

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/25/2002 Time: 15:39:07

Sample: AD31676
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/25/02 15:38 Ended: 1/25/02 15:38 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		101		5.0

Comments for Sample AD31676 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-25-2002 Time: 15:39:36

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\02JAN23\31676.D Vial: 1
Acq On : 23 Jan 2002 2:57 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 24 09:46:44 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	1145052	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	4804374	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2506845	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4228254	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	3728391	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	2727593	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	337138	5.04	ug/L	0.00
Spiked Amount	5.000		Recovery	=	100.80%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	404481	2.44	ug/L	# 56
21) 2,6-Dinitrotoluene	18.34	165	320043	9.91	ug/L	# 17
35) Di-n-butylphthalate	24.86	149	185629	0.68	ug/L	100

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

31676.D SCAN508.M Thu Jan 24 09:46:45 2002

Page 1

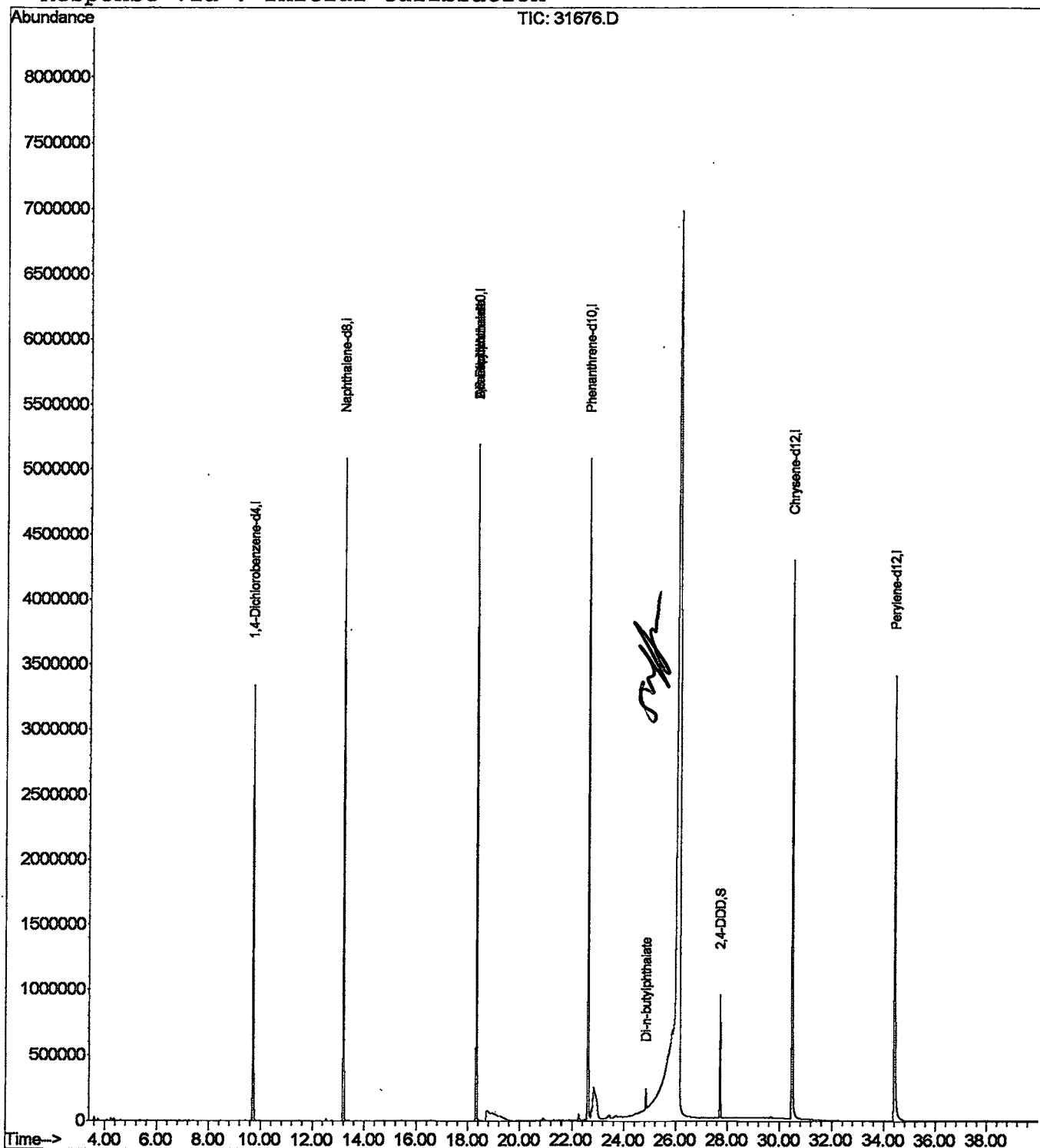
Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
 Acq On : 23 Jan 2002 2:57 pm
 Sample : 508 scan
 Misc : January 22, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 24 9:46 2002

Vial: 1
 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\02JAN23\31676.D
 Acq On : 23 Jan 2002 2:57 pm
 Sample : 508 scan
 Misc : January 22, 2002
 MS Integration Params: LSCINT.P

Vial: 1
 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

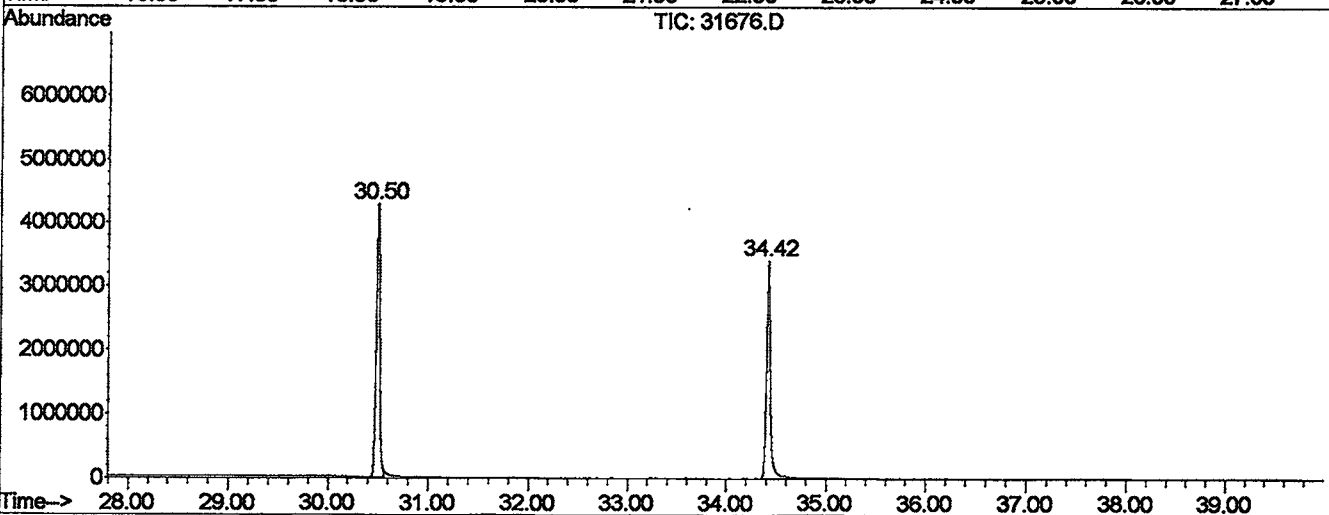
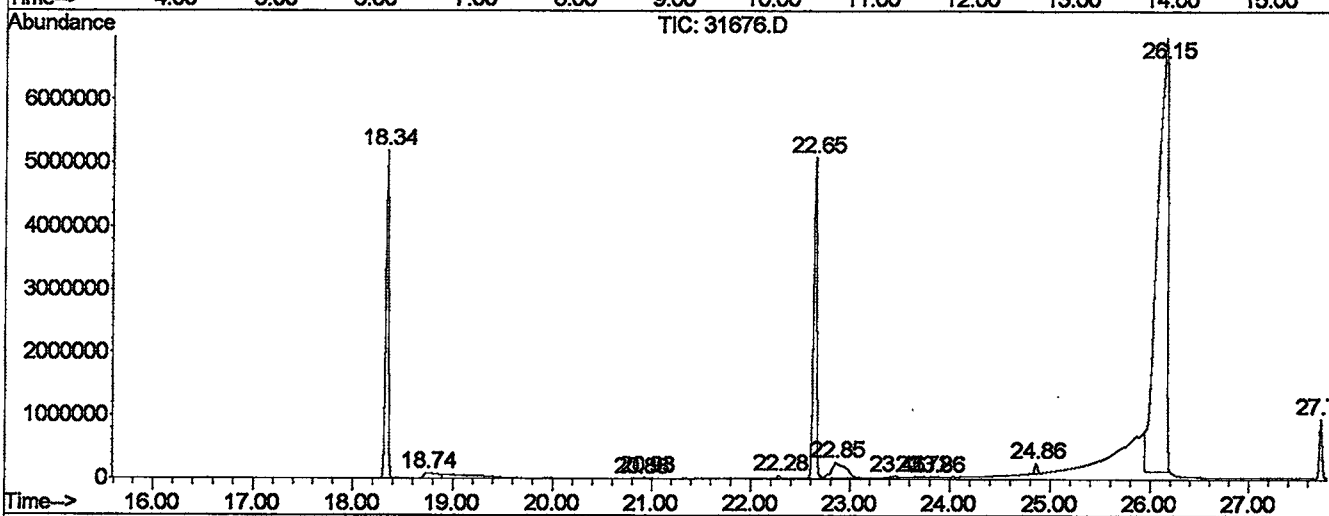
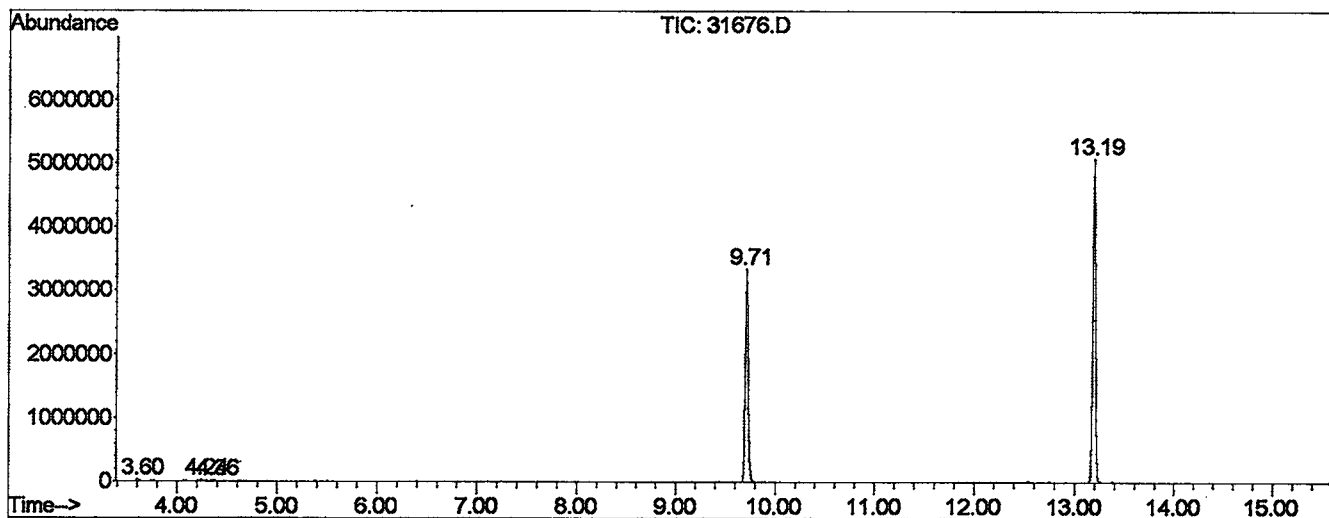
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.602	17	20	25	rVB	27595	46464	0.09%	0.041%
2	4.241	71	76	83	rBV2	21958	52492	0.10%	0.046%
3	4.355	83	86	93	rVB2	16634	35102	0.07%	0.031%
4	9.710	551	555	561	rBV	3335528	6499486	12.96%	5.733%
5	13.192	855	860	865	rBV	5083718	9284727	18.51%	8.189%
6	18.341	1305	1311	1315	rBV	5190169	10223558	20.39%	9.018%
7	18.741	1339	1346	1359	rBV2	80095	784065	1.56%	0.692%
8	20.876	1519	1533	1535	rBV3	5134	33547	0.07%	0.030%
9	20.933	1535	1538	1547	rVV4	19459	59019	0.12%	0.052%
10	22.280	1651	1656	1661	rBV2	45446	84060	0.17%	0.074%
11	22.645	1681	1688	1693	rBV	5074161	11262647	22.46%	9.934%
12	22.851	1695	1706	1731	rVB2	243657	2444024	4.87%	2.156%
13	23.456	1745	1759	1763	rBV5	27851	167872	0.33%	0.148%
14	23.719	1775	1782	1787	rVB4	14440	67028	0.13%	0.059%
15	23.856	1787	1794	1799	rBV6	8514	41686	0.08%	0.037%
16	24.860	1877	1882	1887	rBV	163088	346528	0.69%	0.306%
17	26.150	1977	1995	1999	rVB2	6849919	50149481	100.00%	44.234%
18	27.726	2129	2133	2139	rBV	938932	1685195	3.36%	1.486%
19	30.500	2369	2376	2381	rBV	4286067	10817845	21.57%	9.542%
20	34.416	2713	2719	2755	rBV	3409452	9289600	18.52%	8.194%

Sum of corrected areas: 113374426

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
 Operator :
 Acquired : 23 Jan 2002 2:57 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 22, 2002
 Vial Number: 1
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

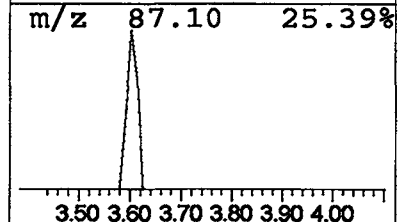
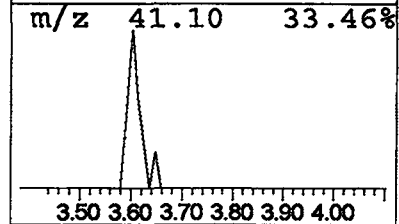
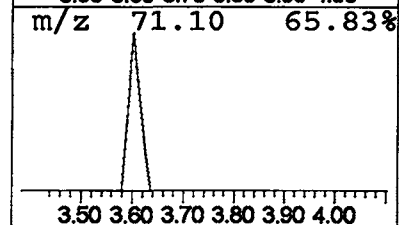
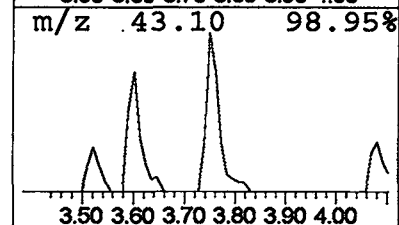
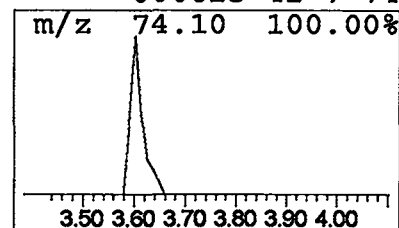
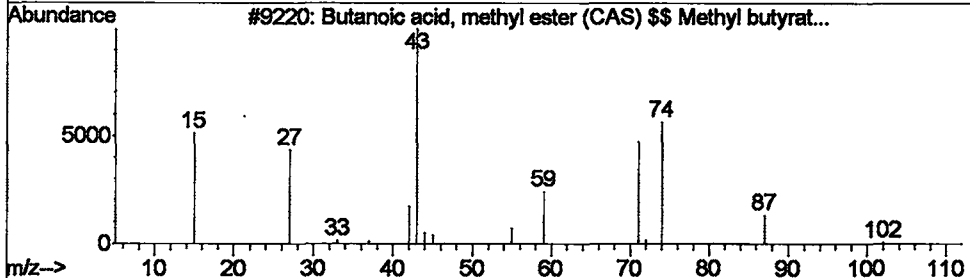
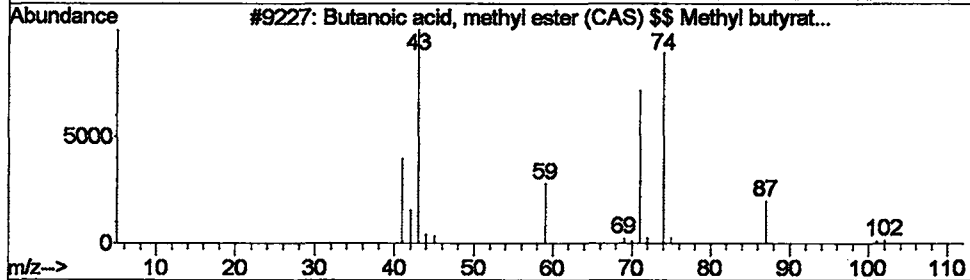
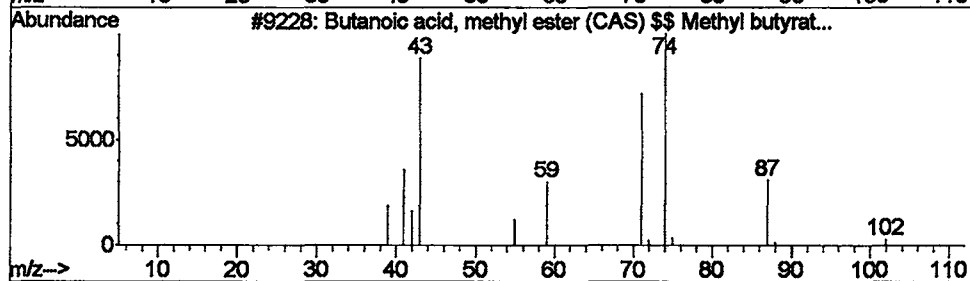
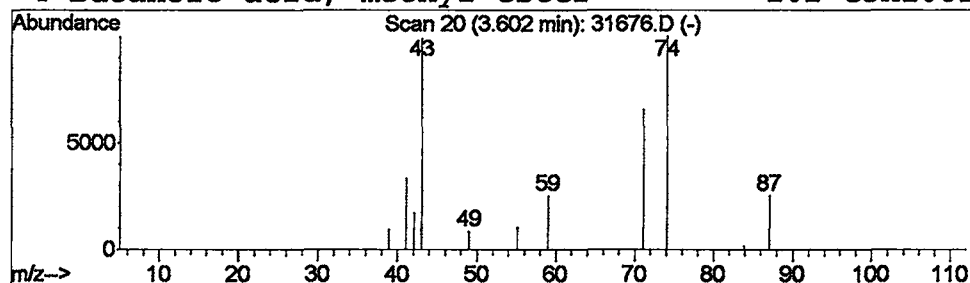
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.14 ug/L	46464	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
2			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
3			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	74



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

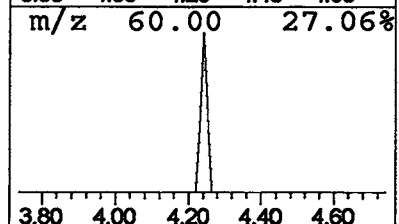
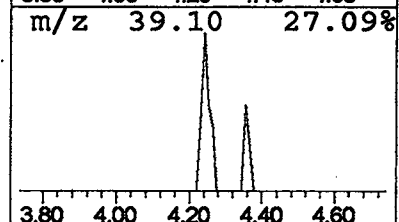
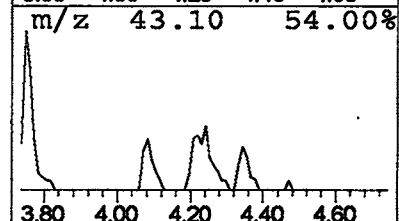
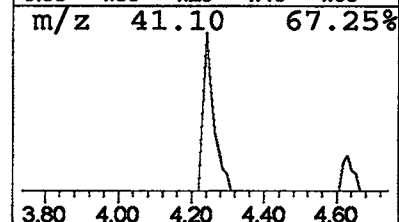
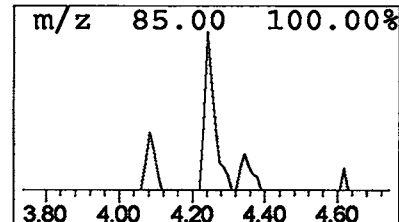
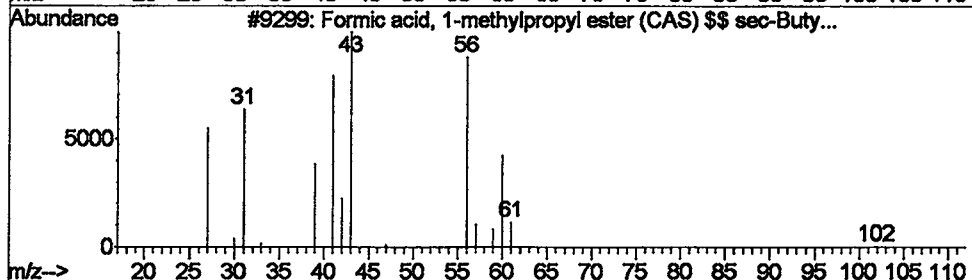
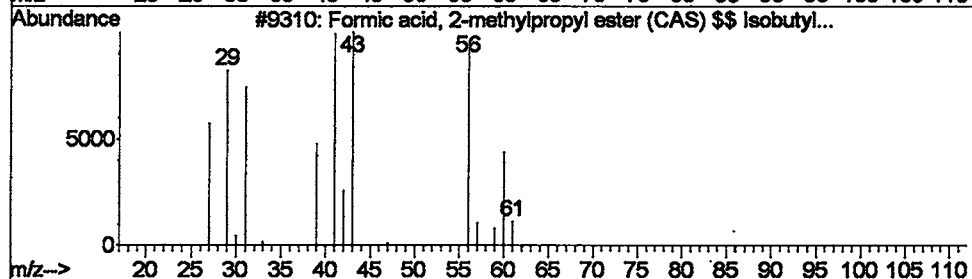
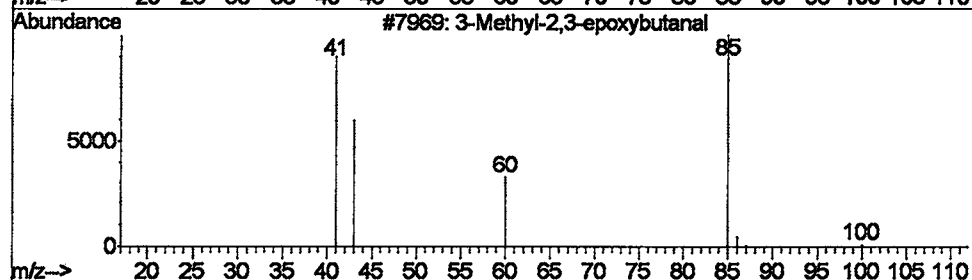
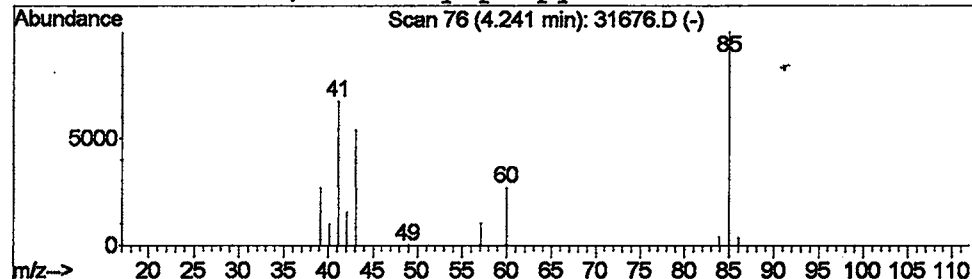
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 2 3-Methyl-2,3-epoxybutanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.16 ug/L	52492	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-2,3-epoxybutanal	100	C5H8O2	000000-00-0	39
2			Formic acid, 2-methylpropyl este...	102	C5H10O2	000542-55-2	22
3			Formic acid, 1-methylpropyl este...	102	C5H10O2	000589-40-2	10
4			Formic acid, 2-methylpropyl este...	102	C5H10O2	000542-55-2	10



Library Search Compound Report

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Acq On : 23 Jan 2002 2:57 pm

Sample : 508 scan

Misc : January 22, 2002

MS Integration Params: LSCINT.P

Vial: 1

Operator:

Inst : Instrumen

Multiplr: 1.00

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

Title : 508 scan method

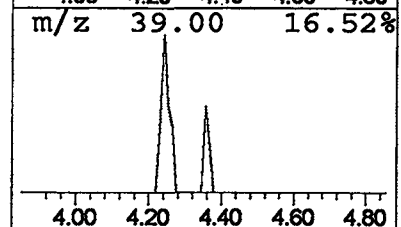
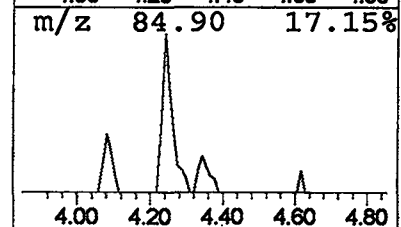
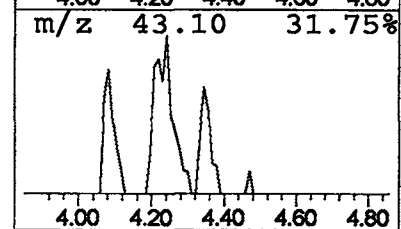
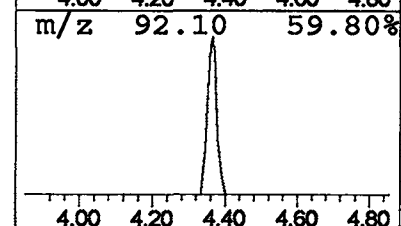
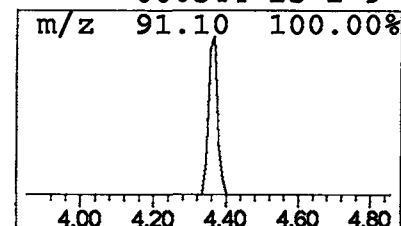
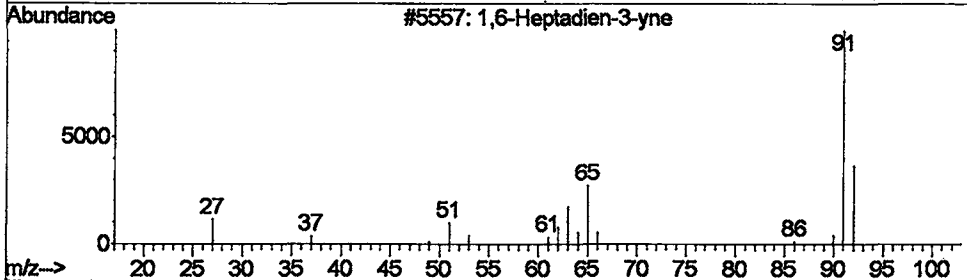
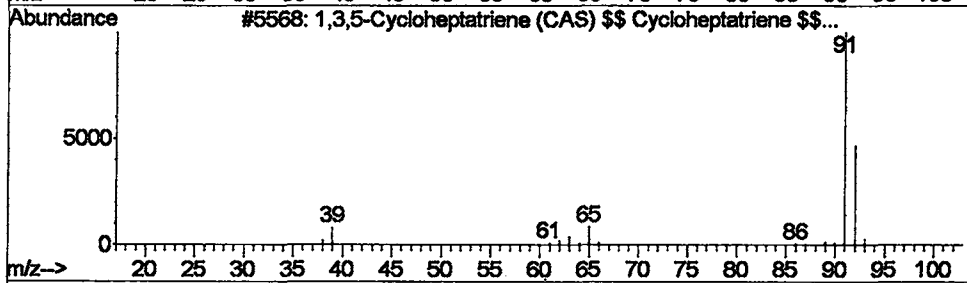
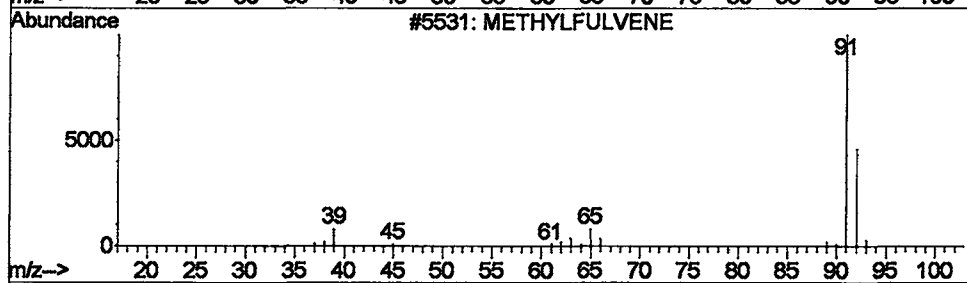
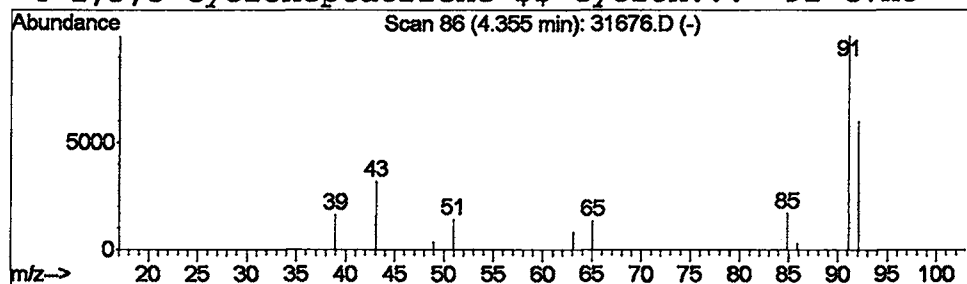
Library : C:\DATABASE\WILEY7N.L

Peak Number 3 METHYLFULVENE

Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	0.11 ug/L	35102	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			METHYLFULVENE	92	C7H8	000000-00-0	42
2			1,3,5-Cycloheptatriene (CAS) \$\$...	92	C7H8	000544-25-2	42
3			1,6-Heptadien-3-yne	92	C7H8	005150-80-1	9
4			1,3,5-Cycloheptatriene \$\$ Cycloh...	92	C7H8	000544-25-2	9



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MS Integration Params: LSCINT.P

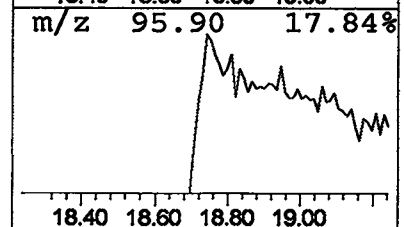
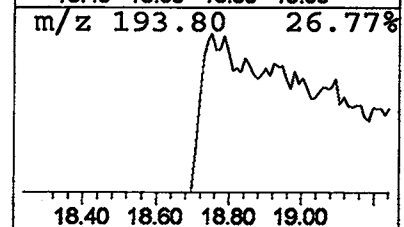
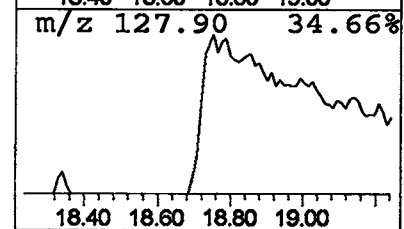
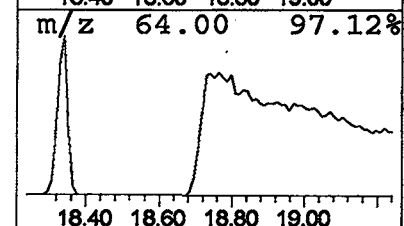
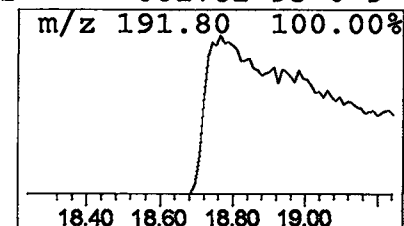
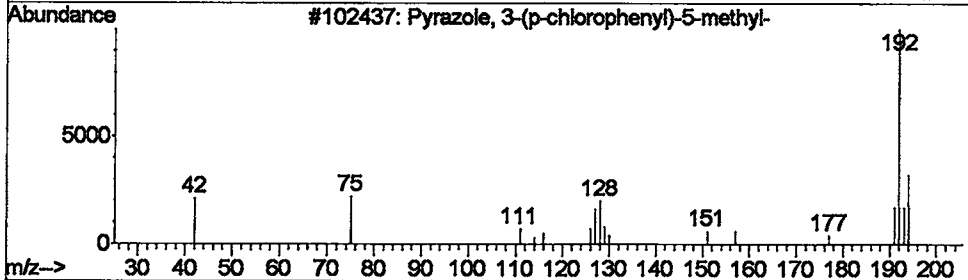
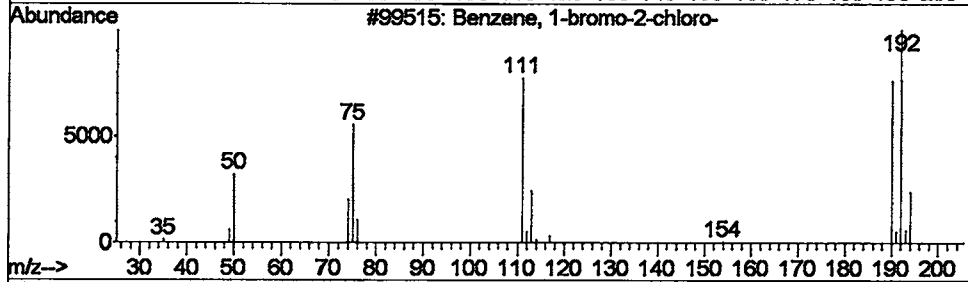
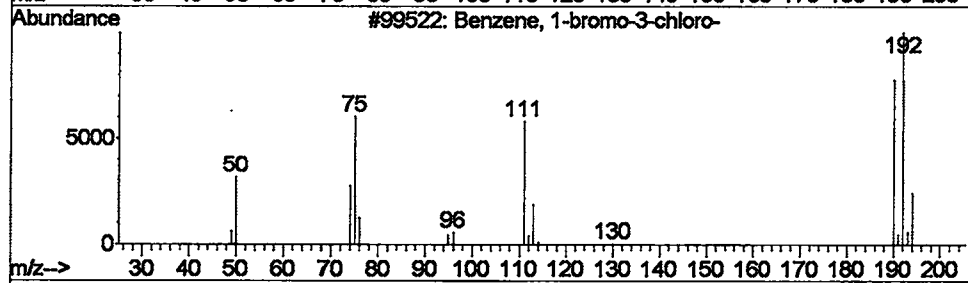
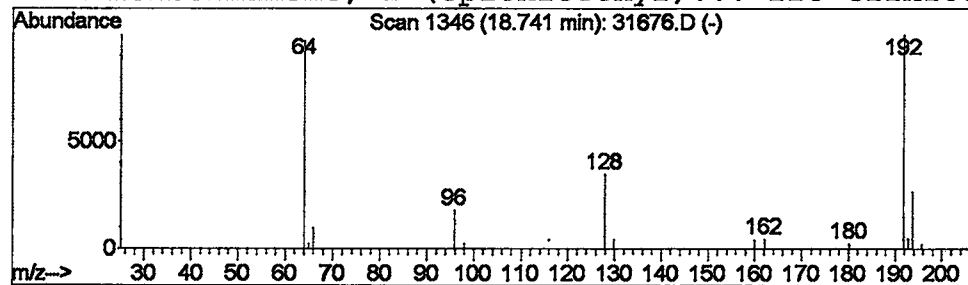
Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 Benzene, 1-bromo-3-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	1.53 ug/L	784065	Acenaphthene-d10	18.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	9
2			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	9
3			Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	9
4			2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	9



Library Search Compound Report

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Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

Vial: 1
Operator:
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Multiplr: 1.00

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

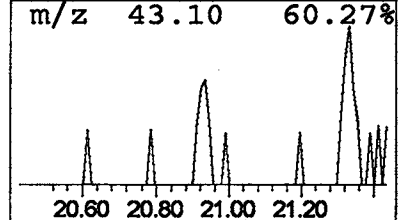
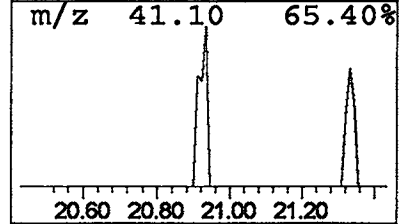
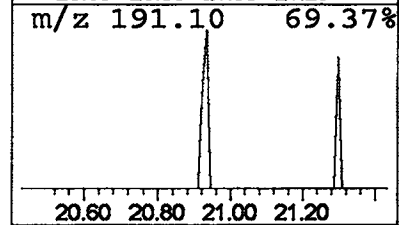
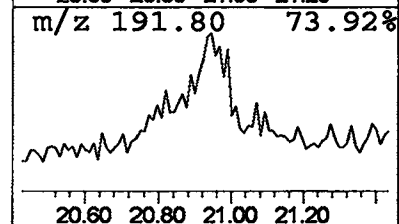
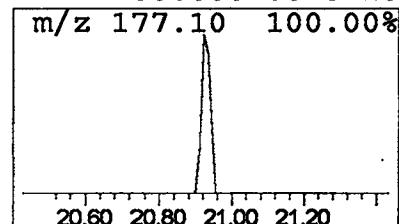
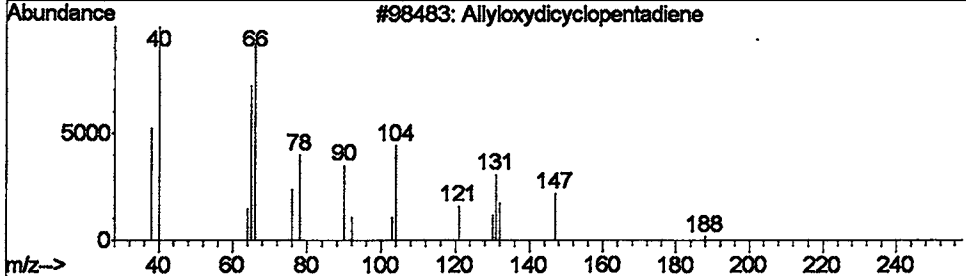
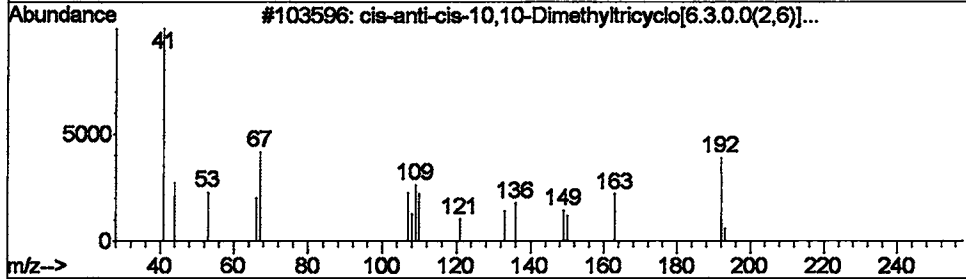
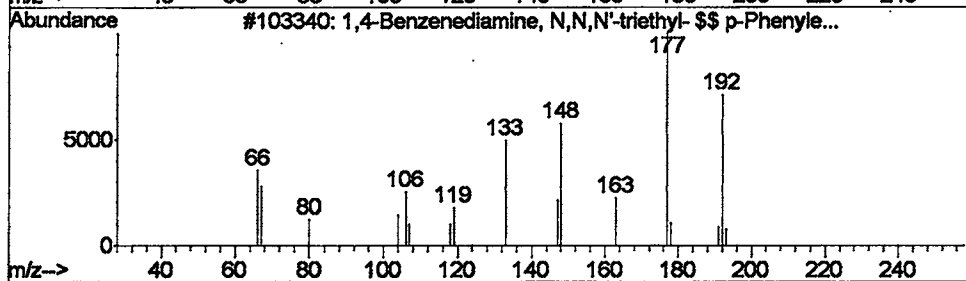
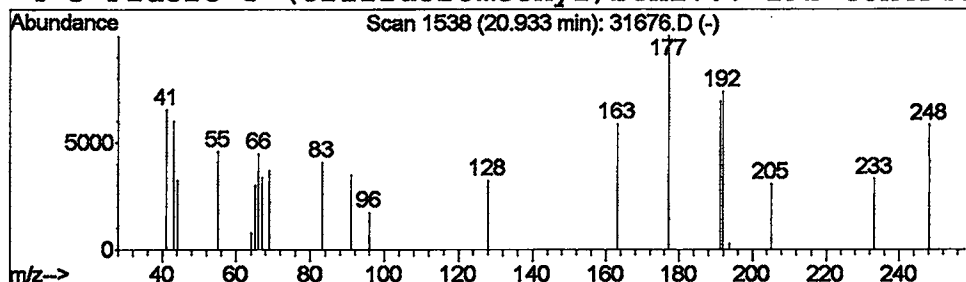
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 5 1,4-Benzenediamine, N,N,N'-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	0.10 ug/L	59019	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenediamine, N,N,N'-trieth...	192	C12H20N2	024340-91-8	47
2			cis-anti-cis-10,10-Dimethyltricy...	192	C13H20O	000000-00-0	23
3			Allyloxydicyclopentadiene	188	C13H16O	000000-00-0	10
4			3-Fluoro-5-(trifluoromethyl)benz...	192	C8H4F4O	000000-00-0	10



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

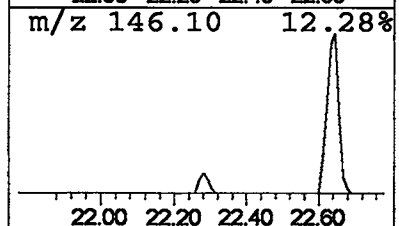
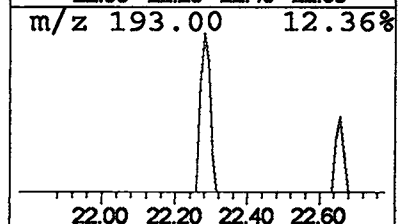
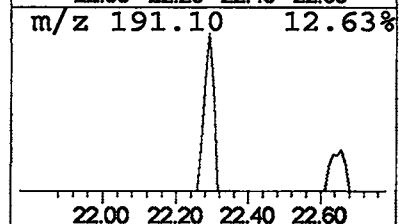
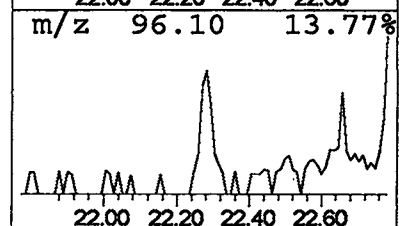
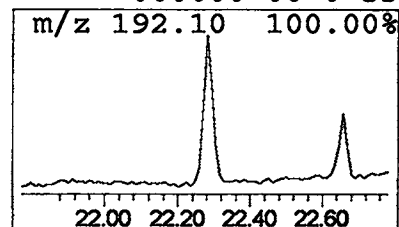
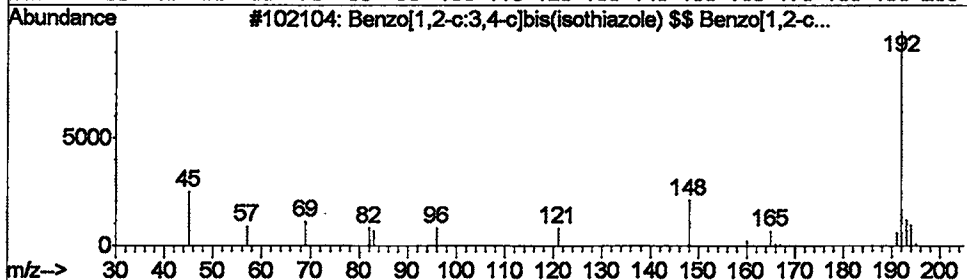
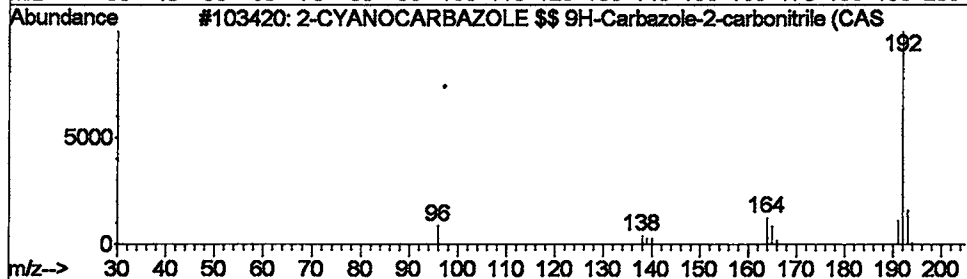
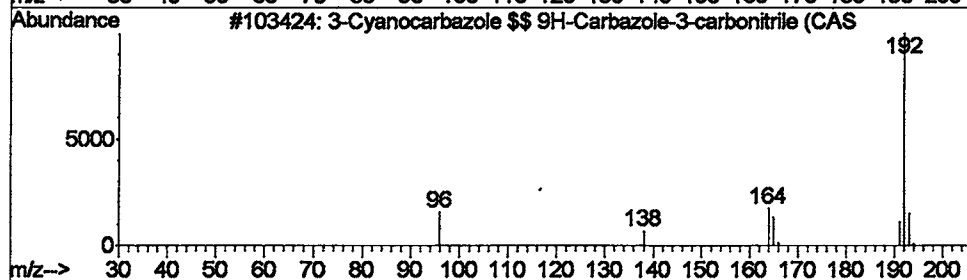
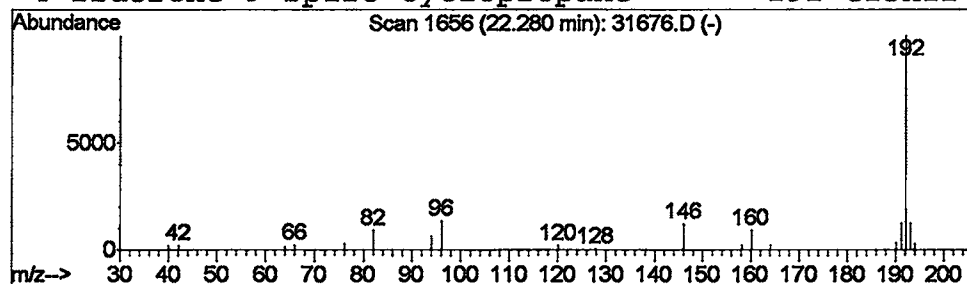
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 6 3-Cyanocarbazole \$\$ 9H-Carb... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	84060	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	72
2			2-CYANOCARBAZOLE \$\$ 9H-Carbazole...	192	C13H8N2	057955-18-7	72
3			Benzo[1,2-c:3,4-c]bis(isothiazol...	192	C8H4N2S2	074960-05-7	64
4			fluorene-9-spiro-cyclopropane	192	C15H12	000000-00-0	53



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

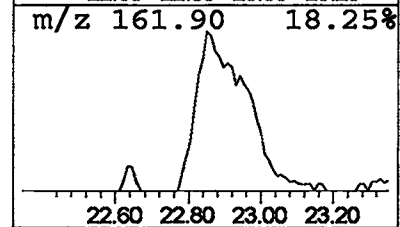
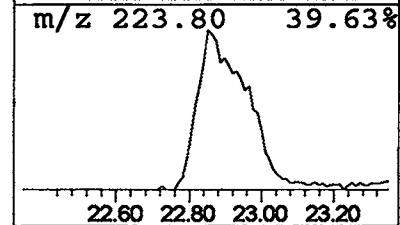
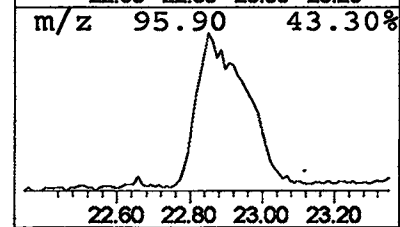
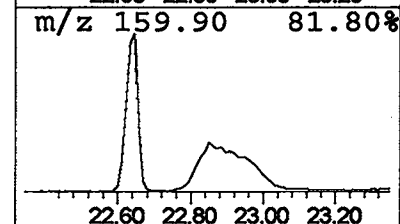
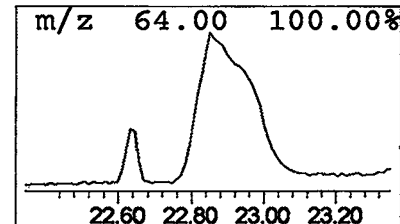
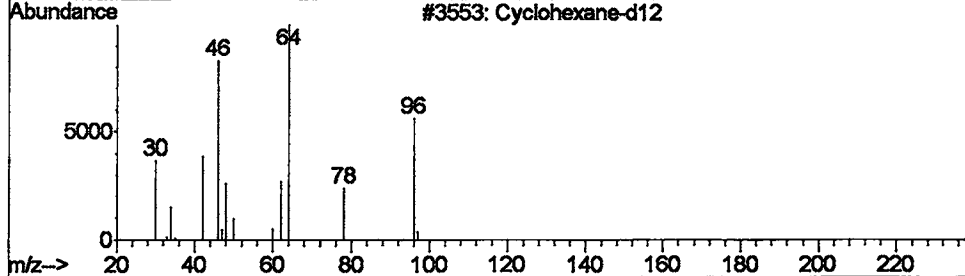
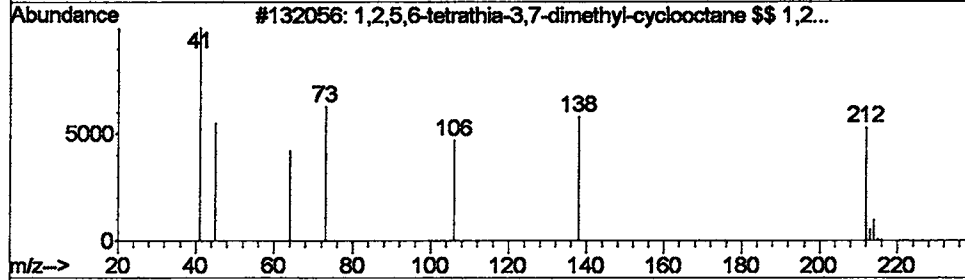
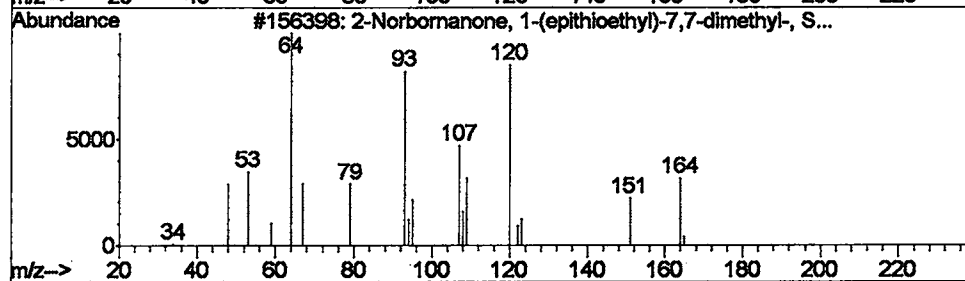
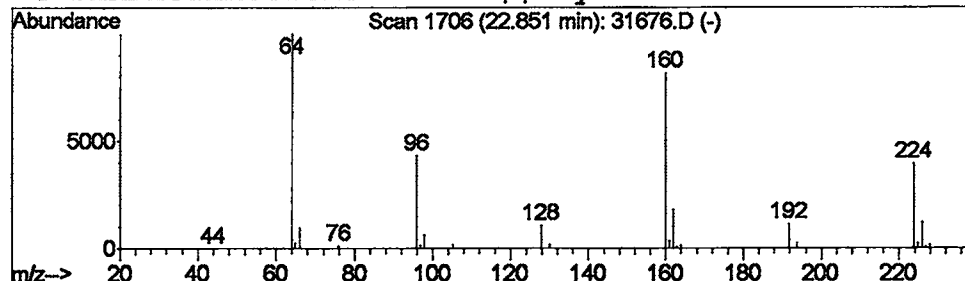
Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 7 2-Norbornanone, 1-(epithioe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.85	4.34 ug/L	2444020	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			1,2,5,6-tetrathia-3,7-dimethyl-c...	212	C6H12S4	116664-31-4	7
3			Cyclohexane-d12	96	C6D12	001735-17-7	7
4			PERDEUTEROCYCLOHEXANE \$\$ Cyclohe...	96	C6D12	001735-17-7	5



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

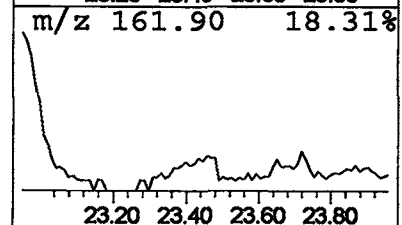
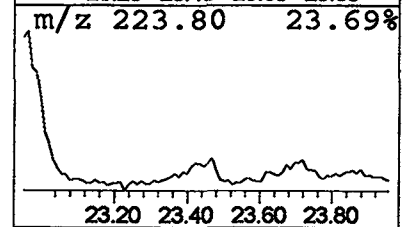
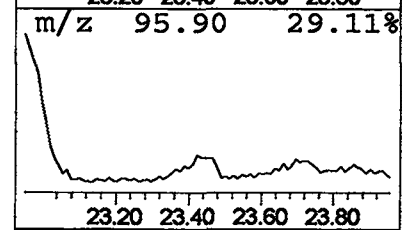
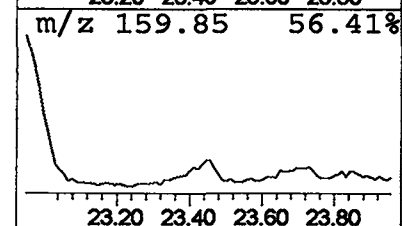
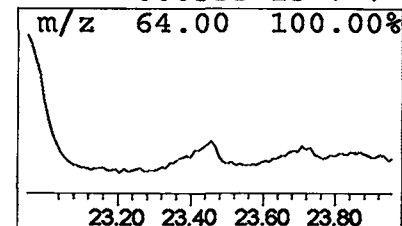
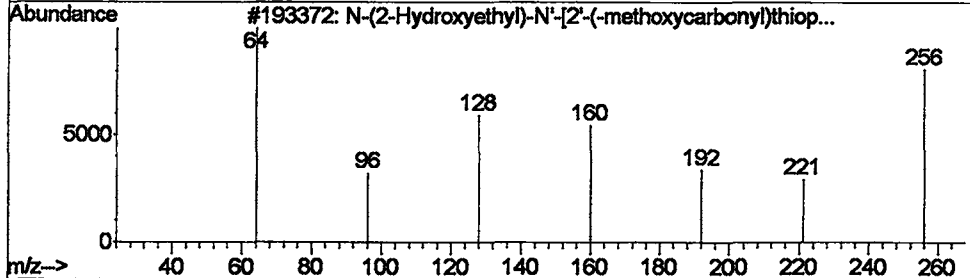
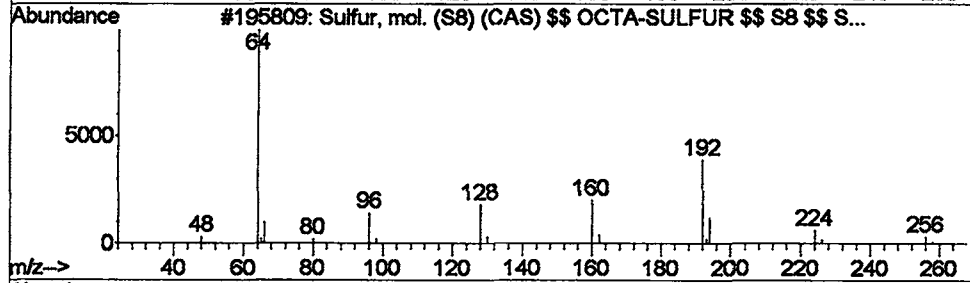
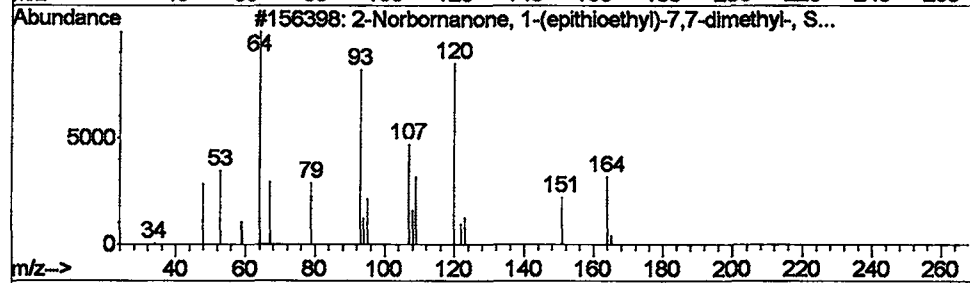
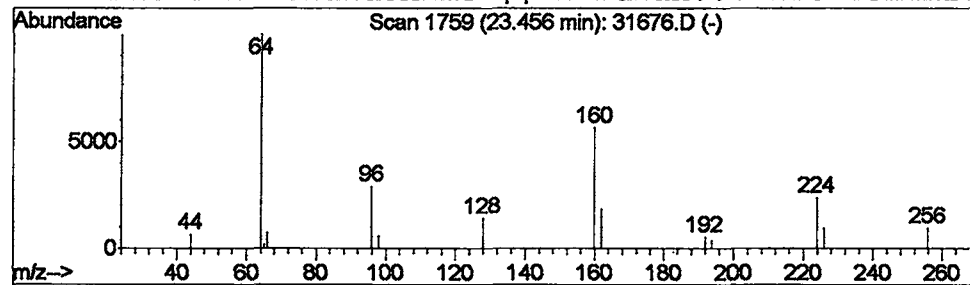
Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 8 2-Norbornanone, 1-(epithioe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	0.30 ug/L	167872	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			Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	9
3			N-(2-Hydroxyethyl)-N'-[2'-(-meth...	255	C10H13N3O3S	000000-00-0	9
4			5-Nitro-2-furaldoxime \$\$ 2-Furan...	156	C5H4N2O4	000555-15-7	7



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

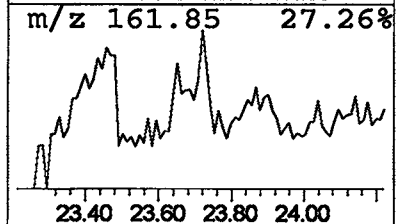
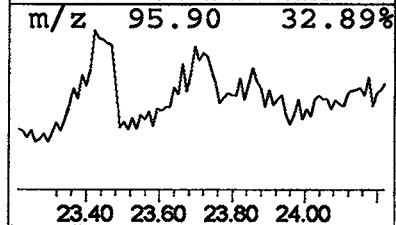
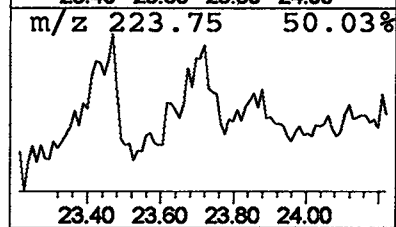
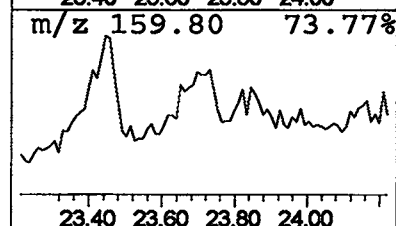
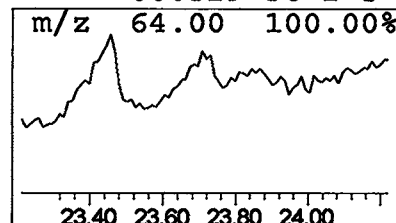
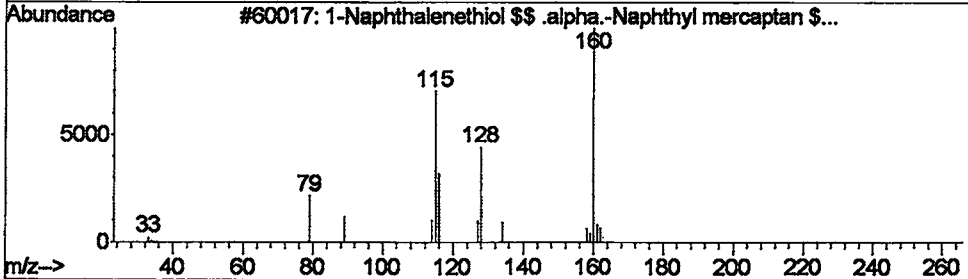
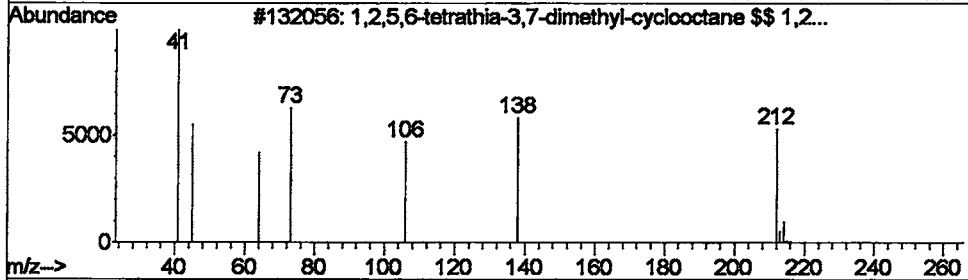
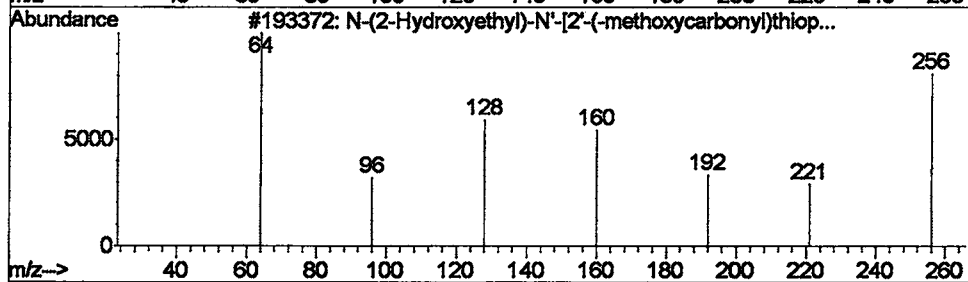
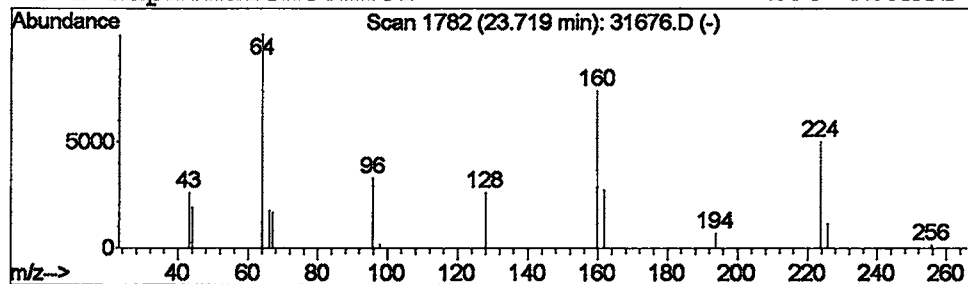
Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 9 N-(2-Hydroxyethyl)-N'-[2'-(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.72	0.12 ug/L	67028	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2-Hydroxyethyl)-N'-[2'-(-meth...	255	C10H13N3O3S	000000-00-0	9
2			1,2,5,6-tetrathia-3,7-dimethyl-c...	212	C6H12S4	116664-31-4	7
3			1-Naphthalenethiol \$\$.alpha.-Na...	160	C10H8S	000529-36-2	5
4			1-Naphthalenethiol	160	C10H8S	000529-36-2	5



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\31676.D
Acq On : 23 Jan 2002 2:57 pm
Sample : 508 scan
Misc : January 22, 2002
MS Integration Params: LSCINT.P

Vial: 1
Operator:
Inst : Instrumen
Multiplr: 1.00

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

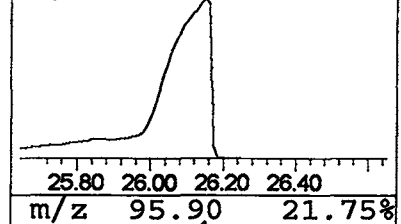
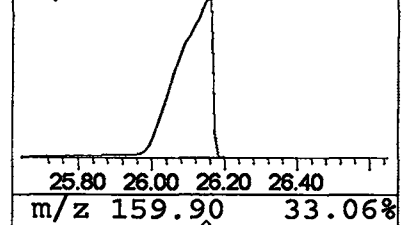
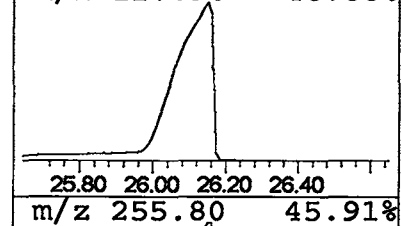
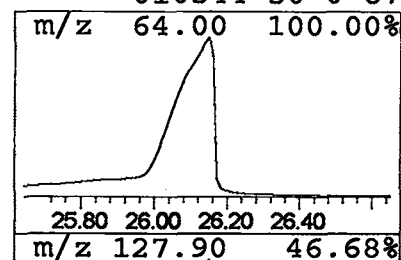
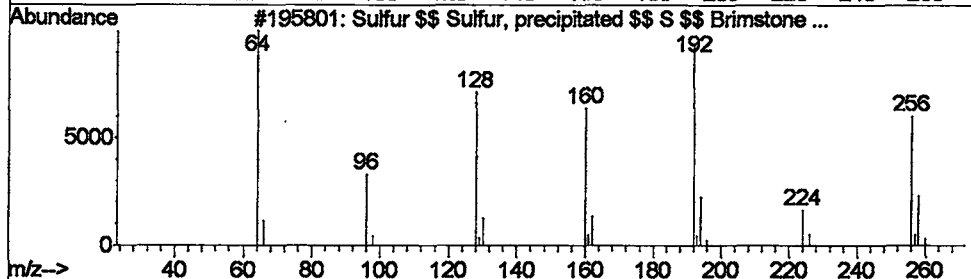
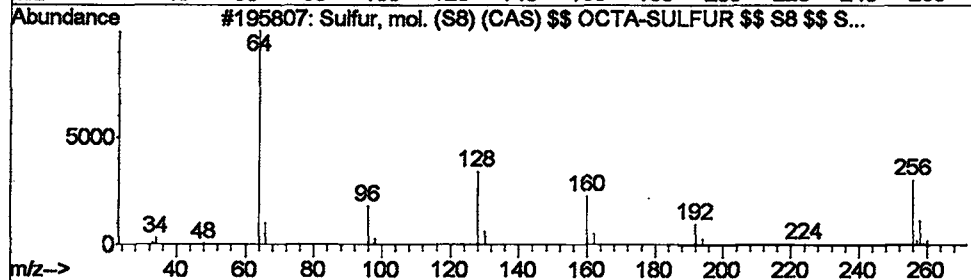
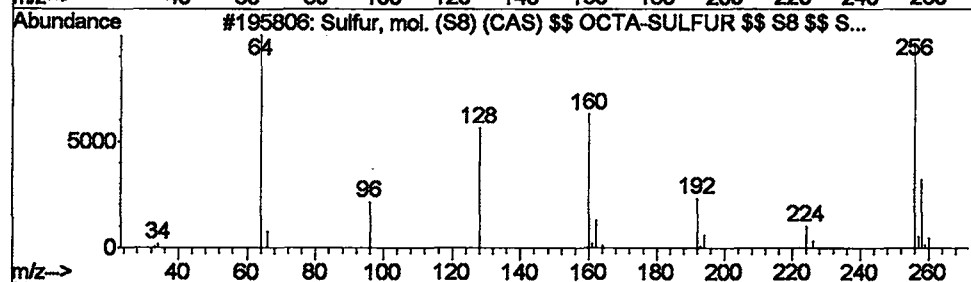
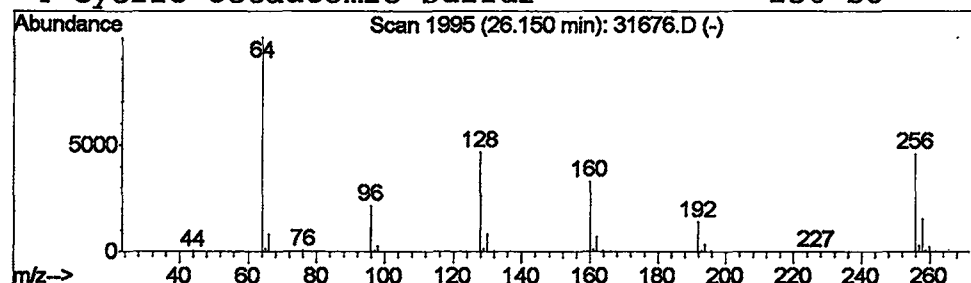
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 10 Sulfur, mol. (S8) (CAS) \$\$... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.15	89.05 ug/L	50149500	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	94
3			Sulfur \$\$ Sulfur, precipitated \$...	256	S8	007704-34-9	87
4			Cyclic octaatomic sulfur	256	S8	010544-50-0	87



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 23 Jan 2002 2:57 pm
Data File: C:\MSDCHEM\1\5973N\02JAN23\31676.D
Name: 508 scan
Misc: January 22, 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...	3.60	0.1	ug/L	46464	1	9.71	6499490	20.0
3-Methyl-2,3-epox...	4.24	0.2	ug/L	52492	1	9.71	6499490	20.0
METHYLFULVENE	4.36	0.1	ug/L	35102	1	9.71	6499490	20.0
Benzene, 1-bromo-...	18.74	1.5	ug/L	784065	3	18.34	10223600	20.0
1,4-Benzenediamin...	20.93	0.1	ug/L	59019	4	22.65	11262600	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	84060	4	22.65	11262600	20.0
2-Norbornanone, 1...	22.85	4.3	ug/L	2444020	4	22.65	11262600	20.0
2-Norbornanone, 1...	23.46	0.3	ug/L	167872	4	22.65	11262600	20.0
N-(2-Hydroxyethyl...	23.72	0.1	ug/L	67028	4	22.65	11262600	20.0
Sulfur, mol. (S8)...	26.15	89.1	ug/L	50149500	4	22.65	11262600	20.0