

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 05/10/2002 Time: 09:03:39

Sample: AE10610
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 5/10/02 09:03 Ended: 5/10/02 09:03 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		76		10.0

Comments for Sample AE10610 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 05-10-2002 Time: 09:03:43

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recovery for 1 of the 43 compounds in the LCS Standard was low.

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
 Acq On : 7 May 2002 10:55 pm
 Sample : 5/3 kb
 Misc :
 MS Integration Params: EVENTS.E
 Quant Time: May 09 09:14:31 2002

Vial: 13
 Operator: Mclean
 Inst : Instrumen
 Multiplr: 1.00

Quant Results File: 050102.RES

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
 Title : 508 Modified GC/MS scan
 Last Update : Wed May 08 09:53:56 2002
 Response via : Initial Calibration
 DataAcq Meth : 508SCAN

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.94	152	5561577	40.00	ug/L	0.00
10) Napthalene-d8	13.43	136	22218257	40.00	ug/L	0.00
17) Acenapthalene-d10	18.57	164	12103766	40.00	ug/L	0.00
29) Phenanthranene-d10	22.96	188	17717259	40.00	ug/L	0.00
37) Chrysene-d12	30.81	240	13825752	40.00	ug/L	0.00
43) Perylene-d12	34.71	264	9461447	40.00	ug/L	0.00

System Monitoring Compounds

27) TCMX	20.54	209	527825	7.55	ug/L	0.00
Spiked Amount	10.000		Recovery	=	75.50%	
50) 2,4-ddd	0.00	235	0	0.00	ug/L	
Spiked Amount	5.000		Recovery	=	0.00%	

Target Compounds

Qvalue

2) n-nitros-dimethyl amine	0.00	74	0	N.D.	
3) bis(2-Chloroethyl) ether	0.00	93	0	N.D.	
4) 1,3-Dichlorobenzene	0.00	146	0	N.D.	
5) 1,4-Dichlorobenzene	0.00	146	0	N.D.	
6) 1,2-Dichlorobenzene	0.00	146	0	N.D.	
7) 2,2'-oxybis(1-Chloropropane	0.00	45	0	N.D.	
8) N-nitroso-di-propylamine	0.00	70	0	N.D.	
9) Hexachloroethane	0.00	117	0	N.D.	
11) Nitrobenzene	0.00	77	0	N.D.	
12) Isophorone	0.00	82	0	N.D.	
13) bis(2-Chloroethoxy) methan	0.00	93	0	N.D.	
14) 1,2,4-Trichlorobenzene	0.00	180	0	N.D.	
15) Napthalene	0.00	128	0	N.D.	
16) Hexachlorobutadiene	0.00	225	0	N.D.	
18) 2-Chloronapthalene	0.00	162	0	N.D.	
19) Dimethylphthalate	0.00	163	0	N.D.	
20) 2,6-Dinitrotoluene	0.00	165	0	N.D.	
21) Acenapthylene	0.00	152	0	N.D.	
22) Acenapthalene	0.00	153	0	N.D.	
23) 2,4-Dinitrotoluene	0.00	165	0	N.D.	
24) Diethylphthalate	0.00	149	0	N.D.	
25) 4-Chlorophenyl-phenylether	0.00	204	0	N.D.	
26) Fluorene	0.00	166	0	N.D.	
28) Azobenzene	0.00	77	0	N.D.	
30) Nnitrosodiphenylamine	0.00	169	0	N.D.	
31) 4-Bromophenyl-phenylether	0.00	248	0	N.D.	
32) Hexachlorobenzene	0.00	284	0	N.D.	
33) Phenanthrene	0.00	178	0	N.D.	

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

10610.D 050102.M Thu May 09 09:14:52 2002

Page 1

Quantitation Report

(QT Reviewed)

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Misc :

Multiplr: 1.00

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Quant Results File: 050102.RES

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)

Title : 508 Modified GC/MS scan

Last Update : Wed May 08 09:53:56 2002

Response via : Initial Calibration

DataAcq Meth : 508SCAN

Compound	R.T.	QIon	Response	Conc	Unit	Qvalue
34) Anthracene	0.00	178	0	N.D.		
35) Di-n-butylphthalate	25.09	149	15771	N.D.		
36) Fluoroanthene	0.00	202	0	N.D.		
38) Pyrene	0.00	202	0	N.D.		
39) Butylbenzylphthalate	0.00	149	0	N.D.		
40) Benzo(a)anthracene	30.81	228	35148	N.D.		
41) Bis(2-ethylhexyl)phthalate	31.38	149	24646	N.D.		
42) Chrysene	0.00	228	0	N.D.		
44) Di-n-octylphthalate	0.00	149	0	N.D.		
45) Benzo(b)fluoranthene	0.00	252	0	N.D.		
46) Benzo(k)fluoranthene	0.00	252	0	N.D.		
47) Benzo(a)pyrene	0.00	252	0	N.D.		
48) Indeno(1,2,3-cd)pyrene	0.00	276	0	N.D.		
49) Dibenz(a,h)anthracene	0.00	278	0	N.D.		
51) Benzo(g,h,i)perylene	0.00	276	0	N.D.		

(#) = qualifier out of range (m) = manual integration (+) = signals summed
10610.D 050102.M Thu May 09 09:14:53 2002 Page 2

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\050702\10610.D

Vial: 13

Acq On : 7 May 2002 10:55 pm

Operator: Mclean

Sample : 5/3 kb

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: EVENTS.E

Quant Time: May 9 9:14 2002

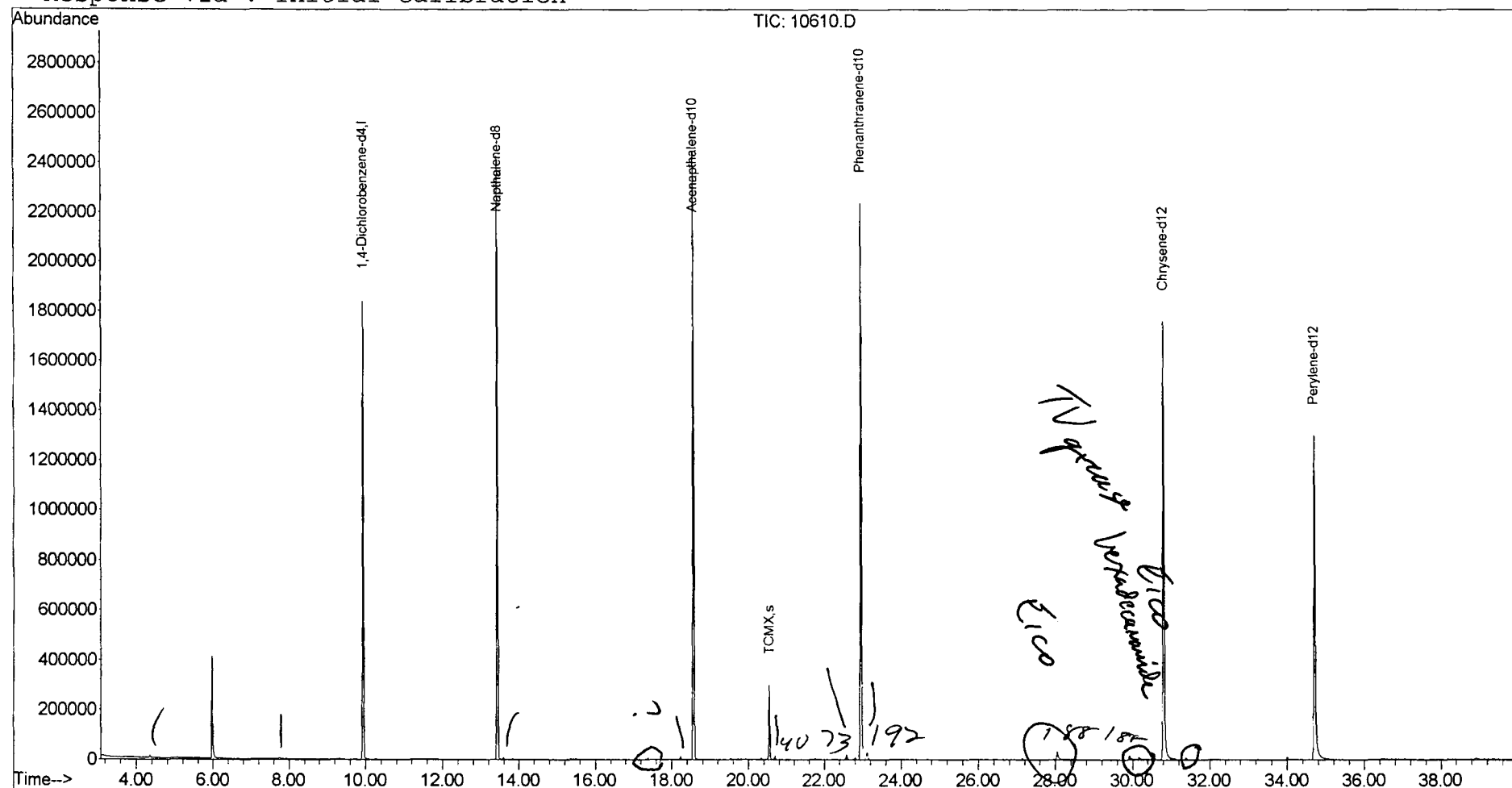
Quant Results File: 050102.RES

Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)

Title : 508 Modified GC/MS scan

Last Update : Wed May 08 09:53:56 2002

Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D

Acq On : 7 May 2002 10:55 pm

Sample : 5/3 kb

Misc :

MS Integration Params: LSCINT.e

Vial: 13

Operator: Mclean

Inst : Instrumen

Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)

Title : 508 Modified GC/MS scan

Signal : TIC

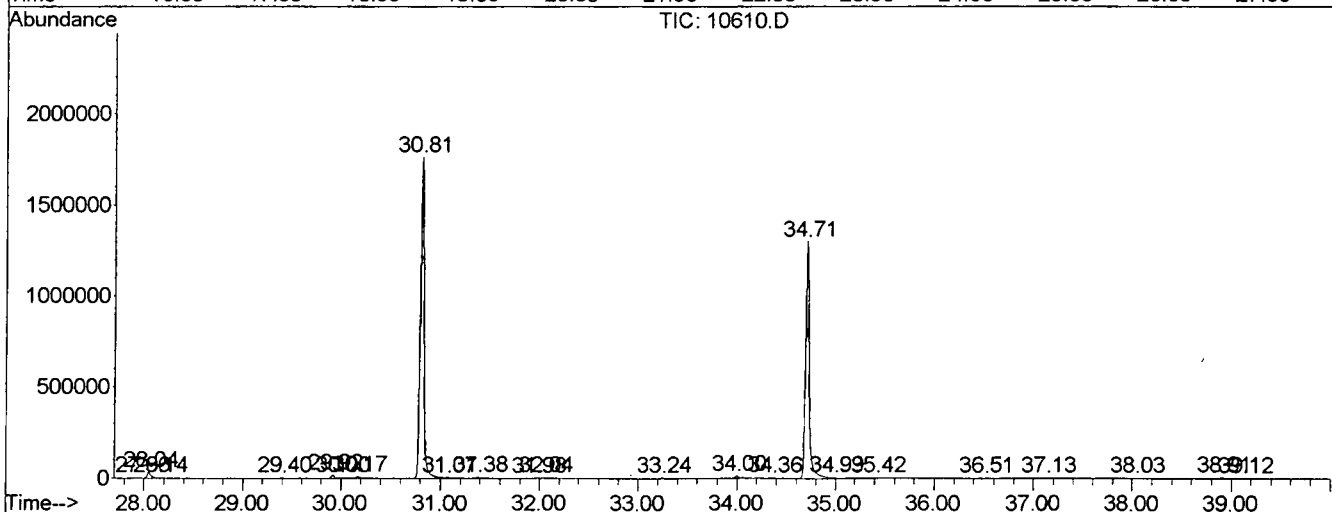
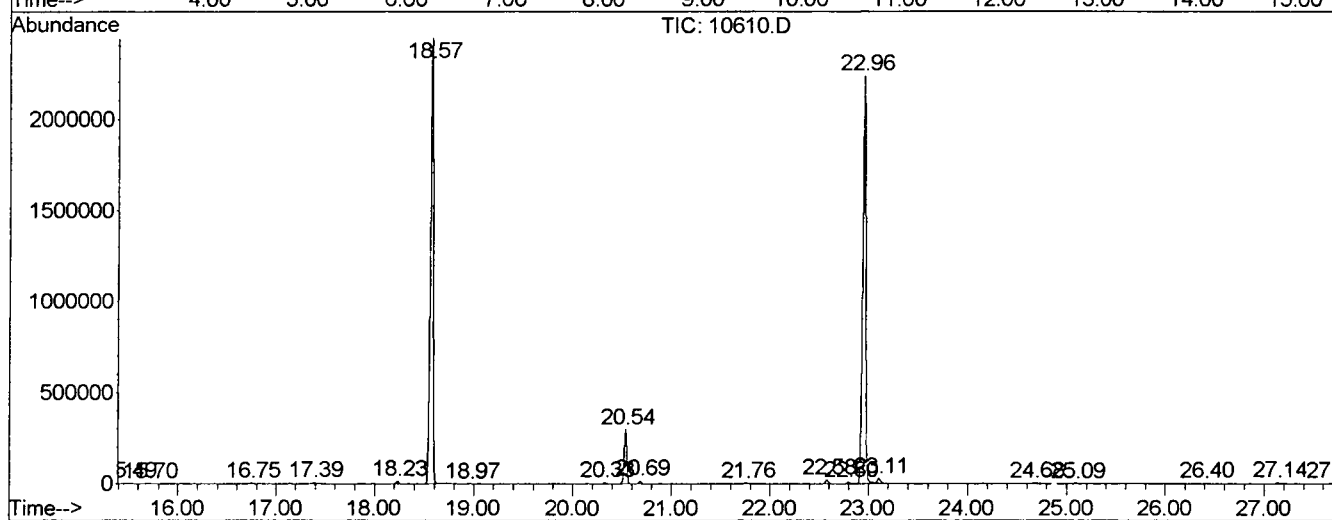
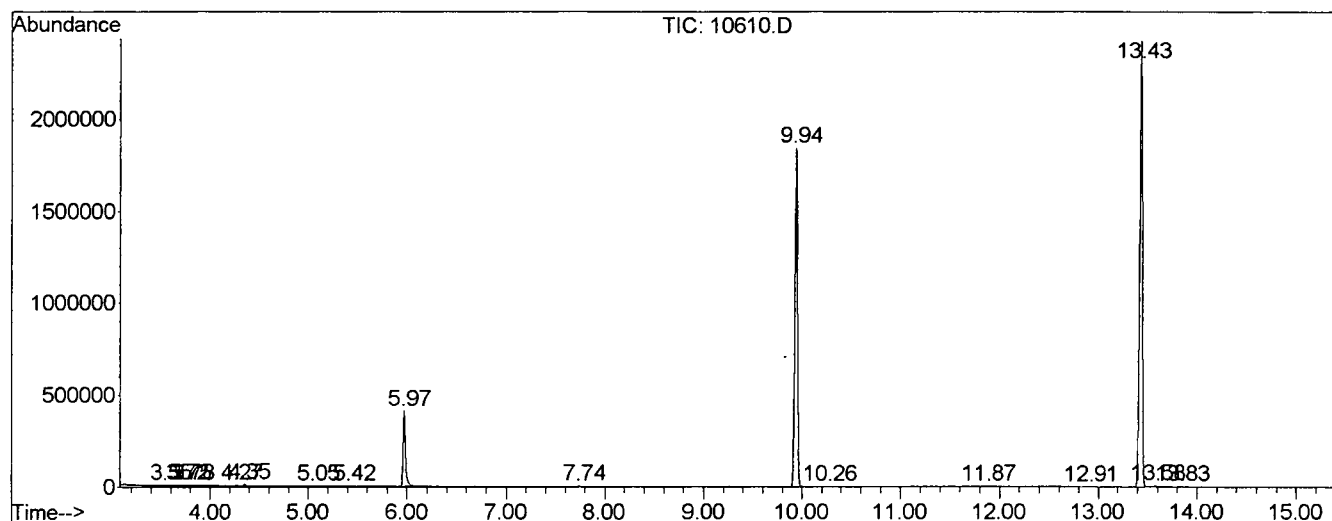
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.555	76	81	88	PV 5	1875	30281	0.06%	0.011%
2	3.714	102	108	112	VV 7	1323	32789	0.07%	0.012%
3	3.749	112	114	117	VV 5	1131	12261	0.02%	0.004%
4	3.779	117	119	121	PV 3	1146	6615	0.01%	0.002%
5	4.272	197	203	209	PV 5	2869	55739	0.11%	0.020%
6	4.354	209	217	228	VV	9381	172105	0.35%	0.063%
7	5.054	331	336	344	PV 6	2300	64066	0.13%	0.023%
8	5.424	395	399	403	VV 3	1780	25949	0.05%	0.009%
9	5.976	481	493	519	PV	399082	6947983	14.02%	2.537%
10	7.739	787	793	801	PV 3	3872	83837	0.17%	0.031%
11	9.936	1158	1167	1184	PV	1806371	33705434	68.01%	12.307%
12	10.265	1216	1223	1232	PV 7	2214	48498	0.10%	0.018%
13	11.869	1490	1496	1503	PV 4	2210	41216	0.08%	0.015%
14	12.909	1664	1673	1679	PV 6	1700	51811	0.10%	0.019%
15	13.432	1747	1762	1778	PV	2394621	45482559	91.77%	16.608%
16	13.585	1781	1788	1795	VV 2	7602	129338	0.26%	0.047%
17	13.832	1818	1830	1836	BV 6	3572	58082	0.12%	0.021%
18	15.489	2105	2112	2123	VV 3	3526	89411	0.18%	0.033%
19	15.700	2143	2148	2155	PV 3	2137	39511	0.08%	0.014%
20	16.746	2316	2326	2334	PV 4	3779	73497	0.15%	0.027%
21	17.386	2430	2435	2445	VV	7978	123420	0.25%	0.045%
22	18.232	2571	2579	2588	VV	13940	212818	0.43%	0.078%
23	18.573	2625	2637	2653	PV	2471099	49562352	100.00%	18.098%
24	18.967	2692	2704	2707	PV 2	1572	23983	0.05%	0.009%
25	20.324	2928	2935	2943	VV 2	6020	109403	0.22%	0.040%
26	20.536	2958	2971	2982	PV	292014	5223424	10.54%	1.907%
27	20.688	2986	2997	3003	VV	16398	259870	0.52%	0.095%
28	21.758	3163	3179	3192	VV 3	5429	124067	0.25%	0.045%
29	22.580	3309	3319	3338	VV 2	20711	396248	0.80%	0.145%
30	22.804	3350	3357	3371	VV	9171	158506	0.32%	0.058%
31	22.956	3371	3383	3403	PV 2	2209535	48411388	97.68%	17.677%
32	23.109	3403	3409	3420	VV 2	27621	602679	1.22%	0.220%
33	24.684	3670	3677	3683	PV	4705	81457	0.16%	0.030%
34	25.095	3741	3747	3756	PV 3	1632	37335	0.08%	0.014%
35	26.400	3964	3969	3975	VV 3	3477	58214	0.12%	0.021%
36	27.140	4083	4095	4102	VV 5	6286	121631	0.25%	0.044%
37	27.674	4176	4186	4194	PV 5	3010	67680	0.14%	0.025%

38	27.962	4225	4235	4242	PV	4	3204	71178	0.14%	0.026%
39	28.045	4242	4249	4264	VV	2	30773	887797	1.79%	0.324%
40	28.145	4264	4266	4279	VV	6	2816	90174	0.18%	0.033%
41	29.402	4474	4480	4485	PV	3	2746	51885	0.10%	0.019%
42	29.919	4560	4568	4576	VV	2	17261	367709	0.74%	0.134%
43	29.995	4576	4581	4584	VV	5	3435	80607	0.16%	0.029%
44	30.172	4602	4611	4621	VV	6	9020	257149	0.52%	0.094%
45	30.812	4705	4720	4761	VV	2	1764120	43154102	87.07%	15.758%
46	31.065	4761	4763	4776	VV	6	5240	188432	0.38%	0.069%
47	31.382	4810	4817	4839	VV	5	7454	272467	0.55%	0.099%
48	31.975	4911	4918	4924	PV	4	2030	37103	0.07%	0.014%
49	32.040	4924	4929	4941	VV	4	2856	64015	0.13%	0.023%
50	33.239	5127	5133	5142	VV	3	2884	61547	0.12%	0.022%
51	33.997	5249	5262	5277	PV	2	12061	263133	0.53%	0.096%
52	34.361	5316	5324	5336	PV	3	2913	74653	0.15%	0.027%
53	34.713	5370	5384	5430	VV	2	1289303	34550933	69.71%	12.616%
54	34.995	5430	5432	5440	VV	8	5075	126720	0.26%	0.046%
55	35.419	5497	5504	5515	VV	8	3140	110271	0.22%	0.040%
56	36.511	5684	5690	5696	VV	5	2845	88761	0.18%	0.032%
57	37.128	5789	5795	5801	VV	4	2906	79000	0.16%	0.029%
58	38.033	5946	5949	5957	VV	6	1567	27312	0.06%	0.010%
59	38.909	6086	6098	6112	PV	8	5291	174964	0.35%	0.064%
60	39.120	6127	6134	6150	PV	8	1769	56549	0.11%	0.021%

Sum of corrected areas: 273861917

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\050702\10610.D
 Operator : Mclean
 Acquired : 7 May 2002 10:55 pm using AcqMethod 508SCAN
 Instrument : Instrumen
 Sample Name: 5/3 kb
 Misc Info :
 Vial Number: 13
 Quant File :050102.RES (Chemstation Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
 Acq On : 7 May 2002 10:55 pm
 Sample : 5/3 kb
 Misc :
 MS Integration Params: LSCINT.e

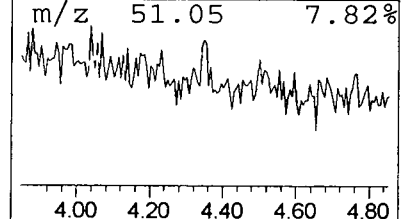
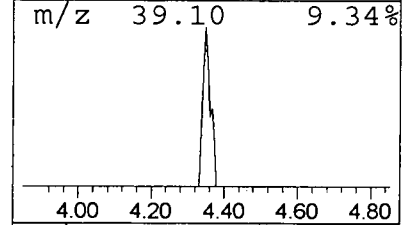
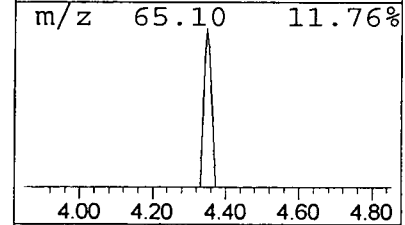
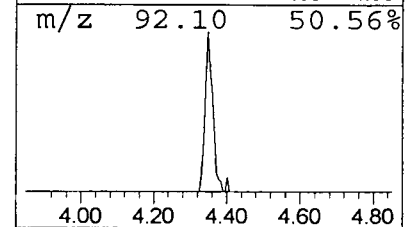
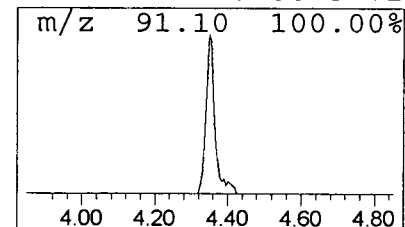
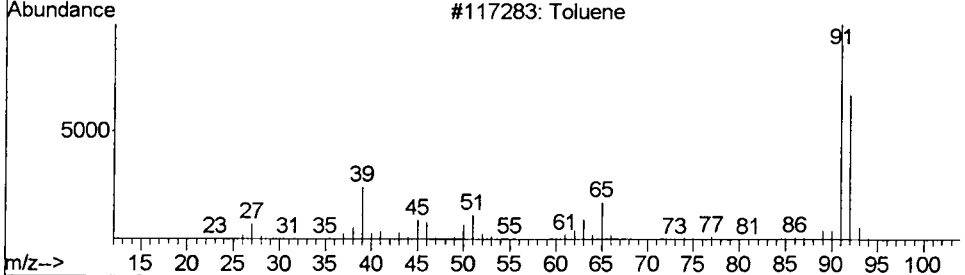
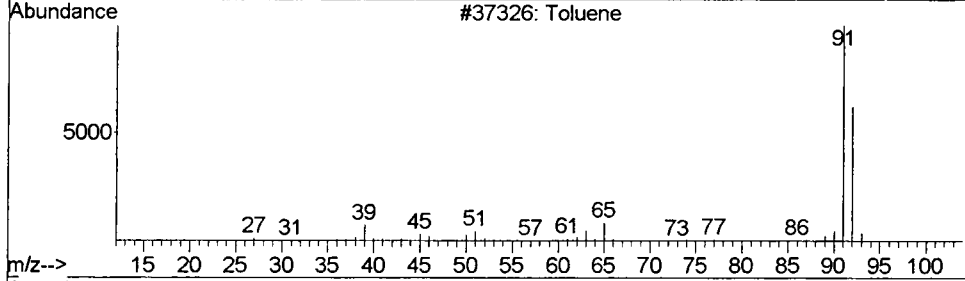
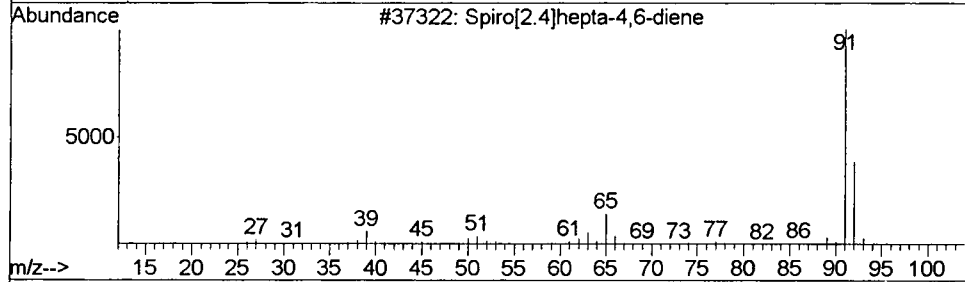
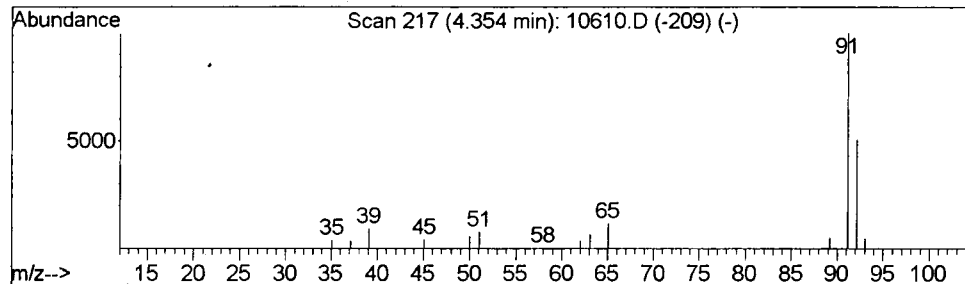
Vial: 13
 Operator: Mclean
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 Spiro[2.4]hepta-4,6-diene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	0.20 ug/L	172105	1,4-Dichlorobenzene-d4	9.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[2.4]hepta-4,6-diene	92	C7H8	000765-46-8	86
2			Toluene	92	C7H8	000108-88-3	80
3			Toluene	92	C7H8	000108-88-3	78
4			Toluene	92	C7H8	000108-88-3	72



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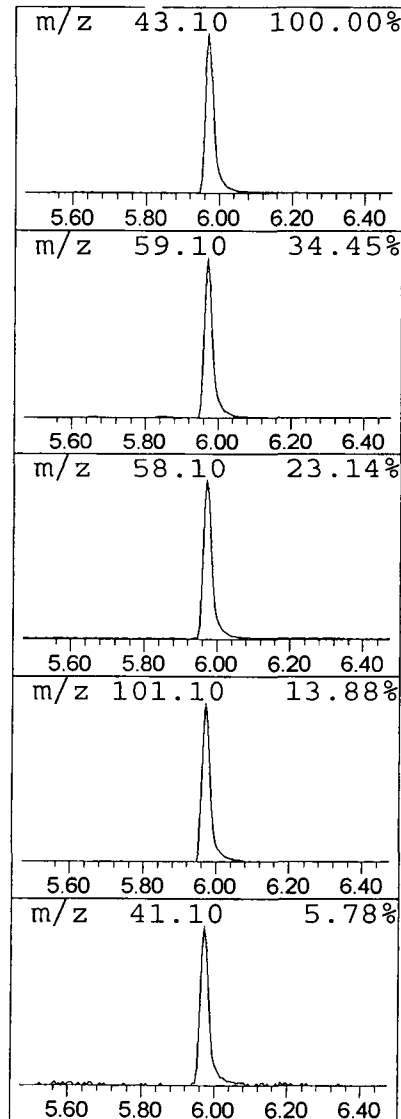
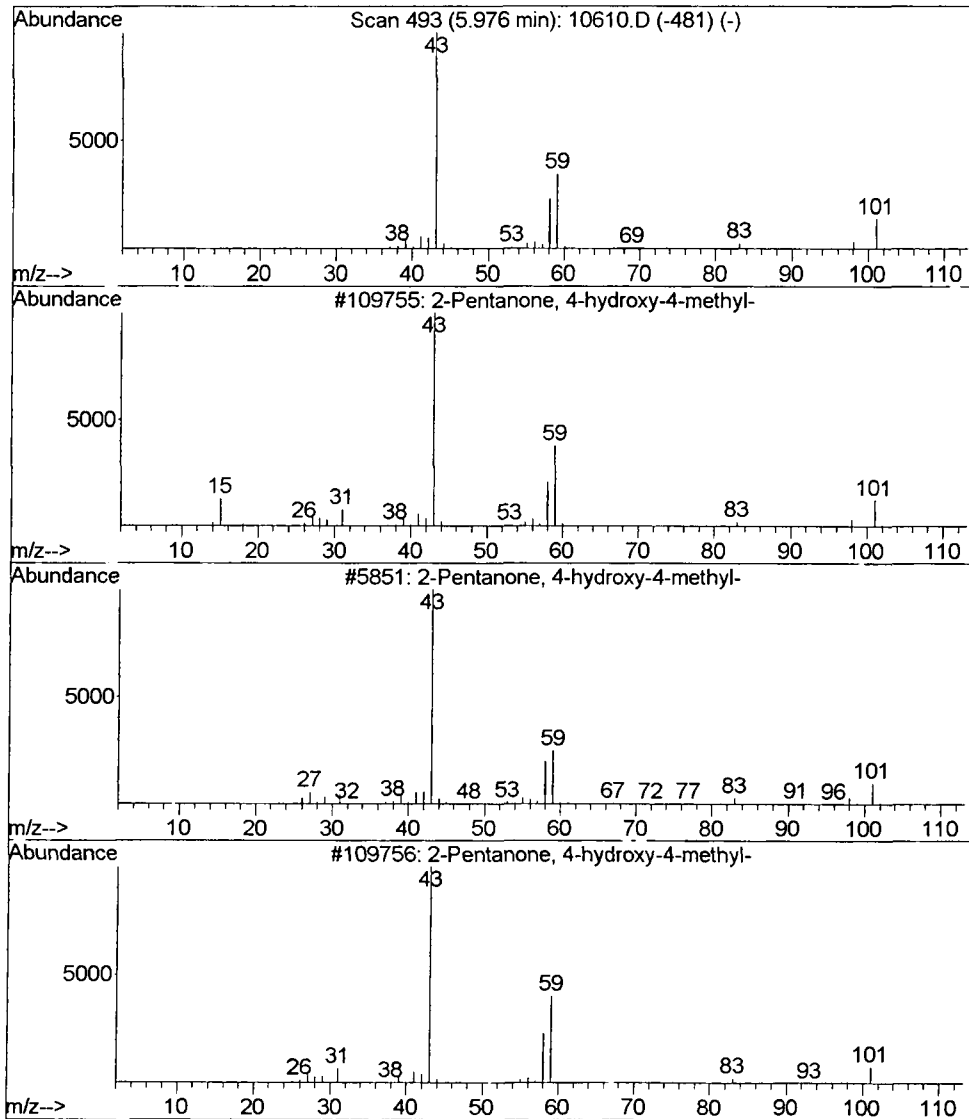
Vial: 13
 Operator: Mclean
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	8.25 ug/L	6947980	1,4-Dichlorobenzene-d4	9.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	90
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
4			Acetone	58	C3H6O	000067-64-1	32



Library Search Compound Report

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 Sample : 5/3 kb
 Misc :
 MS Integration Params: LSCINT.e

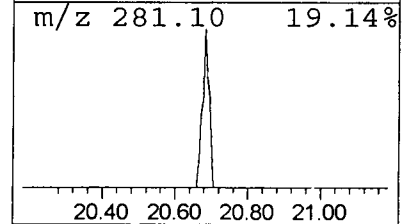
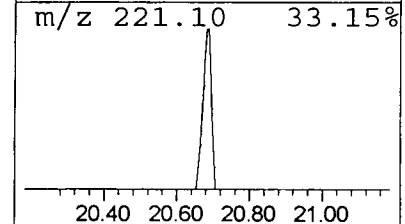
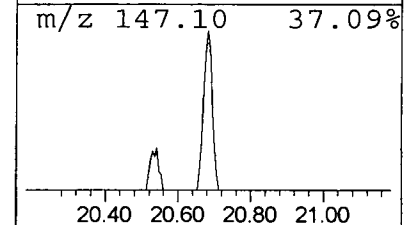
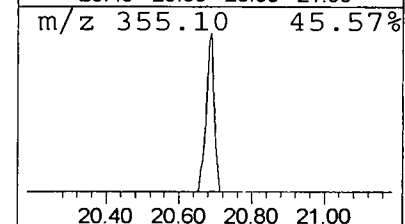
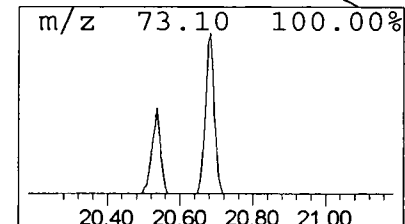
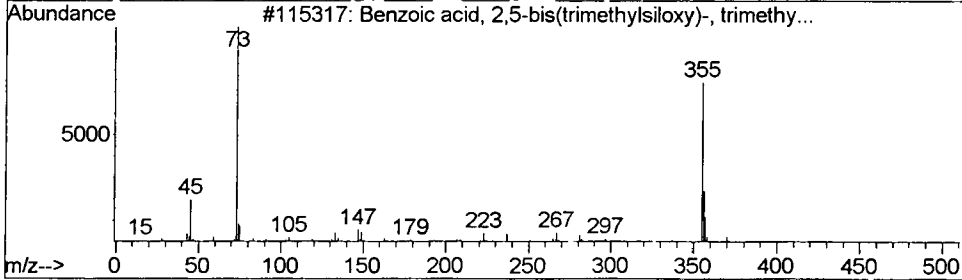
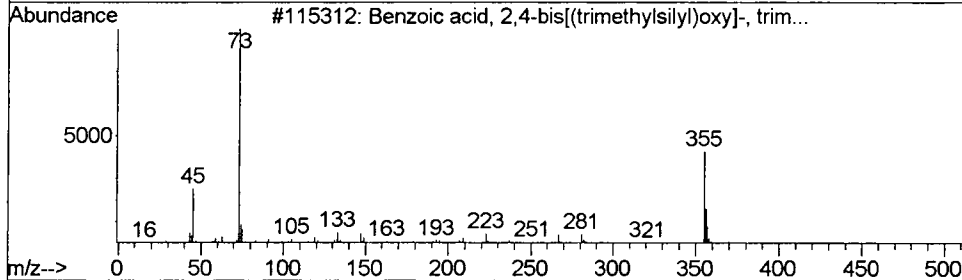
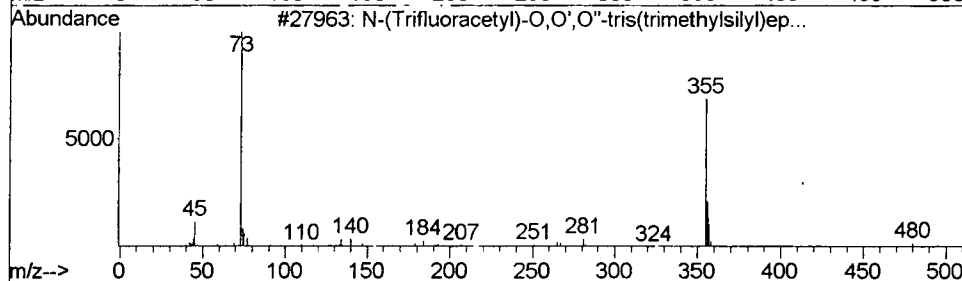
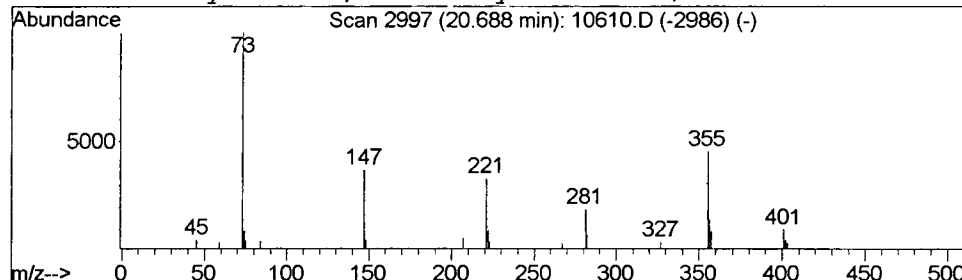
Vial: 13
 Operator: Mclean
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 N-(Trifluoroacetyl)-O,O',O''... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	0.21 ug/L	259870	Acenaphthalene-d10	18.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(Trifluoroacetyl)-O,O',O''-tris...	495	C20H36F3NO4Si3	054135-51-2	25
2			Benzoic acid, 2,4-bis[(trimethyl...	370	C16H30O4Si3	010586-16-0	25
3			Benzoic acid, 2,5-bis(trimethyls...	370	C16H30O4Si3	003618-20-0	17
4			Phenethylamine, N-methyl-.beta.,...	399	C18H37NO3Si3	010538-85-9	16



Library Search Compound Report

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Acq On : 7 May 2002 10:55 pm
Sample : 5/3 kb
Misc :
MS Integration Params: LSCINT.e

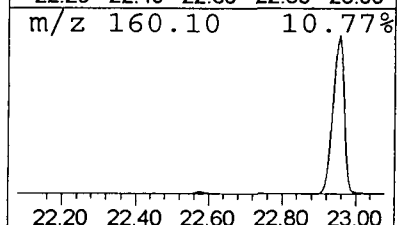
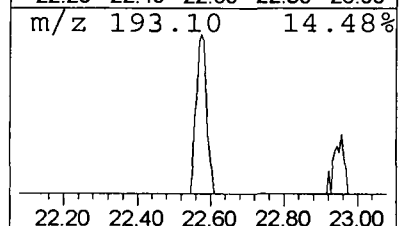
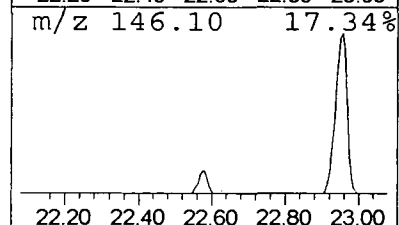
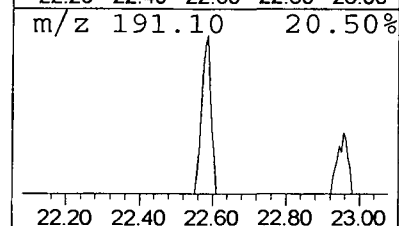
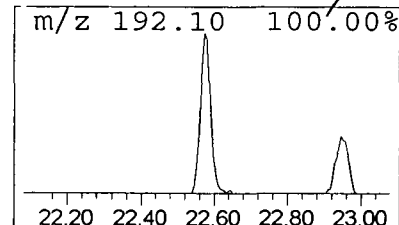
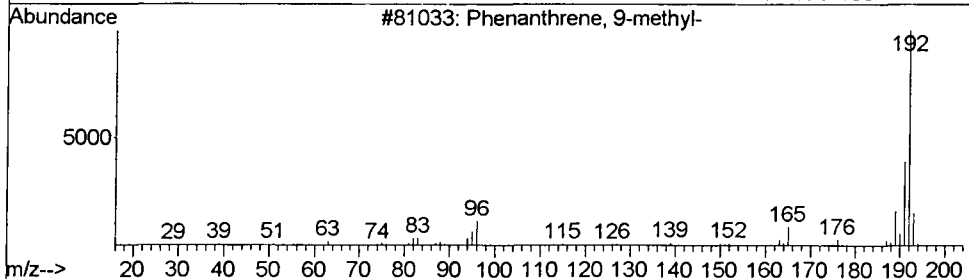
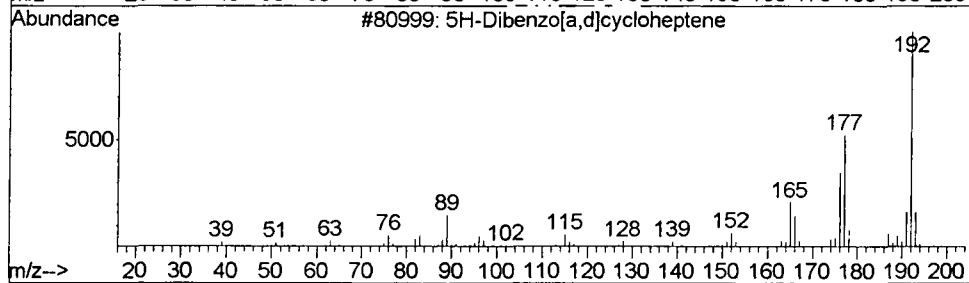
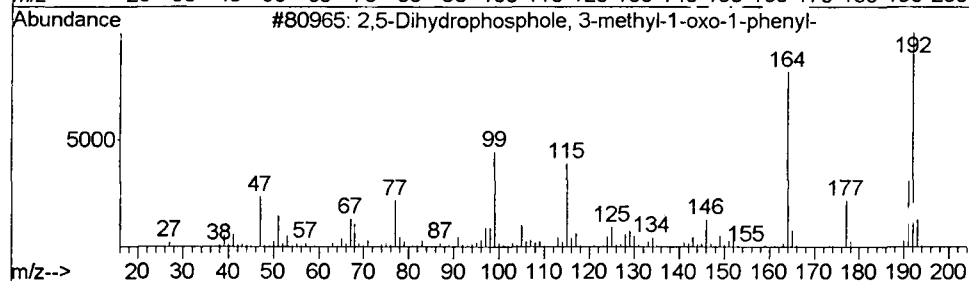
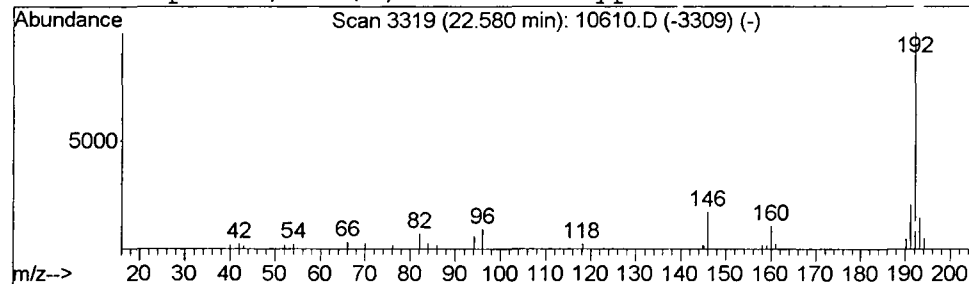
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Operator: Mclean
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 2,5-Dihydrophosphole, 3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	0.33 ug/L	396248	Phenanthranene-d10	22.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Dihydrophosphole, 3-methyl-1...	192	C11H13OP	1000196-97-5	45
2			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	45
3			Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	42
4			2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	42



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
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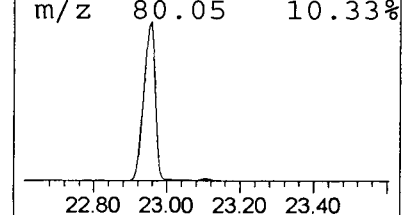
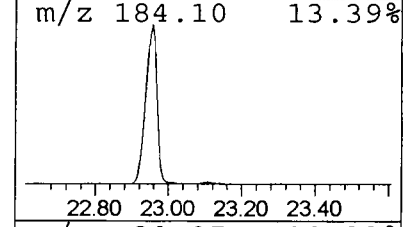
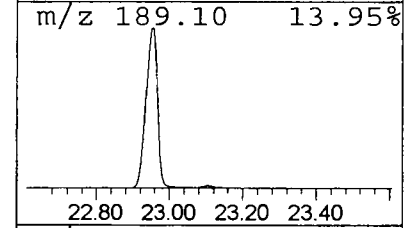
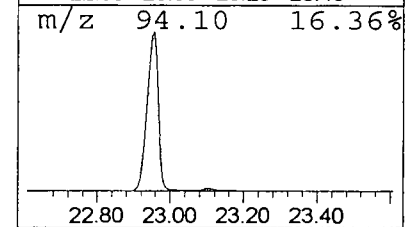
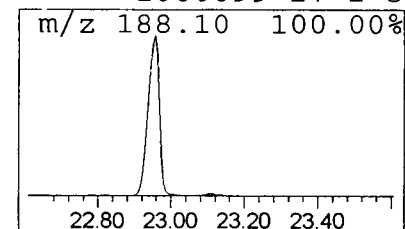
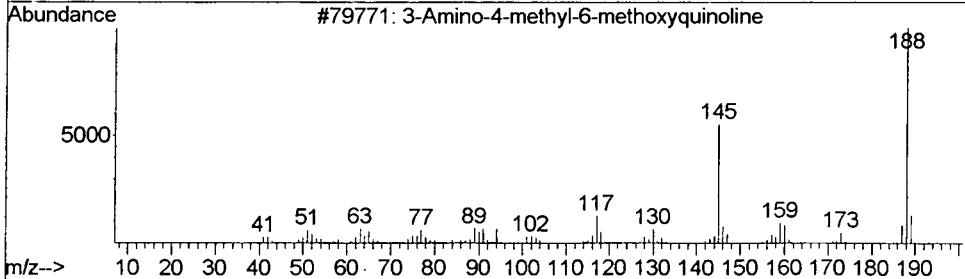
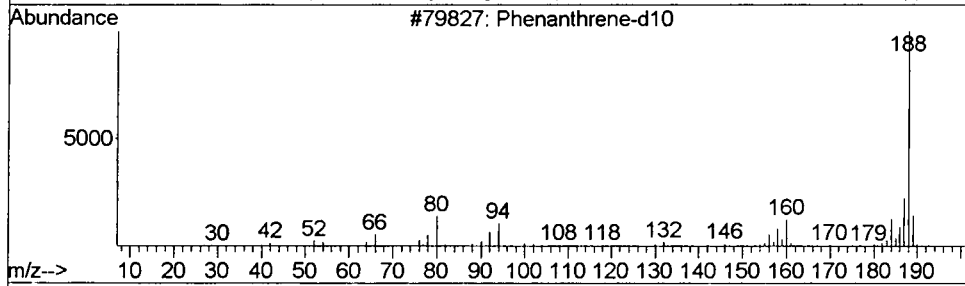
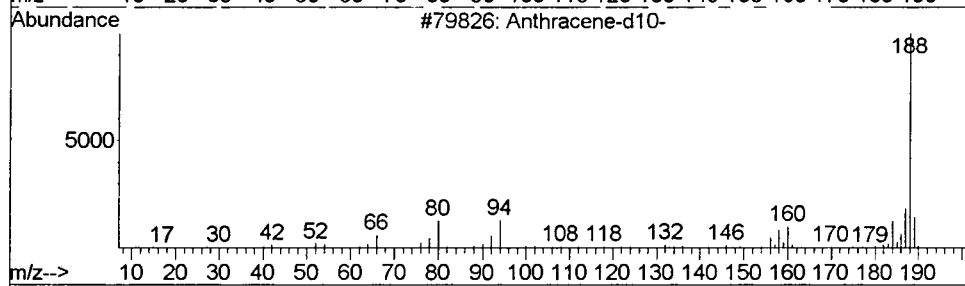
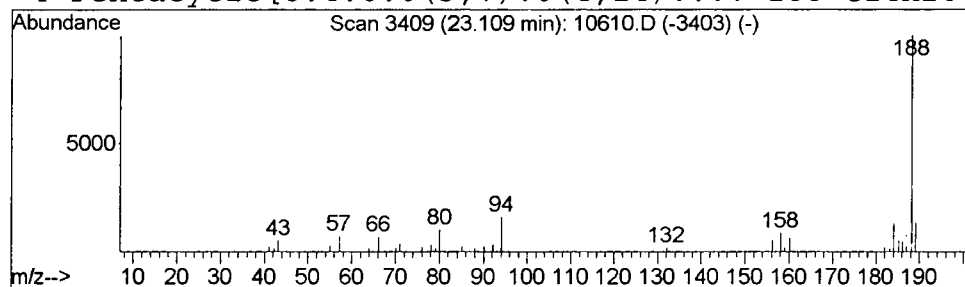
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Operator: Mclean
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 5 Anthracene-d10- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.11	0.50 ug/L	602679	Phenanthranene-d10	22.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene-d10-	188	C14D10	001719-06-8	91
2			Phenanthrene-d10	188	C14D10	001517-22-2	64
3			3-Amino-4-methyl-6-methoxyquinoline	188	C11H12N2O	1000213-71-3	40
4			Pentacyclo[8.4.0.0(3,7).0(4,14)...]	188	C14H20	1000099-27-2	36



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
Acq On : 7 May 2002 10:55 pm
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Misc :
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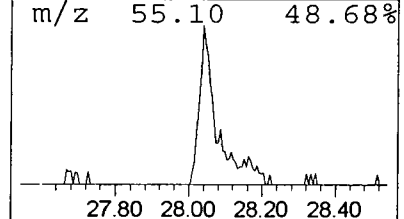
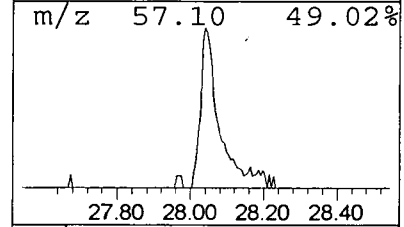
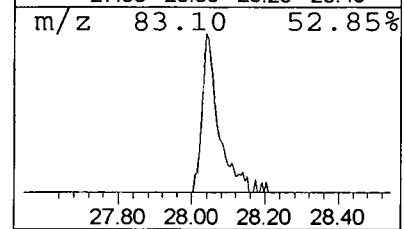
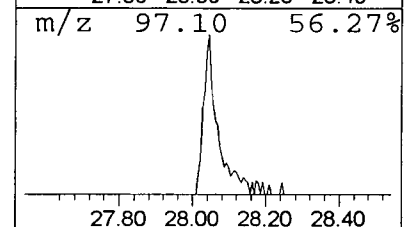
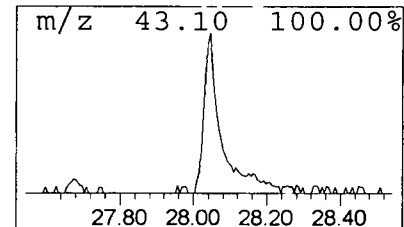
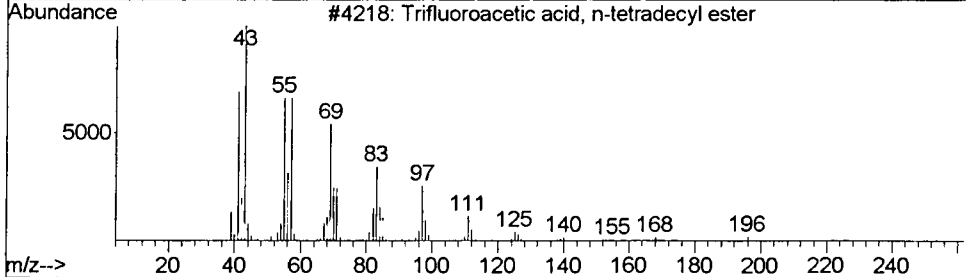
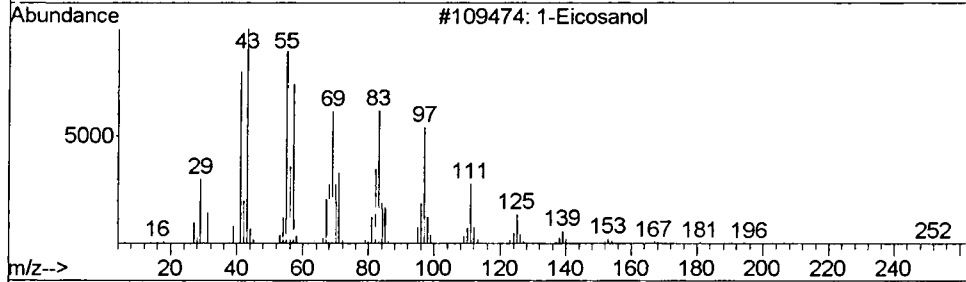
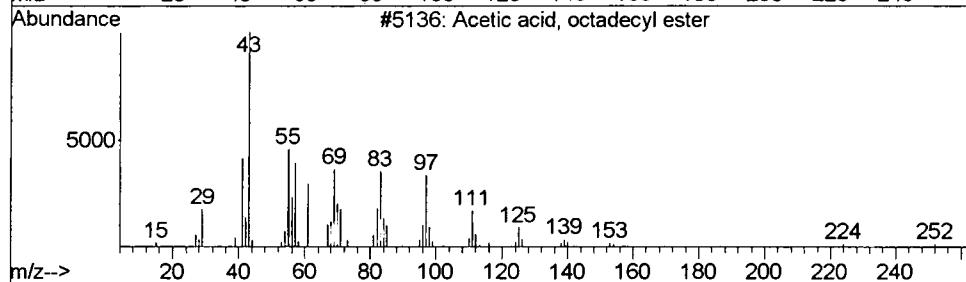
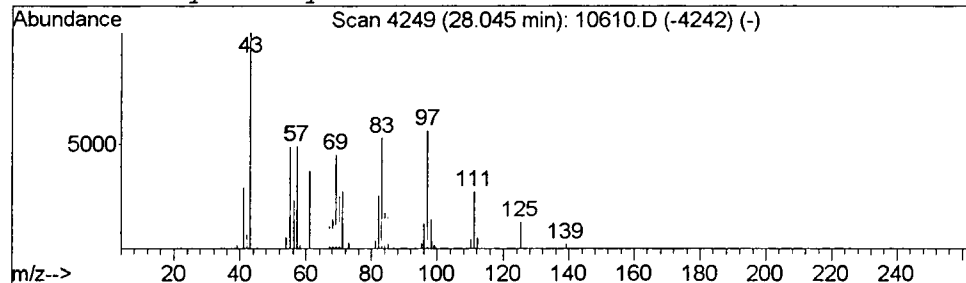
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Multiplr: 1.00

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

Peak Number 6 Acetic acid, octadecyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.04	0.82 ug/L	887797	Chrysene-d12	30.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	91
2			1-Eicosanol	298	C20H42O	000629-96-9	78
3			Trifluoroacetic acid, n-tetradec...	310	C16H29F3O2	1000216-79-0	58
4			Triallylmethylsilane	166	C10H18Si	001112-91-0	43



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
 Acq On : 7 May 2002 10:55 pm
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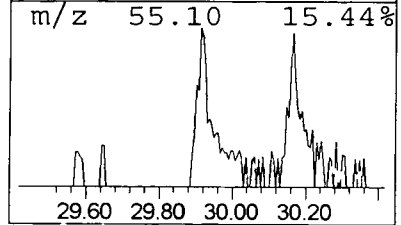
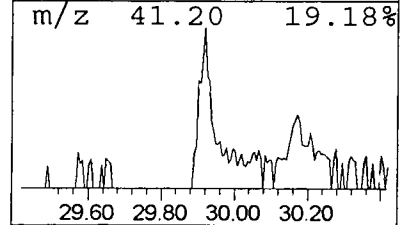
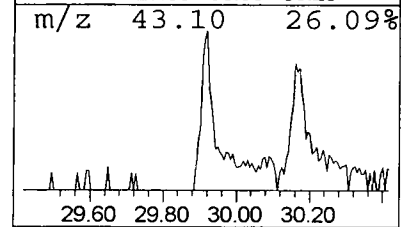
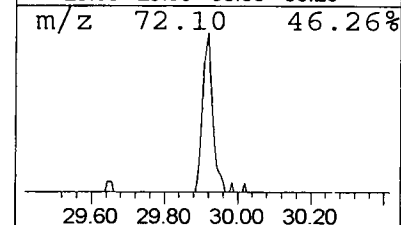
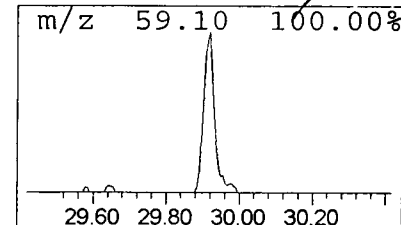
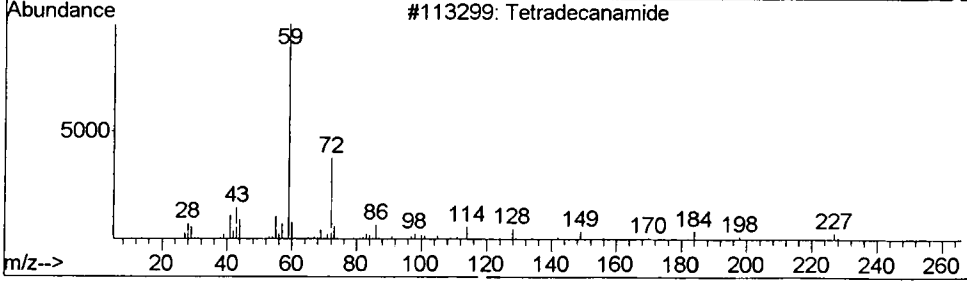
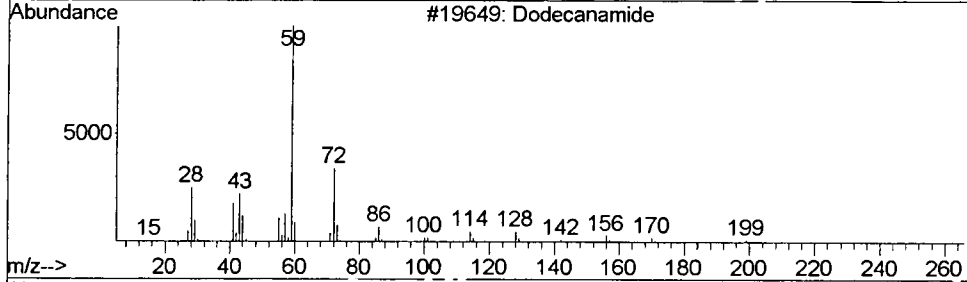
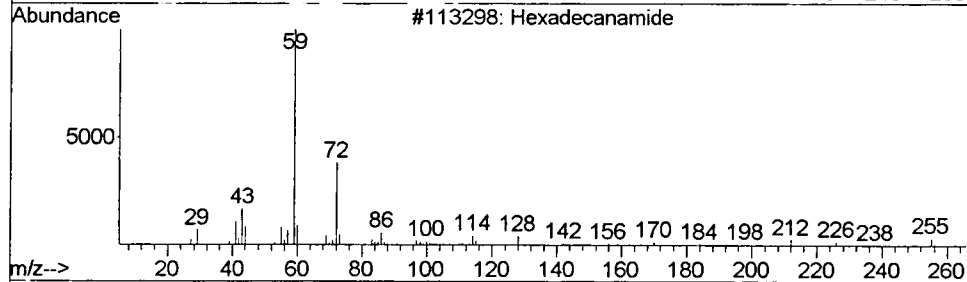
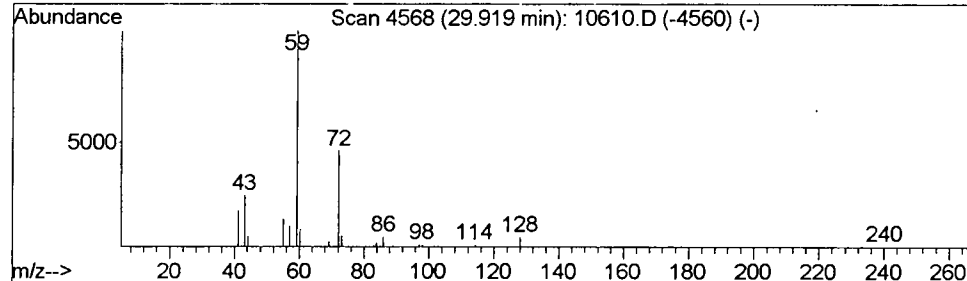
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 Multiplr: 1.00

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

 Peak Number 7 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.92	0.34 ug/L	367709	Chrysene-d12	30.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanamide	255	C16H33NO	000629-54-9	78
2			Dodecanamide	199	C12H25NO	001120-16-7	59
3			Tetradecanamide	227	C14H29NO	000638-58-4	59
4			Tetradecanamide	227	C14H29NO	000638-58-4	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
Acq On : 7 May 2002 10:55 pm
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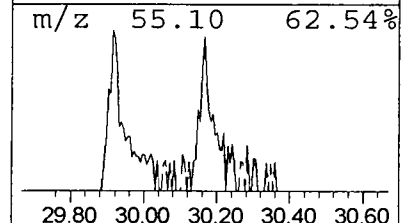
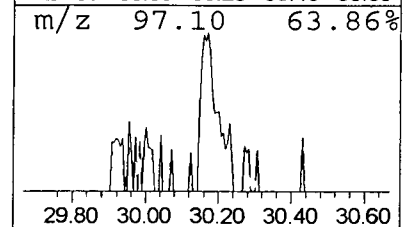
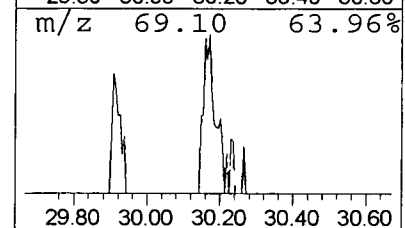
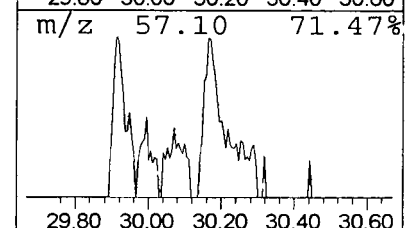
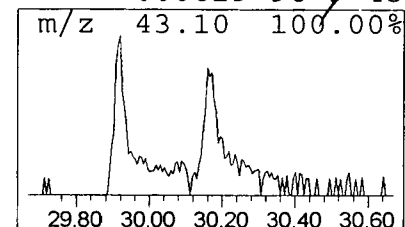
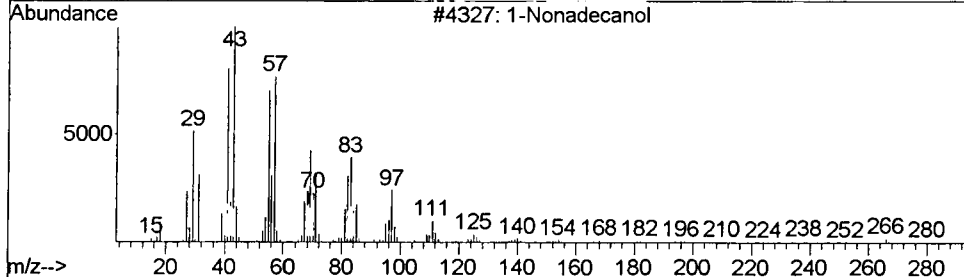
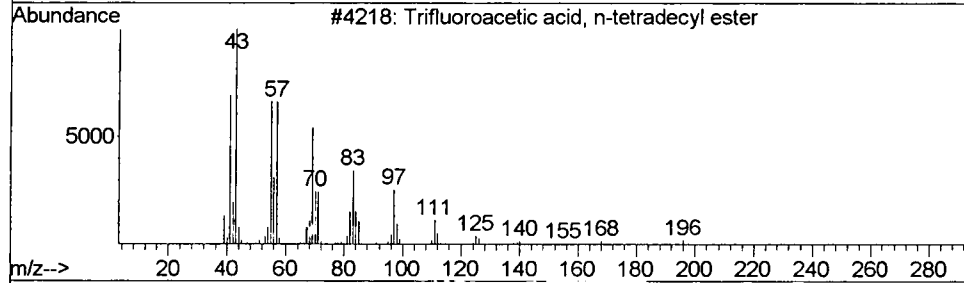
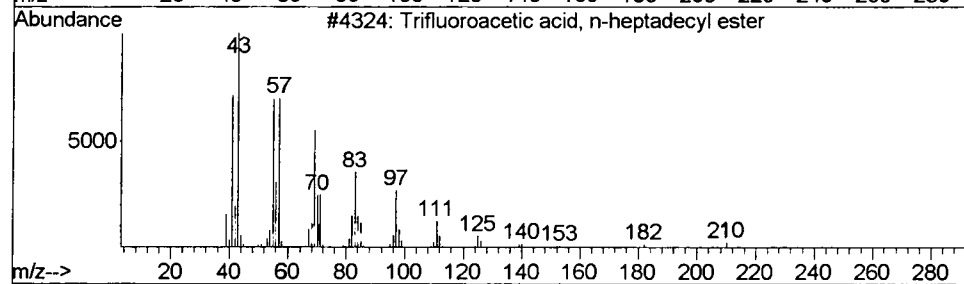
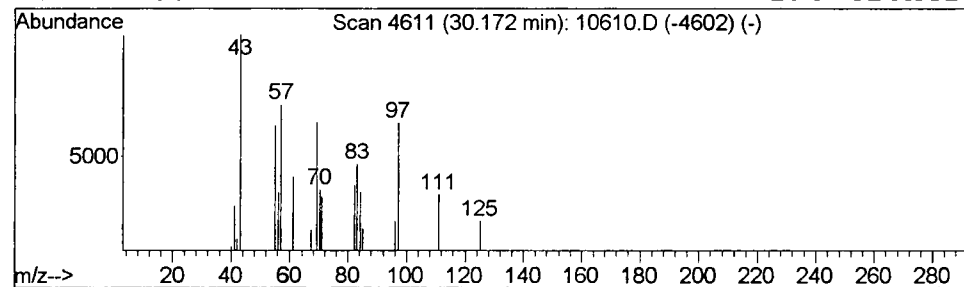
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Operator: Mclean
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 8 Trifluoroacetic acid, n-hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.17	0.24 ug/L	257149	Chrysene-d12	30.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	59
2			Trifluoroacetic acid, n-tetradec...	310	C16H29F3O2	1000216-79-0	59
3			1-Nonadecanol	284	C19H40O	001454-84-8	47
4			1-Eicosanol	298	C20H42O	000629-96-9	43



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
Acq On : 7 May 2002 10:55 pm
Sample : 5/3 kb
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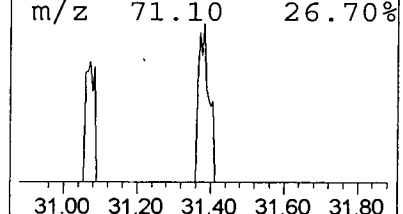
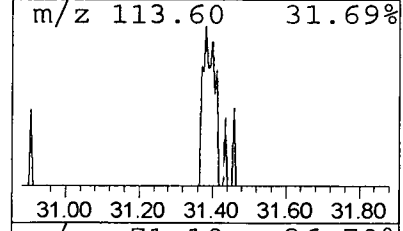
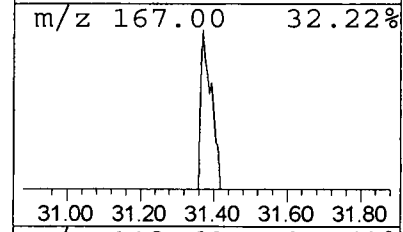
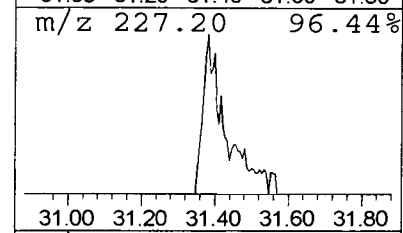
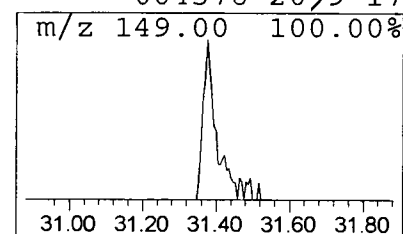
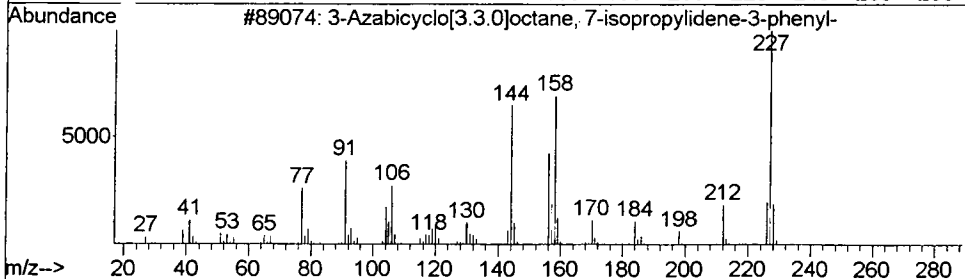
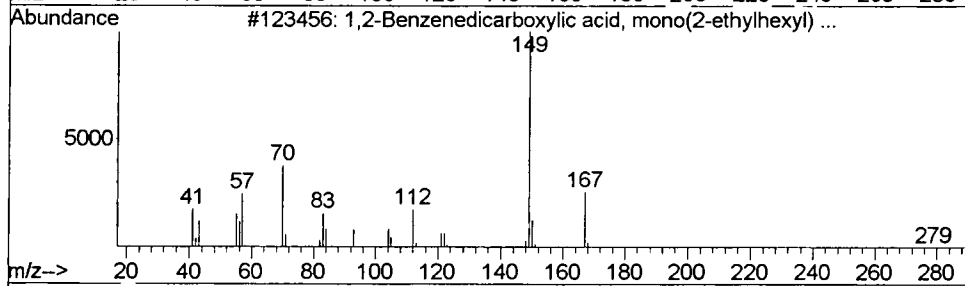
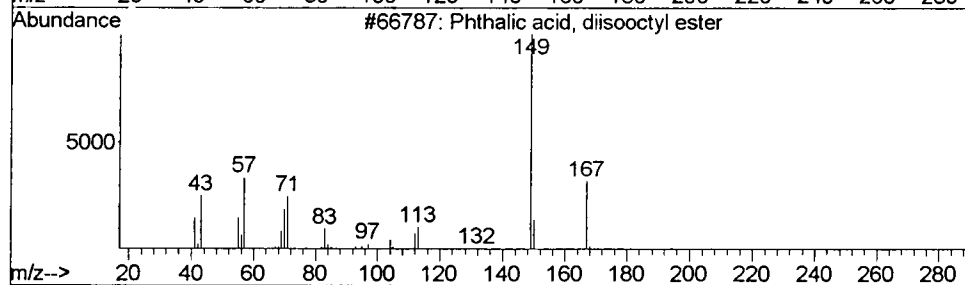
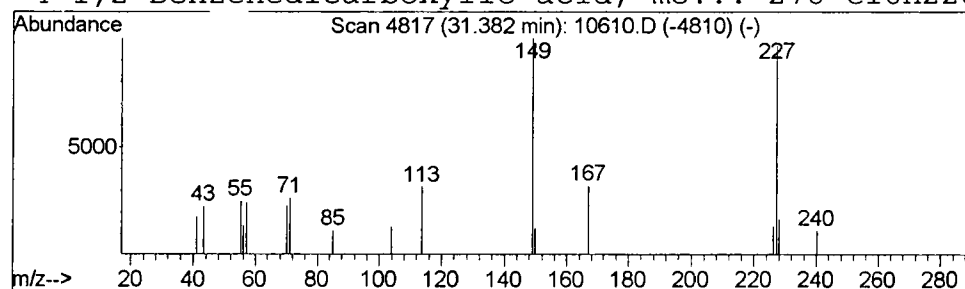
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Multiplr: 1.00

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

Peak Number 9 Phthalic acid, diisooctyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.38	0.25 ug/L	272467	Chrysene-d12	30.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, diisooctyl ester	390	C24H38O4	001330-91-2	38
2			1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	27
3			3-Azabicyclo[3.3.0]octane, 7-iso...	227	C16H21N	1000156-34-8	27
4			1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	17



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D

Acq On : 7 May 2002 10:55 pm

Sample : 5/3 kb

Misc :

MS Integration Params: LSCINT.e

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Operator: Mclean

Inst : Instrumen

Multiplr: 1.00

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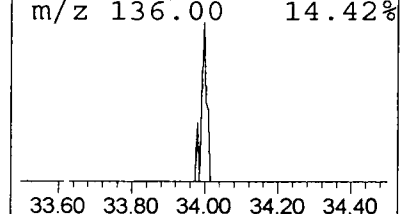
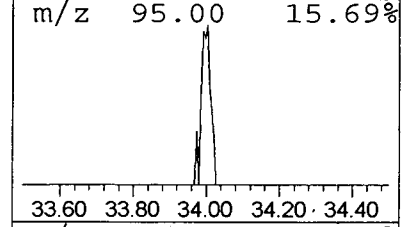
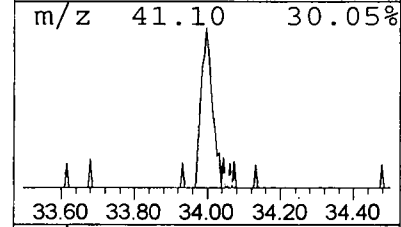
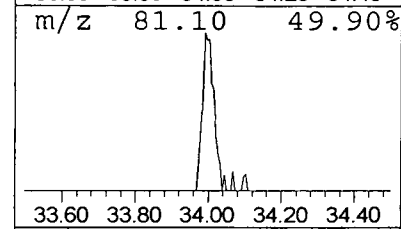
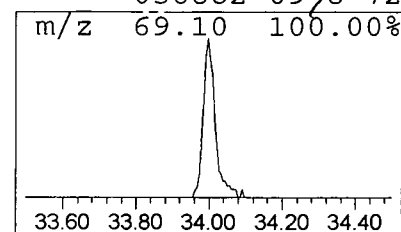
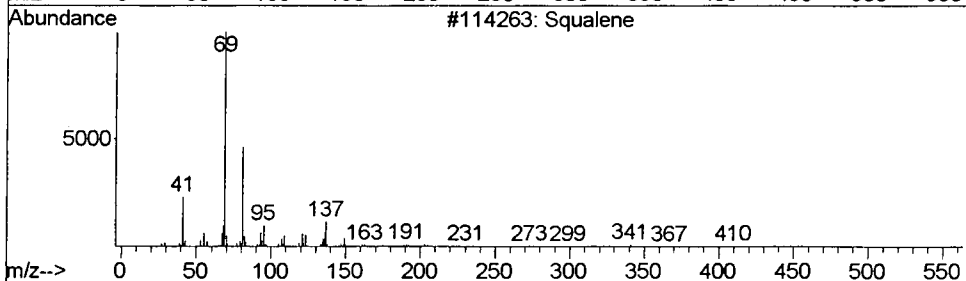
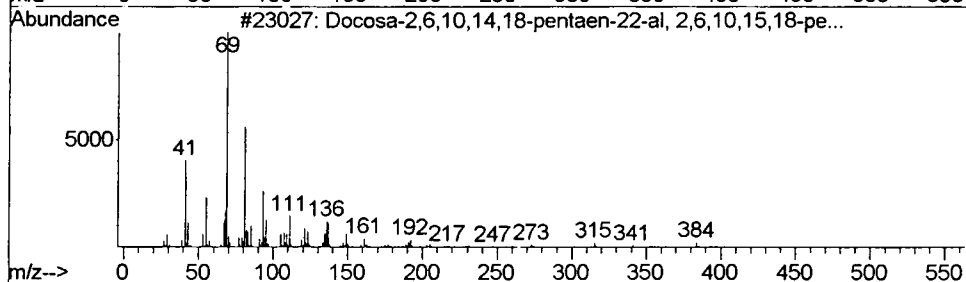
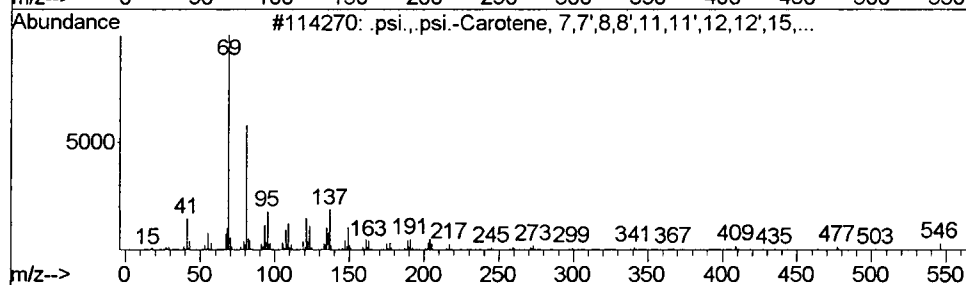
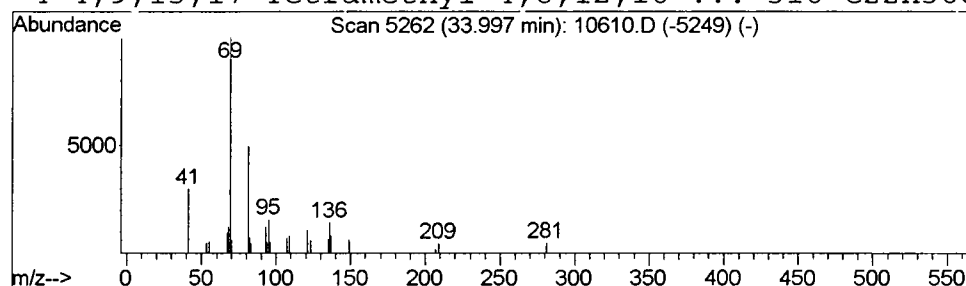
Title : 508 Modified GC/MS scan

Library : C:\DATABASE\NIST98.L

Peak Number 10 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
34.00	0.30 ug/L	263133	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
3			Squalene	410	C30H50	007683-64-9	78
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\050702\10610.D
 Acq On : 7 May 2002 10:55 pm
 Sample : 5/3 kb
 Misc :
 MS Integration Params: LSCINT.e

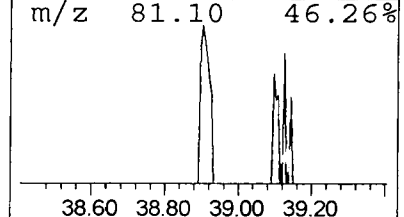
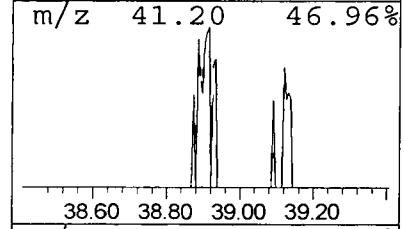
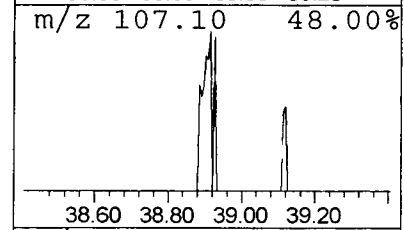
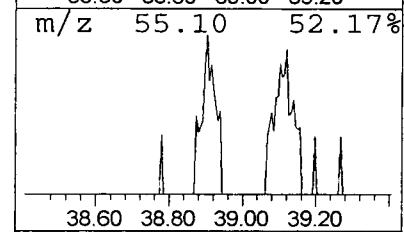
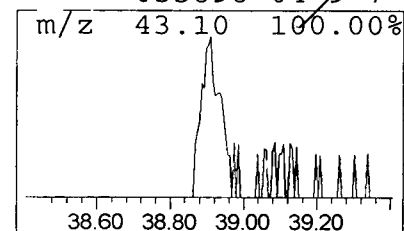
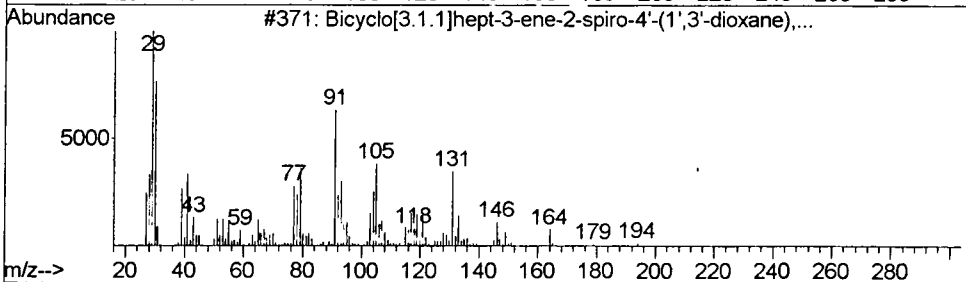
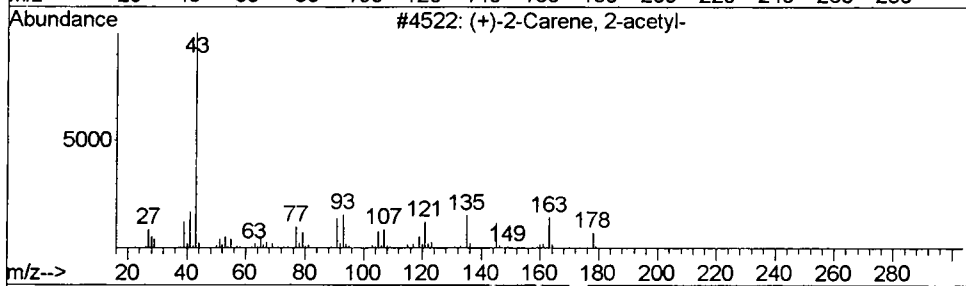
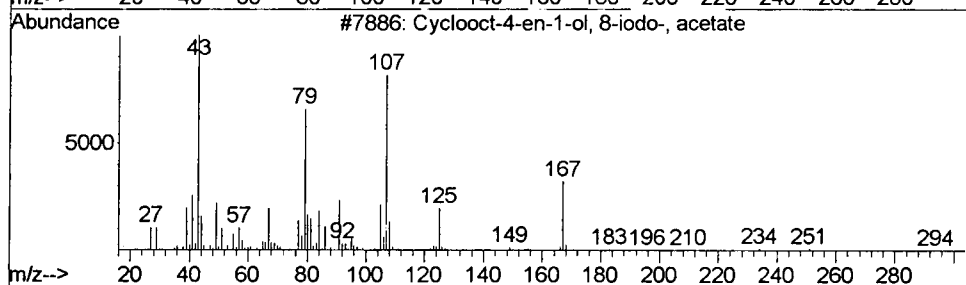
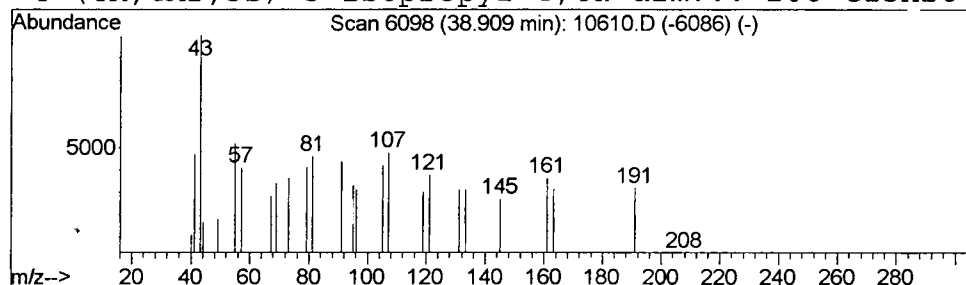
Vial: 13
 Operator: Mclean
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 11 Cyclooct-4-en-1-ol, 8-iodo-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
38.91	0.20 ug/L	174964	Perylene-d12	34.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooct-4-en-1-ol, 8-iodo-, ace...	294	C10H15IO2	1000197-11-8	9
2			(+)-2-Carene, 2-acetyl-	178	C12H18O	1000151-09-7	9
3			Bicyclo[3.1.1]hept-3-ene-2-spiro...	194	C12H18O2	1000149-76-2	9
4			(4R,4Ar,5s)-5-isopropyl-4,4a-dim...	206	C15H26	055898-04-8	7



Tentatively Identified Compound (LSC) summary

Operator ID: Mclean Date Acquired: 7 May 2002 10:55 pm
Data File: C:\MSDCHEM\1\DATA\050702\10610.D
Name: 5/3 kb
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
Spiro[2.4]hepta-4...	4.35	0.2	ug/L	172105	1	9.94	33705400	40.0
2-Pentanone, 4-hy...	5.97	8.2	ug/L	6947980	1	9.94	33705400	40.0
N-(Trifluoracetyl...	20.69	0.2	ug/L	259870	3	18.57	49562400	40.0
2,5-Dihydrophosph...	22.58	0.3	ug/L	396248	4	22.96	48411400	40.0
Anthracene-d10-	23.11	0.5	ug/L	602679	4	22.96	48411400	40.0
Acetic acid, octa...	28.04	0.8	ug/L	887797	5	30.81	43154100	40.0
Hexadecanamide	29.92	0.3	ug/L	367709	5	30.81	43154100	40.0
Trifluoroacetic a...	30.17	0.2	ug/L	257149	5	30.81	43154100	40.0
Phthalic acid, di...	31.38	0.3	ug/L	272467	5	30.81	43154100	40.0
.psi.,.psi.-Carot...	34.00	0.3	ug/L	263133	6	34.71	34550900	40.0
Cyclooct-4-en-1-o...	38.91	0.2	ug/L	174964	6	34.71	34550900	40.0