

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 02/01/2002 Time: 14:24:36

Sample: AE00616
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 2/1/02 14:24 Ended: 2/1/02 14:24 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		87		5.0

Field Blank

Comments for Sample AE00616 - Analysis \$GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 02-04-2002 Time: 13:37:31

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recoveries for 5 of the 43 compounds in the LCS Standard were outside of their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D Vial: 5
 Acq On : 29 Jan 2002 5:59 pm Operator:
 Sample : 508 scan Inst : Instrumen
 Misc : January 29, 2002 Multiplr: 1.00
 MS Integration Params: SPLIT.P
 Quant Time: Jan 30 08:26:00 2002 Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Last Update : Fri Jan 11 13:20:07 2002
 Response via : Initial Calibration
 DataAcq Meth : SCAN508

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1916521	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	8192320	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	4274274	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	7105358	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	6268445	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	4683270	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	487722	4.34	ug/L	0.00
Spiked Amount	5.000		Recovery	=	86.80%	
Target Compounds						
20) Dimethylphthalate	18.34	163	692664	2.45	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	547706	9.95	ug/L #	17
35) Di-n-butylphthalate	24.85	149	134165	0.29	ug/L	98
42) Bis(2-ethylhexyl)phthalate	31.11	149	160771	1.06	ug/L	96

(#) = qualifier out of range (m) = manual integration
 00616.D SCAN508.M Wed Jan 30 08:26:01 2002

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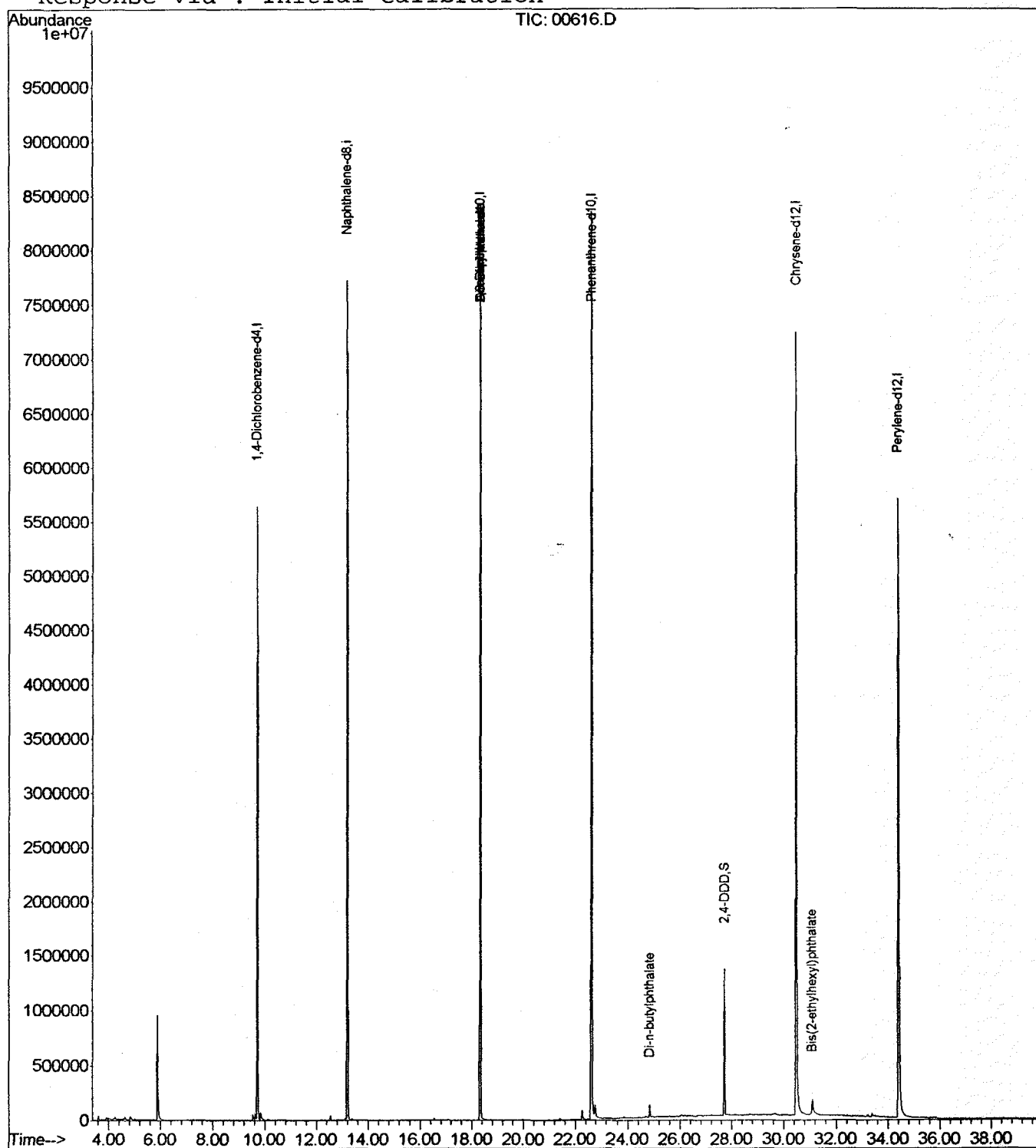
Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
 Misc : January 29, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 30 8:26 2002

Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Last Update : Fri Jan 11 13:20:07 2002
 Response via : Initial Calibration



00616.D SCAN508.M

Wed Jan 30 08:26:01 2002

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LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
 Misc : January 29, 2002
 MS Integration Params: LSCINT.P

Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Smoothing : OFF
 Sampling : 2
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 100 Area counts
 Max Peaks: 20
 Peak Location: TOP

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

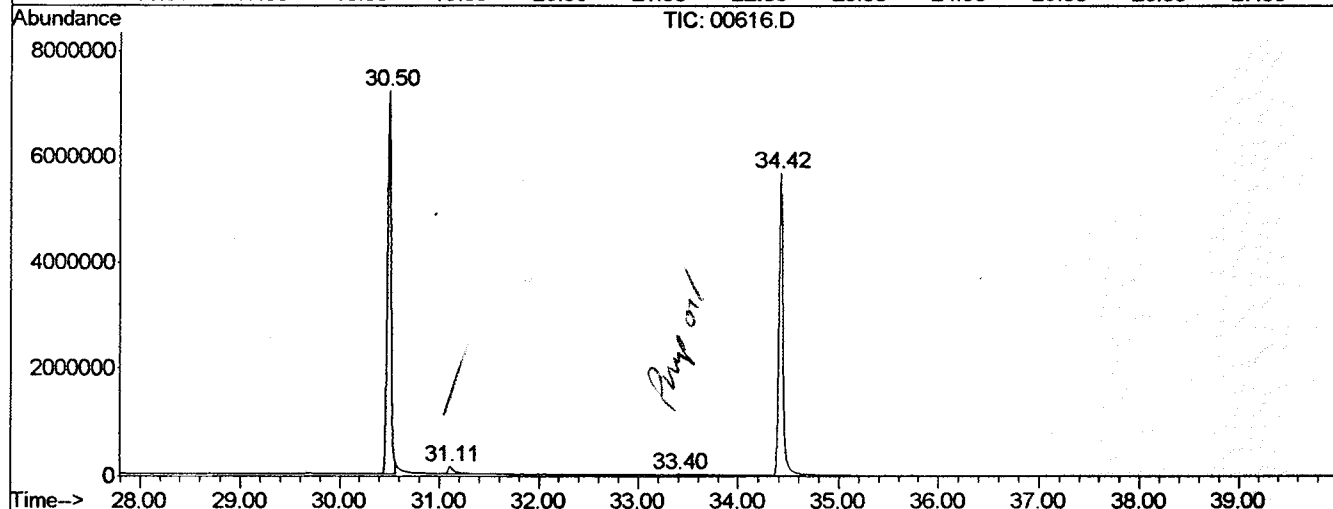
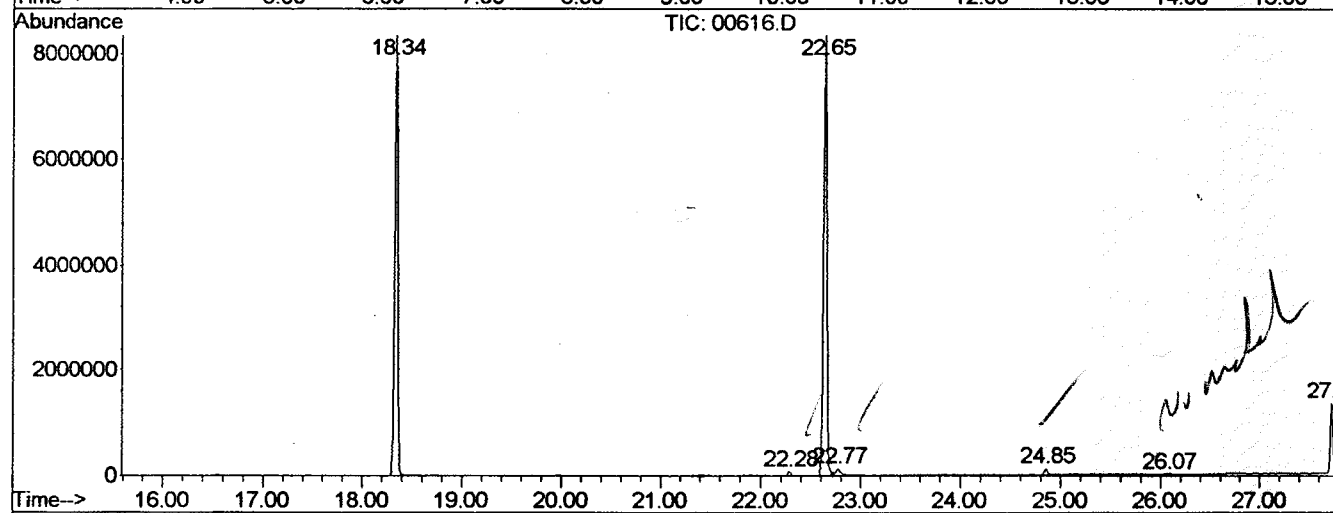
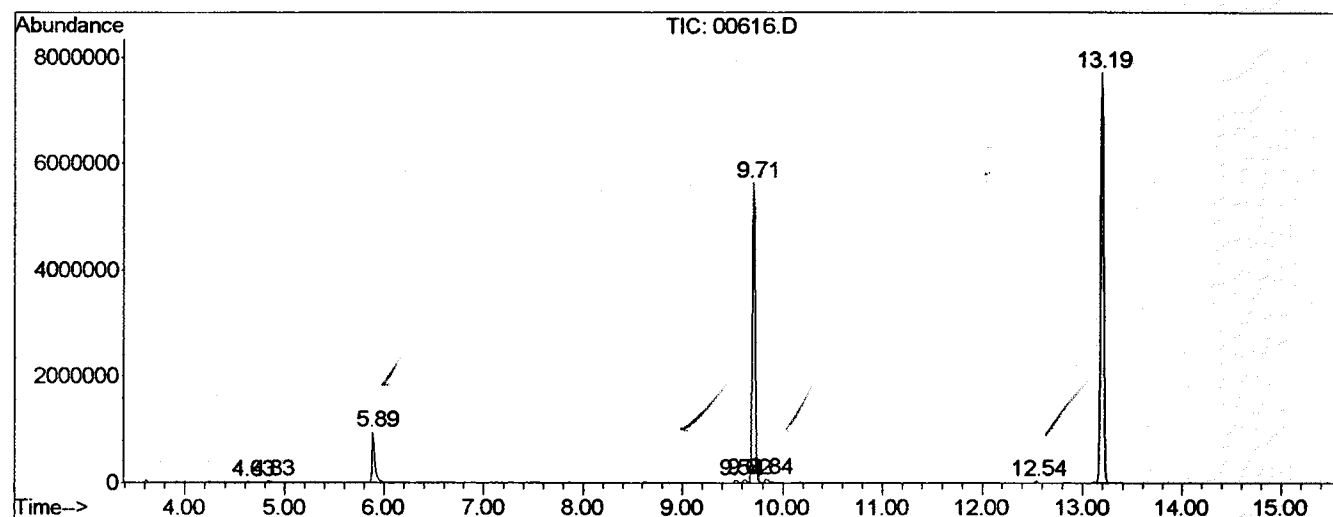
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.629	103	110	119	rBV5	26353	69411	0.37%	0.067%
2	4.835	123	128	141	rBV4	33558	103659	0.55%	0.100%
3	5.885	215	220	241	rBV	951587	1804939	9.55%	1.735%
4	9.539	535	540	545	rBV	50541	123474	0.65%	0.119%
5	9.619	545	547	551	rVV	58037	134496	0.71%	0.129%
6	9.710	551	555	561	rVV	5638436	10979879	58.11%	10.553%
7	9.836	561	566	577	rVV	71127	213817	1.13%	0.206%
8	12.541	799	803	807	rVB	41728	67485	0.36%	0.065%
9	13.192	855	860	865	rBV	7707994	15748830	83.35%	15.137%
10	18.341	1305	1311	1317	rBV	8345140	17513793	92.69%	16.833%
11	22.280	1651	1656	1661	rVV	88075	178700	0.95%	0.172%
12	22.645	1681	1688	1693	rBV2	8348115	18894469	100.00%	18.160%
13	22.771	1695	1699	1725	rVV2	133773	584272	3.09%	0.562%
14	24.849	1877	1881	1887	rVV	117994	225811	1.20%	0.217%
15	26.070	1981	1988	1995	rBV8	13481	68905	0.36%	0.066%
16	27.726	2129	2133	2139	rBV	1335640	2492716	13.19%	2.396%
17	30.500	2369	2376	2381	rBV	7205164	18252856	96.60%	17.544%
18	31.105	2423	2429	2455	rVB	144442	664560	3.52%	0.639%
19	33.400	2625	2630	2635	rBV4	27959	89360	0.47%	0.086%
20	34.416	2713	2719	2741	rBV	5682590	15831499	83.79%	15.216%

Sum of corrected areas: 104042931

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Operator :
 Acquired : 29 Jan 2002 5:59 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 29, 2002
 Vial Number: 5
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D

Acq On : 29 Jan 2002 5:59 pm

Sample : 508 scan

Misc : January 29, 2002

MS Integration Params: LSCINT.P

Vial: 5

Operator:

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

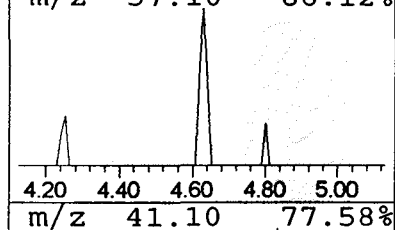
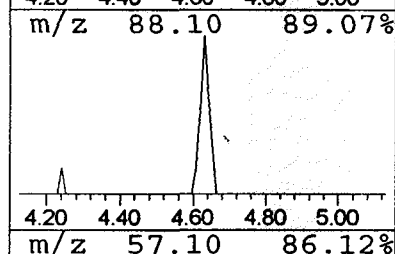
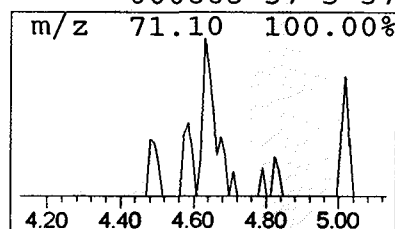
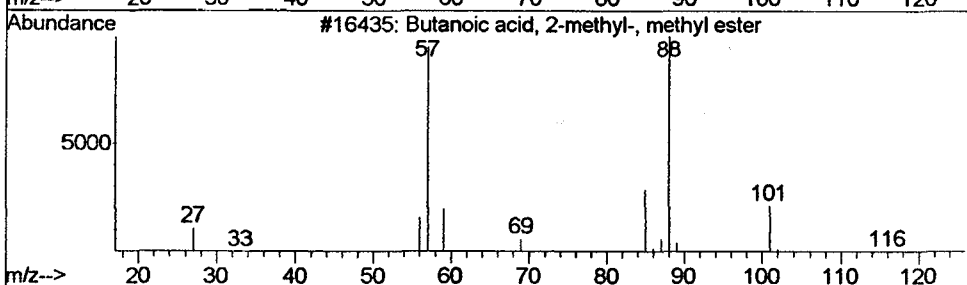
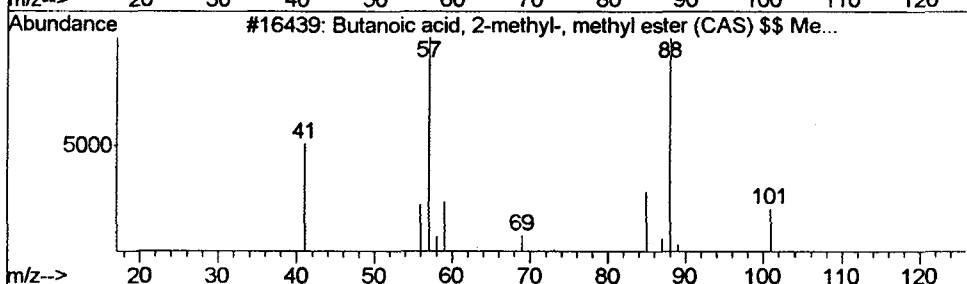
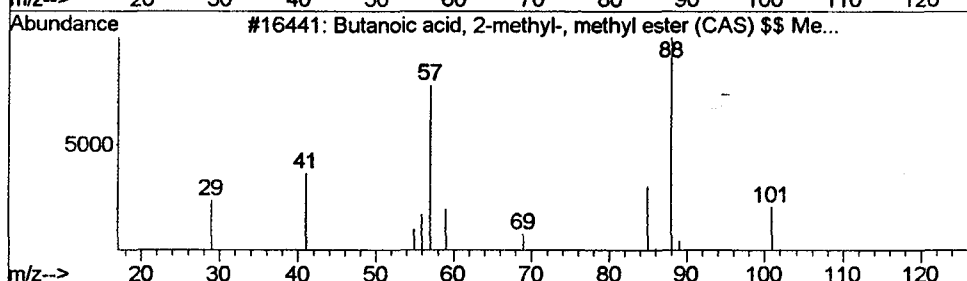
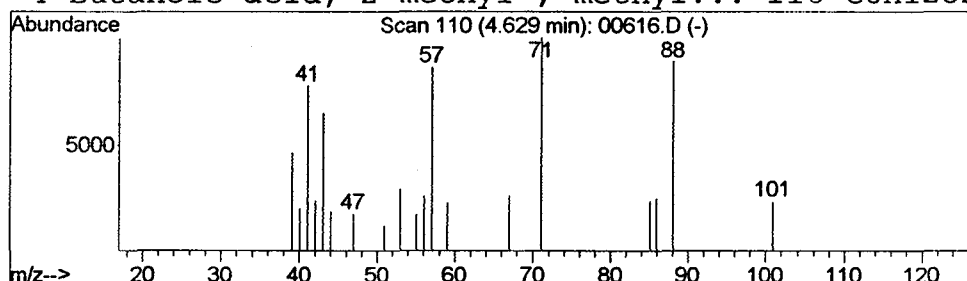
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Butanoic acid, 2-methyl-, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	0.13 ug/L	69411	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	43
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	43
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	43
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	37



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
 Misc : January 29, 2002
 MS Integration Params: LSCINT.P

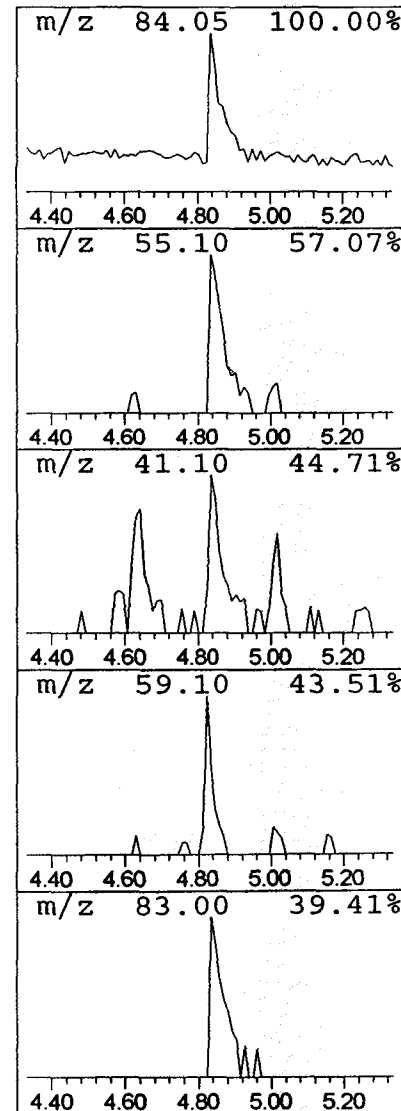
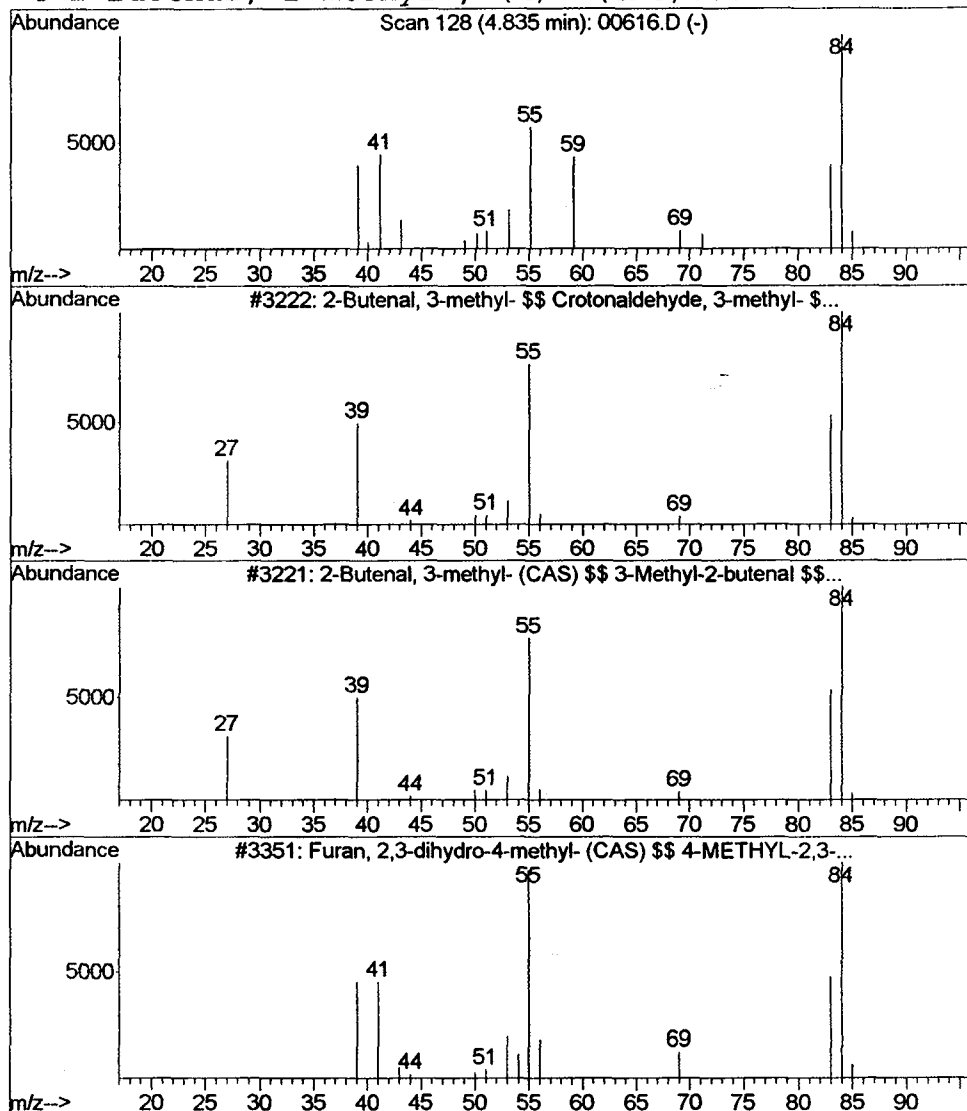
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 2-Butenal, 3-methyl- \$\$ Cro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.19 ug/L	103659	1,4-Dichlorobenzene-d4	9.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl- \$\$ Crotonal...	84	C5H8O	000107-86-8	72	
2	2-Butenal, 3-methyl- (CAS) \$\$ 3-...	84	C5H8O	000107-86-8	72	
3	Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	64	
4	2-Butenal, 2-methyl-, (E)- (CAS)...	84	C5H8O	000497-03-0	50	



Library Search Compound Report

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Acq On : 29 Jan 2002 5:59 pm

Sample : 508 scan

Misc : January 29, 2002

MS Integration Params: LSCINT.P

Vial: 5

Operator:

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

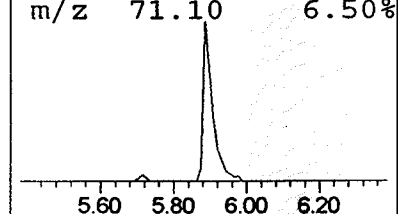
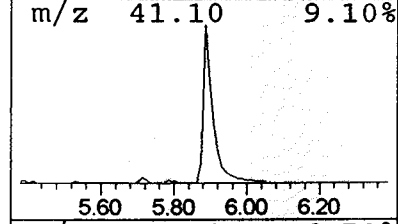
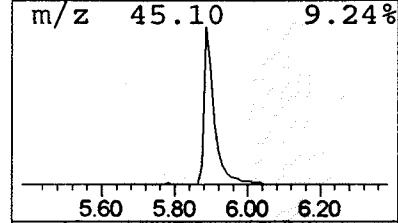
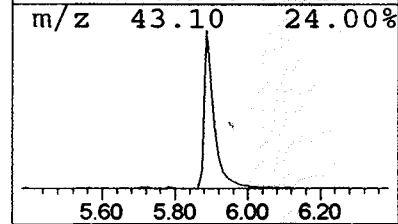
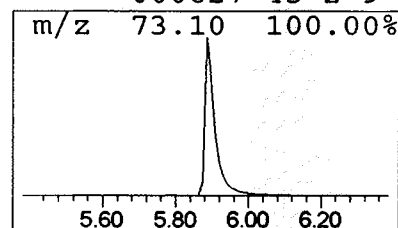
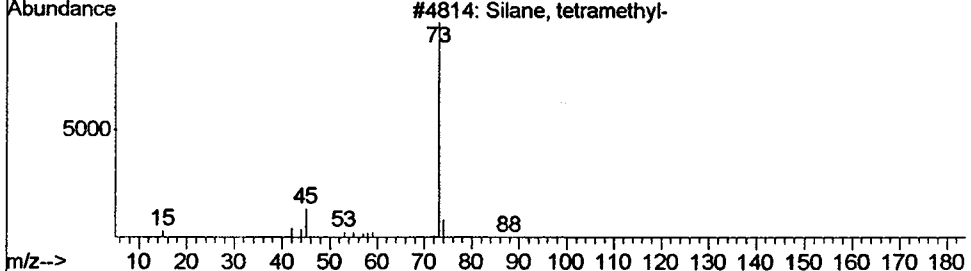
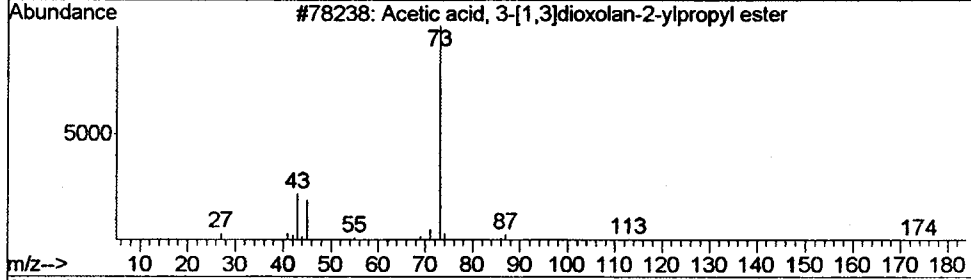
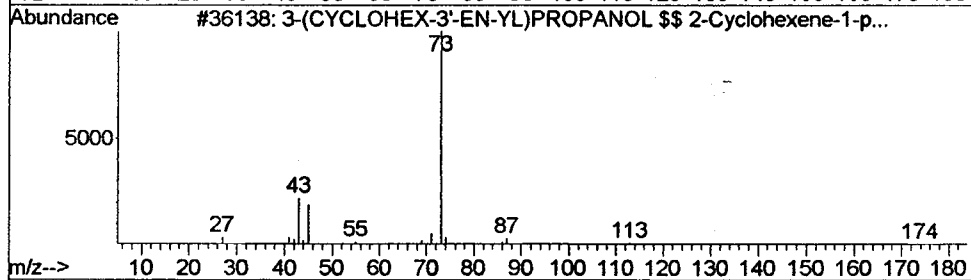
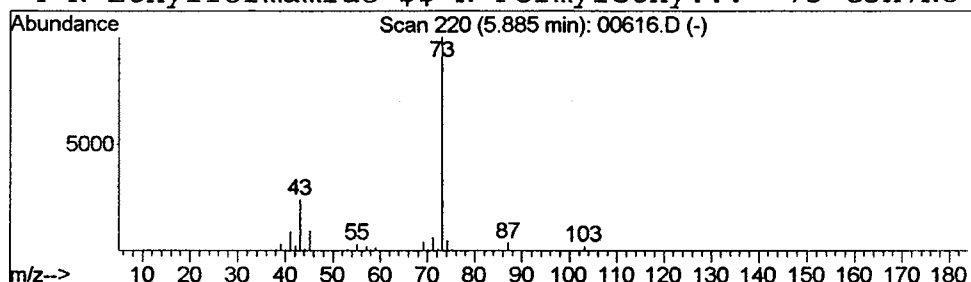
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 3 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	3.29 ug/L	1804940	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	33
2			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9



Library Search Compound Report

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Sample : 508 scan
Misc : January 29, 2002
MS Integration Params: LSCINT.P

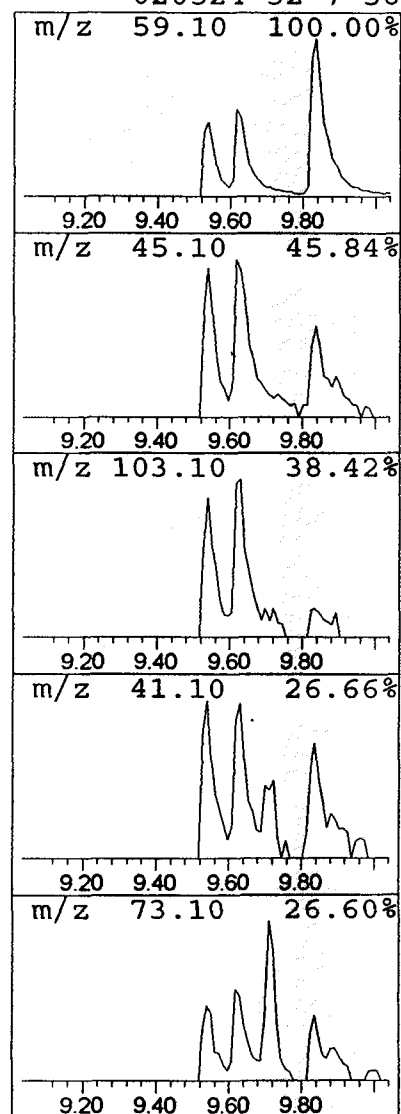
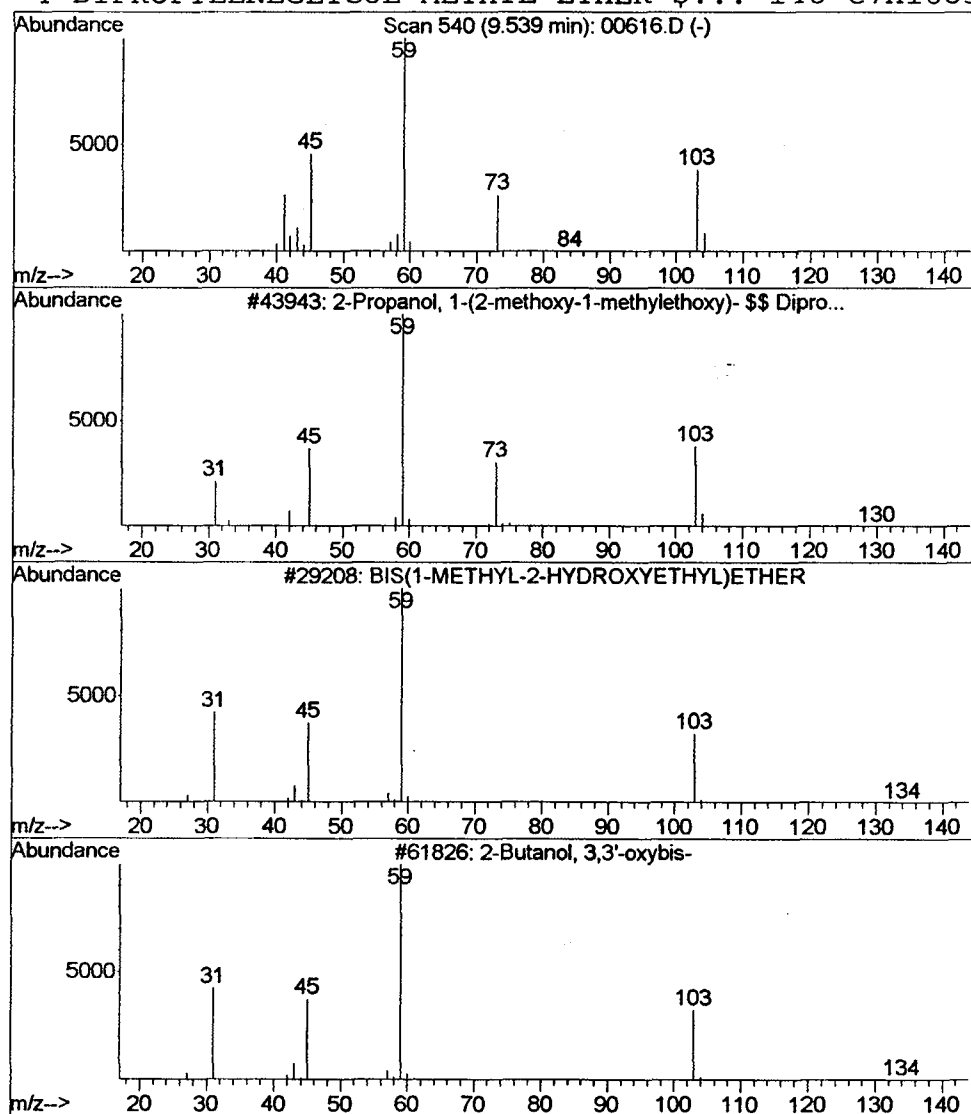
Vial: 5
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	0.22 ug/L	123474	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			BIS(1-METHYL-2-HYDROXYETHYL)ETHER	134	C6H14O3	000000-00-0	72
3			2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	72
4			DIPROPYLENEGLYCOL METHYL ETHER \$...	148	C7H16O3	020324-32-7	56



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D

Acq On : 29 Jan 2002 5:59 pm

Sample : 508 scan

Misc : January 29, 2002

MS Integration Params: LSCINT.P

Vial: 5

Operator:

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

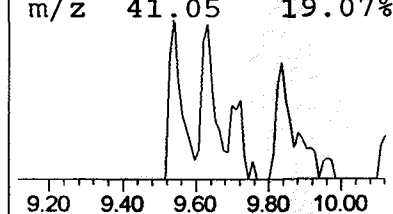
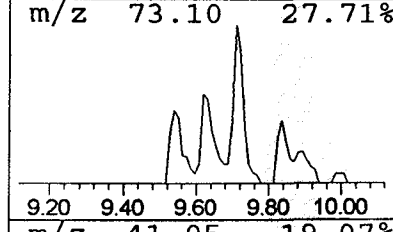
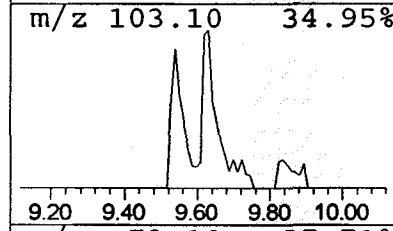
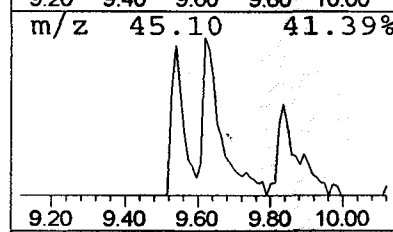
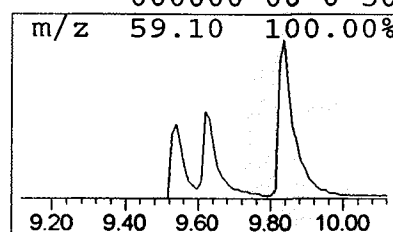
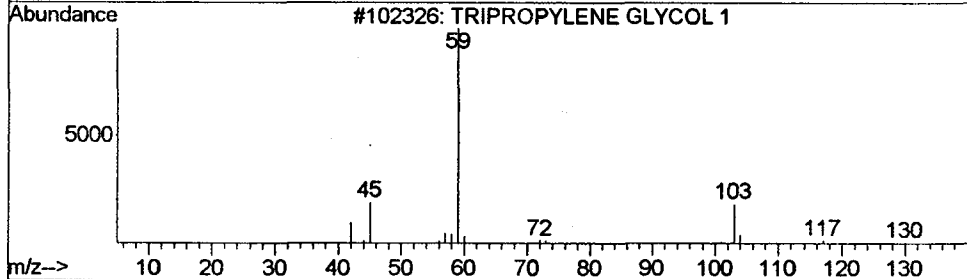
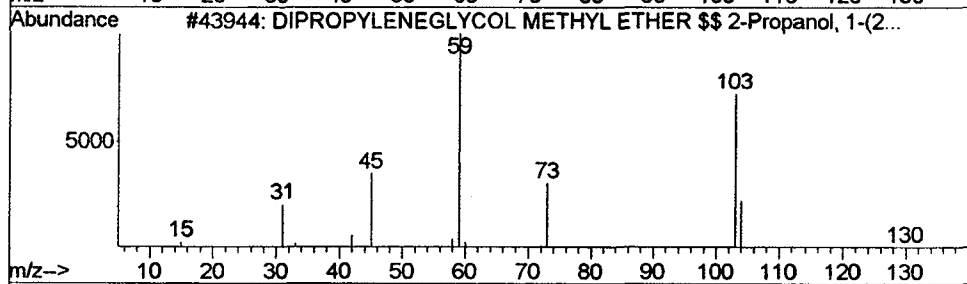
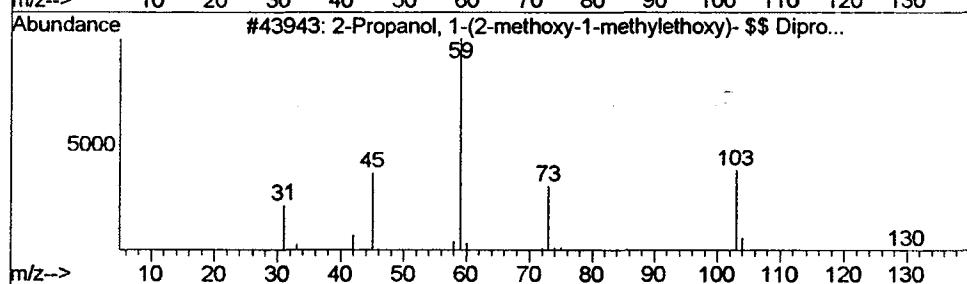
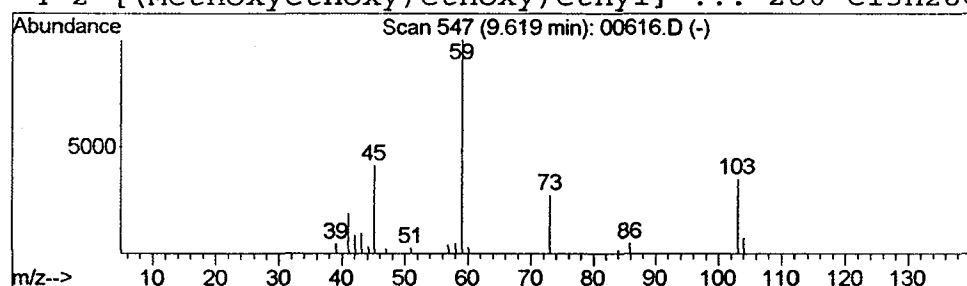
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 5 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	0.24 ug/L	134496	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			DIPROPYLENEGLYCOL METHYL ETHER \$...	148	C7H16O3	020324-32-7	56
3			TRIPROPYLENE GLYCOL 1	192	C9H20O4	000000-00-0	50
4			2-[(Methoxyethoxy)ethoxy)ethyl] ...	280	C13H28O6	000000-00-0	50



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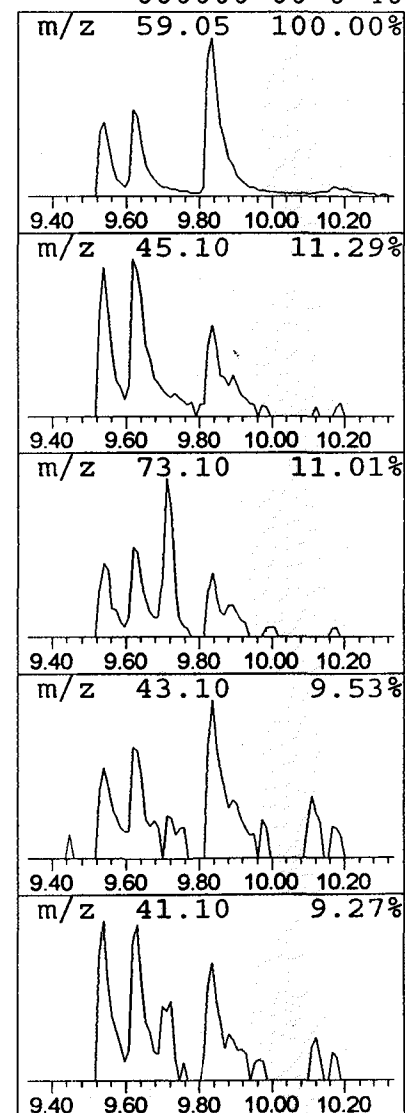
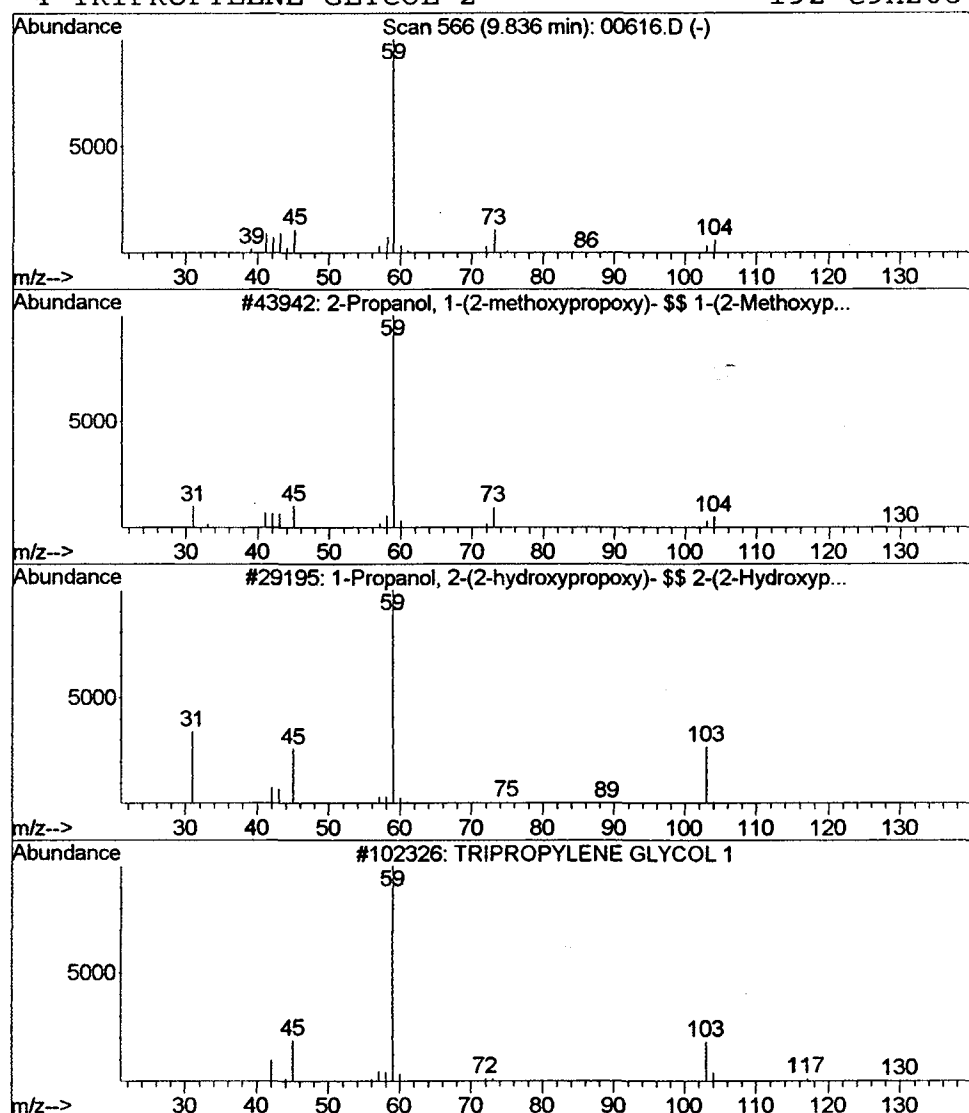
Vial: 5
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 6 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	0.39 ug/L	213817	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	83
2			1-Propanol, 2-(2-hydroxypropoxy)...	134	C6H14O3	000106-62-7	64
3			TRIPROPYLENE GLYCOL 1	192	C9H20O4	000000-00-0	40
4			TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	40



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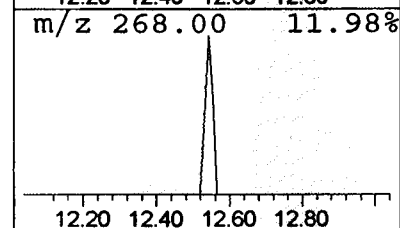
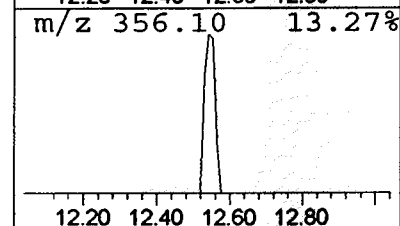
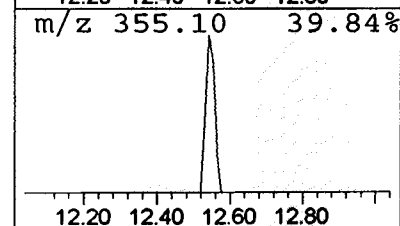
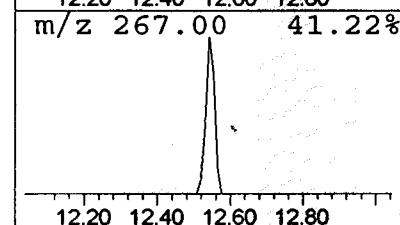
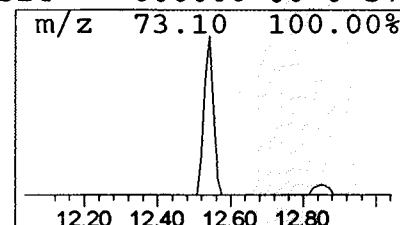
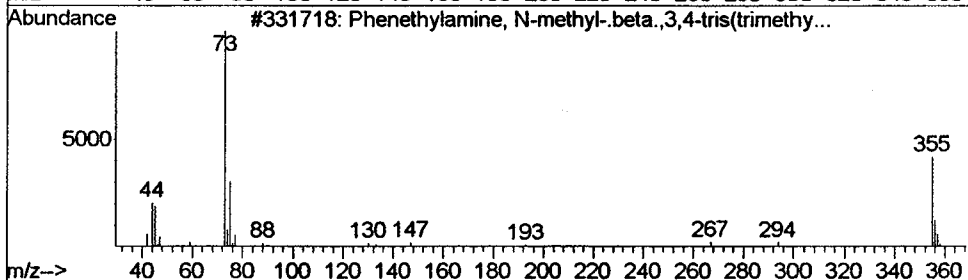
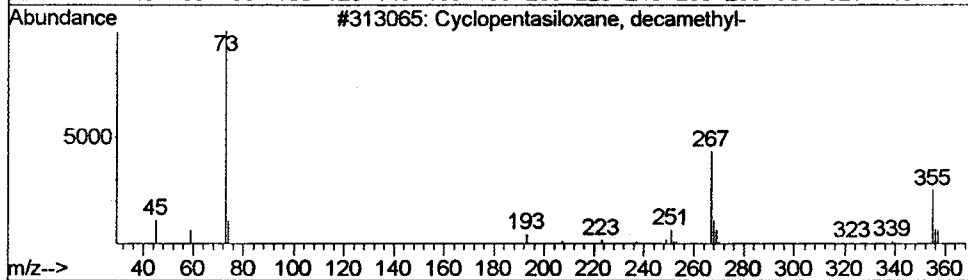
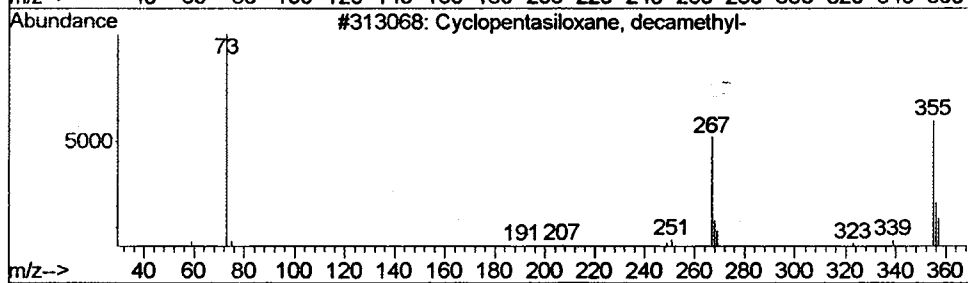
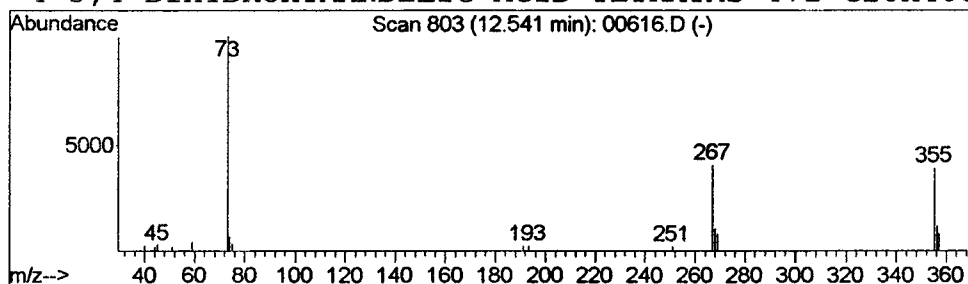
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	0.09 ug/L	67485	Naphthalene-d8	13.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	83
2		Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	45
3		Phenethylamine, N-methyl-.beta.,...	399	C18H37NO3Si3	010538-85-9	37
4		3,4-DIHYDROXYMANDELIC ACID-TETRATMS	472	C20H40O5Si4	000000-00-0	37



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
 Misc : January 29, 2002
 MS Integration Params: LSCINT.P

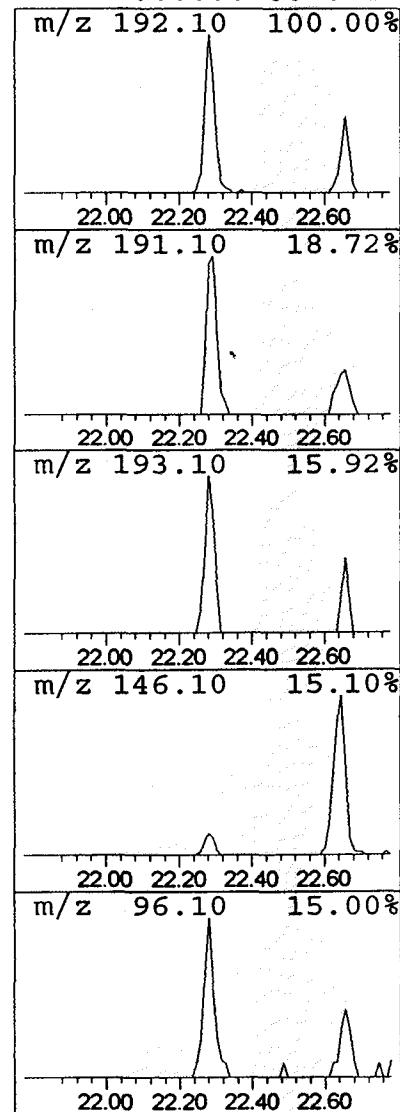
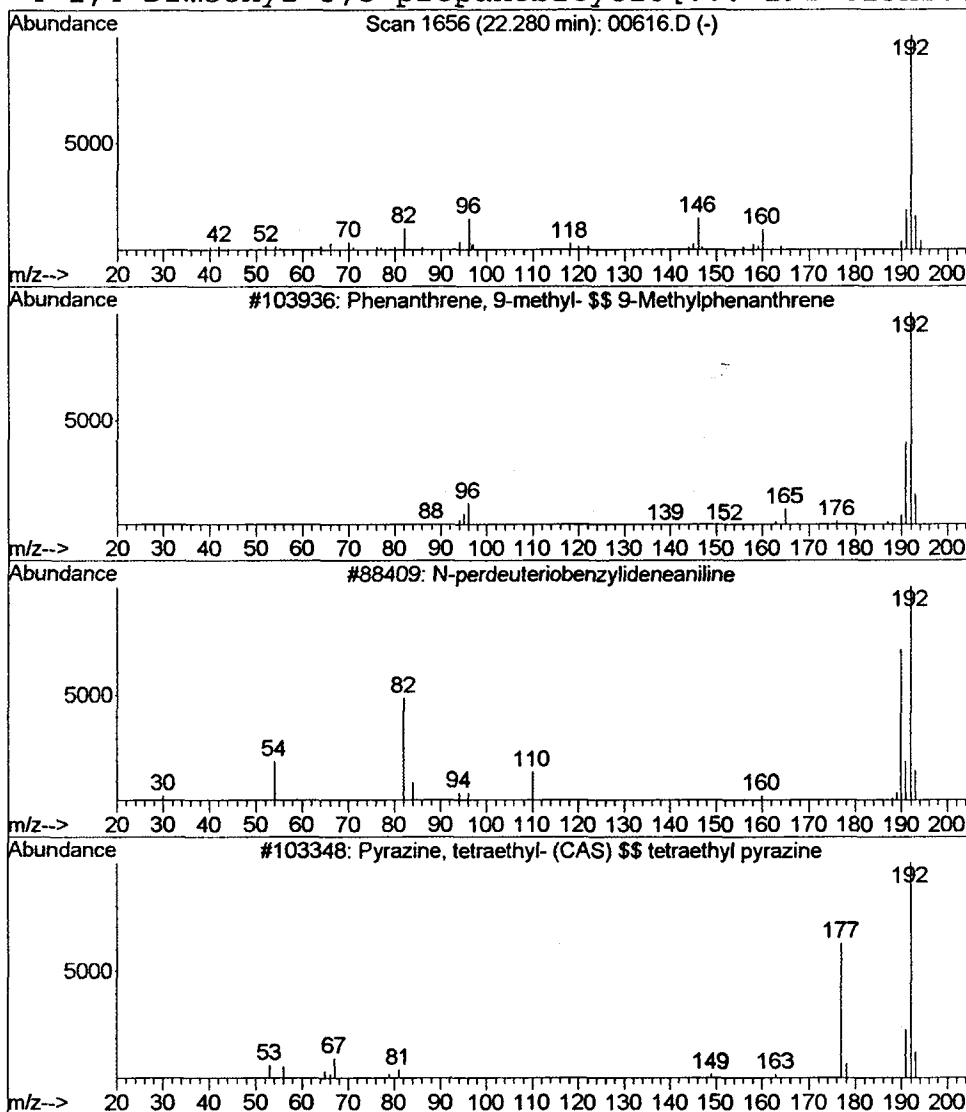
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 8 Phenanthrene, 9-methyl- \$\$... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.19 ug/L	178700	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 9-methyl- \$\$ 9-Met...	192	C15H12	000883-20-5	53
2			N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	53
3			Pyrazine, tetraethyl- (CAS) \$\$ t...	192	C12H20N2	038325-19-8	50
4			1,4-Dimethyl-3,5-propanobicyclo[...	192	C13H20O	000000-00-0	47



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
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 MS Integration Params: LSCINT.P

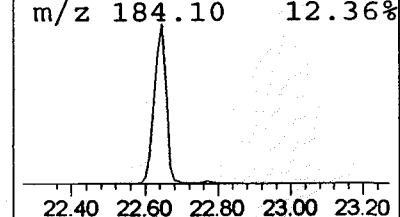
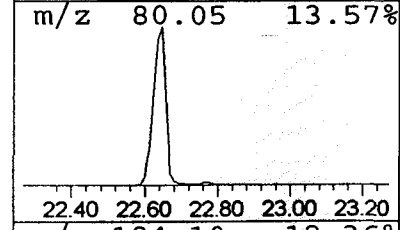
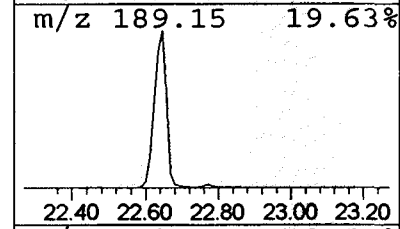
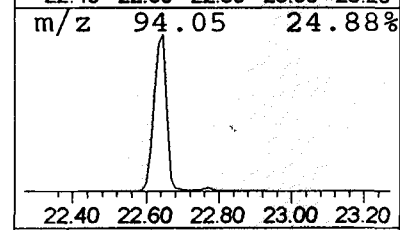
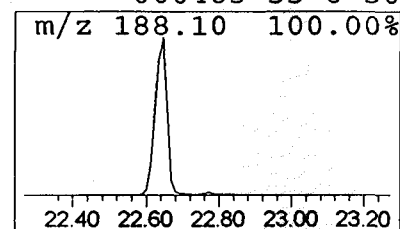
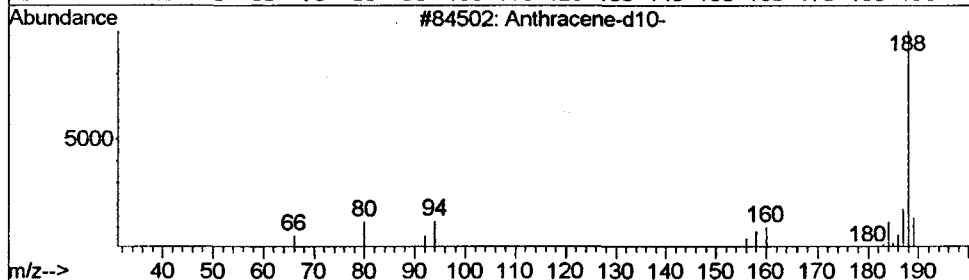
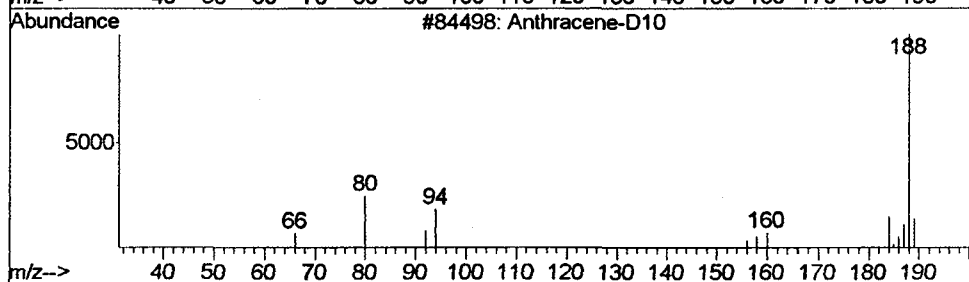
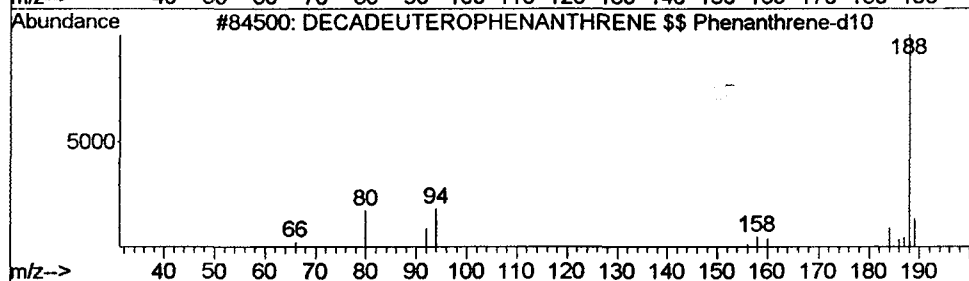
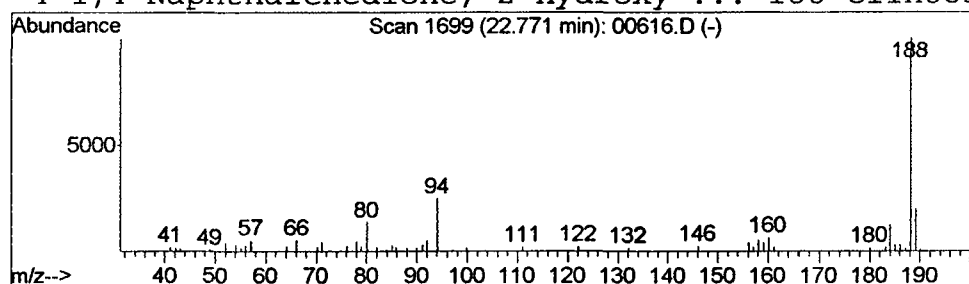
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 9 DECADEUTEROPHENANTHRENE \$\$... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.62 ug/L	584272	Phenanthrene-d10	22.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	83
2		Anthracene-D10	188	C14D10	000000-00-0	74
3		Anthracene-d10-	188	C14D10	001719-06-8	64
4		1,4-Naphthalenedione, 2-hydroxy-...	188	C11H8O3	000483-55-6	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D
 Acq On : 29 Jan 2002 5:59 pm
 Sample : 508 scan
 Misc : January 29, 2002
 MS Integration Params: LSCINT.P

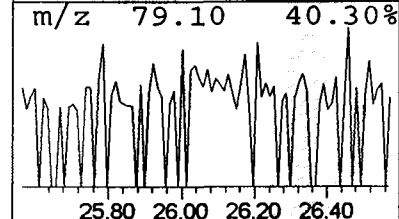
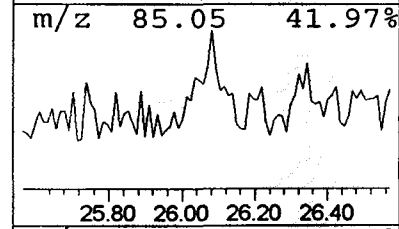
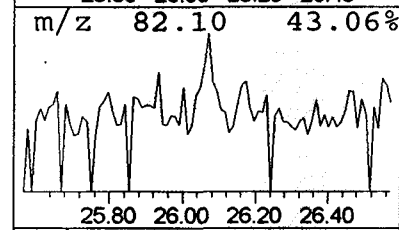
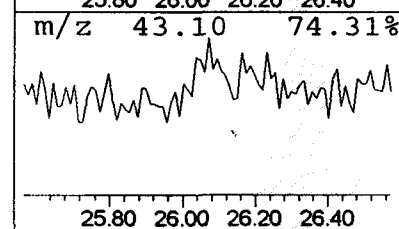
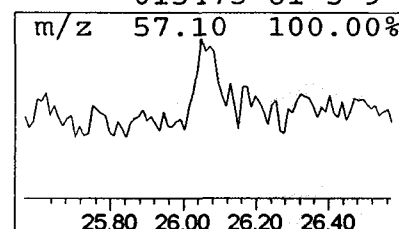
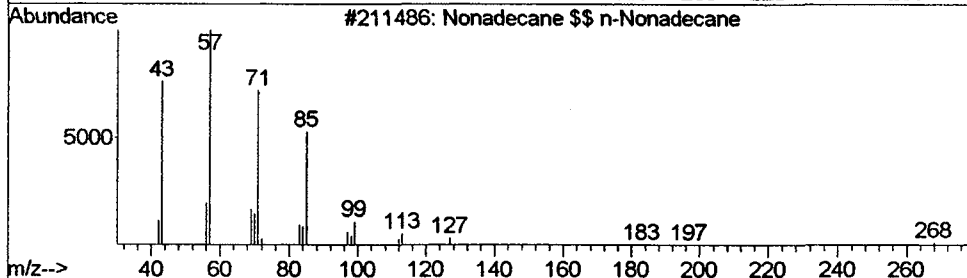
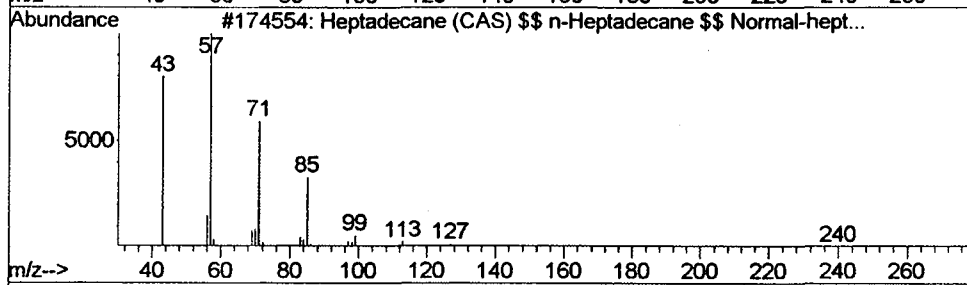
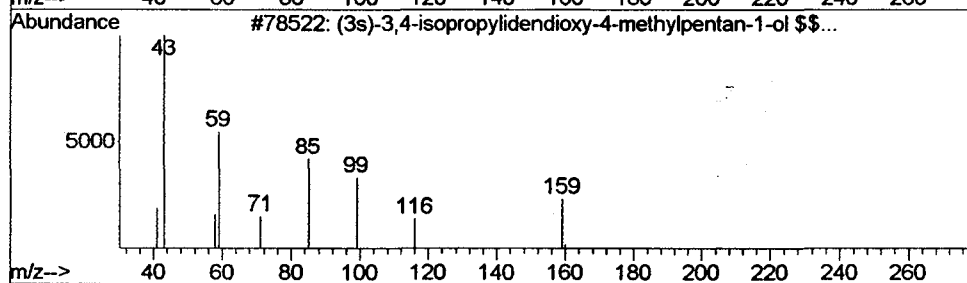
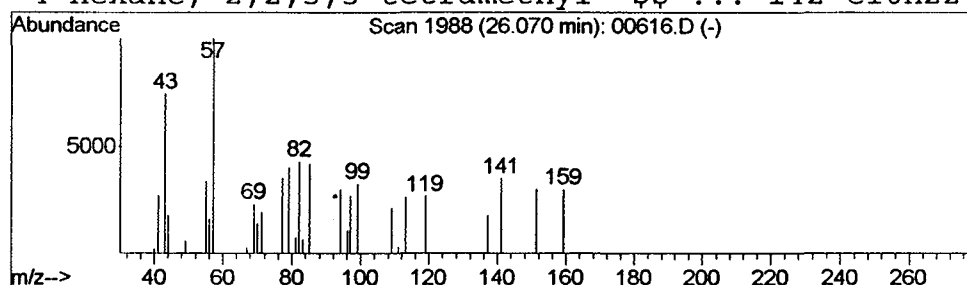
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 10 (3s)-3,4-isopropylidendioxy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.07	0.07 ug/L	68905	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3s)-3,4-isopropylidendioxy-4-me...	174	C9H18O3	067985-68-6	10
2			Heptadecane (CAS) \$\$ n-Heptadeca...	240	C17H36	000629-78-7	9
3			Nonadecane \$\$ n-Nonadecane	268	C19H40	000629-92-5	9
4			Hexane, 2,2,3,3-tetramethyl- \$\$...	142	C10H22	013475-81-5	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN29\00616.D

Acq On : 29 Jan 2002 5:59 pm

Sample : 508 scan

Misc : January 29, 2002

MS Integration Params: LSCINT.P

Vial: 5

Operator:

Inst : Instrumen

Multiplr: 1.00

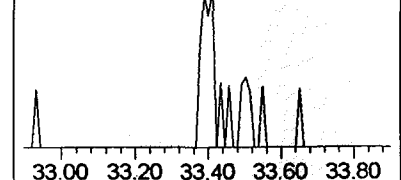
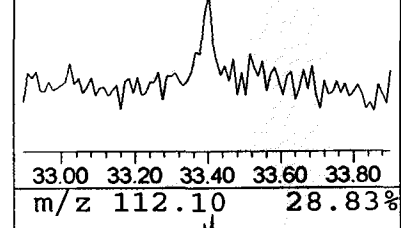
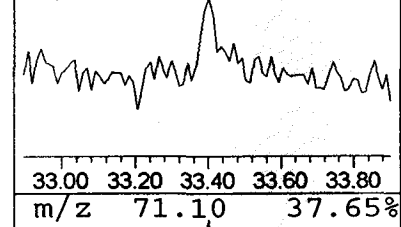
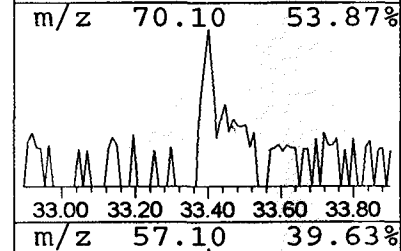
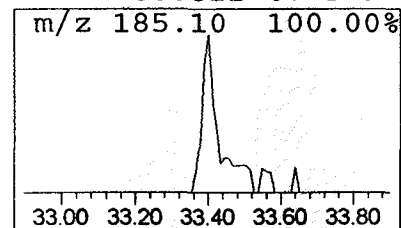
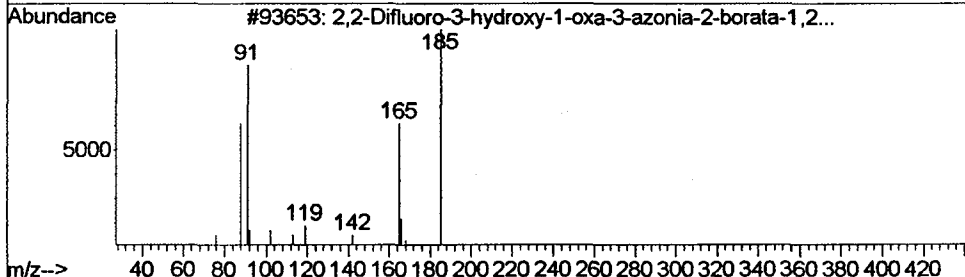
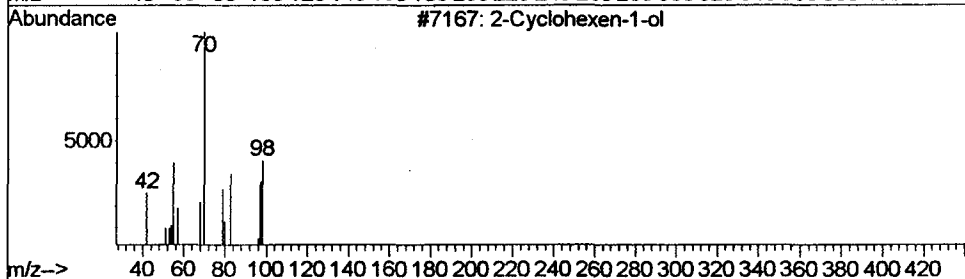
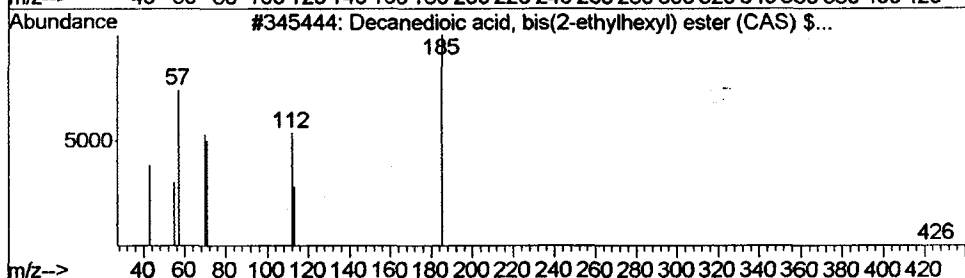
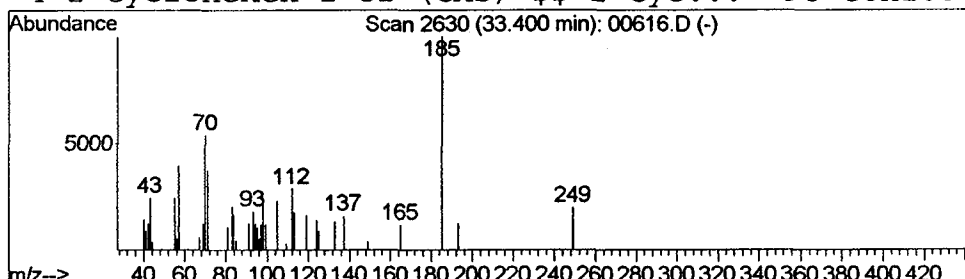
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)

Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 11 Decanedioic acid, bis(2-eth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
33.40	0.11 ug/L	89360	Perylene-d12	34.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	38
2	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	11
3	2,2-Difluoro-3-hydroxy-1-oxa-3-a...	185	C7H6BF2NO2	000000-00-0	9
4	2-Cyclohexen-1-ol (CAS) \$\$ 2-Cyc...	98	C6H10O	000822-67-3	9



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 29 Jan 2002 5:59 pm
Data File: C:\MSDCHEM\1\5973N\02JAN29\00616.D
Name: 508 scan
Misc: January 29, 2002
Method: C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title: 508 scan method
Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, 2-...	4.63	0.1	ug/L	69411	1	9.71	10979900	20.0
2-Butenal, 3-meth...	4.83	0.2	ug/L	103659	1	9.71	10979900	20.0
3-(CYCLOHEX-3'-EN...	5.89	3.3	ug/L	1804940	1	9.71	10979900	20.0
2-Propanol, 1-(2-...	9.54	0.2	ug/L	123474	1	9.71	10979900	20.0
2-Propanol, 1-(2-...	9.62	0.2	ug/L	134496	1	9.71	10979900	20.0
2-Propanol, 1-(2-...	9.84	0.4	ug/L	213817	1	9.71	10979900	20.0
Cyclopentasiloxan...	12.54	0.1	ug/L	67485	2	13.19	15748800	20.0
Phenanthrene, 9-m...	22.28	0.2	ug/L	178700	4	22.65	18894500	20.0
DECADEUTEROPHENAN...	22.77	0.6	ug/L	584272	4	22.65	18894500	20.0
(3s)-3,4-isopropy...	26.07	0.1	ug/L	68905	4	22.65	18894500	20.0
Decanedioic acid,...	33.40	0.1	ug/L	89360	6	34.42	15831500	20.0