

Library Search Compound Report

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Acq On : 20 May 2002 8:37 pm
Sample : 5/16 eh
Misc :
MS Integration Params: LSCINT.e

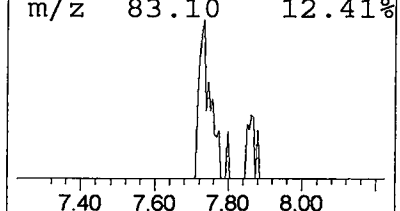
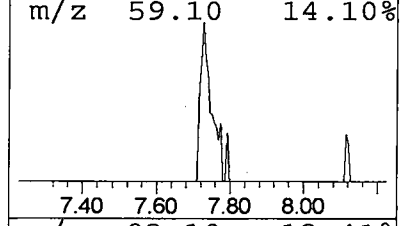
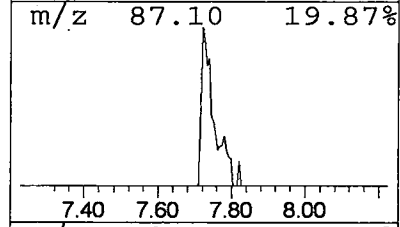
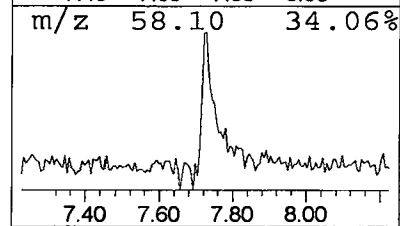
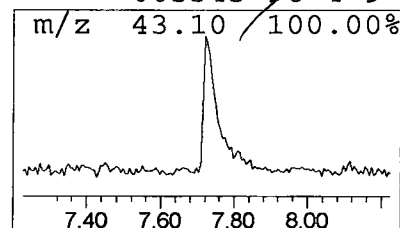
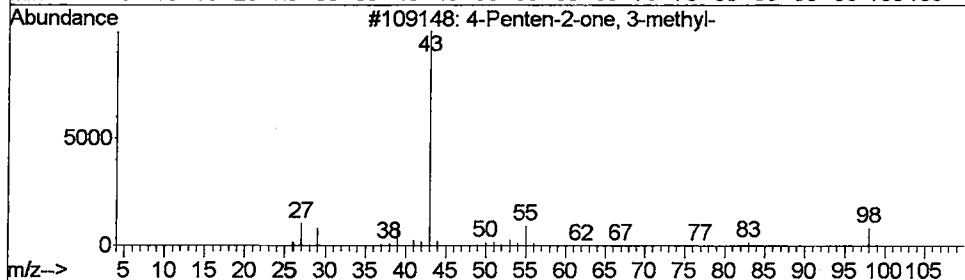
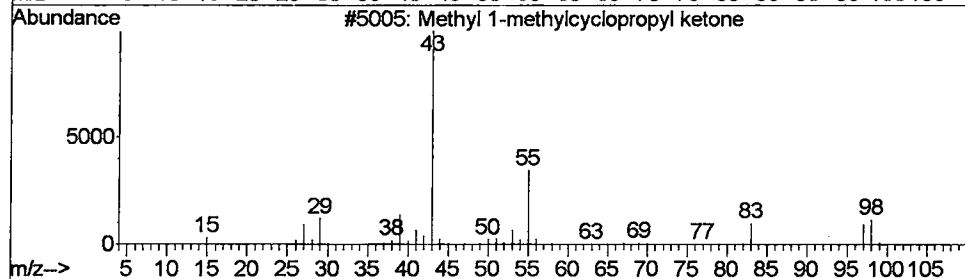
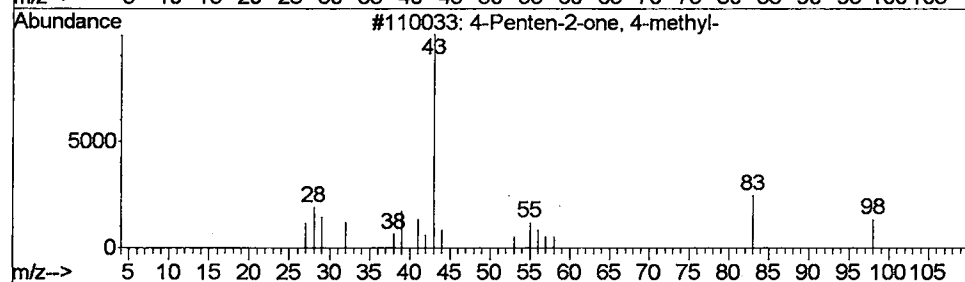
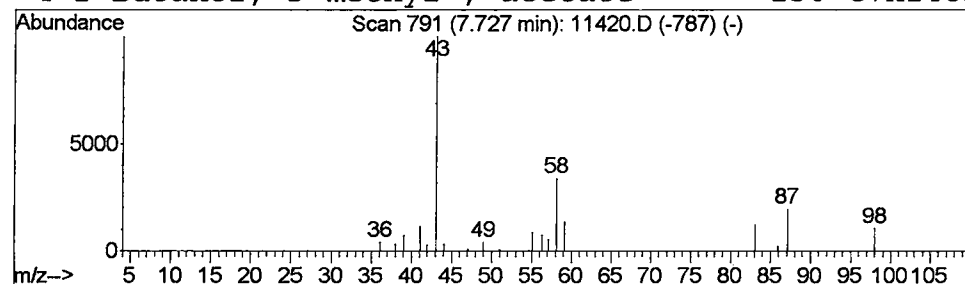
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Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 4 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	0.34 ug/L	328308	1,4-Dichlorobenzene-d4	9.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	12
2			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4			2-Butanol, 3-methyl-, acetate	130	C7H14O2	005343-96-4	9



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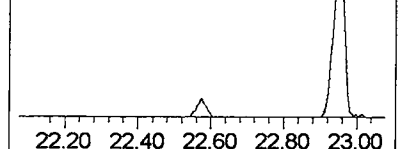
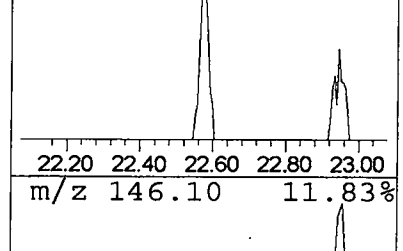
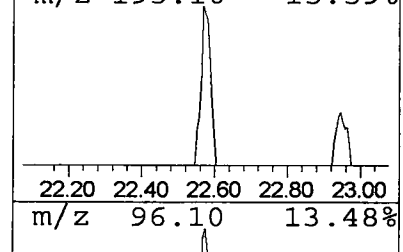
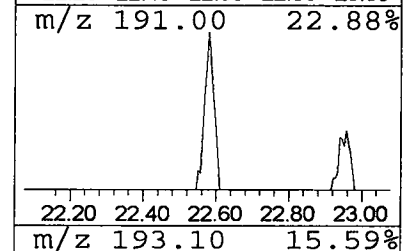
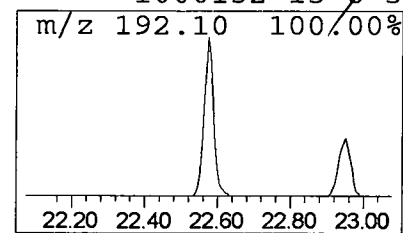
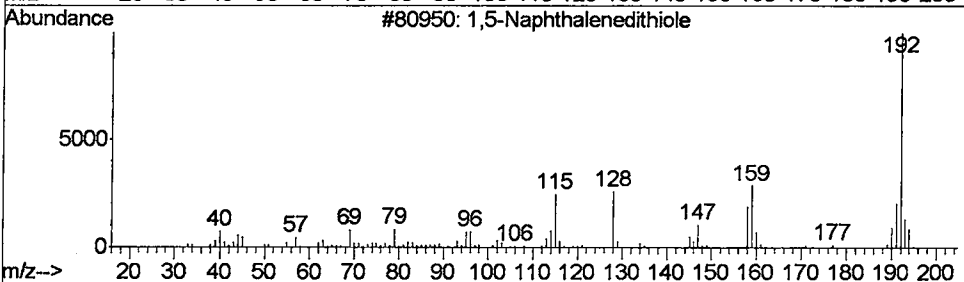
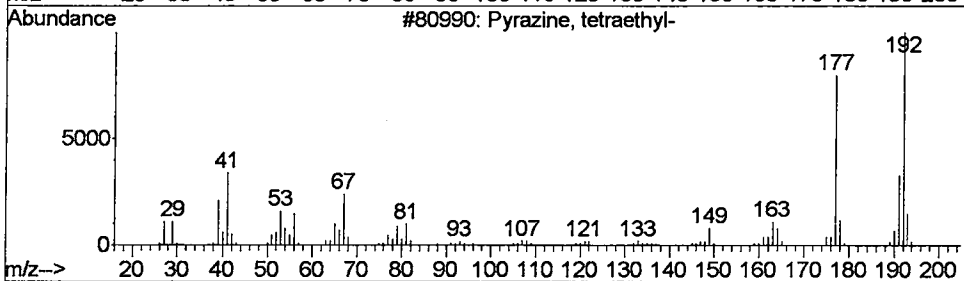
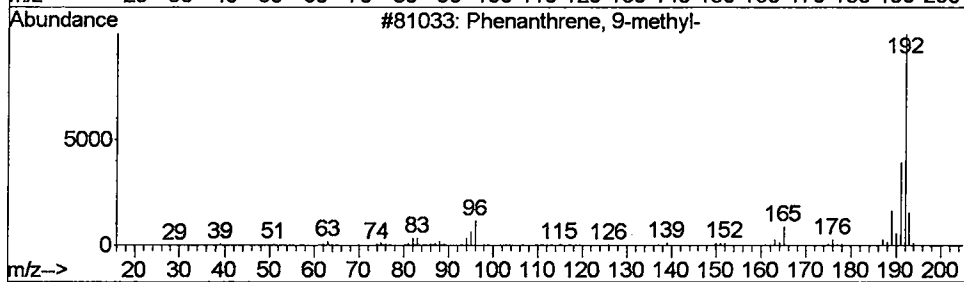
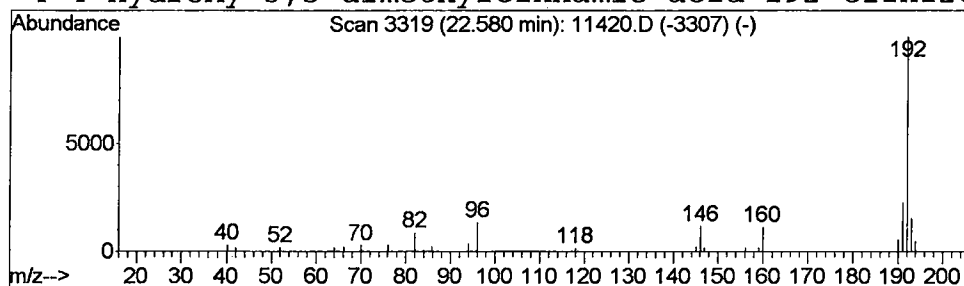
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 Peak Number 5 Phenanthrene, 9-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	0.29 ug/L	403085	Phenanthranene-d10	22.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	53
2		Pyrazine, tetraethyl-	192	C12H20N2	038325-19-8	45
3		1,5-Naphthalenedithiole	192	C10H8S2	1000223-69-5	38
4		4-Hydroxy-3,5-dimethylcinnamic acid	192	C11H12O3	1000132-15-8	38



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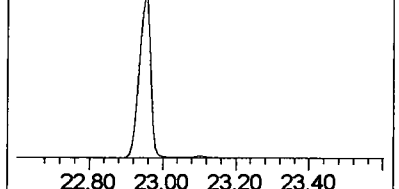
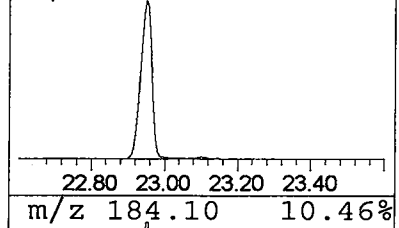
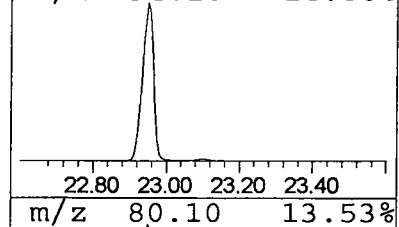
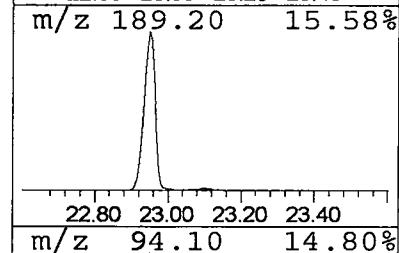
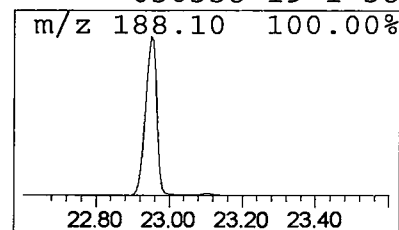
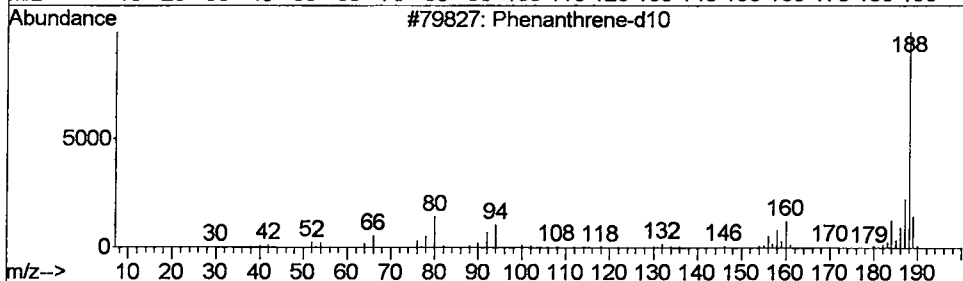
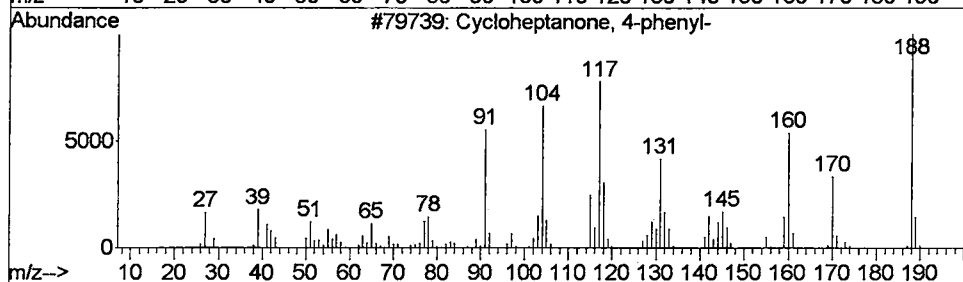
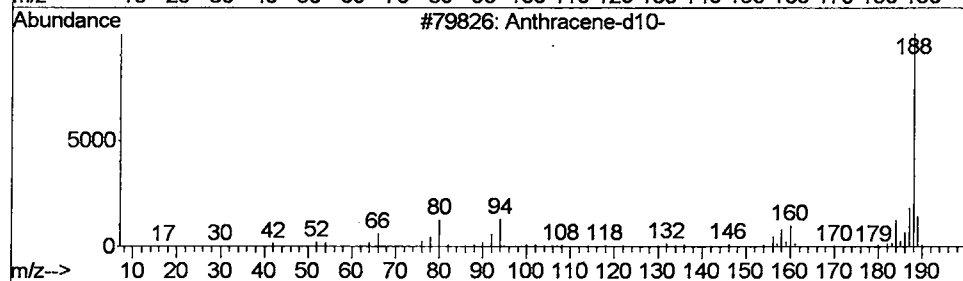
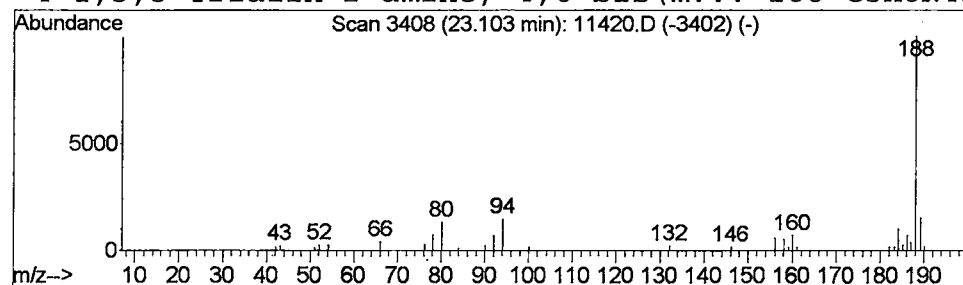
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Multiplr: 1.00

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Peak Number 6 Anthracene-d10- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	0.43 ug/L	583340	Phenanthranene-d10	22.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene-d10-	188	C14D10	001719-06-8	81
2			Cycloheptanone, 4-phenyl-	188	C13H16O	067688-28-2	50
3			Phenanthrene-d10	188	C14D10	001517-22-2	50
4			1,3,5-Triazin-2-amine, 4,6-bis(m...	188	C5H8N4S2	030358-19-1	38



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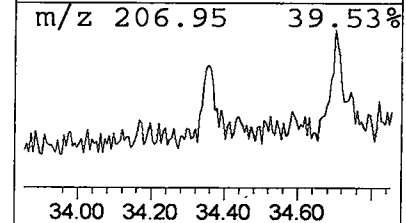
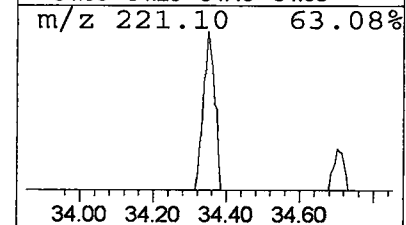
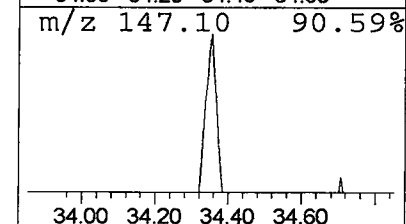
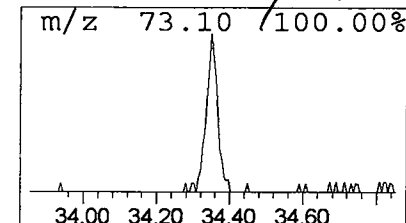
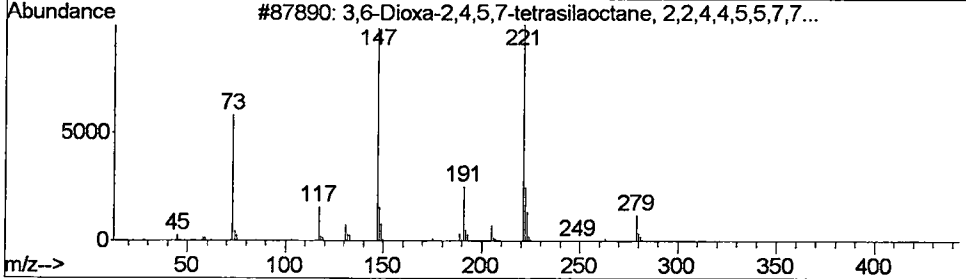
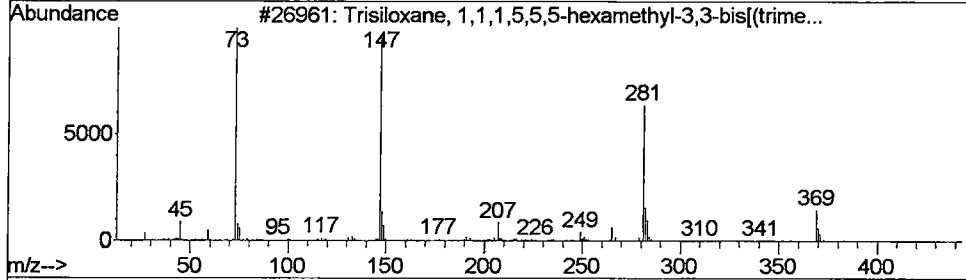
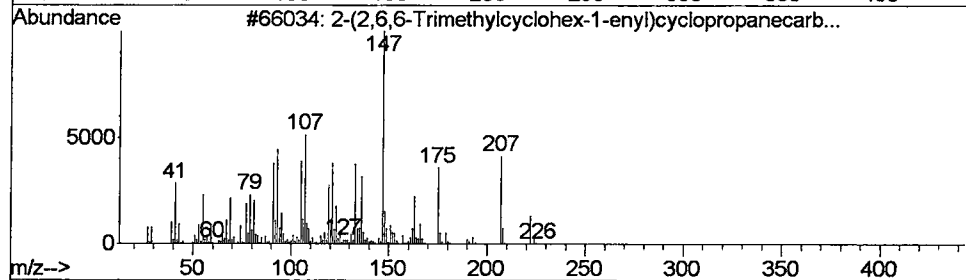
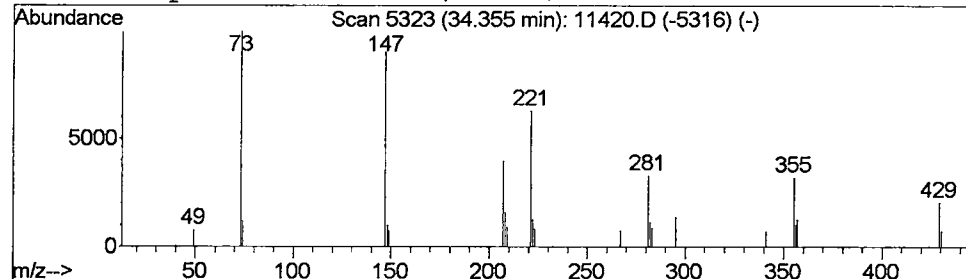
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 Multiplr: 1.00

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 Peak Number 7 2-(2,6,6-Trimethylcyclohex-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
34.35	0.30 ug/L	258709	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2,6,6-Trimethylcyclohex-1-eny...	222	C14H22O2	1000185-64-1	35
2			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
4			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	12



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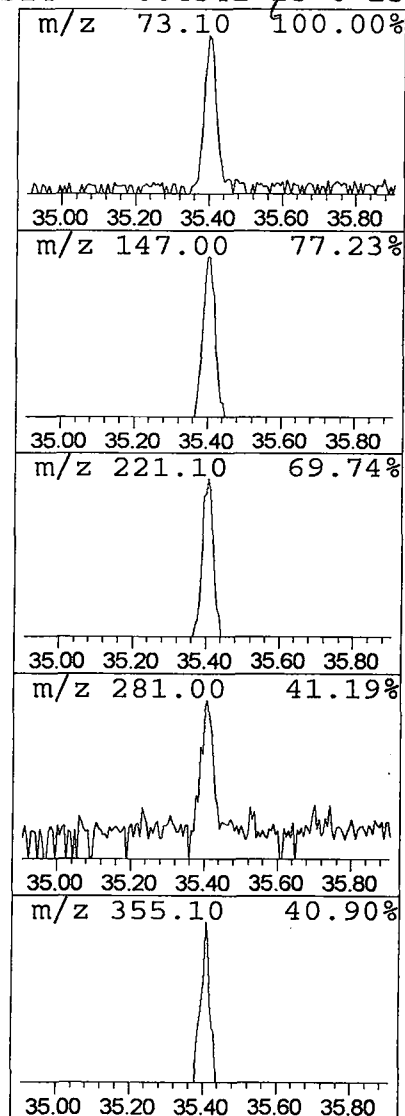
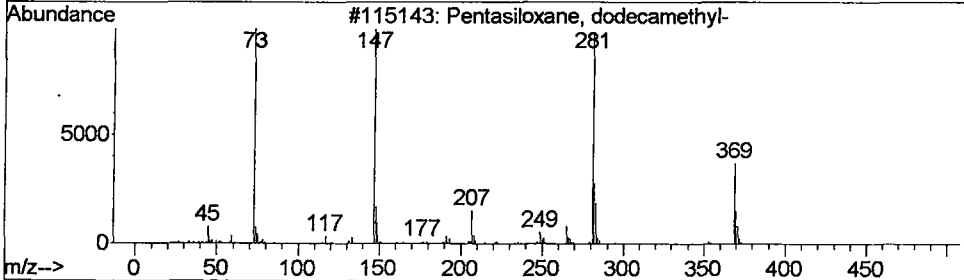
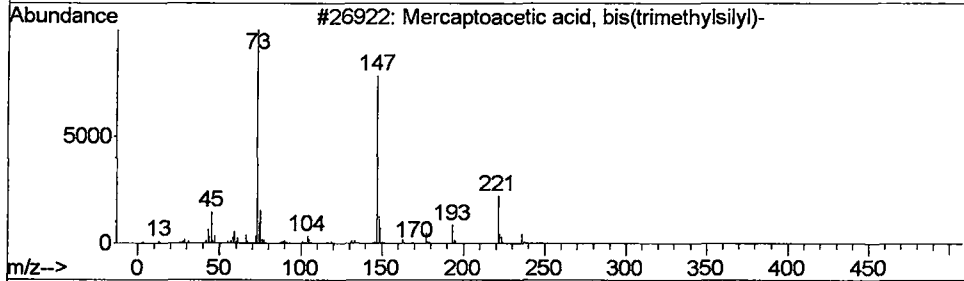
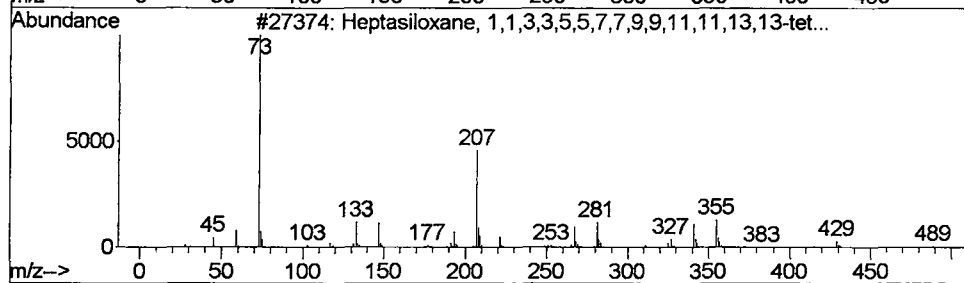
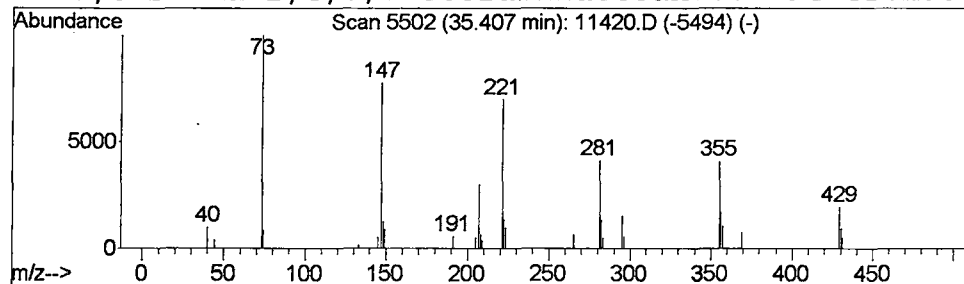
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Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
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 Peak Number 8 Heptasiloxane, 1,1,3,3,5,5,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
35.41	0.43 ug/L	368949	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	37
2			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	35
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25



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Misc :

MS Integration Params: LSCINT.e

Vial: 10

Operator: Mclean

Inst : Instrumen

Multiplr: 1.00

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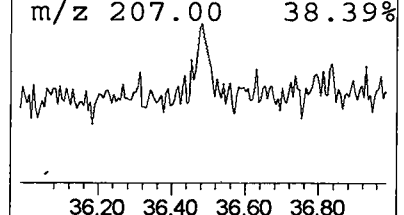
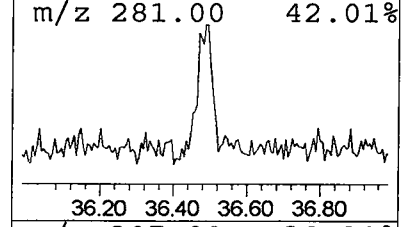
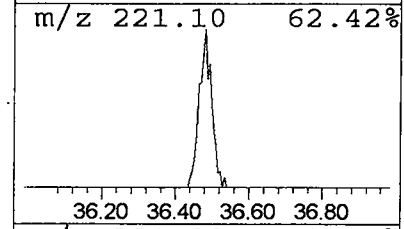
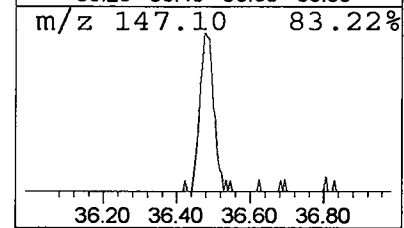
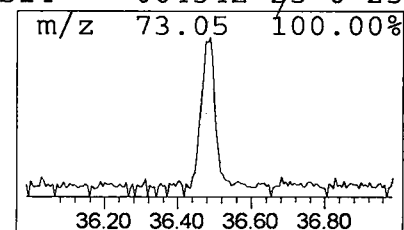
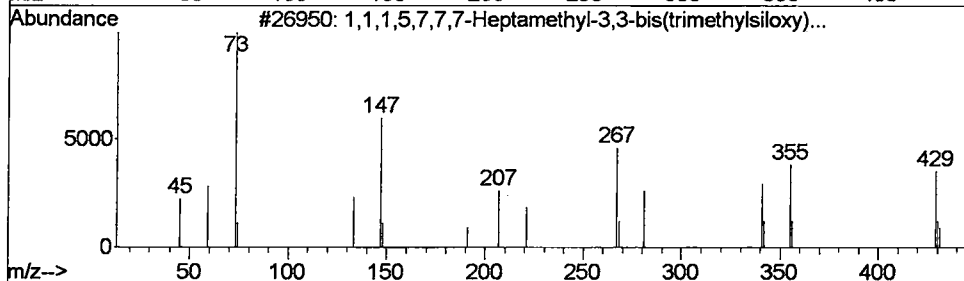
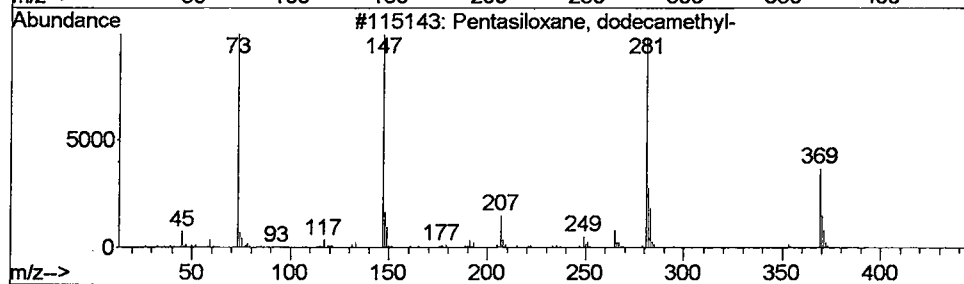
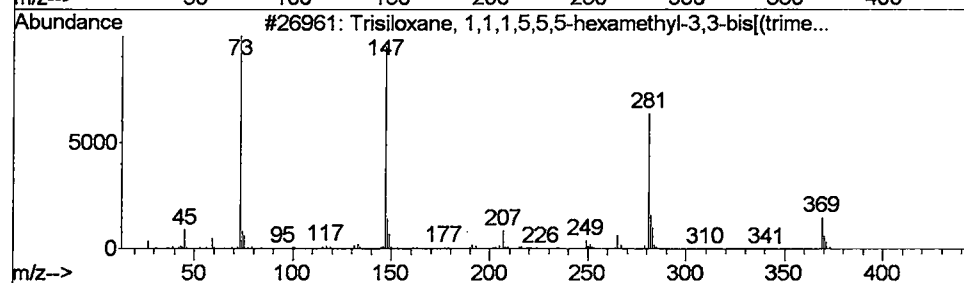
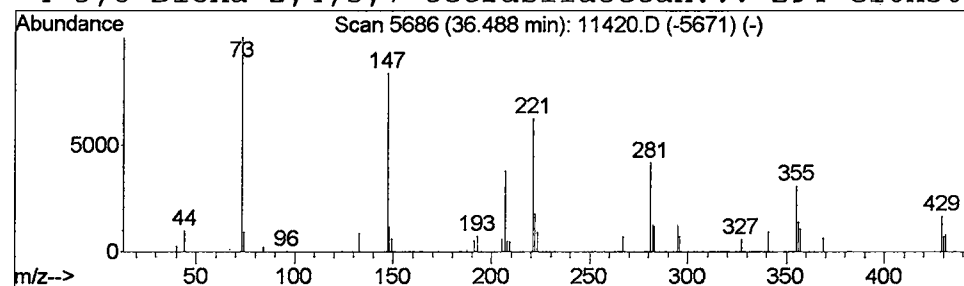
Title : 508 Modified GC/MS scan

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Peak Number 9 Trisiloxane, 1,1,1,5,5,5-he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
36.49	0.43 ug/L	369208	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35
2			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	35
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25



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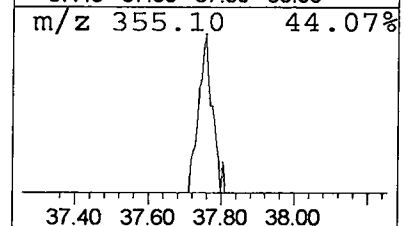
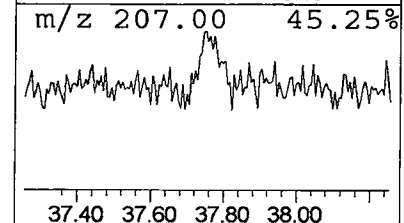
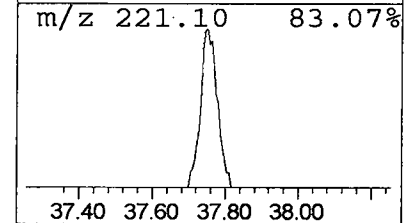
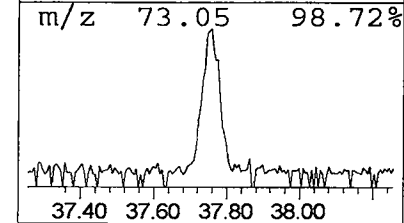
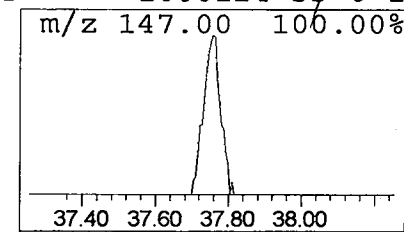
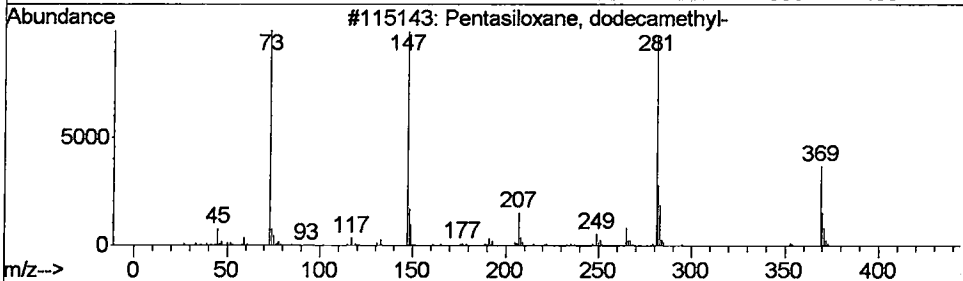
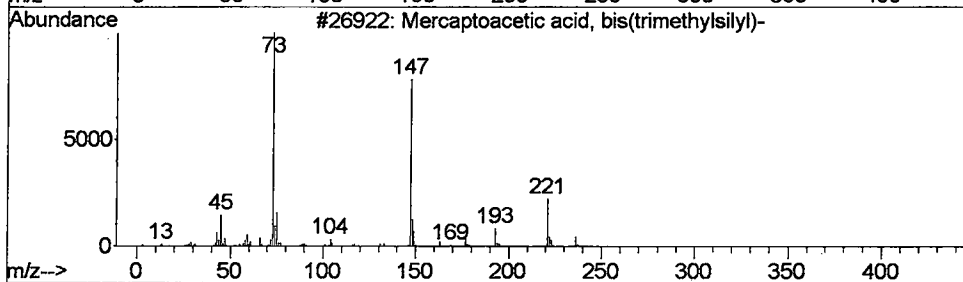
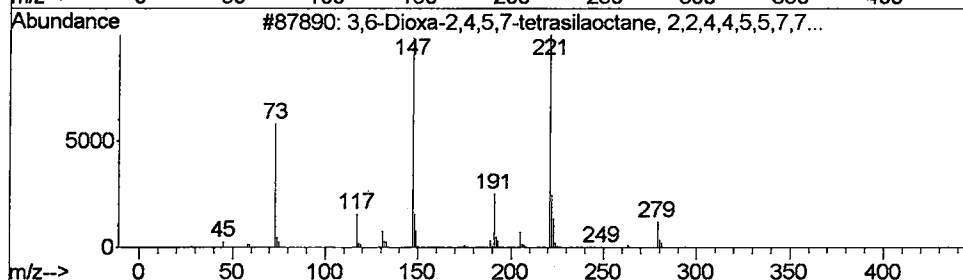
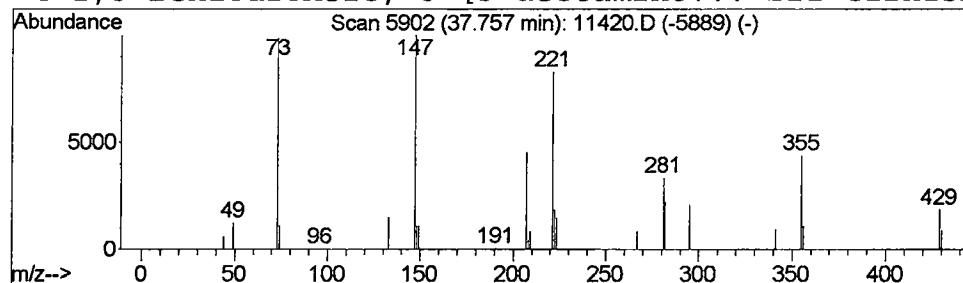
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Peak Number 10 3,6-Dioxa-2,4,5,7-tetrasilaoctane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
37.76	0.41 ug/L	351200	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctane...	294	C10H30O2Si4	004342-25-0	38
2			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	25
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	14
4			1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	11



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MS Integration Params: LSCINT.e

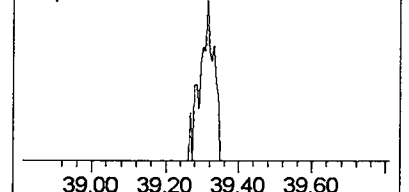
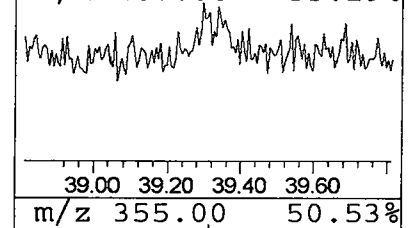
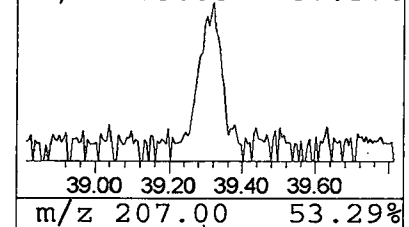
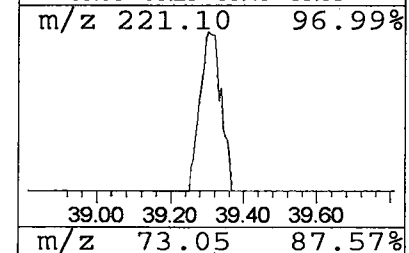
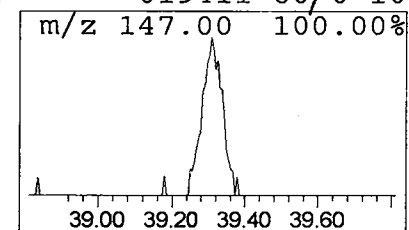
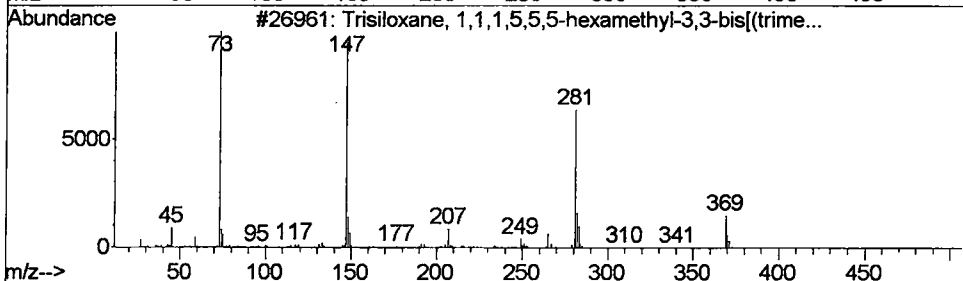
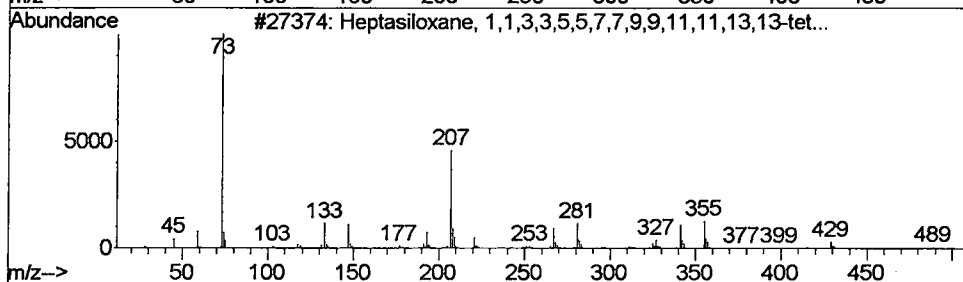
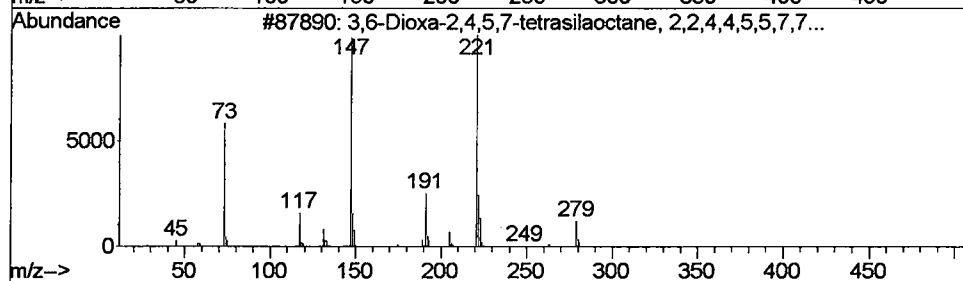
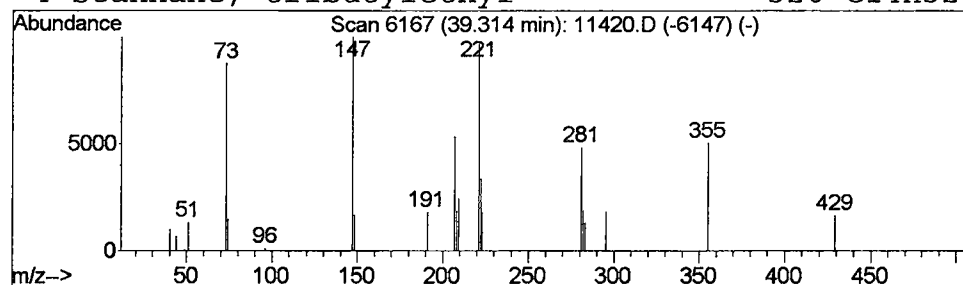
Vial: 10
Operator: Mclean
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

Peak Number 11 3,6-Dioxa-2,4,5,7-tetrasilaoctane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
39.32	0.35 ug/L	304314	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctane...	294	C10H30O2Si4	004342-25-0	38
2			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	25
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	10
4			Stannane, tributylethyl-	320	C14H32Sn	019411-60-0	10



Tentatively Identified Compound (LSC) summary

Operator ID: Mclean Date Acquired: 20 May 2002 8:37 pm
Data File: C:\MSDCHEM\1\DATA\052002\11420.D
Name: 5/16 eh
Misc:
Method: C:\MSDCHEM\1\METHODS\050102.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
Acetonitrile, dic...	3.62	0.3	ug/L	313037	1	9.94	38254500	40.0
Ethyl Chloride	3.75	0.3	ug/L	290057	1	9.94	38254500	40.0
2-Pentanone, 4-hy...	5.98	17.0	ug/L	16297700	1	9.94	38254500	40.0
4-Penten-2-one, 4...	7.73	0.3	ug/L	328308	1	9.94	38254500	40.0
Phenanthrene, 9-m...	22.58	0.3	ug/L	403085	4	22.95	54723600	40.0
Anthracene-d10-	23.10	0.4	ug/L	583340	4	22.95	54723600	40.0
2-(2,6,6-Trimethy...	34.35	0.3	ug/L	258709	6	34.71	34540100	40.0
Heptasiloxane, 1,...	35.41	0.4	ug/L	368949	6	34.71	34540100	40.0
Trisiloxane, 1,1,...	36.49	0.4	ug/L	369208	6	34.71	34540100	40.0
3,6-Dioxa-2,4,5,7...	37.76	0.4	ug/L	351200	6	34.71	34540100	40.0
3,6-Dioxa-2,4,5,7...	39.32	0.4	ug/L	304314	6	34.71	34540100	40.0