

Library Search Compound Report

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Acq On : 10 Jun 2002 6:21 pm
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Misc :
MS Integration Params: LSCINT.e

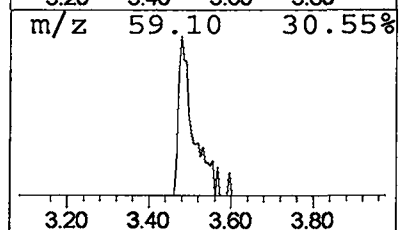
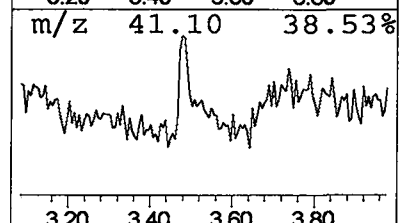
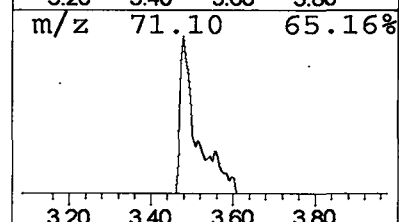
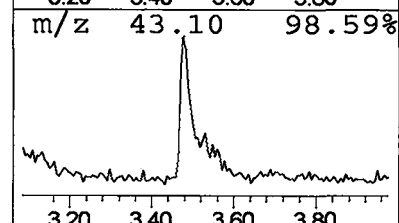
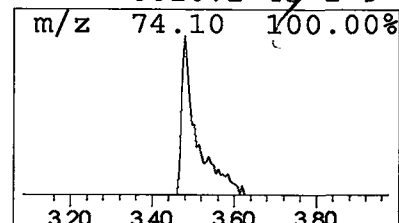
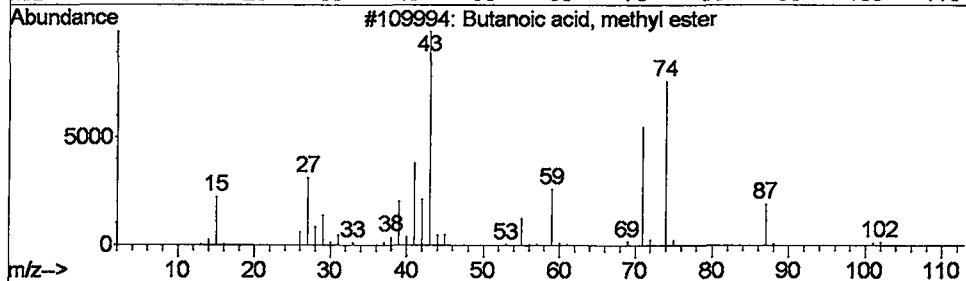
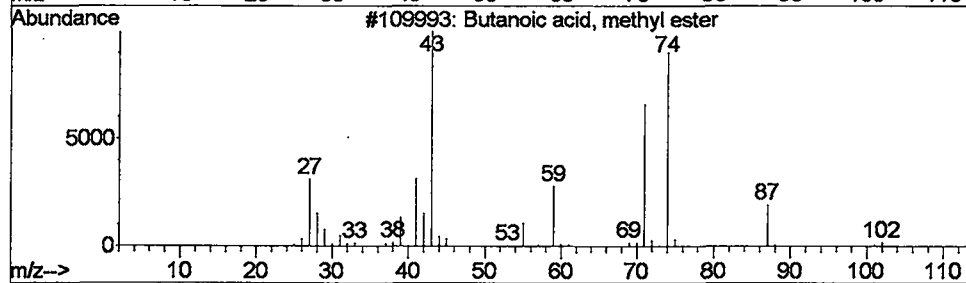
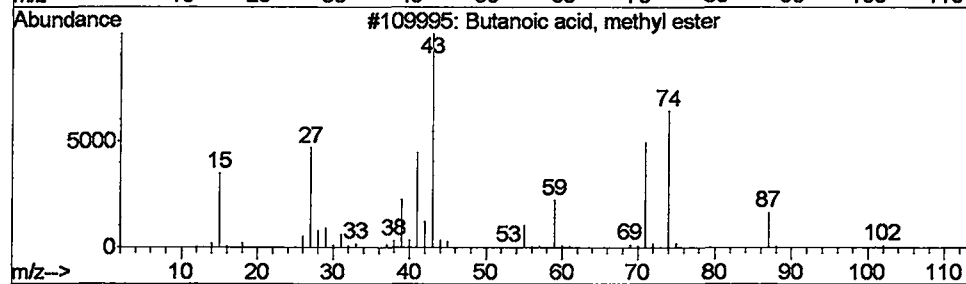
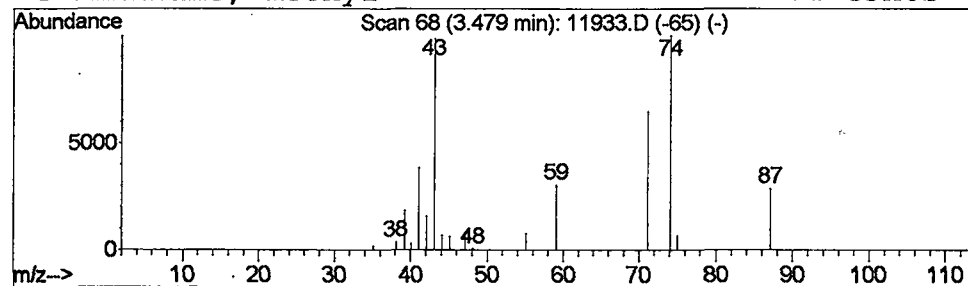
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Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 1 Butanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.48	0.36 ug/L	300922	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	64
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	56
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	45
4			Thiirane, methyl-	74	C3H6S	001072-43-1	9



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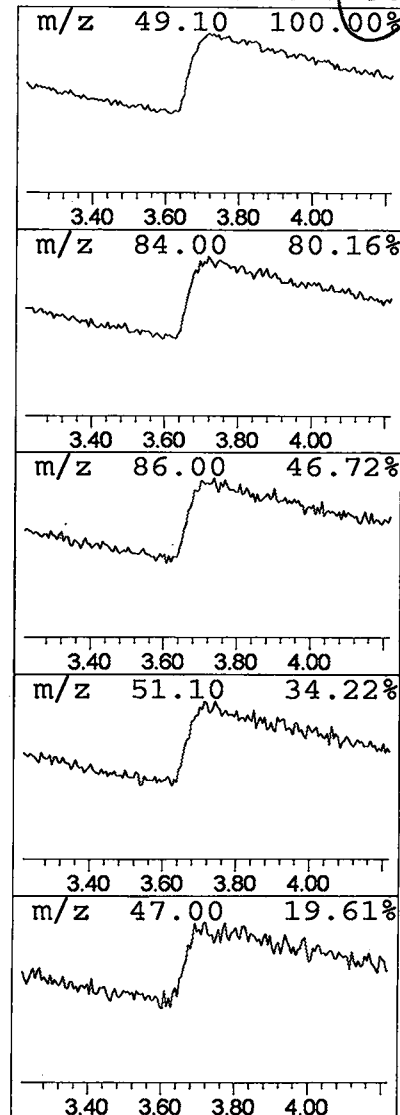
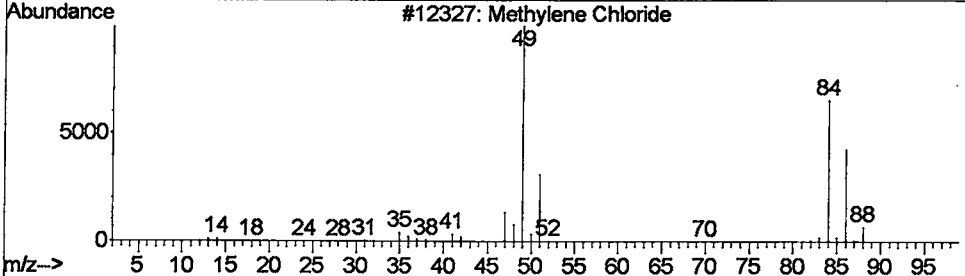
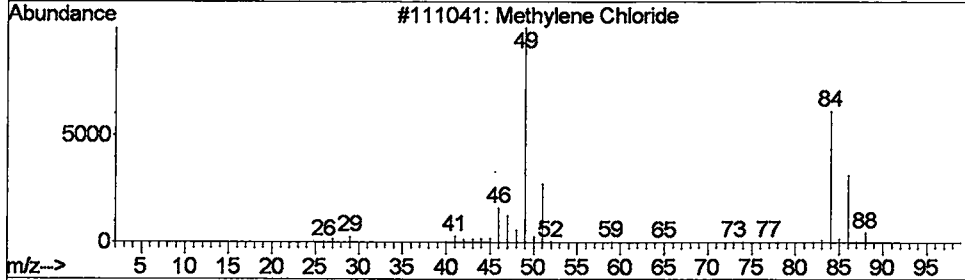
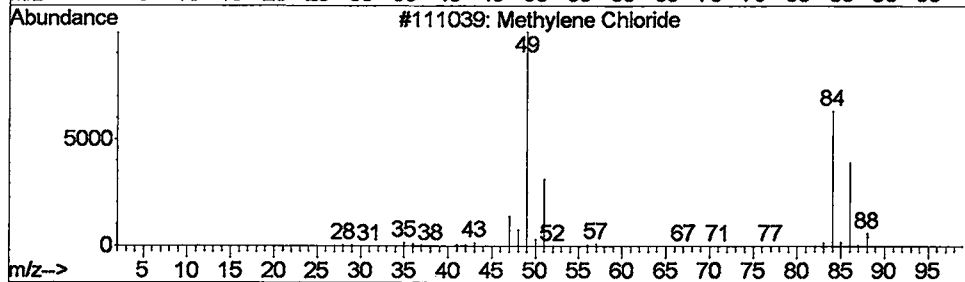
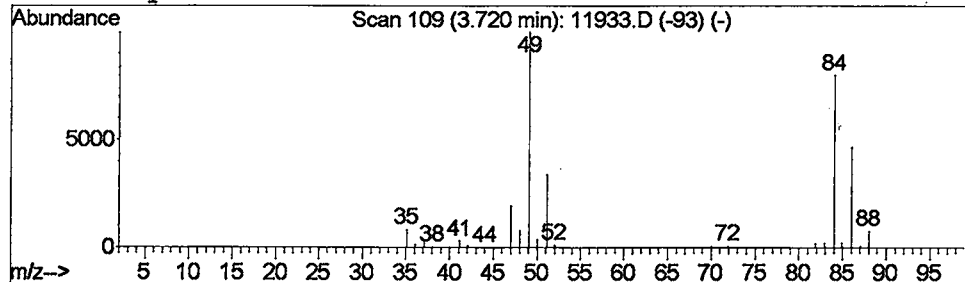
Library : C:\DATABASE\NIST98.L

Peak Number 2 Methylene Chloride

Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	3.20 ug/L	2643260	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylene Chloride	84	CH2Cl2	000075-09-2	95
2			Methylene Chloride	84	CH2Cl2	000075-09-2	91
3			Methylene Chloride	84	CH2Cl2	000075-09-2	91
4			Methylene Chloride	84	CH2Cl2	000075-09-2	90



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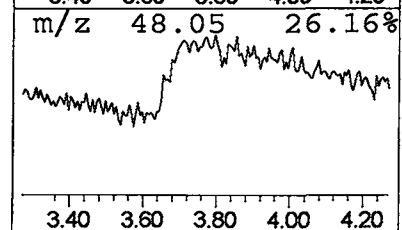
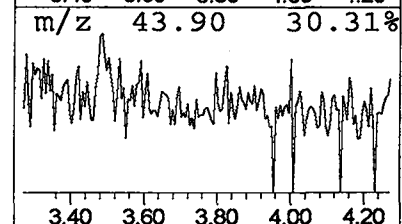
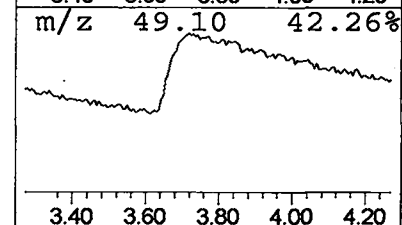
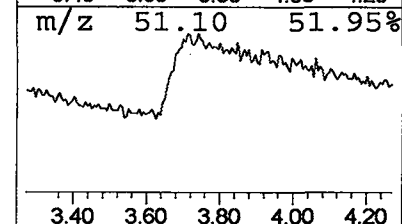
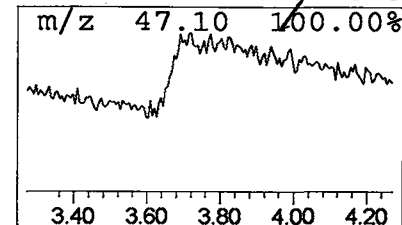
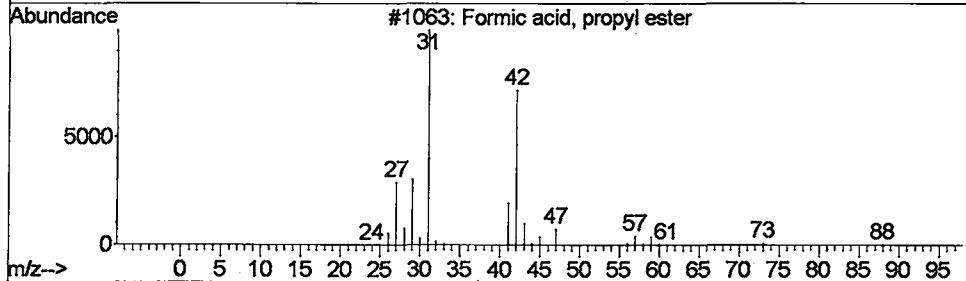
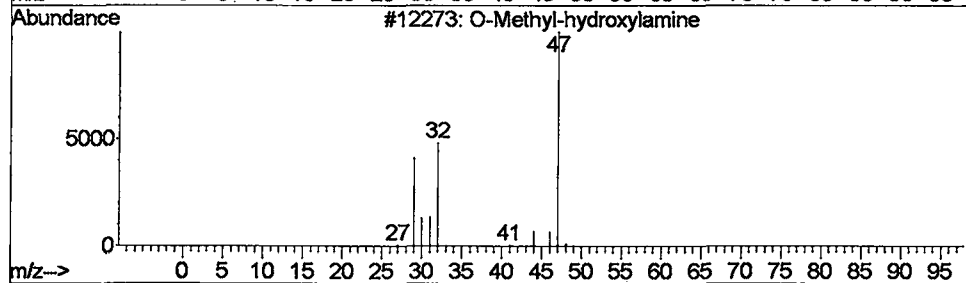
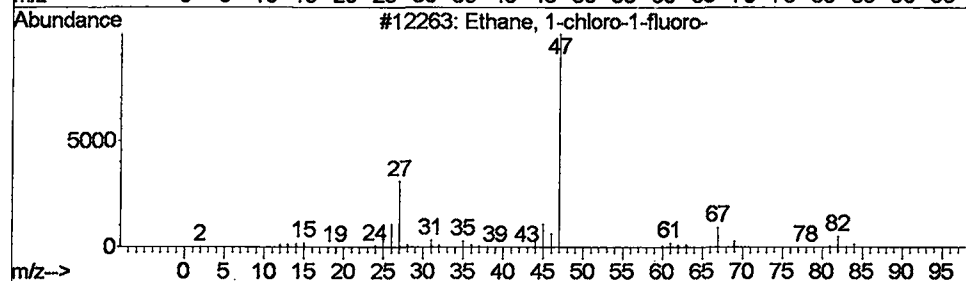
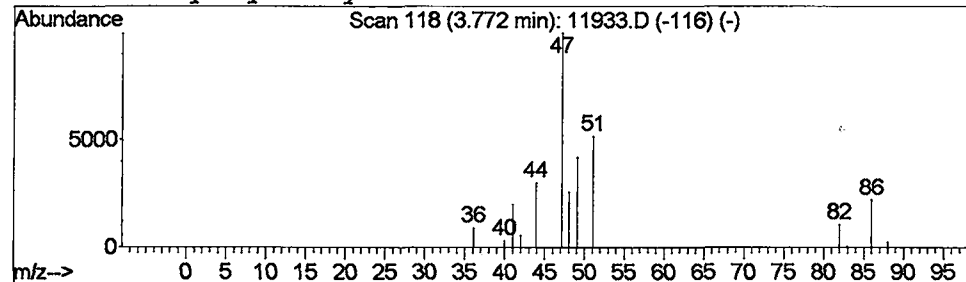
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Peak Number 3 Ethane, 1-chloro-1-fluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.77	1.08 ug/L	889846	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1-fluoro-	82	C2H4ClF	001615-75-4	4
2			O-Methyl-hydroxylamine	47	CH5NO	1000192-49-9	3
3			Formic acid, propyl ester	88	C4H8O2	000110-74-7	3
4			O-Methylhydroxylamine	47	CH5NO	1000202-02-6	3



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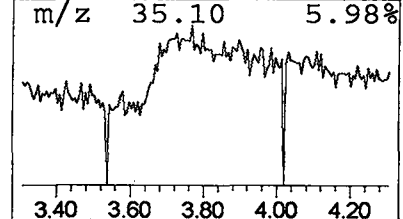
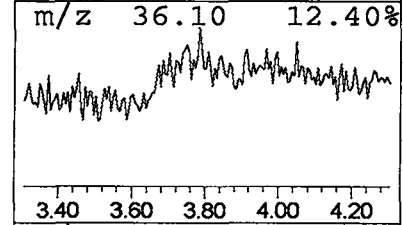
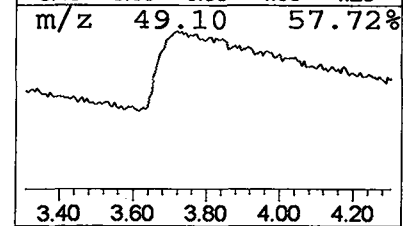
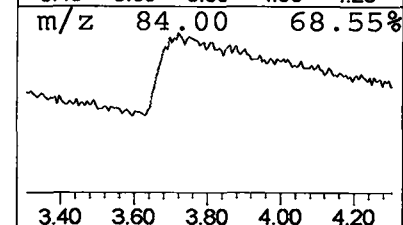
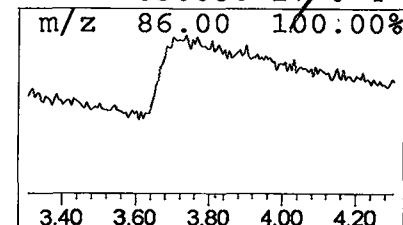
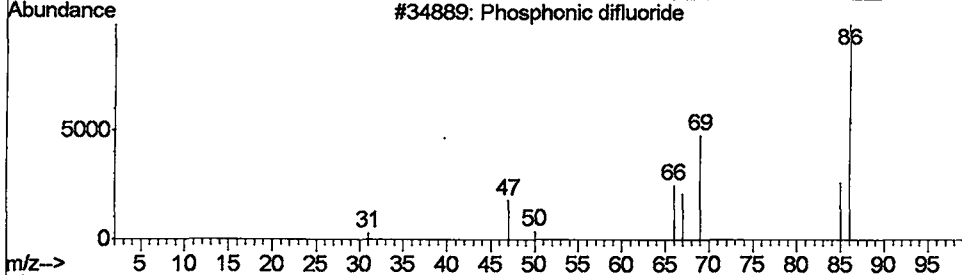
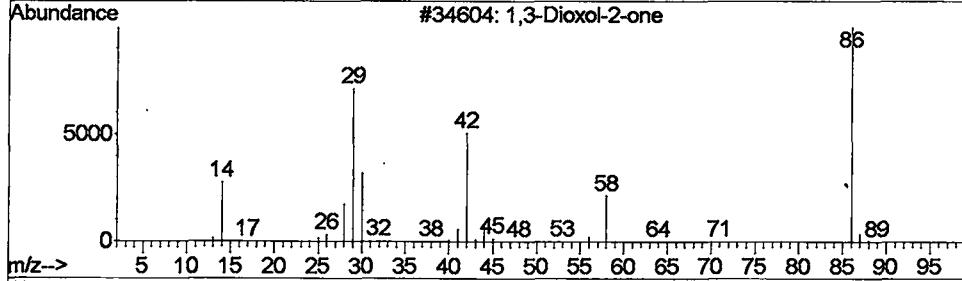
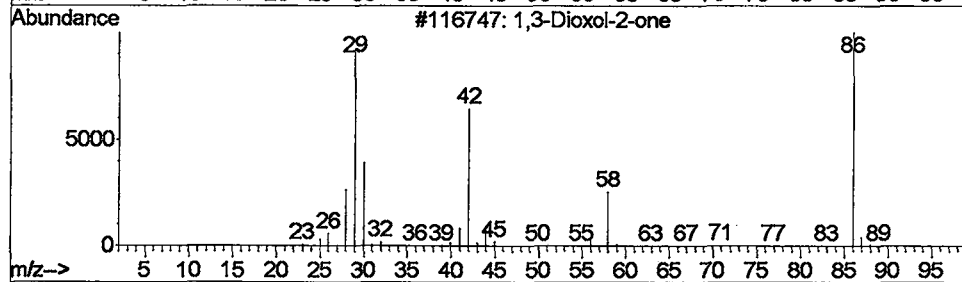
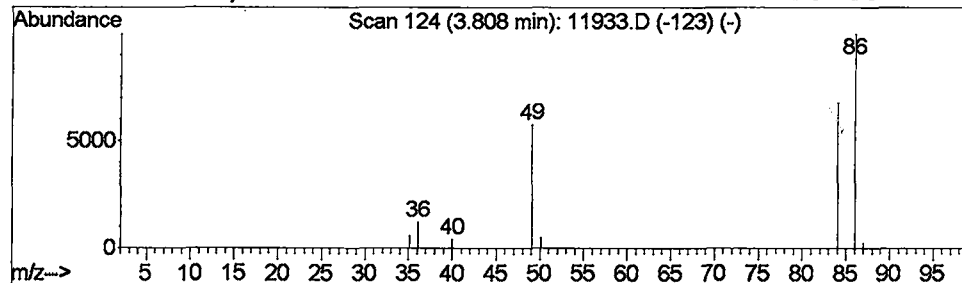
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Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
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Peak Number 4 1,3-Dioxol-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.81	0.50 ug/L	415548	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxol-2-one	86	C3H2O3	000872-36-6	4
2			1,3-Dioxol-2-one	86	C3H2O3	000872-36-6	4
3			Phosphonic difluoride	86	F2HOP	014939-34-5	4
4			Imidazol, 4-fluoro-	86	C3H3FN2	030086-17-0	4



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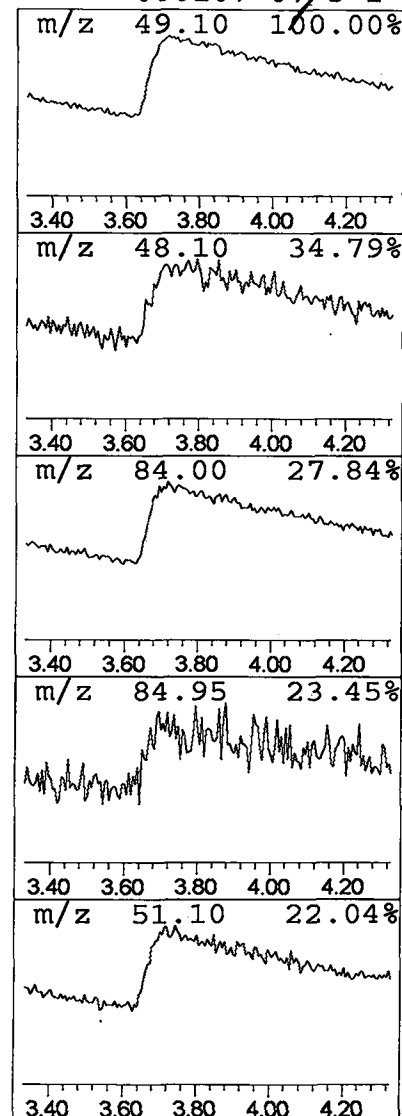
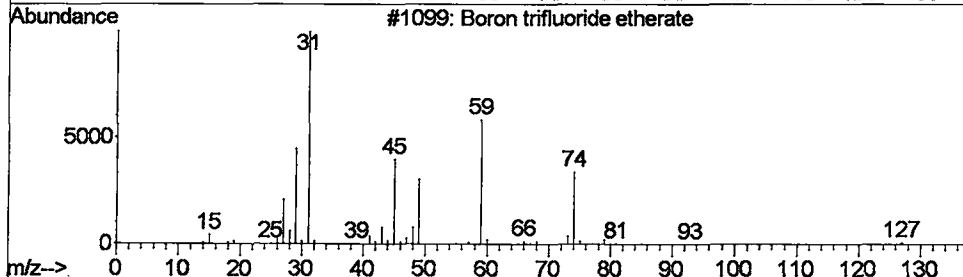
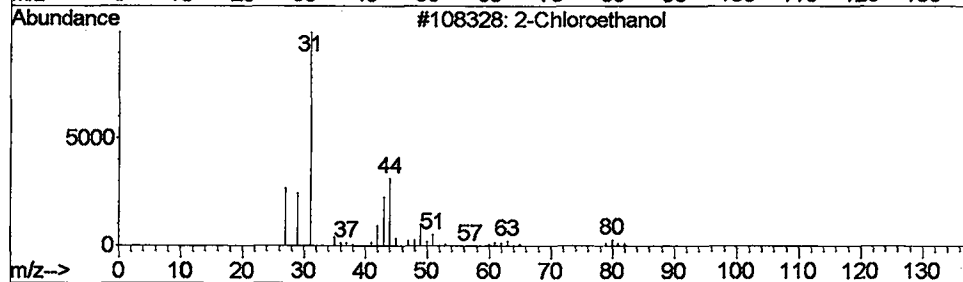
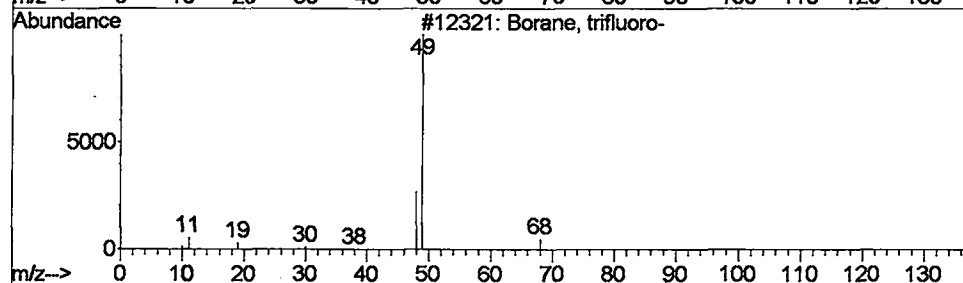
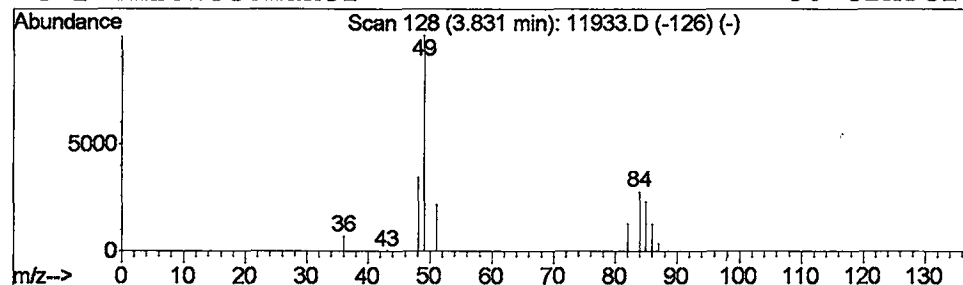
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Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 5 Borane, trifluoro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.83	0.98 ug/L	812169	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Borane, trifluoro-	68	BF3	007637-07-2	2
2			2-Chloroethanol	80	C2H5ClO	000107-07-3	2
3			Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	2
4			2-Chloroethanol	80	C2H5ClO	000107-07-3	2



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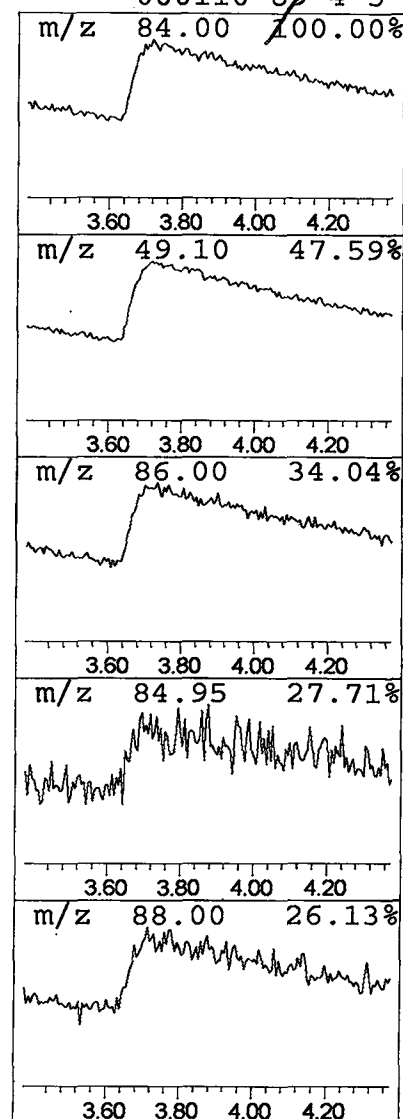
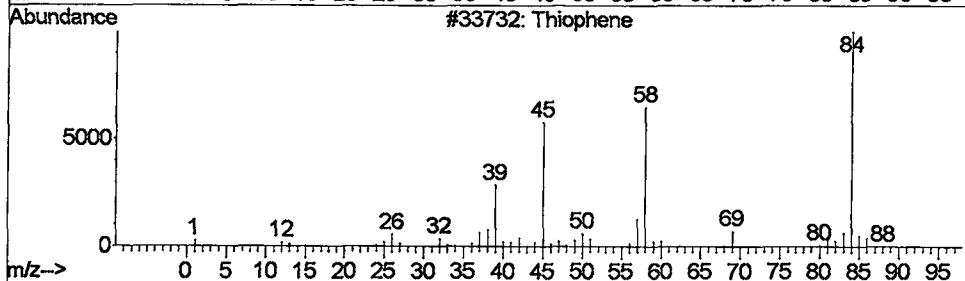
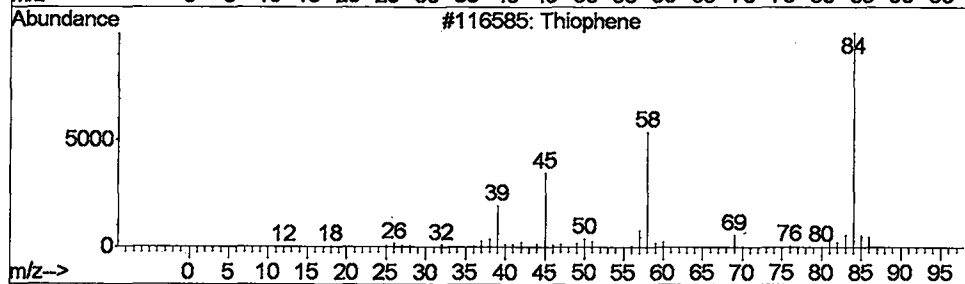
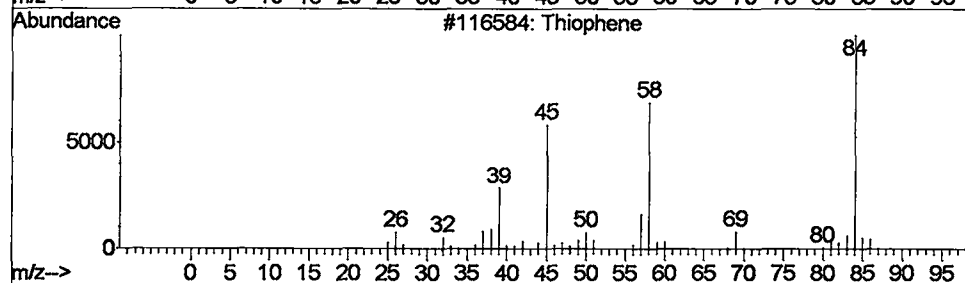
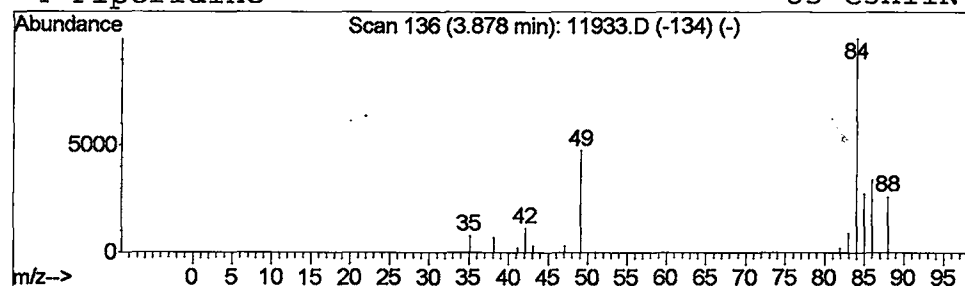
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Library : C:\DATABASE\NIST98.L

Peak Number 6 Thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.88	0.41 ug/L	335342	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene	84	C4H4S	000110-02-1	9
2			Thiophene	84	C4H4S	000110-02-1	9
3			Thiophene	84	C4H4S	000110-02-1	5
4			Piperidine	85	C5H11N	000110-89-4	5



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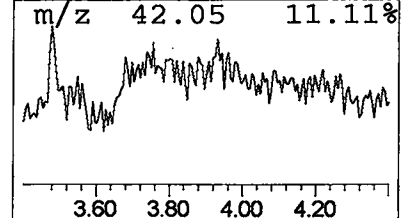
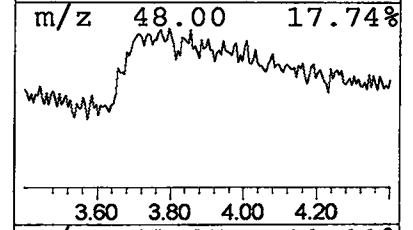
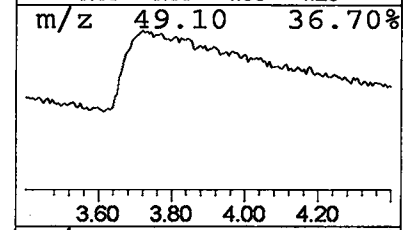
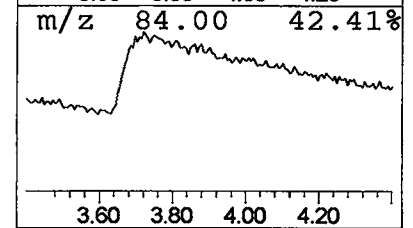
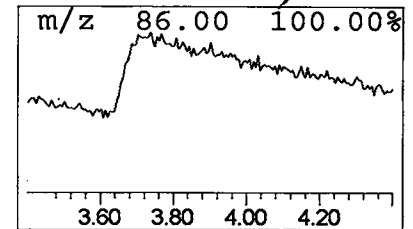
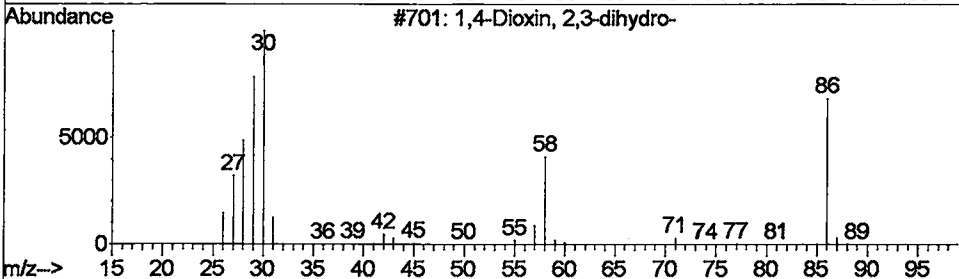
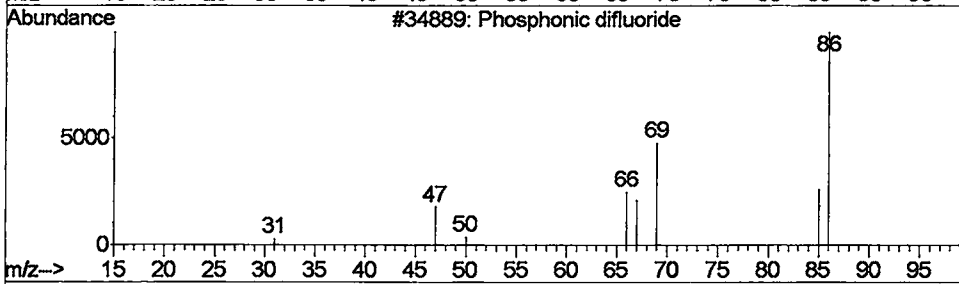
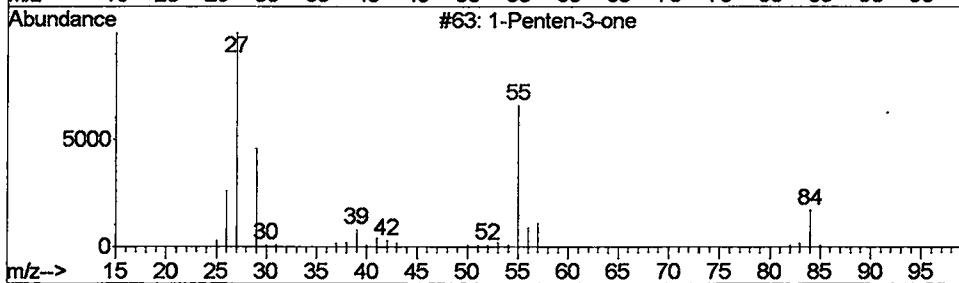
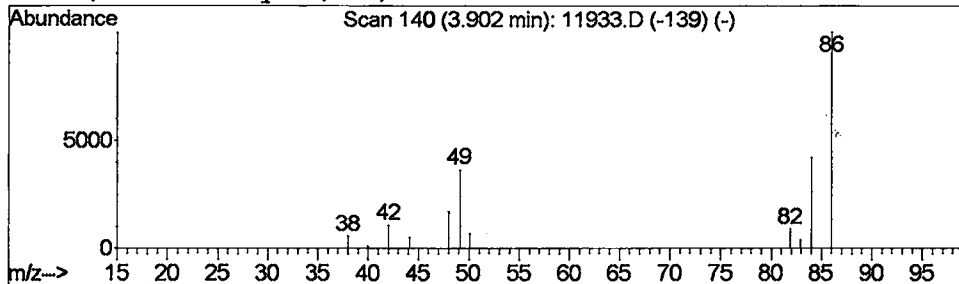
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Peak Number 7 1-Penten-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.90	0.62 ug/L	508579	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Penten-3-one	84	C5H8O	001629-58-9	5
2			Phosphonic difluoride	86	F2HOP	014939-34-5	4
3			1,4-Dioxin, 2,3-dihydro-	86	C4H6O2	000543-75-9	3
4			1,3-Butadiyne, 1,4-difluoro-	86	C4F2	064788-23-4	2



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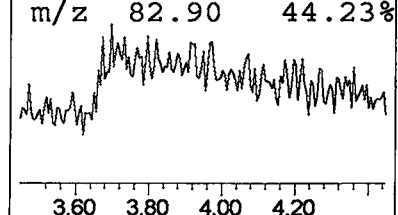
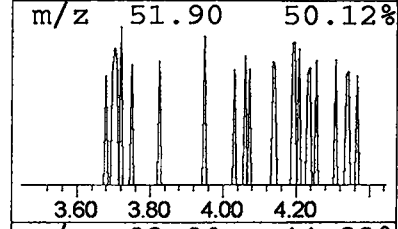
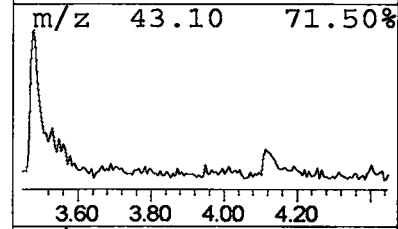
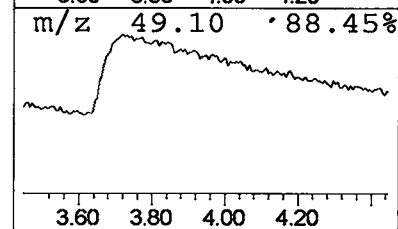
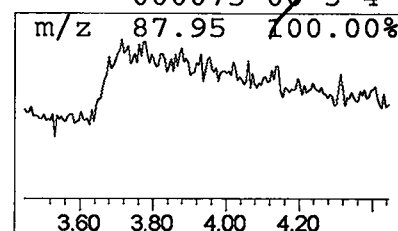
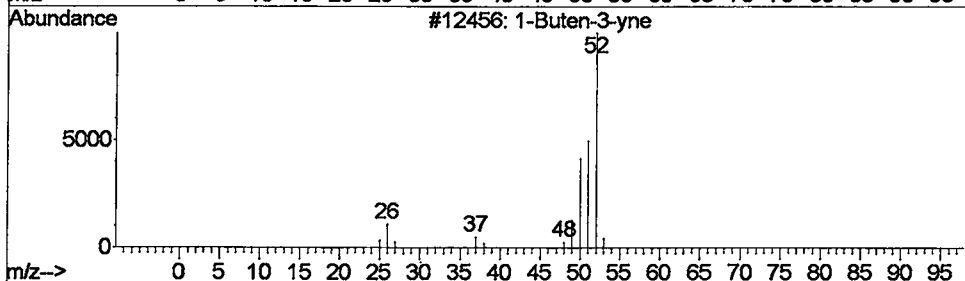
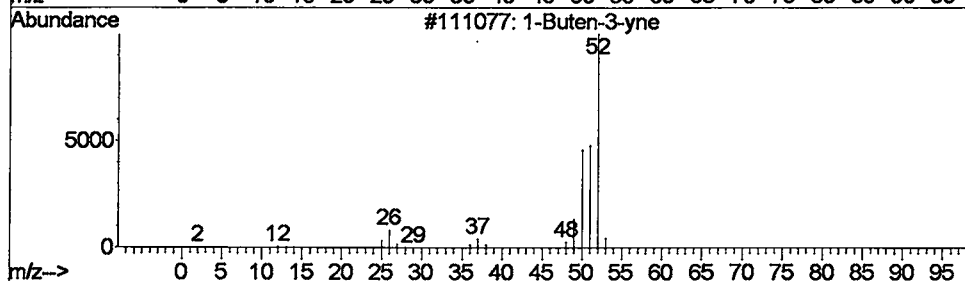
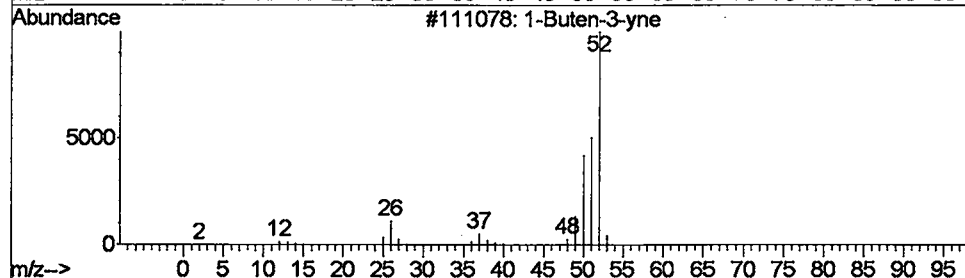
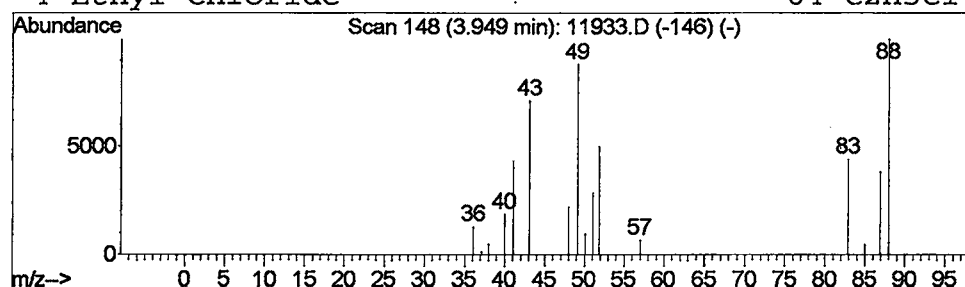
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Peak Number 8 1-Buten-3-yne Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	0.42 ug/L	345661	1,4-dichlorobenzene-d4	9.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Buten-3-yne		52	C4H4	000689-97-4	5
2	1-Buten-3-yne		52	C4H4	000689-97-4	5
3	1-Buten-3-yne		52	C4H4	000689-97-4	5
4	Ethyl Chloride		64	C2H5Cl	000075-00-3	4



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\0610022\11933.D
Acq On : 10 Jun 2002 6:21 pm
Sample : gc/ms scan 6/7 fb
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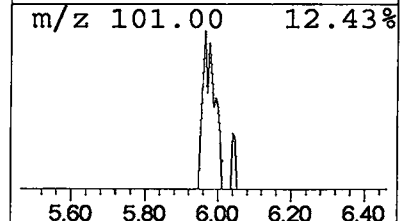
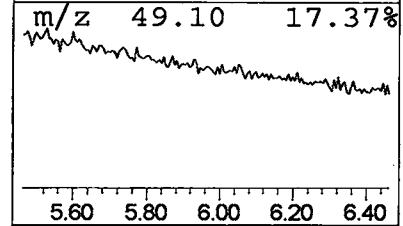
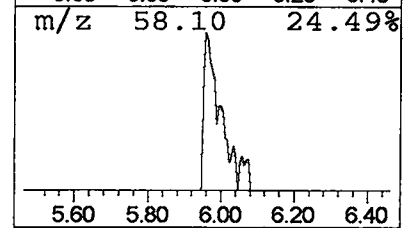
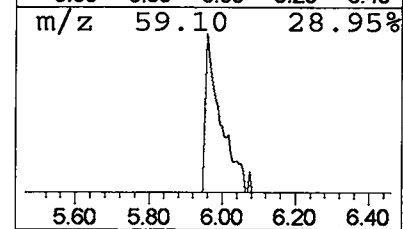
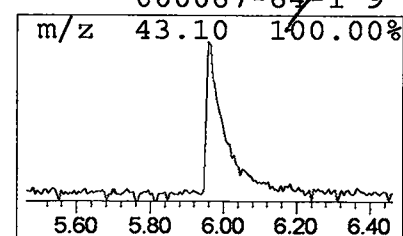
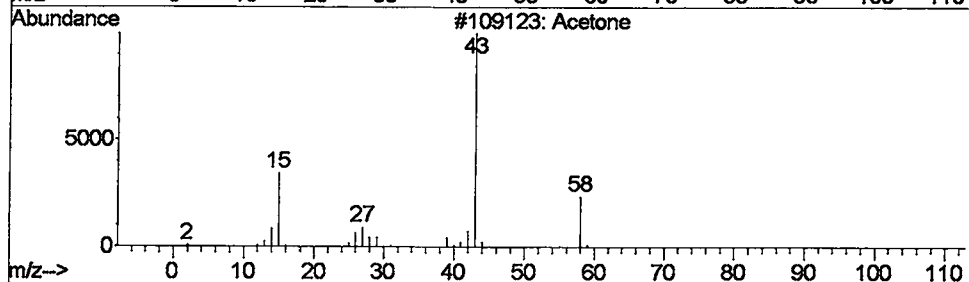
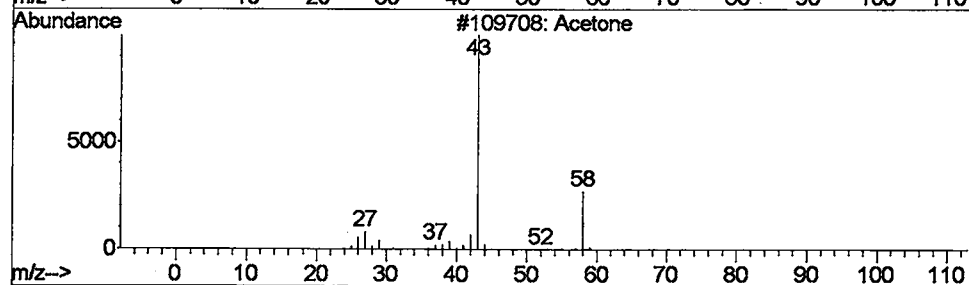
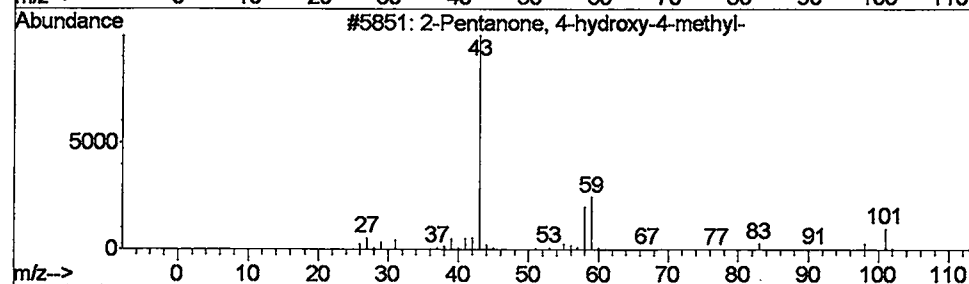
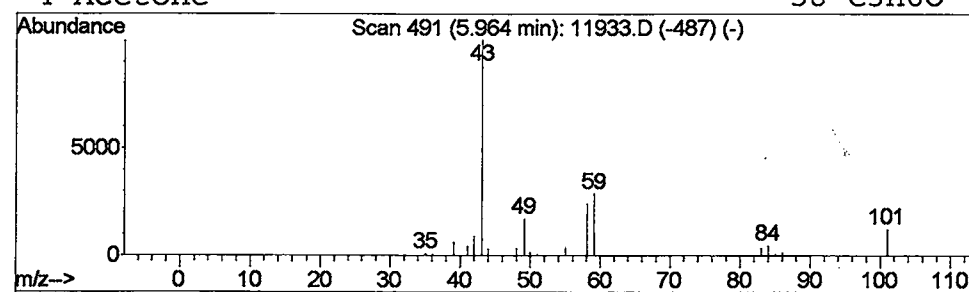
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Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 9 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	0.24 ug/L	194784	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetone	58	C3H6O	000067-64-1	25
3			Acetone	58	C3H6O	000067-64-1	25
4			Acetone	58	C3H6O	000067-64-1	9



Data File : C:\MSDCHEM\1\DATA\0610022\11933.D

Acq On : 10 Jun 2002 6:21 pm

Sample : gc/ms scan 6/7 fb

Misc :

MS Integration Params: LSCINT.e

Vial: 10

Operator:

Inst : Instrumen

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Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)

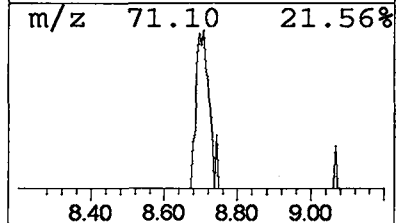
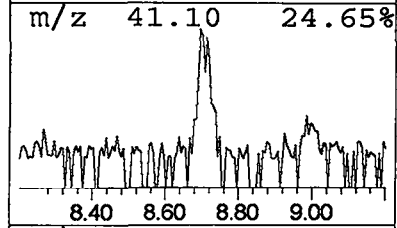
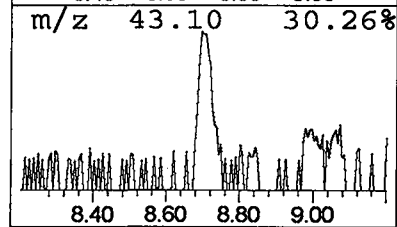
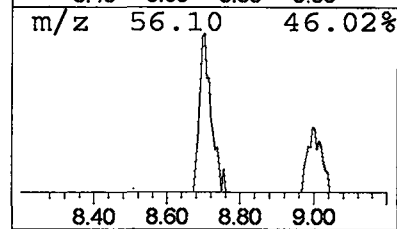
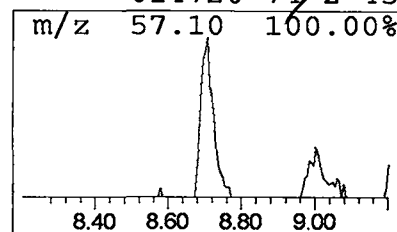
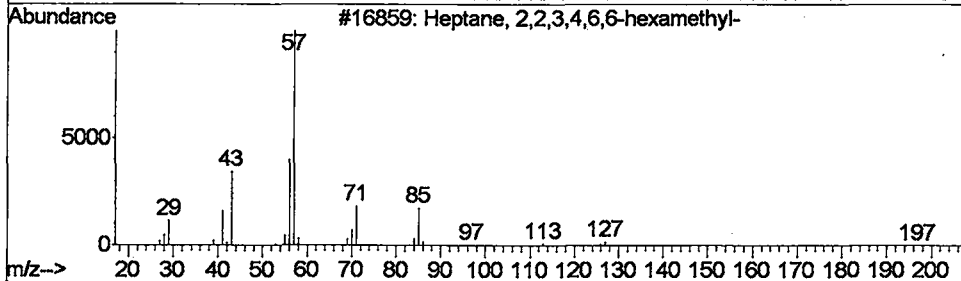
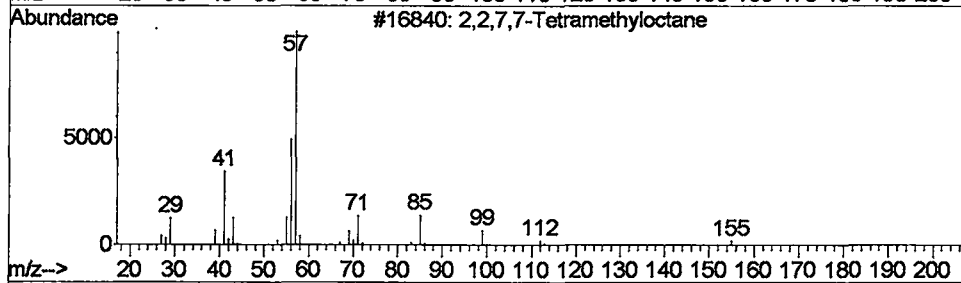
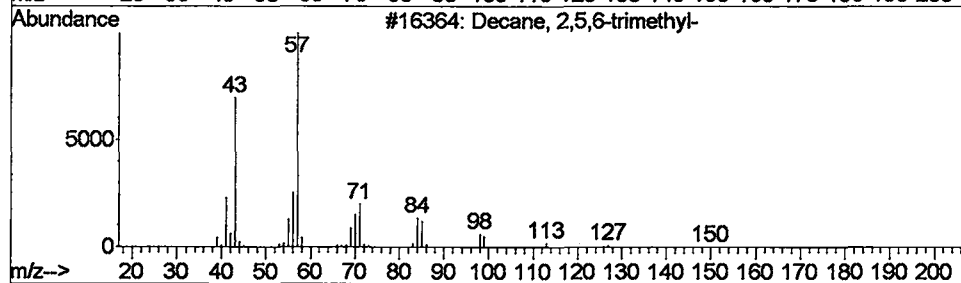
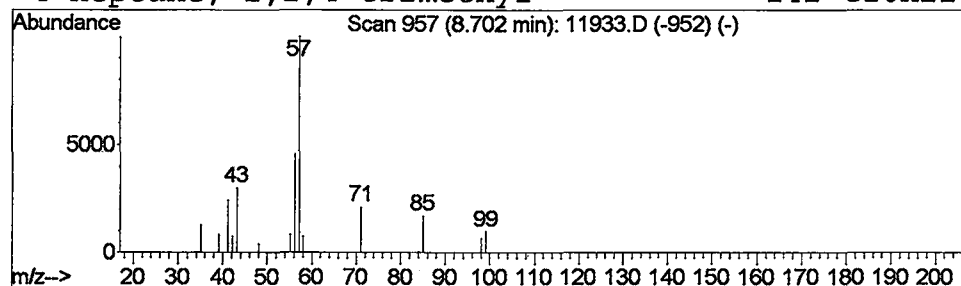
Title : 508 Modified GC/MS scan

Library : C:\DATABASE\NIST98.L

Peak Number 10 Decane, 2,5,6-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	0.21 ug/L	174815	1,4-dichlorobenzene-d4	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	59
2			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	50
3			Heptane, 2,2,3,4,6,6-hexamethyl-	184	C13H28	062108-32-1	45
4			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	45



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\0610022\11933.D
 Acq On : 10 Jun 2002 6:21 pm
 Sample : gc/ms scan 6/7 fb
 Misc :
 MS Integration Params: LSCINT.e

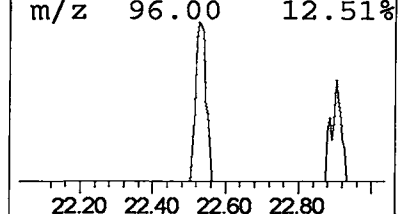
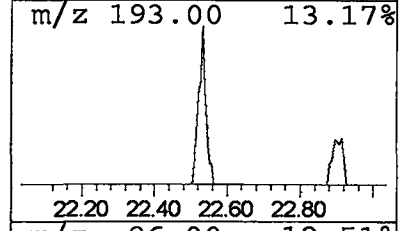
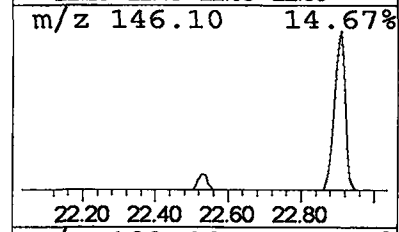
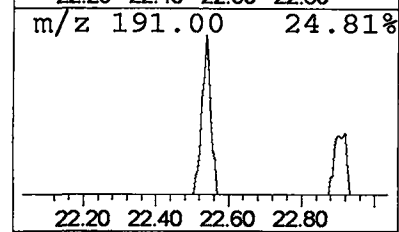
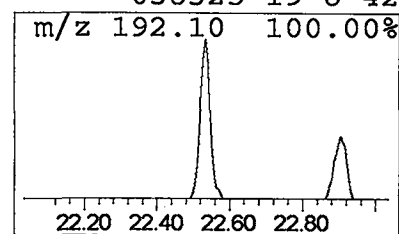
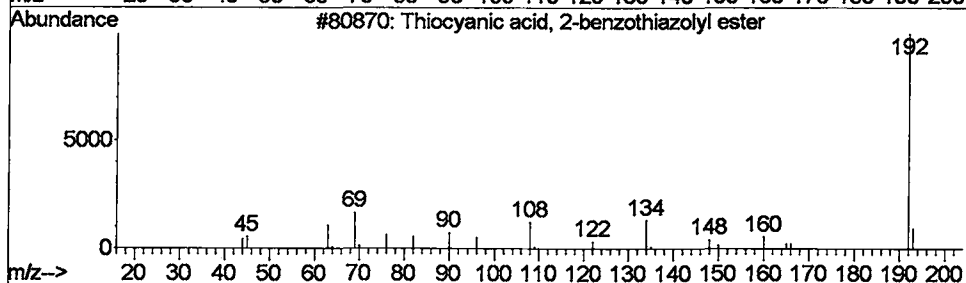
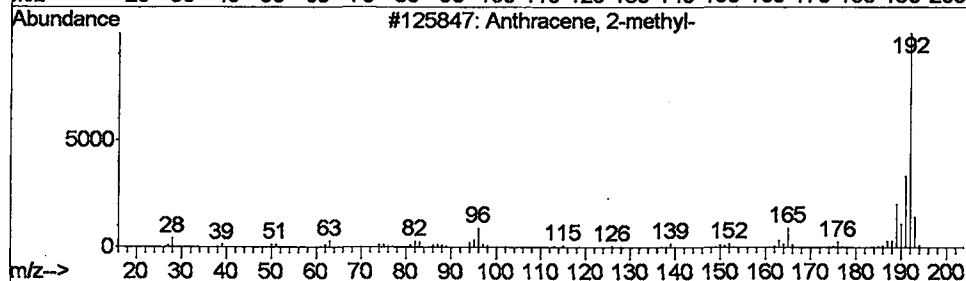
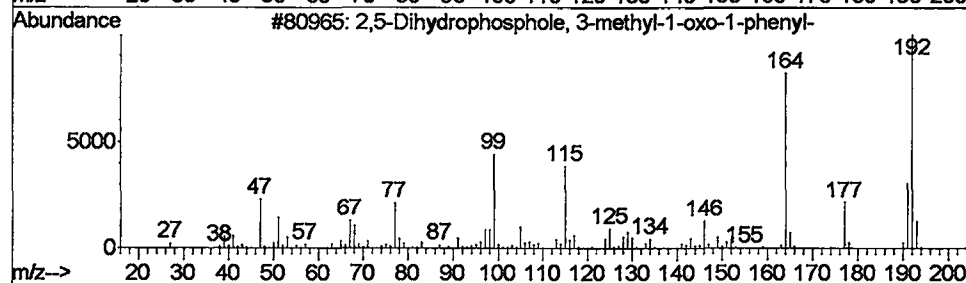
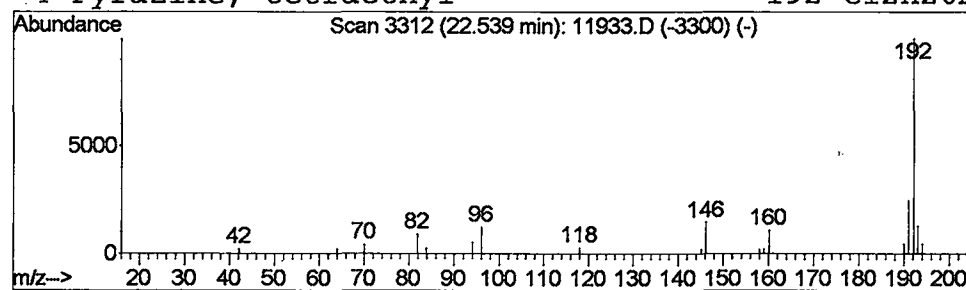
Vial: 10
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
 Title : 508 Modified GC/MS scan
 Library : C:\DATABASE\NIST98.L

 Peak Number 11 2,5-Dihydrophosphole, 3-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	0.25 ug/L	305875	Phenanthranene-d10	22.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Dihydrophosphole, 3-methyl-1...	192	C11H13OP	1000196-97-5	53
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
3			Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	42
4			Pyrazine, tetraethyl-	192	C12H20N2	038325-19-8	42



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\0610022\11933.D
Acq On : 10 Jun 2002 6:21 pm
Sample : gc/ms scan 6/7 fb
Misc :
MS Integration Params: LSCINT.e

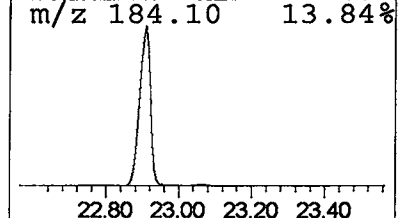
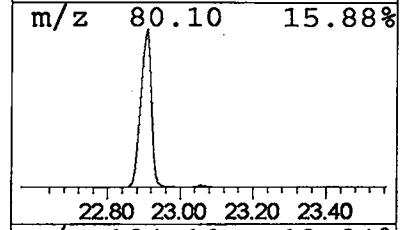
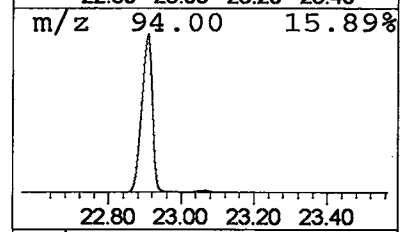
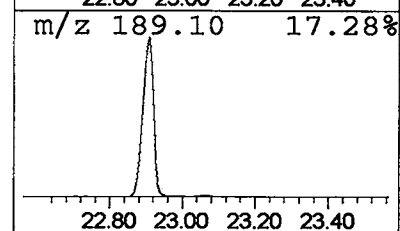
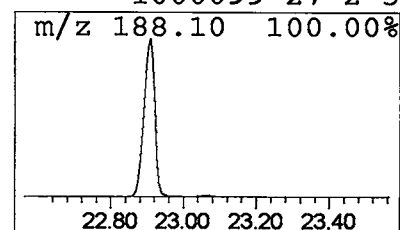
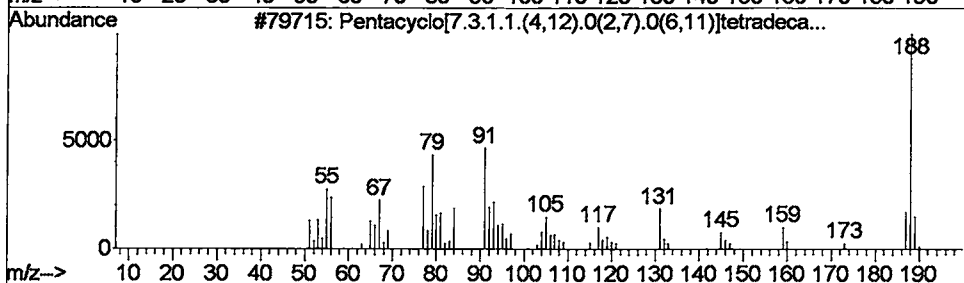
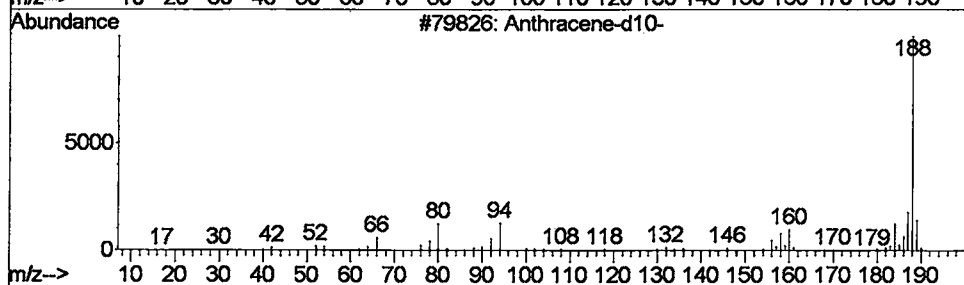
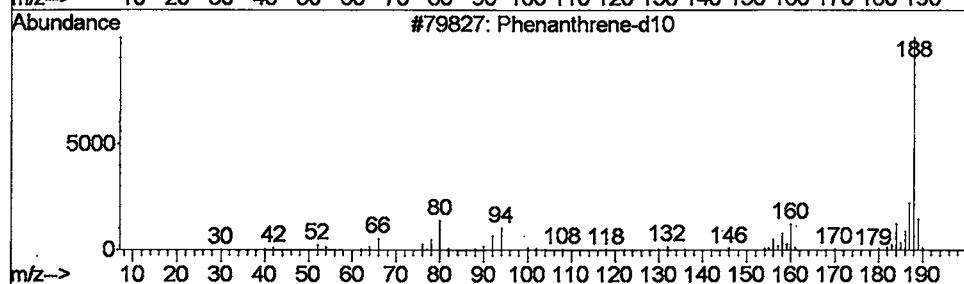
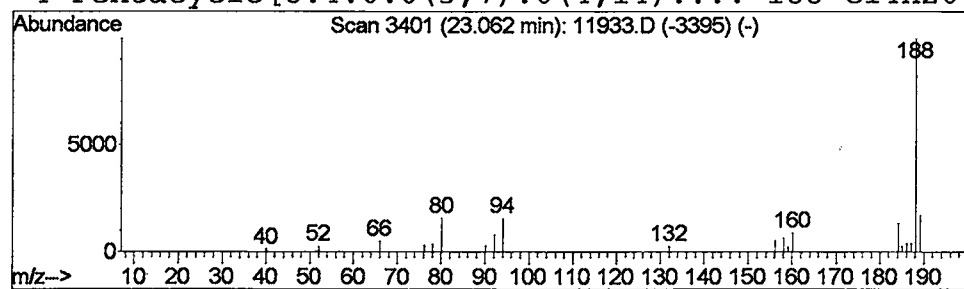
Vial: 10
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 12 Phenanthrene-d10 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.06	0.30 ug/L	360410	Phenanthranene-d10	22.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene-d10	188	C14D10	001517-22-2	86
2		Anthracene-d10-	188	C14D10	001719-06-8	64
3		Pentacyclo[7.3.1.1.(4,12).0(2,7)...]	188	C14H20	1000215-61-8	45
4		Pentacyclo[8.4.0.0(3,7).0(4,14)...]	188	C14H20	1000099-27-2	36



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 10 Jun 2002 6:21 pm
Data File: C:\MSDCHEM\1\DATA\0610022\11933.D
Name: gc/ms scan 6/7 fb
Misc:
Method: C:\MSDCHEM\1\METHODS\060302.M (Chemstation Integrator)
Title: 508 Modified GC/MS scan
Library Searched: C:\DATABASE\NIST98.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, me...	3.48	0.4	ug/L	300922	1	9.90	33036000	40.0
Methylene Chloride	3.72	3.2	ug/L	2643260	1	9.90	33036000	40.0
Ethane, 1-chloro-...	3.77	1.1	ug/L	889846	1	9.90	33036000	40.0
1,3-Dioxol-2-one	3.81	0.5	ug/L	415548	1	9.90	33036000	40.0
Borane, trifluoro-	3.83	1.0	ug/L	812169	1	9.90	33036000	40.0
Thiophene	3.88	0.4	ug/L	335342	1	9.90	33036000	40.0
1-Penten-3-one	3.90	0.6	ug/L	508579	1	9.90	33036000	40.0
1-Buten-3-yne	3.95	0.4	ug/L	345661	1	9.90	33036000	40.0
2-Pentanone, 4-hy...	5.96	0.2	ug/L	194784	1	9.90	33036000	40.0
Decane, 2,5,6-tri...	8.70	0.2	ug/L	174815	1	9.90	33036000	40.0
2,5-Dihydrophosph...	22.54	0.3	ug/L	305875	4	22.91	48422600	40.0
Phenanthrene-d10	23.06	0.3	ug/L	360410	4	22.91	48422600	40.0