

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/24/2002 Time: 10:56:16

Sample: AE00314
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/24/02 10:55 Ended: 1/24/02 10:55 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		88		5.0

Comments for Sample AE00314 - Analysis \$GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-24-2002 Time: 11:29:58

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\02JAN14\00314.D

Vial: 3

Acq On : 14 Jan 2002 12:09 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 14, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 15 08:47:05 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	1243589	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	5281692	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2756804	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4556828	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	3977974	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3004618	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	317110	4.40	ug/L	0.00
Spiked Amount	5.000		Recovery	=	88.00%	

Target Compounds

						Qvalue
2) n-Nitrosodimethylamine	3.61	74	12161	0.23	ug/L #	17
20) Dimethylphthalate	18.34	163	444273	2.44	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	353744	9.96	ug/L #	17
35) Di-n-butylphthalate	24.85	149	26276	0.09	ug/L	88
41) Benzo(a)anthracene	30.49	228	9763	0.04	ug/L #	61
42) Bis(2-ethylhexyl)phthalate	31.11	149	6443	0.58	ug/L #	68
43) Chrysene	30.49	228	9763	0.04	ug/L #	58
48) Benzo(a)pyrene	34.42	252	10207	0.05	ug/L #	1

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

00314.D SCAN508.M

Tue Jan 15 08:47:06 2002

Page 1

Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D

Vial: 3

Acq On : 14 Jan 2002 12:09 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 14, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 15 8:47 2002

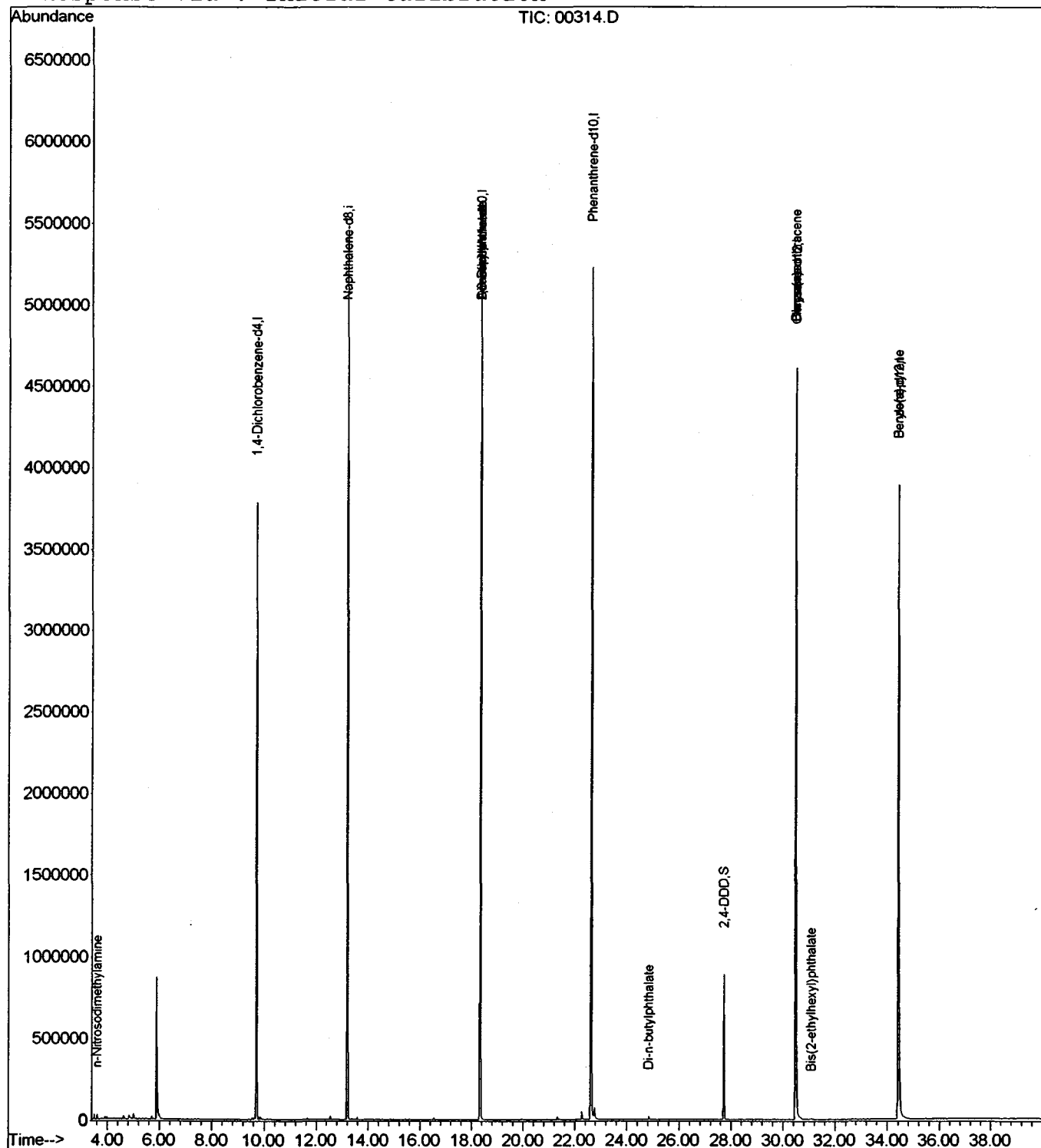
Quant Results File: SCAN508.RE

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



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
 Acq On : 14 Jan 2002 12:09 pm
 Sample : 508 scan
 Misc : January 14, 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

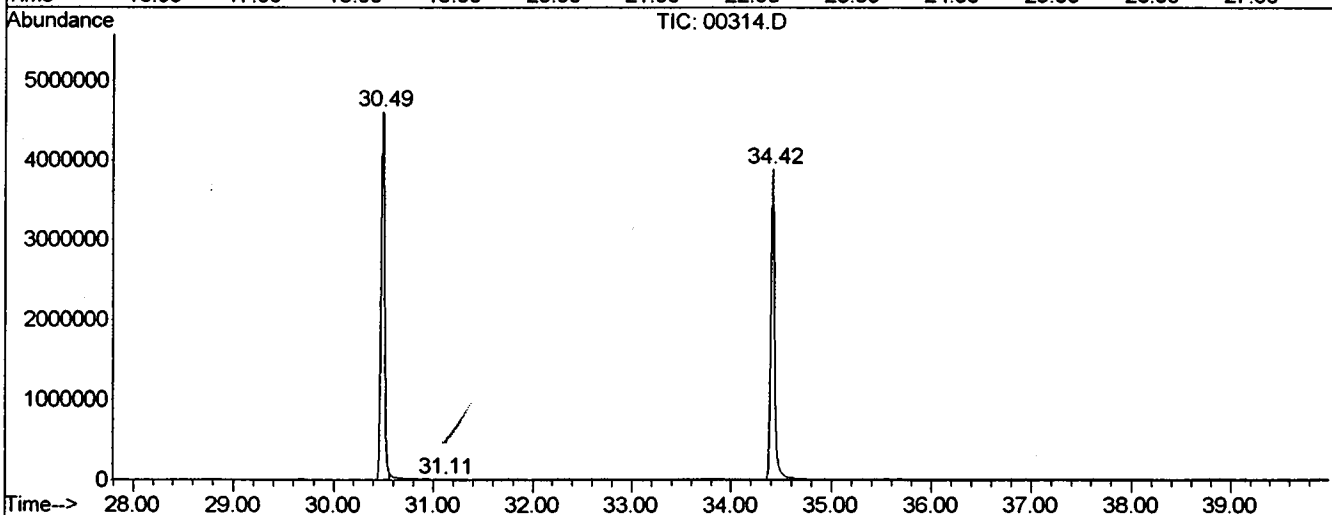
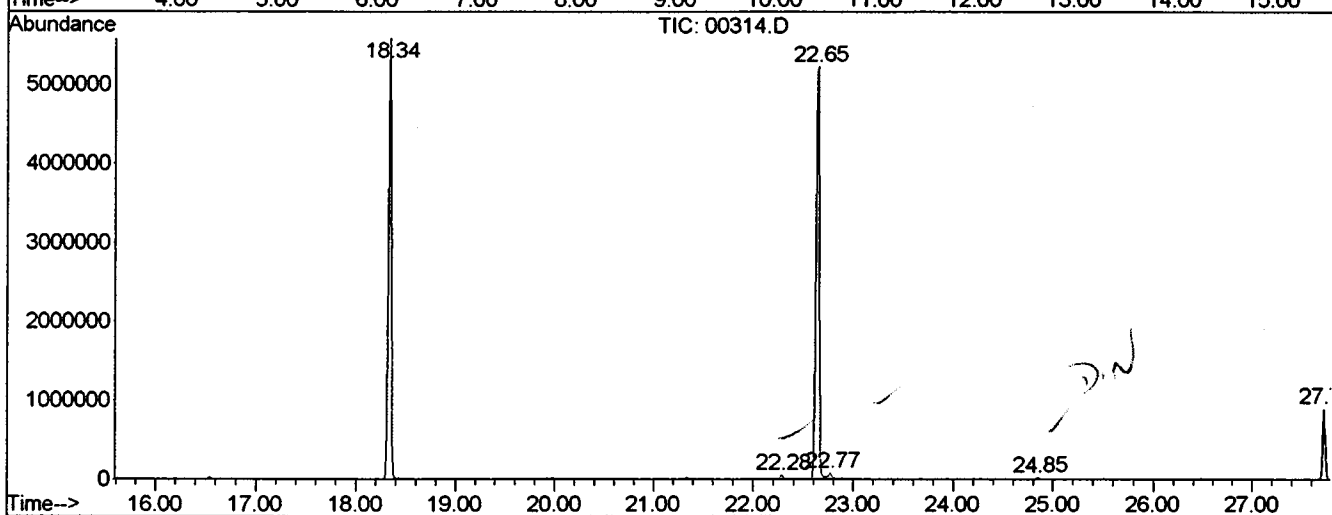
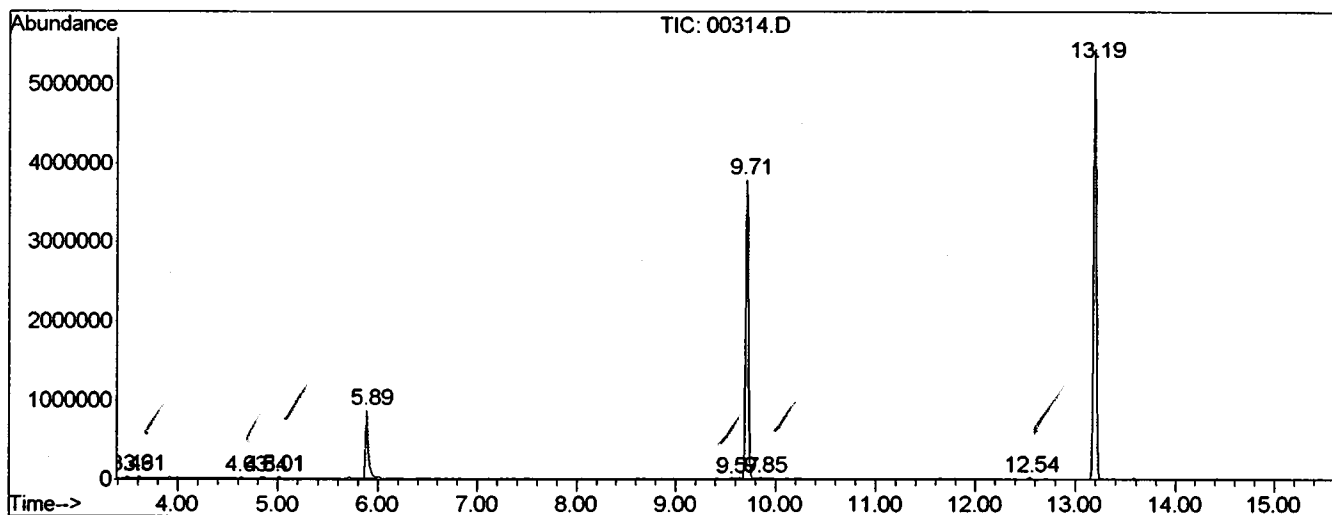
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.488	5	10	13	rBV	29688	45959	0.38%	0.069%
2	3.614	17	21	25	rBV	30405	50274	0.41%	0.076%
3	4.630	103	110	119	rBV5	19464	47666	0.39%	0.072%
4	4.835	125	128	137	rBV3	25893	77319	0.64%	0.116%
5	5.006	141	143	149	rVB	31250	56647	0.47%	0.085%
6	5.885	217	220	229	rBV	868875	1655653	13.66%	2.494%
7	9.573	537	543	547	rVV2	12400	37950	0.31%	0.057%
8	9.710	551	555	561	rVV	3782244	7088714	58.48%	10.679%
9	9.847	565	567	577	rVV	15601	50621	0.42%	0.076%
10	12.542	799	803	807	rVB	25023	41223	0.34%	0.062%
11	13.192	855	860	865	rBV	5437175	10176027	83.95%	15.331%
12	18.341	1305	1311	1315	rBV	5579472	11210979	92.49%	16.890%
13	22.280	1651	1656	1661	rVV	48992	88378	0.73%	0.133%
14	22.645	1681	1688	1693	rVV2	5219364	12121247	100.00%	18.261%
15	22.771	1695	1699	1711	rVB	71554	181744	1.50%	0.274%
16	24.849	1877	1881	1889	rVB	20268	42118	0.35%	0.063%
17	27.726	2129	2133	2137	rBV	885155	1554813	12.83%	2.342%
18	30.489	2369	2375	2381	rBV	4606141	11627466	95.93%	17.517%
19	31.105	2425	2429	2437	rVB3	7759	30234	0.25%	0.046%
20	34.416	2713	2719	2755	rBV	3884980	10191983	84.08%	15.355%

Sum of corrected areas: 66377015

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
Operator :
Acquired : 14 Jan 2002 12:09 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 14, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

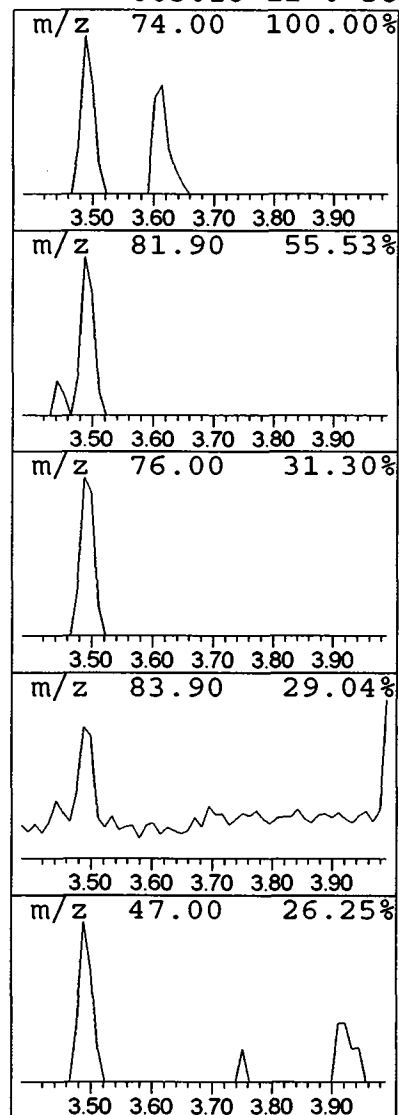
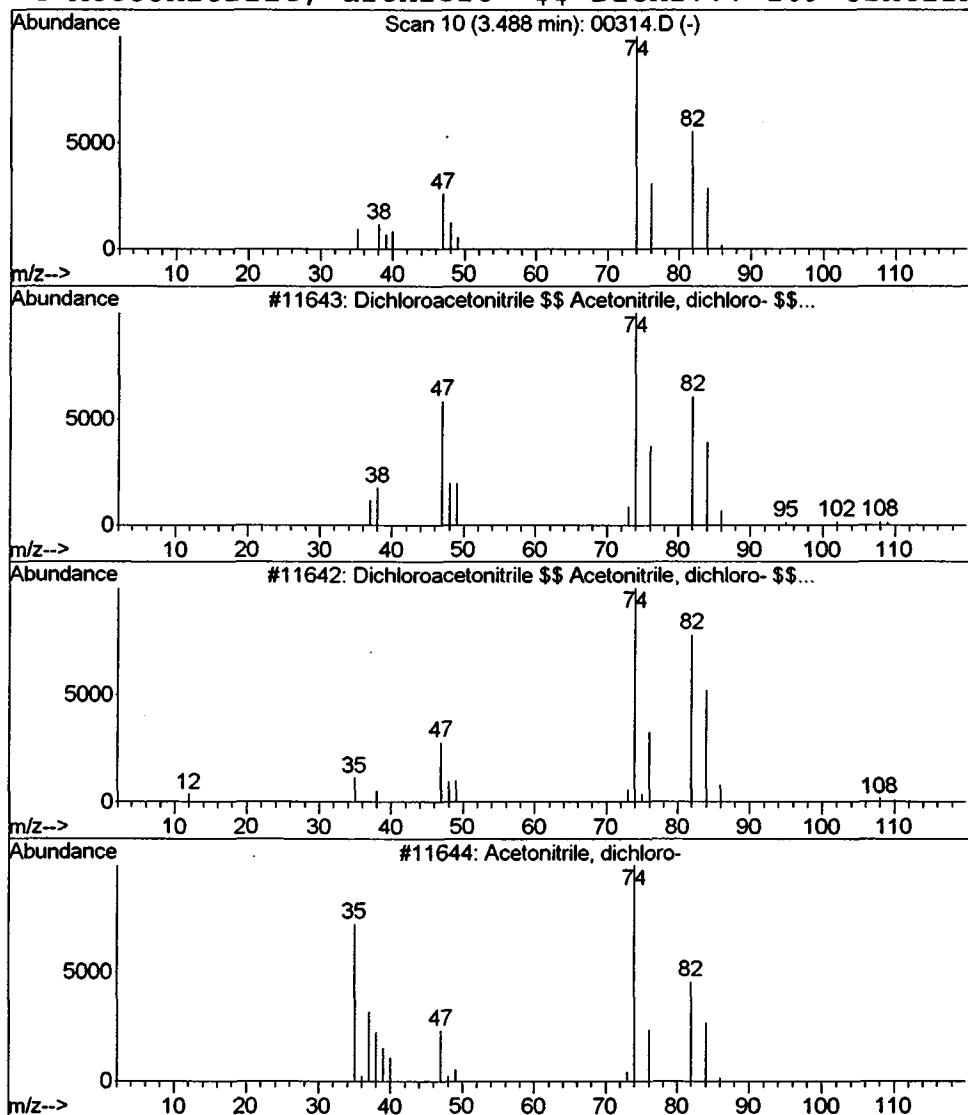
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Dichloroacetonitrile \$\$ Ace... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	0.13 ug/L	45959	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetonitrile \$\$ Acetonit...	109	C2HCl2N	003018-12-0	74
2			Dichloroacetonitrile \$\$ Acetonit...	109	C2HCl2N	003018-12-0	64
3			Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	64
4			Acetonitrile, dichloro- \$\$ Dichl...	109	C2HCl2N	003018-12-0	38



Library Search Compound Report

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Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

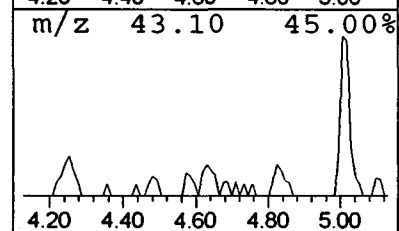
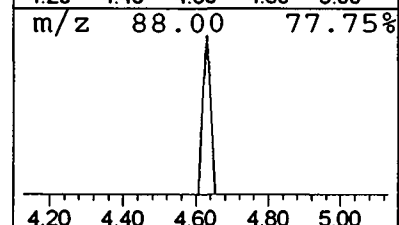
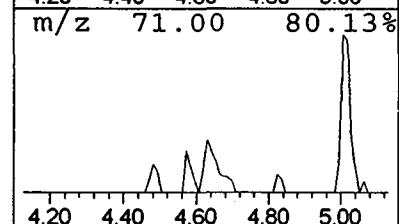
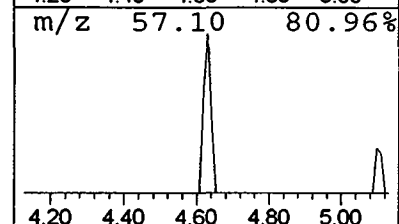
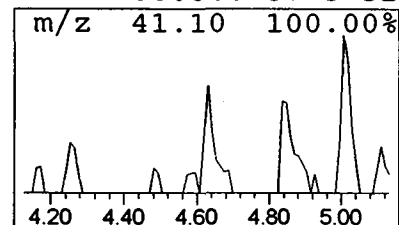
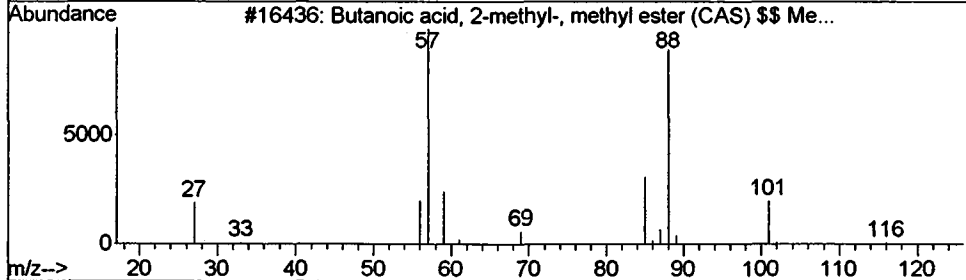
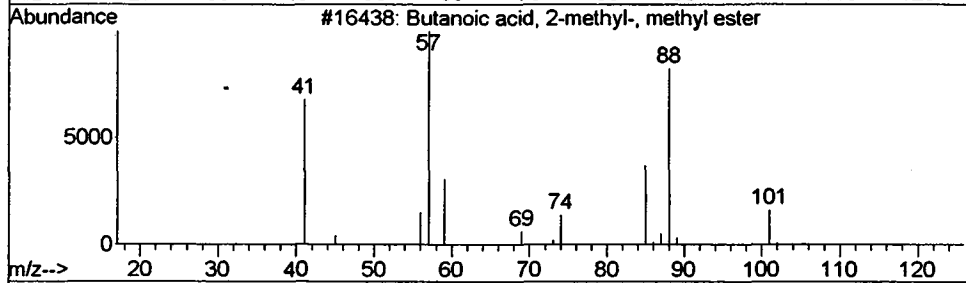
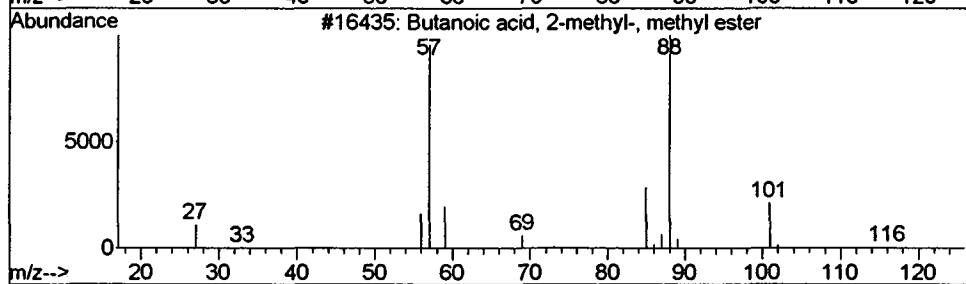
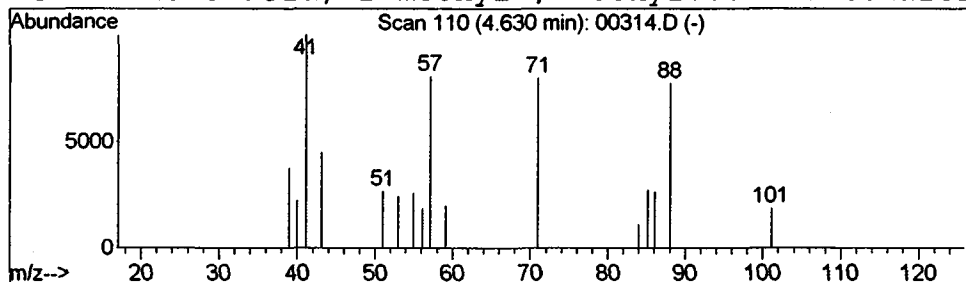
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 2 Butanoic acid, 2-methyl-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	0.13 ug/L	47666	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	38
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	32
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	32



Library Search Compound Report

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Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

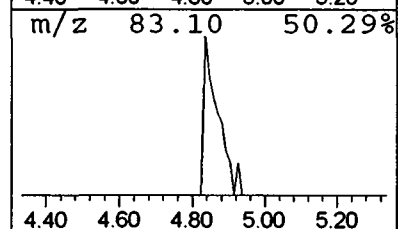
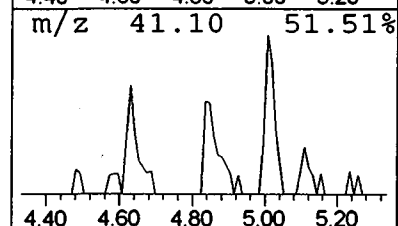
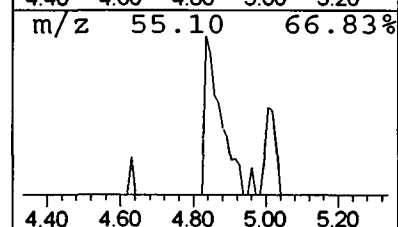
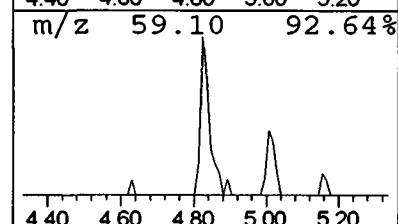
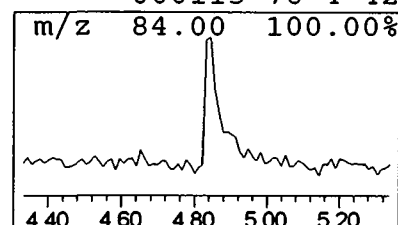
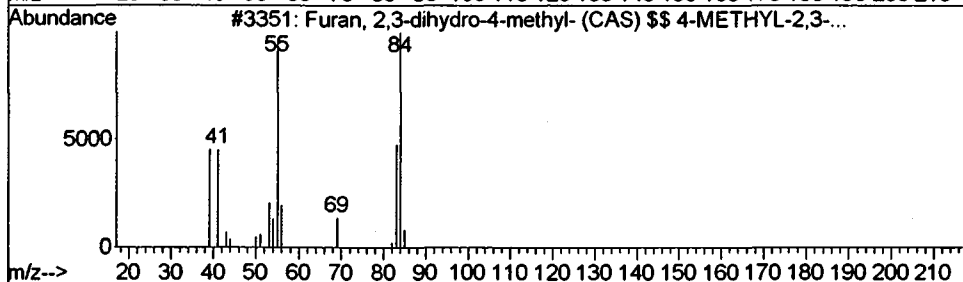
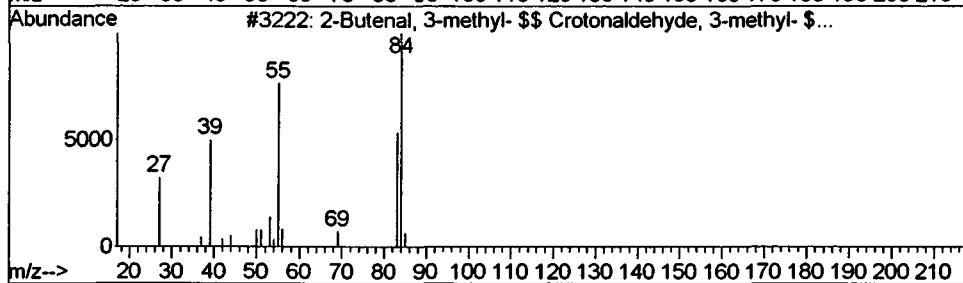
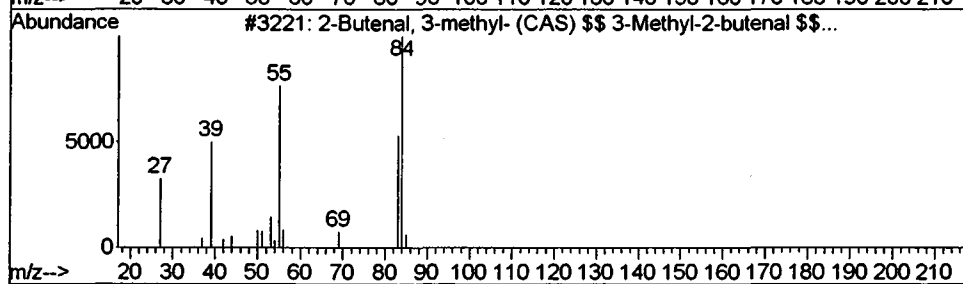
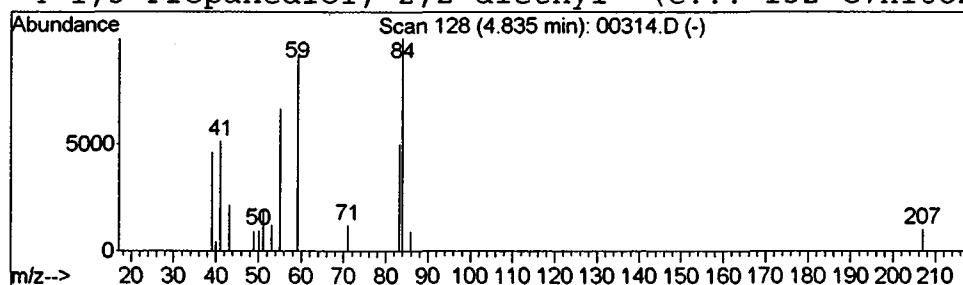
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 3 2-Butenal, 3-methyl- (CAS) ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.22 ug/L	77319	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl- (CAS) \$\$ 3-...	84	C5H8O	000107-86-8	46
2			2-Butenal, 3-methyl- \$\$ Crotonal...	84	C5H8O	000107-86-8	46
3			Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	43
4			1,3-Propanediol, 2,2-diethyl- (C...	132	C7H16O2	000115-76-4	42



Library Search Compound Report

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Misc : January 14, 2002
MS Integration Params: LSCINT.P

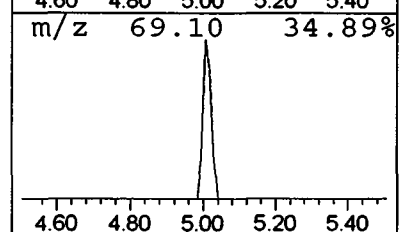
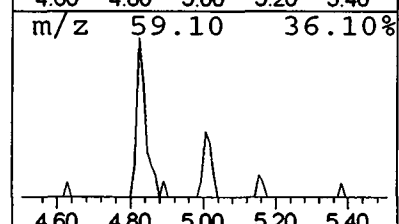
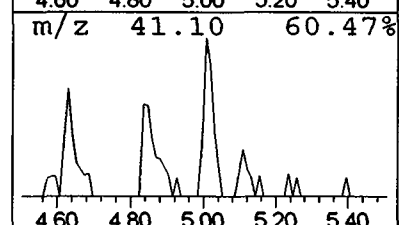
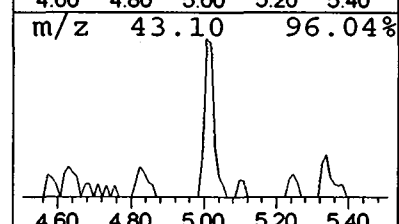
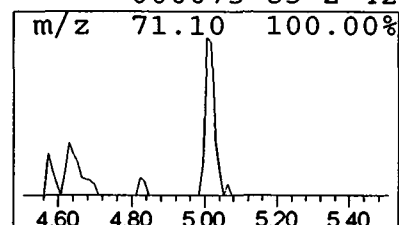
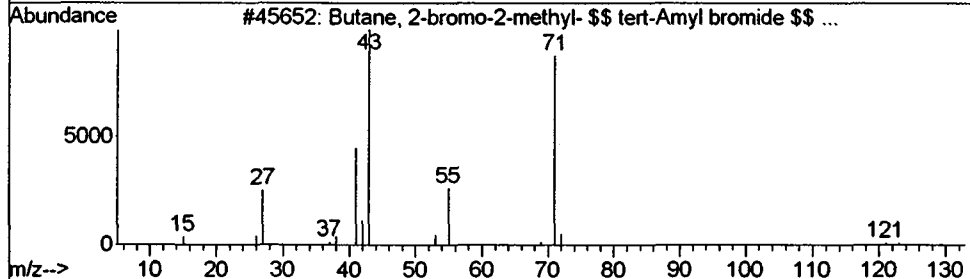
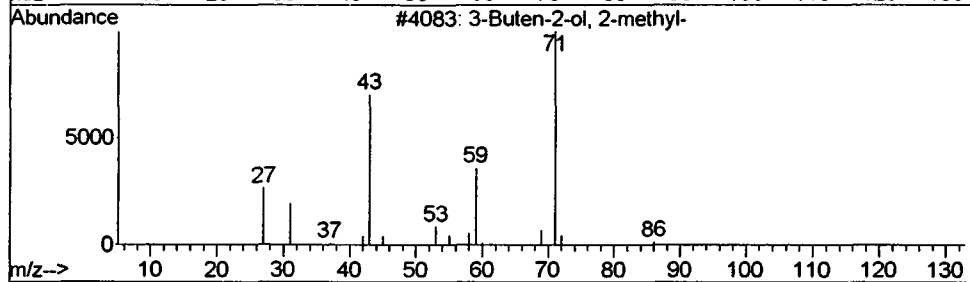
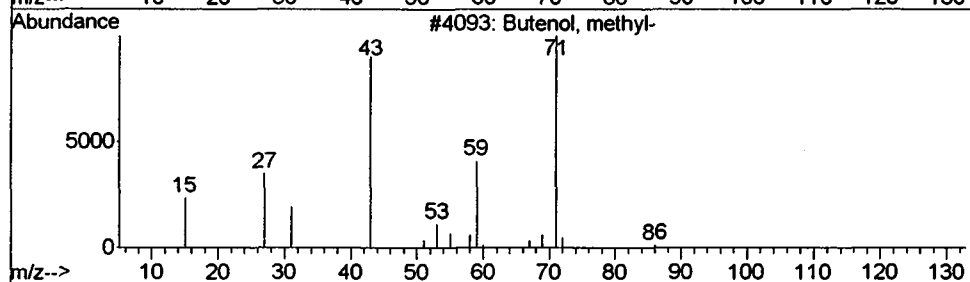
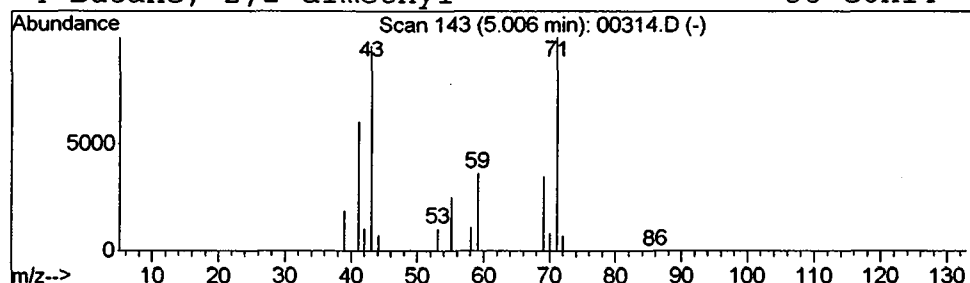
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 Butenol, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.16 ug/L	56647	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butenol, methyl-	86	C5H10O	060766-00-9	78
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	74
3			Butane, 2-bromo-2-methyl- \$\$ ter...	150	C5H11Br	000507-36-8	45
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	42



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Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

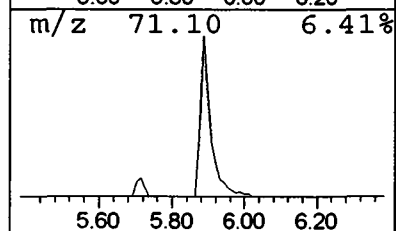
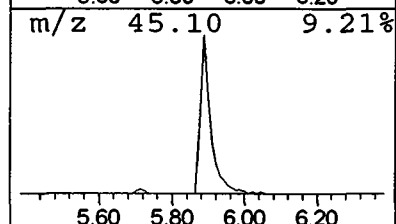
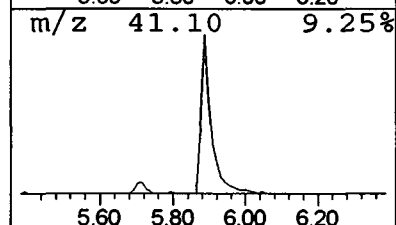
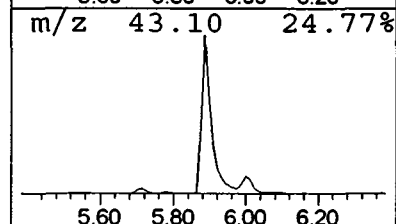
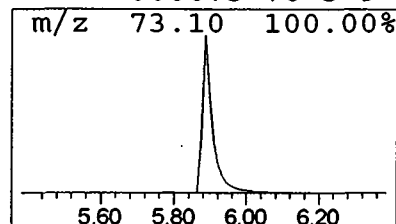
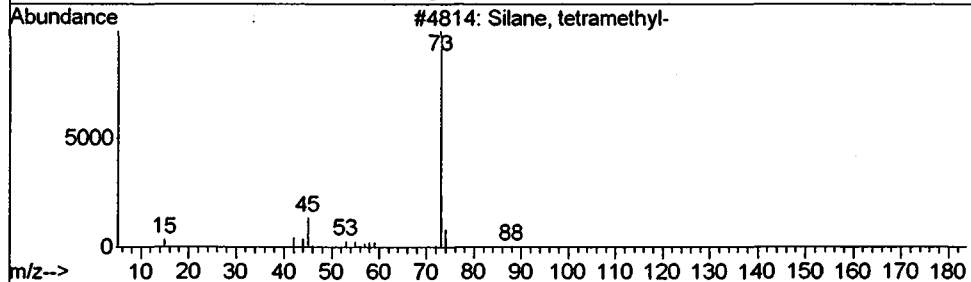
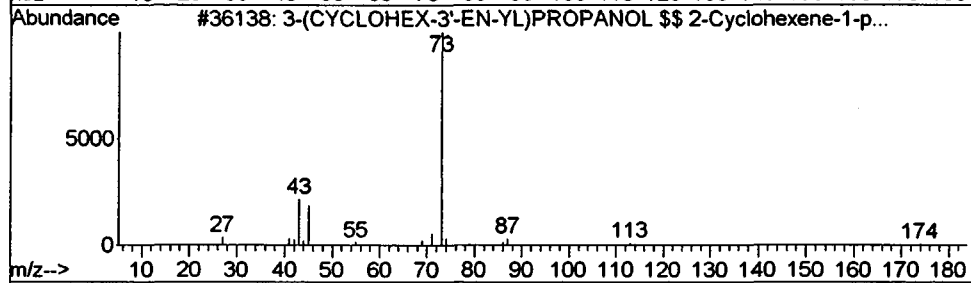
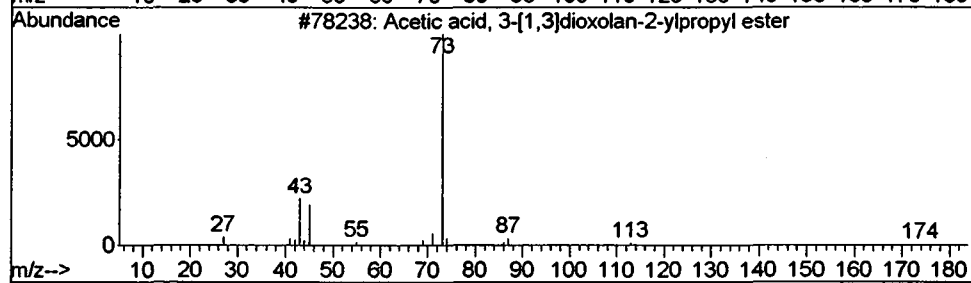
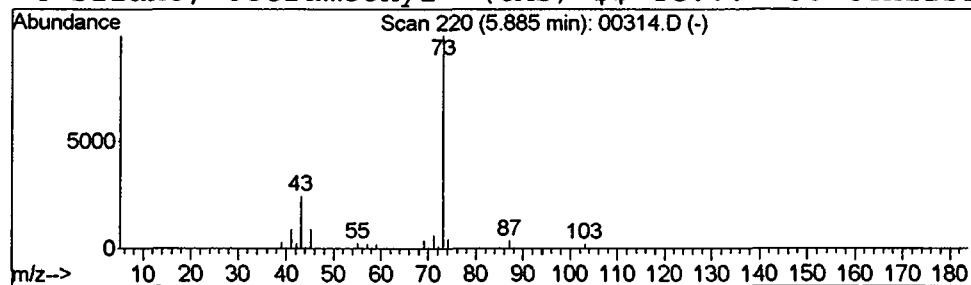
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.67 ug/L	1655650	1,4-Dichlorobenzene-d4	9.71

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



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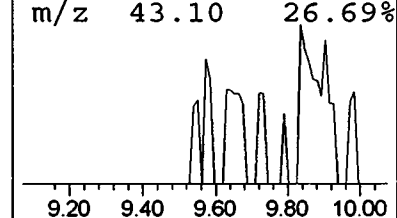
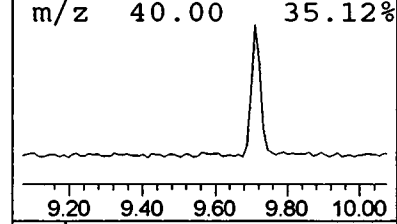
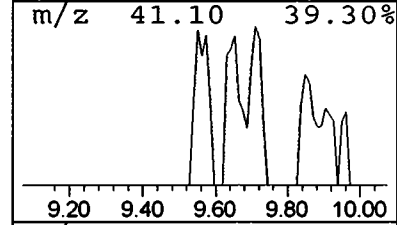
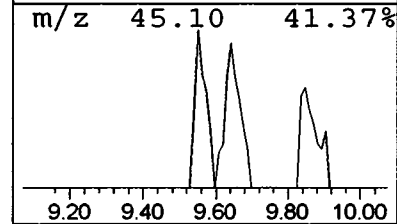
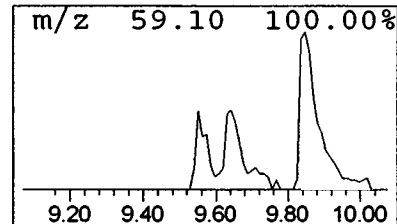
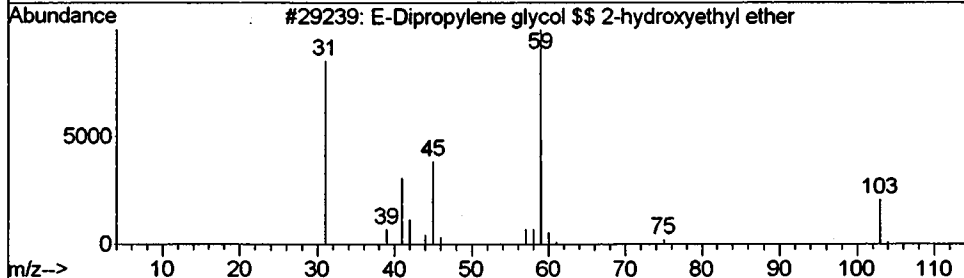
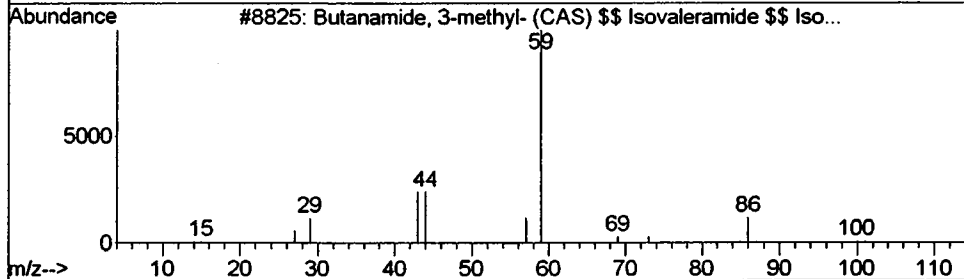
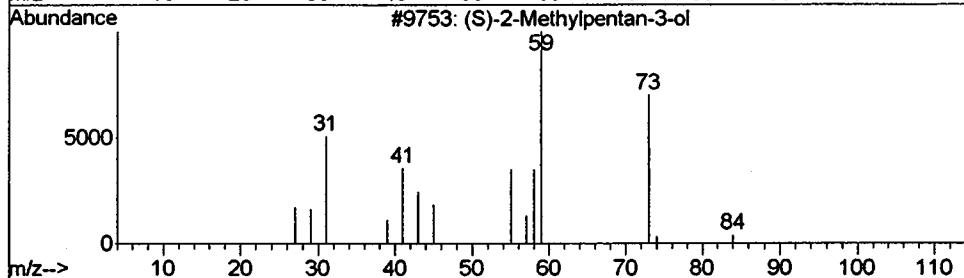
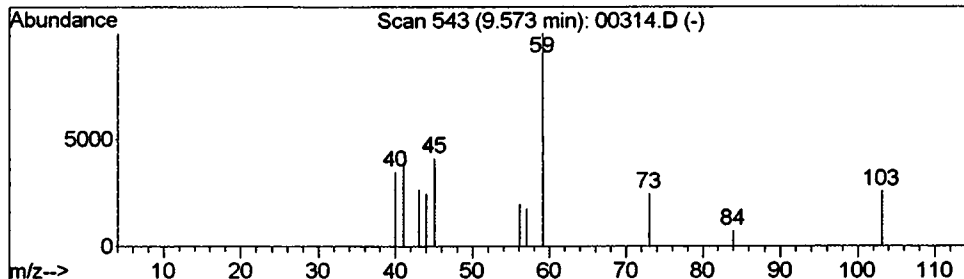
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 6 (S)-2-Methylpentan-3-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	0.11 ug/L	37950	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-2-Methylpentan-3-ol	102	C6H14O	000000-00-0	9
2			Butanamide, 3-methyl- (CAS) \$\$ I...	101	C5H11NO	000541-46-8	9
3			E-Dipropylene glycol \$\$ 2-hydrox...	134	C6H14O3	000000-00-0	9
4			PROPYLENE GLYCOL TRIMER 1	174	C9H18O3	000000-00-0	9



NO GOOD
MATCH

Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

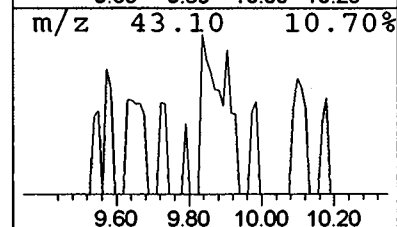
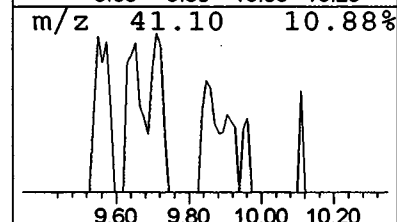
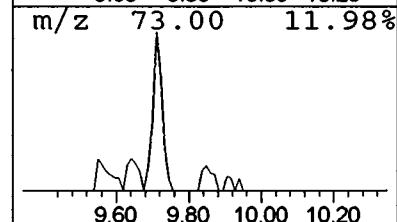
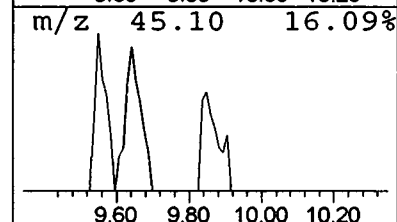
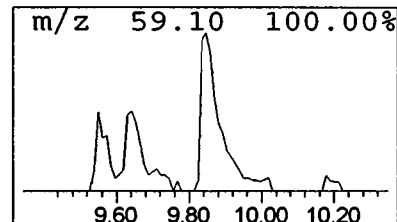
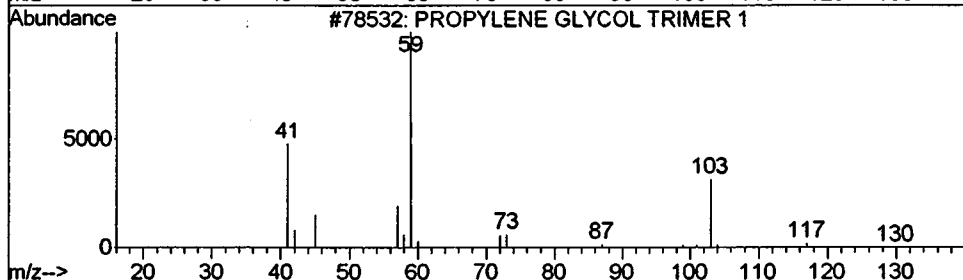
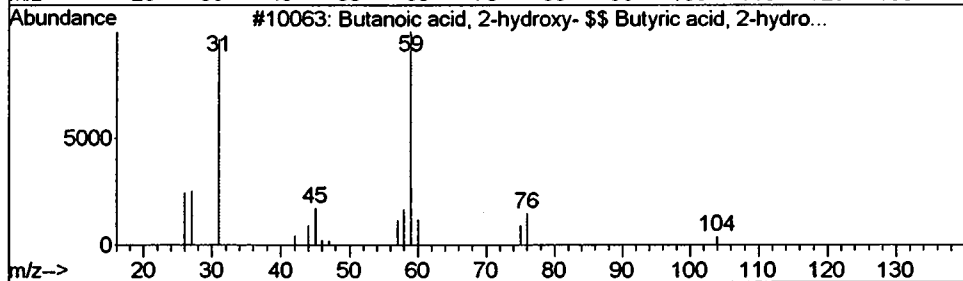
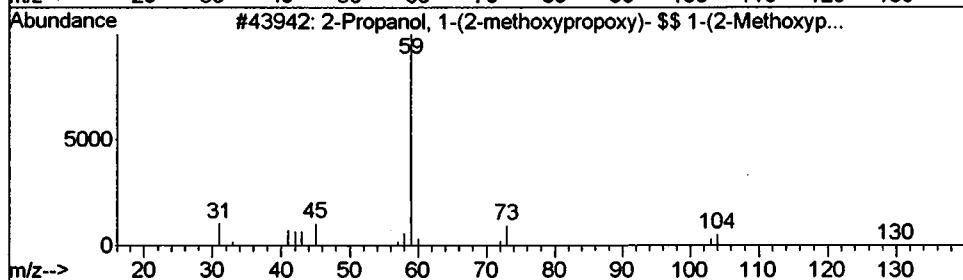
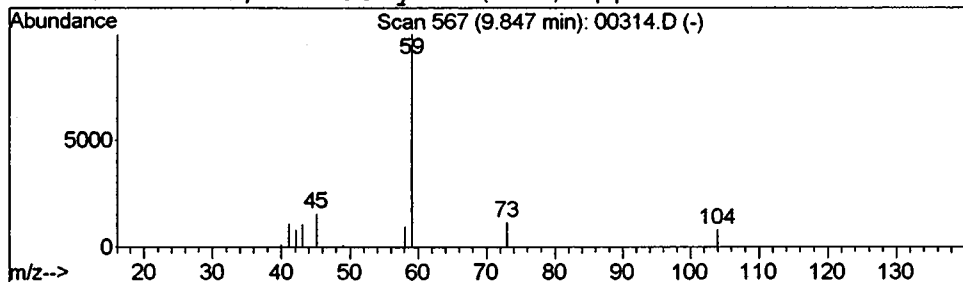
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	0.14 ug/L	50621	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	74
2			Butanoic acid, 2-hydroxy- \$\$ But...	104	C4H8O3	000565-70-8	9
3			PROPYLENE GLYCOL TRIMER 1	174	C9H18O3	000000-00-0	9
4			Formamide, N-methyl- (CAS) \$\$ N...	59	C2H5NO	000123-39-7	4



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

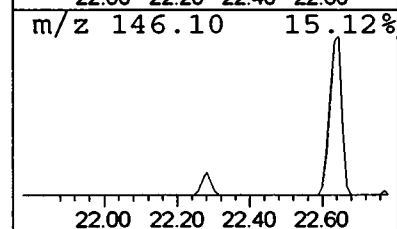
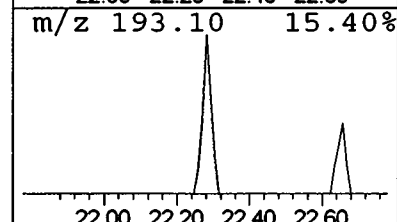
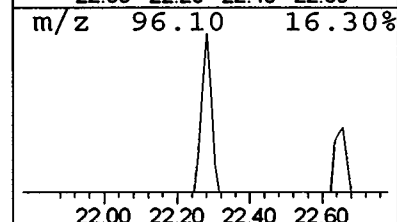
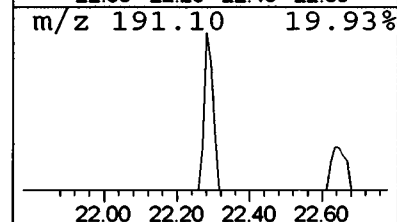
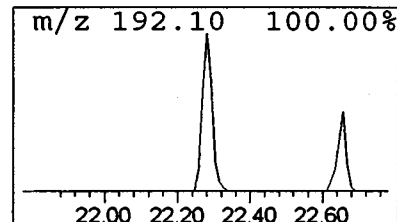
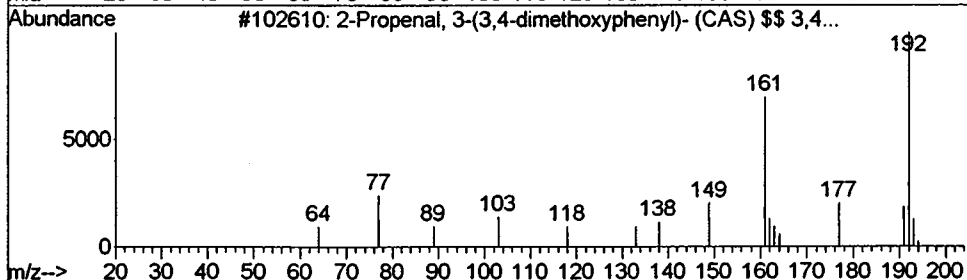
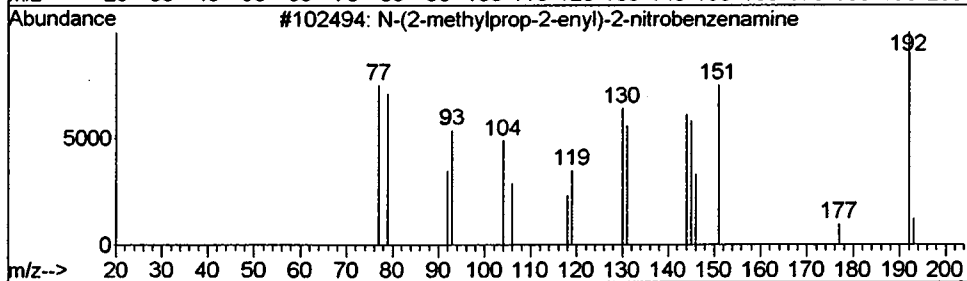
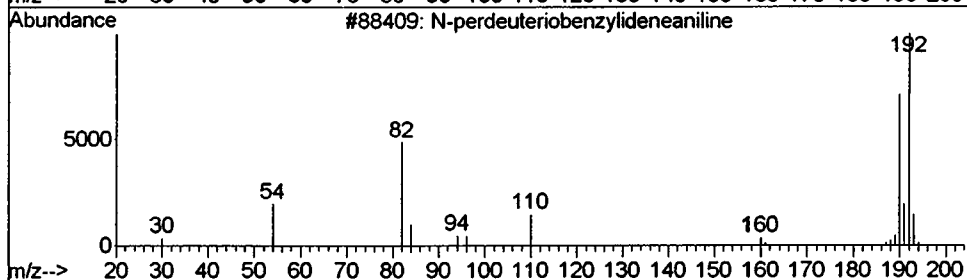
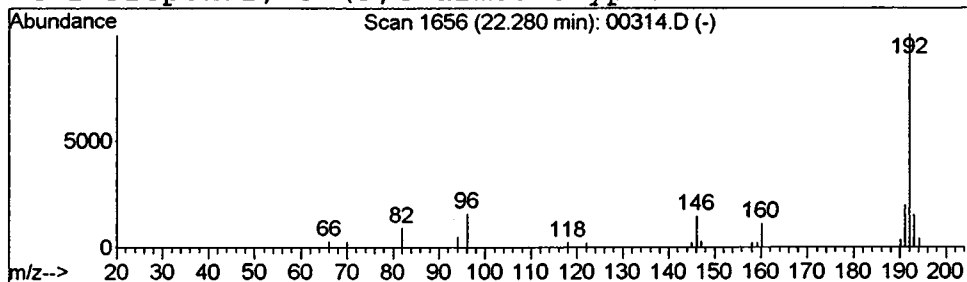
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 8 N-perdeuteriobenzylideneani... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	88378	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	64
2			N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	46
3			2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	42
4			2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	42



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN14\00314.D
Acq On : 14 Jan 2002 12:09 pm
Sample : 508 scan
Misc : January 14, 2002
MS Integration Params: LSCINT.P

Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

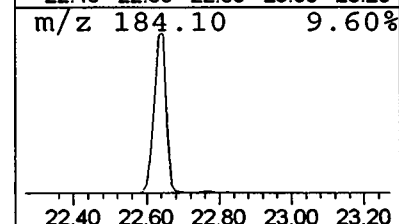
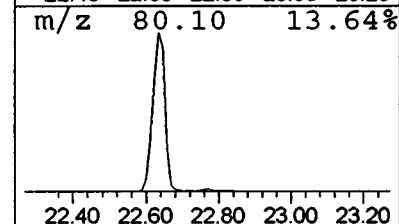
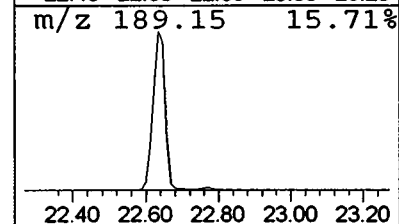
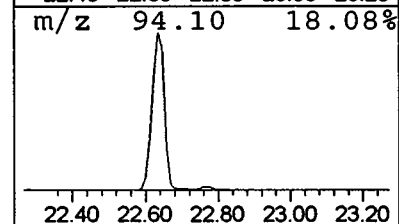
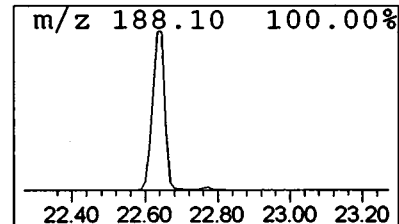
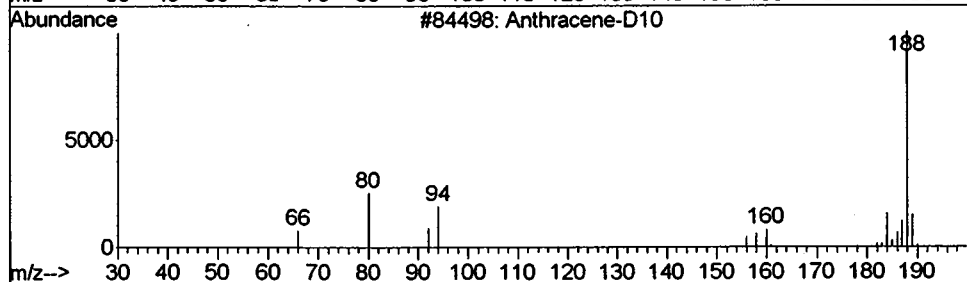
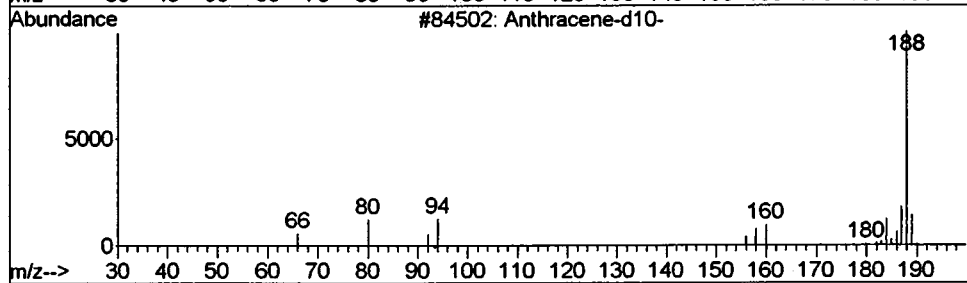
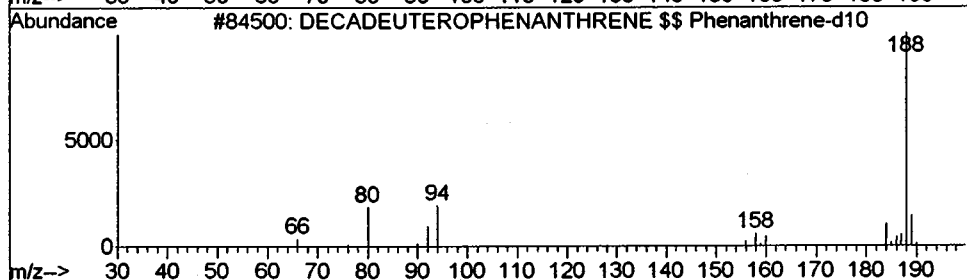
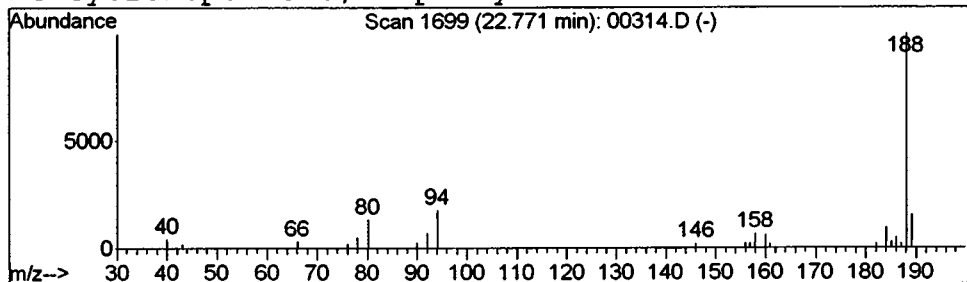
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.30 ug/L	181744	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	94
2			Anthracene-d10-	188	C14D10	001719-06-8	83
3			Anthracene-D10	188	C14D10	000000-00-0	72
4			Cycloheptanone, 4-phenyl-	188	C13H16O	067688-28-2	50



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 14 Jan 2002 12:09 pm
 Data File: C:\MSDCHEM\1\5973N\02JAN14\00314.D
 Name: 508 scan
 Misc: January 14, 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
Dichloroacetonitr...	3.49	0.1	ug/L	45959	1	9.71	7088710	20.0
Butanoic acid, 2-...	4.63	0.1	ug/L	47666	1	9.71	7088710	20.0
2-Butenal, 3-meth...	4.84	0.2	ug/L	77319	1	9.71	7088710	20.0
Butenol, methyl-	5.01	0.2	ug/L	56647	1	9.71	7088710	20.0
Acetic acid, 3-[1...	5.89	4.7	ug/L	1655650	1	9.71	7088710	20.0
(S)-2-Methylpenta...	9.57	0.1	ug/L	37950	1	9.71	7088710	20.0
2-Propanol, 1-(2-...	9.85	0.1	ug/L	50621	1	9.71	7088710	20.0
N-perdeuteriobenz...	22.28	0.1	ug/L	88378	4	22.65	12121200	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	181744	4	22.65	12121200	20.0