

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/18/2002 Time: 13:54:16

Sample: AE00468
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/18/02 13:53 Ended: 1/18/02 13:53 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		92		5.0

5-Nitro-2-furaldoxime
40/100 1.0 ug/2
SSS-15-7

2-Nor
2.2 ug/L 28/100
1782-93-0

NHCDER DEL 18
117 by curcio

FB 365 ~~comon~~
C PAA/PATA

Comments for Sample AE00468 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-18-2002 Time: 14:08:52

The GCMS scan, from 35 to 550 amu, reveals the presence of 5-Nitro-2-furaldoxime at an estimated level of 1.0 ug/L and with a fit of 40 out of 100, and 1-Epithioethyl)-2-Norbornanone at an estimated level of 2.2 ug/L and with a fit of 28 ~~ug/L~~. The recovery for 1 of the 43 compounds in the LCS Standard was above its acceptance range.

Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 11 10:18:54 2002

Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Last Update : Thu Jan 10 11:01:02 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	1166614	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4874107	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2513226	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4115686	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3701613	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2740235	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	298791	4.59	ug/L	0.00
Spiked Amount	5.000		Recovery	=	91.80%	

Target Compounds

	R.T.	QIon	Response	Conc	Units	Qvalue
2) n-Nitroso-dimethylamine	3.60	74	8317	0.17	ug/L #	13
20) Dimethylphthalate	18.34	163	409112	2.46	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	325548	10.06	ug/L #	17
35) Di-n-butylphthalate	24.86	149	18625	0.07	ug/L	94
41) Benzo(a)anthracene	30.49	228	9223	0.04	ug/L #	54
42) Bis(2-ethylhexyl)phthalate	31.12	149	19153	0.65	ug/L	91
43) Chrysene	30.49	228	9223	0.04	ug/L #	51
48) Benzo(a)pyrene	34.42	252	9216	0.05	ug/L #	1

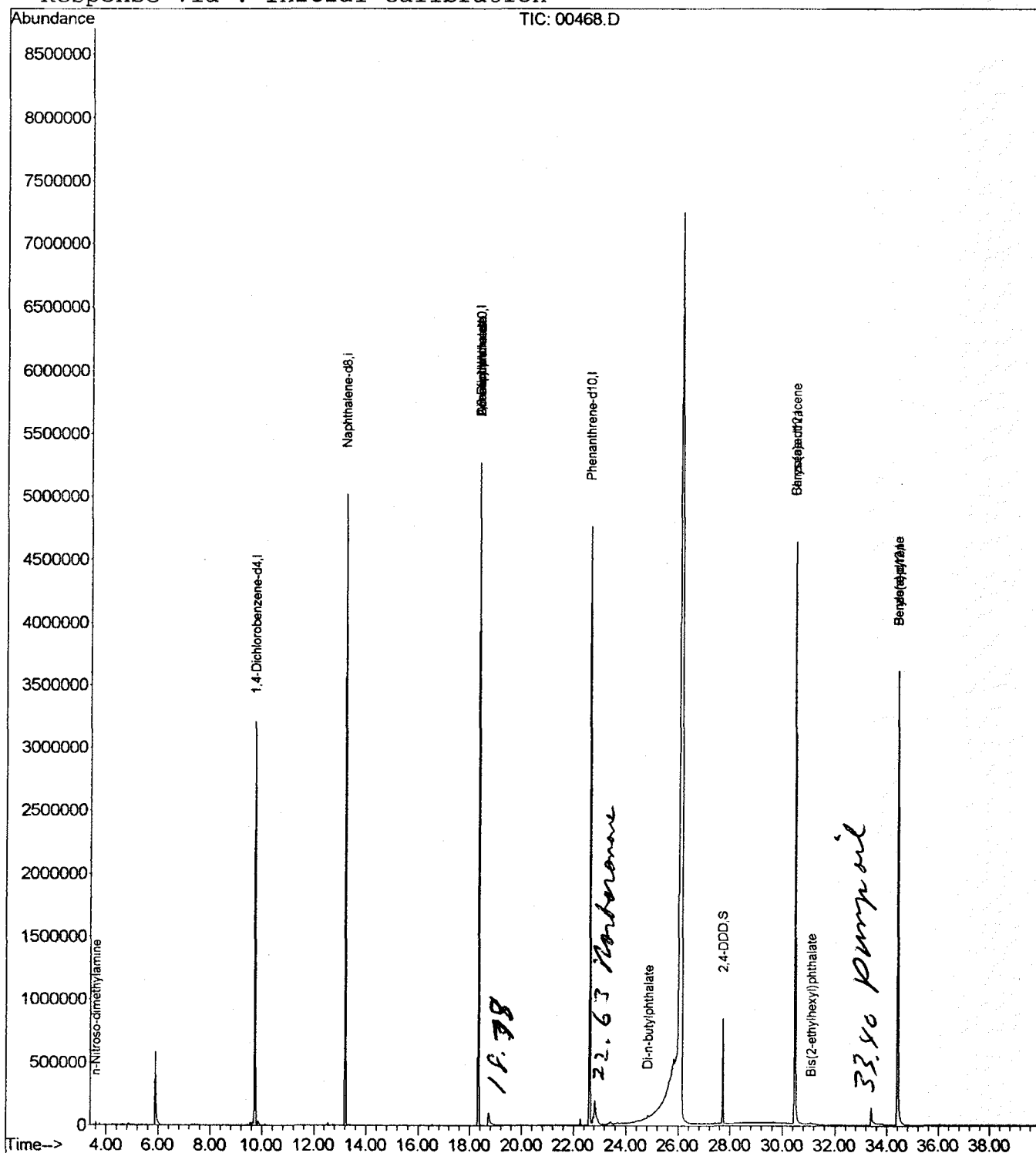
 (#) = qualifier out of range (m) = manual integration
 00468.D SCAN508.M Fri Jan 11 10:18:55 2002

Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 11 10:18 2002

Vial: 5
 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 : Thu Jan 10 11:01:02 2002
 Response via : Initial Calibration



00468.D SCAN508.M

Fri Jan 11 10:18:56 2002

Page 2

Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

Vial: 5
 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

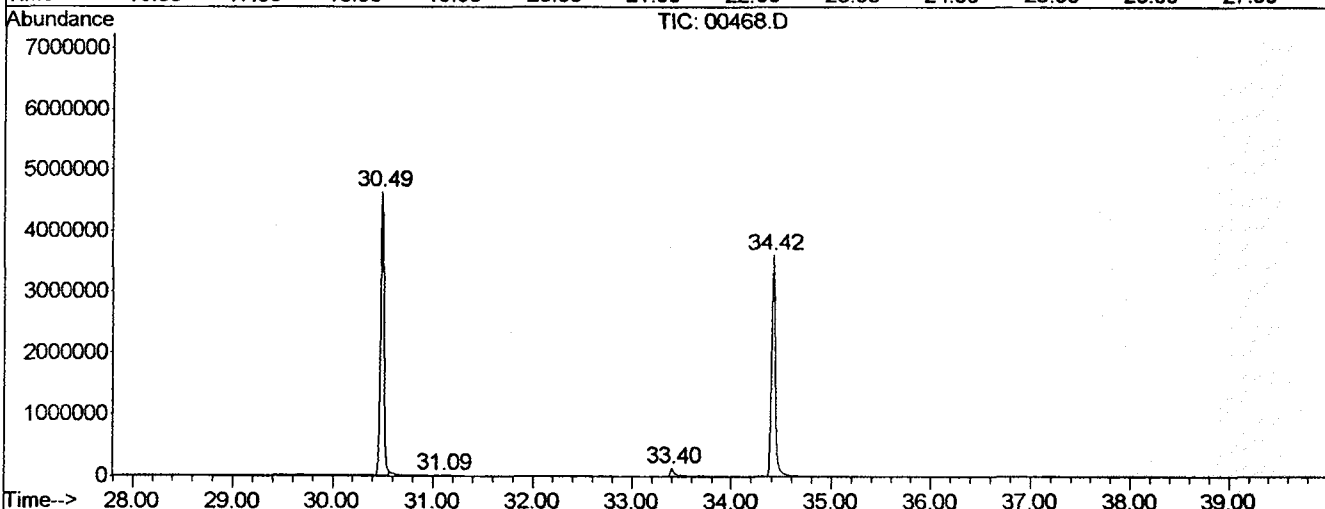
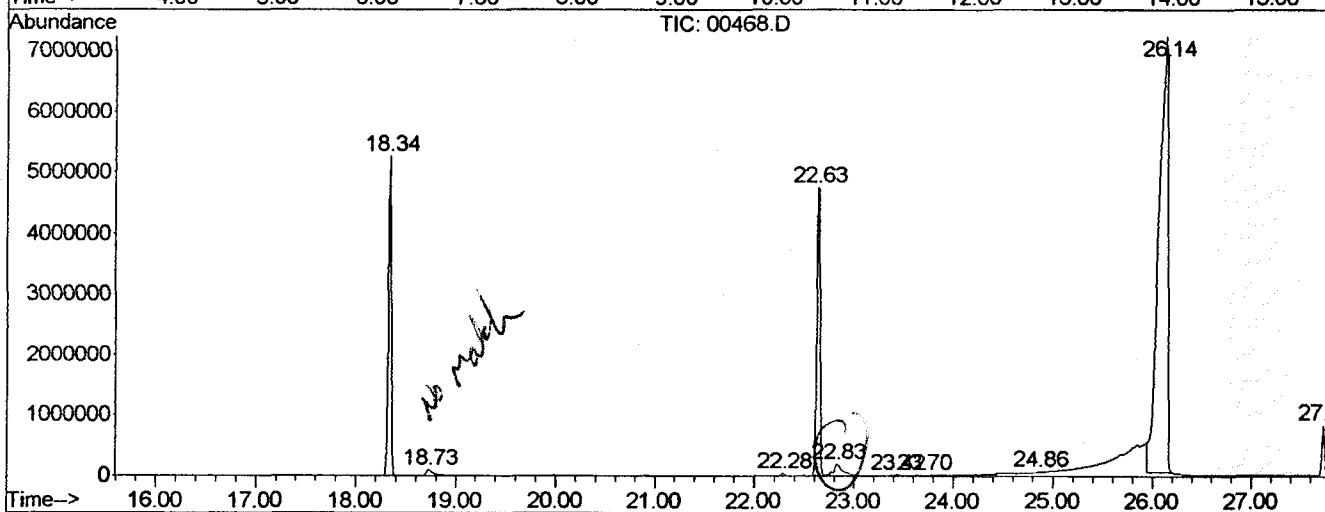
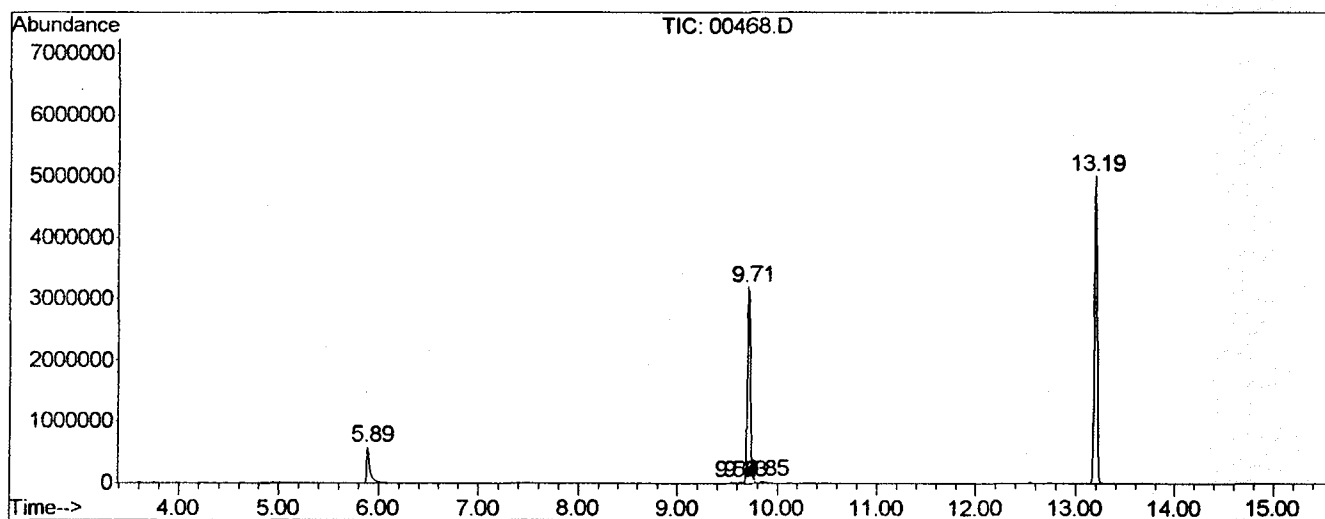
If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.886	217	220	251	rBV	583036	1338078	2.89%	1.220%
2	9.539	539	540	545	rBV2	23945	59307	0.13%	0.054%
3	9.630	545	548	551	rVV	26940	67114	0.14%	0.061%
4	9.710	551	555	563	rVV	3207994	6665000	14.38%	6.076%
5	9.847	563	567	577	rVB2	30438	108727	0.23%	0.099%
6	13.192	855	860	865	rBV	5018847	9381773	20.24%	8.553%
7	18.341	1305	1311	1315	rBV	5271506	10247408	22.11%	9.342%
8	18.730	1339	1345	1367	rBV	100881	529744	1.14%	0.483%
9	22.280	1651	1656	1661	rBV	47409	84948	0.18%	0.077%
10	22.634	1681	1687	1693	rBV2	4758453	10917368	23.56%	9.953%
11	22.828	1693	1704	1727	rVB2	187734	1205380	2.60%	1.099%
12	23.422	1745	1756	1765	rBV3	18618	97397	0.21%	0.089%
13	23.696	1765	1780	1785	rBV6	12128	79691	0.17%	0.073%
14	24.860	1877	1882	1887	rBV2	22864	72651	0.16%	0.066%
15	26.139	1977	1994	1999	rVB	7179827	46345705	100.00%	42.250%
16	27.726	2129	2133	2139	rBV	835385	1492159	3.22%	1.360%
17	30.489	2369	2375	2381	rBV2	4624757	10936407	23.60%	9.970%
18	31.094	2425	2428	2455	rVB7	19213	141370	0.31%	0.129%
19	33.400	2625	2630	2645	rBV	138848	515064	1.11%	0.470%
20	34.416	2713	2719	2745	rBV	3607544	9408958	20.30%	8.577%

Sum of corrected areas: 109694249

File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Operator :
 Acquired : 10 Jan 2002 6:07 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan ext 1/8
 Misc Info : January 10, 2002
 Vial Number: 5
 Quant File :SCAN508.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

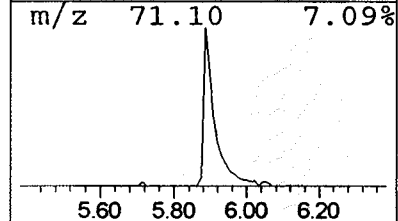
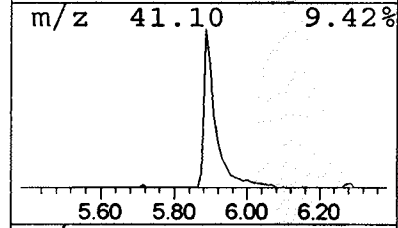
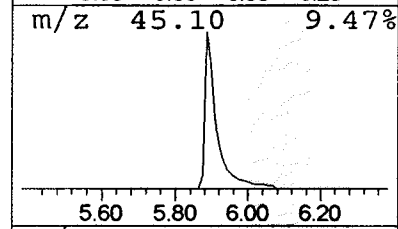
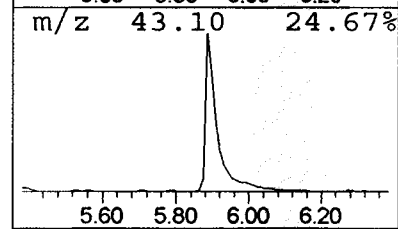
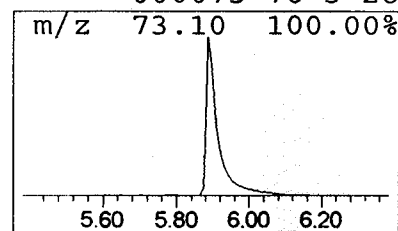
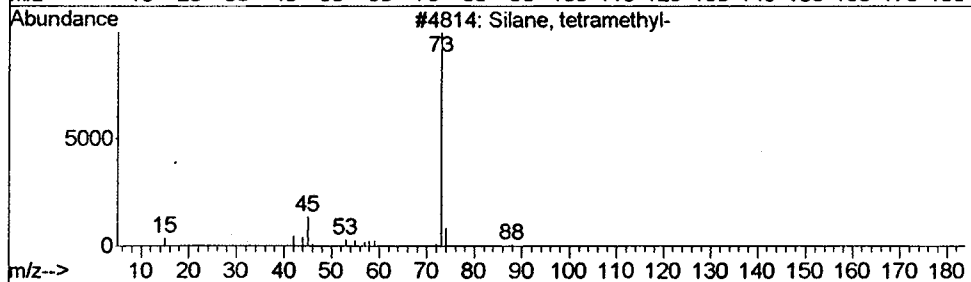
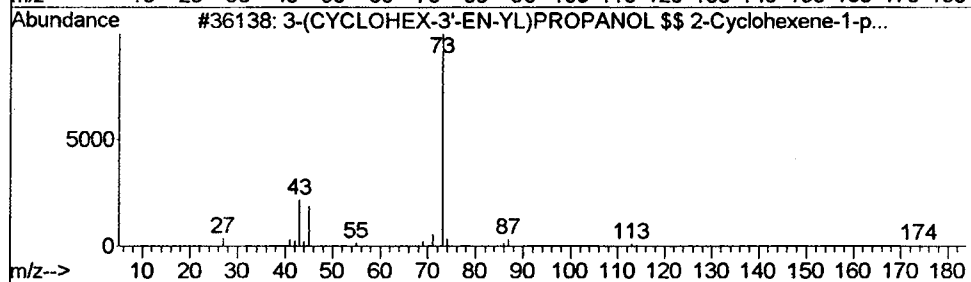
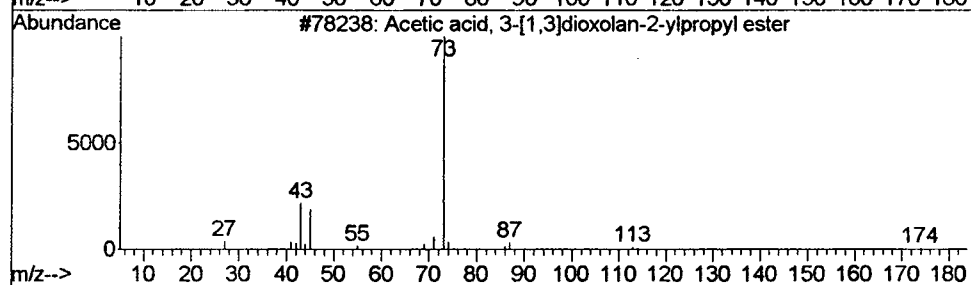
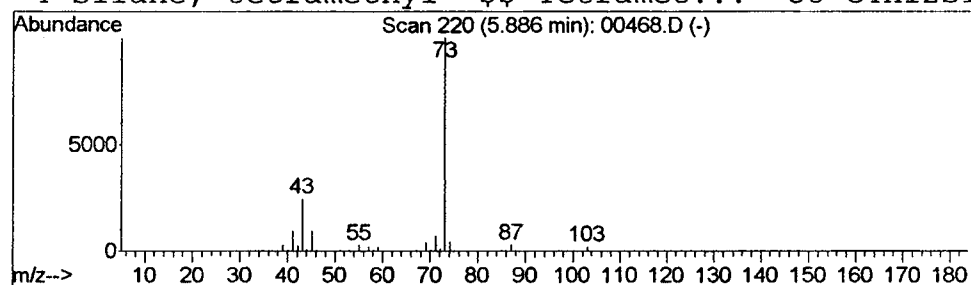
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 Acetic acid, 3-[1,3]dioxola... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.02 ug/L	1338080	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
2			3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	33
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4			Silane, tetramethyl- \$\$ Tetramet...	88	C4H12Si	000075-76-3	28



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

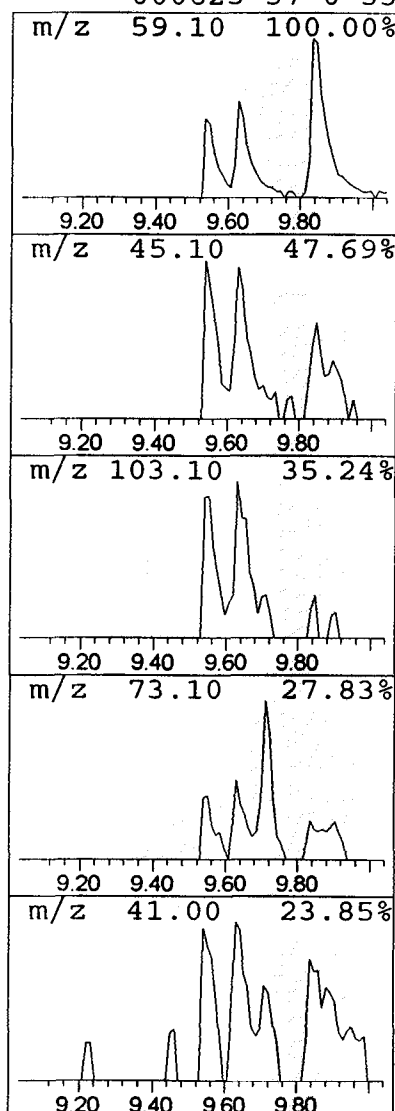
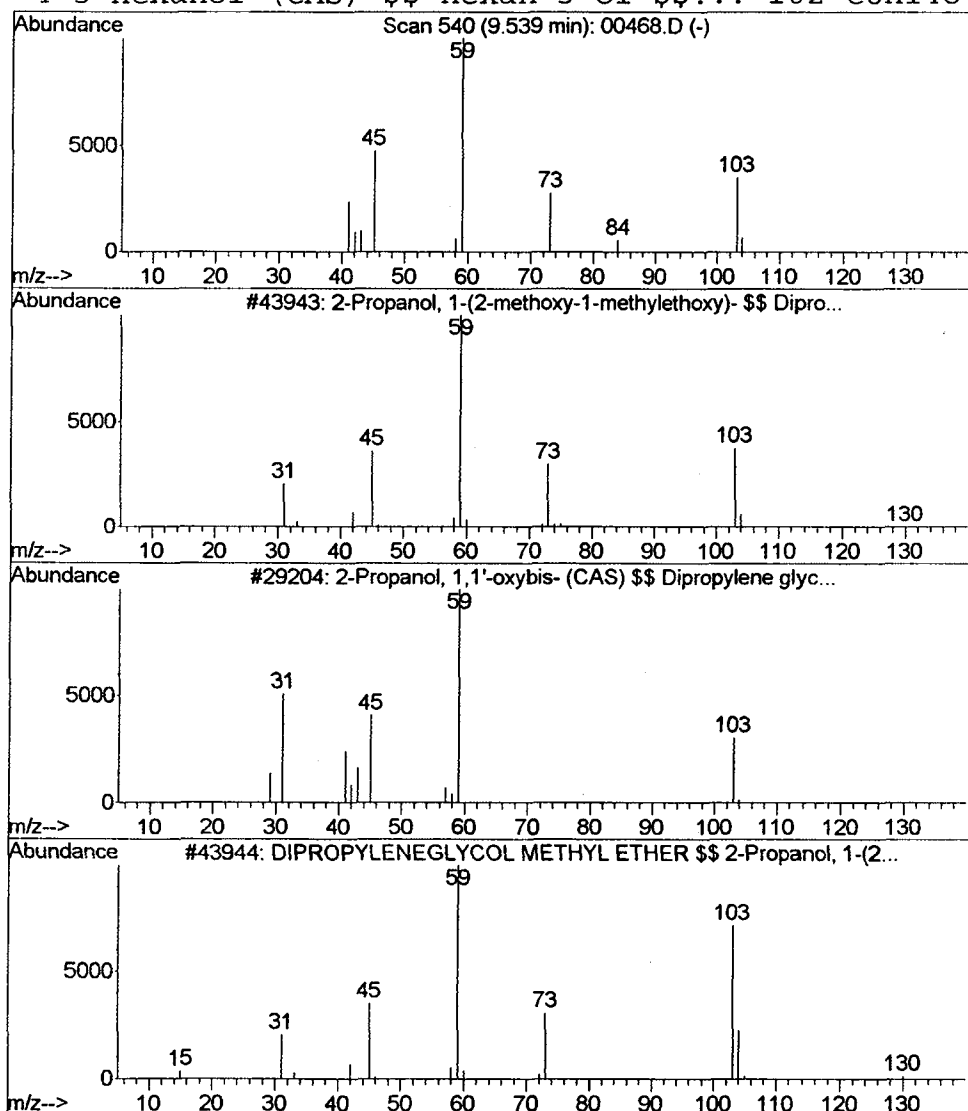
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	0.18 ug/L	59307	1,4-Dichlorobenzene-d4	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
2		2-Propanol, 1,1'-oxybis- (CAS) \$...	134	C6H14O3	000110-98-5	50
3		DIPROPYLENEGLYCOL METHYL ETHER \$...	148	C7H16O3	020324-32-7	39
4		3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$...	102	C6H14O	000623-37-0	33



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

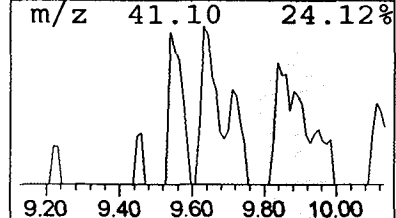
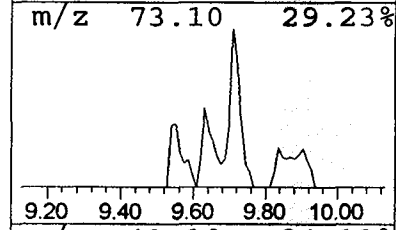
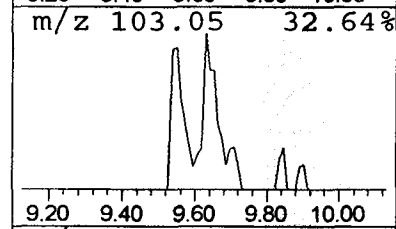
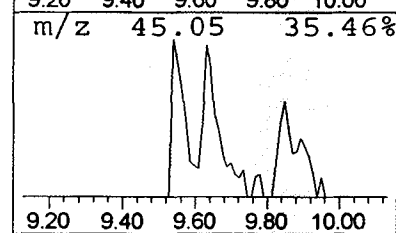
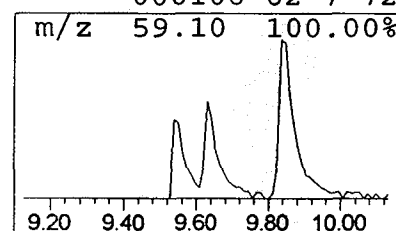
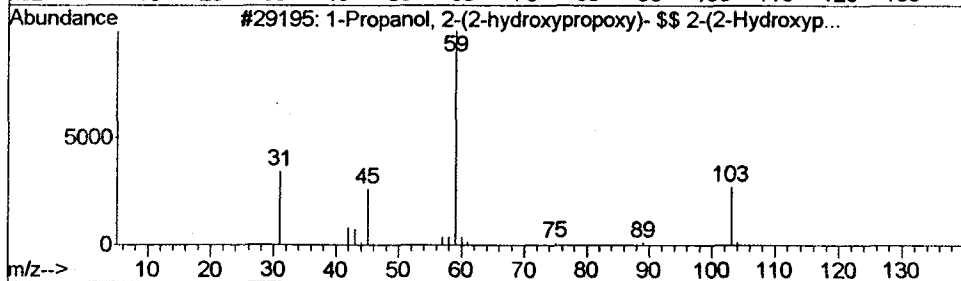
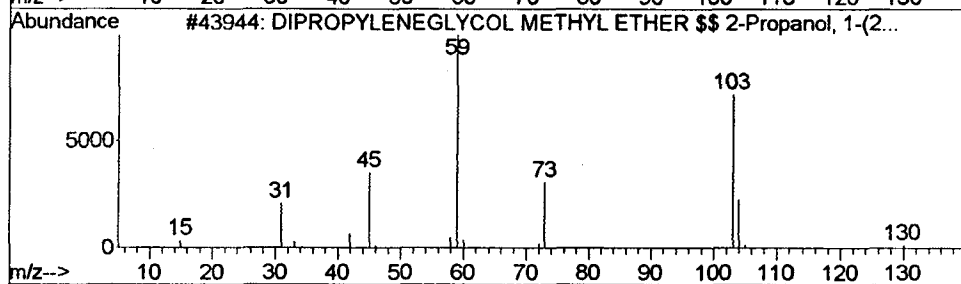
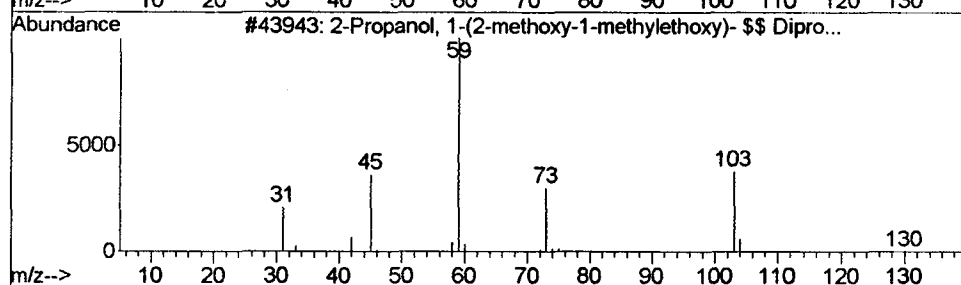
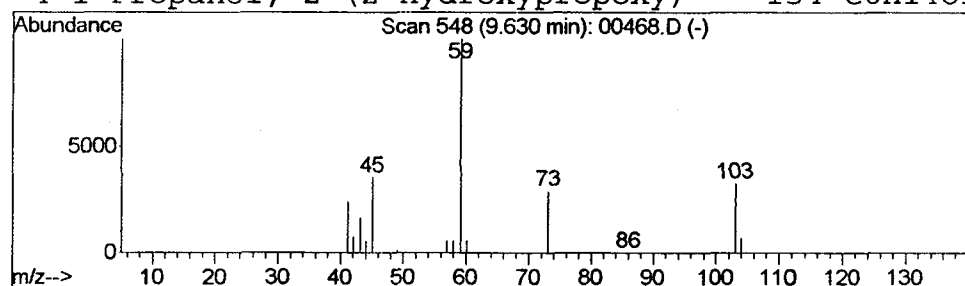
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	0.20 ug/L	67114	1,4-Dichlorobenzene-d4	9.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83	
2	DIPROPYLENEGLYCOL METHYL ETHER \$...	148	C7H16O3	020324-32-7	74	
3	1-Propanol, 2-(2-hydroxypropoxy)...	134	C6H14O3	000106-62-7	72	
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72	



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

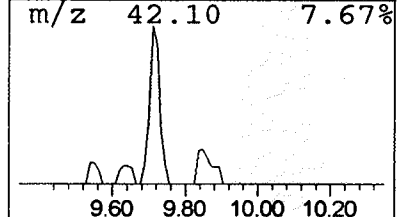
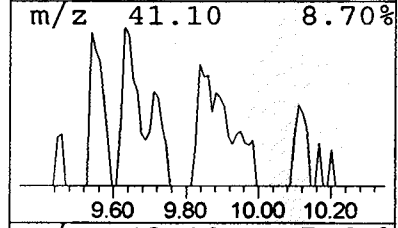
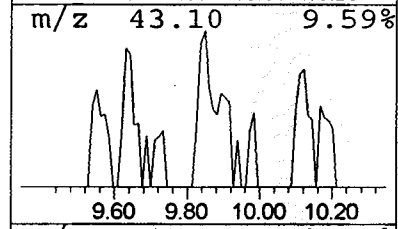
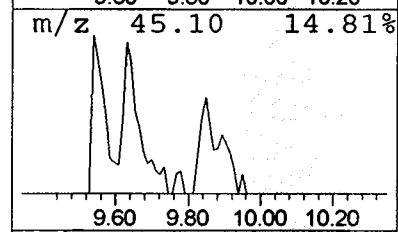
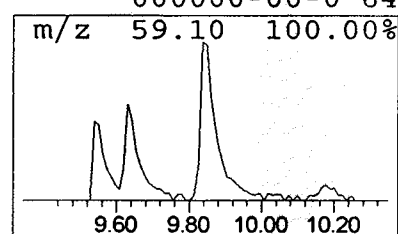
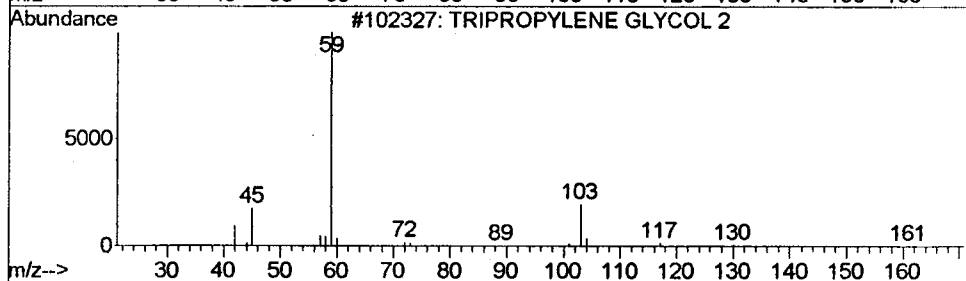
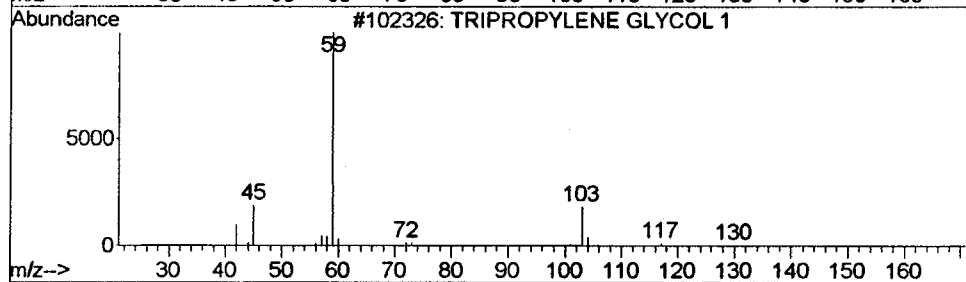
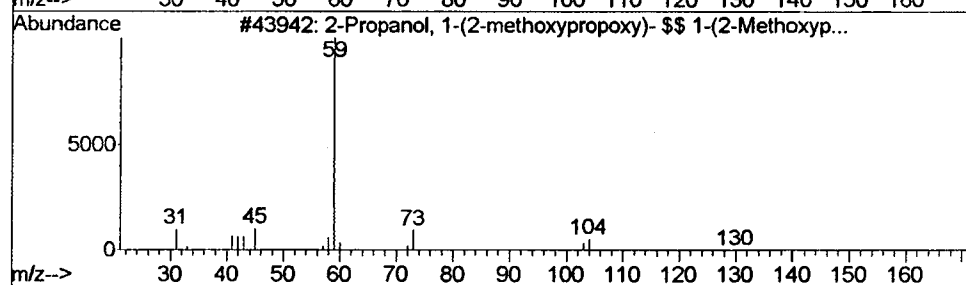
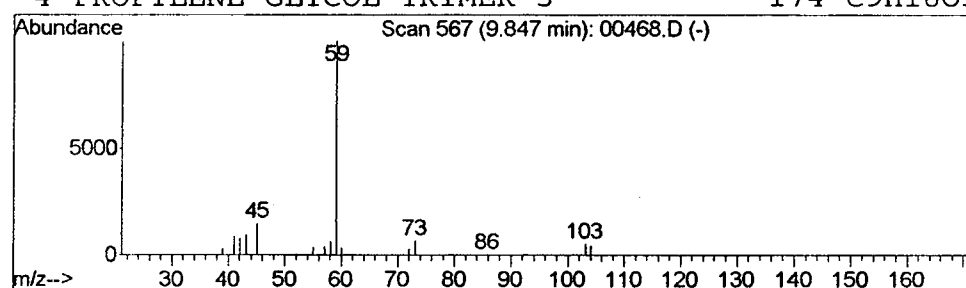
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 4 2-Propanol, 1-(2-methoxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	0.33 ug/L	108727	1,4-Dichlorobenzene-d4	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	78
2		TRIPROPYLENE GLYCOL 1	192	C9H20O4	000000-00-0	78
3		TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	64
4		PROPYLENE GLYCOL TRIMER 3	174	C9H18O3	000000-00-0	64



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Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

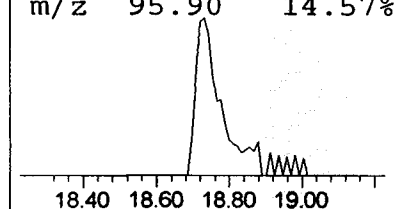
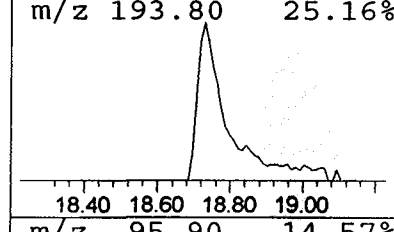
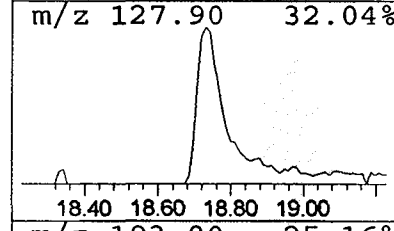
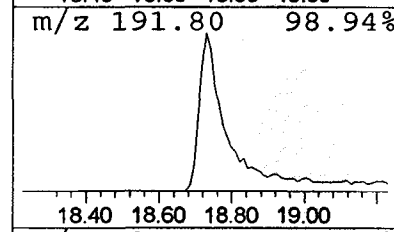
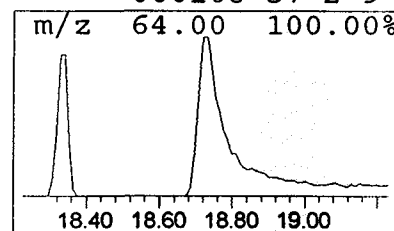
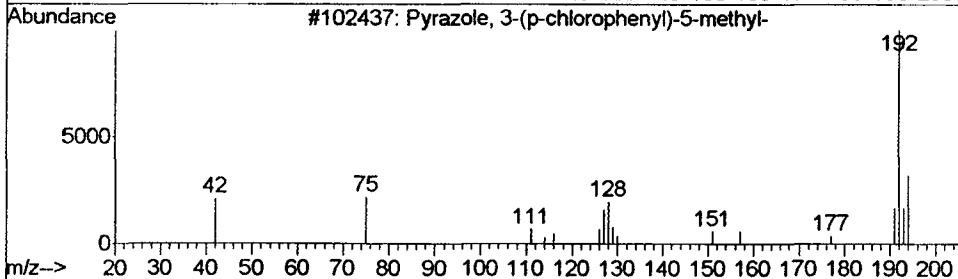
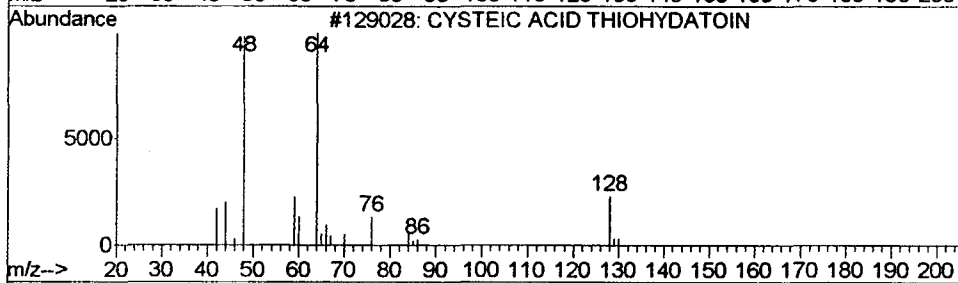
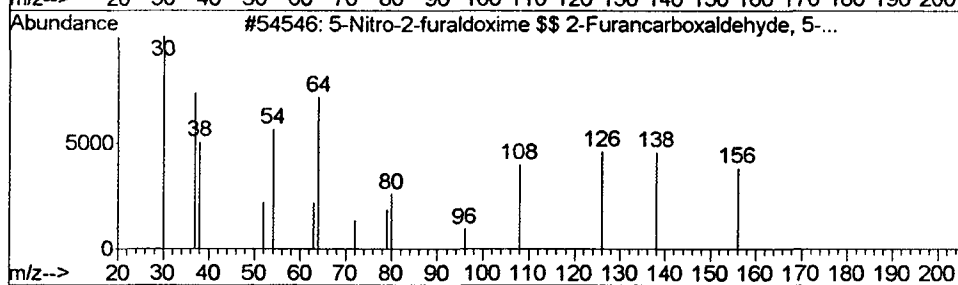
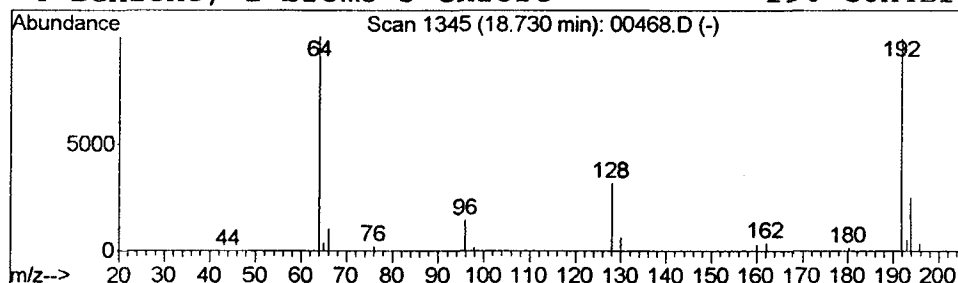
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	1.03 ug/L	529744	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	40
2		CYSTEIC ACID THIOHYDATOIN	210	C4H6N2O4S2	000000-00-0	36
3		Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	9
4		Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	9

NO
 GOOD
 MATCH



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

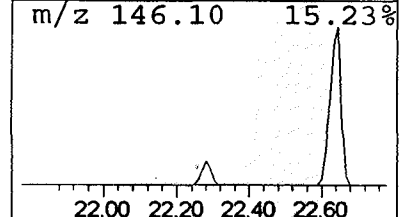
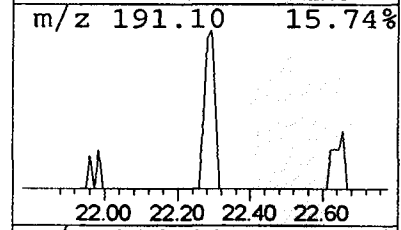
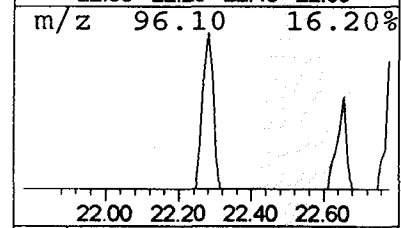
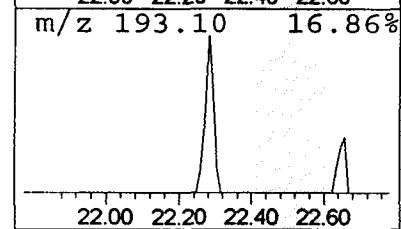
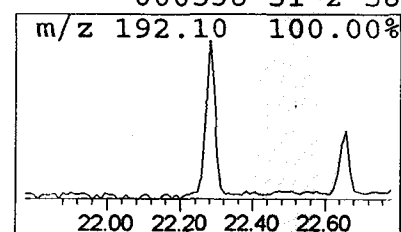
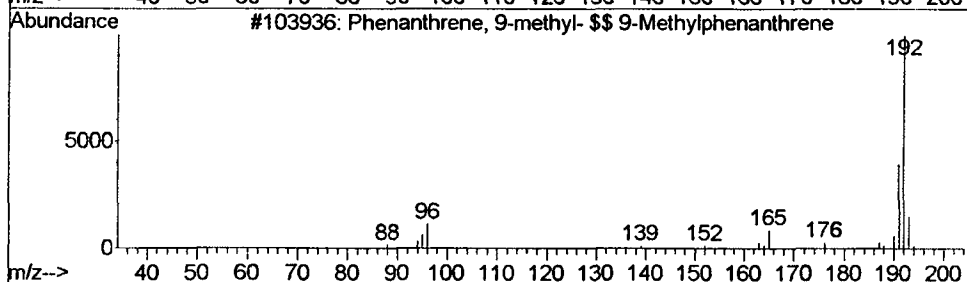
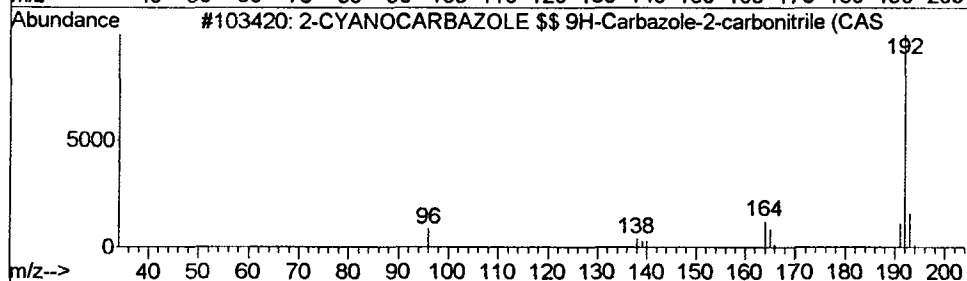
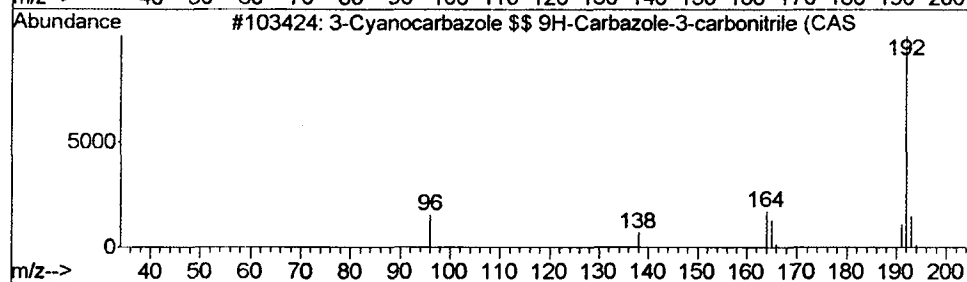
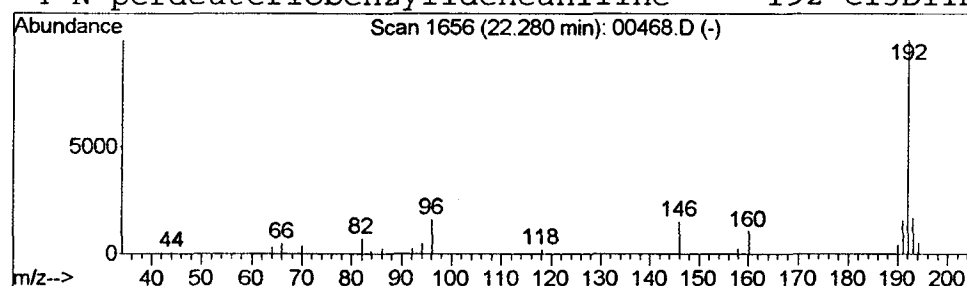
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.16 ug/L	84948	Phenanthrene-d10	22.63

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			Phenanthrene, 9-methyl- \$\$ 9-Met...	192	C15H12	000883-20-5	59
4			N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
Acq On : 10 Jan 2002 6:07 pm
Sample : 508 scan ext 1/8
Misc : January 10, 2002
MS Integration Params: LSCINT.P

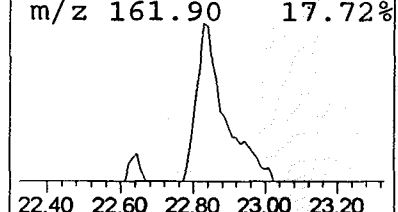
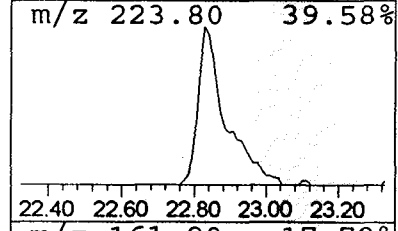
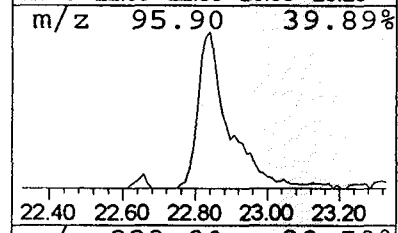
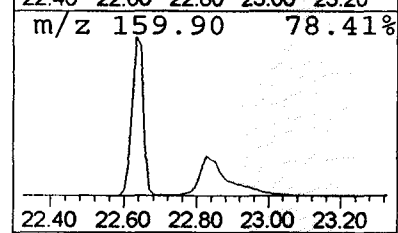
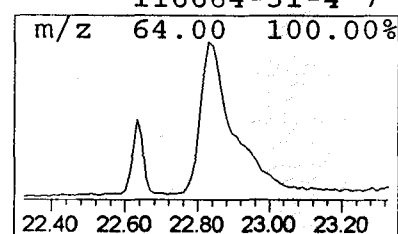
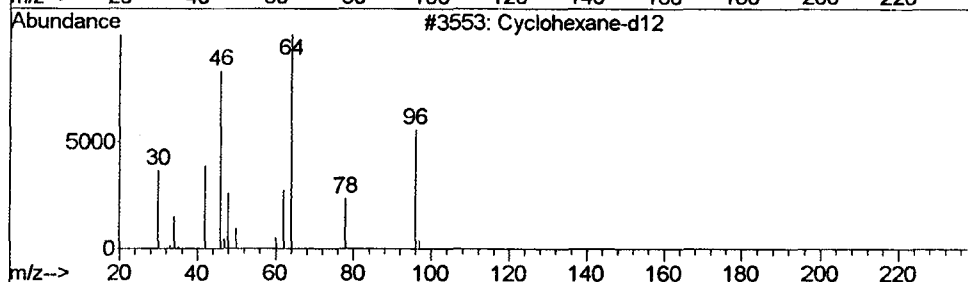
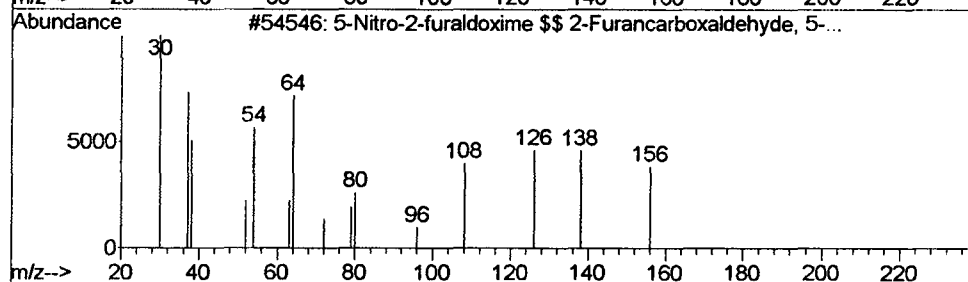
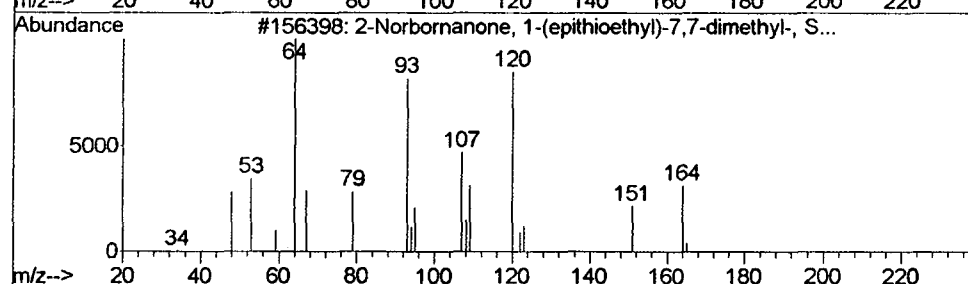
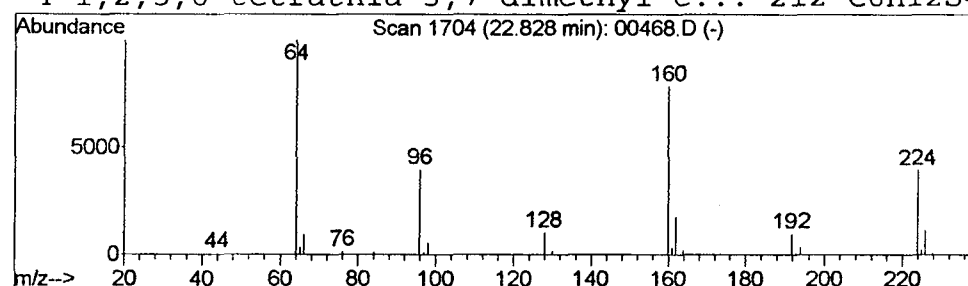
Vial: 5
Operator:
Inst : Instrumen
Multiplr: 1.00

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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.83	2.21 ug/L	1205380	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	28
2		5-Nitro-2-furaldoxime \$\$ 2-Furan...	156	C5H4N2O4	000555-15-7	7
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



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

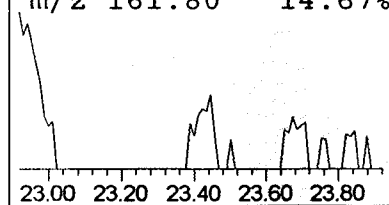
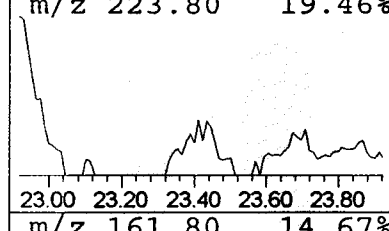
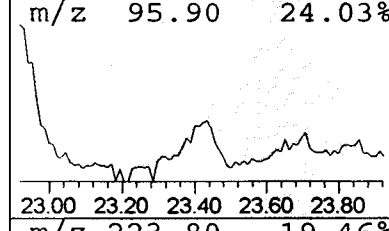
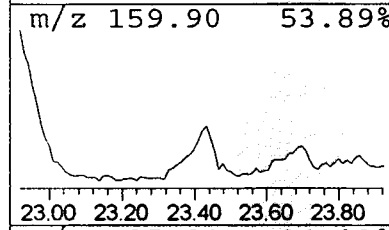
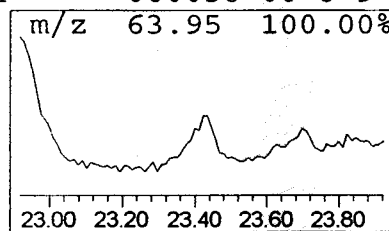
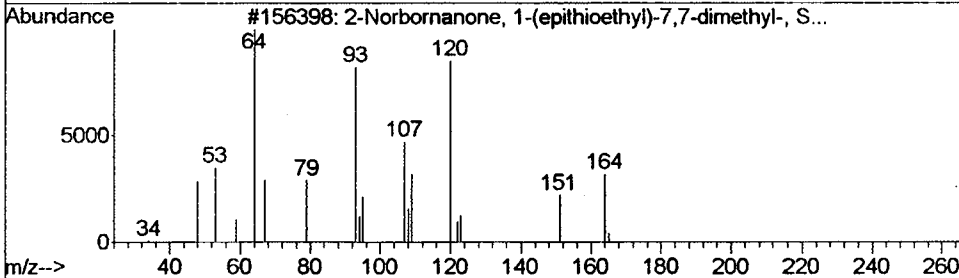
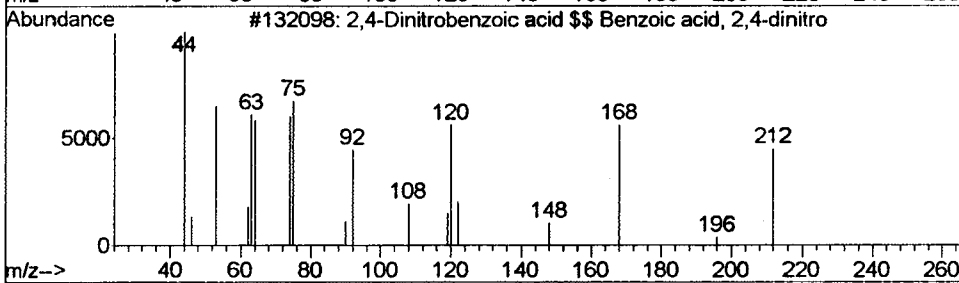
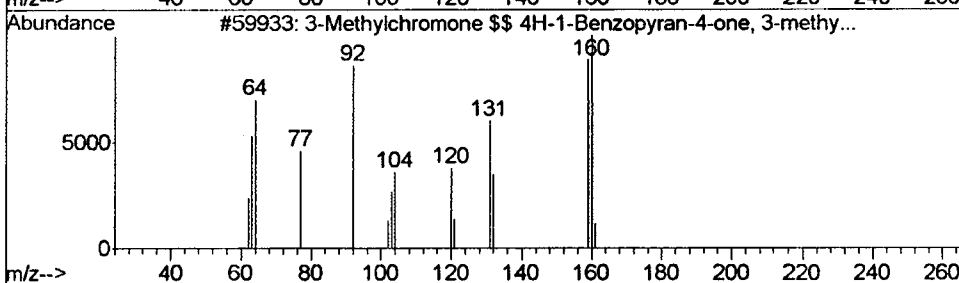
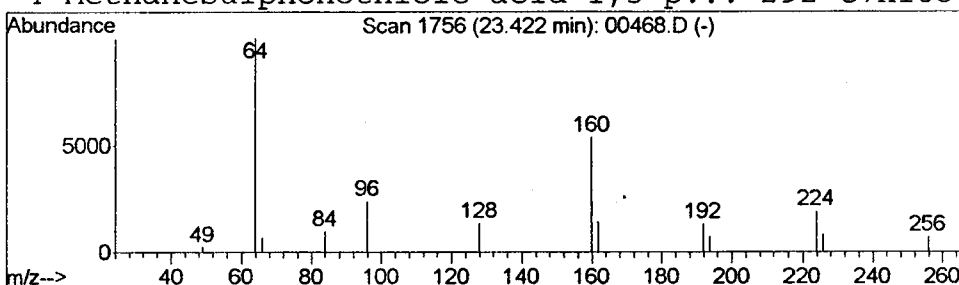
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 8 3-Methylchromone \$\$ 4H-1-Be... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.42	0.18 ug/L	97397	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methylchromone \$\$ 4H-1-Benzopy...	160	C10H8O2	000085-90-5	64
2		2,4-Dinitrobenzoic acid \$\$ Benzo...	212	C7H4N2O6	000610-30-0	36
3		2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	36
4		Methanesulphonothioic acid 1,5-p...	292	C7H16O4S4	000056-00-8	9

NO
 GOOD
 MATCH



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
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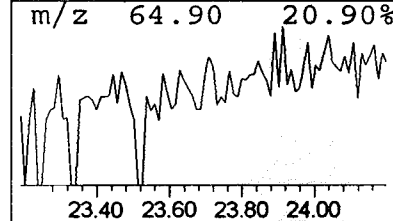
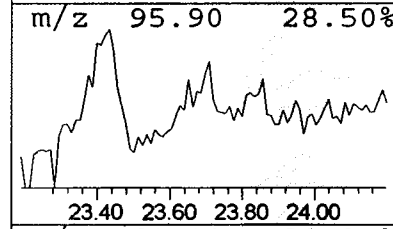
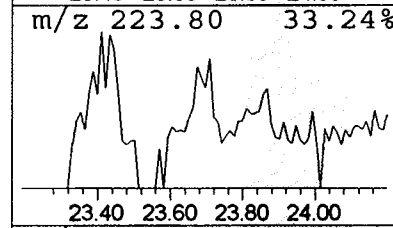
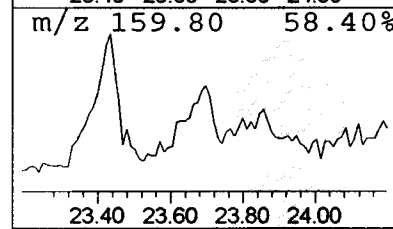
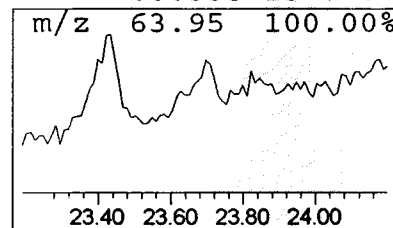
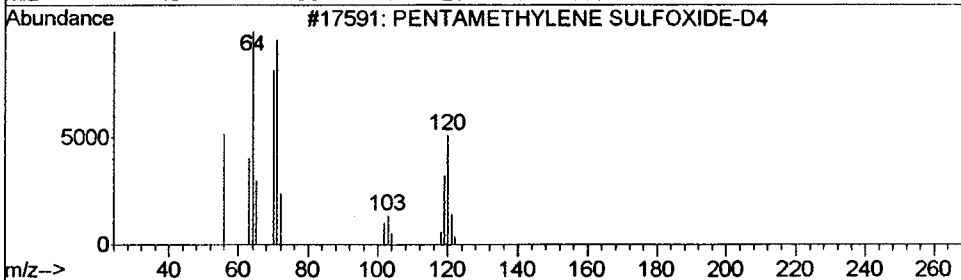
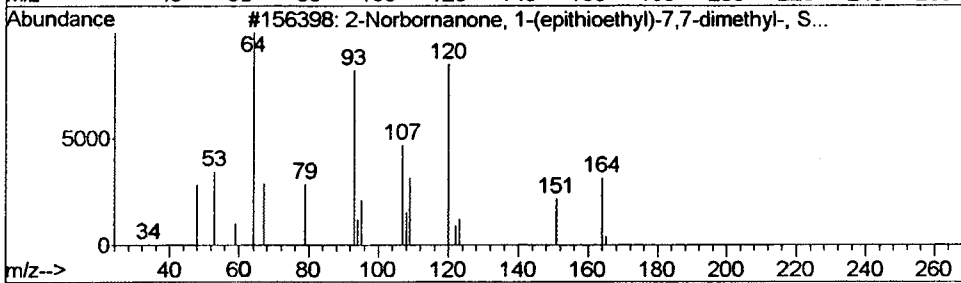
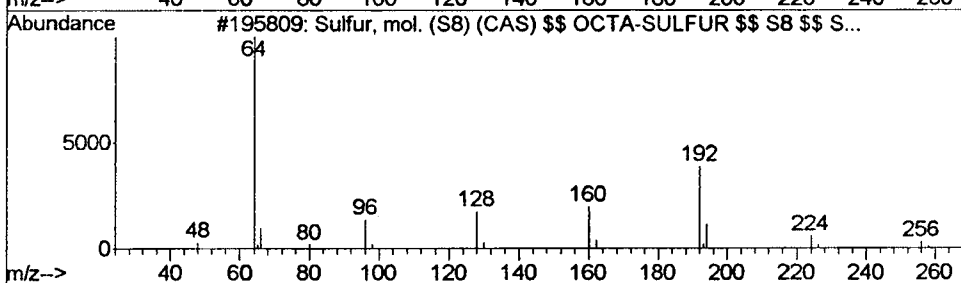
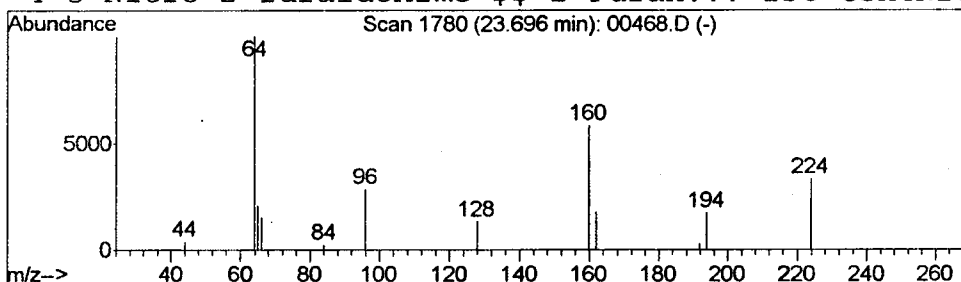
Vial: 5
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 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 9 Sulfur, mol. (S8) (CAS) \$\$... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.70	0.15 ug/L	79691	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	40
2		2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	36
3		PENTAMETHYLENE SULFOXIDE-D4	122	C5H6D4OS	000000-00-0	9
4		5-Nitro-2-furaldoxime \$\$ 2-Furan...	156	C5H4N2O4	000555-15-7	7



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
 Acq On : 10 Jan 2002 6:07 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
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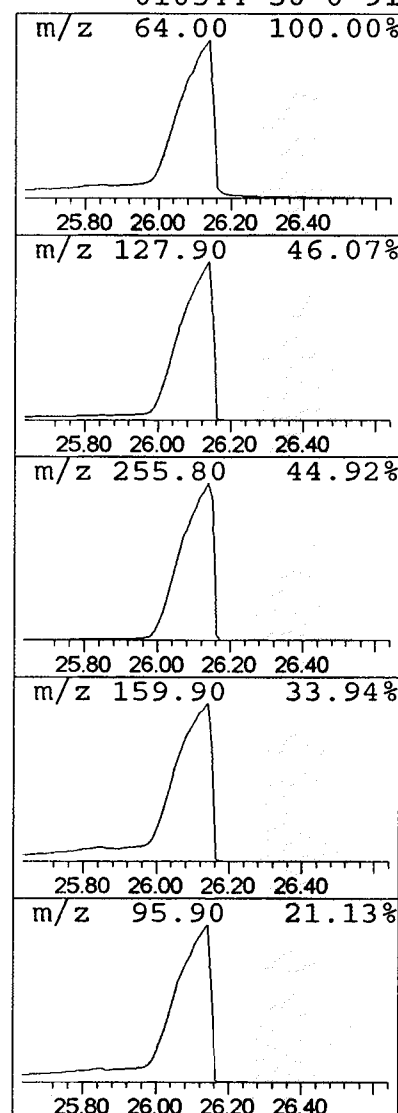
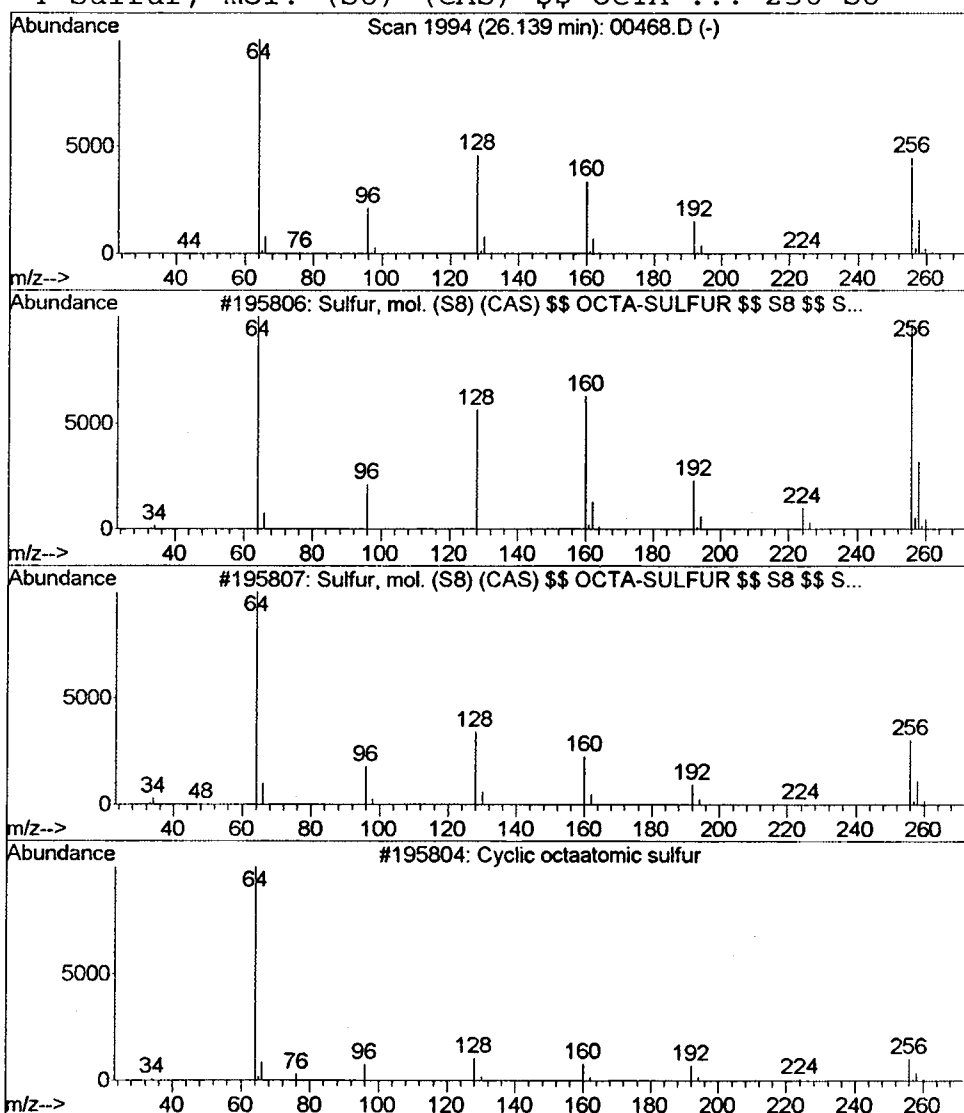
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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.
26.14	84.90 ug/L	46345700	Phenanthrene-d10	22.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	97
2			Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	97
3			Cyclic octaatomic sulfur	256	S8	010544-50-0	91
4			Sulfur, mol. (S8) (CAS) \$\$ OCTA-...	256	S8	010544-50-0	91



Data File : C:\MSDCHEM\1\5973N\02JAN10\00468.D
Acq On : 10 Jan 2002 6:07 pm
Sample : 508 scan ext 1/8
Misc : January 10, 2002
MS Integration Params: LSCINT.P

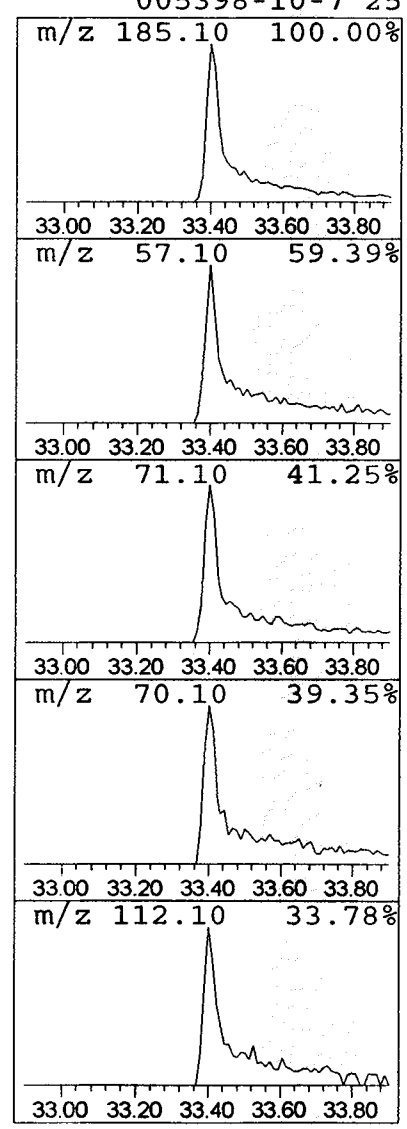
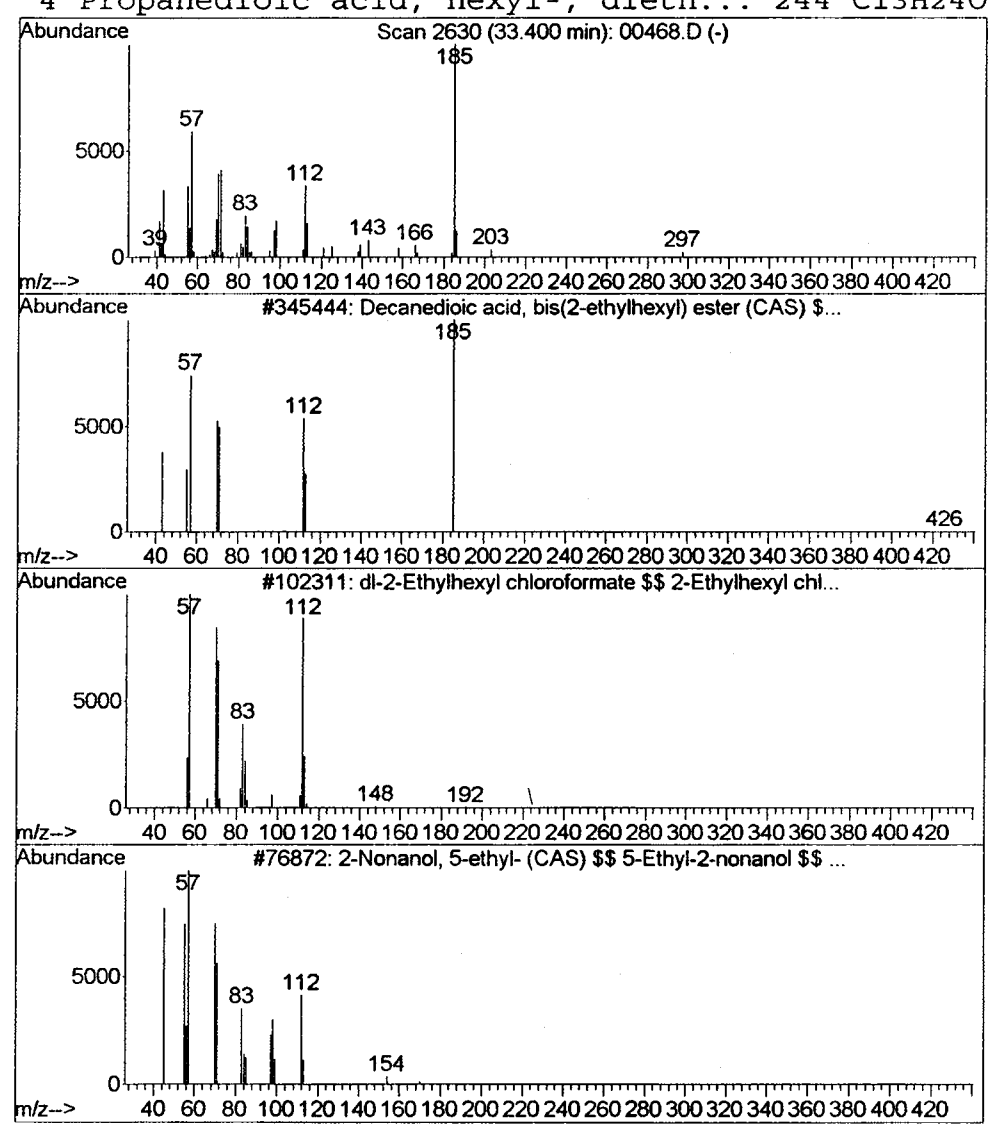
Vial: 5
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 11 Decanedioic acid, bis(2-eth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
33.40	1.09 ug/L	515064	Perylene-d12	34.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	59 <i>NO</i>
2		dl-2-Ethylhexyl chloroformate \$\$...	192	C9H17ClO2	024468-13-1	43 <i>GOOD</i>
3		2-Nonanol, 5-ethyl- (CAS) \$\$ 5-E...	172	C11H24O	000103-08-2	38 <i>MATCH</i>
4		Propanedioic acid, hexyl-, dieth...	244	C13H24O4	005398-10-7	25



Operator ID: Date Acquired: 10 Jan 2002 6:07 pm
Data File: C:\MSDCHEM\1\5973N\02JAN10\00468.D
Name: 508 scan ext 1/8
Misc: January 10, 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
Acetic acid, 3-[1...	5.89	4.0	ug/L	1338080	1	9.72	6665000	20.0
2-Propanol, 1-(2-...	9.54	0.2	ug/L	59307	1	9.72	6665000	20.0
2-Propanol, 1-(2-...	9.63	0.2	ug/L	67114	1	9.72	6665000	20.0
2-Propanol, 1-(2-...	9.85	0.3	ug/L	108727	1	9.72	6665000	20.0
5-Nitro-2-furaldo...	18.73	1.0	ug/L	529744	3	18.34	10247400	20.0
3-Cyanocarbazole ...	22.28	0.2	ug/L	84948	4	22.63	10917400	20.0
2-Norbornanone, 1...	22.83	2.2	ug/L	1205380	4	22.63	10917400	20.0
3-Methylchromone ...	23.42	0.2	ug/L	97397	4	22.63	10917400	20.0
Sulfur, mol. (S8)...	23.70	0.1	ug/L	79691	4	22.63	10917400	20.0
Sulfur, mol. (S8)...	26.14	84.9	ug/L	46345700	4	22.63	10917400	20.0
Decanedioic acid, ...	33.40	1.1	ug/L	515064	6	34.42	9408960	20.0

