	84.95	3	120.00	17
53.80	12	71.25	5	91.00	394	121.00	18
54.55	8	72.15	9	91.95	250	122.00	6
56.45	15	73.00	19	93.00	701	136.05	78
57.25	5	73.20	8	94.00	17	138.90	7
57.70	17	77.00	332	95.00	17		
57.95	19	77.95	15	97.00	5		
63.40	10	79.00	18	98.15	15		
63.90	10	79.95	12	102.30	9		
64.90	62	81.05	8	105.05	160		

CTMP Compounds

Average of 8.304 to 8.337 min.: R0264.D
Converted from RTE data file: >R0264:

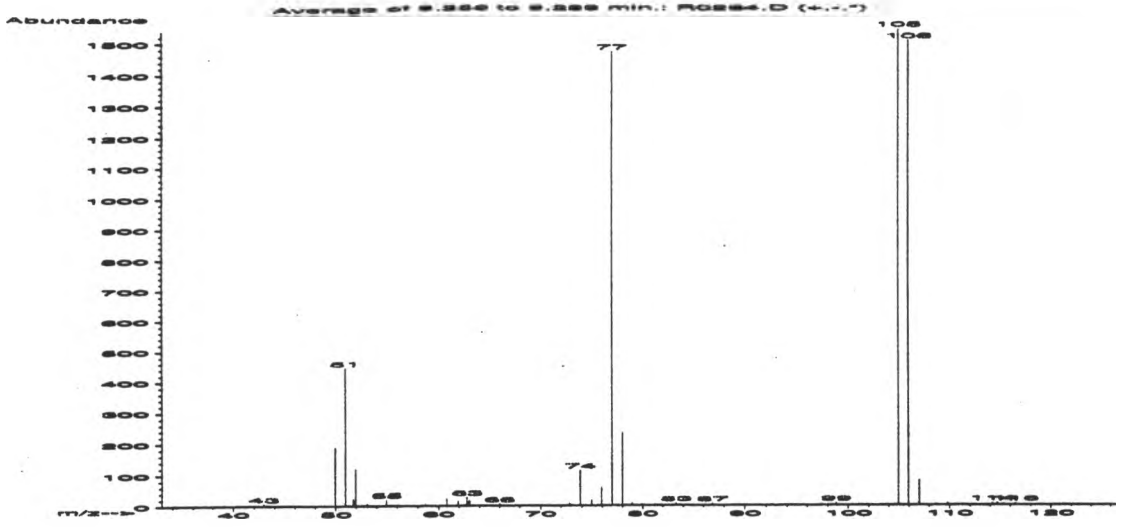
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	72
2.	Bicyclo[3.1.0]hexane, 4-methyl-1-(1-meth	136	C10H16	64
3.	.alpha.-Thujene	136	C10H16	64
4.	.alpha.-Thujene	136	C10H16	64
5.	.alpha.-Thujene	136	C10H16	64
6.	THUJENE	136	C10H16	64
7.	1-Phellandrene	136	C10H16	58
8.	1-Phellandrene	136	C10H16	52
9.	Methylester of 1-Methyl-2,5-cyclohexadie	152	C9H12O2	50
10.	.alpha.-Thujene	136	C10H16	42
11.	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-me	136	C10H16	39
12.	1,3,7-OCTATRIENE, 3,7-DIMETHYL-	136	C10H16	39
13.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	39
14.	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	38
15.	1,4,6-HEPTATRIENE, 3,3,6-TRIMETHYL-	136	C10H16	38
16.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	33
17.	.gamma.-Terpinene	136	C10H16	32
18.	6-(2,3-Butadienyl)-1,4-cycloheptadiene	146	C11H14	23
19.	Tricyclo[3.2.1.0(2,4)]octane, 8-methylen	120	C9H12	22
20.	1,3,5-Cycloheptatriene	92	C7H8	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	003779-61-1	121952	47	70	1	99	11	42	0	39	9852
2.	*64	058037-87-9	8157	35	58	2	88	18	37	0	39	9737
3.	*64	002867-05-2	122057	43	26	2	99	16	37	0	40	9815
4.	*64	002867-05-2	122055	46	42	3	91	16	37	7	40	9653
5.	*64	002867-05-2	122054	33	59	2	99	20	37	11	40	9700
6.	*64	002867-05-2	8156	35	58	2	88	18	37	0	39	9737
7.	*58	000099-83-2	121989	34	53	3	99	29	32	10	43	9628
8.	*52	000099-83-2	121998	35	58	2	65	35	27	23	43	9615
9.	50	059034-54-7	123931	42	3	0	97	20	25	6	35	9766
10.	*42	002867-05-2	8154	34	57	1	74	30	17	2	37	9789
11.	*39	005794-03-6	8150	29	87	2	99	20	15	0	29	9348
12.	*39	000502-99-8	8064	28	85	2	99	16	15	0	29	8774
13.	39	003779-61-1	121953	38	76	2	99	16	15	0	28	9858
14.	*38	029548-02-5	8069	31	84	1	77	23	14	0	26	7966
15.	*38	000000-00-0	8072	31	84	1	77	23	14	0	26	7966
16.	*33	003779-61-1	121950	29	77	2	82	34	10	0	29	8611
17.	*32	000099-85-4	122004	34	67	2	115	50	9	8	37	9631
18.	23	090542-16-8	11507	34	57	0	45	50	6	0	25	8024
19.	*22	038310-48-4	4172	35	51	1	53	64	5	0	39	6347
20.	* 9	000544-25-2	117440	28	57	1	56	80	1	0	33	5064

CTMP Compounds

Peak 1; Benzaldehyde



Average of 9.256 to 9.289 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	7	63.00	16	86.90	6		
49.95	188	66.00	5	98.80	8		
50.95	444	72.80	8	104.95	1539		
51.70	23	73.85	113	105.95	1502		
51.95	118	74.95	18	107.00	81		
53.10	6	75.95	58	109.80	6		
54.95	20	76.95	1465	114.25	7		
58.75	4	78.00	234	114.75	6		
60.75	24	78.95	8	116.50	6		
61.90	16	83.30	8				
62.75	27	85.85	2				

CTMP Compounds

Average of 9.256 to 9.289 min.: R0264.D
Converted from RTE data file: >R0264:

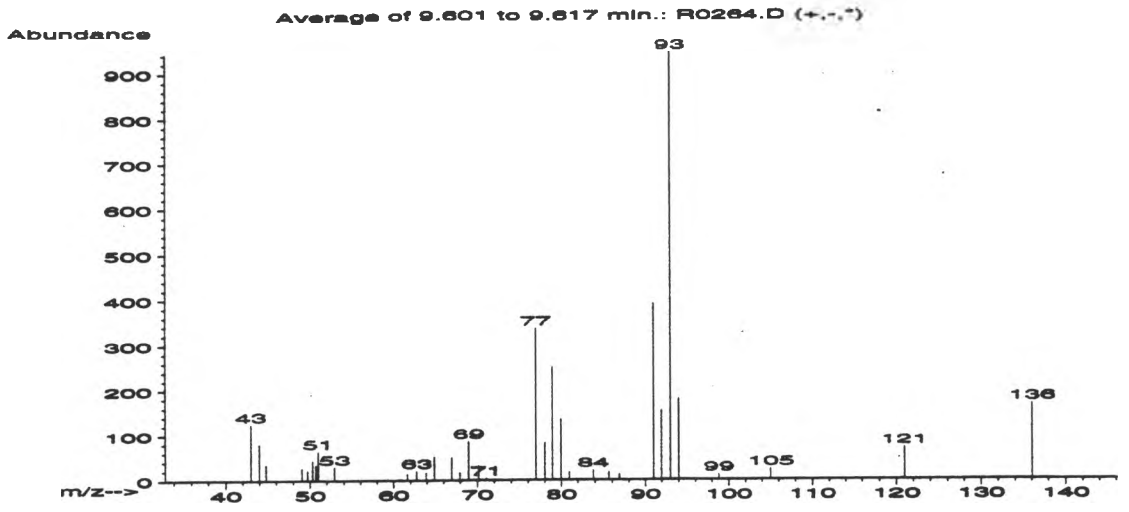
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde	106	C7H6O	91
2.	Benzaldehyde	106	C7H6O	90
3.	Benzaldehyde	106	C7H6O	86
4.	Benzaldehyde	106	C7H6O	72
5.	Benzaldehyde	106	C7H6O	72
6.	Benzaldehyde	106	C7H6O	56
7.	Benzaldehyde	106	C7H6O	56
8.	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	47
9.	1,2-Propanedione, 1-phenyl-	148	C9H8O2	38
10.	PHENYL-GLYOXYLIC ACID	150	C8H6O3	38
11.	Benzaldehyde	106	C7H6O	32
12.	Benzenamine, N-methyl-	107	C7H9N	28
13.	Benzenemethanamine	107	C7H9N	28
14.	2,6-Piperazinedione, 4-benzoyl-, 2-oxime	233	C11H11N3O3	28
15.	1H,6H-PYRROLO(2,3-B)PYRROLE	106	C6H6N2	25
16.	Pyrazine, ethenyl-	106	C6H6N2	23
17.	2,4-Heptadien-6-ynal, (E,E)-	106	C7H6O	12
18.	Pyridine, 2-ethenyl-	105	C7H7N	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000100-52-7	1777	68	29	2	86	3	60	23	58	9965
2.	*90	000100-52-7	118545	63	34	1	68	5	57	22	47	9745
3.	*86	000100-52-7	118550	47	15	0	67	9	53	0	44	9961
4.	*72	000100-52-7	118549	48	31	0	82	14	42	6	41	9940
5.	*72	000100-52-7	118546	56	46	2	74	13	42	0	40	9909
6.	*56	000100-52-7	118552	39	61	3	99	13	30	8	36	9824
7.	*56	000100-52-7	118553	34	69	3	97	15	30	0	35	9814
8.	47	000582-24-1	7806	46	38	2	97	36	20	19	41	8347
9.	38	000579-07-7	11943	41	37	1	99	39	14	2	35	8465
10.	38	000000-00-0	12531	40	41	1	99	39	14	2	35	8514
11.	32	000100-52-7	118551	42	44	2	37	50	9	0	33	9729
12.	28	000100-61-8	118639	37	70	0	86	38	8	0	25	6305
13.	28	000100-46-9	118647	37	73	0	77	38	8	0	25	6335
14.	28	035975-25-8	49406	33	64	0	94	38	8	0	25	8629
15.	*25	058326-34-4	1771	30	47	2	87	42	7	0	29	6836
16.	*23	004177-16-6	118544	28	76	2	97	46	6	0	29	6286
17.	12	007200-04-6	1773	40	48	1	76	64	2	0	33	7642
18.	* 8	000100-69-6	1700	32	67	1	73	69	1	0	27	6905

CTMP Compounds

Peak 25; monoterpene (.beta.-Thujene ??



Average of 9.601 to 9.617 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	125	63.90	16	80.95	17	136.05	168
43.95	80	64.90	52	83.80	21		
44.75	34	66.95	50	85.65	17		
49.05	26	67.95	16	86.90	12		
49.70	21	69.00	86	91.00	391		
50.30	44	70.15	31	91.95	154		
50.70	33	71.05	3	93.00	943		
50.95	64	76.95	337	94.00	179		
52.90	29	78.00	82	98.80	11		
61.65	13	78.95	252	105.05	23		
62.75	20	79.95	135	120.95	71		

CTMP Compounds

Average of 9.601 to 9.617 min.: R0264.D
Converted from RTE data file: >R0264:

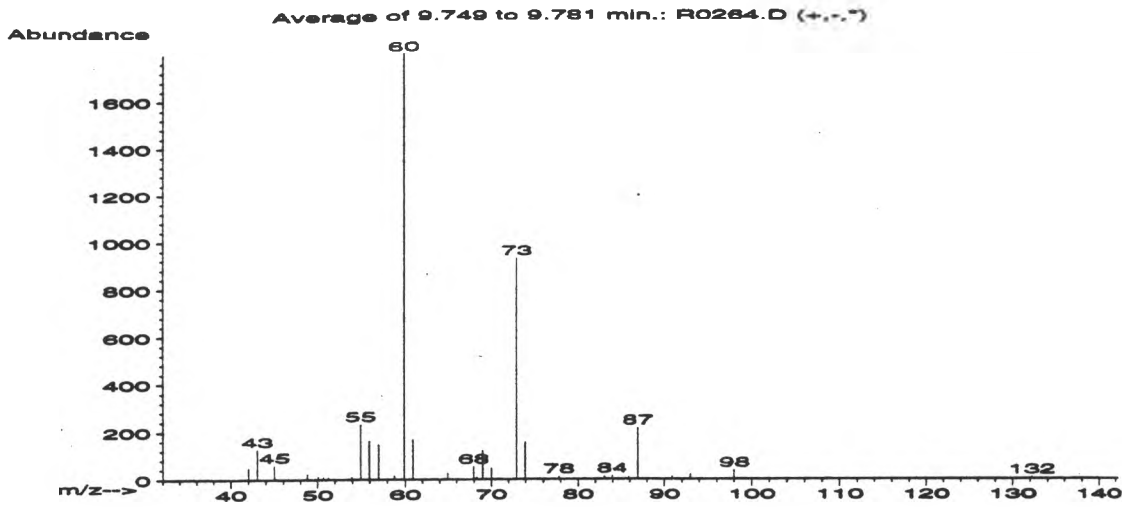
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.beta.-Thujene	136	C10H16	91
2.	Sabinene	136	C10H16	90
3.	.beta.-Phellandrene	136	C10H16	86
4.	.beta.-Phellandrene	136	C10H16	80
5.	Sabinene	136	C10H16	80
6.	.beta.-Terpinene	136	C10H16	78
7.	.beta.-Phellandrene	136	C10H16	78
8.	2-.BETA.-PINENE	136	C10H16	72
9.	Camphene	136	C10H16	64
10.	Camphene	136	C10H16	64
11.	1-Phellandrene	136	C10H16	59
12.	Camphene	136	C10H16	59
13.	Camphene	136	C10H16	59
14.	1-Phellandrene	136	C10H16	58
15.	1-Phellandrene	136	C10H16	58
16.	1-Phellandrene	136	C10H16	53
17.	1-Phellandrene	136	C10H16	53
18.	.beta.-Phellandrene	136	C10H16	53
19.	.beta.-Phellandrene	136	C10H16	46
20.	Sabinene	136	C10H16	45

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	028634-89-1	8155	69	26	2	99	2	62	6	70	9810
2.	*90	003387-41-5	122064	69	28	1	99	8	59	0	76	9882
3.	*86	000555-10-2	122040	57	23	0	81	8	53	0	49	9927
4.	*80	000555-10-2	122038	54	38	0	99	13	48	0	49	9809
5.	*80	003387-41-5	122060	55	46	1	99	13	48	0	47	9363
6.	*78	000099-84-3	8117	48	45	1	82	10	46	2	41	9840
7.	*78	000555-10-2	122039	45	61	1	80	10	46	0	39	9335
8.	*72	000127-91-3	8163	44	67	3	99	13	42	0	40	8858
9.	*64	000079-92-5	122052	46	68	2	70	18	37	0	39	8133
10.	*64	000079-92-5	122050	46	69	2	70	18	37	0	40	8107
11.	*59	000099-83-2	121989	49	39	1	99	24	33	4	39	9687
12.	*59	000079-92-5	122051	47	67	2	99	24	33	0	40	8496
13.	*59	000079-92-5	122046	47	73	2	99	24	33	0	40	8115
14.	*58	000099-83-2	121995	43	45	0	74	28	32	0	44	9619
15.	*58	000099-83-2	121993	44	50	0	81	28	32	0	44	9546
16.	*53	000099-83-2	8088	34	55	1	99	27	28	1	40	9681
17.	*53	000099-83-2	121996	35	31	1	87	29	28	1	40	9617
18.	*53	000555-10-2	122041	34	57	1	74	27	28	0	41	9366
19.	*46	000555-10-2	8118	55	39	1	119	43	20	0	47	9836
20.	*45	003387-41-5	122063	66	32	2	127	48	19	0	58	9831

CTMP Compounds

Peak 26; Hexanoic Acid



Average of 9.749 to 9.781 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	47	58.10	2	77.80	10		
43.00	126	58.80	15	83.05	11		
45.00	59	59.90	1798	83.95	13		
48.80	22	60.90	169	85.85	9		
50.05	12	64.95	26	86.95	216		
50.65	9	67.95	53	90.90	11		
51.20	8	68.30	7	93.00	20		
53.95	10	69.00	120	98.00	36		
54.95	231	70.00	46	132.20	6		
55.95	162	72.95	930				
57.00	145	73.95	156				

CTMP Compounds

Average of 9.749 to 9.781 min.: R0264.D
Converted from RTE data file: >R0264:

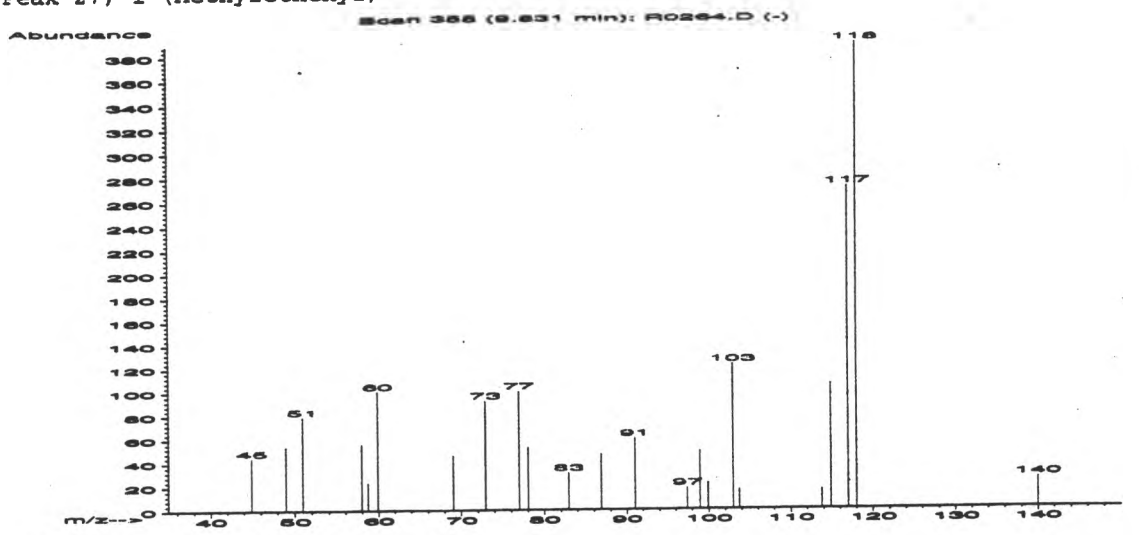
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Hexanoic acid	116	C6H12O2	83
2.	Hexanoic acid	116	C6H12O2	74
3.	Hexanoic acid	116	C6H12O2	74
4.	Hexanoic acid	116	C6H12O2	64
5.	Hexanoic acid	116	C6H12O2	43
6.	Octanoic acid, silver(1+) salt	251	C8H16AgO2	40
7.	Octanoic acid	144	C8H16O2	39
8.	Octanoic acid	144	C8H16O2	38
9.	Octanoic acid	144	C8H16O2	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	83	000142-62-1	3409	43	54	2	72	-1	50	0	39	9971
2.	74	000142-62-1	119466	56	24	1	91	3	44	1	37	9955
3.	74	000142-62-1	119463	53	35	1	72	3	44	16	34	9951
4.	64	000142-62-1	119461	40	43	2	81	10	37	2	31	9938
5.	43	000142-62-1	119462	48	34	2	83	7	18	7	28	9958
6.	40	024927-67-1	56736	37	82	2	67	14	16	1	22	9180
7.	39	000124-07-2	122867	37	68	1	76	17	15	0	20	9881
8.	38	000124-07-2	122871	34	51	0	48	25	14	0	25	9907
9.	28	000124-07-2	122868	36	59	1	52	37	8	0	21	9891

CTMP Compounds

Peak 27; 1-(Methylethenyl)-benzene ??



Scan 355 (9.831 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.90	44	86.90	47	140.00	25		
48.95	54	91.00	60				
50.95	79	97.40	18				
57.95	56	98.95	49				
58.70	23	99.95	22				
59.90	100	102.95	122				
69.05	46	103.70	16				
72.95	92	113.75	16				
76.95	100	114.90	105				
78.05	53	117.00	270				
82.95	31	118.00	389				

CTMP Compounds

Scan 355 (9.831 min): R0264.D

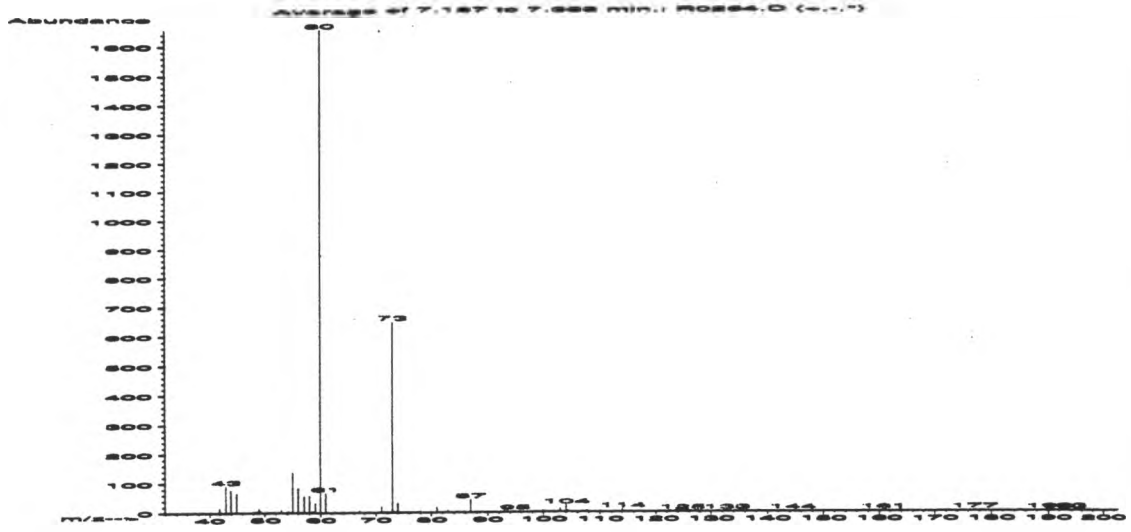
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, (1-methylethenyl)-	118	C9H10	49
2.	Benzene, 1-propenyl-	118	C9H10	47
3.	Benzene, (1-methylethenyl)-	118	C9H10	47
4.	Benzene, (1-methylethenyl)-	118	C9H10	47
5.	Benzene, (1-methylethenyl)-	118	C9H10	47
6.	Benzene, (1-methylethenyl)-	118	C9H10	47
7.	Azetidine, 3-methyl-3-phenyl-	147	C10H13N	38
8.	Benzene, (1-methylethenyl)-	118	C9H10	38
9.	Benzene, (1-methylethenyl)-	118	C9H10	27
10.	Ethane, 2-chloro-1,1,1-trifluoro-	118	C2H2ClF3	27
11.	7-CYANO(15N)-CYCLOHEPTATRIENE	117	C8H715N	23
12.	2-AMINO-ISOINDOLINE	134	C8H10N2	12
13.	Hexanoic acid, hexyl ester	200	C12H24O2	12
14.	Benzene, 2-propenyl-	118	C9H10	10
15.	PROPYL HEXANOATE	158	C9H18O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000098-83-9	119862	57	28	0	76	37	23	21	46	9087
2.	*47	000637-50-3	119853	48	52	0	75	40	20	16	41	9143
3.	*47	000098-83-9	119865	42	57	0	68	40	20	18	40	9132
4.	*47	000098-83-9	119864	48	51	0	80	37	20	6	41	9151
5.	*47	000098-83-9	119859	48	54	0	82	39	20	12	41	9126
6.	*47	000098-83-9	3898	48	50	0	84	40	20	6	41	9101
7.	38	005961-33-1	11712	36	52	0	72	21	14	1	26	9377
8.	*38	000098-83-9	119860	40	61	1	95	40	14	1	36	9247
9.	27	000098-83-9	119861	44	56	0	63	57	8	1	41	9198
10.	*27	000075-88-7	3699	34	76	1	69	57	8	0	39	7514
11.	23	057156-99-7	3693	34	150	0	69	46	6	0	25	8882
12.	12	000000-00-0	7364	33	75	0	85	57	2	0	25	8476
13.	12	006378-65-0	128403	33	96	2	160	60	2	0	22	5037
14.	*10	000300-57-2	3897	29	77	2	122	61	1	0	27	8767
15.	8	000000-00-0	16110	36	80	2	97	70	1	0	22	4708

CTMP Compounds

Peak 28; Pentanoic Acid



Average of 7.187 to 7.368 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.90	16	54.95	137	68.50	2	79.70	3
42.95	92	55.95	84	68.75	3	79.95	2
43.90	76	56.95	56	70.50	3	80.95	17
44.95	66	57.95	58	70.95	20	82.55	2
47.95	4	58.30	2	71.40	5	82.95	6
48.45	4	58.55	5	72.95	647	84.45	3
48.95	14	59.00	33	73.30	3	84.75	1
49.20	6	59.90	1655	73.90	32	84.95	3
50.90	1	60.90	67	76.55	2	85.80	4
52.95	9	62.65	4	77.45	2	86.90	44
54.20	5	67.05	6	77.95	5	88.15	3

Average of 7.187 to 7.368 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
89.15	2	106.45	2	160.80	2		
92.75	2	107.70	4	177.05	3		
93.45	3	110.05	1	190.25	2		
94.90	3	114.00	8	192.65	2		
97.75	2	120.75	2				
98.95	2	121.75	2				
99.85	5	123.65	2				
100.30	1	124.80	2				
102.95	11	126.45	2				
104.00	23	132.80	2				
104.30	3	144.50	2				

CTMP Compounds

Average of 7.187 to 7.368 min.: R0264.D
Converted from RTE data file: >R0264:

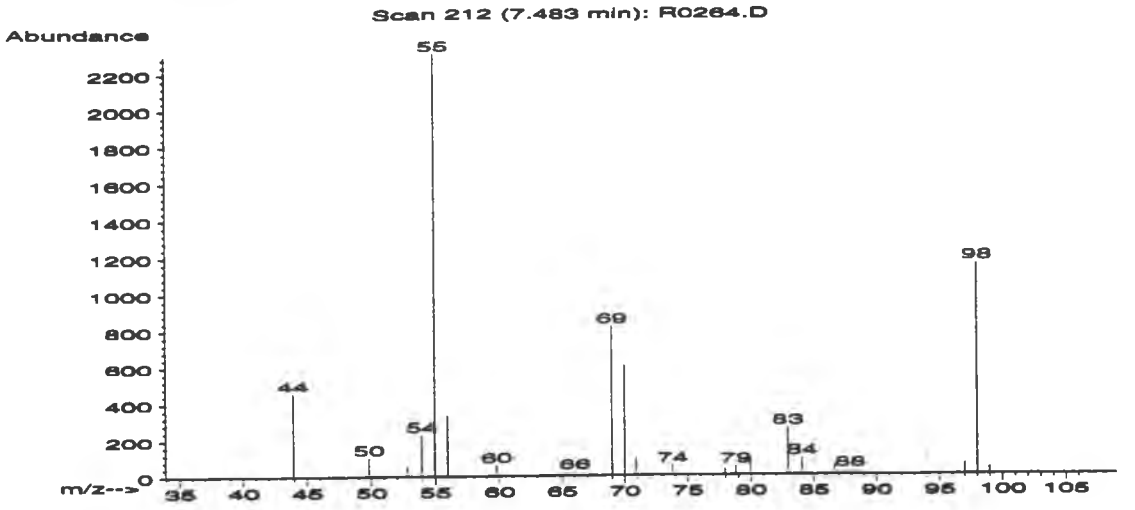
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid	88	C4H8O2	56
2.	Pentanoic acid	102	C5H10O2	56
3.	Butanoic acid	88	C4H8O2	40
4.	Butanoic acid	88	C4H8O2	39

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	56	000107-92-6	117172	38	53	2	87	15	30	0	33	9961
2.	56	000109-52-4	118195	42	46	2	91	13	30	0	33	9978
3.	40	000107-92-6	117171	36	48	3	99	15	16	0	25	9954
4.	39	000107-92-6	117175	34	37	2	67	17	15	1	23	9956

CTMP Compounds

Peak 29; Cyclohexanone



Scan 212 (7.483 min): R0264.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	456	73.80	51	98.95	38		
49.80	102	77.95	33				
52.80	51	78.80	47				
53.95	228	79.95	86				
54.95	2296	82.95	256				
55.95	333	84.05	91				
59.75	59	86.65	47				
66.00	20	87.90	23				
69.00	817	96.40	22				
70.00	601	97.00	62				
70.90	97	98.00	1156				

CTMP Compounds

Scan 212 (7.483 min): R0264.D

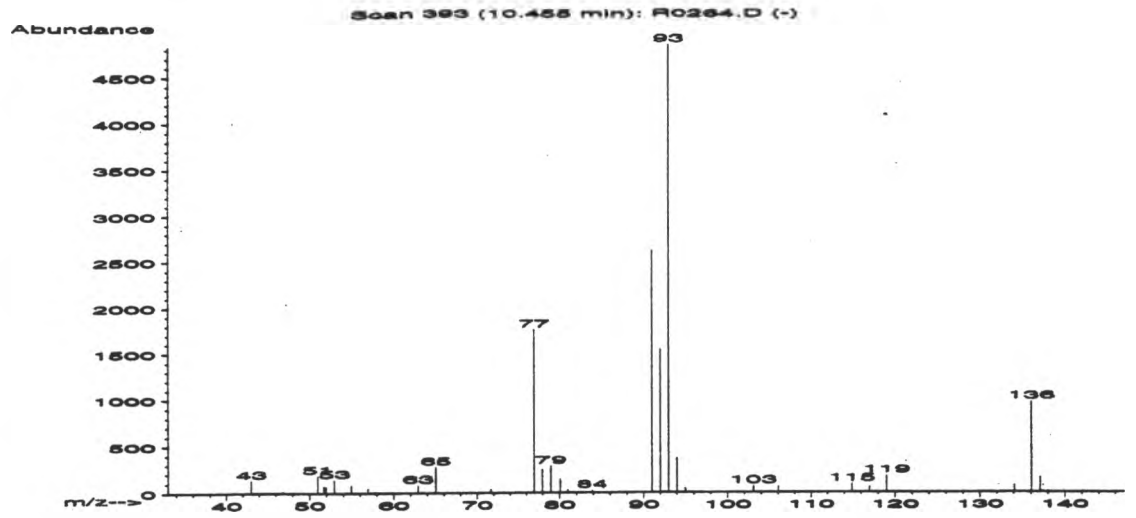
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone	98	C6H10O	64
2.	Cyclohexanone	98	C6H10O	64
3.	Cyclohexanone	98	C6H10O	64
4.	Cyclopentanone, 2-methyl-	98	C6H10O	52
5.	Cyclohexanone	98	C6H10O	50
6.	Cyclopentanone, 2-methyl-	98	C6H10O	47
7.	Cyclohexanone	98	C6H10O	47
8.	Cyclohexanone	98	C6H10O	45
9.	Cyclohexanone	98	C6H10O	45
10.	Cyclohexanol, 1,1'-dioxybis-	230	C12H22O4	42
11.	Cyclopentanone, 2-methyl-	98	C6H10O	38
12.	2-Pentene, 2,3-dimethyl-	98	C7H14	32
13.	2(3H)-Furanone, 5-methyl-	98	C5H6O2	28
14.	1,2,4,5-Tetrazine, 1,2,3,6-tetrahydro-3,	114	C4H10N4	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000108-94-1	117749	50	37	2	99	22	37	0	46	9774
2.	*64	000108-94-1	117747	53	52	3	83	24	37	0	49	8163
3.	*64	000108-94-1	117743	50	39	1	99	22	37	0	44	9778
4.	*52	001120-72-5	816	49	46	1	95	33	27	0	46	9102
5.	50	000108-94-1	819	47	49	1	99	33	25	0	39	9716
6.	*47	001120-72-5	117740	45	52	2	85	40	20	0	40	8713
7.	*47	000108-94-1	117745	37	46	3	260	36	20	0	41	9296
8.	*45	000108-94-1	117746	47	43	1	80	22	19	4	33	9632
9.	*45	000108-94-1	117744	50	47	2	80	22	19	9	35	9644
10.	42	002407-94-5	48328	44	88	2	77	29	17	0	35	9705
11.	*38	001120-72-5	117739	40	57	1	89	36	14	0	33	9517
12.	*32	010574-37-5	117802	33	59	3	99	47	9	0	35	7827
13.	*28	000591-12-8	117674	30	47	1	99	36	8	0	29	9593
14.	10	056051-77-5	2889	33	67	1	62	61	1	0	20	3034

CTMP Compounds

Peak 30; Monoterpene (1-Phellandrene)



Scan 393 (10.455 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	132	71.65	38	95.00	45		
46.80	18	76.95	1763	103.05	65		
50.95	182	77.95	247	106.05	59		
51.70	70	78.95	286	114.90	86		
51.95	70	80.05	141	117.00	54		
52.95	139	80.95	35	119.00	176		
54.95	82	83.90	23	134.05	73		
56.95	47	91.00	2621	136.05	973		
62.90	81	92.00	1544	137.05	158		
65.00	275	93.00	4833				
67.80	11	94.00	371				

BKME 8.

CPMD 14

CTMP Compounds

Scan 393 (10.455 min): R0264.D

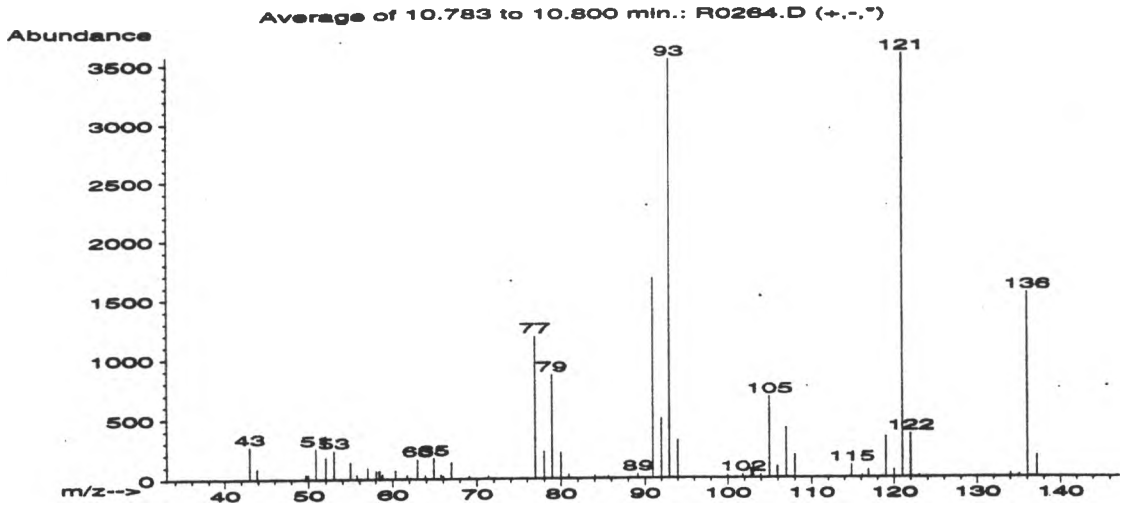
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	l-Phellandrene	136	C10H16	91
2.	l-Phellandrene	136	C10H16	91
3.	l-Phellandrene	136	C10H16	91
4.	l-Phellandrene	136	C10H16	90
5.	l-Phellandrene	136	C10H16	87
6.	l-Phellandrene	136	C10H16	86
7.	l-Phellandrene	136	C10H16	86
8.	l-Phellandrene	136	C10H16	80
9.	.alpha.-Thujene	136	C10H16	78
10.	.DELTA.3-Carene	136	C10H16	78
11.	TRICYCLO[2.2.1.0(2,6)]HEPTANE, 2,3,3-TRI	136	C10H16	72
12.	.DELTA.3-Carene	136	C10H16	72
13.	.DELTA.3-Carene	136	C10H16	72
14.	.DELTA.3-Carene	136	C10H16	64
15.	.alpha.-Thujene	136	C10H16	64
16.	.BETA.-OCIMENE-X	136	C10H16	64
17.	.beta.-Thujene	136	C10H16	64
18.	.beta.-Terpinene	136	C10H16	64
19.	.DELTA.3-Carene	136	C10H16	56
20.	(-)-CIS-2-CARENE	136	C10H16	56

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000099-83-2	121991	74	16	0	90	5	62	0	81	9841
2.	*91	000099-83-2	8088	68	22	0	88	5	62	0	76	9856
3.	*91	000099-83-2	121996	61	8	0	89	5	60	0	56	9974
4.	*90	000099-83-2	121992	64	28	1	99	5	57	8	47	9727
5.	*87	000099-83-2	121989	72	15	0	86	8	54	23	58	9861
6.	*86	000099-83-2	121995	55	33	0	95	8	53	0	49	9764
7.	*86	000099-83-2	121993	34	54	2	99	8	53	4	43	9816
8.	*80	000099-83-2	121990	47	40	0	82	11	48	0	44	9756
9.	*78	002867-05-2	122054	48	44	1	88	8	46	19	40	9844
10.	*78	013466-78-9	122091	44	64	3	99	8	46	0	39	9960
11.	*72	000000-00-0	8189	34	74	2	99	11	42	0	39	8906
12.	*72	013466-78-9	122092	43	65	3	99	13	42	0	39	8969
13.	*72	013466-78-9	122089	37	73	3	99	14	42	0	39	8955
14.	*64	013466-78-9	122094	33	68	2	76	17	37	0	39	9679
15.	64	002867-05-2	122055	47	39	0	69	19	37	0	39	9800
16.	*64	013877-91-3	121956	34	71	2	99	17	37	0	39	8820
17.	*64	028634-89-1	8155	33	59	2	99	20	37	1	40	9487
18.	*64	000099-84-3	8117	34	64	3	92	20	37	0	39	9581
19.	*56	013466-78-9	122088	42	65	3	99	11	30	0	35	8965
20.	*56	005208-49-1	122085	37	67	3	99	14	30	0	35	8943

CTMP Compounds

Peak 31; Monoterpene (.alpha.-Terpinene)



Average of 10.783 to 10.800 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	268	58.45	66	70.95	2	89.15	31
43.90	84	58.80	36	71.40	21	90.95	1676
49.70	36	60.35	68	71.85	2	92.00	495
49.95	36	61.75	29	76.95	1188	93.00	3525
50.85	254	62.95	162	78.00	223	94.00	313
52.00	178	63.90	29	78.95	862	99.95	21
52.95	236	64.90	171	80.00	212	101.80	23
54.95	139	65.75	33	80.95	29	102.80	73
55.70	35	66.00	20	84.05	20	103.05	96
57.00	92	67.00	135	85.15	7	103.95	23
58.05	63	69.05	18	85.65	15	105.00	676

Average of 10.783 to 10.800 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.95	91	134.05	26				
107.00	416	135.05	18				
108.00	188	136.05	1546				
114.85	102	137.15	180				
116.15	15						
116.90	61						
119.00	337						
120.00	58						
121.00	3571						
122.00	361						
123.00	12						

BKME 11
CPMO 17

CTMP Compounds

Average of 10.783 to 10.800 min.: R0264.D
Converted from RTE data file: >R0264:

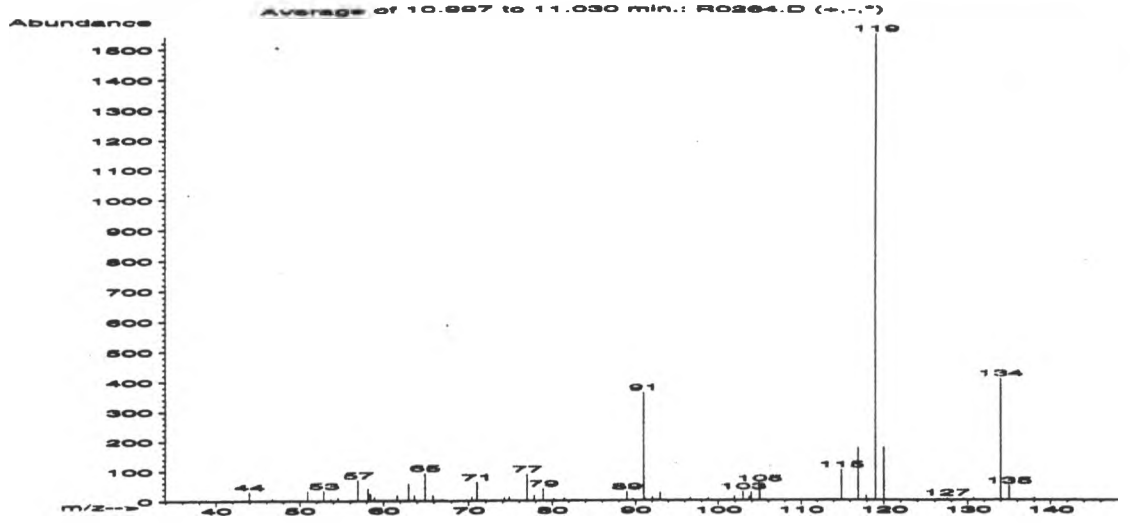
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.alpha.-Terpinene	136	C10H16	97
2.	.alpha.-Terpinene	136	C10H16	95
3.	.alpha.-Terpinene	136	C10H16	95
4.	.alpha.-Terpinene	136	C10H16	94
5.	.ALPHA.-TERPINOLENE	136	C10H16	94
6.	Bornylene	136	C10H16	94
7.	.ALPHA.-TERPINOLENE	136	C10H16	93
8.	.DELTA.-4-CARENE	136	C10H16	93
9.	.DELTA.-4-CARENE	136	C10H16	91
10.	.alpha.-Terpinene	136	C10H16	90
11.	.alpha.-Terpinene	136	C10H16	90
12.	2,2,3-TRIMETHYL-1-VINYL-3-CYCLOPENTENE	136	C10H16	87
13.	.alpha.-Terpinene	136	C10H16	87
14.	Isoterpinolene	136	C10H16	80
15.	.alpha.-Terpinene	136	C10H16	74
16.	.beta.-Terpinene	136	C10H16	70
17.	2-.BETA.-PINENE	136	C10H16	62
18.	.BETA.-OCIMENE-X	136	C10H16	62
19.	2,4,6-Octatriene, 3,4-dimethyl-	136	C10H16	62
20.	.gamma.-Terpinene	136	C10H16	58

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*97	000099-86-5	121981	106	8	0	87	0	78	0	97	9972
2.	*95	000099-86-5	121985	100	12	1	93	1	72	0	93	9971
3.	*95	000099-86-5	8087	99	14	1	89	0	72	0	93	9968
4.	*94	000099-86-5	121986	96	14	1	87	3	70	0	93	9930
5.	*94	000586-62-9	122030	87	20	1	78	5	70	51	90	9823
6.	*94	000464-17-5	8146	79	34	2	92	3	70	0	84	9939
7.	*93	000586-62-9	122035	89	22	1	84	7	66	52	91	9793
8.	*93	000554-61-0	8168	84	28	2	70	7	66	41	90	9844
9.	*91	000554-61-0	122087	92	15	1	76	1	62	6	80	9857
10.	*90	000099-86-5	121983	77	26	2	89	10	59	0	81	9881
11.	*90	000099-86-5	121982	78	37	2	82	10	59	33	72	9575
12.	*87	000000-00-0	8083	71	35	2	79	8	54	14	53	9542
13.	*87	000099-86-5	121984	75	39	3	81	10	54	6	55	9769
14.	*80	000586-63-0	8112	75	37	1	92	12	48	1	50	9838
15.	*74	000099-86-5	121987	78	33	1	97	17	44	0	60	9809
16.	*70	000099-84-3	8117	69	31	0	86	30	41	31	70	8017
17.	*62	000127-91-3	122078	64	42	1	85	28	36	37	58	7990
18.	*62	013877-91-3	8058	64	46	2	98	28	36	0	58	8849
19.	*62	057396-75-5	8066	63	41	2	74	30	36	26	53	8501
20.	*58	000099-85-4	122013	59	40	2	98	32	32	0	51	9001

CTMP Compounds

Peak 32; Monoterpene (Cymene)



Average of 10.997 to 11.030 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	29	61.65	19	76.95	88	98.80	8
46.70	8	63.00	56	77.80	17	101.95	13
50.90	33	63.70	17	78.95	40	102.95	29
52.85	34	64.95	93	80.20	6	103.70	11
53.70	7	65.90	17	81.45	9	103.95	26
54.55	11	67.00	6	88.95	29	104.95	56
56.95	69	69.75	2	89.65	6	114.95	101
58.15	40	70.40	13	91.00	361	116.95	175
58.45	22	71.00	61	92.05	11	117.90	14
58.95	11	74.20	10	93.00	25	119.00	1540
59.45	3	74.80	12	96.65	9	120.00	176

Average of 10.997 to 11.030 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.45	7						
129.45	5						
130.70	7						
134.00	406						
135.00	48						
138.00	8						

BKMB 12.
cPMD 018.

CTMP Compounds

Average of 10.997 to 11.030 min.: R0264.D
Converted from RTE data file: >R0264:

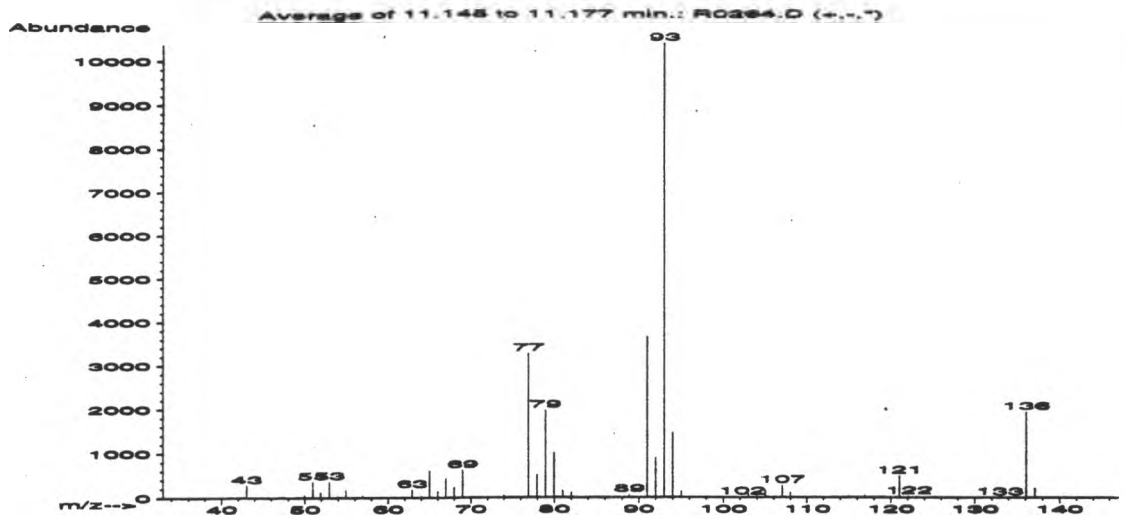
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	91
2.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	91
3.	Benzene, methyl(1-methylethyl)-	134	C10H14	91
4.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	90
5.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	90
6.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	90
7.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	90
8.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	90
9.	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	90
10.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	90
11.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	90
12.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	90
13.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	90
14.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	87
15.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	86
16.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	86
17.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	86
18.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	86
19.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	83
20.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	78

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000535-77-3	121627	63	26	2	98	5	62	0	64	9963
2.	*91	000527-84-4	121625	60	27	2	76	1	60	0	56	9983
3.	*91	025155-15-1	121626	59	31	2	91	5	60	0	51	9981
4.	*90	000535-77-3	121628	50	38	2	79	1	57	0	46	9963
5.	*90	000535-77-3	7446	55	33	2	82	1	57	0	49	9955
6.	*90	000099-87-6	121639	64	26	3	96	5	57	10	47	9959
7.	*90	000099-87-6	121631	54	33	1	76	5	57	0	47	9956
8.	*90	000099-87-6	121636	52	38	2	83	-1	57	0	46	9974
9.	*90	000527-53-7	121673	52	38	2	92	5	57	26	44	9545
10.	*90	000095-93-2	121675	53	36	2	99	5	57	28	46	9567
11.	*90	000535-77-3	121629	55	33	2	76	1	57	0	49	9964
12.	*90	000874-41-9	7452	49	38	1	69	5	57	0	46	9911
13.	*90	000874-41-9	121655	49	37	1	78	5	57	0	44	9906
14.	*87	000099-87-6	121633	58	31	2	99	7	54	0	56	9968
15.	*86	000527-84-4	121624	53	39	3	99	7	53	0	47	9958
16.	*86	000527-84-4	7445	53	36	2	99	7	53	0	47	9958
17.	*86	000099-87-6	121635	53	36	3	98	7	53	0	49	9964
18.	*86	000535-77-3	121630	49	43	3	97	7	53	0	46	9985
19.	*83	001758-88-9	121657	45	45	3	91	3	50	16	43	9901
20.	*78	000933-98-2	121653	47	43	3	96	7	46	8	43	9894

CTMP Compounds

Peak 33; Monoterpene (.beta. ~~Thujene~~ phellandrene)



Average of 11.145 to 11.177 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	275	56.25	10	70.90	7	85.65	18
43.95	10	56.95	55	72.15	13	85.90	10
48.90	28	59.00	4	73.30	9	88.85	73
49.20	24	62.90	183	74.00	49	91.00	3676
49.70	13	64.00	30	76.95	3289	92.00	892
49.95	58	65.00	618	77.95	515	93.00	10366
50.95	355	66.00	142	78.95	1980	94.00	1461
51.90	124	67.00	434	79.95	1006	95.00	138
52.95	369	68.00	222	80.95	149	102.20	13
53.95	31	69.00	622	82.00	110	102.95	60
54.95	184	70.00	21	84.70	5	105.00	140

Average of 11.145 to 11.177 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	268	137.05	208				
107.95	106						
115.00	36						
116.90	47						
117.90	6						
119.00	22						
121.00	493						
122.15	22						
123.00	7						
132.95	5						
136.05	1948						

BKME 15

Cmpd 021.

CTMP Compounds

Average of 11.145 to 11.177 min.: R0264.D
Converted from RTE data file: >R0264:

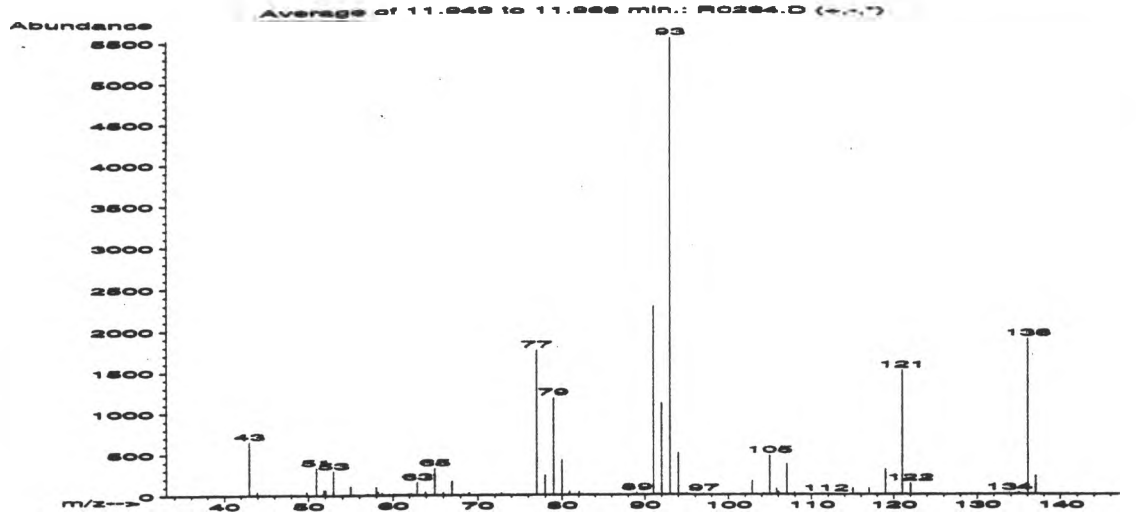
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.beta.-Thujene	136	C10H16	94
2.	.beta.-Phellandrene	136	C10H16	91
3.	Sabinene	136	C10H16	91
4.	.beta.-Phellandrene	136	C10H16	91
5.	Sabinene	136	C10H16	91
6.	.beta.-Terpinene	136	C10H16	91
7.	Sabinene	136	C10H16	91
8.	Sabinene	136	C10H16	91
9.	.beta.-Phellandrene	136	C10H16	90
10.	.beta.-Phellandrene	136	C10H16	86
11.	.beta.-Phellandrene	136	C10H16	83
12.	1-Phellandrene	136	C10H16	74
13.	1-Phellandrene	136	C10H16	72
14.	1-Phellandrene	136	C10H16	72
15.	1-Phellandrene	136	C10H16	72
16.	TRICYCLO[2.2.1.0(2,6)]HEPTANE, 2,3,3-TRI	136	C10H16	72
17.	1-Phellandrene	136	C10H16	72
18.	.alpha.-Thujene	136	C10H16	64
19.	Sabinene	136	C10H16	64
20.	.DELTA.3-Carene	136	C10H16	64

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	028634-89-1	8155	81	11	1	95	1	70	0	93	9982
2.	*91	000555-10-2	122038	76	16	2	91	1	62	0	81	9988
3.	*91	003387-41-5	122064	83	13	1	91	4	62	23	76	9979
4.	*91	000555-10-2	8118	82	9	1	99	1	62	21	66	9966
5.	*91	003387-41-5	122063	76	18	1	95	4	60	12	53	9970
6.	*91	000099-84-3	8117	58	38	2	70	4	60	0	51	9935
7.	*91	003387-41-5	8159	77	16	1	91	4	60	31	53	9945
8.	*91	003387-41-5	122062	72	23	1	87	4	60	13	52	9945
9.	*90	000555-10-2	122039	50	55	2	75	4	57	0	44	9971
10.	*86	000555-10-2	122041	59	37	2	84	9	53	1	47	9801
11.	*83	000555-10-2	122040	67	6	0	69	4	50	8	43	9907
12.	*74	000099-83-2	121991	60	30	1	85	18	44	0	51	9758
13.	*72	000099-83-2	121989	55	36	2	86	19	42	0	49	9775
14.	*72	000099-83-2	8088	50	41	2	99	19	42	0	46	9772
15.	*72	000099-83-2	121995	57	31	2	95	18	42	0	49	9761
16.	*72	000000-00-0	8189	43	61	3	87	13	42	0	40	9684
17.	*72	000099-83-2	121994	54	42	2	86	15	42	20	42	9513
18.	*64	002867-05-2	122055	51	38	2	96	19	37	7	39	9704
19.	*64	003387-41-5	122060	44	56	3	96	19	37	0	40	9968
20.	*64	013466-78-9	122093	34	67	3	69	19	37	0	41	9638

CTMP Compounds

Peak 34; Monoterpine (.gamma.-Terpinene)



Average of 11.949 to 11.966 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	653	58.00	98	69.00	33	92.00	1121
43.95	43	58.20	41	72.80	27	93.00	5529
45.40	9	58.70	25	76.95	1764	94.00	510
49.80	45	60.15	17	77.95	242	95.00	19
50.95	334	61.90	19	78.95	1187	97.00	15
51.80	69	62.25	16	80.00	427	102.85	168
52.05	64	62.90	159	80.90	44	104.20	21
52.95	294	63.90	39	82.05	39	104.95	477
53.95	14	65.00	328	86.90	13	105.80	73
54.95	109	66.00	35	89.00	28	106.05	31
57.05	11	67.00	178	91.00	2289	107.00	375

Average of 11.949 to 11.966 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.95	26						
111.75	10						
115.00	74						
117.00	78						
119.00	306						
121.00	1515						
122.00	138						
133.80	22						
134.95	25						
136.05	1897						
137.00	225						

CTMP Compounds

Average of 11.949 to 11.966 min.: R0264.D
Converted from RTE data file: >R0264:

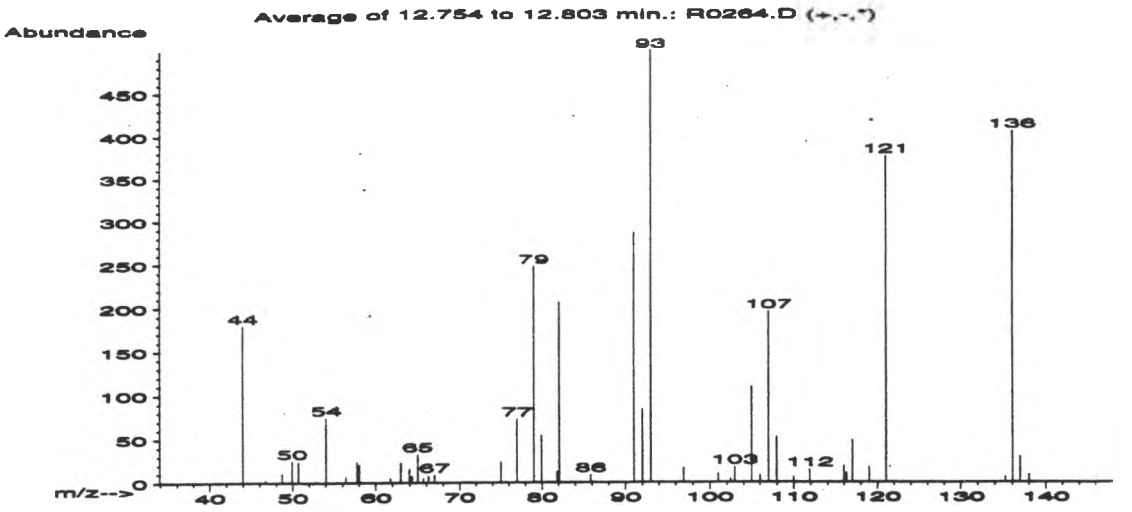
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.gamma.-Terpinene	136	C10H16	95
2.	.gamma.-Terpinene	136	C10H16	95
3.	.gamma.-Terpinene	136	C10H16	94
4.	.DELTA.3-Carene	136	C10H16	94
5.	.gamma.-Terpinene	136	C10H16	94
6.	.gamma.-Terpinene	136	C10H16	94
7.	.gamma.-Terpinene	136	C10H16	93
8.	.DELTA.3-Carene	136	C10H16	91
9.	.gamma.-Terpinene	136	C10H16	91
10.	.DELTA.3-Carene	136	C10H16	91
11.	.gamma.-Terpinene	136	C10H16	91
12.	Cyclofenchene	136	C10H16	91
13.	.DELTA.3-Carene	136	C10H16	91
14.	.gamma.-Terpinene	136	C10H16	90
15.	Tricyclene	136	C10H16	90
16.	.DELTA.3-Carene	136	C10H16	90
17.	.beta.-Terpinene	136	C10H16	87
18.	.DELTA.3-Carene	136	C10H16	86
19.	.ALPHA.-PINENE, (-)-	136	C10H16	80
20.	.ALPHA.-PINENE, (-)-	136	C10H16	80

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000099-85-4	122010	86	10	2	96	0	74	0	94	9987
2.	*95	000099-85-4	122013	86	12	1	77	5	74	0	94	9982
3.	*94	000099-85-4	122004	96	3	0	70	2	70	42	83	9936
4.	*94	013466-78-9	122094	84	19	2	88	0	70	51	90	9860
5.	*94	000099-85-4	122007	85	23	1	74	2	70	0	91	9716
6.	*94	000099-85-4	122006	79	29	2	87	2	70	0	90	9708
7.	*93	000099-85-4	122012	85	13	1	86	7	66	0	91	9893
8.	*91	013466-78-9	122088	81	20	1	73	5	62	47	74	9863
9.	*91	000099-85-4	122008	73	33	2	86	5	62	0	81	9692
10.	*91	013466-78-9	8170	77	30	1	80	0	62	0	74	9970
11.	*91	000099-85-4	8096	77	24	1	90	1	62	0	81	9985
12.	*91	000488-97-1	122100	63	41	3	85	5	60	17	50	9701
13.	*91	013466-78-9	122095	66	38	2	74	5	60	17	53	9890
14.	*90	000099-85-4	122009	75	24	1	74	10	59	0	81	9859
15.	*90	000508-32-7	122098	77	25	1	79	6	59	23	66	9822
16.	*90	013466-78-9	122090	63	40	3	94	2	57	16	47	9830
17.	*87	000099-84-3	8117	65	33	0	80	7	54	10	53	9764
18.	*86	013466-78-9	122089	69	32	1	78	7	53	20	47	9788
19.	*80	000080-56-8	122069	62	41	2	91	13	48	12	45	9348
20.	*80	000080-56-8	122068	62	41	2	91	13	48	12	45	9349

CTMP Compounds

peak35; Monoterpene



Average of 12.754 to 12.803 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	180	61.75	5	79.95	55	105.00	110
46.70	3	62.95	23	81.80	13	106.00	8
48.70	11	63.95	16	82.05	207	107.00	196
49.90	25	64.25	8	85.85	9	107.95	53
50.70	24	64.95	33	91.00	287	109.95	6
52.95	1	65.65	5	92.00	84	111.90	15
54.05	75	66.25	8	93.00	499	115.95	19
56.45	7	66.95	9	96.90	17	116.25	11
57.80	24	75.05	24	100.95	10	117.00	49
58.05	20	76.95	73	102.45	4	119.00	18
58.30	1	79.00	248	102.95	18	121.05	377

Average of 12.754 to 12.803 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.20	6						
136.05	406						
136.95	30						
138.00	9						

CTMP Compounds

Average of 12.754 to 12.803 min.: R0264.D
Converted from RTE data file: >R0264:

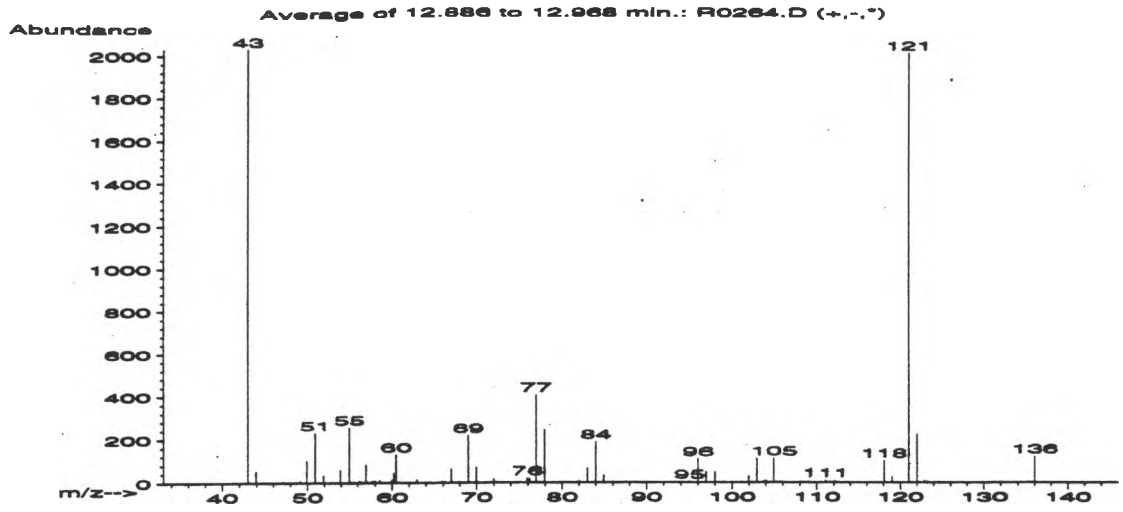
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexene, 5-methyl-3-(1-methylethenyl	136	C10H16	72
2.	.ALPHA.-TERPINOLENE	136	C10H16	59
3.	4-Terpinenyl acetate	196	C12H20O2	53
4.	1-Isopropenyl-2-methylcyclohexene	136	C10H16	53
5.	Benzenemethanol, 3,5-dimethyl-	136	C9H12O	52
6.	p-Menth-1(7)-en-9-ol	154	C10H18O	50
7.	(-)-CIS-CARAN-TRANS-2-OL	154	C10H18O	50
8.	HYDROCINNAMALDEHYDE-.BETA.-D2	134	C9H8D2O	43
9.	.DELTA.-4-CARENE	136	C10H16	43
10.	Phenol, 2,4,6-trimethyl-	136	C9H12O	38
11.	HYDROCINNAMALDEHYDE-2,6-D2	134	C9H8D2O	38
12.	.ALPHA.-PINENE, (-)-	136	C10H16	37
13.	2,5-DIETHYLPYRAZINE	136	C8H12N2	30
14.	Phenol, 3,4,5-trimethyl-	136	C9H12O	27
15.	Phenol, 2,4,5-trimethyl-	136	C9H12O	27
16.	Cycloheptene, 5-ethylidene-1-methyl-	136	C10H16	27
17.	Phenol, 2,4,5-trimethyl-	136	C9H12O	27
18.	Phenol, 2,4,6-trimethyl-	136	C9H12O	27
19.	Phenol, 2,3,5-trimethyl-	136	C9H12O	27
20.	Benzaldehyde, 3-methoxy-	136	C8H8O2	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	056816-08-1	8108	70	50	2	67	17	42	19	48	9398
2.	*59	000586-62-9	8113	45	74	2	96	21	33	0	40	9510
3.	53	004821-04-9	128014	44	86	2	86	29	28	16	38	9186
4.	*53	076480-15-4	8099	43	46	1	99	29	28	0	39	9447
5.	*52	027129-87-9	121916	52	68	2	58	35	27	0	46	8830
6.	50	029548-16-1	14721	44	82	0	61	35	25	12	41	8504
7.	50	006909-21-3	124310	44	63	0	67	31	25	0	39	9173
8.	*43	029372-34-7	7371	48	65	2	81	42	18	14	39	8388
9.	*43	000554-61-0	8168	48	71	3	99	43	18	0	39	9310
10.	*38	000527-60-6	121911	44	54	0	57	54	14	0	44	7040
11.	*38	029372-35-8	7372	34	71	2	72	46	14	18	40	7988
12.	37	000080-56-8	122067	55	61	1	72	43	13	15	37	8007
13.	*30	000000-00-0	7840	48	65	1	65	57	9	0	46	6605
14.	*27	000527-54-8	7911	38	59	0	62	59	8	0	39	6548
15.	*27	000496-78-6	7909	37	58	0	68	59	8	0	41	6524
16.	27	015402-94-5	8128	46	76	0	66	57	8	0	39	9098
17.	*27	000496-78-6	121910	37	57	0	70	59	8	0	41	6503
18.	*27	000527-60-6	121913	38	58	0	59	57	8	0	39	6936
19.	*27	000697-82-5	121906	52	42	0	62	58	8	12	41	6890
20.	*14	000591-31-1	7801	35	70	2	81	67	2	0	39	5357

CTMP Compounds

Peak 36; Nor Monoterpene



Average of 12.886 to 12.968 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2029	57.70	8	67.95	4	82.05	9
43.95	53	58.00	9	69.00	219	83.00	67
47.20	5	58.55	11	69.95	71	84.00	188
49.15	12	59.95	13	72.00	16	84.95	34
49.90	102	60.20	43	72.30	3	86.00	5
50.90	231	60.45	130	75.90	21	87.65	4
51.90	34	62.90	14	76.20	17	95.00	4
53.90	62	65.90	7	76.95	408	96.00	109
54.95	256	66.25	5	77.95	244	96.95	50
56.20	10	66.95	65	79.80	3	98.00	50
56.95	82	67.25	3	81.80	2	98.95	6

Average of 12.886 to 12.968 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.20	4	119.00	27				
101.95	29	121.00	2002				
102.90	110	122.00	221				
103.80	7	122.90	8				
104.05	8	123.25	4				
104.95	111	136.00	122				
108.05	5						
109.05	6						
111.05	12						
112.15	7						
118.05	101						

CTMP Compounds

Average of 12.886 to 12.968 min.: R0264.D
Converted from RTE data file: >R0264:

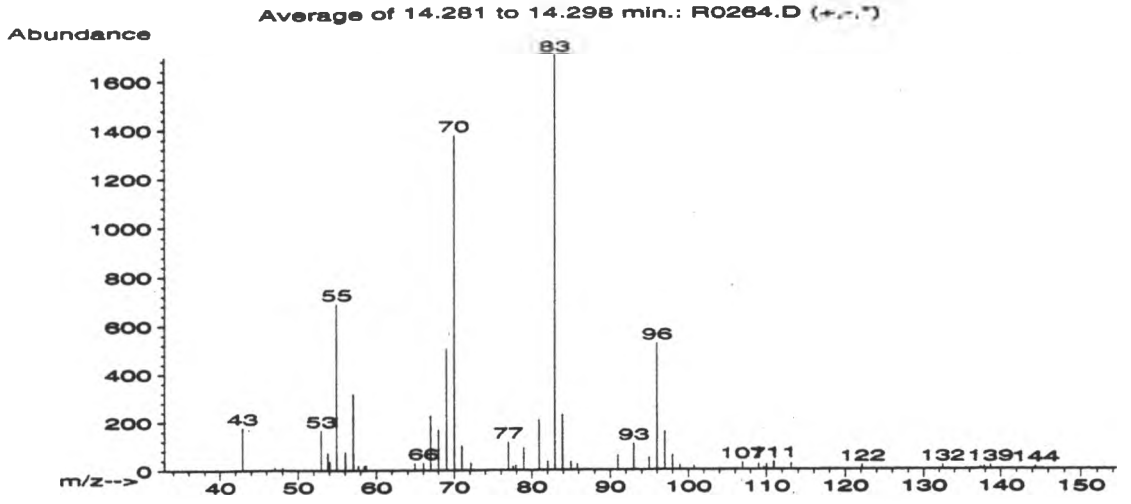
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenemethanol, .alpha.,.alpha.-dimethy	136	C9H12O	80
2.	Benzenemethanol, .alpha.,.alpha.-dimethy	136	C9H12O	74
3.	Benzenamine, 3,5-dimethyl-	121	C8H11N	64
4.	Benzenamine, 2,6-dimethyl-	121	C8H11N	64
5.	Benzenamine, 2,5-dimethyl-	121	C8H11N	59
6.	Benzenamine, 3,4-dimethyl-	121	C8H11N	59
7.	Benzenamine, 3,4-dimethyl-	121	C8H11N	59
8.	Benzenamine, 2,6-dimethyl-	121	C8H11N	59
9.	Pyridine, 2,3,6-trimethyl-	121	C8H11N	53
10.	Benzenamine, 3,5-dimethyl-	121	C8H11N	53
11.	4-Ethyl-3-methylpyridine	121	C8H11N	45
12.	Benzenamine, 2,5-dimethyl-	121	C8H11N	45
13.	Benzenamine, 2,4-dimethyl-	121	C8H11N	45
14.	Benzenamine, 2,4-dimethyl-	121	C8H11N	45
15.	Benzenamine, 3,4-dimethyl-	121	C8H11N	45
16.	Benzene, (1-methoxyethyl)-	136	C9H12O	42
17.	Benzene, (1-methoxyethyl)-	136	C9H12O	42
18.	Benzenamine, 2,3-dimethyl-	121	C8H11N	40
19.	Oxiranecarboxylic acid, 3-phenyl-, methy	178	C10H10O3	36
20.	Oxiranecarboxylic acid, 3-phenyl-, methy	178	C10H10O3	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000617-94-7	7944	55	30	2	121	15	48	0	49	9897
2.	*74	000617-94-7	121928	69	22	0	77	17	44	2	58	9894
3.	*64	000108-69-0	120097	36	47	0	78	23	37	8	43	9840
4.	*64	000087-62-7	120092	43	55	2	78	25	37	0	44	9813
5.	*59	000095-78-3	120091	34	42	0	66	23	33	9	38	9869
6.	*59	000095-64-7	120095	34	68	2	78	25	33	0	39	9812
7.	*59	000095-64-7	4242	36	67	2	98	25	33	0	39	9817
8.	*59	000087-62-7	120094	35	42	0	69	23	33	3	38	9871
9.	*53	001462-84-6	120074	35	66	1	90	28	28	0	39	9803
10.	*53	000108-69-0	4243	28	50	0	87	29	28	1	42	9817
11.	*45	076833-16-4	4222	29	83	0	80	25	19	0	33	9849
12.	*45	000095-78-3	4240	36	71	1	78	21	19	0	35	9869
13.	*45	000095-68-1	120090	39	63	2	79	25	19	0	35	9810
14.	*45	000095-68-1	4239	38	60	1	92	25	19	0	35	9806
15.	*45	000095-64-7	120096	39	64	2	77	21	19	0	35	9834
16.	*42	004013-34-7	121943	40	28	1	91	28	17	0	35	9807
17.	*42	004013-34-7	7961	41	53	3	98	28	17	0	35	9819
18.	*40	000087-59-2	120088	28	49	0	98	31	16	0	33	9793
19.	36	037161-74-3	24597	34	68	2	97	28	12	0	22	9793
20.	36	019190-80-8	24596	36	66	2	98	28	12	0	22	9792

CTMP Compounds

Peak 37; Unidentified Hydrocarbon



Average of 14.281 to 14.298 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	177	58.70	22	77.95	20	96.00	524
47.05	12	64.90	30	78.95	93	97.00	159
48.05	11	66.00	31	80.95	209	98.00	62
52.95	166	66.95	226	82.05	37	98.95	19
53.80	73	68.00	170	82.95	1696	100.70	14
54.05	37	69.00	503	83.95	229	106.95	30
54.95	689	70.00	1369	85.00	35	109.05	23
56.05	76	71.00	102	85.85	24	109.70	9
57.05	316	72.15	29	90.95	62	110.05	20
57.70	19	76.95	118	93.00	110	110.95	32
58.45	18	77.55	17	94.95	51	113.15	24

Average of 14.281 to 14.298 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.15	18						
132.45	18						
137.40	9						
137.90	13						
138.65	16						
144.40	13						

CTMP Compounds

Average of 14.281 to 14.298 min.: R0264.D
Converted from RTE data file: >R0264:

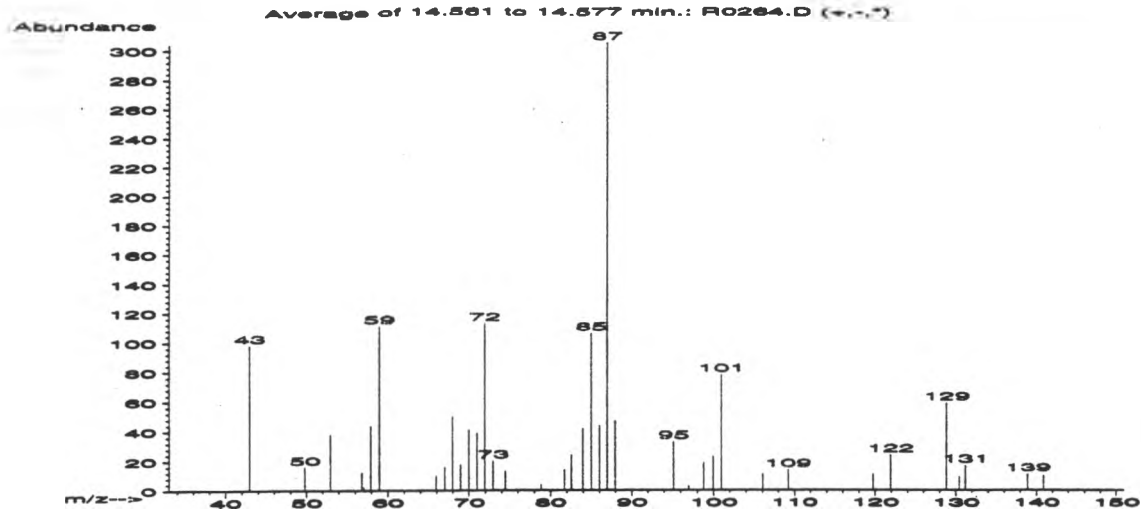
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexane, decyl-	224	C16H32	43
2.	2-Octenal, (E)-	126	C8H14O	36
3.	Heptanol	116	C7H16O	35
4.	1-Heptanol	116	C7H16O	35
5.	1,2-Cyclohexanediol	116	C6H12O2	32
6.	3-Chloro-1-cyclohexyloxy-3-methyl-2-nitr	466	C22H40Cl2N2O4	32
7.	5-Hexyn-1-ol	98	C6H10O	32
8.	Cyclobutane, 2-hexyl-1,1,4-trimethyl-, c	182	C13H26	25
9.	7-Oxabicyclo[4.1.0]heptane	98	C6H10O	25
10.	CYCLOOCTA-1,5-DIEN-7-OL	124	C8H12O	22
11.	2,6-Nonadienal, (E,Z)-	138	C9H14O	22
12.	Cyclohexane, 1,1'-(1,4-butanediyl)bis-	222	C16H30	17
13.	Cyclohexane, 2-propenyl-	124	C9H16	17
14.	BIS(EPOXYCYCLOPENTYL) ETHER	182	C10H14O3	16
15.	Cyclohexane, bromo-	162	C6H11Br	16
16.	Cyclohexane, bromo-	162	C6H11Br	12
17.	Cyclopropane, butyl-	98	C7H14	12
18.	1-Heptanol	116	C7H16O	10
19.	2,2-Dichloro-3,3,4,4-tetramethylcyclobut	194	C8H12Cl2O	10
20.	N,N'-BIS(2,6-DIMETHYL-6-NITROSOHEPT-2-EN	338	C18H30N2O4	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	43	001795-16-0	130034	54	57	1	87	44	18	0	39	7901
2.	36	002548-87-0	120570	38	59	2	81	26	12	7	28	9129
3.	35	053535-33-4	119609	54	40	0	54	55	11	0	39	6880
4.	35	000111-70-6	119606	44	54	0	55	55	11	0	39	6705
5.	32	000931-17-9	119570	39	52	2	76	46	9	9	31	7051
6.	32	086296-67-5	106250	43	99	2	92	48	9	0	35	7602
7.	*32	000928-90-5	117752	40	58	2	59	48	9	9	36	7157
8.	25	049622-19-7	26859	48	41	0	75	53	7	7	36	6504
9.	25	000286-20-4	117777	39	55	2	67	44	7	1	29	8602
10.	22	000000-00-0	4812	43	44	1	80	65	5	0	39	5965
11.	*22	000557-48-2	122258	33	55	1	107	62	5	0	39	6089
12.	17	006165-44-2	129929	47	64	2	69	54	3	3	27	7766
13.	17	002114-42-3	4917	42	57	2	99	53	3	0	29	7645
14.	16	000000-00-0	26567	43	44	2	68	56	3	11	33	7582
15.	16	000108-85-0	17430	40	30	1	99	58	3	10	35	7473
16.	12	000108-85-0	125053	36	41	2	99	58	2	0	25	7465
17.	*12	000930-57-4	931	32	75	2	93	59	2	0	29	6553
18.	10	000111-70-6	3579	38	65	1	53	61	1	0	29	6548
19.	10	066239-90-5	31528	35	37	0	75	61	1	1	26	6051
20.	10	066737-12-0	84991	37	59	0	99	63	1	0	25	7398

CTMP Compounds

Peak 38; Unidentified Hydrocarbon



Average of 14.561 to 14.577 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	98	70.00	41	86.95	304	128.85	59
49.80	16	71.00	39	87.95	47	130.45	9
52.95	38	71.95	113	95.15	33	131.20	17
56.80	12	72.95	20	96.95	3	138.90	11
57.05	2	74.45	13	98.80	19	140.90	10
57.95	44	78.85	4	99.95	23		
58.95	111	81.70	14	100.95	78		
65.90	10	82.55	24	106.05	11		
67.00	16	83.95	42	109.20	14		
67.95	50	85.00	106	119.75	11		
68.95	18	86.00	44	121.90	24		

CTMP Compounds

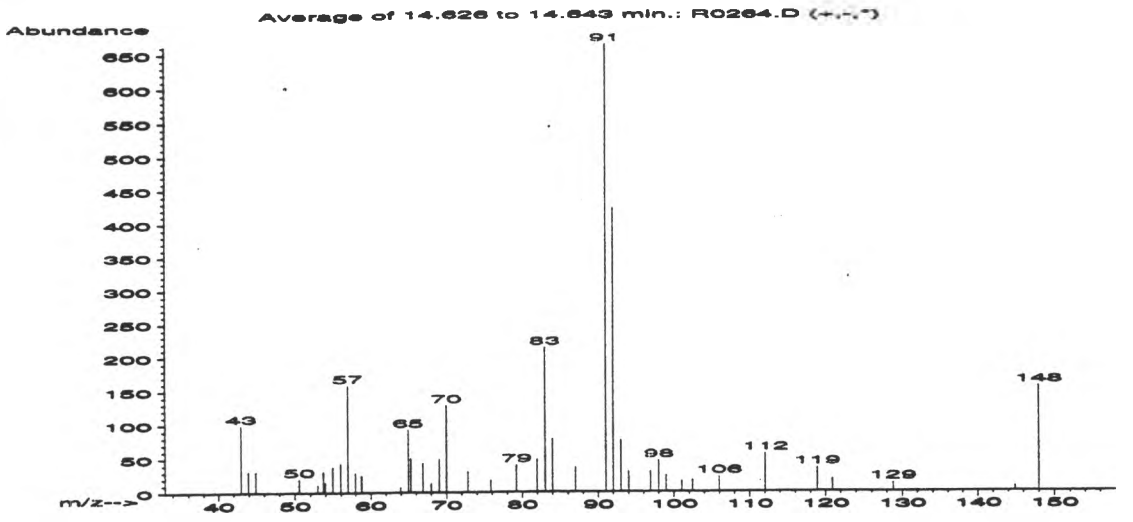
Average of 14.561 to 14.577 min.: R0264.D
Converted from RTE data file: >R0264:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3-Dioxolane-2-propanal, 2-methyl-	144	C7H12O3	47
2.	3,3-D2-HEPTANE	100	C7H14D2	40
3.	Cyclohexane, 1,4-dimethoxy-2-methyl-, st	158	C9H18O2	28
4.	Cyclohexane, 1,4-dimethoxy-2-methyl-, st	158	C9H18O2	28
5.	3,4-DI-O-METHYL-L-ARABINOPYRANOSE	178	C7H14O5	25
6.	1-METHYL MANNOSE ETHYLACETAL	192	C8H16O5	20
7.	1,3-Dioxolane, 2-(1,1-dimethylethyl)-2-m	144	C8H16O2	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	024108-29-0	10591	47	18	0	85	40	20	14	41	8564
2.	40	000000-00-0	1232	41	82	0	68	35	16	0	33	9472
3.	28	030363-88-3	16167	34	72	2	99	40	8	0	22	9014
4.	28	029887-66-9	16168	34	98	3	99	36	8	0	22	9088
5.	25	086049-20-9	24446	41	65	1	72	51	7	5	34	8643
6.	20	000000-00-0	30579	34	112	3	67	50	4	0	18	8430
7.	17	006135-54-2	10713	36	43	1	99	51	3	0	22	8220

CTMP Compounds



Average of 14.626 to 14.643 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	99	58.80	25	81.95	48	101.05	16
43.95	31	63.90	8	83.00	214	102.45	18
44.90	31	64.95	92	84.00	78	105.95	22
50.55	20	65.25	50	87.00	36	112.05	56
53.00	12	66.90	43	91.00	662	118.90	35
53.70	31	68.00	13	92.00	422	120.90	19
53.95	15	69.05	49	93.00	76	128.80	13
54.95	38	69.95	128	94.00	30	144.90	8
55.95	43	72.80	31	96.90	30	148.00	156
56.95	158	75.80	18	98.00	46		
57.95	29	79.20	40	98.95	24		

CTMP Compounds

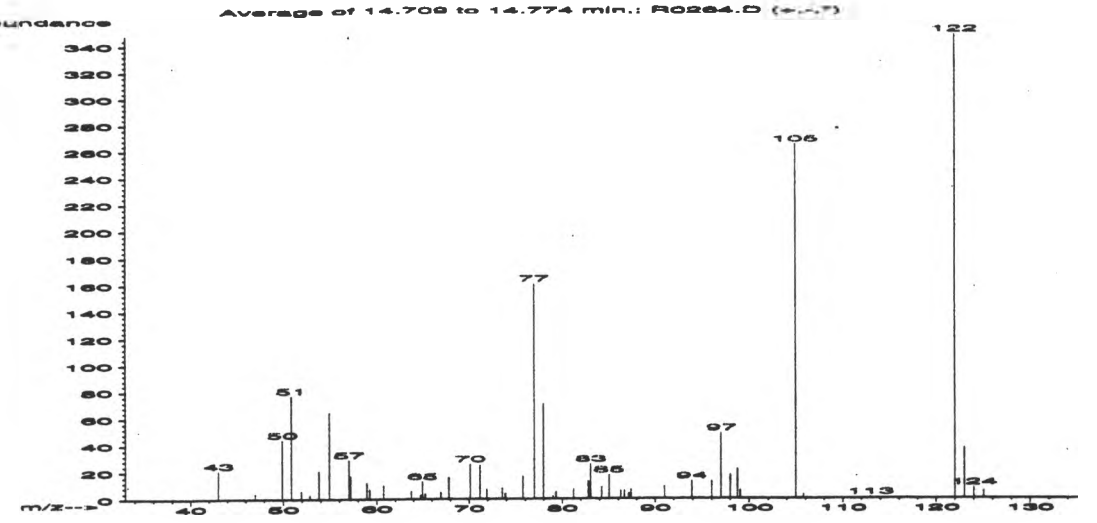
Average of 14.626 to 14.643 min.: R0264.D
Converted from RTE data file: >R0264:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, pentyl-	148	C11H16	49
2.	Benzene, pentyl-	148	C11H16	38
3.	Benzene, pentyl-	148	C11H16	38
4.	TRICYCLO[3.2.1.0(2,4)]OCTANE, 3-METHYLEN	120	C9H12	17
5.	Benzene, methyl-	92	C7H8	16
6.	Benzene, methyl-	92	C7H8	16
7.	Benzene, (3-methylbutyl)-	148	C11H16	10
8.	Benzene, (3-methylbutyl)-	148	C11H16	8
9.	Cyclopentane, propyl-	112	C8H16	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000538-68-1	123433	37	51	0	84	39	23	10	43	9446
2.	*38	000538-68-1	123435	32	53	0	98	37	14	2	35	9459
3.	*38	000538-68-1	12102	32	54	0	91	37	14	2	35	9434
4.	17	000000-00-0	4171	34	73	1	68	54	3	0	21	9153
5.	*16	000108-88-3	117433	31	53	0	73	60	3	0	33	9221
6.	*16	000108-88-3	117431	28	50	0	99	60	3	0	33	9257
7.	*10	002049-94-7	123439	28	71	1	112	63	1	0	27	9115
8.	* 8	002049-94-7	123440	28	64	1	116	69	1	0	27	8635
9.	* 7	002040-96-2	119100	29	68	1	45	72	1	0	27	2998

Peak 40; Benzoic Acid



Average of 14.709 to 14.774 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	21	59.25	7	73.55	8	85.00	18
47.05	4	60.75	10	73.90	4	86.25	6
49.90	44	63.75	6	75.75	17	86.65	6
50.85	77	64.75	3	76.95	161	87.15	4
51.95	6	64.95	13	77.95	71	87.40	7
52.85	3	65.25	4	79.00	2	91.00	9
53.80	21	66.95	5	79.30	5	93.90	13
54.95	65	67.80	16	81.20	7	96.00	13
57.00	29	70.10	26	82.80	13	97.00	49
57.20	17	71.15	25	83.05	26	98.00	18
58.95	12	71.90	7	84.20	9	98.75	22

Average of 14.709 to 14.774 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	6						
104.95	265						
105.80	3						
112.95	1						
122.00	348						
123.00	38						
124.00	8						
125.05	6						

CTMP Compounds

Average of 14.709 to 14.774 min.: R0264.D
Converted from RTE data file: >R0264:

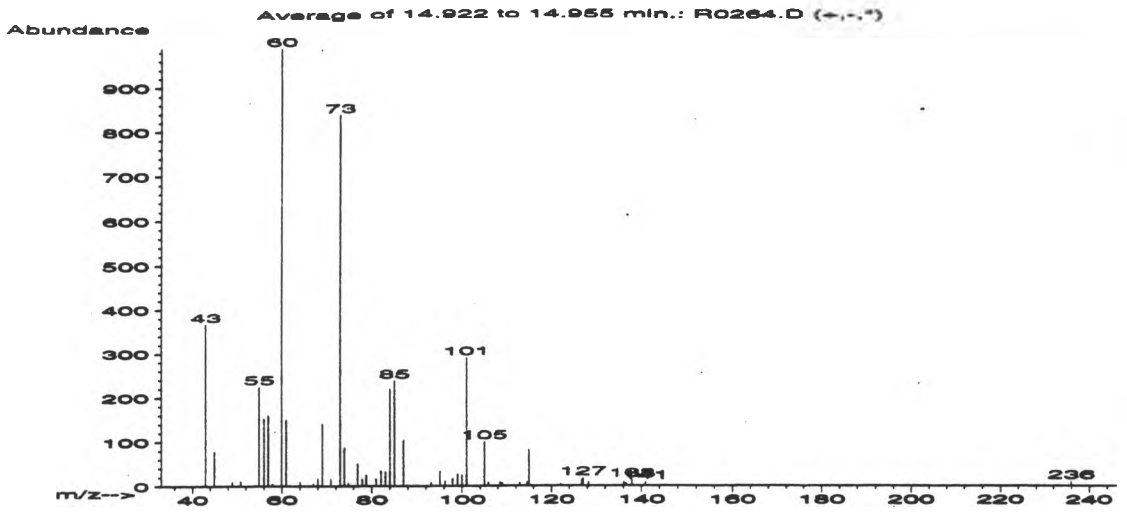
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzoic acid	122	C7H6O2	72
2.	Benzoic acid	122	C7H6O2	72
3.	Benzoic acid	122	C7H6O2	72
4.	3-Pyridinecarboxaldehyde, oxime, (E)-	122	C6H6N2O	64
5.	Benzoic acid	122	C7H6O2	64
6.	Phenol, 2,6-dimethyl-	122	C8H10O	64
7.	Phenol, 2,6-dimethyl-	122	C8H10O	64
8.	Benzoic acid	122	C7H6O2	64
9.	Benzoic acid	122	C7H6O2	58
10.	Benzene, 1-methoxy-4-methyl-	122	C8H10O	53
11.	Benzoic acid, silver(1+) salt	228	C7H5AgO2	50
12.	Benzoic acid, silver(1+) salt	229	C7H6AgO2	50
13.	Benzene, 1-methoxy-4-methyl-	122	C8H10O	50
14.	Benzene, 1-methoxy-4-methyl-	122	C8H10O	50
15.	Benzene, 1-methoxy-3-methyl-	122	C8H10O	50
16.	Benzene, 1-methoxy-2-methyl-	122	C8H10O	50
17.	Benzene, 1-methoxy-4-methyl-	122	C8H10O	45
18.	1,2-Cyclononadiene	122	C9H14	45
19.	Cyclohexane, 1,2-propadienyl-	122	C9H14	45
20.	2-Pyridinecarboxaldehyde, oxime, (E)-	122	C6H6N2O	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	000065-85-0	120160	62	30	2	86	18	42	10	49	9635
2.	*72	000065-85-0	120154	55	33	2	80	18	42	10	43	9591
3.	*72	000065-85-0	4328	65	33	2	75	18	42	10	47	9454
4.	*64	051892-16-1	4316	37	59	3	99	18	37	0	39	8490
5.	*64	000065-85-0	120156	57	36	2	76	19	37	3	38	9555
6.	*64	000576-26-1	120221	37	75	2	99	20	37	0	39	8200
7.	*64	000576-26-1	120219	37	76	2	99	20	37	0	39	8211
8.	*64	000065-85-0	120159	57	38	3	77	18	37	21	39	9096
9.	*58	000065-85-0	120155	55	42	2	75	27	32	24	46	9374
10.	*53	000104-93-8	120269	35	66	2	97	30	28	0	39	8097
11.	50	000532-31-0	130178	52	68	1	78	19	25	4	33	9374
12.	50	000532-31-0	47319	52	64	2	77	19	25	7	36	9374
13.	*50	000104-93-8	120267	38	71	2	94	20	25	0	35	8257
14.	*50	000104-93-8	120264	40	72	1	83	20	25	0	33	8252
15.	*50	000100-84-5	120259	40	74	1	99	20	25	0	33	8252
16.	*50	000578-58-5	120256	39	74	1	93	20	25	0	35	8254
17.	*45	000104-93-8	120266	30	71	2	92	25	19	0	33	8226
18.	*45	001123-11-1	120280	31	95	0	99	23	19	0	33	8063
19.	*45	005664-17-5	120279	31	91	0	99	23	19	0	33	8063
20.	*43	001193-96-0	4315	33	59	2	99	44	18	5	40	7974

CTMP Compounds

Peak 41; Octanoic Acid



Average of 14.922 to 14.955 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	366	64.00	10	80.95	16	100.00	25
44.95	78	67.00	7	82.00	35	100.95	290
48.95	10	67.95	18	83.00	32	104.95	100
50.85	11	69.00	141	84.00	220	105.80	8
54.25	1	70.95	17	85.00	238	108.45	9
54.95	224	72.95	837	87.00	104	108.95	7
56.00	153	73.90	87	93.15	8	112.90	8
56.95	160	74.80	7	95.05	34	114.50	9
57.90	5	76.95	51	96.25	11	115.00	82
59.90	989	77.95	16	97.90	17	122.05	5
60.90	150	78.80	25	98.95	27	126.70	14

Average of 14.922 to 14.955 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	18						
128.30	8						
136.05	8						
136.55	6						
137.90	13						
140.90	8						
235.95	10						

CTMP Compounds

Average of 14.922 to 14.955 min.: R0264.D
Converted from RTE data file: >R0264:

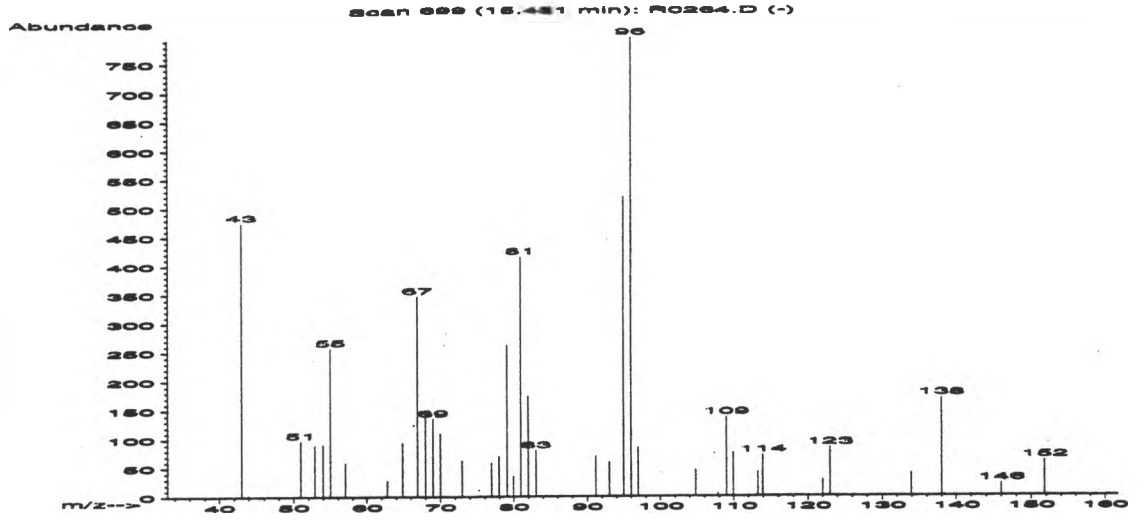
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Octanoic acid	144	C8H16O2	72
2.	Octanoic acid	144	C8H16O2	64
3.	Octanoic acid	144	C8H16O2	64
4.	Octanoic acid, silver(1+) salt	251	C8H16AgO2	56
5.	Octanoic acid	144	C8H16O2	56
6.	1H-Indole-2,3-dione, 5-methyl-	161	C9H7NO2	50
7.	Dodecanoic acid	200	C12H24O2	45
8.	Dodecanoic acid	200	C12H24O2	43
9.	Hexanoic acid	116	C6H12O2	43
10.	Glycine, N-methyl-N-(1-oxododecyl)-	271	C15H29NO3	42
11.	Dodecanoic acid	200	C12H24O2	40
12.	Decanoic acid	172	C10H20O2	38
13.	Hexanoic acid	116	C6H12O2	37
14.	Hexanoic acid	116	C6H12O2	37
15.	Hexanoic acid	116	C6H12O2	37
16.	Dodecanoic acid	200	C12H24O2	36
17.	Undecanoic acid	186	C11H22O2	36
18.	Octanoic acid, 1,2,3-propanetriyl ester	470	C27H50O6	36
19.	Tridecanoic acid	214	C13H26O2	33
20.	Decanoic acid	172	C10H20O2	33

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000124-07-2	122868	55	49	1	75	13	42	6	38	9831
2.	64	000124-07-2	122867	53	48	0	68	18	37	5	41	9826
3.	64	000124-07-2	10653	64	38	0	72	8	37	8	37	9780
4.	56	024927-67-1	56736	63	78	3	85	13	30	0	36	9907
5.	56	000124-07-2	122871	63	44	2	89	13	30	0	36	9857
6.	50	000608-05-9	124979	45	49	1	75	31	25	10	38	9703
7.	45	000143-07-7	128389	43	94	1	73	21	19	0	35	9829
8.	43	000143-07-7	128386	43	78	0	63	44	18	12	41	9794
9.	43	000142-62-1	119462	43	40	0	96	44	18	16	41	9083
10.	42	000097-78-9	63887	45	100	2	78	29	17	0	35	9677
11.	40	000143-07-7	128385	45	85	1	78	31	16	0	37	9693
12.	38	000334-48-5	126157	40	70	2	84	36	14	4	31	9513
13.	37	000142-62-1	119466	39	43	1	99	44	13	2	31	9027
14.	37	000142-62-1	119463	43	58	1	94	44	13	0	37	9046
15.	37	000142-62-1	3409	41	45	1	86	44	13	9	31	9082
16.	36	000143-07-7	128387	34	101	2	84	26	12	0	22	9771
17.	36	000112-37-8	127364	40	88	2	84	29	12	0	29	9774
18.	36	000538-23-8	136794	63	40	1	86	29	12	1	28	9873
19.	33	000638-53-9	129335	34	85	1	70	31	10	4	26	9648
20.	33	000334-48-5	126152	31	67	1	99	35	10	1	22	9608

CTMP Compounds

Peak 42; Unidentified Terpene



Scan 699 (15.481 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	474	69.00	135	93.00	59	123.00	84
43.90	3	70.00	110	95.00	517	133.90	39
50.95	97	72.95	62	96.00	791	138.00	168
52.80	90	76.90	58	96.95	85	146.00	21
53.95	91	77.95	69	104.80	45	151.80	61
54.95	257	79.05	262	107.85	5		
57.00	59	79.95	36	109.00	137		
62.80	28	80.95	414	109.95	75		
64.90	94	81.95	173	113.25	42		
66.90	346	83.05	80	113.90	71		
68.00	142	91.15	70	122.00	28		

CTMP Compounds

Scan 699 (15.481 min): R0264.D

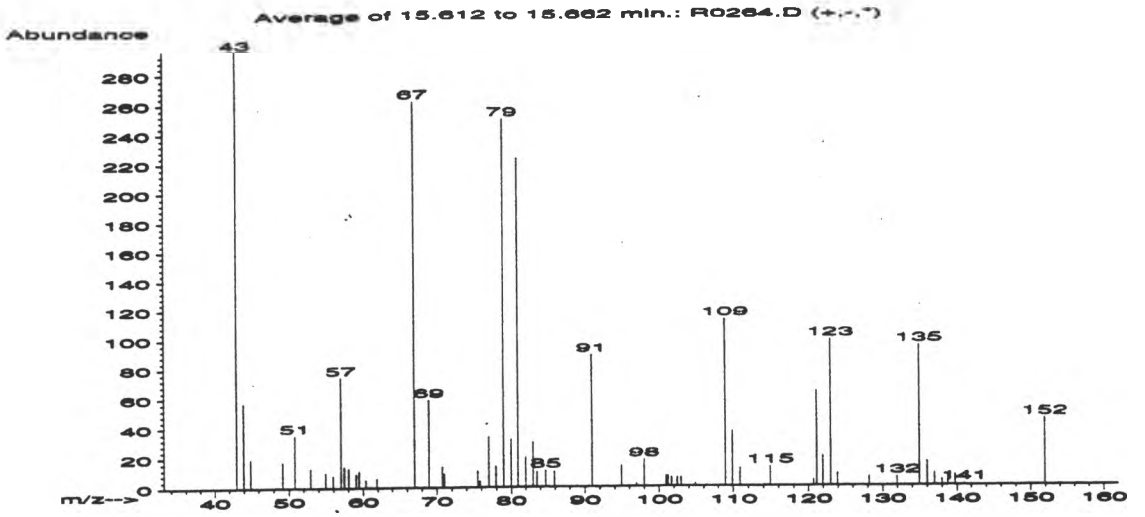
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Spiro[4.5]decane	138	C10H18	72
2.	2-Cyclohexen-1-one, 4,4,5-trimethyl-	138	C9H14O	50
3.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	49
4.	Cyclohexane, 1-methyl-4-(1-methylethenyl	138	C10H18	46
5.	Cyclohexane, 1-methyl-4-(1-methylethylid	138	C10H18	46
6.	Cyclohexene, 1-methyl-4-(1-methylethyl)-	138	C10H18	46
7.	Cyclohexane, 1-methyl-4-(1-methylethylid	138	C10H18	46
8.	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	43
9.	1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	43
10.	Cyclohexane, 1-methyl-3-(1-methylethylid	138	C10H18	43
11.	Spiro[3.4]octan-1-one, 5-methyl-, cis-	138	C9H14O	43
12.	2-Cyclohexen-1-one, 4,4,6-trimethyl-	138	C9H14O	38
13.	1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	38
14.	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	138	C10H18	38
15.	1H-Imidazole-4-ethanamine, 5-methyl-	125	C6H11N3	38
16.	5-Eicosyne	278	C20H38	35
17.	(-)-NEOMENTHYLACETATE	198	C12H22O2	35
18.	Naphthalene, decahydro-, cis-	138	C10H18	35
19.	Cyclohexene, 1-isopentyl-	152	C11H20	27
20.	CYCLOBUTENE, 1,2,3,4-TETRAMETHYL-	110	C8H14	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	000176-63-6	8822	76	35	1	77	18	42	28	50	8913
2.	*50	017429-29-7	8623	49	48	1	99	33	25	1	41	9397
3.	*49	002758-18-1	117591	50	58	1	77	38	23	0	44	9164
4.	*46	001879-07-8	8808	57	57	1	50	45	20	0	49	8183
5.	*46	001124-27-2	8812	56	52	1	65	44	20	0	49	7345
6.	*46	029350-67-2	122304	64	52	1	60	44	20	0	50	7555
7.	*46	001124-27-2	122319	64	51	1	60	44	20	0	50	7495
8.	*43	061177-16-0	13884	45	54	0	65	48	18	0	44	7461
9.	*43	000694-31-5	560	45	47	0	90	46	18	0	44	8971
10.	*43	013828-34-7	8811	60	39	0	65	42	18	2	41	6963
11.	*43	065147-55-9	8649	46	73	0	52	46	18	0	44	7081
12.	*38	013395-73-8	8624	35	67	0	60	48	14	0	41	9207
13.	*38	000694-48-4	559	37	56	0	90	46	14	0	41	8976
14.	38	000554-59-6	8831	47	58	0	51	46	14	2	41	7306
15.	38	036376-47-3	4985	47	38	0	84	46	14	8	41	8979
16.	35	074685-31-7	66578	57	69	0	36	54	11	12	41	8153
17.	35	000000-00-0	33967	45	69	0	55	52	11	19	41	6726
18.	*35	000493-01-6	122333	37	65	0	42	51	11	0	41	8116
19.	*27	003983-04-8	124044	36	46	0	45	57	8	0	41	8819
20.	*25	003200-65-5	2267	52	43	0	52	61	7	22	44	6344

CTMP Compounds

Peak 43; Unidentified Terpene



Average of 15.612 to 15.662 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	296	59.05	9	77.90	14	96.95	2
43.95	57	59.45	11	78.95	249	98.00	18
44.90	19	60.40	5	79.95	32	100.95	7
49.20	17	61.90	6	80.90	223	101.20	7
50.80	35	67.00	261	82.00	20	101.70	6
52.90	13	68.95	59	83.00	30	102.45	6
54.90	10	70.75	14	83.55	10	102.95	6
55.90	8	71.00	9	84.70	11	104.90	2
57.00	74	75.45	11	85.90	10	108.95	113
57.45	14	75.75	4	90.95	89	109.90	37
58.05	13	76.95	34	94.95	14	110.90	12

Average of 15.612 to 15.662 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.90	13	137.95	4				
120.70	4	138.75	6				
121.10	64	139.75	7				
121.95	20	141.00	1				
123.00	99	151.95	45				
123.90	8						
128.20	6						
131.95	6						
134.95	95						
136.00	16						
136.95	8						

CTMP Compounds

Average of 15.612 to 15.662 min.: R0264.D
Converted from RTE data file: >R0264:

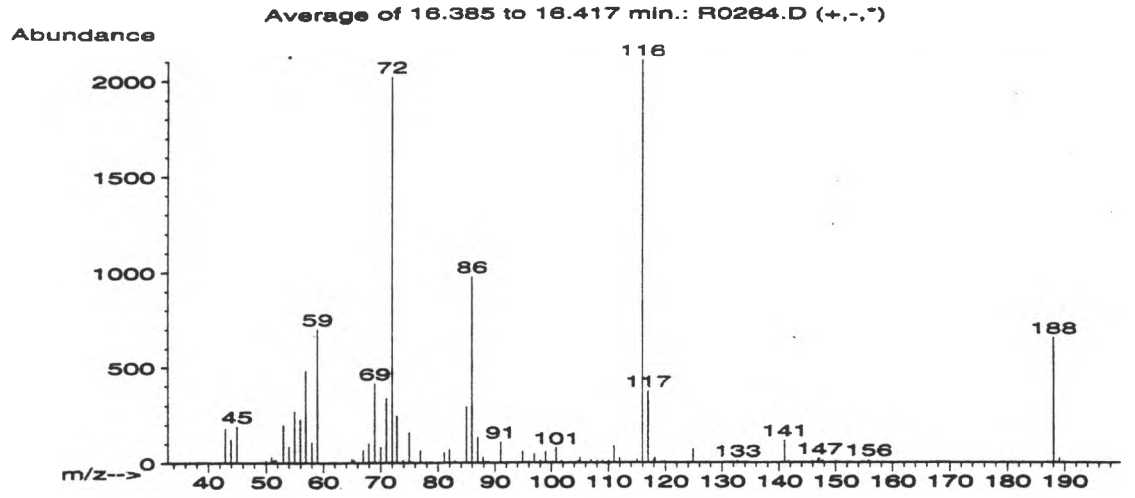
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,4-Undecadiene, (Z)-	152	C11H20	53
2.	6-Formyl-2-oxabicyclo[3.3.0]oct-6-en-3-o	152	C8H8O3	46
3.	VINYLCYCLOOCTANE	138	C10H18	43
4.	Cyclooctane, ethenyl-	138	C10H18	43
5.	ETHYLIDENECYCLOOCTANE	138	C10H18	37
6.	Ethylidenecyclooctane	138	C10H18	37
7.	Pulegone	152	C10H16O	37
8.	1-Methylcyclooctyl isocyanide	151	C10H17N	23
9.	cis[2-[(1E,3Z)-1,3-Butadienyl]cyclopenty	152	C10H16O	17
10.	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimet	152	C10H16O	14
11.	Fenchone	152	C10H16O	14
12.	Fenchone	152	C10H16O	14
13.	Cyclohexanol, 4-sec-butyl-	156	C10H20O	12
14.	Fenchone	152	C10H16O	10
15.	Cyclohexene, 3-bromo-	160	C6H9Br	10
16.	1,4-Cyclononadiene	122	C9H14	10
17.	Bicyclo[3.1.0]hexan-2-ol, acetate, (1.al	140	C8H12O2	10
18.	1H-Pyrrole, 1-butyl-	123	C8H13N	10
19.	1H-Pyrrole, 1-butyl-	123	C8H13N	9
20.	1H-Purine-2,6-dione, 3,7-dihydro-	152	C5H4N4O2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	055976-14-2	13855	44	79	2	87	28	28	0	39	8975
2.	*46	042186-08-3	13374	54	45	1	84	42	20	0	49	8096
3.	*43	013151-62-7	8837	45	78	2	68	43	18	0	39	7576
4.	*43	061142-41-4	122320	45	78	2	68	43	18	0	39	7576
5.	37	019780-51-9	8838	38	71	2	68	43	13	2	31	8139
6.	37	000000-00-0	8814	38	71	2	68	43	13	2	31	8139
7.	*37	000089-82-7	123989	36	70	2	75	41	13	6	35	8058
8.	23	086559-22-0	13192	38	29	1	76	49	6	0	29	7623
9.	*17	090542-13-5	13641	31	81	2	84	52	3	0	29	7666
10.	*14	004695-62-9	13780	40	44	0	57	69	2	11	38	5587
11.	*14	001195-79-5	124016	41	43	0	67	69	2	9	38	5656
12.	*14	001195-79-5	13781	48	41	0	72	69	2	6	41	5292
13.	12	006292-20-2	15569	42	58	1	69	58	2	0	29	6657
14.	*10	001195-79-5	124012	33	58	1	75	69	1	0	35	5316
15.	10	001521-51-3	16576	35	46	1	75	69	1	11	33	6310
16.	*10	027538-12-1	4474	35	69	3	118	70	1	0	35	6477
17.	*10	000698-56-6	9253	33	67	3	256	74	1	0	39	4355
18.	*10	000589-33-3	120322	39	59	2	74	68	1	0	35	5856
19.	* 9	000589-33-3	120321	34	64	2	52	71	1	7	36	4695
20.	* 9	000069-89-6	13237	29	72	0	52	71	1	0	33	6266

CTMP Compounds

Peak 44; Unidentified Hydrocarbon



Average of 16.385 to 16.417 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	179	56.90	481	72.85	244	86.95	134
43.90	122	58.00	109	73.90	12	87.90	28
44.95	192	58.95	701	74.95	158	91.00	108
49.95	12	65.00	21	76.90	63	92.95	1
50.90	33	65.40	16	77.95	5	94.90	59
51.30	15	67.00	66	81.05	53	96.00	6
51.70	16	67.95	100	81.95	68	97.00	47
52.95	198	69.00	414	82.95	10	98.00	12
53.95	85	70.00	82	84.00	2	98.95	56
54.95	268	70.95	336	84.95	293	100.20	7
55.95	227	72.00	2015	85.90	977	100.85	78

Average of 16.385 to 16.417 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.80	11	115.95	2104	141.75	9	189.05	23
104.30	8	116.95	373	145.75	6	189.75	6
104.70	9	117.90	17	146.00	8		
105.00	27	118.15	26	146.90	21		
106.95	14	119.40	6	147.15	21		
108.05	11	119.90	7	147.75	12		
109.00	12	124.00	7	150.00	6		
110.05	11	124.85	71	155.80	14		
111.00	88	127.05	6	158.20	5		
111.95	24	132.70	10	187.05	6		
115.00	20	141.00	117	188.05	659		

CTMP Compounds

Average of 16.385 to 16.417 min.: R0264.D
Converted from RTE data file: >R0264:

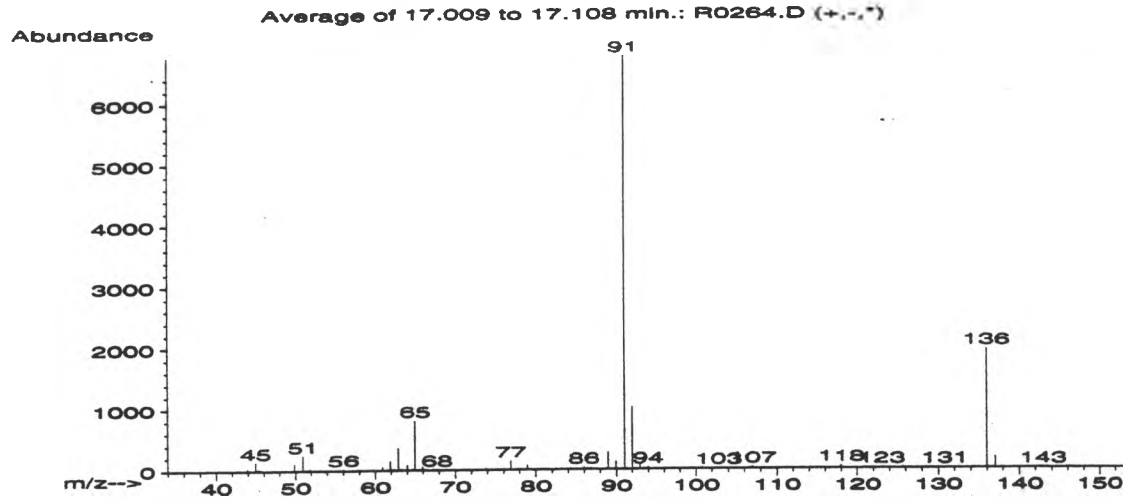
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,2-DIMETHYL-1-OXA-2-SILACYCLOHEXANONE-6	144	C6H12O2Si	36
2.	Thiourea, tetraethyl-	188	C9H20N2S	16
3.	1,1,2-TRIMETHYL-1-SILACYCLOBUTANE	114	C6H14Si	16
4.	Thiourea, tetraethyl-	188	C9H20N2S	12
5.	2(3H)-Furanone, dihydro-	86	C4H6O2	9
6.	2-(TRIMETHYLSILOXY)ETHYL ESTER-THIOCYANI	175	C6H13NOSSi	8
7.	Methanetricarboxaldehyde	100	C4H4O3	8
8.	1,5-Hexadiene-3,4-diol, 2,5-dimethyl-	142	C8H14O2	8
9.	L-Valine	117	C5H11NO2	8
10.	3-Dodecanone	184	C12H24O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	36	015129-96-1	10538	40	67	2	95	27	12	4	25	9196
2.	*16	004274-15-1	29076	34	79	1	68	57	3	7	36	7385
3.	16	030681-90-4	3075	43	66	2	68	58	3	0	31	7033
4.	*12	004274-15-1	127473	30	85	2	78	57	2	0	29	7379
5.	* 9	000096-48-0	117007	29	61	2	118	80	1	0	33	3344
6.	8	000000-00-0	23305	39	54	2	99	66	1	0	28	6584
7.	8	018655-47-5	1042	42	51	3	90	67	1	0	29	6207
8.	8	004723-10-8	122654	33	55	2	67	70	1	0	25	6197
9.	8	000072-18-4	119670	34	46	2	85	68	1	4	26	6211
10.	7	001534-27-6	127228	37	75	2	73	78	1	0	25	6209

CTMP Compounds

Peak 45; Benzeneacetic Acid



Average of 17.009 to 17.108 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	37	57.95	8	76.05	4	88.95	279
44.95	138	59.70	13	76.90	139	89.95	127
45.15	15	60.90	51	77.80	9	91.00	6763
45.40	18	61.90	146	78.05	17	92.00	1021
48.20	4	62.90	355	79.00	68	92.95	72
49.85	107	64.00	76	84.30	7	93.50	9
50.95	243	65.00	811	85.50	6	93.95	29
51.85	27	65.95	57	85.95	29	96.50	6
53.20	11	67.75	3	86.15	5	98.15	4
55.55	5	73.85	26	86.45	12	99.45	4
56.00	18	75.00	9	86.85	18	99.95	8

Average of 17.009 to 17.108 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.55	3	118.00	45	138.00	6		
100.80	9	121.00	3	141.00	3		
102.80	10	121.95	6	142.90	3		
104.85	9	123.00	12				
106.70	5	124.15	2				
107.00	24	125.95	5				
107.95	7	129.55	4				
111.05	8	130.80	7				
114.00	3	135.00	14				
114.75	3	135.95	1967				
115.00	3	137.00	184				

CTMP Compounds

Average of 17.009 to 17.108 min.: R0264.D
Converted from RTE data file: >R0264:

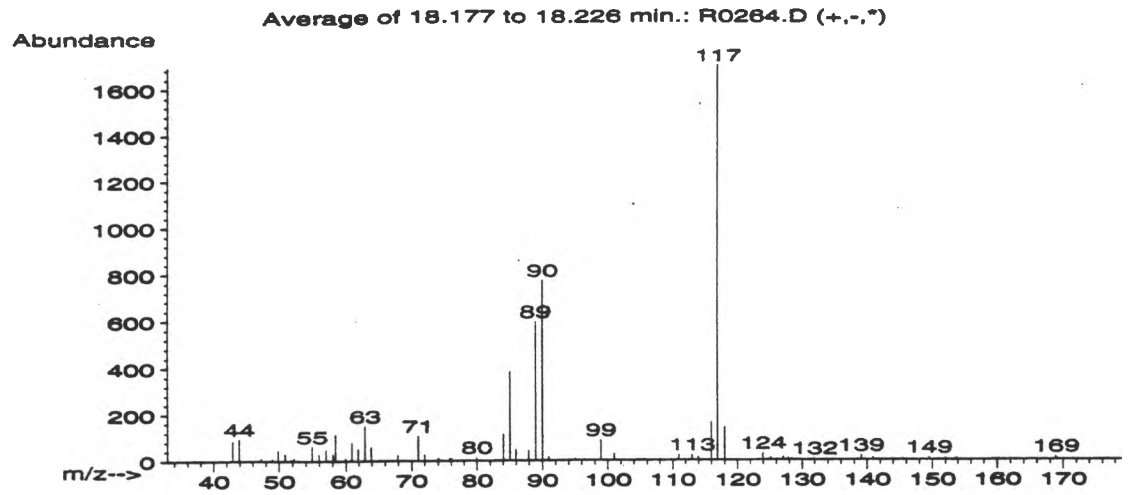
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzeneacetic acid	136	C8H8O2	91
2.	Benzeneacetic acid	136	C8H8O2	91
3.	Benzeneacetic acid	136	C8H8O2	83
4.	Benzeneacetic acid	136	C8H8O2	80
5.	Propanedioic acid, phenyl-	180	C9H8O4	53
6.	Benzoic acid, 3-methyl-	136	C8H8O2	50
7.	Benzeneacetaldehyde	120	C8H8O	47
8.	Benzene, (iodomethyl)-	218	C7H7I	47
9.	Benzene, methyl-	92	C7H8	46
10.	1,3,5-Cycloheptatriene	92	C7H8	43
11.	Phosphonous dichloride, (phenylmethyl)-	192	C7H7Cl2P	40
12.	SPIRO(2,4)HEPTADIENE-(2,4)	92	C7H8	40
13.	Benzene, methyl-	92	C7H8	38
14.	Spiro[3.3]hepta-1,5-diene	92	C7H8	38
15.	Cycloheptatrienylium, iodide	218	C7H7I	38
16.	Benzene, methyl-	92	C7H8	35
17.	Tetracyclo[4.1.0.0(2,4).0(3,5)]heptane	92	C7H8	32
18.	Benzenemethanesulfonamide	171	C7H9NO2S	32
19.	Benzene, methyl-	92	C7H8	30
20.	1,3,5-Cycloheptatriene	92	C7H8	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000103-82-2	7792	71	10	0	83	0	62	0	76	9983
2.	*91	000103-82-2	121830	68	12	0	69	0	62	0	76	9974
3.	*83	000103-82-2	121834	58	17	2	43	15	50	0	56	9653
4.	*80	000103-82-2	121833	53	33	2	64	15	48	0	47	9969
5.	53	002613-89-0	25412	46	40	2	61	28	28	3	38	9950
6.	*50	000099-04-7	7790	41	40	1	42	18	25	0	33	9506
7.	47	000122-78-1	119981	43	28	0	59	40	20	2	41	9484
8.	47	000620-05-3	42507	44	39	1	70	37	20	0	39	9593
9.	*46	000108-88-3	117430	50	18	0	17	43	20	26	44	8395
10.	*43	000544-25-2	117441	35	27	0	39	46	18	10	43	9369
11.	40	004545-85-1	30522	42	42	1	86	34	16	2	35	9584
12.	*40	000000-00-0	418	40	31	1	95	31	16	0	35	9575
13.	*38	000108-88-3	117431	42	25	1	30	50	14	9	38	8827
14.	*38	022635-78-5	420	37	27	1	48	46	14	0	39	9493
15.	38	001316-80-9	42508	45	30	2	92	37	14	4	37	8471
16.	*35	000108-88-3	117429	37	26	0	25	53	11	11	38	8748
17.	*32	050861-26-2	424	31	3	0	80	50	9	2	35	9581
18.	32	004563-33-1	21753	39	46	1	55	50	9	0	33	9543
19.	*30	000108-88-3	117433	36	22	0	20	59	9	23	43	8353
20.	*27	000544-25-2	416	35	34	0	31	59	8	0	41	9198

CTMP Compounds

Peak 46; Indole



Average of 18.177 to 18.226 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	87	58.05	30	72.00	26	87.95	44
43.90	95	58.45	113	73.85	3	88.95	594
47.30	11	59.95	13	74.05	11	90.00	770
48.95	8	60.90	79	75.80	12	90.95	17
49.85	45	61.90	51	76.10	8	95.00	8
50.90	29	62.95	149	78.30	4	96.40	3
51.80	5	63.90	58	78.95	4	98.95	87
52.20	11	65.05	2	79.95	14	100.95	27
54.95	63	67.95	24	84.05	113	105.55	5
55.95	27	70.05	2	85.05	383	108.05	5
57.00	49	71.00	105	85.95	49	110.05	1

Average of 18.177 to 18.226 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.95	22	127.80	8				
113.00	23	128.30	4				
113.90	14	130.95	3				
116.00	164	131.95	5				
116.95	1691	139.10	19				
118.00	141	140.90	11				
123.95	29	145.50	5				
124.90	4	149.50	11				
125.20	10	151.95	7				
126.05	3	153.80	8				
127.05	14	168.90	14				

CTMP Compounds

Average of 18.177 to 18.226 min.: R0264.D
Converted from RTE data file: >R0264:

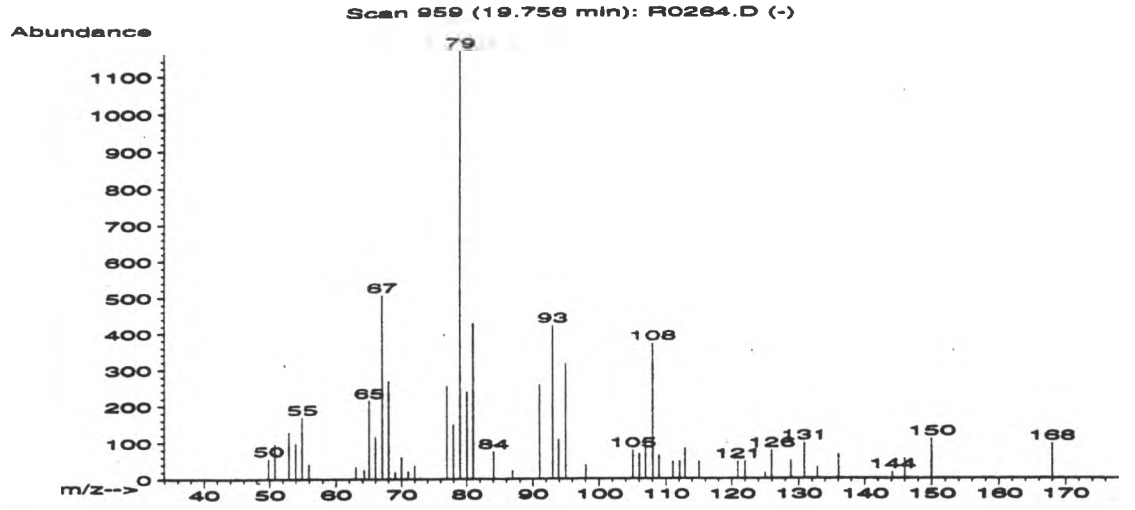
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Indole	117	C8H7N	81
2.	(E)-1-Azido-2-phenylethene	145	C8H7N3	74
3.	1H-Indole	117	C8H7N	72
4.	Benzeneacetonitrile	117	C8H7N	64
5.	1H-Indole	117	C8H7N	64
6.	1H-Indole	117	C8H7N	64
7.	1H-Indole	117	C8H7N	64
8.	Benzene, (isocyanomethyl)-	117	C8H7N	53
9.	1H-Indole	117	C8H7N	50
10.	Benzonitrile, 2-methyl-	117	C8H7N	45
11.	Benzeneacetonitrile	117	C8H7N	45
12.	1H-Indole	117	C8H7N	45
13.	1H-Indole	117	C8H7N	45
14.	Benzonitrile, 4-methyl-	117	C8H7N	45
15.	Benzonitrile, 4-methyl-	117	C8H7N	45
16.	8-Quinolinol	145	C9H7NO	45
17.	1H-Indole	117	C8H7N	45
18.	Benzene, (3-chloro-1-propenyl)-	152	C9H9Cl	38
19.	Benzeneacetonitrile	117	C8H7N	38
20.	2A,7-DIHYDRO[1,2]DIAZETO[4,1-A]ISOINDOLE	144	C9H8N2	37

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*81	000120-72-9	119700	65	25	1	88	16	49	0	64	9781
2.	74	018756-03-1	11002	32	14	1	70	3	44	11	33	9730
3.	*72	000120-72-9	119695	62	27	2	93	20	42	3	49	9771
4.	*64	000140-29-4	119686	53	44	2	76	23	37	0	49	9542
5.	*64	000120-72-9	119697	43	47	2	97	20	37	0	39	9662
6.	*64	000120-72-9	119694	46	50	2	88	17	37	0	39	9740
7.	*64	000120-72-9	3695	37	50	1	69	19	37	6	39	9575
8.	*53	010340-91-7	3688	43	49	2	90	28	28	15	38	9401
9.	*50	000120-72-9	119699	46	25	2	90	17	25	3	33	9729
10.	*45	000529-19-1	3675	43	54	3	87	23	19	4	30	9179
11.	*45	000140-29-4	119684	44	52	2	86	25	19	4	30	9400
12.	*45	000120-72-9	119698	33	62	3	99	21	19	0	35	9752
13.	*45	000120-72-9	119696	33	76	3	91	25	19	0	30	9506
14.	*45	000104-85-8	119682	44	54	3	88	23	19	9	35	8828
15.	*45	000104-85-8	3677	44	54	3	88	23	19	9	35	8828
16.	45	000148-24-3	123033	41	58	2	84	23	19	10	31	9698
17.	*45	000120-72-9	119701	42	29	1	91	23	19	1	30	9583
18.	38	002687-12-9	13410	43	40	1	71	48	14	16	41	8590
19.	*38	000140-29-4	119685	31	76	3	86	23	14	0	26	9448
20.	37	059523-17-0	10840	47	55	1	57	43	13	2	37	9288

CTMP Compounds

Peak 47; Unidentified Terpene



Scan 959 (19.756 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	2	67.00	505	84.05	74	108.05	370
49.80	56	68.00	268	86.85	23	108.95	63
50.80	96	69.00	19	91.00	256	111.05	47
52.95	129	70.00	59	93.00	420	112.10	48
53.95	97	71.00	21	93.90	108	112.90	83
54.95	169	72.00	37	95.00	314	115.00	47
55.95	40	76.95	254	98.05	38	120.90	47
63.00	34	77.95	149	98.95	1	122.00	48
64.25	26	78.95	1160	105.05	78	124.95	15
65.00	214	80.05	238	106.05	68	125.95	76
66.00	116	80.95	427	106.95	95	128.80	49

Scan 959 (19.756 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.80	96						
132.80	31						
136.05	65						
144.15	18						
146.00	54						
150.00	108						
168.00	95						

CTMP Compounds

Scan 959 (19.756 min): R0264.D

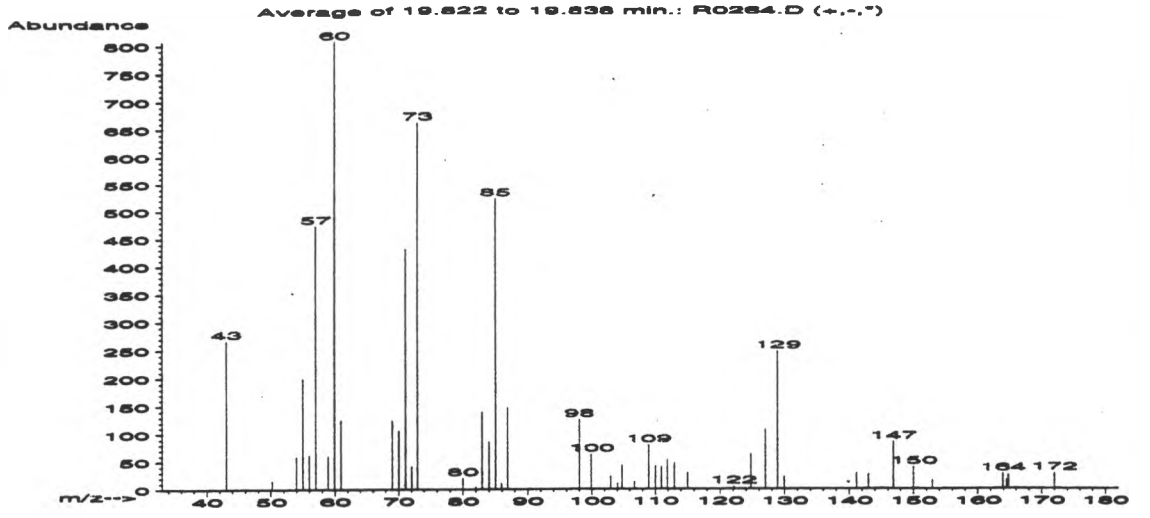
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Cyclohexyl-1-butyne	136	C10H16	59
2.	1,3-Cyclooctadiene	108	C8H12	58
3.	Bicyclo[4.2.0]oct-1(8)-ene	108	C8H12	53
4.	6-Nonynoic acid, methyl ester	168	C10H16O2	53
5.	3-Undecen-5-yne, (Z)-	150	C11H18	52
6.	3-Undecen-5-yne, (E)-	150	C11H18	52
7.	3-Heptadecen-5-yne, (Z)-	234	C17H30	50
8.	1,4-Cyclooctadiene, (Z,Z)-	108	C8H12	43
9.	1,3-Cyclooctadiene, (Z,Z)-	108	C8H12	43
10.	BICYCLO[3.2.0]HEPTANE, 2-METHYLENE-	108	C8H12	43
11.	Cyclopropane, 1-ethenyl-2-hexenyl-, [1.a	150	C11H18	43
12.	4-Ethylidenecyclohexene	108	C8H12	38
13.	cis-4,5-Bis-(cyanomethyl)cyclohexene	160	C10H12N2	38
14.	Tricyclodecanedimethanol	196	C12H20O2	35
15.	3-Methylene-1,6-hexadiene	108	C8H12	35
16.	5-Dodecen-7-yne, (Z)-	164	C12H20	35
17.	6-BUTYL-1,4-CYCLOHEPTADIENE	150	C11H18	30
18.	5-Undecen-3-yne, (E)-	150	C11H18	27
19.	CIS-3-BUTYL-4-VINYL-CYCLOPENTENE	150	C11H18	27
20.	Dispiro[2.1.2.2]nonan-8-one	136	C9H12O	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	057497-06-0	8121	62	56	2	75	21	33	0	39	9353
2.	*58	001700-10-3	1980	67	46	1	68	29	32	0	50	9276
3.	*53	003642-23-7	2008	59	55	1	70	38	28	0	51	8990
4.	53	020731-17-3	20306	61	57	3	99	30	28	0	39	8358
5.	*52	074744-27-7	12908	51	59	2	74	34	27	0	46	9220
6.	*52	074744-29-9	12909	52	58	2	70	33	27	0	46	9244
7.	50	074744-55-1	50158	62	54	0	56	33	25	18	39	9297
8.	*43	016327-22-3	1983	55	47	1	49	45	18	0	40	9033
9.	*43	003806-59-5	1981	60	59	2	64	45	18	0	41	9195
10.	*43	000000-00-0	2002	66	41	1	72	46	18	0	44	8417
11.	*43	022822-99-7	12912	57	40	1	76	44	18	0	40	9011
12.	*38	016631-66-6	1973	35	62	2	92	47	14	7	40	8806
13.	38	000000-00-0	16890	47	42	0	85	46	14	4	41	8584
14.	35	026896-48-0	33029	45	82	0	33	55	11	0	39	8664
15.	35	016626-48-5	1950	58	51	0	51	51	11	0	43	9010
16.	35	016336-83-7	125375	46	52	0	44	55	11	0	39	8851
17.	*30	022735-58-6	12981	52	44	0	35	57	9	0	46	8779
18.	*27	074744-31-3	12907	35	48	0	49	59	8	0	41	8537
19.	27	093779-52-3	12980	43	55	0	32	58	8	0	39	8679
20.	*27	074685-57-7	8039	51	39	1	45	57	8	17	39	8689

CTMP Compounds

Peak 48; Decanoic Acid



Average of 19.822 to 19.838 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	267	71.05	431	99.90	63	122.10	5
50.20	16	72.00	41	102.95	23	124.75	63
53.95	59	72.90	660	104.05	11	127.00	107
54.95	199	79.95	20	104.80	43	128.95	247
56.00	62	82.00	4	106.70	14	129.95	22
57.00	473	82.95	140	108.95	80	141.15	28
58.90	60	84.00	86	110.00	41	143.00	26
59.90	807	85.00	523	111.00	40	146.90	85
60.90	125	85.90	11	111.90	53	150.00	40
69.00	124	86.90	147	113.00	47	152.95	16
70.00	106	98.00	126	115.00	29	163.90	27

Average of 19.822 to 19.838 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
164.50	16						
164.75	24						
172.00	28						

CTMP Compounds

Average of 19.822 to 19.838 min.: R0264.D
Converted from RTE data file: >R0264:

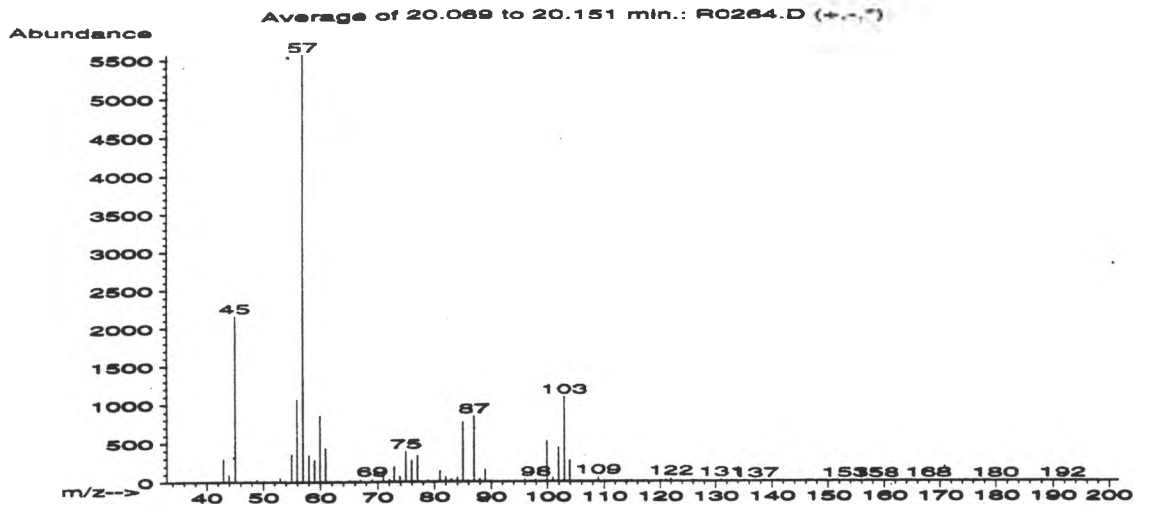
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Decanoic acid	172	C10H20O2	90
2.	Decanoic acid	172	C10H20O2	70
3.	Decanoic acid, silver(1+) salt	279	C10H20AgO2	64
4.	Dodecanamide, N,N-bis(2-hydroxyethyl)-	287	C16H33NO3	47
5.	Decanoic acid	172	C10H20O2	46
6.	D-Glucose, 4-O-.alpha.-D-glucopyranosyl-	342	C12H22O11	40
7.	Nonanoic acid	158	C9H18O2	38
8.	Decanoic acid	172	C10H20O2	38
9.	Decanoic acid	172	C10H20O2	37
10.	Octanoic acid, silver(1+) salt	251	C8H16AgO2	32
11.	Nonanoic acid	158	C9H18O2	25
12.	Nonadecane	268	C19H40	22
13.	Heptane	100	C7H16	14
14.	Octadecane	254	C18H38	12
15.	Octacosane	394	C28H58	12
16.	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	10
17.	Hexadecane, 7,9-dimethyl-	254	C18H38	10
18.	Decane, 5-ethyl-5-methyl-	184	C13H28	10
19.	Octacosane	394	C28H58	10
20.	Nonane, 5-propyl-	170	C12H26	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000334-48-5	126152	79	35	0	91	36	57	0	93	8937
2.	*70	000334-48-5	126151	75	38	2	91	30	41	0	74	8983
3.	64	013126-67-5	66612	87	69	2	73	25	37	0	45	9322
4.	47	000120-40-1	69540	55	88	1	81	40	20	3	39	9282
5.	*46	000334-48-5	22282	44	71	0	67	44	20	0	44	8849
6.	40	000069-79-4	85910	45	119	3	134	34	16	0	37	9152
7.	38	000112-05-0	124679	70	38	1	93	46	14	0	38	8386
8.	*38	000334-48-5	126156	35	31	0	69	48	14	0	41	8754
9.	37	000334-48-5	126153	57	50	2	88	41	13	2	37	8751
10.	32	024927-67-1	56736	46	90	2	97	48	9	15	37	8035
11.	25	000112-05-0	124677	44	58	1	67	55	7	0	37	8164
12.	22	000629-92-5	132089	53	79	1	55	61	5	17	38	5150
13.	14	000142-82-5	118108	44	46	2	60	67	2	10	38	5271
14.	12	000593-45-3	131492	45	67	1	49	61	2	8	37	5285
15.	12	000630-02-4	96901	53	97	1	58	61	2	3	37	5119
16.	10	000638-36-8	132694	53	76	1	53	70	1	8	37	4955
17.	10	021164-95-4	58320	51	51	0	46	73	1	4	38	4971
18.	10	017312-74-2	27768	47	58	1	53	71	1	1	38	4737
19.	10	000630-02-4	135948	44	102	0	58	73	1	0	39	5237
20.	10	000998-35-6	126026	45	49	1	53	78	1	17	38	4187

CTMP Compounds

Peak 7; Unidentifed Oxyhydrocarbon



Average of 20.069 to 20.151 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	293	55.95	1066	69.00	35	79.95	12
43.95	96	56.95	5571	70.05	14	81.00	143
45.00	2163	58.00	346	71.00	184	82.00	60
48.85	30	58.95	282	71.95	27	83.00	36
49.95	5	59.90	861	72.15	23	84.00	56
51.30	4	60.90	437	72.90	198	85.00	773
51.75	9	61.75	14	73.90	73	85.90	25
52.30	7	62.95	19	74.95	389	87.00	850
52.95	54	64.95	23	75.95	271	87.95	38
53.90	17	66.00	15	77.00	339	88.95	157
54.95	361	66.95	31	78.90	17	90.95	7

Average of 20.069 to 20.151 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.00	28	111.00	11	128.85	3	165.90	3
97.95	32	112.70	2	131.05	22	167.65	5
99.95	524	114.00	12	132.95	14	167.90	7
100.95	54	114.95	21	137.05	6	168.40	5
101.95	439	116.90	7	137.40	4	170.00	5
102.95	1098	120.00	11	140.90	5	171.95	1
103.95	272	121.00	28	151.05	4	179.80	4
105.90	1	121.65	7	152.95	7	182.05	3
106.30	4	121.95	42	153.95	2	191.65	3
108.95	55	123.75	1	158.55	3		
110.00	14	126.00	14	165.00	5		

CTMP Compounds

Average of 20.069 to 20.151 min.: R0264.D
Converted from RTE data file: >R0264:

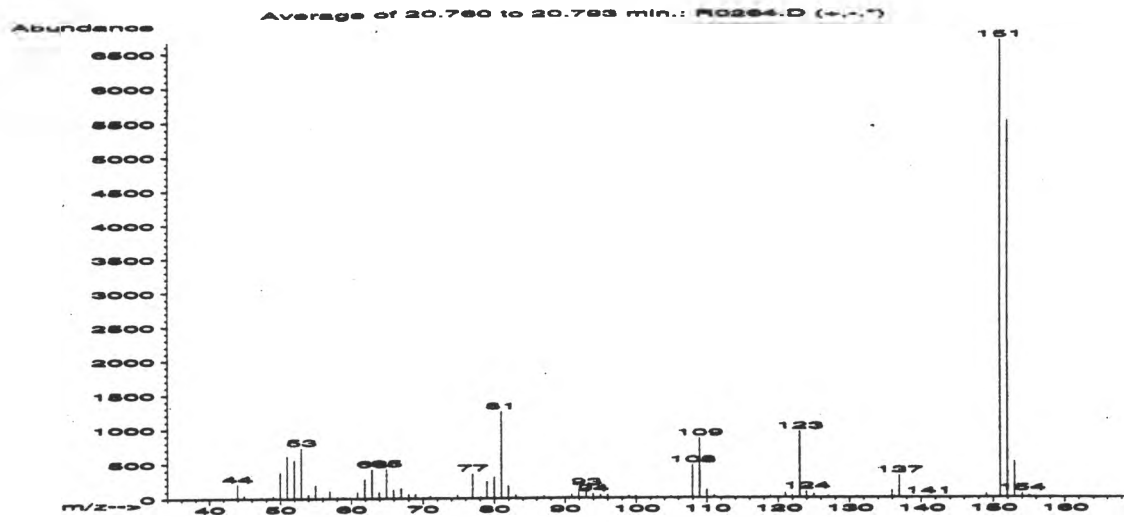
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Butanoic acid, 4-butoxy-	160	C8H16O3	38
2.	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	38
3.	Ethanol, 2-butoxy-	118	C6H14O2	38
4.	Propene, 3-tert-butoxy-2-(methoxymethyl)	158	C9H18O2	37
5.	2-Deoxy-D-ribose	134	C5H10O4	33
6.	Ethanol, 2-butoxy-	118	C6H14O2	32
7.	Ethanol, 2-butoxy-	118	C6H14O2	32
8.	Ethanol, 2-butoxy-	118	C6H14O2	32
9.	Ethanol, 2-butoxy-	118	C6H14O2	28
10.	L-Threonine	119	C4H9NO3	25
11.	Butane, 1,1'-oxybis-	130	C8H18O	22
12.	2-Propanol, 1-amino-	75	C3H9NO	12
13.	Pentane, 1-butoxy-	144	C9H20O	10
14.	Butane, 1,1'-oxybis-	130	C8H18O	10
15.	Butanoic acid, 3-methyl-, 2-methylpropyl	158	C9H18O2	10
16.	Butanoic acid, 3-methyl-, butyl ester	158	C9H18O2	8
17.	Butane, 1-butoxy-2-methyl-	144	C9H20O	7
18.	Butane, 1,1'-oxybis-	130	C8H18O	7
19.	Propanoic acid, butyl ester	130	C7H14O2	7
20.	Propanoic acid, 2-methylpropyl ester	130	C7H14O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	055724-73-7	16725	40	71	2	73	25	14	0	29	8426
2.	38	013343-98-1	6932	45	48	2	99	40	14	0	37	9583
3.	38	000111-76-2	119789	49	40	2	99	40	14	0	35	9605
4.	37	023230-86-6	16144	39	55	2	99	43	13	10	31	9599
5.	33	000533-67-5	121502	35	72	1	43	33	10	0	21	8901
6.	32	000111-76-2	119793	47	32	2	76	48	9	0	37	9575
7.	32	000111-76-2	119786	41	39	2	99	46	9	14	35	9604
8.	32	000111-76-2	3837	41	37	1	85	48	9	2	31	9578
9.	28	000111-76-2	119788	38	43	2	89	36	8	0	25	9585
10.	25	000072-19-5	119886	35	63	2	99	41	7	0	22	9533
11.	22	000142-96-1	121217	45	23	0	89	65	5	12	41	9066
12.	*12	000078-96-6	116616	28	72	1	94	60	2	0	29	3947
13.	10	018636-66-3	10872	34	59	1	99	63	1	0	22	9113
14.	10	000142-96-1	121218	34	41	1	84	65	1	0	25	9052
15.	10	000589-59-3	124708	40	59	3	99	65	1	0	29	7855
16.	8	000109-19-3	16118	39	67	2	69	68	1	0	28	7829
17.	7	062238-03-3	10874	37	48	1	74	75	1	0	22	9103
18.	7	000142-96-1	121220	34	38	1	84	71	1	4	26	9061
19.	7	000590-01-2	121118	34	44	3	96	80	1	0	25	8818
20.	7	000540-42-1	121123	41	32	1	97	80	1	0	28	8934

CTMP Compounds

Peak 2; Vanillin



Average of 20.760 to 20.793 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	203	58.05	16	68.95	59	81.95	178
44.90	42	58.80	16	70.05	10	83.05	44
48.95	33	59.80	5	71.00	33	85.00	1
49.95	373	60.90	92	71.95	8	86.00	13
50.95	614	61.90	272	74.80	45	86.85	1
51.95	551	62.90	414	75.95	5	87.00	29
52.95	728	63.90	86	76.95	349	90.95	53
53.95	60	64.95	423	78.05	19	91.95	119
54.95	190	65.95	120	78.95	237	93.00	147
56.00	20	67.00	141	79.95	305	93.95	58
56.95	107	68.00	54	80.95	1253	95.00	45

Average of 20.760 to 20.793 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.00	50	117.90	8	135.95	100		
98.95	30	118.90	23	136.95	314		
99.95	27	119.90	8	137.95	5		
103.00	17	121.00	64	141.00	12		
104.95	16	121.95	34	149.05	50		
106.95	11	123.00	957	150.95	6663		
107.95	468	123.95	88	151.95	5495		
108.95	861	125.00	52	152.95	514		
110.00	110	126.00	3	154.00	57		
111.00	31	127.00	22	155.00	23		
112.90	1	134.95	13	158.20	6		

CTMP Compounds

Average of 20.760 to 20.793 min.: R0264.D
Converted from RTE data file: >R0264:

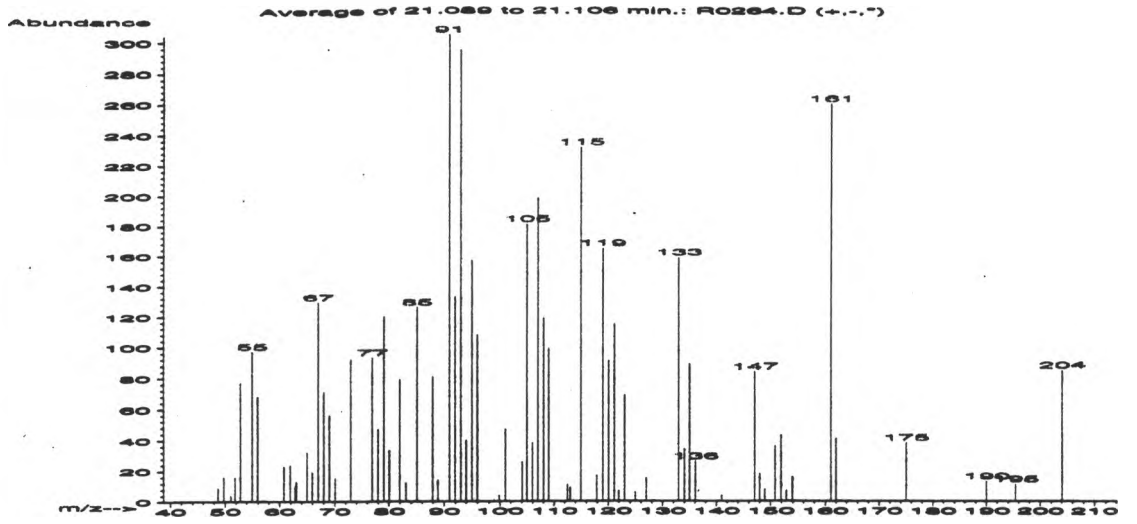
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	95
2.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	95
3.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	94
4.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	89
5.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	87
6.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	76
7.	N-HEXYLIMIDAZOLE	152	C9H16N2	64
8.	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	64
9.	Benzaldehyde, 2,4-dihydroxy-6-methyl-	152	C8H8O3	64
10.	Benzaldehyde, 3-(chloroacetoxy)-4-methox	228	C10H9ClO4	59
11.	Benzaldehyde, 4-(methylthio)-	152	C8H8OS	56
12.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	53
13.	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	38
14.	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	38
15.	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	38
16.	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	37
17.	cis-Hydrindane-2,5-dione	152	C9H12O2	35
18.	P-FORMANISIDINE	151	C8H9NO2	35
19.	6H-Purin-6-one, 2-amino-1,7-dihydro-	151	C5H5N5O	35
20.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	32

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000121-33-5	13356	91	5	1	78	4	72	54	93	9825
2.	*95	000121-33-5	123903	97	0	0	83	4	72	46	93	9852
3.	*94	000121-33-5	123901	99	0	0	71	4	70	54	93	9825
4.	*89	000121-33-5	123902	78	22	1	61	23	56	0	90	9806
5.	*87	000121-33-5	123898	76	18	1	73	9	54	30	59	9830
6.	*76	000121-33-5	123900	72	31	1	57	23	45	0	68	9806
7.	*64	000000-00-0	13553	33	51	2	91	17	37	4	39	9165
8.	*64	000673-22-3	13357	46	37	2	85	18	37	5	40	9749
9.	*64	000487-69-4	13353	33	35	1	91	23	37	8	43	9759
10.	59	066267-38-7	47410	76	44	1	65	22	33	0	41	9811
11.	*56	003446-89-7	13330	47	62	3	82	13	30	0	35	9805
12.	*53	000121-33-5	123899	38	47	1	70	30	28	0	39	9643
13.	*38	002634-33-5	13018	36	55	2	99	48	14	0	39	8187
14.	38	000621-59-0	13355	59	40	1	57	47	14	0	39	9913
15.	*38	000621-59-0	123897	30	56	1	69	39	14	4	30	9609
16.	*37	000148-53-8	13354	36	72	2	55	44	13	0	30	8411
17.	*35	092464-21-6	13494	33	76	0	65	55	11	0	41	6312
18.	*35	023896-88-0	13108	37	68	2	90	51	11	0	39	6746
19.	*35	000073-40-5	123751	34	66	1	69	53	11	0	39	8150
20.	32	000498-02-2	125552	56	25	1	88	50	9	6	37	8124

CTMP Compounds

Peak 49; Unidentified Sesquiterpene



Average of 21.089 to 21.106 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.70	9	63.00	13	80.05	33	95.95	108
49.80	16	64.95	32	81.95	79	98.95	1
51.00	4	65.90	19	83.05	12	99.85	4
51.80	16	67.00	129	85.05	126	100.95	47
52.80	77	68.00	71	87.95	81	104.05	26
54.95	97	69.00	56	88.90	14	104.95	181
55.95	68	70.05	15	90.95	304	105.95	38
56.95	1	72.90	92	91.95	133	107.00	198
60.75	23	76.90	93	93.00	294	108.05	119
61.90	24	77.95	47	94.00	40	109.00	99
62.75	10	79.00	120	95.00	157	112.50	11

Average of 21.089 to 21.106 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.05	9	134.05	34	161.05	259		
115.00	231	135.00	89	162.00	41		
117.90	17	136.05	26	175.00	38		
119.00	165	141.00	4	190.00	13		
120.10	91	147.10	84	195.40	11		
121.10	115	148.00	18	204.05	85		
121.90	7	148.95	8				
123.00	69	150.85	36				
124.95	6	151.95	43				
126.95	15	152.90	7				
132.95	159	153.95	16				

CTMP Compounds

Average of 21.089 to 21.106 min.: R0264.D
Converted from RTE data file: >R0264:

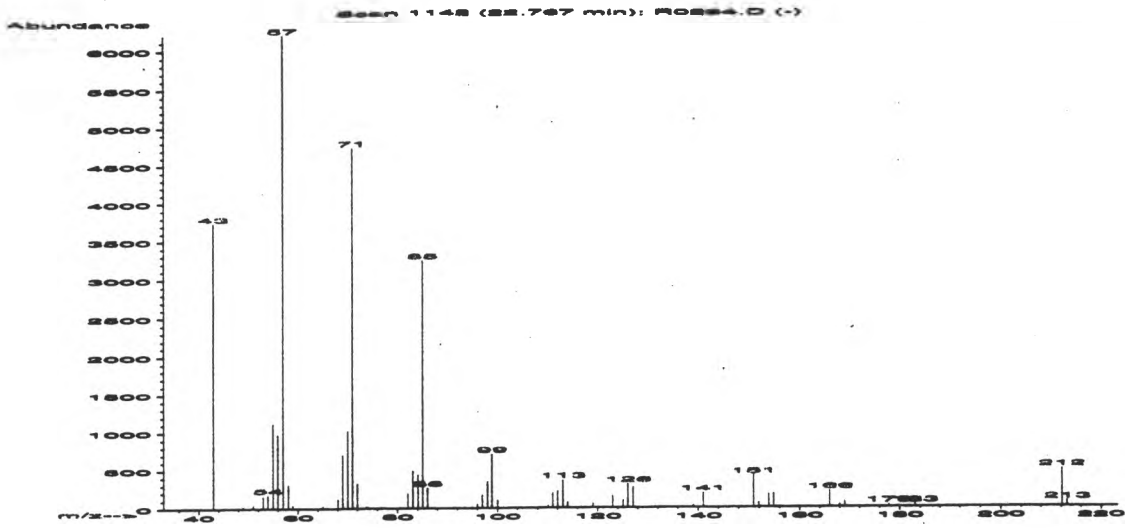
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Junipene	204	C15H24	86
2.	TRICYCLO[4.1.0.0(3,5)]HEPTANE, 2-ISOBUTE	204	C15H24	22
3.	1,4,4,7a-Tetramethyl-5,6,7,7a-tetrahydro	176	C13H20	22
4.	Tricyclo[4.1.0.0(2,4)]heptane, 3,3,7,7-t	204	C15H24	22
5.	Farnesene	204	C15H24	14
6.	Bicyclo[2.2.2]oct-2-ene, 1,2,3,6-tetrame	164	C12H20	14
7.	.ALPHA.-PINENE, (-)-	136	C10H16	11
8.	.ALPHA.-PINENE, (-)-	136	C10H16	11
9.	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	11
10.	1,4,6-HEPTATRIENE, 3,3,6-TRIMETHYL-	136	C10H16	11
11.	3-Carbomethoxy-5-methylenecyclohex-1-ene	152	C9H12O2	11
12.	Spiro[2.4]heptane, 4-methylene-	108	C8H12	11
13.	1,3,6-Heptatriene, 5-methyl-, (E)-	108	C8H12	11
14.	1-Phenyl-3-amino-2-pyrazoline	161	C9H11N3	11
15.	3-Carbomethoxy-4-methylenecyclohex-1-ene	152	C9H12O2	11
16.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	11
17.	.ALPHA.-PINENE, (-)-	136	C10H16	10
18.	THREO-1,2-DIPHENYLETHAN-2-D-OL	198	C14H13DO	10
19.	Cyclohexene, 4-ethenyl-3-(1-methyl-1-pro	162	C12H18	10
20.	Benzene, [(2-propenyloxy)methyl]-	148	C10H12O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000475-20-7	128709	85	66	3	151	30	53	0	87	8667
2.	22	000000-00-0	36784	58	90	1	76	63	5	0	39	6455
3.	22	051595-84-7	24065	46	44	0	73	65	5	21	41	5740
4.	22	056348-21-1	36783	58	90	1	76	63	5	0	39	6455
5.	14	000502-61-4	128650	58	79	2	113	70	2	0	39	6723
6.	14	062376-14-1	18765	62	66	2	66	66	2	0	39	6627
7.	*11	000080-56-8	122066	51	50	0	94	75	2	0	46	5483
8.	*11	000080-56-8	122065	51	54	0	90	75	2	0	46	5475
9.	*11	029548-02-5	8069	56	59	1	67	77	2	0	49	6100
10.	*11	000000-00-0	8072	56	59	1	67	77	2	0	49	6100
11.	*11	071436-03-8	13486	53	10	0	77	76	2	0	49	5292
12.	*11	024308-54-1	118772	34	38	0	70	76	2	17	43	5282
13.	*11	000818-48-4	1948	34	62	0	65	75	2	22	43	5509
14.	*11	003314-35-0	17232	44	62	0	85	80	2	0	44	4768
15.	*11	071436-02-7	13485	53	7	0	78	76	2	0	49	5297
16.	*11	003779-61-1	121952	48	67	1	69	79	2	0	44	5461
17.	*10	000080-56-8	122067	34	67	0	68	78	1	0	41	5917
18.	10	006932-62-3	34106	46	60	1	90	72	1	8	41	6271
19.	*10	061142-15-2	17863	37	62	0	88	73	1	0	41	5789
20.	10	014593-43-2	12046	61	46	0	76	80	1	0	43	4267

CTMP Compounds

Peak 50; Pentadecane



Scan 1142 (22.767 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3736	68.00	118	85.05	3241	112.00	222
48.95	28	69.00	703	86.00	265	113.00	366
50.95	49	70.00	1018	95.00	9	113.90	72
52.95	157	71.00	4718	96.00	52	119.00	56
53.95	176	72.00	326	97.00	165	122.00	11
54.95	1119	73.70	18	98.00	349	123.00	147
55.95	977	73.95	20	98.95	713	125.05	97
56.95	6191	80.95	9	100.05	101	126.05	312
58.05	310	82.05	189	107.85	1	127.05	267
58.95	43	83.05	495	110.05	31	139.00	29
64.95	32	84.05	442	111.05	196	141.00	192

Scan 1142 (22.767 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.40	15	212.20	500				
150.95	419	213.20	69				
151.95	59						
153.95	166						
154.95	175						
166.00	214						
168.00	33						
169.00	69						
177.80	32						
179.80	19						
183.05	32						

CTMP Compounds

Scan 1142 (22.767 min): R0264.D

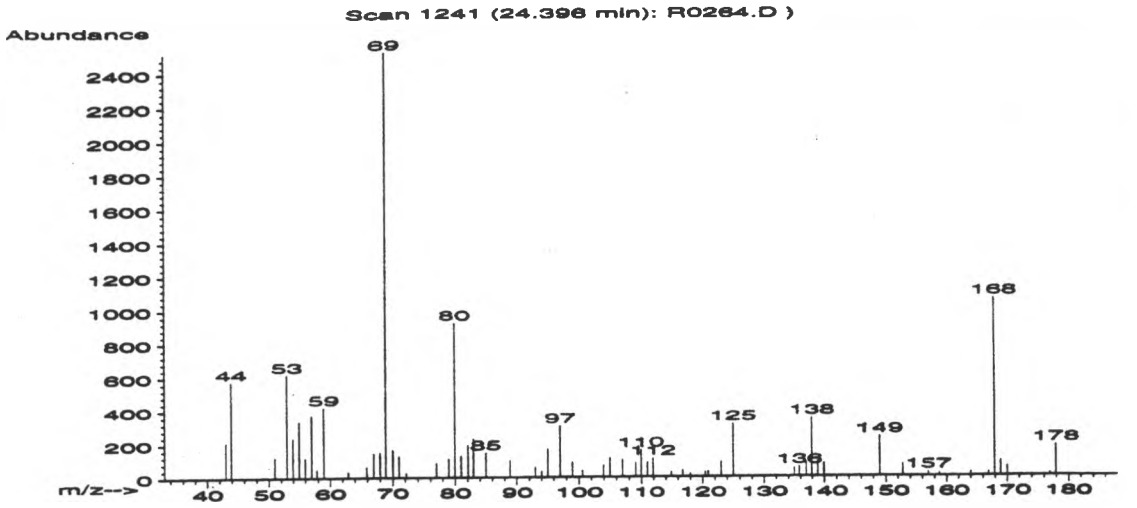
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Pentadecane	212	C15H32	93
2.	Hexatriacontane	507	C36H74	80
3.	Tetradecane	198	C14H30	80
4.	Heptadecane	240	C17H36	72
5.	Hexadecane	226	C16H34	64
6.	Pentadecane	212	C15H32	64
7.	Tetradecane	198	C14H30	59
8.	Nonadecane	268	C19H40	58
9.	Dodecane, 2,6,11-trimethyl-	212	C15H32	53
10.	Dodecane, 2,7,10-trimethyl-	212	C15H32	53
11.	Tetradecane	198	C14H30	50
12.	Pentadecane	212	C15H32	49
13.	Docosane	310	C22H46	46
14.	Pentadecane	212	C15H32	45
15.	Heptane, 5-ethyl-2-methyl-	142	C10H22	43
16.	Pentadecane	212	C15H32	38
17.	Octacosane	394	C28H58	38
18.	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	35
19.	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	35
20.	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	000629-62-9	40628	92	27	1	85	9	66	0	92	9929
2.	80	000630-06-8	136998	78	75	3	93	11	48	0	43	9883
3.	80	000629-59-4	128276	78	36	1	87	12	48	0	43	9890
4.	72	000629-78-7	130830	70	45	2	99	12	42	0	42	9840
5.	64	000544-76-3	46975	74	35	3	137	23	37	0	45	9670
6.	64	000629-62-9	129232	82	25	2	125	22	37	0	43	9760
7.	59	000629-59-4	128275	77	31	2	122	22	33	0	41	9731
8.	58	000629-92-5	132085	82	35	2	126	26	32	0	43	9698
9.	53	031295-56-4	40639	68	38	0	77	29	28	0	42	9715
10.	53	074645-98-0	40640	62	46	1	84	30	28	0	43	9715
11.	50	000629-59-4	128278	75	36	0	67	32	25	5	42	9767
12.	*49	000629-62-9	129237	58	54	1	99	43	23	0	56	9834
13.	46	000629-97-0	133781	98	33	1	69	45	20	18	49	9933
14.	*45	000629-62-9	129233	72	41	0	62	46	19	13	50	9688
15.	43	013475-78-0	10261	53	33	0	69	42	18	23	43	9270
16.	*38	000629-62-9	129238	60	56	0	58	60	14	0	56	9889
17.	38	000630-02-4	96901	68	71	2	79	46	14	0	42	9878
18.	35	007225-67-4	128292	60	43	0	82	53	11	0	43	9144
19.	35	054833-48-6	72677	62	68	1	64	52	11	0	43	9942
20.	35	007225-67-4	34144	62	43	0	69	53	11	0	43	9137

CTMP Compounds

Peak 51; Unidentified Monterpene



Scan 1241 (24.396 min): R0264.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	213	65.90	66	82.05	194	104.95	113
43.90	576	67.00	146	82.95	232	106.95	101
50.95	120	68.00	149	84.95	147	109.05	83
52.95	617	68.90	2518	88.90	99	109.95	160
53.95	237	70.00	164	93.00	59	110.95	87
54.95	336	71.00	126	94.00	35	111.90	112
55.95	117	72.15	26	95.00	171	114.90	30
56.95	373	76.95	84	97.00	306	116.75	38
57.80	49	78.95	111	98.95	88	118.00	17
58.95	421	79.95	923	100.55	38	120.40	29
62.90	34	80.95	128	103.95	69	120.90	32

Scan 1241 (24.396 min): R0264.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.00	90	158.80	17				
124.95	316	164.00	23				
134.95	49	166.90	24				
135.80	56	167.90	1066				
136.95	83	168.90	90				
137.90	350	170.00	56				
138.90	89	176.95	16				
139.90	76	177.95	183				
149.00	237						
152.80	72						
156.95	23						

CTMP Compounds

Scan 1241 (24.396 min): R0264.D

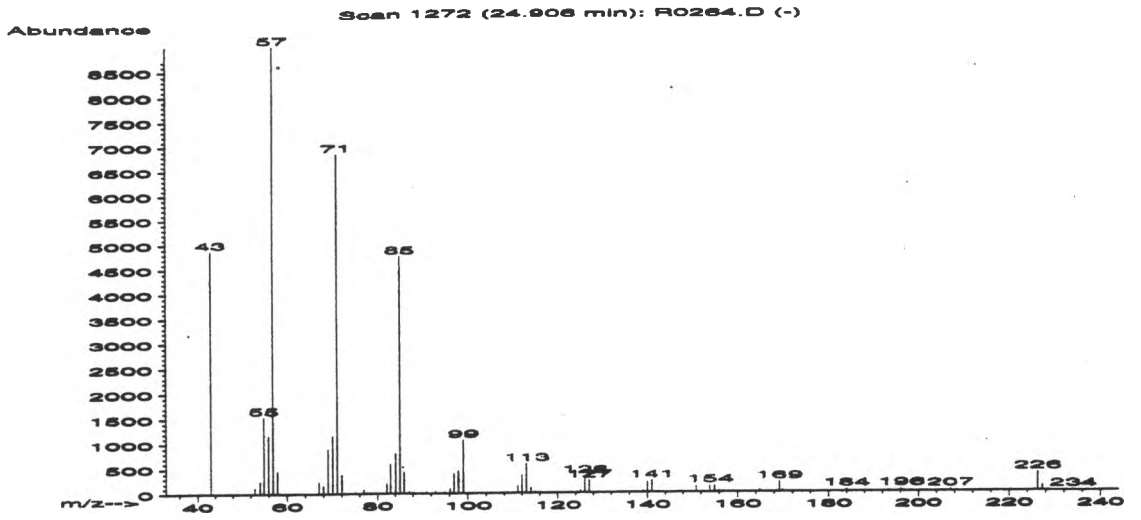
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	(erythro-2-Bromo-1-methylpropyl)cyanamid	176	C5H9BrN2	32
2.	2,5-Dimethoxy-1,4-benzoquinone	168	C8H8O4	28
3.	Methanone, dicyclopropyl-	110	C7H10O	22
4.	Butyraldehyde, 3-methyl-2-methylene-, is	154	C9H18N2	17
5.	Cyclopentane, 1-butyl-2-propyl-	168	C12H24	17
6.	3-ETHYL-5-METHYL-1-PROPYL-CYCLOHEXANE	168	C12H24	17
7.	1-BUTENE, 3-CHLORO-3-METHYL-	104	C5H9Cl	17
8.	Geranyl acetate	196	C12H20O2	17
9.	2-Pentene, 4-bromo-	148	C5H9Br	17
10.	3-HEPTENE, 2-METHYL-	112	C8H16	12
11.	3-Heptene, 2-methyl-, (E)-	112	C8H16	12
12.	2-Pentene, 4,4'-oxybis-	154	C10H18O	12
13.	Methanone, dicyclopropyl-	110	C7H10O	12
14.	1,3-Benzodioxol-2-one, hexahydro-, trans	142	C7H10O3	12
15.	DIETHYLISOPROPYL-BORANE	112	C7H17B	12
16.	1,6-Octadiene, 2,7-dimethyl-	138	C10H18	10
17.	2,6-Octadiene, 2,7-dimethyl-	138	C10H18	10
18.	3-Butyn-2-ol, 2-methyl-	84	C5H8O	10
19.	2-METHOXY-3,5,5-TRIMETHYL-2-CYCLOHEXENON	168	C10H16O2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	32	085782-20-3	23562	38	14	0	99	50	9	0	33	8186
2.	28	003117-03-1	20117	36	52	1	78	40	8	0	21	8792
3.	*22	001121-37-5	118863	33	42	1	85	65	5	1	40	8150
4.	17	033063-81-9	14527	33	67	1	81	52	3	0	22	8388
5.	17	062199-50-2	20759	40	68	2	81	54	3	0	29	8388
6.	17	000000-00-0	20772	39	57	2	76	54	3	0	29	8409
7.	*17	002190-48-9	118428	29	47	1	99	55	3	0	29	8374
8.	17	000105-87-3	128005	34	73	2	117	54	3	0	21	8572
9.	17	001809-26-3	11773	35	59	1	74	55	3	0	22	8436
10.	12	000692-96-6	2654	39	57	2	79	58	2	0	29	8348
11.	12	000692-96-6	2653	34	62	2	79	58	2	0	22	8348
12.	12	052867-34-2	14613	34	54	1	76	60	2	0	20	8311
13.	*12	001121-37-5	2198	38	31	1	89	65	2	7	36	8130
14.	12	020192-66-9	9902	33	52	1	72	60	2	0	22	8306
15.	*12	000000-00-0	2638	32	39	1	71	63	2	1	30	8340
16.	10	040195-09-3	122294	34	48	1	79	61	1	0	22	8253
17.	10	016736-42-8	8736	33	54	1	95	61	1	0	20	8253
18.	10	000115-19-5	116867	35	37	0	99	63	1	0	25	8206
19.	9	005682-76-8	20402	44	62	2	51	80	1	15	33	8710

CTMP Compounds

Peak 52; Hexadecane



Scan 1272 (24.906 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4879	71.00	6848	87.15	37	112.00	360
52.95	117	72.00	383	88.00	21	113.00	585
54.05	248	72.85	16	91.00	31	114.00	110
54.95	1530	75.05	32	93.00	40	114.90	27
55.95	1157	76.95	73	95.00	27	122.90	19
56.95	9011	80.95	13	96.15	94	125.05	52
57.95	453	82.05	195	97.00	399	126.05	340
67.00	241	82.95	585	98.00	458	127.05	251
68.00	161	84.05	809	99.05	1067	139.15	33
69.00	893	85.05	4759	109.05	6	140.00	211
70.00	1162	86.00	432	111.05	146	141.00	236

Scan 1272 (24.906 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.95	122	226.25	374				
154.05	139	227.25	109				
155.05	129	233.95	20				
156.00	26						
157.05	29						
164.90	39						
169.15	203						
169.90	34						
184.00	47						
196.15	55						
207.05	40						

CTMP Compounds

Scan 1272 (24.906 min): R0264.D

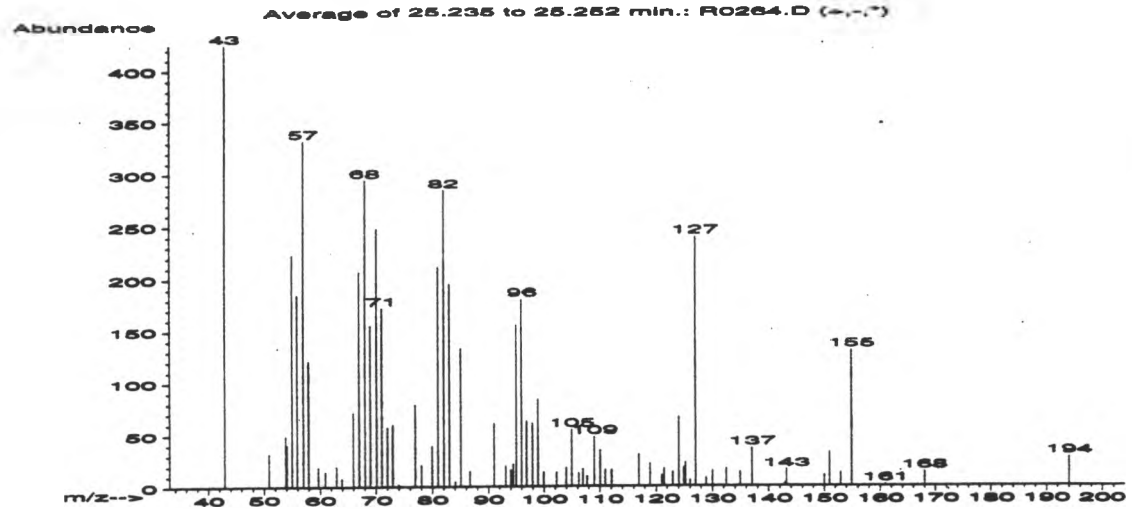
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Hexadecane	226	C16H34	91
2.	Hexadecane	226	C16H34	91
3.	Dodecane, 4-methyl-	184	C13H28	86
4.	Pentadecane	212	C15H32	86
5.	Iron, tricarbonyl[N-(phenyl-2-pyridinylm	398	C21H14FeN2O3	86
6.	Hexadecane	226	C16H34	83
7.	Nonane, 3,7-dimethyl-	156	C11H24	83
8.	Hexadecane	226	C16H34	81
9.	Heptadecane	240	C17H36	72
10.	Dodecane, 2,7,10-trimethyl-	212	C15H32	53
11.	Hexadecane	226	C16H34	53
12.	Nonane, 2,6-dimethyl-	156	C11H24	52
13.	Heptane, 3-ethyl-5-methyl-	142	C10H22	50
14.	1-Decene, 4-methyl-	154	C11H22	49
15.	Undecane, 2,4-dimethyl-	184	C13H28	49
16.	Nonadecane	268	C19H40	38
17.	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	35
18.	Undecane, 3,5-dimethyl-	184	C13H28	30
19.	Hexane, 2,4-dimethyl-	114	C8H18	30
20.	PENTADECANE, 2,6,10-TRIMETHYL-	254	C18H38	30

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000544-76-3	130125	73	44	2	98	5	62	0	81	9917
2.	*91	000544-76-3	46975	94	25	2	99	12	62	45	90	9693
3.	*86	006117-97-1	27734	51	56	2	103	9	53	0	46	9892
4.	86	000629-62-9	129234	86	23	1	99	7	53	0	45	9905
5.	86	074764-11-7	97422	84	53	2	93	9	53	0	47	9935
6.	*83	000544-76-3	130126	78	37	0	60	52	50	0	93	9869
7.	*83	017302-32-8	15631	69	26	2	99	15	50	19	58	9830
8.	*81	000544-76-3	130127	77	39	1	103	18	49	0	74	9862
9.	72	000629-78-7	130827	85	27	2	116	18	42	0	45	9848
10.	53	074645-98-0	40640	62	46	0	70	26	28	0	43	9733
11.	*53	000544-76-3	130128	64	53	1	81	40	28	0	58	9873
12.	*52	017302-28-2	15630	48	42	1	88	35	27	0	44	9398
13.	50	052896-90-9	10260	57	29	0	74	35	25	9	43	9280
14.	*49	013151-29-6	14800	60	40	2	71	42	23	0	56	9189
15.	*49	017312-80-0	27743	49	54	2	132	39	23	0	44	9665
16.	38	000629-92-5	132085	60	55	0	83	49	14	0	43	9715
17.	35	007225-67-4	128290	62	33	1	92	54	11	0	43	9013
18.	*30	017312-81-1	27752	45	52	1	80	57	9	0	44	9235
19.	*30	000589-43-5	119377	44	45	2	134	59	9	0	44	8969
20.	30	000000-00-0	58329	75	40	0	69	57	9	0	45	9682

CTMP Compounds

Peak 53; Unidentified Hydrocarbon



Average of 25.235 to 25.252 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	425	62.90	20	76.90	79	94.00	16
50.85	32	63.90	8	78.00	21	94.40	22
53.80	49	65.90	72	79.95	39	95.00	156
54.05	40	66.95	207	81.00	211	96.00	181
54.95	223	68.00	294	82.00	284	96.90	63
55.90	185	69.00	155	83.00	195	97.95	61
57.00	332	70.10	248	84.05	5	98.95	84
57.90	121	71.00	172	85.05	133	99.95	14
58.90	1	72.00	57	86.65	15	102.20	14
59.65	19	72.90	60	91.00	61	103.95	18
60.90	15	73.95	2	93.05	20	104.95	55

Average of 25.235 to 25.252 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.20	13	122.95	14	142.90	3		
106.95	17	124.05	67	143.15	16		
107.70	10	124.90	18	150.00	11		
109.00	48	125.20	23	150.95	33		
110.05	35	126.05	6	152.95	13		
110.95	16	127.00	240	154.95	131		
112.05	16	128.95	8	160.95	2		
116.95	31	130.05	15	168.00	14		
118.90	22	132.45	17	194.00	28		
121.00	11	134.95	14				
121.40	17	137.05	37				

CTMP Compounds

Average of 25.235 to 25.252 min.: R0264.D
Converted from RTE data file: >R0264:

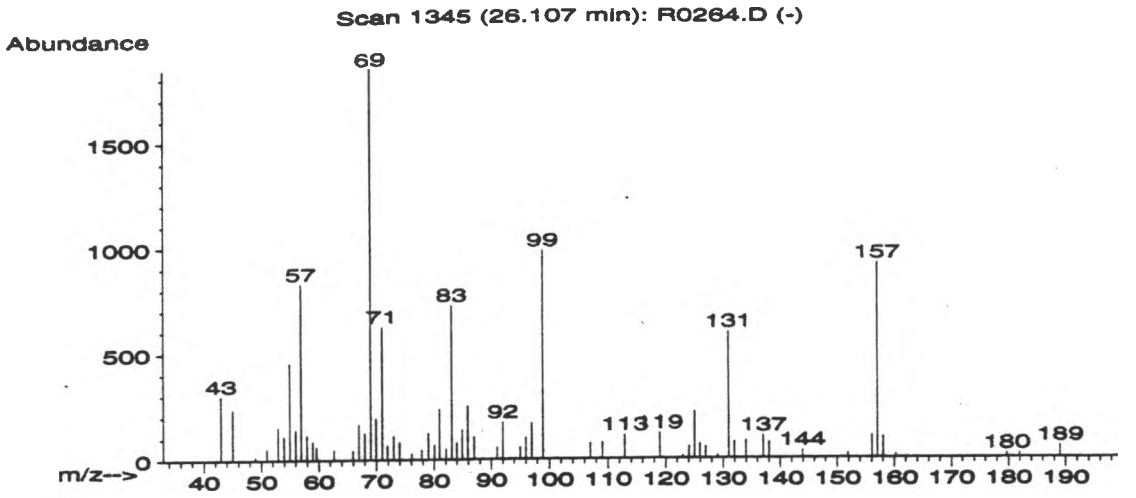
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,14-Tetradecanediol	230	C14H30O2	27
2.	TROPINE-N-OXIDE B	157	C8H15NO2	27
3.	Pentadecanal	226	C15H30O	27
4.	(R)-(-)-(E)-14-Methyl-8-hexadecen-1-ol	254	C17H34O	27
5.	E5-DODECENYLACETATE	226	C14H26O2	22
6.	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	22
7.	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	22
8.	5-Undecene, 9-methyl-, (Z)-	168	C12H24	15
9.	2-TRIDECEN-1-OL	198	C13H26O	14
10.	1,9-Nonanediol, dimethanesulfonate	316	C11H24O6S2	14
11.	1-Decanol	158	C10H22O	14
12.	3-CYCLOHEXYL-PROPANOL	142	C9H18O	14
13.	1,1'-Bicyclopentyl	138	C10H18	14
14.	1,1'-Bicyclopentyl	138	C10H18	14
15.	1,1'-Bicyclopentyl	138	C10H18	10
16.	1,12-Dodecanediol	202	C12H26O2	10
17.	1,5-HEXADIENE, 3-DEUTEROMETHYL-4-METHYL-	110	C8H13D	10
18.	Tridecanal	198	C13H26O	10
19.	1,1'-Bicyclopentyl	138	C10H18	10
20.	4-Undecene, 9-methyl-, (Z)-	168	C12H24	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	27	019812-64-7	48475	75	67	2	92	59	8	0	41	7207
2.	27	032663-71-1	15772	58	64	1	58	59	8	0	39	6753
3.	27	000000-00-0	130116	47	31	0	78	56	8	2	41	6994
4.	27	000000-00-0	58302	55	40	0	53	56	8	6	41	.7244
5.	22	000000-00-0	46800	59	82	3	118	65	5	0	39	6642
6.	22	018645-10-8	124045	47	60	0	58	65	5	24	41	6597
7.	22	018645-10-8	13875	70	41	0	66	65	5	14	41	6597
8.	*15	074630-65-2	20724	58	48	0	58	78	2	0	56	5451
9.	14	000000-00-0	34079	50	26	0	78	68	2	4	41	6083
10.	14	004248-77-5	78725	61	107	1	52	70	2	0	39	7088
11.	14	000112-30-1	124754	43	62	0	56	69	2	19	41	6194
12.	14	001124-63-6	10228	43	60	0	50	67	2	19	41	6444
13.	14	001636-39-1	122325	44	35	0	50	68	2	17	41	6055
14.	14	001636-39-1	8819	57	48	0	63	67	2	7	40	6383
15.	10	001636-39-1	122326	57	47	0	56	73	1	7	40	6391
16.	10	005675-51-4	128530	43	69	0	49	71	1	2	41	6794
17.	*10	000000-00-0	2250	44	47	0	42	71	1	18	40	6643
18.	10	010486-19-8	128240	43	22	0	58	75	1	12	41	5538
19.	10	001636-39-1	122324	57	47	0	57	73	1	7	40	6345
20.	*10	074630-56-1	20712	44	59	1	57	71	1	0	40	5649

CTMP Compounds

Peak 54; Unidentified Hydrocarbon



Scan 1345 (26.107 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	301	59.65	60	76.05	28	91.00	56
45.00	236	62.65	46	77.80	48	92.00	173
48.95	15	65.90	44	78.95	126	95.05	56
50.95	52	67.00	166	80.05	70	96.00	101
52.95	153	68.00	125	80.95	237	97.00	169
53.95	111	69.00	1844	82.05	51	98.95	985
54.95	455	69.90	192	83.05	727	106.95	73
55.95	141	71.00	625	83.95	81	109.05	77
56.95	831	71.90	66	84.95	139	112.90	112
57.95	115	72.95	111	85.90	252	119.00	120
58.95	86	73.95	82	87.00	106	123.00	14

Scan 1345 (26.107 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	58	151.90	23				
125.05	219	156.05	108				
125.95	70	157.05	922				
126.95	55	158.05	99				
129.00	15	160.30	18				
130.95	598	179.70	21				
131.95	76	181.95	21				
133.95	82	189.05	57				
137.00	107						
138.00	76						
143.90	38						

CTMP Compounds

Scan 1345 (26.107 min): R0264.D

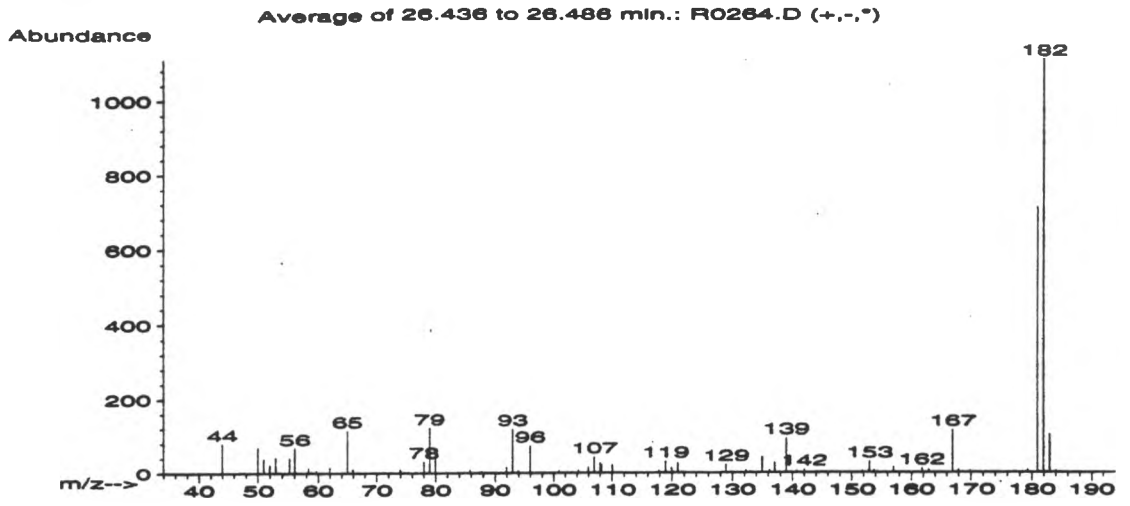
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	38
2.	METHYL 2-HYDROXYDECANOATE	202	C11H22O3	35
3.	1-METHYL-3-PROPYL-CYCLOOCTANE	168	C12H24	32
4.	4-Octene, 2,3,6,7-tetramethyl-	168	C12H24	32
5.	Zinc, bis[2-(1,1-dimethylethyl)-3,3-dime	314	C18H34Zn	25
6.	1R,2T,4C,5C-1,2,4,5-TETRAMETHYLCYCLOHEXA	140	C10H20	23
7.	1,5-Heptadiene, 3,6-dimethyl-	124	C9H16	18
8.	2,6-HEPTADIENE, 2,5-DIMETHYL-	124	C9H16	18
9.	1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	14
10.	1-Dodecyn-4-ol	182	C12H22O	12
11.	1-Nonanol, 4,8-dimethyl-	172	C11H24O	12
12.	Silane, (3-methyl-1,2-propadien-1-yl-3-y	270	C13H30Si3	10
13.	Cyclohexane, 1,1'-(1-methylethylidene)bi	208	C15H28	9
14.	1,2,6,7-HEPTANTETROL, 1,2:6,7-DI-O-(ETHY	240	C11H22B2O4	9
15.	1,3,2-Dioxaborolane, 4,4'-(1,3-propanedi	240	C11H22B2O4	9
16.	Farnesol	222	C15H26O	8
17.	Farnesol	222	C15H26O	8
18.	2,6-OCTADIENE, 2,6-DIMETHYL-	138	C10H18	8
19.	2-Pentene, 4,4'-oxybis-	154	C10H18O	8
20.	1,4-Hexadiene, 3,3,5-trimethyl-	124	C9H16	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	061142-70-9	14850	57	29	0	67	50	14	5	40	7750
2.	35	071271-24-4	35534	44	56	1	89	53	11	5	38	7893
3.	32	000000-00-0	20780	54	38	1	76	47	9	7	34	7763
4.	32	063830-66-0	20743	42	52	2	98	47	9	16	37	7878
5.	25	074793-36-5	78306	50	80	3	77	53	7	0	31	6791
6.	23	019899-40-2	9528	37	56	2	88	50	6	4	25	7344
7.*	18	034891-10-6	4886	48	35	1	94	69	3	0	46	7353
8.*	18	000000-00-0	4893	48	34	1	94	69	3	0	46	7353
9.	14	067682-47-7	4884	46	27	0	67	69	2	6	41	7353
10.	12	074646-36-9	26783	44	46	1	99	65	2	0	37	7937
11.	12	033933-80-1	22410	41	80	2	77	58	2	0	28	7890
12.	10	024295-79-2	63375	39	70	1	77	66	1	10	31	7581
13.	9	054934-90-6	38781	55	55	1	54	78	1	17	37	6897
14.	9	000000-00-0	52366	47	60	1	36	77	1	0	35	4079
15.	9	074810-64-3	52365	47	60	1	36	77	1	0	35	4079
16.	8	004602-84-0	129873	38	79	2	80	69	1	0	27	7353
17.	8	004602-84-0	129872	38	78	2	77	69	1	0	27	7353
18.*	8	002609-23-6	122297	31	52	2	99	69	1	0	29	7353
19.	8	052867-34-2	14613	39	42	1	82	68	1	7	29	7372
20.*	8	074753-00-7	4897	28	60	2	90	69	1	0	29	7353

CTMP Compounds

Peak 55a; Syringaldehyde



Average of 26.436 to 26.486 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	80	64.95	115	95.95	75	121.00	27
50.00	70	65.95	11	100.95	7	121.90	3
50.95	39	73.95	10	104.30	8	128.95	22
51.95	22	77.95	32	105.95	15	129.75	2
52.90	42	78.95	123	106.95	44	132.30	7
55.20	41	79.95	39	107.95	27	132.95	3
56.05	68	85.75	9	108.20	21	135.00	42
58.30	14	87.65	5	110.05	22	136.20	6
58.85	3	91.95	16	117.90	7	137.00	27
59.65	6	92.95	120	118.95	32	138.95	94
61.95	15	93.95	6	119.95	13	140.75	5

Average of 26.436 to 26.486 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
142.00	8	169.90	5				
151.80	5	179.30	8				
152.80	7	180.95	708				
153.00	31	181.95	1108				
153.75	6	183.00	104				
154.30	4	183.95	5				
157.05	15						
161.80	12						
162.95	8						
166.95	116						
168.00	7						

CTMP Compounds

Average of 26.436 to 26.486 min.: R0264.D
Converted from RTE data file: >R0264:

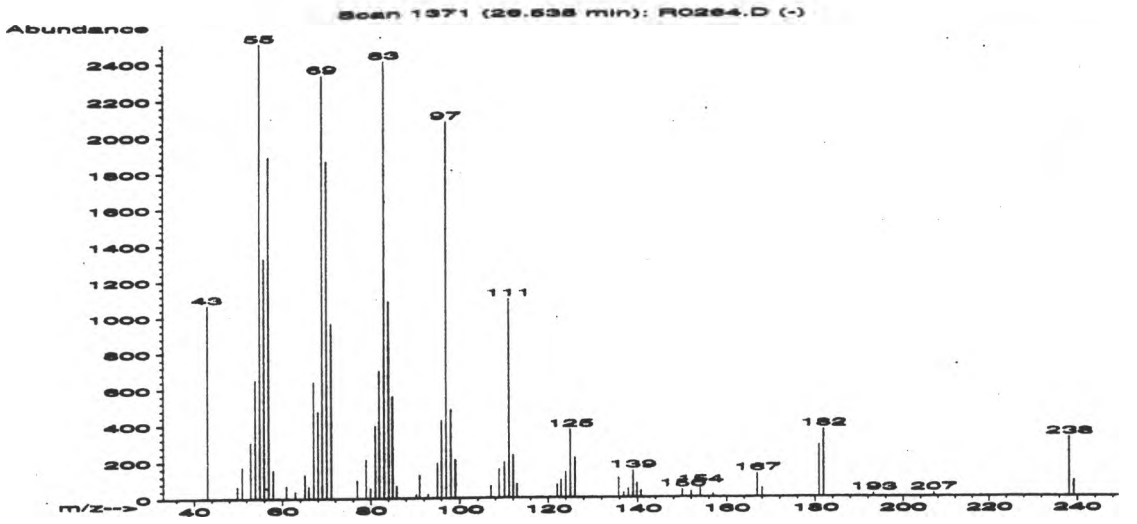
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	C9H10O4	86
2.	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	C9H10O4	37
3.	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	C9H10O4	37
4.	2-AMINO-5-NITRONICOTINAMIDE	182	C6H6N4O3	37
5.	3-(2-Methylprop-2-enyl)-5,5-dimethylimid	182	C9H14N2O2	28
6.	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	C9H10O4	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000134-96-3	126989	67	38	2	91	8	53	8	47	9906
2.	37	000134-96-3	126987	51	67	2	66	41	13	0	31	9869
3.	37	000134-96-3	26404	43	75	2	60	44	13	0	37	9837
4.	*37	000000-00-0	26241	40	51	3	88	44	13	8	35	8383
5.	*28	059004-93-2	26431	29	57	2	77	38	8	0	29	8087
6.	12	000134-96-3	126988	43	59	3	109	64	2	8	35	9873

CTMP Compounds

Peak 55b; Heptadecene



Scan 1371 (26.535 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1068	65.00	129	81.95	701	97.00	2072
49.85	67	65.90	68	83.05	2402	98.00	487
50.95	173	67.00	641	84.05	1089	99.05	210
52.95	306	68.00	476	84.95	560	106.95	68
53.95	650	69.00	2333	85.90	67	108.80	159
54.95	2504	70.00	1865	90.25	21	110.05	194
55.95	1326	71.00	967	91.00	127	111.05	1102
56.95	1888	76.95	98	93.00	23	112.00	234
57.95	155	78.95	211	94.10	1	112.90	77
60.90	69	79.95	55	95.00	192	122.00	72
62.90	38	81.05	398	96.00	426	122.90	98

Scan 1371 (26.535 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.00	138	154.05	63				
125.05	373	156.95	19				
126.05	219	166.90	128				
135.80	109	168.00	50				
136.95	26	180.95	284				
138.00	50	181.95	371				
139.00	147	193.25	19				
139.90	78	207.05	20				
140.75	37	238.20	322				
150.00	42	239.20	86				
151.95	32						

CTMP Compounds

Scan 1371 (26.535 min): R0264.D

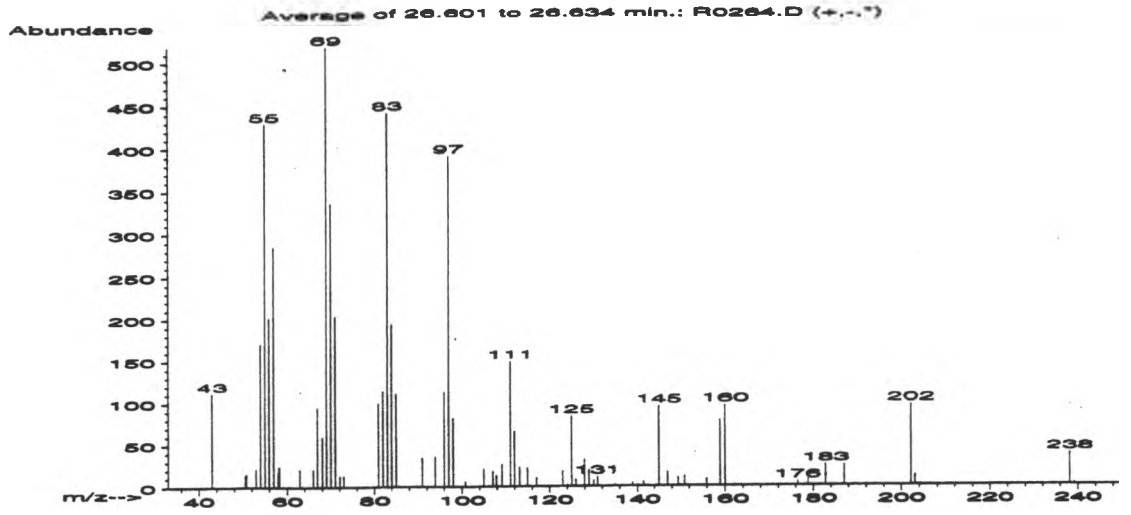
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Heptadecene	238	C17H34	86
2.	5-Octadecene, (E)-	252	C18H36	86
3.	3-Hexadecene, (Z)-	224	C16H32	86
4.	7-Hexadecene, (Z)-	224	C16H32	86
5.	9-Octadecene, (E)-	252	C18H36	80
6.	1-Heptadecene	238	C17H34	72
7.	6-Tridecene	182	C13H26	64
8.	1-Tridecene	182	C13H26	62
9.	9-Eicosene, (E)-	280	C20H40	58
10.	3-Eicosene, (E)-	280	C20H40	58
11.	Cyclopropane, 1-methyl-1-(2-methylpropyl	238	C17H34	49
12.	Cyclopropane, 1-methyl-1-(2-methylpropyl	238	C17H34	49
13.	5-Eicosene, (E)-	280	C20H40	49
14.	4-Nonene, 5-butyl-	182	C13H26	49
15.	4-Nonene, 5-butyl-	182	C13H26	38
16.	1-Tridecene	182	C13H26	38
17.	2,4-(D2)MENTH-2-ENE	138	C10H16D2	30
18.	1,1-Di(1,1-dimethylethyl)cyclopropane	154	C11H22	25
19.	2-Undecene, 2,5-dimethyl-	182	C13H26	18
20.	1-Hexene, 2,5,5-trimethyl-	126	C9H18	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	006765-39-5	51970	91	61	1	111	28	53	0	89	8628
2.	86	007206-21-5	57573	129	31	1	86	6	53	4	49	9886
3.	86	034303-81-6	46061	110	33	1	93	6	53	11	46	9713
4.	86	035507-09-6	46062	129	27	1	92	6	53	4	49	9836
5.	80	007206-25-9	57574	126	35	0	77	14	48	2	49	9872
6.	*72	006765-39-5	130749	97	64	1	94	16	42	7	50	9881
7.	*64	024949-38-0	127045	104	38	1	79	32	37	42	81	8157
8.	*62	002437-56-1	26848	75	57	2	95	30	36	18	59	8488
9.	58	074685-29-3	67214	88	80	0	75	28	32	0	49	9892
10.	58	074685-33-9	67216	111	55	1	98	26	32	0	43	9803
11.	*49	041977-41-7	51964	61	91	3	133	42	23	0	51	9503
12.	*49	041977-41-7	130745	67	85	3	133	44	23	0	58	9370
13.	49	074685-30-6	67215	115	45	0	72	38	23	11	50	8601
14.	*49	007367-38-6	127047	69	63	2	84	42	23	21	58	8836
15.	*38	007367-38-6	26857	66	62	2	89	52	14	18	45	8600
16.	*38	002437-56-1	127044	51	76	1	113	51	14	0	46	8267
17.	*30	005256-68-8	8797	55	53	2	82	60	9	21	43	5940
18.	*25	080816-10-0	124361	61	43	0	75	63	7	20	49	7473
19.	*18	049622-16-4	26852	46	75	0	61	67	3	0	44	7688
20.	*18	062185-56-2	5435	37	56	0	69	69	3	10	43	7126

CTMP Compounds

Peak 56; 1-Heptadecene ??



Average of 26.601 to 26.634 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	112	65.95	21	84.00	193	109.05	26
50.55	15	66.95	95	85.00	111	111.05	149
50.80	16	68.00	60	91.00	35	112.00	66
52.90	22	69.00	518	93.95	36	113.15	23
53.95	171	70.00	335	96.00	113	114.95	22
54.95	429	71.00	203	97.00	389	116.95	10
55.95	202	72.05	13	98.00	82	123.00	18
56.95	285	72.95	13	100.70	6	124.10	2
57.95	18	80.95	100	104.95	21	125.00	84
58.20	24	82.00	114	107.05	18	126.00	8
62.90	21	83.05	440	107.80	13	127.95	32

Average of 26.601 to 26.634 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
128.95	19	155.95	8	239.20	3		
130.05	7	158.95	78	283.45	5		
130.95	11	160.05	96				
135.00	2	166.90	1				
138.95	4	176.40	5				
140.10	2	178.80	9				
141.40	5	182.80	25				
145.00	95	187.05	24				
147.00	16	202.15	96				
149.40	10	203.05	12				
150.90	12	238.15	38				

CTMP Compounds

Average of 26.601 to 26.634 min.: R0264.D
Converted from RTE data file: >R0264:

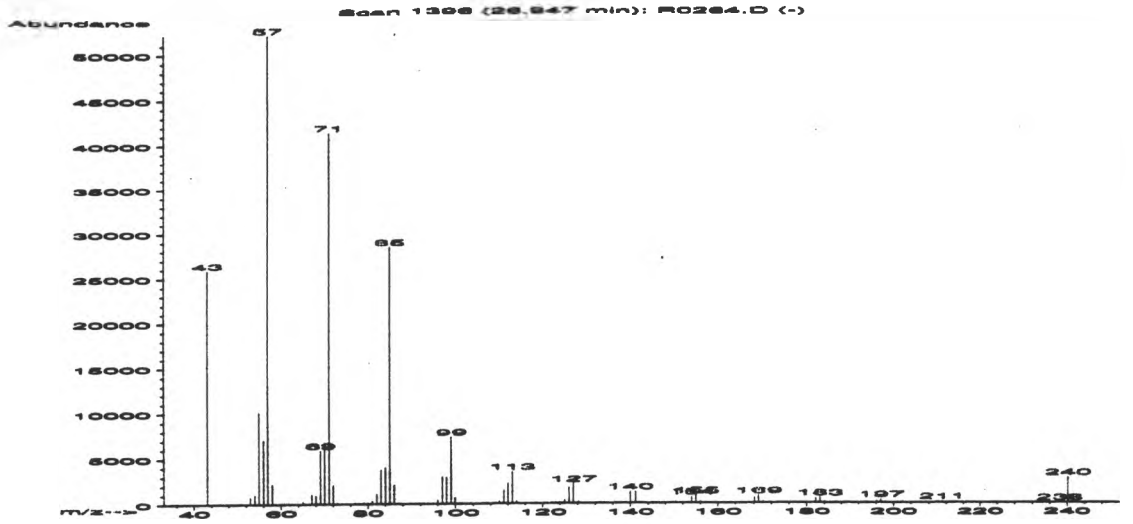
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Heptadecene	238	C17H34	94
2.	3-Octadecene, (E)-	252	C18H36	90
3.	1-Heptadecene	238	C17H34	86
4.	9-Eicosene, (E)-	280	C20H40	80
5.	1-Hexadecene	224	C16H32	72
6.	Cyclotetradecane	196	C14H28	72
7.	9-Octadecene, (E)-	252	C18H36	64
8.	5-Octadecene, (E)-	252	C18H36	64
9.	1-Heptadecene	238	C17H34	60
10.	7-Tetradecene	196	C14H28	53
11.	1-Octadecene	252	C18H36	43
12.	1-Undecene	154	C11H22	35
13.	Silane, trichloroeicosyl-	414	C20H41Cl3Si	35
14.	Cyclopentane, 1-butyl-2-propyl-	168	C12H24	35
15.	CYCLOPROPANE, 1-(2-BUTYL)-1-(2-METHYLBUT	168	C12H24	27
16.	Cycloheptane, methyl-	112	C8H16	27
17.	Tridecanol	200	C13H28O	27
18.	4-Decene, 6-methyl-, (E)-	154	C11H22	27
19.	CYCLOOCTANE, 1,2-DIMETHYL-	140	C10H20	27
20.	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimet	152	C10H16O	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	006765-39-5	130749	104	51	2	70	3	70	47	83	9685
2.	90	007206-19-1	57572	116	44	0	68	3	57	1	50	9834
3.	*86	006765-39-5	51970	83	68	1	84	26	53	0	91	8252
4.	80	074685-29-3	67214	111	57	2	82	12	48	0	49	9851
5.	72	000629-73-2	130027	106	52	1	82	11	42	0	42	9821
6.	72	000295-17-0	128073	78	70	2	98	18	42	0	43	9711
7.	64	007206-25-9	57574	104	53	1	72	20	37	10	42	9720
8.	64	007206-21-5	57573	109	51	0	61	23	37	10	47	9741
9.	*60	006765-39-5	130747	64	84	1	84	38	35	0	64	8153
10.	53	010374-74-0	128059	43	88	0	69	29	28	8	41	9599
11.	43	000112-88-9	131398	75	93	1	54	42	18	0	41	9787
12.	35	000821-95-4	124353	43	72	0	55	55	11	19	41	8620
13.	35	018733-57-8	99977	45	100	0	46	51	11	19	41	9629
14.	35	062199-50-2	20759	45	57	1	93	52	11	20	41	8296
15.	27	000000-00-0	20754	46	65	0	56	60	8	5	41	6891
16.	*27	004126-78-7	2728	36	68	0	77	59	8	0	41	8294
17.	27	026248-42-0	34900	45	92	0	65	56	8	2	41	9626
18.	27	036229-57-9	14819	46	60	0	82	59	8	19	41	8096
19.	27	000000-00-0	9535	44	75	0	52	59	8	12	41	8326
20.	27	015358-88-0	124028	45	60	0	74	58	8	2	41	7948

CTMP Compounds

Peak 57; Heptadecane



Scan 1396 (26.947 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	25858	60.65	32	79.05	172	95.00	66
49.95	23	65.00	281	79.95	45	96.00	441
50.95	92	67.00	1030	80.95	349	97.00	3003
51.80	65	68.00	921	82.05	1102	98.00	2955
52.95	740	69.00	5893	83.05	3758	99.05	7393
53.95	1059	70.00	6777	84.05	4003	99.95	688
54.95	10117	71.00	41351	85.05	28486	100.95	55
55.95	7076	72.00	2100	86.00	2122	104.80	52
56.95	52128	72.95	89	86.90	52	106.80	43
57.95	2188	76.95	98	90.95	20	109.05	71
59.90	45	77.80	33	92.00	38	110.05	262

Scan 1396 (26.947 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.05	1456	128.20	169	151.95	71	184.20	76
112.00	2248	131.05	24	154.05	718	194.00	39
113.00	3521	132.20	20	155.05	868	196.15	177
114.00	303	132.95	35	156.05	131	197.15	395
122.00	35	135.05	77	159.05	16	198.15	54
122.40	32	138.00	63	168.15	608	207.55	20
123.00	68	139.00	123	169.15	831	210.20	119
124.00	105	140.00	1310	170.15	131	211.20	134
125.05	442	141.15	1285	176.80	38	238.30	26
126.05	1749	142.15	144	182.05	492	240.20	2790
127.05	2167	143.00	32	183.05	574	241.30	459

Scan 1396 (26.947 min): R0264.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
242.00	48						

CTMP Compounds

Scan 1396 (26.947 min): R0264.D

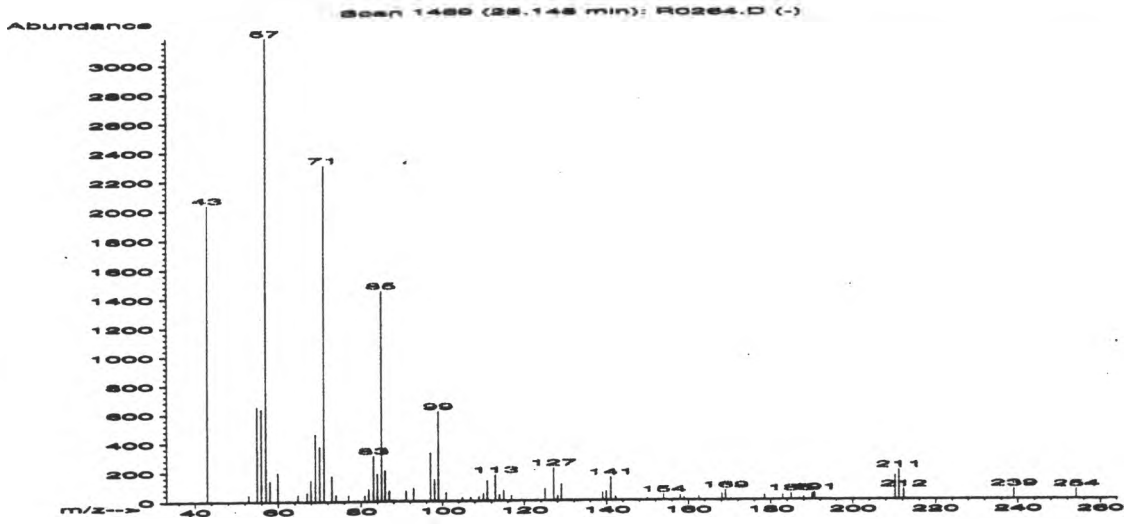
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Heptadecane	240	C17H36	94
2.	Heptadecane	240	C17H36	94
3.	Octadecane	254	C18H38	90
4.	Hexadecane	226	C16H34	90
5.	Pentadecane	212	C15H32	86
6.	Tridecane	184	C13H28	83
7.	Pentadecane	212	C15H32	83
8.	Decane, 2,3,5-trimethyl-	184	C13H28	78
9.	Tetracosane	338	C24H50	78
10.	Nonane, 3,7-dimethyl-	156	C11H24	74
11.	Heptadecane	240	C17H36	72
12.	Iron, tricarbonyl[N-(phenyl-2-pyridinylm	398	C21H14FeN2O3	49
13.	Eicosane	282	C20H42	47
14.	Tetradecane, 2-methyl-	212	C15H32	43
15.	Docosane	310	C22H46	43
16.	Nonadecane	268	C19H40	38
17.	Octadecane	254	C18H38	38
18.	Nonacosane	408	C29H60	27
19.	Octadecane	254	C18H38	27
20.	Eicosane, 10-methyl-	296	C21H44	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000629-78-7	130827	107	18	1	94	5	70	42	87	9812
2.	*94	000629-78-7	130828	90	26	2	96	2	70	0	89	9862
3.	90	000593-45-3	131494	98	19	0	67	5	57	6	49	9876
4.	90	000544-76-3	130130	104	13	0	75	2	57	5	45	9817
5.	86	000629-62-9	129234	86	23	2	99	8	53	0	47	9861
6.	83	000629-50-5	127254	98	11	0	80	5	50	2	41	9771
7.	83	000629-62-9	129232	108	6	0	80	2	50	2	42	9733
8.	78	062238-11-3	27778	74	29	3	93	9	46	0	41	9859
9.	78	000646-31-1	134673	82	54	3	92	8	46	0	41	9900
10.	*74	017302-32-8	15631	69	26	1	90	16	44	17	52	9780
11.	*72	000629-78-7	52777	65	57	2	111	16	42	0	50	9867
12.	49	074764-11-7	97422	85	50	2	69	38	23	0	45	9916
13.	47	000112-95-8	67905	75	50	2	69	38	20	0	41	9917
14.	43	001560-95-8	129239	78	16	0	78	44	18	10	41	8978
15.	43	000629-97-0	133781	73	59	0	58	44	18	3	42	9962
16.	38	000629-92-5	132085	72	45	1	99	47	14	0	42	9647
17.	38	000593-45-3	131492	86	38	1	54	52	14	0	47	9899
18.	27	000630-03-5	99234	57	45	0	49	58	8	16	41	9960
19.	27	000593-45-3	131490	53	64	0	51	58	8	5	41	9904
20.	27	054833-23-7	72672	54	68	0	51	59	8	13	41	9891

CTMP Compounds

Peak 58; methylheptadecane



Scan 1469 (28.148 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2036	69.00	463	85.90	207	110.05	48
43.90	3	70.00	376	86.90	69	111.05	136
52.95	40	71.00	2307	90.95	67	113.00	176
54.95	649	72.95	173	92.90	87	114.00	38
55.95	635	73.95	46	97.00	328	115.00	68
57.05	3185	76.95	41	98.00	146	116.90	33
58.05	139	80.95	39	98.95	615	124.95	80
59.90	197	81.95	84	100.85	54	127.05	223
64.75	45	83.05	310	104.95	21	128.05	31
66.95	61	84.05	186	106.95	22	128.95	112
67.90	146	85.05	1450	108.95	27	139.00	51

Scan 1469 (28.148 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
139.90	61	182.95	33				
141.00	156	184.95	44				
142.15	24	187.00	6				
149.85	9	188.05	17				
153.95	36	190.15	44				
158.05	31	190.65	47				
158.95	16	210.20	163				
162.55	23	211.20	201				
168.15	42	212.30	68				
169.00	66	239.05	70				
178.55	30	254.15	65				

CTMP Compounds

Scan 1469 (28.148 min): R0264.D

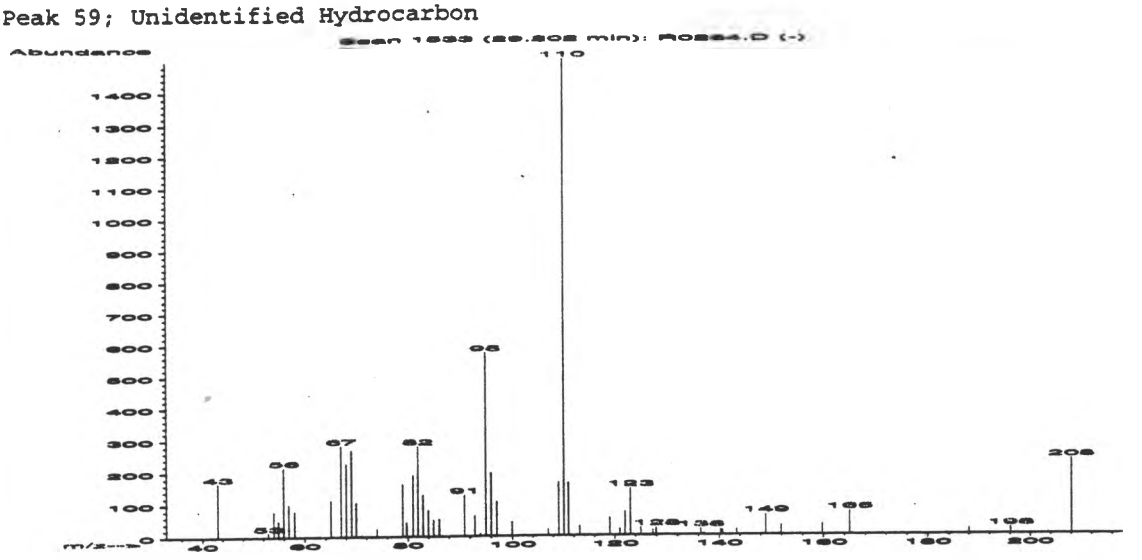
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Heptadecane, 2-methyl-	254	C18H38	87
2.	Tetradecane, 2-methyl-	212	C15H32	86
3.	Hexatriacontane	507	C36H74	86
4.	Octadecane	254	C18H38	81
5.	Pentadecane	212	C15H32	76
6.	Octadecane	254	C18H38	76
7.	Pentacosane	352	C25H52	74
8.	Eicosane	282	C20H42	72
9.	Tricosane	324	C23H48	72
10.	Heptadecane, 2-methyl-	254	C18H38	68
11.	Octacosane	394	C28H58	64
12.	Dodecane, 2-methyl-	184	C13H28	64
13.	Docosane	310	C22H46	64
14.	Heptadecane	240	C17H36	64
15.	Octacosane	394	C28H58	58
16.	Pentadecane	212	C15H32	58
17.	Tetracosane, 2,6,10,15,19,23-hexamethyl-	422	C30H62	58
18.	Dodecane, 1-iodo-	296	C12H25I	50
19.	Tetradecane, 1-iodo-	324	C14H29I	50
20.	Hexatriacontane	507	C36H74	49

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	001560-89-0	58319	74	60	2	88	12	54	0	81	9916
2.	*86	001560-95-8	129240	56	66	3	99	10	53	0	47	9910
3.	86	000630-06-8	136998	102	50	1	89	9	53	0	46	9919
4.	*81	000593-45-3	131492	72	54	1	83	16	49	0	68	9919
5.	*76	000629-62-9	129232	76	38	0	74	24	45	31	68	9799
6.	*76	000593-45-3	131490	69	51	1	80	25	45	0	76	9911
7.	74	000629-99-2	135023	97	46	1	93	16	44	0	51	9919
8.	72	000112-95-8	132690	78	52	1	97	18	42	0	43	9901
9.	72	000638-67-5	134294	80	54	1	96	16	42	0	43	9918
10.	*68	001560-89-0	131485	59	69	2	124	24	40	0	51	9884
11.	64	000630-02-4	96901	85	55	1	84	21	37	0	47	9917
12.	64	001560-97-0	127257	54	48	1	85	18	37	15	43	9791
13.	64	000629-97-0	133781	95	48	1	69	21	37	0	48	9837
14.	64	000629-78-7	130830	81	34	1	94	24	37	0	43	9859
15.	58	000630-02-4	135948	76	70	0	67	30	32	0	45	9833
16.	*58	000629-62-9	129234	56	52	0	76	28	32	0	49	9859
17.	58	000111-01-3	136351	78	72	2	76	30	32	0	43	9906
18.	50	004292-19-7	72273	55	62	0	79	33	25	16	43	9897
19.	50	019218-94-1	134271	55	70	0	84	34	25	4	43	9822
20.	49	000630-06-8	136996	75	82	0	71	36	23	0	45	9904

CTMP Compounds

Peak 59; Unidentified Hydrocarbon



Scan 1533 (29.202 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	167	69.95	105	91.00	128	113.15	31
52.90	13	71.00	5	92.95	64	119.00	55
54.05	79	74.05	23	94.00	7	121.00	20
54.95	50	79.05	161	95.00	574	122.00	74
55.95	215	79.80	44	96.00	197	123.00	146
56.95	100	81.05	191	97.05	107	125.00	24
58.05	79	81.95	281	99.95	44	127.30	17
65.00	112	83.00	129	107.00	20	127.95	24
67.00	282	83.95	81	109.05	167	136.45	20
68.00	226	85.00	51	110.05	1497	137.00	5
69.00	268	86.10	54	110.95	164	140.25	17

Scan 1533 (29.202 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.65	15						
143.40	18						
149.00	63						
151.95	30						
159.80	34						
165.00	73						
188.05	19						
196.15	21						
208.05	233						

CTMP Compounds

Scan 1533 (29.202 min): R0264.D

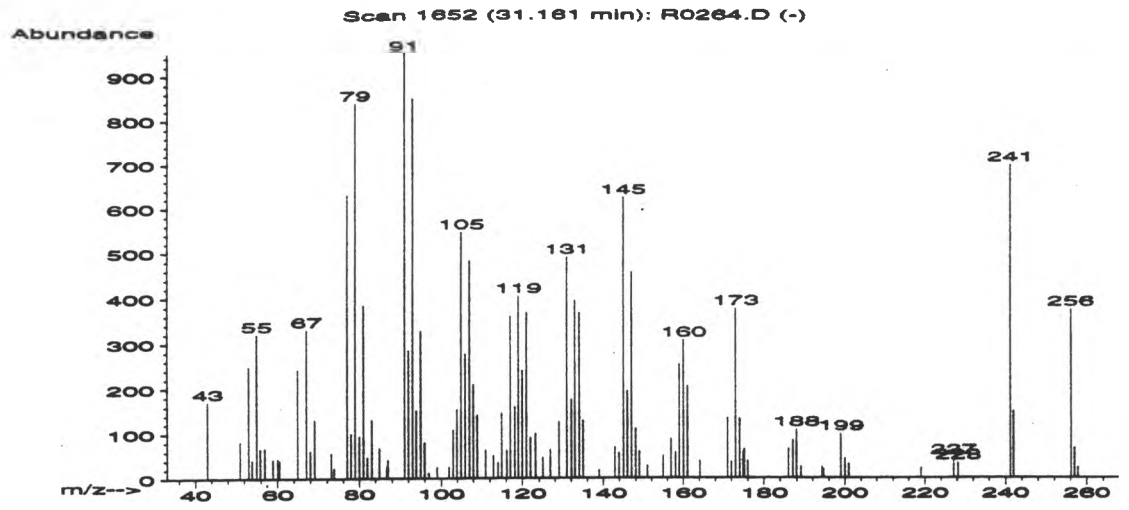
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	5-Methyl-2-pyrimidone	110	C5H6N2O	72
2.	6-Methyl-2-pyrimidone	110	C5H6N2O	64
3.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	64
4.	2-Cyclohexen-1-one, 5,5-dimethyl-3-(1-me	166	C11H18O	56
5.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	53
6.	1,10-ANHYDRO-6-DEOXY-7,8-DIHYDRO-7,8-DIH	184	C9H12O4	50
7.	1,3,7,7-TETRAMETHYL-2,11-DIOXA-10-BICYCL	226	C13H22O3	50
8.	Phenol, 4-(heptyloxy)-	208	C13H20O2	49
9.	7-Azabicyclo[4.1.0]heptane, 2-methyl-5-(	153	C10H19N	45
10.	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-,	170	C9H14O3	45
11.	5-Methyl-2-pyrimidone	110	C5H6N2O	43
12.	5-Methoxypyrimidine	110	C5H6N2O	43
13.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	43
14.	1,4-Benzenediol	110	C6H6O2	43
15.	1,4-Benzenediol	110	C6H6O2	43
16.	3-Methyl-5-methyliden-2(5H)-furanone	110	C6H6O2	38
17.	1,3-Benzenediol	110	C6H6O2	38
18.	Pyrazine, methyl-, 4-oxide	110	C5H6N2O	38
19.	Pyrrolidine, 1-(1-pentenyl)-	139	C9H17N	37
20.	N-METHYL-N-(2-PROPENYL)-CYCLOHEXYLAMINE	153	C10H19N	37

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	041398-85-0	118819	49	53	1	71	20	42	0	46	9752
2.	*64	015231-48-8	118820	48	47	1	71	23	37	0	46	9747
3.	*64	001072-91-9	2139	48	53	1	95	25	37	0	46	9709
4.	56	028017-79-0	19596	44	69	1	69	15	30	0	31	9761
5.	*53	001072-91-9	118843	42	56	2	99	26	28	0	39	8401
6.	50	000000-00-0	27319	47	85	3	89	16	25	0	37	9817
7.	50	070412-58-7	46714	56	62	3	85	16	25	0	36	9832
8.	*49	013037-86-0	38513	50	51	2	93	36	23	0	46	9325
9.	45	055854-39-2	14129	44	66	2	90	22	19	0	35	9813
10.	45	006994-95-2	21260	57	51	3	93	22	19	1	37	9774
11.	*43	041398-85-0	2112	44	28	1	83	41	18	0	40	9294
12.	*43	031458-33-0	2118	33	33	0	90	50	18	14	43	9081
13.	*43	013750-81-7	2107	45	32	0	76	44	18	3	38	9129
14.	*43	000123-31-9	118838	34	43	1	68	44	18	9	38	9141
15.	*43	000123-31-9	2131	34	55	1	99	44	18	0	39	9139
16.	*38	061892-54-4	2128	33	33	1	84	50	14	13	39	9080
17.	*38	000108-46-3	118835	33	53	0	82	48	14	0	41	9145
18.	*38	025594-37-0	2120	36	70	1	99	50	14	0	39	9081
19.	37	013937-90-1	8970	34	47	0	79	41	13	14	36	9365
20.	37	000000-00-0	14125	42	44	1	67	44	13	10	31	9160

CTMP Compounds

Peak 60; Unidentified terpenoid



Scan 1652 (31.161 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	171	67.00	330	83.05	130	98.95	25
50.95	82	68.00	61	84.95	67	101.95	26
53.00	249	69.00	130	86.70	26	102.95	108
53.85	41	73.05	57	87.00	41	103.95	155
54.95	321	73.80	24	91.00	950	104.95	546
55.85	66	76.95	630	92.00	284	105.95	277
56.95	68	77.95	100	93.00	848	107.05	483
58.95	43	78.95	838	93.90	152	107.95	210
60.15	44	79.95	94	95.00	328	108.95	141
60.50	39	81.05	384	96.00	80	111.00	63
64.90	242	81.95	47	97.00	12	112.90	51

Scan 1652 (31.161 min): R0264.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.00	36	126.80	64	146.00	194	164.15	39
114.90	146	129.05	126	147.00	458	171.00	134
116.15	63	130.95	491	148.00	110	172.00	37
117.00	361	132.05	175	149.00	59	173.00	377
118.15	160	132.95	394	150.95	28	174.00	132
119.00	405	134.05	366	154.95	50	174.90	58
120.00	240	135.00	128	156.95	88	175.15	64
121.00	368	139.00	18	158.05	57	176.00	38
122.00	91	142.90	69	159.05	254	185.95	65
123.15	100	143.90	56	160.05	308	187.05	85
124.95	47	145.00	626	161.05	205	187.95	108

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
189.05	25	256.05	375				
194.25	25	256.95	66				
194.65	20	257.80	24				
199.00	99						
200.00	43						
201.00	32						
219.00	23						
227.15	45						
228.25	34						
241.20	699						
242.00	149						

Scan 1652 (31.161 min): R0264.D

CTMP Compounds

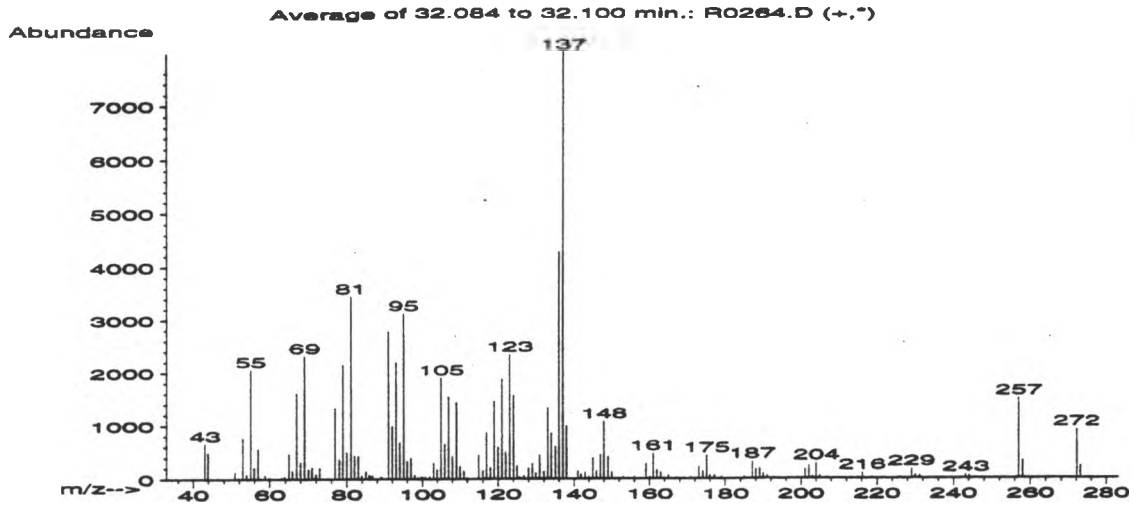
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	CYCLOPENTAN-3'-SPIROTRICYCLO[3.1.0.0(2,4	188	C14H20	68
2.	CIS/TRANS-7-BICYCLO[4.1.0]HEPT-7-YLIDENE	188	C14H20	60
3.	1-PHENYL-3,5-DIMETHYL-4,5,67(8H)-TETRAHY	256	C14H16N4O	25
4.	Pyrimidine, 2,4-bis[(trimethylsilyl)oxy]	256	C10H20N2O2Si2	22
5.	Phenol, 4,4'-(1-methylethylidene)bis[2-m	256	C17H20O2	22
6.	Mixture of trans,trans-1,3-Dimethylenecy	188	C14H20	11
7.	3,5-Dimethylbenzaldehyde	134	C9H10O	10
8.	7-(7-Methylnorbornadiene)carbaldehyde	134	C9H10O	10
9.	trans-Caryophyllene	204	C15H24	10
10.	Silane, methoxydimethyl(pentafluoropheny	256	C9H9F5OSi	10
11.	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	10
12.	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	10
13.	Farnesene	204	C15H24	10
14.	4,4-DIDEUTERIO-1,2,3,4-TETRAHYDROCARBAZO	171	C12H11D2N	10
15.	Dispiro[2.1.2.4]undecane, 8-methylene-	162	C12H18	10
16.	1H-Pyrrole, 3-ethyl-5-[(4-ethyl-3,5-dime	256	C17H24N2	10
17.	Cyclohexane, 1,5-diethenyl-3-methyl-2-me	162	C12H18	10
18.	1,7-OCTADIENE, 2,7-DIMETHYL-3,6-DIMETHYL	162	C12H18	10
19.	1-Dibenzofurancarboxylic acid, 1,9b-dihy	256	C16H16O3	10
20.	trans-7,7-Dimethyl-6-methylidenetricyclo	188	C14H20	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*68	078578-93-5	29438	88	55	0	81	70	40	0	95	6241
2.	*60	000000-00-0	29441	79	65	0	78	70	35	0	93	7034
3.	*25	064899-15-6	58840	65	100	2	59	72	7	0	64	6175
4.	*22	010457-14-4	58667	64	77	2	72	62	5	1	40	6089
5.	*22	000079-97-0	59059	50	55	1	70	63	5	14	39	5409
6.	*11	066405-18-3	29413	55	31	0	98	75	2	0	49	6150
7.	*10	000000-00-0	7382	43	34	0	56	79	1	7	40	4160
8.	*10	082478-38-4	7415	33	48	1	116	77	1	0	39	4383
9.	10	000087-44-5	128693	57	88	0	92	79	1	0	39	5725
10.	*10	023761-74-2	131533	44	118	3	115	75	1	0	40	7007
11.	10	000630-20-6	125449	57	46	0	42	72	1	2	41	4946
12.	10	000630-20-6	19061	45	58	0	42	72	1	0	39	4911
13.	10	000502-61-4	36639	43	90	2	89	79	1	4	38	4545
14.	*10	065342-65-6	21912	36	53	1	64	80	1	0	39	4817
15.	10	051567-08-9	17903	61	61	1	86	75	1	0	39	5049
16.	*10	002407-83-2	59075	33	115	1	73	72	1	0	39	5222
17.	10	074742-35-1	17868	73	59	1	78	72	1	17	39	5500
18.	10	000000-00-0	17825	52	65	0	84	72	1	4	38	5867
19.	*10	040801-40-9	58996	33	129	2	69	72	1	0	39	5229
20.	*10	082078-83-9	29440	58	71	0	80	77	1	14	41	5950

CTMP Compounds

Peak 61; Diterpene (Sandaracopimaradiene)



Average of 32.084 to 32.100 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	663	58.80	67	71.00	219	83.00	426
43.90	490	60.00	26	71.75	37	83.95	59
46.45	10	60.65	12	72.00	92	85.00	142
50.90	131	63.00	28	72.95	212	85.90	71
51.95	30	63.75	47	75.05	21	86.50	53
52.95	765	64.95	467	76.95	1335	86.75	62
54.00	86	65.90	159	78.00	365	88.90	37
54.95	2055	67.00	1606	78.95	2151	89.25	25
55.95	212	68.00	308	80.00	497	91.00	2772
56.95	562	69.00	2311	81.05	3428	92.00	987
57.80	13	70.05	182	82.00	433	93.00	2190
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
94.00	678	103.00	300	116.00	153	126.80	59
95.00	3110	103.95	174	117.00	867	127.95	203
96.00	327	104.95	1896	118.00	213	129.00	277
97.00	387	105.95	648	119.00	1454	129.95	104
98.00	74	107.00	1537	120.00	587	130.95	445
98.95	30	108.00	414	121.00	1873	132.00	134
99.70	44	109.05	1427	122.05	506	133.05	1330
99.95	26	110.05	229	123.10	2334	133.95	855
100.20	26	111.05	148	124.10	1556	135.05	598
100.80	39	111.90	21	125.00	235	136.05	4263
101.90	52	114.95	440	125.80	24	137.05	7961

Average of 32.084 to 32.100 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
138.00	986	152.95	33	169.00	18	188.05	170
141.00	141	155.95	36	171.00	33	189.05	180
141.90	86	159.05	274	172.15	17	190.00	91
143.00	121	160.05	38	173.10	216	191.00	47
144.00	39	161.00	466	174.15	135	199.00	21
145.00	387	162.00	159	175.10	429	201.15	176
146.00	146	163.05	109	176.00	61	202.15	236
147.00	449	163.90	20	177.05	52	203.05	36
148.00	1075	165.00	67	179.05	39	204.05	286
149.05	405	166.90	22	185.05	34	205.05	51
150.05	124	168.00	16	187.05	315	206.80	14

Average of 32.084 to 32.100 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
207.05	15	244.10	50				
212.95	17	253.25	8				
215.05	24	257.05	1492				
216.10	102	258.05	323				
218.50	15	272.15	903				
218.90	9	273.15	223				
229.05	172						
230.05	58						
231.10	57						
238.95	15						
243.15	62						

Average of 32.084 to 32.100 min.: R0264.D
Converted from RTE data file: >R0264:

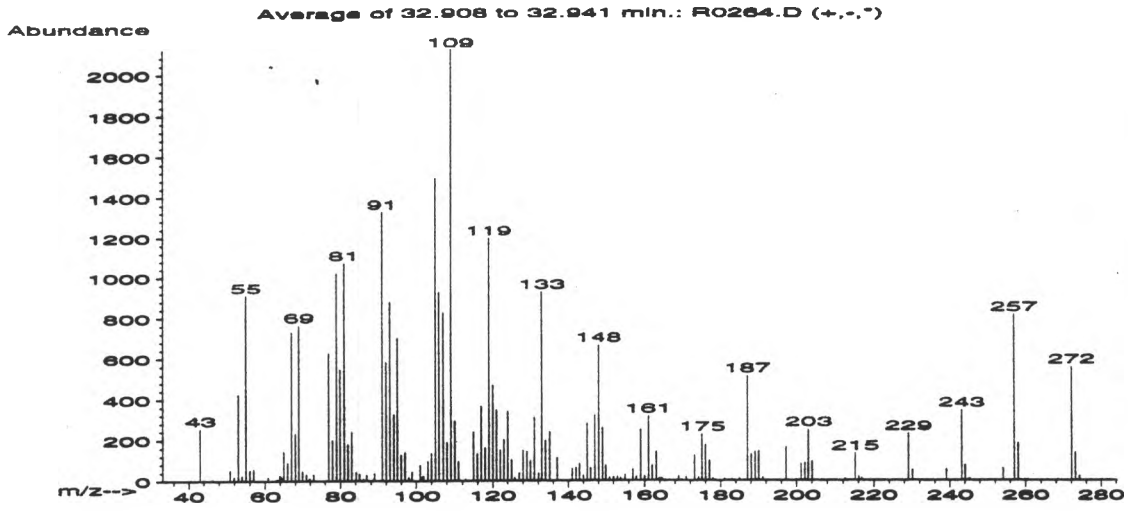
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Sandaracopimaradiene	272	C20H32	94
2.	4a(2H)-Naphthalenecarboxylic acid, octah	196	C12H20O2	43
3.	(X-BUTENYL)-BIS(X-CHLOROBUTYL) ESTER OF	316	C12H23Cl2O3P	43
4.	1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethy	236	C15H24O2	38
5.	cis-anti-cis-Tricyclo[7.3.0.0(2,6)]dodec	178	C12H18O	38
6.	Phosphonic acid, bicyclo[2.2.1]hept-2-yl	204	C9H17O3P	38
7.	1-Chlorobicyclo[3.3.1]nonan-3-one	172	C9H13ClO	37
8.	Cyclopenta[c]pyran, 3,4,4a,5,6,7-hexahyd	152	C10H16O	35
9.	1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethy	236	C15H24O2	32
10.	BORNYL ESTER OF 3-ISOPROPYLIDENE-CYCLOPE	290	C19H30O2	32
11.	3,5-Octadiene, 2,2,4,5,7,7-hexamethyl-,	194	C14H26	27
12.	BICYCLO[3.3.1]NON-1-BROMO-3-ONE	216	C9H13BrO	25
13.	Phenol, 3-(dimethylamino)-	137	C8H11NO	22
14.	Pyrazine, 2-methoxy-3-(1-methylethyl)-	152	C8H12N2O	16
15.	BICYCLO[3.3.1]NON-1-BROMO-3-ONE	216	C9H13BrO	14
16.	PYRIDINE-4-AMIDOXIME	137	C6H7N3O	14
17.	2(1H)-Pyridinone, 1-ethyl-6-methyl-	137	C8H11NO	14
18.	Benzaldehyde, 3-hydroxy-, oxime	137	C7H7NO2	14
19.	Benzeneacetic acid, .alpha.-hydroxy-2-me	182	C9H10O4	12
20.	.alpha.-Chamigrene	204	C15H24	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	001686-56-2	132292	112	48	2	81	3	70	33	91	9890
2.	43	062338-25-4	33008	43	74	2	69	44	18	17	38	9072
3.	43	000000-00-0	78743	56	83	1	77	45	18	9	38	8890
4.	38	021730-91-6	50874	43	83	3	86	47	14	0	39	8641
5.	38	073306-76-0	24911	58	60	2	95	50	14	0	39	8457
6.	38	031061-88-8	36247	53	72	3	80	50	14	11	38	8391
7.	37	066921-77-5	22156	54	55	2	73	45	13	15	37	8965
8.	35	075222-59-2	13737	60	57	1	80	52	11	0	39	8377
9.	32	021730-91-6	130642	56	64	1	68	46	9	6	37	8670
10.	32	000000-00-0	70699	45	111	3	99	47	9	0	37	8686
11.	27	055712-52-2	32145	59	60	0	60	56	8	6	39	8800
12.	25	066077-98-3	129423	56	62	1	76	52	7	15	37	8157
13.	22	000099-07-0	8296	48	48	0	53	65	5	9	38	8241
14.	16	025773-40-4	13395	45	49	1	96	57	3	0	37	8114
15.	*14	066077-98-3	41754	34	54	1	53	68	2	0	39	8034
16.	*14	001594-57-6	8226	33	86	3	99	68	2	0	39	7741
17.	*14	019038-36-9	8283	37	78	3	67	66	2	0	39	7997
18.	*14	022241-18-5	8270	33	52	1	69	67	2	0	39	7822
19.	12	010408-29-4	126984	43	73	2	72	65	2	0	35	7758
20.	*11	019912-83-5	128680	55	53	1	43	78	2	0	47	5312

Peak 62; Diterpene (Isopimaradiene)

CTMP Compounds



Average of 32.908 to 32.941 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	256	62.95	3	71.75	12	84.20	43
43.95	4	63.25	8	72.00	10	85.00	33
46.30	7	63.90	29	72.95	32	85.75	1
50.85	53	64.25	23	76.95	626	86.00	10
51.85	19	64.95	144	77.95	200	86.90	28
52.95	423	65.95	87	78.95	1020	88.75	9
53.95	26	67.00	731	79.95	546	88.95	36
54.95	910	68.00	231	81.00	1071	91.00	1327
55.95	53	69.00	763	81.95	177	92.00	581
57.00	57	69.95	48	83.00	239	93.00	878
60.90	19	71.00	34	84.00	5	94.00	327

Average of 32.908 to 32.941 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.00	699	104.95	1492	117.95	161	129.00	142
96.00	126	105.95	925	119.00	1196	130.00	95
97.00	139	107.05	825	120.00	471	131.00	310
98.00	18	108.05	188	121.00	347	132.05	36
98.90	44	109.05	2118	122.00	150	132.95	929
100.95	77	110.05	293	123.00	201	134.00	196
101.30	15	111.05	93	124.05	340	135.05	237
101.70	22	112.90	10	125.05	101	137.05	110
101.95	22	114.95	239	125.90	15	141.00	59
103.00	94	115.95	132	126.95	38	142.00	64
103.95	136	117.00	366	128.00	147	143.00	83
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.00	26	154.95	29	169.00	23	187.05	513
145.00	282	156.95	54	170.95	20	188.05	127
145.95	60	157.95	19	173.10	125	189.10	142
147.00	321	159.00	249	174.25	16	190.05	143
148.05	665	160.05	21	175.10	226	191.15	14
149.05	258	161.05	316	176.05	174	197.15	164
149.95	73	162.05	74	177.00	96	199.90	7
150.95	15	163.10	141	177.95	10	201.15	83
151.95	18	163.80	10	181.05	9	202.15	85
152.95	19	164.15	12	183.00	7	203.05	249
153.85	13	164.65	11	184.95	12	204.05	94

Average of 32.908 to 32.941 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

207.95	3	245.25	8
212.55	9	254.10	59
215.20	132	257.05	816
216.15	19	258.05	184
216.90	12	272.15	556
229.10	229	273.15	135
230.15	51	274.20	23
239.05	55		
243.15	346		
244.10	75		
245.00	7		

Average of 32.908 to 32.941 min.: R0264.D
Converted from RTE data file: >R0264:

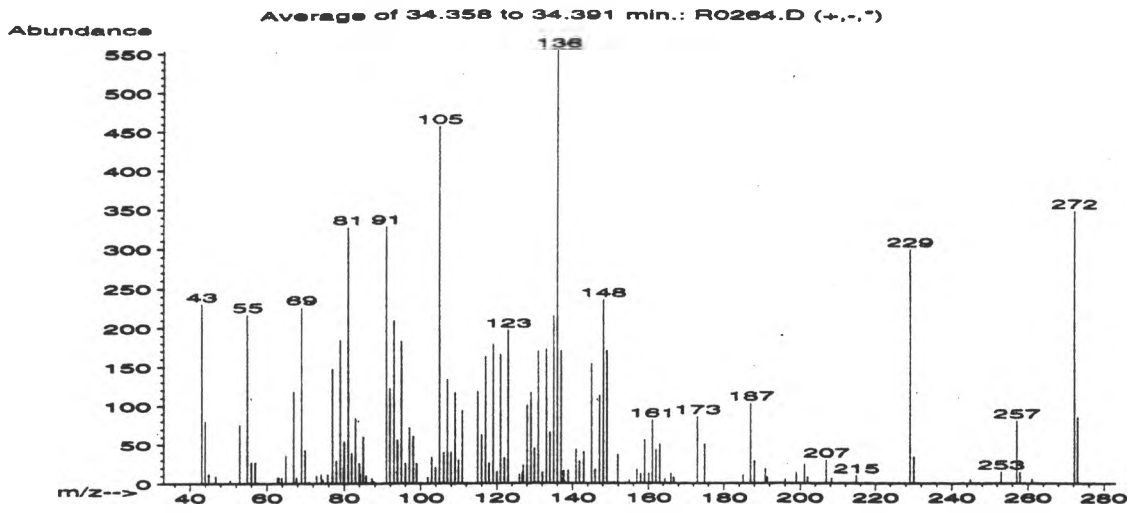
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Isopimaradiene	272	C20H32	96
2.	Trachylobane	272	C20H32	49
3.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	15
4.	8-ETHYLCYCLO-OCTA-2,4,6-TRIENONE	148	C10H12O	14
5.	2-Cyclopenten-1-one, 3,4,4-trimethyl-	124	C8H12O	11
6.	trans-Caryophyllene	204	C15H24	11
7.	Cyclohexanecarboxylic acid, 4-(chloromet	204	C10H17ClO2	11
8.	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	10
9.	(1R*,2S*,5R*)-1,4,4-Trimethylbicyclo[3.2	190	C13H18O	10
10.	3,5-Heptadien-2-one, 6-methyl-, (E)-	124	C8H12O	10
11.	Bicyclo[2.2.1]heptane, 7-methylene-2-(1-	148	C11H16	10
12.	Benzene, 1-ethyl-4-fluoro-	124	C8H9F	10
13.	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	10
14.	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	10
15.	2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	10
16.	2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	10
17.	Phenol, 3-amino-	109	C6H7NO	10
18.	Benzamide, 2-hydroxy-N-(4-hydroxyphenyl)	229	C13H11NO3	10
19.	2-CARENE, 4-.ALPHA.-ISOPROPENYL-, (+)-	176	C13H20	10
20.	2,8-Decadiyne	134	C10H14	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	001686-66-4	132293	137	54	2	76	5	76	0	95	9932
2.	*49	005282-35-9	64471	84	111	3	59	38	23	21	43	6594
3.	*15	020070-61-5	132290	78	91	1	46	75	2	0	60	7107
4.	*14	061775-57-3	12053	34	37	0	62	70	2	0	41	5258
5.	*11	030434-65-2	4785	34	54	0	75	77	2	21	43	6690
6.	*11	000087-44-5	128690	50	76	0	44	80	2	0	46	6724
7.	*11	055590-77-7	36282	48	79	2	74	77	2	0	46	6723
8.	*10	003277-26-7	7206	37	65	0	50	76	1	0	41	4873
9.	*10	081532-23-2	30154	35	43	0	63	72	1	0	39	5735
10.	*10	016647-04-4	4765	45	52	1	73	77	1	0	40	6676
11.	*10	066929-97-3	12140	33	71	0	50	76	1	0	41	4750
12.	*10	000459-47-2	4751	45	38	0	84	77	1	14	43	6678
13.	10	000116-02-9	122724	45	52	3	77	77	1	18	38	6625
14.	*10	003277-26-7	121492	37	62	0	56	76	1	0	41	4868
15.	*10	000694-85-9	118786	36	44	2	83	77	1	5	40	6625
16.	*10	000694-85-9	2043	33	69	3	99	77	1	0	39	6625
17.	*10	000591-27-5	118800	44	49	2	99	77	1	0	40	6625
18.	*10	000526-18-1	47981	43	64	3	93	77	1	0	40	6659
19.	*10	000000-00-0	24060	61	71	1	73	76	1	0	41	5743
20.	10	004116-93-2	7429	43	72	1	57	73	1	4	38	5282

CTMP Compounds

Peak 63; unidentified Diterpene



Average of 34.358 to 34.391 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	230	63.15	8	75.80	11	85.00	60
43.95	80	63.90	7	76.95	147	85.75	10
44.95	12	64.90	36	77.95	29	87.25	6
46.70	9	66.95	118	79.00	184	87.70	2
50.50	4	67.75	7	79.85	21	91.00	328
52.95	76	69.00	226	80.00	54	91.95	122
54.95	217	69.95	43	81.00	327	93.00	209
55.95	27	70.95	2	81.95	39	94.00	56
57.00	27	72.90	10	83.00	84	95.00	183
61.40	1	74.05	12	83.95	26	96.00	26
62.75	7	74.50	4	84.20	12	97.00	72

Average of 34.358 to 34.391 min.: R0264.D
Converted from RTE data file: >R0264:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.05	61	111.00	94	125.95	11	136.05	554
99.00	26	114.95	118	126.70	14	137.05	171
101.95	8	116.00	63	126.95	23	137.75	16
102.90	34	116.95	163	127.95	101	138.00	3
103.95	21	117.95	26	129.00	117	138.95	17
104.95	456	119.00	179	129.95	45	140.90	44
106.05	40	120.00	15	130.95	170	141.90	29
107.00	134	121.00	166	132.05	14	142.95	41
107.95	40	122.00	33	133.05	173	145.00	154
109.00	117	123.00	197	134.00	66	145.90	18
110.00	30	124.90	1	135.00	216	147.15	113

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.10	236	163.05	51	194.95	1	253.00	15
149.05	171	164.40	6	196.05	5	257.05	81
150.95	2	166.00	13	198.90	14	257.95	14
151.95	37	166.75	8	201.15	25	261.05	6
154.90	4	173.00	86	202.00	8	272.10	349
156.95	18	174.95	51	206.90	30	273.00	85
157.95	12	185.05	11	208.30	7		
158.95	56	187.00	103	214.95	10		
160.05	13	188.00	29	229.05	300		
161.00	82	190.90	19	230.05	34		
162.05	43	191.40	8	244.90	5		

CTMP Compounds

Average of 34.358 to 34.391 min.: R0264.D
Converted from RTE data file: >R0264:

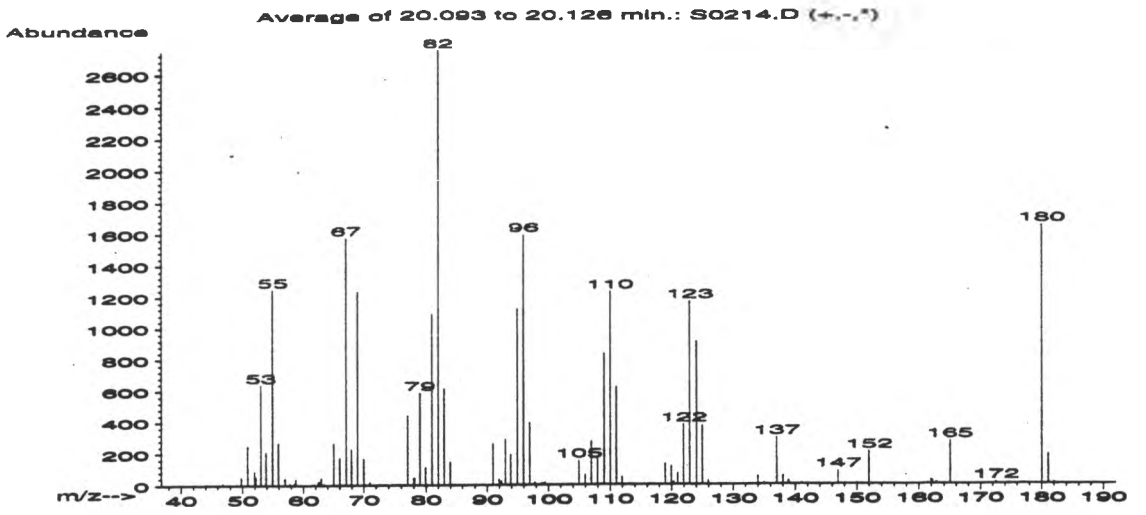
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,5-CYCLOOCTADIENE-(1-ETHYLBORINATO)-COB	272	C15H22BCo	43
2.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	42
3.	Androst-5-en-4-one	272	C19H28O	35
4.	4,5-DIMETHYL-O-PHENYLENDIAMINE	136	C8H12N2	27
5.	Perylene, eicosahydro-	272	C20H32	25
6.	(3.alpha.,6a.alpha.,6b.beta.,10.beta.,12	272	C18H24O2	25
7.	3.BETA.-HYDROXY-ANDROST-5,16-ENE	272	C19H28O	25
8.	Ketone, methyl 3-pyridyl, O-acetyloxime	178	C9H10N2O2	22
9.	Benzaldehyde, 2-methoxy-	136	C8H8O2	22
10.	Androst-16-en-3-one, (5.alpha.)-	272	C19H28O	20
11.	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	137	C9H15N	18
12.	Cembrene-C	272	C20H32	16
13.	Podocarpa-6,13-diene, 13-isopropyl-	272	C20H32	11
14.	ZINC, BIS(4-PENTENYL)-	202	C10H18Zn	11
15.	Benzenemethanol, 3,5-dimethyl-	136	C9H12O	10
16.	BICYCLO(3,2,2)NON-6-EN-3-ONE	136	C9H12O	10
17.	6-METHYL-4,5-DIPHENYL-6H-CYCLOPENTA[B]FU	272	C20H16O	10
18.	Acetic acid, (2-benzothiazolyloxy)-	209	C9H7NO3S	10
19.	Benzocyclododecene, 2,3-diethyl-4a,5,6,7	272	C20H32	10
20.	VULGAROL A	220	C15H24O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	000000-00-0	64205	46	137	0	77	43	18	7	40	8243
2.	*42	020070-61-5	64458	97	99	2	62	60	17	38	78	5973
3.	*35	013583-72-7	64398	78	98	1	53	66	11	0	78	5598
4.	*27	000000-00-0	7858	36	54	1	90	60	8	0	39	7161
5.	*25	047041-72-5	132296	52	108	0	58	65	7	0	46	6618
6.	*25	071370-29-1	64348	89	84	2	53	72	7	48	70	5499
7.	*25	000000-00-0	64406	66	126	3	59	72	7	0	64	4772
8.	22	003240-21-9	24539	44	73	2	99	62	5	16	38	7097
9.	*22	000135-02-4	121851	43	74	2	71	62	5	4	39	7083
10.	*20	018339-16-7	132275	60	111	2	55	68	4	0	51	5425
11.	*18	007148-07-4	8325	54	42	0	68	68	3	0	49	6909
12.	16	064363-64-0	64437	57	105	2	92	56	3	0	36	8318
13.	*11	005939-62-8	64460	61	124	2	62	80	2	0	46	5007
14.	*11	000000-00-0	35460	56	68	2	98	80	2	0	47	4298
15.	*10	027129-87-9	7919	35	60	2	72	72	1	17	40	6923
16.	*10	000934-62-3	8043	34	68	2	99	71	1	13	40	6868
17.	*10	086738-91-2	64429	38	91	0	46	80	1	0	39	5056
18.	10	002875-32-3	38875	46	60	1	83	73	1	9	38	6763
19.	*10	061141-65-9	64463	57	110	2	62	74	1	0	40	4952
20.	10	011056-03-4	44015	58	84	3	249	72	1	0	39	3822

CTMP Compounds

Peak 64; Monoterpene acetate



Average of 20.093 to 20.126 min.: S0214.D
Converted from RTE data file: >S0214:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.80	12	57.75	10	67.05	1571	79.90	110
49.05	6	58.50	13	67.95	226	80.95	1090
49.80	50	58.75	38	68.95	1230	82.00	2747
50.85	248	61.20	4	70.80	166	82.95	615
51.95	87	61.80	6	71.00	18	83.95	148
52.20	52	62.40	20	75.30	6	90.95	263
53.00	637	62.65	21	75.80	7	91.95	36
53.85	208	62.90	44	77.00	443	92.30	24
54.95	1243	63.40	7	77.95	44	92.95	290
55.90	269	65.00	267	78.20	44	93.85	193
56.95	43	66.00	171	79.00	586	94.95	1123

Average of 20.093 to 20.126 min.: S0214.D
Converted from RTE data file: >S0214:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.95	1594	110.00	1232	124.05	914	146.95	86
96.95	398	111.00	624	125.00	373	148.00	5
97.80	16	111.95	50	125.95	24	149.95	8
98.75	7	113.00	2	127.85	4	151.95	206
99.05	13	116.50	8	128.90	6	161.40	9
99.45	16	118.95	133	133.95	54	161.90	26
104.95	153	119.95	114	135.00	11	162.15	25
105.95	63	120.30	17	137.00	298	162.75	12
106.95	277	121.00	72	138.00	54	165.00	274
107.95	176	121.95	382	138.90	25	172.55	12
109.00	837	122.95	1169	141.05	11	179.00	4

Average of 20.093 to 20.126 min.: S0214.D
Converted from RTE data file: >S0214:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
180.00	1652						
181.05	186						
182.00	11						

CTMP Compounds

Average of 20.093 to 20.126 min.: S0214.D
Converted from RTE data file: >S0214:

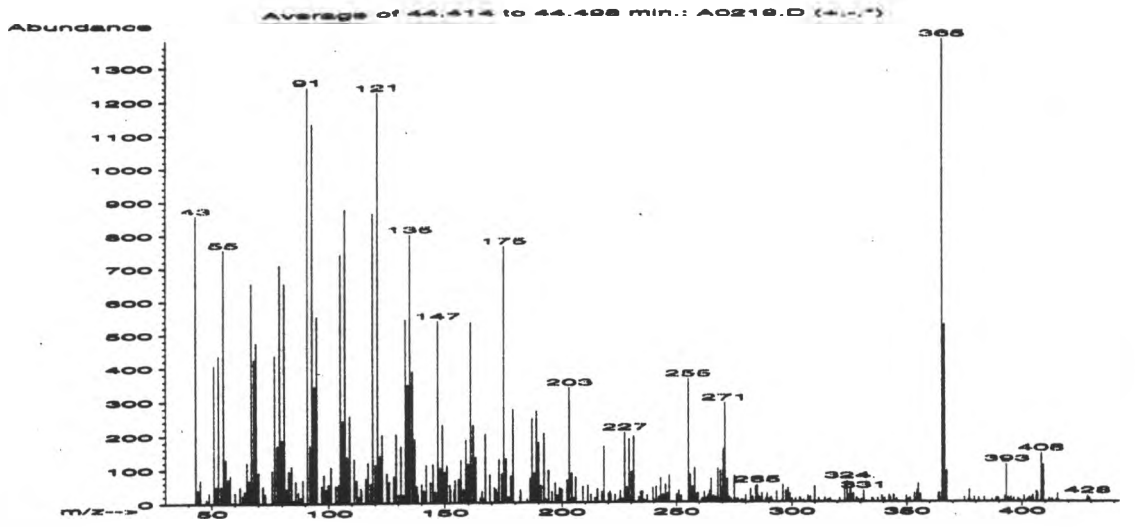
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Carone	152	C10H16O	38
2.	TRANS-5,10-DIMETHYLDECALONE-2	180	C12H20O	35
3.	3-Octyne, 2-methyl-	124	C9H16	35
4.	d-Isothujone	152	C10H16O	30
5.	3-Octyne, 7-methyl-	124	C9H16	27
6.	2(1H)-Pyridinone, 1-ethyl-	123	C7H9NO	25
7.	7-CHLORO-2-METHYL-2,3-HEPTADIENE	144	C8H13Cl	22
8.	Theobromine	180	C7H8N4O2	15
9.	P-METHOXYPHENYL GLYCIDYL ETHER	180	C10H12O3	14
10.	HEX-1-ENE-5-IMINE	97	C6H11N	14
11.	2,4-DIMETHYLFURAN	96	C6H8O	14
12.	Theobromine	180	C7H8N4O2	14
13.	3-Octyne	110	C8H14	14
14.	(ACETYLETHYL)PHENYLTHIOL	180	C10H12OS	11
15.	(1R*,5.ALPHA.,6.BETA.)-5-HYDROXY-6-METHY	180	C11H16O2	10
16.	2-Cyclohexen-1-one, 3-methyl-6-(1-methyl	152	C10H16O	10
17.	1-Pyrrolidinecarbonitrile	96	C5H8N2	10
18.	1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	10
19.	CIS-DIMETHYL-ISOPROPYLIDENE CYCLOPROPANE	110	C8H14	10
20.	Pyridine, 1-ethyl-1,2,3,6-tetrahydro-	111	C7H13N	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000497-62-1	13726	43	57	0	69	49	14	25	43	8041
2.	*35	000000-00-0	25805	49	87	3	85	55	11	0	39	6005
3.	35	055402-15-8	120437	46	58	0	59	55	11	19	41	6877
4.	*30	000471-15-8	13717	56	65	3	65	59	9	0	47	6559
5.	27	037050-06-9	4876	44	53	3	173	58	8	16	41	6095
6.	*25	013337-79-6	4557	53	53	1	51	65	7	0	47	5169
7.	22	065041-85-2	10640	45	53	0	84	65	5	0	39	7103
8.	*15	000083-67-0	126770	58	59	1	54	72	2	0	51	6894
9.	*14	002211-94-1	25533	44	63	1	41	70	2	0	40	5182
10.	*14	000000-00-0	688	36	69	2	93	68	2	0	39	6872
11.	*14	000000-00-0	591	61	34	0	56	68	2	2	41	5415
12.	*14	000083-67-0	126769	57	72	1	52	68	2	0	40	6952
13.	*14	015232-76-5	118878	35	54	0	47	70	2	0	41	5810
14.	*11	006110-01-6	25463	48	29	0	55	71	2	0	46	5245
15.	*10	030841-58-8	25693	44	57	2	49	71	1	0	39	5496
16.	*10	000089-81-6	123973	33	64	0	50	73	1	0	41	7178
17.	*10	001530-88-7	567	37	55	1	57	76	1	11	40	4632
18.	*10	000694-31-5	560	41	47	0	57	78	1	0	39	4205
19.	10	000000-00-0	2261	46	60	0	75	72	1	0	39	5030
20.	*10	006972-40-3	2369	33	60	0	45	80	1	0	41	4522

CTMP Compounds

Peak 65; Triterpene



Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	859	56.95	72	68.05	424	82.05	43
43.95	40	57.90	82	68.95	474	83.00	97
44.90	70	59.00	2	70.00	92	84.05	109
47.80	12	59.95	32	72.00	51	85.05	9
48.85	31	62.05	49	73.00	29	85.95	66
51.00	408	63.15	23	75.95	98	87.00	33
51.95	50	63.45	12	77.00	439	87.95	18
52.95	437	64.00	35	78.05	172	89.00	70
54.00	51	64.95	120	79.05	710	89.90	3
54.95	755	66.05	68	80.05	187	91.00	1242
56.00	131	67.00	654	81.05	654	92.05	171

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.05	1133	105.05	742	114.15	36	126.00	63
93.95	344	106.00	243	116.00	75	128.00	80
95.00	553	107.00	878	117.05	119	129.00	204
97.00	52	108.00	137	118.05	57	130.05	24
98.00	85	109.00	257	118.95	865	131.05	168
99.00	41	110.05	2	120.00	112	132.05	24
99.85	56	111.05	130	121.05	1224	133.00	543
100.05	11	112.05	68	122.05	139	134.00	349
101.00	107	112.65	21	123.05	202	135.00	800
103.00	52	113.65	19	124.05	2	136.05	388
104.20	56	113.95	44	125.05	88	137.10	187

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
138.05	50	150.05	92	161.05	537	172.05	30
138.40	25	151.00	110	162.10	230	173.05	129
140.15	56	152.20	54	163.05	134	174.25	86
141.10	36	152.55	39	165.05	14	175.05	766
142.05	112	154.00	39	165.75	34	176.10	130
143.95	62	154.45	68	166.20	12	177.00	16
145.00	114	156.00	72	167.15	203	178.00	80
146.00	32	157.05	129	169.05	83	178.55	54
147.05	540	158.05	40	170.00	2	179.05	275
148.00	103	159.05	185	171.05	45	181.90	20
149.00	231	160.10	115	171.70	39	182.20	38

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
185.05	10	197.10	58	209.00	48	223.10	23
186.20	73	197.80	21	211.10	52	224.40	6
187.05	249	198.45	21	212.40	24	225.30	34
188.10	88	199.10	43	214.10	15	226.25	10
189.05	270	199.85	39	215.15	38	227.25	208
190.05	178	202.15	67	215.40	40	228.15	45
191.00	50	203.15	340	217.15	32	229.15	187
192.20	205	204.10	3	218.15	167	230.30	91
193.10	10	204.25	88	220.05	27	231.10	196
194.20	96	205.10	13	220.80	32	233.40	15
195.70	31	205.95	76	221.05	25	233.65	10

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
233.95	13	244.10	23	256.05	83	263.40	14
234.20	31	244.35	21	257.05	47	263.85	23
234.65	18	245.15	53	258.05	102	264.15	18
235.05	32	246.10	27	258.95	26	264.50	36
235.95	7	246.55	19	259.45	28	265.05	71
237.10	21	246.90	80	261.05	8	265.75	16
239.65	43	248.15	1	261.40	12	266.25	19
240.10	10	250.10	23	261.75	8	267.05	16
241.20	47	251.05	35	262.15	31	268.05	101
242.25	17	252.20	19	262.40	14	269.20	94
243.10	73	255.20	365	262.65	12	270.05	43

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
270.25	158	278.35	8	286.95	26	298.25	41
271.10	294	279.05	6	288.60	10	298.55	12
271.60	25	280.05	21	289.15	25	299.00	25
272.25	70	282.15	39	289.90	9	299.95	9
273.10	15	283.00	16	290.90	12	300.50	1
273.95	9	284.20	48	291.15	14	301.55	10
275.15	80	284.75	16	293.40	31	303.45	13
275.70	10	284.95	52	295.60	7	303.70	9
276.70	11	285.50	16	296.10	51	305.15	6
277.55	2	285.75	16	297.30	33	307.10	19
277.85	5	286.05	12	297.55	13	308.15	15

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
309.95	46	325.90	42	337.40	10	353.25	27
311.85	11	326.25	11	339.20	18	353.55	10
314.50	12	326.65	19	340.40	10	354.15	5
315.15	2	326.95	26	342.25	21	354.50	36
315.90	6	328.40	12	342.80	13	355.00	55
316.65	9	329.20	6	344.30	21	355.95	23
320.95	11	330.40	8	345.55	8	356.25	3
323.25	58	331.40	34	349.70	18	357.05	2
324.30	63	332.45	1	350.15	5	363.60	26
325.20	21	334.90	10	350.80	9	364.25	27
325.55	34	335.50	9	351.45	12	365.30	1380

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
366.25	527	388.15	1	396.55	11	408.30	144
367.20	92	388.40	2	398.35	10	409.25	108
375.05	13	388.75	11	399.25	5	411.75	10

376.70	8	389.10	5	400.65	2	413.15	7
377.10	36	389.50	12	401.00	17	414.90	7
377.85	4	389.85	6	402.30	7	415.45	24
379.20	13	391.30	4	403.20	13	415.85	4
381.25	12	392.45	17	404.15	12	422.25	1
383.50	13	393.20	112	404.80	20	428.20	10
384.50	1	394.20	12	406.30	31	428.45	18
386.90	9	395.20	15	406.65	28	429.20	11

Average of 44.414 to 44.498 min.: A0219.D
Converted from RTE data file: >A0219:

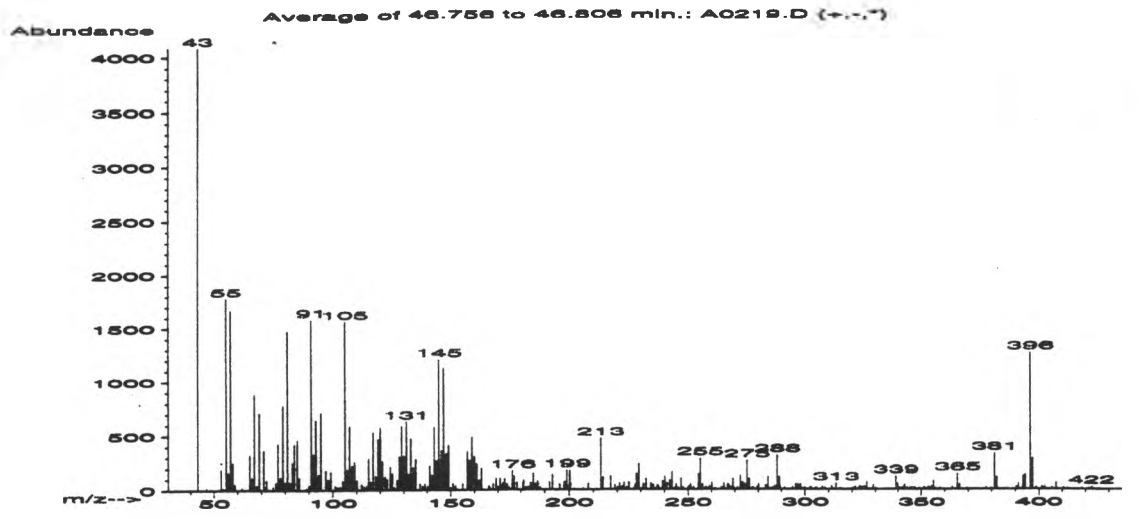
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Octacosane, 2-methyl-	408	C29H60	72
2.	Benzaldehyde, 2,4-dimethoxy-5-[3-(4-meth	326	C19H18O5	22
3.	1,5-Cycloundecadiene, 8,8-dimethyl-9-met	190	C14H22	15
4.	BIS(PENTAMETHYLCYCLOPENTADIENYL)MANGANES	325	C20H30Mn	15
5.	Benzene, (1-methyl-1-propylpentyl)-	204	C15H24	11
6.	6-METHYL-6-(3'-ISOPROPENYL-CYCLOPROP-1'-	206	C14H22O	11
7.	.alpha.-Ylangene	204	C15H24	11
8.	CIS,CIS,TRANS-3,3,6,6,9,9-HEXAMETHYL-TET	204	C15H24	10
9.	Acetonitrile, (3,5,5-trimethyl-2-cyclohe	161	C11H15N	10
10.	Acetonitrile, (3,5,5-trimethyl-2-cyclohe	161	C11H15N	10
11.	(2,6-XYLYLOXY)ACETONITRILE	161	C10H11NO	10
12.	3,3,7,7-TETRAMETHYL-5-(2-METHYL-1-PROPEN	204	C15H24	10
13.	2-(N,N-Dimethylaminomethyleneamino)-3-cy	365	C23H19N5	10
14.	Carbonic acid, methyl 3,4-xylyl ester	180	C10H12O3	10
15.	2H-1-Benzopyran-2-one, 7-amino-4-methyl-	175	C10H9NO2	10
16.	BREVIANAMIDE A	365	C21H23N3O3	10
17.	Cobalt, [(3,4,5,6-.eta.)-1,2-dihydro-1-p	366	C22H21B2Co	10
18.	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	136	C10H16	10
19.	(+)-Aromadendrene	204	C15H24	9
20.	(4R,4aS,6S)-6-(1'-Hydroxy-1'-methylethyl	236	C15H24O2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	001560-98-1	99232	54	129	3	72	15	42	0	40	5776
2.	*22	065621-11-6	81705	33	69	0	88	65	5	2	39	5619
3.	*15	062338-54-9	30226	70	83	1	58	80	2	30	59	5928
4.	*15	067506-86-9	81486	68	93	1	62	74	2	21	53	6505
5.	*11	054932-91-1	36648	50	63	3	172	74	2	0	46	5167
6.	*11	059744-13-7	37593	48	70	1	106	73	2	0	46	5228
7.	*11	014912-44-8	128768	51	67	1	42	80	2	0	44	4634
8.	10	000000-00-0	36802	46	91	0	86	73	1	0	39	5324
9.	*10	069697-22-9	17331	47	73	1	51	78	1	0	40	4762
10.	*10	069697-21-8	17332	29	64	1	40	80	1	3	38	4673
11.	*10	000000-00-0	17238	38	50	0	66	73	1	0	39	5238
12.	*10	067843-59-8	36785	54	60	0	54	71	1	9	40	4878
13.	*10	093031-34-6	91410	34	66	1	98	73	1	1	40	5746
14.	10	031268-81-2	25516	44	71	0	72	80	1	0	39	5323
15.	*10	026093-31-2	23409	33	66	2	43	80	1	0	39	4419
16.	*10	023402-09-7	135360	44	100	3	87	68	1	3	36	6142
17.	*10	070181-50-9	91632	34	130	3	73	71	1	0	39	6122
18.	*10	003338-55-4	8056	54	48	0	75	80	1	1	40	5290
19.	9	000489-39-4	128755	57	97	1	52	73	1	2	37	5277
20.	9	085184-35-6	50904	53	56	1	58	71	1	10	37	5294

CTMP Compounds

Peak 66; Unidentified Sterol



Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4086	61.85	21	76.00	72	89.00	14
46.80	20	65.05	325	77.00	428	89.95	41
48.75	4	66.05	116	77.95	120	90.15	43
52.00	3	67.05	882	79.05	780	91.00	1577
52.95	193	68.05	41	80.05	71	92.00	330
54.00	16	69.00	708	81.05	1473	93.00	644
55.00	1777	70.95	368	82.00	75	94.00	144
56.00	162	71.80	32	83.00	253	95.00	712
56.95	1664	72.15	90	83.85	418	97.00	181
57.90	248	73.90	1	85.05	462	98.00	98
58.95	53	74.95	31	85.95	117	99.05	170

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.00	40	112.00	55	121.00	262	130.00	312
102.00	28	112.25	40	122.05	123	131.05	631
103.00	29	113.05	30	123.00	99	132.00	148
104.05	86	113.40	9	124.00	7	133.00	473
105.05	1561	114.25	38	124.25	216	134.15	208
106.00	189	115.00	289	124.70	76	135.00	284
107.00	586	116.00	77	125.00	151	137.05	58
108.00	225	117.00	531	126.05	23	138.05	35
109.00	256	118.05	132	127.05	95	139.05	57
110.10	88	119.00	472	128.05	306	140.15	36
111.05	6	120.00	574	129.05	594	141.05	225

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
142.10	140	153.05	7	167.15	3	177.05	124
143.05	580	155.10	59	168.05	56	178.30	68
144.00	274	157.00	358	169.20	107	180.90	67
145.00	1211	158.05	274	170.10	31	181.15	90
146.00	365	159.00	488	171.00	107	182.15	23
147.00	1130	160.10	308	172.05	41	183.05	26
148.05	338	161.05	240	172.20	62	184.05	67
149.00	411	162.05	94	173.00	102	185.10	153
150.05	24	163.05	200	174.10	54	186.05	53
151.00	59	166.05	37	175.05	22	187.10	77
152.05	40	166.50	26	176.20	176	188.10	21

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.90	73	213.20	475	227.15	18	236.50	17
193.15	141	214.15	114	227.70	46	237.15	43
196.20	48	216.15	5	228.30	146	237.75	25
198.05	74	217.20	124	229.25	236	238.20	4
199.05	182	219.10	42	230.05	8	239.20	81
200.25	175	220.15	23	231.10	54	240.25	121
200.55	59	221.05	57	232.25	102	241.10	60
202.10	10	222.10	31	234.35	59	242.20	87
205.90	16	223.05	67	234.95	9	242.40	24
208.00	56	224.10	21	235.20	45	243.20	163
211.10	7	225.05	70	235.65	4	244.20	4

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
244.45	19	252.30	25	264.15	24	274.05	54
245.05	49	254.25	146	265.10	59	275.15	267
245.35	15	255.15	288	265.40	23	276.15	103
245.70	19	256.05	49	266.75	52	277.05	14
247.10	109	257.05	15	267.40	48	277.70	21
247.80	20	257.65	24	268.30	23	278.00	13
248.05	1	258.05	12	269.20	103	279.40	25
249.00	1	259.00	37	269.70	15	279.70	28
250.10	28	260.05	62	271.05	21	280.15	52
250.45	31	261.65	11	272.30	127	283.10	38
251.05	54	263.95	11	273.25	69	284.20	119

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
284.55	13	292.95	7	302.80	19	320.05	8
285.05	3	293.95	1	304.45	9	320.80	17
285.65	15	294.70	25	305.00	14	321.05	10
286.15	13	296.05	47	307.25	27	321.40	28
287.00	29	297.05	45	308.40	16	322.65	12
287.25	24	298.10	48	311.20	34	323.40	32
288.20	315	298.50	10	312.10	4	323.70	5
289.20	116	299.15	9	313.25	58	324.30	23
289.50	23	299.70	12	314.90	3	325.30	31
291.10	4	300.05	14	315.20	14	326.40	65
291.40	17	302.30	24	318.80	10	328.35	4

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
329.15	42	343.70	11	353.15	26	369.20	6
330.15	11	344.20	12	353.55	10	369.70	13
337.15	1	345.45	16	354.30	31	377.65	22
339.05	122	346.20	15	354.90	22	379.55	9
339.70	48	347.20	16	355.20	81	380.20	10
340.10	15	349.05	10	355.90	9	381.25	334
340.40	1	349.45	10	357.40	9	382.25	114
340.65	16	351.05	17	358.00	9	386.75	13
341.80	16	351.40	18	363.15	24	389.00	7
342.10	11	352.20	7	365.50	147	390.40	26
342.85	41	352.70	12	366.45	44	390.75	21

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
391.35	54	410.40	18				
393.30	124	410.75	10				
394.20	140	412.15	9				

396.35	1269	418.10	3
397.30	285	418.30	13
398.70	22	421.30	13
401.25	27	422.40	25
402.45	21	422.85	14
405.25	13		
405.55	15		
407.30	61		

Average of 46.756 to 46.806 min.: A0219.D
Converted from RTE data file: >A0219:

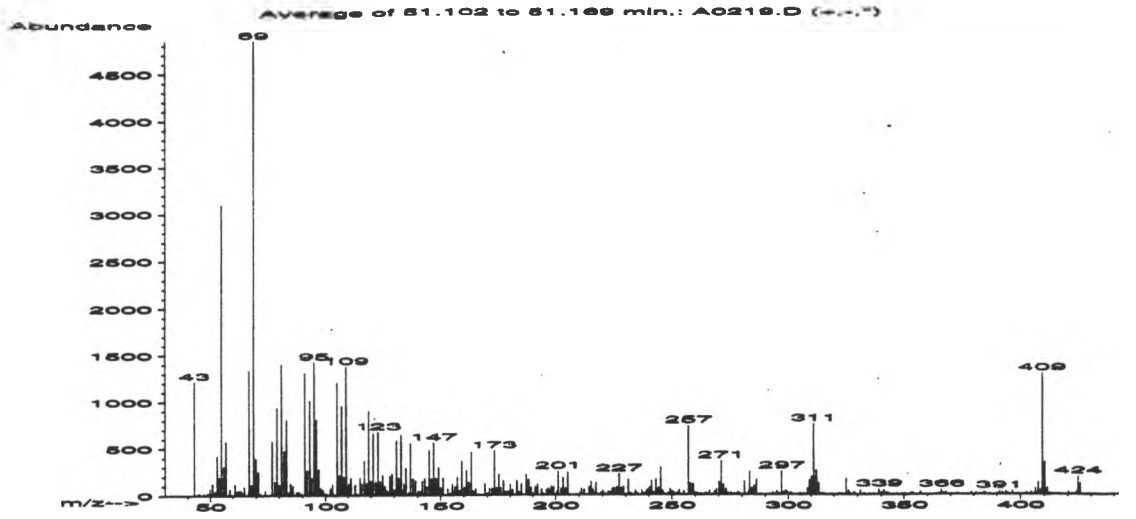
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Stigmast-5-en-3-ol, (3.beta.)-	414	C29H50O	14
2.	19-Norpregn-4-ene-3,20-dione, 10-vinyl-	326	C22H30O2	10
3.	(23E)-3.beta.-Acetoxy-27-nor-5,23-choles	426	C28H42O3	9
4.	5.alpha.-Cholest-8-en-3-one, 6.alpha.-hy	456	C30H48O3	7
5.	Octanoic acid, 8-(octylthio)-	288	C16H32O2S	7
6.	2-METHYL-1,5-(4H)-DIHYDROPYRIDO[2,3-B]-1	175	C9H9N3O	7
7.	3-BROMO-1,2,4-TRIAZINE 2-OXIDE	175	C3H2BrN3O	7
8.	(-)-2.BETA.-ACETOXY-11.ALPHA.-HYDROXYVER	348	C22H36O3	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	14	000083-46-5	100190	60	96	0	15	69	2	0	43	9494
2.	10	013258-85-0	81871	46	126	3	107	66	1	0	34	7038
3.	9	083872-51-9	101759	43	14	1	92	77	1	8	30	5587
4.	7	005259-17-6	105344	40	99	1	27	77	1	0	24	6000
5.*	7	056909-05-8	69876	48	57	1	20	72	1	1	23	5698
6.	7	017260-05-8	23366	38	79	3	107	77	1	0	28	5214
7.	7	061178-02-7	23282	34	59	0	15	77	1	1	26	7638
8.	6	068420-38-2	87644	34	117	3	88	77	1	0	18	3285

CTMP Compounds

Peak 67; Unidentified Triterpene



Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1214	55.00	3097	67.00	1332	80.05	109
44.95	22	56.00	306	68.00	116	81.05	1400
47.05	12	56.95	569	69.00	4851	82.05	475
48.55	16	58.00	7	70.00	383	83.05	809
48.85	20	58.75	65	71.00	248	84.05	33
49.85	70	61.00	118	71.95	16	84.95	127
50.20	21	62.00	45	74.00	43	85.85	99
50.90	122	62.85	46	76.05	5	87.00	1
51.95	43	63.50	42	77.00	580	87.50	32
53.00	418	64.00	27	78.00	142	87.95	1
54.00	192	64.95	88	79.05	938	88.15	12

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
88.45	36	98.80	49	110.05	120	121.00	660
89.05	12	99.45	13	111.05	181	122.10	141
89.75	13	100.00	8	112.95	108	123.05	677
91.00	1307	100.35	17	113.75	14	124.05	143
92.00	265	102.00	70	114.10	3	125.05	217
93.10	1016	103.00	111	115.05	189	126.00	93
94.00	180	105.05	1204	116.00	120	126.80	50
95.00	1426	106.05	213	117.05	369	127.05	32
95.95	809	107.00	953	118.05	127	128.05	206
97.00	274	108.00	191	119.00	900	129.05	233
98.00	70	109.00	1376	120.00	149	130.05	59

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.05	586	141.05	40	153.05	60	163.15	456
131.95	183	142.05	149	154.00	18	164.00	40
133.00	645	143.10	186	155.00	112	165.10	64
133.95	51	144.00	90	155.55	28	169.00	121
134.15	111	145.05	477	156.05	85	170.05	16
135.05	290	146.00	175	157.00	194	170.20	16
136.10	28	147.00	564	158.05	46	171.00	63
137.05	553	148.00	179	159.00	362	172.10	69
138.05	174	149.05	294	160.10	77	173.05	474
139.15	155	150.05	79	161.10	261	174.10	74
140.35	38	151.05	182	162.05	135	175.05	220

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
175.75	73	187.10	215	197.05	74	212.15	55
177.00	149	188.20	162	198.10	91	214.30	86
178.00	34	189.15	79	199.10	82	215.15	143
178.25	21	190.05	19	200.55	29	215.90	50
179.00	37	191.10	85	201.10	255	216.20	8
180.05	105	192.20	114	202.25	65	216.45	16
180.55	32	194.00	58	203.15	183	217.20	130
181.15	54	194.55	14	204.10	68	219.10	24
183.05	152	195.05	3	205.15	241	220.20	43
183.95	34	196.05	50	210.40	23	221.05	9
185.10	116	196.40	49	211.10	67	222.45	33

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
222.75	13	231.15	160	239.50	48	246.80	8
223.20	27	232.10	16	240.15	82	248.00	8
224.00	31	234.05	47	241.20	152	248.25	19
224.20	63	234.90	20	241.50	26	249.10	62
225.05	70	235.15	8	242.15	25	249.65	40
226.15	86	237.05	46	243.10	165	250.00	17
226.55	15	237.65	13	244.05	42	250.25	3
227.20	222	237.90	20	244.25	74	250.70	31
228.25	67	238.65	17	245.15	290	251.05	9
229.10	83	238.90	39	246.00	40	252.00	1
230.10	3	239.20	55	246.45	4	252.20	22

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
253.15	52	265.50	14	273.25	60	281.00	145
255.15	37	266.10	47	273.80	1	281.75	10
257.10	738	267.95	1	274.05	21	282.75	37
257.90	118	268.15	37	274.60	6	283.20	247
258.15	113	268.80	20	275.30	18	284.05	66
259.15	113	269.00	60	276.70	11	285.00	68
259.95	20	270.10	135	277.00	4	285.25	96
261.00	21	270.45	25	278.10	25	285.65	17
262.50	16	271.05	361	278.50	19	286.20	161
264.15	12	272.10	102	279.25	9	288.15	4
264.50	23	273.00	22	279.60	7	292.95	2

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
293.30	21	299.15	44	311.10	756	323.25	10
294.00	2	299.70	20	312.15	257	324.05	3
295.05	38	300.20	7	313.15	119	325.15	166
295.85	13	301.15	22	314.05	10	326.05	3
296.20	1	305.10	19	314.25	14	326.25	43
297.05	249	306.75	10	315.25	17	326.95	11
297.65	19	307.15	7	315.65	7	328.05	12
298.00	23	308.25	63	318.80	9	328.50	21
298.20	27	309.10	156	319.30	7	328.75	24
298.55	9	309.50	41	321.80	12	331.20	49
298.80	33	310.15	194	322.45	5	333.00	15

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
335.15	10	343.35	8	364.55	12	382.75	9
336.15	7	346.95	17	365.55	21	384.35	29
336.90	7	349.00	6	366.15	50	384.90	10

339.15	59	349.65	4	366.55	13	385.25	11
340.10	22	350.70	8	367.20	12	386.95	6
340.90	10	352.55	8	368.05	22	389.75	9
341.20	46	353.05	18	372.70	10	390.25	9
341.75	12	353.70	17	372.95	9	391.05	38
342.40	15	354.20	6	377.00	3	391.40	4
342.75	13	356.85	30	379.00	25	392.25	26
343.00	15	359.15	5	380.95	19	393.70	28

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
393.95	35	406.20	63	416.15	7		
394.50	14	406.75	11	420.25	28		
396.50	37	407.55	127	422.00	13		
396.85	11	407.90	31	422.40	2		
398.70	13	408.25	42	423.45	22		
401.80	6	409.25	1296	424.05	32		
402.30	15	410.30	343	424.35	192		
402.55	16	411.15	9	425.25	116		
402.80	8	411.45	65	426.45	6		
404.35	12	412.15	4	429.00	5		
404.55	25	414.25	5				

Average of 51.102 to 51.169 min.: A0219.D
Converted from RTE data file: >A0219:

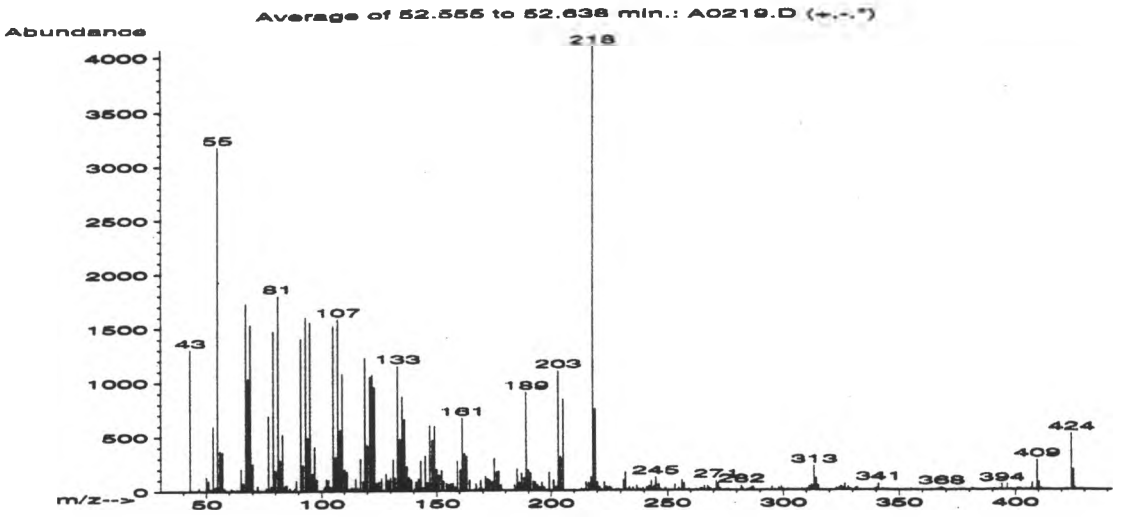
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cycloprop[7,8]ergost-22-en-3-one, 3',7-d	410	C29H46O	53
2.	1,3-Dioxane, 2,2,4,5-tetramethyl-6-(1-me	410	C27H54O2	33
3.	d-Nerolidol	222	C15H26O	30
4.	2-METHOXY-13C-3-METHYLPYRAZINE	124	C513CH8N2O	9
5.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	9
6.	TRANS-3,7-DIMETHYL-2,4,6-OCTATRIENE-1-OL	152	C10H16O	7
7.	METHYL ENT-16-KAUREN-19-OATE	316	C21H32O2	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	053755-18-3	99497	64	117	3	71	29	28	0	41	9606
2.	33	056324-82-4	99474	41	143	3	69	35	10	0	24	9333
3.	30	000142-50-7	129864	41	110	2	101	35	9	0	14	9429
4.	9	034061-82-0	4673	46	108	2	38	78	1	11	33	3790
5.	9	002847-30-5	120355	44	71	1	58	77	1	0	35	3624
6.	7	089155-85-1	13599	33	79	2	156	72	1	0	21	3844
7.	6	005524-25-4	79043	36	136	2	43	78	1	0	11	3705

CTMP Compounds

Peak 68; Unidentified Triterpene



Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1301	60.95	21	73.00	1	86.20	27
46.75	25	61.85	10	75.95	27	88.00	8
50.00	129	63.45	13	77.00	694	88.40	27
51.05	98	63.95	7	78.00	45	89.10	99
52.05	19	65.00	205	79.00	1471	91.00	1406
52.95	598	66.00	78	80.05	189	92.00	241
54.00	39	67.05	1725	81.05	1797	93.05	1595
54.95	3181	68.05	1034	81.95	286	94.00	492
56.00	369	69.00	1527	83.05	525	95.05	1552
57.00	357	70.00	248	84.15	51	96.00	161
58.00	20	72.20	46	85.05	58	97.05	408

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.00	103	109.00	1075	118.10	90	128.00	153
99.80	3	110.05	197	119.00	1222	129.05	97
100.95	20	111.10	172	119.95	423	130.05	119
101.25	37	112.05	15	121.05	1050	131.05	289
102.00	109	112.95	30	122.05	1068	131.95	120
103.05	100	113.80	1	123.00	953	133.00	1150
104.00	38	114.05	27	124.05	74	134.00	476
105.05	1518	114.25	11	125.00	82	135.00	869
106.05	314	115.00	111	126.05	113	136.05	659
107.00	1581	116.00	30	126.40	4	137.00	76
108.05	564	117.00	296	127.05	13	137.15	225

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
138.05	125	149.05	598	160.20	192	171.05	131
139.05	100	150.10	200	161.10	671	172.00	108
140.30	18	151.05	144	162.10	341	173.05	97
141.05	86	152.10	188	163.05	319	174.20	84
141.95	113	153.00	90	164.20	99	175.05	298
143.05	278	154.25	69	166.05	10	176.10	173
144.00	32	155.05	55	167.05	60	177.00	179
145.05	326	156.05	61	168.40	17	178.00	52
146.05	76	157.00	69	169.00	94	179.05	7
147.00	603	158.00	34	169.70	15	180.00	2
148.05	469	159.00	277	169.95	11	181.95	5

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
184.05	57	194.00	53	204.15	316	221.05	32
184.40	22	194.30	14	205.15	845	221.70	9
185.15	199	194.80	11	209.95	16	223.10	75
186.15	75	195.00	30	213.10	22	224.10	34
187.05	156	196.05	75	214.20	13	225.30	33
188.15	115	197.00	31	215.15	79	225.95	21
189.10	910	198.40	2	216.25	70	226.30	6
190.05	191	199.20	167	217.20	124	228.20	13
191.05	160	201.15	98	218.10	4070	229.15	13
192.20	87	202.10	35	219.15	751	231.20	92
193.05	78	203.15	1104	220.10	76	231.50	19

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
232.10	167	241.20	33	249.05	24	262.50	13
233.15	4	242.10	43	250.45	7	264.15	22
233.50	12	242.60	9	253.05	56	265.00	21
233.80	30	243.15	88	254.80	27	266.10	40
235.25	26	244.20	36	256.20	96	267.50	38
236.95	47	245.00	121	257.10	64	267.75	26
237.20	11	245.20	86	258.15	6	268.05	22
237.65	8	246.25	55	258.65	2	268.90	15
238.25	11	247.00	12	259.15	17	270.30	13
238.65	9	247.20	5	259.40	6	271.20	89
239.65	26	248.80	4	261.90	10	272.05	65

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
272.80	13	284.60	10	298.05	25	312.05	6
273.05	20	284.95	16	299.00	3	312.20	50
274.60	3	285.65	14	299.20	33	313.25	222
275.45	10	286.20	30	299.95	12	313.85	46
276.05	7	286.75	6	300.55	3	314.30	111
276.35	9	287.05	33	302.20	13	315.20	45
276.75	7	293.00	5	305.00	6	323.00	23
278.20	6	295.00	5	308.00	16	323.20	20
278.95	1	295.20	31	310.10	14	324.30	27
282.00	43	296.30	6	311.00	4	325.00	42
282.50	24	297.30	1	311.20	42	325.60	26

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
326.05	16	339.65	13	355.00	15	368.45	12
326.45	23	340.40	24	356.00	6	369.20	12
326.70	62	341.15	63	356.95	4	377.30	7
327.45	2	342.50	4	357.65	3	377.80	9
328.05	33	342.75	14	363.25	4	380.65	6
328.70	5	343.55	7	365.50	2	381.20	2
329.10	13	344.10	6	365.90	11	381.50	17
331.10	21	344.75	5	366.50	2	381.75	1
332.00	26	345.80	6	367.15	15	387.50	2
333.40	8	348.95	6	367.45	18	390.75	16
339.40	8	353.05	9	368.05	24	393.20	12

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
394.10	51	404.20	3	421.70	7		
396.40	54	404.80	6	422.75	6		
396.85	5	406.75	18	424.30	517		

CTMP Compounds

397.70	4	407.30	61	425.30	188
398.00	12	409.35	273	425.70	24
399.15	4	410.05	14	426.05	13
399.55	6	410.25	70	428.70	9
401.00	18	410.65	11	428.95	7
401.20	9	411.00	15		
401.95	10	411.25	4		
402.25	12	412.05	4		

Average of 52.555 to 52.638 min.: A0219.D
Converted from RTE data file: >A0219:

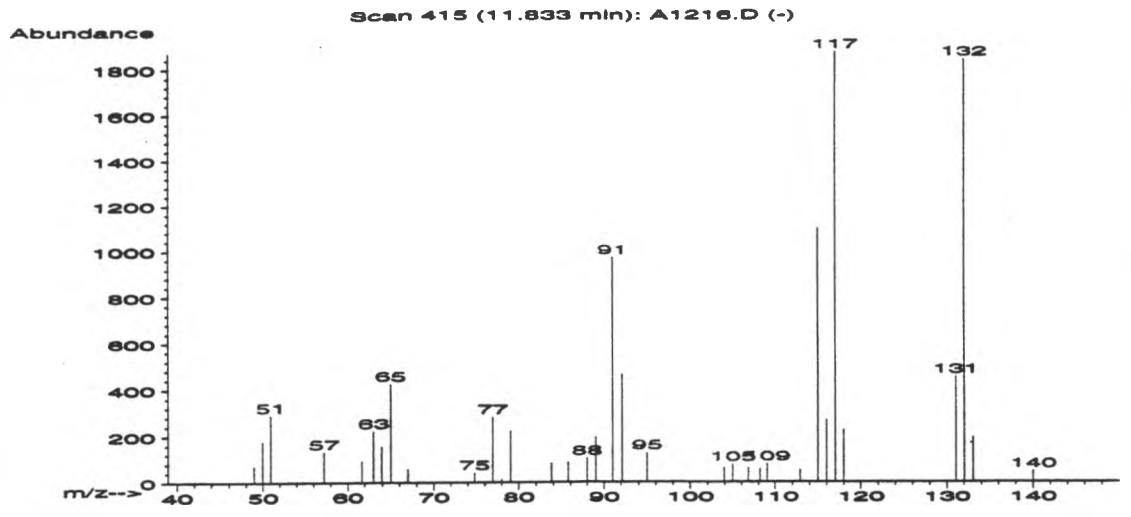
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-KETO-URS-12-ENE	424	C30H48O	96
2.	.beta.-Amyrin	426	C30H50O	64
3.	D:C-Friedooleanan-3-one	424	C30H48O	58
4.	METHYL COMMATE E	502	C31H50O5	58
5.	Pyrene, hexadecahydro-	218	C16H26	50
6.	6-Acetyl-5-hydroxy-1,8-dimethyl-1,2,3,4-	218	C14H18O2	47
7.	1,2,3,3a,5,6,6a,7-Octahydro-1,3a,6-trime	218	C15H22O	46
8.	NORUNS-12-ENE	396	C29H48	46
9.	2,2-Dimethyl-6-(prop-2-enyl)benzofuran-4	218	C13H14O3	45
10.	Butanoic acid, 3-oxo-2-(phenylmethylene)	218	C13H14O3	43
11.	TETRAHYDRO-3,6,8,8-TETRAMETHYL-7-METHANO	218	C15H22O	43
12.	4,5'-Bipyrimidine, 4',6-dimethoxy-	218	C10H10N4O2	41
13.	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	38
14.	2-Isopropenyl-5-acetyl-6-hydroxy-2,3-dih	218	C13H14O3	38
15.	(-)-Lepidozenal	218	C15H22O	38
16.	Aristolone	218	C15H22O	38
17.	Aristolone	218	C15H22O	35
18.	1,4-Methanonaphthalene, 1,4-dihydro-9-ph	218	C17H14	30
19.	1,4-Naphthoquinone, 6-ethyl-2,5-dihydrox	218	C12H10O4	27
20.	1,4-Naphthalenedione, 5,8-dihydroxy-2,3-	218	C12H10O4	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000000-00-0	101578	116	83	0	66	22	76	45	96	9700
2.	*64	000559-70-6	101804	78	92	1	75	34	37	27	66	8844
3.	*58	005945-53-9	101572	64	130	3	97	27	32	0	44	8420
4.	58	000000-00-0	108319	139	53	1	75	35	32	1	52	9002
5.	*50	002435-85-0	43086	71	79	3	99	50	25	0	68	8922
6.	*47	069611-14-9	42903	37	31	2	99	37	20	11	40	7870
7.	*46	071583-68-1	43034	55	23	0	77	44	20	21	46	7870
8.	46	000000-00-0	97230	81	102	3	99	42	20	0	43	9460
9.	*45	087386-32-1	42807	64	75	2	81	50	19	34	51	8806
10.	*43	000620-80-4	42797	53	104	2	82	46	18	0	49	9111
11.	*43	000000-00-0	43003	80	70	1	71	48	18	11	46	8818
12.	*41	059549-37-0	42609	64	80	3	96	53	16	0	58	8440
13.	*38	000243-42-5	43062	76	49	2	99	46	14	2	42	8541
14.	*38	006906-88-3	42817	51	36	1	93	54	14	16	45	7487
15.	*38	074033-93-5	42992	72	71	2	76	51	14	26	47	8515
16.	*38	006831-17-0	129615	78	66	2	93	64	14	40	72	8317
17.	*35	006831-17-0	43029	67	99	3	78	69	11	0	64	7739
18.	*30	055028-73-4	43093	50	89	2	70	59	9	0	46	8486
19.	*27	013378-87-5	42704	53	64	2	93	59	8	0	40	8435
20.	*25	021418-10-0	42705	51	79	3	92	65	7	0	44	8335

CTMP Compounds

Peak 69; Monoterpene



Scan 415 (11.833 min): A1216.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.95	71	76.95	281	104.95	77	133.05	193
49.95	179	78.00	13	106.80	60	140.00	45
50.95	289	79.05	222	108.20	56		
53.00	6	83.80	82	109.05	78		
57.20	133	85.75	86	112.90	51		
61.65	94	88.00	104	115.00	1100		
63.00	221	89.00	194	116.00	268		
63.95	155	91.00	971	117.00	1869		
65.00	423	92.15	463	118.00	224		
67.00	58	95.00	127	131.05	454		
74.80	42	103.95	62	132.05	1839		

CTMP Compounds

Scan 415 (11.833 min): A1216.D

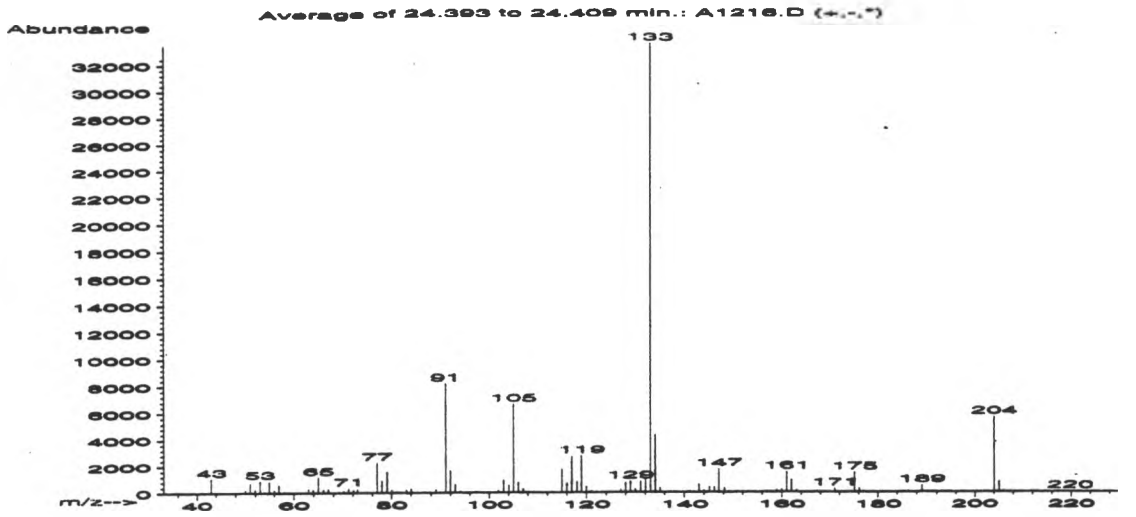
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	96
2.	BENZENE, 1-ISOPROPENYL-?-METHYL-	132	C10H12	91
3.	Benzene, (2-methyl-1-propenyl)-	132	C10H12	87
4.	Benzene, 1-methyl-4-(1-methylethenyl)-	132	C10H12	87
5.	Benzene, (2-methyl-2-propenyl)-	132	C10H12	83
6.	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	81
7.	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	81
8.	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	81
9.	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	80
10.	Benzene, methyl(1-methylethenyl)-	132	C10H12	80
11.	Benzene, (1-methyl-1-propenyl)-, (E)-	132	C10H12	76
12.	(E)-4-(1'-PROPENYL)TOLUENE	132	C10H12	76
13.	(Z)-4-(1'-PROPENYL)TOLUENE	132	C10H12	76
14.	1R-METHYL-2T-PHENYLCYCLOPROPANE	132	C10H12	74
15.	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	74
16.	Benzene, (2-methyl-2-propenyl)-	132	C10H12	72
17.	Benzene, (2-methyl-2-propenyl)-	132	C10H12	64
18.	Benzene, (2-methyl-1-propenyl)-	132	C10H12	64
19.	Benzene, (2-methyl-2-propenyl)-	132	C10H12	64
20.	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	58

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	001587-04-8	121407	94	20	0	85	3	76	0	96	9947
2.	*91	026444-18-8	7009	74	36	0	88	3	62	20	66	9865
3.	*87	000768-49-0	121403	78	33	1	97	11	54	25	72	9684
4.	*87	001195-32-0	121408	84	30	0	75	13	54	33	74	9889
5.	*83	003290-53-7	6997	64	41	0	92	15	50	18	53	9424
6.	*81	000824-63-5	121419	68	38	0	77	19	49	31	70	9494
7.	*81	001587-04-8	7007	71	40	2	92	16	49	37	76	9489
8.	*81	002039-90-9	7013	63	48	0	81	20	49	0	64	9755
9.	*80	002039-89-6	7012	64	48	0	73	15	48	11	47	9755
10.	*80	026444-18-8	121411	55	49	0	90	12	48	0	49	9685
11.	*76	000768-00-3	6995	68	36	0	79	23	45	27	70	9500
12.	*76	002077-30-7	7005	63	42	1	93	22	45	0	64	9661
13.	*76	002077-29-4	7003	63	42	1	99	22	45	0	64	9676
14.	*74	005070-01-9	7019	61	44	2	99	19	44	26	55	9207
15.	*74	027831-13-6	7014	64	43	1	99	17	44	7	53	9570
16.	*72	003290-53-7	121405	58	45	0	99	16	42	12	47	9415
17.	*64	003290-53-7	121404	57	48	2	99	23	37	3	49	9393
18.	*64	000768-49-0	6996	49	57	1	99	23	37	0	44	9561
19.	*64	003290-53-7	121406	58	41	0	99	16	37	4	43	9377
20.	*58	005379-20-4	7015	48	55	1	98	26	32	0	44	9459

CTMP Compounds

Peak 3; Unidentified Sesquiterpene



Average of 24.393 to 24.409 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1101	58.05	89	69.10	108	80.05	206
49.00	11	59.00	81	70.10	162	81.00	44
49.95	221	59.90	66	71.10	363	82.05	84
50.95	758	60.90	33	72.10	209	83.05	225
51.95	274	61.90	51	72.95	263	84.05	291
53.00	918	63.00	331	73.85	35	86.00	20
53.95	92	63.95	260	74.90	37	87.05	56
54.95	857	65.00	1189	76.00	33	87.90	34
56.00	212	66.00	252	77.00	2261	89.00	263
56.95	593	67.00	292	78.00	874	90.00	37
57.90	28	68.00	42	79.05	1569	91.00	8207
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
92.00	1681	103.00	950	118.05	815	130.00	216
93.00	602	104.05	566	119.00	2772	131.05	831
94.10	109	105.05	6665	120.00	443	132.05	968
95.10	9	106.05	761	121.00	122	133.05	33464
96.10	44	107.05	273	122.05	14	134.05	4360
97.05	50	108.00	36	124.00	10	135.05	318
98.00	10	109.05	30	124.95	24	136.95	34
98.95	6	113.00	48	126.00	43	138.00	36
99.95	38	115.00	1770	127.00	230	139.00	11
100.95	17	116.00	673	128.00	715	141.00	115
101.95	155	117.00	2743	129.00	846	142.00	76
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.00	593	159.00	172	176.95	91	194.00	37
144.00	143	160.05	203	178.00	26	202.10	82
145.10	394	161.05	1554	179.00	8	204.05	5648
146.10	360	162.05	921	180.55	17	205.10	763
147.05	1774	163.05	158	184.05	14	206.00	93
148.15	294	166.00	12	185.05	20	206.85	16
149.10	47	168.00	24	186.20	103	219.75	19
151.00	81	171.00	264	189.05	514		
152.00	55	172.00	83	190.05	47		
154.05	3	175.15	1509	191.00	28		
157.00	111	176.15	271	191.75	35		

CTMP Compounds

Average of 24.393 to 24.409 min.: A1216.D
Converted from RTE data file: >A1216:

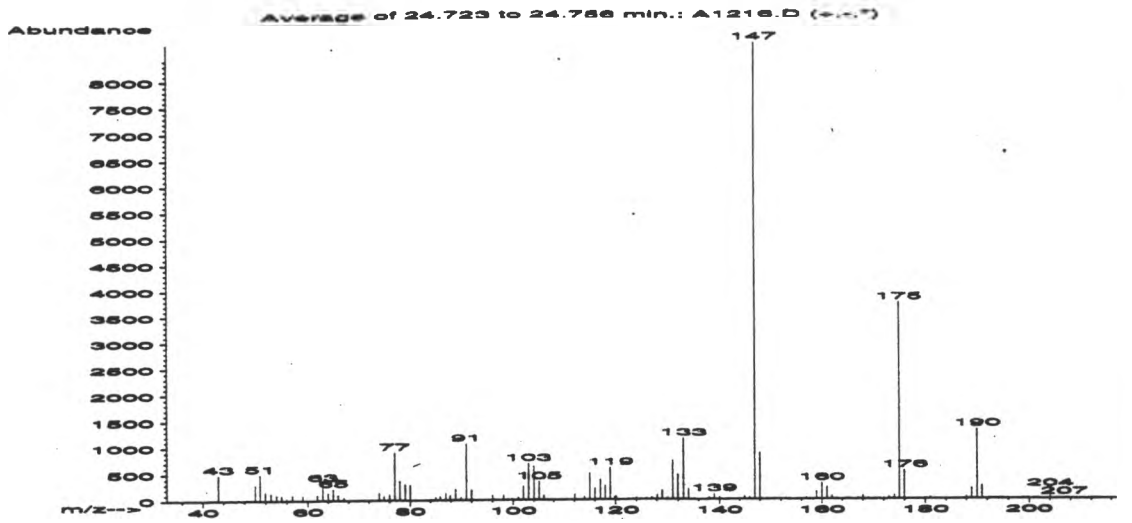
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	59
2.	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	59
3.	1-Propanone, 2-chloro-1-(2,4-dimethylphe	210	C12H15ClO	59
4.	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-e	266	C20H26	59
5.	3-METHYL-1,2,4-BENZOXAZINONE	161	C9H7NO2	53
6.	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	148	C11H16	50
7.	BENZENE, 1,3,5-TRIMETHYL-2-PROPYL-	162	C12H18	50
8.	1-Propanone, 2-chloro-1-(2,5-dimethylphe	210	C12H15ClO	50
9.	Benzene, 1-(1,1-dimethylethyl)-3-methyl-	148	C11H16	47
10.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	45
11.	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	148	C11H16	45
12.	M-TOLYL-DIMETHYLACETALDEHYDE	162	C11H14O	45
13.	Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	45
14.	1-Propanone, 3-cyclopentyl-1-(2,4-dimeth	230	C16H22O	45
15.	Disiloxane, 1,1,3,3-tetramethyl-1,3-bis[	362	C16H34O5Si2	42
16.	2,5-Octadiyne, 4,4-diethyl-	162	C12H18	42
17.	Benzoxazole, 2-methyl-	133	C8H7NO	42
18.	Benzene, 2,4-dimethyl-1-(1-methylpropyl)	162	C12H18	40
19.	Benzene, (1,1-dimethylethyl)methyl-	148	C11H16	40
20.	1H-Indol-5-ol	133	C8H7NO	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	000098-51-1	12112	44	46	2	67	21	33	0	39	9757
2.	*59	004706-90-5	123452	48	34	2	91	25	33	17	39	9736
3.	59	054965-53-6	39356	61	31	1	75	23	33	3	39	9778
4.	59	000734-17-8	62220	44	65	3	99	21	33	0	39	9779
5.	*53	007653-60-3	17201	38	42	2	70	26	28	17	38	8008
6.	50	004706-89-2	12116	45	42	0	68	31	25	0	39	9735
7.	*50	000000-00-0	17850	60	29	1	88	20	25	1	33	9693
8.	50	054965-52-5	39357	61	37	1	69	20	25	0	36	9766
9.	47	001075-38-3	12111	40	42	3	73	36	20	11	39	9721
10.	45	000098-51-1	123446	42	37	2	78	25	19	4	37	9772
11.	45	000098-51-1	123448	49	39	2	99	21	19	0	35	9790
12.	45	000000-00-0	17722	43	43	2	67	21	19	6	34	9619
13.	*45	000622-58-2	7114	41	63	3	98	25	19	0	35	9762
14.	45	055191-11-2	48547	43	62	2	85	25	19	5	37	9774
15.	42	000126-80-7	90620	48	72	3	88	28	17	9	36	8530
16.	*42	061227-87-0	17824	43	24	1	99	26	17	0	35	9755
17.	*42	000095-21-6	7127	39	51	2	70	30	17	0	35	9736
18.	40	001483-60-9	17844	44	39	1	76	31	16	10	37	9651
19.	40	027138-21-2	12113	45	47	2	99	35	16	0	35	9707
20.	*38	001953-54-4	7129	34	49	3	99	36	14	12	35	9758

CTMP Compounds

Peak 70; Unidentified Sesquiterpene



Average of 24.723 to 24.756 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	481	59.05	85	74.95	72	88.95	207
48.80	11	59.85	10	75.95	109	90.00	48
50.00	288	61.90	99	76.95	902	91.00	1069
50.95	489	62.95	335	78.00	360	92.00	184
51.95	154	64.00	141	79.05	295	96.05	85
53.00	128	65.00	215	80.00	283	98.15	84
54.05	96	65.95	102	81.00	8	98.95	15
55.00	83	67.05	48	85.05	54	99.90	25
55.95	31	71.10	13	85.95	71	101.00	45
57.05	99	73.00	2	87.00	135	102.00	257
58.00	11	74.00	138	87.90	88	103.00	693

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.05	637	119.90	55	134.05	184	160.00	302
105.05	347	120.15	58	137.95	38	161.05	221
106.00	82	124.05	35	139.00	97	162.05	56
109.05	9	126.00	19	140.00	39	165.00	14
112.05	101	127.00	37	145.00	56	167.05	25
113.95	58	128.05	78	146.00	37	168.00	69
115.00	504	129.00	168	147.00	8705	169.00	17
116.00	216	130.05	34	148.00	875	173.00	35
117.05	383	131.05	735	153.00	32	174.05	80
118.00	265	132.00	463	157.00	28	175.00	3765
119.00	603	133.05	1160	159.00	131	176.00	537

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
180.15	7	207.00	7				
180.95	28						
188.00	40						
189.00	193						
190.05	1322						
191.00	247						
194.10	6						
194.95	7						
196.00	17						
204.05	171						
206.70	17						

CTMP Compounds

Average of 24.723 to 24.756 min.: A1216.D
Converted from RTE data file: >A1216:

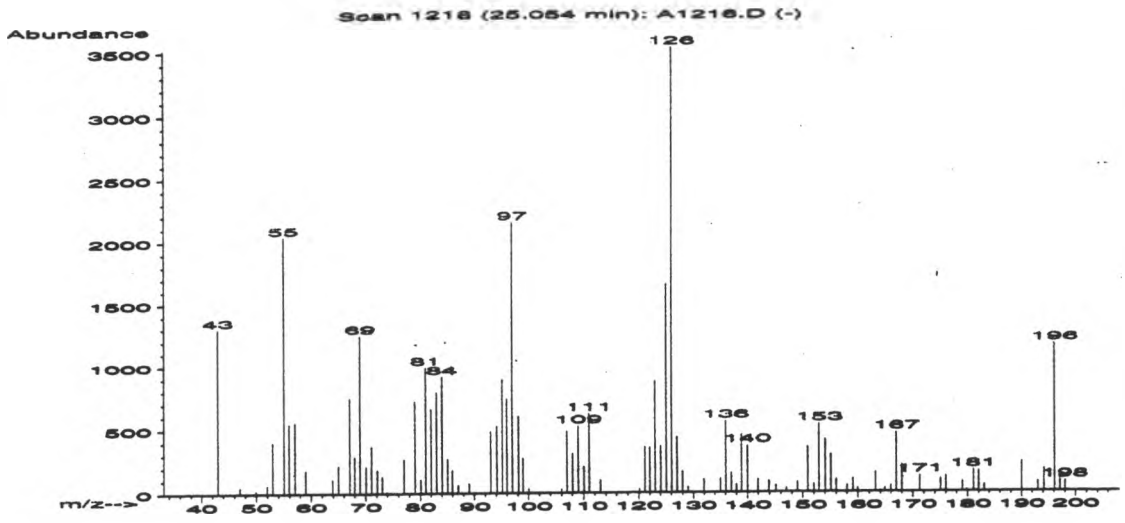
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Benzoxazolamine, N,N-diethyl-	190	C11H14N2O	53
2.	2-(2',4',5'-TRIMETHYLPHENYL)-PROPAN-1-OL	178	C12H18O	43
3.	Benzene, 1,2,4-trimethyl-5-(1-methylethy	162	C12H18	38
4.	Disiloxane, hexamethyl-	162	C6H18OSi2	38
5.	1-Naphthalenamine, 5,6,7,8-tetrahydro-	147	C10H13N	38
6.	1-Butanone, 1-(2,3,4,5-tetramethylphenyl	204	C14H20O	38
7.	Pyrido[3,4-d]pyrimidin-4(3H)-one	147	C7H5N3O	38
8.	DEWARBENZENE, HEXAMETHYL-	162	C12H18	37
9.	Ethanone, 1-[4-(1-methylethyl)phenyl]-	162	C11H14O	37
10.	Benzene, 1,4-bis(1-methylethyl)-	162	C12H18	37
11.	Benzene, 1,4-bis(1-methylethyl)-	162	C12H18	37
12.	Bicyclo[2.2.0]hexa-2,5-diene, 1,2,3,4,5,	162	C12H18	37
13.	2-Naphthalenamine, 5,6,7,8-tetrahydro-	147	C10H13N	37
14.	1-(6-Methyl-2-pyrazyl)-1-heptene	190	C12H18N2	33
15.	Ethanone, 1-(2,4,6-trimethylphenyl)-	162	C11H14O	32
16.	Ethanone, 1-(2,4,6-trimethylphenyl)-	162	C11H14O	32
17.	Pyrido[2,3-d]pyrimidin-4(1H)-one	147	C7H5N3O	32
18.	Benzoic acid, 2-ethoxy-, methyl ester	180	C10H12O3	32
19.	Benzene, 1,3-bis(1-methylethyl)-	162	C12H18	25
20.	Benzene, 1,3-bis(1-methylethyl)-	162	C12H18	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	020852-38-4	29988	39	76	3	99	27	28	18	40	9431
2.	43	062528-64-7	24820	43	23	0	77	42	18	0	39	9003
3.	38	010222-95-4	17851	48	33	1	71	38	14	2	37	9032
4.	*38	000107-46-0	125060	34	61	3	98	48	14	0	39	8986
5.	*38	002217-41-6	11725	28	59	3	99	50	14	9	38	8330
6.	38	069855-49-8	36568	59	48	3	90	47	14	0	43	8968
7.	*38	019178-25-7	11604	33	74	3	73	48	14	0	39	8928
8.	37	000000-00-0	17883	46	55	2	66	41	13	0	34	8998
9.	37	000645-13-6	17732	41	49	0	75	41	13	0	33	9015
10.	37	000100-18-5	17861	45	54	2	79	41	13	0	34	8858
11.	37	000100-18-5	125186	39	46	2	82	41	13	11	31	8798
12.	37	007641-77-2	17884	46	55	2	66	41	13	0	34	8998
13.	*37	002217-43-8	123301	30	57	2	72	42	13	9	34	7631
14.	*33	083568-42-7	30083	29	91	3	66	34	10	0	29	9284
15.	32	001667-01-2	125158	49	46	2	73	47	9	0	31	8104
16.	32	001667-01-2	17734	44	52	2	87	48	9	0	37	8250
17.	*32	024410-19-3	11600	31	63	3	76	48	9	0	33	8844
18.	32	003686-55-3	25484	41	20	0	67	47	9	6	35	8971
19.	25	000099-62-7	125184	39	61	2	79	44	7	0	29	8457
20.	25	000099-62-7	17860	40	61	2	71	45	7	0	29	8694

CTMP Compounds

Peak 71; Unidentified Hydrocarbon



Scan 1218 (25.054 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1300	63.90	113	79.00	725	94.10	533
46.95	51	65.00	218	80.05	111	95.10	899
49.95	25	67.05	751	81.05	993	96.00	743
50.95	1	68.00	292	82.05	664	97.00	2146
51.95	68	69.00	1246	83.05	798	98.15	607
52.95	405	70.05	213	84.05	920	99.00	275
55.00	2033	71.05	372	85.05	274	100.05	34
55.95	546	72.15	188	85.95	184	102.95	4
57.05	561	73.00	134	87.00	65	106.00	32
59.00	184	73.95	11	89.00	79	107.05	488
59.90	4	77.00	270	93.00	488	108.05	314

Scan 1218 (25.054 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	528	127.00	436	143.90	94	159.05	110
110.05	209	128.00	168	145.10	56	159.90	31
111.00	625	129.00	46	147.00	35	163.10	155
113.00	103	131.95	108	149.05	82	164.00	10
120.10	32	135.05	113	150.95	356	164.85	33
121.10	363	136.05	562	152.00	68	166.00	50
122.00	356	137.05	155	152.95	535	167.00	464
123.05	877	138.00	66	154.05	415	168.00	212
124.05	367	138.95	458	155.05	296	171.25	126
125.05	1651	140.00	371	156.00	100	175.05	105
126.05	3519	141.95	104	157.95	55	176.00	124

Scan 1218 (25.054 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
179.05	82	198.00	83				
179.85	13						
181.05	168						
182.05	161						
183.05	58						
190.05	238						
192.00	4						
193.05	81						
194.15	178						
196.15	1163						
197.10	146						

CTMP Compounds

Scan 1218 (25.054 min): A1216.D

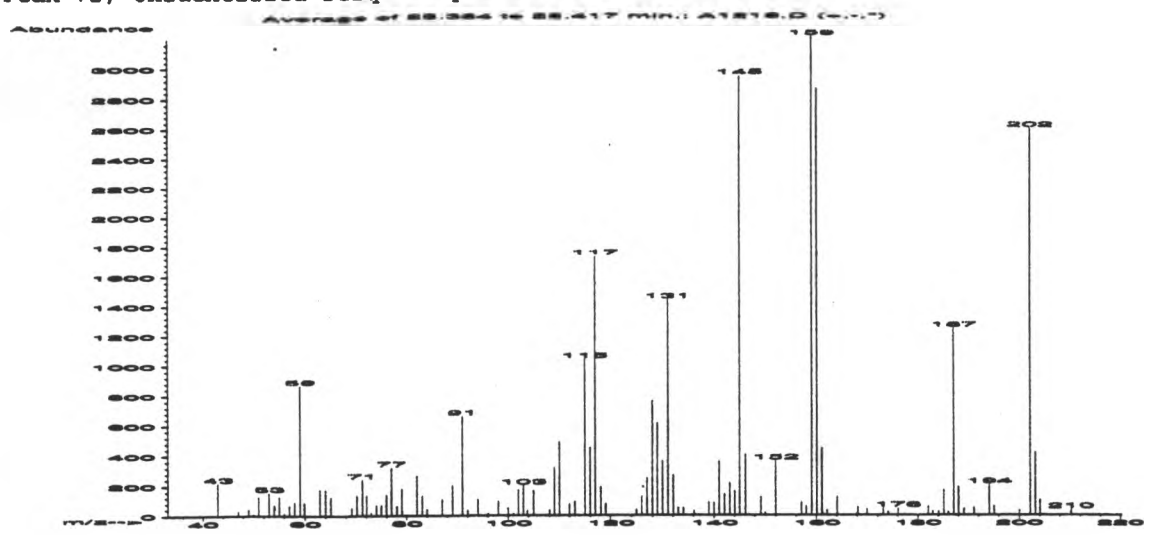
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 2-isopropyl-2,5-dimethyl-	168	C11H20O	49
2.	Phenol, o-(propylthio)-	168	C9H12OS	43
3.	8-Thiabicyclo[3.2.1]oct-2-ene	126	C7H10S	41
4.	Phenol, o-(isopentylthio)-	196	C11H16OS	38
5.	2-Hydroxybenzenethiole	126	C6H6OS	38
6.	1,3-Cyclopentanedione, 2-ethyl-	126	C7H10O2	38
7.	3H-Pyrazol-3-one, 2,4-dihydro-4,4,5-trim	126	C6H10N2O	35
8.	1,1-DIFLUOROCYCLOPROPABENZENE	126	C7H4F2	35
9.	3H-Pyrazol-3-one, 2,4-dihydro-4,4,5-trim	126	C6H10N2O	30
10.	2,4-PENTADIENOIC ACID, 3,4-DIMETHYL-, IS	168	C10H16O2	30
11.	ETHYL CYCLOPENTENOLONE	126	C7H10O2	30
12.	3-ethylcyclohexanone	126	C8H14O	27
13.	1,1-DIFLUOROCYCLOPROPABENZENE	126	C7H4F2	27
14.	Benzenemethanol, 3-fluoro-.alpha.-methyl	140	C8H9FO	27
15.	2-Cyclohexen-1-one, 6-butyl-3-methoxy-	182	C11H18O2	25
16.	1H-Pyrazole-1-carboxaldehyde, 4-ethyl-4,	168	C9H16N2O	25
17.	Guanidine, [2-(hexahydro-1(2H)-azocinyl)	198	C10H22N4	22
18.	Cyclohexanone, 2-isopropyl-2,5-dimethyl-	168	C11H20O	20
19.	Talbutal	224	C11H16N2O3	14
20.	Methyl cinnamate	126	C6H6O3	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	020144-44-9	20619	71	40	2	87	45	23	23	58	8910
2.	*43	024362-86-5	20190	53	43	0	79	49	18	17	46	8805
3.	*41	040698-01-9	5253	61	57	2	74	52	16	0	56	8534
4.	*38	029549-67-5	32815	53	61	0	86	55	14	0	49	8281
5.	*38	000000-00-0	5117	57	44	0	80	52	14	0	49	8640
6.	*38	000823-36-9	5208	35	53	0	75	52	14	4	43	8387
7.	*35	003201-20-5	120525	45	65	2	167	52	11	0	40	8723
8.	*35	018238-55-6	120528	38	45	2	99	55	11	1	40	7902
9.	*30	003201-20-5	5157	54	55	1	85	60	9	0	47	8525
10.	*30	000000-00-0	20319	55	55	2	94	56	9	0	49	7886
11.	*30	000000-00-0	5203	52	45	1	76	60	9	0	46	8051
12.	*27	022461-89-8	5360	55	51	1	83	56	8	0	40	8362
13.	*27	018238-55-6	5168	38	43	2	95	56	8	1	40	7883
14.	*27	000402-63-1	9162	43	67	1	60	56	8	0	40	6392
15.	*25	053690-81-6	26667	49	60	1	97	65	7	0	46	7802
16.	*25	054411-09-5	20257	49	55	0	58	65	7	18	47	5524
17.	22	000055-65-2	33766	45	61	0	99	63	5	13	41	7519
18.	*20	020144-44-9	125776	58	58	0	57	70	4	0	56	5609
19.	14	000115-44-6	129978	44	55	0	32	67	2	20	41	3543
20.	*14	061892-88-4	5130	33	67	2	99	67	2	0	41	7798

CTMP Compounds

Peak 72; Unidentified Sesquiterpene



Average of 25.384 to 25.417 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	216	59.05	865	74.95	69	92.05	35
46.95	30	59.90	86	75.95	139	94.00	109
49.00	44	62.95	176	77.00	318	96.05	12
49.95	11	64.00	174	78.05	65	98.05	94
50.95	125	65.00	121	79.05	180	100.00	52
53.00	153	69.10	51	82.00	267	101.00	15
54.00	69	70.10	133	83.05	131	102.00	174
55.00	125	71.15	237	84.00	44	103.00	198
56.00	15	72.05	134	87.00	107	103.80	32
57.00	67	72.95	16	89.00	204	105.00	167
58.00	89	74.00	69	91.00	660	108.05	37

Average of 25.384 to 25.417 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	319	126.00	130	140.00	80	157.00	85
110.05	491	127.00	248	141.00	359	158.00	58
112.00	76	128.00	763	142.00	141	159.05	3199
113.00	90	129.00	612	143.05	217	160.05	2851
115.00	1042	130.00	362	144.05	162	161.05	444
116.00	452	131.05	1441	145.00	2933	162.00	32
117.00	1730	132.05	267	146.15	403	164.05	121
118.10	190	133.05	49	149.10	120	167.95	15
119.05	77	134.05	50	150.00	18	168.15	53
121.00	2	136.05	29	152.05	359	169.95	41
125.00	38	139.00	87	155.00	1	173.15	42

Average of 25.384 to 25.417 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
174.15	23	194.10	201				
176.05	43	195.10	60				
182.05	55	200.00	33				
182.95	25	202.15	2589				
184.05	24	203.15	417				
185.05	169	204.05	100				
185.95	21	210.20	35				
187.05	1247						
188.00	191						
189.05	44						
191.10	50						

CTMP Compounds

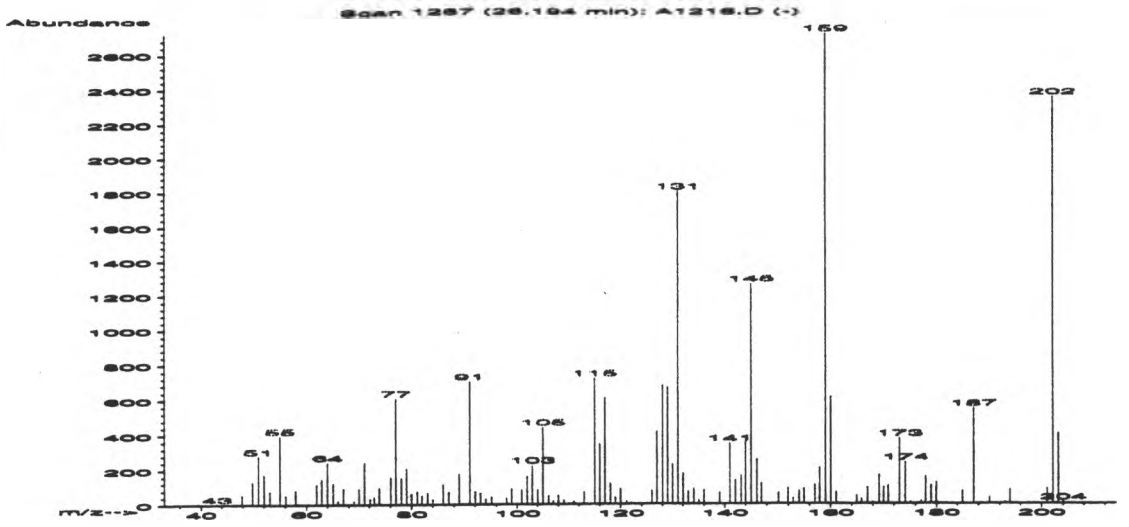
Average of 25.384 to 25.417 min.: A1216.D
Converted from RTE data file: >A1216:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-(2-butenyl)-2,3-dimethyl-	160	C12H16	59
2.	3-Buten-2-one, 3-methyl-4-phenyl-	160	C11H12O	55
3.	(1-p-Anisylmethylene)cyclopropane	160	C11H12O	53
4.	Naphthalene, 1,2,3,4-tetrahydro-6,7-dime	160	C12H16	50
5.	Naphthalene, 1,2,3,4-tetrahydro-5,7-dime	160	C12H16	50
6.	2,4-Cyclohexadien-1-one, 4,6-dimethyl-6-	160	C11H12O	49
7.	6-N-BUTYL-1,2,3,4-TETRAHYDRONAPHTHALENE	188	C14H20	48
8.	Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E	160	C12H16	46
9.	Benzene, (1,3-dimethyl-2-butenyl)-	160	C12H16	42
10.	Benzene, 1,2,4-trimethyl-5-(1-methylethe	160	C12H16	42
11.	.ALPHA.,2,4,6-TETRAMETHYL-STYRENE	160	C12H16	41
12.	Benzene, 1,2,4-trimethyl(1-methylethenyl	160	C12H16	38
13.	2,4,6-TRIMETHYLINDANE	160	C12H16	38
14.	Naphthalene, 1,2,3,4-tetrahydro-6,7-dime	160	C12H16	38
15.	Naphthalene, 1,2,3,4-tetrahydro-1,6-dime	202	C15H22	38
16.	6-N-BUTYL-1,2,3,4-TETRAHYDRONAPHTHALENE	188	C14H20	35
17.	1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	160	C12H16	30
18.	(E)-2-(1'-PROPENYL)MESITYLENE	160	C12H16	30
19.	Benzene, 1-(1-methylethenyl)-2-(1-methyl	160	C12H16	30
20.	2-Phenyl-3-propen-2-yloxirane	160	C11H12O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	054340-85-1	17012	79	40	1	89	54	33	61	90	6703
2.	*55	001901-26-4	16930	74	27	0	81	42	29	47	66	7915
3.	*53	055088-84-1	16965	59	12	0	98	38	28	8	55	7617
4.	*50	001076-61-5	17057	75	47	2	88	49	25	55	81	7034
5.	*50	021693-54-9	17056	75	47	2	89	48	25	46	81	6989
6.	*49	051738-15-9	124920	62	56	3	99	41	23	0	56	8288
7.	*48	000000-00-0	29429	97	33	1	68	64	22	57	86	5466
8.	*46	054340-86-2	17013	71	50	2	91	53	20	54	76	6734
9.	*42	050704-01-3	17008	71	39	0	70	57	17	47	76	6212
10.	*42	054340-84-0	17021	63	50	3	89	58	17	0	64	6809
11.	*41	014679-13-1	17022	62	51	2	64	55	16	0	56	6900
12.	*38	054340-83-9	17023	60	9	0	85	58	14	0	56	6427
13.	*38	065001-56-1	17042	57	18	0	82	52	14	19	49	6714
14.	*38	001076-61-5	124946	61	54	2	91	58	14	0	51	6704
15.	*38	000483-77-2	35797	63	62	0	62	63	14	39	64	6262
16.	*35	000000-00-0	127531	79	49	2	84	66	11	38	74	5521
17.	*30	002613-76-5	124938	62	49	1	69	59	9	14	47	5939
18.	*30	002077-41-0	17017	68	36	1	85	58	9	12	48	6560
19.	*30	005557-93-7	17018	68	45	2	91	56	9	30	50	6098
20.	*25	053274-96-7	16960	53	23	0	77	62	7	11	46	6465

Peak 73; Unidentified Sesquiterpene



Scan 1287 (26.194 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4	64.00	244	77.05	609	91.00	706
47.80	55	65.10	122	78.05	155	92.05	76
49.85	131	66.00	22	79.05	208	93.00	66
50.95	279	67.00	95	80.00	63	94.00	33
51.95	172	69.00	22	81.05	78	95.10	43
53.05	79	70.05	94	81.95	53	98.00	38
54.95	396	71.10	243	83.05	69	98.95	91
56.05	56	72.10	34	84.05	30	100.95	85
57.95	85	72.95	46	86.00	116	101.95	164
61.90	115	73.85	98	87.00	73	102.95	226
62.90	147	76.05	160	89.00	179	104.05	85

Scan 1287 (26.194 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.05	443	118.00	120	132.05	178	146.15	256
106.15	51	119.00	41	133.05	73	147.00	120
107.05	20	120.00	90	134.05	93	150.15	65
108.05	52	121.15	18	135.05	23	151.95	92
109.05	26	122.00	8	136.05	82	152.95	32
110.05	4	125.95	79	139.00	66	154.05	75
111.05	17	126.95	417	141.00	351	154.95	89
113.00	71	128.05	683	142.00	140	157.05	112
115.00	724	129.05	669	143.15	168	157.95	211
116.00	349	130.05	228	144.00	368	159.05	2717
117.00	611	131.05	1806	145.00	1267	160.05	616

Scan 1287 (26.194 min): A1216.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
161.05	69	177.10	18	203.15	404		
165.00	49	177.95	159	204.05	10		
165.95	28	178.95	107				
167.00	97	179.95	124				
168.00	13	184.95	76				
169.15	167	187.05	548				
170.00	97	190.10	39				
170.90	108	193.00	10				
173.00	376	194.00	84				
174.15	240	201.00	91				
175.10	10	202.15	2350				

CTMP Compounds

Scan 1287 (26.194 min): A1216.D

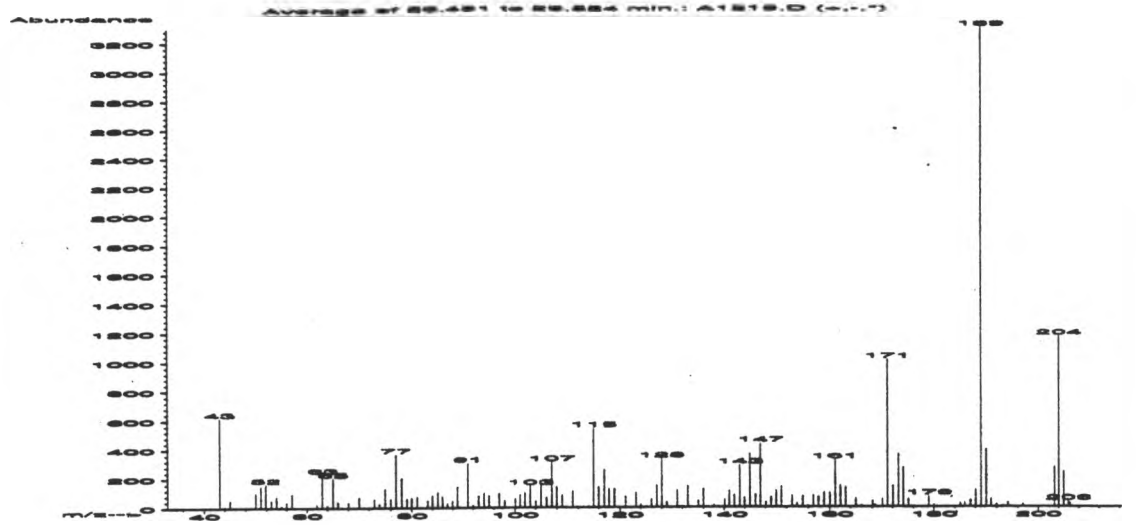
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	CYCLOISOLONGIFOLENE	202	C15H22	64
2.	1,8-Dihydro-5H-pyrazolo[4,3-g]quinolin-5	202	C9H6N4O2	58
3.	8,9-DEHYDRO-NEOISOLONGIFOLENE	202	C15H22	52
4.	1H-Indene, 5-hexyl-2,3-dihydro-	202	C15H22	50
5.	4-Isopropyl-6-methyl-1,2,3,4-tetrahydron	202	C14H18O	50
6.	Naphthalene, 1,2,3,4-tetrahydro-2,5,8-tr	174	C13H18	35
7.	Naphthalene, 1,2,3,4-tetrahydro-1,5,7-tr	174	C13H18	30
8.	8-Quinolinol, 2-methyl-	159	C10H9NO	25
9.	4(1H)-Quinolinone, 1-methyl-	159	C10H9NO	25
10.	5-ETHYL-8-NITROQUINOLINE	202	C11H10N2O2	25
11.	2-Quinolinemethanol	159	C10H9NO	22
12.	8-Quinolinemethanol	159	C10H9NO	22
13.	3H-5-(3-Indazolyl)-1,3,4-oxadiazol-2-one	202	C9H6N4O2	18
14.	Unknown name	202	C11H10N2O2	14
15.	4,6,6-Trimethyl-3-chloro-2-methoxycycloh	202	C10H15ClO2	14
16.	2H,3H-Triazino-1,2,4[4,5-b]indazole-1,4-	202	C9H6N4O2	14
17.	1-ETHYL-4-METHYL-5-PHENYL-4-IMIDAZOLIN-2	202	C12H14N2O	14
18.	2,4-Dichlorophenetole	190	C8H8Cl2O	11
19.	1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetr	160	C11H12O	11
20.	8-Quinolinol, 7-methyl-	159	C10H9NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	028380-07-6	35806	46	107	3	95	20	37	0	40	9732
2.	*58	073908-01-7	35299	37	4	1	99	27	32	10	43	9021
3.	*52	000000-00-0	35793	52	86	2	116	35	27	0	46	8603
4.	*50	054889-55-3	35782	66	59	1	69	50	25	42	64	5866
5.	*50	057494-10-7	35725	51	39	2	99	34	25	11	39	8486
6.	35	030316-17-7	23263	62	72	1	98	51	11	0	39	7452
7.	*30	021693-55-0	23264	62	60	3	83	58	9	23	45	6959
8.	*25	000826-81-3	124796	48	57	2	99	62	7	0	44	7365
9.	*25	000083-54-5	16467	52	57	2	72	62	7	0	44	7424
10.	*25	065745-67-7	35499	49	100	3	86	62	7	0	46	5850
11.	*22	001780-17-2	16472	46	70	3	77	62	5	0	40	6839
12.	*22	016032-35-2	16473	46	48	1	97	62	5	0	40	7371
13.	*18	086795-48-4	35298	33	70	2	78	67	3	14	43	5961
14.	*14	000000-00-0	35504	47	75	1	78	70	2	0	40	5694
15.	*14	084883-39-6	35379	47	61	0	73	68	2	13	40	5461
16.	*14	068767-71-5	35297	34	69	2	68	67	2	0	41	6089
17.	*14	071624-04-9	35585	36	84	3	69	67	2	0	41	6121
18.	*11	000000-00-0	127586	50	70	1	69	75	2	0	44	6169
19.	*11	001198-20-5	124926	61	46	1	55	73	2	8	47	4694
20.	*10	005541-68-4	16471	34	66	3	99	71	1	13	40	6704

CTMP Compounds

Peak 74; Unidentified Sesquiterpene



Average of 26.491 to 26.524 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	617	61.95	25	76.00	61	87.95	47
44.00	9	63.00	232	77.00	368	88.95	143
45.00	51	64.00	19	78.05	206	91.00	305
49.95	104	65.00	203	79.05	64	92.00	19
50.95	149	66.00	43	80.00	70	93.05	82
51.90	164	68.00	39	81.00	76	94.10	101
53.00	53	70.05	74	83.05	53	95.10	84
54.00	79	71.05	5	84.00	87	97.05	99
55.00	14	72.95	61	85.05	108	98.10	49
56.00	39	73.90	27	86.00	78	100.05	63
57.05	96	74.95	130	86.95	29	101.00	90

Average of 26.491 to 26.524 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.95	103	116.00	141	129.00	36	143.05	290
102.95	147	117.05	259	131.00	117	143.95	66
104.00	45	118.00	128	132.00	1	145.00	369
105.00	156	119.00	128	133.05	146	146.05	88
106.05	70	121.05	77	135.05	47	147.00	439
107.05	311	123.05	100	136.05	128	148.05	36
108.00	140	124.00	18	138.00	16	149.05	73
109.05	86	125.00	7	139.00	8	150.05	114
111.05	114	126.05	57	140.10	55	151.00	140
114.00	7	127.00	152	141.00	114	153.00	78
115.00	544	128.00	335	142.00	85	153.95	28

Average of 26.491 to 26.524 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
155.00	77	168.15	44	185.05	27	203.15	276
156.00	9	168.65	11	185.95	33	204.05	1169
156.95	81	170.00	56	187.05	50	205.05	244
158.00	73	171.00	1009	188.05	119	205.95	37
159.05	104	172.05	145	189.05	3298	206.30	27
160.05	99	173.10	362	190.05	398		
161.05	322	174.00	272	190.95	57		
162.05	150	175.05	56	192.00	22		
163.05	134	176.05	5	193.00	9		
164.95	60	179.00	73	194.10	33		
166.00	9	179.95	14	197.00	23		

CTMP Compounds

Average of 26.491 to 26.524 min.: A1216.D
Converted from RTE data file: >A1216:

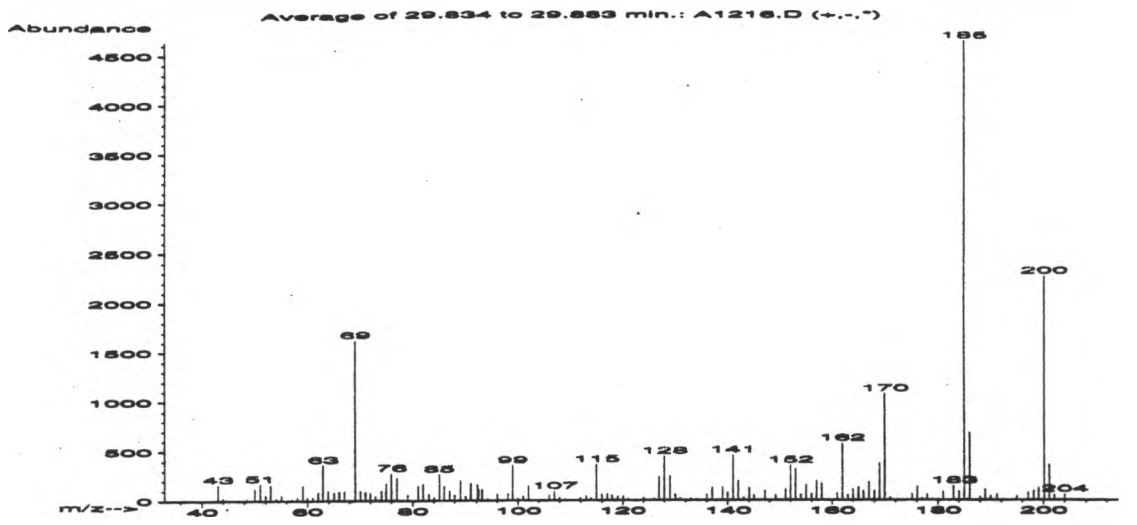
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-Methyl-2-methoxymethyl-4-chromone	204	C12H12O3	83
2.	1-H-2,5-DIMETHYL-3-ACETYLPYRROLO(3,2-B)P	204	C11H12N2O2	50
3.	ACETOPHENONE, 2,4,5-TRIETHYL-	204	C14H20O	47
4.	2-CYCLOPENTYL-4-ISOPROPYLPHENOL	204	C14H20O	47
5.	.beta.-Selinene	204	C15H24	47
6.	1,4-Benzoxazepin-5(2H)-one, 3,4-dihydro-	189	C11H11NO2	43
7.	1,4-Benzoxazepin-5(2H)-one, 3,4-dihydro-	189	C11H11NO2	43
8.	N-METHYL-3-PHENYL-4-METHYLISOXAZOL-5-ONE	189	C11H11NO2	43
9.	3-METHYL-1-PHENYL-PYRROLIDIN-2,5-DIONE	189	C11H11NO2	43
10.	Thiazole, 2-ethyl-4-phenyl-	189	C11H11NS	38
11.	Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	38
12.	2-Butenimidic acid, 3-methyl-N-phenyl-,	189	C12H15NO	38
13.	2-Nitro-1-naphthol	189	C10H7NO3	38
14.	4-METHYLENE-3-P-TOLYL-1,3-OXAZOLIDIN-2-O	189	C11H11NO2	37
15.	Pyrido[3,4-d]pyrimidin-4(3H)-one, 2,6,8-	189	C10H11N3O	37
16.	Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	37
17.	2-(5-METHYL-3-ISOXAZOYL)-4-ACETYL-5-METH	204	C11H12N2O2	35
18.	1-(P-NITROPHENYL)IMIDAZOLE	189	C9H7N3O2	32
19.	INDOLE, 5,7-DIFORMYL-2,3-DIHYDRO-N-METHY	189	C11H11NO2	32
20.	.DELTA.-SELINENE	204	C15H24	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	082366-89-0	36428	42	9	1	93	4	50	13	42	9404
2.	*50	068576-22-7	36359	43	44	2	67	33	25	11	38	9247
3.	*47	000000-00-0	36570	51	45	1	79	37	20	10	39	9407
4.	*47	000000-00-0	36582	45	61	3	99	36	20	0	39	9435
5.	*47	017066-67-0	128731	37	92	3	75	38	20	0	39	9337
6.	*43	066362-41-2	127561	36	46	2	91	44	18	14	40	8908
7.	*43	066362-41-2	29609	36	46	2	91	44	18	14	40	8908
8.	*43	007713-65-7	29584	43	78	3	77	45	18	0	39	8883
9.	*43	000000-00-0	29590	34	93	3	91	43	18	0	39	8916
10.	*38	019968-50-4	29616	44	71	3	77	50	14	0	40	8639
11.	*38	000717-74-8	128659	42	65	2	71	36	14	14	36	9014
12.	*38	056830-02-5	29629	43	89	3	69	50	14	0	40	8686
13.	*38	000607-24-9	29546	34	30	1	78	48	14	0	39	8846
14.	*37	066568-57-8	127548	38	18	1	88	44	13	9	36	8845
15.	*37	022378-52-5	29560	47	50	3	89	45	13	2	37	8931
16.	*37	000717-74-8	36651	38	67	2	95	41	13	2	37	8996
17.	*35	068576-18-1	36346	56	50	1	49	52	11	0	40	9151
18.	*32	002301-25-9	29519	38	52	2	90	50	9	10	35	8871
19.	*32	000000-00-0	29602	33	63	1	93	48	9	10	37	8375
20.	*25	028624-28-4	36735	41	77	2	40	55	7	0	35	8160

CTMP Compounds

Peak 75; Unidentified Hydrocarbon



Average of 29.834 to 29.883 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	163	58.05	31	69.10	1622	81.05	150
44.00	21	59.05	149	70.15	98	82.00	168
48.45	12	59.95	28	71.05	88	83.05	65
49.95	118	60.95	29	72.00	70	84.05	31
51.00	170	62.00	88	72.95	37	85.05	266
52.05	54	62.95	359	74.05	100	85.95	145
52.95	154	63.90	101	75.00	170	87.00	96
54.00	23	65.00	83	76.00	277	87.95	56
55.00	50	66.00	90	77.00	227	89.00	200
56.05	1	67.05	98	78.05	4	90.00	42
57.05	11	68.05	6	79.05	55	91.00	174

Average of 29.834 to 29.883 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
92.20	159	106.05	47	119.05	35	133.00	19
92.40	112	107.00	94	120.05	39	134.00	8
93.05	105	108.00	29	121.05	17	136.00	60
94.10	17	109.05	1	124.05	28	137.05	125
96.00	63	111.95	25	126.00	18	139.00	128
98.05	69	113.00	43	127.00	236	140.00	76
98.95	355	113.95	23	128.00	446	141.00	454
100.00	20	115.00	362	129.05	242	142.00	195
100.95	41	116.00	59	130.05	60	143.05	26
102.00	147	117.05	65	131.00	19	144.05	122
105.00	4	118.00	48	132.05	1	145.00	48
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.05	93	161.00	72	174.05	5	186.05	677
148.10	7	161.95	574	175.05	64	188.00	31
149.10	51	163.00	53	176.05	135	189.00	105
151.00	111	164.00	111	177.00	20	190.00	40
151.95	352	165.00	130	177.95	58	191.15	55
152.95	315	165.95	91	179.05	10	195.00	42
154.00	53	167.00	185	180.00	1	197.10	77
154.95	155	168.00	92	181.00	83	198.15	92
156.00	64	169.00	370	183.05	146	199.10	124
157.00	196	170.00	1075	184.05	87	200.15	2263
158.00	169	171.05	26	185.05	4632	201.10	353
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
202.05	54						
204.00	58						

CTMP Compounds

Average of 29.834 to 29.883 min.: A1216.D
Converted from RTE data file: >A1216:

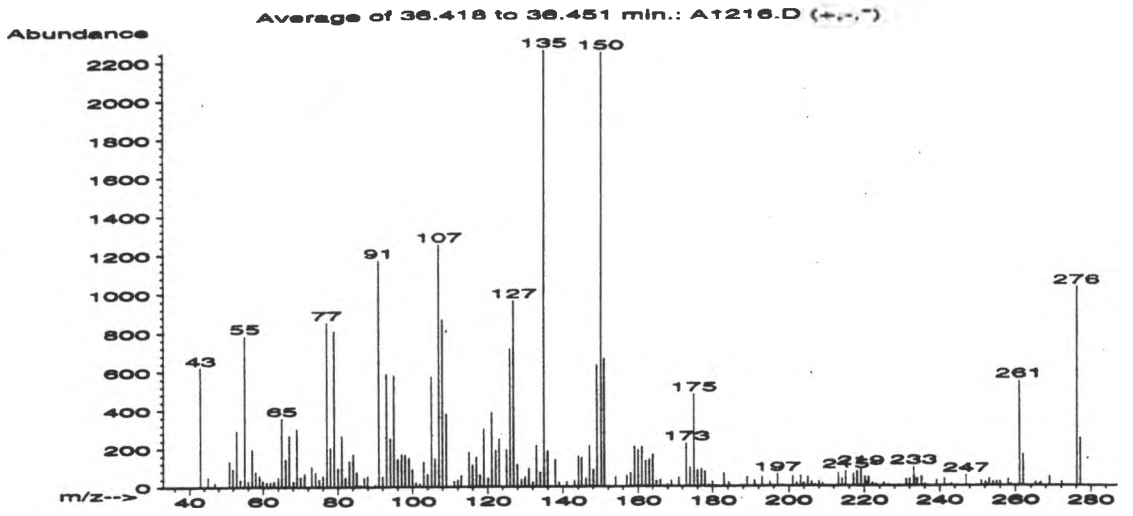
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3,6-Trimethyl-8-ethyl-2,7-naphthyridin	200	C13H16N2	83
2.	6-Methoxy-1-acetonaphthone	200	C13H12O2	83
3.	Ethyl 5'5'-Dimethyl-4'-thia-1'-cyclopent	200	C10H16O2S	53
4.	2-CHLOROPHENOL,O-TRIMETHYLSILYL	200	C9H13ClOSi	53
5.	4-CHLOROPHENOL-TRIMETHYL-SILYL-ETHER	200	C9H13ClOSi	53
6.	Cyclohexanone, 4-methyl-, thiosemicarbaz	185	C8H15N3S	43
7.	3-p-Methoxyphenyl-pyridine	185	C12H11NO	43
8.	2,3,4,5,6-d5-Stilbene	180	C14H7D5	43
9.	2-Pyrimidinamine, 4-methyl-6-phenyl-	185	C11H11N3	43
10.	Benzene, 1-fluoro-3-(1-phenylethyl)-	200	C14H13F	42
11.	Bicyclo[2.2.2]octane, 1-iodo-4-phenyl-	312	C14H17I	37
12.	Naphthalene, 2-isothiocyanato-	185	C11H7NS	35
13.	6-ETHOXY-2,2'-BIPYRIDYL	200	C12H12N2O	33
14.	[1,1'-Biphenyl]-4-ol, 3-amino-	185	C12H11NO	32
15.	1,7-TRIMETHYLENE-2,3-DIMETHYLINDOLE	185	C13H15N	32
16.	Silane, trimethyl-1-naphthalenyl-	200	C13H16Si	27
17.	4-Methyl-2-(2'-methyl-1'propenyl)-4-(2''	200	C14H16O	17
18.	2(3H)-Benzothiazolone, 5-chloro-	185	C7H4ClNOS	17
19.	5-Thiazolecarboxylic acid, 2,4-dimethyl-	185	C8H11NO2S	17
20.	1,2-Naphthalenedione, 3,8-dimethyl-5-(1-	228	C15H16O2	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	088300-64-5	34881	33	31	0	99	3	50	0	41	9665
2.	*83	058149-89-6	34848	37	5	0	99	1	50	5	38	9547
3.	*53	056700-55-1	34559	38	73	2	99	28	28	0	39	9657
4.	*53	017881-65-1	128362	47	57	3	70	28	28	7	40	9617
5.	*53	000000-00-0	128360	37	66	2	96	28	28	10	39	9577
6.	*43	022397-22-4	27924	35	49	1	99	46	18	14	43	7396
7.	*43	005958-02-1	28020	50	26	1	68	42	18	16	39	8699
8.	*43	000000-00-0	25891	48	66	2	79	50	18	0	44	8281
9.	*43	015755-15-4	27994	51	61	2	84	47	18	0	46	6747
10.	*42	074764-42-4	34913	39	77	3	78	26	17	1	36	9733
11.	37	055044-15-0	77473	59	82	3	86	42	13	13	31	8695
12.	*35	001636-33-5	27992	49	40	2	92	51	11	16	39	8743
13.	*33	054015-97-3	34767	32	107	3	99	31	10	0	26	9595
14.	*32	001134-36-7	28026	45	63	2	99	47	9	0	35	8707
15.	*32	005825-43-4	28082	35	88	3	99	47	9	0	30	6719
16.	27	018052-80-7	34893	44	54	0	38	56	8	6	41	9641
17.	*17	093518-42-4	34922	29	101	2	37	52	3	0	23	9151
18.	*17	020600-44-6	27878	28	103	2	77	52	3	0	29	8669
19.	*17	007210-77-7	27904	28	114	2	70	52	3	0	27	8679
20.	16	005574-34-5	47769	50	62	1	36	60	3	0	31	9500

CTMP Compounds

Peak 76; Unidentified Hydrocarbon



Average of 36.418 to 36.451 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	621	59.05	59	70.10	52	81.05	267
45.00	51	59.95	31	71.05	70	82.05	48
46.95	21	60.95	25	72.05	2	83.05	133
50.95	133	61.95	25	73.00	105	84.05	170
51.95	94	62.90	30	74.00	76	85.05	77
52.95	294	64.00	49	75.00	38	86.00	8
54.00	37	65.00	359	75.95	60	87.00	49
55.05	784	66.00	145	77.00	851	87.95	57
56.00	31	67.00	269	78.00	204	90.00	12
57.05	196	68.05	29	79.00	808	91.00	1166
58.00	78	69.05	303	80.05	98	92.00	55

Average of 36.418 to 36.451 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.05	584	104.00	66	117.05	156	129.05	39
94.05	251	105.05	573	118.00	62	130.00	51
95.00	576	106.05	149	119.00	301	131.00	96
96.05	145	107.05	1248	120.10	45	132.05	24
97.10	170	108.00	866	121.10	387	133.00	214
98.05	165	109.05	381	122.05	189	134.05	75
99.00	151	111.05	29	123.05	249	135.05	2248
100.00	91	112.00	36	125.00	193	136.05	185
100.95	22	113.00	61	126.00	716	138.00	140
102.00	15	115.00	183	126.95	958	139.00	21
103.00	130	116.00	114	127.95	115	141.00	25

Average of 36.418 to 36.451 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.00	29	158.05	72	171.00	49	184.30	20
144.10	159	159.05	208	173.05	225	188.05	1
145.00	152	160.00	189	174.05	99	189.00	47
146.10	44	161.05	206	175.05	477	191.00	30
147.00	211	162.05	133	176.05	83	193.00	49
148.10	89	163.05	143	177.05	90	195.00	23
149.05	630	164.00	165	178.00	77	197.00	62
150.10	2236	165.00	28	179.00	10	198.00	5
150.95	664	166.00	37	180.00	24	201.05	52
154.00	50	167.95	11	181.00	2	202.10	16
157.05	59	169.00	33	183.00	66	203.15	53

CTMP Compounds

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
204.00	17	219.10	93	233.00	97	253.05	39
205.00	48	220.10	46	233.20	48	254.15	20
206.05	22	220.40	19	234.00	38	255.10	23
206.95	8	221.10	49	235.10	49	256.00	25
208.00	24	222.10	14	236.05	10	258.05	35
209.00	14	223.05	8	239.15	29	258.80	10
213.15	68	225.10	18	241.20	38	261.05	543
214.15	39	226.15	3	243.10	12	262.05	162
215.10	77	229.10	4	247.00	55	265.20	20
217.10	61	231.05	35	251.00	26	266.20	8
218.05	77	232.00	39	252.15	20	266.55	16
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
268.90	49						
272.05	19						
276.10	1020						
277.10	246						

Average of 36.418 to 36.451 min.: A1216.D
Converted from RTE data file: >A1216:

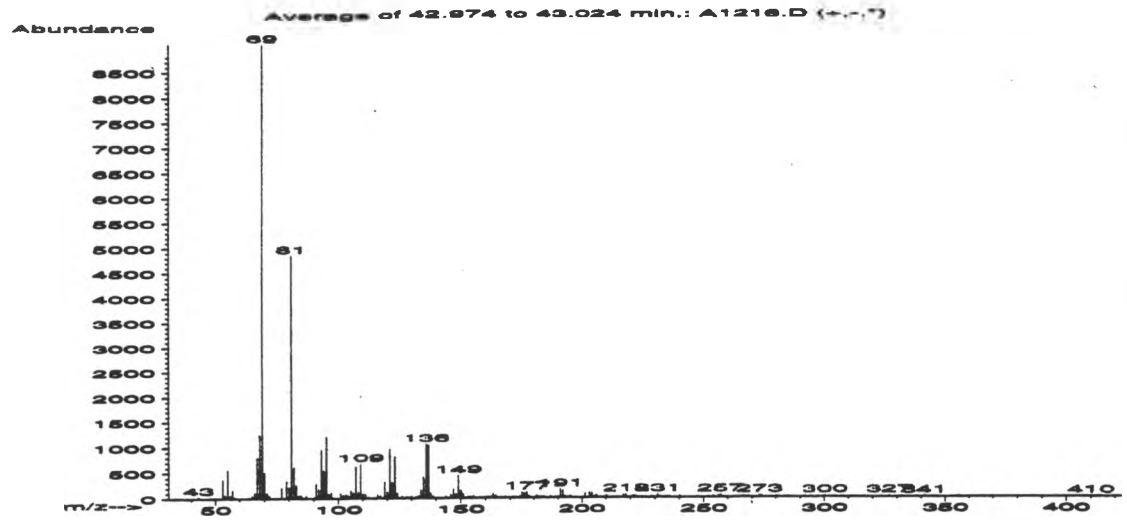
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Methyl-cis-bicyclo[4.3.0]non-7-en-2-on	150	C10H14O	43
2.	2,3,4,5-TETRAHYDROBENZOXEPIN-5,5-D2	148	C10H10D2O	38
3.	Benzene, 2-methoxy-1,3,4-trimethyl-	150	C10H14O	38
4.	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6	150	C10H14O	30
5.	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	30
6.	O-TOLYL VINYL SULFIDE	150	C9H10S	27
7.	1H-Indole, 5-fluoro-	135	C8H6FN	22
8.	Benzenemethanol, 4-(1-methylethyl)-	150	C10H14O	22
9.	Thiocyanic acid, phenyl ester	135	C7H5NS	18
10.	Adenine	135	C5H5N5	18
11.	Adenine	135	C5H5N5	18
12.	1,2-Benzisothiazole	135	C7H5NS	18
13.	Benzothiazole	135	C7H5NS	18
14.	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	14
15.	Ethanamine, 1-(2,4-cyclopentadien-1-ylid	135	C9H13N	14
16.	2,5-CYCLOHEXADIENE, 1,4-DIETHYL-1,4-DIME	164	C12H20	14
17.	Adenine	135	C5H5N5	11
18.	Adenine	135	C5H5N5	11
19.	1-Pentyn-3-ol, 3-methyl-, 4-nitrobenzoat	247	C13H13NO4	11
20.	Phenol, 4-methyl-	108	C7H8O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	077494-79-2	12818	48	45	2	103	46	18	0	44	8785
2.	*38	041807-17-4	12074	48	77	2	89	51	14	0	46	8482
3.	*38	021573-36-4	12758	52	54	1	78	55	14	0	44	8316
4.	*30	000116-26-7	12776	66	42	1	87	62	9	23	50	6115
5.	*30	000527-35-5	12735	55	50	0	70	56	9	17	43	8185
6.	*27	007297-72-5	12652	33	40	0	74	57	8	0	41	8201
7.	*22	000399-52-0	7540	44	47	1	69	64	5	0	40	6766
8.	22	000536-60-7	123695	57	51	0	69	64	5	5	40	8436
9.	*18	005285-87-0	7525	48	52	2	90	69	3	0	46	6130
10.	*18	000073-24-5	121689	53	38	1	92	68	3	0	49	6196
11.	*18	000073-24-5	7506	53	40	1	81	68	3	0	47	6223
12.	*18	000272-16-2	121700	57	34	2	70	68	3	10	49	6149
13.	*18	000095-16-9	121697	49	46	3	78	67	3	8	47	6008
14.	*14	002380-63-4	7511	36	45	3	99	69	2	0	41	6109
15.	*14	014469-77-3	7590	54	58	1	81	69	2	0	40	6149
16.	*14	000000-00-0	18721	31	58	0	66	68	2	20	42	5763
17.	*11	000073-24-5	121690	52	36	1	83	76	2	0	46	6138
18.	*11	000073-24-5	121686	53	35	2	90	73	2	0	49	6148
19.	*11	056009-23-5	55094	50	82	3	71	78	2	0	46	5861
20.	*11	000106-44-5	118728	48	55	1	50	79	2	14	47	3875

CTMP Compounds

Peak 77; Squalene



Average of 42.974 to 43.024 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	34	68.05	1247	83.05	249	95.10	1213
49.95	17	69.10	9055	84.10	54	96.05	82
53.00	367	70.10	500	85.05	63	97.05	114
54.00	61	71.10	102	86.00	7	100.95	93
55.00	556	72.00	49	87.00	51	102.00	61
56.05	56	75.95	7	87.95	12	103.00	75
57.05	156	77.00	209	90.00	26	104.00	40
57.95	17	79.05	341	91.00	281	105.05	150
65.05	54	80.05	217	92.05	177	106.00	102
66.00	107	81.05	4852	93.05	958	107.05	618
67.05	799	82.05	609	94.05	549	108.05	105

Average of 42.974 to 43.024 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	672	124.10	87	138.00	95	155.00	36
110.05	73	126.20	29	139.00	29	158.00	4
111.05	68	128.00	21	144.05	38	160.00	17
112.00	6	129.00	1	146.05	70	161.05	29
116.00	70	130.00	28	147.05	169	162.05	22
117.05	42	132.00	14	148.10	77	163.05	80
119.00	315	133.05	41	149.05	442	164.00	44
120.05	112	134.00	157	150.10	147	165.00	10
121.05	959	135.05	406	150.95	78	166.00	8
122.10	300	136.05	1060	153.00	22	168.00	20
123.15	810	137.05	1033	154.00	22	171.10	18

Average of 42.974 to 43.024 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
172.05	22	187.05	24	205.10	25	223.95	8
174.15	20	188.05	3	206.00	53	225.15	9
175.10	105	189.10	22	209.70	15	228.15	19
176.00	91	190.05	15	210.05	46	229.10	20
177.05	116	191.00	168	215.00	14	230.05	2
178.00	31	192.05	142	217.05	53	231.05	62
181.05	50	193.00	32	218.10	63	232.05	16
181.95	20	195.15	38	220.15	11	233.15	8
182.95	17	201.20	79	221.10	41	234.00	6
183.95	25	203.10	104	222.05	35	234.20	11
186.45	18	204.05	95	223.00	7	235.00	25

CTMP Compounds

Average of 42.974 to 43.024 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
236.00	29	262.20	10	273.15	44	302.15	10
240.15	40	263.20	9	274.10	37	326.90	28
247.00	16	265.05	3	278.00	9	330.90	16
247.90	12	265.45	13	280.15	22	331.15	6
250.00	11	266.00	6	281.00	18	331.75	9
251.90	13	266.30	18	283.45	11	341.15	18
252.15	16	266.95	26	285.05	25	341.80	11
254.00	28	267.95	19	291.95	17	354.75	13
256.10	36	269.00	20	294.20	11	356.00	9
257.00	55	270.00	13	298.90	11	410.15	11
259.05	11	272.00	9	300.10	29	410.40	10

Average of 42.974 to 43.024 min.: A1216.D
Converted from RTE data file: >A1216:

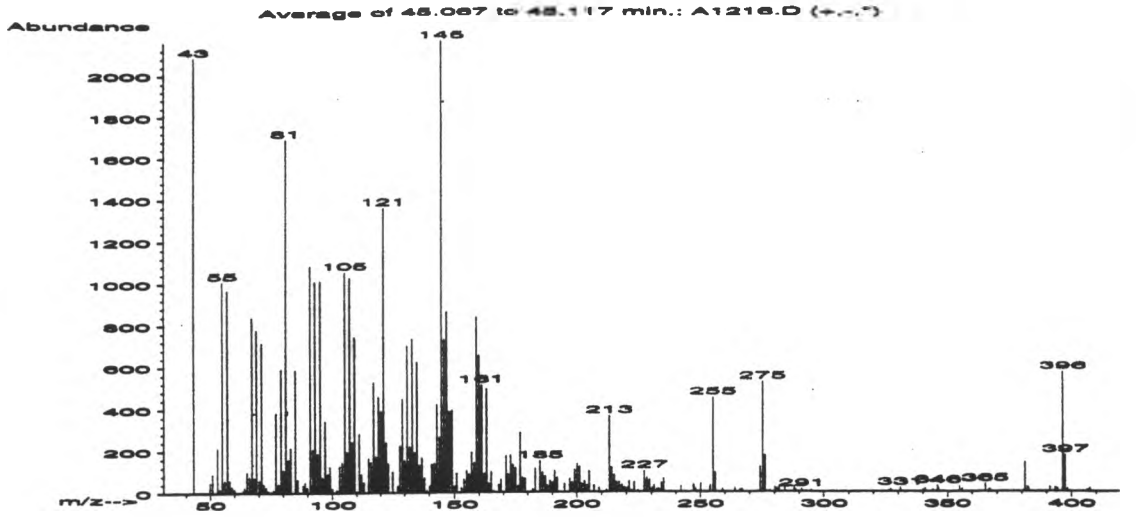
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,6,10,15,19,23-HEXAMETHYL-2,6,10,14,18,	410	C30H50	91
2.	10-DEMETHYLSQUALENE	396	C29H48	90
3.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	86
4.	Lycopersen	547	C40H66	78
5.	6,10,14-Hexadecatrien-1-ol, 3,7,11,15-te	292	C20H36O	72
6.	trans-Farnesol	222	C15H26O	56
7.	Farnesol	222	C15H26O	56
8.	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	47
9.	Farnesol	222	C15H26O	45
10.	cis-Farnesol	222	C15H26O	45
11.	Geraniol formate	182	C11H18O2	42
12.	Linalool	154	C10H18O	42
13.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	38
14.	Cyclohexane, 1,1-dimethyl-2,4-bis(1-meth	192	C14H24	11
15.	Cyclohexane, 3,4-bis(1-methylethenyl)-1,	192	C14H24	11
16.	2,5-Furandione, 3-(dodecenyl)dihydro-	266	C16H26O3	10
17.	11-METHYLSQUALENE	424	C31H52	10
18.	5-Hexen-1-one, 1-(1H-imidazol-2-yl)-4,4-	192	C11H16N2O	10
19.	2H-Benzocyclohepten-2-one, 1,4a,5,6,7,8,	178	C12H18O	10
20.	4-(2',6',6'-TRIMETHYLCYCLOHEX-1'-EN-1'-Y	210	C14H26O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	91	000000-00-0	99541	102	29	1	85	3	60	0	56	9963
2.	90	059681-06-0	97232	88	50	3	88	5	57	0	49	9962
3.	86	007683-64-9	99537	87	49	3	99	10	53	0	45	9961
4.	78	000502-62-5	110625	80	62	2	71	8	46	13	40	9919
5.	72	036237-66-8	71334	61	58	2	72	14	42	3	39	9909
6.	56	000106-28-5	44954	53	56	3	83	15	30	0	36	9914
7.	56	004602-84-0	129877	60	65	3	115	12	30	0	36	9882
8.	*47	035387-63-4	8748	38	43	2	95	36	20	0	39	9757
9.	45	004602-84-0	129871	44	73	1	80	21	19	1	35	9918
10.	45	003790-71-4	44953	45	72	2	71	22	19	0	35	9901
11.	42	000105-86-2	127006	53	47	2	92	26	17	19	37	9796
12.	42	000078-70-6	124213	43	58	3	99	29	17	0	35	9824
13.	*38	007683-64-9	136174	33	71	0	20	48	14	0	41	2398
14.	*11	062337-98-8	31101	50	50	0	14	75	2	0	46	9418
15.	*11	061142-74-3	31100	50	50	0	14	75	2	0	46	9418
16.	*10	025377-73-5	62058	34	76	1	17	71	1	0	39	9297
17.	10	063424-36-2	101597	43	85	1	39	68	1	0	37	9904
18.	*10	069393-40-4	30773	34	50	0	12	75	1	0	41	7065
19.	10	017429-26-4	24883	43	29	0	12	78	1	16	41	1922
20.	10	054344-90-0	39643	47	36	0	10	78	1	0	39	1894

CTMP Compounds

Peak 78; Unidentified Triterpene



Average of 45.067 to 45.117 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2087	63.40	9	74.00	8	85.95	64
49.90	49	63.95	26	75.00	4	88.15	34
50.95	92	65.00	99	75.95	15	88.95	51
53.00	214	66.00	77	77.00	382	89.90	25
54.00	18	67.05	838	78.05	41	91.00	1082
55.00	1008	68.05	72	79.05	591	92.05	208
56.00	58	69.00	779	80.05	109	93.05	1008
57.05	968	70.10	58	81.05	1691	94.10	188
58.00	60	71.05	715	82.05	158	95.05	1013
58.95	29	72.00	41	83.05	216	96.05	73
60.00	17	73.00	25	85.05	586	97.05	342
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.10	90	110.05	7	122.15	239	135.05	624
99.05	124	111.05	280	123.10	138	136.05	131
100.00	20	112.00	89	125.00	101	137.05	167
102.00	14	113.00	50	127.00	33	138.05	71
103.00	127	115.00	164	128.00	224	139.10	11
104.00	145	116.00	146	129.00	448	140.25	31
105.05	1054	117.00	529	130.00	154	141.00	137
106.05	196	118.00	172	131.05	700	142.00	141
107.05	1027	119.00	457	132.00	221	143.05	422
108.05	242	120.10	389	133.05	735	144.10	266
109.05	744	121.10	1360	134.00	193	145.00	2160
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.05	733	158.05	142	171.05	176	185.05	151
147.05	866	159.05	840	172.05	88	186.10	97
148.10	389	160.05	655	173.10	178	187.10	76
149.10	395	161.05	515	174.05	132	188.05	32
150.10	30	162.10	90	175.10	118	189.10	57
150.95	93	163.05	496	176.10	30	190.10	47
152.95	23	164.05	43	177.05	286	191.00	104
154.00	62	164.95	100	177.95	71	192.05	70
155.00	106	166.00	8	179.00	65	195.00	40
156.00	89	168.05	37	182.00	16	197.15	66
157.05	194	169.00	65	183.05	115	198.10	47
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
199.15	111	214.10	119	224.50	9	247.10	36
200.10	136	215.10	83	227.15	102	247.40	30
201.15	122	216.05	49	228.15	67	248.15	14
202.15	40	217.10	48	229.20	58	248.95	5
203.20	54	218.15	34	230.10	17	250.15	42

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
204.05	31	219.15	24	231.10	32	253.75	24
205.00	99	220.00	16	232.20	13	254.10	31
206.95	31	220.25	18	233.00	14	255.20	452
209.00	19	221.05	54	234.05	44	256.10	93
212.05	11	222.00	9	235.05	64	259.05	15
213.15	364	223.05	48	242.15	27	264.05	17
266.05	13	288.00	25	346.00	29	391.30	23
267.00	13	288.55	12	346.30	15	393.25	11
273.10	5	291.05	13	354.95	26	393.45	21
274.15	121	295.00	8	355.90	13	393.95	13
275.20	527	326.25	8	365.25	38	394.30	14
276.20	175	327.15	11	366.80	12	396.45	573
278.00	9	331.00	19	367.20	10	397.35	175
280.15	22	340.05	9	381.35	140	398.45	13
281.00	17	340.70	10	382.30	5	406.30	9
281.95	21	340.95	16	382.50	23	406.75	9
284.10	26	344.05	10	382.75	12	407.30	17

Average of 45.067 to 45.117 min.: A1216.D
Converted from RTE data file: >A1216:

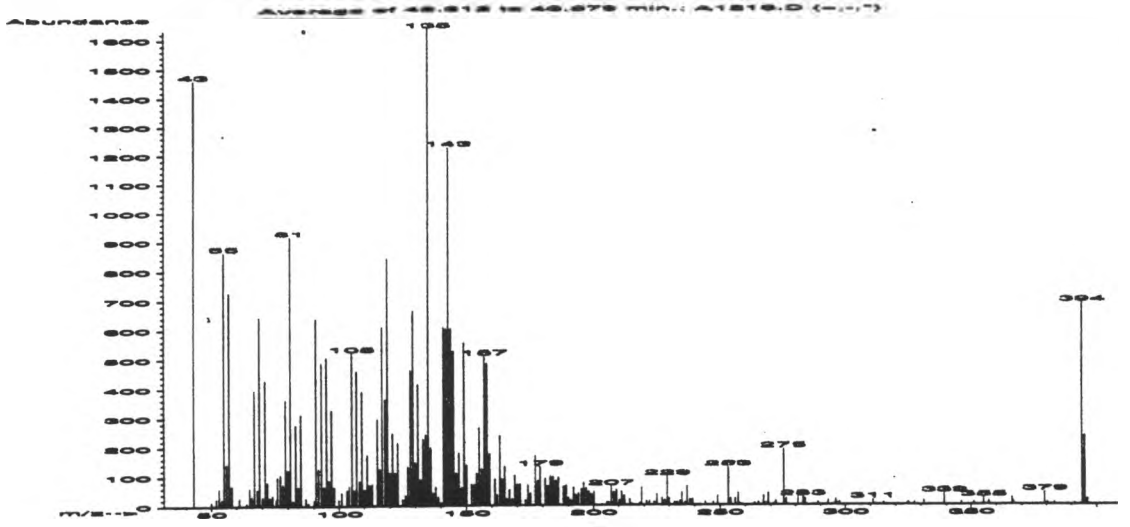
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Pyrrolo[2,3-b]pyridine, 2-(1-methylet	160	C10H12N2	11
2.	Benzene, 1-(1,1-dimethylethyl)-4-ethenyl	160	C12H16	11
3.	2,3-Dimethyl-3-phenylhex-1-ene	188	C14H20	10
4.	6,7-Dihydro-7-hydroxy-7-methyl-5H-pyrrol	163	C10H13NO	10
5.	Benzene, (2,2-dimethyl-1-methylenepropyl	160	C12H16	10
6.	8-Isopropyliden-4-methyl-anti-tricyclo[3	160	C12H16	10
7.	Naphthalene, 1,2,3,4-tetrahydro-1,5-dime	160	C12H16	10
8.	(1S,2E,4S,6R,7E,11S)-2,7,12(20)-Cembratr	304	C20H32O2	10
9.	1H-Indene, 2,3-dihydro-4,5,7-trimethyl-	160	C12H16	10
10.	1,3-Dioxan-5-ol, 2-pentadecyl-, acetate,	356	C21H40O4	10
11.	1,3,5-Trisilacyclohexane, 1,1-dimethyl-	160	C5H16Si3	10
12.	4-ISOQUINOLINOL	145	C9H7NO	10
13.	Propanedioic acid, dipropyl-, dimethyl e	216	C11H20O4	9
14.	Quinoline, 2-(2-methylpropoxy)-	201	C13H15NO	9
15.	Benzene, (1,3-dimethyl-2-butenyl)-	160	C12H16	9
16.	Benzene, 1-(1-methylethenyl)-2-(1-methyl	160	C12H16	9
17.	5-AMINO-15N-ISOQUINOLINE	144	C9H8N15N	9
18.	1,3-Dioxan-5-ol, 2-pentadecyl-, acetate,	356	C21H40O4	9
19.	Benzenamine, N-(2,2-dimethyl-4,4-dipheny	327	C23H21NO	9
20.	5.EPSILON.-METHOXYCARBONYL-5.EPSILON.-ME	317	C14H23NO7	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*11	027257-18-7	16897	50	47	1	70	79	2	0	46	6296
2.	*11	001746-23-2	17025	43	52	1	99	80	2	0	44	6204
3.	10	071491-58-2	29407	53	61	0	97	78	1	0	39	6396
4.	*10	082217-83-2	18096	52	64	2	71	72	1	17	39	6704
5.	10	005676-29-9	124934	57	48	0	67	80	1	10	43	6204
6.	*10	093958-98-6	17073	34	63	1	94	80	1	0	39	6222
7.	*10	021564-91-0	17050	43	59	1	81	80	1	0	39	6204
8.	10	057688-98-9	133611	53	81	1	70	80	1	4	38	6453
9.	*10	006682-06-0	17043	43	58	1	76	78	1	0	40	6441
10.	*10	030889-23-7	135108	37	89	2	87	79	1	0	39	6271
11.	*10	054424-15-6	16562	45	73	3	99	77	1	0	39	6846
12.	*10	000000-00-0	11056	37	56	0	75	80	1	0	41	6229
13.	9	016644-05-6	41851	54	76	1	67	78	1	0	32	6358
14.	* 9	056273-37-1	35178	45	58	2	72	80	1	4	37	6204
15.	* 9	050704-01-3	17008	39	63	1	78	80	1	3	30	6204
16.	* 9	005557-93-7	17018	46	62	2	99	80	1	0	35	6204
17.	9	057174-26-2	10830	39	90	2	67	80	1	0	33	6204
18.	* 9	030889-26-0	89440	40	87	2	81	79	1	0	35	6296
19.	9	055470-95-6	82062	58	69	1	74	80	1	3	30	6204
20.	9	063535-48-8	79189	46	110	2	99	80	1	0	35	6204

CTMP Compounds

Peak 79; Unidentified Triterpene



Average of 46.812 to 46.879 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1459	65.00	60	75.95	97	87.95	9
50.00	14	66.00	32	77.00	107	89.95	1
51.90	25	67.00	395	78.00	72	90.15	20
53.00	58	68.05	55	79.05	361	91.00	637
54.05	22	69.05	642	80.00	122	92.00	125
55.00	863	70.10	29	81.05	914	93.05	487
56.00	141	71.15	428	82.00	17	94.10	65
57.05	726	72.10	79	83.05	274	95.10	506
58.00	67	73.00	28	84.00	63	96.00	86
60.95	26	73.95	35	85.10	312	97.10	326
63.85	10	75.55	23	86.95	26	98.10	63

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.90	21	111.95	70	124.05	2	135.05	1631
101.00	45	113.00	74	125.05	22	136.05	198
103.00	52	115.00	295	126.00	35	137.10	43
104.00	68	116.00	125	127.00	132	138.05	65
105.05	520	117.00	610	128.00	463	139.00	29
106.05	54	118.05	363	129.05	665	140.10	12
107.05	459	119.00	842	130.00	146	141.05	609
108.10	84	120.05	112	131.05	414	142.00	603
109.05	390	121.05	247	132.05	89	143.00	1220
110.05	55	122.05	112	133.05	228	144.00	603
111.10	174	123.10	216	134.05	244	145.05	527

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.05	111	158.05	484	170.00	71	184.00	97
147.10	180	159.05	176	171.05	71	185.10	83
148.05	60	161.10	90	173.10	18	186.05	94
149.10	556	162.00	36	174.10	69	188.10	64
150.10	136	163.10	238	175.15	40	189.10	67
152.00	72	164.05	89	177.05	170	190.10	25
153.00	71	165.05	132	178.00	84	191.05	17
153.95	110	166.00	22	179.00	130	192.05	59
155.00	265	166.95	54	181.00	90	193.00	35
156.00	124	168.00	22	181.95	66	194.00	40
157.05	508	169.00	102	183.05	100	195.10	55

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
196.00	77	210.20	17	227.10	25	238.55	9
197.10	58	211.10	46	228.20	17	239.15	20
198.05	46	212.10	32	229.20	97	244.15	12
199.15	37	214.30	21	230.00	23	247.15	11
200.15	45	215.20	4	232.00	9	249.00	31

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
203.15	1	218.10	7	233.05	9	253.15	127
205.05	12	219.05	60	234.15	15	254.15	22
206.05	11	221.10	14	235.00	43	256.05	22
207.00	62	222.25	13	236.20	8	257.10	40
208.00	45	224.10	11	237.00	63	258.05	4
209.00	53	225.10	36	238.10	19	263.80	7
265.20	11	289.05	9	331.05	15	383.20	8
267.20	32	293.15	16	339.20	37	391.20	5
268.05	6	295.90	8	343.20	2	394.30	687
269.15	41	296.20	19	346.20	11	395.30	236
271.10	4	296.50	8	351.15	10	396.35	19
272.00	15	297.75	9	355.00	22		
275.20	190	310.95	16	357.00	12		
276.25	23	312.10	1	366.20	24		
280.95	47	315.05	8	366.70	11		
283.00	26	324.75	11	379.25	41		
283.75	22	327.25	9	380.40	7		

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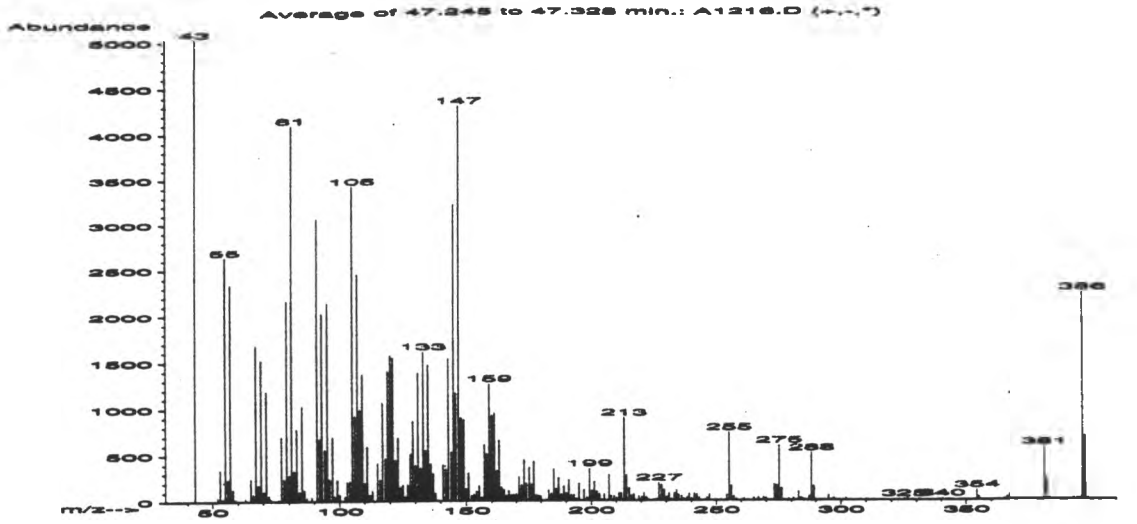
	Name	MolWt	Formula	Qual
1.	Cholesta-4,6-dien-3-ol, benzoate, (3.bet	488	C34H48O2	47
2.	Cholesta-4,6-dien-3-ol, (3.beta.)-	384	C27H44O	46
3.	1,2-Dihydro-1,3-dimethyl-naphthalene	158	C12H14	14
4.	Quinoline, 4-methyl-	143	C10H9N	11
5.	2H-Imidazo[4,5-b]pyridin-2-one, 1,3-dihy	135	C6H5N3O	11
6.	1H-Indole, 5-fluoro-	135	C8H6FN	11
7.	Quinoline, 5-methyl-	143	C10H9N	10
8.	Tricyclo[3.3.1.1(3,7)]decane-1-carboxyli	287	C11H16AgO2	10
9.	Benzene, 1-(1,3-dimethyl-3-butenyl)-4-me	190	C13H18O	10
10.	Oxiranecarboxylic acid, 2-ethyl-3-phenyl	220	C13H16O3	10
11.	Quinoline, 6-methyl-	143	C10H9N	10
12.	Quinoline, 6-methyl-	143	C10H9N	10
13.	Quinoline, 7-methyl-	143	C10H9N	10
14.	Quinoline, 4-methyl-	143	C10H9N	10
15.	P-FLUOROBENZYLIDENE CHLORIDE	178	C7H5Cl2F	10
16.	1,2,3,4-TETRAHYDROQUINOLINE-2,2-D2	133	C9H9D2N	10
17.	Quinoline, 8-methyl-	143	C10H9N	10
18.	Tricyclo[3.3.1.13,7]decane, 2-bromo-	214	C10H15Br	10
19.	Benzenemethanol, .alpha.,.alpha.,4-trime	150	C10H14O	10
20.	3,4-METHYLENEDIOXYBENZYL METHYL KETONE	178	C10H10O3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	025485-34-1	108133	97	114	3	86	36	20	0	41	9398
2.	46	014214-69-8	95098	79	125	0	72	41	20	0	47	9388
3.	*14	000000-00-0	16325	34	52	0	59	70	2	0	41	5355
4.	*11	000491-35-0	122801	33	42	0	65	77	2	10	43	4725
5.	*11	016328-62-4	7518	35	48	2	99	77	2	4	43	6317
6.	*11	000399-52-0	7540	47	45	2	91	77	2	0	44	6317
7.	*10	007661-55-4	10421	34	60	1	64	77	1	0	41	4725
8.	10	075112-78-6	69448	59	65	0	67	77	1	0	43	6365
9.	10	074672-05-2	30132	54	53	2	96	77	1	10	43	6353
10.	10	054852-65-2	43670	55	60	2	93	77	1	22	40	6350
11.	*10	000091-62-3	122808	35	60	1	56	77	1	0	41	4725
12.	*10	000091-62-3	122807	45	54	1	57	77	1	2	43	4725
13.	*10	000612-60-2	122810	38	58	2	64	77	1	1	42	4725
14.	*10	000491-35-0	122805	33	59	1	65	77	1	0	41	4725
15.	*10	000000-00-0	24392	35	52	0	52	77	1	0	41	4739
16.	*10	020668-18-2	7159	36	81	3	99	75	1	1	40	6652
17.	*10	000611-32-5	122814	39	52	1	54	77	1	0	39	4725
18.	*10	007314-85-4	41073	37	70	2	99	77	1	0	41	6317
19.	*10	001197-01-9	123699	51	52	2	94	76	1	10	39	6469
20.	*10	004676-39-5	24601	37	46	1	89	77	1	13	40	6317

CTMP Compounds

Peak 80; Unidentified triterpene



Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	5030	59.00	18	76.00	19	87.00	38
47.05	10	62.95	25	77.05	697	89.00	43
49.80	9	65.00	245	78.00	239	91.00	3062
51.00	1	66.00	77	79.05	2156	92.00	672
52.00	42	67.00	1674	80.05	281	93.00	2019
53.00	343	68.10	178	81.05	4090	94.05	553
54.00	28	69.10	1518	82.05	330	95.10	2130
55.00	2633	70.10	105	83.05	779	96.00	237
56.00	237	71.10	1179	84.05	102	97.15	691
57.05	2333	72.15	62	85.05	1021	98.05	53
58.00	128	72.95	23	85.95	122	99.05	230

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.95	67	111.05	586	123.10	682	133.05	1613
100.30	6	112.05	67	124.10	148	134.05	546
102.00	53	113.10	107	125.05	176	135.05	1468
103.00	208	115.00	406	126.00	49	136.05	401
104.00	215	116.00	230	126.20	20	137.05	298
105.05	3417	117.00	1059	127.00	179	138.00	81
106.05	915	118.05	460	128.00	508	139.05	10
107.05	2446	119.00	1397	129.00	865	141.00	395
108.05	983	120.05	1568	130.05	384	142.00	345
109.05	1366	121.10	1545	131.05	1382	143.00	1539
110.05	198	122.05	441	132.05	357	144.10	529

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
145.00	3220	156.05	38	167.05	112	178.00	65
146.00	1166	157.05	609	168.05	64	179.05	59
147.10	4291	158.05	509	169.05	75	180.00	48
148.15	899	159.05	1264	170.05	70	182.00	16
149.15	878	160.10	921	171.05	259	183.05	113
150.10	129	161.05	952	172.10	174	184.00	80
151.00	300	162.10	324	173.10	445	185.05	342
152.05	58	163.05	656	174.10	186	186.10	127
153.00	72	164.00	148	175.15	365	187.05	246
154.05	103	165.00	117	176.10	180	188.10	72
155.00	165	165.95	62	177.00	431	189.10	155

CTMP Compounds

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
190.10	81	200.20	106	212.10	84	222.65	14
191.00	227	201.15	204	213.20	895	223.10	3
192.05	62	202.15	99	214.15	271	225.15	15
192.40	23	203.15	73	215.20	136	226.15	22
193.00	64	204.05	11	216.15	50	227.20	196
194.05	25	205.10	72	217.10	67	228.20	172
195.15	189	207.00	283	219.10	50	229.20	116
196.05	3	207.95	52	220.20	40	230.20	39
197.05	118	209.05	49	221.10	86	231.10	83
198.15	37	210.05	30	222.15	36	231.95	10
199.15	348	211.10	79	222.40	12	232.20	19

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
233.15	87	245.10	13	260.15	5	274.20	168
234.15	113	246.20	36	261.10	26	275.20	594
235.05	63	247.20	68	261.55	5	276.20	130
236.10	46	250.05	4	262.95	8	277.15	7
237.05	22	251.65	9	265.00	31	279.05	22
238.20	32	254.15	62	266.55	14	280.15	10
239.10	77	255.20	736	267.00	35	281.00	25
240.10	24	256.10	159	269.00	35	282.00	10
241.15	79	257.10	43	270.10	28	283.05	94
242.20	63	258.05	14	271.05	6	284.00	28
243.10	29	258.20	9	273.20	175	284.45	5

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
285.10	16	299.25	9	331.05	15	355.15	30
285.95	10	302.00	26	339.45	9	363.20	8
287.05	44	302.25	6	340.45	20	365.25	18
287.25	45	310.05	12	341.95	6	366.30	38
288.20	510	310.95	3	344.00	1	367.30	61
289.20	152	323.10	7	344.20	10	378.15	6
290.70	6	325.05	14	346.15	3	379.30	4
293.20	7	326.15	11	348.00	7	381.35	568
295.05	54	326.55	15	353.25	6	382.30	227
296.50	5	328.25	8	354.25	109	383.15	20
297.10	26	328.75	4	354.80	37	383.40	11

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
392.55	6						
393.05	30						
394.35	42						
395.30	31						
396.35	2241						
397.40	686						
398.30	155						

CTMP Compounds

Average of 47.245 to 47.328 min.: A1216.D
Converted from RTE data file: >A1216:

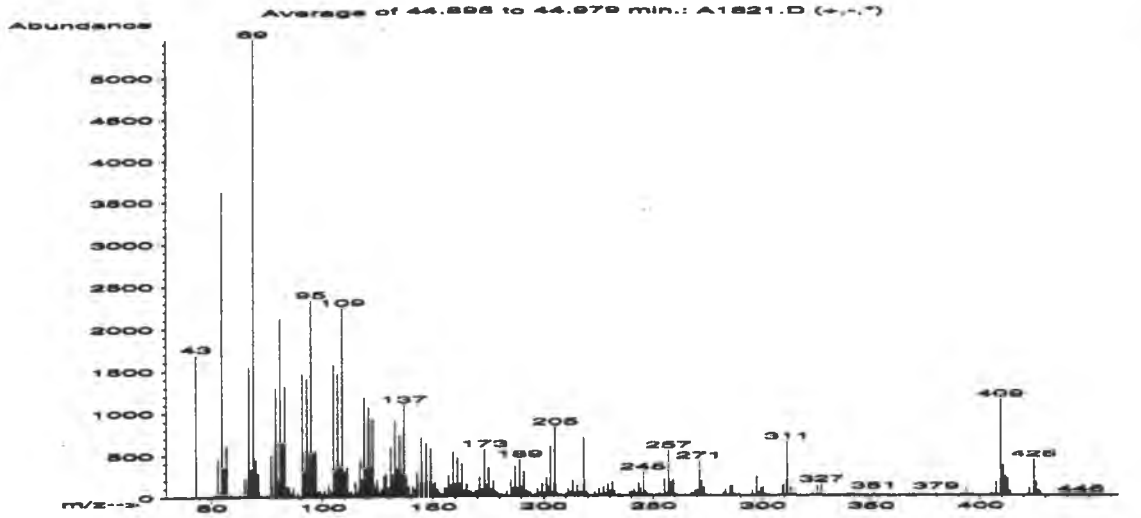
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	STIGMASTA-4,22-DIENE	396	C29H48	43
2.	3-BROMO-1,2,4-TRIAZINE 2-OXIDE	175	C3H2BrN3O	16
3.	2-Pentenoic acid, 5-phenyl-, (E)-	176	C11H12O2	10
4.	6-AMINO-2,4-DIMETHYLNICOTINONITRILE	147	C8H9N3	10
5.	2H-Benzotriazole, 2-ethyl-	147	C8H9N3	10
6.	ENDO-FENCHOL	154	C10H18O	10
7.	13-METHYL-13-CARBINALPODOCARP-7-EN-3B,X-	306	C19H30O3	10
8.	1,2-Diheptylcyclopropene	236	C17H32	10
9.	2-Phenanthrenecarboxaldehyde, 1,2,3,4,4a	306	C19H30O3	10
10.	9,10-Secoergosta-5,7,22-trien-3-ol, (3.b	398	C28H46O	10
11.	Cyclopentaneethanol, 2-(hydroxymethyl)-.	172	C10H20O2	10
12.	1-Naphthalenepropanol, .alpha.-ethenylde	306	C20H34O2	9
13.	Isotrixagoyl oxide	288	C20H32O	9
14.	BENZENE, 1-FLUORO-4-(2-CYANOETHENYL)-, (	147	C9H6FN	9
15.	Quinoline, 1,2,3,4-tetrahydro-6-methyl-	147	C10H13N	9
16.	KAUREN-19-OL	288	C20H32O	9
17.	5-AMINO-1-METHYL-1H-INDAZOLE	147	C8H9N3	9
18.	1-(6-Methyl-2-pyrazyl)-1-heptene	190	C12H18N2	9
19.	3,8,11-Trioxatetracyclo[4.4.1.0(2,4).0(7	154	C8H10O3	9
20.	N-ISOPENTYLIDENE FURFURYL AMINE	165	C10H15NO	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	076866-92-7	97237	74	127	2	55	43	18	12	42	8305
2.	*16	061178-02-7	126402	36	53	0	57	60	3	13	37	6706
3.	*10	055320-96-2	23813	35	45	0	60	77	1	0	41	5175
4.	*10	000000-00-0	11620	33	57	2	57	77	1	0	39	5520
5.	*10	016584-04-6	11632	36	63	1	58	77	1	0	41	5429
6.	*10	000000-00-0	14757	34	73	1	81	75	1	0	39	5620
7.	10	000000-00-0	75871	66	101	3	89	71	1	3	38	5533
8.	10	035365-53-8	51031	46	90	2	61	66	1	0	35	5834
9.	10	072088-19-8	75872	66	101	3	89	71	1	3	38	5533
10.	10	000067-96-9	97597	47	107	0	39	76	1	19	41	7803
11.	10	000485-42-7	22351	46	78	2	75	66	1	0	35	5794
12.	9	004549-12-6	75934	60	87	2	45	77	1	4	35	7146
13.	* 9	083631-61-2	70049	41	58	2	67	75	1	15	35	5211
14.	* 9	071750-12-4	11638	36	62	3	85	77	1	5	34	5535
15.	* 9	000091-61-2	11721	40	74	2	81	76	1	0	33	5714
16.	9	000000-00-0	70086	55	97	1	48	75	1	17	37	7186
17.	* 9	000000-00-0	11635	39	75	2	85	77	1	0	33	5429
18.	9	083568-42-7	30083	58	63	3	85	76	1	0	36	5808
19.	* 9	050267-11-3	14334	34	66	1	64	77	1	0	35	5294
20.	* 9	000000-00-0	18995	40	32	1	62	77	1	0	35	5175

CTMP Compounds

Peak 81; Unidentified Sterol



Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1693	57.00	615	69.00	5456	82.05	649
47.15	7	58.00	5	70.05	435	83.05	1313
47.40	7	59.00	32	71.10	273	84.05	119
49.80	15	60.95	19	72.00	12	85.05	126
50.90	13	61.50	3	72.20	57	86.10	49
51.80	6	62.05	6	75.00	19	87.05	107
52.00	28	62.95	36	76.95	503	88.15	9
52.95	451	64.95	221	77.95	144	89.00	48
53.95	64	66.00	99	79.00	1290	89.80	8
54.95	3628	67.00	1546	80.00	191	91.00	1469
56.00	348	68.00	329	81.00	2120	92.00	307

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.00	1408	104.00	78	115.00	178	126.05	66
94.05	300	105.05	1573	115.95	65	127.05	86
95.00	2332	106.00	317	117.00	433	128.05	247
96.00	527	107.05	1465	117.95	202	129.10	273
97.05	545	108.05	361	119.00	1188	130.00	108
98.05	62	109.05	2239	120.05	345	131.05	581
99.10	73	110.05	296	121.10	1069	132.05	252
99.95	33	111.05	349	122.15	367	133.05	912
101.00	77	112.00	42	123.15	926	134.05	337
102.00	25	113.00	66	124.10	124	135.05	729
102.90	148	113.95	20	125.10	201	136.05	265

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.05	1095	148.10	183	159.10	531	169.05	74
138.05	255	149.15	573	160.10	152	170.10	66
139.10	124	150.10	140	161.05	459	171.05	226
140.05	26	151.10	171	162.10	153	172.20	88
141.05	119	152.10	89	163.10	390	173.15	562
142.10	82	153.00	48	164.05	70	174.10	130
143.00	295	154.05	30	165.10	147	175.10	348
144.10	157	155.10	109	166.15	66	176.10	86
145.00	707	156.10	99	167.05	63	177.10	187
146.05	163	157.00	249	168.05	39	178.10	59
147.10	634	158.10	134	168.20	8	178.50	16

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
178.95	38	189.15	438	199.15	156	211.15	85
179.15	2	190.15	111	200.15	45	212.10	52
180.10	23	191.05	293	201.20	217	213.15	186
181.15	22	192.25	67	202.20	110	214.20	35
181.80	1	192.50	49	203.20	596	215.25	127
182.15	17	193.15	46	204.20	151	216.15	48
183.15	60	194.05	34	205.25	822	217.25	131
185.05	193	195.10	13	206.20	35	218.25	700
186.10	102	196.10	26	207.10	18	219.25	180
187.05	364	197.10	83	208.10	19	220.00	12
188.05	102	198.10	43	210.20	27	220.20	29

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
221.95	12	232.20	55	242.25	31	251.10	16
223.20	46	233.40	14	243.25	156	252.15	16
224.05	11	234.10	21	244.25	90	252.75	19
225.20	91	234.65	5	245.25	283	253.20	37
226.15	24	234.90	13	246.25	56	254.15	8
227.20	113	235.15	11	247.10	29	255.20	204
228.15	33	237.15	2	247.45	10	256.20	43
229.15	149	238.35	3	248.25	11	257.15	538
230.15	59	239.15	52	248.80	13	258.05	9
230.50	11	240.20	52	249.15	14	258.20	153
231.20	165	241.20	79	249.95	5	259.20	189

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
260.20	23	264.85	9	273.30	97	282.10	38
260.65	13	265.50	3	274.00	10	282.50	19
261.05	6	265.85	10	274.20	11	283.10	75
261.40	7	267.30	33	275.05	4	284.15	16
261.65	2	268.10	30	275.30	1	284.60	3
262.15	2	268.45	4	276.20	12	285.25	118
263.20	1	269.15	65	277.70	2	286.25	123
263.40	2	270.20	66	278.50	4	287.20	26
263.75	7	271.20	413	279.05	7	287.95	2
264.00	4	272.25	183	279.35	14	288.25	15
264.35	2	273.05	5	279.65	9	288.60	7

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
289.25	24	298.30	41	309.20	124	315.15	45
289.75	3	299.15	89	309.40	22	316.15	1
290.90	5	299.35	29	310.15	180	316.45	3
291.85	1	300.20	103	310.40	31	318.00	3
293.15	3	301.30	25	311.20	642	318.95	2
294.80	1	302.25	4	312.25	182	319.30	2
295.20	64	306.65	3	313.25	95	320.85	1
295.80	6	307.15	2	313.65	20	321.30	4
296.15	11	307.45	2	314.15	17	322.20	2
297.25	227	307.70	12	314.50	14	323.25	53
298.05	7	308.40	9	314.85	5	324.35	9

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
325.25	114	331.80	5	342.55	3	347.95	5
325.55	17	333.90	2	342.85	5	348.20	1
325.95	8	334.25	4	343.15	10	351.35	53

CTMP Compounds

326.20	14	337.90	4	343.70	2	352.20	5
326.50	22	338.30	4	344.15	11	352.75	6
326.70	30	339.20	45	344.50	7	353.35	16
327.25	131	339.45	40	344.95	8	353.70	6
328.75	6	340.35	23	345.20	2	353.95	3
329.00	10	340.65	6	345.60	1	354.55	6
331.10	3	341.45	28	346.70	2	354.80	2
331.55	2	342.20	16	347.15	12	355.45	9

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
356.45	8	369.05	18	380.45	4	390.25	5
357.05	8	369.45	28	381.25	5	391.15	15
359.45	3	369.85	17	381.55	2	391.55	44
361.15	3	370.25	3	381.95	4	392.20	9
362.15	3	371.50	3	382.95	4	393.50	93
363.25	5	372.25	3	383.20	3	394.30	25
365.25	3	373.30	4	383.75	8	394.65	37
365.90	5	374.55	4	385.70	10	395.40	26
367.40	22	376.05	2	386.20	10	396.40	29
368.30	4	379.20	6	387.40	2	397.05	3
368.70	1	379.55	43	388.60	1	397.45	6

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
398.35	7	406.25	15	421.65	2	433.45	1
398.65	7	407.45	158	422.50	87	437.30	4
399.20	6	408.30	18	423.25	7	438.55	3
399.75	1	409.50	1151	424.65	431	445.95	8
400.95	4	410.55	361	425.50	159	449.65	2
401.50	7	411.55	226	426.55	62		
402.30	3	412.55	199	427.50	42		
404.30	4	413.30	9	428.80	4		
404.85	19	413.60	54	429.20	7		
405.35	20	418.65	2	429.75	7		
406.05	11	421.25	4	431.80	2		

CTMP Compounds

Average of 44.895 to 44.979 min.: A1821.D
Converted from RTE data file: >A1821:

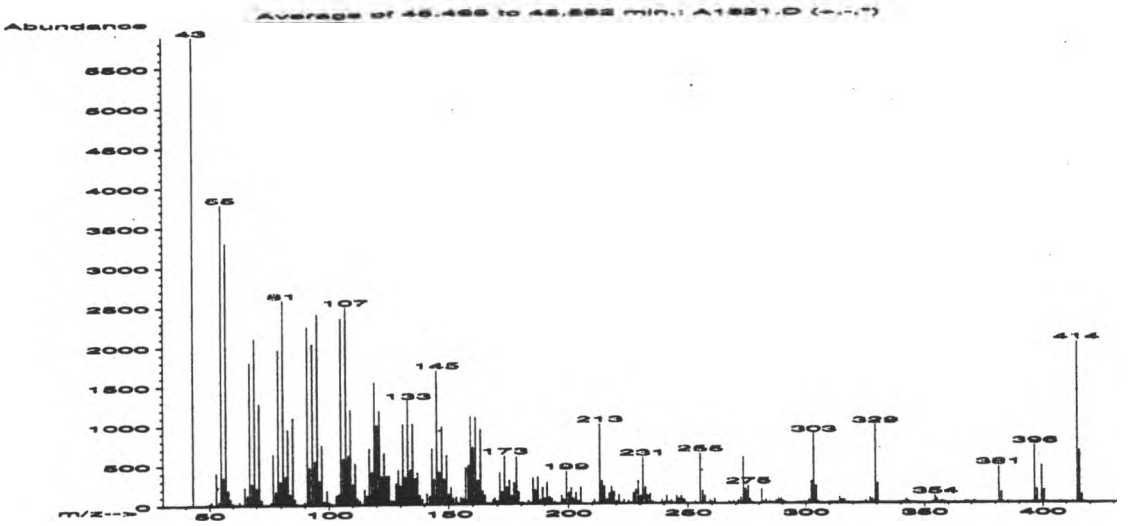
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3-Dioxane, 2,2,4,5-tetramethyl-6-(1-me	410	C27H54O2	38
2.	Cycloprop[7,8]ergost-22-en-3-one, 3',7-d	410	C29H46O	38
3.	9,19-Cyclolanost-24-en-3-ol, (3.beta.)-	426	C30H50O	28
4.	d-Nerolidol	222	C15H26O	28
5.	trans-Geraniol	154	C10H18O	25
6.	MENTHONE-8-THIOL	186	C10H18OS	25
7.	P-MENTHON-8-THIOL	186	C10H18OS	23
8.	24-Norcholane, 23-[2-methyl-1-(1-methyle	412	C30H52	17
9.	1-Anthracenecarboxaldehyde, 5,8,8a,9,10,	410	C25H30O5	10
10.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	10
11.	METHYL 2-HYDROXYDECANOATE	202	C11H22O3	10
12.	4-Pyridinol, acetate (ester)	137	C7H7NO2	8
13.	D:B-Friedo-18,19-secolup-19-ene, 3,10-ep	426	C30H50O	7
14.	Gorgostane, (5.alpha.)-	412	C30H52	7
15.	Ergost-25-ene-3,5,6,12-tetrol, (3.beta.,	448	C28H48O4	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	056324-82-4	99474	42	143	3	90	25	14	0	27	9661
2.	38	053755-18-3	99497	53	107	3	71	39	14	5	37	9584
3.	28	000469-38-5	101816	91	81	2	81	37	8	8	25	9618
4.	28	000142-50-7	129864	40	96	2	84	40	8	5	25	9302
5.*	25	000106-24-1	124204	50	49	2	70	64	7	0	44	8396
6.	25	035117-86-3	28348	33	106	3	92	44	7	0	22	9201
7.	23	033281-91-3	28351	33	106	2	70	42	6	0	18	9328
8.	17	053755-13-8	99863	34	162	3	47	53	3	0	20	8684
9.	10	064960-69-6	99438	50	76	2	99	64	1	4	26	8098
10.	10	002847-30-5	120355	35	80	2	92	65	1	0	21	4849
11.	10	071271-24-4	35534	41	69	2	72	64	1	0	29	8319
12.*	8	014210-20-9	8251	28	70	1	52	70	1	0	29	4540
13.	7	035060-26-5	101808	33	171	2	60	77	1	0	21	7483
14.	7	056143-37-4	99864	41	151	2	30	74	1	0	24	4843
15.	6	056052-97-2	104522	54	125	1	45	70	1	0	17	9446

CTMP Compounds

Peak 82; Unidentified triterpene



Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	5887	55.95	351	67.00	1802	80.00	294
46.00	3	57.00	3305	68.05	267	81.00	2579
48.50	10	58.00	186	69.00	2104	82.05	361
48.75	14	59.00	83	70.05	217	83.05	951
49.00	6	60.05	25	71.05	1279	84.00	139
49.55	3	61.00	8	71.95	18	85.05	1102
50.00	23	62.05	6	72.15	64	86.05	78
50.90	46	62.80	45	75.95	31	87.00	17
52.95	414	63.50	3	76.95	642	88.15	4
53.95	45	64.95	227	78.00	172	88.95	12
54.95	3789	66.00	121	79.00	1969	89.90	31

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
91.00	2255	100.95	17	112.05	83	123.15	648
92.00	469	102.30	6	113.05	52	124.05	363
93.00	2041	103.00	121	114.00	5	125.10	371
94.05	547	104.00	141	115.05	196	126.05	49
95.05	2406	105.00	2359	115.95	113	126.50	11
96.00	299	106.00	583	116.95	714	127.10	54
97.00	755	107.05	2492	118.00	420	128.10	269
98.05	45	108.05	625	119.00	1545	129.05	441
99.10	182	109.05	1201	120.00	1004	130.00	235
99.75	8	110.05	259	121.05	1187	131.05	1022
100.10	30	111.10	523	122.05	356	132.00	350

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	1317	144.05	321	154.05	24	165.05	114
134.05	443	145.10	1702	155.05	84	165.80	7
135.05	1021	146.05	410	156.05	75	166.10	19
136.10	335	147.05	985	157.05	472	167.05	19
137.05	405	148.05	319	158.05	496	167.95	9
138.10	120	149.15	622	159.05	1115	168.20	57
139.10	68	150.10	134	160.05	721	169.05	76
140.30	21	151.10	215	161.05	1105	170.00	22
141.05	141	152.05	78	162.10	301	170.20	41
142.10	105	152.65	8	163.10	948	171.05	404
143.00	711	153.20	95	164.10	168	172.10	159

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.15	609	182.05	10	192.15	91	201.20	208
174.10	214	183.10	51	193.10	65	202.15	70
175.10	299	183.95	22	194.30	28	202.50	7
176.10	109	185.10	328	195.30	15	203.20	146
177.10	267	186.05	180	195.85	2	204.20	42
178.15	595	187.10	347	196.15	14	205.25	210
179.15	155	188.05	32	196.40	12	206.10	9
180.15	23	188.20	58	197.15	111	210.25	26
180.40	14	189.10	206	198.15	59	211.05	59
180.65	1	190.15	72	199.15	414	212.25	20
181.10	20	191.05	274	200.20	146	213.20	1005

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
214.20	288	222.50	11	231.20	579	239.15	50
215.20	223	222.70	2	232.20	208	240.25	23
216.20	59	223.25	50	233.25	106	240.65	2
217.20	133	224.80	5	234.30	126	241.20	97
218.20	216	225.15	44	235.25	25	242.15	16
219.25	151	226.15	15	235.45	25	242.55	9
219.80	14	227.20	140	236.55	11	243.15	43
220.20	29	227.40	27	236.95	1	243.80	6
220.45	3	228.15	184	237.85	1	244.20	7
221.25	114	229.20	290	238.15	3	244.45	5
222.20	6	230.20	102	238.45	3	245.25	92

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
246.25	66	255.20	634	261.25	63	268.75	7
247.25	93	256.20	160	262.50	5	269.25	23
248.10	50	257.15	98	263.00	4	270.45	9
248.45	46	258.05	4	263.20	4	271.20	39
248.70	14	258.30	8	263.50	3	272.20	75
249.15	10	258.65	5	263.75	2	273.25	579
251.10	14	259.15	39	264.00	4	274.05	24
252.10	3	259.95	5	265.20	4	274.30	185
253.15	30	260.20	25	267.20	30	275.35	223
254.10	2	260.50	9	268.20	7	276.20	48
254.40	4	261.05	2	268.45	2	276.45	7

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
276.95	5	287.30	38	292.25	1	300.15	9
277.20	11	287.70	4	295.40	9	300.35	9
277.55	3	288.30	58	295.85	4	301.05	10
279.25	1	288.65	9	296.60	2	301.30	45
281.15	176	289.15	27	297.10	14	302.35	278
282.05	18	289.50	56	297.40	15	303.30	874
283.10	41	290.00	9	297.70	3	304.35	219
284.25	11	290.20	24	298.10	7	305.35	20
284.40	5	290.50	25	298.50	5	306.75	2
285.15	14	290.75	5	298.75	5	307.25	3
286.20	9	291.50	11	299.40	16	309.25	2

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
309.60	1	316.25	40	328.25	45	340.15	1
310.20	11	317.25	11	329.40	988	340.40	10
310.45	2	318.00	3	330.35	246	341.20	16

310.80	9	319.95	5	331.60	9	341.40	10
311.25	13	322.45	2	332.30	3	341.65	9
312.30	13	322.95	3	332.90	3	342.00	3
313.30	8	324.30	3	333.50	2	342.25	44
314.40	78	325.30	32	337.70	4	342.70	18
315.10	22	325.80	3	338.00	2	342.95	7
315.35	40	326.70	4	339.15	11	343.25	24
316.05	1	327.25	70	339.40	8	344.35	5

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
344.95	1	354.90	38	359.00	5	370.15	2
345.45	7	355.25	57	359.55	4	370.50	12
346.30	4	355.50	26	360.40	3	370.90	5
346.50	12	355.90	11	360.65	3	371.35	29
348.50	1	356.25	2	363.35	4	372.50	2
352.20	2	356.45	9	365.40	6	372.90	3
353.25	11	357.25	28	367.30	21	376.05	2
353.50	16	357.50	27	367.65	15	376.45	2
353.75	18	357.75	9	368.35	18	378.35	2
354.20	11	358.40	14	368.95	7	379.25	9
354.55	92	358.75	12	369.40	8	379.90	1

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
380.40	7	389.70	2	399.55	469	406.55	4
381.50	459	390.40	4	400.55	157	406.90	6
382.50	137	390.65	2	401.35	3	407.40	22
383.40	3	391.50	7	401.70	5	408.50	10
384.25	2	392.70	6	401.95	4	408.90	2
384.55	2	395.00	4	402.65	2	409.50	7
384.85	2	395.40	18	404.30	2	409.85	4
385.30	17	396.55	726	404.65	1	410.25	1
386.20	5	397.45	58	405.10	7	410.60	6
386.50	6	397.65	171	405.45	2	411.85	2
386.95	6	398.45	12	405.75	6	412.65	16

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
412.90	12						
414.50	2033						
415.50	653						
416.65	104						
417.45	12						
417.75	1						
418.40	5						
418.70	6						

CTMP Compounds

Average of 45.465 to 45.582 min.: A1821.D
Converted from RTE data file: >A1821:

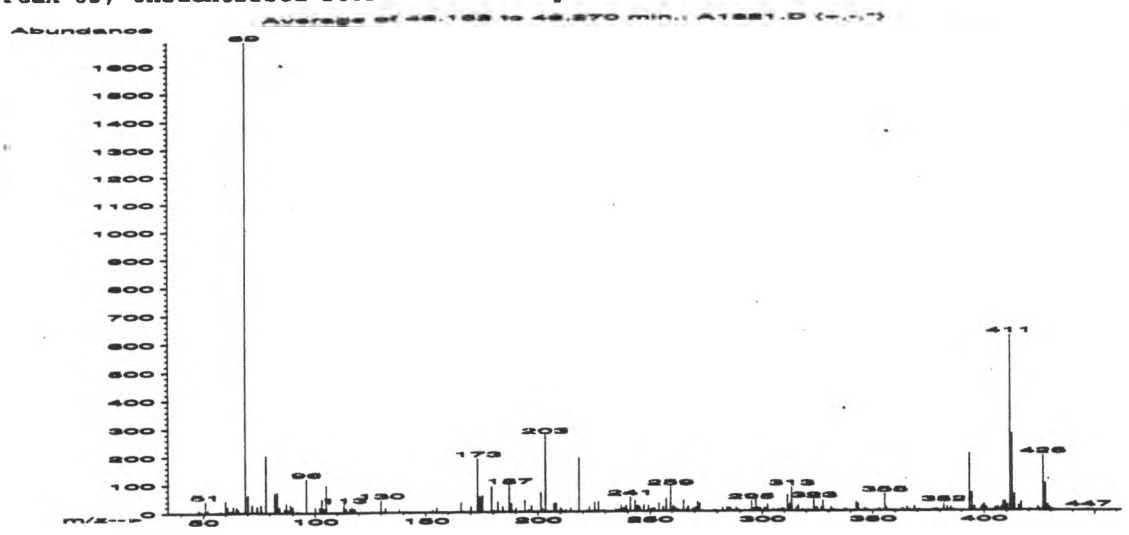
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	24.XI.-ETHYLCHOLEST-5-EN-3.BETA.-OL	414	C29H50O	91
2.	Stigmast-5-en-3-ol, (3.beta.,24S)-	414	C29H50O	91
3.	Stigmast-5-en-3-ol, (3.beta.,24S)-	414	C29H50O	87
4.	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	60
5.	ERGOST-5-EN-3.BETA.-OL	400	C28H48O	52
6.	Cholest-7-en-3-ol, 4,4-dimethyl-, (3.bet	414	C29H50O	51
7.	Ergosta-5,7-dien-3-ol, (3.beta.)-	398	C28H46O	32
8.	Ergostane-3,12-diol, (3.alpha.,5.beta.,1	418	C28H50O2	32
9.	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	25
10.	A-Norcholestan-3-one, 5-ethenyl-, (5.bet	398	C28H46O	22
11.	24-Oxo-24-homocholesterol	414	C28H46O2	15
12.	Stigmastan-7-one	414	C29H50O	14
13.	Stigmast-5-en-3-ol, (3.beta.)-	414	C29H50O	12
14.	(20S)-6.beta.-Methoxy-3.alpha.,5-cyclo-5	400	C28H48O	12
15.	Benzene, 1,3,5-tris(2,2-dimethylpropyl)-	414	C21H35I	10
16.	Ergost-22-en-3-ol, (3.alpha.,5.beta.,22E	400	C28H48O	10
17.	Ergosta-5,24(28)-dien-3-ol, (3.beta.)-	398	C28H46O	10
18.	KAUREN-19-YL-ACETATE	330	C22H34O2	10
19.	Benzofuran, 7-(2,4-dinitrophenoxy)-2,3-d	388	C19H20N2O7	10
20.	Cholestan-2,3-dione-2-oxime	415	C27H45NO2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	019044-06-5	100201	129	57	3	99	15	62	26	86	8651
2.	*91	000083-47-6	136254	144	53	1	92	5	60	7	60	9730
3.	*87	000083-47-6	100193	139	58	2	88	10	54	7	60	9918
4.	*60	026047-31-4	97994	77	75	3	91	40	35	47	68	8401
5.	52	000000-00-0	98006	86	106	2	84	31	27	0	45	8436
6.	*51	006384-28-7	100204	94	65	2	93	63	26	68	90	7176
7.	32	000516-79-0	97590	52	107	3	115	47	9	13	32	8284
8.	32	056052-70-1	100875	46	134	3	118	50	9	0	35	7905
9.	25	004651-51-8	97973	77	128	0	55	63	7	0	45	8438
10.	22	019594-90-2	97586	61	113	2	47	63	5	0	39	7539
11.	*15	083511-95-9	100184	62	76	1	41	76	2	0	51	4965
12.	*14	055331-88-9	100197	44	120	2	37	69	2	0	40	7588
13.	12	000083-46-5	100190	39	122	0	22	64	2	0	33	9412
14.	12	084985-77-3	98011	42	107	2	87	63	2	5	34	7742
15.	*10	025347-04-0	99985	40	114	3	126	80	1	0	39	4911
16.	10	055527-92-9	97982	53	90	2	38	78	1	22	39	6939
17.	*10	000474-63-5	97582	48	99	2	47	67	1	1	35	7182
18.	*10	000000-00-0	83050	52	113	3	87	63	1	6	28	7785
19.	10	062059-48-7	95700	44	113	3	83	77	1	0	39	5606
20.	* 9	006901-58-2	100309	40	80	3	92	73	1	15	37	4232

CTMP Compounds

Peak 83; Unidentified Sterol or Triterpene



Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.60	3	62.40	5	76.20	2	92.00	3
47.95	11	62.85	1	78.05	204	96.05	120
48.85	4	63.65	23	82.05	68	100.15	18
50.20	4	63.95	3	83.05	71	102.15	17
50.90	42	65.00	18	84.00	18	102.95	47
52.00	11	65.75	11	86.30	11	103.95	15
58.00	5	69.00	1686	87.05	33	105.00	95
60.00	42	70.05	62	88.20	9	113.20	28
60.85	22	72.00	27	88.95	26	114.05	14
61.85	1	74.20	22	89.70	2	115.95	13
62.15	5	75.85	27	89.90	19	117.00	17

Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.05	12	168.50	2	187.10	93	210.15	14
126.10	3	170.20	19	188.15	28	210.50	6
130.00	44	173.10	191	190.10	12	212.30	5
132.05	15	174.10	55	194.15	40	214.55	12
138.10	10	175.15	57	196.00	8	218.25	192
141.05	3	179.20	91	197.10	20	221.80	6
153.05	10	180.40	3	201.25	68	222.90	16
154.95	16	181.10	1	202.00	10	224.15	3
157.05	2	181.75	2	203.25	273	225.15	33
165.80	34	182.05	35	207.15	28	225.65	4
166.70	3	184.20	18	208.10	31	227.00	34

Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
228.20	2	239.00	7	249.50	3	259.25	86
229.25	7	239.20	20	249.85	1	260.40	17
234.50	7	239.80	4	250.15	4	260.75	2
234.70	9	241.20	51	250.55	5	261.25	14
235.65	4	243.20	37	250.80	9	262.25	7
236.00	4	244.40	20	251.35	9	262.90	4
236.25	4	245.00	17	252.20	10	264.05	2
236.50	7	245.45	11	254.10	27	265.05	39
237.10	22	247.30	22	255.95	16	266.70	9
238.15	10	248.65	3	257.20	45	267.05	17
238.45	10	249.20	20	258.40	3	267.30	12

Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
269.15	10	286.25	6	297.15	55	307.50	3
269.80	6	287.70	3	297.80	12	307.90	2
270.30	13	288.35	13	298.30	4	308.20	2
271.25	33	289.25	3	298.95	11	309.20	9
272.20	26	289.40	4	299.25	7	310.05	6
278.25	3	291.95	2	301.00	11	311.40	55
279.20	4	294.30	5	301.85	8	312.40	24
282.25	14	295.20	35	302.45	24	313.00	18
284.25	13	295.45	10	304.95	2	313.30	84
284.45	12	296.05	1	305.25	5	315.50	11
285.50	12	296.30	9	307.25	3	316.35	19

Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
318.00	3	327.50	36	343.35	24	363.25	8
318.40	2	331.30	12	343.90	3	363.55	5
318.65	2	331.50	9	346.30	9	365.40	12
320.20	3	331.80	2	347.45	5	366.75	5
321.20	2	332.75	3	351.45	2	368.65	16
321.70	2	334.90	1	352.25	4	370.20	1
323.45	40	337.30	4	353.25	7	371.00	4
323.80	3	337.60	7	355.35	60	376.20	2
324.20	10	338.40	4	355.70	5	377.00	6
324.95	12	339.90	2	356.05	12	377.55	3
326.80	12	342.45	30	358.20	2	378.35	7

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
379.05	3	395.85	15	407.85	14	416.70	30
379.75	3	398.75	8	408.55	32	420.45	4
381.25	3	399.00	14	408.85	14	421.90	1
381.90	25	399.70	22	409.50	32	423.90	3
383.50	14	400.20	22	409.70	5	424.20	14
384.55	3	401.00	11	410.30	19	424.95	5
385.10	12	403.95	2	411.55	622	426.60	197
386.05	2	404.80	4	412.55	273	427.50	95
386.50	2	405.20	11	413.60	59	428.70	21
393.50	205	406.30	12	415.65	17	429.60	10
394.70	64	407.50	6	416.10	13	430.10	1

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
430.95	4						
431.20	2						
447.25	6						
448.90	2						

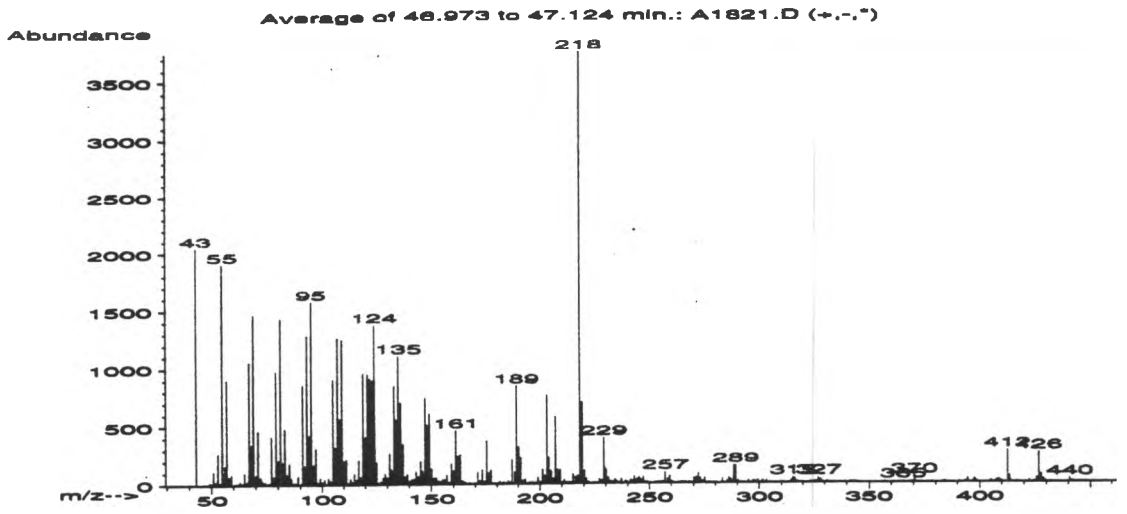
Average of 46.152 to 46.270 min.: A1821.D
Converted from RTE data file: >A1821:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,3-Dioxane, 2,2,4,5-tetramethyl-6-(1-me	410	C27H54O2	45
2.	(25.xi.)-26,26-Dimethyl-5,23-ergostadien	426	C30H50O	40
3.	9,19-Cyclolanost-24-en-3-ol, (3.beta.)-	426	C30H50O	36
4.	Lup-20(29)-en-3-ol, (3.beta.)-	426	C30H50O	33
5.	1,3-Benzenediol, 5-methyl-2-(3,7,11-trim	412	C26H36O4	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*45	056324-82-4	99474	43	100	1	68	25	19	6	33	9602
2.	*40	090195-41-8	101836	35	142	1	68	35	16	0	35	9291
3.	*36	000469-38-5	101816	32	187	3	89	28	12	0	29	9623
4.	*33	000545-47-1	101799	30	159	2	83	32	10	0	29	9375
5.	*28	052104-23-1	99753	29	150	2	99	38	8	0	26	9267

CTMP Compounds



Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2047	54.00	15	65.00	100	75.55	5
46.50	3	54.95	1904	65.95	5	76.05	7
47.75	3	56.00	161	66.20	23	76.95	410
48.00	2	57.00	904	67.00	1057	78.00	69
48.55	3	57.90	64	68.00	341	79.05	974
49.00	15	59.00	87	69.00	1464	80.05	208
49.25	16	61.20	5	70.05	82	81.05	1428
50.25	11	62.35	10	71.05	461	82.05	192
50.95	113	62.90	24	72.10	60	83.05	478
51.95	25	63.40	2	73.00	25	84.05	86
52.95	272	64.00	8	74.25	16	85.05	177

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
86.00	49	97.05	308	108.05	562	119.05	958
87.20	13	98.05	16	109.05	1247	120.05	409
88.25	11	99.05	51	110.00	197	121.05	949
88.95	71	100.15	18	111.05	212	122.10	910
90.15	3	100.40	6	112.00	12	123.10	897
91.00	854	101.10	41	113.00	47	124.10	1373
92.00	159	102.95	48	114.05	19	125.10	190
93.00	1287	104.00	31	115.00	93	126.05	14
94.00	422	105.05	908	116.00	41	127.10	21
95.00	1571	106.00	321	117.00	210	128.05	55
96.00	166	107.05	1264	118.00	62	129.05	91

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.00	61	141.05	42	152.15	56	161.10	463
131.00	267	142.10	46	153.10	23	162.15	244
132.00	129	143.00	109	153.65	7	163.10	255
133.05	847	144.05	70	154.20	20	164.10	31
134.05	555	145.05	201	155.10	41	165.05	17
135.05	1106	146.05	117	156.10	43	165.75	9
136.10	699	147.10	744	157.05	81	167.20	11
137.05	343	148.10	513	157.80	15	168.00	2
138.05	65	149.05	608	158.05	10	170.00	6
139.10	87	150.10	132	159.05	177	171.05	102
140.10	24	151.05	54	160.05	119	172.10	30

Average of 46.973 to 47.124 min.: A1821.D

Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.10	122	183.10	14	193.10	38	203.25	763
174.10	20	184.05	3	194.55	3	204.15	225
175.15	372	185.10	24	195.30	10	205.20	115
176.10	94	186.05	14	195.95	2	206.20	43
177.05	120	187.05	206	196.30	8	207.15	576
178.10	2	188.25	103	197.05	7	208.15	122
179.05	8	189.15	847	198.15	10	209.20	120
180.10	2	190.20	319	199.10	54	210.15	10
180.75	4	191.10	227	200.15	13	211.15	32
181.10	18	192.10	28	201.25	121	212.20	10
182.10	6	192.45	8	202.20	72	212.45	8

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
212.70	5	221.20	44	230.25	117	236.45	2
213.20	14	222.25	16	231.20	51	237.25	39
214.15	8	223.75	1	232.15	7	239.00	22
214.45	6	224.10	1	232.45	19	239.70	5
215.15	83	224.40	3	233.20	5	240.00	11
216.30	57	225.15	11	233.50	10	241.40	29
217.25	73	226.55	1	233.75	6	242.10	21
218.25	3745	227.20	38	234.25	32	243.15	61
219.30	703	228.10	26	234.50	11	243.65	4
220.25	114	229.20	395	235.10	12	244.30	40
220.70	10	230.00	12	235.75	5	245.30	56

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
245.70	3	254.50	3	264.20	6	272.25	89
246.10	35	255.20	9	264.65	15	273.15	44
247.20	59	256.15	19	265.20	7	274.10	18
248.15	10	257.20	98	266.15	9	275.25	47
248.45	2	258.35	39	267.75	6	276.45	4
248.80	6	259.25	64	268.05	4	276.70	1
249.10	12	259.50	4	268.30	6	277.00	1
250.45	2	260.25	16	268.70	7	277.25	7
251.90	3	261.20	3	270.20	50	277.95	2
253.10	13	263.40	2	271.15	43	279.20	1
254.25	13	263.95	1	271.35	51	280.05	5

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
283.25	40	291.75	2	298.70	2	307.15	2
284.20	3	292.65	1	299.35	27	307.50	1
285.25	21	292.95	4	300.45	5	308.40	1
285.75	1	293.45	1	300.70	2	309.15	4
286.20	49	295.00	23	301.40	24	310.20	8
287.20	34	295.75	7	301.75	4	310.65	4
287.40	10	296.15	1	302.15	8	310.95	4
288.40	153	296.90	7	303.35	22	312.40	1
289.30	153	297.25	22	304.60	2	312.70	3
290.20	18	297.45	8	305.00	3	313.00	2
290.50	15	298.15	17	305.75	2	313.60	7

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
314.15	4	318.20	5	325.50	9	331.15	16
314.55	31	319.40	4	325.80	1	331.95	2
315.25	48	319.85	2	326.05	8	332.50	4
315.45	21	321.25	6	326.50	7	333.25	1

CTMP Compounds

315.70	12	321.55	3	326.80	15	334.00	1
316.20	42	322.25	2	327.25	46	334.50	1
316.45	16	322.70	2	327.75	6	337.00	1
316.75	4	323.25	10	328.15	29	337.25	3
317.00	4	323.50	6	328.45	18	338.00	5
317.25	7	324.70	6	329.05	6	338.40	2
317.70	5	325.25	10	330.30	3	339.40	8

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
339.75	7	349.30	1	363.20	1	370.35	54
341.40	13	351.05	2	363.50	2	370.55	36
341.85	8	352.95	1	364.50	4	370.95	9
342.20	6	355.55	3	365.30	12	371.15	5
342.45	5	356.15	5	365.50	5	371.50	4
342.65	11	356.45	4	365.85	2	372.00	2
343.60	11	357.25	8	367.25	1	372.70	1
343.90	3	358.15	2	367.50	1	376.30	2
344.65	5	360.75	2	367.90	5	376.85	4
344.95	2	361.65	1	368.80	10	377.30	5
345.45	5	362.15	2	369.45	7	378.10	1

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
382.90	2	396.00	7	404.30	3	412.50	277
383.40	9	397.05	19	405.00	15	413.50	59
384.00	9	397.30	20	405.35	9	413.75	23
384.40	6	397.65	34	406.60	6	416.50	6
386.05	2	398.30	19	407.35	11	416.75	5
390.75	6	398.65	11	407.65	26	417.75	4
391.15	2	399.70	1	408.25	15	418.30	1
393.25	10	400.30	2	408.70	26	420.00	1
393.70	15	401.20	1	408.95	2	420.50	1
394.55	37	403.15	3	409.65	13	420.75	4
395.75	4	404.05	2	409.90	7	422.45	18

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
424.00	2	430.15	3	446.80	4		
424.25	4	430.45	1	447.35	1		
424.55	3	430.75	3	447.75	1		
425.25	3	430.95	1	448.65	1		
425.55	40	431.45	2				
425.75	22	435.45	3				
426.60	261	440.60	32				
427.30	19	441.55	10				
427.60	73	442.50	2				
428.70	30	444.40	1				
429.20	13	445.90	2				

CTMP Compounds

Average of 46.973 to 47.124 min.: A1821.D
Converted from RTE data file: >A1821:

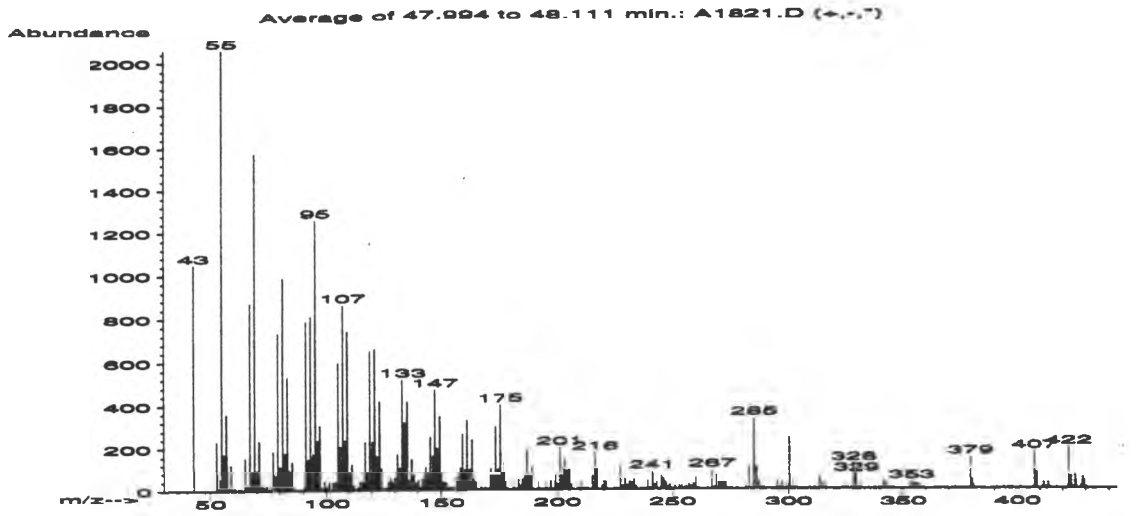
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Viminalol	426	C30H50O	99
2.	.beta.-Amyrin	426	C30H50O	70
3.	2,2-Dimethyl-6-(prop-2-enyl)benzofuran-4	218	C13H14O3	64
4.	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	55
5.	Viminalol	426	C30H50O	55
6.	1,2,3,3a,5,6,6a,7-Octahydro-1,3a,6-trime	218	C15H22O	47
7.	2,6-Diisopropylidene-3-methyl-3-vinylcyc	218	C15H22O	46
8.	(13S)-8a,13:13,20-Diepoxy-5.beta.,9.beta	278	C18H30O2	46
9.	(E)-2-Methyl-4-(2',6',6'-trimethyl-3'-me	218	C15H22O	43
10.	Aristolone	218	C15H22O	41
11.	(4R,4aS,6S)-6-Isopropenyl-4,4a-dimethyl-	218	C15H22O	41
12.	3.BETA.-HYDROXY-16-OXO-12-EN-28-NOROLEAN	426	C29H46O2	38
13.	2,3-Dihydroxanthotoxin	218	C12H10O4	35
14.	4,5'-Bipyrimidine, 4',6-dimethoxy-	218	C10H10N4O2	30
15.	1,4-Naphthalenedione, 5,8-dihydroxy-2,3-	218	C12H10O4	30
16.	4-HYDROXY-6-(P-METHOXYPHENYL)-3-PYRIDAZO	218	C11H10N2O3	30
17.	3-p-Anisyl-2-hydroxycyclohex-2-en-1-one	218	C13H14O3	27
18.	Naphthalene, 1-(phenylmethyl)-	218	C17H14	27
19.	cis-2-(4-Methoxyphenyl)-4-methylcyclohex	218	C14H18O2	25
20.	2,1,3-Benzothiadiazole, 5,7-dichloro-4-m	218	C7H4Cl2N2S	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*99	000638-95-9	101805	142	34	0	76	26	80	23	99	8782
2.	*70	000559-70-6	101804	96	80	1	81	30	41	22	78	8762
3.	*64	087386-32-1	42807	78	62	2	82	32	37	48	72	8617
4.	*55	000243-42-5	43062	86	41	3	82	44	29	33	72	8412
5.	*55	000638-95-9	136390	86	81	2	73	44	29	16	72	8384
6.	*47	071583-68-1	43034	53	29	2	85	36	20	10	40	7748
7.	*46	069366-06-9	42971	49	79	3	90	44	20	0	44	7570
8.	46	067010-57-5	66519	79	112	2	56	44	20	0	43	9083
9.	*43	077822-46-9	42989	76	84	3	73	46	18	30	50	8208
10.	*41	006831-17-0	129615	81	61	1	77	51	16	26	58	8001
11.	*41	053768-26-6	43013	68	62	3	99	52	16	32	58	7898
12.	*38	071545-19-2	101771	56	117	2	66	53	14	0	47	8417
13.	*35	000000-00-0	42715	45	73	2	98	55	11	0	40	8233
14.	*30	059549-37-0	42609	48	96	3	99	56	9	0	46	8382
15.	*30	021418-10-0	42705	48	82	3	99	60	9	0	44	8268
16.	*30	058884-19-8	42652	47	70	0	99	56	9	0	44	8243
17.	*27	070871-47-5	42801	43	30	2	99	60	8	0	40	8070
18.	*27	000611-45-0	43091	44	111	3	99	60	8	0	40	7918
19.	*25	084736-51-6	42891	37	72	0	68	63	7	8	43	7354
20.	*25	002160-26-1	42491	37	102	3	99	62	7	13	43	8128

CTMP Compounds

Peak 85; Unidentified Triterpenes Unresolved



Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1047	60.20	11	70.05	95	83.05	531
47.20	7	60.55	10	71.00	235	84.05	95
50.00	4	61.75	4	72.15	19	85.05	135
50.55	10	62.50	12	73.00	14	86.45	9
52.95	231	62.95	20	74.15	21	90.15	15
54.00	54	63.95	2	76.95	187	91.00	784
54.95	2058	64.95	155	78.00	69	92.00	147
56.00	173	66.00	25	79.00	734	93.00	810
56.95	359	67.00	868	80.00	115	94.05	173
58.20	13	68.05	92	81.00	986	95.05	1258
58.95	122	69.00	1572	82.05	176	96.00	235

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.05	304	106.00	207	116.00	37	126.25	9
98.00	10	107.05	861	117.00	228	126.50	6
99.15	44	108.05	236	117.95	80	127.20	37
100.00	18	109.05	739	119.00	649	128.05	56
100.45	1	110.00	80	120.05	230	129.10	34
101.15	39	111.10	123	121.05	659	129.95	56
102.95	36	112.10	21	122.10	162	131.05	170
103.55	11	113.05	1	123.15	420	132.00	107
103.80	39	113.30	5	124.10	102	133.05	518
104.00	17	114.05	15	125.10	12	134.00	319
105.00	597	115.00	43	126.05	4	135.05	417

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.10	43	145.00	252	153.65	5	163.95	49
137.05	146	146.10	162	154.25	17	164.30	10
138.15	73	147.05	472	155.05	13	165.05	35
139.10	29	148.05	199	156.10	12	167.10	15
139.80	4	149.10	347	157.00	63	167.80	6
140.10	46	150.05	75	158.10	105	168.05	4
140.80	13	151.10	37	159.05	266	169.15	9
141.55	1	152.20	35	160.10	97	169.55	3
142.00	55	152.65	12	161.05	329	170.05	5
143.05	110	153.00	5	162.10	98	171.10	103
144.00	78	153.25	6	163.05	238	172.10	68

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.10	299	186.10	63	197.10	46	210.20	30
174.10	98	187.10	186	197.95	5	211.00	2
175.20	400	188.05	62	199.15	69	211.20	18
176.15	76	189.15	105	200.05	27	211.55	2
177.05	131	191.75	4	201.15	197	211.80	7
178.10	33	192.10	37	202.20	66	212.05	11
181.15	28	193.05	2	203.20	144	213.20	5
181.80	3	194.00	7	204.20	91	215.25	68
183.25	49	195.25	26	205.25	103	216.25	171
184.00	19	195.80	4	206.20	23	217.25	100
185.10	48	196.15	2	209.10	19	219.45	19

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
220.20	41	231.25	37	240.95	10	248.30	17
220.55	11	232.20	34	241.20	83	248.45	7
220.80	12	233.30	52	242.15	23	248.80	5
221.20	35	233.90	14	242.45	4	249.10	22
224.10	4	234.20	8	243.30	35	250.10	5
225.10	5	236.25	4	245.05	13	251.20	17
227.20	115	237.15	4	245.25	67	253.05	17
228.15	17	237.95	5	246.30	48	254.00	3
229.20	62	238.60	5	246.80	7	254.15	15
230.30	22	239.25	43	247.15	34	255.15	8
230.65	3	240.20	5	247.75	5	256.10	14

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
256.70	7	261.75	5	270.20	33	277.45	4
257.15	24	262.15	3	270.65	3	277.80	8
257.40	8	262.40	3	271.25	34	278.10	6
257.65	5	263.25	4	271.55	8	281.75	19
258.05	9	263.65	2	272.30	33	283.15	104
258.35	16	265.00	6	272.80	5	285.25	332
258.65	3	265.20	10	273.15	30	286.25	102
259.15	31	267.15	89	273.55	4	287.30	34
260.25	58	268.10	6	274.45	4	288.45	9
261.00	1	268.40	10	274.75	6	288.75	2
261.25	5	269.10	67	275.80	4	289.05	1

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
289.25	6	297.25	33	305.35	3	314.95	22
289.55	5	297.95	4	306.05	4	315.25	29
290.15	4	298.40	1	306.50	1	316.05	5
290.65	2	299.25	21	306.90	3	316.25	5
291.30	1	299.50	11	307.25	2	317.75	2
292.55	1	300.25	242	308.50	3	319.10	2
292.80	3	301.15	6	309.25	9	319.30	4
295.00	21	301.40	57	311.10	6	319.80	3
295.25	39	302.05	2	311.35	14	320.20	4
296.25	6	302.35	6	313.30	62	322.15	1
297.00	15	303.30	14	314.45	20	323.10	12

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
323.40	6	331.05	24	341.30	43	352.05	3
323.70	2	334.85	7	341.65	22	353.20	22
324.15	11	337.15	7	342.35	31	353.55	33

CTMP Compounds

324.65	1	337.40	2	342.70	25	354.60	23
325.20	25	337.65	3	342.95	9	355.30	26
325.45	4	338.00	5	343.65	1	355.50	16
326.55	3	339.25	5	344.45	11	356.30	23
327.15	7	339.70	1	344.70	10	357.30	19
328.30	119	340.00	2	345.85	8	357.60	9
329.35	68	340.30	14	347.20	3	358.35	9
330.75	2	340.65	1	350.80	2	358.75	4

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
359.10	6	373.55	1	384.90	1	392.25	2
364.75	3	376.05	3	385.40	1	392.95	2
366.00	3	376.50	3	385.70	3	393.25	3
367.15	3	377.15	3	387.50	2	393.50	4
367.40	2	378.70	3	387.95	1	393.95	6
367.95	5	379.50	148	388.65	3	395.05	5
368.95	9	380.40	42	389.25	3	395.75	4
370.50	2	380.70	18	390.00	6	396.55	21
371.10	4	381.00	7	390.75	2	397.15	5
372.80	10	381.25	8	391.15	5	397.45	13
373.15	3	383.55	1	391.90	1	398.00	5

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
398.35	2	408.50	76	418.25	2	428.50	37
399.40	3	410.75	6	421.25	3	428.75	55
400.50	1	411.50	29	422.25	17	429.20	1
400.85	4	412.20	3	422.55	193	429.45	36
401.25	8	412.55	6	423.40	14	429.70	5
401.45	2	413.20	3	423.65	58	430.05	1
404.05	2	413.50	29	424.10	11	430.40	6
404.55	4	413.75	2	425.40	65	430.70	4
405.35	1	414.15	3	425.70	37		
406.55	3	414.50	7	425.95	14		
407.50	173	417.35	7	427.85	14		

CTMP Compounds

Average of 47.994 to 48.111 min.: A1821.D
Converted from RTE data file: >A1821:

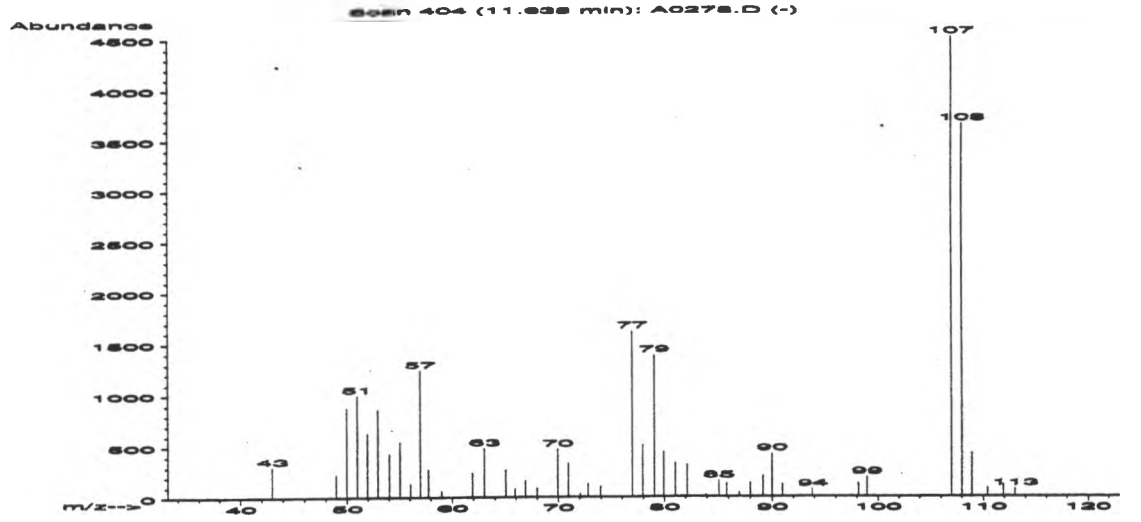
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cycloeucalenol	426	C30H50O	47
2.	Lupanol	428	C30H52O	43
3.	D:B-Friedo-18,19-secolup-19-ene, 3,10-ep	426	C30H50O	38
4.	9,19-Cyclolanost-24-en-3-ol, (3.beta.)-	426	C30H50O	38
5.	Epi-.psi.-Taraxastanonol	442	C30H50O2	37
6.	Bicyclo[2.2.1]heptan-2-ol, 3,3-dimethyl-	140	C9H16O	37
7.	.beta.-Serratan-3.alpha.-ol	428	C30H52O	32
8.	d-Nerolidol	222	C15H26O	32
9.	PERFLUORO-4-METHYLPENTENE-2	300	C6F12	27
10.	Bicyclo[5.1.0]octane, 8-(1-methylethylid	150	C11H18	25
11.	PERFLUORO-2,4 DIMETHYLBUTENE-1	300	C6F12	16
12.	4-ENDO,8-ENDO-DICHLORO-1,3,5,7-TETRAMETH	260	C12H14Cl2O2	12
13.	METHYL 2-HYDROXYDECANOATE	202	C11H22O3	12
14.	Gorgosterol	426	C30H50O	10
15.	D:A-Friedooleanane-1,24-diol	444	C30H52O2	10
16.	Trifluoroacetyl derivative of octopamine	441	C14H8F9NO5	10
17.	Cholest-7-en-3-ol, acetate, (3.beta.)-	428	C29H48O2	10
18.	24-Isopropyl-5,23-cholestadien-3.beta.-o	426	C30H50O	10
19.	.alpha.-Anomer of 3-azido-4,5-isopropyli	599	C36H61N3O4	9
20.	6-(2,5-DIHYDROXY-3-METHYLPHENYL)-1-[1,2-	426	C27H38O4	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	000469-39-6	101815	76	106	2	69	39	20	3	39	9644
2.	*43	003186-86-5	102144	58	35	0	63	45	18	12	43	8806
3.	38	035060-26-5	136392	55	157	3	76	25	14	0	22	9612
4.	38	000469-38-5	101816	80	101	2	65	36	14	6	35	9384
5.	37	000000-00-0	103861	94	96	2	52	42	13	16	36	6741
6.	37	000515-28-6	9414	44	90	3	83	45	13	0	34	7917
7.	*32	000000-00-0	102146	62	107	1	63	50	9	4	33	9634
8.	32	000142-50-7	129864	43	101	2	63	50	9	0	37	8721
9.	*27	000000-00-0	73633	37	90	2	53	59	8	0	39	7022
10.	25	054166-47-1	123743	41	93	3	93	45	7	0	27	8891
11.	*16	000000-00-0	73632	41	82	2	53	59	3	0	33	7022
12.	*12	061605-34-3	59490	43	48	1	70	63	2	0	35	6944
13.	12	071271-24-4	35534	42	69	2	76	62	2	0	33	7053
14.	10	029782-65-8	101786	49	164	3	83	65	1	0	22	6717
15.	10	056816-62-7	104086	78	51	1	47	71	1	15	39	5556
16.	10	000000-00-0	136548	38	114	3	76	63	1	0	27	6944
17.	10	017137-70-1	102096	42	163	3	110	63	1	0	29	6429
18.	10	090195-40-7	101834	45	82	2	77	63	1	7	27	7001
19.	9	084961-07-9	137305	46	96	2	48	75	1	0	34	7570
20.	* 9	097743-94-7	101750	33	86	1	41	77	1	12	36	8674

CTMP Compounds

Peak 86; 4-Methylphenol



Scan 404 (11.638 min): A0278.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	305	59.00	66	73.95	110	88.00	142
48.95	228	61.90	241	76.95	1620	89.15	211
49.95	879	63.00	488	77.95	512	90.00	427
50.95	997	65.00	274	79.05	1384	91.00	126
51.95	631	65.90	82	79.95	445	93.80	77
52.95	862	66.90	167	81.05	334	98.15	136
54.05	432	68.00	92	82.15	315	98.95	196
55.05	546	69.95	474	83.90	23	107.00	4503
56.05	139	70.95	337	85.10	164	108.00	3647
57.00	1242	72.05	35	85.80	136	108.90	425
57.75	276	72.80	133	87.00	47	110.40	90

Scan 404 (11.638 min): A0278.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.90	116						
113.00	80						

CTMP Compounds

Scan 404 (11.638 min): A0278.D

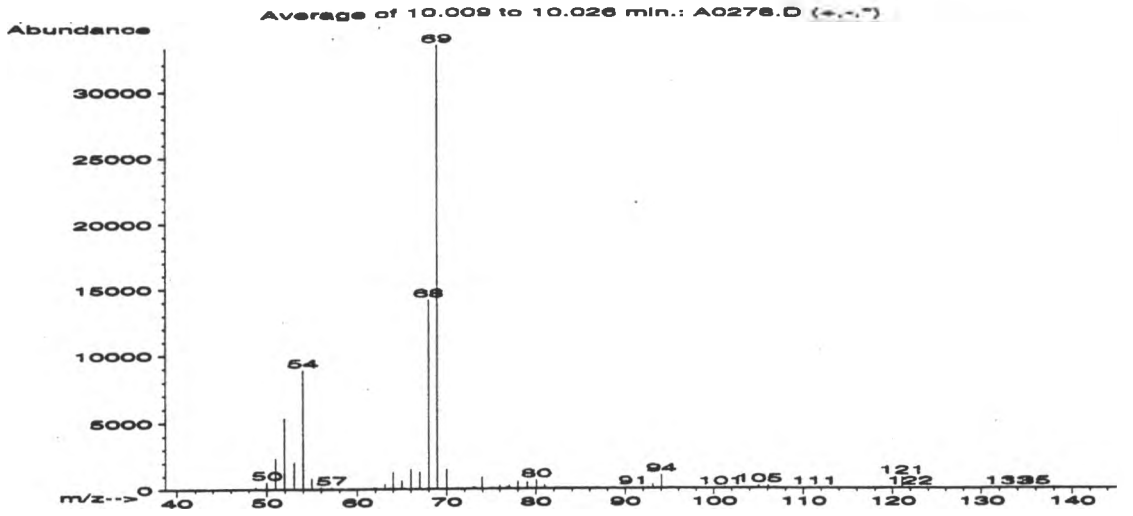
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-methyl-	108	C7H8O	97
2.	Phenol, 3-methyl-	108	C7H8O	95
3.	Phenol, 4-methyl-	108	C7H8O	95
4.	Phenol, 4-methyl-	108	C7H8O	95
5.	Phenol, 4-methyl-	108	C7H8O	94
6.	Phenol, 4-methyl-	108	C7H8O	91
7.	Phenol, 4-methyl-	108	C7H8O	83
8.	Phenol, 2-methyl-	108	C7H8O	68
9.	Phenol, 2-methyl-	108	C7H8O	68
10.	(E,E)-6-(Dimethylamino)-3-methyl-3,5-hex	153	C9H15NO	64
11.	Phenol, 3-methyl-	108	C7H8O	64
12.	Phenol, 2-methyl-	108	C7H8O	62
13.	BENZYLAMINE-.ALPHA.-D1	107	C7H8DN	59
14.	Phenol, 3-methyl-	108	C7H8O	59
15.	Benzenemethanol	108	C7H8O	58
16.	Phenol, 2-methyl-	108	C7H8O	52
17.	Pyrazine, ethyl-	108	C6H8N2	50
18.	Pyrazine, ethyl-	108	C6H8N2	50
19.	Pyridine, 3-ethyl-	107	C7H9N	46
20.	Pyridine, 4-ethyl-	107	C7H9N	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*97	000106-44-5	118730	99	10	1	77	0	78	46	95	9872
2.	*95	000108-39-4	118722	98	13	0	78	3	74	18	94	9804
3.	*95	000106-44-5	118731	99	10	1	87	0	74	18	94	9876
4.	*95	000106-44-5	118727	93	16	0	80	3	72	29	93	9911
5.	*94	000106-44-5	118729	92	16	1	77	0	70	44	83	9831
6.	*91	000106-44-5	118726	78	29	1	75	3	62	17	81	9913
7.	*83	000106-44-5	118728	60	44	1	93	12	50	0	56	9935
8.	*68	000095-48-7	118717	72	41	1	80	24	40	0	53	9619
9.	*68	000095-48-7	118715	70	41	1	80	24	40	0	53	9698
10.	64	075847-94-8	14069	57	0	0	80	18	37	2	41	9711
11.	*64	000108-39-4	118724	63	38	1	70	31	37	0	64	9701
12.	*62	000095-48-7	118716	64	47	1	80	27	36	0	58	9587
13.	*59	004397-68-6	1831	33	73	2	99	24	33	5	40	9719
14.	*59	000108-39-4	118721	47	59	1	80	24	33	0	40	9756
15.	*58	000100-51-6	118742	58	49	1	69	32	32	0	51	8878
16.	*52	000095-48-7	118719	48	62	2	73	32	27	0	46	9676
17.	*50	013925-00-3	118681	44	51	2	97	31	25	0	40	9199
18.	*50	013925-00-3	118680	46	57	1	72	34	25	0	39	9107
19.	*46	000536-78-7	118606	48	59	1	97	43	20	0	46	8241
20.	*43	000536-75-4	118610	43	68	2	78	44	18	0	40	8285

CTMP Compounds

Peak 87; PBM hit 2,2'Azobis[2-methyl-propanenitrile 74



Average of 10.009 to 10.026 min.: A0278.D
Converted from RTE data file: >A0278:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.75	147	62.15	72	73.20	78	82.15	59
50.00	549	63.10	396	73.95	887	83.40	29
50.95	2352	64.00	1326	74.95	118	85.50	48
51.95	5309	65.00	646	75.20	72	85.75	45
53.00	2059	66.00	1485	76.00	244	86.75	45
54.00	8865	67.00	1308	76.80	121	88.75	36
54.95	850	68.00	14156	77.05	255	90.90	74
55.95	183	68.95	33256	78.00	563	91.80	25
57.15	154	70.00	1494	79.00	526	92.00	51
60.90	23	71.00	23	80.05	636	93.10	302
61.90	116	72.95	144	80.95	265	94.05	1017

Average of 10.009 to 10.026 min.: A0278.D
Converted from RTE data file: >A0278:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
94.80	75	111.25	23				
95.20	113	113.30	10				
97.70	24	118.25	20				
98.40	3	118.95	34				
100.80	37	121.05	847				
101.30	31	121.95	37				
103.95	39	132.90	24				
105.00	218	135.00	40				
106.05	204						
106.75	50						
107.00	48						

CTMP Compounds

Average of 10.009 to 10.026 min.: A0278.D
Converted from RTE data file: >A0278:

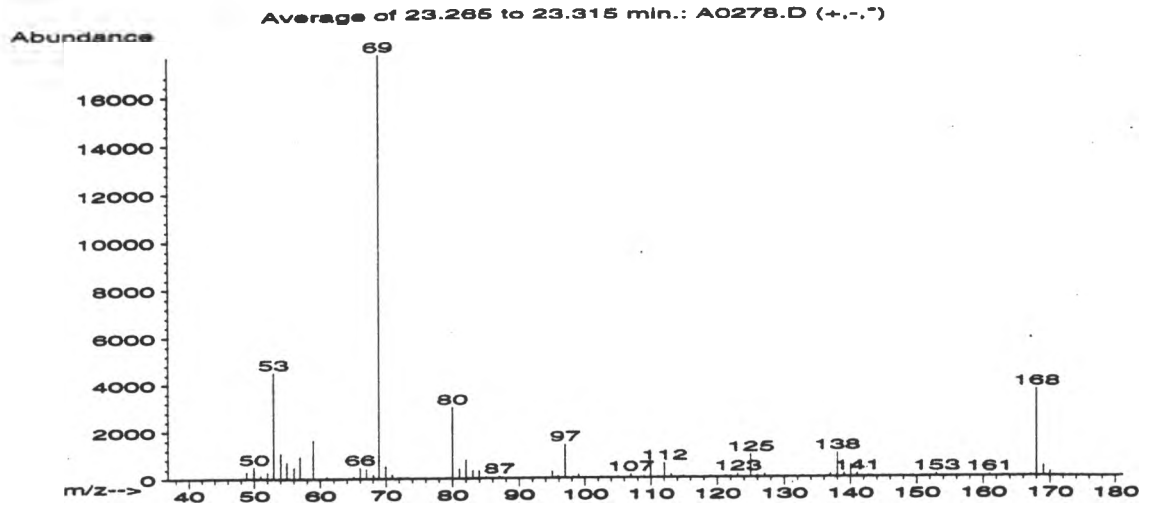
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Propanenitrile, 2,2'-azobis[2-methyl-	164	C8H12N4	74
2.	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	25
3.	3-Butyn-2-ol, 2-methyl-	84	C5H8O	23
4.	3-Butyn-2-ol, 2-methyl-	84	C5H8O	23

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	74	000078-67-1	18324	57	35	2	74	2	44	0	32	9940
2.	25	018476-57-8	8737	33	40	1	79	44	7	0	22	9248
3.	23	000115-19-5	116867	34	38	1	91	47	6	0	22	8891
4.	23	000115-19-5	116864	33	38	1	67	50	6	0	25	8849

CTMP Compounds

Peak 51; Unidentified Monoterpene Acid



Average of 23.265 to 23.315 min.: A0278.D
Converted from RTE data file: >A0278:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.80	32	58.95	1648	71.85	24	83.95	334
47.70	11	59.75	9	72.05	60	85.05	59
48.85	308	60.95	102	73.20	76	86.00	29
49.95	495	62.15	35	74.65	35	87.00	90
51.00	138	65.05	86	74.95	13	87.50	18
52.00	265	66.00	464	78.00	44	88.85	1
52.95	4508	67.00	409	79.05	35	89.25	28
54.00	1065	68.05	171	80.00	3009	92.00	14
54.95	717	68.95	17655	81.00	418	93.05	52
56.00	492	69.95	534	82.00	777	94.30	36
56.95	939	71.00	170	83.00	332	94.95	286

Average of 23.265 to 23.315 min.: A0278.D
Converted from RTE data file: >A0278:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.55	50	109.95	499	119.75	29	131.40	12
95.90	91	111.00	43	120.25	35	132.75	24
96.95	1423	112.05	606	121.20	54	132.95	27
98.20	62	113.05	123	121.55	43	135.00	18
99.00	154	114.25	18	122.00	57	135.25	49
101.95	11	114.50	18	123.05	138	135.65	24
102.45	22	114.95	65	125.00	938	136.95	124
105.05	18	117.40	10	125.95	75	138.00	1015
106.95	139	118.50	21	127.10	127	139.05	163
108.00	9	119.05	84	129.05	42	140.05	501
109.00	46	119.45	26	129.85	12	141.05	145

Average of 23.265 to 23.315 min.: A0278.D
Converted from RTE data file: >A0278:
Modified:added subtracted scaled clipped

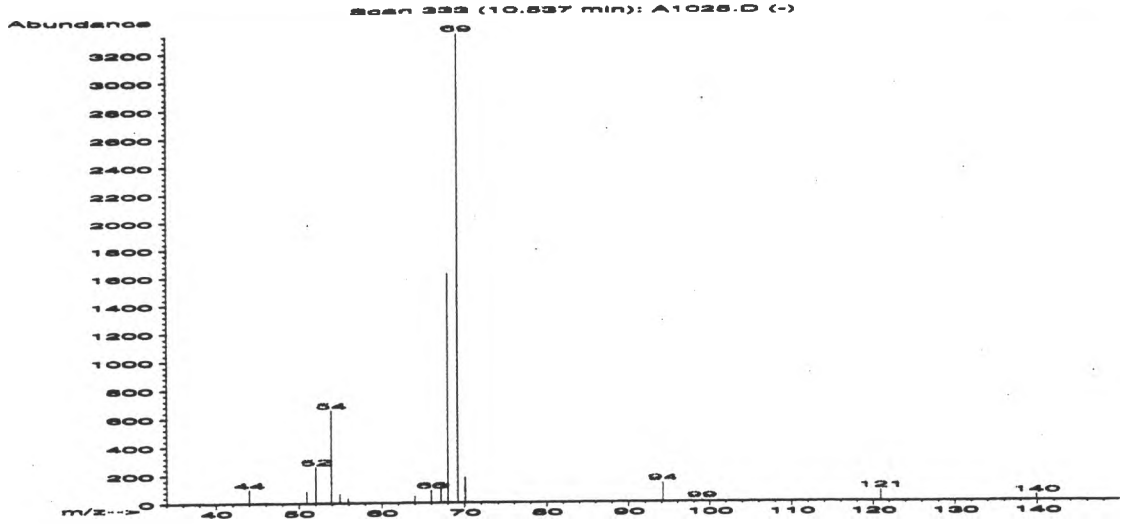
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
142.50	16	156.90	21	170.80	20		
143.00	21	157.15	27	171.05	16		
143.40	22	158.15	10				
144.95	30	158.90	33				
146.55	11	160.95	85				
146.90	1	165.15	17				
148.45	11	167.15	64				
149.95	2	168.00	3666				
152.95	118	169.00	442				
153.95	9	170.00	190				
156.00	15	170.55	30				

CTMP Compounds

No Hits

CTMP Compounds

Peak 87; 2,2'-azobis[2-methyl-propanenitrile



Scan 333 (10.537 min): A1025.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	98	70.05	181				
50.95	86	94.15	139				
52.05	260	99.00	11				
53.95	653	120.95	80				
54.95	65	139.90	41				
55.95	33						
64.00	51						
66.00	91						
67.15	143						
68.00	1626						
69.15	3326						

- Blowing agent for elastomers and plastics
- Initiator for free radical reaction.

may be from resin repair work.
High concentration and reliable ID.

CTMP Compounds

Scan 333 (10.537 min): A1025.D

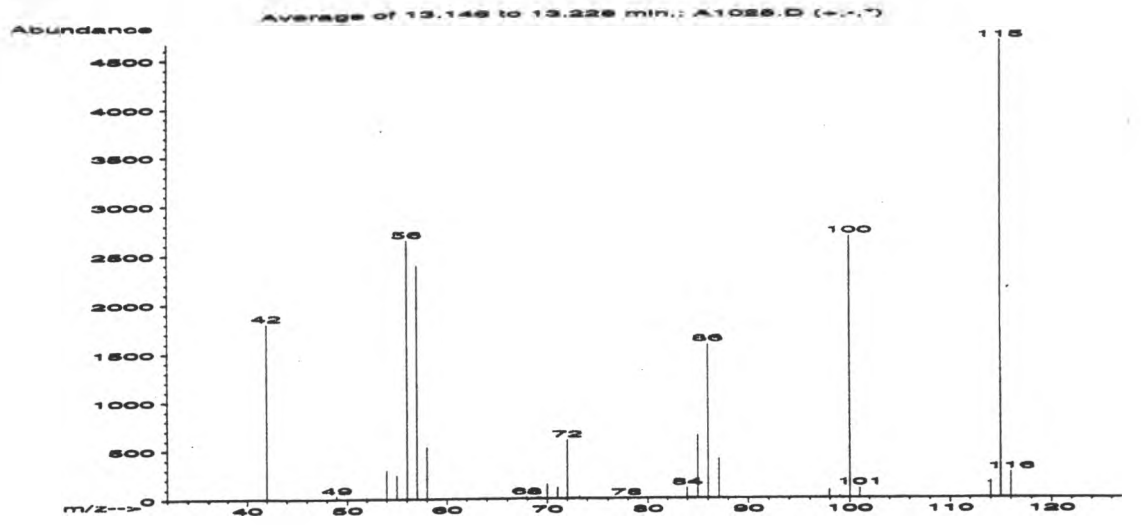
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Propanenitrile, 2,2'-azobis[2-methyl-	164	C8H12N4	43
2.	Tetramethylsuccinonitrile	136	C8H12N2	40
3.	Propanenitrile, 2,2'-azobis[2-methyl-	164	C8H12N4	39

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	43	000078-67-1	125265	34	55	1	80	10	18	0	22	9968
2.	40	003333-52-6	7834	34	43	1	99	12	16	4	26	9968
3.	39	000078-67-1	18324	38	54	1	66	19	15	0	24	9899

CTMP Compounds

Peak 88; Unidentified Amine



Average of 13.146 to 13.228 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1802	70.00	147	100.00	2681		
48.95	34	71.00	111	101.00	101		
51.95	14	72.00	599	102.05	6		
54.00	295	73.20	22	114.00	170		
55.00	240	77.85	3	115.00	4669		
56.05	2640	83.95	106	116.00	262		
57.00	2388	85.00	642	117.00	10		
58.00	536	86.00	1582				
67.95	18	87.10	401				
69.05	19	97.95	78				
69.30	13	99.00	20				

CTMP Compounds

Average of 13.146 to 13.228 min.: A1025.D
Converted from RTE data file: >A1025:

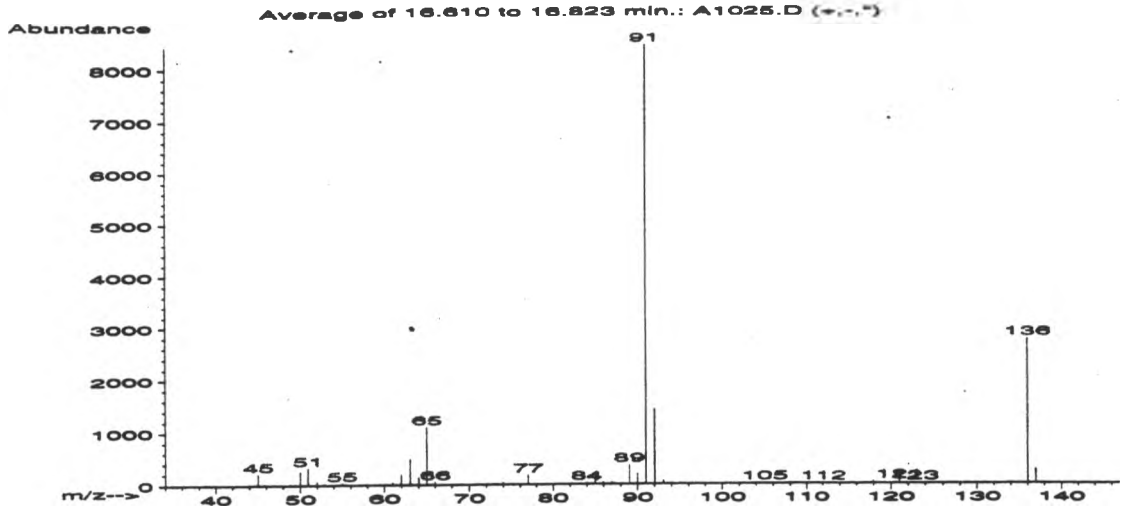
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	.ALPHA.-METHYLTETRONIC ACID-D1	114	C5H5DO3	40
2.	2,5-Pyrrolidinedione, 1-hydroxy-	115	C4H5NO3	28
3.	Morpholine	87	C4H9NO	12
4.	Hexane	86	C6H14	12
5.	1,5-Pentanediamine	102	C5H14N2	10
6.	3-Hexanamine, 3-ethyl-	129	C8H19N	8
7.	Pyrrolidine, 1-nitroso-	100	C4H8N2O	8
8.	5-[1(R,S),2-DIHYDROXYETHYL]TETRAZOLE	130	C3H6N4O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*40	000000-00-0	2903	39	56	3	224	31	16	0	35	8824
2.	*28	006066-82-6	119390	32	77	1	99	40	8	0	26	7952
3.	12	000110-91-8	117142	33	70	3	140	60	2	0	25	4314
4.	*12	000110-54-3	117109	32	57	2	109	58	2	0	27	5485
5.	10	000462-94-2	118272	45	56	1	56	70	1	0	37	4925
6.	8	056667-17-5	120985	36	56	2	56	70	1	0	22	5259
7.	* 8	000930-55-2	117892	32	60	1	58	67	1	0	29	5086
8.	8	084348-17-4	6237	35	62	0	56	66	1	0	25	5182

CTMP Compounds

Peak 45; Benzeneacetic acid



Average of 16.610 to 16.823 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	24	52.95	18	66.00	51	85.95	37
44.85	1	55.00	28	72.20	5	86.95	30
45.05	213	55.30	4	72.95	16	87.20	8
45.80	3	58.10	2	73.45	1	89.05	363
48.30	3	59.85	4	74.00	48	90.00	190
48.55	3	60.95	40	74.80	3	91.00	8422
48.85	21	61.95	188	75.00	17	92.05	1435
49.30	3	63.00	487	77.00	172	93.05	59
50.00	251	63.75	6	78.05	4	94.00	11
50.95	323	64.00	134	83.95	20	95.00	7
52.00	59	65.00	1099	84.95	84	95.45	3

Average of 16.610 to 16.823 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.00	11						
110.00	4						
111.25	3						
112.00	4						
117.95	33						
121.00	37						
122.80	2						
136.00	2777						
136.95	271						

CTMP Compounds

Average of 16.610 to 16.823 min.: A1025.D
Converted from RTE data file: >A1025:

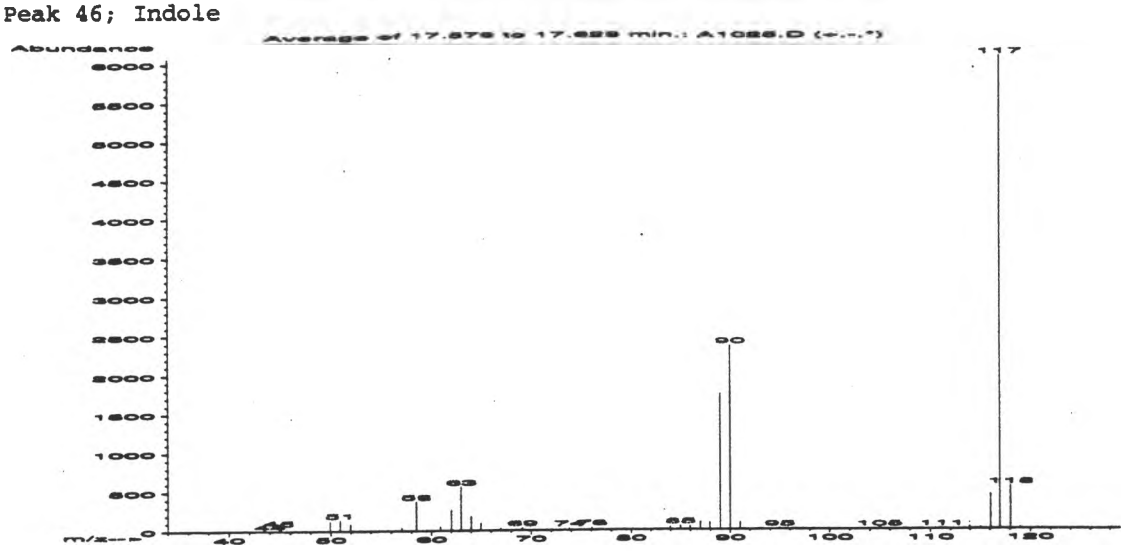
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzeneacetic acid	136	C8H8O2	91
2.	Benzeneacetic acid	136	C8H8O2	91
3.	Benzeneacetic acid	136	C8H8O2	91
4.	Benzeneacetic acid	136	C8H8O2	87
5.	Benzoic acid, 3-methyl-	136	C8H8O2	64
6.	Benzeneacetaldehyde	120	C8H8O	47
7.	Propanedioic acid, phenyl-	180	C9H8O4	45
8.	Benzene, (iodomethyl)-	218	C7H7I	40
9.	SPIRO(2,4)HEPTADIENE-(2,4)	92	C7H8	40
10.	Formic acid, phenylmethyl ester	136	C8H8O2	40
11.	Bicyclo[6.1.0]nona-5,8-dien-4-one	134	C9H10O	40
12.	Benzene, methyl-	92	C7H8	38
13.	Spiro[3.3]hepta-1,5-diene	92	C7H8	38
14.	Oxirane, phenyl-	120	C8H8O	38
15.	SPIRO[2.4]HEPTA-2,6-DIENE	92	C7H8	37
16.	Benzene, methyl-	92	C7H8	32
17.	Tetracyclo[4.1.0.0(2,4).0(3,5)]heptane	92	C7H8	32
18.	Benzene, methyl-	92	C7H8	32
19.	1,3,5-Cycloheptatriene	92	C7H8	27
20.	Benzene, methyl-	92	C7H8	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000103-82-2	7792	71	10	0	94	0	62	0	76	9994
2.	*91	000103-82-2	121830	69	12	0	78	0	62	0	76	9989
3.	*91	000103-82-2	121833	70	15	2	76	0	60	15	58	9979
4.	*87	000103-82-2	121834	66	24	1	50	15	54	0	64	9748
5.	*64	000099-04-7	7790	37	44	2	48	18	37	0	39	9610
6.	47	000122-78-1	119981	43	28	0	53	40	20	4	41	9416
7.	45	002613-89-0	25412	43	33	2	46	25	19	0	37	9961
8.	40	000620-05-3	42507	41	40	1	88	31	16	2	35	9482
9.	*40	000000-00-0	418	40	31	1	99	31	16	0	35	9456
10.	*40	000104-57-4	121868	33	87	1	50	31	16	0	30	7782
11.	40	056666-74-1	7422	40	40	2	67	34	16	13	35	9499
12.	*38	000108-88-3	117431	41	26	0	27	50	14	1	38	8801
13.	*38	022635-78-5	420	33	47	1	54	46	14	0	39	9424
14.	38	000096-09-3	119997	36	15	0	69	37	14	5	30	9465
15.	37	000000-00-0	419	45	33	3	92	43	13	0	35	9324
16.	*32	000108-88-3	117433	36	32	1	27	50	9	17	37	8353
17.	*32	050861-26-2	424	31	3	0	77	50	9	2	35	9484
18.	32	000108-88-3	117434	39	40	2	86	46	9	0	33	8020
19.	*27	000544-25-2	117441	33	37	1	36	56	8	0	41	9315
20.	25	000108-88-3	117429	44	39	3	63	53	7	0	37	8728

CTMP Compounds

Peak 46; Indole



Average of 17.579 to 17.628 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	2	64.00	180	76.05	34	94.95	12
44.90	51	64.95	92	80.15	8	96.45	9
49.95	123	66.95	29	83.95	37	104.95	10
50.95	139	67.90	5	85.00	49	111.15	13
51.95	85	69.00	16	85.95	47	113.95	34
53.00	15	69.15	31	87.00	96	115.00	24
57.05	43	71.55	12	87.95	87	116.05	447
58.50	374	72.00	8	89.00	1743	117.00	6068
60.90	51	72.85	8	90.00	2368	118.05	549
62.00	268	73.80	24	91.00	92	119.00	16
62.95	559	74.95	8	93.00	2		

CTMP Compounds

Average of 17.579 to 17.628 min.: A1025.D
Converted from RTE data file: >A1025:

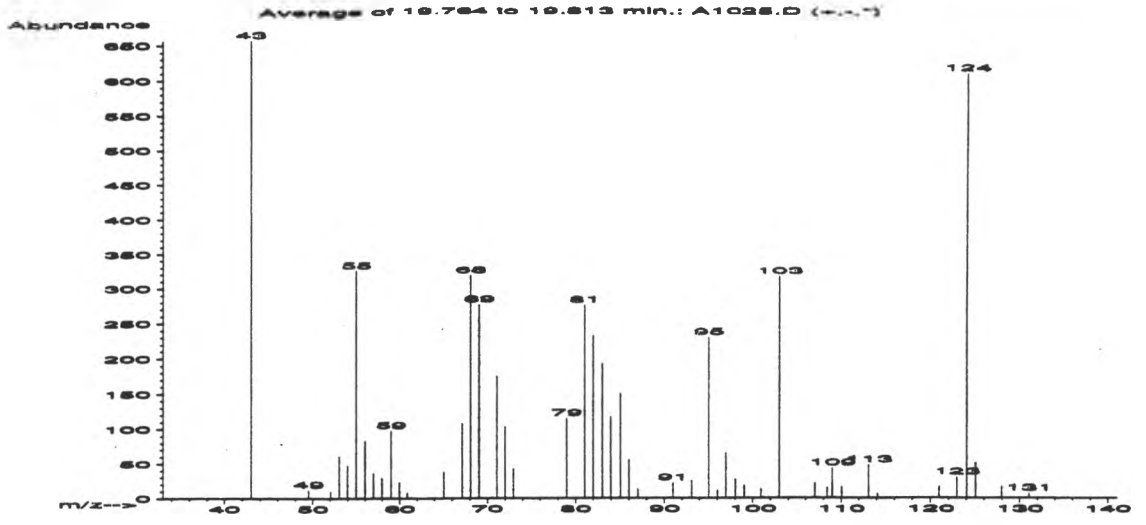
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1H-Indole	117	C8H7N	94
2.	1H-Indole	117	C8H7N	91
3.	Benzeneacetonitrile	117	C8H7N	90
4.	Benzeneacetonitrile	117	C8H7N	86
5.	1H-Indole	117	C8H7N	86
6.	Benzene, 1-isocyano-2-methyl-	117	C8H7N	83
7.	Benzeneacetonitrile	117	C8H7N	83
8.	1H-Indole	117	C8H7N	83
9.	1H-Indole	117	C8H7N	83
10.	(E)-1-Azido-2-phenylethene	145	C8H7N3	74
11.	Benzene, (isocyanomethyl)-	117	C8H7N	72
12.	Benzeneacetonitrile	117	C8H7N	72
13.	Benzene, 1-isocyano-3-methyl-	117	C8H7N	72
14.	Benzonitrile, 3-methyl-	117	C8H7N	64
15.	Benzonitrile, 3-methyl-	117	C8H7N	64
16.	Benzonitrile, 4-methyl-	117	C8H7N	64
17.	Benzonitrile, 2-methyl-	117	C8H7N	59
18.	1H-Indole	117	C8H7N	45
19.	1H-Indole	117	C8H7N	43
20.	Benzeneacetonitrile	117	C8H7N	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000120-72-9	119700	80	10	1	73	0	70	0	90	9972
2.	*91	000120-72-9	119697	59	30	2	94	2	60	0	56	9961
3.	*90	000140-29-4	3678	59	33	2	78	5	57	20	49	9651
4.	*86	000140-29-4	119683	53	44	2	71	9	53	0	49	9693
5.	*86	000120-72-9	119698	66	23	1	71	9	53	17	47	9973
6.	*83	010468-64-1	3685	62	36	3	73	4	50	18	43	9180
7.	*83	000140-29-4	119686	54	38	3	97	5	50	11	40	9723
8.	*83	000120-72-9	119699	57	11	1	92	4	50	9	38	9973
9.	*83	000120-72-9	119694	58	33	2	83	4	50	6	41	9973
10.	74	018756-03-1	11002	33	13	1	96	4	44	11	33	9934
11.	*72	010340-91-7	3688	40	54	3	97	12	42	20	40	9491
12.	*72	000140-29-4	119685	51	43	2	73	12	42	15	40	9626
13.	*72	020600-54-8	3686	37	29	2	70	13	42	1	40	8425
14.	*64	000620-22-4	119679	46	52	3	67	7	37	7	33	9118
15.	*64	000620-22-4	3676	46	52	3	67	7	37	7	33	9118
16.	*64	000104-85-8	119681	46	54	3	74	7	37	9	34	9075
17.	*59	000529-19-1	3675	33	67	3	69	22	33	0	39	9395
18.	45	000120-72-9	3695	67	35	1	52	25	19	0	36	9604
19.	43	000120-72-9	119695	43	46	1	60	42	18	2	41	9916
20.	40	000140-29-4	119684	50	45	2	62	32	16	10	36	9630

CTMP Compounds

Peak 89; Unidentified Hydrocarbon



Average of 19.764 to 19.813 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	656	60.90	8	83.00	192	99.05	18
49.55	12	65.05	38	83.95	117	100.95	13
52.05	10	67.15	108	85.05	150	103.00	315
53.00	61	68.10	318	86.00	55	107.00	21
53.95	48	69.05	276	87.00	13	108.40	15
55.00	325	71.05	175	91.00	22	109.00	43
56.00	83	72.00	103	93.10	25	110.05	16
56.95	36	73.00	42	95.05	229	113.10	48
57.95	29	79.00	115	96.05	11	114.10	6
59.00	98	81.05	275	97.00	65	120.95	16
59.95	23	82.00	232	98.05	27	122.95	30

Average of 19.764 to 19.813 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	607						
125.05	51						
127.95	16						
131.05	7						

CTMP Compounds

Average of 19.764 to 19.813 min.: A1025.D
Converted from RTE data file: >A1025:

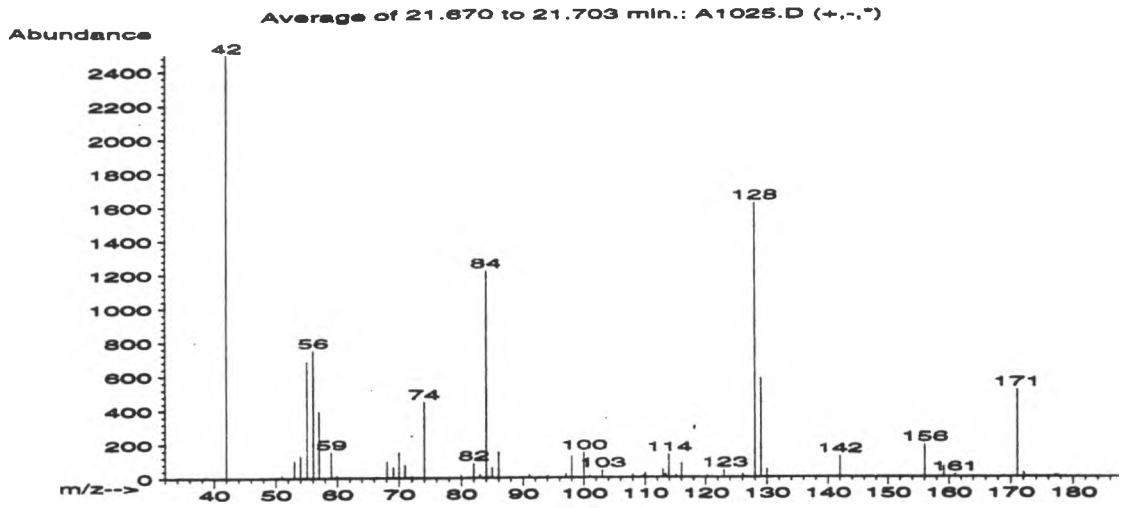
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3,6-DIMETHYL-2H-PYRAN-2-ONE	124	C7H8O2	37
2.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	32
3.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	32
4.	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	27
5.	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	22
6.	5,6-Dimethyl-2-pyrone	124	C7H8O2	22
7.	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	22
8.	Octadecanal	268	C18H36O	22
9.	Phenol, 3-methoxy-	124	C7H8O2	22
10.	Pyrazine, 2-methoxy-6-methyl-	124	C6H8N2O	16
11.	1,4-Benzenediol, 2-methyl-	124	C7H8O2	12
12.	Phenol, 3-methoxy-	124	C7H8O2	12
13.	Phenol, 4-methoxy-	124	C7H8O2	12
14.	5-Tetradecen-1-ol, acetate, (Z)-	254	C16H30O2	12
15.	4-Methoxy-5-methylpyridazine	124	C6H8N2O	10
16.	Phenol, 2-methoxy-	124	C7H8O2	10
17.	PHYTOL ACETATE	338	C22H42O2	10
18.	2-Methoxy-5-methylpyrimidine	124	C6H8N2O	10
19.	E3-TETRADECENYLACETATE	254	C16H30O2	10
20.	Propanal, 2,2-dimethyl-, oxime	101	C5H11NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*37	053034-20-1	4694	38	79	3	92	44	13	3	36	8479
2.	*32	002847-30-5	4672	38	86	3	79	48	9	0	35	8248
3.	*32	002847-30-5	120355	53	62	1	88	48	9	0	35	8247
4.	*27	001004-36-0	120371	37	45	2	79	57	8	0	39	7682
5.	*22	001004-36-0	4698	33	59	0	74	63	5	0	41	7392
6.	*22	004209-44-3	4696	43	63	2	92	61	5	0	39	7413
7.	*22	001004-36-0	120369	37	32	1	80	62	5	0	39	7408
8.	22	000638-66-4	132074	44	93	1	65	62	5	9	38	5803
9.	*22	000150-19-6	120384	45	59	1	92	62	5	0	39	7423
10.	*16	002882-21-5	4676	36	65	1	79	58	3	0	35	7861
11.	*12	000095-71-6	4704	35	67	2	92	62	2	10	37	7426
12.	*12	000150-19-6	4706	36	74	1	92	62	2	0	35	7401
13.	*12	000150-76-5	4707	36	75	2	76	62	2	0	30	7425
14.	12	035153-13-0	131474	45	89	3	93	64	2	0	37	5862
15.	*10	094693-85-3	4662	29	7	0	75	70	1	4	37	6949
16.	*10	000090-05-1	120378	33	62	2	67	68	1	0	35	7125
17.	10	000000-00-0	85178	55	26	1	66	66	1	0	36	6834
18.	*10	017758-07-5	4668	37	56	1	74	66	1	12	35	7824
19.	10	000000-00-0	58220	39	95	3	99	65	1	0	29	5700
20.	*10	000637-91-2	1287	38	60	0	37	78	1	0	39	3537

CTMP Compounds

Peak 90; Unidentified Amine



Average of 21.670 to 21.703 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	2500	70.00	151	91.05	20	113.00	47
51.00	17	70.95	78	94.00	15	113.40	19
53.00	104	72.05	11	97.05	25	113.95	136
54.00	130	73.00	5	98.00	128	115.15	14
55.05	684	74.00	450	100.00	149	116.05	84
56.05	749	79.95	17	101.00	12	120.30	12
57.00	392	82.00	87	103.00	45	120.95	5
59.00	152	83.00	19	108.00	20	123.05	44
59.90	15	84.00	1222	109.00	3	126.05	19
68.05	98	84.95	63	109.75	14	128.05	1623
69.10	66	86.00	155	110.00	26	129.05	582

Average of 21.670 to 21.703 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.05	49						
142.00	125						
156.05	193						
159.15	61						
161.00	16						
171.05	515						
172.05	25						
177.05	13						
177.45	11						

CTMP Compounds

Average of 21.670 to 21.703 min.: A1025.D
Converted from RTE data file: >A1025:

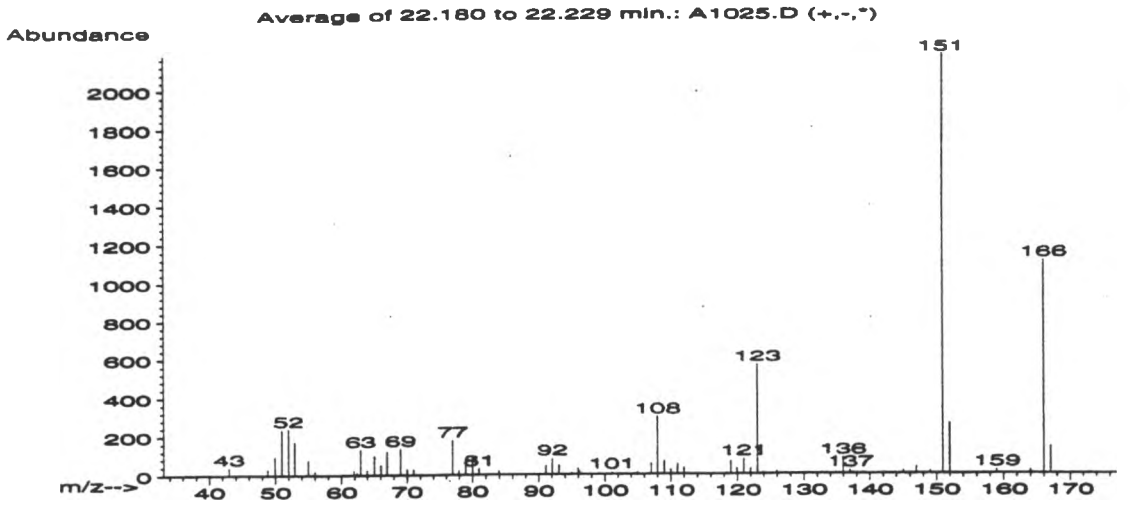
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Norvaline, N-methyl-2-propyl-, ethyl est	201	C11H23NO2	38
2.	4-Piperidinone, 1-nitroso-	128	C5H8N2O2	38
3.	4-TRIDEUTERIOMETHYLQUINUCLIDINE	125	C8H12D3N	37
4.	3-Imidazoline(1-N)-3-oxide-1-oxyl, 2,2,4	171	C8H15N2O2	32
5.	1-Piperidinecarboxylic acid, ethyl ester	157	C8H15NO2	32
6.	2,4,6(1H,3H,5H)-Pyrimidinetrione	128	C4H4N2O3	32
7.	Pyrrolidine, 2,5-dimethyl-1-nitroso-	128	C6H12N2O	28
8.	3-Imidazoline-3-oxide-1-oxyl, 2,2,4,5,5-	171	C8H15N2O2	27
9.	Aziridine, 2,2,3,3-tetramethyl-	99	C6H13N	23
10.	6-Azabicyclo[3.2.1]octan-8-ol, 5-methoxy	171	C9H17NO2	12
11.	6-Azabicyclo[3.2.1]octan-8-ol, 5-methoxy	171	C9H17NO2	12
12.	1,2-BIS(2,6-DIMETHYL-4-MORPHOLINYL)ETHAN	256	C14H28N2O2	8
13.	2-Pentene, 3-methyl-, (E)-	84	C6H12	8
14.	2-PENTENE, 3-METHYL- (CIS/TRANS)	84	C6H12	8
15.	1-METHOXYCARBONYL-1,4-DIAMINOBUTANE	146	C6H14N2O2	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	006141-44-2	35097	46	70	3	219	50	14	0	39	6869
2.	*38	055556-91-7	5701	29	61	1	99	39	14	11	37	8839
3.	*37	000000-00-0	5041	30	53	2	99	45	13	5	30	8639
4.	*32	072960-74-8	21798	37	45	1	93	47	9	10	37	7690
5.	32	005325-94-0	124611	39	55	0	51	47	9	16	37	8530
6.	*32	000067-52-7	120730	30	47	2	99	46	9	0	33	8658
7.	*28	055556-86-0	5758	25	68	3	94	39	8	6	23	9052
8.	*27	018796-04-8	21797	34	78	2	99	58	8	0	39	7211
9.	23	005910-14-5	1016	34	62	2	99	48	6	3	23	8224
10.	*12	039077-13-9	126054	29	53	1	49	59	2	0	29	5003
11.	*12	039077-13-9	21819	29	53	1	49	59	2	0	29	5003
12.	8	000000-00-0	58876	33	83	2	64	66	1	0	21	7120
13.	* 8	000616-12-6	116908	29	66	2	92	70	1	0	27	6468
14.	* 8	000000-00-0	116905	29	66	2	99	66	1	0	27	7111
15.	8	000056-87-1	123115	37	64	1	118	68	1	0	25	6329

CTMP Compounds

Peak 91; Acetovanillone



Average of 22.180 to 22.229 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	41	62.95	132	79.00	88	104.95	9
44.00	2	63.95	26	80.00	93	107.00	55
48.85	31	65.10	98	81.00	31	108.00	297
49.95	96	66.05	51	83.95	21	109.00	68
51.00	234	67.00	121	91.05	45	110.00	23
52.00	237	69.05	135	92.05	82	111.00	52
52.95	172	70.00	30	93.05	48	112.00	31
55.00	77	71.00	28	95.00	8	119.00	66
56.00	20	75.00	2	95.95	33	119.95	29
61.90	24	77.00	178	96.20	16	120.95	77
62.40	11	77.95	22	101.05	12	122.00	28

Average of 22.180 to 22.229 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.00	567	164.00	19				
123.95	5	166.00	1115				
125.95	12	167.05	139				
135.95	83						
137.00	19						
145.05	16						
147.00	36						
149.05	13						
150.95	2182						
151.95	260						
159.00	21						

CTMP Compounds

Average of 22.180 to 22.229 min.: A1025.D
Converted from RTE data file: >A1025:

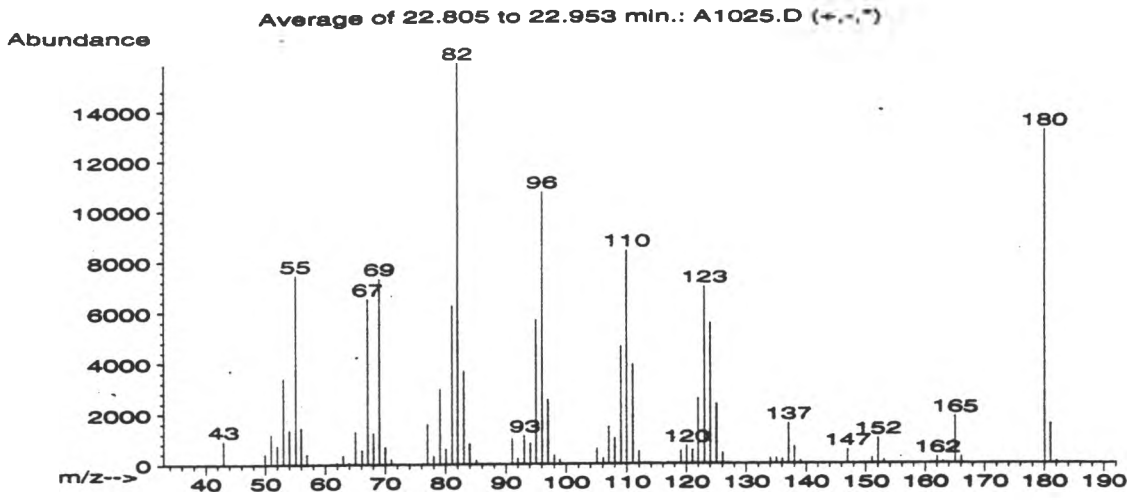
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	91
2.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	91
3.	4-(METHYLTHIO)ACETOPHENONE	166	C9H10OS	91
4.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	90
5.	1,2-Benzenediol, 4-(1,1-dimethylethyl)-	166	C10H14O2	86
6.	4,7,7-Trimethylbicyclo[3.3.0]octan-2-one	166	C11H18O	83
7.	Ethanone, 1-(2-hydroxy-5-methoxyphenyl)-	166	C9H10O3	80
8.	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	166	C9H10O3	72
9.	2-METHOXY-4-ETHYL-6-METHYLPHENOL	166	C10H14O2	64
10.	2,3-DIHYDROXY-5-METHYL-ACETOPHENONE	166	C9H10O3	64
11.	Benzenethiol, 4-(1,1-dimethylethyl)-	166	C10H14S	59
12.	2,2-Dimethyl-1,3-benzoxathiole	166	C9H10OS	59
13.	2,4-Dimethyl-3-acetyl-5-ethylfuran	166	C10H14O2	58
14.	2,3-DIHYDROXY-4-METHYL-ACETOPHENONE	166	C9H10O3	53
15.	2,5-DIHYDROXY-4-METHYL-ACETOPHENONE	166	C9H10O3	53
16.	3',4'-DIHYDROXY-2'-METHYLACETOPHENONE	166	C9H10O3	53
17.	Benzaldehyde, 3-methoxy-, oxime	151	C8H9NO2	47
18.	P-FORMANISIDINE	151	C8H9NO2	47
19.	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	43
20.	1,4 Benzodioxan-6-amine	151	C8H9NO2	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000498-02-2	125553	76	20	3	96	5	62	32	68	9952
2.	*91	000498-02-2	125550	80	15	2	75	5	62	25	66	9966
3.	*91	000000-00-0	19251	60	43	2	96	5	60	0	56	9965
4.	*90	000498-02-2	19319	71	25	2	99	8	59	0	76	9964
5.	*86	000098-29-3	125560	48	53	3	99	9	53	19	47	9793
6.	*83	060064-73-5	19639	42	11	0	99	0	50	13	42	9292
7.	*80	000705-15-7	19315	57	44	1	70	13	48	0	49	9798
8.	*72	000552-41-0	19313	55	38	1	99	17	42	0	49	9686
9.	*64	000000-00-0	19410	40	56	2	95	18	37	3	38	9771
10.	*64	069751-80-0	19309	35	22	0	99	21	37	10	43	9729
11.	*59	002396-68-1	19537	37	55	2	99	21	33	15	40	9760
12.	*59	000000-00-0	19252	41	44	1	99	25	33	0	39	9683
13.	*58	071041-34-4	19381	35	8	0	99	27	32	10	43	9634
14.	*53	069751-81-1	19308	37	30	3	99	27	28	0	39	9643
15.	*53	054698-17-8	19310	47	18	1	99	27	28	5	40	9647
16.	*53	066296-84-2	19311	39	44	2	89	27	28	0	39	9834
17.	*47	038489-80-4	13105	45	33	1	84	40	20	14	43	8684
18.	*47	023896-88-0	13108	45	37	2	93	40	20	0	39	7443
19.	*43	002634-33-5	13018	37	54	2	99	43	18	0	39	8791
20.	*43	022013-33-8	13118	43	52	2	88	45	18	0	40	8609

CTMP Compounds

Peak 64; Unidentified Monoterpene



Average of 22.805 to 22.953 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	934	57.90	6	69.00	7317	85.05	154
48.05	7	59.00	23	70.00	676	86.00	12
48.70	9	60.90	11	71.00	174	87.00	4
49.95	404	61.65	5	77.00	1591	87.50	4
51.00	1202	61.95	79	78.00	322	89.00	22
52.00	747	63.00	354	79.05	2973	91.05	1022
53.00	3388	63.95	60	80.05	594	92.00	229
54.00	1334	65.00	1282	81.05	6254	93.10	1129
55.05	7438	66.10	556	82.00	15868	94.10	814
56.00	1434	67.05	6504	83.00	3676	95.00	5694
56.95	395	68.05	1223	84.00	797	96.05	10721

Average of 22.805 to 22.953 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.00	2553	111.00	3937	124.05	5569	139.05	116
98.00	338	112.05	482	125.05	2359	140.00	8
99.00	144	113.00	24	126.05	419	144.00	4
103.00	29	114.00	5	127.00	27	147.00	551
104.05	5	115.00	5	131.05	11	148.00	39
105.10	605	117.00	41	132.95	11	148.95	5
106.10	208	119.05	512	134.05	207	149.20	4
107.00	1471	120.05	707	135.05	217	151.05	231
108.00	1042	121.00	546	136.05	170	152.05	1004
109.00	4656	122.00	2584	137.05	1591	153.05	142
110.00	8422	123.05	7011	138.05	661	154.05	4

Average of 22.805 to 22.953 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.00	11	181.05	1571				
161.00	36	182.05	98				
162.05	250						
163.00	73						
164.00	18						
165.05	1868						
166.10	253						
167.10	4						
177.00	1						
178.80	7						
180.05	13191						

CTMP Compounds

Average of 22.805 to 22.953 min.: A1025.D
Converted from RTE data file: >A1025:

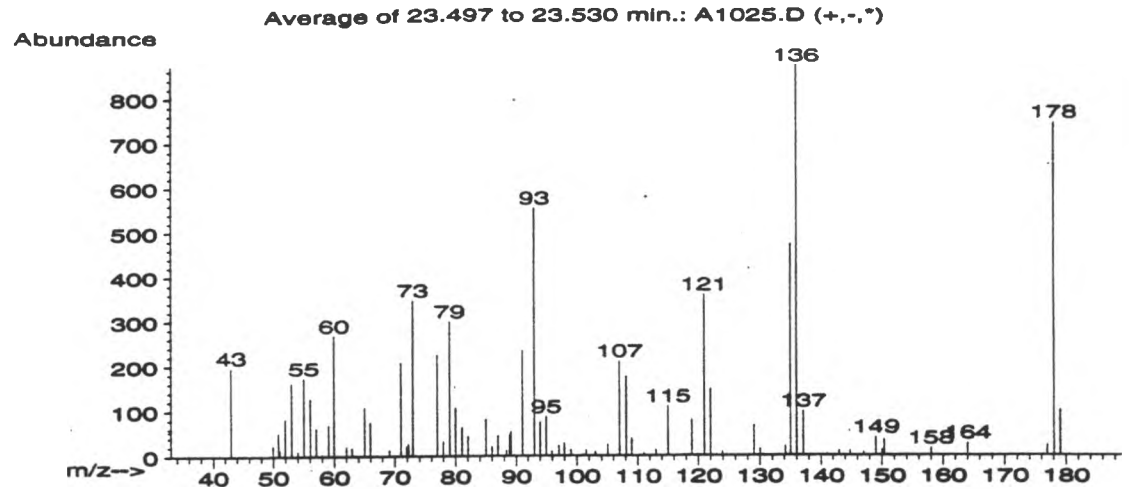
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethyl-3-iminomethyl-4-methyl-6-hydroxy-2	180	C9H12N2O2	83
2.	(+)-(3a,R,7aS)-3a,7a-Dimethylindan-1,5-d	180	C11H16O2	59
3.	(-)-7-2-EXO.3-EXO-DIMETHYLBORNANE	166	C12H22	27
4.	Theobromine	180	C7H8N4O2	25
5.	7-CHLORO-2-METHYL-2,3-HEPTADIENE	144	C8H13Cl	14
6.	Theobromine	180	C7H8N4O2	14
7.	1,2,4-Cyclopentanetrione, 3-(2-pentenyl)	180	C10H12O3	14
8.	5,9,9-TRIMETHYLSPIRO[3.6]DECANE	180	C13H24	12
9.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	11
10.	Benzaldehyde, 6-hydroxy-4-methoxy-2,3-di	180	C10H12O3	11
11.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	10
12.	5-Ethyl-5-isopropyl-2-cyclopenten-1-one	152	C10H16O	10
13.	trans-4-Methyl-5-isopropylcyclopent-2-en	138	C9H14O	10
14.	9H-Purine, 9-methyl-6-(methylthio)-	180	C7H8N4S	10
15.	2-N-BUTYL-4-VINYLCYCLOPENTANONE	166	C11H18O	10
16.	7H-Purinium, 6-mercapto-7,9-dimethyl-, h	180	C7H8N4S	10
17.	1-AZA-2-BORACYCLOPENTANE, 2-ETHYL-1-METH	111	C6H14BN	10
18.	CYCLOBUTANE, 1-CIS-2-CIS-3-TRANS-4-TRANS	360	C28H24	10
19.	1,4,4,7a-Tetramethyl-5,6,7,7a-tetrahydro	180	C13H24	10
20.	(4R*,5R*)-5-Isopropyl-4,5-dimethyl-2-cyc	152	C10H16O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000000-00-0	25425	40	26	2	83	0	50	0	39	4652
2.	*59	079897-27-1	25659	51	22	1	89	22	33	16	40	8304
3.	27	059581-85-0	19763	45	35	2	99	60	8	20	41	6551
4.	*25	000083-67-0	25334	49	57	1	83	63	7	0	46	6588
5.	14	065041-85-2	10640	48	39	0	73	66	2	16	41	6148
6.	*14	000083-67-0	126772	36	65	1	83	66	2	0	39	6459
7.	*14	054644-27-8	25482	36	73	2	77	69	2	10	40	5522
8.	12	000000-00-0	25867	45	18	1	99	64	2	0	37	6622
9.	*11	002758-18-1	594	37	50	0	55	77	2	10	43	4730
10.	*11	034883-12-0	25524	33	68	2	64	78	2	16	43	4846
11.	*10	002758-18-1	117592	42	25	0	58	74	1	3	38	5006
12.	*10	081825-26-5	13617	40	20	0	45	76	1	0	39	4150
13.	*10	081825-21-0	8608	37	38	1	67	73	1	0	41	5050
14.	*10	001127-75-9	25344	33	61	2	83	80	1	17	40	4702
15.	*10	054973-10-3	19584	41	11	1	51	71	1	13	38	3927
16.	*10	005752-11-4	25336	39	57	3	81	80	1	15	40	4652
17.	*10	000000-00-0	2358	36	53	1	48	72	1	0	39	6513
18.	10	000000-00-0	90418	56	75	1	58	80	1	0	39	4652
19.	10	085329-81-3	25873	44	40	1	31	80	1	10	41	5860
20.	*10	081825-25-4	13618	38	33	0	53	77	1	0	39	5917

CTMP Compounds

Peak 92; Unidentified



Average of 23.497 to 23.530 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	196	59.05	69	77.00	224	89.15	54
49.95	23	59.95	267	78.00	32	91.05	234
50.80	51	62.00	20	79.05	300	93.05	553
51.05	13	62.90	17	80.00	106	94.00	74
51.95	81	65.00	107	81.05	63	95.00	86
53.00	161	65.95	74	82.05	44	95.95	9
54.00	10	69.10	13	85.00	82	97.05	22
55.00	172	71.00	207	86.00	19	97.95	27
56.05	127	71.95	21	86.95	45	99.05	12
57.00	61	72.20	26	88.40	11	101.05	3
57.95	3	72.95	347	88.90	47	101.55	11

Average of 23.497 to 23.530 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.00	8	123.95	8	147.05	7		
105.05	25	129.05	66	149.05	40		
107.00	210	130.05	14	150.05	11		
108.10	175	132.95	1	150.35	35		
109.00	38	134.15	20	158.00	16		
111.00	5	135.00	473	164.00	27		
113.00	12	136.00	871	176.95	22		
115.00	109	137.10	98	178.05	743		
119.00	79	141.00	3	179.05	101		
121.00	360	143.00	10				
122.00	147	144.80	9				

CTMP Compounds

Average of 23.497 to 23.530 min.: A1025.D
Converted from RTE data file: >A1025:

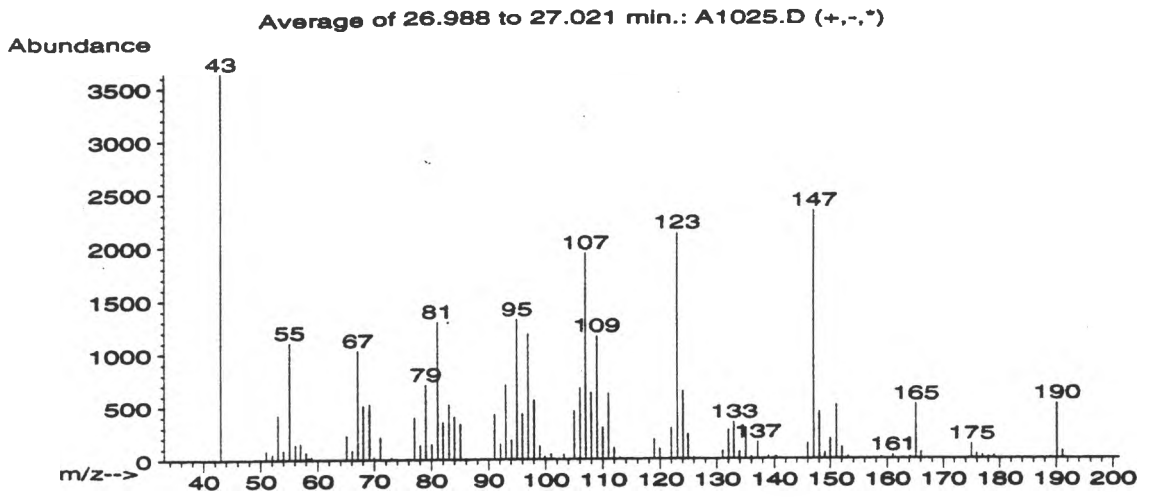
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2,2-Dimethylbenzofuran-4,7(2H,3H)-dione	178	C10H10O3	50
2.	.ALPHA.-TERPINOLENE	136	C10H16	41
3.	1,3-Dimethyl-adamantan-2-one	178	C12H18O	38
4.	Cyclohexene, 1-methyl-4-(1-methylethenyl	136	C10H16	38
5.	N-(2',3',3'-TRIDEUTERO-ALLYL)ANILINE	133	C9H8D3N	35
6.	2(1H)-Naphthalenone, 3,4,5,6,7,8-hexahyd	178	C12H18O	30
7.	Benzaldehyde, 2-methoxy-	136	C8H8O2	30
8.	Cyclohexene, 5-methyl-3-(1-methylethenyl	136	C10H16	30
9.	.gamma.-Terpinene	136	C10H16	30
10.	m-Mentha-4,8-diene, (1S,3S)-(+)-	136	C10H16	27
11.	2,4(1H,3H)-Pteridinedione, 8-methyl-	178	C7H6N4O2	27
12.	4(3H)-Pteridinone, 3-hydroxy-6-methyl-	178	C7H6N4O2	22
13.	4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-d	136	C5H4N4O	18
14.	4(3H)-Pteridinone, 3-hydroxy-2-methyl-	178	C7H6N4O2	18
15.	Benzene, 1,2-dimethoxy-4-(1-propenyl)-	178	C11H14O2	18
16.	Benzaldehyde, 4-methoxy-	136	C8H8O2	18
17.	8-Methyl-9-oxatetracyclo[5.4.0.0(3,10).0	178	C11H14O2	14
18.	Benzaldehyde, 4-methoxy-	136	C8H8O2	14
19.	9H-Fluorene, 9-methylene-	178	C14H10	14
20.	Benzaldehyde, 4-(dimethylamino)-, O-meth	178	C10H14N2O	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	084428-21-7	24602	65	64	1	85	48	25	0	64	6451
2.	*41	000586-62-9	122033	76	41	2	82	51	16	29	60	7116
3.	*38	052719-85-4	24900	34	52	2	82	50	14	1	40	6814
4.	*38	007705-14-8	122027	42	32	0	86	49	14	14	40	6791
5.	*35	000000-00-0	7140	33	42	0	74	54	11	0	41	7048
6.	*30	001609-25-2	24876	36	80	1	82	59	9	21	43	7379
7.	*30	000135-02-4	121852	37	58	0	87	57	9	17	43	7058
8.	*30	056816-08-1	8108	66	40	0	67	57	9	22	47	7057
9.	*30	000099-85-4	122009	59	41	0	93	57	9	12	47	6130
10.	*27	005208-51-5	8100	62	49	0	75	56	8	20	41	7252
11.	*27	013300-38-4	24403	44	65	1	85	59	8	0	40	7005
12.	*22	018106-59-7	24405	43	69	1	60	65	5	0	40	6402
13.	*18	000315-30-0	121780	43	49	0	76	68	3	0	44	6658
14.	*18	018106-58-6	24404	49	68	1	76	69	3	0	44	5717
15.	*18	000093-16-3	126632	35	69	0	61	69	3	10	43	5714
16.	*18	000123-11-5	121856	33	65	3	116	68	3	21	43	6454
17.	*14	086516-45-2	24768	37	70	1	61	68	2	5	40	6324
18.	*14	000123-11-5	121857	39	55	2	98	66	2	14	40	6717
19.	*14	004425-82-5	24969	34	63	3	68	70	2	0	41	5264
20.	*14	019293-74-4	24631	37	47	1	84	70	2	1	40	5265

CTMP Compounds

Peak 93; Coeluting Compounds



Average of 26.988 to 27.021 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3638	65.05	227	80.05	146	95.05	1321
50.95	81	66.05	84	81.05	1302	96.00	432
52.05	51	67.05	1034	82.00	356	97.00	1187
53.00	422	68.05	515	83.00	522	98.05	564
54.00	84	69.10	528	84.00	403	99.00	128
55.05	1107	69.95	23	85.00	336	99.90	27
56.10	141	71.05	211	85.95	7	100.85	1
57.00	148	73.00	20	91.05	425	101.00	48
57.95	66	77.05	398	92.10	147	103.20	46
58.50	17	78.05	133	93.10	704	105.05	457
58.95	27	79.05	713	94.10	184	106.05	674

Average of 26.988 to 27.021 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	1932	124.05	640	140.15	20	161.00	34
108.00	625	124.95	233	140.40	20	163.00	9
109.00	1165	125.95	14	146.00	145	164.10	19
110.00	301	131.05	77	147.05	2312	165.15	515
111.00	619	132.05	274	148.05	441	166.05	57
112.00	105	133.00	348	149.00	60	175.05	138
113.00	15	133.95	67	150.00	190	175.95	44
119.00	187	135.00	292	151.05	505	176.95	31
119.95	96	136.00	22	152.05	107	178.05	15
122.00	295	137.10	157	153.05	18	178.95	25
123.05	2116	139.00	29	159.00	15	189.00	13

Average of 26.988 to 27.021 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
190.10	521						
191.05	71						

CTMP Compounds

Average of 26.988 to 27.021 min.: A1025.D
Converted from RTE data file: >A1025:

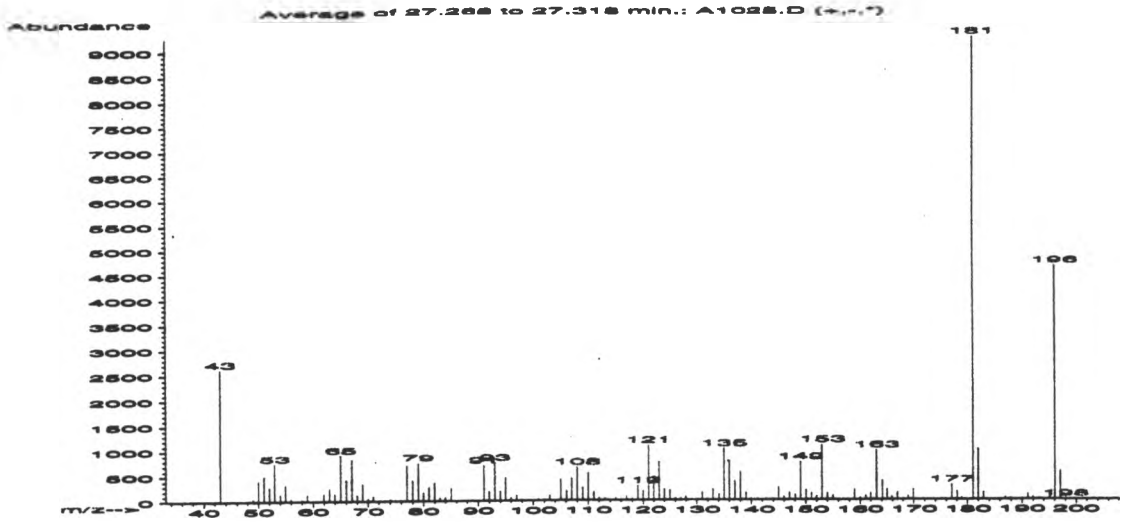
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 2,5-dimethyl-2-(1-methyle	166	C11H18O	38
2.	(4R,6R,7R,9S)-4,7-Epoxy-5(11)-megastigme	210	C13H22O2	35
3.	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	27
4.	(4R,6R,7R,9R)-4,7-Epoxy-5(11)-megastigme	210	C13H22O2	16
5.	Cyclohexanone, 2,5-dimethyl-2-(1-methyle	166	C11H18O	16
6.	(E)-5-Isopropyl-2,6-dimethyl-5,6-epoxy-1	180	C12H20O	12
7.	3,8-Nonadien-2-one, (E)-	138	C9H14O	12
8.	1H-1-Silaindene, 2,3-dihydro-1-methyl-1-	190	C12H18Si	11
9.	(E)-4,8-Dimethyl-3,8-nonadien-2-one	166	C11H18O	11
10.	Benzenamine, N-methyl-2-(2-propenyl)-	147	C10H13N	10
11.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	10
12.	1,3,5-TRIMETHYL-2-OXABICYCLO(3.3.1)NON-3	166	C11H18O	10
13.	BENZENE, 1-FLUORO-4-(2-CYANOETHENYL)-, (	147	C9H6FN	10
14.	Bicyclo[2.2.2]octane, 1-bromo-4-methyl-	202	C9H15Br	10
15.	2,4-Cycloheptadien-1-one, 2,6,6-trimethy	150	C10H14O	10
16.	BENZENE, 1-FLUORO-4-(2-CYANOETHENYL)-, (	147	C9H6FN	10
17.	3-CAREN-10-AL	150	C10H14O	10
18.	Pentalene, octahydro-1-(2-octyldecyl)-	362	C26H50	10
19.	2-Nitro-2-(3-oxobutyl)cyclooctanone	241	C12H19NO4	10
20.	2-Butyne-1,4-diamine, N,N,N',N'-tetramet	140	C8H16N2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	006711-26-8	125589	73	35	2	57	61	14	44	66	6331
2.	35	072505-41-0	39575	62	68	1	36	54	11	0	39	7327
3.	27	051504-54-2	8754	59	47	0	58	59	8	4	39	6034
4.	16	072523-53-6	39574	56	57	1	46	59	3	6	37	6995
5.	16	006711-26-8	19588	43	68	2	51	56	3	8	37	7316
6.	12	077822-44-7	25746	46	69	2	51	63	2	0	37	5928
7.	12	055282-90-1	8595	57	46	1	78	65	2	0	37	5461
8.	*11	061141-64-8	30106	53	58	1	63	71	2	0	47	5653
9.	*11	000000-00-0	19558	48	49	1	39	72	2	0	46	6032
10.	*10	041652-73-7	11703	34	70	3	57	77	1	0	41	5378
11.	10	000080-57-9	12854	46	61	0	42	77	1	0	39	5312
12.	*10	037709-65-2	19687	34	42	0	60	77	1	14	39	5275
13.	*10	027530-50-3	11637	34	69	2	59	76	1	0	39	5502
14.	10	000697-40-5	35343	53	42	0	44	78	1	1	40	5390
15.	*10	000503-93-5	12794	39	42	0	38	78	1	16	38	4858
16.	*10	071750-12-4	11638	34	69	2	59	76	1	0	39	5491
17.	*10	000000-00-0	12814	49	30	0	42	80	1	16	41	4537
18.	10	055401-65-5	90867	56	110	2	64	68	1	18	37	6573
19.	10	086572-28-3	52904	45	90	3	188	72	1	0	39	6150
20.	*10	000111-53-5	9294	33	72	1	32	80	1	0	39	4097

CTMP Compounds

Peak 94; Syringone 1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanone



Average of 27.268 to 27.318 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2616	60.90	5	74.00	36	83.95	75
49.00	57	61.95	155	74.20	23	85.00	255
50.00	413	63.00	254	74.95	18	89.00	13
51.00	501	63.95	149	75.95	16	89.40	10
52.00	289	65.00	913	77.00	713	90.00	20
52.95	746	66.00	429	78.00	411	91.05	707
54.00	136	67.00	833	79.05	757	92.00	186
55.00	326	68.00	133	80.00	175	93.00	761
56.00	54	69.00	344	81.00	283	94.05	192
58.00	33	70.00	56	82.00	364	94.95	464
58.95	137	71.00	99	83.00	76	96.00	71

Average of 27.268 to 27.318 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.00	113	109.00	262	121.05	1099	132.95	220
98.00	2	110.00	545	122.00	475	134.05	120
99.95	8	111.00	178	123.00	762	135.00	1024
100.95	34	112.00	56	124.00	220	136.00	782
101.80	10	113.00	39	125.00	203	137.00	376
102.05	13	115.00	48	126.00	46	138.00	561
103.00	106	116.00	17	127.00	42	139.00	152
105.05	415	117.00	82	128.00	74	139.95	27
106.10	195	118.00	39	130.05	13	141.10	28
107.00	441	119.00	292	131.00	157	143.95	39
108.00	662	120.00	191	131.90	32	145.00	256

Average of 27.268 to 27.318 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.00	76	156.90	16	169.00	72	187.90	28
147.00	154	158.95	208	169.95	208	190.00	20
148.05	106	160.00	43	172.55	14	191.05	114
149.05	760	161.05	85	175.00	3	192.05	47
150.05	201	162.00	136	177.05	303	192.80	5
151.05	140	163.05	993	178.05	181	193.00	20
152.05	82	164.10	376	178.95	41	195.05	104
153.05	1100	165.00	216	181.05	9261	196.05	4684
154.00	139	165.90	65	182.00	1012	197.05	567
155.05	90	166.95	150	182.95	155	198.05	18
156.05	8	168.00	11	187.00	47		

CTMP Compounds

Average of 27.268 to 27.318 min.: A1025.D
Converted from RTE data file: >A1025:

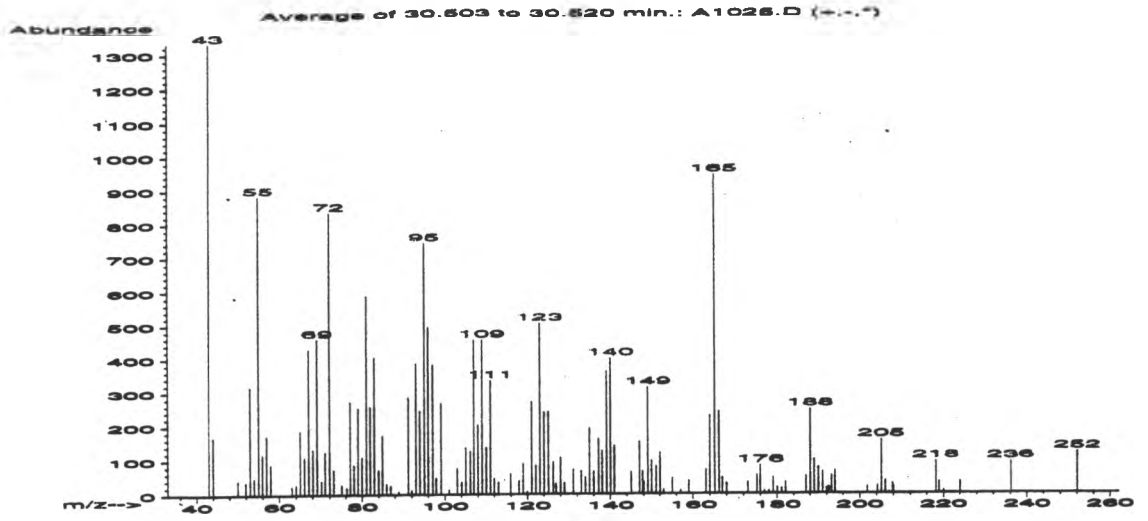
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphen	196	C10H12O4	90
2.	3,4-DIMETHOXYBENZALDEHYDE OXIME	181	C9H11NO3	49
3.	9H-Fluoren-2-amine	181	C13H11N	46
4.	Benzaldehyde, 3,4,5-trimethoxy-	196	C10H12O4	43
5.	Silane, (3-methoxyphenoxy)trimethyl-	196	C10H16O2Si	42
6.	Ethanone, 1-[1,1'-biphenyl]-4-yl-	196	C14H12O	40
7.	3-METHYLCARBAZOLE	181	C13H11N	38
8.	Benzenamine, N-(phenylmethylene)-	181	C13H11N	38
9.	Benzenamine, N-(phenylmethylene)-	181	C13H11N	38
10.	2,3,4,5,6-PENTAFLUOROBENZYL-PENTACHLOROP	444	C13H2Cl5F5O	38
11.	ETHYL ESTER OF N-P-HYDROXYPHENYLCARBAMIC	181	C9H11NO3	38
12.	2-Hydroxy-4,5-dimethoxyacetophenone	196	C10H12O4	37
13.	3,5,6-Trimethyl-6-nitrocylcohexa-2,4-die	181	C9H11NO3	37
14.	9H-Carbazole, 2-methyl-	181	C13H11N	32
15.	9H-Carbazole, 2-methyl-	181	C13H11N	32
16.	9H-Fluoren-2-amine	181	C13H11N	32
17.	Benzaldehyde, 2,4,5-trimethoxy-	196	C10H12O4	16
18.	Benzaldehyde, 3,4,5-trimethoxy-	196	C10H12O4	16
19.	2-(5'-Hydroxy-1',1',5'-trimethylhexyl)-3	224	C14H24O2	14
20.	Benzeneacetic acid, 2,5-dimethoxy-	196	C10H12O4	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	002478-38-8	32719	94	21	1	93	19	59	38	83	9834
2.	*49	002169-98-4	26049	52	62	2	69	39	23	0	46	8839
3.	*46	000153-78-6	26191	48	59	2	67	42	20	0	46	8799
4.	*43	000086-81-7	32715	38	61	1	43	42	18	12	39	7983
5.	*42	033285-71-1	32772	38	48	1	70	26	17	0	35	9781
6.	*40	000092-91-1	128050	36	75	3	91	34	16	0	35	9393
7.	*38	004630-20-0	126939	36	71	2	82	47	14	0	39	8771
8.	*38	000538-51-2	126930	34	56	2	74	50	14	1	40	8747
9.	*38	000538-51-2	26181	35	53	2	68	50	14	1	40	8747
10.	38	000000-00-0	103944	44	68	3	93	50	14	2	41	8730
11.	*38	000000-00-0	26034	46	76	3	70	39	14	0	35	8842
12.	*37	020628-06-2	32718	36	34	2	50	42	13	0	35	9690
13.	*37	000000-00-0	26041	38	39	2	69	45	13	0	35	7709
14.	*32	003652-91-3	126936	42	68	2	72	49	9	0	33	8763
15.	*32	003652-91-3	126934	42	68	2	72	49	9	0	33	8763
16.	*32	000153-78-6	126942	35	72	3	89	47	9	0	35	8793
17.	*16	004460-86-0	32714	46	79	2	39	58	3	0	35	8004
18.	*16	000086-81-7	127962	36	82	3	44	57	3	0	35	8435
19.	14	090165-05-2	45904	44	57	2	38	69	2	21	38	8775
20.	*14	001758-25-4	32701	45	62	2	50	69	2	15	38	4907

CTMP Compounds

Peak 95; Unidentified Sequiterpene



Average of 30.503 to 30.520 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1332	64.00	29	76.20	21	87.00	25
44.00	169	65.00	187	77.05	273	88.95	9
49.95	43	66.00	110	78.00	87	91.15	286
51.95	37	67.05	429	79.00	254	92.05	13
53.00	317	68.05	133	80.00	110	93.00	387
53.95	47	69.10	460	81.05	588	94.00	246
55.00	883	70.05	42	82.00	259	95.05	744
55.95	118	70.95	125	83.00	405	96.00	495
56.95	173	72.00	834	84.00	71	97.05	383
57.95	88	73.05	73	85.00	173	97.95	48
63.00	25	74.95	28	86.00	30	99.05	269

Average of 30.503 to 30.520 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.05	14	113.00	35	126.95	30	140.05	402
103.00	77	115.95	60	128.05	107	141.00	142
104.05	36	118.00	39	128.95	33	143.00	1
105.05	138	119.00	90	131.05	72	145.00	63
106.15	127	119.95	7	133.00	67	147.05	154
107.00	458	121.05	273	134.00	49	147.80	65
108.00	204	122.05	84	135.00	194	148.05	35
109.00	458	123.05	507	136.00	66	149.05	316
110.00	137	124.05	242	137.15	162	150.00	98
111.00	337	125.05	243	138.00	127	151.05	81
112.00	45	126.20	94	139.15	363	152.05	121

Average of 30.503 to 30.520 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
152.95	11	175.15	55	190.00	78	207.75	29
155.05	46	176.00	83	191.05	64	208.00	21
157.00	10	177.00	8	192.00	17	218.15	95
159.00	38	178.05	8	192.50	20	218.95	33
163.05	71	179.05	47	193.15	53	220.05	8
164.00	230	180.05	19	194.05	67	224.05	34
165.15	945	181.05	16	201.80	21	236.15	94
166.15	242	182.00	33	204.20	24	252.10	121
167.00	47	186.95	51	205.10	158		
168.00	30	188.05	250	206.05	37		
173.00	33	189.00	100	207.00	4		

CTMP Compounds

Average of 30.503 to 30.520 min.: A1025.D
Converted from RTE data file: >A1025:

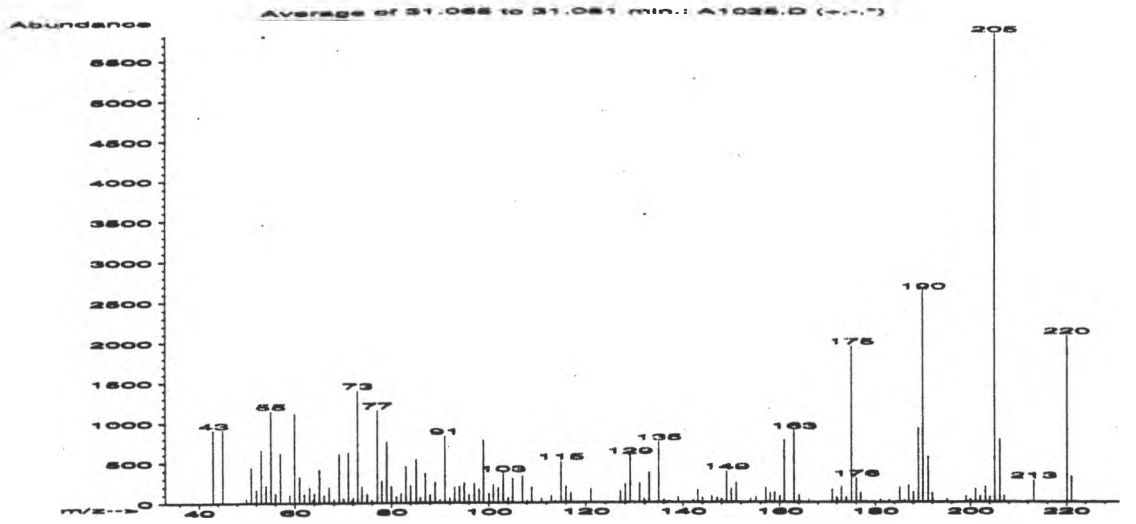
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	7(S)-10-OXO-4X1-METHYL-7-ISOPROPYL-5E-UN	252	C15H24O3	38
2.	5,5-Epoxymethano-2,2,6-trimethyl-7-oxabi	208	C12H16O3	38
3.	8-Acetyl-3,3-epoxymethano-6,6,7-trimethy	236	C14H20O3	35
4.	3-HEXEN-2-ONE, 3-CYCLOHEXYL-4-ETHYL-	208	C14H24O	25
5.	2-HEXANONE, 3-CYCLOHEXYLIDEN-4-ETHYL-	208	C14H24O	22
6.	5,5-DIMETHYL-7,8-EPOXYSPIRO[3.5]NONAN-1-	180	C11H16O2	18
7.	Ethane, (methylseleno)-	124	C3H8Se	18
8.	Spiro[cyclobutane-1,3'-[7]oxabicyclo[4.1	180	C11H16O2	14
9.	2-Propanone, 1-phenylthio-1-(1-methyleth	242	C12H15ClOS	14
10.	4-ETHOXYPYRIDINE	123	C7H9NO	14
11.	Ethynyl (1R*,2R*,5S*)-5,8,8-trimethylbic	204	C14H20O	11
12.	(Z)-4-(5',5'-Epoxymethano-1',2',2'-trime	236	C14H20O3	11
13.	(4R,5R,9S)-5,9-DIMETHYLSPIRO(3.5)NONAN-1	166	C11H18O	10
14.	(1S*,2S*,5R*,7S*)-2,4-Dimethyl-7-ethyl-6	168	C10H16O2	10
15.	6H-Purin-6-one, 1,7-dihydro-2-(methylami	165	C6H7N5O	10
16.	3,8-Nonadien-2-one, (E)-	138	C9H14O	10
17.	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	138	C10H18	10
18.	2-CHLORO-1-METHYLINDOLE	165	C9H8ClN	10
19.	6-(3'-ACETYL-1'-CYCLOPROPEN-1'-YL)-6-MET	208	C13H20O2	10
20.	Cyclohexane, 1-methyl-4-(1-methylethylid	138	C10H18	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	057213-51-1	57329	64	101	3	99	61	14	0	64	6040
2.	*38	091186-45-7	38450	70	75	3	93	65	14	0	76	7369
3.	*35	091186-43-5	50791	110	40	2	98	69	11	32	81	5202
4.	*25	000000-00-0	38687	59	79	1	72	65	7	0	46	7237
5.	22	000000-00-0	38688	61	75	2	66	65	5	0	39	7215
6.	*18	067920-67-6	25646	60	54	1	41	68	3	0	46	5434
7.	18	037773-04-9	4625	81	34	0	51	69	3	5	43	5203
8.	*14	075314-18-0	25681	60	62	2	42	68	2	0	41	5446
9.	14	069798-67-0	53200	60	83	0	64	67	2	0	43	6323
10.	*14	033399-46-1	4570	35	39	0	41	69	2	0	41	5161
11.	*11	085544-99-6	36595	49	38	0	40	76	2	0	46	5153
12.	*11	091200-98-5	50777	48	112	3	70	80	2	0	44	6632
13.	*10	000000-00-0	19624	52	59	2	40	80	1	0	39	5010
14.	*10	091860-89-8	20484	48	70	1	53	78	1	0	39	4888
15.	*10	010030-78-1	125388	41	54	0	70	80	1	0	39	5848
16.	*10	055282-90-1	8595	43	65	3	139	76	1	0	39	5089
17.	*10	000554-59-6	8831	41	50	0	45	80	1	0	39	4800
18.	*10	065610-58-4	18872	32	68	3	70	77	1	12	39	5637
19.	10	065868-83-9	38501	58	69	0	54	75	1	0	43	6617
20.	*10	001124-27-2	8812	37	54	0	43	79	1	0	41	4941

CTMP Compounds

Peak 96; Unidentified



Average of 31.065 to 31.081 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	910	59.95	1120	70.05	57	80.00	199
44.95	914	60.95	321	71.05	624	81.05	72
49.95	58	61.95	112	71.80	33	82.00	116
50.95	441	63.00	193	72.05	62	83.00	458
52.00	163	63.75	44	73.00	1398	84.00	211
53.00	663	64.00	121	73.95	195	85.10	535
54.05	218	65.00	414	75.00	111	86.00	65
55.00	1147	66.00	97	75.95	37	87.00	366
56.00	119	67.00	194	77.05	1153	88.00	98
57.00	619	68.00	46	78.05	269	89.00	258
58.95	103	69.10	604	79.05	761	90.00	41

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
91.00	834	102.00	182	116.00	198	135.00	752
92.00	60	103.00	362	117.05	115	136.05	30
93.00	188	104.05	58	121.05	165	137.05	17
94.05	201	105.05	296	126.00	1	139.05	62
94.95	245	107.00	327	127.05	145	142.05	30
95.95	101	108.05	22	128.05	230	143.10	150
97.05	237	109.00	190	129.05	582	144.05	61
98.05	169	111.00	46	130.05	13	146.00	81
98.95	782	113.05	84	131.00	238	147.05	57
100.05	114	113.90	17	131.95	45	148.00	39
101.00	222	115.00	508	133.00	371	148.95	384

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.00	171	164.05	87	178.05	17	195.05	35
151.00	241	166.15	33	181.05	31	199.10	76
152.05	2	167.00	13	182.90	33	200.05	37
153.95	44	171.05	161	185.10	179	201.05	162
155.00	63	171.95	61	186.10	22	202.05	75
157.10	181	172.20	31	187.00	210	203.10	191
158.00	111	173.00	193	188.00	122	204.05	62
159.00	125	174.00	66	189.05	930	205.05	5819
160.05	80	175.05	1944	190.00	2630	206.15	782
161.00	777	176.05	298	191.15	567	207.00	79
163.00	894	177.00	114	192.00	112	213.15	267

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
220.05	2073						
221.05	312						

CTMP Compounds

Average of 31.065 to 31.081 min.: A1025.D
Converted from RTE data file: >A1025:

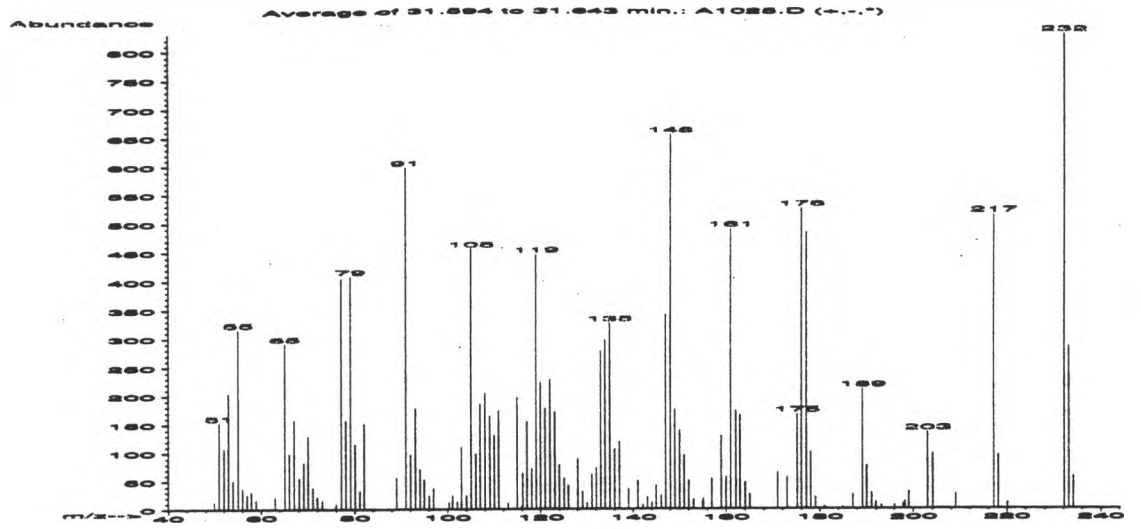
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-TRIMETHYLSILYL-5-METHOXYMETHYLBENZOCYC	220	C13H20OSi	64
2.	4-Methoxy-3-methylthioquinoline	205	C11H11NOS	56
3.	9-Phenanthrenecarbonitrile, 9,10-dihydro	205	C15H11N	53
4.	3-Methoxy-2-(methylthio)quinoline	205	C11H11NOS	52
5.	2-Amino-6-(3,5-dimethylpyrazoloyl)pyrimi	205	C9H11N5O	50
6.	6-Hydroxymethylidene-7-isopropylidene-4-	220	C13H16O3	43
7.	Benzeneacetonitrile, .alpha.-(phenylmeth	205	C15H11N	43
8.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	38
9.	Benzeneacetonitrile, .alpha.-(phenylmeth	205	C15H11N	38
10.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	35
11.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	35
12.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	35
13.	(4S,4aS,6R,8aR)-6-Isopropenyl-4,8a-dimet	220	C15H24O	35
14.	8-Allyl-2-amino-6-methylimidazo[1,5-a]-1	205	C9H11N5O	32
15.	PROPYL ESTER OF P-TERT-BUTYLBENZOIC ACID	220	C14H20O2	27
16.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	25
17.	Pyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione	205	C10H11N3O2	25
18.	5-ETHYL-4-PHENYL-3-MERCAPTO-1,2,4-TRIAZO	205	C10H11N3S	22
19.	Pyridine, 3,5-dichloro-4-methoxy-2,6-dim	205	C8H9Cl2NO	22
20.	3,5-Di-tert-butyl-1-methoxybenzene	220	C15H24O	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000000-00-0	43706	50	23	0	72	25	37	11	44	8941
2.	*56	083936-11-2	36910	39	9	1	86	12	30	0	35	8724
3.	*53	056666-55-8	128797	38	45	0	85	26	28	0	39	8721
4.	*52	035524-68-6	36909	43	80	3	90	32	27	0	44	8695
5.	*50	080081-91-0	36873	35	25	1	99	32	25	0	39	8690
6.	*43	094239-81-3	43669	33	97	3	97	45	18	0	39	7052
7.	*43	016610-80-3	37019	43	103	2	86	41	18	17	38	8551
8.	*38	000128-37-0	129737	56	62	1	83	52	14	0	47	8486
9.	*38	002510-95-4	37020	33	104	3	90	40	14	0	35	8810
10.	*35	000128-37-0	129736	57	61	2	99	55	11	0	40	8449
11.	*35	000128-37-0	129733	48	62	1	73	52	11	4	39	8507
12.	*35	000128-37-0	129735	55	55	1	83	52	11	5	38	8518
13.	*35	086921-22-4	44003	52	43	1	71	54	11	0	39	8418
14.	*32	078109-18-9	36872	38	12	2	92	50	9	9	36	8020
15.	27	000000-00-0	43735	47	68	1	88	56	8	16	38	8153
16.	*25	000128-37-0	129734	37	67	1	82	52	7	10	36	8490
17.	*25	016953-81-4	36892	33	46	1	94	62	7	8	43	7941
18.	*22	029448-76-8	128781	43	86	3	70	62	5	0	39	7938
19.	*22	051050-42-1	36859	35	91	2	99	61	5	0	39	7972
20.	*18	068039-43-0	43908	44	31	1	49	70	3	0	44	8342

CTMP Compounds

Peak 97; Unidentified Sesquiterpene



Average of 31.594 to 31.643 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.95	13	65.05	290	78.05	157	96.05	24
50.95	153	66.00	98	79.05	407	97.05	37
52.00	107	67.10	157	80.05	115	100.30	12
53.00	204	68.10	55	81.05	32	101.05	24
53.95	51	69.05	83	82.05	151	102.05	13
55.05	315	70.00	129	89.00	56	103.00	110
56.00	36	71.00	38	91.05	596	104.05	24
56.95	25	71.95	21	92.05	97	105.05	455
57.85	31	73.00	15	93.10	178	106.05	98
58.95	16	75.95	9	94.10	71	106.95	185
63.00	21	77.05	404	95.00	53	108.00	205

Average of 31.594 to 31.643 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	165	121.00	178	133.00	278	146.05	24
110.00	131	122.00	228	134.00	297	147.00	340
111.00	174	123.05	171	135.00	325	148.05	652
113.00	11	124.00	78	136.05	106	149.00	175
115.00	197	125.05	55	137.05	119	150.05	139
115.95	5	126.00	42	139.00	36	151.00	95
116.15	64	128.05	89	141.00	50	152.00	50
117.05	155	129.05	30	142.15	8	153.05	17
118.10	72	130.05	11	143.10	21	155.00	15
119.05	445	131.05	61	144.05	12	155.20	19
120.05	223	132.05	73	144.95	42	156.95	54

Average of 31.594 to 31.643 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.00	129	177.05	481	196.00	7	233.15	283
160.00	57	178.00	100	197.85	9	234.10	57
161.00	488	179.05	20	198.20	13		
162.10	172	181.00	5	199.05	30		
163.00	165	184.95	4	203.00	135		
164.05	47	187.05	25	204.10	98		
165.05	26	189.15	210	208.95	26		
171.00	64	190.05	76	217.15	513		
173.00	56	191.05	28	218.15	95		
175.10	166	192.00	12	220.05	11		
176.05	523	193.15	7	232.15	830		

CTMP Compounds

Average of 31.594 to 31.643 min.: A1025.D
Converted from RTE data file: >A1025:

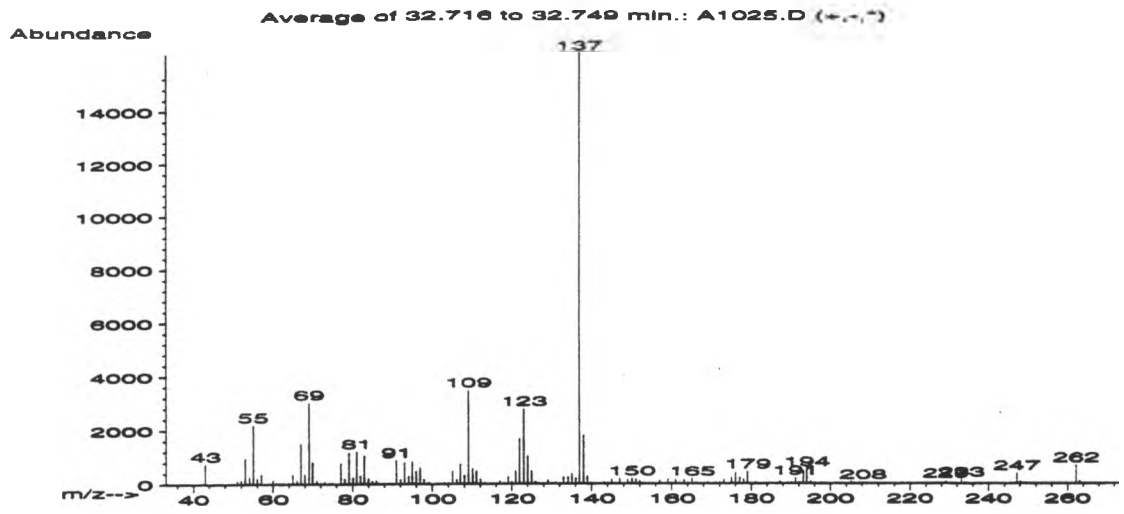
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	MEGASTIGMA-4,6(E),8(Z)-TRIENE	176	C13H20	35
2.	6-(BUT-2'-ENYLIDENE)-1,5,5-TRIMETHYLCYCL	176	C13H20	35
3.	VULGARONE B	218	C15H22O	35
4.	(+)-(4R,4aS,6S)-1-Hydroxy-6-isopropenyl-	232	C15H20O2	30
5.	3,8-.alpha.-Furanether	232	C15H20O2	30
6.	2H-1-Benzopyran-2-one, 7-hydroxy-4-methy	176	C10H8O3	25
7.	Furan, 2-[(2-ethoxy-3,4-dimethyl-2-cyclo	232	C15H20O2	20
8.	MEGASTIGMA-4,6(Z),8(Z)-TRIENE	176	C13H20	18
9.	Aromadendrene	204	C15H24	18
10.	Pyrido[3,2-d]pyrimidin-4(3H)-one, 3-hydr	177	C8H7N3O2	15
11.	MEGASTIGMA-4,6(Z),8(E)-TRIENE	176	C13H20	15
12.	MEGASTIGMA-4,6(E),8(E)-TRIENE	176	C13H20	15
13.	3,6-Dimethylspiro[4.5]deca-2,6-dien-1-on	176	C12H16O	15
14.	(6Z,2'E)-6-(BUT-2'-ENYLIDENE)-1,5,5-TRIM	176	C13H20	15
15.	(6E,2'E)-6-(BUT-2'-ENYLIDENE)-1,5,5-TRIM	176	C13H20	15
16.	Nootkatone	218	C15H22O	15
17.	Benzene, 1-methoxy-4-(2-propenyl)-	148	C10H12O	11
18.	Isolongifolene	204	C15H24	11
19.	Benzene, 1-methoxy-4-(1-propenyl)-	148	C10H12O	11
20.	Benzene, 1-methoxy-4-(1-propenyl)-	148	C10H12O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	000000-00-0	24054	78	57	0	54	70	11	37	72	5826
2.	*35	071186-24-8	24049	78	57	0	54	70	11	37	72	5826
3.	*35	064180-68-3	43053	77	88	0	50	67	11	25	66	6034
4.	*30	086917-83-1	49251	49	68	1	99	58	9	0	44	6919
5.	*30	076601-35-5	49255	55	113	3	96	60	9	0	49	7120
6.	*25	000090-33-5	23771	49	63	1	58	61	7	6	47	5806
7.	*20	055162-49-7	49232	69	61	1	84	70	4	19	50	6683
8.	*18	071186-25-9	24052	63	73	0	54	68	3	14	47	6075
9.	*18	000489-39-4	36770	67	90	2	112	69	3	28	47	5439
10.	*15	003303-23-9	24133	58	55	1	40	79	2	0	56	4831
11.	*15	000000-00-0	24053	70	65	0	54	76	2	26	59	5729
12.	*15	000000-00-0	24055	70	65	0	54	76	2	24	59	5749
13.	*15	085620-39-9	23973	63	50	1	128	78	2	0	58	4977
14.	*15	051468-85-0	24047	70	65	0	54	76	2	26	59	5729
15.	*15	051468-86-1	24048	70	65	0	54	76	2	24	59	5749
16.	*15	004674-50-4	43011	69	80	1	34	80	2	12	53	5646
17.	*11	000140-67-0	123419	58	65	1	60	73	2	0	46	4541
18.	*11	001135-66-6	128737	56	77	0	53	79	2	19	46	5151
19.	*11	000104-46-1	123412	53	55	0	70	73	2	0	49	4524
20.	*11	000104-46-1	123411	56	58	0	66	73	2	0	49	4524

CTMP Compounds

Peak 98; Unidentified sesquiterpene



Average of 32.716 to 32.749 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	742	62.40	16	75.00	26	88.90	25
50.00	20	63.95	55	77.05	770	91.00	868
51.00	112	65.00	361	78.00	190	92.05	156
52.00	133	66.05	114	79.05	1156	93.05	803
53.00	972	67.00	1496	80.05	222	94.10	292
54.05	262	68.05	347	81.05	1192	95.05	835
55.00	2195	69.05	3035	82.00	301	96.00	484
56.00	197	69.95	808	83.00	1051	97.00	605
57.00	359	71.00	102	84.00	190	97.95	167
59.95	129	72.05	12	85.00	90	99.20	56
60.90	36	73.05	71	85.95	111	102.05	22

Average of 32.716 to 32.749 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.00	38	115.00	3	126.00	71	137.00	16103
103.95	28	116.00	11	127.00	6	138.05	1804
105.05	464	117.00	97	128.05	1	139.05	288
106.05	149	118.00	46	129.05	129	140.00	30
107.00	736	119.05	267	130.05	7	141.05	12
108.00	310	119.95	83	131.05	52	143.10	60
109.00	3475	121.00	493	131.95	12	144.00	13
110.05	585	122.05	1678	133.00	236	145.00	137
111.05	481	123.05	2783	134.10	251	146.05	17
112.10	171	124.05	1024	135.10	383	147.05	168
113.05	34	125.00	469	136.05	196	149.05	148

Average of 32.716 to 32.749 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.05	185	164.00	15	179.05	448	196.05	14
151.05	159	165.10	181	180.05	10	196.95	13
152.00	90	166.10	34	181.05	40	198.05	15
153.00	28	169.00	38	187.15	81	201.20	32
154.05	17	171.00	42	189.10	51	205.15	81
157.00	100	172.05	45	190.15	48	206.05	19
159.10	171	173.05	144	191.15	206	208.15	41
159.95	27	175.05	230	192.15	49	208.95	3
161.00	140	176.05	397	193.15	455	211.00	19
162.05	26	177.05	209	194.05	533	218.15	20
163.05	127	178.05	141	195.05	81	219.95	6

CTMP Compounds

Average of 32.716 to 32.749 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
226.05	16						
229.05	86						
233.10	144						
234.05	41						
247.15	379						
248.10	80						
262.15	679						
263.15	95						

Average of 32.716 to 32.749 min.: A1025.D
Converted from RTE data file: >A1025:

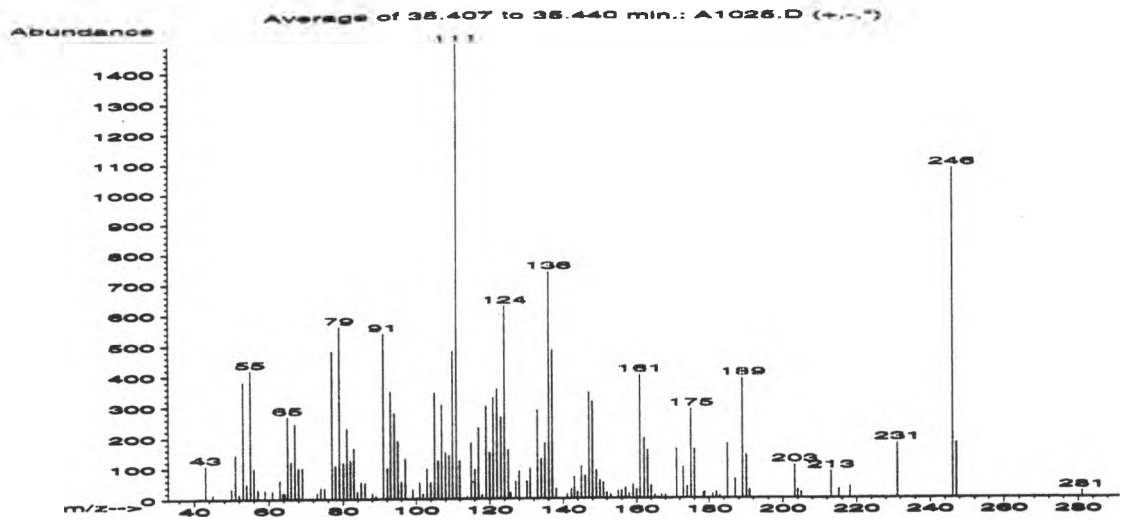
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3,6-DIMETHYL-2,3,3A,4,5,7A-HEXAHYDROBENZ	152	C10H16O	64
2.	2-Butanone, 4-(4-hydroxy-3-methoxyphenyl	194	C11H14O3	53
3.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	53
4.	Benzeneacetic acid, 4-hydroxy-3-methoxy-	182	C9H10O4	50
5.	Benzaldehyde, 4-[(4-hydroxy-3-methoxyphe	288	C16H16O5	50
6.	2(1H)-Pyridinone, 1,4,6-trimethyl-	137	C8H11NO	50
7.	Benzeneacetic acid, 4-hydroxy-3-methoxy-	182	C9H10O4	42
8.	Benzeneacetic acid, 4-hydroxy-3-methoxy-	196	C10H12O4	42
9.	4-Nitroso-3-methylphenol	137	C7H7NO2	42
10.	3-(3-HYDROXY-4-METHOXYPHENYL)-L-ALANINE	247	C10H14ClNO4	40
11.	Benzeneacetic acid, 4-hydroxy-3-methoxy-	182	C9H10O4	38
12.	Silane, trimethyl(4-methyl-3-penten-1-yn	152	C9H16Si	38
13.	(E)-4-(2',6',6'-Trimethyl-1',2'-epoxycyc	222	C14H22O2	38
14.	ETHAN, 1,2-BIS(PHENYLMERCAPTO)-	246	C14H14S2	36
15.	2-AMINO-4,5,6,7-D4-BENZIMIDAOLE	133	C7H3D4N3	36
16.	TRANS-1-TRIMETHYLSILYLHEX-3-EN-1-YNE	152	C9H16Si	33
17.	BORNYL ESTER OF 3-ISOPROPYLIDENE-CYCLOPE	290	C19H30O2	32
18.	Benzaldehyde, 3-hydroxy-, oxime	137	C7H7NO2	28
19.	Benzeneacetic acid, 4-hydroxy-3-methoxy-	182	C9H10O4	27
20.	BUTANE, 1,2-DIDEUTERO-2-(P-ANISYL)-	164	C11H14D2O	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	070786-44-6	13847	57	36	3	95	20	37	14	41	9786
2.	*53	000122-48-5	31742	59	39	3	95	28	28	20	41	8881
3.	*53	002785-89-9	13455	41	38	2	82	30	28	17	39	9657
4.	50	000306-08-1	126983	43	58	2	72	31	25	0	39	9636
5.	50	077745-46-1	69846	48	74	3	68	18	25	9	37	9913
6.	*50	015031-89-7	8286	36	62	2	96	18	25	0	35	9825
7.	42	000306-08-1	126982	50	40	2	68	28	17	8	36	9703
8.	42	015964-80-4	32692	48	60	2	97	30	17	0	35	9671
9.	*42	000615-01-0	8262	34	32	2	99	30	17	6	35	9770
10.	40	035296-56-1	55027	54	73	1	87	31	16	0	36	9660
11.	38	000306-08-1	26394	48	46	2	94	38	14	5	33	9610
12.	38	062338-12-9	13564	39	54	2	78	38	14	0	33	9621
13.	38	089128-12-1	44868	43	51	1	76	36	14	0	37	9643
14.	36	000000-00-0	54771	38	90	3	90	30	12	0	29	9727
15.	*36	000000-00-0	7100	31	62	3	90	30	12	6	29	9768
16.	33	060216-43-5	13562	40	55	2	76	35	10	0	29	9702
17.	32	000000-00-0	70699	55	61	2	61	50	9	5	33	8868
18.	*28	022241-18-5	8270	30	58	2	99	38	8	0	27	9452
19.	27	000306-08-1	126981	54	48	2	63	58	8	0	39	9646
20.	*22	000000-00-0	18598	29	47	2	58	63	5	11	39	9600

CTMP Compounds

Peak 99; Unidentified



Average of 35.407 to 35.440 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	110	61.00	27	71.95	5	83.95	24
44.95	14	63.00	61	73.00	21	85.00	55
49.95	34	63.75	18	73.95	36	86.00	52
51.00	144	64.05	20	75.00	35	88.00	19
51.95	16	64.25	17	77.00	482	89.00	10
53.00	382	65.05	269	78.00	110	91.00	539
54.00	49	66.00	121	79.05	562	92.10	100
55.05	419	67.10	244	80.05	118	93.05	349
56.00	100	68.00	100	81.05	229	94.05	279
57.00	31	69.05	101	82.00	125	95.00	189
58.95	30	71.05	5	83.00	166	96.00	56

Average of 35.407 to 35.440 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.00	131	109.00	141	121.00	329	134.10	131
99.05	31	110.00	482	122.00	358	135.00	183
100.00	5	111.00	1487	123.05	265	136.05	742
101.00	54	112.00	123	124.05	629	137.05	484
101.95	17	113.95	8	125.05	159	138.10	32
103.00	99	115.00	183	125.70	19	141.05	15
104.00	53	116.05	96	127.05	57	142.15	31
105.05	345	117.05	231	128.05	90	143.05	72
106.05	125	118.00	13	130.10	57	143.95	22
107.00	307	119.00	300	131.00	100	145.00	105
108.00	151	120.00	151	133.05	290	146.05	75

Average of 35.407 to 35.440 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.05	347	159.05	45	172.95	101	189.10	391
148.05	315	160.00	29	174.00	39	190.15	140
149.05	91	161.00	402	175.05	291	191.00	27
150.00	60	162.10	197	176.00	160	203.15	108
151.00	51	163.05	157	178.45	18	204.05	28
152.00	18	164.00	43	178.80	21	204.95	19
153.00	12	165.05	11	181.05	14	209.05	1
155.00	24	166.00	4	182.00	21	213.05	87
155.95	26	166.90	12	183.00	8	215.15	28
157.00	34	168.00	11	185.00	178	218.15	37
158.00	15	171.05	162	187.05	63	224.00	5

CTMP Compounds

Average of 35.407 to 35.440 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
231.20	179						
246.15	1086						
247.20	180						
281.05	22						

Average of 35.407 to 35.440 min.: A1025.D
Converted from RTE data file: >A1025:

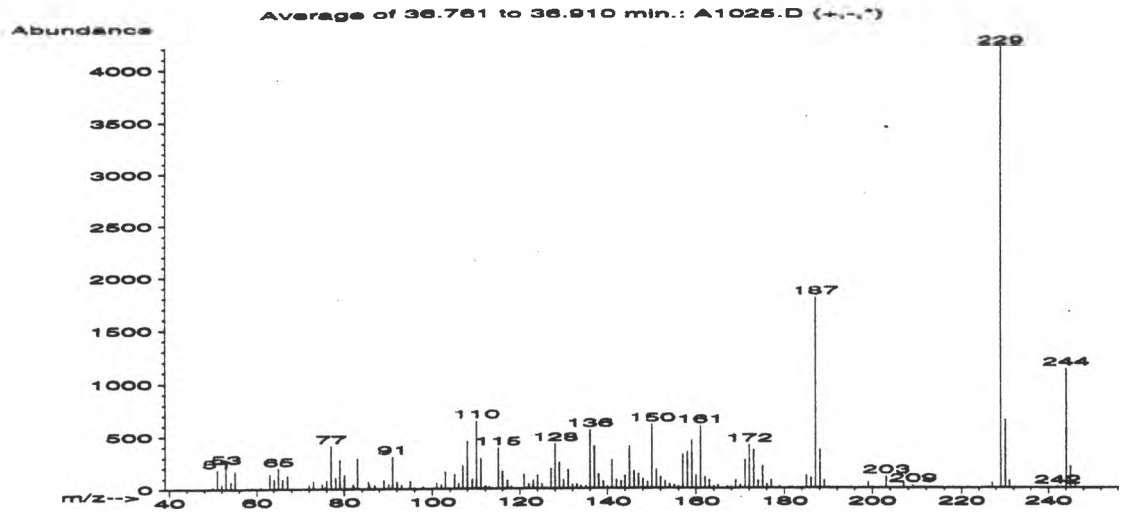
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	8-METHYL-5-METHYLBENZO(1,2-B:5,4-B')DIFU	246	C13H10O5	64
2.	Benzo[1,2-b:5,4-b']difuran-4,8-dione, 2,	246	C14H14O4	35
3.	Chrysene, octadecahydro-	246	C18H30	11
4.	METHYL 3-THIOPHENECARBOXYLATE	142	C6H6O2S	11
5.	3-MERCAPTOPYRIDINE	111	C5H5NS	11
6.	4,4-DI-N-PROPYL-1-PHENYLTHIO-1-CYCLOBUTE	246	C16H22S	11
7.	TRIDEUTERIOMETHOXYBENZENE	108	C7H5D3O	11
8.	11,12-Dehydrolupanine	246	C15H22N2O	10
9.	Pimpinellin	246	C13H10O5	10
10.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
11.	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	10
12.	5-Hydroxy-11-oxo-benzo[a]fluorene	246	C17H10O2	10
13.	N2-PHENYLSULFONYL-N1-PENTANETHYLENEFORMA	252	C12H16N2O2S	9
14.	3-PHENYLTHIO-4-N-PROPYLHEPTA-1,3-DIENE	246	C16H22S	9
15.	6,8-Dimethoxy-1,2,3,4-tetrahydrodibenzof	246	C14H14O4	9
16.	METHYL 2-THIOPHENECARBOXYLATE	142	C6H6O2S	9
17.	(E)-9-((2'S,3'R)-3-HYDROXY-6'-((E)-2''-H	352	C21H36O4	9
18.	(+)-Methyl-4-[(1'R)-2'-methyl-3'-oxocycl	212	C12H20O3	9
19.	3-METHYL-(2,6-DIMETHYLHEPTYL)-2-PENTEN-5	238	C15H26O2	9
20.	Cyclohexane, 1,4-dimethyl-2-octadecyl-	364	C26H52	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	068454-45-5	54690	35	34	0	68	22	37	4	43	5096
2.	*35	027304-03-6	54756	64	106	2	54	66	11	0	64	5701
3.	*11	002090-14-4	131135	50	116	3	77	74	2	0	44	6059
4.	*11	000000-00-0	9797	34	34	0	87	74	2	18	43	6657
5.	*11	016133-26-9	2327	35	51	2	82	74	2	2	43	6657
6.	*11	000000-00-0	54920	56	79	3	107	74	2	0	47	5852
7.	*11	004019-63-0	1919	34	49	0	77	74	2	2	43	6657
8.	*10	035611-60-0	54864	44	96	1	58	77	1	0	39	5525
9.	*10	000131-12-4	54685	45	101	2	73	72	1	0	40	5426
10.	*10	000071-30-7	118914	41	40	2	88	74	1	11	38	6657
11.	*10	000071-30-7	118913	39	47	1	80	74	1	0	39	6657
12.	*10	000000-00-0	54935	39	23	0	48	77	1	1	40	5221
13.	9	000000-00-0	57129	39	43	0	74	74	1	0	33	6657
14.	* 9	000000-00-0	54922	58	109	2	63	74	1	0	37	5261
15.	* 9	095361-60-7	54763	39	87	1	51	80	1	0	35	5188
16.	* 9	000000-00-0	9796	31	42	0	71	74	1	2	35	6657
17.	9	071117-50-5	88544	48	100	3	90	71	1	11	33	6726
18.	9	090898-60-5	40328	49	59	2	99	72	1	6	33	6765
19.	9	053042-71-0	51785	40	46	2	99	74	1	12	34	6657
20.	9	055282-02-5	91309	47	82	1	76	74	1	0	35	6657

CTMP Compounds

Peak 100; Unidentified



Average of 36.761 to 36.910 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.00	9	63.00	138	77.05	410	86.95	35
49.90	20	64.05	95	78.05	111	87.95	4
51.00	181	65.00	197	79.05	279	89.00	83
52.00	44	66.00	93	80.10	133	90.10	44
53.00	225	67.05	125	81.05	9	91.00	308
54.05	71	72.00	38	81.95	44	92.05	72
55.00	170	73.00	76	82.15	34	93.10	37
57.90	8	75.00	50	83.00	294	94.05	1
58.95	11	75.45	5	85.50	71	95.05	77
59.95	9	75.70	11	85.75	45	96.00	12
60.90	19	76.00	85	86.00	9	98.00	21

Average of 36.761 to 36.910 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.95	1	110.00	648	122.00	42	133.00	42
100.30	8	111.05	289	123.05	84	133.95	28
101.00	58	112.00	26	124.00	129	135.05	29
102.05	40	112.20	17	125.00	43	136.00	561
103.00	162	113.00	19	126.00	3	137.05	404
103.95	5	114.00	1	127.05	192	138.05	138
105.05	138	115.00	389	128.05	427	139.05	71
106.00	48	116.00	165	129.05	249	140.00	20
106.95	225	117.05	80	130.00	87	141.00	274
108.00	456	118.00	22	131.05	179	142.05	87
109.05	94	121.00	136	132.00	37	143.05	71

Average of 36.761 to 36.910 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.00	123	155.05	34	167.05	20	178.00	2
145.00	400	156.00	20	168.00	19	179.00	19
146.00	166	157.00	326	168.95	84	180.00	1
146.95	138	158.00	351	170.00	34	181.20	11
148.00	91	159.00	460	171.05	275	181.90	8
149.00	64	160.00	122	172.05	414	182.95	2
150.00	610	161.00	594	173.05	367	184.00	6
151.00	179	162.05	109	174.00	74	185.05	124
152.00	112	163.00	83	175.05	213	186.05	100
153.00	73	164.05	21	176.05	39	187.05	1804
154.00	40	165.00	33	177.00	81	188.10	366

CTMP Compounds

Average of 36.761 to 36.910 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
189.05	74	200.05	7	228.05	4		
190.25	5	200.30	4	229.10	4208		
190.95	2	202.05	9	230.10	652		
192.00	8	203.10	111	231.10	75		
193.05	5	207.00	48	242.10	11		
193.95	6	209.05	29	243.20	10		
195.10	12	209.75	5	244.05	1132		
197.05	2	211.15	5	245.05	207		
197.95	6	217.15	5	246.10	26		
199.05	62	218.20	6				
199.55	3	227.10	48				

Average of 36.761 to 36.910 min.: A1025.D
Converted from RTE data file: >A1025:

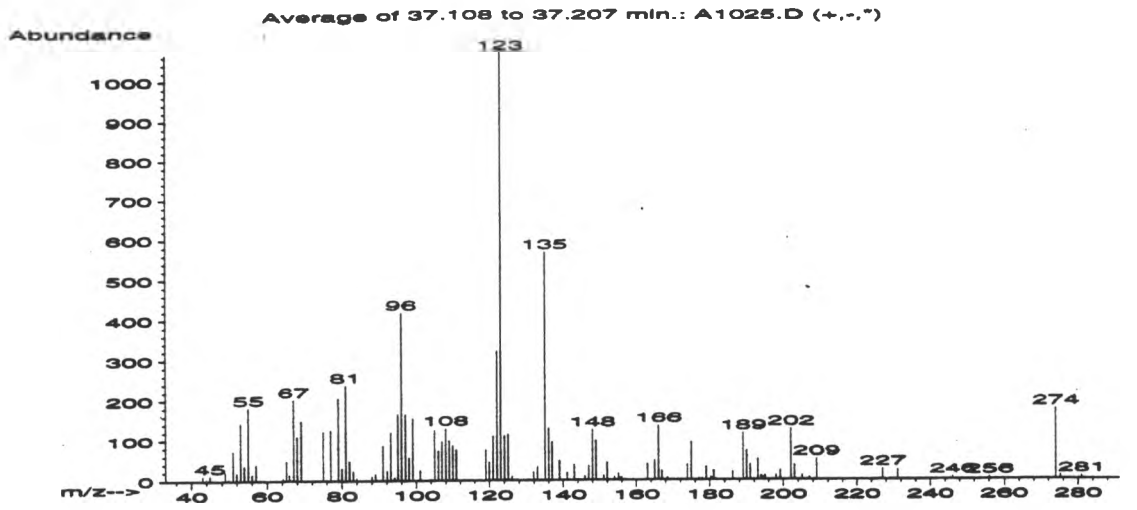
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-(2-Methylphenyl)-3-aldoximido-2(1H)-py	244	C13H12N2OS	83
2.	5-ACETYL-1,1,2,3,3,6-HEXAMETHYL INDAN	244	C17H24O	49
3.	2,3,6,7,10,11-HEXAHYDRO-1H,5H,9H-(1)BENZ	229	C16H7NO	38
4.	Naphthalene, 2,6-bis(1,1-dimethylethyl)-	244	C18H28	38
5.	Suberosin	244	C15H16O3	35
6.	10H-Phenothiazine, 1-methoxy-	229	C13H11NOS	35
7.	2,2-DIMETHYL-3-METHOXYCARBONYL-5-PHENYL-	229	C14H15NO2	35
8.	TETRAISOPROPYLIDENE-CYCLOPENTANONE	244	C17H24O	35
9.	4-D3-METHOXYXANTHONE	226	C14H7D3O3	35
10.	Benzo[a]acridine	229	C17H11N	35
11.	Benzo[a]acridine	229	C17H11N	35
12.	Evolitine	229	C13H11NO3	35
13.	1,1,3,3,5-PENTAMETHYL-6-T-BUTYL-2,3-DIHY	244	C18H28	32
14.	6,7-METHYLENDIOXYTHIENO(2,3-B)QUINOLINE	229	C12H7NO2S	32
15.	1,1,3,3,4-PENTAMETHYL-6-T-BUTYL-2,3-DIHY	244	C18H28	32
16.	Styrene, 2,3,4,5,6-pentaethyl-	244	C18H28	27
17.	Naphthalene, 6,7-diethyl-1,2,3,4-tetrahy	244	C18H28	25
18.	METHYL N-(2,4-DIMETHYL-1-NAPHTHYL)CARBAM	229	C14H15NO2	25
19.	Cyclopenta[c][1]benzopyran-4(1H)-one, 7-	229	C14H15NO2	25
20.	BENZO(c)ACRIDINE	229	C17H11N	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	091540-40-8	54001	34	11	1	96	0	50	0	39	9011
2.	*49	000000-00-0	54260	51	34	1	83	37	23	0	46	9483
3.	*38	000000-00-0	48057	43	65	1	79	50	14	0	40	8734
4.	*38	042981-76-0	54291	50	90	2	99	40	14	0	30	9401
5.	*35	000581-31-7	54152	37	88	1	62	55	11	11	40	8525
6.	*35	001576-70-1	47974	42	74	3	76	55	11	0	39	8700
7.	*35	063405-40-3	48002	39	84	2	92	55	11	0	39	8699
8.	*35	000000-00-0	54250	43	78	1	45	52	11	0	39	9235
9.	*35	041977-78-0	46758	37	83	3	99	55	11	0	41	8700
10.	*35	000225-11-6	130295	37	88	2	81	55	11	0	41	8695
11.	*35	000225-11-6	48072	33	88	2	80	55	11	0	39	8694
12.	*35	000000-00-0	47984	37	78	2	98	53	11	0	39	8761
13.	32	000000-00-0	54287	43	82	3	99	50	9	0	35	8989
14.	*32	062638-09-9	47946	41	69	3	89	50	9	7	36	8733
15.	32	000000-00-0	54286	40	77	2	79	47	9	0	33	8969
16.	*27	002715-34-6	131033	49	87	3	62	60	8	0	39	9010
17.	25	055741-10-1	54294	42	88	3	78	43	7	2	29	9167
18.	*25	063953-45-7	48012	30	20	1	79	55	7	2	35	8697
19.	*25	062669-74-3	48024	33	83	2	85	53	7	6	35	8730
20.	*25	000000-00-0	48071	42	73	1	77	53	7	0	35	8713

CTMP Compounds

Peak 101; Unidentified Diterpene



Average of 37.108 to 37.207 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	12	57.00	39	81.05	237	96.00	418
43.95	4	64.25	6	82.00	48	97.00	165
44.90	12	65.10	48	83.00	22	98.00	57
48.90	20	65.95	14	84.00	5	99.00	154
49.90	3	67.05	202	88.00	9	101.00	25
51.00	74	68.00	109	88.95	16	104.10	3
52.00	18	69.05	148	91.00	87	105.00	125
53.00	143	75.00	122	92.10	23	106.05	74
54.00	36	77.00	125	93.10	120	107.00	97
55.00	182	79.05	205	94.10	7	108.00	130
56.00	15	80.00	31	95.00	165	109.00	99

Average of 37.108 to 37.207 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	87	131.95	20	149.00	98	168.50	5
111.00	75	133.00	33	151.05	11	173.95	38
113.95	1	135.00	569	152.00	44	175.00	94
119.00	75	136.05	129	154.05	7	177.05	4
120.00	45	137.05	95	155.20	15	178.00	3
121.00	110	139.05	49	155.80	5	179.00	33
122.05	322	141.10	18	156.05	5	180.30	6
123.05	1067	143.05	38	163.00	40	181.00	23
124.05	111	145.95	9	165.05	49	186.20	20
125.05	115	147.00	36	166.10	136	189.05	117
126.05	9	148.05	126	167.00	22	190.05	72

Average of 37.108 to 37.207 min.: A1025.D
Converted from RTE data file: >A1025:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.00	38	209.00	52				
193.10	51	227.05	26				
193.95	9	231.15	24				
194.30	7	246.20	6				
195.00	11	256.15	5				
198.05	10	274.05	177				
199.20	23	275.20	10				
202.10	127	281.00	8				
203.05	37						
205.05	11						
207.00	5						

CTMP Compounds

Average of 37.108 to 37.207 min.: A1025.D
Converted from RTE data file: >A1025:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	32
2.	(t-2-Isopropenyl-c-5-methyl-r-1-cyclopen	166	C11H18O	30
3.	2-Pyrimidinamine, N,N-dimethyl-	123	C6H9N3	30
4.	Phenol, 4-amino-2-methyl-	123	C7H9NO	30
5.	Phenol, 3-amino-2-methyl-	123	C7H9NO	27
6.	Benzenemethanol, 3-amino-	123	C7H9NO	27
7.	3-Isopropenyl-6-methyl-5-hepten-2-one	166	C11H18O	25
8.	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	22
9.	2,2,3,4,5,5-HEXAMETHYL-2,5-DIHYDROTHIOPH	202	C10H18O2S	22
10.	3-Heptyne, 5,5-diethyl-	152	C11H20	22
11.	(Z,1'R*,3'S*,6'R*)-4-(3',4',4'-Trimethyl	220	C14H20O2	14
12.	CIS-1-TRIMETHYLSILYLPENT-3-EN-1-YNE	138	C8H14Si	14
13.	(Z,1'R*,3'R*,6'R*)-4-(3',4',4'-Trimethyl	220	C14H20O2	14
14.	TRANS-2-HYDROXYMETHYL-3-ISOPROPYLIDEN-1-	154	C10H18O	14
15.	trans-DL-Chrysanthemumic acid	168	C10H16O2	12
16.	cis-Chrysanthemic acid	168	C10H16O2	12
17.	TRANS-.BETA.-IONON-5,6-EPOXIDE	208	C13H20O2	12
18.	Ethyl chrysanthemumate	196	C12H20O2	12
19.	Pyrethrin I	328	C21H28O3	10
20.	Bicyclo[2.2.2]octane, 1-methyl-4-(methyl	202	C10H18O2S	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*32	000767-15-7	4538	42	51	2	90	50	9	0	35	8405
2.	*30	074063-72-2	19585	65	49	3	81	62	9	0	58	7915
3.	*30	005621-02-3	4537	57	60	3	99	57	9	0	49	8228
4.	*30	002835-96-3	4588	34	50	2	93	58	9	14	43	8199
5.	*27	053222-92-7	4586	40	41	2	78	58	8	15	38	8171
6.	*27	001877-77-6	4580	52	37	1	99	58	8	2	41	8176
7.	*25	026533-38-0	19563	56	57	3	74	62	7	0	47	7914
8.	22	051504-54-2	8754	59	45	0	73	64	5	0	43	8058
9.	*22	000000-00-0	35388	43	51	1	69	62	5	18	39	7689
10.	22	061228-06-6	13862	46	56	3	85	62	5	0	39	8093
11.	14	090242-89-0	43770	43	30	0	90	66	2	0	39	7853
12.	14	062170-41-6	122254	50	34	1	83	66	2	9	38	7853
13.	14	090242-91-4	43769	44	27	2	68	66	2	6	41	7853
14.	14	013012-42-5	14643	43	37	2	99	66	2	0	39	7853
15.	12	000705-16-8	20340	46	52	2	80	64	2	3	37	8084
16.	12	015259-78-6	20339	45	56	2	87	65	2	7	35	8001
17.	12	023267-57-4	38551	44	63	1	85	62	2	0	35	8387
18.	12	000097-41-6	32943	44	77	3	97	64	2	0	35	7939
19.	10	000121-21-1	82395	43	107	2	82	66	1	0	37	7853
20.	10	069855-48-7	35391	59	51	3	96	66	1	0	36	7854

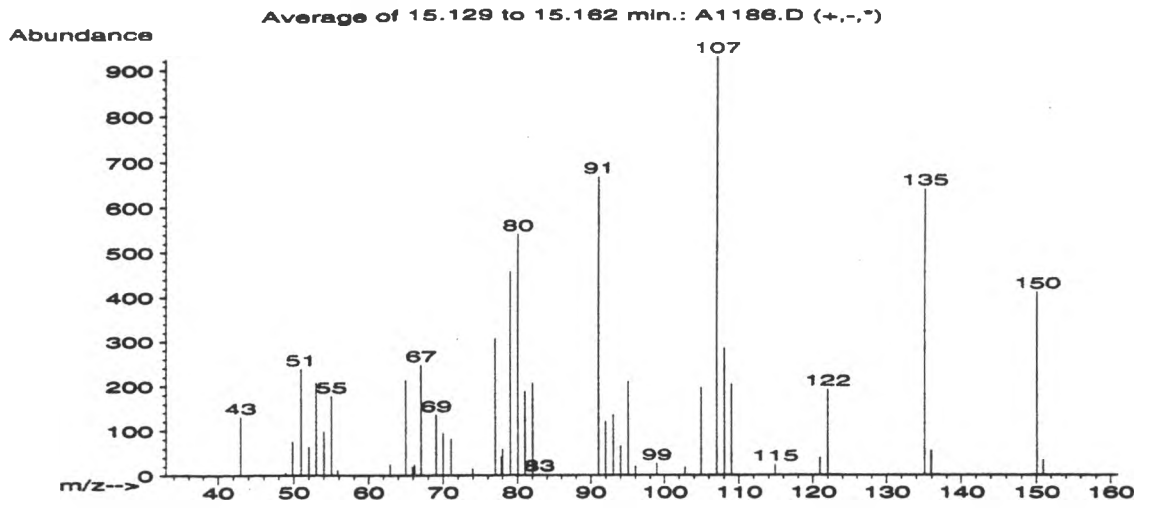
Pages 267 through 274 are not available in printed form

(CTMP Compounds - Peaks 102 through 105)

To view the data from these pages please see the mass spectral database contained on the diskettes included with NRBS Project Report No. 138, "Broad Spectrum Analysis of Municipal and Industrial Effluents Discharged into the Peace, Athabasca and Slave River Basins, Evaluation of Surface Waters"

CTMP Compounds

Peak 106; Monoterpene (4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one)



Average of 15.129 to 15.162 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	130	65.90	19	80.05	538	102.80	18
48.90	6	66.15	24	81.00	187	104.95	195
49.85	75	67.05	247	82.05	206	107.05	924
50.95	238	69.10	135	82.95	2	108.05	283
52.00	64	70.00	94	91.00	662	109.00	202
52.95	207	71.05	81	91.95	120	110.95	2
54.00	98	73.95	14	93.00	134	114.90	23
55.00	177	77.00	306	94.00	65	120.95	40
55.80	11	77.80	42	95.00	208	122.00	190
62.90	24	78.00	59	96.00	20	135.05	636
65.00	212	79.00	456	98.95	26	135.95	55

Average of 15.129 to 15.162 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.10	409						
150.90	34						

CTMP Compounds

Average of 15.129 to 15.162 min.: A1186.D
Converted from RTE data file: >A1186:

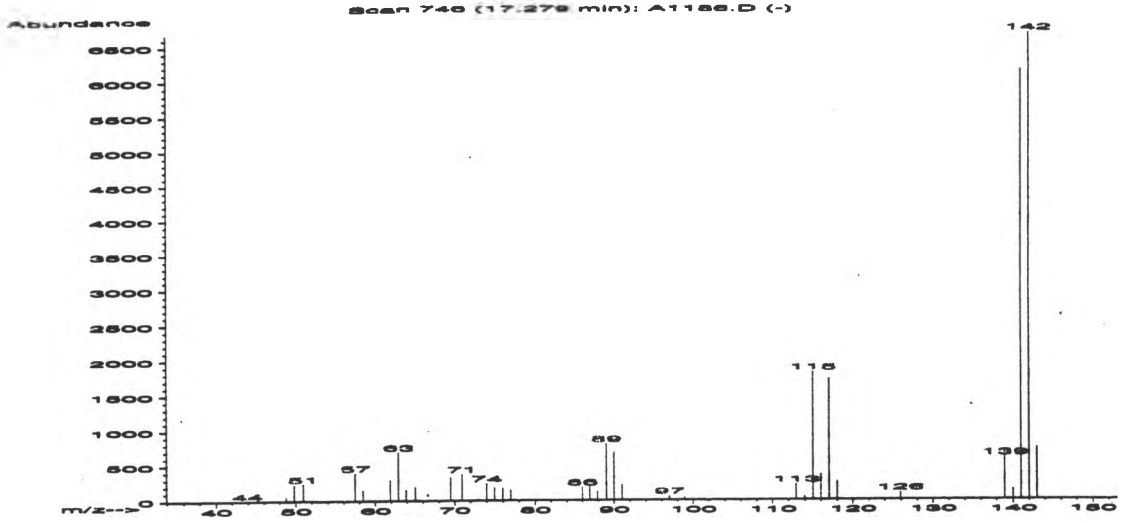
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	94
2.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	87
3.	1,3-Dimethylbicyclo[3.3.0]oct-3-en-2-one	150	C10H14O	83
4.	2-Cyano-1,3,4-trimethyl-3-piperidine	150	C9H14N2	83
5.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	81
6.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	62
7.	2-Cyclohexen-1-one, 3-methyl-6-(1-methyl	150	C10H14O	49
8.	2,4-Cycloheptadien-1-one, 2,6,6-trimethy	150	C10H14O	49
9.	1-Phenyl-1-butanol	150	C10H14O	38
10.	BENZENE, 1-ETHOXY-4-ETHYL-	150	C10H14O	35
11.	1,5-Hexadiene, 2,5-dimethyl-3-methylene-	122	C9H14	35
12.	Pyridine, 3,5-dimethyl-	107	C7H9N	27
13.	Phenol, 4-butyl-	150	C10H14O	25
14.	Benzenemethanol, .alpha.-methyl-	122	C8H10O	18
15.	Benzenemethanol, .alpha.-methyl-	122	C8H10O	18
16.	2-PINENE-9-AL	150	C10H14O	18
17.	BICYCLO(3.3.1)NON-2-ENE	122	C9H14	14
18.	Ethanamine, 1-(2,4-cyclopentadien-1-ylid	135	C9H13N	11
19.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	10
20.	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	150	C9H10O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	018309-32-5	12853	82	53	1	77	5	70	0	84	9882
2.	*87	000080-57-9	12854	78	36	1	96	11	54	16	72	9810
3.	*83	070640-02-7	12804	36	13	0	48	0	50	0	41	5276
4.	*83	073657-70-2	12678	31	8	0	50	0	50	9	42	5113
5.	*81	000080-57-9	123741	75	20	1	99	17	49	39	66	9679
6.	*62	000080-57-9	123740	69	24	1	88	29	36	36	58	9400
7.	*49	000491-09-8	123725	68	50	1	75	38	23	18	47	8350
8.	*49	000503-93-5	123728	64	49	1	99	39	23	0	50	8496
9.	*38	000000-00-0	12746	43	54	0	96	47	14	15	40	7435
10.	*35	000000-00-0	12763	34	59	0	87	55	11	0	41	7935
11.	*35	059131-13-4	4462	49	53	2	83	51	11	12	39	7018
12.	*27	000591-22-0	118623	43	90	2	67	58	8	0	39	7757
13.	*25	001638-22-8	12720	61	42	1	73	61	7	6	47	6878
14.	*18	000098-85-1	120231	48	46	1	46	66	3	0	46	7121
15.	*18	000098-85-1	120234	49	40	0	46	68	3	0	46	7080
16.	*18	069855-03-4	12851	50	53	2	47	66	3	0	44	5166
17.	*14	006671-66-5	4497	44	51	2	46	68	2	0	39	5367
18.	*11	014469-77-3	7590	46	66	0	58	76	2	0	44	5431
19.	*10	000089-83-8	123683	33	70	3	194	76	1	0	41	6119
20.	*10	001450-72-2	12615	36	59	0	51	72	1	0	41	6315

CTMP Compounds

Peak 107; Methylnaphthalene with Indole impurity



Scan 746 (17.279 min): A1186.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	5	70.95	368	91.00	216	140.00	144
48.80	57	72.95	16	97.00	52	141.00	6148
49.80	228	73.95	241	98.95	40	142.00	6675
50.95	241	74.95	181	112.90	223	143.00	738
57.45	394	75.95	171	113.95	43		
58.45	145	76.95	142	115.00	1815		
61.90	294	86.00	185	116.00	359		
62.90	691	86.90	193	117.00	1722		
63.90	151	87.90	117	118.00	259		
65.00	190	89.00	801	125.95	101		
69.50	329	90.00	681	139.00	603		

CTMP Compounds

Scan 746 (17.279 min): A1186.D

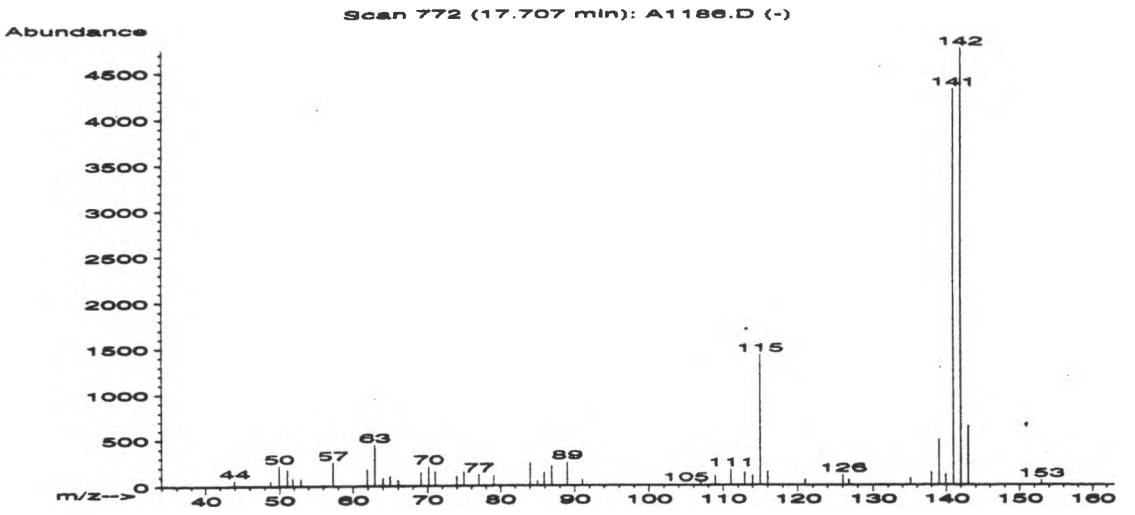
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Naphthalene, 2-methyl-	142	C11H10	81
2.	Naphthalene, 1-methyl-	142	C11H10	81
3.	Naphthalene, 1-methyl-	142	C11H10	81
4.	Naphthalene, 2-methyl-	142	C11H10	74
5.	Naphthalene, 2-methyl-	142	C11H10	74
6.	Naphthalene, 1-methyl-	142	C11H10	74
7.	Naphthalene, 1-methyl-	142	C11H10	74
8.	Naphthalene, 1-methyl-	142	C11H10	74
9.	VINYLINDENE	142	C11H10	72
10.	Naphthalene, 2-methyl-	142	C11H10	72
11.	Naphthalene, 1-methyl-	142	C11H10	72
12.	Naphthalene, 1-methyl-	142	C11H10	72
13.	Naphthalene, 2-methyl-	142	C11H10	64
14.	Naphthalene, 2-methyl-	142	C11H10	64
15.	7H-BENZOCYCLOHEPTENE	142	C11H10	64
16.	AZULENE, 1- AND 2-METHYL-,	142	C11H10	64
17.	1H-Indene, 1-ethylidene-	142	C11H10	58
18.	Naphthalene, 1-methyl-	142	C11H10	58
19.	Naphthalene, 1-methyl-	142	C11H10	52
20.	Naphthalene, 2-methyl-	142	C11H10	50

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*81	000091-57-6	122763	68	25	1	90	17	49	26	70	9739
2.	*81	000090-12-0	122759	68	25	1	88	17	49	21	70	9744
3.	*81	000090-12-0	122757	84	10	0	87	17	49	37	80	9644
4.	*74	000091-57-6	122764	69	30	1	91	16	44	0	53	9751
5.	*74	000091-57-6	10279	66	27	2	90	17	44	5	56	9676
6.	*74	000090-12-0	122758	62	37	2	96	20	44	0	51	9704
7.	*74	000090-12-0	122756	65	26	1	93	17	44	7	56	9736
8.	*74	000090-12-0	122755	63	32	1	78	18	44	4	51	9771
9.	*72	063927-06-0	10275	63	39	3	81	20	42	13	45	9702
10.	*72	000091-57-6	122761	51	42	1	95	18	42	0	44	9694
11.	*72	000090-12-0	122754	64	35	1	89	17	42	0	50	9699
12.	*72	000090-12-0	122753	50	50	3	98	20	42	0	46	9767
13.	*64	000091-57-6	122762	52	36	0	76	22	37	0	46	9738
14.	*64	000091-57-6	122760	48	50	3	99	22	37	0	44	9764
15.	*64	000000-00-0	10280	52	46	2	92	24	37	0	46	9726
16.	*64	000000-00-0	10277	51	32	1	91	21	37	0	46	9682
17.	*58	002471-83-2	10276	64	33	1	89	26	32	0	44	9561
18.	*58	000090-12-0	122752	58	39	1	75	33	32	0	51	9692
19.	*52	000090-12-0	10278	57	38	1	82	33	27	0	47	9714
20.	*50	000091-57-6	122765	54	44	1	79	32	25	0	40	9702

CTMP Compounds

Peak 108; Methylnaphthalene



Scan 772 (17.707 min): A1186.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	64	64.00	84	85.00	52	115.00	1422
48.80	52	64.95	106	85.90	143	116.00	148
49.95	220	66.00	63	86.90	216	121.00	56
51.05	179	69.10	149	89.00	254	126.05	109
51.80	87	70.15	207	91.00	64	126.80	54
52.95	75	71.00	161	104.95	11	135.05	70
54.00	7	73.95	101	106.95	42	136.05	1
56.00	6	74.95	153	108.95	99	137.05	12
57.30	256	77.00	120	111.05	171	137.95	138
61.90	179	79.05	110	112.90	137	139.00	492
62.90	446	84.05	250	114.00	102	139.90	115

Scan 772 (17.707 min): A1186.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
141.00	4305						
142.00	4751						
143.00	642						
152.95	50						

CTMP Compounds

Scan 772 (17.707 min): A1186.D

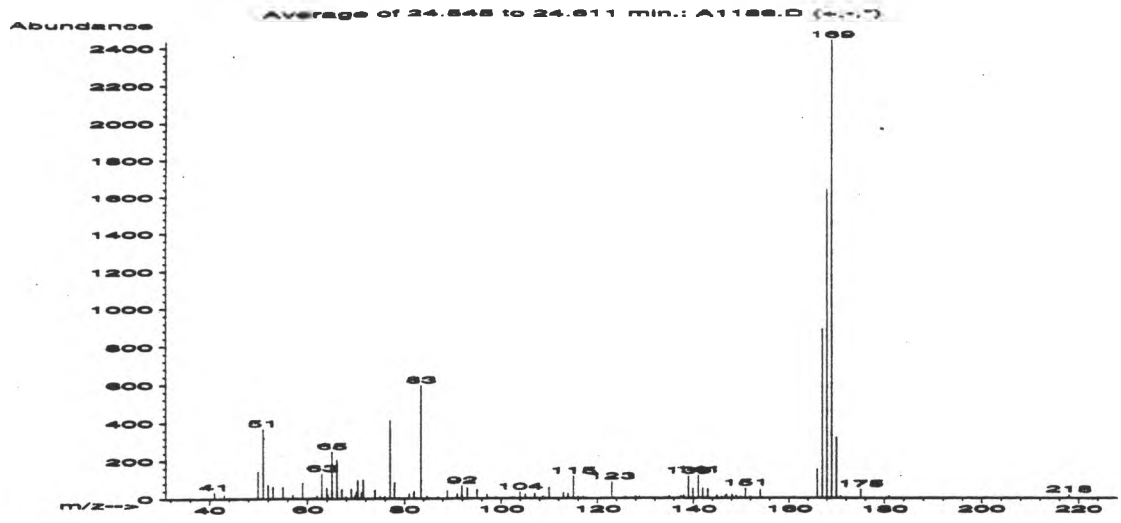
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Naphthalene, 2-methyl-	142	C11H10	94
2.	Naphthalene, 1-methyl-	142	C11H10	94
3.	Naphthalene, 2-methyl-	142	C11H10	91
4.	Naphthalene, 1-methyl-	142	C11H10	91
5.	Naphthalene, 1-methyl-	142	C11H10	91
6.	Naphthalene, 1-methyl-	142	C11H10	91
7.	Naphthalene, 2-methyl-	142	C11H10	90
8.	Naphthalene, 2-methyl-	142	C11H10	90
9.	Naphthalene, 1-methyl-	142	C11H10	90
10.	Naphthalene, 1-methyl-	142	C11H10	90
11.	Naphthalene, 1-methyl-	142	C11H10	90
12.	Naphthalene, 2-methyl-	142	C11H10	87
13.	7H-BENZOCYCLOHEPTENE	142	C11H10	87
14.	1,4-Methanonaphthalene, 1,4-dihydro-	142	C11H10	86
15.	Naphthalene, 2-methyl-	142	C11H10	86
16.	BENZOCYCLOHEPTATRIENE	142	C11H10	83
17.	AZULENE, 1- AND 2-METHYL-,	142	C11H10	80
18.	Naphthalene, 1-methyl-	142	C11H10	78
19.	Naphthalene, 2-methyl-	142	C11H10	76
20.	Naphthalene, 1-methyl-	142	C11H10	76

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000091-57-6	122764	81	18	2	99	4	70	0	90	9955
2.	*94	000090-12-0	122752	90	8	1	95	4	70	1	91	9908
3.	*91	000091-57-6	10279	78	14	1	95	4	62	17	81	9884
4.	*91	000090-12-0	122757	85	10	0	96	5	62	37	80	9868
5.	*91	000090-12-0	122755	74	21	1	88	5	62	8	76	9973
6.	*91	000090-12-0	10278	75	21	1	99	4	62	0	81	9926
7.	*90	000091-57-6	122763	74	19	1	98	6	59	20	76	9936
8.	*90	000091-57-6	122760	71	26	2	82	6	59	2	70	9958
9.	*90	000090-12-0	122759	73	20	1	98	6	59	0	81	9941
10.	*90	000090-12-0	122754	69	31	3	99	6	59	0	68	9902
11.	*90	000090-12-0	122753	70	29	2	83	6	59	0	76	9962
12.	*87	000091-57-6	122761	68	25	1	98	6	54	2	58	9896
13.	*87	000000-00-0	10280	75	21	1	84	6	54	20	59	9914
14.	*86	004453-90-1	10281	63	34	2	90	6	53	12	47	9926
15.	*86	000091-57-6	122762	66	25	1	93	6	53	6	45	9915
16.	*83	000264-09-5	10284	69	25	0	68	11	50	25	58	9596
17.	*80	000000-00-0	10277	57	26	1	89	12	48	0	49	9840
18.	*78	000090-12-0	122756	61	30	2	96	7	46	2	41	9916
19.	*76	000091-57-6	122765	70	27	1	67	24	45	0	68	9916
20.	*76	000090-12-0	122758	75	21	1	83	24	45	0	81	9909

CTMP Compounds

Peak 109; N-Phenylbenzamine



Average of 24.545 to 24.611 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.00	34	61.90	15	70.30	99	83.50	596
43.00	19	62.95	131	71.15	31	84.70	12
43.95	8	63.95	55	71.45	100	87.00	9
49.90	145	64.15	20	73.85	45	88.95	43
50.95	369	65.00	248	74.95	11	91.00	27
51.95	72	66.00	204	75.95	11	91.95	68
53.00	63	67.00	48	77.00	413	93.00	57
55.00	61	67.90	9	77.95	85	95.00	46
57.00	19	69.00	52	79.00	2	97.05	19
58.25	1	69.80	15	81.00	24	98.90	5
59.00	85	70.05	35	82.00	40	102.30	8

Average of 24.545 to 24.611 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.95	33	125.80	11	141.05	123	151.95	9
105.00	21	127.00	1	141.95	53	154.00	43
107.00	26	127.90	13	143.05	49	165.95	154
108.70	12	128.80	9	144.90	16	167.00	892
110.00	58	130.95	2	145.90	7	168.00	1641
112.95	30	134.95	13	146.75	16	169.00	2433
113.90	25	136.95	4	147.00	19	170.00	321
115.00	118	137.45	13	148.10	20	170.90	10
116.00	9	138.00	16	149.00	12	175.05	47
117.00	11	138.95	118	149.90	7	180.95	13
123.00	89	139.90	52	150.95	52	218.00	17

CTMP Compounds

Average of 24.545 to 24.611 min.: A1186.D
Converted from RTE data file: >A1186:

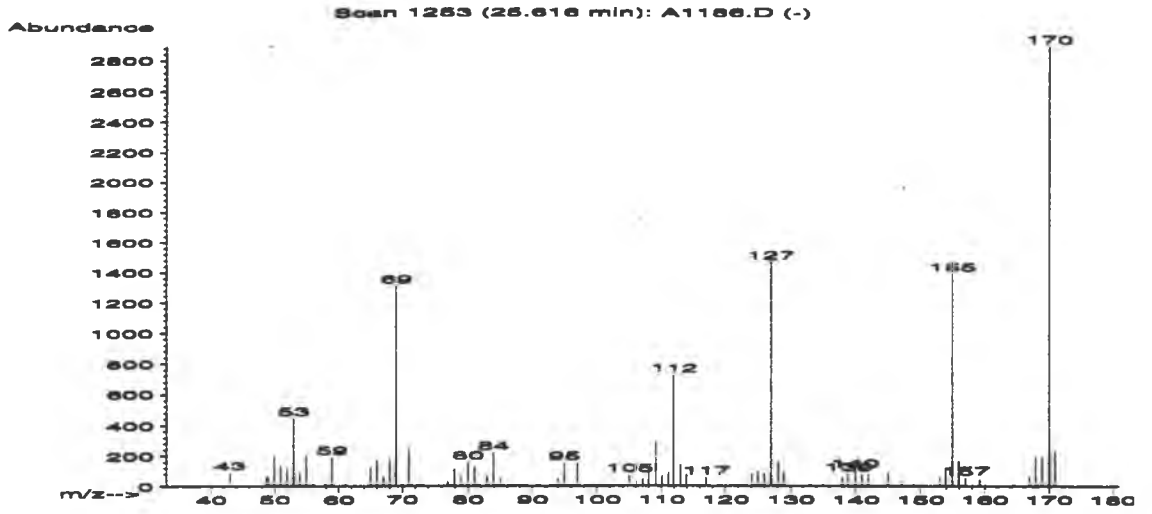
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenamine, N-phenyl-	169	C12H11N	95
2.	Hydrazine, 1,1-diphenyl-2-(2,4,6-trinitr	395	C18H13N5O6	90
3.	Benzenamine, N-phenyl-	169	C12H11N	76
4.	Benzenamine, N-phenyl-	169	C12H11N	76
5.	Pyridine, 4-(phenylmethyl)-	169	C12H11N	76
6.	Benzenamine, N-phenyl-	169	C12H11N	76
7.	Hydrazinecarboxamide, N,N-diphenyl-	227	C13H13N3O	72
8.	Benzenamine, N-phenyl-	169	C12H11N	70
9.	Benzenamine, N-phenyl-	169	C12H11N	70
10.	Benzenamine, N-phenyl-	169	C12H11N	68
11.	[1,1'-Biphenyl]-2-amine	169	C12H11N	64
12.	[1,1'-Biphenyl]-2-amine	169	C12H11N	64
13.	Benzenamine, N-phenyl-	169	C12H11N	64
14.	Benzenamine, N-phenyl-	169	C12H11N	58
15.	Urea, N,N'-diphenyl-	212	C13H12N2O	53
16.	[1,1'-Biphenyl]-4-amine	169	C12H11N	50
17.	[1,1'-Biphenyl]-3-amine	169	C12H11N	46
18.	Benzenamine, N-nitroso-N-phenyl-	198	C12H10N2O	38
19.	Benzyl benzoate	212	C14H12O2	35
20.	1,1'-Biphenyl, 2-methyl-	168	C13H12	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000122-39-4	125853	90	5	1	94	14	74	0	95	9583
2.	90	001707-75-1	96920	110	27	1	91	9	59	0	64	9964
3.	*76	000122-39-4	125849	72	25	1	95	22	45	0	76	9479
4.	*76	000122-39-4	125854	77	16	0	74	24	45	24	66	9386
5.	*76	002116-65-6	21014	75	14	2	84	24	45	35	66	9347
6.	*76	000122-39-4	21015	66	27	1	99	25	45	0	64	9202
7.	72	000603-51-0	47143	81	37	1	67	14	42	1	40	9813
8.	*70	000122-39-4	125852	74	16	1	94	29	41	10	66	9307
9.	*70	000122-39-4	125847	69	26	1	81	27	41	0	76	9294
10.	*68	000122-39-4	125848	58	38	1	86	25	40	0	56	9286
11.	*64	000090-41-5	125855	47	35	2	82	25	37	0	44	9340
12.	*64	000090-41-5	21016	65	25	2	82	24	37	18	47	9347
13.	*64	000122-39-4	125846	86	10	0	75	35	37	45	80	9150
14.	*58	000122-39-4	125850	44	36	1	99	27	32	0	44	9179
15.	53	000102-07-8	129195	73	46	1	74	29	28	0	41	9671
16.	*50	000092-67-1	125856	43	50	2	96	33	25	0	40	8845
17.	*46	002243-47-2	21017	48	43	2	77	44	20	0	44	8772
18.	38	000086-30-6	128187	57	59	1	58	49	14	6	41	8598
19.	35	000120-51-4	40479	47	65	1	59	51	11	5	41	8633
20.	*35	000643-58-3	125814	43	47	2	45	55	11	0	40	6889

CTMP Compounds

Peak 110; Unidentified Hydrocarbon



Scan 1253 (25.616 min): A1186.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	92	58.95	191	77.95	111	105.95	30
48.70	55	61.00	35	78.95	64	107.05	47
49.05	56	65.00	122	80.05	160	107.95	112
49.95	201	66.00	173	81.05	128	109.05	295
50.95	128	67.00	61	82.95	66	110.05	64
51.95	112	68.00	179	83.95	222	111.05	85
52.95	444	69.00	1308	85.05	43	111.90	726
53.95	86	70.05	20	93.95	46	113.00	140
54.95	205	71.00	244	95.00	152	113.90	73
56.05	25	72.95	9	97.00	148	117.00	58
57.95	36	76.95	29	105.00	75	121.00	10

Scan 1253 (25.616 min): A1186.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.00	12	139.95	107	159.20	44		
124.05	79	141.00	78	166.90	61		
124.95	94	142.00	76	167.90	196		
125.95	80	145.00	87	168.90	192		
126.95	1472	147.10	41	170.00	2891		
128.05	168	149.00	14	170.90	236		
128.95	96	153.05	55				
132.95	17	153.95	106				
135.05	33	154.95	1396				
138.00	69	155.95	168				
138.90	80	157.05	55				

CTMP Compounds

Scan 1253 (25.616 min): A1186.D

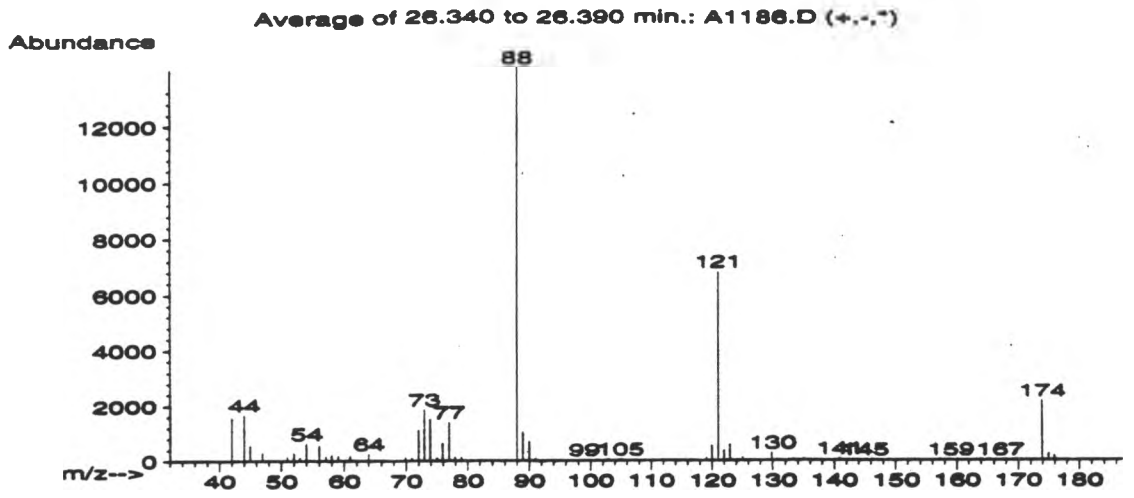
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	6-(Dimethylamino)-5.5-dimethyl-4,5-dihyr	170	C7H14N4O	47
2.	N-Methylbarbital	198	C9H14N2O3	40
3.	Naphthalene, 1,6,7-trimethyl-	170	C13H14	38
4.	Naphthalene, 2,3,6-trimethyl-	170	C13H14	38
5.	Naphthalene, 2,3,6-trimethyl-	170	C13H14	37
6.	AZULENE, 2,4,6-TRIMETHYL-	170	C13H14	22
7.	5-HYDROXYMETHYL-1,3-DIMETHYL-URACIL	170	C7H10N2O3	17
8.	Benzoic acid, 3,4,5-trihydroxy-	170	C7H6O5	16
9.	Thiazole, 4-ethyl-2-propyl-	155	C8H13NS	14
10.	TRIETHYL(1-PENTENYL)-SILANE	184	C11H24Si	12
11.	1-Isoquinolinecarbonitrile, 2-oxide	170	C10H6N2O	12
12.	Naphthalene, 2,3,6-trimethyl-	170	C13H14	10
13.	(TRIFLUOROACETAMIDO)SULPHUR PENTAFLUORID	239	C2HF8NOS	10
14.	2-BUTYL-4,5-DIMETHYLTHIAZOLE	169	C9H15NS	10
15.	Isothiazole, trimethyl-	127	C6H9NS	10
16.	Thiazole, 2-ethyl-5-methyl-	127	C6H9NS	10
17.	4,5-DIMETHYL-2-ISOBUTYLTHIAZOLE	169	C9H15NS	9
18.	3-Pentenoic acid, 2,2-diethyl-	156	C9H16O2	9
19.	3-NITRO-4-METHYLPYRAZOLE	127	C4H5N3O2	9
20.	4(5)-METHYL-5(4)-NITROIMIDAZOLE	127	C4H5N3O2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	068765-44-6	21118	38	19	0	84	39	20	1	40	8773
2.	40	000050-11-3	128153	39	79	2	79	34	16	7	34	8898
3.	*38	002245-38-7	126033	38	67	3	74	39	14	1	32	8848
4.	*38	000829-26-5	126035	55	48	2	69	40	14	4	31	8939
5.	*37	000829-26-5	21690	30	69	3	99	43	13	2	31	8800
6.	22	000000-00-0	21680	46	52	1	50	63	5	13	38	8990
7.	*17	000000-00-0	21111	31	90	2	75	51	3	0	26	7639
8.	*16	000149-91-7	21077	36	59	2	90	59	3	0	35	8010
9.	14	041981-68-4	14985	45	61	2	50	69	2	18	38	4931
10.	12	000000-00-0	27610	50	52	1	46	60	2	0	27	5571
11.	*12	006969-11-5	125912	28	85	2	67	58	2	0	27	8254
12.	10	000829-26-5	126034	44	48	0	26	73	1	13	41	8892
13.	10	080409-41-2	51995	45	71	1	50	76	1	0	39	6356
14.	*10	000000-00-0	20939	43	40	2	39	79	1	9	38	4070
15.	*10	039228-36-9	5557	37	69	2	50	72	1	0	39	4493
16.	*10	019961-53-6	5551	34	61	1	42	76	1	0	39	4470
17.	* 9	000000-00-0	20940	39	49	2	46	77	1	0	35	4198
18.	* 9	038477-07-5	15337	37	63	2	50	76	1	0	35	4122
19.	* 9	038858-90-1	120655	33	52	1	35	80	1	0	30	4065
20.	* 9	014003-66-8	5495	33	42	1	44	76	1	7	37	4117

CTMP Compounds

Peak 111; Unidentified Sulpher containing hydrocarbon



Average of 26.340 to 26.390 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1545	59.00	163	73.95	1515	91.00	80
44.00	1664	60.90	165	74.95	98	98.95	28
44.95	559	63.90	250	75.95	657	102.95	43
46.90	279	65.00	20	76.95	1396	104.95	52
50.90	147	66.00	12	77.90	123	108.00	5
51.95	276	68.00	2	79.00	128	119.00	84
52.95	124	69.00	26	83.00	4	119.95	563
54.00	625	69.95	111	85.80	4	121.00	6767
56.00	556	71.00	93	88.00	14003	121.95	370
57.00	148	72.00	1120	88.95	1029	122.95	583
58.00	210	72.95	1850	90.00	695	125.00	87

Average of 26.340 to 26.390 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.95	11	152.95	7				
127.95	11	158.95	12				
129.85	268	161.95	13				
130.70	25	163.20	20				
131.00	5	167.00	24				
133.20	14	173.95	2143				
133.55	15	175.00	230				
134.10	22	175.95	169				
135.00	50	177.00	10				
140.95	71						
145.00	14						

CTMP Compounds

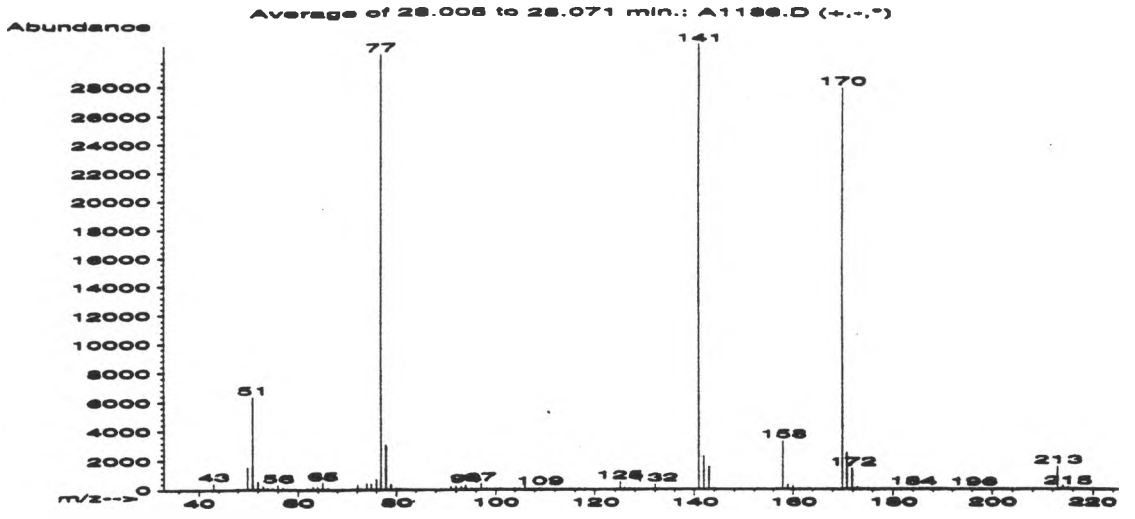
Average of 26.340 to 26.390 min.: A1186.D
Converted from RTE data file: >A1186:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Propene, 3-(methylthio)-	88	C4H8S	50
2.	METHYL 2,3,4-TRI-O-METHYL-6-DEOXY-.ALPHA	220	C10H20O5	40
3.	Phosphoric acid, methylsilylene P,P'-bis	462	C17H40O8P2Si	39
4.	2-Propanol, 1,1'-iminobis-	133	C6H15NO2	37
5.	PROPYL N,N-DIMETHYLDITHIOCARBAMATE	163	C6H13NS2	36
6.	.beta.-D-Glucopyranoside, methyl 2,3,4,6	250	C11H22O6	33
7.	Heptanoic acid, 2,4-dimethyl-, methyl es	172	C10H20O2	33
8.	Thietane, 2-methyl-	88	C4H8S	33
9.	Carbamodithioic acid, dimethyl-, methyl	135	C4H9NS2	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*50	010152-76-8	117228	37	62	0	95	31	25	0	41	8886
2.	40	072983-16-5	43493	39	56	1	94	34	16	10	31	8874
3.	39	019097-77-9	105870	52	110	2	79	20	15	0	27	9787
4.	*37	000110-97-4	7087	35	62	2	86	41	13	0	35	8800
5.	36	000000-00-0	17951	47	42	1	77	27	12	5	27	9748
6.	33	003149-65-3	56238	33	94	2	76	32	10	0	22	8880
7.	33	018450-78-7	22289	34	76	1	99	34	10	0	22	8873
8.	*33	017837-41-1	225	28	91	1	85	31	10	0	27	8884
9.	*22	003735-92-0	7501	34	56	1	62	62	5	18	40	8850

Peak 112; N-Butyl-benzenesulphonamide



Average of 28.005 to 28.071 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	427	57.95	20	74.00	445	91.00	225
47.80	26	61.90	87	74.95	393	91.95	261
48.95	34	62.95	191	76.00	712	93.00	189
49.95	1553	63.95	166	76.95	30133	94.00	283
50.95	6353	65.00	455	78.00	3066	95.10	82
52.00	525	66.00	127	79.00	330	96.00	43
53.00	189	68.05	3	80.00	54	97.00	370
53.90	70	69.00	63	81.00	56	98.00	17
55.00	52	71.05	53	82.00	24	98.15	12
56.00	310	72.05	338	84.00	1	98.95	2
57.00	103	72.95	66	85.95	32	101.00	19

Average of 28.005 to 28.071 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.95	14	115.90	8	132.00	346	147.95	5
103.95	108	116.95	89	133.00	47	152.95	12
105.00	60	118.05	52	134.00	44	154.05	8
106.05	311	119.00	42	135.00	24	156.95	48
107.00	68	120.05	16	136.00	13	157.95	3286
108.05	33	124.15	12	137.95	17	158.95	315
109.00	101	124.95	516	140.90	30760	159.95	196
110.20	19	125.95	69	141.90	2286	163.20	15
111.05	22	127.00	49	142.95	1558	168.90	46
113.00	2	127.95	5	143.90	87	169.95	27843
115.00	11	130.95	10	145.00	7	170.95	2507

Average of 28.005 to 28.071 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
171.95	1409	204.95	9				
172.95	106	206.45	7				
175.05	10	213.05	1541				
180.00	10	214.00	194				
184.00	67	215.05	95				
187.00	42						
188.05	15						
188.95	14						
189.20	10						
195.90	10						
196.15	11						

CTMP Compounds

Scan 1393 (27.923 min): A1186.D

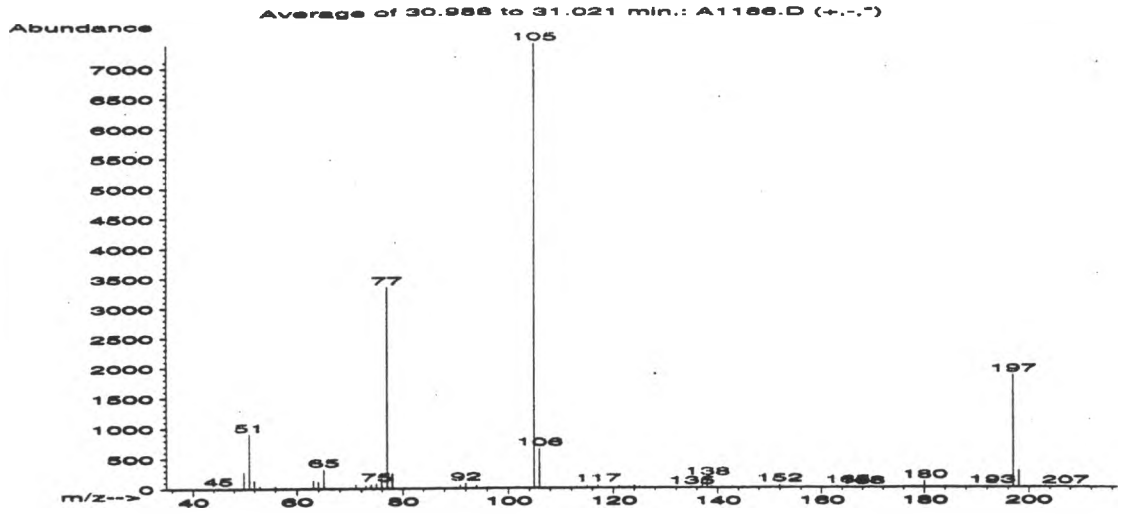
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	97
2.	N-PROPYL BENZENESULFONAMIDE	199	C9H13NO2S	50
3.	CYCLOBUTA(1,2-D)BENZYNE	170	C12H10O	50
4.	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	43
5.	P-CHLORO MANDELIC ACID	186	C8H7ClO3	38
6.	O-[L-2-(Benzolsulfonyloxy)propionyl]-ace	301	C13H19NO5S	33
7.	3,3-Dimethyl-1-phenyltriazene	149	C8H11N3	22
8.	DIPYRIDYL-(2)-AMINE	171	C10H9N3	17
9.	BIS(4-PYRIDYL)METHANE	170	C11H10N2	12
10.	[1,1'-Biphenyl]-4-ol, acetate	212	C14H12O2	10
11.	4-BENZOLSULFONAMIDE-1,2,4-TRIAZOL	224	C8H8N4O2S	10
12.	Benzene, 1-(ethenylsulfonyl)-4-nitro-	213	C8H7NO4S	8
13.	5-Nonanone, 2-(dimethylamino)-1-phenyl-	261	C17H27NO	8
14.	DIETHYLPARABANATE	170	C7H10N2O3	8
15.	5-Nitro-2-furaldehyde	141	C5H3NO4	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*97	003622-84-2	129253	108	10	1	89	2	78	14	95	9903
2.	50	000000-00-0	34217	47	67	1	65	35	25	0	39	9921
3.	*50	059817-14-0	21644	30	28	2	87	16	25	1	30	7878
4.	*43	003622-84-2	40734	43	59	0	44	47	18	0	44	9962
5.	38	000000-00-0	28166	39	87	2	86	37	14	2	31	8454
6.	33	000000-00-0	74134	34	27	1	75	35	10	0	22	8473
7.	22	007227-91-0	12260	47	29	1	68	65	5	9	38	6109
8.	17	001202-34-2	126058	36	38	2	58	55	3	0	22	4771
9.	*12	000000-00-0	21590	43	63	1	59	62	2	12	37	5552
10.	10	000148-86-7	40477	38	56	1	59	70	1	0	33	5563
11.	10	029982-62-5	45486	45	55	0	62	76	1	0	39	7342
12.	8	005535-55-7	40684	33	83	3	61	67	1	0	22	5897
13.	8	027820-12-8	60078	33	69	3	67	70	1	0	21	5279
14.	* 8	000000-00-0	21108	28	81	1	65	70	1	0	26	5279
15.	* 7	000698-63-5	122522	29	75	1	83	72	1	0	27	5851

CTMP Compounds

Peak 113, N-Phenylbenzamide



Average of 30.988 to 31.021 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.90	14	72.95	47	90.00	12	119.00	5
49.95	273	73.80	24	90.95	58	121.00	35
50.95	906	74.00	68	92.00	87	123.00	21
51.95	137	74.95	80	94.05	51	124.00	43
53.00	42	75.95	164	96.00	3	124.95	29
55.95	45	77.00	3346	104.95	7388	126.00	12
57.90	15	78.00	246	105.95	657	128.90	12
63.00	136	80.05	13	111.90	4	135.00	12
63.90	114	81.00	2	113.00	20	137.05	60
65.00	315	85.05	6	115.00	38	138.00	163
71.05	63	86.90	19	117.00	52	138.90	30

Average of 30.988 to 31.021 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.95	8	180.00	105				
142.85	29	192.95	15				
144.95	5	197.00	1866				
151.00	8	198.05	273				
151.90	46	203.15	15				
158.05	7	207.00	8				
162.00	7						
163.05	12						
165.00	20						
167.90	4						
175.10	3						

CTMP Compounds

Average of 30.988 to 31.021 min.: A1186.D
Converted from RTE data file: >A1186:

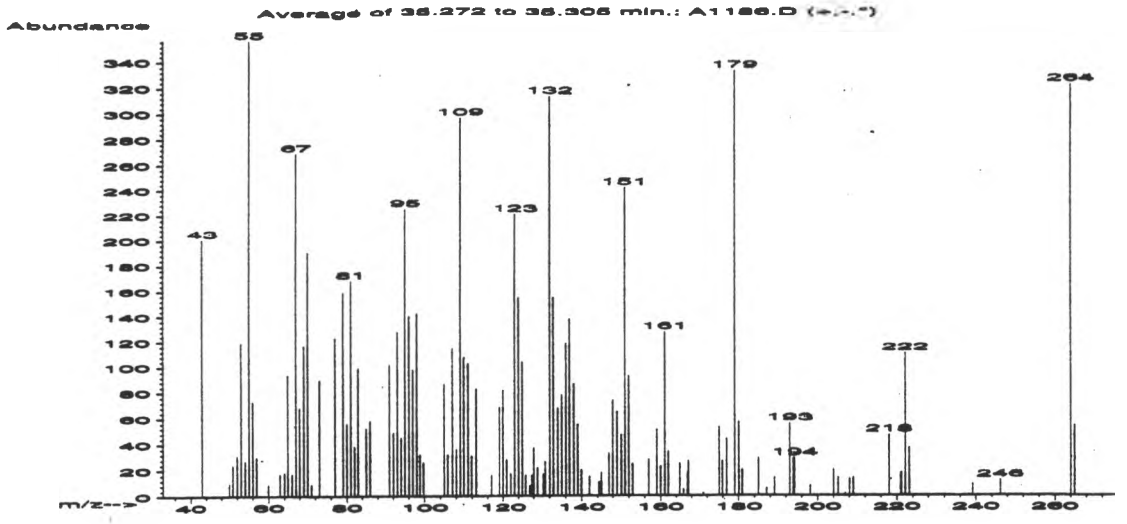
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Benzamide, N-phenyl-	197	C13H11NO	90
2.	Benzamide, N-phenyl-	197	C13H11NO	87
3.	1-BENZOYLOXY-2-FORMYLOXYBENZENE	242	C14H10O4	72
4.	Benzamide, N-phenyl-	197	C13H11NO	72
5.	Benzamide, N-benzoyl-N-phenyl-	301	C20H15NO2	64
6.	Benzoic acid, phenyl ester	198	C13H10O2	64
7.	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	64
8.	.beta.-D-Ribofuranose, 1-acetate 2,3,5-t	504	C28H24O9	53
9.	Benzenepentanoic acid, .delta.-oxo-	192	C11H12O3	53
10.	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	53
11.	Ethanedione, diphenyl-	210	C14H10O2	53
12.	DIPHENYL-PROPANTRIONE	238	C15H10O3	53
13.	Ethanone, 2-chloro-1,2-diphenyl-	230	C14H11ClO	50
14.	Benzamide, N-phenyl-	197	C13H11NO	47
15.	.BETA. BIS-DEUTERO-PHENYLSULFONYIMETHYLK	260	C14H10D2O3S	45
16.	Benzoic acid, phenyl ester	198	C13H10O2	43
17.	METHYL ESTER OF 3-BENZOYL-PROPIONIC ACID	192	C11H12O3	42
18.	1-Propanone, 2-methyl-1-phenyl-	148	C10H12O	42
19.	1,2-Propanedione, 1-phenyl-	148	C9H8O2	42
20.	Benzoic acid, phenyl ester	198	C13H10O2	42

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000093-98-1	33399	76	21	0	84	6	59	0	81	9985
2.	*87	000093-98-1	128102	69	31	0	59	13	54	0	76	9924
3.	72	797922-93-1	53323	47	59	2	99	15	42	9	38	9821
4.	*72	000093-98-1	128101	41	18	0	92	13	42	0	39	9959
5.	64	003027-01-8	133512	57	35	0	69	6	37	11	36	9755
6.	*64	000093-99-2	34022	56	30	1	84	25	37	9	46	9725
7.	*64	000070-11-1	128136	43	43	2	88	25	37	0	44	9704
8.	53	006974-32-9	108430	61	50	0	88	29	28	4	39	9672
9.	53	001501-05-9	30728	45	44	1	80	29	28	0	39	9729
10.	53	000582-24-1	7806	53	23	0	70	29	28	4	43	9700
11.	53	000134-81-6	39597	46	31	1	92	29	28	2	41	9732
12.	53	000000-00-0	51730	44	44	1	82	29	28	0	39	9720
13.	50	000447-31-4	48422	43	44	2	76	31	25	0	39	9725
14.	47	000093-98-1	128103	44	52	0	64	40	20	2	41	9964
15.	45	056667-00-6	59593	52	59	2	93	22	19	15	36	9756
16.	*43	000093-99-2	128221	38	45	1	73	43	18	0	39	9723
17.	42	000000-00-0	30719	48	35	1	98	29	17	6	35	9719
18.	42	000611-70-1	123401	50	21	0	82	29	17	3	36	9703
19.	42	000579-07-7	123378	50	28	1	70	29	17	0	35	9658
20.	42	000093-99-2	128225	46	13	1	73	29	17	0	37	9728

CTMP Compounds

Peak 114, Unidentified



Average of 35.272 to 35.305 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	201	64.00	18	79.00	159	95.05	225
49.95	10	64.95	94	80.00	56	96.05	140
50.85	24	66.00	17	81.05	168	97.05	98
51.95	31	67.00	269	82.05	38	98.05	143
53.00	119	68.00	68	83.00	99	98.90	32
54.00	27	69.00	117	85.00	52	99.80	26
55.00	357	70.05	190	86.00	58	105.05	87
56.00	73	71.00	9	91.00	102	105.95	32
57.00	30	73.05	90	92.10	49	107.05	115
59.95	9	74.95	1	93.05	128	108.05	36
62.90	17	77.00	123	94.05	45	109.05	296

Average of 35.272 to 35.305 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.95	108	125.05	104	135.00	78	149.05	65
111.00	103	125.95	16	136.05	119	150.10	47
111.90	31	127.00	8	137.00	138	151.00	242
113.05	83	127.45	16	138.05	87	152.00	93
117.00	16	127.95	37	139.00	55	152.95	25
119.05	69	128.95	22	139.90	20	157.00	28
120.05	82	130.45	17	142.00	15	159.00	51
121.00	28	130.95	27	144.40	11	160.05	23
122.05	17	132.05	313	145.00	18	161.10	128
123.05	221	133.00	155	146.95	33	162.00	34
124.05	155	134.00	68	148.00	74	164.95	25

Average of 35.272 to 35.305 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
165.95	5	187.05	6	218.05	47		
166.90	18	189.05	14	220.90	17		
167.15	27	192.95	56	221.15	18		
171.00	2	193.90	29	222.15	111		
175.10	53	194.15	29	223.15	37		
175.90	27	198.10	8	239.20	9		
176.95	44	204.05	20	246.15	12		
179.00	333	205.20	14	264.05	323		
180.10	57	206.95	2	265.05	54		
180.95	20	208.05	13				
185.00	29	209.05	14				

CTMP Compounds

Average of 35.272 to 35.305 min.: A1186.D
Converted from RTE data file: >A1186:

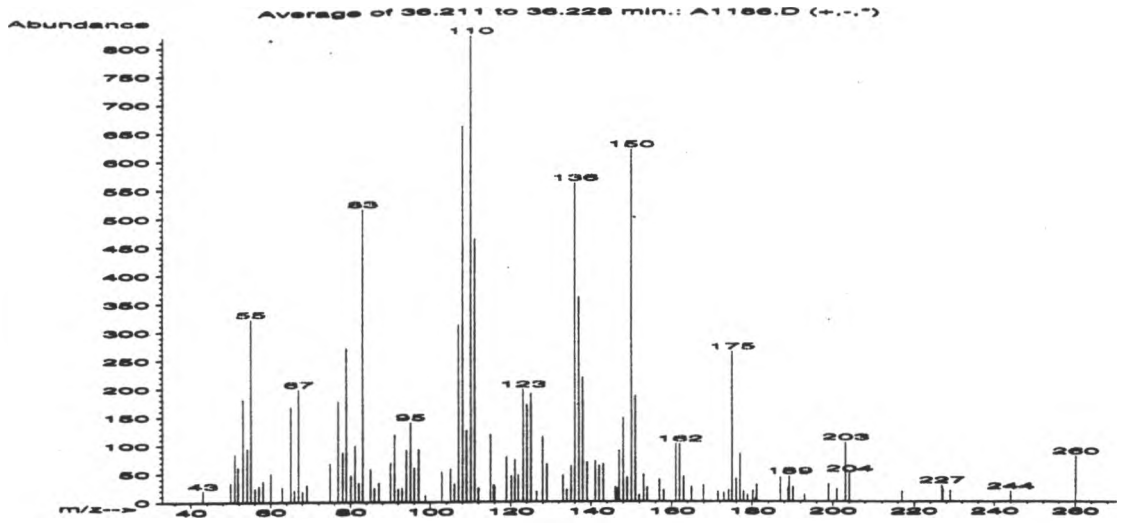
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	6-Phenyl(deuterate)-2,3,4,5-tetrahydro-3	174	C10H5D5N2O	47
2.	PHTHALAZINO(2,3-B)PHTHALAZINE-5,12-(7H,1	264	C16H12N2O2	30
3.	DIHYDROEDULAN IA	194	C13H22O	15
4.	EXO-4-ISOPROPYL-1-METHYL-7-METHYLENEBICY	222	C14H22O2	15
5.	Spiro[2-ethylidene-3-methylcyclohexane]o	208	C14H24O	14
6.	1,8(2H,5H)-Isoquinolinedione, 6,7-dihydr	179	C9H9NO3	11
7.	(1S*,3.ALPHA.,6.ALPHA.)-3-METHYLTRICYCLO	194	C12H18O2	11
8.	Tricyclo[4.3.1.1(3,8)]undecane, 3-methox	180	C12H20O	11
9.	1,4-Undecadiene, (Z)-	152	C11H20	11
10.	2-OXO-8-EPI-12-NORAMBRIENOLIDE	264	C16H24O3	11
11.	3-PHENYLTHIOHEPTAN-2-ONE	222	C13H18OS	10
12.	2,5-Furandione, 3-(dodecenyl)dihydro-	266	C16H26O3	10
13.	DIHYDROEDULAN IIA	194	C13H22O	10
14.	Thiazolo[3,2-a]pyridinium, 8-hydroxy-3,5	179	C9H9NOS	10
15.	Phenol, 2-methoxy-	124	C7H8O2	10
16.	7,7-Dimethyl-6-methylidene-5-(2'-oxo-1'-	236	C14H20O3	10
17.	3-Cyclohexene-1-carboxaldehyde, 1,3,4-tr	152	C10H16O	10
18.	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	10
19.	Spiro[5.6]dodecane-1,7-dione	194	C12H18O2	10
20.	Dihyrodebromospirolaurenone	222	C15H26O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*47	055999-93-4	23022	84	56	2	97	68	21	64	90	5758
2.	*30	021626-89-1	61254	58	86	1	87	62	9	0	56	6181
3.	*15	063335-66-0	32083	66	75	1	85	77	2	0	58	5439
4.	*15	071328-12-6	44879	61	83	2	76	75	2	0	56	5161
5.	*14	075750-99-1	38707	52	37	1	103	70	2	0	39	6290
6.	*11	037704-54-4	25052	49	53	0	71	75	2	0	46	5786
7.	*11	062617-75-8	31973	52	22	0	77	74	2	0	46	5717
8.	*11	021898-92-0	25836	46	71	0	61	80	2	0	44	4884
9.	*11	055976-14-2	13855	49	75	3	157	77	2	0	46	4814
10.	*11	029065-00-7	61286	68	105	2	75	75	2	0	47	5242
11.	*10	062870-24-0	44702	33	6	0	91	78	1	6	39	4562
12.	10	025377-73-5	62058	58	106	3	162	74	1	0	39	5896
13.	*10	000000-00-0	32085	49	83	2	126	79	1	0	39	6362
14.	*10	030277-00-0	25032	35	86	2	63	77	1	0	39	5349
15.	*10	000090-05-1	120383	41	50	0	63	77	1	0	39	4329
16.	10	091186-55-9	50768	75	71	3	166	77	1	0	41	5187
17.	*10	040702-26-9	13655	36	91	1	69	72	1	0	39	5360
18.	*10	031396-33-5	13138	47	57	1	80	77	1	0	39	4950
19.	*10	050803-80-0	127868	70	90	2	74	77	1	0	41	5108
20.	*10	030925-31-6	44985	36	42	0	56	74	1	0	41	6641

CTMP Compounds

Peak 115; Unidentified



Average of 36.211 to 36.228 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	20	62.90	26	80.05	47	94.00	92
49.95	34	65.00	168	81.05	100	95.05	141
50.95	84	66.00	20	82.05	34	96.05	60
51.80	61	67.05	198	83.05	516	97.10	93
53.00	181	68.10	18	85.05	58	98.85	12
54.00	94	69.10	30	86.00	25	102.90	54
55.00	322	72.95	1	87.10	34	105.00	59
56.05	23	74.90	68	90.00	69	105.95	32
57.00	29	76.95	178	91.00	120	107.00	313
58.05	37	78.00	88	92.00	23	108.05	660
59.95	50	78.95	272	92.95	25	109.05	127

Average of 36.211 to 36.228 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.05	818	124.10	172	139.00	70	151.95	11
111.05	465	125.05	192	141.00	72	153.05	48
111.95	24	126.45	18	142.00	64	153.95	25
114.95	120	127.95	116	143.05	67	156.95	39
115.75	30	129.00	67	146.00	26	157.95	20
116.00	28	133.00	47	146.40	23	161.05	102
119.00	80	134.00	22	147.00	91	162.00	102
120.15	46	135.00	64	148.00	148	163.00	44
121.05	75	136.00	562	149.00	43	164.95	26
121.95	47	137.05	362	150.00	620	167.90	29
123.10	199	138.00	220	151.00	187	171.50	18

Average of 36.211 to 36.228 min.: A1186.D
Converted from RTE data file: >A1186:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.00	15	188.95	24	229.00	19		
174.15	20	189.20	45	244.00	18		
175.00	265	190.15	26	260.05	80		
176.00	40	193.00	12				
177.00	85	199.00	31				
177.90	18	201.00	22				
178.85	11	203.10	105				
180.20	19	204.05	49				
180.85	6	217.00	18				
181.05	30	226.90	29				
187.05	43	227.15	22				

CTMP Compounds

Average of 36.211 to 36.228 min.: A1186.D
Converted from RTE data file: >A1186:

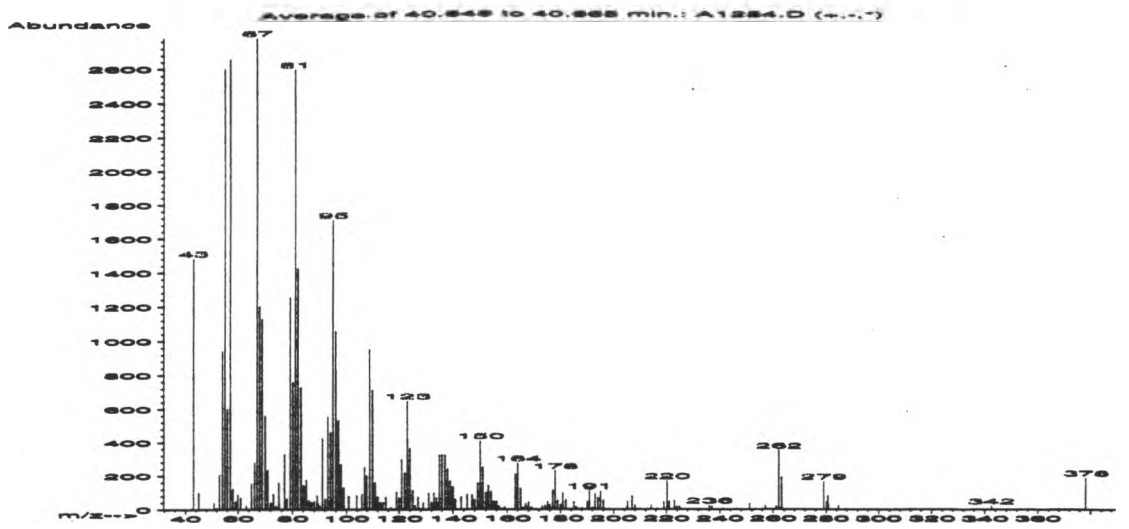
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Acetamide, N-(4-aminophenyl)-	150	C8H10N2O	41
2.	4-METHYL-4-PROPYL-2,5-CYCLOHEXADIEN-1-ON	150	C10H14O	38
3.	2-AMINOACETANILIDE	150	C8H10N2O	35
4.	N-Acetyl-N'-phenylhydrazine	150	C8H10N2O	27
5.	Ethane, bromo-	108	C2H5Br	25
6.	3-Ethenyl-4-methylcyclohex-2-en-1-one	136	C9H12O	25
7.	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimet	150	C10H14O	22
8.	2-ACETAMIDO-4-PICOLINE	150	C8H10N2O	22
9.	Acetamide, N-(3-aminophenyl)-	150	C8H10N2O	22
10.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	22
11.	Benzene, 1-ethoxy-3-methyl-	136	C9H12O	22
12.	Bicyclo[3.1.0]hex-3-en-2-one, 4-methyl-1	150	C10H14O	22
13.	Phenol, 3-(2-aminoethyl)-	137	C8H11NO	22
14.	Phenol, 3-butyl-	150	C10H14O	14
15.	2-Pyridinamine, 3-methyl-N-nitro-	153	C6H7N3O2	11
16.	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimet	150	C10H14O	11
17.	2H-Quinolizine, 1,3,4,6,7,9a-hexahydro-	137	C9H15N	11
18.	1-Propanol, 2,3-dibromo-	216	C3H6Br2O	10
19.	Glycine, N-[(phenylmethoxy)carbonyl]-	209	C10H11NO4	10
20.	1-DEUTERO-1-PHENYL-1-PROPANOL	136	C9H11DO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*41	000122-80-5	12565	61	44	1	61	54	16	0	51	6280
2.	*38	061783-86-6	12774	43	21	0	57	54	14	22	47	5907
3.	*35	034801-09-7	12573	45	44	2	80	54	11	0	40	6251
4.	*27	000114-83-0	12559	51	55	2	63	58	8	2	39	5893
5.	*25	000074-96-4	118652	37	47	1	80	63	7	10	43	6855
6.	*25	000000-00-0	7967	58	64	2	79	63	7	0	46	6102
7.	*22	000494-90-6	123734	48	53	0	66	62	5	8	43	5246
8.	*22	000000-00-0	12545	42	53	1	60	62	5	13	39	5186
9.	*22	000102-28-3	12564	36	58	1	77	62	5	5	40	6064
10.	*22	000621-32-9	7956	57	43	0	75	63	5	5	39	5883
11.	*22	000621-32-9	121937	52	43	0	68	63	5	6	41	5903
12.	*22	024545-81-1	12800	62	56	2	76	64	5	14	41	5156
13.	*22	000588-05-6	8299	60	35	0	62	64	5	2	41	5304
14.	*14	004074-43-5	12719	29	68	0	67	66	2	17	42	5460
15.	*11	018344-53-1	13918	52	67	2	62	80	2	0	44	4651
16.	*11	000494-90-6	123733	49	38	2	239	80	2	0	46	5231
17.	*11	001004-90-6	8334	50	59	2	66	77	2	0	46	5560
18.	10	000096-13-9	129409	47	79	2	80	73	1	0	39	5639
19.	10	001138-80-3	129034	60	62	2	56	73	1	0	39	4751
20.	*10	032047-42-0	7926	35	46	1	77	72	1	19	40	4648

CTMP Compounds

Peak 116; Ester of Linoleic Acid



Average of 40.649 to 40.665 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1483	59.90	92	73.00	91	85.00	173
45.00	102	60.90	71	74.00	19	85.95	54
50.95	40	63.00	23	75.00	157	87.00	41
51.85	10	65.00	152	77.00	330	87.95	48
53.00	208	66.05	280	77.95	64	88.85	9
54.05	945	67.00	2781	79.05	1254	89.00	83
55.00	2601	68.00	1204	80.05	759	89.50	30
55.95	602	69.00	1131	81.05	2594	90.00	21
57.05	2658	70.00	559	82.00	1425	91.00	425
58.00	123	71.05	235	83.05	729	92.00	62
59.00	48	72.05	40	84.05	142	93.00	555

Average of 40.649 to 40.665 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
94.05	462	109.05	955	122.05	218	134.00	70
95.00	1709	110.05	714	123.10	652	134.20	42
96.00	1058	111.10	159	124.05	365	135.05	325
97.00	532	112.00	74	125.05	114	136.05	328
98.05	268	113.00	39	125.95	22	137.05	323
98.90	129	114.00	42	127.05	75	138.00	240
100.95	78	115.00	74	128.00	7	139.05	169
103.95	86	116.95	11	129.00	42	139.95	136
106.00	94	119.00	107	131.00	98	141.00	58
107.05	253	120.05	71	131.95	44	143.00	76
107.95	199	121.00	298	133.00	101	145.15	91

Average of 40.649 to 40.665 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.00	89	157.90	4	175.15	47	188.00	10
147.95	58	159.05	16	176.00	26	190.10	48
149.05	160	163.05	212	177.00	118	190.95	111
150.05	412	164.00	276	178.00	231	192.00	12
150.95	251	165.00	125	178.95	53	193.00	95
152.05	100	166.00	12	180.00	26	194.15	71
153.00	143	166.90	33	180.95	98	195.05	106
154.00	108	168.00	44	181.95	57	196.10	56
155.00	47	169.00	13	185.05	46	198.00	4
155.95	45	173.00	19	185.95	17	204.95	22
156.95	18	174.15	25	186.95	1	205.20	49

Average of 40.649 to 40.665 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
206.95	79	237.05	18	284.70	22		
208.05	25	241.05	8	342.45	20		
213.05	2	251.15	34	378.25	187		
214.20	25	257.05	22				
219.00	44	261.20	20				
220.20	170	262.15	351				
221.15	48	263.20	190				
223.00	53	279.10	165				
224.05	19	280.15	44				
225.00	19	280.65	84				
236.05	25	280.90	27				

Average of 40.649 to 40.665 min.: A1284.D
Converted from RTE data file: >A1284:

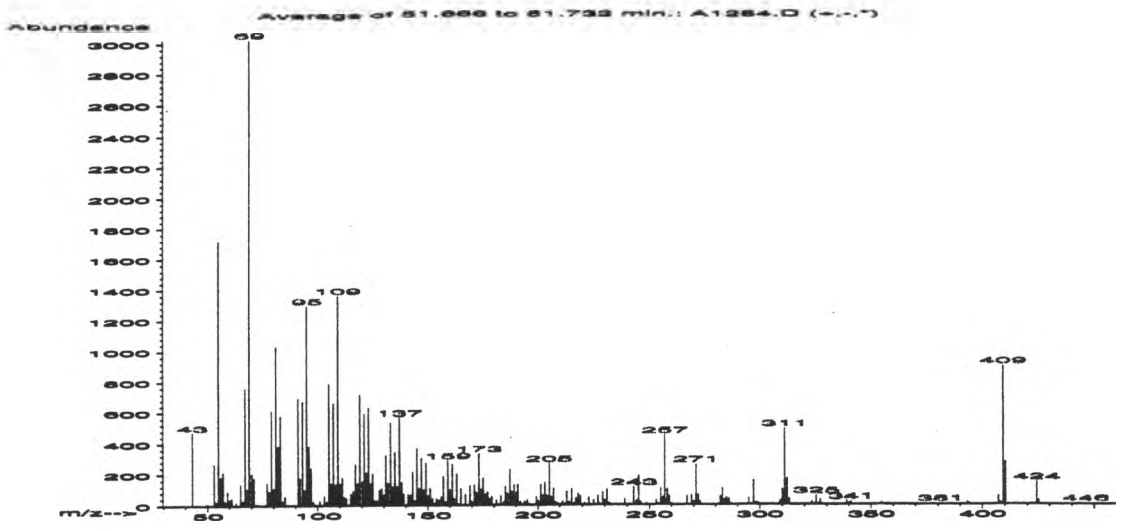
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	87
2.	9,12-Octadecadienoic acid (Z,Z)-, methyl	294	C19H34O2	87
3.	9,12-Octadecadienoic acid (Z,Z)-, 2-hydr	354	C21H38O4	80
4.	5-Eicosyne	278	C20H38	80
5.	9,12-Octadecadienoic acid (Z,Z)-, 2,3-di	354	C21H38O4	74
6.	11-Octadecynenitrile	261	C18H31N	72
7.	3,4-Octadiene, 7-methyl-	124	C9H16	62
8.	9,17-Octadecadienal, (Z)-	264	C18H32O	53
9.	Methylenecyclononane	138	C10H18	49
10.	9,12-Octadecadienoic acid, methyl ester,	294	C19H34O2	49
11.	Ethanol, 2-(9,12-octadecadienyloxy)-, (Z	310	C20H38O2	43
12.	1,13-Tetradecadiene	194	C14H26	42
13.	1,12-Tridecadiene	180	C13H24	42
14.	1,E-8,Z-10-TRIDECATRIENE	178	C13H22	38
15.	3BETA-METHYL-TRANS-HEXAHYDROPHTHALIDE	154	C9H14O2	30
16.	TRICYCLO[5.2.1.0(2,6)]DECANE	136	C10H16	30
17.	Myrcenol	154	C10H18O	25
18.	Oxirane, 5-hexenyl-	126	C8H14O	18
19.	1,E-11,Z-13-OCTADECATRIENE	248	C18H32	18
20.	Bicyclo[5.1.0]octane	110	C8H14	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000060-33-3	132609	94	83	3	72	14	54	41	78	9880
2.	87	000112-63-0	133235	149	21	0	68	14	54	10	78	9810
3.	80	003443-82-1	89015	111	69	3	90	11	48	16	47	9694
4.	80	074685-31-7	66578	82	76	1	93	14	48	0	43	9771
5.	74	002277-28-3	89014	103	90	2	82	17	44	0	59	9431
6.	*72	056599-92-9	60104	59	110	3	84	20	42	0	46	9734
7.	*62	037050-05-8	4880	72	38	1	81	28	36	12	58	9226
8.	53	056554-35-9	61434	123	27	2	95	36	28	21	56	7929
9.	*49	056133-38-1	8815	48	25	1	99	36	23	0	44	9333
10.	49	002566-97-4	133240	129	37	2	93	44	23	16	53	7813
11.	43	017367-08-7	77158	81	99	0	64	50	18	0	47	9873
12.	*42	021964-49-8	32141	70	58	1	82	57	17	0	76	9717
13.	*42	021964-48-7	25852	77	46	0	62	60	17	39	66	8022
14.	*38	080625-30-5	24966	74	45	1	90	58	14	18	53	7385
15.	*30	002205-25-6	14502	53	56	1	96	58	9	0	47	8560
16.	*30	000000-00-0	8195	63	54	2	78	57	9	16	47	7413
17.	*25	000543-39-5	14602	54	56	3	186	61	7	0	49	7153
18.	*18	019600-63-6	5404	57	53	3	122	68	3	0	49	6706
19.	18	080625-36-1	55839	84	62	3	135	66	3	0	47	7650
20.	*11	000286-43-1	118912	37	67	0	64	71	2	4	43	8852

CTMP Compounds

Peak 117; Unidentified Triterpene



A

verage of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	470	59.00	88	73.00	3	91.00	694
49.95	13	59.95	39	77.00	144	92.00	176
50.90	1	60.90	48	78.00	89	93.05	674
51.85	1	62.95	20	79.00	612	94.05	99
53.00	267	64.95	136	80.00	107	95.05	1294
54.00	27	66.05	29	81.05	1031	96.00	380
55.00	1718	67.05	759	82.00	382	97.05	239
56.00	181	68.00	106	83.05	576	98.00	24
57.05	212	69.00	3025	84.00	26	99.00	3
57.95	27	70.05	202	85.05	57	101.00	28
58.30	13	71.05	172	88.95	2	102.95	62

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.00	25	115.95	91	127.00	31	138.05	146
105.00	788	117.00	266	128.00	98	139.00	73
106.00	140	118.05	140	129.00	111	140.95	71
107.05	662	119.00	719	130.00	67	142.00	66
108.05	134	120.10	154	131.00	324	143.05	217
109.05	1360	121.05	592	132.00	141	143.95	28
110.05	137	122.05	209	133.05	537	144.15	27
111.00	175	123.10	632	134.00	118	145.00	367
111.95	54	124.15	138	135.05	344	146.00	110
112.95	45	125.00	201	136.05	121	147.05	304
115.00	72	125.85	30	137.05	568	148.05	101

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
149.10	274	158.30	18	171.05	130	183.00	59
150.05	62	159.05	289	172.00	83	184.30	19
150.95	110	160.00	101	173.10	332	185.05	121
151.85	9	161.05	266	174.05	101	186.00	75
152.00	43	162.00	43	175.10	173	187.05	230
153.00	12	163.05	202	176.00	70	188.10	88
153.95	45	164.00	8	177.00	82	189.15	130
155.00	34	164.95	108	178.00	40	190.10	78
156.00	58	167.00	70	178.95	55	190.95	132
157.00	188	169.00	127	181.05	33	192.00	21
158.00	21	170.00	25	182.00	5	194.00	24

CTMP Compounds

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
194.95	15	207.00	108	216.40	7	231.10	101
195.15	34	208.00	20	217.05	46	232.05	11
199.15	54	209.00	12	218.10	75	239.10	39
200.05	28	210.00	5	219.10	59	240.95	1
201.20	132	211.05	25	221.05	14	241.20	8
202.10	64	212.30	10	222.95	49	243.05	114
203.15	146	213.00	87	225.05	32	244.10	28
203.95	62	213.80	9	227.00	61	245.10	187
204.20	37	214.05	20	227.25	22	246.00	20
205.10	267	215.15	103	229.15	83	248.65	11
206.00	54	216.00	10	230.10	32	253.00	33

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
253.95	10	271.10	260	286.00	42	323.25	23
255.10	109	272.15	67	286.95	8	325.00	18
256.05	54	272.65	8	295.05	46	325.25	60
257.00	449	273.00	24	297.10	159	326.85	20
258.05	101	280.95	6	298.15	13	327.10	37
259.00	57	282.05	58	299.00	14	339.00	31
260.05	7	283.05	108	309.05	28	339.30	14
267.00	57	283.95	38	310.00	99	340.20	9
269.05	63	284.95	49	311.15	493	341.00	21
269.50	11	285.20	18	312.10	169	354.75	16
270.00	27	285.55	12	313.15	39	355.00	2

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
365.20	5	424.30	146				
366.55	8	425.20	29				
381.25	8	446.20	7				
393.30	18						
394.20	9						
405.15	7						
407.20	58						
407.90	13						
408.20	16						
409.35	900						
410.35	278						

CTMP Compounds

Average of 51.666 to 51.732 min.: A1284.D
Converted from RTE data file: >A1284:

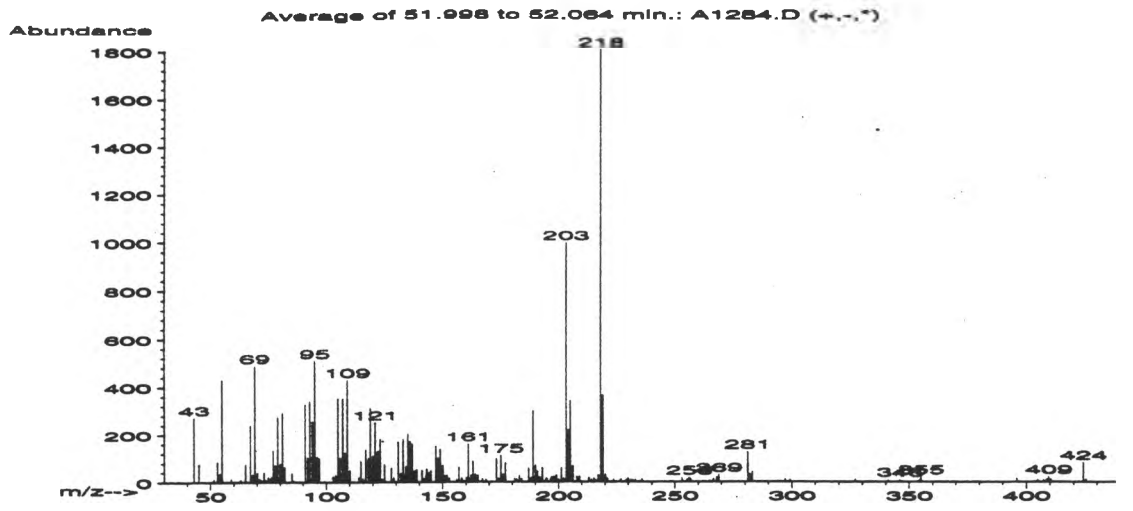
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	(+,-)-(E)-Dihydrofarnesal	222	C15H26O	38
2.	Chola-5,22-dien-3-ol, (3.beta.,22Z)-	342	C24H38O	25
3.	E and Z isomers of 2,6,10-Trimethyl-2,6,	234	C17H30	23
4.	(+,-)-(Z)-Dihydrofarnesal	222	C15H26O	23
5.	4-(6',6'-DIMETHYL-2'-METHYLIDENCYCLOHEX-	196	C13H24O	16
6.	6-Methyl-2,6-heptadienal	124	C8H12O	14
7.	4,8-DIMETHYLNONA-1,7-DIENE	152	C11H20	12
8.	3-HEXENE, 3,4-BIS(DIETHYLBORYL)-	220	C14H30B2	8
9.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	8
10.	METHYL 2-HYDROXYDECANOATE	202	C11H22O3	8
11.	2-METHOXY-13C-3-METHYLPYRAZINE	124	C513CH8N2O	7
12.	METHYL ENT-16-KAUREN-19-OATE	316	C21H32O2	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	069659-93-4	44957	48	24	0	92	39	14	15	36	8782
2.	25	057597-14-5	86228	75	67	1	67	54	7	10	32	8723
3.	23	068965-67-3	50164	42	46	1	88	47	6	10	28	9272
4.	23	069659-92-3	44956	32	36	0	99	47	6	1	26	8564
5.	16	000000-00-0	33110	47	90	3	44	58	3	0	31	9012
6.	*14	094705-04-1	4757	39	10	0	55	69	2	10	39	4808
7.	*12	062108-28-5	13858	41	61	2	85	61	2	0	35	8916
8.	8	000000-00-0	43851	35	90	3	99	69	1	0	22	7763
9.	8	002847-30-5	120355	41	74	1	79	68	1	0	28	5124
10.	8	071271-24-4	35534	35	77	2	99	68	1	0	21	7828
11.	7	034061-82-0	4673	33	121	2	32	72	1	2	23	5170
12.	6	005524-25-4	79043	33	162	2	52	73	1	0	11	5121

CTMP Compounds

Peak 117; Unidentified Triterpene



Average of 51.998 to 52.064 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	272	68.05	32	77.95	72	94.10	255
44.95	76	69.00	488	79.00	275	95.05	509
50.95	4	70.05	39	80.00	78	96.15	106
51.55	12	71.05	14	81.00	292	97.05	100
53.00	86	71.90	8	82.00	62	102.95	24
54.00	35	73.00	41	83.05	1	104.00	29
55.00	429	73.95	8	85.10	36	105.05	352
58.95	14	74.95	21	85.95	5	106.00	103
62.90	11	75.95	13	91.00	328	107.05	351
65.00	74	76.20	21	92.05	102	108.10	123
67.05	240	76.95	133	93.00	340	109.05	429

Average of 51.998 to 52.064 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.05	48	124.05	12	136.05	172	148.05	102
113.95	20	125.05	74	137.05	160	149.05	137
114.95	90	127.95	59	138.05	47	150.10	70
115.95	13	129.00	19	138.95	53	150.95	26
116.95	137	130.00	2	141.15	50	151.95	28
118.05	101	131.00	170	142.05	15	152.90	15
119.00	312	132.00	38	143.00	27	156.00	9
120.05	110	132.95	182	143.15	55	157.00	62
121.05	251	134.00	30	144.20	39	158.20	16
122.05	131	134.20	66	144.95	49	159.00	5
123.10	180	135.05	205	147.05	152	160.20	19

Average of 51.998 to 52.064 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
161.05	161	175.60	6	190.10	70	199.10	30
162.00	15	176.00	33	190.95	45	200.00	9
162.20	29	177.00	81	191.65	15	201.10	60
163.05	87	181.00	15	191.95	19	202.15	13
164.00	32	182.00	11	193.00	60	203.15	998
165.15	27	183.00	26	194.40	11	204.15	220
167.00	14	184.05	12	194.95	15	205.05	343
168.65	11	187.00	58	196.65	12	206.05	67
173.15	98	188.00	7	197.00	20	207.95	22
174.05	15	188.20	18	197.95	23	208.95	22
175.10	112	189.05	301	198.50	12	213.05	18

CTMP Compounds

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
214.05	9	226.90	11	256.00	17	297.15	11
215.20	15	229.15	10	256.55	13	299.15	8
215.55	8	229.70	8	256.85	6	326.95	10
216.05	5	229.95	16	264.70	4	340.80	8
217.00	30	231.05	8	265.00	5	346.05	10
218.15	1804	231.95	8	266.45	12	354.25	9
219.10	366	232.95	8	267.95	19	355.00	20
220.10	31	235.00	2	268.90	30	396.05	15
221.05	13	235.95	11	281.15	127	404.65	8
223.75	10	253.00	16	282.00	32	407.15	7
226.50	7	255.15	11	283.00	42	408.30	5

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
408.50	12						
409.40	22						
410.40	8						
424.20	82						
425.20	10						

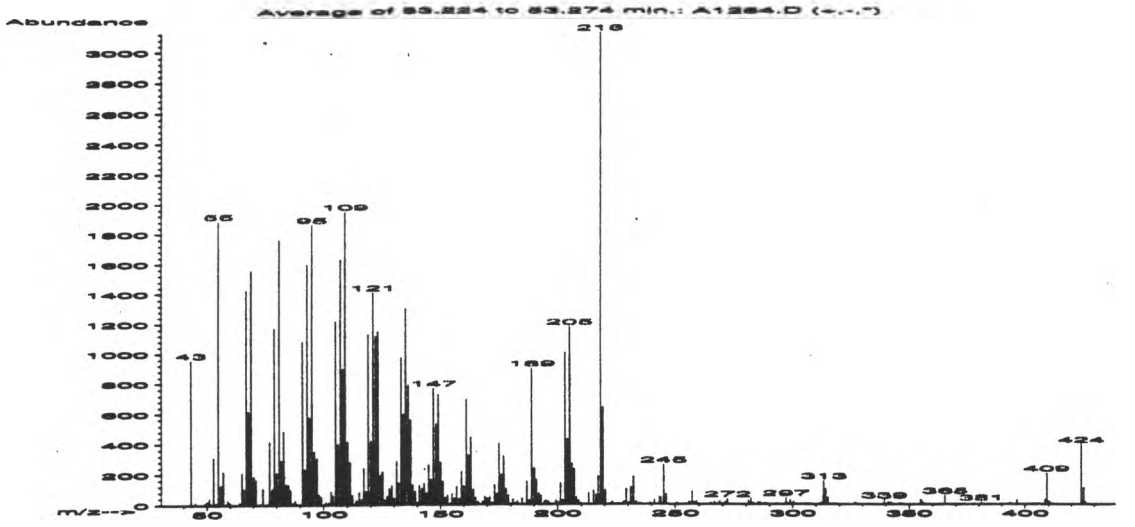
Average of 51.998 to 52.064 min.: A1284.D
Converted from RTE data file: >A1284:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1,1'-Biphenyl, 3-chloro-4-methoxy-	218	C13H11ClO	72
2.	2-Chloro-p-methoxybiphenyl	218	C13H11ClO	72
3.	1,2,3,3a,5,6,6a,7-Octahydro-1,3a,6-trime	218	C15H22O	72
4.	3-Chloro-4'-methoxybiphenyl	218	C13H11ClO	72
5.	3-Acetyl-1-fluoro-7-methoxynaphthalene	218	C13H11FO2	64
6.	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	64
7.	2-Isopropenyl-5-acetyl-6-hydroxy-2,3-dih	218	C13H14O3	53
8.	Olean-12-ene	410	C30H50	53
9.	Naphthalene, 1-(phenylmethyl)-	218	C17H14	52
10.	1,1'-Biphenyl, 4-chloro-4'-methoxy-	218	C13H11ClO	50
11.	2,6-Diisopropylidene-3-methyl-3-vinylcyc	218	C15H22O	50
12.	Ethanone, 1,1'-(6-hydroxy-2,7-benzofuran	218	C12H10O4	49
13.	(Z)-1,3,4,5-Tetrahydro-3,3,3',4'-tetrame	218	C13H18N2O	49
14.	Urs-12-ene	410	C30H50	47
15.	1-[5-[1-dimethylhydrazono)ethyl]-2-methy	218	C13H18N2O	46
16.	4-HYDROXY-6-(P-METHOXYPHENYL)-3-PYRIDAZO	218	C11H10N2O3	45
17.	D:C-Friedooleanan-3-one	424	C30H48O	38
18.	5-Oxo-isolongifolene	218	C15H22O	35
19.	4(eq)-acetimidoadamantane-2(eq)-carbonit	218	C13H18N2O	35
20.	Trimethyl ether, methyl ester of 5-Hydro	249	C14H19NO3	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	021424-83-9	42775	45	36	1	84	14	42	3	43	9377
2.	*72	074428-82-3	42780	45	36	1	84	14	42	3	43	9377
3.	*72	071583-68-1	43034	58	19	0	91	11	42	14	41	9320
4.	*72	074447-84-0	42781	45	36	1	84	14	42	3	43	9377
5.	*64	071493-39-5	42792	37	53	1	87	17	37	10	40	8818
6.	*64	000243-42-5	43062	78	41	1	72	35	37	26	72	8600
7.	*53	006906-88-3	42817	52	36	2	98	29	28	16	39	9127
8.	53	000471-68-1	136171	59	102	3	85	26	28	0	39	9694
9.	*52	000611-45-0	43091	52	103	3	96	35	27	0	46	9378
10.	*50	058970-19-7	129583	55	67	2	97	35	25	15	40	9279
11.	*50	069366-06-9	42971	54	54	2	87	31	25	19	40	9148
12.	*49	055682-72-9	42698	34	44	1	87	40	23	14	43	8128
13.	*49	095863-75-5	42832	63	62	1	68	36	23	22	47	9381
14.	47	000464-97-1	136172	59	115	3	67	40	20	0	39	9413
15.	*46	090909-71-0	42831	34	54	2	99	44	20	10	43	9358
16.	*45	058884-19-8	42652	60	57	1	99	49	19	0	56	8770
17.	*38	005945-53-9	101572	70	117	2	60	58	14	0	53	8948
18.	*35	074842-31-2	43022	40	40	3	99	54	11	14	40	8245
19.	*35	081601-56-1	42844	36	44	1	99	54	11	0	41	8241
20.	35	000000-00-0	55990	38	72	2	67	55	11	22	43	8349

Peak 118; Unidentified Triterpene



Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	958	57.05	217	72.95	1	85.05	131
44.90	14	58.95	28	74.00	106	85.95	96
49.05	10	59.95	15	75.95	4	86.95	10
49.45	14	64.10	12	76.95	414	87.90	27
50.20	22	65.00	209	78.00	102	88.15	12
50.90	42	65.90	104	79.05	1169	91.00	1079
51.95	1	67.00	1423	80.00	210	92.00	234
52.95	312	68.00	616	81.05	1760	93.00	1594
54.00	10	69.05	1555	82.05	292	94.00	575
55.00	1887	70.10	180	83.05	484	95.05	1860
56.00	126	71.05	163	84.05	135	96.00	350

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.05	307	109.05	1949	119.00	1131	130.00	45
98.00	69	110.05	413	120.05	417	131.05	285
98.95	54	111.10	281	121.05	1409	132.00	143
100.90	15	112.00	62	122.10	1115	133.05	972
101.95	13	113.40	13	123.10	1147	134.05	595
103.00	88	113.85	27	124.15	192	135.05	1305
103.95	60	115.00	81	125.00	216	136.05	787
105.05	1216	115.95	31	126.00	31	137.05	561
106.00	398	116.15	38	127.00	55	138.05	129
107.05	1628	117.00	239	127.95	108	138.80	11
108.05	898	118.00	87	129.00	126	139.10	88

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.00	14	151.00	152	162.05	326	171.10	51
140.95	125	151.95	46	163.05	444	172.05	12
142.00	107	153.00	62	164.15	99	173.00	5
143.00	141	154.00	8	164.95	15	173.15	129
143.95	77	154.95	73	165.15	45	174.10	72
145.00	264	155.95	45	166.15	20	175.10	403
145.95	167	157.00	119	168.00	22	176.10	195
147.00	768	158.00	43	168.25	13	177.00	316
148.10	534	159.05	218	169.00	53	178.00	100
149.10	729	160.05	121	169.65	22	178.55	18
150.05	281	161.05	695	170.00	42	179.00	60

CTMP Compounds

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
179.95	4	192.95	56	203.15	1007	217.10	186
180.95	35	194.40	17	204.15	431	218.15	3122
181.90	8	195.00	28	205.10	1180	219.10	640
183.00	20	195.65	14	206.05	267	220.00	28
185.05	40	195.95	18	206.95	232	220.20	95
187.00	152	196.25	9	208.00	47	222.00	1
188.10	29	199.10	28	208.95	23	222.80	6
189.05	902	200.00	17	210.00	8	223.10	20
190.10	238	201.15	141	213.05	74	227.90	13
191.00	160	202.00	27	215.10	92	228.15	19
192.00	73	202.25	25	216.20	61	229.10	101

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
230.30	13	246.05	66	268.05	9	285.55	8
231.10	113	250.75	14	268.90	23	286.05	11
232.15	179	251.00	3	270.00	6	288.20	9
233.20	10	255.80	19	271.15	18	297.10	42
233.45	20	256.05	8	271.40	11	297.65	9
234.80	9	256.55	11	271.90	12	298.95	27
239.30	13	257.15	86	272.15	36	300.25	16
241.15	33	257.95	13	281.00	28	312.05	11
243.15	49	259.00	21	282.05	41	313.05	55
243.95	45	265.00	13	282.85	11	313.25	155
245.10	261	266.70	19	285.05	12	314.15	100

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
315.05	45	365.25	57	425.35	106		
326.65	12	381.15	13	426.15	12		
327.00	9	393.45	11				
339.20	29	396.45	30				
340.95	15	406.15	8				
341.20	12	408.45	35				
342.20	12	409.30	204				
346.05	10	410.15	17				
354.95	32	410.40	11				
355.25	26	410.75	13				
356.00	9	424.25	395				

CTMP Compounds

Average of 53.224 to 53.274 min.: A1284.D
Converted from RTE data file: >A1284:

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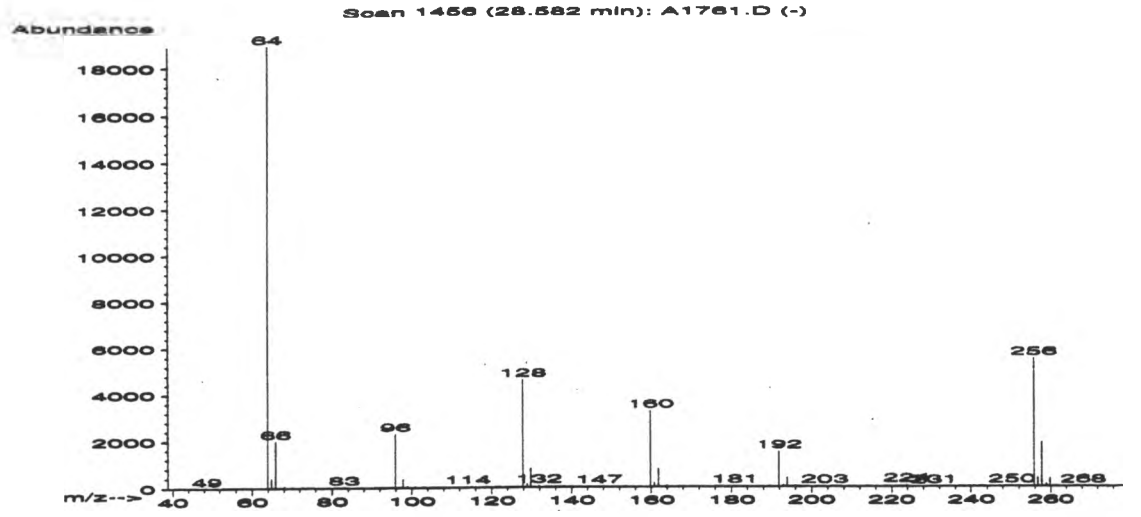
	Name	MolWt	Formula	Qual
1.	3-KETO-URS-12-ENE	424	C30H48O	90
2.	D:C-Friedooleanan-3-one	424	C30H48O	64
3.	2-((Z)-3'-Methyl-1',3'-butadien-1'-yl)-2	220	C14H20O2	56
4.	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	55
5.	TETRAHYDRO-3,6,8,8-TETRAMETHYL-7-METHANO	218	C15H22O	50
6.	1,2,3,3a,5,6,6a,7-Octahydro-1,3a,6-trime	218	C15H22O	47
7.	(13S)-8a,13:13,20-Diepoxy-5.beta.,9.beta	278	C18H30O2	46
8.	.delta.-Guaiene	204	C15H24	44
9.	2,6-Diisopropylidene-3-methyl-3-vinylcyc	218	C15H22O	43
10.	Epi-.psi.-Taraxastanonol	442	C30H50O2	43
11.	Viminalol	426	C30H50O	41
12.	.beta.-Amyrin	426	C30H50O	38
13.	Pyrene, hexadecahydro-	218	C16H26	30
14.	(+)-Aromadendrene	204	C15H24	25
15.	Cyclododecanecarbonitrile	193	C13H23N	25
16.	cis-2-(4-Methoxyphenyl)-4-methylcyclohex	218	C14H18O2	25
17.	Aristolone	218	C15H22O	25
18.	(4R,4aS,6S)-6-Isopropenyl-4,4a-dimethyl-	218	C15H22O	14
19.	.gamma.-Gurjunene	204	C15H24	11
20.	.delta.-Guaiene	204	C15H24	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000000-00-0	101578	128	80	2	82	20	59	52	91	8852
2.	*64	005945-53-9	101572	55	139	3	93	25	37	0	47	7393
3.	*56	088354-60-3	43768	98	63	0	50	74	30	45	94	5728
4.	*55	000243-42-5	43062	85	51	3	86	42	29	30	70	7204
5.	*50	000000-00-0	43003	76	84	2	82	49	25	39	68	7796
6.	*47	071583-68-1	43034	43	38	1	85	38	20	10	43	6474
7.	46	067010-57-5	66519	80	112	3	75	42	20	0	43	8599
8.	*44	003691-11-0	36708	82	80	1	52	71	18	0	90	6123
9.	*43	069366-06-9	42971	52	76	3	93	48	18	0	44	7242
10.	43	000000-00-0	103861	142	78	1	58	46	18	4	47	7215
11.	*41	000638-95-9	136390	75	93	2	81	52	16	33	60	6750
12.	*38	000559-70-6	101804	80	97	2	99	55	14	17	46	7233
13.	*30	002435-85-0	43086	55	95	2	99	58	9	0	47	7508
14.	*25	000489-39-4	128755	69	81	1	88	77	7	0	68	5301
15.	*25	069300-13-6	31373	63	49	2	61	61	7	0	50	6011
16.	*25	084736-51-6	42891	52	86	2	90	65	7	0	46	6678
17.	*25	006831-17-0	129615	62	88	1	93	63	7	0	46	7358
18.	*14	053768-26-6	43013	70	65	2	93	68	2	14	41	6669
19.	*11	022567-17-5	128698	70	83	1	56	80	2	25	48	5495
20.	*11	003691-11-0	128700	65	79	0	40	77	2	6	47	5936

CTMP Compounds

Peak 119, Sulpher S8



Scan 1456 (28.582 min): A1761.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.70	10	78.95	28	95.90	2292	119.15	8
52.95	22	80.40	25	97.00	53	121.00	20
53.80	37	81.05	18	97.90	370	122.10	46
56.95	16	82.00	20	99.00	53	125.00	29
63.90	18882	83.05	32	100.90	44	125.90	18
64.90	413	84.95	3	102.05	9	126.15	31
65.90	1989	91.00	27	105.05	15	126.95	11
67.00	18	91.95	34	109.00	5	127.90	4634
68.10	84	93.00	6	112.05	31	128.95	147
70.10	51	93.90	30	113.95	47	129.80	813
73.90	11	95.00	38	115.00	19	130.80	41

Scan 1456 (28.582 min): A1761.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.80	68	151.05	24	176.65	32	193.95	392
133.95	14	152.95	5	177.15	34	195.05	29
135.00	21	159.80	3270	178.00	31	195.95	57
136.05	25	160.80	197	179.00	38	197.25	5
137.05	19	161.80	762	180.15	31	198.75	15
138.20	55	162.90	18	180.40	33	203.25	41
139.95	42	163.20	38	180.90	47	205.15	34
143.25	19	163.95	78	189.45	38	207.10	24
144.75	23	167.20	48	189.80	25	215.05	22
146.90	33	173.00	12	191.80	1510	220.05	10
148.00	31	176.15	45	192.95	82	223.80	95

Scan 1456 (28.582 min): A1761.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
230.75	15	259.75	342				
234.15	8	261.00	37				
247.05	23	261.40	23				
248.20	10	263.40	37				
249.55	13	268.30	19				
250.20	33						
251.90	8						
255.75	5494						
256.75	369						
257.75	1892						
258.90	129						

CTMP Compounds

Scan 1456 (28.582 min): A1761.D

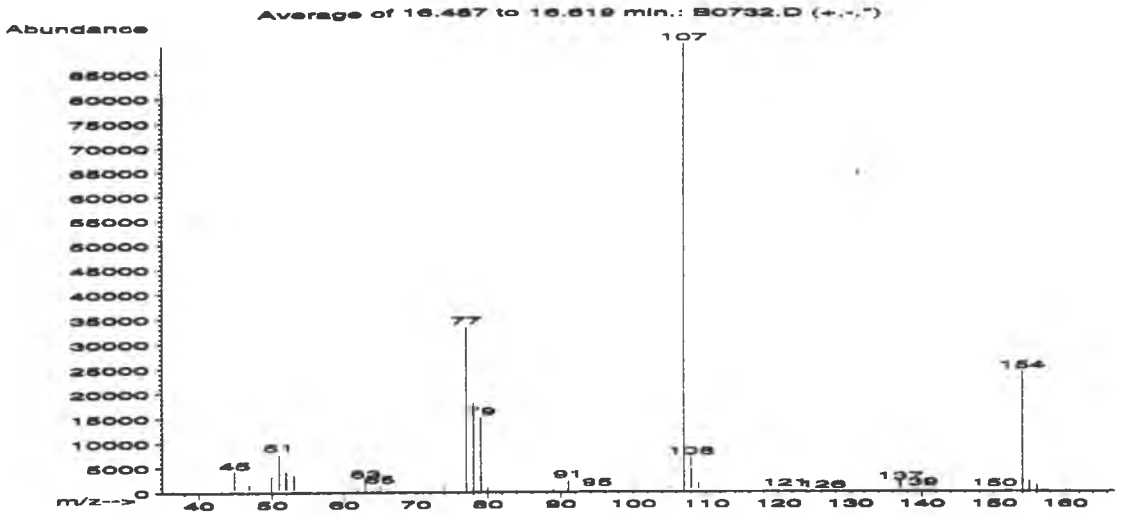
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Sulfur, mol. (S8)	256	S8	94
2.	Sulfur, mol. (S8)	256	S8	94
3.	Sulfur, mol. (S8)	256	S8	40
4.	CYSTEIC ACID THIOHYDATOIN	210	C4H6N2O4S2	40
5.	Manganese, [[1,2-ethanediylbis[carbamodi	265	C4H6MnN2S4	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	010544-50-0	131606	107	24	1	80	0	70	51	92	9001
2.	*94	010544-50-0	131605	87	43	2	67	4	70	0	87	9939
3.	40	010544-50-0	131607	54	76	1	86	11	16	0	22	9246
4.	40	000000-00-0	39082	33	84	2	94	14	16	1	26	9377
5.	10	012427-38-2	61467	71	69	0	30	75	1	0	42	9164

CTMP Compounds

Peak 120; Substituted phenol



Average of 16.487 to 16.619 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.90	4318	61.95	950	79.05	15118	95.00	720
45.90	366	63.00	2498	80.00	839	96.05	122
46.95	1619	63.95	476	81.00	280	97.05	115
49.95	3459	65.00	1407	81.95	218	100.00	7
50.95	7899	66.00	906	84.00	326	102.00	3
51.95	4123	67.00	393	89.00	423	104.05	806
53.00	3494	72.95	33	90.10	112	105.00	1111
54.00	90	74.00	999	91.00	2330	107.00	90579
55.00	415	75.00	693	92.05	218	108.00	7009
58.90	64	77.05	33372	92.95	175	109.00	1793
60.95	751	78.05	17919	94.00	354	110.00	638

Average of 16.487 to 16.619 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.10	130	132.65	8	142.30	5	154.00	24364
116.95	1	133.00	17	142.95	12	155.00	2152
117.90	13	133.25	4	143.30	6	156.00	1237
119.00	54	134.05	54	143.80	5	157.05	72
120.00	254	135.00	37	144.10	36		
121.00	514	135.15	8	147.20	5		
122.00	44	137.00	1840	148.05	8		
125.10	29	138.05	462	150.05	424		
126.20	90	139.05	608	151.05	76		
131.90	4	140.10	27	152.05	19		
132.25	7	141.05	1	152.70	10		

CTMP Compounds

Average of 16.487 to 16.619 min.: B0732.D
Converted from RTE data file: >B0732:

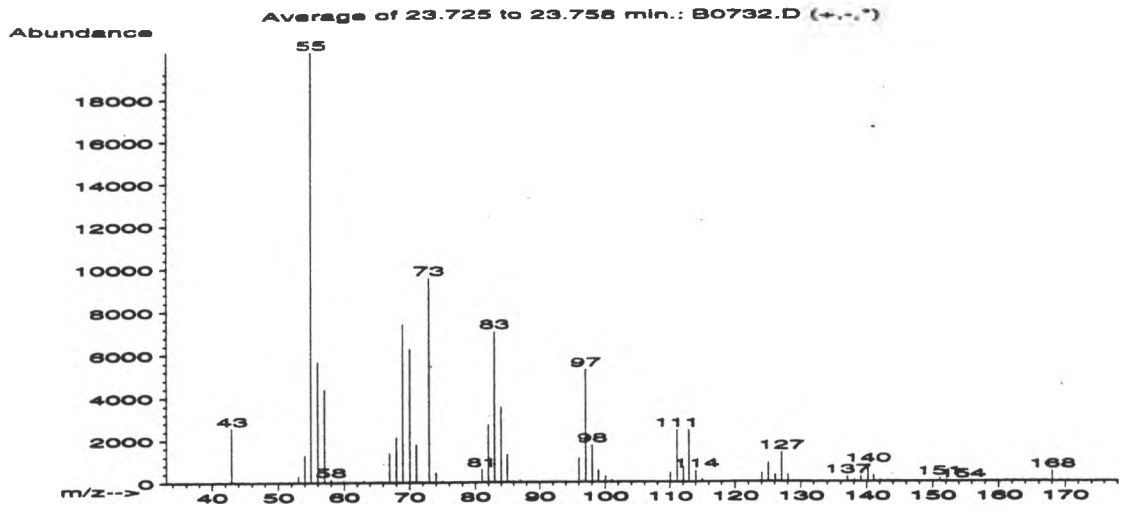
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-chloro-6-methyl-	142	C7H7ClO	64
2.	4-Pyridinecarboxaldehyde	107	C6H5NO	50
3.	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	47
4.	1-PHENYL-1-PROPANOL-1-13C	136	C813CH12O	40
5.	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	38
6.	.ALPHA.,.BETA.,.BETA.-D3-STYRENE	104	C8H5D3	38
7.	Pyridine, 2,4-dimethyl-	107	C7H9N	38
8.	Pyridine, 3,4-dimethyl-	107	C7H9N	37
9.	Benzenemethanol, .alpha.-ethyl-	136	C9H12O	36
10.	Phenol, 2-ethyl-	122	C8H10O	36
11.	Phenol, 4-propyl-	136	C9H12O	28
12.	Pyridine, 2,3-dimethyl-	107	C7H9N	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	000087-64-9	122597	54	28	2	92	18	37	20	40	9693
2.	*50	000872-85-5	1808	37	42	0	74	34	25	10	39	8920
3.	47	000156-38-7	13348	44	41	0	69	40	20	0	39	9310
4.	40	056248-23-8	7928	51	77	2	92	35	16	0	31	9100
5.	38	000156-38-7	123893	40	47	0	69	36	14	0	33	9525
6.	*38	003814-93-5	1667	31	59	2	85	39	14	0	33	9058
7.	*38	000108-47-4	118615	40	51	2	66	40	14	13	35	9176
8.	*37	000583-58-4	118621	35	57	3	72	43	13	0	35	9232
9.	36	000093-54-9	121920	38	51	2	69	30	12	0	29	9178
10.	36	000090-00-6	120201	35	54	2	87	27	12	0	21	9635
11.	28	000645-56-7	121890	36	43	2	83	37	8	0	25	9260
12.	*25	000583-61-9	118611	29	64	2	68	43	7	0	29	9093

CTMP Compounds

Peak 121; Cyclododecane or Dodecene



Average of 23.725 to 23.758 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2558	61.75	25	75.00	64	95.05	16
48.45	18	62.95	79	80.00	36	96.05	1137
51.95	9	65.00	45	81.00	615	97.05	5313
53.05	294	66.00	21	82.00	2719	98.05	1764
54.00	1289	67.00	1384	83.00	7080	99.00	544
54.95	20222	68.00	2152	84.00	3562	100.05	255
56.00	5679	69.00	7429	85.00	1305	101.05	96
57.00	4371	70.05	6274	86.00	72	101.95	28
58.00	145	71.05	1787	87.00	97	102.20	24
58.95	23	72.95	9560	88.40	16	106.00	43
59.90	77	74.00	477	88.95	34	110.05	449

Average of 23.725 to 23.758 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.10	2467	128.05	323	143.95	30		
112.10	686	128.95	35	150.20	40		
113.00	2461	129.90	43	151.05	158		
114.05	545	130.15	21	152.10	70		
115.05	124	137.05	255	154.25	22		
116.00	26	138.10	96	154.50	24		
117.80	24	139.10	273	157.00	13		
124.05	412	140.15	773	158.25	16		
125.05	891	141.05	293	162.15	33		
126.10	327	142.00	81	167.00	70		
127.05	1403	142.95	54	168.05	486		

CTMP Compounds

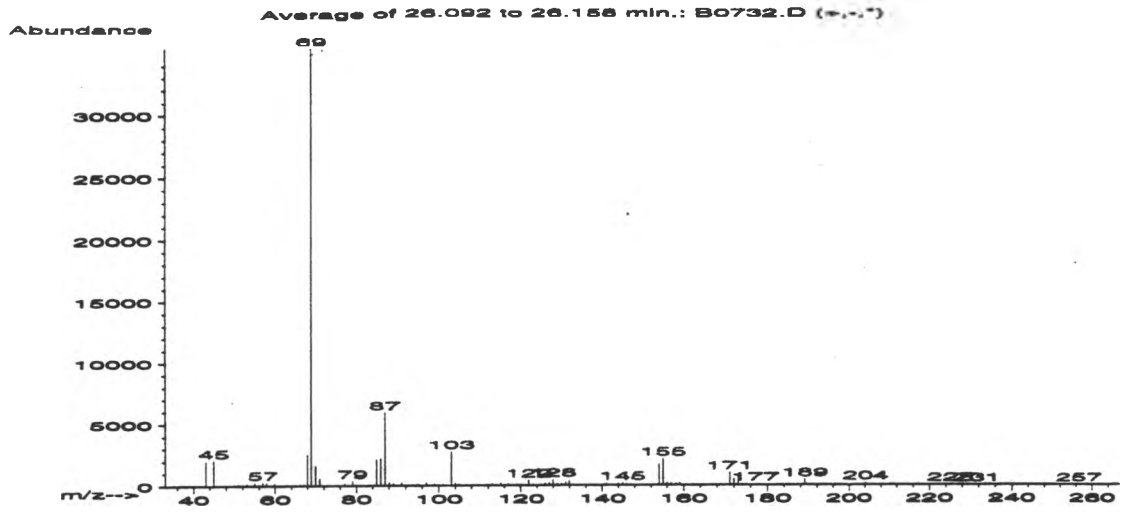
Average of 23.725 to 23.758 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclododecane	168	C12H24	64
2.	Cyclododecane	168	C12H24	58
3.	Cyclododecane	168	C12H24	58
4.	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	53
5.	3-Heptene, 4-ethyl-	126	C9H18	52
6.	Cyclododecane	168	C12H24	52
7.	Silane, trichloroeicosyl-	414	C20H41Cl3Si	50
8.	5-Decene	140	C10H20	49
9.	1-Undecanol	172	C11H24O	47
10.	3-Nonene, 3-methyl-, (E)-	140	C10H20	47
11.	4-Undecene, 4-methyl-	168	C12H24	47
12.	Cyclotetradecane	196	C14H28	47
13.	1-Decene	140	C10H20	46
14.	1-Dodecanol	186	C12H26O	43
15.	Cyclododecane	168	C12H24	43
16.	1-Hexyn-3-ol	98	C6H10O	38
17.	Cyclopropane, octyl-	154	C11H22	38
18.	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	38
19.	TRANS NONENE-3	126	C9H18	38
20.	1-Hexadecanol	242	C16H34O	35

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	000294-62-2	125805	87	19	1	37	24	37	0	45	8566
2.	*58	000294-62-2	125806	53	44	0	38	27	32	0	49	8810
3.	*58	000294-62-2	20781	62	39	0	35	31	32	0	56	8755
4.	53	002207-01-4	2722	47	44	0	68	27	28	20	41	8846
5.	*52	033933-74-3	5427	52	32	1	93	31	27	18	47	8937
6.	*52	000294-62-2	125807	57	46	0	31	34	27	0	49	8654
7.	50	018733-57-8	99977	73	85	3	120	31	25	0	40	9213
8.	*49	019689-19-1	9442	34	65	0	53	39	23	15	43	8715
9.	47	000112-42-5	126223	70	43	0	32	37	20	0	42	8333
10.	*47	069405-42-1	9445	51	37	1	78	37	20	4	41	8853
11.	*47	061142-40-3	20706	61	35	0	71	37	20	4	40	8953
12.	47	000295-17-0	33202	60	54	0	42	37	20	0	43	8903
13.	*46	000872-05-9	122495	33	62	0	30	41	20	22	43	7986
14.	43	000112-53-8	127407	54	55	0	34	41	18	6	41	8447
15.	43	000294-62-2	125809	46	52	0	27	44	18	10	41	8944
16.	*38	000105-31-7	117755	37	55	0	92	50	14	0	41	8774
17.	*38	001472-09-9	14829	46	49	0	32	46	14	19	40	8474
18.	*38	001678-97-3	5467	34	59	0	37	55	14	4	43	8626
19.	*38	000000-00-0	5412	48	40	0	36	48	14	2	41	8692
20.	35	036653-82-4	130923	69	57	0	31	51	11	0	42	8853

Peak 122; Unidentified Alkoxy compound



Average of 26.092 to 26.158 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1986	58.95	46	69.95	1648	83.05	88
44.95	2082	59.95	201	71.00	595	84.00	34
49.95	80	60.95	80	73.95	7	85.00	2160
50.95	144	61.90	39	75.00	17	86.00	2269
52.00	84	62.95	142	76.00	1	87.00	5926
53.00	156	64.00	22	77.05	212	88.05	260
54.05	64	65.00	96	78.00	53	89.00	162
55.00	254	66.20	147	79.05	382	91.00	244
56.00	115	67.10	150	80.00	91	92.05	37
56.95	297	68.00	2544	81.00	60	93.00	31
57.95	270	68.95	35436	82.05	54	93.95	131

Average of 26.092 to 26.158 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.00	135	108.05	75	122.00	437	135.00	10
96.00	43	109.05	53	123.05	78	136.10	23
97.00	238	110.05	60	125.05	89	140.05	73
98.00	37	112.05	92	126.05	168	141.00	172
99.00	137	113.05	176	127.05	228	141.95	48
100.00	61	114.05	87	128.00	476	143.00	70
101.00	54	115.10	206	129.00	109	144.00	148
103.05	2752	116.05	29	130.05	120	145.00	188
104.05	190	117.00	133	131.05	257	146.05	84
105.00	119	119.05	126	131.95	322	147.05	89
107.05	66	121.00	66	134.00	6	149.00	11

Average of 26.092 to 26.158 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

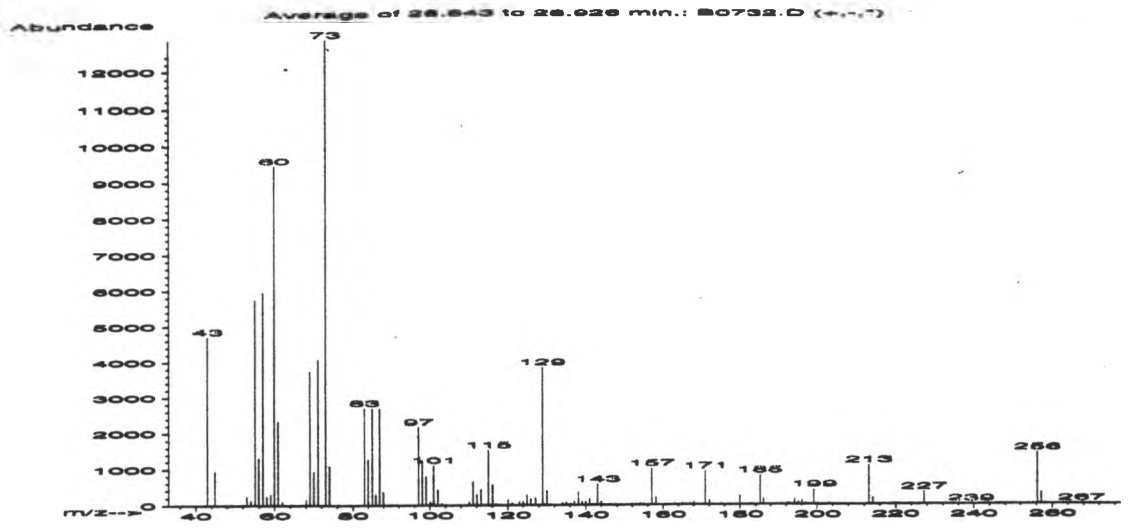
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.00	3	165.10	49	177.95	22	191.00	6
154.00	1708	166.95	7	182.15	13	193.45	20
155.00	2143	168.95	46	183.00	18	194.80	20
156.00	186	170.05	2	183.25	13	197.05	46
157.00	183	171.05	1042	184.25	9	197.95	13
158.10	142	172.05	483	185.00	34	198.20	17
159.10	204	173.05	765	185.25	15	203.20	9
160.05	6	174.05	49	187.05	14	204.10	184
160.95	2	175.05	63	188.10	49	205.15	17
162.10	94	176.30	13	189.05	449	205.50	12
163.20	62	177.10	85	189.95	47	206.10	23

Average of 26.092 to 26.158 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
207.10	19						
208.10	5						
209.65	7						
224.25	5						
225.15	31						
231.50	7						
231.95	1						
256.70	2						

No Library Hits

Peak 123; Hexadecanoic Acid



Average of 28.843 to 28.926 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4710	59.00	298	74.00	1075	99.05	791
44.95	934	59.95	9439	76.20	21	100.05	90
46.95	9	60.95	2322	83.00	2706	101.00	1103
48.80	7	61.95	91	84.00	1264	102.05	422
51.95	24	64.20	33	85.05	2697	103.05	53
53.00	252	65.05	19	86.00	287	107.05	17
54.00	129	68.00	153	87.00	2674	110.05	101
55.00	5742	69.00	3740	88.00	358	111.05	657
55.95	1313	70.00	934	89.05	4	112.05	289
57.00	5946	71.05	4067	97.05	2163	113.15	430
58.00	252	73.00	12847	98.05	1238	114.05	23

Average of 28.843 to 28.926 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.05	1532	129.00	3832	141.70	14	156.15	27
116.10	569	130.05	381	142.10	21	157.10	1004
117.00	34	131.05	22	143.05	576	158.10	206
117.80	6	134.05	58	144.00	102	163.10	37
120.05	151	135.05	83	147.80	10	164.10	11
121.05	72	136.10	40	149.05	18	165.10	48
123.05	96	137.05	100	151.10	20	165.80	13
124.05	96	138.10	347	152.10	36	167.05	32
125.05	283	139.10	94	153.10	26	168.10	69
126.05	168	140.05	92	154.05	49	171.05	924
127.15	194	141.00	163	155.00	22	172.10	106

Average of 28.843 to 28.926 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
175.20	39	192.30	44	203.75	8	227.20	331
177.10	10	192.95	34	204.25	10	234.75	6
177.75	14	194.10	130	209.00	20	239.30	11
179.00	1	195.10	75	213.20	1076	250.00	1
180.00	244	196.15	107	214.20	182	256.15	1418
182.40	8	197.10	45	215.05	10	257.20	302
183.15	8	197.80	14	216.05	10	258.00	11
185.15	803	199.20	411	219.00	14	258.25	8
186.10	152	200.25	45	219.70	6	267.45	7
190.30	1	201.45	9	220.10	20		
190.70	10	203.10	31	220.70	8		

CTMP Compounds

Average of 28.843 to 28.926 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Pentadecanoic acid	242	C15H30O2	87
2.	Tetradecanoic acid	228	C14H28O2	87
3.	Pentadecanoic acid	242	C15H30O2	86
4.	Hexadecanoic acid	256	C16H32O2	83
5.	Undecanoic acid	186	C11H22O2	83
6.	Dodecanamide, N,N-bis(2-hydroxyethyl)-	287	C16H33NO3	80
7.	Tetradecanoic acid	228	C14H28O2	74
8.	Dodecanoic acid	200	C12H24O2	72
9.	Tridecanoic acid	214	C13H26O2	72
10.	Decanoic acid	172	C10H20O2	64
11.	Decanoic acid	172	C10H20O2	64
12.	Decanoic acid, silver(1+) salt	279	C10H20AgO2	53
13.	Tridecanoic acid	214	C13H26O2	53
14.	Dodecanoic acid	200	C12H24O2	53
15.	Dodecanoic acid	200	C12H24O2	53
16.	Dodecanoic acid	200	C12H24O2	50
17.	Tetradecanoic acid	228	C14H28O2	45
18.	Undecanoic acid	186	C11H22O2	43
19.	Nonanoic acid	158	C9H18O2	43
20.	Decanoic acid	172	C10H20O2	42

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	87	001002-84-2	130901	96	60	2	77	9	54	0	51	9888
2.	87	000544-63-8	130226	98	45	1	79	9	54	0	51	9892
3.	86	001002-84-2	130903	99	63	2	67	9	53	0	46	9881
4.	*83	000057-10-3	131575	83	53	1	75	14	50	23	56	8264
5.	83	000112-37-8	127362	101	30	2	75	13	50	0	56	9742
6.	80	000120-40-1	69540	90	60	1	71	15	48	0	47	9855
7.	74	000544-63-8	130228	101	37	2	82	18	44	0	56	9807
8.	72	000143-07-7	128389	86	49	2	69	20	42	0	45	9674
9.	72	000638-53-9	129335	91	47	3	75	18	42	0	47	9736
10.	64	000334-48-5	126157	75	40	2	78	18	37	22	39	9611
11.	64	000334-48-5	126151	76	37	2	69	20	37	4	39	9547
12.	53	013126-67-5	66612	60	92	3	54	27	28	0	39	9847
13.	53	000638-53-9	41267	71	61	0	50	29	28	21	41	6419
14.	53	000143-07-7	128386	74	62	2	69	29	28	0	41	9656
15.	53	000143-07-7	128387	70	62	2	59	29	28	0	38	9727
16.	50	000143-07-7	128385	55	67	1	63	34	25	5	40	9573
17.	45	000544-63-8	130227	72	72	1	63	22	19	0	37	9883
18.	43	000112-37-8	127364	87	41	2	90	50	18	0	45	9682
19.	*43	000112-05-0	124678	35	66	0	57	44	18	0	41	9387
20.	42	000334-48-5	126153	78	31	2	83	29	17	11	37	9451

CTMP Compounds

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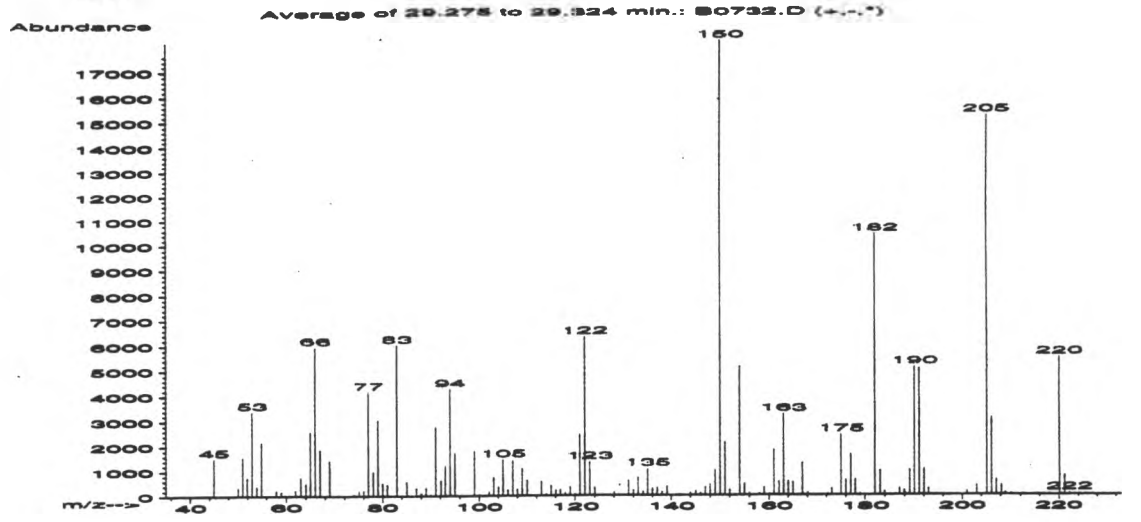
Peak ~~193~~; Unidentified Sesquiterpene



Average of 29.275 to 29.324 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	1502	64.00	500	80.00	502	93.00	1196
50.00	337	65.00	2572	81.00	453	94.00	4269
50.95	1538	66.00	5933	83.00	6006	95.00	1699
51.95	734	67.00	1836	85.00	575	99.00	1783
52.95	3370	68.95	1414	86.00	22	100.00	52
54.00	395	74.00	69	87.00	307	101.05	21
55.00	2152	75.05	207	88.00	120	102.05	170
58.00	217	76.00	204	89.00	320	103.05	759
59.00	176	77.05	4152	90.00	57	104.05	349
61.95	235	78.05	977	91.05	2748	105.00	1454
63.00	746	79.05	3028	92.10	624	106.00	236

Average of 29.275 to 29.324 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	1399	120.05	73	133.00	722	146.00	97
108.00	276	121.00	2443	134.05	164	146.20	47
109.00	1093	122.00	6325	135.00	1080	147.00	333
110.00	622	123.00	1344	136.05	279	148.00	447
113.00	577	124.05	310	137.05	311	149.05	1012
114.05	62	127.20	59	138.05	147	150.05	18166
115.05	400	128.05	127	139.10	364	151.00	2133
116.05	222	129.00	42	141.00	1	152.00	222
116.95	253	130.00	18	141.90	41	154.00	5126
118.00	102	131.00	615	144.00	105	155.00	459
119.00	348	132.00	205	145.05	169	156.00	93

Average of 29.275 to 29.324 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
158.05	72	169.05	6	183.05	983	195.45	9
159.00	307	172.20	65	183.95	158	198.45	10
160.10	49	173.05	263	186.20	27	198.95	16
161.00	1810	174.05	17	187.00	261	201.05	160
162.10	553	175.05	2424	187.95	181	202.00	6
163.00	3234	176.05	598	188.15	69	203.05	385
164.00	560	177.05	1631	189.05	1006	203.75	21
165.00	524	178.00	630	190.05	5110	205.10	15214
166.05	33	179.00	68	191.05	5051	206.15	3098
166.95	1301	180.05	4	192.05	1063	207.10	608
168.05	101	182.00	10461	193.00	265	208.15	390

CTMP Compounds

Average of 29.275 to 29.324 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
208.95	87						
209.15	29						
210.10	36						
214.95	18						
217.95	22						
218.20	13						
220.10	5505						
221.15	786						
222.15	81						
223.05	16						

Average of 29.275 to 29.324 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	4-Methoxy-3-methylthioquinoline	205	C11H11NOS	59
2.	Benzoic acid, 2,4-dihydroxy-6-methyl-, m	182	C9H10O4	45
3.	2,5-Methano-1H-inden-7(4H)-one, hexahydr	150	C10H14O	27
4.	6-Hydroxymethylidene-7-isopropylidene-4-	220	C13H16O3	22
5.	2H-1-Benzopyran, 6,7-dimethoxy-2,2-dimet	220	C13H16O3	18
6.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	15
7.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	15
8.	Benzothiazole, 2-(sec-butylamino)-	206	C11H14N2S	11
9.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	11
10.	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	11
11.	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	11
12.	5-METHYL-2-(N-METHYLPHENYLAMINO)-2-THIAZ	206	C11H14N2S	11
13.	2,4,6-Tri-isopropyl-phenol	220	C15H24O	11
14.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	11
15.	[1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-	150	C6H6N4O	10
16.	Benzonitrile, 3-(2-phenylethenyl)-, (E)-	205	C15H11N	10
17.	Phenol, 2,6-bis(1,1-dimethylethyl)-4-met	220	C15H24O	10
18.	6H-Purin-6-one, 1,7-dihydro-1-methyl-	150	C6H6N4O	10
19.	5-PHENYLISOQUINOLINE	205	C15H11N	10
20.	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	083936-11-2	36910	30	16	0	77	23	33	9	42	5611
2.	*45	003187-58-4	126976	74	49	2	97	48	19	0	58	7361
3.	*27	027567-85-7	12863	59	44	3	96	57	8	14	41	6375
4.	*22	094239-81-3	43669	43	86	3	83	64	5	0	40	5438
5.	*18	000644-06-4	43695	68	50	2	59	70	3	1	47	5698
6.	*15	000128-37-0	129736	62	55	1	83	71	2	0	56	5580
7.	*15	000128-37-0	129734	61	55	2	83	71	2	0	56	5600
8.	*11	028291-73-8	37313	57	56	3	94	76	2	0	47	6300
9.	*11	000128-37-0	129732	49	64	3	83	71	2	0	46	5584
10.	*11	000611-01-8	123596	50	65	3	87	78	2	0	46	6336
11.	*11	000611-01-8	12583	50	66	3	88	79	2	0	46	6180
12.	*11	029604-93-1	37318	51	76	2	58	76	2	0	46	5268
13.	*11	000000-00-0	43903	44	24	0	83	71	2	0	44	5572
14.	*11	000128-37-0	129737	50	68	2	83	71	2	0	46	5592
15.	*10	002503-56-2	12451	37	48	1	99	74	1	13	40	6598
16.	*10	014064-35-8	37016	33	86	3	73	71	1	11	40	5565
17.	*10	000128-37-0	129735	43	69	2	83	71	1	0	40	5607
18.	*10	001125-39-9	12452	35	61	3	99	73	1	11	40	6497
19.	*10	024464-35-5	128793	33	74	3	73	76	1	14	40	5280
20.	*10	000603-79-2	12582	36	47	1	73	79	1	5	40	6180

CTMP Compounds

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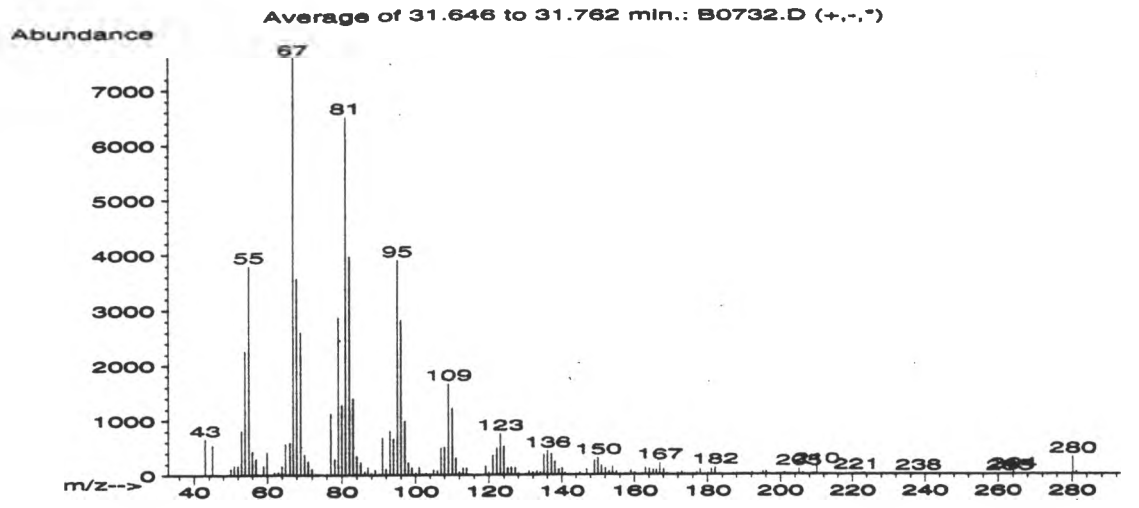
Peak 124; Linoleic Acid



Average of 31.646 to 31.762 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	660	59.00	174	71.00	251	83.00	1399
44.95	544	59.95	421	72.00	110	84.00	351
50.05	121	62.00	46	72.95	14	85.00	233
50.95	170	63.00	56	74.00	10	86.05	62
52.05	164	64.00	166	76.00	22	87.00	148
53.00	814	65.00	564	77.05	1134	87.95	36
54.00	2263	66.10	595	78.05	295	89.00	93
55.00	3793	67.00	7599	79.05	2865	90.15	19
56.00	433	68.00	3561	80.00	1283	91.00	681
57.00	293	69.00	2596	81.00	6507	92.00	117
57.95	8	70.05	378	82.00	3959	93.00	814

Average of 31.646 to 31.762 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
94.00	669	105.00	102	117.00	15	131.00	79
95.05	3891	106.05	76	119.05	163	132.05	54
96.05	2810	107.00	500	120.00	46	133.05	63
97.05	989	108.00	512	121.05	368	134.05	46
98.05	223	109.05	1664	122.05	497	135.00	379
99.05	137	110.10	1221	123.05	763	136.10	443
100.05	37	111.10	313	124.05	526	137.15	388
101.05	146	112.05	57	125.10	131	138.10	247
102.00	16	113.00	128	126.05	142	139.10	105
103.00	36	114.00	130	127.05	139	140.15	126
104.05	17	115.10	9	128.05	29	141.00	34

Average of 31.646 to 31.762 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.80	1	155.05	63	168.05	102	178.00	108
144.00	6	155.95	10	169.05	16	179.05	11
145.00	48	158.15	11	172.00	30	180.15	40
146.05	2	159.15	80	172.20	8	181.00	107
147.00	108	160.05	34	173.05	62	182.10	129
149.05	267	162.05	26	173.85	18	183.15	17
150.05	311	163.10	126	174.15	2	184.40	5
151.05	174	164.10	111	175.05	13	186.05	2
152.10	124	165.15	88	175.80	6	187.10	19
153.05	63	166.05	87	176.10	22	188.00	24
154.05	142	167.00	218	177.10	48	189.05	11

CTMP Compounds

Average of 31.646 to 31.762 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
189.95	5	209.10	39	228.00	5	276.25	5
191.00	5	210.10	138	233.25	7	280.20	323
192.20	49	213.00	9	236.00	7	281.15	55
194.10	1	213.30	4	236.50	11	283.00	5
195.15	65	219.20	7	238.15	11		
196.05	65	221.10	30	251.25	6		
197.00	7	222.00	7	263.05	7		
201.05	40	222.45	17	263.50	12		
204.05	4	223.05	8	263.80	6		
205.10	104	223.25	29	264.15	45		
206.15	39	224.70	5	269.20	5		

Average of 31.646 to 31.762 min.: B0732.D
Converted from RTE data file: >B0732:

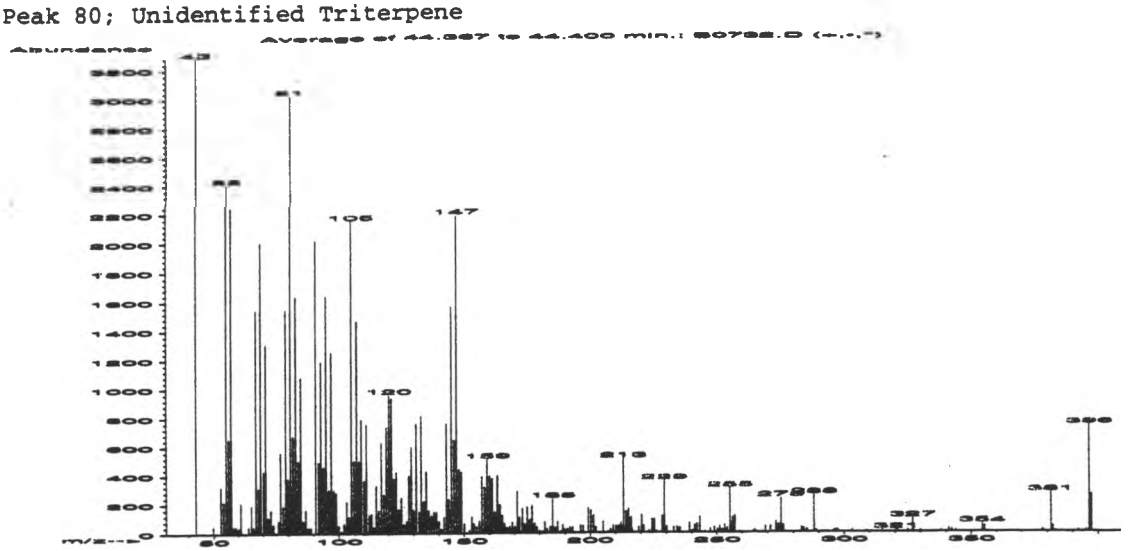
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	7-Hexadecyne	222	C16H30	93
2.	11-Octadecynoic acid, methyl ester	294	C19H34O2	91
3.	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	90
4.	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	86
5.	3,4-Octadiene, 7-methyl-	124	C9H16	81
6.	5-Eicosyne	278	C20H38	78
7.	Cyclodecene	138	C10H18	64
8.	1-Hexadecyne	222	C16H30	64
9.	Cyclodecene	138	C10H18	64
10.	3-Octadecyne	250	C18H34	58
11.	11,14-Eicosadienoic acid, methyl ester	322	C21H38O2	58
12.	3-Hexadecyne	222	C16H30	53
13.	9,17-Octadecadienal, (Z)-	264	C18H32O	52
14.	4-METHYL-4-(ISO-BUTEN-1-YL)CYCLOBUTANONE	138	C9H14O	52
15.	3-Dodecyne	166	C12H22	49
16.	1,E-8,Z-10-TRIDECATRIENE	178	C13H22	46
17.	Cyclohexane, ethenyl-	110	C8H14	43
18.	Oxacycloheptadec-8-en-2-one	252	C16H28O2	43
19.	Pentalene, octahydro-, cis-	110	C8H14	35
20.	TRANS-BICYCLO[5.1.0]OCTANE	110	C8H14	30

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*93	074685-28-2	45100	84	53	1	91	8	66	0	91	9891
2.	91	026543-37-3	71930	103	71	3	81	4	60	0	59	9924
3.	*90	000060-33-3	132609	78	97	3	82	5	57	4	43	9974
4.	86	000060-33-3	67138	90	88	3	68	10	53	0	49	9631
5.	*81	037050-05-8	4880	68	43	1	99	17	49	0	76	9558
6.	78	074685-31-7	66578	79	79	2	85	10	46	0	41	9794
7.	*64	003618-12-0	122323	73	45	1	83	21	37	16	44	9944
8.	*64	000629-74-3	45097	63	82	2	61	25	37	0	50	9805
9.	*64	003618-12-0	122322	73	45	1	83	21	37	16	44	9944
10.	58	061886-64-4	56712	90	54	1	74	30	32	0	47	9684
11.	58	002463-02-7	80740	124	37	1	71	30	32	11	49	8525
12.	53	061886-62-2	45098	82	51	1	93	30	28	0	41	9685
13.	52	056554-35-9	61434	91	56	2	85	33	27	0	49	8455
14.	*52	000000-00-0	8602	43	24	0	118	34	27	0	44	8845
15.	*49	006790-27-8	19712	58	49	3	197	44	23	0	56	9290
16.	*46	080625-30-5	24966	73	40	1	78	44	20	28	50	8181
17.	43	000695-12-5	118900	58	52	2	193	41	18	0	43	8442
18.	43	000123-69-3	57479	73	76	1	47	44	18	0	41	9614
19.	*35	001755-05-1	118910	36	56	0	83	55	11	0	41	7727
20.	*30	021370-66-1	2299	36	64	0	57	58	9	18	43	9445

CTMP Compounds

Peak 80; Unidentified Triterpene



Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3281	63.95	44	76.05	86	87.00	159
49.75	47	65.05	190	77.05	557	88.05	37
52.95	319	66.05	41	78.00	187	89.00	39
54.00	215	67.00	1544	79.05	1548	91.00	2016
55.05	2405	68.00	308	80.00	378	92.05	493
56.00	649	69.00	1999	81.00	3021	93.00	1184
57.00	2240	70.05	426	82.00	672	94.05	457
58.00	44	71.05	1306	83.00	1637	95.05	1638
59.00	46	72.05	114	84.00	498	96.05	298
59.95	36	73.00	158	85.05	1078	97.05	1253
60.95	208	74.00	62	86.00	84	98.05	292

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	275	110.10	359	121.05	933	132.05	147
100.00	52	111.05	754	122.05	375	133.00	811
101.00	14	112.10	124	123.05	423	134.05	221
102.00	67	113.10	134	124.05	164	135.05	425
103.05	214	114.10	42	125.05	245	136.10	155
104.00	115	115.00	327	126.05	65	137.10	121
105.00	2148	116.05	157	127.10	83	138.10	147
106.00	502	117.00	628	128.05	397	139.15	143
107.00	1464	118.05	267	129.00	597	140.15	83
108.05	499	119.05	735	129.95	157	141.05	28
109.00	787	120.05	954	131.00	758	142.05	113

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.05	758	155.05	45	166.05	67	177.05	189
144.05	235	156.05	85	167.00	37	178.05	66
145.05	1567	157.05	393	168.05	49	179.00	41
146.05	646	158.05	315	169.05	75	180.10	18
147.05	2182	159.10	509	170.05	44	181.10	14
148.10	442	160.05	394	171.05	285	182.10	75
149.05	424	161.10	374	172.00	110	183.05	26
150.10	66	162.10	143	173.10	169	184.15	44
152.00	21	163.15	398	174.05	61	185.15	232
153.10	114	164.15	192	175.10	177	186.05	38
154.00	66	165.10	121	176.05	92	187.10	80

CTMP Compounds

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
188.20	12	201.25	119	214.20	146	227.15	3
189.15	57	202.15	39	215.15	163	228.20	118
190.05	24	205.15	80	216.15	105	229.20	358
191.05	30	207.00	12	216.55	22	230.15	42
192.05	41	208.10	28	219.20	43	233.05	42
193.05	40	209.10	54	220.30	122	234.25	43
194.05	3	210.05	6	221.10	49	235.20	31
196.15	53	210.25	49	223.10	18	235.40	33
197.15	48	211.20	49	224.25	95	236.15	1
199.20	170	212.15	71	225.20	95	239.15	68
200.25	155	213.15	507	226.20	11	240.00	10

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
240.45	16	253.05	56	273.20	75	297.30	17
241.20	54	254.10	33	274.20	55	303.15	18
242.05	61	255.20	302	275.15	233	309.25	11
243.20	109	256.00	67	276.05	49	315.20	11
245.10	9	256.20	105	283.10	35	320.70	11
247.25	29	257.15	117	284.05	29	324.90	5
249.00	40	258.90	6	285.25	20	325.20	13
250.30	24	264.45	13	288.15	253	327.00	90
251.15	45	264.95	19	289.15	16	328.20	5
251.50	19	269.05	42	296.05	16	330.00	13
252.25	19	271.15	41	296.70	14	330.40	4

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
338.20	11	383.25	7				
341.10	26	392.20	14				
341.95	2	395.30	14				
342.30	18	396.45	736				
343.80	14	397.35	255				
354.30	53						
355.25	43						
378.15	18						
381.40	266						
382.00	34						
382.25	37						

CTMP Compounds

Average of 44.367 to 44.400 min.: B0732.D
Converted from RTE data file: >B0732:

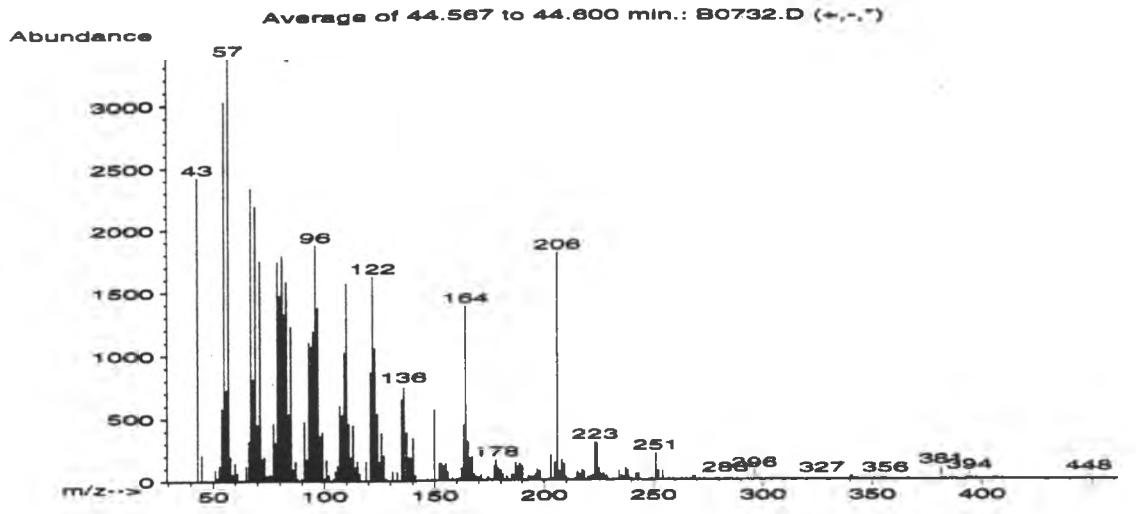
PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	3-Nonyn-2-ol	140	C9H16O	18
2.	Silane, trichloro-3-cyclohexen-1-yl-	214	C6H9Cl3Si	11
3.	Cyclohexane, 1,4-dibromo-	240	C6H10Br2	11
4.	1-Nitrobicyclo[6.1.0]nonane	169	C9H15NO2	10
5.	Cyclohexane, 1,4-dibromo-	240	C6H10Br2	10
6.	Cyclopentanecarboxylic acid, 3-methylene	140	C8H12O2	10
7.	CYCLOPENTANE, 1-ISOBUTYLIDEN-3-METHYL-	138	C10H18	10
8.	5.alpha.-Androst-15-en-17.beta.-ol, 17-m	288	C20H32O	10
9.	4.beta.,7.beta.-Epidioxy-3a.alpha.,7a.al	166	C9H10O3	10
10.	1,3,7-OCTATRIENE, 2,7-DIMETHYL-	136	C10H16	10
11.	Cyclohexane, 1,1-dichloro-	152	C6H10Cl2	10
12.	Cyclohexane, 1,2-dibromo-	240	C6H10Br2	10
13.	Cyclopentanol, 3,?-dimethyl-	114	C7H14O	10
14.	CYCLOPENTANE, 1-HYDROXYMETHYL-3-METHYL-	114	C7H14O	10
15.	Cyclohexane, 1,3-dibromo-	240	C6H10Br2	10
16.	3-BROMO-1,2,4-TRIAZINE 2-OXIDE	175	C3H2BrN3O	10
17.	Androst-5-en-17-one, 3-hydroxy-, (3.beta	288	C19H28O2	10
18.	Cyclopentaneethanol, 2-(hydroxymethyl)-.	172	C10H20O2	10
19.	3-Cyclohexene-1-acetic acid, .alpha.-oxo	168	C9H12O3	9
20.	N-PHENYL-4H-5,7A-EPOXYISOINDOLINE	211	C14H13NO	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*18	026547-25-1	9352	52	69	1	79	69	3	0	46	7133
2.	*11	010137-69-6	40935	45	60	1	75	76	2	0	44	6190
3.	*11	035076-92-7	52248	54	48	0	78	77	2	0	49	6050
4.	10	091923-58-9	20933	56	41	0	72	77	1	3	40	6050
5.	*10	035076-92-7	130771	41	56	0	75	77	1	0	39	6050
6.	*10	037575-80-7	9210	36	58	2	66	76	1	0	39	6144
7.	10	000000-00-0	8779	46	61	2	92	66	1	0	34	6810
8.	*10	013864-65-8	70076	39	115	3	92	69	1	18	36	7001
9.	*10	056411-68-8	19332	45	41	1	75	75	1	0	40	6492
10.	*10	000000-00-0	8062	43	63	1	90	75	1	0	39	6399
11.	*10	002108-92-1	123840	33	48	1	63	77	1	0	39	6050
12.	*10	005401-62-7	52246	38	56	0	71	77	1	0	39	6050
13.	10	074664-15-6	3167	44	56	0	68	71	1	19	41	6677
14.	10	000000-00-0	3170	44	56	0	68	71	1	19	41	6677
15.	*10	003725-17-5	52247	40	56	0	87	77	1	0	39	6050
16.	10	061178-02-7	23282	58	90	0	34	77	1	0	43	5537
17.	10	000053-43-0	132993	74	89	1	54	77	1	15	39	4732
18.	10	000485-42-7	22351	63	66	3	91	66	1	0	36	6820
19.	9	077846-83-4	20227	44	43	2	92	77	1	7	34	6050
20.	9	000000-00-0	39967	45	66	2	73	77	1	0	35	6050

CTMP Compounds

CTMP Peak ~~125~~ 26; Unidentified triterpene



Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2425	58.95	53	72.00	176	83.00	1580
44.95	209	59.95	141	73.00	190	84.00	534
46.90	1	60.95	62	74.00	41	85.00	1226
51.00	90	62.90	4	75.00	43	86.00	91
51.95	24	65.00	118	76.00	48	87.00	152
53.00	126	66.10	320	77.05	458	88.00	17
54.00	582	67.00	2334	78.05	307	89.90	21
55.05	3029	68.00	815	79.05	1740	91.05	472
56.00	729	69.05	2191	80.00	1471	92.05	172
57.00	3375	70.05	450	81.00	1788	93.05	1101
57.95	193	71.05	1748	82.00	1323	94.05	1069

Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.05	1188	107.00	602	121.05	869	136.05	760
96.05	1870	108.00	528	122.05	1620	137.15	390
97.05	1371	109.00	1020	123.05	1054	138.15	187
98.05	360	110.10	1567	124.05	537	139.10	183
99.05	390	111.05	456	125.10	150	140.15	340
100.05	20	112.10	188	126.05	384	141.05	44
101.05	168	113.00	445	127.10	201	150.05	570
102.05	49	114.05	111	128.05	15	152.05	135
104.00	21	115.05	158	131.00	75	153.05	135
105.00	79	116.05	56	133.05	69	154.10	116
106.00	125	119.00	154	135.05	648	155.15	139

Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
156.00	67	169.05	27	182.10	3	195.10	29
158.05	18	170.00	26	182.95	34	196.20	52
160.10	14	171.05	48	185.15	46	197.10	89
161.15	15	174.15	27	186.10	46	198.20	72
162.15	99	175.05	10	187.10	147	202.15	12
163.15	445	177.10	115	188.10	107	203.15	205
164.15	1385	178.00	168	189.15	137	204.15	9
165.15	312	179.05	96	190.10	113	205.15	142
166.05	177	179.75	44	192.05	7	206.15	1805
167.00	192	180.05	77	193.05	34	207.05	69
168.05	48	181.10	46	194.05	24	208.10	163

CTMP Compounds

Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
209.15	124	224.20	296	237.25	97	259.10	12
210.05	25	225.20	93	238.20	71	262.95	29
214.20	15	226.25	43	239.10	12	265.00	43
215.20	70	227.20	50	240.10	7	266.95	13
216.10	49	228.50	32	242.05	48	268.00	24
217.20	85	233.20	6	243.15	51	268.30	19
218.15	68	234.15	73	249.10	29	269.30	34
220.15	24	235.25	35	251.10	213	271.20	13
221.15	27	235.50	29	252.25	75	273.20	12
222.15	37	236.25	22	254.15	68	278.90	14
223.10	300	236.75	20	257.15	19	279.45	6

Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
279.65	21	327.15	28	366.45	18	448.50	39
282.75	34	339.25	4	381.45	94		
284.05	7	340.20	27	382.40	3		
284.50	12	340.95	16	393.35	19		
285.10	15	341.20	23	394.30	51		
296.15	70	342.95	22	395.30	12		
297.25	30	343.20	24	397.55	36		
299.05	14	351.15	13	405.40	17		
311.15	17	354.40	7	406.35	9		
325.10	14	355.10	25	407.25	12		
326.90	13	355.90	27	409.40	14		

CTMP Compounds

Average of 44.567 to 44.600 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	(7)(3,5)PYRAZOLOPHANE	164	C10H16N2	25
2.	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	25
3.	.beta.-Patchoulane	206	C15H26	22
4.	2-Ethyl-3-methyl-1-(phenylthio)but-2-ene	206	C13H18S	22
5.	2-Methyl-3-phenylthiopropene	164	C10H12S	14
6.	1,E-11,Z-13-HEXADECATRIENE	220	C16H28	12
7.	(E)-9,11-Dodecadien-1-yl acetate	224	C14H24O2	11
8.	9-PROPYL-9-BORABICYCLO[3.3.1]NONANE	164	C11H21B	11
9.	Tetradecanal	212	C14H28O	10
10.	2-ETHYL-5-PENTYL-1-PYRROLINE	167	C11H21N	10
11.	Hexadecanal	240	C16H32O	10
12.	10-Heptadecen-8-ynoic acid, methyl ester	278	C18H30O2	10
13.	Tetradecanal	212	C14H28O	10
14.	3,6-Dodecadienoic acid, methyl ester	210	C13H22O2	10
15.	4-Penten-2-ynylamine, N,N,4-trimethyl-	123	C8H13N	10
16.	CIS-P-MENTHAN-9-OL	156	C10H20O	10
17.	ISOPROPYL N-BUTYL DISULPHIDE	164	C7H16S2	10
18.	TRANS,TRANS-NONA-2,4-DIENOL	140	C9H16O	10
19.	Ethanol, 2-(9,12-octadecadienyloxy)-, (Z	310	C20H38O2	10
20.	Bicyclo[3.3.1]nonan-2-ol, exo-	140	C9H16O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*25	037072-10-9	18554	51	59	1	44	63	7	0	46	6343
2.	*25	064566-18-3	131394	63	105	3	128	64	7	0	50	6977
3.	*22	020478-88-0	37752	59	91	2	46	61	5	0	41	7125
4.	*22	066165-26-2	37539	36	26	1	70	61	5	14	40	6179
5.	*14	000702-00-1	125345	33	85	3	89	67	2	1	40	5683
6.	12	080634-97-5	44092	61	87	3	149	63	2	6	37	6886
7.	*11	050767-78-7	45890	50	81	1	69	79	2	0	46	5299
8.	*11	000000-00-0	18702	48	74	1	39	79	2	0	46	5387
9.	10	000124-25-4	40571	58	89	3	99	79	1	0	39	5953
10.	*10	061772-95-0	19966	37	56	1	40	70	1	14	37	6111
11.	10	000629-80-1	52760	85	76	2	74	72	1	0	39	6217
12.	10	016714-85-5	66504	58	119	3	121	79	1	0	39	4497
13.	10	000124-25-4	129222	59	86	3	115	73	1	0	39	5968
14.	10	016106-01-7	39470	67	67	0	45	79	1	0	38	4512
15.	*10	019837-34-4	4590	37	71	2	42	79	1	0	39	5078
16.	10	005113-95-1	15609	47	69	0	58	80	1	12	41	5481
17.	*10	072437-53-7	18278	33	56	1	244	75	1	0	39	4878
18.	*10	064576-90-5	9353	50	46	1	44	80	1	16	39	4884
19.	10	017367-08-7	77158	59	119	0	58	76	1	0	43	7729
20.	*10	010036-15-4	122489	34	81	0	38	77	1	0	41	6521

CTMP Compounds

CTMP Compounds

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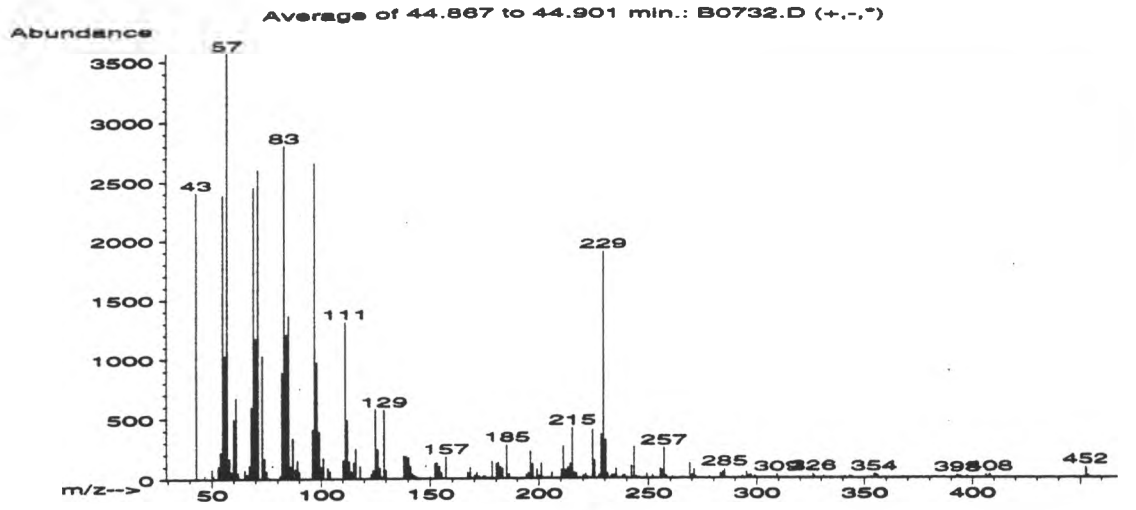
Peak 126; Tetradeanoic acid, hexadecyl ester



Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2407	59.95	493	73.00	1028	88.15	80
46.80	30	61.00	672	74.00	167	89.00	149
50.00	83	61.95	48	75.00	64	90.00	58
50.95	23	62.95	4	75.95	9	96.05	409
53.00	109	65.00	73	81.00	29	97.05	2654
54.00	221	66.05	40	82.00	890	98.05	968
55.05	2386	67.05	112	83.00	2800	99.05	388
56.00	1027	67.95	598	84.05	1203	100.05	99
57.00	3569	69.00	2454	85.00	1363	101.00	171
58.00	169	70.05	1173	86.00	104	103.05	86
58.95	58	71.05	2599	87.00	332	104.10	60

Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.10	156	126.05	241	143.05	26	168.20	93
111.15	1306	127.05	88	144.05	15	170.10	26
112.05	485	128.05	11	149.05	5	171.10	47
113.05	143	129.00	570	150.10	12	172.10	16
114.00	61	130.00	71	152.10	124	173.05	7
115.05	131	135.00	2	153.05	131	174.05	19
116.05	246	138.15	187	154.05	100	175.05	18
118.05	104	139.15	181	155.00	46	177.05	3
123.05	39	140.20	171	157.00	179	178.15	140
124.05	71	141.00	102	167.05	56	180.15	123
125.10	578	142.00	37	168.00	21	181.10	131

Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
182.10	93	201.20	122	217.10	42	231.15	41
183.05	83	202.10	9	218.20	3	232.90	20
185.10	276	204.15	9	220.15	26	233.25	28
186.20	35	206.00	48	221.15	36	234.20	28
190.10	6	210.20	72	222.20	12	235.20	79
194.05	32	211.20	263	224.30	398	238.15	22
195.10	49	212.15	71	225.15	148	238.45	26
196.20	222	213.20	90	227.20	30	239.15	22
197.15	119	214.20	122	228.20	362	241.15	1
199.20	74	215.15	416	229.25	1896	242.15	100
200.20	23	216.15	46	230.25	313	243.25	257

CTMP Compounds

Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
244.30	17	264.60	6	295.20	51	340.00	10
244.55	17	265.90	1	296.20	24	341.15	14
245.70	11	269.10	123	297.20	29	343.20	16
249.15	40	270.10	28	299.05	18	344.05	14
251.90	27	271.05	71	309.25	31	353.00	12
252.20	7	271.70	13	311.05	4	354.40	33
255.40	83	278.15	15	326.15	36	355.15	31
256.15	68	283.15	43	326.65	18	356.15	22
257.20	249	284.15	53	329.30	2	392.70	22
258.15	22	285.05	74	331.00	13	393.40	13
260.90	13	293.30	18	339.15	4	394.25	15

Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
397.40	13						
406.25	27						
407.65	20						
408.15	30						
452.40	87						
452.65	71						
453.65	21						

CTMP Compounds

Average of 44.867 to 44.901 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

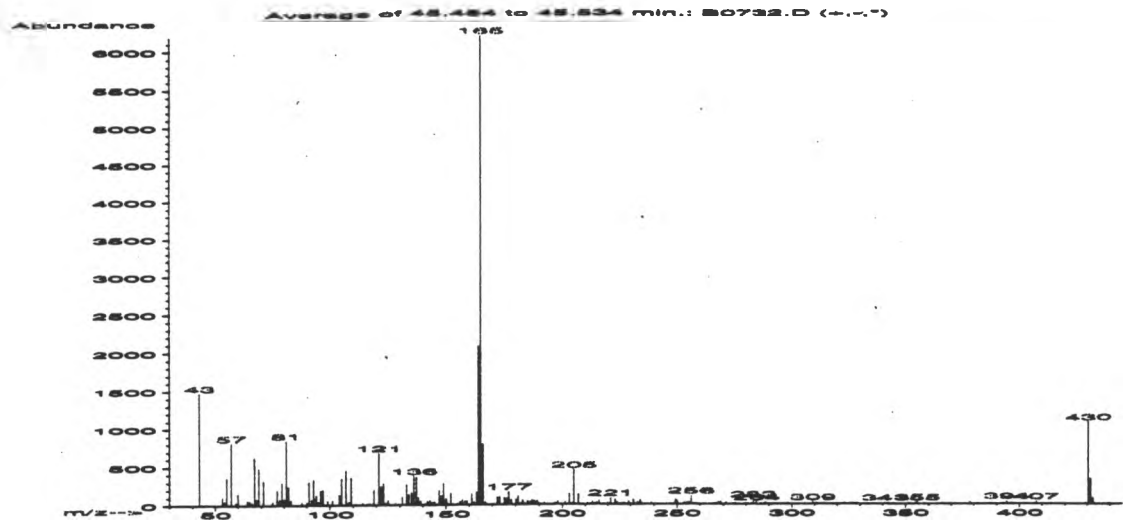
	Name	MolWt	Formula	Qual
1.	Tetradecanoic acid, hexadecyl ester	452	C30H60O2	98
2.	1-Hexadecene	224	C16H32	86
3.	1-Hexadecene	224	C16H32	86
4.	7-Heptadecene, 1-chloro-	272	C17H33Cl	83
5.	1-Nonadecene	266	C19H38	72
6.	Cyclohexadecane	224	C16H32	70
7.	1-Dotriacontanol	467	C32H66O	64
8.	Hexadecanoic acid, tetradecyl ester	452	C30H60O2	58
9.	1-Hexadecene	224	C16H32	58
10.	Tetradecanoic acid, tetradecyl ester	424	C28H56O2	58
11.	1,2-Octadecanediol	286	C18H38O2	52
12.	5-Octadecene, (E)-	252	C18H36	46
13.	2-Octadecenal	266	C18H34O	43
14.	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-,	224	C15H28O	38
15.	4-Octadecenal	266	C18H34O	25
16.	1-Hexadecanol	242	C16H34O	25
17.	Cycloundecane, (1-methylethyl)-	196	C14H28	20
18.	Thiophene, 2-decyl-	224	C14H24S	18
19.	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-,	224	C15H28O	18
20.	3-Decen-5-one	154	C10H18O	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*98	002599-01-1	104932	137	56	0	56	13	79	59	98	8399
2.	*86	000629-73-2	130027	121	42	1	68	29	53	49	84	8944
3.	*86	000629-73-2	130032	79	72	2	101	29	53	0	90	8962
4.	*83	056554-78-0	64326	92	76	1	59	35	50	48	83	8818
5.	72	018435-45-5	132005	116	40	1	95	18	42	0	45	9093
6.	*70	000295-65-8	46076	93	68	0	56	45	41	32	83	8735
7.	64	006624-79-9	106313	83	97	2	110	21	37	0	45	9143
8.	58	004536-26-9	104931	98	101	3	89	35	32	0	56	9318
9.	*58	000629-73-2	130029	61	87	2	112	32	32	0	56	9012
10.	58	003234-85-3	101543	120	79	1	51	27	32	12	45	8904
11.	52	020294-76-2	69289	102	56	2	93	31	27	0	46	8001
12.	*46	007206-21-5	57573	63	98	1	53	45	20	25	47	9005
13.	*43	056554-96-2	62186	54	108	2	71	50	18	0	47	8966
14.	*38	020576-58-3	46007	63	85	2	58	64	14	0	64	6735
15.	*25	056554-98-4	62188	60	99	1	59	61	7	0	46	8777
16.	25	029354-98-1	130926	76	85	0	55	61	7	0	45	9051
17.	*20	062338-56-1	33199	74	62	1	72	68	4	0	58	7028
18.	*18	024769-39-9	130011	44	60	0	72	66	3	0	44	5372
19.	*18	020576-56-1	46008	53	88	2	65	67	3	0	47	6610
20.	*18	032064-73-6	14556	46	47	0	72	69	3	0	44	5669

CTMP Compounds

18

Peak 127; Vitamin E



Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1474	67.05	620	83.00	60	101.05	59
52.00	1	67.95	80	87.95	37	104.05	136
53.00	103	69.00	476	89.95	40	105.00	349
54.00	50	71.00	321	91.00	304	107.00	450
55.00	359	75.00	43	92.10	69	108.10	40
57.00	814	77.00	190	93.00	330	109.05	358
59.00	36	78.10	72	94.05	123	111.05	8
59.95	151	79.05	291	95.05	44	114.05	27
63.95	61	80.00	79	96.05	191	116.05	17
65.00	53	81.00	844	97.05	201	117.00	16
66.00	29	82.00	238	99.00	51	118.05	12

Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	201	135.10	166	147.05	192	159.05	50
121.05	680	136.10	378	148.05	120	161.10	146
122.05	241	137.15	361	149.05	279	162.10	36
123.05	279	138.05	92	150.10	82	163.15	165
124.05	22	139.05	45	151.05	14	164.10	2087
125.05	54	141.00	19	152.10	154	165.10	6186
128.05	21	142.05	45	153.05	9	166.05	798
131.00	102	143.05	59	155.05	15	167.00	31
132.00	7	144.05	28	156.05	44	172.10	92
133.00	262	145.05	40	157.00	62	173.10	101
134.05	139	146.05	4	158.10	48	175.10	88

Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
176.10	85	188.15	48	207.05	132	221.20	86
177.05	169	189.15	46	208.05	5	223.15	63
178.05	64	190.00	19	211.15	24	224.00	26
180.05	69	192.10	26	212.20	5	224.30	14
181.05	111	196.25	13	213.20	37	226.00	3
182.05	14	197.10	21	214.15	14	226.20	14
183.05	54	198.10	42	215.10	28	227.15	22
184.00	4	201.20	33	216.15	53	229.10	42
185.15	47	203.15	145	218.20	13	231.15	60
186.20	35	204.20	16	219.80	23	232.90	27
187.15	62	205.15	458	220.20	3	233.25	16

CTMP Compounds

Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
234.15	56	257.15	14	279.15	8	298.05	17
234.65	13	258.00	10	279.65	18	309.25	27
239.00	27	258.50	10	281.00	10	311.15	11
248.45	9	264.45	10	283.10	65	323.20	15
248.80	13	265.95	11	284.15	15	325.15	14
249.25	65	267.05	15	284.50	24	326.35	22
250.00	51	267.95	34	286.15	9	327.10	6
253.05	25	268.80	37	288.20	21	327.40	10
254.10	28	271.15	30	288.95	13	328.25	12
255.15	29	274.20	15	293.80	9	329.00	11
256.05	116	275.15	19	296.45	13	340.90	18

Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
342.05	12	396.40	15				
342.45	13	407.35	34				
354.40	18	429.15	12				
355.10	22	430.40	1075				
366.30	11	431.45	329				
378.25	30	432.35	71				
378.65	9						
381.35	9						
386.95	10						
392.45	9						
394.45	37						

CTMP Compounds

Average of 45.484 to 45.534 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

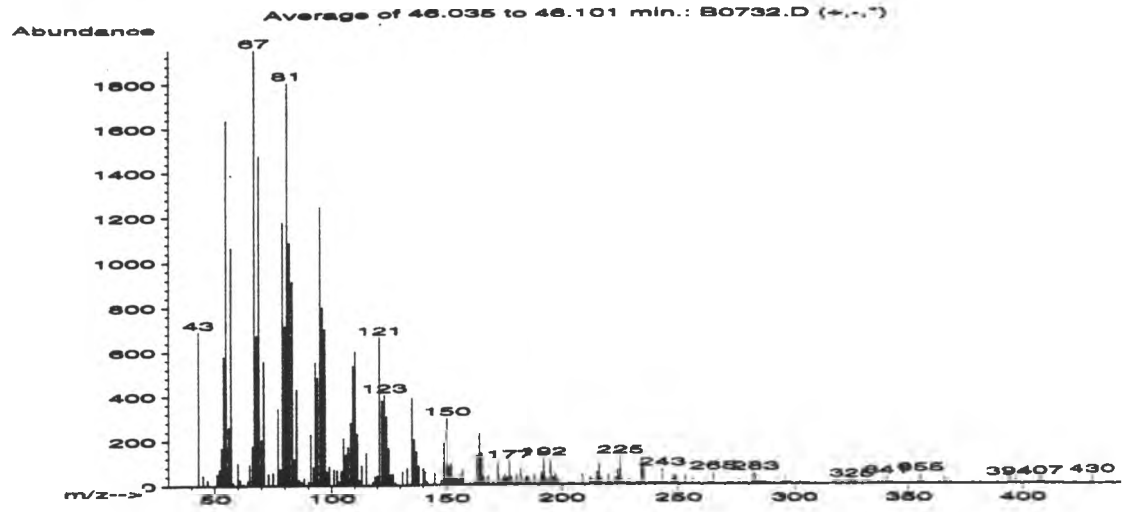
	Name	MolWt	Formula	Qual
1.	Vitamin E	430	C29H50O2	90
2.	Thiazolidine, 2-phenyl-	165	C9H11NS	64
3.	2-Amino-8-methylimidazo[1,5-a]-1,3,5-tri	165	C6H7N5O	59
4.	1H-Purin-2-amine, 6-methoxy-	165	C6H7N5O	59
5.	2H-1,4-Benzothiazin-3(4H)-one	165	C8H7NOS	47
6.	o-METHOXYPHENYLISOTHIOCYANATE	165	C8H7NOS	47
7.	Benzoic acid, 2-hydroxy-4-[(2-hydroxy-4-	346	C18H18O7	40
8.	TERTIO BUTYL HYDROXY ANISOLE	180	C11H16O2	40
9.	6H-Purin-6-one, 1,7-dihydro-2-(methylami	165	C6H7N5O	40
10.	3-(3,4-DIMETHOXYPHENYL)-2-(4-FORMYL-2-(M	432	C22H24O9	38
11.	4,5-Diamino-2,1-benzisothiazole	165	C7H7N3S	38
12.	6H-Purin-6-one, 2-amino-1,7-dihydro-1-me	165	C6H7N5O	38
13.	Carbamic acid, phenyl-, ethyl ester	165	C9H11NO2	38
14.	Zectane	222	C12H18N2O2	33
15.	Arsenous acid, triethyl ester	210	C6H15AsO3	33
16.	Guanosine, N-methyl-	297	C11H15N5O5	33
17.	2-PHENYL-D(5)-THIOPHENE	160	C10H3D5S	33
18.	6-Amino-2-benzimidazolethiol	165	C7H7N3S	33
19.	1,3-Dithiane, 2-(1,1-dimethylethyl)-5-(m	222	C9H18S3	28
20.	Tetrahydrosorbilin	236	C14H20O3	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000059-02-9	102430	92	52	3	88	10	59	46	76	9879
2.	*64	004569-82-8	18981	34	51	0	83	24	37	14	43	9838
3.	*59	070187-88-1	18818	32	11	1	99	22	33	0	39	9804
4.	*59	020535-83-5	18804	44	73	3	68	24	33	0	39	9788
5.	*47	005325-20-2	125390	43	58	3	99	37	20	0	40	9294
6.	*47	000000-00-0	18841	36	63	1	99	37	20	0	39	9297
7.	40	003542-22-1	86938	40	82	2	89	31	16	7	35	9628
8.	40	000121-00-6	25603	44	61	3	99	34	16	0	35	9330
9.	*40	010030-78-1	125388	33	52	2	70	34	16	7	37	9505
10.	38	065479-33-6	102563	44	85	3	83	37	14	0	34	9295
11.	*38	074801-74-4	18832	32	43	1	91	24	14	2	29	9796
12.	*38	000938-85-2	125386	34	42	2	99	36	14	7	36	9346
13.	*38	000101-99-5	125412	28	48	1	99	37	14	1	30	9295
14.	33	000315-18-4	44659	39	94	2	86	31	10	0	27	9496
15.	33	003141-12-6	39113	41	89	3	75	31	10	0	29	9239
16.	33	002140-77-4	72722	38	115	3	80	34	10	0	29	9514
17.	*33	020637-42-7	16877	30	65	3	93	34	10	0	29	9474
18.	*33	000000-00-0	18837	30	37	3	99	31	10	0	29	9556
19.	28	068449-94-5	44453	35	99	2	88	37	8	0	25	9288
20.	28	088924-67-8	50760	33	73	2	89	37	8	0	25	9293

CTMP Compounds

29

Peak 128; Unidentified Triterpene



Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	691	59.95	100	73.00	52	86.05	25
44.95	46	60.95	26	74.95	57	87.05	17
46.85	24	62.40	7	77.05	345	88.15	33
51.00	51	64.15	22	78.05	74	90.00	18
52.00	74	65.00	94	79.05	1178	91.00	228
53.00	169	66.10	178	80.00	717	92.10	82
54.00	580	67.00	1952	81.00	1804	93.00	553
55.00	1637	67.95	674	82.00	1086	94.00	484
56.00	262	69.00	1475	83.00	914	95.05	1245
57.00	1066	70.00	206	84.00	117	96.05	801
58.00	12	71.05	556	85.05	430	97.05	701

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.00	62	110.10	602	124.10	309	137.10	150
99.05	83	111.05	230	125.05	166	138.10	86
101.00	72	112.00	23	126.05	49	139.10	1
102.20	67	113.05	88	127.05	52	140.15	75
103.05	19	115.05	145	128.05	11	140.40	36
104.00	64	118.00	17	129.00	2	141.00	58
105.00	213	119.05	40	131.00	63	142.00	14
106.00	138	120.00	46	133.05	77	145.05	51
107.00	172	121.05	664	134.05	4	148.05	23
108.05	283	122.05	380	135.10	393	149.05	188
109.05	536	123.05	405	136.10	207	150.10	302

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.10	85	165.15	140	178.10	35	193.05	29
152.15	95	166.00	33	180.10	44	194.10	13
153.05	36	168.05	36	181.05	8	195.10	101
154.00	29	170.05	14	182.05	71	196.10	32
155.05	25	172.05	97	184.25	35	197.10	45
156.10	43	172.30	41	185.15	34	198.10	22
157.10	63	173.05	7	186.10	19	203.15	9
160.10	6	174.10	29	188.15	42	204.10	7
162.10	8	175.10	46	190.10	3	205.15	15
163.15	130	176.10	29	191.00	54	209.05	46
164.15	236	177.10	103	192.10	117	212.20	31

CTMP Compounds

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
213.20	22	226.15	20	238.55	16	249.45	15
214.15	9	226.50	13	240.05	11	250.05	5
215.15	56	228.15	15	241.15	13	252.10	3
216.15	93	229.20	28	242.15	6	253.10	39
217.15	27	231.90	7	243.15	69	256.15	22
218.20	1	232.50	8	244.30	15	258.65	9
220.10	48	233.25	15	245.05	9	263.00	14
221.10	9	234.20	119	247.20	22	264.30	15
223.15	30	235.10	73	248.20	40	265.05	51
224.15	64	235.40	22	248.75	35	271.20	13
225.20	125	237.20	9	249.10	32	272.80	8

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
275.95	22	294.70	7	326.75	14	356.15	5
277.90	7	295.05	10	336.95	8	365.55	24
278.25	8	295.30	15	338.80	9	366.30	18
279.25	5	296.20	27	340.45	15	368.20	8
282.05	46	297.10	12	340.70	30	378.15	11
283.10	48	298.15	4	341.80	9	381.40	15
283.90	11	298.55	5	342.20	7	388.80	7
284.90	12	298.95	2	342.70	11	389.25	2
286.25	7	302.40	8	354.25	17	393.70	23
287.15	12	325.10	15	355.25	42	394.10	2
289.20	7	326.50	10	355.75	13	394.30	13

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
394.55	17	429.90	11				
396.45	14	430.35	32				
397.30	23						
398.40	10						
406.50	10						
406.95	21						
407.60	25						
407.90	11						
408.15	4						
409.35	7						
422.50	9						

CTMP Compounds

Average of 46.035 to 46.101 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

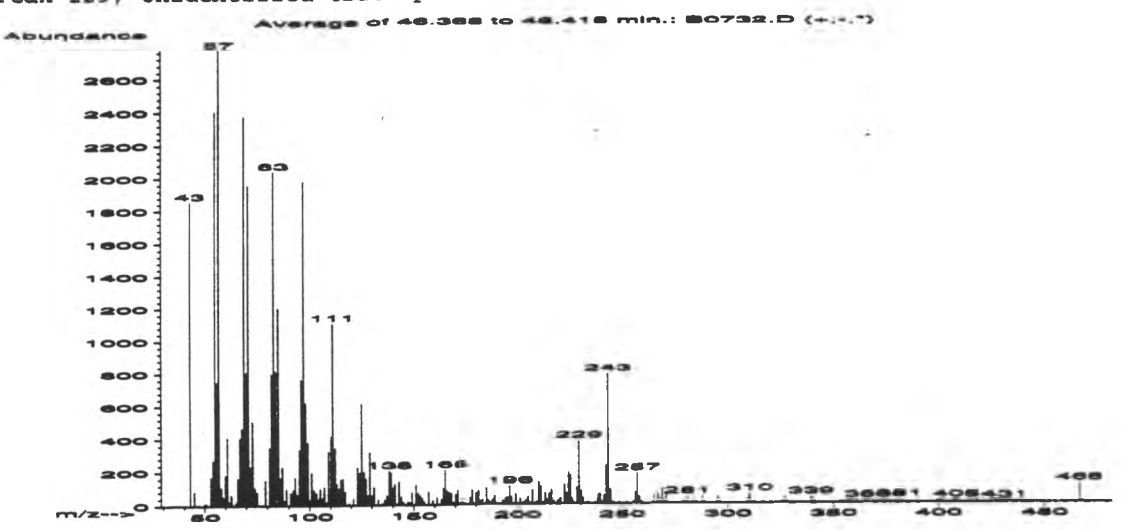
	Name	MolWt	Formula	Qual
1.	5-Octadecyne	250	C18H34	60
2.	Cyclopropaneoctanoic acid, 2-[[2-[(2-eth	334	C22H38O2	58
3.	Bicyclo[4.3.1]decan-10-one	152	C10H16O	53
4.	9-Eicosyne	278	C20H38	52
5.	9,12-Octadecadienoic acid (Z,Z)-, methyl	294	C19H34O2	49
6.	7-Tetradecyne	194	C14H26	49
7.	5-Undecyne	152	C11H20	49
8.	5,10-Pentadecadien-1-ol, (E,Z)-	224	C15H28O	46
9.	Bicyclo[3.3.1]nonan-2-ol, exo-	140	C9H16O	46
10.	4-CHLORO-2,2-DIMETHYL-OCT-7-ENONITRILE	185	C10H16ClN	43
11.	Naphthalene, decahydro-	138	C10H18	43
12.	CIS-1-ETHINYL-2-METHYL-1-CYCLOHEXANOL	138	C9H14O	43
13.	1H-Indene, 1-(1,5-dimethyl-2-hexenyl)oct	248	C18H32	41
14.	9,12-Octadecadienoyl chloride, (Z,Z)-	298	C18H31ClO	38
15.	Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-3	178	C13H22	38
16.	2-HYDROXY-(Z)9-PENTADECENYL PROPANOATE	298	C18H34O3	38
17.	(-)-TRANS PINANE	138	C10H18	35
18.	1(2H)-Naphthalenone, octahydro-4-methoxy	182	C11H18O2	30
19.	1,12-Tridecadiene	180	C13H24	30
20.	p-Menth-8(10)-en-9-ol, cis-	154	C10H18O	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*60	071899-42-8	56713	71	80	1	79	38	35	0	68	8813
2.	58	010152-71-3	84215	104	76	2	96	28	32	0	47	8902
3.	*53	020440-21-5	124035	65	55	2	96	40	28	34	56	8600
4.	52	071899-38-2	66577	86	79	1	77	33	27	0	45	8865
5.	49	000112-63-0	133235	101	74	0	63	41	23	0	56	8949
6.	*49	035216-11-6	32140	60	67	1	86	39	23	0	46	8827
7.	*49	002294-72-6	13854	57	60	1	99	36	23	0	47	9083
8.	*46	064275-56-5	46004	50	41	0	92	45	20	0	46	8492
9.	*46	010036-15-4	122489	66	52	1	85	45	20	25	45	7109
10.	*43	000000-00-0	27961	53	78	2	92	46	18	0	47	8263
11.	*43	000091-17-8	122340	63	50	1	77	46	18	24	46	8462
12.	*43	036144-41-9	8632	50	29	0	53	49	18	0	46	7400
13.	*41	054411-95-9	55830	70	84	2	68	52	16	0	53	8153
14.	38	007459-33-8	73230	114	49	2	85	52	14	29	50	7145
15.	*38	050746-55-9	24961	69	60	2	156	57	14	0	53	6888
16.	*38	077899-00-4	73238	52	94	3	222	52	14	0	46	7486
17.	*35	000473-55-2	8827	64	53	1	76	70	11	0	64	6689
18.	*30	021727-79-7	26712	63	79	1	73	57	9	17	45	7905
19.	*30	021964-48-7	25852	69	56	0	65	63	9	18	58	7247
20.	*25	015714-13-3	14722	63	59	2	92	61	7	29	46	6615

CTMP Compounds

130

Peak ~~129~~; Unidentified triterpenoid



Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1858	58.00	107	70.05	804	84.00	815
44.95	85	58.95	52	71.05	1954	85.10	1199
46.80	4	59.95	181	72.00	230	86.00	161
49.95	12	61.00	409	73.00	505	87.00	228
50.30	10	61.85	22	74.00	105	87.95	29
50.95	11	62.95	61	75.00	77	89.00	96
53.00	171	65.05	16	77.05	1	91.00	76
54.00	272	66.05	162	79.05	150	92.10	94
55.05	2406	67.00	407	81.00	347	93.00	166
55.95	746	68.00	465	82.00	797	94.00	66
57.00	2778	69.05	2374	83.00	2040	95.05	333

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.05	762	106.05	43	117.00	80	131.00	107
97.05	1978	107.00	110	119.00	15	133.05	32
98.05	619	108.00	18	121.05	39	135.00	13
99.05	375	109.00	322	123.05	226	136.05	31
99.80	33	110.10	417	124.05	195	137.15	57
100.10	30	111.10	1106	125.10	612	138.15	207
101.00	194	112.10	341	126.10	199	139.10	193
102.05	91	113.10	128	127.10	157	140.15	102
103.05	73	114.15	103	128.05	60	141.00	126
104.05	35	115.00	155	129.00	317	142.05	6
105.00	98	116.05	157	130.00	57	143.05	139

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.05	47	159.10	26	172.05	2	187.15	12
145.05	17	161.10	43	173.05	36	187.90	22
147.05	19	163.15	33	174.10	9	188.20	29
148.05	16	164.15	99	177.05	40	189.15	54
149.05	75	165.10	210	178.10	85	193.00	24
151.10	121	166.00	83	180.10	70	194.15	39
152.15	72	167.00	75	181.10	82	195.15	38
153.10	54	168.05	67	182.05	20	196.20	111
154.00	38	169.05	14	183.10	27	197.15	44
155.00	17	170.05	61	185.15	99	199.15	62
157.05	78	171.05	86	186.10	24	201.20	33

CTMP Compounds

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
203.20	13	216.15	86	227.10	2	239.10	61
204.15	24	217.15	17	228.20	98	240.00	5
205.15	46	218.20	4	229.20	382	240.45	11
207.05	87	219.15	20	230.20	76	241.15	50
209.10	15	220.15	23	231.20	32	242.25	232
210.20	132	220.50	35	233.20	10	243.20	793
211.10	105	222.25	116	234.10	2	244.20	82
212.20	7	223.10	64	236.15	2	245.20	9
213.20	66	224.25	200	237.20	11	248.20	9
214.15	26	225.20	172	238.25	39	248.55	11
215.15	62	226.15	26	238.45	53	251.90	16

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
255.10	14	271.10	59	288.05	38	328.00	12
256.10	70	273.20	3	289.20	9	332.00	10
257.15	183	274.15	3	295.10	39	339.30	38
258.15	41	278.65	13	296.05	23	339.55	24
259.15	12	278.95	7	309.20	29	340.05	16
265.05	45	279.20	27	310.20	58	340.40	27
267.00	67	279.65	14	311.25	10	340.95	8
268.10	26	281.00	41	325.10	4	353.15	9
268.45	20	283.05	15	325.50	12	354.55	2
269.10	92	284.10	26	325.80	7	357.25	10
270.45	10	285.05	17	327.05	33	366.05	14

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
375.75	13	429.40	10				
378.40	4	431.25	10				
379.15	12	466.55	115				
381.40	18	467.80	11				
394.25	9	468.05	11				
397.05	17						
399.50	11						
401.15	11						
407.30	10						
408.15	15						
422.25	1						

CTMP Compounds

Average of 46.368 to 46.418 min.: B0732.D
Converted from RTE data file: >B0732:

PBM Search of library F:\LIBRARY.L

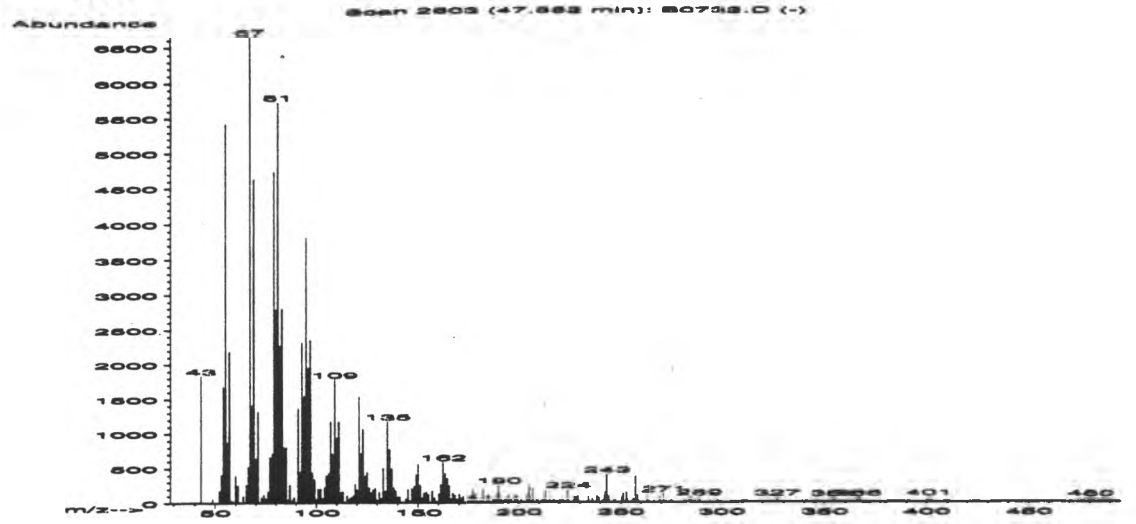
	Name	MolWt	Formula	Qual
1.	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	83
2.	1-Heptadecene	238	C17H34	58
3.	1-Hentetracontanol	593	C41H84O	58
4.	1-Octadecanol	270	C18H38O	49
5.	1-Hexadecene	224	C16H32	46
6.	1-Dotriacontanol	467	C32H66O	46
7.	1-Hexadecene	224	C16H32	43
8.	Cycloundecane, (1-methylethyl)-	196	C14H28	43
9.	1-Hexadecene	224	C16H32	43
10.	1-Hexadecene	224	C16H32	43
11.	TRANS-2-TRIDECENAL	196	C13H24O	38
12.	TRANS-2-DODECENAL	182	C12H22O	38
13.	2,2-DIDEUTERO OCTADECANAL	268	C18H34D2O	38
14.	1-Hexadecene	224	C16H32	38
15.	11-Dodecen-1-ol, 2,4,6-trimethyl-, (R,R,	226	C15H30O	30
16.	Cyclotetradecane	196	C14H28	25
17.	1-Tetradecene	196	C14H28	25
18.	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-,	224	C15H28O	20
19.	Cyclopentadecanone	224	C15H28O	18
20.	Nonacosane	408	C29H60	15

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000822-28-6	132080	80	58	2	122	32	50	0	84	9448
2.	*58	006765-39-5	130749	68	86	1	66	26	32	0	47	9567
3.	58	040710-42-7	112195	100	94	1	99	31	32	0	51	8087
4.	49	000112-92-5	132223	83	80	3	96	36	23	0	45	7910
5.	*46	000629-73-2	130029	59	89	2	119	45	20	0	46	7845
6.	46	006624-79-9	106313	98	82	1	99	42	20	0	46	8008
7.	*43	000629-73-2	130032	71	79	2	91	49	18	0	47	7867
8.	*43	062338-56-1	33199	62	76	3	93	47	18	0	46	7966
9.	*43	000629-73-2	46060	74	83	1	66	50	18	15	45	7699
10.	*43	000629-73-2	130027	68	92	2	66	46	18	16	47	9587
11.	*38	071277-06-0	33087	81	55	2	55	61	14	30	66	6450
12.	*38	081149-96-4	26777	65	66	2	114	64	14	0	64	6355
13.	*38	056555-07-8	62961	59	100	2	105	53	14	0	46	7647
14.	*38	000629-73-2	130028	64	82	1	91	54	14	0	50	7617
15.	*30	027829-54-5	130118	51	90	3	65	60	9	0	46	8528
16.	*25	000295-17-0	33202	48	87	2	86	64	7	0	46	7357
17.	*25	001120-36-1	33169	54	80	2	99	63	7	0	49	7535
18.	*20	020576-58-3	46007	59	70	2	49	69	4	0	51	8373
19.	*18	000502-72-7	46030	56	96	2	84	67	3	0	49	7404
20.	*15	000630-03-5	136146	60	85	1	105	79	2	0	51	6977

CTMP Compounds

131

Peak ~~130~~; Unidentified Triterpenoid



Scan 2603 (47.552 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1835	61.00	257	74.95	63	86.15	46
48.70	63	63.75	95	76.05	162	87.00	258
52.05	183	65.10	264	77.05	662	88.00	36
52.95	406	66.05	522	78.05	712	89.00	78
53.95	1680	67.00	6655	79.05	4734	91.00	1359
55.05	5418	67.95	1409	80.00	2787	92.00	446
55.95	873	69.00	4626	81.00	5721	92.95	2315
57.00	2183	70.00	636	82.00	2269	94.05	1543
58.00	29	71.05	1315	83.00	2809	95.05	3806
59.00	13	72.95	70	84.00	803	96.05	1949
59.95	395	74.05	116	85.10	797	97.05	2344

Scan 2603 (47.552 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.00	430	109.05	1782	120.05	190	131.00	155
99.05	335	110.15	941	121.05	1535	132.15	61
100.00	50	111.05	1170	122.05	707	133.00	498
101.00	199	112.10	152	123.05	1062	134.05	168
102.05	203	113.10	164	124.05	384	135.00	1171
103.05	68	114.00	6	125.05	434	136.10	766
104.20	224	115.00	102	126.20	218	137.15	484
105.00	392	116.15	52	127.10	144	138.10	215
106.05	426	116.95	82	128.05	186	139.05	173
107.00	1172	118.05	109	129.00	209	140.15	82
108.00	704	119.05	268	130.00	39	141.00	80

Scan 2603 (47.552 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.05	59	155.00	122	167.05	140	179.95	6
145.05	195	157.00	173	168.00	107	181.00	57
146.05	27	158.00	67	169.05	54	182.00	199
147.05	207	159.05	14	170.20	128	183.10	4
148.05	243	160.10	133	171.05	66	184.15	108
149.05	403	161.10	266	172.10	89	185.10	97
150.05	555	162.15	582	175.05	76	187.15	69
151.05	257	163.15	418	176.05	104	188.10	40
152.15	68	164.15	349	177.10	181	189.15	139
153.05	145	165.05	246	178.15	132	190.05	246
154.10	160	166.05	57	179.00	65	191.00	69

CTMP Compounds

Scan 2603 (47.552 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
192.15	27	207.00	202	220.30	46	239.20	72
193.10	40	209.10	58	221.10	85	241.25	29
194.00	87	210.10	12	222.15	24	242.20	146
195.05	94	211.20	15	223.15	14	243.20	402
196.15	57	211.90	73	224.30	180	244.20	86
197.20	3	213.20	174	227.20	78	247.20	60
198.20	116	214.20	13	228.15	75	250.45	71
199.20	83	215.20	34	229.20	85	251.15	137
201.20	45	217.10	49	234.15	86	252.75	145
204.15	109	218.10	17	236.15	57	255.15	11
205.15	234	219.15	17	238.40	97	256.15	49

Scan 2603 (47.552 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
257.25	374	310.50	57	480.50	52		
258.15	99	311.95	40				
263.20	89	327.00	60				
269.10	12	341.10	17				
269.30	99	354.50	59				
271.30	123	366.30	61				
275.15	54	367.20	57				
284.15	64	391.20	39				
285.00	82	401.25	67				
289.05	71	408.45	12				
298.20	42	410.30	41				

CTMP Compounds

Scan 2603 (47.552 min): B0732.D

PBM Search of library F:\LIBRARY.L

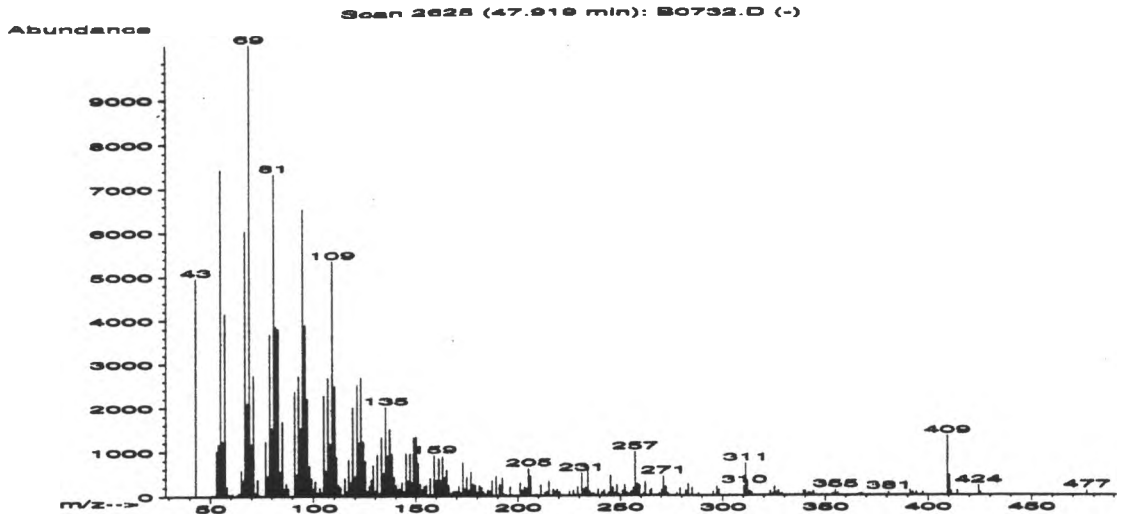
	Name	MolWt	Formula	Qual
1.	anti(10,11)-Tricyclo[4.3.1.1(2,5)]-undec	164	C11H16O	53
2.	(1R,4S)-1-Methoxymyodesertan	184	C11H20O2	53
3.	5-Dodecyne	166	C12H22	53
4.	(1S,7aS)-1-Methoxymyodesertan	184	C11H20O2	52
5.	1,E-11,Z-13-HEPTADECATRIENE	234	C17H30	50
6.	4,5-Nonadiene, 2-methyl-	138	C10H18	49
7.	1,5-Cyclododecadiene, (Z,Z)-	164	C12H20	46
8.	Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-3	178	C13H22	46
9.	Cyclohexane, 1,2-diethenyl-, cis-	136	C10H16	43
10.	1,5-Cyclododecadiene, (E,Z)-	164	C12H20	41
11.	3-Octyne, 2,2,7-trimethyl-	152	C11H20	38
12.	Cyclopentane, 1,3-dimethyl-2-(1-methylet	138	C10H18	30
13.	Bicyclo[5.1.0]oct-3-ene	108	C8H12	30
14.	Cyclohexane, 1,2-diethenyl-, cis-	136	C10H16	30
15.	Cyclohexene, 3-ethenyl-4-(1-methyletheny	148	C11H16	25
16.	endo-cis-Bicyclo[3.3.0]octane-2-one	124	C8H12O	18
17.	3-Tridecen-1-yne, (Z)-	178	C13H22	18
18.	1,E-6,Z-10-HEXADECATRIENE	220	C16H28	18
19.	(-)-TRANS PINANE	138	C10H18	18
20.	D-Fenchyl alcohol	154	C10H18O	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	085219-11-0	18681	72	56	3	86	37	28	42	59	8151
2.	*53	075281-28-6	27585	58	67	3	96	37	28	0	51	8734
3.	*53	019780-12-2	19713	60	58	2	88	36	28	0	51	8567
4.	*52	075281-31-1	27587	49	91	3	99	35	27	0	46	8788
5.	*50	080625-35-0	50170	86	61	1	84	50	25	36	72	7899
6.	*49	055956-32-6	8722	50	68	2	90	38	23	0	46	8679
7.	*46	031821-17-7	18740	64	62	2	89	51	20	0	64	7790
8.	*46	050746-55-9	24961	53	76	3	172	45	20	0	49	7349
9.	*43	001004-84-8	8126	59	72	2	71	49	18	0	46	7799
10.	*41	019428-99-0	18741	69	55	2	87	52	16	0	53	7696
11.	*38	055402-13-6	13860	53	56	1	66	53	14	0	49	7629
12.	*30	061142-31-2	8781	36	65	0	62	58	9	15	43	7823
13.	*30	000659-84-7	2009	49	73	2	99	60	9	0	44	7173
14.	*30	001004-84-8	122042	63	52	3	97	60	9	24	45	6422
15.	*25	061142-61-8	12125	72	34	1	50	78	7	0	68	4607
16.	*18	032405-37-1	4840	33	68	0	57	70	3	22	43	7541
17.	*18	037981-62-7	24937	56	75	3	54	67	3	0	47	6910
18.	*18	083489-23-0	44095	55	73	2	99	70	3	0	47	6346
19.	*18	000473-55-2	122329	50	70	1	51	70	3	0	46	6468
20.	*18	001632-73-1	124316	46	63	0	61	66	3	0	44	6312

CTMP Compounds

132

CTMP Peak 131



Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4953	60.95	48	73.05	363	86.00	162
51.00	39	63.00	30	74.00	17	87.00	269
52.00	22	63.95	77	77.00	1228	88.00	170
53.00	1016	65.00	571	78.05	445	91.00	2363
54.00	1172	66.10	360	79.05	3665	92.05	481
55.05	7423	67.00	6021	80.00	1529	92.95	2714
55.95	1226	68.00	2086	81.00	7318	94.05	1532
57.00	4140	69.05	10189	82.00	3840	95.05	6519
57.95	213	70.05	1173	83.00	3789	96.05	3876
58.95	39	71.05	2726	84.00	542	97.05	2196
59.95	34	72.00	73	85.05	1682	98.05	663

Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	390	110.15	2471	121.05	2505	132.05	67
100.10	162	111.00	872	122.05	1200	133.10	1327
101.00	325	112.05	252	123.05	2686	134.05	514
102.00	77	113.00	193	124.05	1224	135.10	2011
103.05	179	114.10	28	125.05	773	136.05	899
104.05	82	115.00	396	126.10	111	137.05	1504
105.00	2265	116.00	104	127.05	228	138.10	946
106.00	562	116.95	811	128.05	367	139.15	420
107.00	2669	118.00	298	129.00	689	140.05	238
108.05	1169	119.00	1995	130.00	114	141.05	151
109.00	5325	120.05	449	131.00	930	142.00	167

Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.05	311	154.00	211	165.15	575	176.20	131
144.00	100	155.00	237	166.05	240	177.05	526
145.05	960	156.10	39	167.00	62	178.15	254
146.10	337	157.05	406	168.05	99	179.00	237
147.05	951	158.10	35	169.05	108	180.10	78
148.10	303	159.00	914	170.00	106	181.15	227
149.05	1308	160.10	357	171.05	222	182.00	167
150.05	1334	161.15	834	172.10	84	183.05	85
151.10	723	162.15	343	173.05	739	184.15	45
152.20	261	163.10	886	174.10	170	185.15	125
153.10	145	164.15	415	175.05	414	186.15	107

CTMP Compounds

Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
187.15	346	202.05	116	217.25	138	232.15	137
188.15	5	203.15	191	218.20	85	233.15	184
189.20	436	204.15	160	219.20	142	234.25	660
191.05	251	205.25	611	220.45	81	235.20	99
192.15	395	206.15	431	223.15	16	236.30	42
193.05	46	208.10	20	225.15	94	237.15	44
194.15	29	209.15	30	227.20	118	239.20	140
196.20	195	211.10	226	228.20	18	241.05	81
197.20	20	213.20	64	229.15	196	242.20	114
199.20	7	214.15	84	230.20	16	244.25	68
201.20	283	215.10	314	231.25	498	245.20	437

Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
246.20	176	258.25	264	277.65	51	312.05	322
247.30	59	259.25	229	279.15	167	313.20	101
248.30	230	261.15	52	281.90	109	314.05	75
249.20	27	262.15	290	283.15	251	323.20	95
251.10	112	264.45	104	285.15	168	324.40	39
252.15	230	265.05	144	288.20	55	325.25	194
253.15	61	269.15	57	295.25	99	326.25	71
254.15	38	270.30	132	297.20	201	327.15	112
255.20	98	271.20	427	298.30	130	328.75	46
256.25	178	272.20	201	310.25	212	339.30	97
257.15	979	273.15	55	311.25	717	340.20	94

Scan 2625 (47.919 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
341.55	48	381.00	76	424.40	209		
341.80	57	391.30	108	425.25	66		
342.45	49	392.55	71	476.65	95		
343.20	38	393.35	7				
344.20	98	394.30	74				
353.75	47	396.45	6				
354.90	119	397.40	67				
356.15	57	409.40	1326				
366.45	47	410.30	439				
367.70	39	411.20	78				
367.95	40	414.30	104				

CTMP Compounds

Scan 2625 (47.919 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	E and Z isomers of 2,6,10-Trimethyl-2,6,	234	C17H30	40
2.	Ergost-25-ene-3,5,6-triol, (3.beta.,5.al	432	C28H48O3	40
3.	Cyclopropane, 1,1-dimethyl-2-(2-methyl-2	124	C9H16	35
4.	7-Heptadecyne, 17-chloro-	270	C17H31Cl	25
5.	Isogeraniol	154	C10H18O	22
6.	(4R,5R,9S)-5,9-DIMETHYLSPIRO(3.5)NONAN-1	166	C11H18O	18
7.	(E)- and (Z)-15-Acetonyl-8.alpha.,17-epo	346	C23H38O2	16
8.	5-OXO-CAMPHOR	168	C10H16O2	14
9.	2-Naphthalenamine, 1,2,4a,5,6,7,8,8a-oct	165	C11H19N	14
10.	2H-Inden-2-one, octahydro-3a-methyl-, tr	152	C10H16O	14
11.	9,12-Octadecadienoic acid (Z,Z)-, methyl	294	C19H34O2	14
12.	Ethynyl (1R*,2R*,5S*)-5,8,8-trimethylbic	204	C14H20O	12
13.	Hexane, 1-(isopropylidenecyclopropyl)-	166	C12H22	11
14.	Moronic acid	454	C30H46O3	10
15.	1.BETA.,4,4-TRIMETHYL-BICYCLO(3.2.0)HEPT	152	C10H16O	10
16.	.DELTA.9(12)-CAPNELLENE-10.ALPHA.-OL-8-O	234	C15H22O2	10
17.	2-Propen-1-one, 1-(2,2-dimethylcycloprop	124	C8H12O	10
18.	6-Methoxy-4,8,8-trimethyl-7-oxatetracycl	168	C10H16O2	10
19.	trans-Geraniol	154	C10H18O	10
20.	N-Butyl-N-cyanomethylaminodimethylborane	152	C8H17BN2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	40	068965-67-3	50164	65	29	0	99	34	16	1	37	9268
2.	40	056143-28-3	102681	46	168	2	88	34	16	0	37	9282
3.	*35	069147-03-1	4904	44	59	1	125	51	11	0	39	8384
4.	*25	056554-75-7	63662	68	84	2	58	74	7	0	76	6202
5.	22	005944-20-7	14595	47	70	3	119	63	5	19	38	6015
6.	*18	000000-00-0	19624	34	67	0	38	70	3	18	43	6390
7.	16	088034-07-5	87170	61	86	1	59	58	3	0	36	9001
8.	*14	000000-00-0	20472	35	61	0	43	68	2	0	41	8762
9.	14	056053-03-3	19054	57	63	0	51	70	2	0	39	5196
10.	*14	020379-99-1	13744	50	53	0	45	70	2	22	41	6056
11.	14	000112-63-0	133235	95	79	1	52	69	2	0	41	6338
12.	12	085544-99-6	36595	60	41	2	71	61	2	17	37	6292
13.	*11	024524-53-6	19735	44	58	0	40	75	2	0	44	5621
14.	10	006713-27-5	105109	58	130	0	18	72	1	0	43	8342
15.	10	014590-79-5	13735	47	67	0	52	72	1	0	39	5344
16.	10	054707-39-0	50027	48	77	0	50	70	1	18	36	6575
17.	*10	077846-92-5	4774	37	62	2	403	78	1	0	41	8552
18.	10	073433-67-7	20516	49	49	0	40	72	1	11	38	5761
19.	10	000106-24-1	124204	54	46	1	77	66	1	0	36	7484
20.	*10	064602-37-5	13404	43	64	1	54	80	1	0	40	8308

CTMP Compounds

CTMP Compounds

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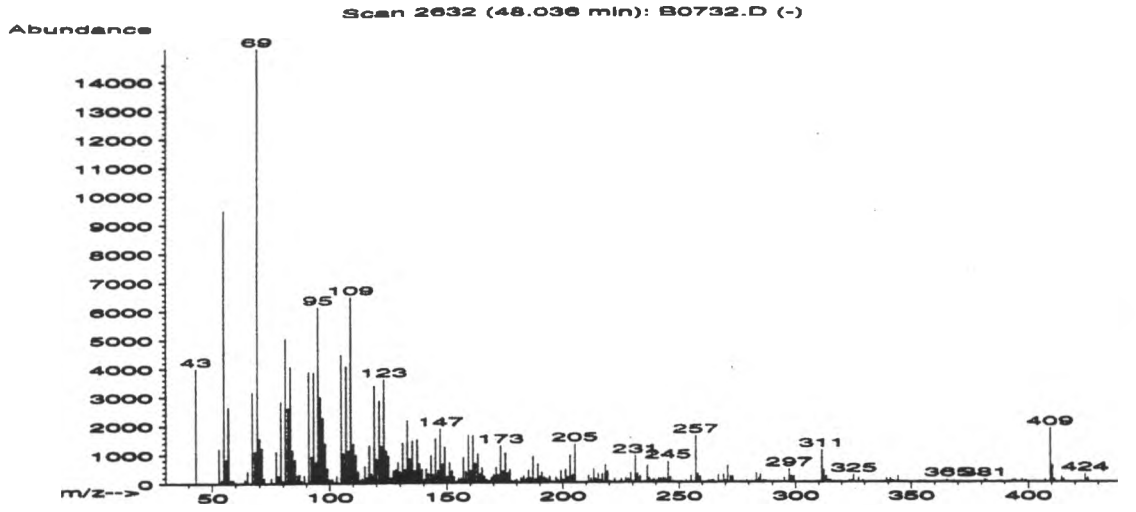
Peak ~~132~~; Unidentified Triterpene



Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3991	66.05	9	80.00	73	92.10	925
53.00	1197	67.00	3165	81.00	5041	93.05	3845
54.05	125	68.05	1096	82.00	2604	94.00	720
55.05	9481	69.05	15152	83.00	4054	95.05	6130
56.00	833	70.05	1553	84.00	1133	96.05	2982
57.00	2641	71.05	1221	85.05	816	97.05	2263
58.00	133	72.05	173	86.15	277	98.05	1384
59.00	112	75.05	172	87.00	302	99.00	506
59.95	39	77.05	1101	87.95	81	100.05	143
63.90	130	78.05	265	89.15	262	101.05	151
65.00	418	79.05	2834	91.00	3861	102.05	34

Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.05	246	115.10	595	126.10	188	137.15	1518
105.00	4473	116.00	211	127.05	425	138.15	671
106.00	1031	117.00	1317	128.05	473	139.15	470
107.00	4057	117.95	327	129.00	721	140.20	112
108.10	1128	119.00	3385	130.00	398	141.00	480
109.00	6466	120.05	848	131.00	1394	142.00	324
110.05	1359	121.05	2862	132.00	478	143.05	961
111.15	969	122.05	1285	133.00	2166	144.05	290
112.15	394	123.05	3594	134.00	849	145.05	1542
113.05	91	124.05	1111	135.00	1454	146.05	442
114.00	147	125.05	937	136.05	429	147.05	1882

Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.05	651	159.15	1654	169.95	283	182.00	174
149.05	1248	160.15	426	171.05	538	183.10	244
150.05	231	161.15	1640	172.10	260	184.15	131
151.05	701	162.15	670	173.05	1279	185.15	426
152.15	423	163.15	998	174.15	408	186.10	165
153.05	203	164.15	304	175.10	1037	187.15	906
154.05	53	165.00	520	176.20	339	188.15	124
155.00	162	166.00	221	177.05	454	189.15	646
156.00	164	167.05	98	178.00	61	190.10	219
157.05	891	168.05	59	179.10	65	191.00	347
158.10	383	169.05	181	180.00	111	192.05	184

CTMP Compounds

Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
193.05	127	204.15	259	220.20	41	234.25	6
194.20	220	205.15	1334	222.25	126	235.15	39
195.10	33	211.15	253	224.30	24	236.25	594
196.10	23	212.25	131	225.20	132	237.20	161
197.05	188	213.25	479	227.15	161	238.25	74
197.95	84	214.20	117	228.15	118	239.15	133
199.25	412	215.20	298	229.15	337	240.20	66
200.10	96	216.15	82	230.20	29	241.20	167
201.20	446	217.10	299	231.15	929	242.20	139
202.15	194	218.25	609	232.15	311	243.20	155
203.15	955	219.20	385	233.25	221	244.15	123

Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
245.20	730	259.15	211	273.20	200	299.30	206
246.20	187	262.25	46	279.15	75	311.25	1117
247.20	60	263.05	68	281.05	18	312.20	415
248.80	37	264.05	87	283.15	327	313.20	201
250.35	33	264.95	78	284.25	127	314.20	67
251.15	35	267.05	253	285.00	262	315.05	59
252.10	4	268.15	63	286.20	56	323.25	84
253.10	81	269.20	270	287.25	60	324.25	57
255.15	247	270.20	71	295.20	165	325.15	253
257.15	1618	271.05	584	297.20	448	327.25	152
258.15	290	272.30	206	298.20	215	329.15	70

Scan 2632 (48.036 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
339.30	123	394.45	77	415.30	94		
340.60	51	396.45	11	424.35	280		
341.05	127	397.25	106	425.50	138		
342.05	52	398.40	43				
344.30	204	398.75	43				
354.00	37	399.15	53				
365.45	96	407.25	92				
368.20	49	409.40	1875				
381.40	93	410.30	581				
382.15	58	411.30	107				
393.30	82	414.30	184				

CTMP Compounds

Scan 2632 (48.036 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Ergost-22-en-3-one, (5.beta.,22E)-	398	C28H46O	45
2.	4,8-DIMETHYLNONA-1,7-DIENE	152	C11H20	43
3.	5-OXO-CAMPHOR	168	C10H16O2	38
4.	E and Z isomers of 2,6,10-Trimethyl-2,6,	234	C17H30	37
5.	(+,-)-(E)-Dihydrofarnesal	222	C15H26O	37
6.	(+,-)-(Z)-Dihydrofarnesal	222	C15H26O	37
7.	1,3-Dioxane, 2,2,4,5-tetramethyl-6-(1-me	410	C27H54O2	36
8.	1,6-Heptadiene, 3,5-dimethyl-	124	C9H16	27
9.	Z-Citral	152	C10H16O	25
10.	Cyclopropane, 1,1-dimethyl-2-(2-methyl-2	124	C9H16	23
11.	Cyclohexanone, 2-(1-mercapto-2-methyleth	186	C10H18OS	17
12.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	16
13.	9,19-Cyclocholest-24-en-3-ol, 14-methyl-	398	C28H46O	12
14.	4-(6',6'-DIMETHYL-2'-METHYLIDENCYCLOHEX-	196	C13H24O	12
15.	Isogeraniol	154	C10H18O	10
16.	N-Butyl-N-cyanomethylaminodimethylborane	152	C8H17BN2	10
17.	P-MENTHON-8-THIOL	186	C10H18OS	9
18.	1-Anthracenecarboxaldehyde, 5,8,8a,9,10,	410	C25H30O5	8
19.	3-HEXENE, 3,4-BIS(DIETHYLBORYL)-	220	C14H30B2	8
20.	4(1H)-Pyrimidinone, 2-(ethylthio)-	156	C6H8N2OS	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	45	018865-44-6	97587	45	156	2	87	22	19	0	34	9533
2.	*43	062108-28-5	13858	33	69	3	123	44	18	0	39	9195
3.	*38	000000-00-0	20472	41	55	1	68	38	14	4	37	8949
4.	37	068965-67-3	50164	43	47	1	85	45	13	10	35	9409
5.	*37	069659-93-4	44957	28	46	0	82	45	13	0	33	9021
6.	37	069659-92-3	44956	41	28	0	93	45	13	14	35	8755
7.	36	056324-82-4	99474	49	136	3	91	30	12	0	22	9391
8.	*27	068701-99-5	4890	36	57	1	141	60	8	0	39	8852
9.	25	000106-26-3	123949	43	67	3	196	53	7	0	35	9256
10.	*23	069147-03-1	4904	29	74	3	125	48	6	0	29	8920
11.	17	035117-86-3	28347	32	76	1	82	51	3	5	26	8769
12.	16	002847-30-5	120355	45	70	1	90	59	3	0	34	5168
13.	12	068654-82-0	97606	71	74	1	63	61	2	6	33	9310
14.	12	000000-00-0	33110	46	91	3	45	61	2	0	37	9231
15.	10	005944-20-7	14595	55	39	0	30	76	1	16	40	5020
16.	*10	064602-37-5	13404	36	56	2	38	78	1	0	39	8630
17.	9	033281-91-3	28351	44	91	1	51	74	1	0	37	9262
18.	8	064960-69-6	99438	36	132	2	91	68	1	0	21	7744
19.	8	000000-00-0	43851	45	54	1	89	68	1	5	26	7956
20.	8	006965-19-1	15123	33	94	2	63	68	1	0	21	4044

CTMP Compounds

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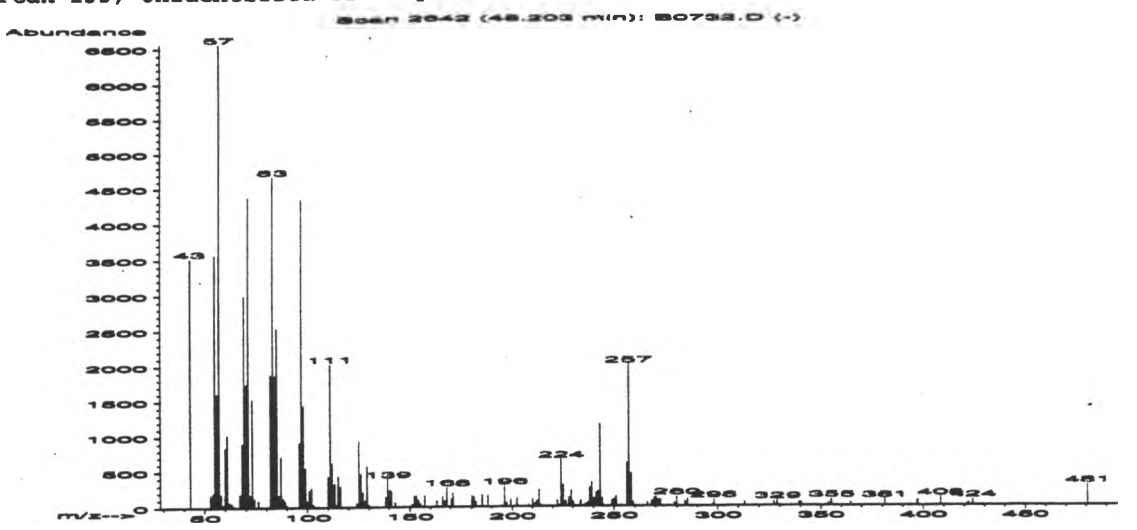
Peak ~~133~~; Unidentified Triterpene



Scan 2642 (48.203 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3512	63.00	55	82.00	1875	98.00	1430
52.95	178	63.95	22	83.00	4671	99.05	554
54.00	202	67.00	190	84.00	1859	99.95	87
55.00	3566	68.05	898	85.00	2525	101.00	238
56.00	1608	69.05	2997	86.05	165	101.95	269
57.00	6563	70.05	1740	87.05	707	103.00	32
57.90	183	71.05	4379	88.15	123	110.10	436
59.00	34	72.05	175	89.00	90	111.15	2026
60.00	838	73.05	1524	89.85	27	112.00	622
60.90	1016	74.00	124	96.05	918	113.15	327
61.90	72	76.05	92	97.05	4344	114.05	31

Scan 2642 (48.203 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.00	438	140.25	238	163.15	82	188.00	157
116.05	287	141.05	216	166.05	145	194.15	14
124.05	59	143.00	62	167.05	83	195.15	15
125.05	929	150.05	10	168.05	272	196.20	289
126.05	467	151.05	40	170.30	111	197.15	53
127.05	204	152.05	150	171.05	195	199.20	98
128.05	94	153.05	155	180.25	158	202.15	115
129.00	577	154.10	92	181.15	134	208.00	24
130.05	31	155.10	37	182.15	69	210.15	102
138.15	140	157.10	155	185.15	167	211.20	42
139.15	391	162.05	10	186.05	6	212.15	78

Scan 2642 (48.203 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
213.20	238	229.15	225	243.30	1167	268.05	74
214.15	22	230.20	60	244.20	108	269.15	116
217.10	9	233.65	62	245.20	10	270.20	134
220.20	8	234.00	82	249.05	82	271.20	91
222.20	77	236.20	34	250.05	92	272.20	82
223.15	16	237.20	50	251.00	139	279.00	49
224.20	663	238.25	264	256.15	609	280.15	134
225.20	301	239.20	336	257.15	2009	284.00	60
226.30	63	240.20	110	258.25	462	285.25	102
226.50	67	241.30	186	259.15	52	295.10	10
228.15	124	242.20	211	266.05	53	297.10	24

CTMP Compounds

Scan 2642 (48.203 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
298.05	88	381.25	83				
313.05	58	397.05	75				
327.15	69	397.25	68				
328.50	22	408.50	116				
328.75	69	421.75	35				
339.30	47	422.15	40				
340.30	48	424.25	84				
353.50	38	480.65	285				
354.75	68						
355.15	87						
364.55	45						

CTMP Compounds

Scan 2642 (48.203 min): B0732.D

PBM Search of library F:\LIBRARY.L

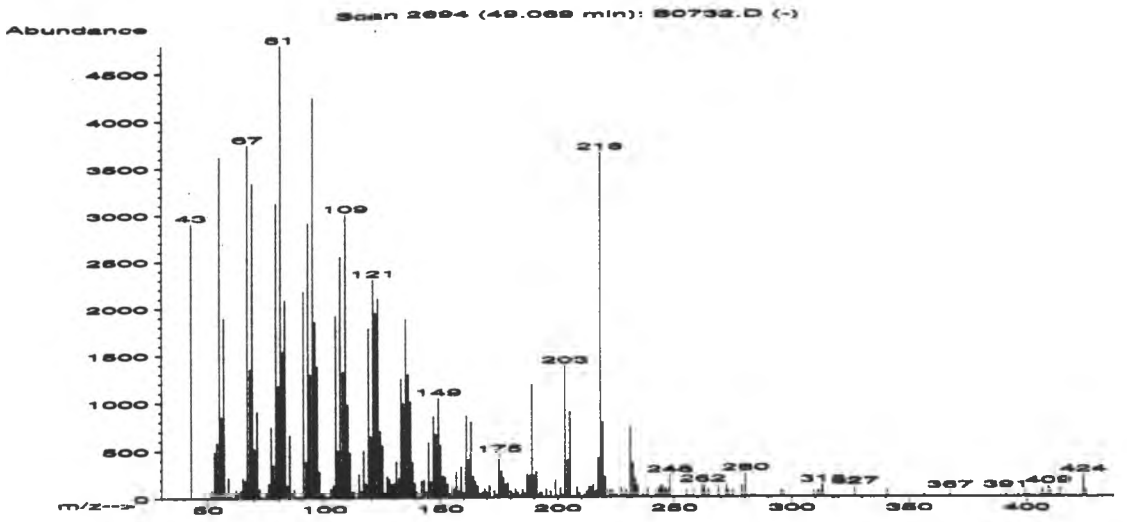
	Name	MolWt	Formula	Qual
1.	Cyclohexadecane	224	C16H32	91
2.	1-Nonadecene	266	C19H38	83
3.	Hexadecanoic acid, tetradecyl ester	452	C30H60O2	83
4.	7-Heptadecene, 1-chloro-	272	C17H33Cl	78
5.	Cyclotetradecane	196	C14H28	78
6.	1,2-Octadecanediol	286	C18H38O2	64
7.	5-Eicosene, (E)-	280	C20H40	60
8.	1-Hexadecene	224	C16H32	60
9.	1-Hexadecene	224	C16H32	53
10.	3-Eicosene, (E)-	280	C20H40	53
11.	1-Heptadecene	238	C17H34	49
12.	1-Dotriacontanol	467	C32H66O	49
13.	3-Hexadecene, (Z)-	224	C16H32	49
14.	Nonacosanol	424	C29H60O	49
15.	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	42
16.	Cyclotetradecane	196	C14H28	38
17.	1-Heptadecene	238	C17H34	30
18.	Ethane, 1,1,2,2-tetrachloro-	166	C2H2Cl4	25
19.	Heptadecane	240	C17H36	11
20.	Pentadecane	212	C15H32	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000295-65-8	46076	111	46	0	52	40	62	42	95	9186
2.	*83	018435-45-5	132005	98	57	1	78	31	50	0	84	9369
3.	83	004536-26-9	104931	116	67	2	89	14	50	18	53	8456
4.	*78	056554-78-0	64326	89	82	1	51	36	46	49	83	9192
5.	*78	000295-17-0	33202	78	58	2	116	40	46	0	90	8751
6.	64	020294-76-2	69289	88	70	2	95	22	37	0	47	9425
7.	*60	074685-30-6	67215	88	67	1	104	40	35	0	81	9312
8.	*60	000629-73-2	130032	71	80	3	111	40	35	0	76	9312
9.	*53	000629-73-2	130029	74	74	2	118	40	28	0	58	9302
10.	*53	074685-33-9	67216	91	75	2	87	36	28	0	56	9368
11.	*49	006765-39-5	130749	68	86	1	61	40	23	0	47	9269
12.	49	006624-79-9	106313	83	98	3	129	40	23	0	45	9371
13.	*49	034303-81-6	46061	60	89	3	112	40	23	0	46	9251
14.	49	025154-56-7	101559	87	90	3	105	40	23	0	47	9357
15.	*42	000822-28-6	132080	73	65	3	112	57	17	0	74	8734
16.	*38	000295-17-0	128073	72	61	0	47	59	14	9	50	9023
17.	*30	006765-39-5	130747	55	92	0	53	57	9	0	49	9242
18.	*25	000079-34-5	125456	50	61	0	52	63	7	0	46	7049
19.	*11	000629-78-7	130830	52	62	2	86	79	2	0	46	3659
20.	*11	000629-62-9	129232	50	56	1	99	78	2	0	46	3931

CTMP Compounds

135

Peak ~~134~~; Unidentified triterpene



Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2908	62.15	93	75.00	48	86.10	41
48.95	41	62.95	38	76.05	162	87.00	94
51.95	90	64.00	84	77.05	746	88.95	13
53.00	489	65.00	215	78.05	352	91.00	2178
53.95	588	66.05	191	79.05	3122	92.00	380
55.05	3619	67.00	3747	80.00	1175	92.95	2911
56.00	855	68.00	1350	81.00	4786	94.05	1296
57.00	1892	69.05	3334	82.00	1535	95.05	4244
57.95	12	70.05	516	83.00	2082	96.05	1851
59.00	217	71.05	901	84.00	135	97.05	1377
59.95	20	72.05	98	85.00	662	98.05	279

Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	31	111.15	474	123.05	2099	134.00	991
100.00	51	112.10	70	124.05	698	135.10	1877
101.05	21	113.00	69	125.05	548	136.15	1294
103.00	104	115.05	251	126.00	59	137.15	1006
104.05	139	116.05	79	127.05	224	138.15	370
105.00	1911	117.00	499	128.05	201	139.15	157
106.00	501	118.05	158	129.00	146	140.05	66
107.00	2550	119.05	1784	130.00	153	140.95	2
108.10	1323	120.05	647	131.00	380	142.05	182
109.10	3002	121.05	2303	132.05	213	143.05	191
110.15	977	122.05	1946	133.00	1244	144.05	68

Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
145.05	581	156.00	93	167.00	43	179.00	149
146.00	175	157.05	266	168.05	54	180.15	66
147.05	851	158.05	67	169.05	93	181.00	33
148.05	668	159.05	325	169.95	55	182.10	84
149.15	1040	160.05	50	171.05	126	183.15	50
150.05	552	161.15	853	173.15	67	184.05	20
151.10	227	162.15	392	174.10	25	185.15	81
152.05	215	163.15	789	175.05	449	186.00	41
153.10	149	164.15	223	176.15	271	187.15	241
154.00	43	165.05	165	177.05	200	188.25	225
155.00	13	166.05	118	178.05	131	189.15	1182

CTMP Compounds

Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
190.05	220	203.15	1376	216.15	62	229.20	79
191.00	265	204.15	384	217.20	417	230.05	3
192.15	42	205.15	896	218.20	3653	231.15	747
193.05	53	208.15	106	219.20	781	232.15	362
195.15	85	209.15	43	220.15	212	233.15	189
196.15	5	210.05	5	222.20	65	234.15	115
197.05	66	211.20	29	223.05	68	236.50	47
199.15	176	212.15	64	224.15	27	238.25	64
200.00	12	213.20	120	225.05	46	238.55	90
201.15	100	214.15	109	227.15	106	242.05	58
202.15	26	215.15	130	228.15	39	243.20	92

Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
244.05	128	264.70	81	284.20	35	340.80	72
245.20	115	269.05	113	295.20	65	354.95	6
246.45	90	271.15	5	296.20	54	356.15	50
247.30	69	272.30	124	297.20	5	367.20	60
248.20	227	272.80	55	309.25	60	391.30	62
255.20	72	273.20	68	311.25	73	394.30	3
256.20	15	275.15	80	312.05	46	396.45	24
257.05	15	279.00	122	313.05	121	398.75	35
258.15	66	280.40	245	313.30	123	399.40	65
262.15	130	281.00	19	327.00	103	400.90	46
263.05	107	283.00	32	340.55	70	406.50	72

Scan 2694 (49.069 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
407.25	53						
408.45	19						
409.45	105						
410.20	77						
413.20	43						
414.30	91						
424.40	224						
425.25	72						

CTMP Compounds

Scan 2694 (49.069 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Epi-.psi.-Taraxastanonol	442	C30H50O2	59
2.	Stigmast-5-en-3-ol, (3.beta.)-	414	C29H50O	50
3.	1,2,3,3a,5,6,6a,7-Octahydro-1,3a,6-trime	218	C15H22O	50
4.	Pyrene, hexadecahydro-	218	C16H26	42
5.	D:C-Friedooleanan-3-one	424	C30H48O	42
6.	INDOLOPURIDOCOLINE	218	C15H10N2	38
7.	Cyclohexane, 1,2,3,4,5,6-hexachloro-	288	C6H6Cl6	32
8.	TETRAHYDRO-3,6,8,8-TETRAMETHYL-7-METHANO	218	C15H22O	30
9.	Benzenesulfinothioic acid, S-phenyl este	234	C12H10OS2	27
10.	Cholestan-3-one, 4,4-dimethyl-, (5.alpha	414	C29H50O	27
11.	Cyclohexane, 1,1'-(1,3-butadiene-1,4-diy	218	C16H26	16
12.	1-Oxo-1,2,3,4,4e,9e-hexahydrothioxanthen	218	C13H14OS	14
13.	Dendrolasin	218	C15H22O	14
14.	METHYL COMMATE E	502	C31H50O5	12
15.	Urs-12-ene	410	C30H50	12
16.	9-OXA-11-AZABICYCLO(6.2.1)UNDEC-1(11)-EN	233	C11H17F2NO2	12
17.	D-Norandrostan-16-ol, (5.alpha.,16.beta.	262	C18H30O	11
18.	2,6-Diisopropylidene-3-methyl-3-vinylcyc	218	C15H22O	11
19.	Aristolone	218	C15H22O	10
20.	2,10-DIMETHYL-7-ISOPROPENYL-BICYCLO(4.4.	218	C15H22O	10

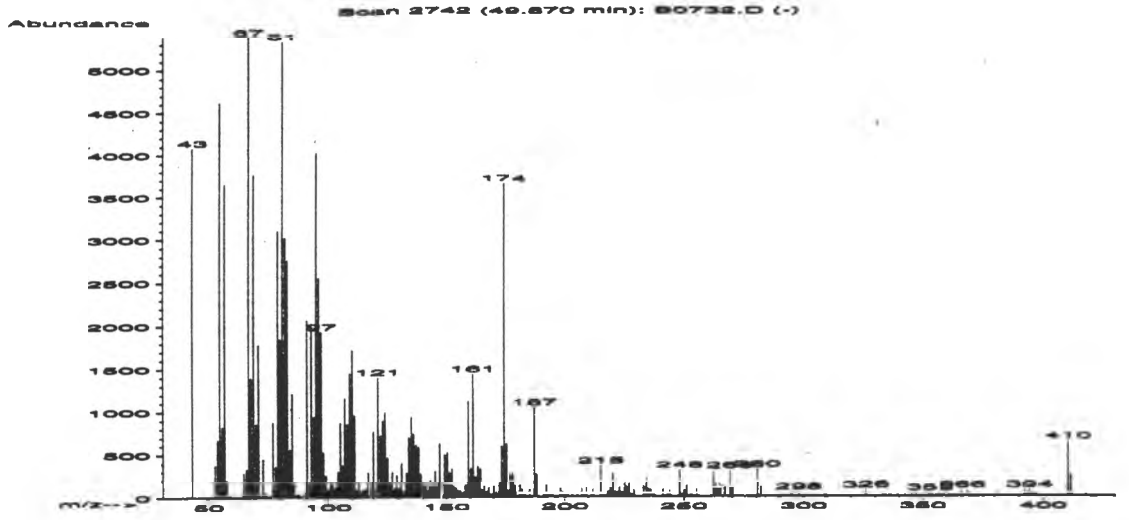
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	000000-00-0	103861	123	75	2	85	25	33	1	39	8176
2.	*50	000083-46-5	136252	96	71	1	78	46	25	58	78	8243
3.	*50	071583-68-1	43034	50	33	1	67	33	25	11	40	3672
4.	*42	002435-85-0	43086	91	75	3	65	57	17	41	70	5864
5.	*42	005945-53-9	101572	78	99	2	42	60	17	25	66	4178
6.	*38	000000-00-0	42948	48	47	2	74	50	14	13	39	4156
7.	32	000608-73-1	132959	45	121	3	62	50	9	0	37	4685
8.	*30	000000-00-0	43003	87	77	2	54	62	9	6	56	5919
9.	27	001208-20-4	49768	44	62	1	53	57	8	20	38	4689
10.	27	002097-85-0	100195	60	137	3	115	60	8	0	39	6421
11.	16	055712-53-3	43079	46	105	1	53	59	3	19	37	6312
12.	*14	084559-53-5	42796	47	63	3	76	70	2	0	40	4103
13.	14	023262-34-2	42953	43	113	3	93	70	2	9	38	6579
14.	12	000000-00-0	108319	97	112	1	55	61	2	5	36	8165
15.	12	000464-97-1	99533	61	129	3	197	64	2	0	36	6211
16.	12	055087-32-6	49412	44	98	1	81	63	2	0	37	7780
17.	*11	035575-61-2	60640	50	117	2	57	74	2	0	46	6345
18.	*11	069366-06-9	42971	48	79	1	54	72	2	0	44	4710
19.	*10	006831-17-0	43029	58	108	3	76	80	1	0	39	4570
20.	*10	061187-89-1	43020	56	106	3	122	71	1	0	40	7466

CTMP Compounds

CTMP Compounds

136

Peak ~~135~~; Unidentified Triterpene



Scan 2742 (49.870 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4078	67.95	1394	81.00	5336	93.00	1990
52.95	375	69.00	3760	82.00	3015	94.05	941
54.05	676	70.05	857	83.00	2759	95.05	4019
55.00	4618	71.05	1783	84.00	557	96.05	2551
56.00	825	73.00	449	85.00	1211	97.05	1927
57.00	3649	74.05	58	86.00	144	98.05	524
57.95	199	76.05	6	87.00	24	99.05	253
59.10	24	77.05	880	88.00	38	100.00	86
65.00	282	78.05	360	89.90	72	101.05	168
66.05	330	79.05	3096	91.05	2066	101.95	147
67.00	5390	80.00	1847	92.00	145	103.00	117

Scan 2742 (49.870 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.05	302	115.10	94	128.05	93	139.15	269
105.00	871	116.15	98	129.00	255	140.15	158
106.00	376	117.00	290	130.05	114	141.00	145
107.00	1161	119.05	772	131.00	394	142.05	80
108.05	856	121.05	1402	132.00	64	143.05	198
109.00	1450	122.05	722	133.00	281	144.00	128
110.00	1720	123.05	894	134.00	700	145.05	306
111.00	954	124.05	993	135.10	939	146.05	147
112.10	91	125.05	464	136.10	742	147.05	631
113.15	178	126.05	153	137.15	608	149.05	495
114.10	66	127.05	288	138.15	581	150.15	522

Scan 2742 (49.870 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.05	286	162.00	235	173.05	594	185.15	91
152.15	328	163.15	358	174.05	3654	187.15	1054
153.05	129	164.15	329	175.05	620	188.15	262
154.15	111	165.00	82	176.10	80	191.05	26
155.00	77	166.00	131	177.05	254	192.15	145
156.00	71	167.15	65	178.00	276	193.05	19
157.00	48	168.05	114	179.10	131	194.05	24
158.00	148	169.05	28	180.15	11	195.05	22
159.00	1124	170.05	129	181.05	141	196.15	13
160.15	334	171.05	53	182.00	87	197.05	11
161.05	1444	172.30	165	183.10	53	198.20	103

CTMP Compounds

Scan 2742 (49.870 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
199.20	62	216.05	21	227.20	149	248.20	313
200.20	38	217.20	10	228.15	29	249.20	25
201.10	37	218.20	68	229.15	78	250.20	74
203.15	47	219.20	99	233.15	121	251.15	131
205.15	29	220.20	265	234.25	228	253.05	42
207.10	94	221.15	61	235.10	83	255.25	92
208.05	23	222.30	52	236.25	81	262.15	291
209.10	104	223.10	110	237.20	36	263.20	152
211.15	38	224.20	49	241.20	91	264.05	96
212.00	89	225.20	160	243.20	28	265.05	144
215.20	363	226.05	114	244.20	77	267.00	111

Scan 2742 (49.870 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
269.10	304	368.70	60				
270.20	100	381.40	49				
280.50	319	389.20	37				
281.90	118	392.30	64				
294.95	59	394.30	72				
298.05	54	396.45	31				
309.15	35	410.30	645				
326.15	77	411.45	248				
333.40	40	418.05	50				
353.00	40						
366.30	72						

CTMP Compounds

Scan 2742 (49.870 min): B0732.D

PBM Search of library F:\LIBRARY.L

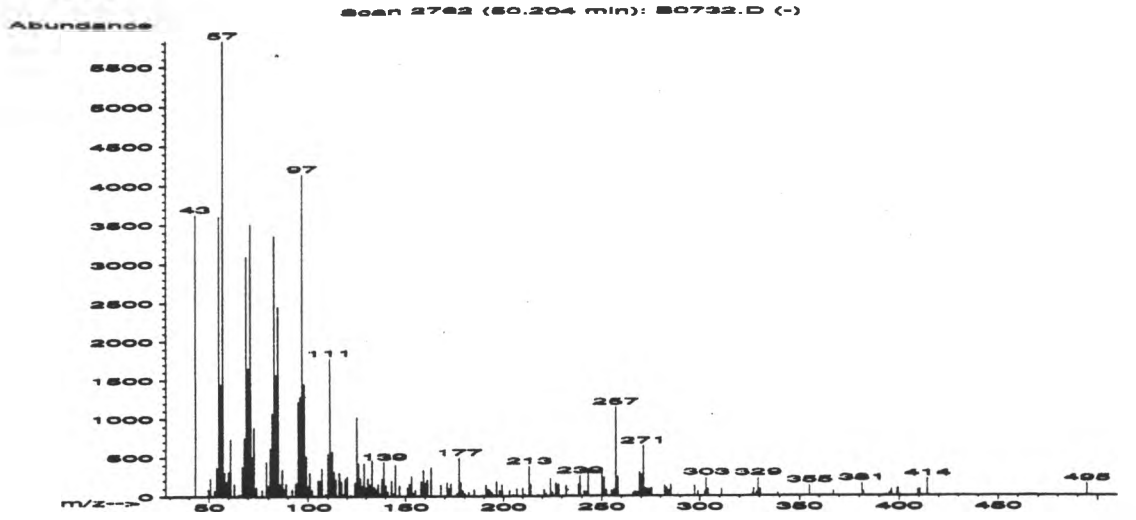
	Name	MolWt	Formula	Qual
1.	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	62
2.	7-Heptadecyne, 1-chloro-	270	C17H31Cl	53
3.	9-Eicosyne	278	C20H38	53
4.	Methylenecyclononane	138	C10H18	49
5.	(Z)-Octadec-9-en-18-olide	280	C18H32O2	49
6.	1,E-8,Z-10-TRIDECATRIENE	178	C13H22	46
7.	9,12-Octadecadienoic acid (Z,Z)-, 2-hydr	354	C21H38O4	46
8.	9,12-Octadecadienoyl chloride, (Z,Z)-	298	C18H31ClO	44
9.	Pentalene, octahydro-2-methyl-	124	C9H16	43
10.	5,10-Pentadecadien-1-ol, (E,E)-	224	C15H28O	43
11.	5,10-Pentadecadien-1-ol, (E,E)-	224	C15H28O	43
12.	Cyclohexane, 1,2-diethenyl-, cis-	136	C10H16	30
13.	9,12-Octadecadienoic acid, methyl ester,	294	C19H34O2	20
14.	1H-Pyrazole, 3,4-dimethyl-	96	C5H8N2	18
15.	1-(Isopropylamino-2,2-dimethylcyclopropa	152	C9H16N2	15
16.	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	14
17.	4.beta.,7.beta.-Epidioxy-3a.alpha.,7a.al	166	C9H10O3	14
18.	(Z)14-TRICOSENYL FORMATE	366	C24H46O2	11
19.	5,10-Undecadienoic acid, 2-methylene-, m	208	C13H20O2	11
20.	Stigmasta-3,5-dien-7-one	410	C29H46O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*62	000060-33-3	132609	98	85	2	77	29	36	17	53	8940
2.	53	056554-74-6	63665	76	74	2	97	29	28	0	41	8984
3.	53	071899-38-2	66577	80	84	1	74	29	28	0	41	9021
4.	*49	056133-38-1	8815	50	23	0	93	39	23	0	46	8641
5.	*49	068985-15-9	67147	91	48	1	114	39	23	8	49	8643
6.	*46	080625-30-5	24966	70	54	0	66	54	20	41	70	6951
7.	46	003443-82-1	89015	83	104	3	91	44	20	0	45	8904
8.	*44	007459-33-8	73230	81	81	3	136	79	18	0	90	7032
9.	*43	003868-64-2	4923	56	55	1	98	46	18	0	47	8215
10.	*43	064275-46-3	46005	45	40	0	89	49	18	0	44	8499
11.	*43	064275-46-3	130023	45	63	1	89	49	18	0	44	8499
12.	*30	001004-84-8	122042	76	42	1	78	59	9	9	44	5866
13.	20	002566-97-4	133240	100	53	3	124	69	4	0	51	7052
14.	*18	002820-37-3	568	33	58	0	57	69	3	14	43	4766
15.	*15	081803-26-1	13550	58	54	1	61	79	2	0	56	4050
16.	14	064566-18-3	131394	58	109	0	60	67	2	0	43	8977
17.	*14	056411-68-8	19332	37	49	0	86	68	2	0	41	6210
18.	11	077899-10-6	91683	98	88	1	58	79	2	0	46	6027
19.	*11	051788-60-4	38495	52	70	2	99	79	2	0	46	5431
20.	*11	002034-72-2	99496	65	88	2	45	75	2	10	47	3766

CTMP Compounds

137

Peak ~~126~~: Unidentified triterpene



Scan 2762 (50.204 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3625	61.00	739	74.05	110	87.95	95
49.80	95	63.00	160	77.05	85	89.00	160
50.95	224	65.05	22	79.05	440	92.10	86
53.00	72	66.00	21	80.00	136	94.00	172
54.05	370	67.00	377	81.00	616	95.05	1217
55.05	3605	67.95	755	82.00	1067	96.05	1286
56.00	1442	69.05	3099	83.00	3348	97.05	4132
57.00	5831	70.00	1652	84.00	1561	98.05	1445
57.95	302	71.05	3506	85.00	2444	99.00	513
59.00	183	72.05	503	85.95	155	100.10	126
59.95	311	72.95	887	87.10	337	101.00	301

Scan 2762 (50.204 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.10	78	117.00	183	130.00	112	141.00	58
105.00	203	118.00	26	131.00	227	143.05	195
106.00	191	119.05	228	132.00	150	144.05	32
107.00	359	120.05	250	133.00	461	145.05	404
109.00	29	122.05	17	134.15	116	147.05	129
110.00	546	124.15	172	135.00	82	151.05	110
111.00	1779	125.05	1023	136.10	160	152.05	156
112.15	573	126.05	418	137.05	31	153.15	257
113.15	314	127.10	227	138.15	221	154.00	39
114.00	211	128.05	133	139.15	439	155.10	72
116.00	300	129.00	425	140.15	136	157.10	6

Scan 2762 (50.204 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
158.10	189	177.20	496	194.05	50	214.15	149
159.15	334	178.10	173	195.10	17	217.20	12
160.10	166	179.05	72	196.30	185	218.20	16
161.15	209	180.05	36	197.95	74	221.05	87
163.15	372	182.15	52	199.20	142	222.20	32
168.00	148	184.05	4	203.05	74	224.20	223
169.05	6	185.00	84	205.15	22	225.20	48
171.05	171	189.15	14	207.00	92	227.10	166
172.05	94	191.00	140	210.05	104	228.25	147
173.05	155	192.05	85	211.20	22	232.15	133
176.10	36	193.00	73	213.25	381	238.20	148

CTMP Compounds

Scan 2762 (50.204 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
239.15	257	257.15	1142	275.25	101	326.40	37
241.20	60	258.25	243	282.15	131	327.00	99
242.20	47	266.05	43	283.10	101	328.50	49
243.20	341	267.05	59	284.25	70	329.35	228
248.20	3	268.05	54	285.25	138	330.50	85
250.20	287	269.20	305	297.30	130	339.05	38
251.15	234	270.45	271	299.05	62	355.00	132
252.25	72	271.30	641	302.50	61	367.20	66
253.15	9	272.25	96	303.25	232	381.40	156
255.15	71	273.20	87	304.15	84	382.15	51
256.20	84	274.20	90	311.00	86	393.25	15

Scan 2762 (50.204 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
395.20	39						
396.20	81						
399.15	93						
399.40	99						
409.45	77						
410.30	76						
414.30	215						
494.70	149						

CTMP Compounds

Scan 2762 (50.204 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	1-Hexadecene	224	C16H32	78
2.	1-Heptacosanol	396	C27H56O	64
3.	1-Hentetracontanol	593	C41H84O	58
4.	1-Octadecene	252	C18H36	53
5.	Nonacosanol	424	C29H60O	52
6.	Cyclopentane, (4-octyldodecyl)-	350	C25H50	46
7.	1-Heptadecene	238	C17H34	42
8.	1-Heptadecene	238	C17H34	41
9.	5-Eicosene, (E)-	280	C20H40	38
10.	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	38
11.	1-Hexadecene	224	C16H32	38
12.	1-Nonadecene	266	C19H38	38
13.	Phosphonic acid, dioctadecyl ester	587	C36H75O3P	30
14.	Hexacosanolide	394	C26H50O2	27
15.	4,4-DIDEUTERO HEPTADECANAL	254	C17H32D2O	22
16.	Ethane, 2,2-dichloro-1,1,1-trifluoro-	152	C2HCl2F3	18
17.	1-Hexadecene	224	C16H32	18
18.	Eicosane	282	C20H42	15
19.	Heptane, 3-methyl-	114	C8H18	11
20.	Nonadecane	268	C19H40	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	000629-73-2	130027	78	77	2	61	40	46	0	84	9222
2.	64	002004-39-9	97211	85	85	2	124	22	37	0	45	9638
3.	58	040710-42-7	137292	84	105	2	95	26	32	0	45	9547
4.	*53	000112-88-9	131396	79	83	1	54	40	28	28	59	9405
5.	52	025154-56-7	101559	90	88	2	111	34	27	0	47	9584
6.	46	005638-09-5	134961	89	66	2	78	42	20	0	47	8833
7.	*42	006765-39-5	130747	65	82	0	53	59	17	0	64	9005
8.	*41	006765-39-5	130749	62	72	1	42	53	16	0	56	9192
9.	38	074685-30-6	67215	73	82	2	121	48	14	0	41	9353
10.	*38	000822-28-6	132080	66	72	2	91	51	14	0	50	8986
11.	*38	000629-73-2	130031	49	95	3	152	55	14	0	46	9167
12.	*38	018435-45-5	132005	73	81	1	73	53	14	0	45	9356
13.	30	019047-85-9	112020	83	111	2	52	58	9	0	45	9336
14.	27	057951-54-9	96878	59	41	0	55	59	8	0	43	8165
15.	22	056554-50-8	58295	59	74	0	44	61	5	0	43	8828
16.	*18	000306-83-2	13202	49	49	1	51	67	3	0	46	6074
17.	*18	000629-73-2	130028	43	102	0	52	67	3	0	44	8991
18.	*15	000112-95-8	67905	59	66	1	69	79	2	0	56	4661
19.	*11	000589-81-1	119373	45	28	0	58	75	2	0	44	4254
20.	*11	000629-92-5	132085	48	69	2	117	79	2	0	44	4660

CTMP Compounds

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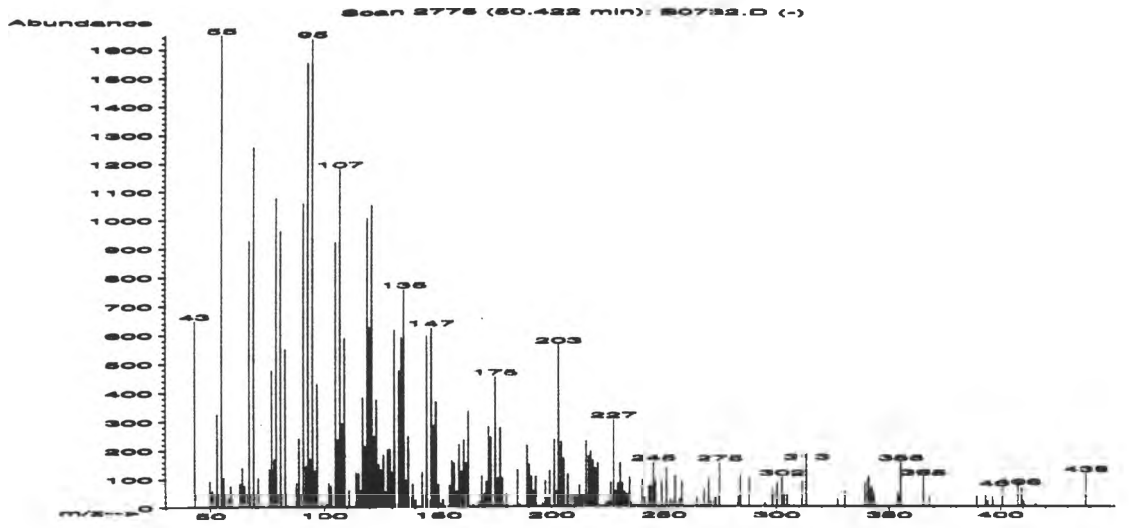
Peak ~~127~~; Unidentified triterpene



Scan 2775 (50.422 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	647	64.00	138	83.00	548	99.05	18
50.05	93	65.00	75	84.00	46	101.05	11
51.00	57	67.00	928	87.90	86	102.10	85
52.05	39	69.05	1257	89.00	239	103.00	74
53.00	325	70.05	6	91.00	1058	105.00	921
54.05	21	71.05	103	92.10	145	106.00	237
55.05	1647	76.05	134	93.05	1551	107.00	1178
56.00	104	77.05	475	94.00	168	108.00	291
58.00	33	78.10	167	95.05	1634	109.00	587
59.00	74	79.05	1077	96.05	128	111.05	58
63.00	83	81.00	960	97.05	429	114.00	121

Scan 2775 (50.422 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.10	119	126.05	183	137.15	247	150.05	78
116.10	59	127.05	55	138.15	32	151.05	12
117.00	383	128.05	201	139.15	80	152.15	25
118.05	213	129.00	202	140.20	24	155.00	76
119.00	1004	130.00	122	143.05	122	156.00	163
120.05	625	131.00	615	144.05	41	157.00	154
121.05	1049	132.00	9	145.05	595	158.15	55
122.05	249	133.00	475	146.05	22	159.15	218
123.05	374	134.00	590	147.05	622	160.15	125
124.05	149	135.05	755	148.05	285	161.15	235
125.05	131	136.15	95	149.05	367	162.10	154

Scan 2775 (50.422 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.15	334	178.00	101	198.00	30	213.25	40
165.15	6	180.00	44	199.20	127	214.15	23
167.95	21	185.10	130	201.20	235	215.20	229
169.05	109	186.05	8	202.15	54	216.25	176
170.20	47	189.20	216	203.00	562	217.20	194
171.05	90	190.05	148	204.15	226	218.20	162
172.05	280	191.05	106	205.15	169	219.20	135
173.10	244	192.05	56	207.00	114	220.30	153
175.05	451	193.05	107	210.15	32	224.10	17
176.20	102	196.10	12	211.20	29	225.20	18
177.15	277	197.15	91	212.15	75	226.05	86

CTMP Compounds

Scan 2775 (50.422 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
227.25	303	240.05	95	257.15	26	295.10	12
228.20	55	241.20	32	258.15	88	298.30	58
229.15	82	243.20	72	265.00	32	300.25	83
230.15	153	244.05	75	268.20	58	302.40	102
231.15	83	245.20	154	270.30	96	303.20	42
232.20	51	246.20	92	271.15	20	304.65	49
233.15	43	248.95	92	273.20	33	311.25	89
234.25	102	251.15	136	275.15	153	313.05	157
235.05	12	253.05	25	283.20	36	326.95	27
237.15	9	254.15	17	284.25	111	330.15	54
239.15	6	255.15	110	288.05	98	339.20	85

Scan 2775 (50.422 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
340.55	102	389.30	37	438.30	116		
340.95	107	393.35	38				
341.25	61	394.35	19				
342.20	67	396.45	34				
342.80	41	400.65	65				
343.20	44	401.00	47				
353.90	46	407.75	71				
354.45	27	409.25	61				
355.25	154	409.45	65				
365.30	103	410.25	18				
368.05	33	415.35	11				

CTMP Compounds

Scan 2775 (50.422 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	(5'Z,8'Z,11'Z)-6-(Heptadeca-5',8',11'-tr	330	C22H34O2	86
2.	LEDENE	204	C15H24	46
3.	Naphthalene, decahydro-1,6-bis(methylene	204	C15H24	45
4.	.epsilon.-Muurolene	204	C15H24	45
5.	(1R,3S,4S,7E,11E)-3,4-Epoxycembra-7,11,1	288	C20H32O	45
6.	Stigmast-5-en-3-ol, (3.beta.,24S)-	414	C29H50O	43
7.	.delta.-Guaiene	204	C15H24	41
8.	.beta.-Myrcene	136	C10H16	30
9.	1,5-Cycloundecadiene, 8,8-dimethyl-9-met	190	C14H22	30
10.	.beta.-Myrcene	136	C10H16	27
11.	.beta.-Myrcene	136	C10H16	27
12.	.alpha.-Bergamotene	204	C15H24	25
13.	.alpha.-Guaiene	204	C15H24	18
14.	Acetamide, N-phenyl-	135	C8H9NO	18
15.	TRICYCLO[6.3.1.0(1,5)]DODECAN-10-ONE	178	C12H18O	15
16.	3-Cyclohexen-1-ol, 5-methylene-6-(1-meth	150	C10H14O	11
17.	Cyclohexane, 1,2-dimethyl-3,5-bis(1-meth	192	C14H24	11
18.	VULGAROL A	220	C15H24O	11
19.	3-ACETOXYPYRIDINE	137	C7H7NO2	11
20.	Phosphonic acid, ethyl-,ethyl phenyl est	230	C10H15O2PS	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	86	081575-28-2	83058	90	79	3	95	9	53	0	49	7626
2.	*46	021747-46-6	36772	77	73	3	71	52	20	49	68	7103
3.	*45	054932-90-0	36742	70	92	3	96	47	19	34	52	8194
4.	*45	030021-46-6	36749	70	92	3	96	47	19	34	52	8194
5.	*45	079897-31-7	70091	74	95	3	111	46	19	14	55	8869
6.	43	000083-47-6	136253	85	130	2	58	47	18	0	45	8495
7.	*41	003691-11-0	128700	70	90	2	70	52	16	0	53	8355
8.	*30	000123-35-3	8068	43	60	0	95	57	9	0	44	6512
9.	*30	062338-54-9	30226	68	79	2	88	60	9	6	47	6985
10.	*27	000123-35-3	121974	36	64	0	92	57	8	0	41	6492
11.	*27	000123-35-3	121973	36	64	0	90	57	8	0	41	6385
12.	*25	017699-05-7	36758	48	76	0	65	63	7	19	44	6840
13.	*18	003691-12-1	128699	78	75	1	64	69	3	18	46	8404
14.	*18	000103-84-4	121706	37	41	1	94	68	3	2	43	5540
15.	*15	063072-63-9	24908	71	69	1	60	76	2	33	50	7589
16.	*11	054274-41-8	12790	52	74	1	50	77	2	0	44	6834
17.	*11	062337-99-9	31106	49	75	0	48	80	2	0	46	7196
18.	*11	011056-03-4	44015	51	87	3	169	73	2	0	46	5425
19.	*11	017747-43-2	122116	36	40	0	99	78	2	4	43	5255
20.	*11	007526-28-5	48214	37	69	0	85	78	2	22	43	5149

CTMP Compounds

CTMP Compounds

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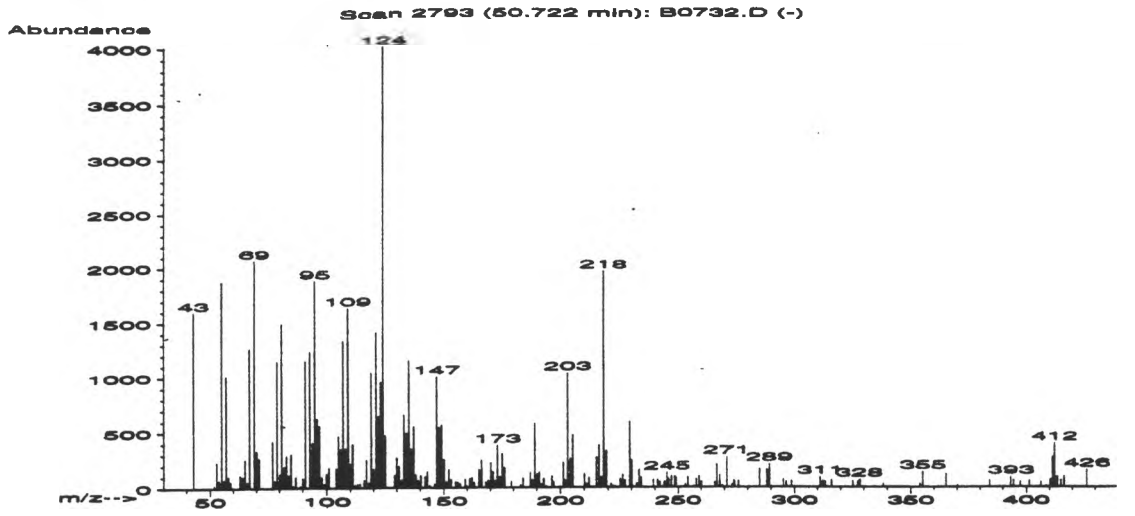
Peak ~~130~~; Unidentified Triterpene



Scan 2793 (50.722 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1596	65.00	254	82.00	194	95.05	1883
51.90	28	66.05	51	83.00	289	96.05	622
52.95	234	67.00	1264	84.00	117	97.05	559
53.95	71	69.05	2070	85.00	306	98.00	98
55.00	1875	69.95	330	86.00	19	99.05	37
56.00	75	71.05	267	87.00	99	99.95	130
57.00	1010	77.05	423	89.00	20	101.00	183
58.00	103	78.05	69	90.00	90	104.05	174
58.95	58	79.05	1144	91.05	1150	105.00	469
63.00	118	80.10	127	93.05	1236	106.00	355
63.90	104	81.00	1494	94.05	407	107.00	1337

Scan 2793 (50.722 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	359	120.05	168	133.00	661	144.05	26
109.00	1635	121.05	1411	134.05	496	146.05	36
110.10	220	122.05	649	135.05	1154	147.05	1006
111.05	391	123.05	958	136.05	352	148.05	547
112.15	24	124.05	4014	137.15	555	149.05	573
113.10	34	125.05	468	138.15	120	150.05	257
114.00	36	126.05	5	139.15	65	151.15	55
116.05	72	129.00	120	140.25	111	152.20	166
117.00	255	130.00	271	141.05	3	153.05	75
118.00	47	131.00	194	142.05	103	155.00	56
119.05	1044	132.10	72	143.00	147	156.05	47

Scan 2793 (50.722 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
157.05	38	170.20	229	188.20	69	203.15	1040
159.15	77	171.05	146	189.15	582	204.20	259
160.00	15	172.05	64	190.20	121	205.15	475
161.15	85	173.05	384	191.05	139	210.15	123
162.05	93	174.15	99	192.15	34	211.15	34
163.15	47	175.10	307	193.05	82	212.15	88
164.15	3	176.05	185	194.05	12	215.15	275
165.15	167	179.00	56	196.45	104	216.20	381
166.20	250	183.05	26	197.20	45	217.20	96
168.05	52	184.15	86	201.25	226	218.20	1971
169.05	68	187.15	135	202.05	66	219.25	331

CTMP Compounds

Scan 2793 (50.722 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
221.20	34	234.20	90	253.10	28	271.05	276
222.25	14	239.20	70	254.15	94	273.20	29
223.00	7	241.20	70	256.25	6	274.05	62
225.15	78	242.20	48	257.15	10	274.45	51
226.20	115	243.20	3	258.00	76	276.15	58
227.20	65	244.15	54	259.15	105	285.00	165
229.25	595	245.20	134	260.15	51	288.10	159
230.15	244	245.95	79	266.05	49	289.20	210
231.15	6	247.20	105	266.80	207	295.20	71
232.20	38	248.55	101	268.05	111	296.45	50
233.20	161	249.05	87	269.15	20	298.70	58

Scan 2793 (50.722 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
311.15	92	354.00	33	410.30	72		
312.30	58	355.15	139	411.30	276		
313.20	55	365.30	123	412.30	399		
314.25	8	370.25	20	413.30	94		
316.05	67	384.25	62	413.55	96		
325.25	56	393.25	94	415.05	63		
327.20	52	394.45	66	416.45	102		
327.90	69	397.40	52	426.40	156		
328.25	67	401.25	61				
338.30	33	406.25	47				
341.05	1	408.45	13				

CTMP Compounds

Scan 2793 (50.722 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	53
2.	2-HYDROXY-4,6-DIMETHYLPYRIMIDINE-HYDROCH	124	C6H8N2O	43
3.	Phenol, 4-methoxy-	124	C7H8O2	38
4.	Phenol, 2-methoxy-, acetate	166	C9H10O3	38
5.	Benzene, 1-ethoxy-3-methoxy-	152	C9H12O2	38
6.	3-ISOPROPENYLTHIOPHENE	124	C7H8S	38
7.	Benzene, (methylthio)-	124	C7H8S	35
8.	2-(1-METHYLVINYL)THIOPHENE	124	C7H8S	35
9.	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	35
10.	1,4-Benzenediol, 2-methyl-	124	C7H8O2	35
11.	Benzene, (methylthio)-	124	C7H8S	35
12.	Benzene, (methylthio)-	124	C7H8S	35
13.	Benzene, (methylthio)-	124	C7H8S	35
14.	Tricyclo[8.6.0.0(2,9)]hexadeca-8,16,head	248	C16H24O2	32
15.	Pregn-4-ene-3,20-dione, (9.beta.,10.alph	314	C21H30O2	30
16.	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	27
17.	Benzene, 1-(1,1-dimethylethoxy)-4-methox	180	C11H16O2	25
18.	Benzene, 1-(1,1-dimethylethoxy)-4-methox	180	C11H16O2	25
19.	1,4,4,7a-Tetramethyl-5,6,7,7a-tetrahydro	180	C13H24	25
20.	6,8-Diazabicyclo[3.2.1]oct-6-ene-6-oxide	198	C10H18N2O2	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	002847-30-5	120355	61	54	1	94	37	28	0	51	8926
2.	*43	000108-79-2	120352	41	66	2	99	45	18	5	38	8835
3.	*38	000150-76-5	4707	43	69	3	94	50	14	0	40	8599
4.	*38	000613-70-7	19294	47	47	0	73	51	14	0	44	8261
5.	38	025783-45-3	13475	44	65	3	99	49	14	4	41	8596
6.	*38	000000-00-0	4724	51	45	1	99	52	14	0	46	8218
7.	*35	000100-68-5	120399	36	66	1	99	52	11	0	39	8228
8.	*35	030616-73-0	4734	44	37	0	84	52	11	9	38	7831
9.	*35	001004-36-0	120369	44	22	1	98	52	11	14	43	8315
10.	*35	000095-71-6	4704	49	63	2	99	52	11	0	39	8379
11.	*35	000100-68-5	120396	37	70	1	91	52	11	0	39	8225
12.	*35	000100-68-5	120397	36	65	1	88	52	11	0	39	8220
13.	*35	000100-68-5	4730	36	70	1	89	52	11	0	39	8222
14.	32	000000-00-0	55755	56	106	3	99	49	9	0	36	8675
15.	30	002755-10-4	133961	83	83	1	91	60	9	0	45	8305
16.	*27	001004-36-0	120371	35	41	1	71	60	8	1	40	8337
17.	25	015360-00-6	25625	47	44	1	92	52	7	0	37	8225
18.	25	015360-00-6	126839	43	56	2	85	52	7	0	37	8215
19.	25	085329-81-3	25873	47	56	2	64	52	7	0	37	8294
20.	16	077719-84-7	33755	45	94	3	81	60	3	0	37	8477

CTMP Compounds

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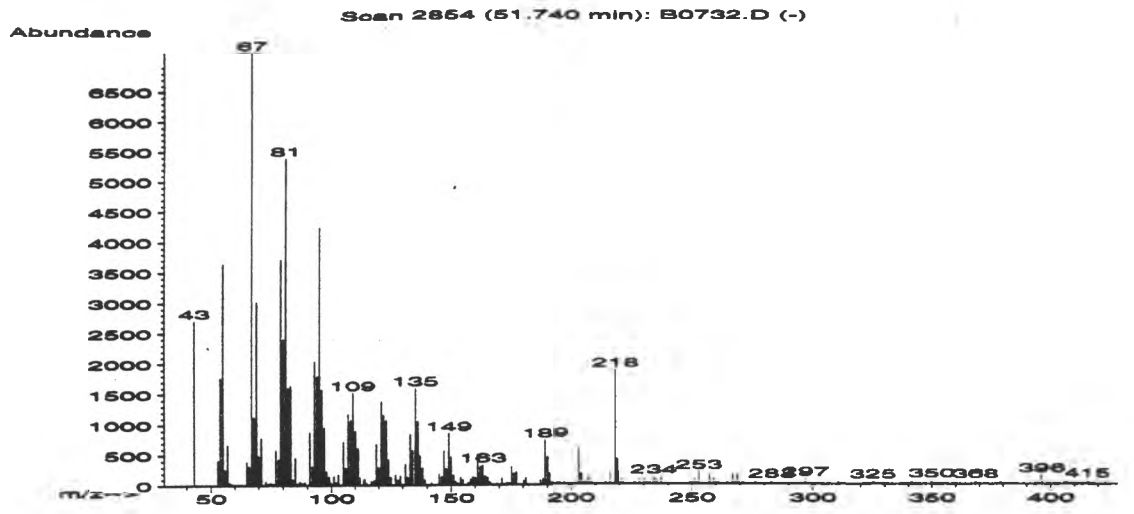
Peak ~~139~~; Unidentified Triterpene



Scan 2854 (51.740 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2702	67.95	1123	80.00	2403	92.15	316
53.05	411	69.05	3013	81.00	5391	93.05	2037
53.95	1770	70.00	479	82.00	1598	94.05	1792
55.00	3635	71.00	776	83.00	1634	95.05	4236
56.00	256	73.00	60	84.00	98	96.05	1570
57.00	666	74.00	28	85.10	449	97.05	949
58.00	45	74.95	40	86.10	29	98.05	227
59.00	25	76.00	29	87.00	59	99.05	140
65.00	385	77.05	578	87.90	40	100.05	34
66.00	315	78.05	427	89.00	52	101.05	153
67.00	7152	79.05	3707	91.00	871	102.05	49

Scan 2854 (51.740 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.05	178	115.00	32	128.05	80	141.00	12
105.00	716	117.05	66	129.00	159	142.00	38
106.00	288	118.05	83	131.00	349	145.05	185
107.00	1170	119.05	677	132.00	134	146.05	141
108.05	1070	120.00	296	133.00	839	147.05	573
109.00	1517	121.05	1377	134.00	574	148.05	275
110.15	890	122.05	1149	135.15	1591	149.05	853
111.15	602	123.05	1071	136.15	1051	150.05	461
112.00	123	124.05	415	137.15	474	151.05	155
113.75	93	125.05	132	138.15	286	152.10	59
114.15	105	127.00	173	139.10	85	153.05	27

Scan 2854 (51.740 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
154.10	134	166.00	48	180.10	67	197.05	41
155.05	83	167.05	7	181.00	120	200.25	7
157.15	41	167.95	7	183.15	1	203.15	596
158.10	99	169.05	24	187.15	79	204.15	177
159.05	142	171.10	116	188.25	104	205.20	38
160.05	123	172.10	11	189.15	737	207.00	115
161.10	503	173.05	37	190.15	458	208.05	68
162.10	306	174.05	32	191.05	190	210.15	14
163.15	333	175.10	300	192.05	46	214.10	37
164.15	148	176.10	186	194.00	26	216.05	197
165.10	126	177.05	208	195.15	56	218.20	1887

CTMP Compounds

Scan 2854 (51.740 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
219.20	411	237.15	113	266.95	156	325.15	49
219.95	182	243.20	16	268.95	150	325.65	38
221.20	78	249.15	47	271.15	31	329.20	15
226.20	66	250.70	47	273.20	2	341.30	53
228.15	103	251.25	83	276.25	36	349.75	64
230.00	93	252.90	205	281.05	11	368.45	57
231.10	30	255.15	1	283.15	57	378.90	40
232.15	56	257.25	153	297.05	90	396.20	152
233.25	5	259.15	87	297.30	9	405.65	33
234.15	127	260.90	42	310.65	42	406.25	48
235.20	81	264.55	59	313.05	20	406.50	48

Scan 2854 (51.740 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
408.40	21						
410.35	2						
415.45	66						
416.05	41						

CTMP Compounds

Scan 2854 (51.740 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	Cyclopropaneoctanoic acid, 2-[[2-[(2-eth	334	C22H38O2	74
2.	Ethanol, 2-(9,12-octadecadienyloxy)-, (Z	310	C20H38O2	64
3.	5-Dodecyne	166	C12H22	58
4.	7-Hexadecyne	222	C16H30	53
5.	Cyclohexane, 1,1'-(1,3-butadiene-1,4-diy	218	C16H26	46
6.	Cyclohexane, 1,2-diethenyl-, cis-	136	C10H16	43
7.	Cyclododecyne	164	C12H20	43
8.	Methylenecyclononane	138	C10H18	38
9.	2-Cyclohexylmethylenecyclopropane	136	C10H16	38
10.	1-Propanone, 1-(4-cycloocten-1-yl)-	166	C11H18O	30
11.	1-TERT-BUTYL-1,5-CYCLOOCTADIENE	164	C12H20	30
12.	5,10-Undecadienoic acid, 2-methylene-, m	208	C13H20O2	30
13.	6,6-Dimethyl-2,3-diazabicyclo[3.1.0]hex-	110	C6H10N2	22
14.	1,E-6,Z-10-HEXADECATRIENE	220	C16H28	22
15.	9,12-Octadecadienoyl chloride, (Z,Z)-	298	C18H31ClO	14
16.	Cyclobutane, 1-ethyl-3-methylene-	96	C7H12	14
17.	Cyclobuta[1,2:3,4]dicyclooctene, 1,2,5,6	216	C16H24	11
18.	Ethane, 2-bromo-1,1,2-trifluoro-1-methox	192	C3H4BrF3O	11
19.	TRICYCLO[8.6.0.0(2,9)]HEXADECA-5,13-DIEN	216	C16H24	11
20.	4-(1-Methylethenyl)cyclohex-2-enone	136	C9H12O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_l	Tilt	R_IV	XCORR
1.	74	010152-71-3	84215	94	86	3	99	16	44	0	51	9725
2.	64	017367-08-7	77158	92	89	2	86	19	37	0	40	9686
3.	*58	019780-12-2	19713	67	51	2	77	34	32	0	58	9019
4.	53	074685-28-2	45100	76	61	2	87	29	28	0	40	9224
5.	*46	055712-53-3	43079	67	75	2	83	44	20	6	47	7857
6.	*43	001004-84-8	122042	74	41	2	73	50	18	11	50	6888
7.	*43	001129-90-4	18739	65	54	1	71	47	18	0	44	8215
8.	*38	056133-38-1	8815	48	24	0	55	55	14	0	46	8583
9.	38	057497-09-3	8141	43	54	0	72	50	14	4	41	7599
10.	*30	054703-58-1	19618	68	52	2	55	62	9	0	53	7713
11.	*30	000000-00-0	18734	59	50	1	48	65	9	0	56	7132
12.	*30	051788-60-4	128974	59	68	1	79	64	9	0	51	7311
13.	*22	068914-93-2	2146	47	63	2	97	61	5	0	40	7655
14.	22	083489-23-0	44095	62	65	0	85	62	5	0	43	7193
15.	14	007459-33-8	73230	57	83	0	37	70	2	23	41	8422
16.	*14	056335-70-7	634	35	47	0	85	68	2	0	41	7009
17.	*11	061277-43-8	42175	75	64	2	37	75	2	0	45	7026
18.	*11	000679-90-3	30477	35	57	1	55	77	2	14	43	4713
19.	*11	000000-00-0	42186	75	64	2	37	75	2	0	45	7026
20.	*10	062702-87-8	7966	44	33	0	36	75	1	14	43	4126

CTMP Compounds

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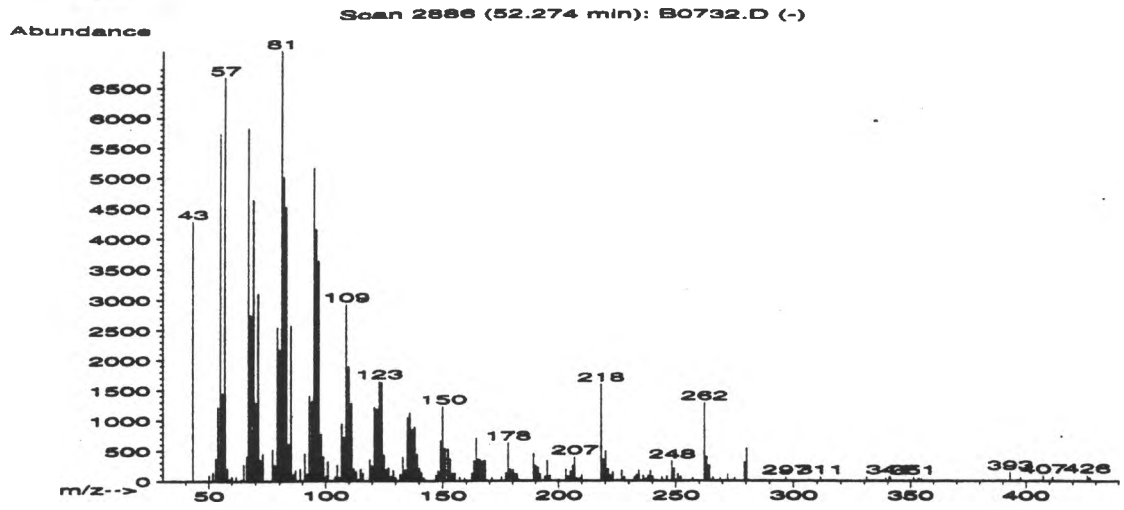
Peak ~~140~~; Unidentified triterpene



Scan 2886 (52.274 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4275	61.75	68	77.00	518	89.15	199
50.05	100	63.95	23	78.05	262	91.00	451
51.80	143	65.00	272	79.05	2551	92.05	114
53.00	369	66.15	405	80.00	2179	92.95	1410
54.00	1220	67.00	5822	81.00	7106	94.05	1316
55.05	5733	68.00	2745	82.00	5011	95.05	5160
56.00	1452	69.05	4633	83.00	4515	96.05	4151
57.00	6667	70.05	1297	84.05	608	97.05	3629
57.95	201	71.05	3103	85.00	2583	98.05	769
59.00	27	71.95	342	86.15	106	99.05	395
60.00	68	73.05	452	87.00	172	100.15	80

Scan 2886 (52.274 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.05	315	114.15	20	127.05	215	139.15	440
104.05	67	115.00	195	128.05	79	140.15	203
105.00	257	116.00	123	129.00	169	141.05	131
106.00	57	119.05	352	130.00	49	142.05	42
107.00	949	120.05	250	132.00	108	147.05	95
108.00	719	121.05	1221	133.05	396	148.05	163
109.00	2926	122.05	1190	134.05	183	149.15	662
110.05	1889	123.05	1648	135.10	1047	150.05	1225
111.15	1286	124.05	1629	136.05	1128	151.05	533
112.10	203	125.05	423	137.15	848	152.20	524
113.10	154	126.10	187	138.15	884	153.10	356

Scan 2886 (52.274 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
154.05	121	167.05	321	183.10	16	205.15	155
155.00	124	168.05	331	189.15	445	206.15	255
157.10	59	168.95	4	190.15	246	207.00	391
159.15	46	171.05	52	191.05	220	208.00	41
160.15	16	175.20	62	192.05	110	209.15	41
161.15	7	177.10	129	194.20	69	210.05	95
162.20	131	178.00	624	195.20	327	218.20	1598
163.15	335	179.00	191	196.20	82	219.20	348
164.15	712	180.15	177	200.20	20	220.15	489
165.15	361	181.10	119	203.15	191	221.20	196
166.05	343	182.05	110	204.15	70	222.10	87

CTMP Compounds

Scan 2886 (52.274 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
223.15	139	240.05	70	264.20	256	311.40	67
225.15	6	244.05	64	265.05	16	331.00	64
227.00	172	246.20	76	265.95	58	339.20	45
228.15	61	248.30	321	267.15	2	340.70	68
232.40	63	249.30	204	269.05	41	341.20	60
233.15	104	250.05	12	272.20	104	351.25	62
234.20	175	251.00	112	275.15	56	353.50	38
236.15	90	252.25	73	279.25	304	354.80	32
237.15	36	257.20	39	280.25	538	393.05	144
238.15	90	262.25	1292	281.15	11	396.35	26
239.20	172	263.15	399	296.80	64	397.65	54

Scan 2886 (52.274 min): B0732.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
407.40	85						
411.20	64						
426.25	94						
427.40	49						

CTMP Compounds

Scan 2886 (52.274 min): B0732.D

PBM Search of library F:\LIBRARY.L

	Name	MolWt	Formula	Qual
1.	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	90
2.	1,13-Tetradecadiene	194	C14H26	62
3.	9,12-Octadecadienoic acid (Z,Z)-, methyl	294	C19H34O2	62
4.	7-Tetradecyne	194	C14H26	58
5.	Naphthalene, decahydro-	138	C10H18	52
6.	Naphthalene, decahydro-, cis-	138	C10H18	52
7.	6,11-UNDECADIENE, 1-ACETOXY-3,7-DIMETHYL	252	C16H28O2	50
8.	Methylenecyclononane	138	C10H18	46
9.	p-Menth-8(10)-en-9-ol, cis-	154	C10H18O	45
10.	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	43
11.	Cyclopropane, 1-(1-methylethyl)-2-(2-met	152	C11H20	43
12.	Spiro[4.5]decane	138	C10H18	38
13.	2,2-Dimethyl-1-isopropenyl-cyclopentane	138	C10H18	30
14.	Iridomyrmecin	168	C10H16O2	30
15.	1,E-8,Z-10-TRIDECATRIENE	178	C13H22	30
16.	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	30
17.	(Z)14-TRICOSENYL FORMATE	366	C24H46O2	25
18.	13-Oxabicyclo[10.1.0]tridecane	182	C12H22O	25
19.	2,5-Furandione, 3-(dodecenyl)dihydro-	266	C16H26O3	25
20.	3,9-Dodecadiene	166	C12H22	20

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000060-33-3	132609	98	85	2	73	17	59	44	84	9352
2.	*62	021964-49-8	32141	78	63	2	92	28	36	28	59	9648
3.	62	000112-63-0	133235	105	73	1	70	28	36	0	59	9374
4.	*58	035216-11-6	32140	50	77	2	81	29	32	0	46	9320
5.	*52	000091-17-8	122340	70	47	1	89	35	27	27	47	9157
6.	*52	000493-01-6	122337	69	47	1	90	35	27	25	47	9133
7.	*50	000000-00-0	57460	73	69	0	99	47	25	0	81	8792
8.	*46	056133-38-1	8815	62	15	0	79	42	20	22	47	8376
9.	*45	015714-13-3	14722	81	42	2	93	48	19	22	58	8100
10.	*43	064566-18-3	57551	45	18	0	93	48	18	0	44	8336
11.	*43	056259-17-7	13869	43	56	0	92	50	18	0	44	8207
12.	*38	000176-63-6	8822	35	79	0	58	55	14	16	43	9075
13.	*30	072535-87-6	8783	50	57	3	120	60	9	0	46	6647
14.	*30	000485-43-8	125756	59	66	1	58	64	9	0	56	8757
15.	*30	080625-30-5	24966	68	63	2	81	64	9	21	50	6342
16.	*30	064566-18-3	131394	61	106	0	61	61	9	0	56	9639
17.	25	077899-10-6	91683	112	78	0	59	61	7	18	47	7430
18.	*25	000286-99-7	26828	48	81	0	80	62	7	0	46	7273
19.	*25	025377-73-5	62058	74	85	1	54	80	7	0	81	6345
20.	*20	054764-65-7	19716	62	48	1	66	69	4	0	56	8163