

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/29/2002 Time: 11:56:01

Sample: AE00739
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/29/02 11:55 Ended: 1/29/02 11:55 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		103		5.0

Comments for Sample AE00739 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-29-2002 Time: 11:56:05

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.

The recoveries for 15 of the 43 compounds in the LCS Standard were outside of their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D Vial: 7
 Acq On : 16 Jan 2002 8:07 pm Operator:
 Sample : 508scan Inst : Instrumen
 Misc : January 16, 2002 Multiplr: 1.00
 MS Integration Params: SPLIT.P
 Quant Time: Jan 17 08:12:25 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	1300604	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	5588695	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2912323	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4760249	20.00	ug/L	-0.02
38) Chrysene-d12	30.49	240	4024900	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2952703	20.00	ug/L	0.00

System Monitoring Compounds
 37) 2,4-DDD 27.73 235 385930 5.13 ug/L 0.00
 Spiked Amount 5.000 Recovery = 102.60%

Target Compounds	R.T.	QIon	Response	Conc	Units	Qvalue
2) n-Nitrosodimethylamine	3.60	74	11618	0.21	ug/L #	15
20) Dimethylphthalate	18.34	163	467822	2.43	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	371847	9.91	ug/L #	17
35) Di-n-butylphthalate	24.85	149	9108	0.03	ug/L	95
41) Benzo(a)anthracene	30.50	228	9090	0.04	ug/L #	48
42) Bis(2-ethylhexyl)phthalate	31.10	149	8450	0.59	ug/L	91
43) Chrysene	30.50	228	9090	0.04	ug/L #	46
48) Benzo(a)pyrene	34.42	252	10276	0.05	ug/L #	1

(#) = qualifier out of range (m) = manual integration
 00739.D SCAN508.M Thu Jan 17 08:12:26 2002

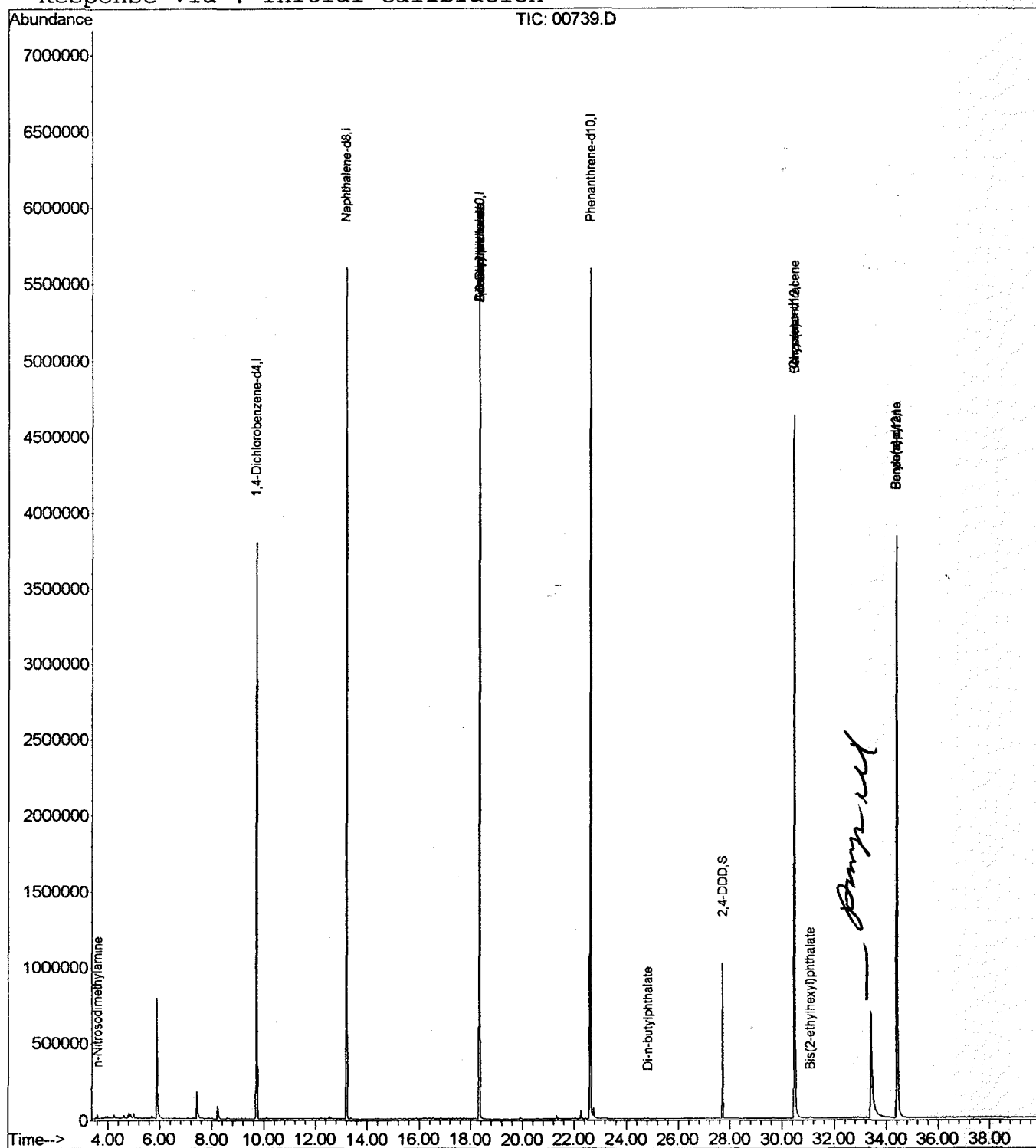
quantitation report (not reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 17 8:12 2002

Vial: 7
 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



00739.D SCAN508.M

Thu Jan 17 08:12:26 2002

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Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

Vial: 7
 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

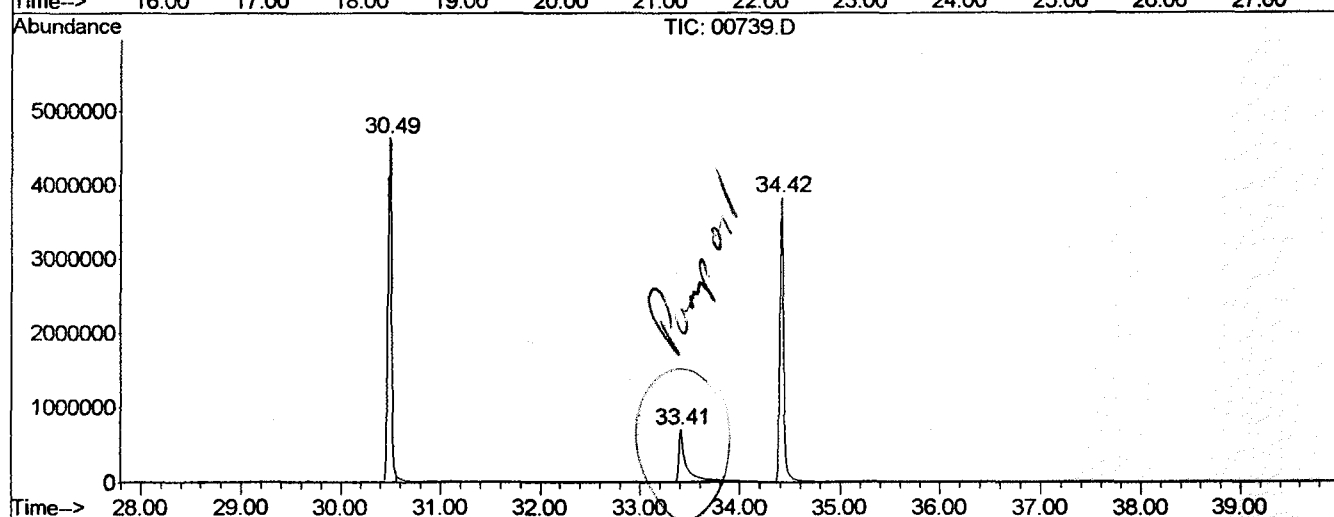
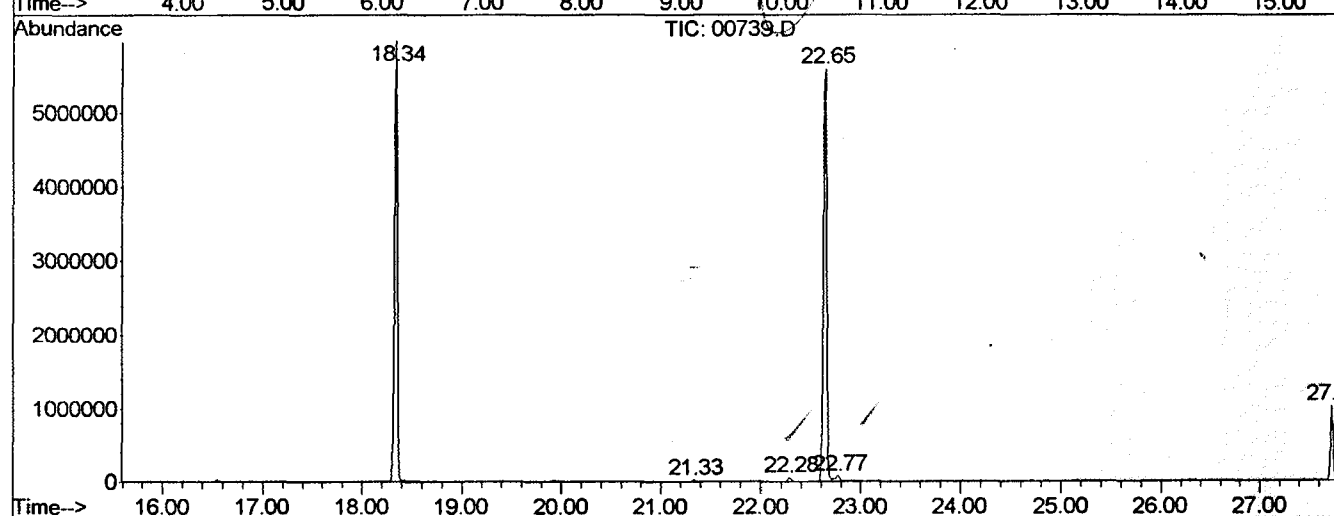
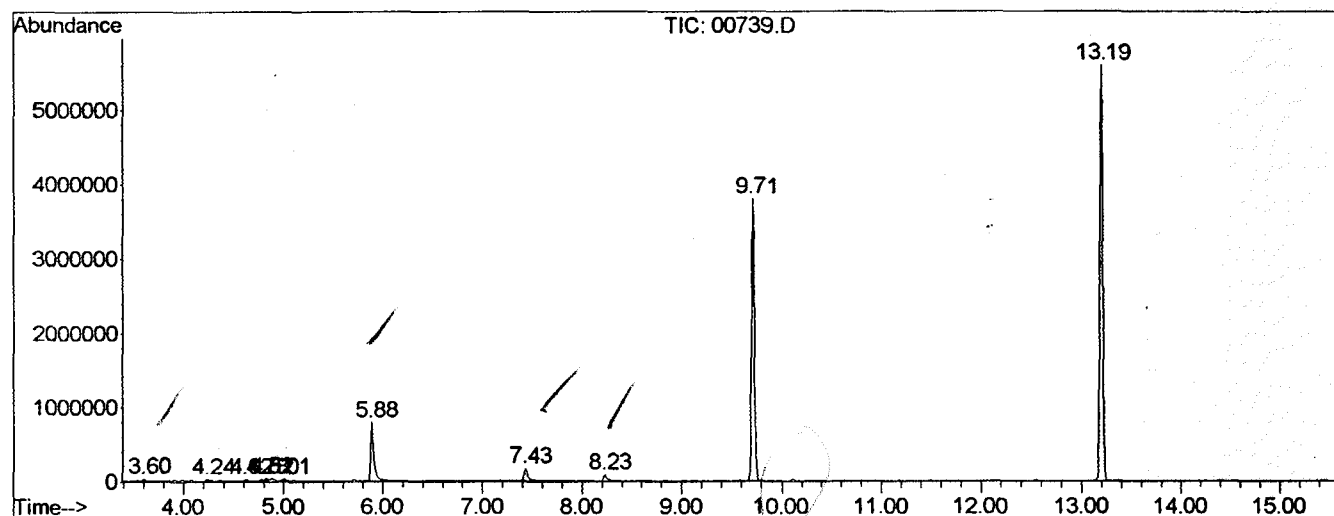
Signal : TIC

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	rVB2	27846	45388	0.36%	0.063%
2	4.241	71	76	83	rVV5	22808	57922	0.46%	0.080%
3	4.618	107	109	119	rVB2	20201	42724	0.34%	0.059%
4	4.778	119	123	125	rBV	23205	34771	0.28%	0.048%
5	4.823	125	127	129	rBV2	31055	50048	0.40%	0.069%
6	5.006	139	143	147	rVB2	31924	66918	0.53%	0.092%
7	5.885	217	220	243	rVB	786235	1707025	13.53%	2.356%
8	7.426	351	355	367	rBV	168975	440565	3.49%	0.608%
9	8.225	423	425	435	rBV	85494	198407	1.57%	0.274%
10	9.710	551	555	561	rBV	3790843	7353050	58.27%	10.150%
11	13.192	855	860	865	rBV	5590370	10700619	84.80%	14.771%
12	18.341	1305	1311	1315	rBV	5963307	11810093	93.59%	16.303%
13	21.332	1569	1573	1577	rVV	22399	40506	0.32%	0.056%
14	22.280	1653	1656	1661	rVB2	53828	95686	0.76%	0.132%
15	22.645	1681	1688	1693	rVV2	5588865	12618743	100.00%	17.419%
16	22.771	1693	1699	1715	rVV	72195	236093	1.87%	0.326%
17	27.726	2129	2133	2139	rBV	1018346	1855871	14.71%	2.562%
18	30.488	2369	2375	2381	rBV	4627972	11707624	92.78%	16.161%
19	33.411	2625	2631	2679	rBV	694660	3449454	27.34%	4.762%
20	34.416	2713	2719	2737	rBV	3825997	9930026	78.69%	13.708%

Sum of corrected areas: 72441533

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Operator :
 Acquired : 16 Jan 2002 8:07 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508scan
 Misc Info : January 16, 2002
 Vial Number: 7
 Quant File :SCAN508.RES (RTE Integrator)



00739.D SCAN508.M

Thu Jan 17 08:17:51 2002

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Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

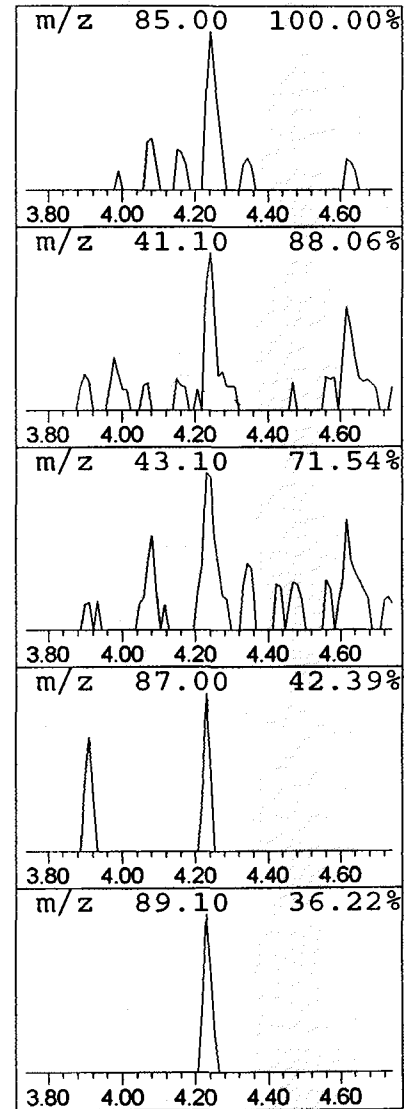
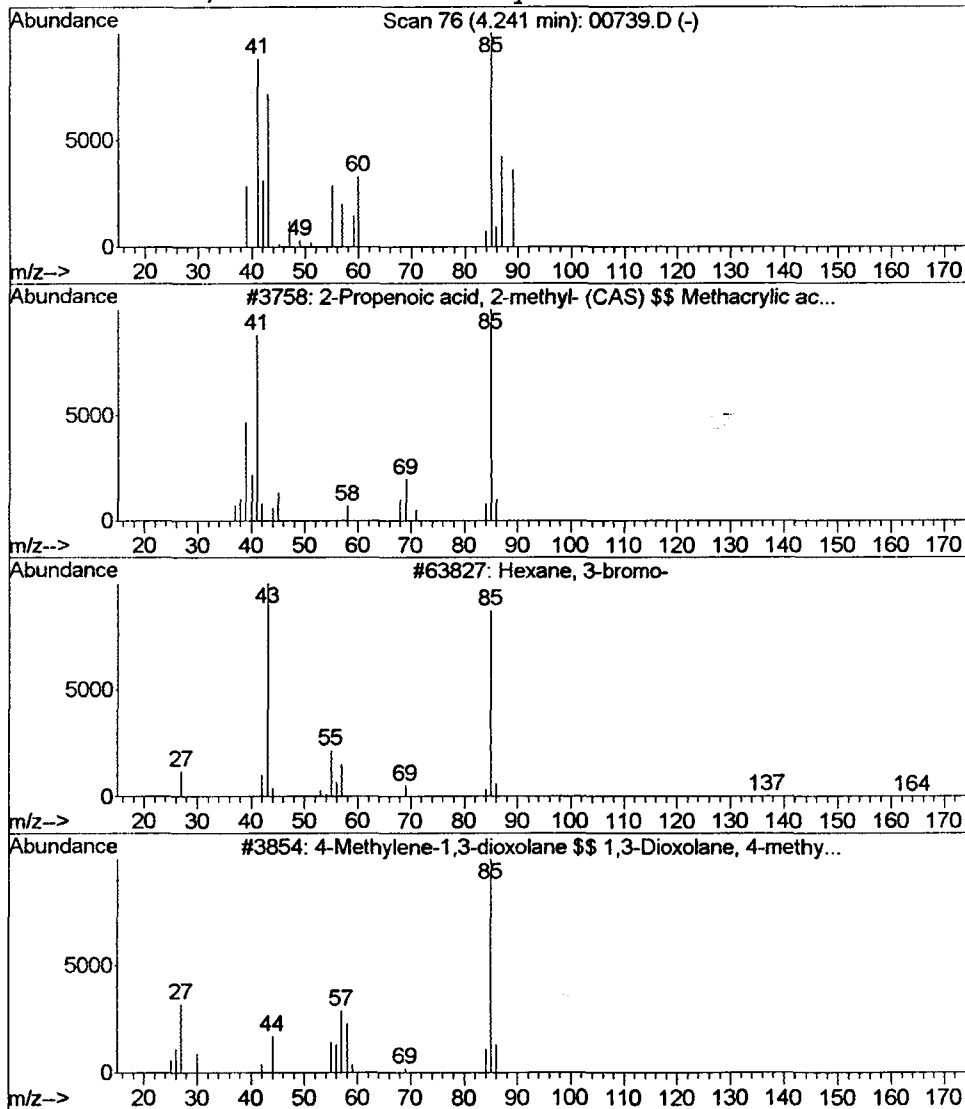
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 2-Propenoic acid, 2-methyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.16 ug/L	57922	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 2-methyl- (CAS...	86	C4H6O2	000079-41-4	35
2		Hexane, 3-bromo-	164	C6H13Br	003377-87-5	25
3		4-Methylene-1,3-dioxolane \$\$ 1,3...	86	C4H6O2	004362-24-7	25
4		Pentane, 2-bromo-4-methyl-	164	C6H13Br	030310-22-6	23



-----, REPORT COMPOUND REPORT

Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

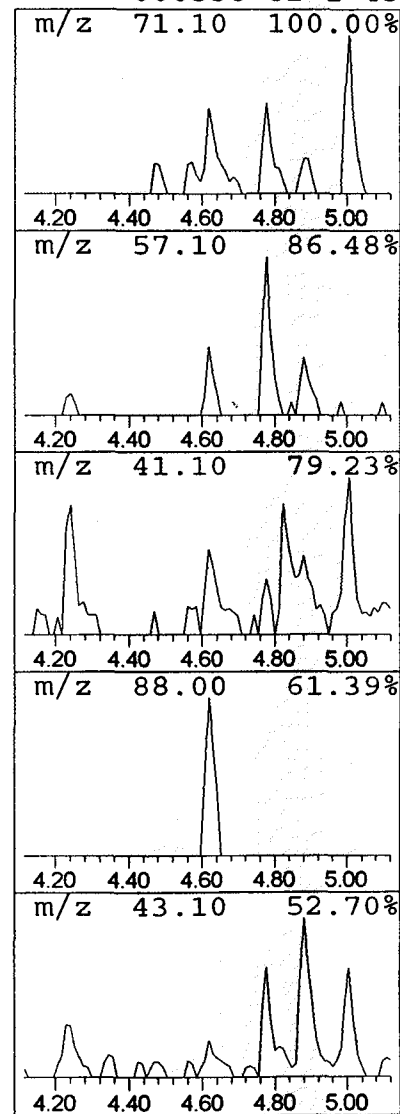
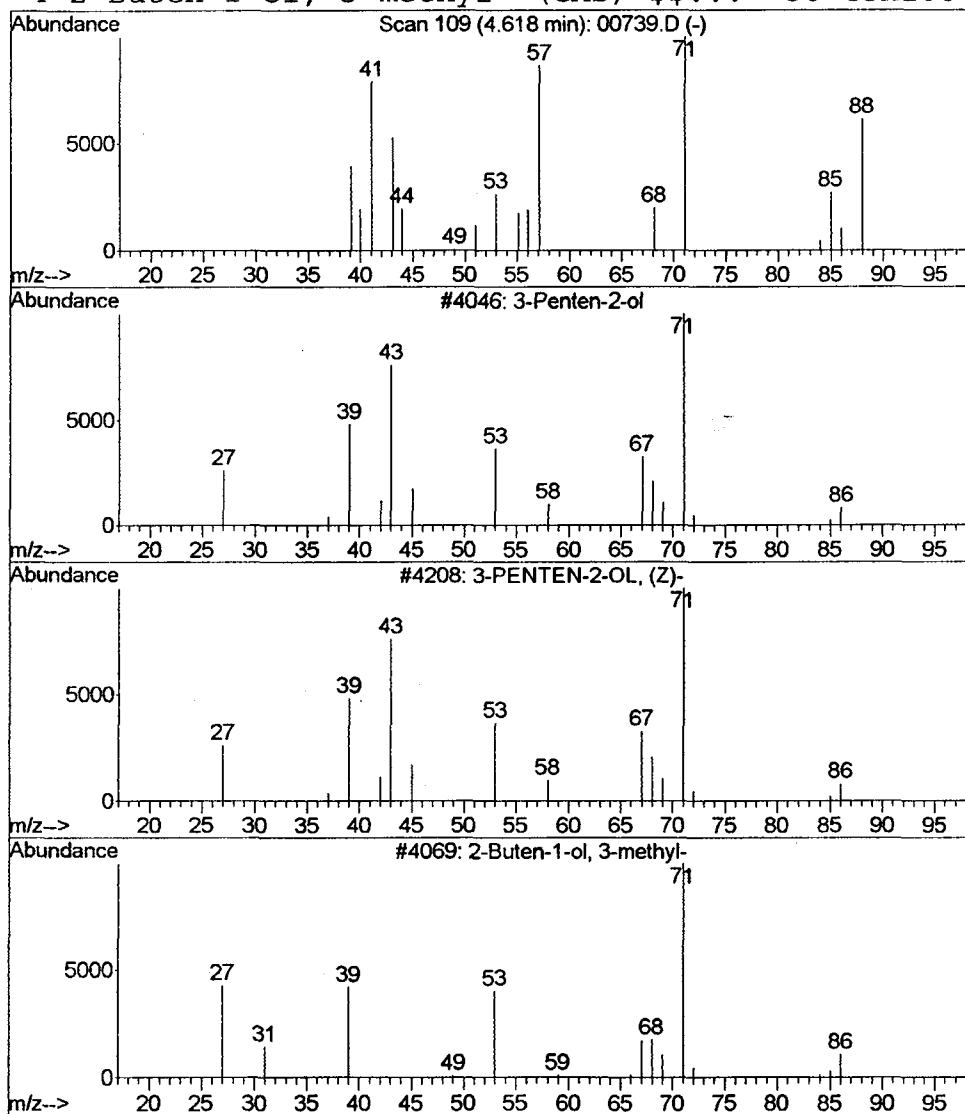
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 3-Penten-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	0.12 ug/L	42724	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	49
2			3-PENTEN-2-OL, (Z)-	86	C5H10O	024652-50-4	49
3			2-Buten-1-ol, 3-methyl-	86	C5H10O	000556-82-1	43
4			2-Buten-1-ol, 3-methyl- (CAS) \$\$...	86	C5H10O	000556-82-1	43



Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

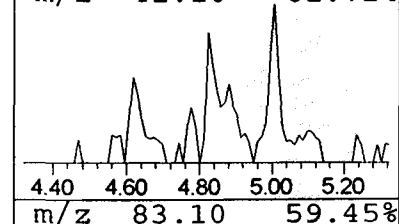
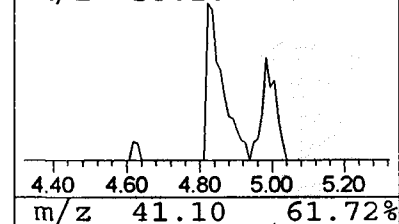
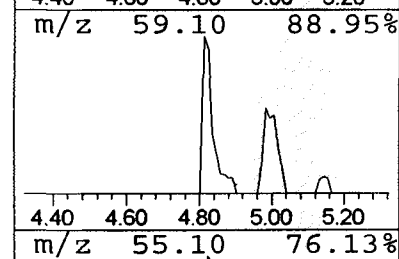
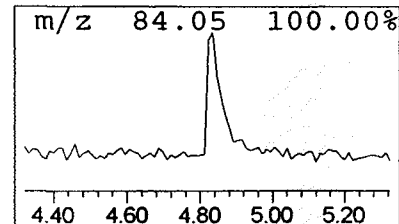
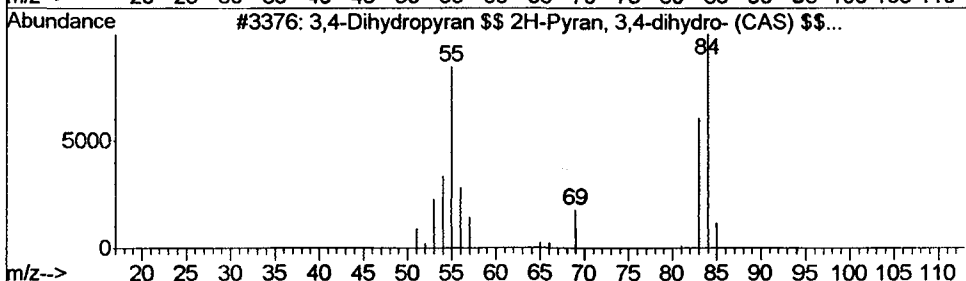
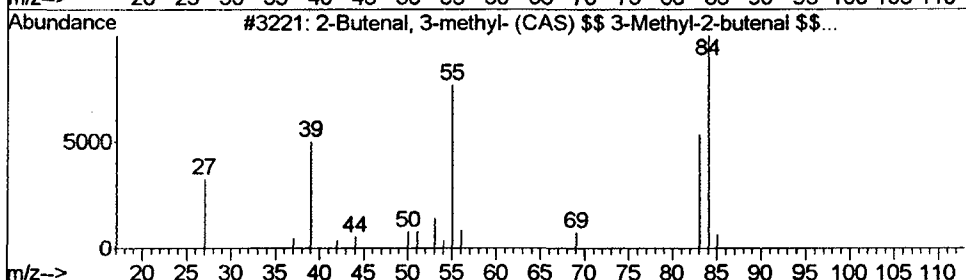
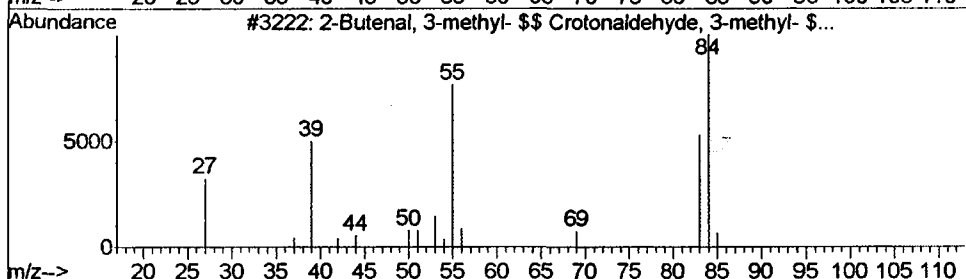
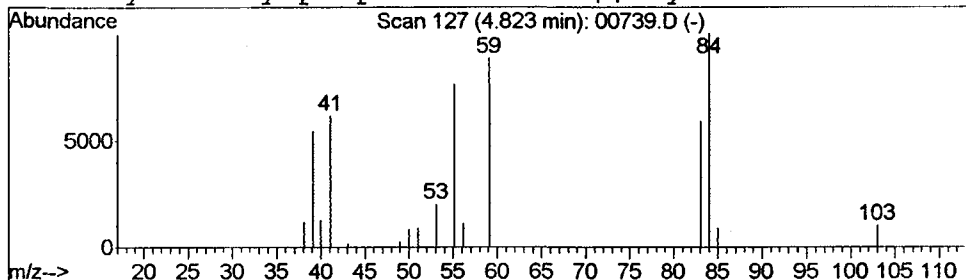
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 2-Butenal, 3-methyl- \$\$ Cro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	0.14 ug/L	50048	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenal, 3-methyl- \$\$ Crotonal...	84	C5H8O	000107-86-8	62
2		2-Butenal, 3-methyl- (CAS) \$\$ 3-...	84	C5H8O	000107-86-8	62
3		3,4-Dihydropyran \$\$ 2H-Pyran, 3,...	84	C5H8O	000110-87-2	50
4		2-Cyclobutylprop-2-en-1-ol \$\$ Cy...	112	C7H12O	116203-80-6	50



Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Acq On : 16 Jan 2002 8:07 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

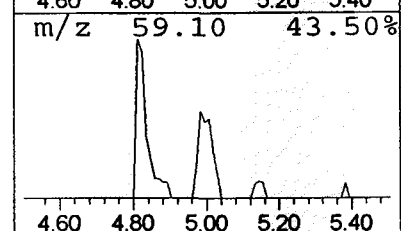
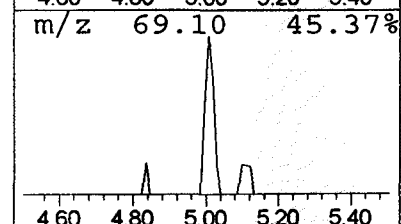
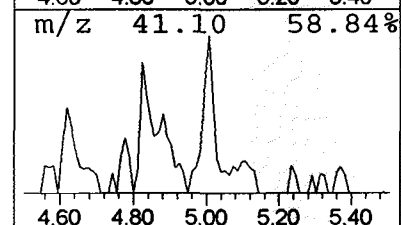
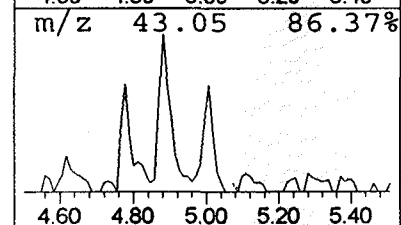
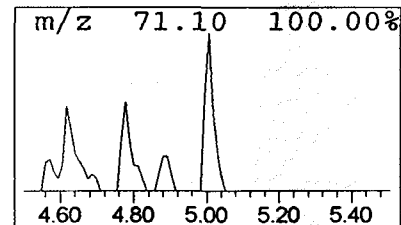
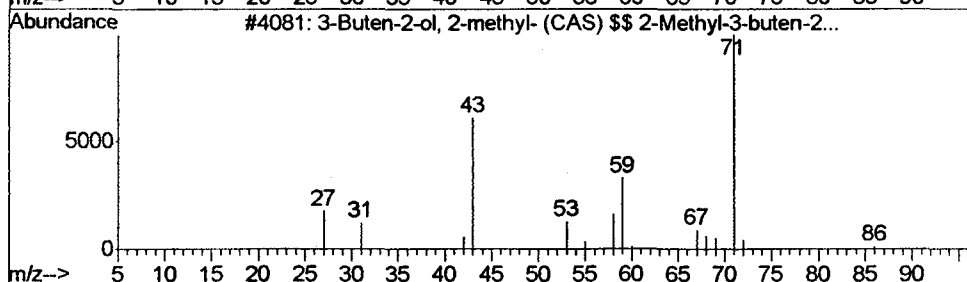
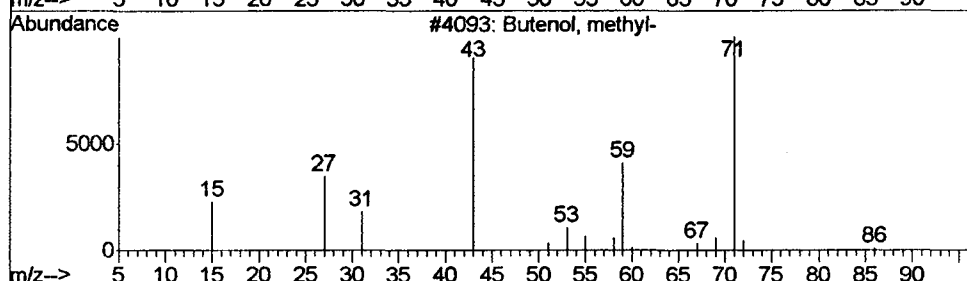
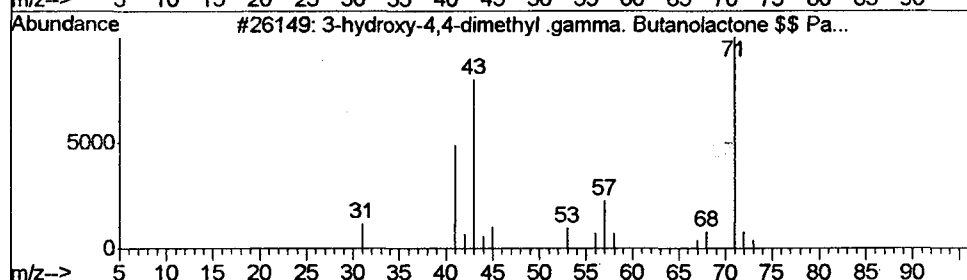
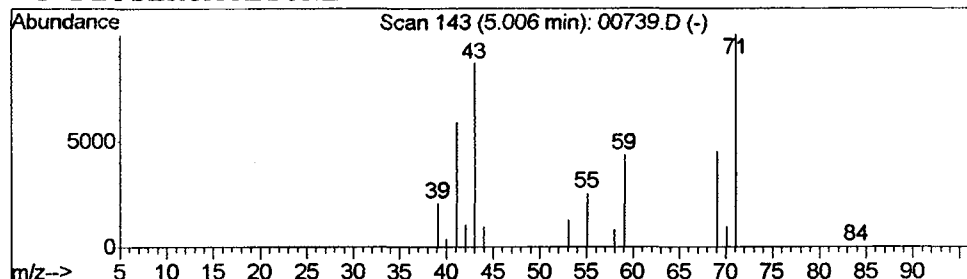
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.18 ug/L	66918	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-hydroxy-4,4-dimethyl .gamma. B...	130	C6H10O3	052126-90-6	53
2		Butenol, methyl-	86	C5H10O	060766-00-9	50
3		3-Buten-2-ol, 2-methyl- (CAS) \$\$...	86	C5H10O	000115-18-4	40
4		DEUTEROACETONE	59	C3H5DO	004468-52-4	12



Library Search Compound Report

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MS Integration Params: LSCINT.P

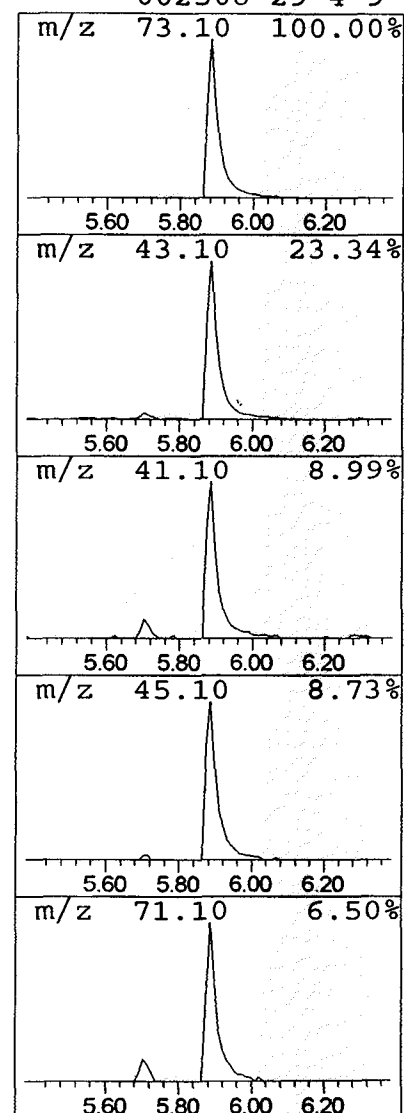
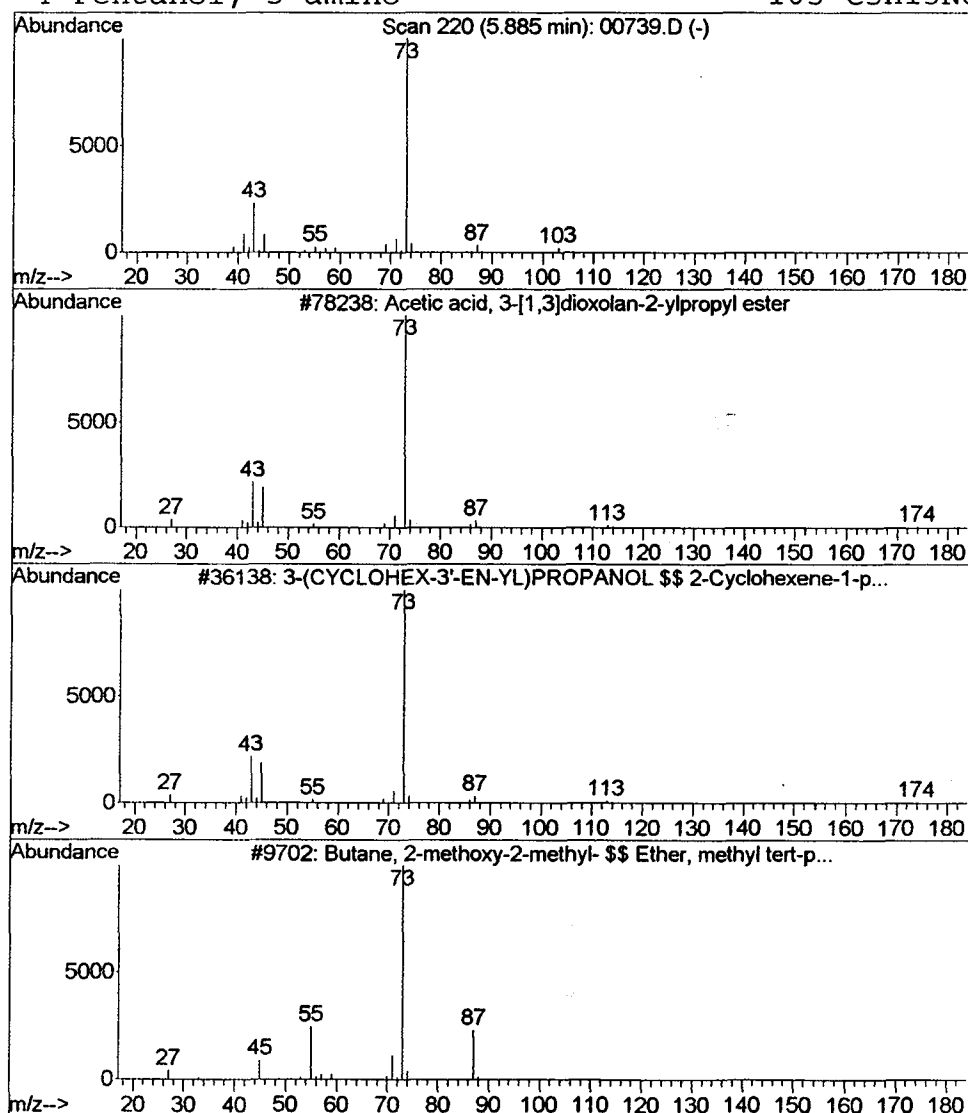
Vial: 7
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 5 Acetic acid, 3-[1,3]dioxola... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.88	4.64 ug/L	1707030	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	36
2		3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	36
3		Butane, 2-methoxy-2-methyl- \$\$ E...	102	C6H14O	000994-05-8	33
4		Pentanol, 5-amino-	103	C5H13NO	002508-29-4	9



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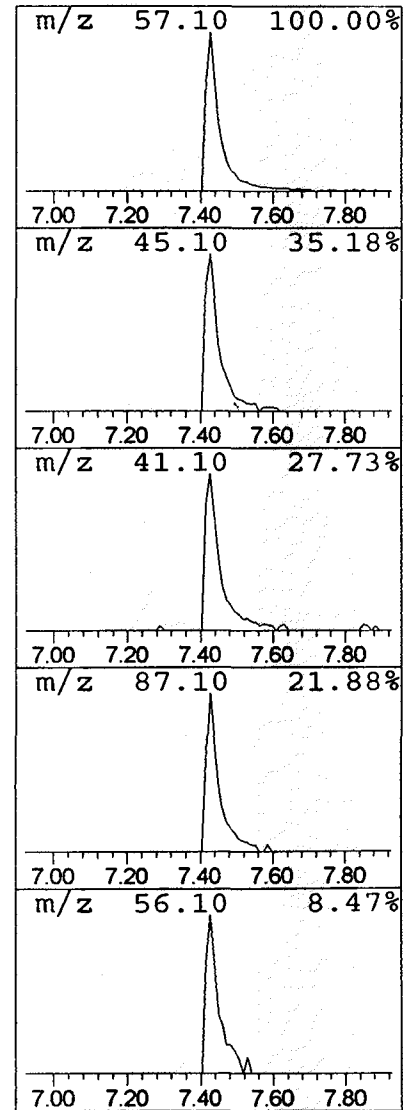
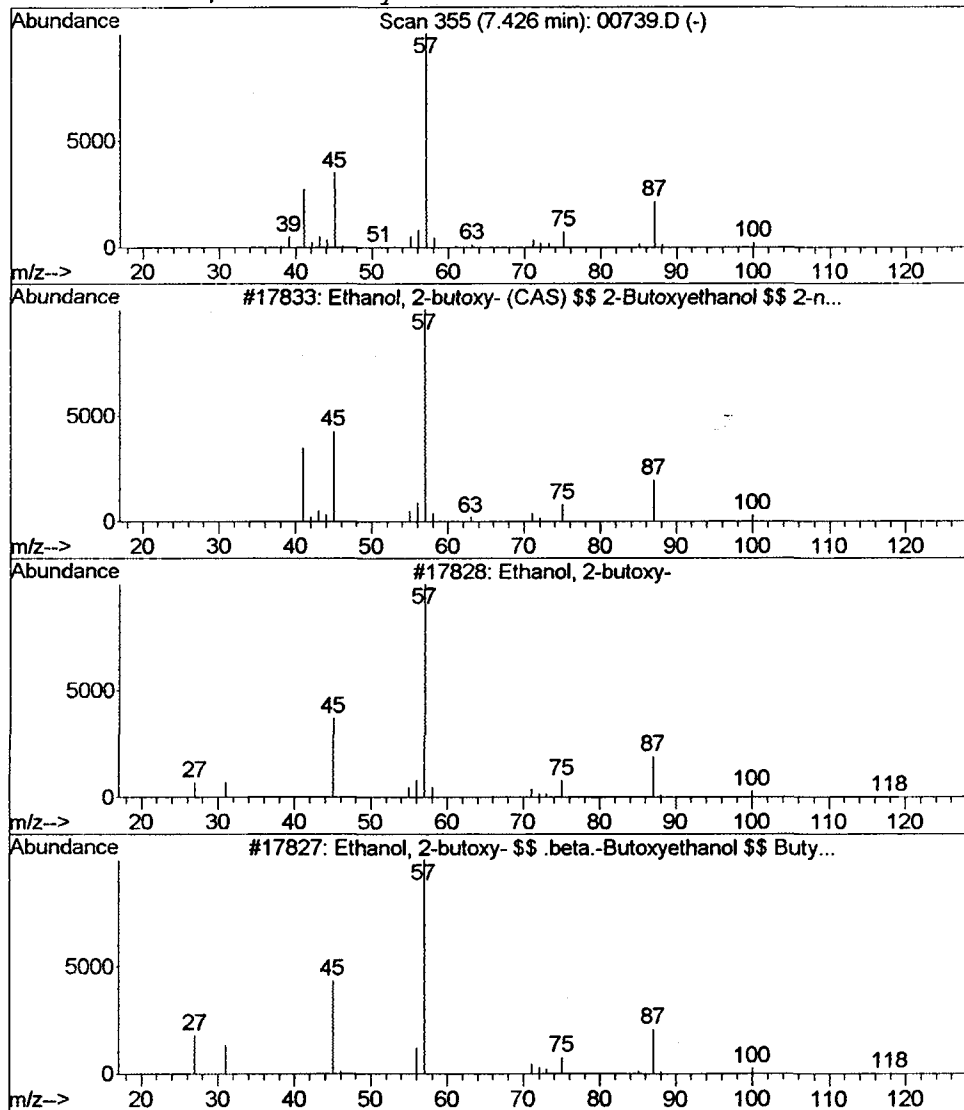
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 6 Ethanol, 2-butoxy- (CAS) \$\$... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	1.20 ug/L	440565	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy- (CAS) \$\$ 2-Bu...	118	C6H14O2	000111-76-2	86
2		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
3		Ethanol, 2-butoxy- \$\$.beta.-But...	118	C6H14O2	000111-76-2	72
4		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	72



Library Search Compound Report

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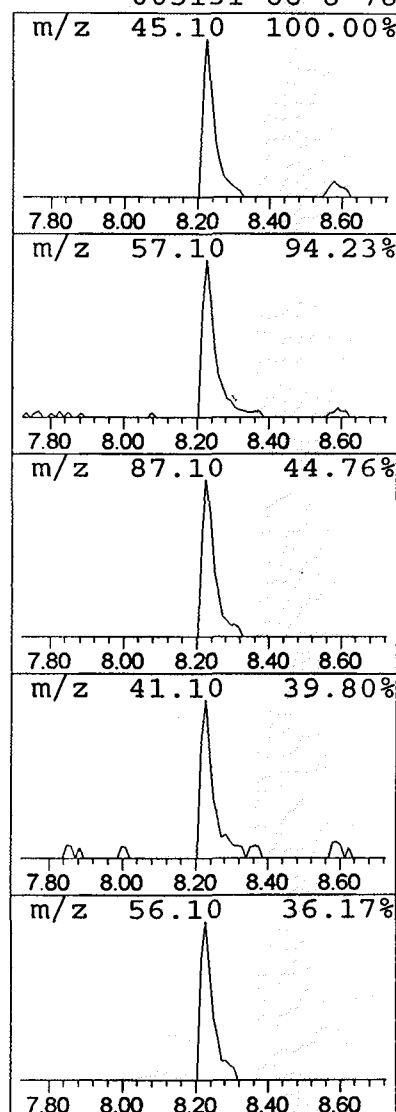
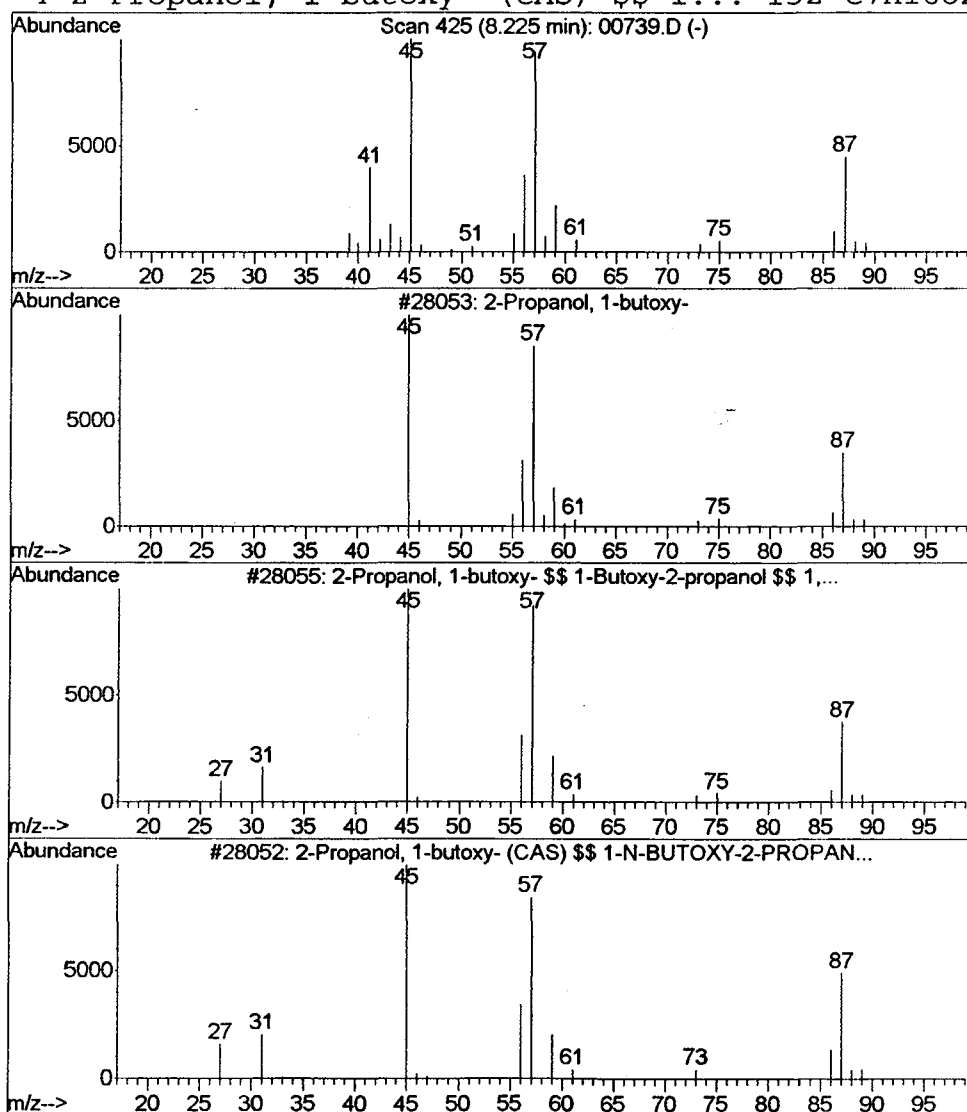
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 7 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	0.54 ug/L	198407	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-			132	C7H16O2	005131-66-8	90
2	2-Propanol, 1-butoxy-	\$\$	1-Butox...	132	C7H16O2	005131-66-8	90
3	2-Propanol, 1-butoxy-	(CAS)	\$\$ 1...	132	C7H16O2	005131-66-8	83
4	2-Propanol, 1-butoxy-	(CAS)	\$\$ 1...	132	C7H16O2	005131-66-8	78



Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
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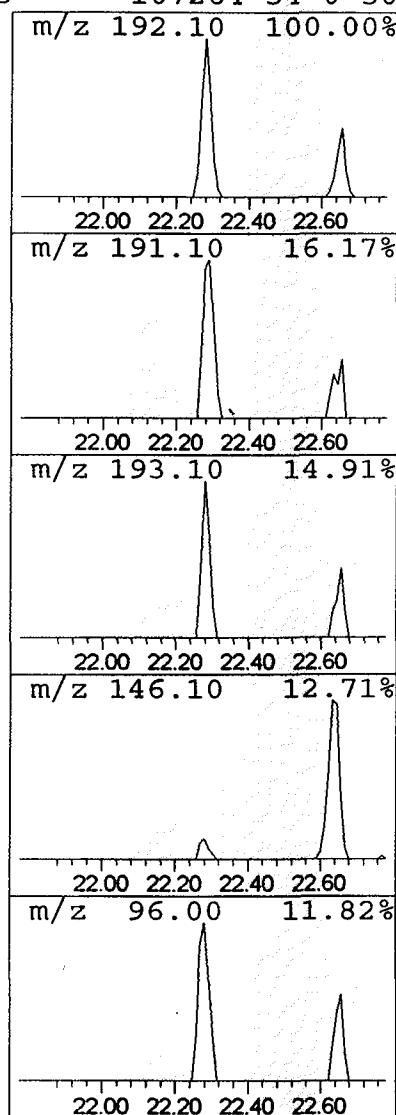
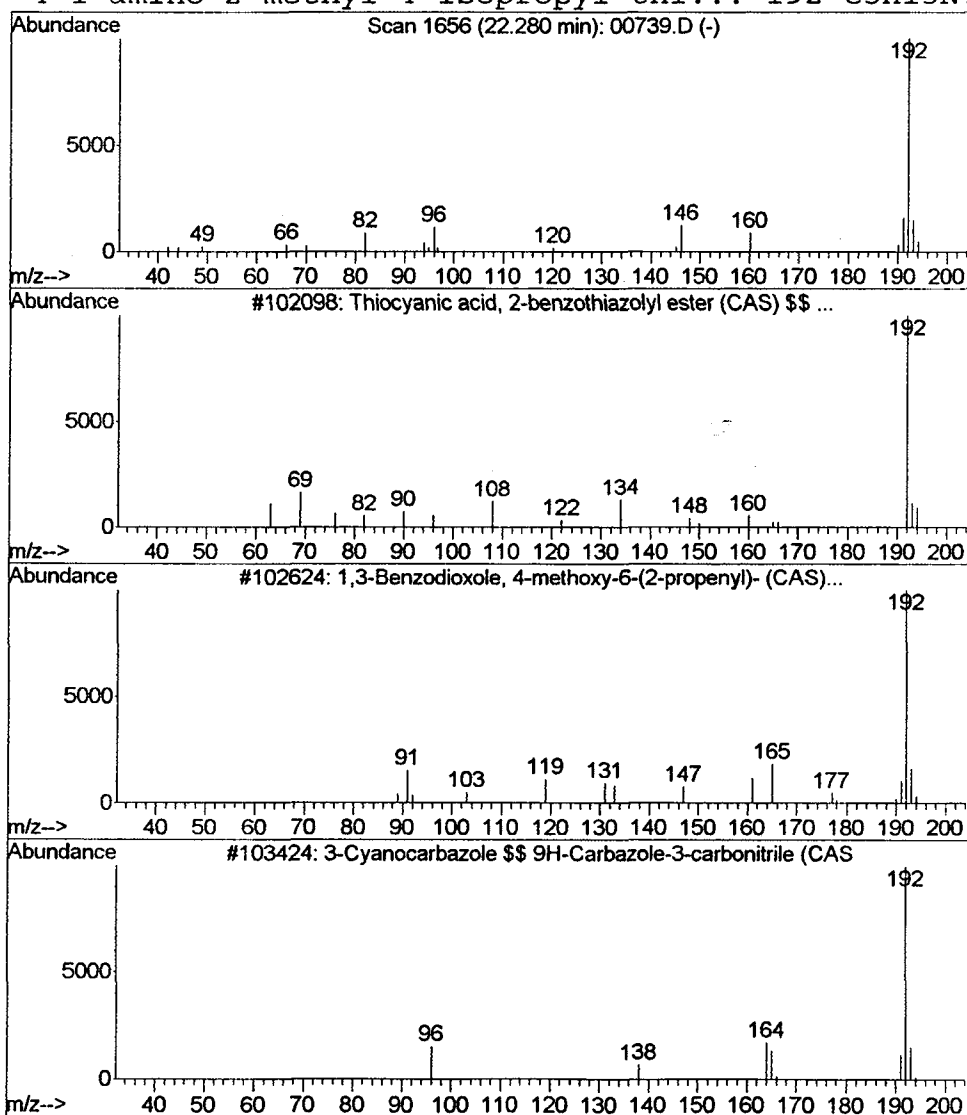
Vial: 7
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Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
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 Peak Number 8 Thiocyanic acid, 2-benzothi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	95686	Phenanthrene-d10	22.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	59
2		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	58
3		3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	56
4		1-amino-2-methyl-4-isopropyl-thi...	192	C5H13N4PS	107264-54-0	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
Acq On : 16 Jan 2002 8:07 pm
Sample : 508scan
Misc : January 16, 2002
MS Integration Params: LSCINT.P

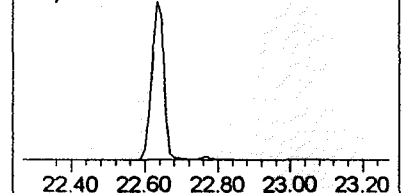
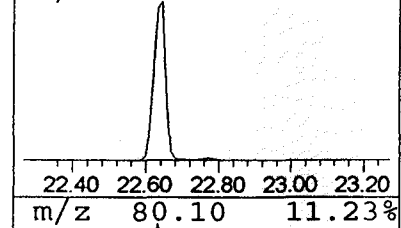
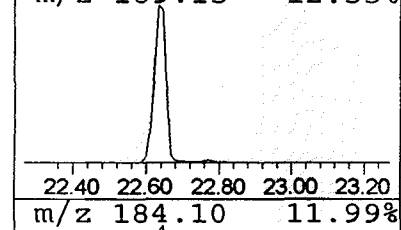
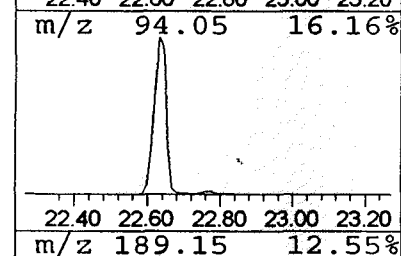
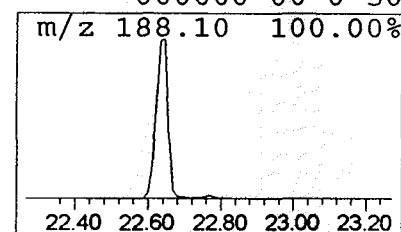
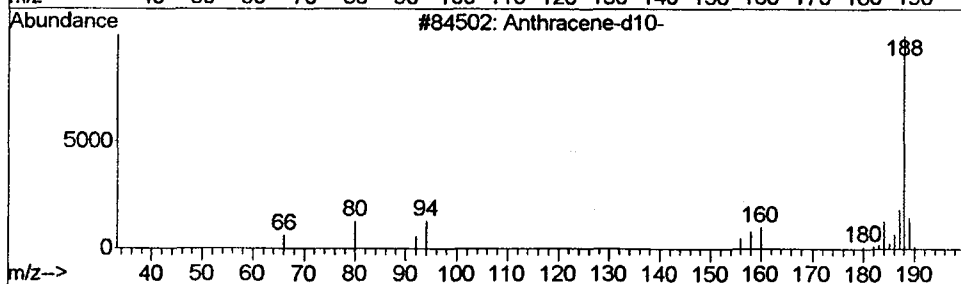
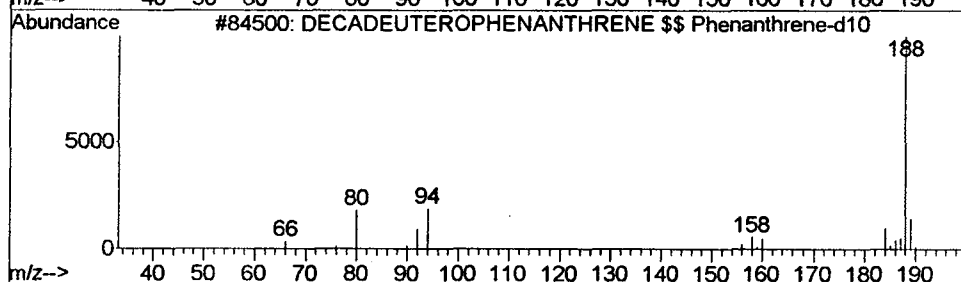
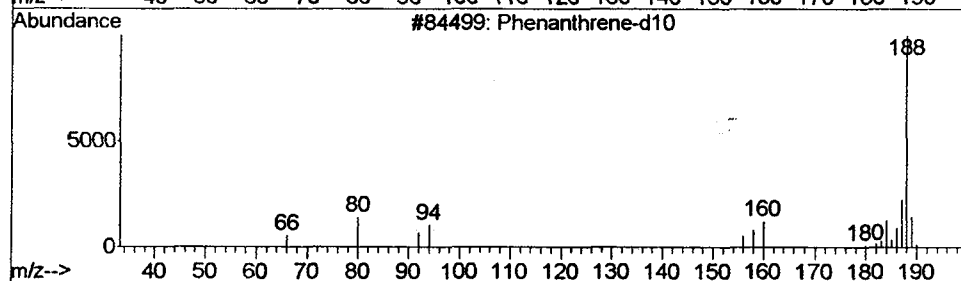
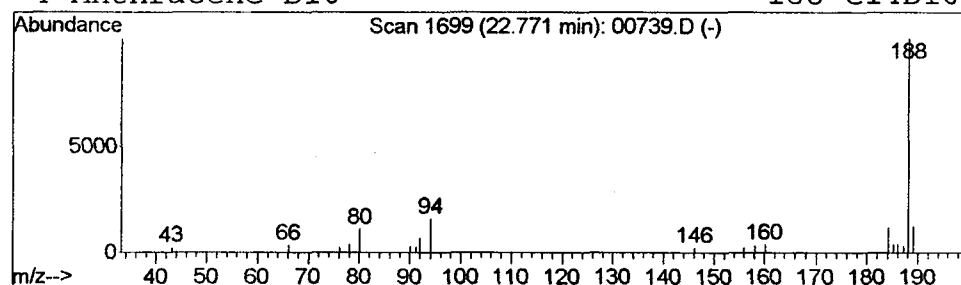
Vial: 7
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 9 Phenanthrene-d10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.37 ug/L	236093	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene-d10	188	C14D10	001517-22-2	86
2			DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	83
3			Anthracene-d10-	188	C14D10	001719-06-8	56
4			Anthracene-D10	188	C14D10	000000-00-0	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00739.D
Acq On : 16 Jan 2002 8:07 pm
Sample : 508scan
Misc : January 16, 2002
MS Integration Params: LSCINT.P

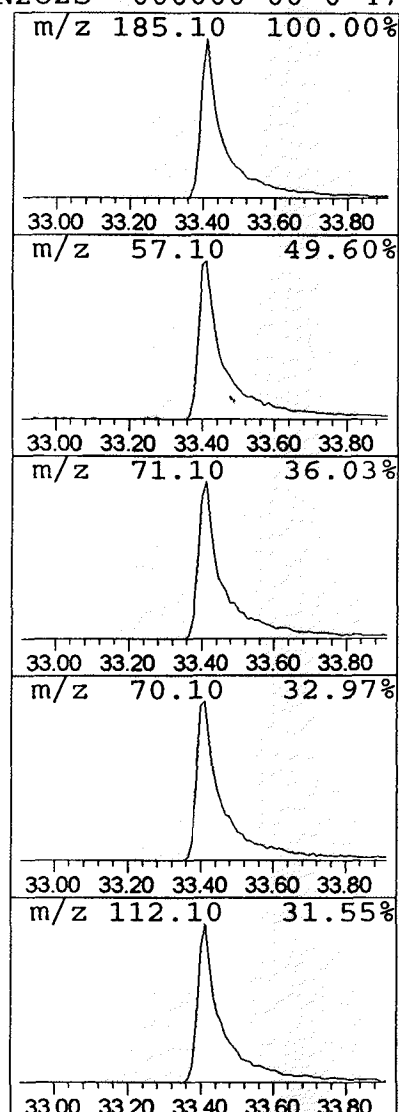
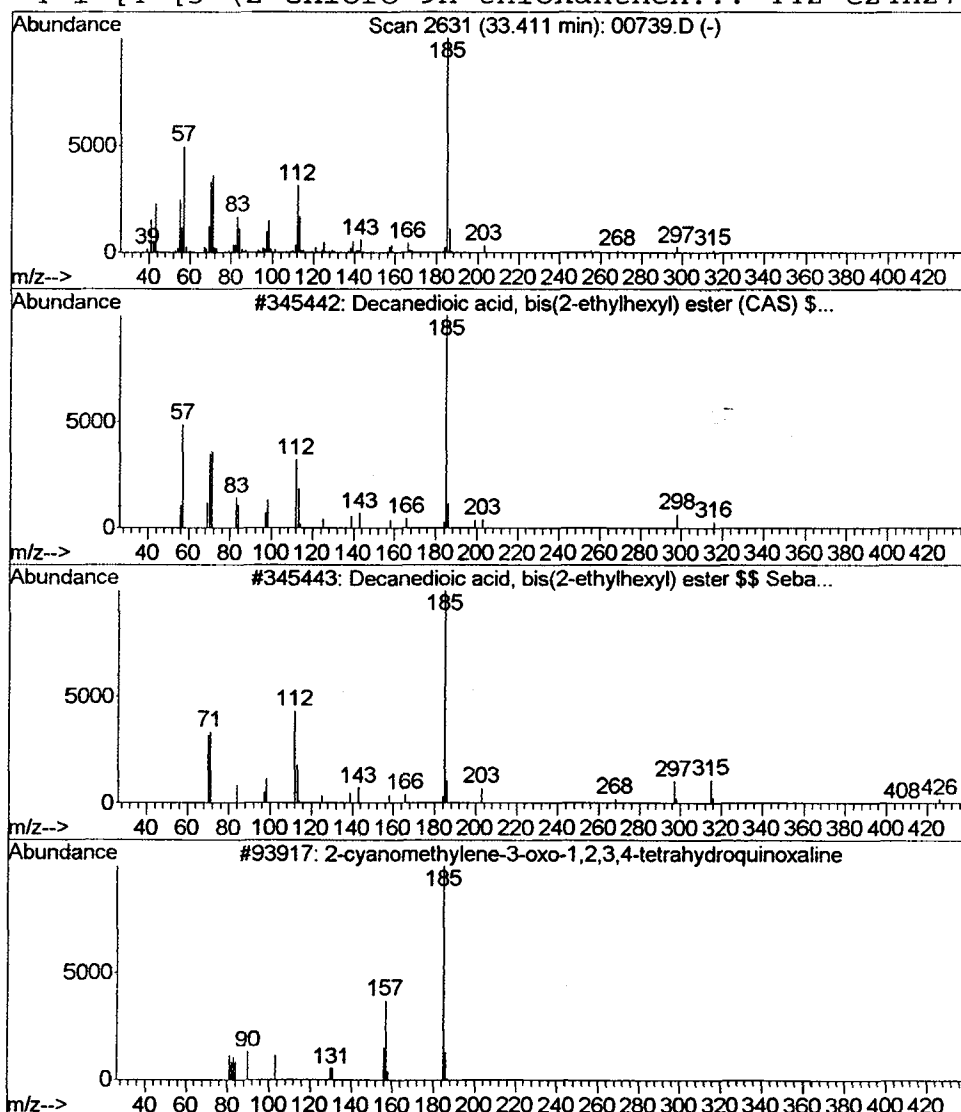
Vial: 7
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 10 Decanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
33.41	6.95 ug/L	3449450	Perylene-d12	34.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	94
2			Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	91
3			2-cyanomethylene-3-oxo-1,2,3,4-t...	185	C10H7N3O	000000-00-0	50
4			1-[4-[3-(2-chloro-9H-thioxahthen...	442	C24H27ClN2O2S	000000-00-0	47



Identified Compounds (2007 Summary)

Operator ID: Date Acquired: 16 Jan 2002 8:07 pm
 Data File: C:\MSDCHEM\1\5973N\02JAN16\00739.D
 Name: 508scan
 Misc: January 16, 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
2-Propenoic acid, ...	4.24	0.2	ug/L	57922	1	9.71	7353050	20.0
3-Penten-2-ol	4.62	0.1	ug/L	42724	1	9.71	7353050	20.0
2-Butenal, 3-meth...	4.82	0.1	ug/L	50048	1	9.71	7353050	20.0
3-hydroxy-4,4-dim...	5.01	0.2	ug/L	66918	1	9.71	7353050	20.0
Acetic acid, 3-[1...	5.88	4.6	ug/L	1707030	1	9.71	7353050	20.0
Ethanol, 2-butoxy...	7.43	1.2	ug/L	440565	1	9.71	7353050	20.0
2-Propanol, 1-but...	8.23	0.5	ug/L	198407	1	9.71	7353050	20.0
Thiocyanic acid, ...	22.28	0.2	ug/L	95686	4	22.65	12618700	20.0
Phenanthrene-d10	22.77	0.4	ug/L	236093	4	22.65	12618700	20.0
Decanedioic acid, ...	33.41	6.9	ug/L	3449450	6	34.42	9930030	20.0