

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/25/2002 Time: 15:34:31

Sample: AD31675

Analysis: \$GCMS GCMS Scan For Unknowns

Units: ug

Started: 1/25/02 15:34 Ended: 1/25/02 15:34 Analyst: DLV

Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		96		5.0

Comments for Sample AD31675 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-25-2002 Time: 15:37:32

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.

The recoveries for 9 of the 43 compounds in the LCS Standard were above their acceptance ranges. The pH of this sample when received was less than 2.

Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN22\31675.D

Vial: 1

Acq On : 22 Jan 2002 4:20 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 22, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 16:55:28 2002

Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

Title : 508 scan method

Last Update : Fri Jan 11 13:20:07 2002

Response via : Initial Calibration

DataAcq Meth : SCAN508

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1360704	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	5803482	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	3010850	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4863465	20.00	ug/L	-0.02
38) Chrysene-d12	30.49	240	3988739	20.00	ug/L	-0.02
44) Perylene-d12	0.00	264	0	0.00	ug/L	-34.42

System Monitoring Compounds

37) 2,4-DDD	27.73	235	370347	4.82	ug/L	0.00
Spiked Amount	5.000		Recovery	=	96.40%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	486047	2.44	ug/L	# 56
21) 2,6-Dinitrotoluene	18.34	165	386061	9.95	ug/L	# 17
35) Di-n-butylphthalate	24.86	149	211596	0.67	ug/L	# 97
42) Bis(2-ethylhexyl)phthalate	31.09	149	5213	0.57	ug/L	# 44

 (#) = qualifier out of range (m) = manual integration

31675.D SCAN508.M

Tue Jan 22 16:55:28 2002

Page 1

Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN22\31675.D

Vial: 1

Acq On : 22 Jan 2002 4:20 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 22, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 16:55 2002

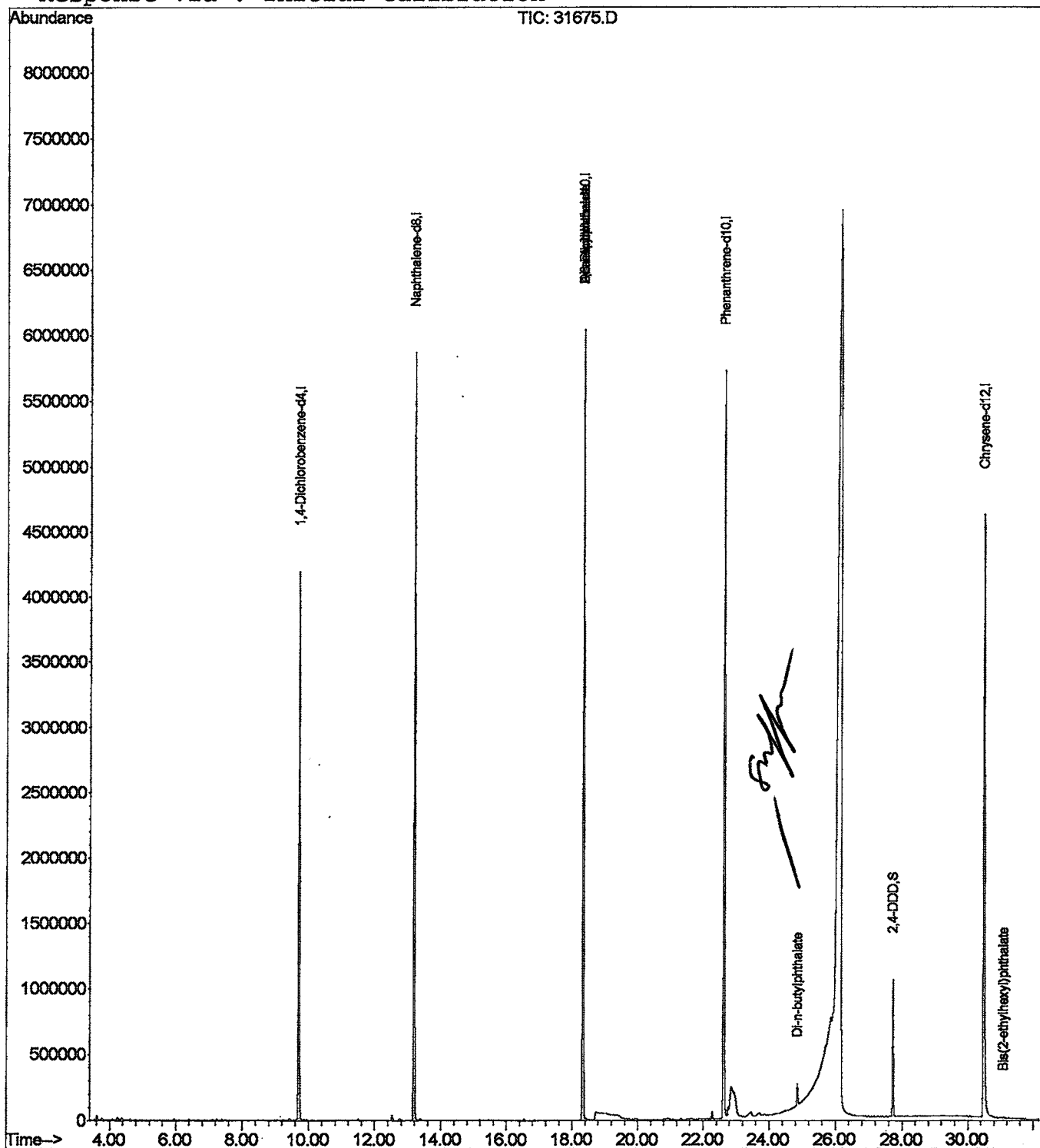
Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)

Title : 508 scan method

Last Update : Fri Jan 11 13:20:07 2002

Response via : Initial Calibration



Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D

Vial: 2

Acq On : 24 Jan 2002 12:31 pm

Operator:

Sample : 508scan; re-inj

Inst : Instrumen

Misc : January 24, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 24 13:39:07 2002

Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

Title : 508 scan method

Last Update : Fri Jan 11 13:20:07 2002

Response via : Initial Calibration

DataAcq Meth : SCAN508

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev (Min)
1) 1,4-Dichlorobenzene-d4	9.72	152	1460658	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	6191419	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	3192767	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	5209941	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	4501606	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3306770	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	420743	5.11	ug/L	0.00
Spiked Amount	5.000		Recovery	=	102.20%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	510475	2.42	ug/L	# 57
21) 2,6-Dinitrotoluene	18.34	165	399892	9.72	ug/L	# 17
35) Di-n-butylphthalate	24.86	149	217729	0.65	ug/L	# 97
42) Bis(2-ethylhexyl)phthalate	31.11	149	9896	0.59	ug/L	# 44

(#) = qualifier out of range (m) = manual integration

31675A.D SCAN508.M Thu Jan 24 13:39:08 2002

Page 1

Quantitation Report

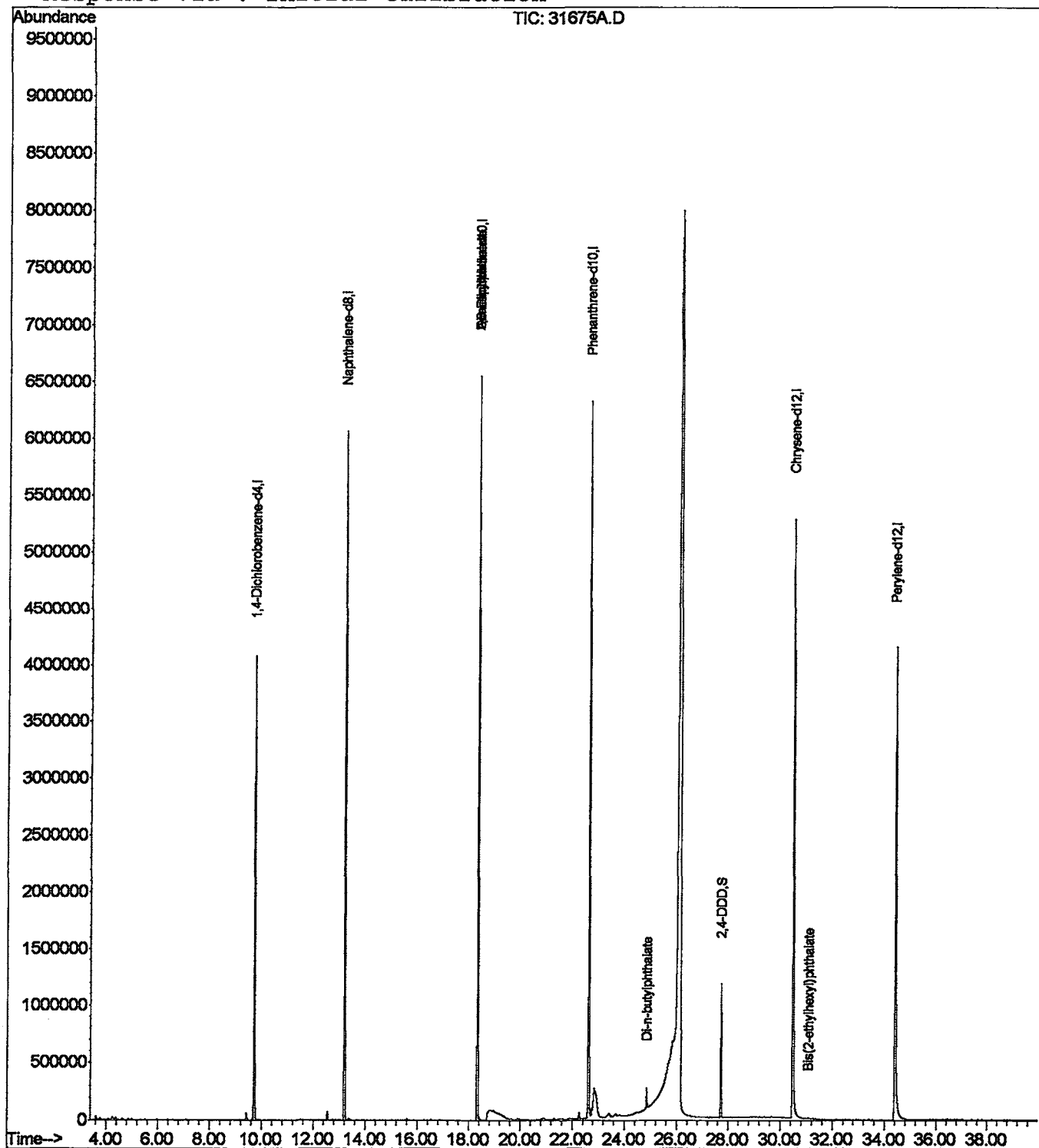
(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: SPLIT.P
Quant Time: Jan 24 13:39 2002

Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D

Vial: 2

Acq On : 24 Jan 2002 12:31 pm

Operator:

Sample : 508scan; re-inj

Inst : Instrumen

Misc : January 24, 2002

Multiplr: 1.00

MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)

Title : 508 scan method

Smoothing : OFF

Filtering: 5

Sampling : 2

Min Area: 100 Area counts

Start Thrs: 0.2

Max Peaks: 20

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

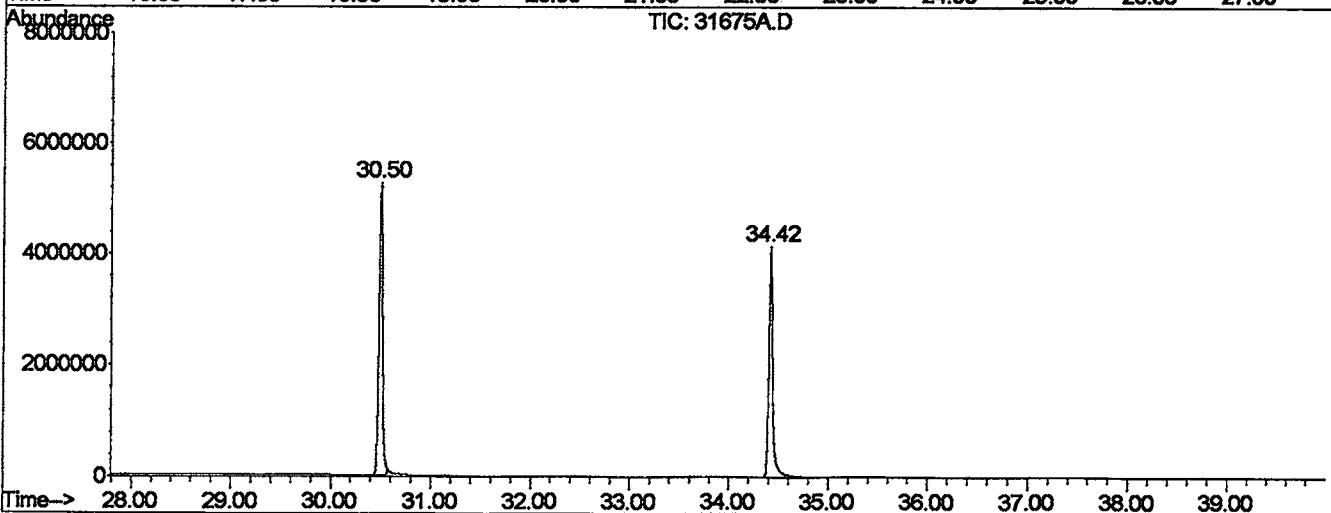
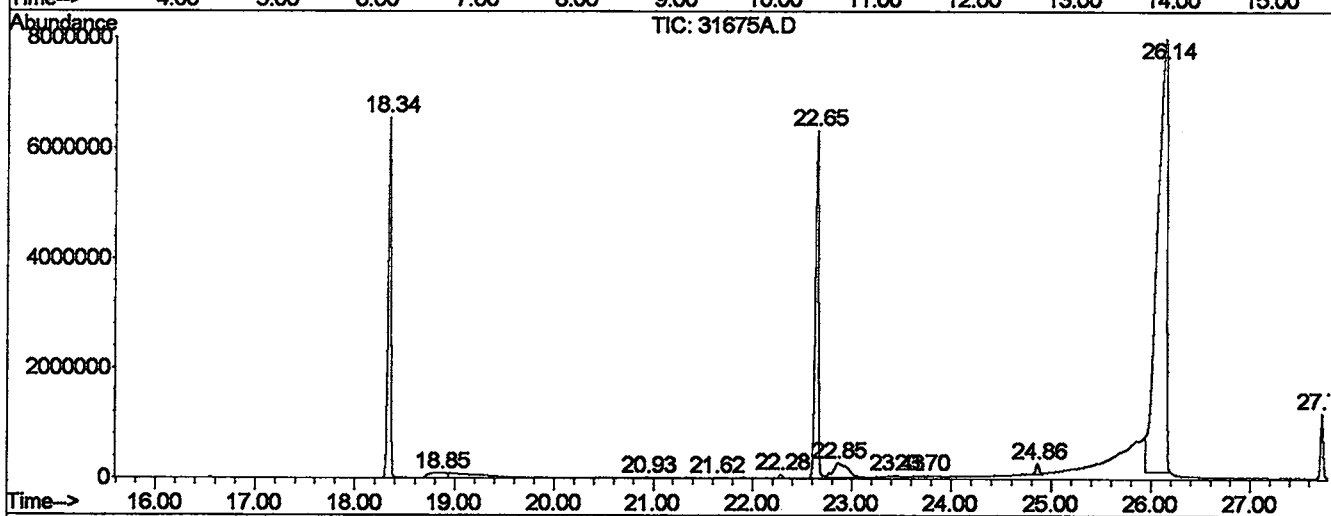
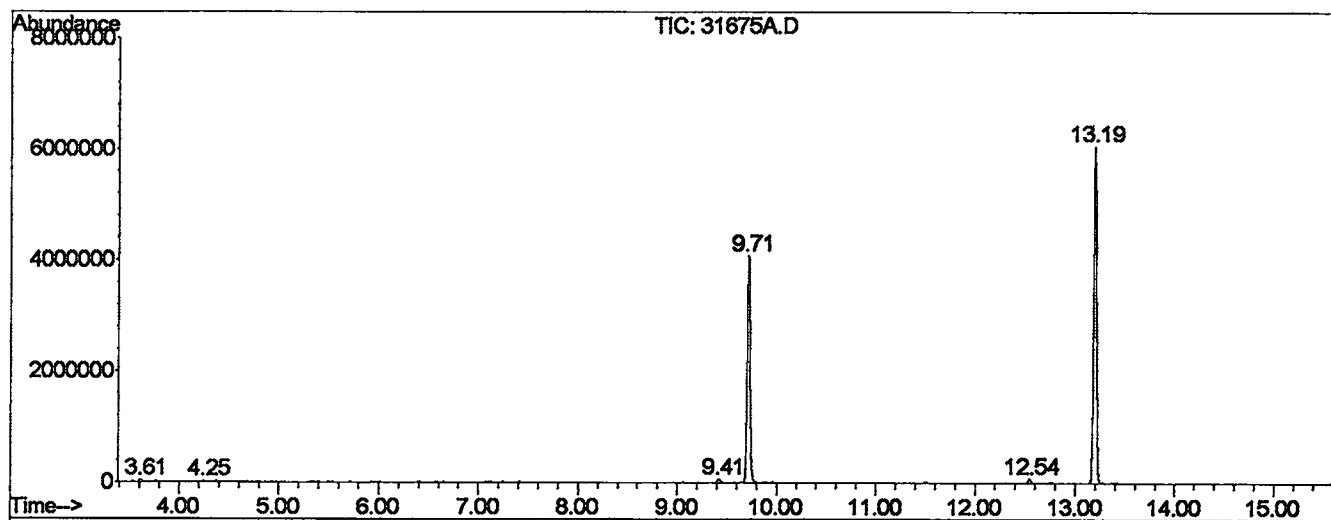
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.613	17	21	25	rBV	37530	67677	0.12%	0.051%
2	4.253	71	77	83	rVV3	21800	59657	0.11%	0.045%
3	9.413	525	529	535	rVV	61370	124919	0.23%	0.094%
4	9.710	551	555	561	rVV	4078393	8362916	15.30%	6.270%
5	12.541	799	803	807	rBV	77173	134458	0.25%	0.101%
6	13.192	855	860	865	rBV	6064602	11972886	21.90%	8.977%
7	18.341	1305	1311	1315	rBV	6551871	12997127	23.77%	9.744%
8	18.855	1339	1356	1363	rBV5	89505	1121229	2.05%	0.841%
9	20.933	1523	1538	1547	rVB4	14505	84607	0.15%	0.063%
10	21.618	1589	1598	1607	rVB5	8980	68310	0.12%	0.051%
11	22.280	1651	1656	1661	rBV	60694	117825	0.22%	0.088%
12	22.645	1681	1688	1693	rVV	6313371	13917013	25.46%	10.434%
13	22.851	1695	1706	1733	rVB2	257561	2594033	4.74%	1.945%
14	23.433	1745	1757	1765	rBV2	32960	176620	0.32%	0.132%
15	23.696	1769	1780	1785	rBV6	26510	149615	0.27%	0.112%
16	24.860	1877	1882	1887	rBV	186692	405828	0.74%	0.304%
17	26.139	1977	1994	1999	rVB	7869866	54671113	100.00%	40.989%
18	27.726	2127	2133	2139	rBV	1166327	2116185	3.87%	1.587%
19	30.500	2369	2376	2381	rBV	5267673	12990976	23.76%	9.740%
20	34.416	2713	2719	2749	rBV	4148573	11246204	20.57%	8.432%

Sum of corrected areas: 133379198

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Operator :
 Acquired : 24 Jan 2002 12:31 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508scan; re-inj
 Misc Info : January 24, 2002
 Vial Number: 2
 Quant File :SCAN508.RES (RTE Integrator)



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Smoothing : OFF
 Sampling : 2
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 100 Area counts
 Max Peaks: 20
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

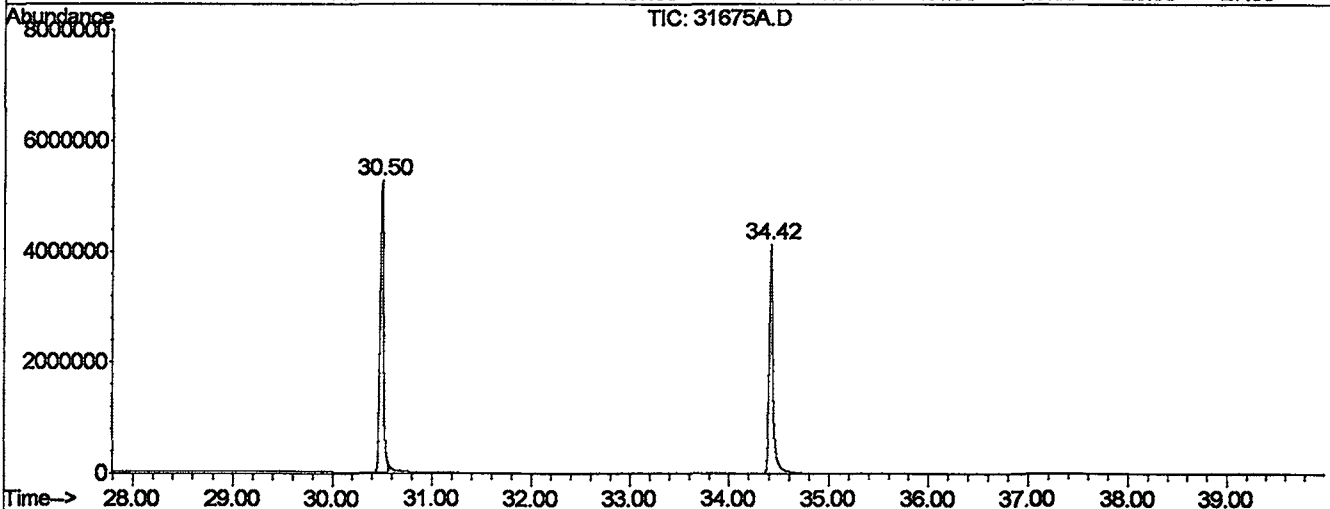
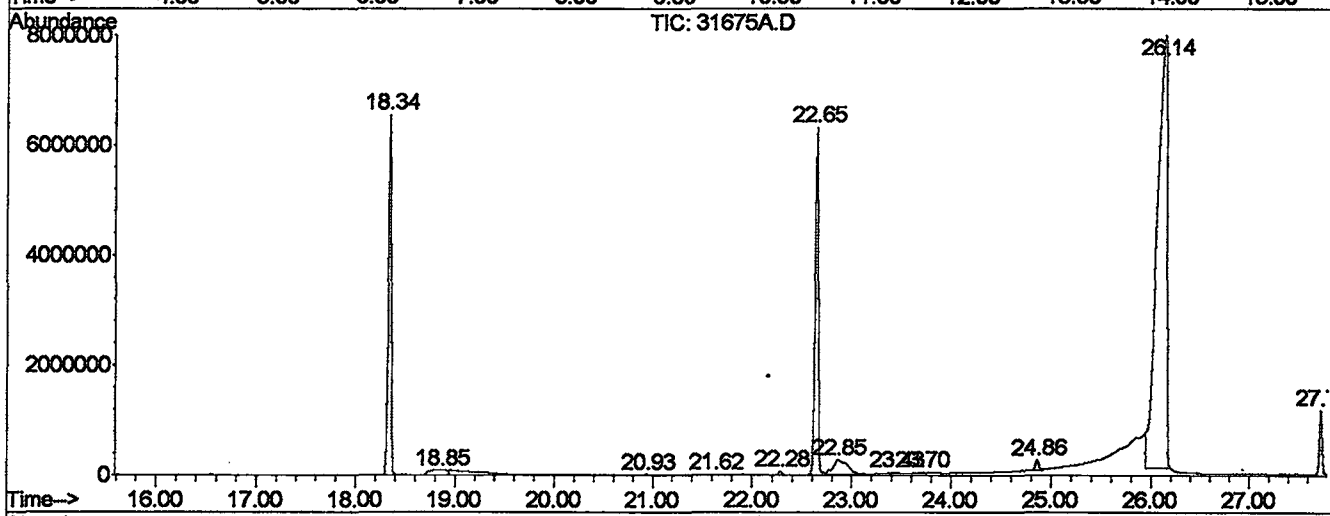
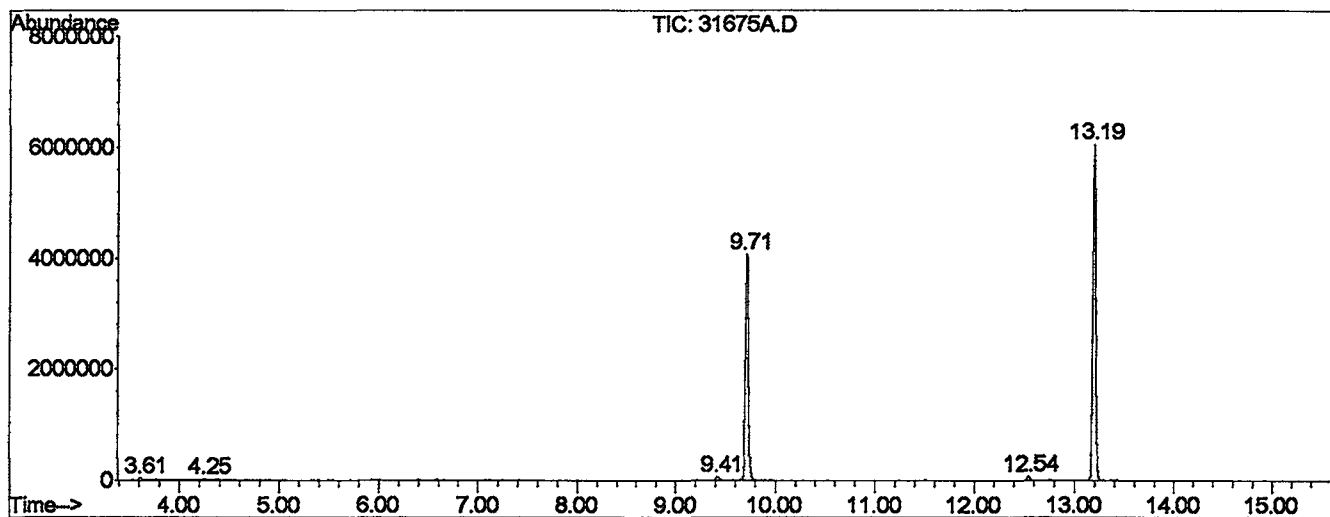
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.613	17	21	25	rBV	37530	67677	0.12%	0.051%
2	4.253	71	77	83	rVV3	21800	59657	0.11%	0.045%
3	9.413	525	529	535	rVV	61370	124919	0.23%	0.094%
4	9.710	551	555	561	rVV	4078393	8362916	15.30%	6.270%
5	12.541	799	803	807	rBV	77173	134458	0.25%	0.101%
6	13.192	855	860	865	rBV	6064602	11972886	21.90%	8.977%
7	18.341	1305	1311	1315	rBV	6551871	12997127	23.77%	9.744%
8	18.855	1339	1356	1363	rBV5	89505	1121229	2.05%	0.841%
9	20.933	1523	1538	1547	rVB4	14505	84607	0.15%	0.063%
10	21.618	1589	1598	1607	rVB5	8980	68310	0.12%	0.051%
11	22.280	1651	1656	1661	rBV	60694	117825	0.22%	0.088%
12	22.645	1681	1688	1693	rVV	6313371	13917013	25.46%	10.434%
13	22.851	1695	1706	1733	rVB2	257561	2594033	4.74%	1.945%
14	23.433	1745	1757	1765	rBV2	32960	176620	0.32%	0.132%
15	23.696	1769	1780	1785	rBV6	26510	149615	0.27%	0.112%
16	24.860	1877	1882	1887	rBV	186692	405828	0.74%	0.304%
17	26.139	1977	1994	1999	rVB	7869866	54671113	100.00%	40.989%
18	27.726	2127	2133	2139	rBV	1166327	2116185	3.87%	1.587%
19	30.500	2369	2376	2381	rBV	5267673	12990976	23.76%	9.740%
20	34.416	2713	2719	2749	rBV	4148573	11246204	20.57%	8.432%

Sum of corrected areas: 133379198

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Operator :
 Acquired : 24 Jan 2002 12:31 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508scan; re-inj
 Misc Info : January 24, 2002
 Vial Number: 2
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

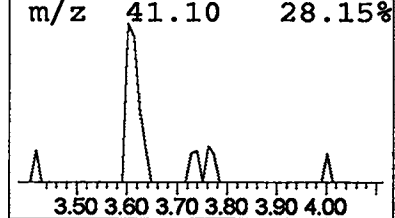
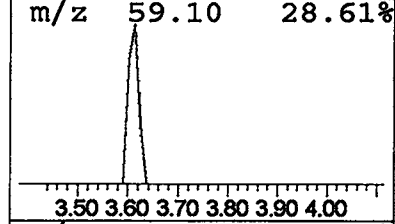
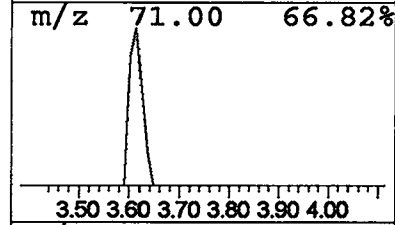
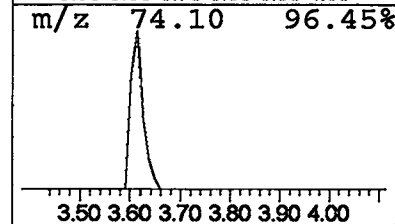
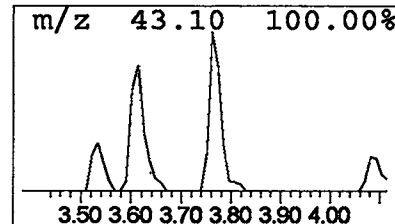
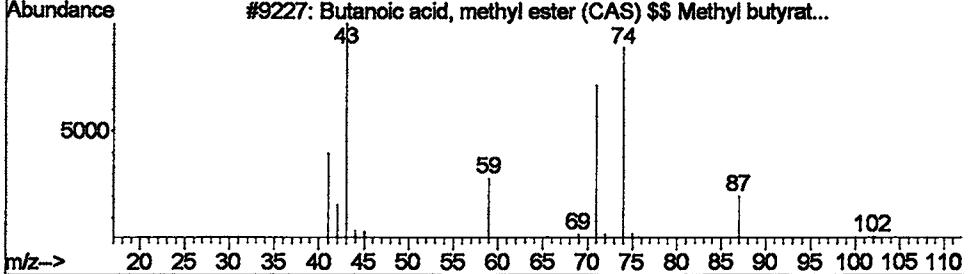
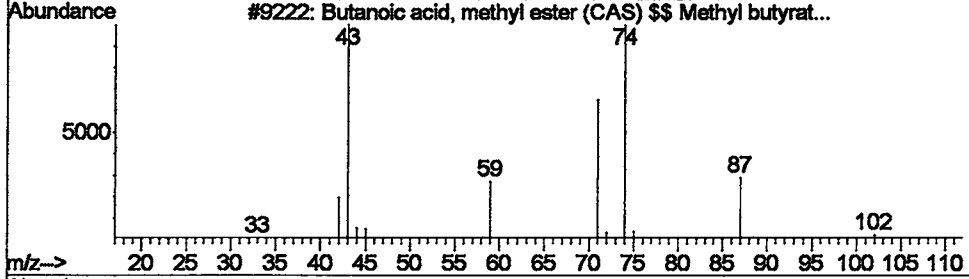
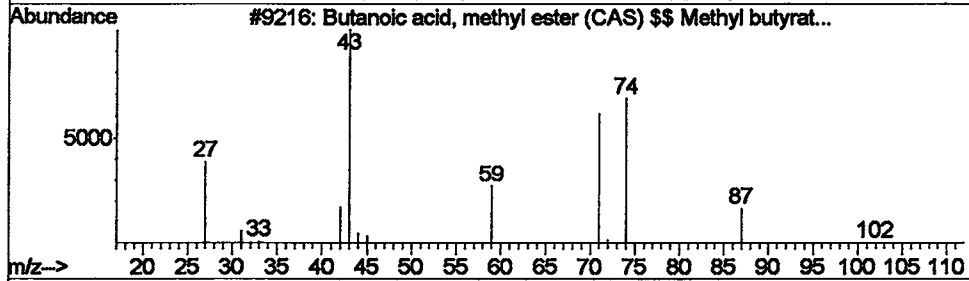
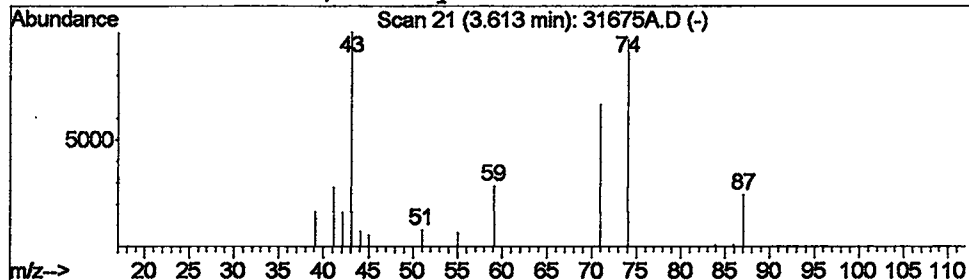
Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	0.16 ug/L	67677	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
2			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
3			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: LSCINT.P

Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

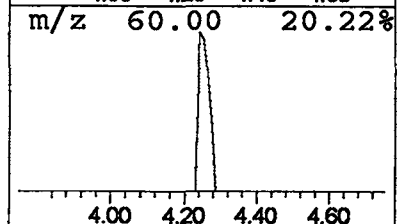
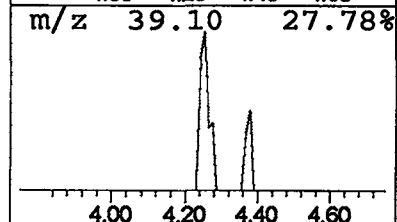
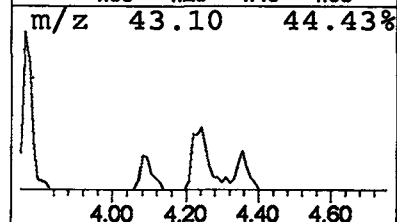
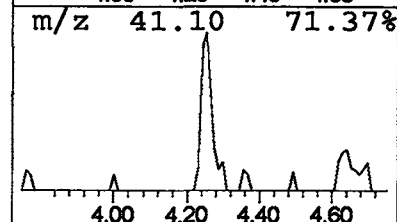
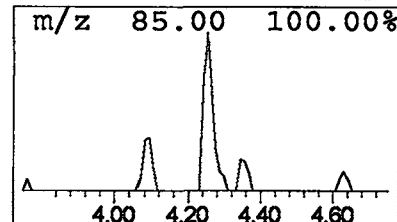
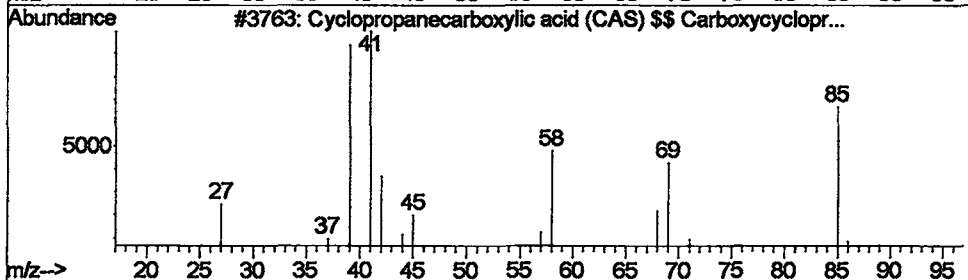
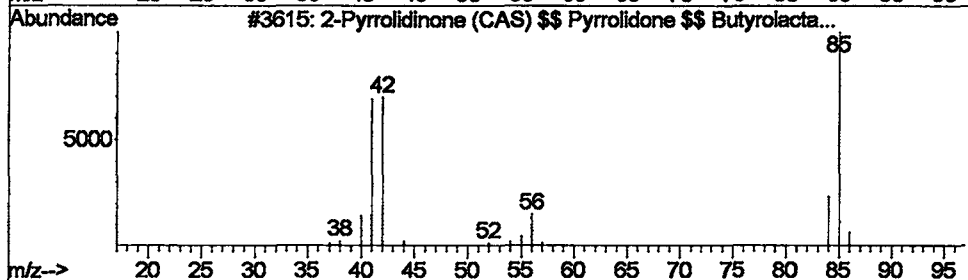
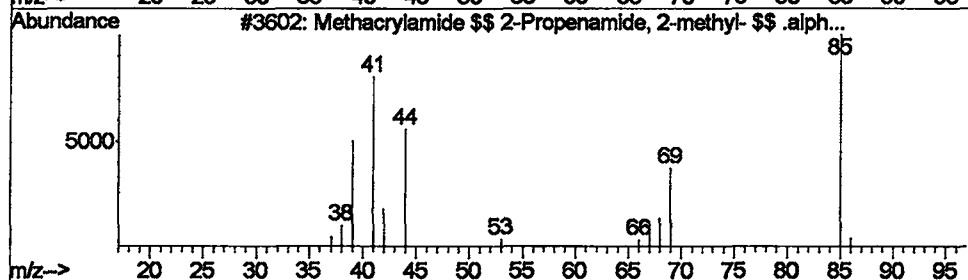
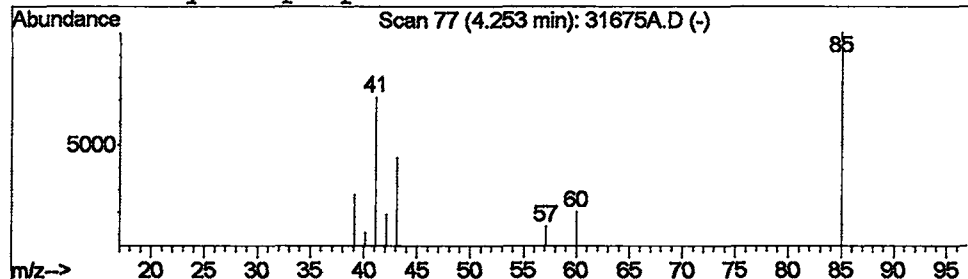
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 2 Methacrylamide \$\$ 2-Propena... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	0.14 ug/L	59657	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methacrylamide \$\$ 2-Propenamide,...	85	C4H7NO	000079-39-0	36
2			2-Pyrrolidinone (CAS) \$\$ Pyrroli...	85	C4H7NO	000616-45-5	9
3			Cyclopropanecarboxylic acid (CAS...	86	C4H6O2	001759-53-1	9
4			3-Methyl-2-propenamide	85	C4H7NO	000000-00-0	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

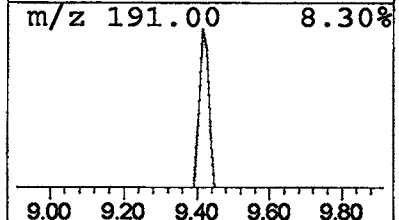
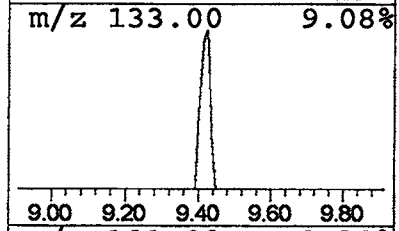
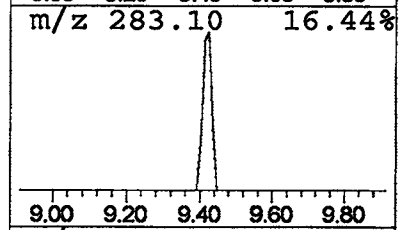
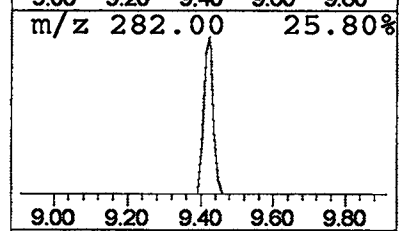
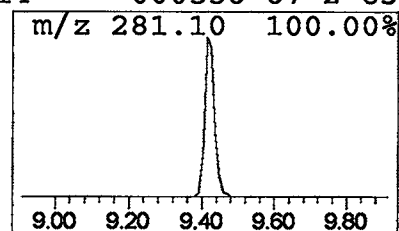
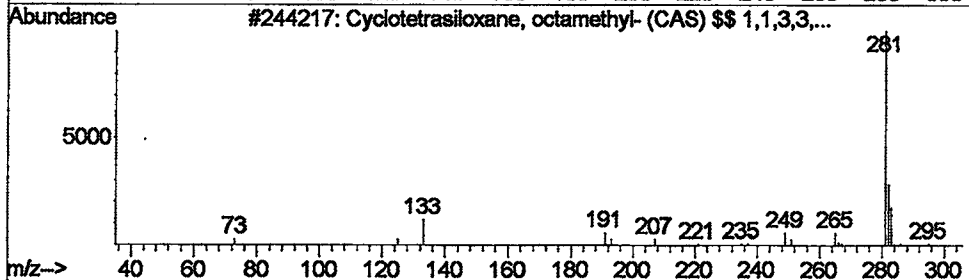
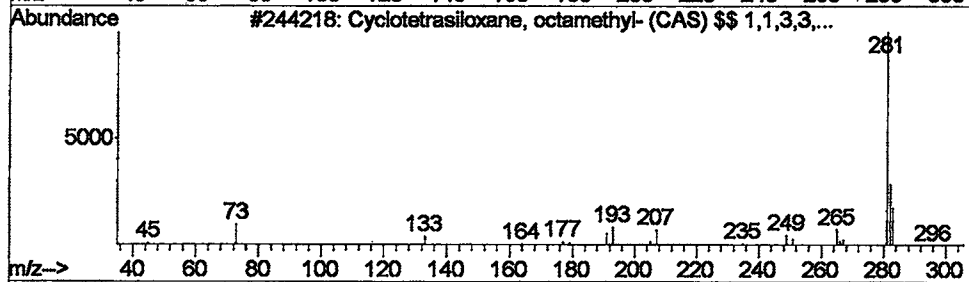
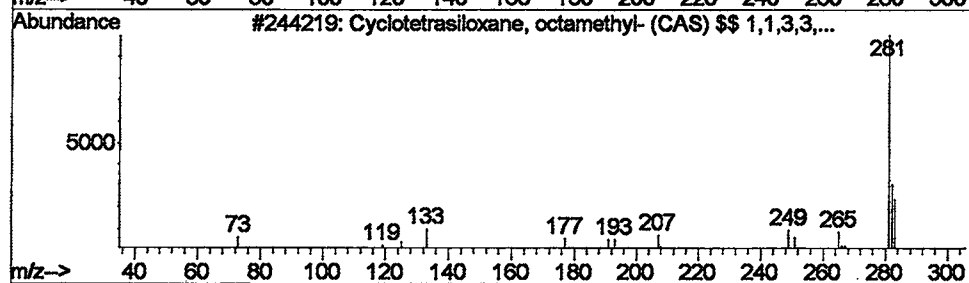
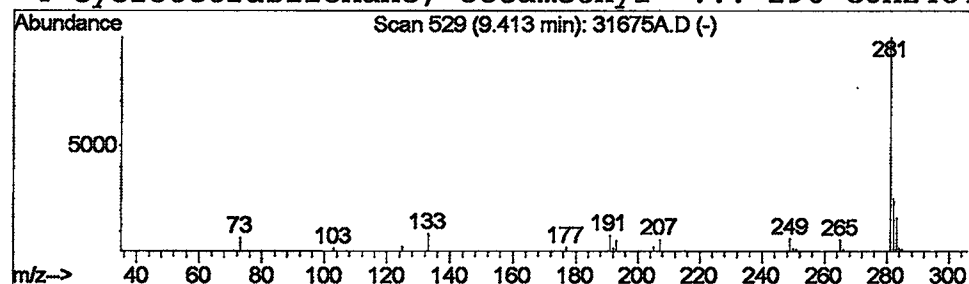
Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 3 Cyclotetrasiloxane, octamet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	0.30 ug/L	124919	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetrasiloxane, octamethyl- ...	296	C8H24O4Si4	000556-67-2	90
2	Cyclotetrasiloxane, octamethyl- ...	296	C8H24O4Si4	000556-67-2	86
3	Cyclotetrasiloxane, octamethyl- ...	296	C8H24O4Si4	000556-67-2	83
4	Cyclotetrasiloxane, octamethyl- ...	296	C8H24O4Si4	000556-67-2	83



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: LSCINT.P

Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

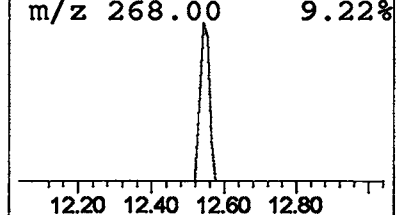
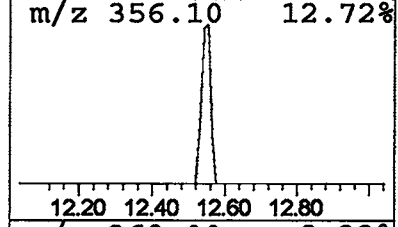
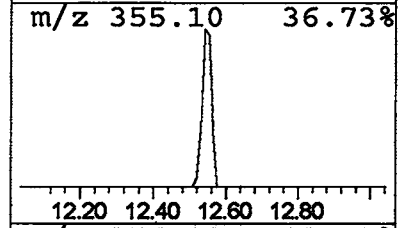
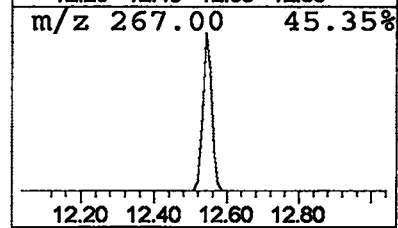
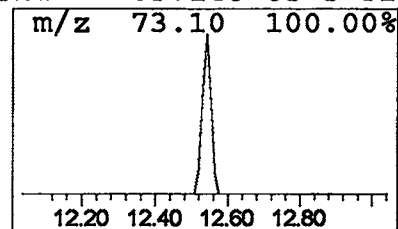
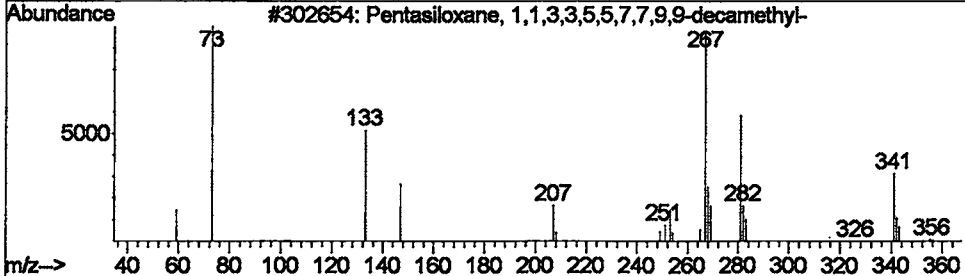
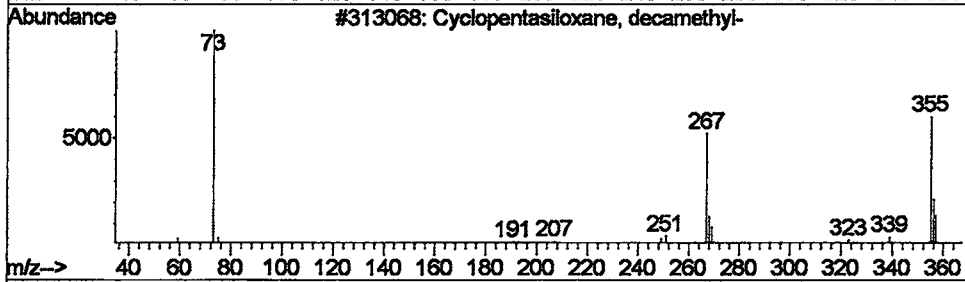
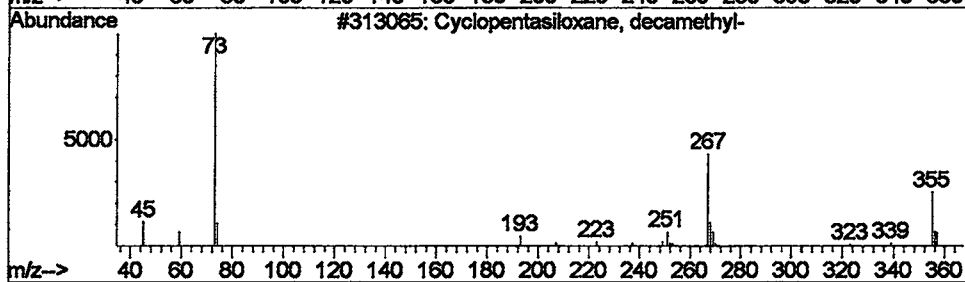
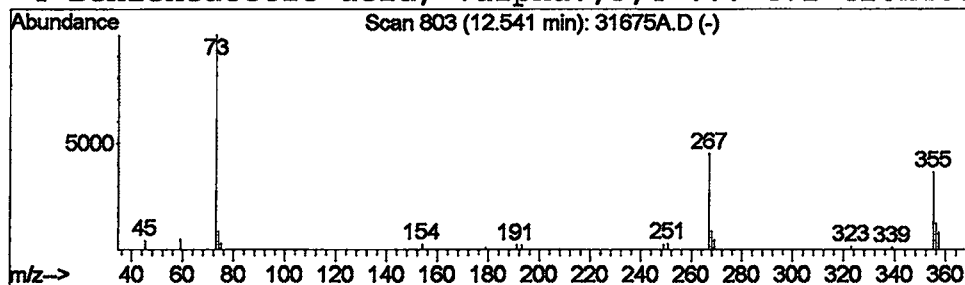
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 4 Cyclopentasiloxane, decamet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	0.22 ug/L	134458	Naphthalene-d8	13.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	64	
2	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	59	
3	Pentasiloxane, 1,1,3,3,5,5,7,7,9...	356	C10H32O4Si5	000995-83-5	40	
4	Benzeneacetic acid, .alpha.,3,4-...	472	C20H40O5Si4	037148-65-5	32	



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

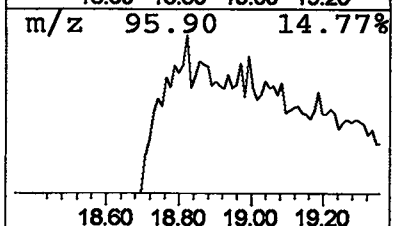
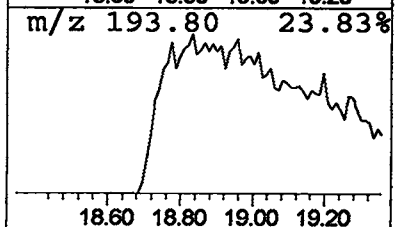
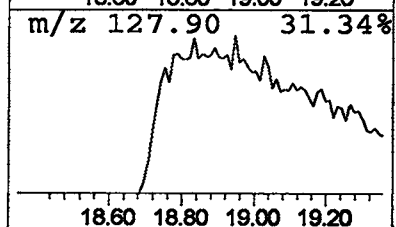
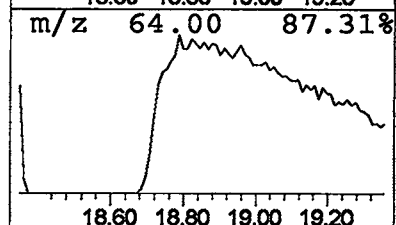
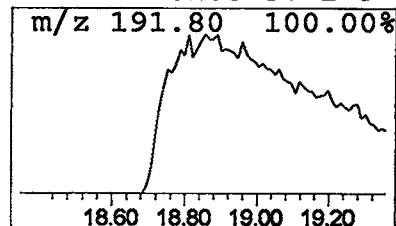
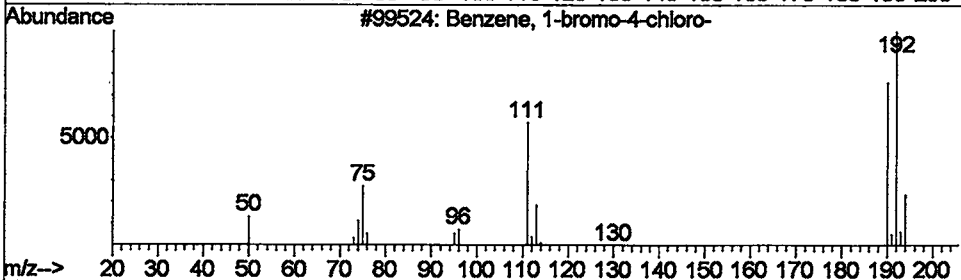
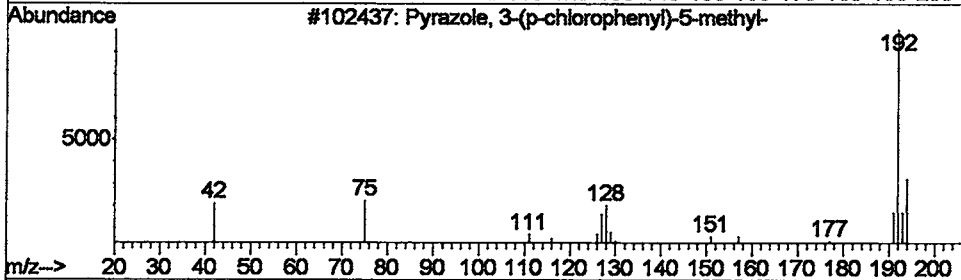
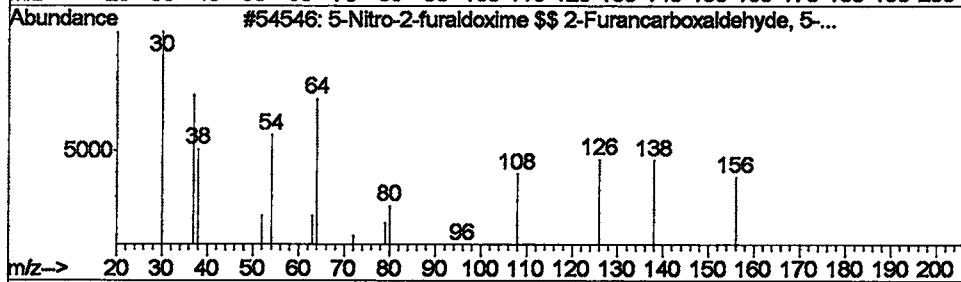
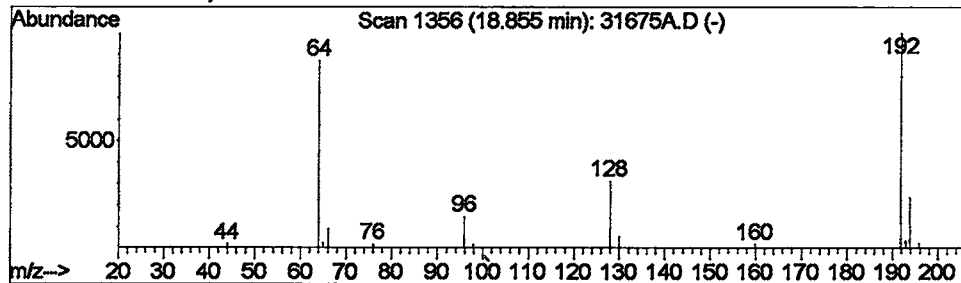
Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 5 5-Nitro-2-furaldoxime \$\$ 2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.85	1.73 ug/L	1121230	Acenaphthene-d10	18.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Nitro-2-furaldoxime \$\$ 2-Furan...	156	C5H4N2O4	000555-15-7	42
2		Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	9
3		Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	9
4		Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	9



NO
 GOOD
 MATCH

Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

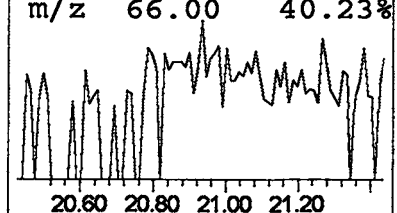
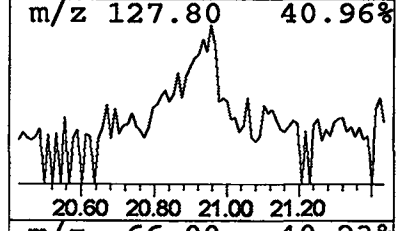
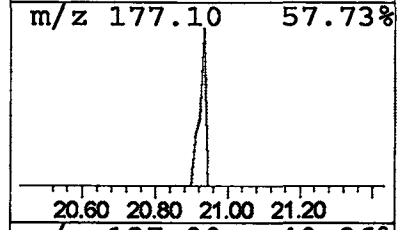
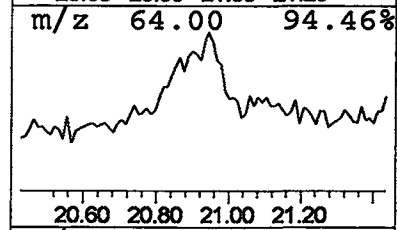
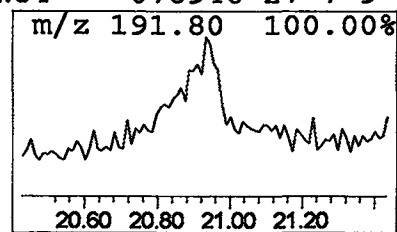
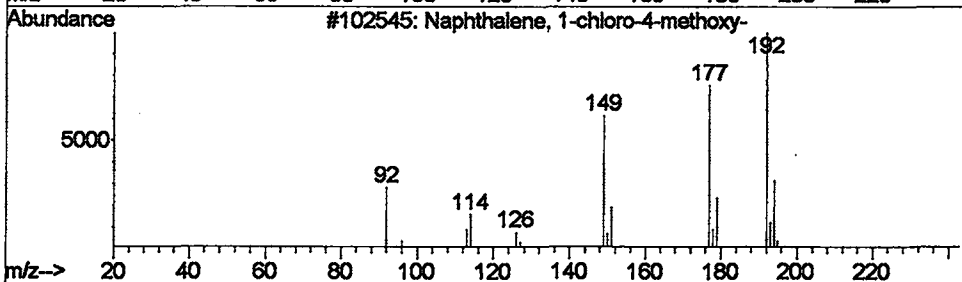
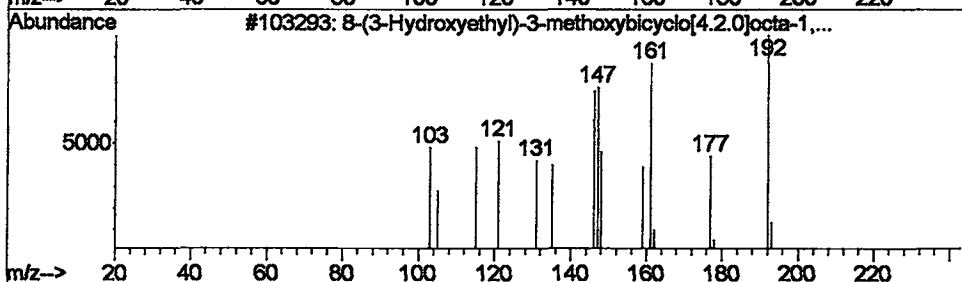
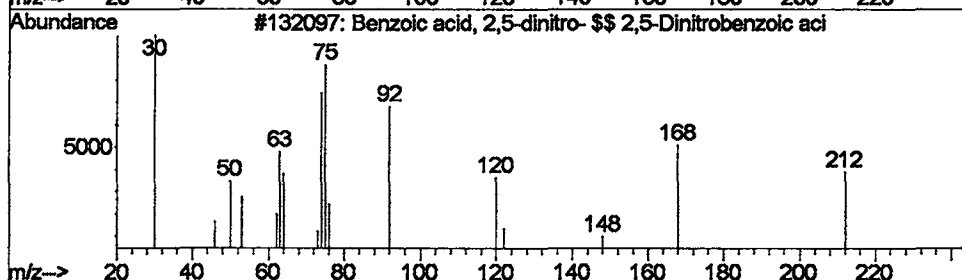
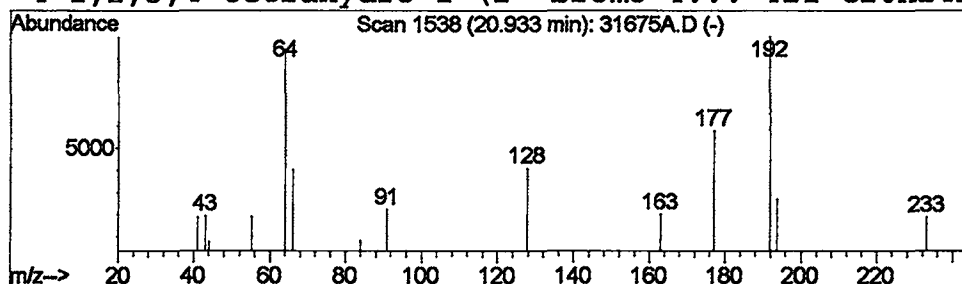
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 6 Benzoic acid, 2,5-dinitro- ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	0.12 ug/L	84607	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,5-dinitro- \$\$ 2,...	212	C7H4N2O6	000610-28-6	35
2			8-(3-Hydroxyethyl)-3-methoxybicy...	192	C12H16O2	000000-00-0	12
3			Naphthalene, 1-chloro-4-methoxy-	192	C11H9ClO	010443-43-3	10
4			1,2,3,4-tetrahydro-1-(2'-bromo-4...	421	C20H24BrNO4	078946-27-7	9

NO
 Gsm
 m/m/c



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

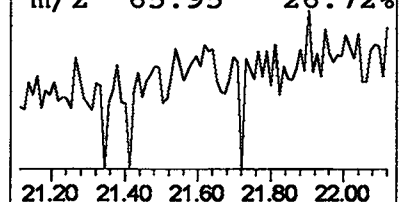
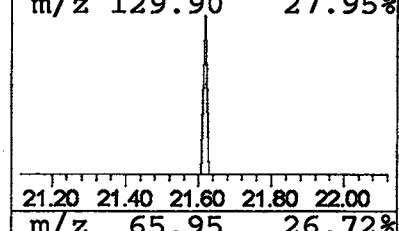
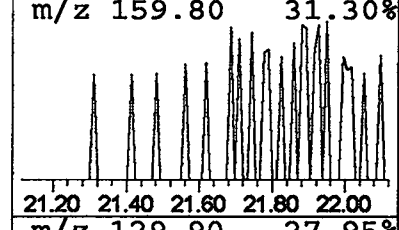
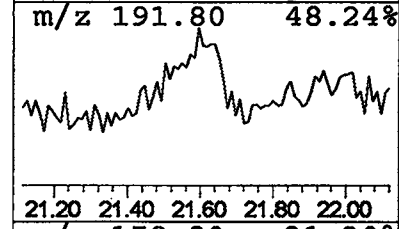
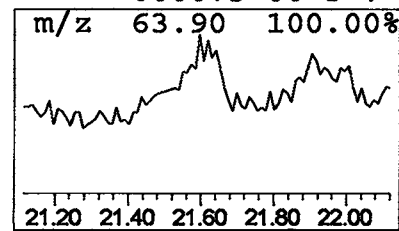
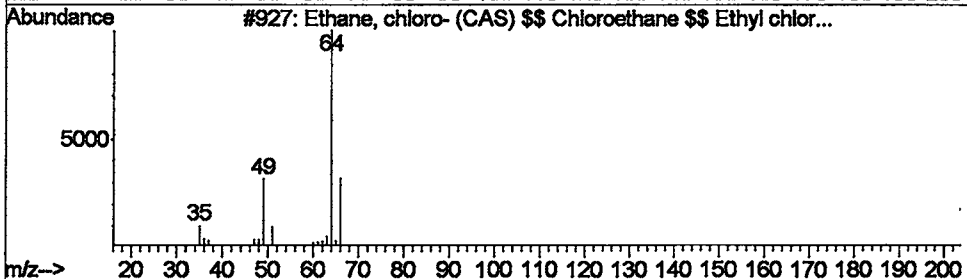
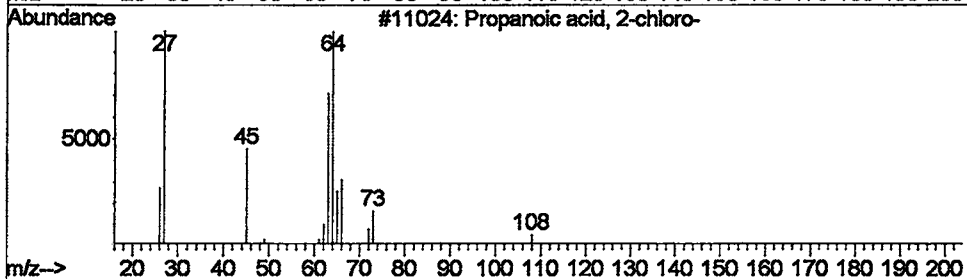
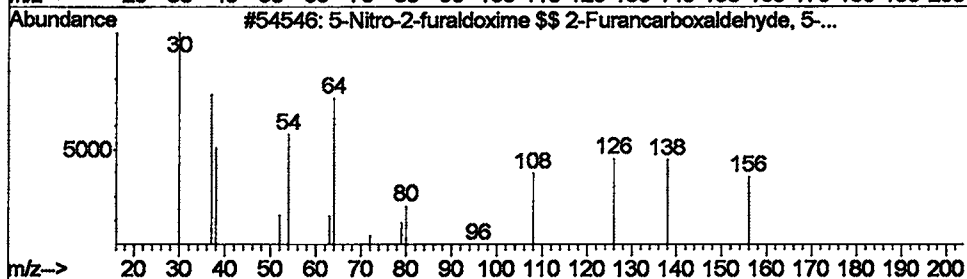
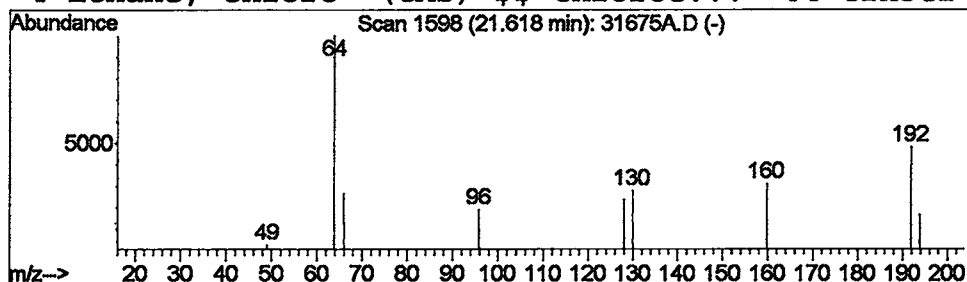
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 7 5-Nitro-2-furaldoxime \$\$ 2-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.62	0.10 ug/L	68310	Phenanthrene-d10	22.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Nitro-2-furaldoxime \$\$ 2-Furan...	156	C5H4N2O4	000555-15-7	40
2		Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	9
3		Ethane, chloro- (CAS) \$\$ Chloroe...	64	C2H5Cl	000075-00-3	7
4		Ethane, chloro- (CAS) \$\$ Chloroe...	64	C2H5Cl	000075-00-3	7

NO
 Good
 match



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

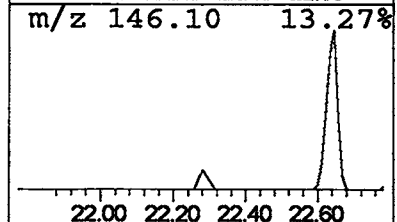
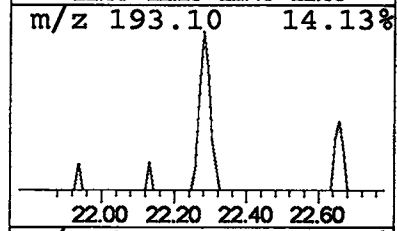
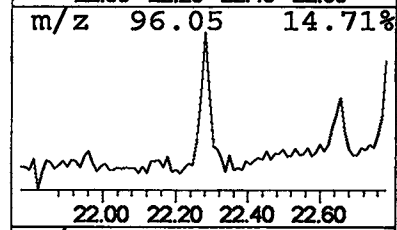
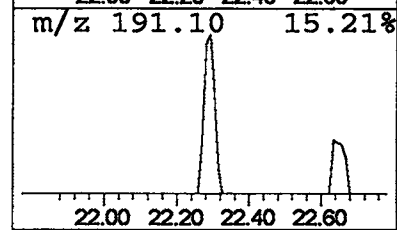
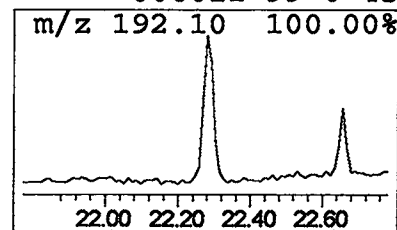
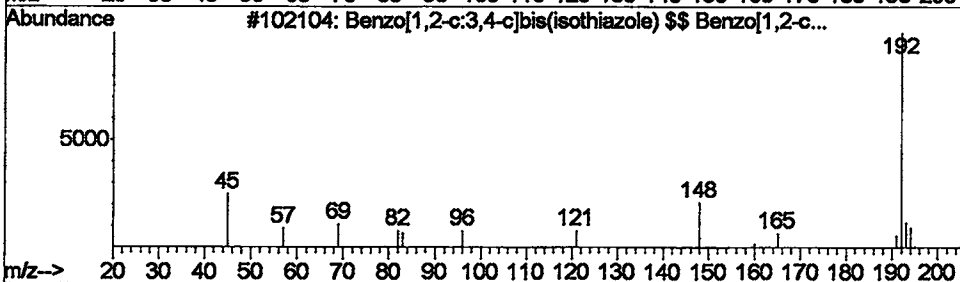
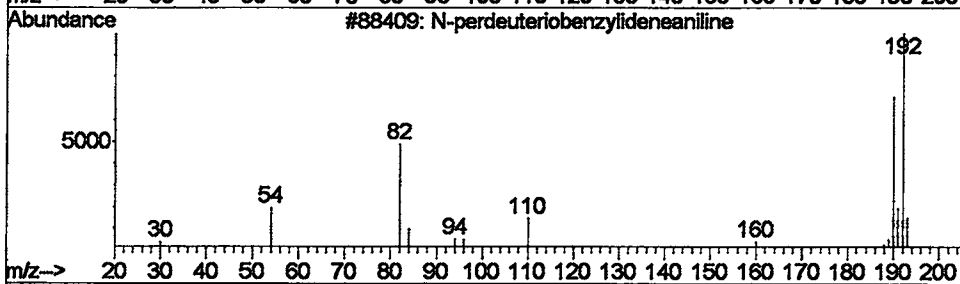
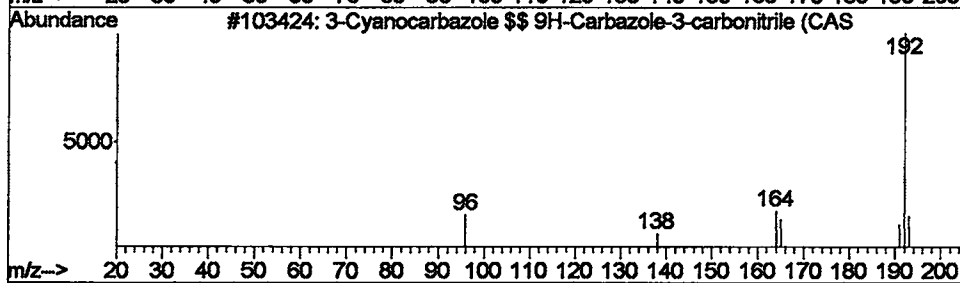
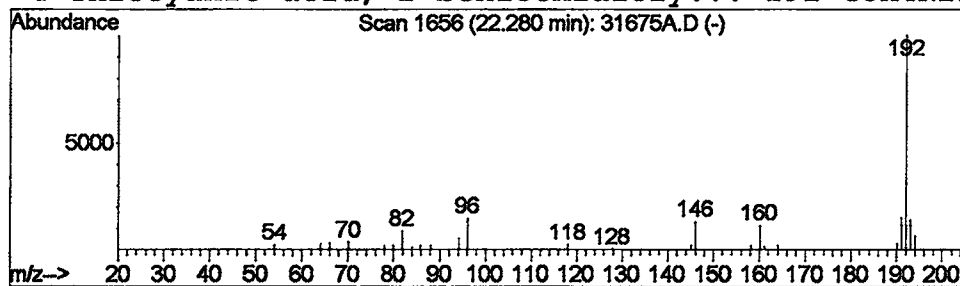
Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 8 3-Cyanocarbazole \$\$ 9H-Carb... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.17 ug/L	117825	Phenanthrene-d10	22.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	64	
2	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	59	
3	Benzo[1,2-c:3,4-c]bis(isothiazol...	192	C8H4N2S2	074960-05-7	45	
4	Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	45	



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: LSCINT.P

Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

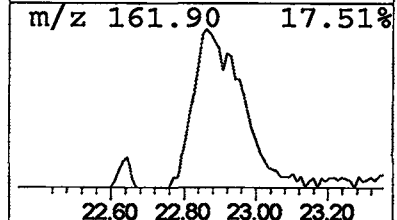
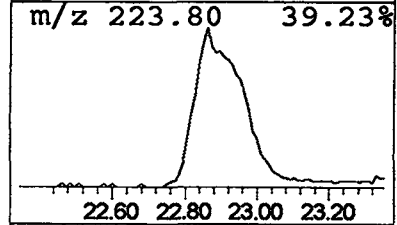
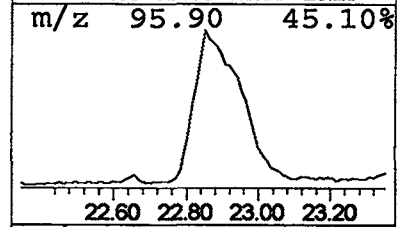
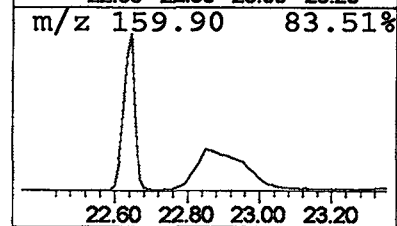
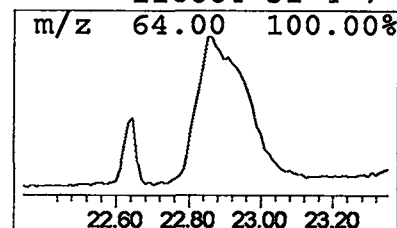
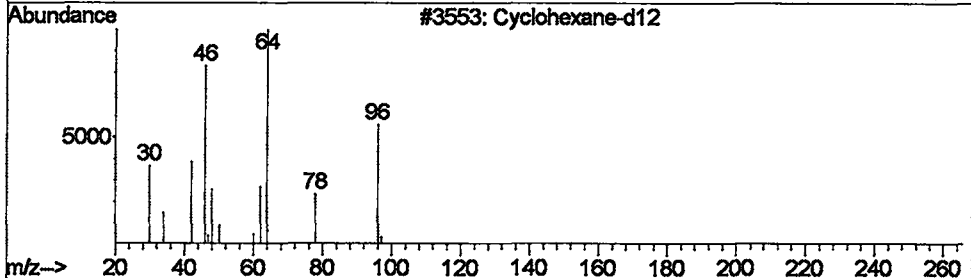
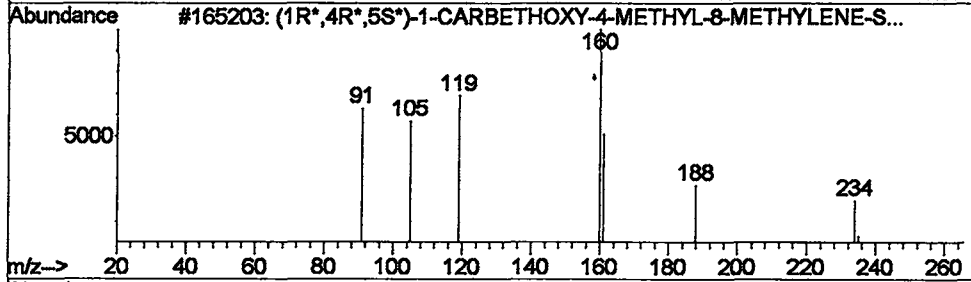
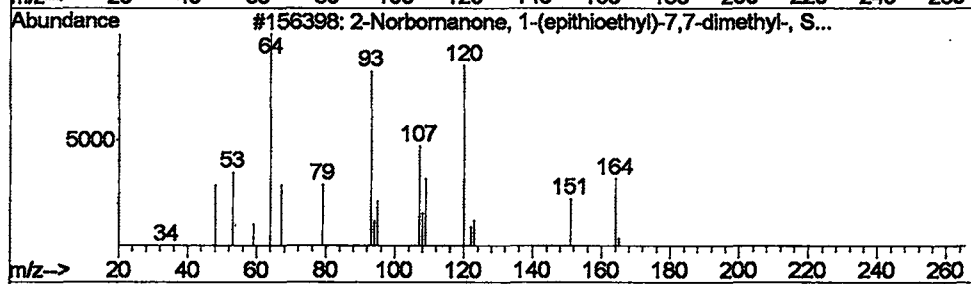
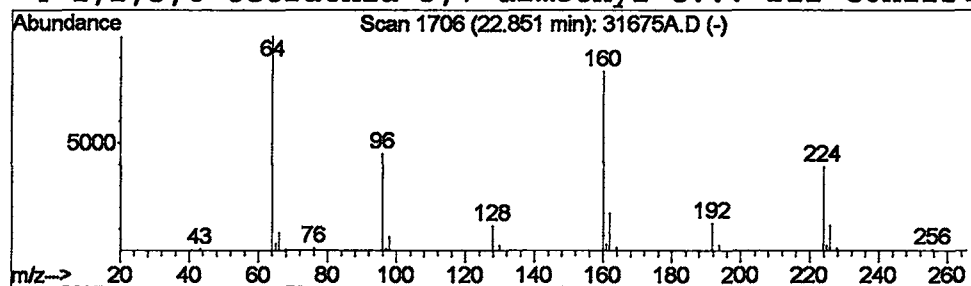
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 9 2-Norbornanone, 1-(epithioe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.85	3.73 ug/L	2594030	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	28
2			(1R*,4R*,5S*)-1-CARBETHOXY-4-MET...	234	C15H22O2	043219-76-7	9
3			Cyclohexane-d12	96	C6D12	001735-17-7	7
4			1,2,5,6-tetrathia-3,7-dimethyl-c...	212	C6H12S4	116664-31-4	7



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Acq On : 24 Jan 2002 12:31 pm
 Sample : 508scan; re-inj
 Misc : January 24, 2002
 MS Integration Params: LSCINT.P

Vial: 2
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

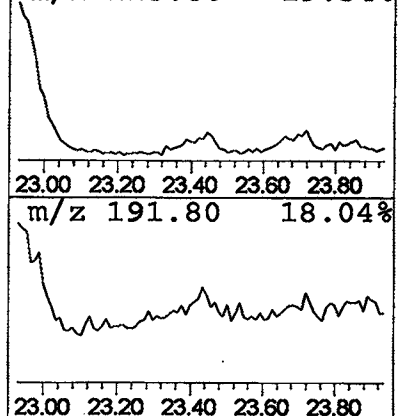
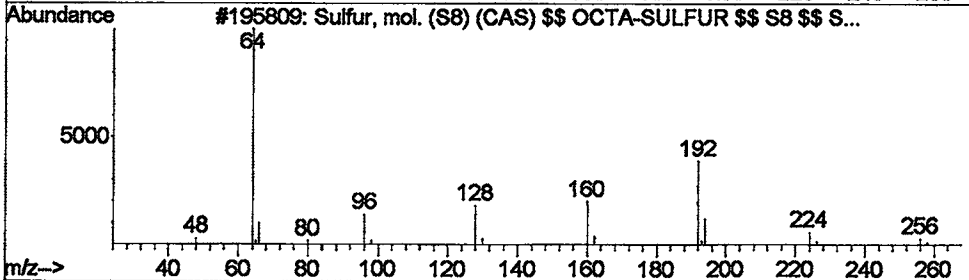
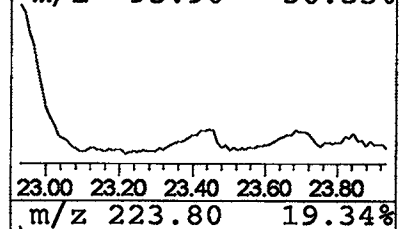
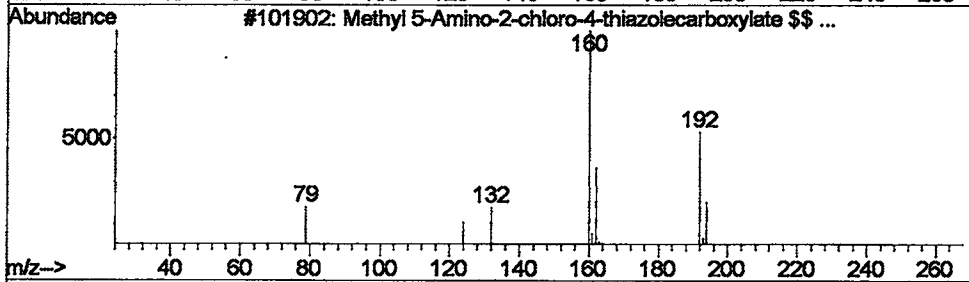
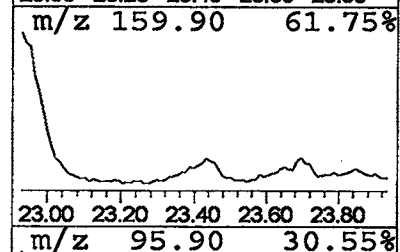
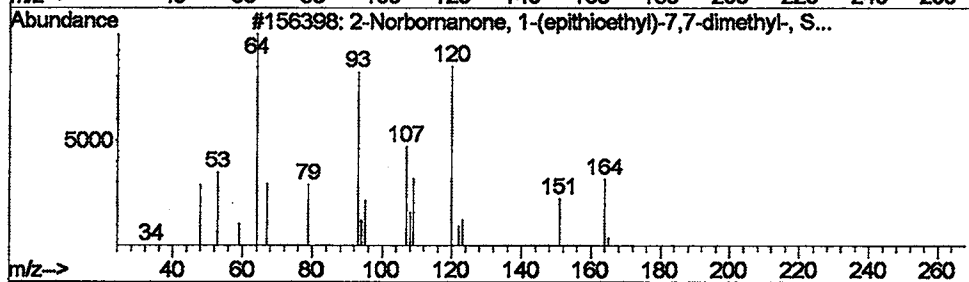
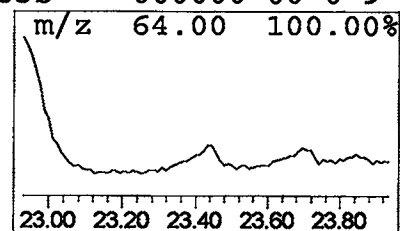
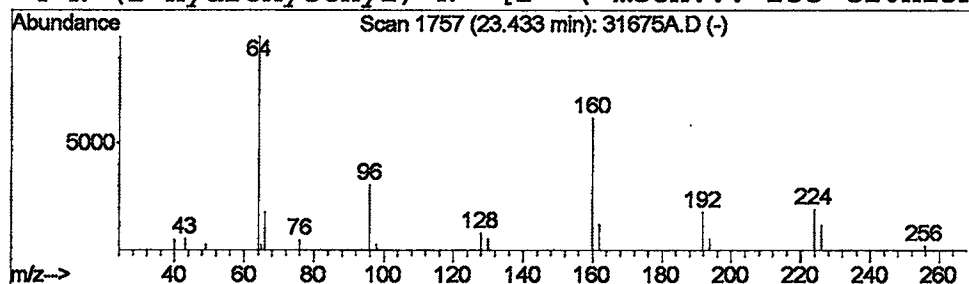
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 10 2-Norbornanone, 1-(epithioe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.43	0.25 ug/L	176620	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	36
2	Methyl 5-Amino-2-chloro-4-thiazo...	192	C5H5ClN2O2S	000000-00-0	9
3	Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	9
4	N-(2-Hydroxyethyl)-N'-[2'-(-meth...	255	C10H13N3O3S	000000-00-0	9

NO
 GOOD
 MATCH



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: LSCINT.P

Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

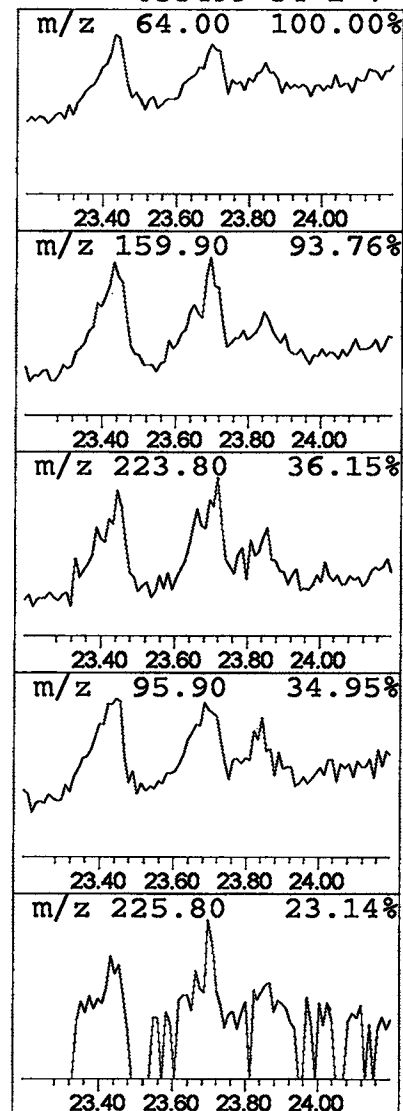
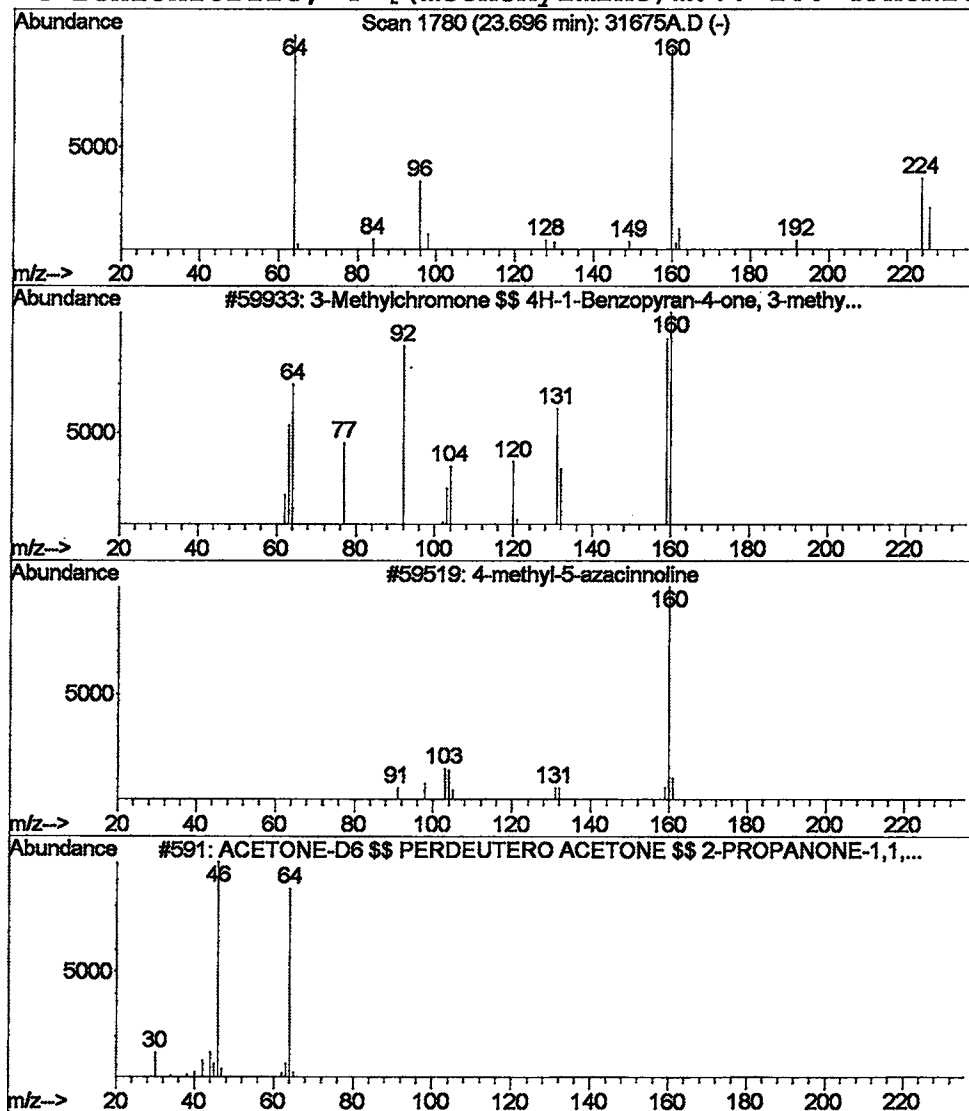
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

Peak Number 11 3-Methylchromone \$\$ 4H-1-Be... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.70	0.22 ug/L	149615	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylchromone \$\$ 4H-1-Benzopy...	160	C10H8O2	000085-90-5	50
2			4-methyl-5-azacinnoline	160	C8H8N4	000000-00-0	7
3			ACETONE-D6 \$\$ PERDEUTERO ACETONE...	64	C3D6O	000666-52-4	7
4			Benzonitrile, 4-[(methoxyimino)m...	160	C9H8N2O	033499-34-2	7

NO
GOOD
MATCH



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN24\31675A.D
Acq On : 24 Jan 2002 12:31 pm
Sample : 508scan; re-inj
Misc : January 24, 2002
MS Integration Params: LSCINT.P

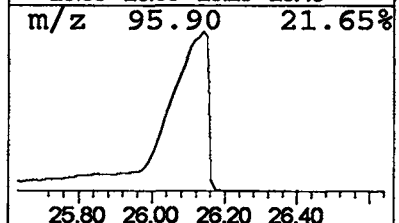
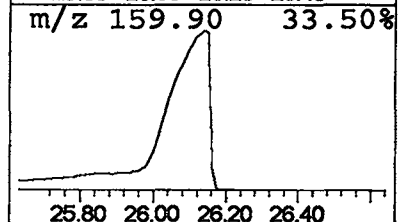
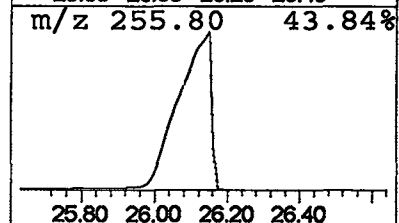
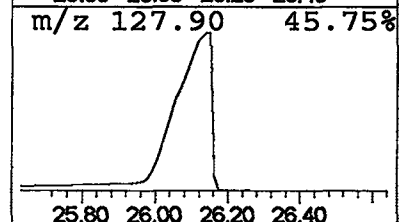
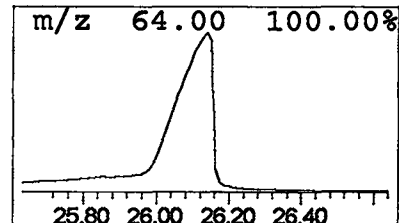
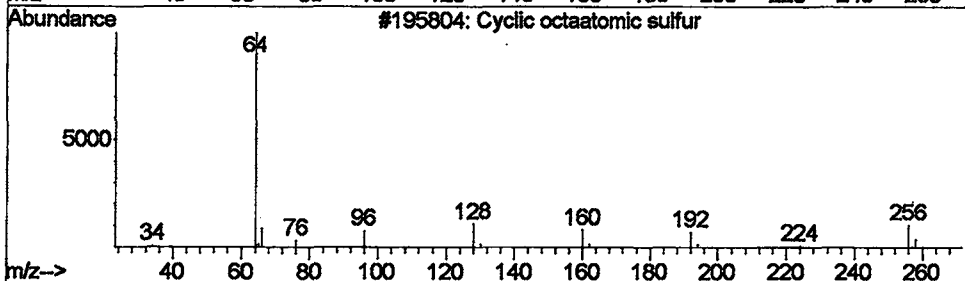
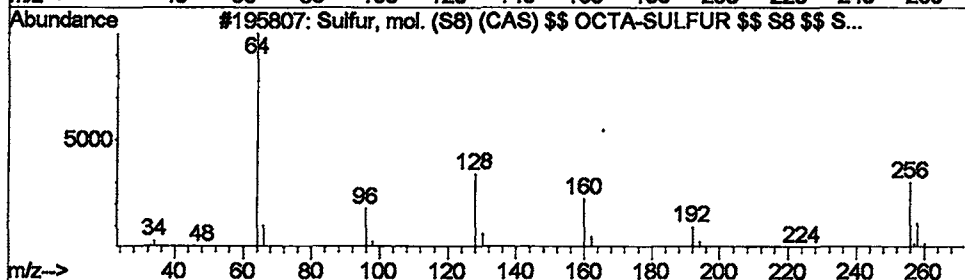
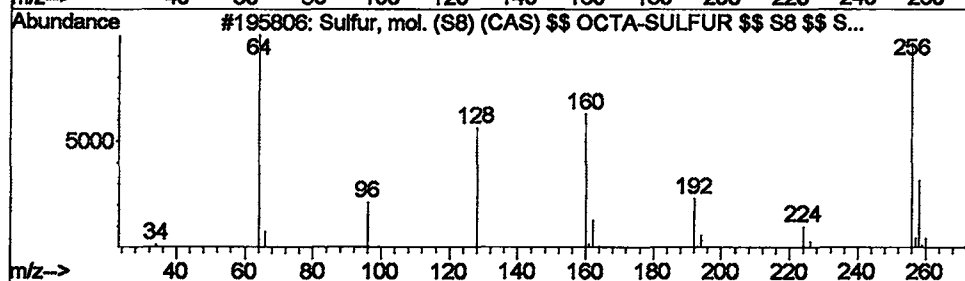
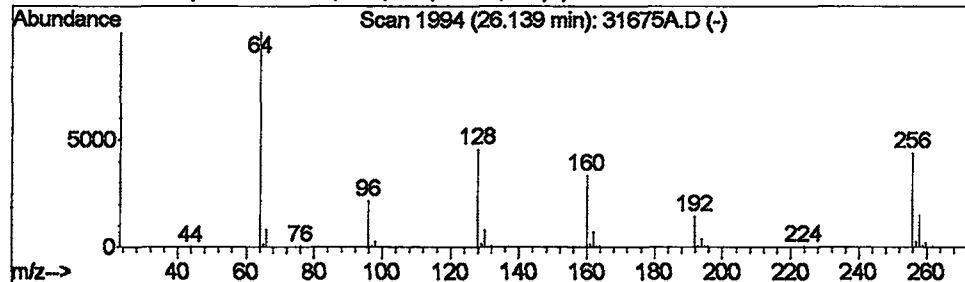
Vial: 2
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

Peak Number 12 Sulfur, mol. (S8) (CAS) \$\$... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.14	78.57 ug/L	54671100	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur, mol. (S8) (CAS) \$\$	OCTA-...	256	S8	010544-50-0	96	
2	Sulfur, mol. (S8) (CAS) \$\$	OCTA-...	256	S8	010544-50-0	95	
3	Cyclic octaatomic sulfur		256	S8	010544-50-0	91	
4	Sulfur, mol. (S8) (CAS) \$\$	OCTA-...	256	S8	010544-50-0	90	



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 24 Jan 2002 12:31 pm
 Data File: C:\MSDCHEM\1\5973N\02JAN24\31675A.D
 Name: 508scan; re-inj
 Misc: January 24, 2002
 Method: C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
 Title: 508 scan method
 Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard---			
					#	RT	Resp	Conc
Butanoic acid, me...	3.61	0.2	ug/L	67677	1	9.72	8362920	20.0
Methadrylamide \$\$...	4.25	0.1	ug/L	59657	1	9.72	8362920	20.0
Cyclotetrasiloxan...	9.41	0.3	ug/L	124919	1	9.72	8362920	20.0
Cyclopentasiloxan...	12.54	0.2	ug/L	134458	2	13.19	11972900	20.0
5-Nitro-2-furaldo...	18.85	1.7	ug/L	1121230	3	18.34	12997100	20.0
Benzoic acid, 2,5...	20.93	0.1	ug/L	84607	4	22.65	13917000	20.0
5-Nitro-2-furaldo...	21.62	0.1	ug/L	68310	4	22.65	13917000	20.0
3-Cyanocarbazole ...	22.28	0.2	ug/L	117825	4	22.65	13917000	20.0
2-Norbornanone, 1...	22.85	3.7	ug/L	2594030	4	22.65	13917000	20.0
2-Norbornanone, 1...	23.43	0.3	ug/L	176620	4	22.65	13917000	20.0
3-Methylchromone ...	23.70	0.2	ug/L	149615	4	22.65	13917000	20.0
Sulfur, mol. (S8)...	26.14	78.6	ug/L	54671100	4	22.65	13917000	20.0