

Library Search Compound Report

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Acq On : 7 Jun 2002 11:02 am
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Misc :
MS Integration Params: LSCINT.e

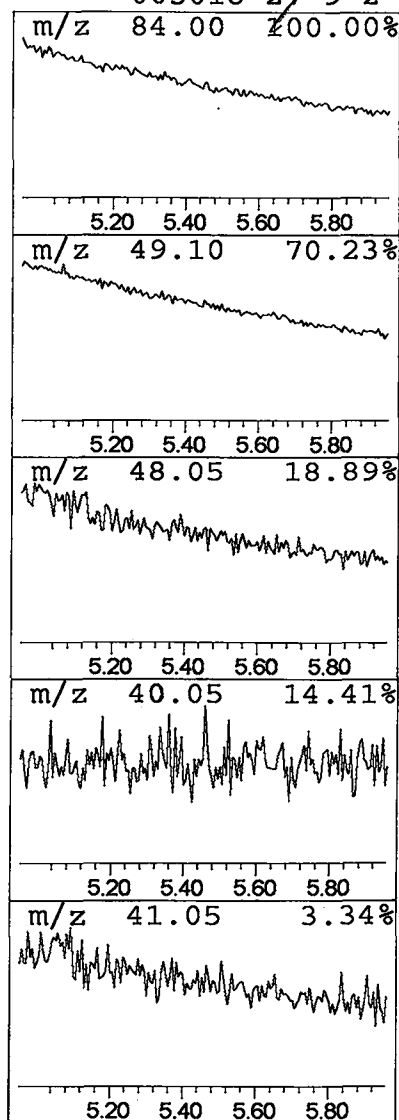
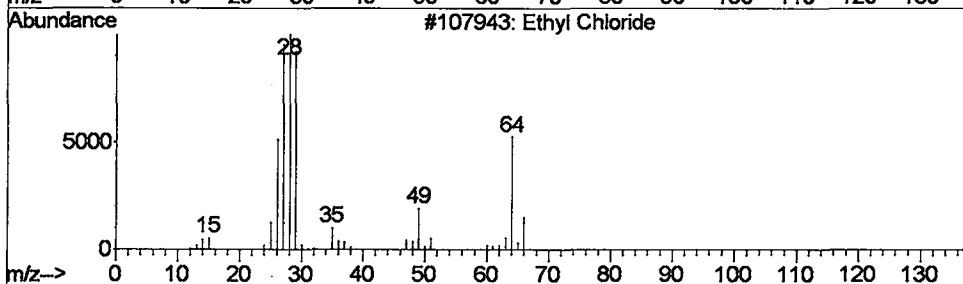
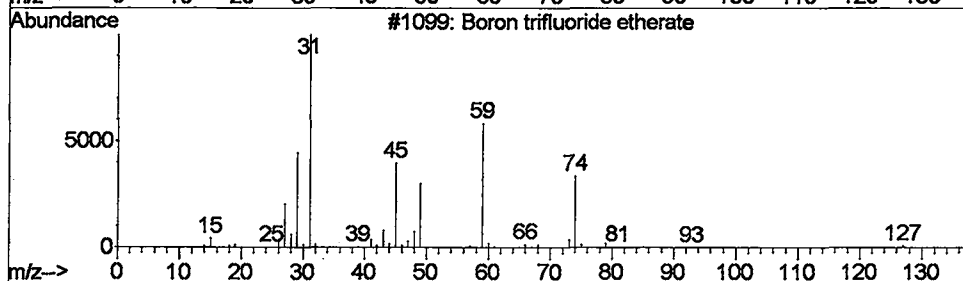
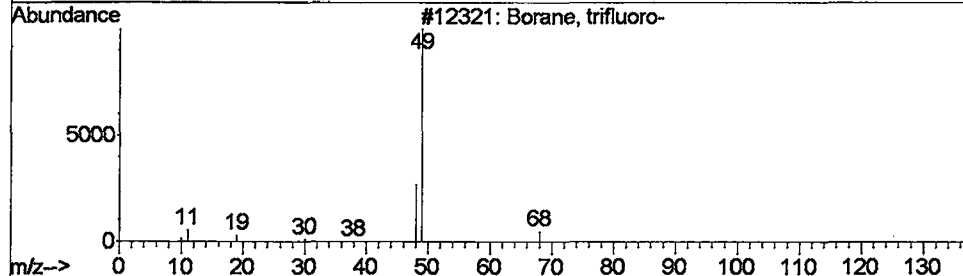
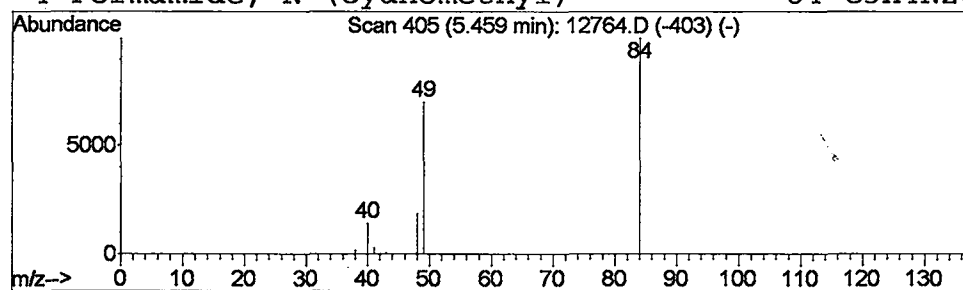
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Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 15 Borane, trifluoro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.46	0.40 ug/L	236789	1,4-dichlorobenzene-d4	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Borane, trifluoro-	68	BF3	007637-07-2	2
2		Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	2
3		Ethyl Chloride	64	C2H5Cl	000075-00-3	2
4		Formamide, N-(cyanomethyl)-	84	C3H4N2O	005018-27-9	2



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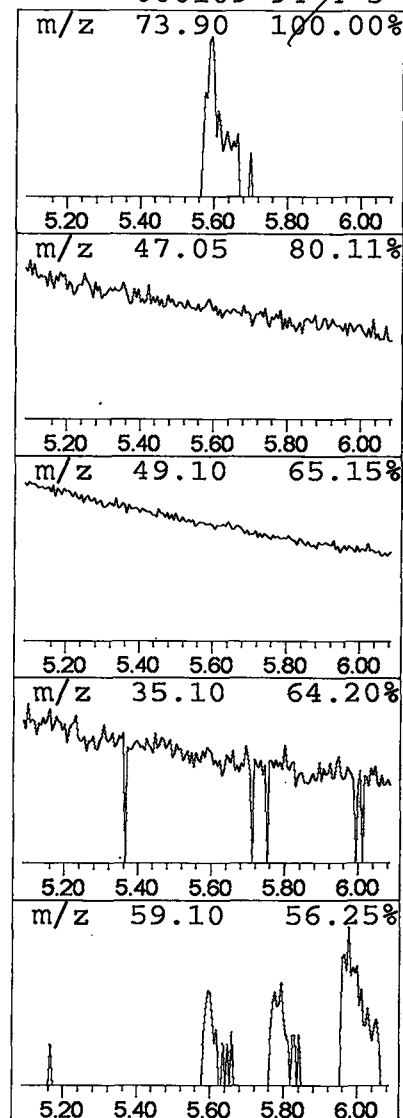
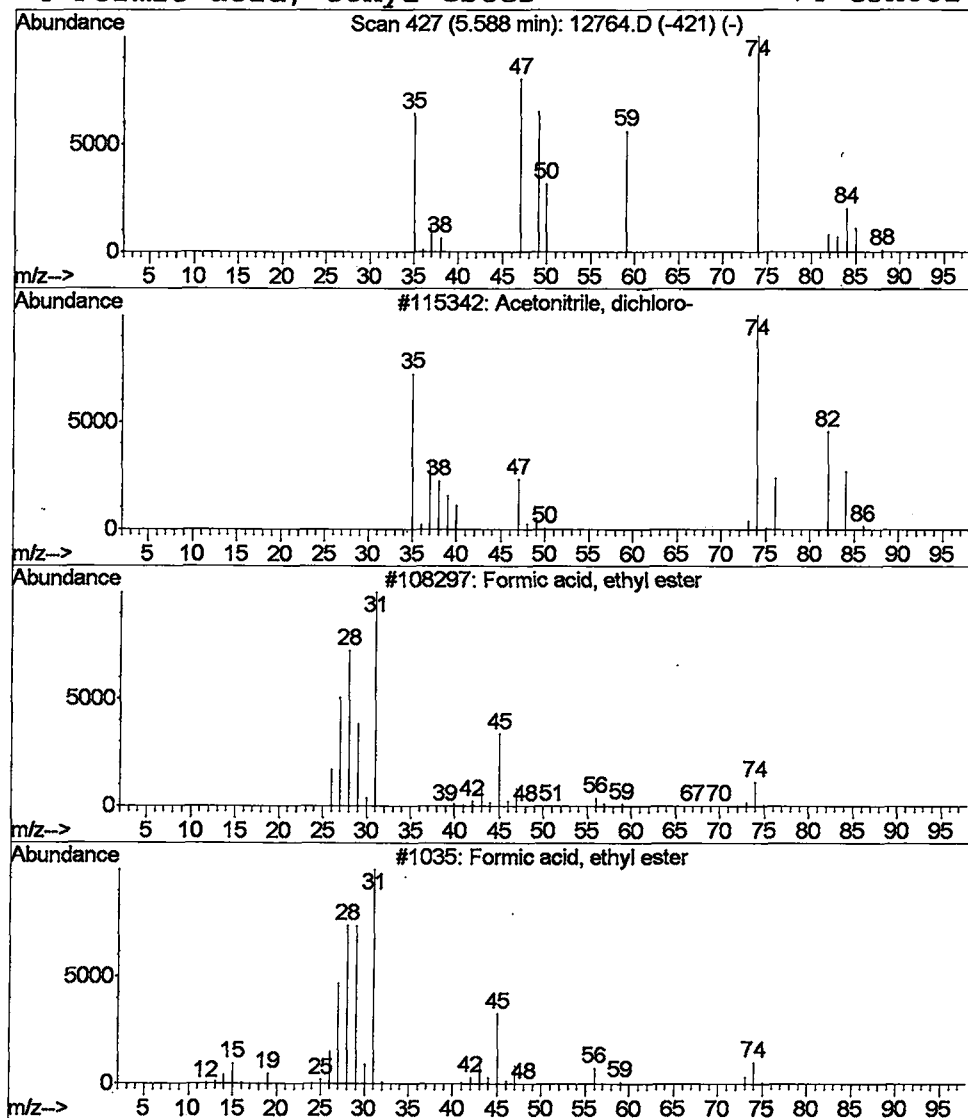
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Multiplr: 1.00

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Peak Number 16 Acetonitrile, dichloro- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	0.47 ug/L	278438	1,4-dichlorobenzene-d4	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	9
2		Formic acid, ethyl ester	74	C3H6O2	000109-94-4	3
3		Formic acid, ethyl ester	74	C3H6O2	000109-94-4	3
4		Formic acid, ethyl ester	74	C3H6O2	000109-94-4	3



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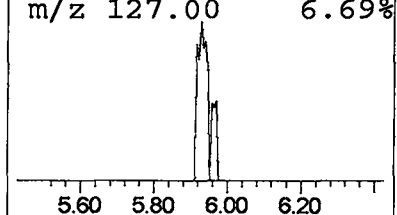
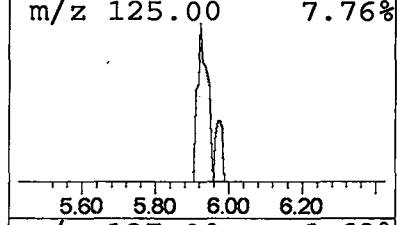
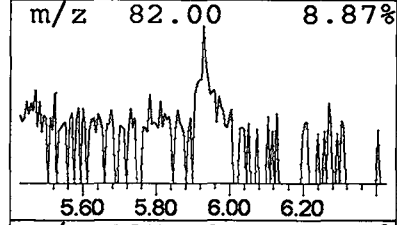
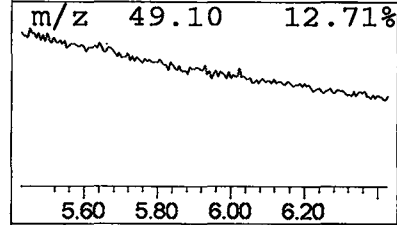
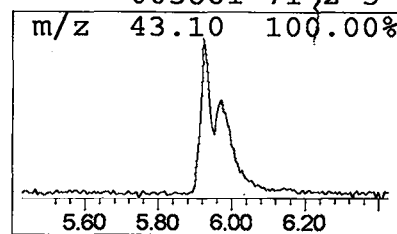
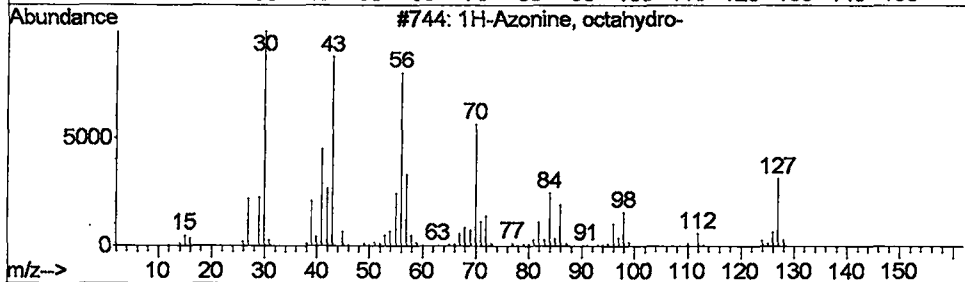
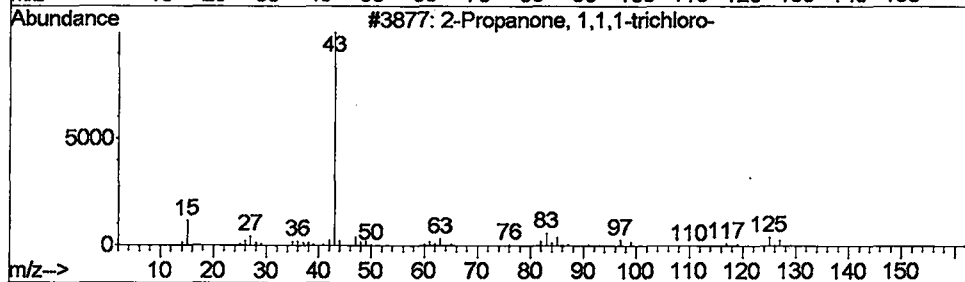
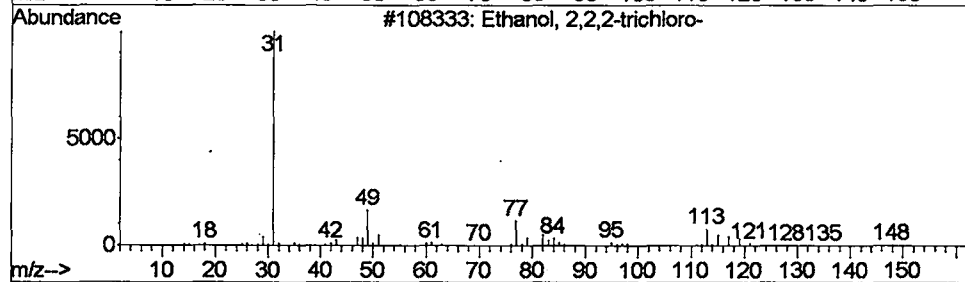
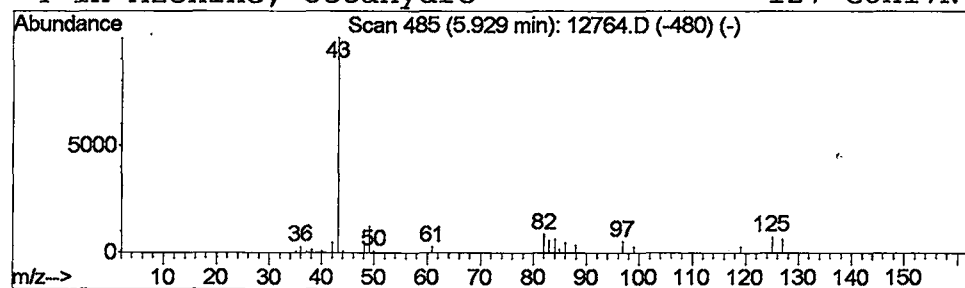
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Peak Number 17 Ethanol, 2,2,2-trichloro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	0.39 ug/L	232376	1,4-dichlorobenzene-d4	9.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2,2,2-trichloro-	148	C2H3Cl3O	000115-20-8	9
2			2-Propanone, 1,1,1-trichloro-	160	C3H3Cl3O	000918-00-3	9
3			1H-Azonine, octahydro-	127	C8H17N	005661-71-2	7
4			1H-Azonine, octahydro-	127	C8H17N	005661-71-2	5



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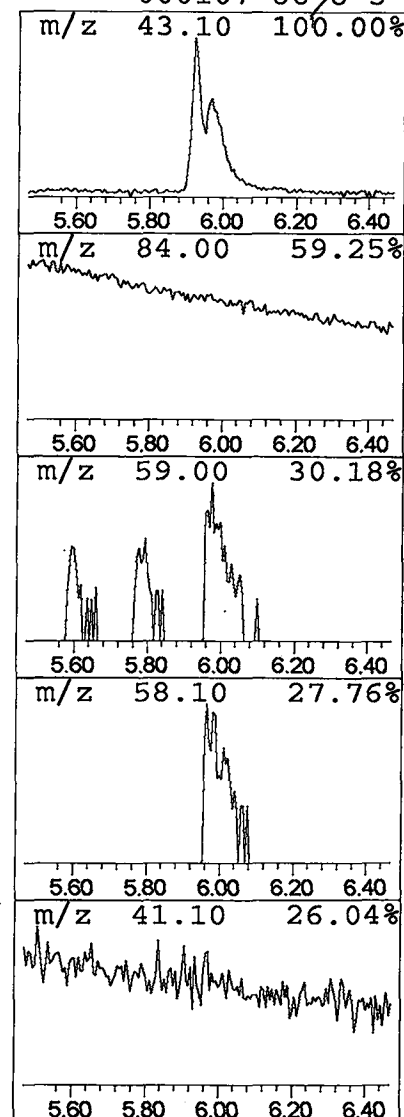
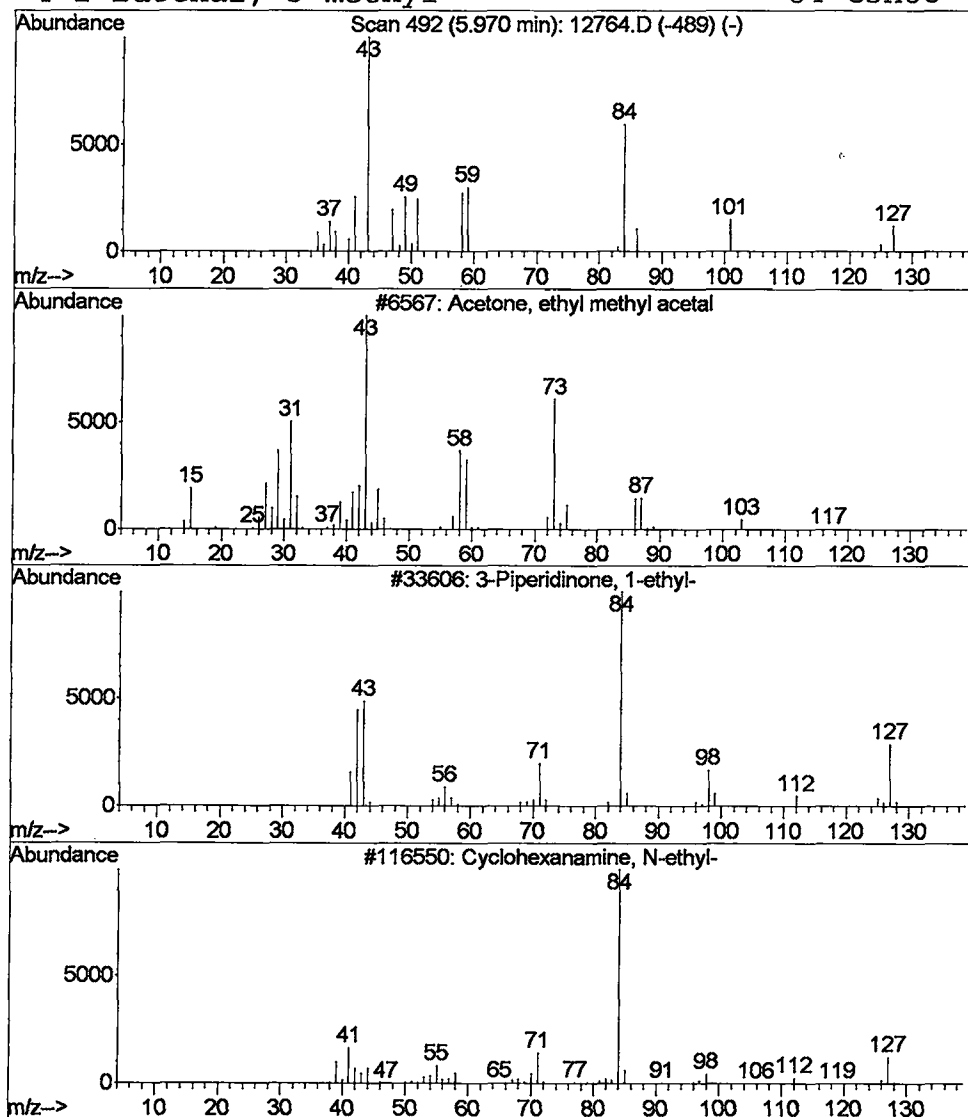
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 18 Acetone, ethyl methyl acetal Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	0.30 ug/L	179801	1,4-dichlorobenzene-d4	9.89

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone, ethyl methyl acetal	118	C6H14O2	029328-22-1	9
2	3-Piperidinone, 1-ethyl-	127	C7H13NO	043152-93-8	7
3	Cyclohexanamine, N-ethyl-	127	C8H17N	005459-93-8	5
4	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	5



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MS Integration Params: LSCINT.e

Vial: 4

Operator:

Inst : Instrumen

Multiplr: 1.00

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

Title : 508 Modified GC/MS scan

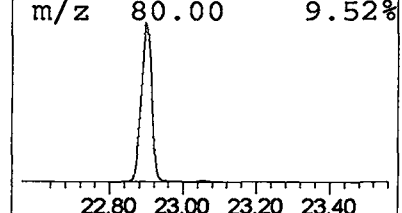
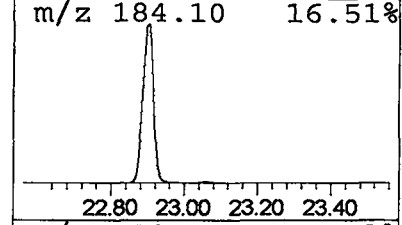
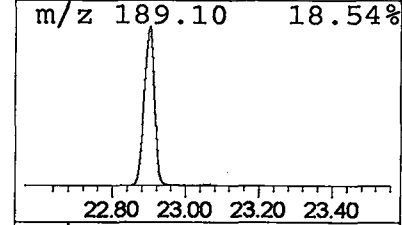
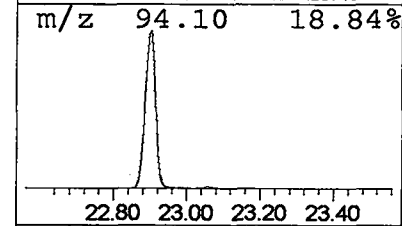
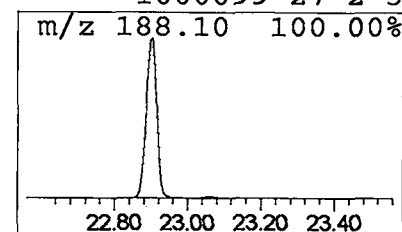
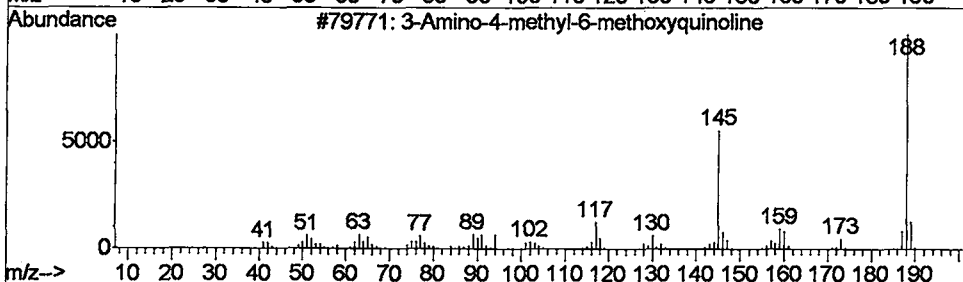
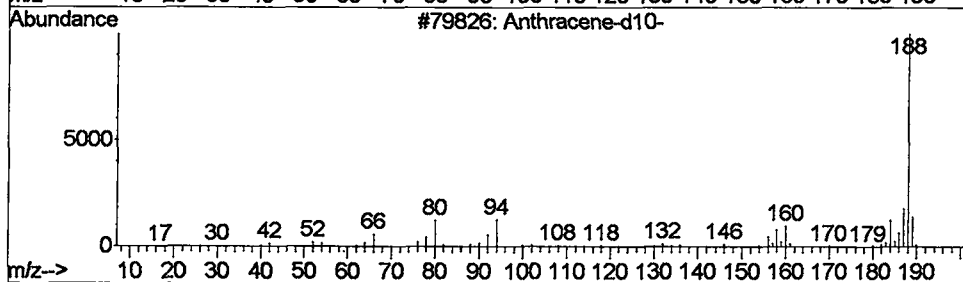
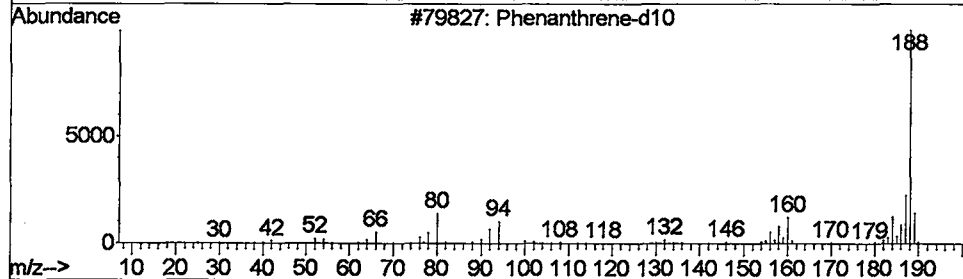
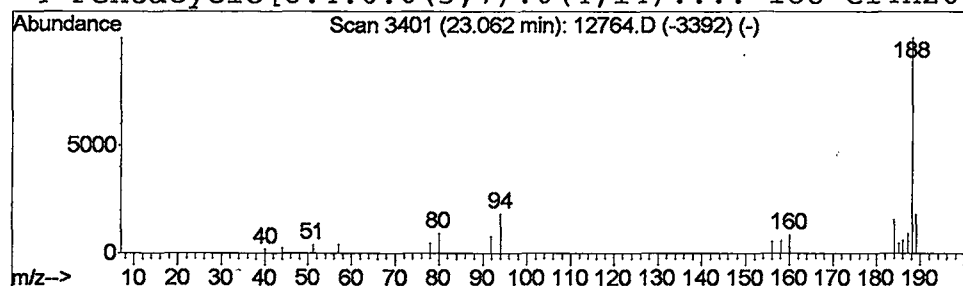
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Peak Number 19 Phenanthrene-d10

Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.06	0.27 ug/L	244987	Phenanthranene-d10	22.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene-d10	188	C14D10	001517-22-2	90
2		Anthracene-d10-	188	C14D10	001719-06-8	80
3		3-Amino-4-methyl-6-methoxyquinoline	188	C11H12N2O	1000213-71-3	42
4		Pentacyclo[8.4.0.0(3,7).0(4,14)....	188	C14H20	1000099-27-2	36



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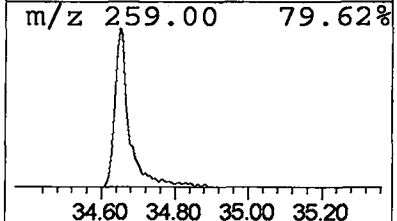
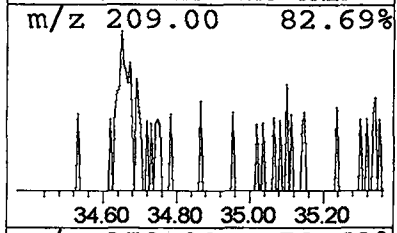
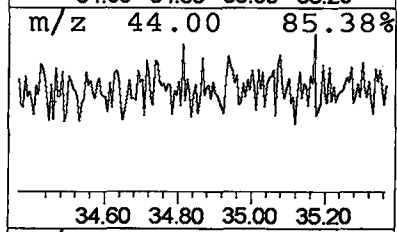
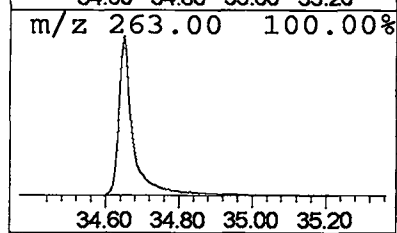
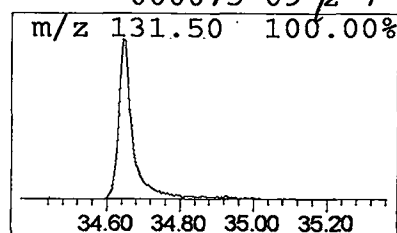
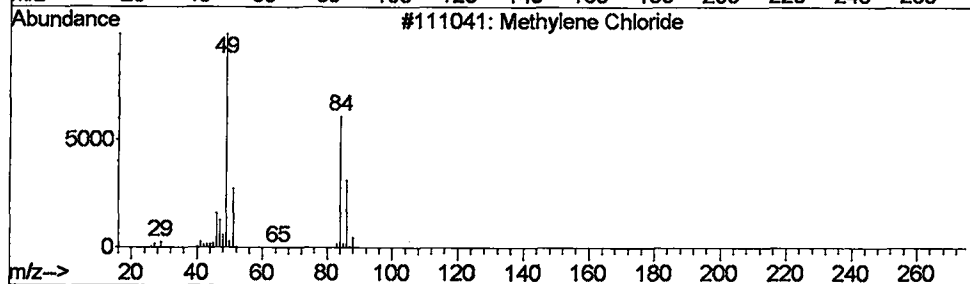
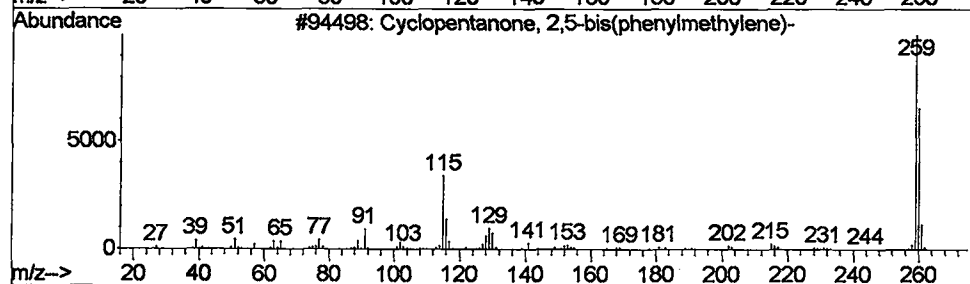
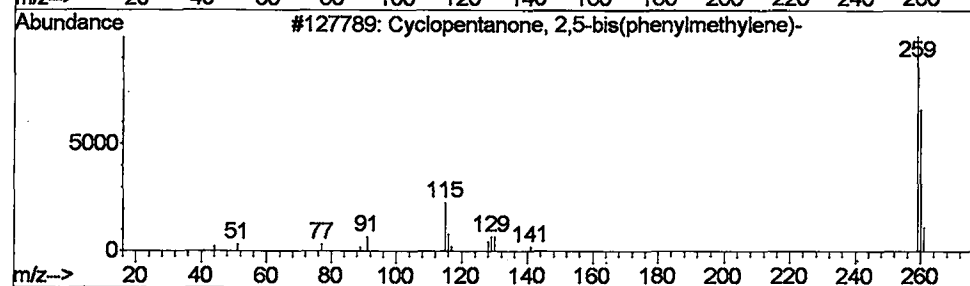
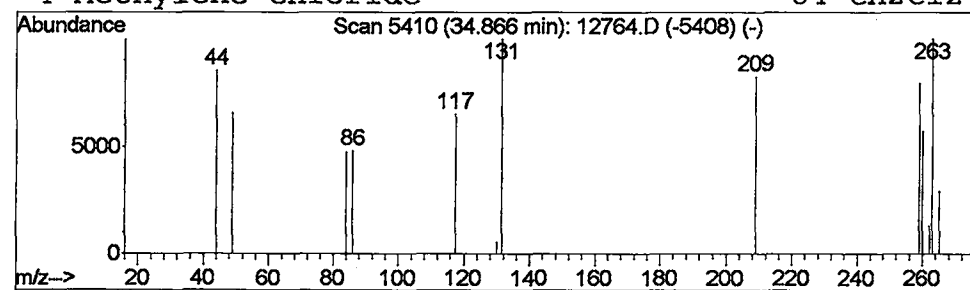
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Peak Number 20 Cyclopentanone, 2,5-bis(phe... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
34.86	0.42 ug/L	138911	Perylene-d12	34.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentanone, 2,5-bis(phenylme...	260	C19H16O	000895-80-7	9
2		Cyclopentanone, 2,5-bis(phenylme...	260	C19H16O	000895-80-7	9
3		Methylene Chloride	84	CH2Cl2	000075-09-2	7
4		Methylene Chloride	84	CH2Cl2	000075-09-2	7



tentatively identified compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Methylene Chloride	3.72	8.7 ug/L		5172260	1	9.89	23874100	40.0
Borane, trifluoro-	3.75	3.8 ug/L		2260540	1	9.89	23874100	40.0
Methylene Chloride	3.78	10.0 ug/L		5985130	1	9.89	23874100	40.0
Propiolonitrile	3.87	4.9 ug/L		2904310	1	9.89	23874100	40.0
1-Penten-3-one	3.93	10.3 ug/L		6170120	1	9.89	23874100	40.0
1-Buten-3-yne, 2-...	4.04	4.0 ug/L		2409610	1	9.89	23874100	40.0
Methylene Chloride	4.09	7.9 ug/L		4732180	1	9.89	23874100	40.0
Acetic acid, chlo...	4.24	7.9 ug/L		4736040	1	9.89	23874100	40.0
1-Propyne, 1-(met...	4.49	1.0 ug/L		585816	1	9.89	23874100	40.0
Methylene Chloride	4.52	3.1 ug/L		1878960	1	9.89	23874100	40.0
2-Butenal, 3-methyl-	4.79	1.8 ug/L		1096390	1	9.89	23874100	40.0
Methylene Chloride	4.87	2.2 ug/L		1341470	1	9.89	23874100	40.0
2-Chloro-4-aminop...	5.00	1.4 ug/L		835092	1	9.89	23874100	40.0
4H-1,2,4-Triazol-...	5.26	0.3 ug/L		154273	1	9.89	23874100	40.0
Borane, trifluoro-	5.46	0.4 ug/L		236789	1	9.89	23874100	40.0
Acetonitrile, dic...	5.59	0.5 ug/L		278438	1	9.89	23874100	40.0
Ethanol, 2,2,2-tr...	5.93	0.4 ug/L		232376	1	9.89	23874100	40.0
Acetone, ethyl me...	5.97	0.3 ug/L		179801	1	9.89	23874100	40.0
Phenanthrene-d10	23.06	0.3 ug/L		244987	4	22.90	36564300	40.0
Cyclopentanone, 2...	34.86	0.4 ug/L		138911	6	34.65	13178400	40.0