

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/24/2002 Time: 11:46:24

Sample: AE00329
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/24/02 11:46 Ended: 1/24/02 11:46 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		85		5.0

Comments for Sample AE00329 - Analysis \$GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-24-2002 Time: 11:46:29

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recoveries for 31 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D

Vial: 3

Acq On : 11 Jan 2002 3:46 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 11, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 14 10:32:31 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	9.72	152	1080871	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4527529	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2421299	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4210523	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	3815201	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	2849235	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	282411	4.24	ug/L	0.00
Spiked Amount	5.000		Recovery	=	84.80%	

Target Compounds

	R.T.	QIon	Response	Conc	Units	Qvalue
2) n-Nitrosodimethylamine	3.60	74	9888	0.21	ug/L #	12
20) Dimethylphthalate	18.34	163	389092	2.43	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	309632	9.93	ug/L #	17
35) Di-n-butylphthalate	24.85	149	20231	0.07	ug/L	96
41) Benzo(a)anthracene	30.50	228	13039	0.06	ug/L #	74
42) Bis(2-ethylhexyl)phthalate	31.11	149	21550	0.06	ug/L	88
43) Chrysene	30.50	228	10101	0.05	ug/L #	72
48) Benzo(a)pyrene	34.42	252	11773	0.06	ug/L #	1

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

00329.D SCAN508.M Mon Jan 14 10:32:32 2002

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Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D

Vial: 3

Acq On : 11 Jan 2002 3:46 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 11, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 14 10:32 2002

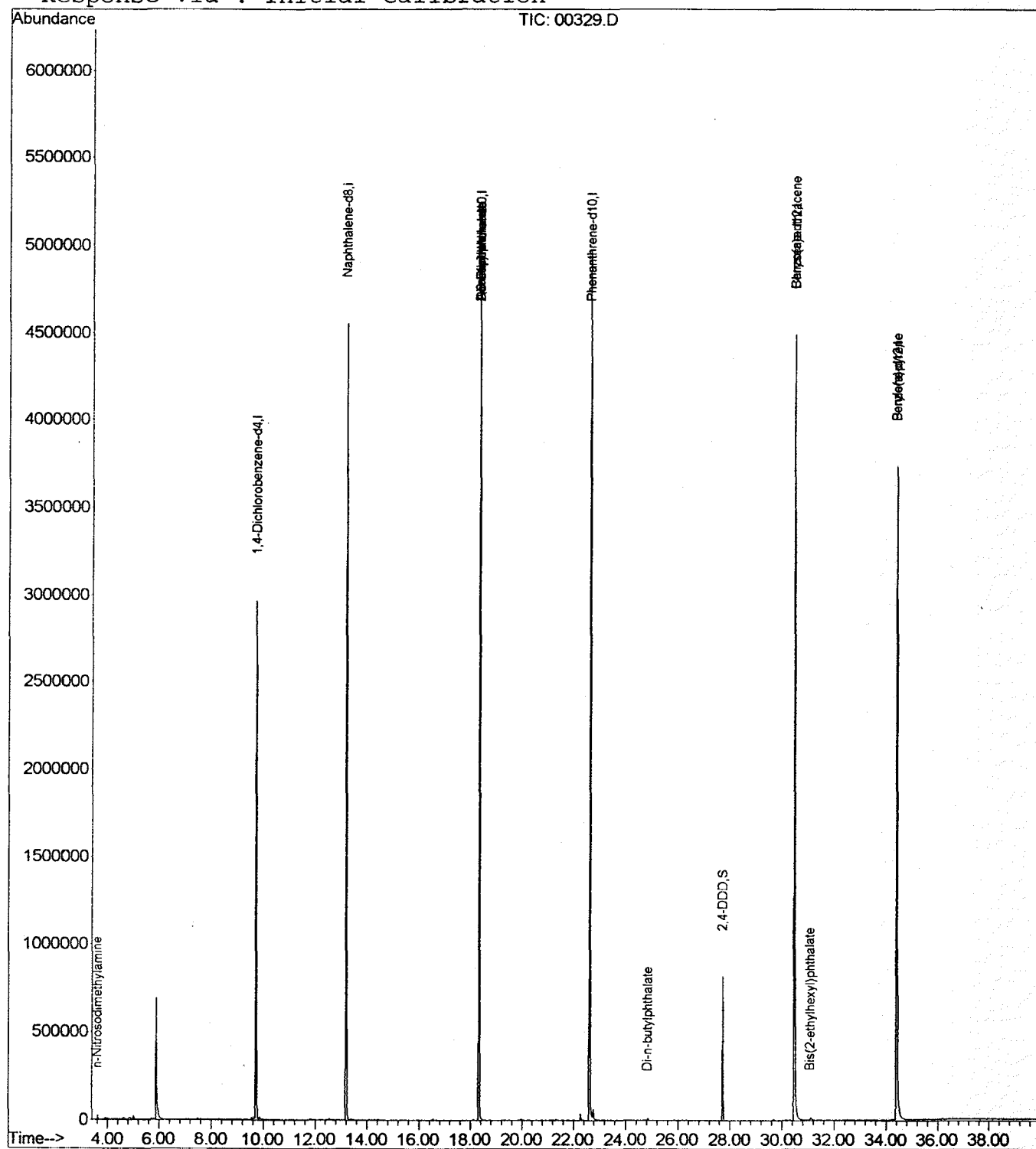
Quant Results File: SCAN508.RE

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



00329.D SCAN508.M

Mon Jan 14 10:32:32 2002

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LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
Acq On : 11 Jan 2002 3:46 pm
Sample : 508 scan
Misc : January 11, 2002
MS Integration Params: LSCINT.P

Vial: 3
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

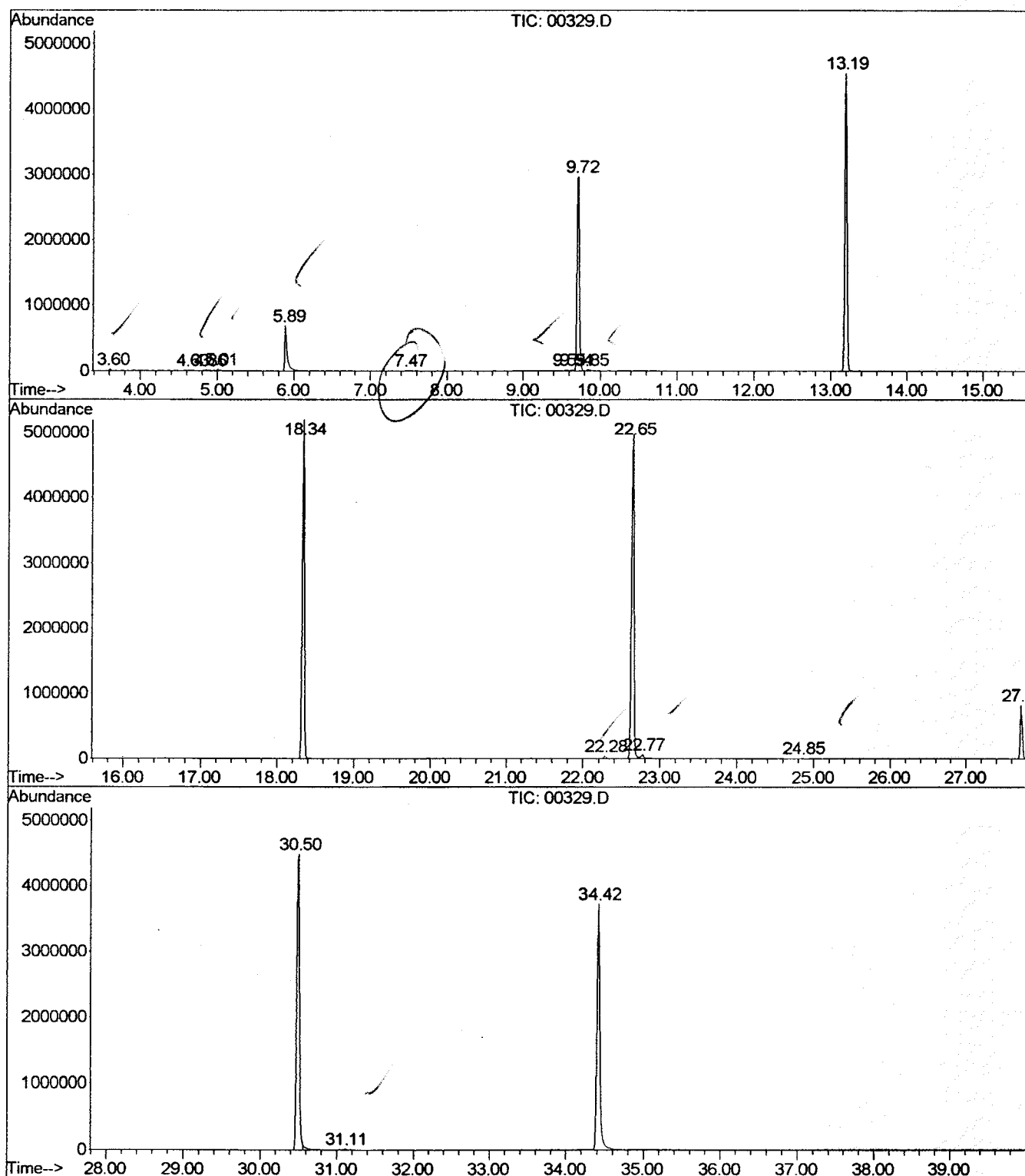
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.602	17	20	25	rVV	26020	38578	0.35%	0.064%
2	4.629	107	110	123	rVB2	12227	27086	0.24%	0.045%
3	4.858	123	130	141	rBV3	12113	42616	0.38%	0.071%
4	5.006	141	143	149	rVB2	20893	40707	0.37%	0.068%
5	5.885	217	220	247	rBV	687863	1467876	13.21%	2.450%
6	7.472	357	359	367	rBV	6431	22696	0.20%	0.038%
7	9.550	539	541	547	rBV2	15513	38463	0.35%	0.064%
8	9.641	547	549	551	rVV	16574	30589	0.28%	0.051%
9	9.721	551	556	561	rVV	2965398	6108053	54.96%	10.193%
10	9.847	561	567	577	rVB	16193	48682	0.44%	0.081%
11	13.192	855	860	865	rBV	4553699	8686074	78.15%	14.495%
12	18.341	1305	1311	1315	rBV	5198388	9828733	88.43%	16.402%
13	22.280	1651	1656	1661	rBV	37996	73628	0.66%	0.123%
14	22.645	1681	1688	1693	rBV	4975516	11036888	99.30%	18.418%
15	22.771	1695	1699	1715	rVB	62759	171046	1.54%	0.285%
16	24.849	1877	1881	1887	rVB	13560	28058	0.25%	0.047%
17	27.726	2129	2133	2139	rVV	817603	1422422	12.80%	2.374%
18	30.500	2369	2376	2381	rBV	4488675	11114265	100.00%	18.547%
19	31.105	2425	2429	2439	rVB4	17010	60122	0.54%	0.100%
20	34.416	2713	2719	2749	rVV	3730637	9637630	86.71%	16.083%

Sum of corrected areas: 59924212

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Operator :
 Acquired : 11 Jan 2002 3:46 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 11, 2002
 Vial Number: 3
 Quant File :SCAN508.RES (RTE Integrator)



00329.D SCAN508.M

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Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
 Misc : January 11, 2002
 MS Integration Params: LSCINT.P

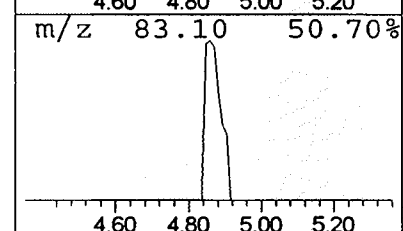
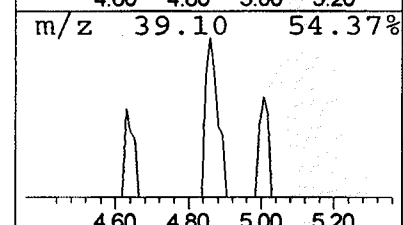
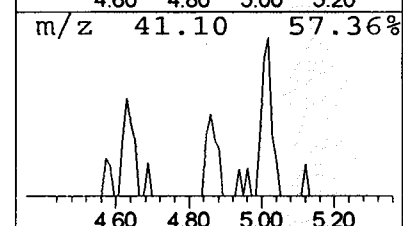
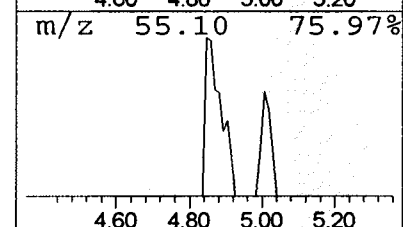
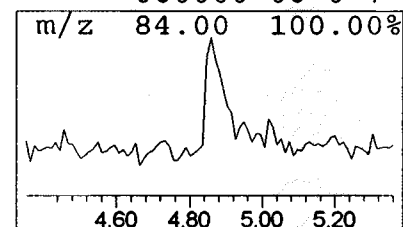
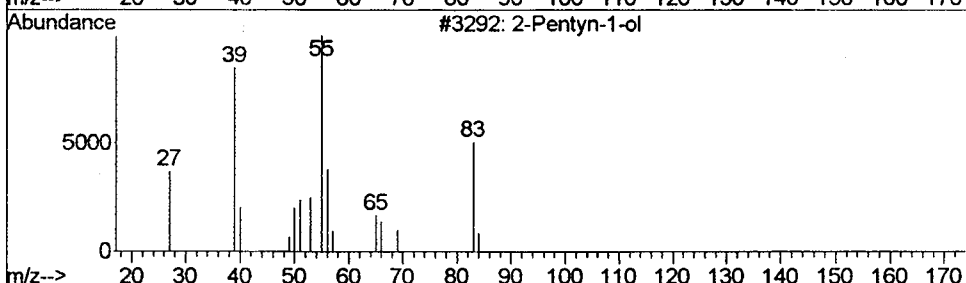
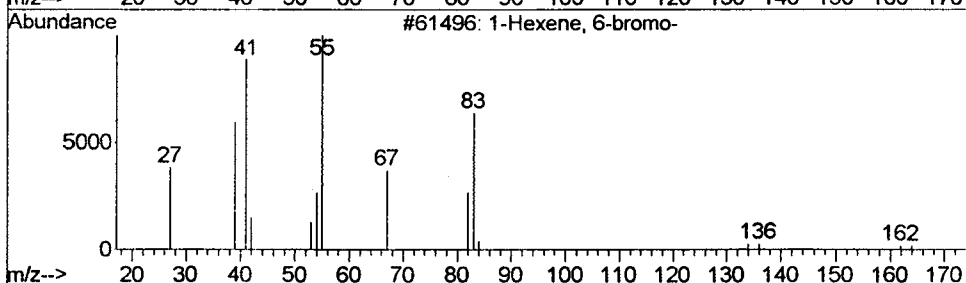
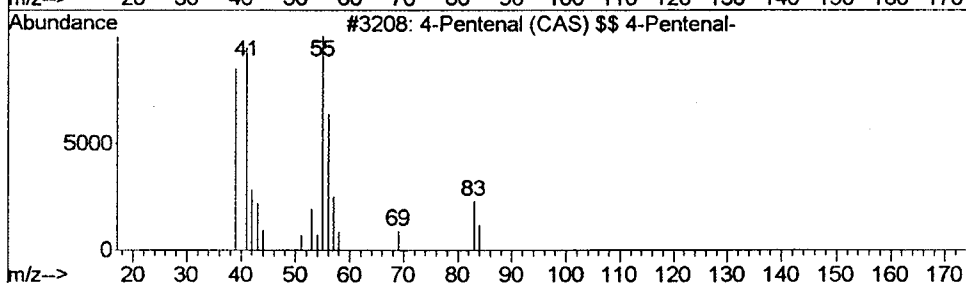
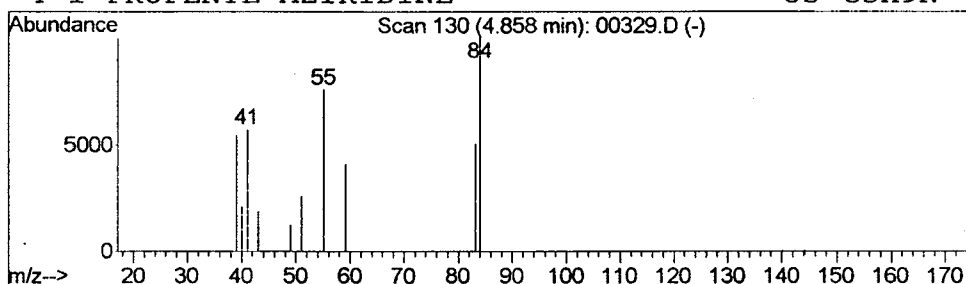
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 4-Pentenal (CAS) \$\$ 4-Pente... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	0.14 ug/L	42616	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pentenal (CAS) \$\$ 4-Pentenal-	84	C5H8O	002100-17-6	9
2			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	9
3			2-Pentyn-1-ol	84	C5H8O	006261-22-9	9
4			1-PROPENYL-AZIRIDINE	83	C5H9N	000000-00-0	7



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
 Misc : January 11, 2002
 MS Integration Params: LSCINT.P

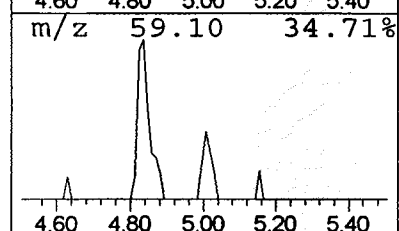
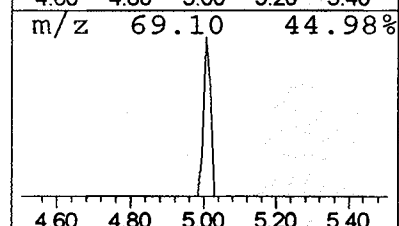
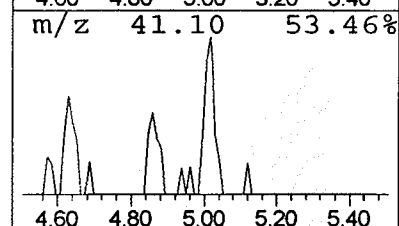
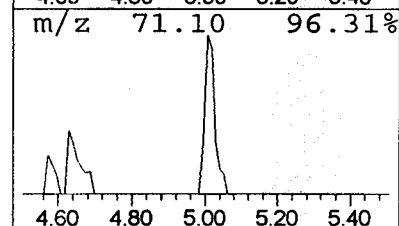
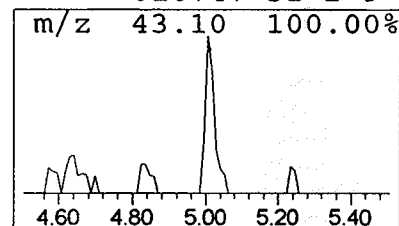
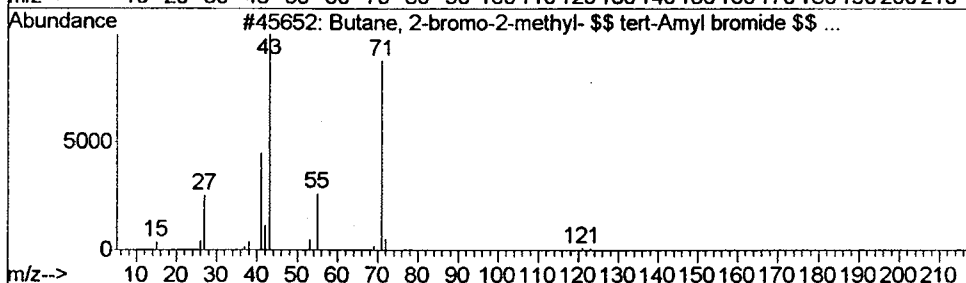
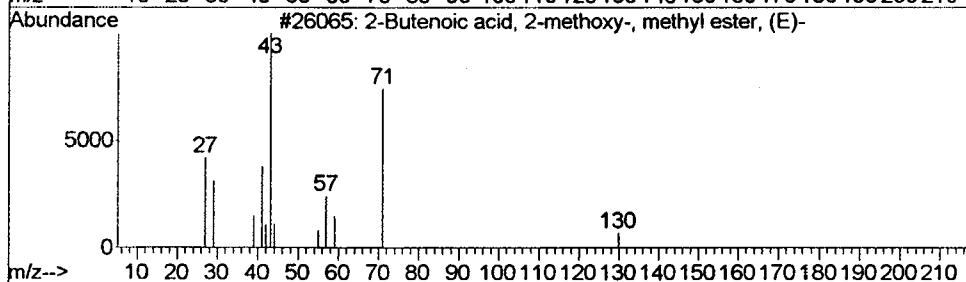
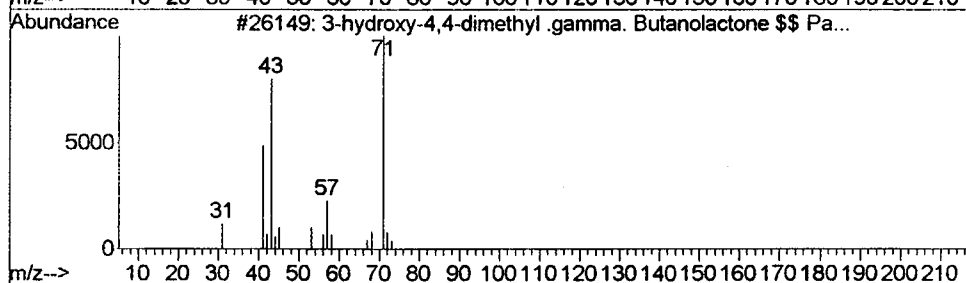
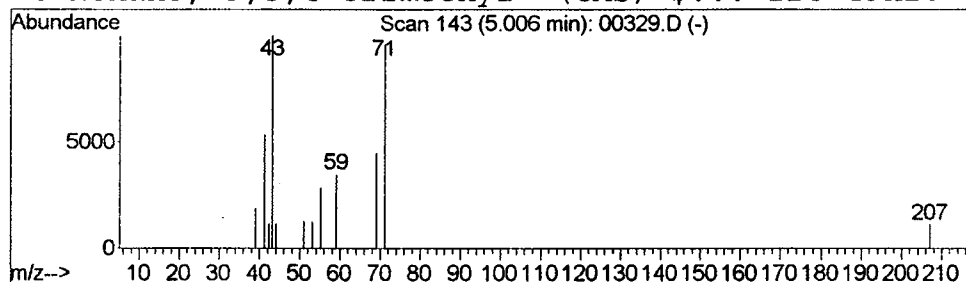
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 3-hydroxy-4,4-dimethyl .gam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.13 ug/L	40707	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-hydroxy-4,4-dimethyl .gamma. B...	130	C6H10O3	052126-90-6	42
2			2-Butenoic acid, 2-methoxy-, met...	130	C6H10O3	056009-29-1	36
3			Butane, 2-bromo-2-methyl- \$\$ ter...	150	C5H11Br	000507-36-8	28
4			Hexane, 3,3,4-trimethyl- (CAS) \$...	128	C9H20	016747-31-2	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
 Misc : January 11, 2002
 MS Integration Params: LSCINT.P

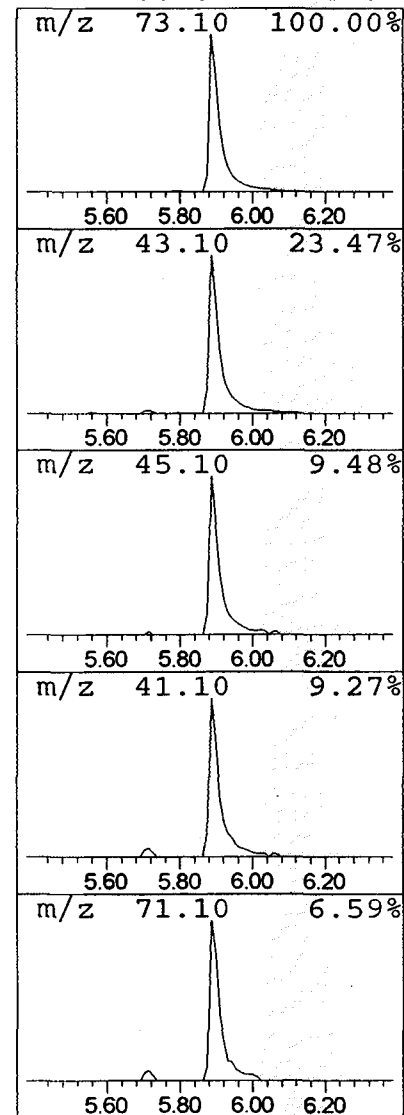
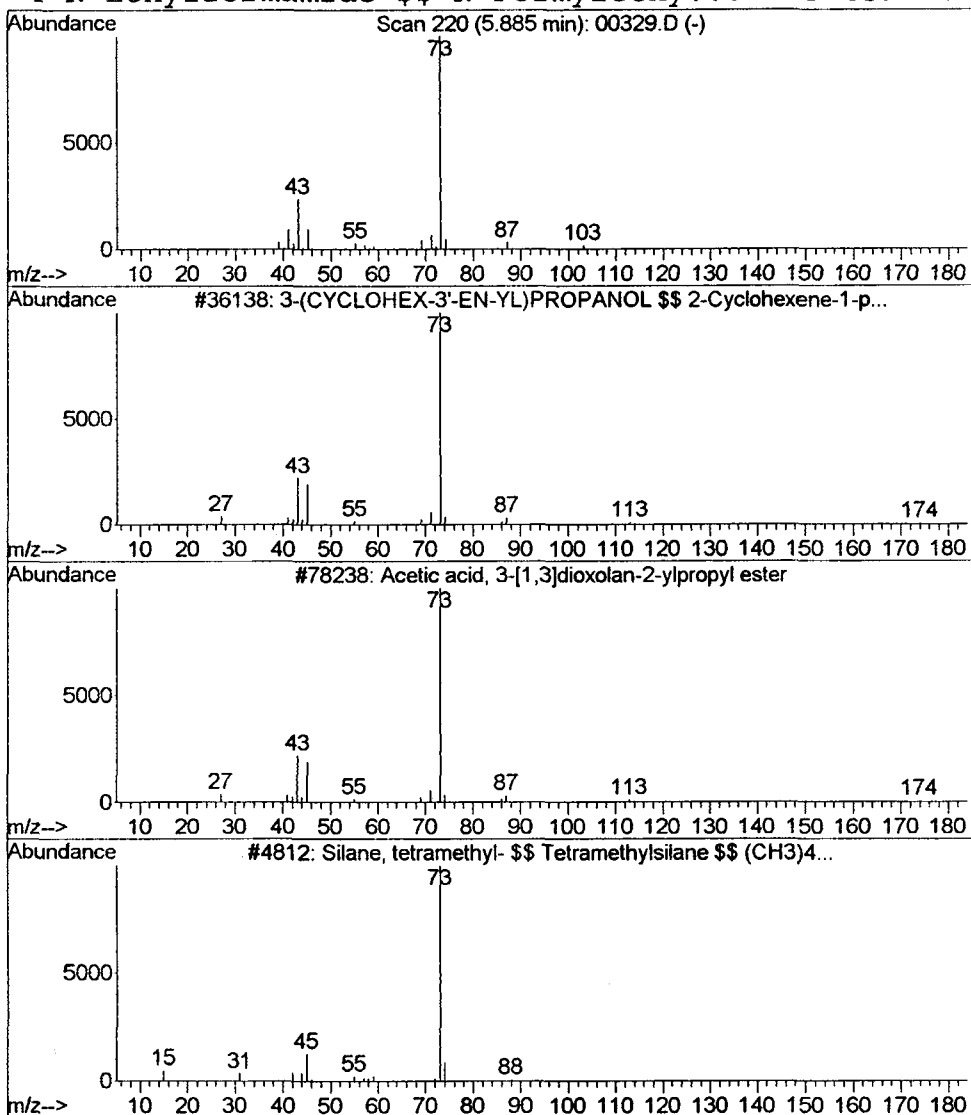
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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	4.81 ug/L	1467880	1,4-Dichlorobenzene-d4	9.72

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- \$\$ Tetramet...	88	C4H12Si	000075-76-3	28
4		N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
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 MS Integration Params: LSCINT.P

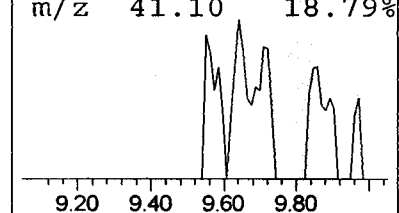
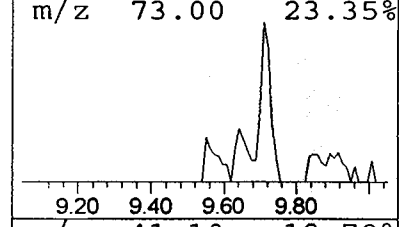
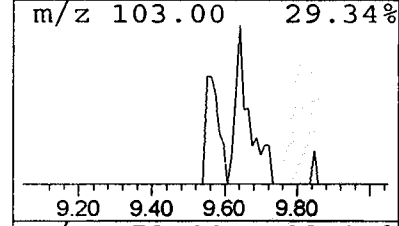
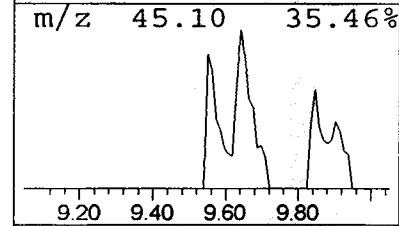
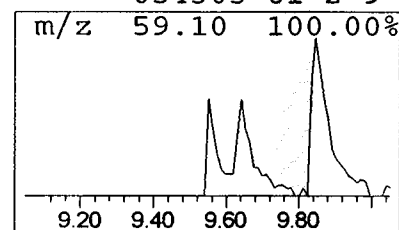
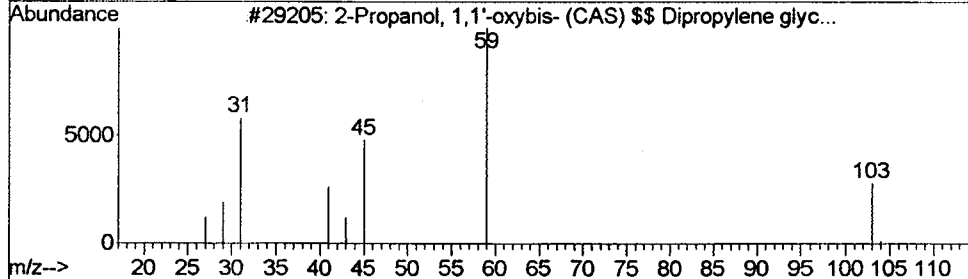
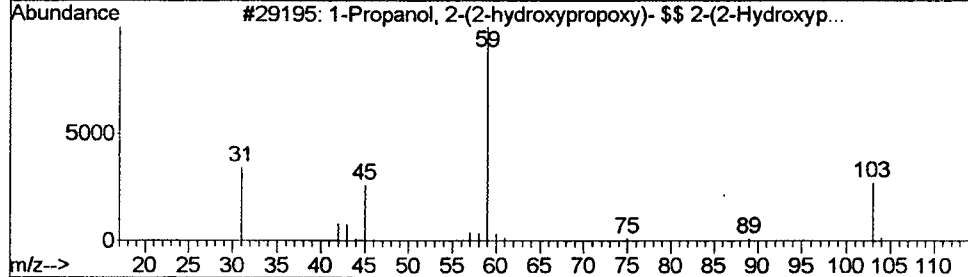
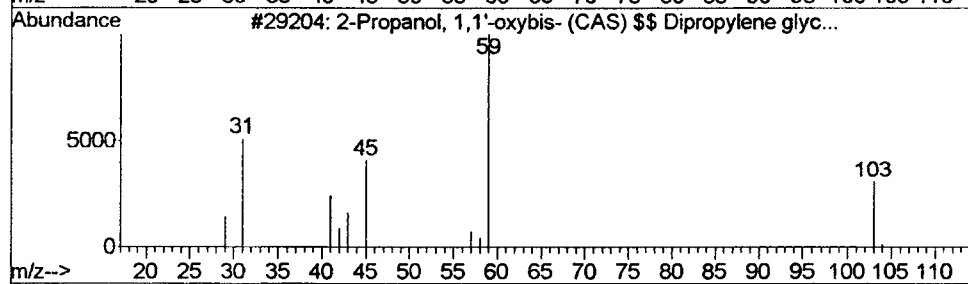
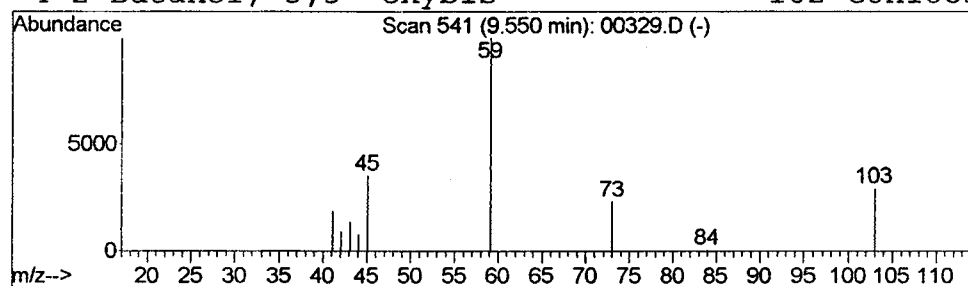
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 4 2-Propanol, 1,1'-oxybis- (C... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	0.13 ug/L	38463	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1,1'-oxybis- (CAS) \$...	134	C6H14O3	000110-98-5	50
2			1-Propanol, 2-(2-hydroxypropoxy)...	134	C6H14O3	000106-62-7	40
3			2-Propanol, 1,1'-oxybis- (CAS) \$...	134	C6H14O3	000110-98-5	38
4			2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	9



Library Search Compound Report

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 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
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 MS Integration Params: LSCINT.P

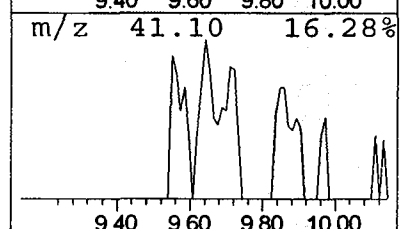
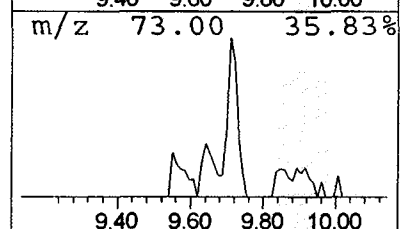
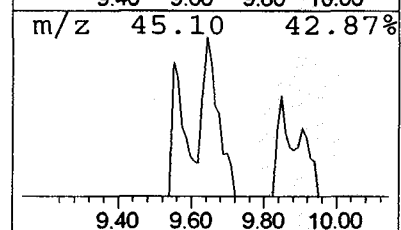
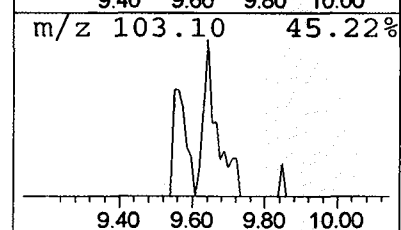
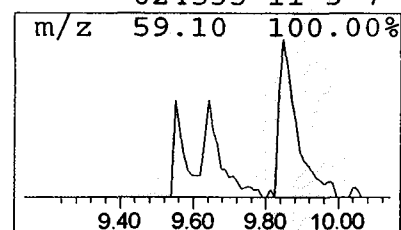
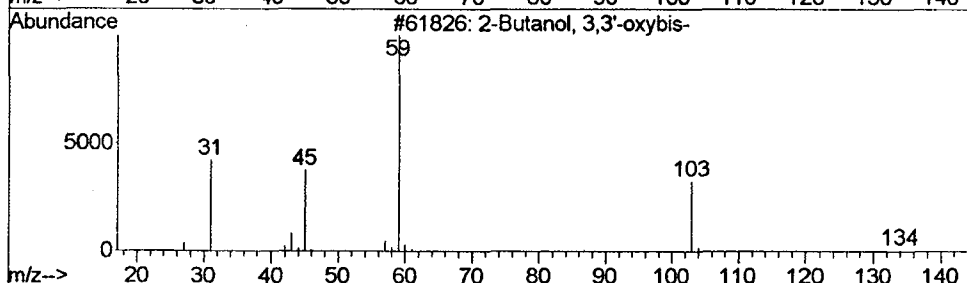
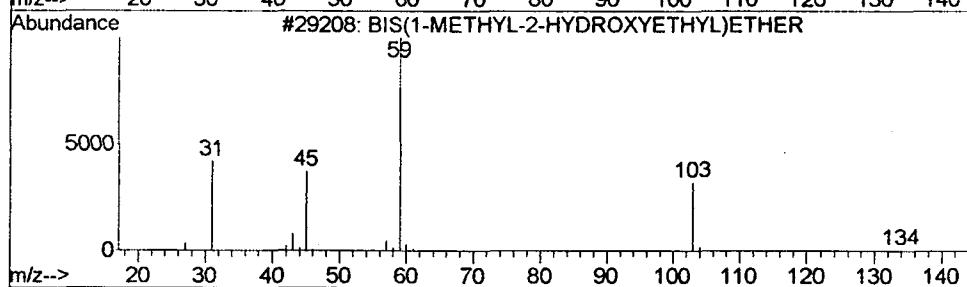
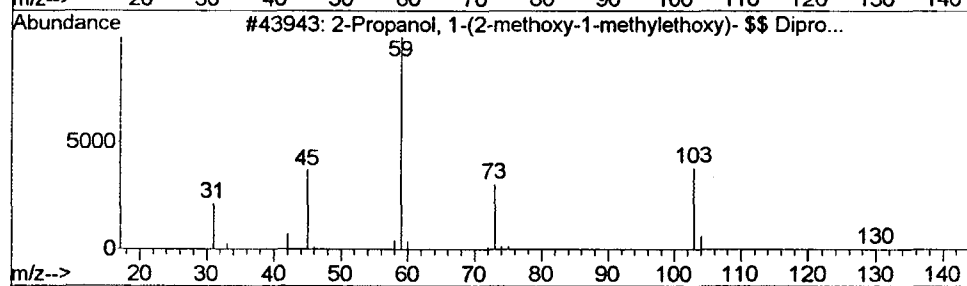
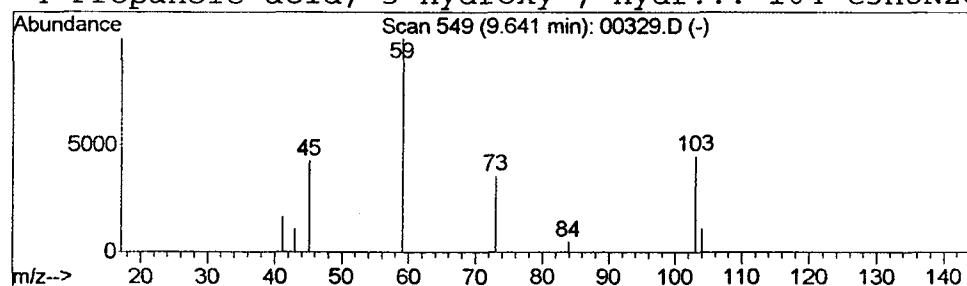
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.64	0.10 ug/L	30589	1,4-Dichlorobenzene-d4	9.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
2		BIS(1-METHYL-2-HYDROXYETHYL) ETHER	134	C6H14O3	000000-00-0	9
3		2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	9
4		Propanoic acid, 3-hydroxy-, hydr...	104	C3H8N2O2	024535-11-3	7



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D

Acq On : 11 Jan 2002 3:46 pm

Sample : 508 scan

Misc : January 11, 2002

MS Integration Params: LSCINT.P

Vial: 3

Operator:

Inst : Instrumen

Multiplr: 1.00

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

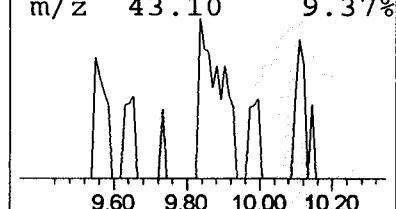
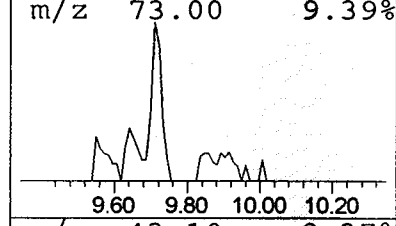
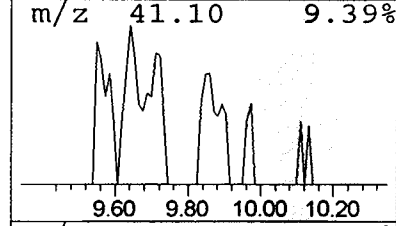
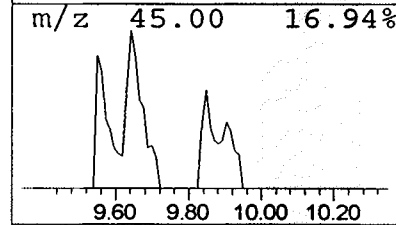
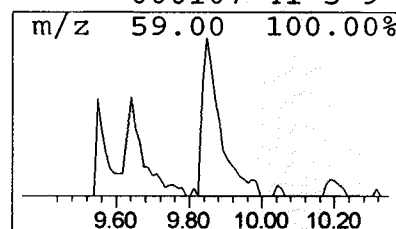
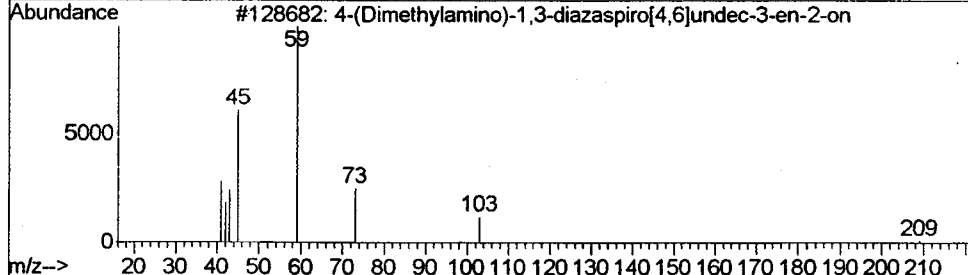
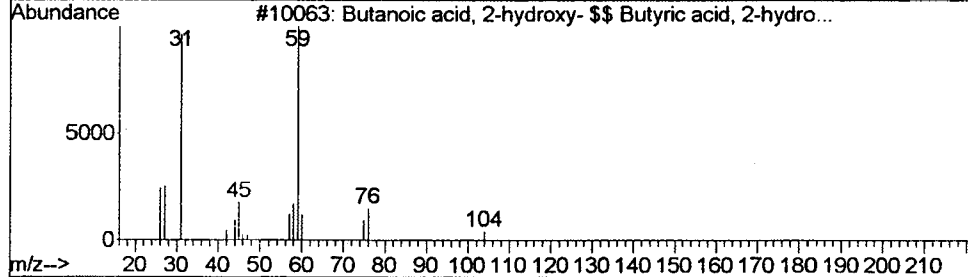
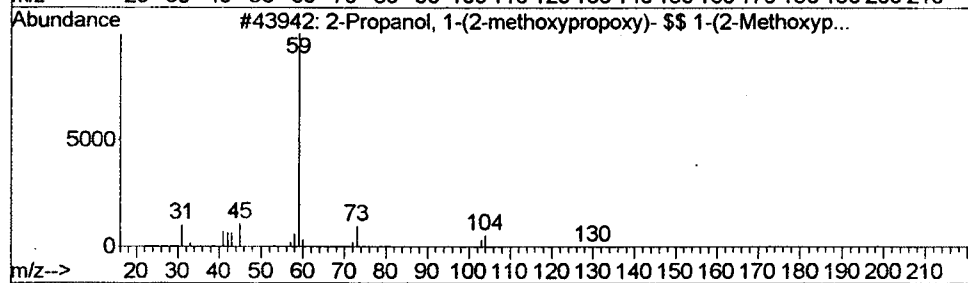
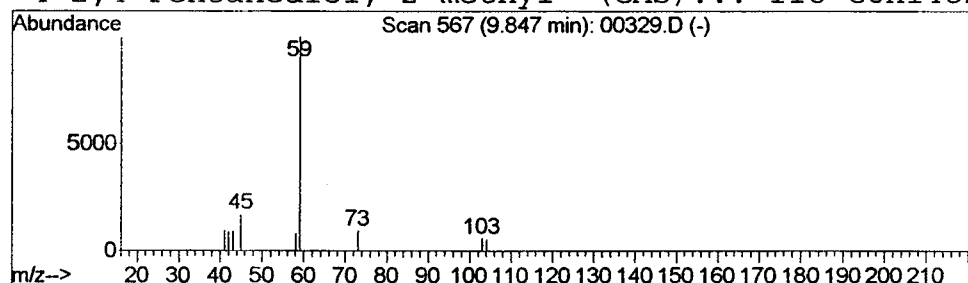
Title : 508 scan method

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.
9.85	0.16 ug/L	48682	1,4-Dichlorobenzene-d4	9.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	83
2		Butanoic acid, 2-hydroxy- \$\$ But...	104	C4H8O3	000565-70-8	9
3		4-(Dimethylamino)-1,3-diazaspiro...	209	C11H19N3O	000000-00-0	9
4		2,4-Pentanediol, 2-methyl- (CAS)...	118	C6H14O2	000107-41-5	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
 Misc : January 11, 2002
 MS Integration Params: LSCINT.P

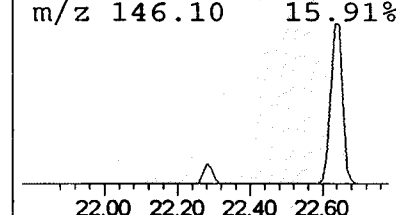
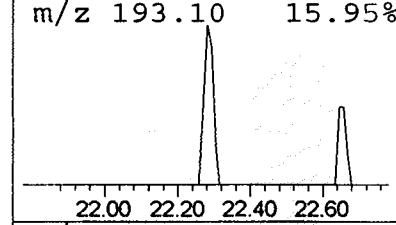
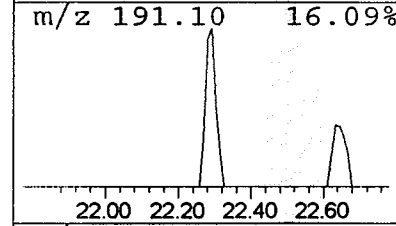
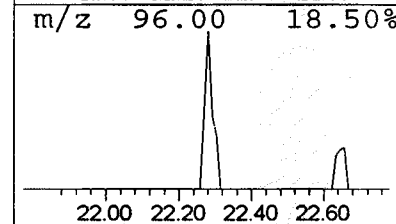
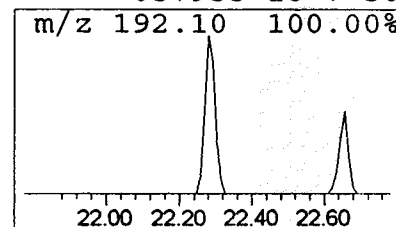
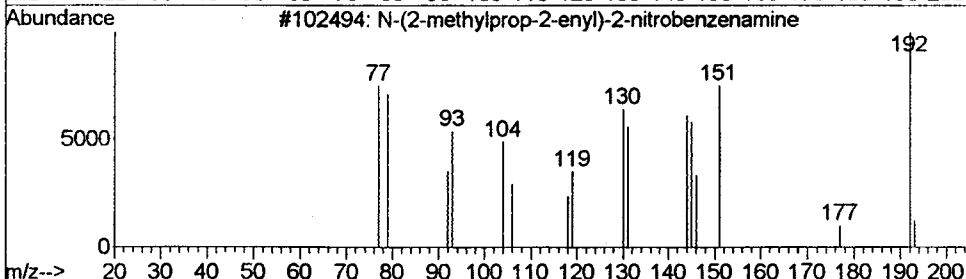
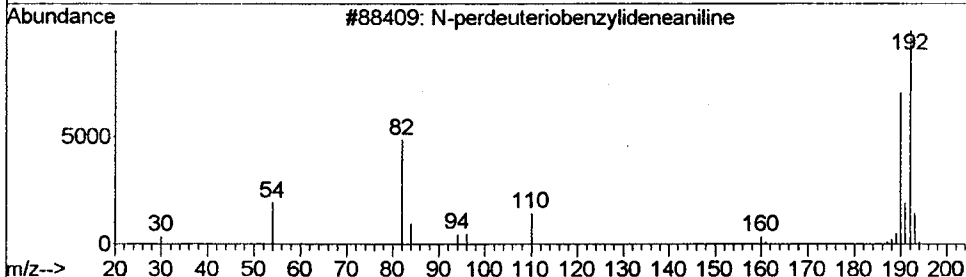
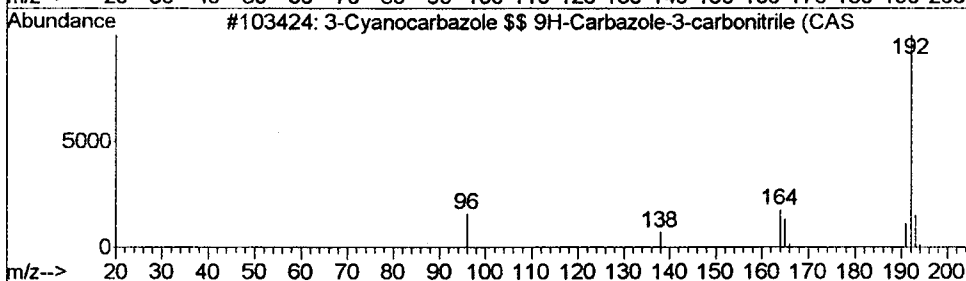
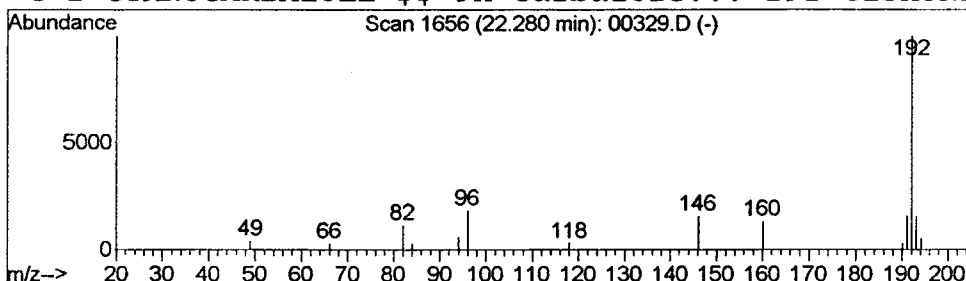
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 7 3-Cyanocarbazole \$\$ 9H-Carb... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.13 ug/L	73628	Phenanthrene-d10	22.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	64
2		N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58
3		N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	52
4		2-CYANOCARBAZOLE \$\$ 9H-Carbazole...	192	C13H8N2	057955-18-7	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN11\00329.D
 Acq On : 11 Jan 2002 3:46 pm
 Sample : 508 scan
 Misc : January 11, 2002
 MS Integration Params: LSCINT.P

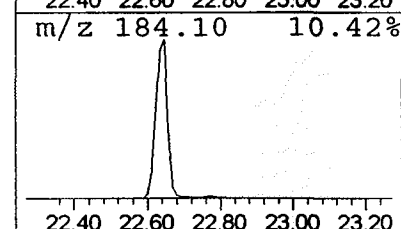
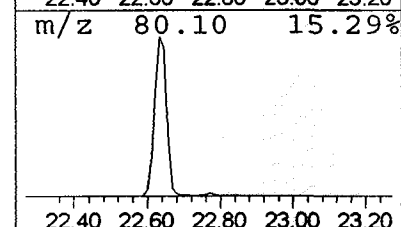
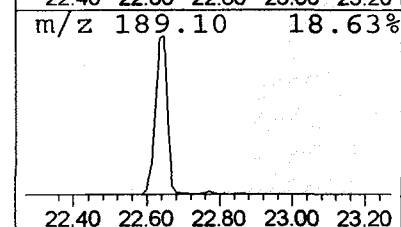
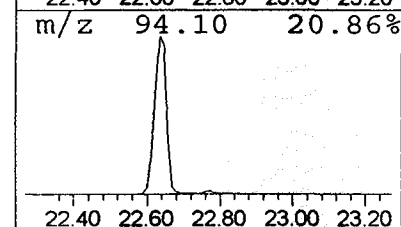
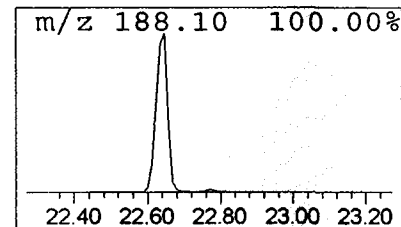
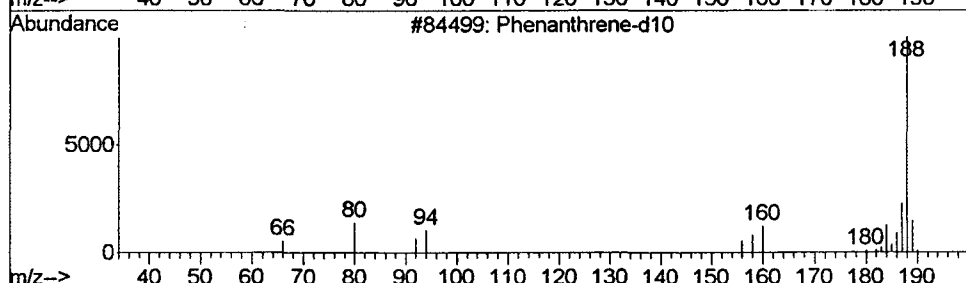
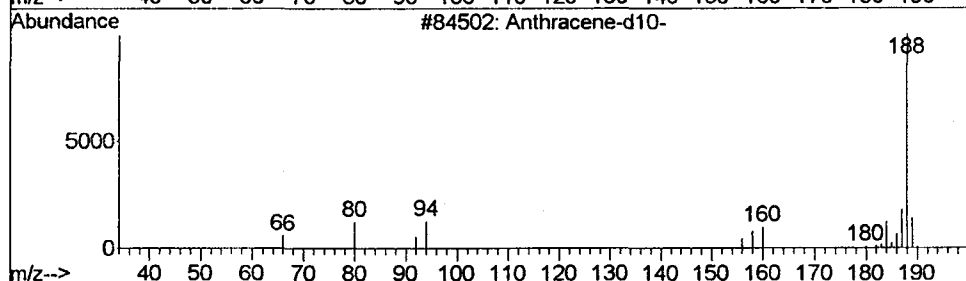
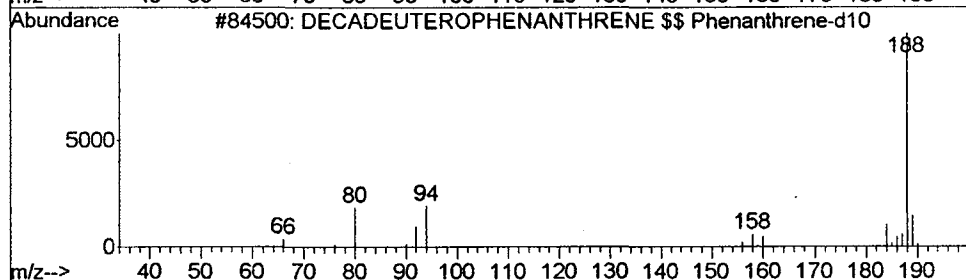
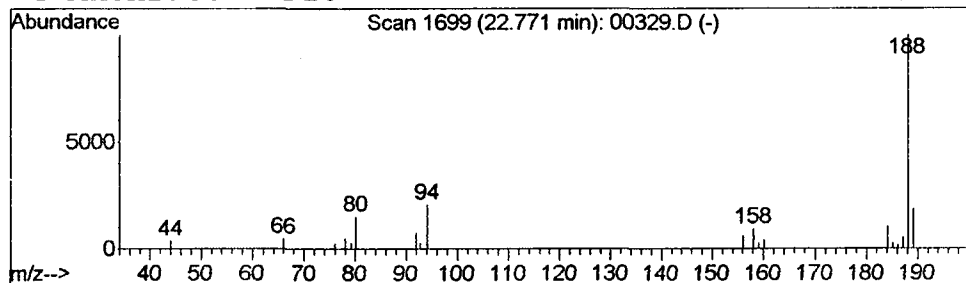
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 8 DECADEUTEROPHENANTHRENE \$\$... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.31 ug/L	171046	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	91
2			Anthracene-d10-	188	C14D10	001719-06-8	72
3			Phenanthrene-d10	188	C14D10	001517-22-2	72
4			Anthracene-D10	188	C14D10	000000-00-0	50



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 11 Jan 2002 3:46 pm
Data File: C:\MSDCHEM\1\5973N\02JAN11\00329.D
Name: 508 scan
Misc: January 11, 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
4-Pentenal (CAS) ...	4.86	0.1	ug/L	42616	1	9.72	6108050	20.0
3-hydroxy-4,4-dim...	5.01	0.1	ug/L	40707	1	9.72	6108050	20.0
3-(CYCLOHEX-3'-EN...	5.89	4.8	ug/L	1467880	1	9.72	6108050	20.0
2-Propanol, 1,1'-...	9.55	0.1	ug/L	38463	1	9.72	6108050	20.0
2-Propanol, 1-(2-...	9.64	0.1	ug/L	30589	1	9.72	6108050	20.0
2-Propanol, 1-(2-...	9.85	0.2	ug/L	48682	1	9.72	6108050	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	73628	4	22.65	11036900	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	171046	4	22.65	11036900	20.0