

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/28/2002 Time: 15:28:20

Sample: AD31638
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/28/02 15:27 Ended: 1/28/02 15:27 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		82		5.0

Comments for Sample AD31638 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-28-2002 Time: 15:28:31

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

The recoveries for 2 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Data File : C:\MSDCHEM\1\5973N\02JAN17\31638.D

Vial: 5

Acq On : 17 Jan 2002 1:32 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 17, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 08:30:08 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	1114973	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4700646	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2452402	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4060540	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3485941	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2465990	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	263058	4.10	ug/L	0.00
Spiked Amount	5.000		Recovery	=	82.00%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	394215	2.43	ug/L	# 56
21) 2,6-Dinitrotoluene	18.34	165	307838	9.74	ug/L	# 17
35) Di-n-butylphthalate	24.85	149	84516	0.32	ug/L	98

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

31638.D SCAN508.M

Tue Jan 22 08:30:09 2002

Page 1

Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31638.D

Vial: 5

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Sample : 508 scan

Inst : Instrumen

Misc : January 17, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 8:30 2002

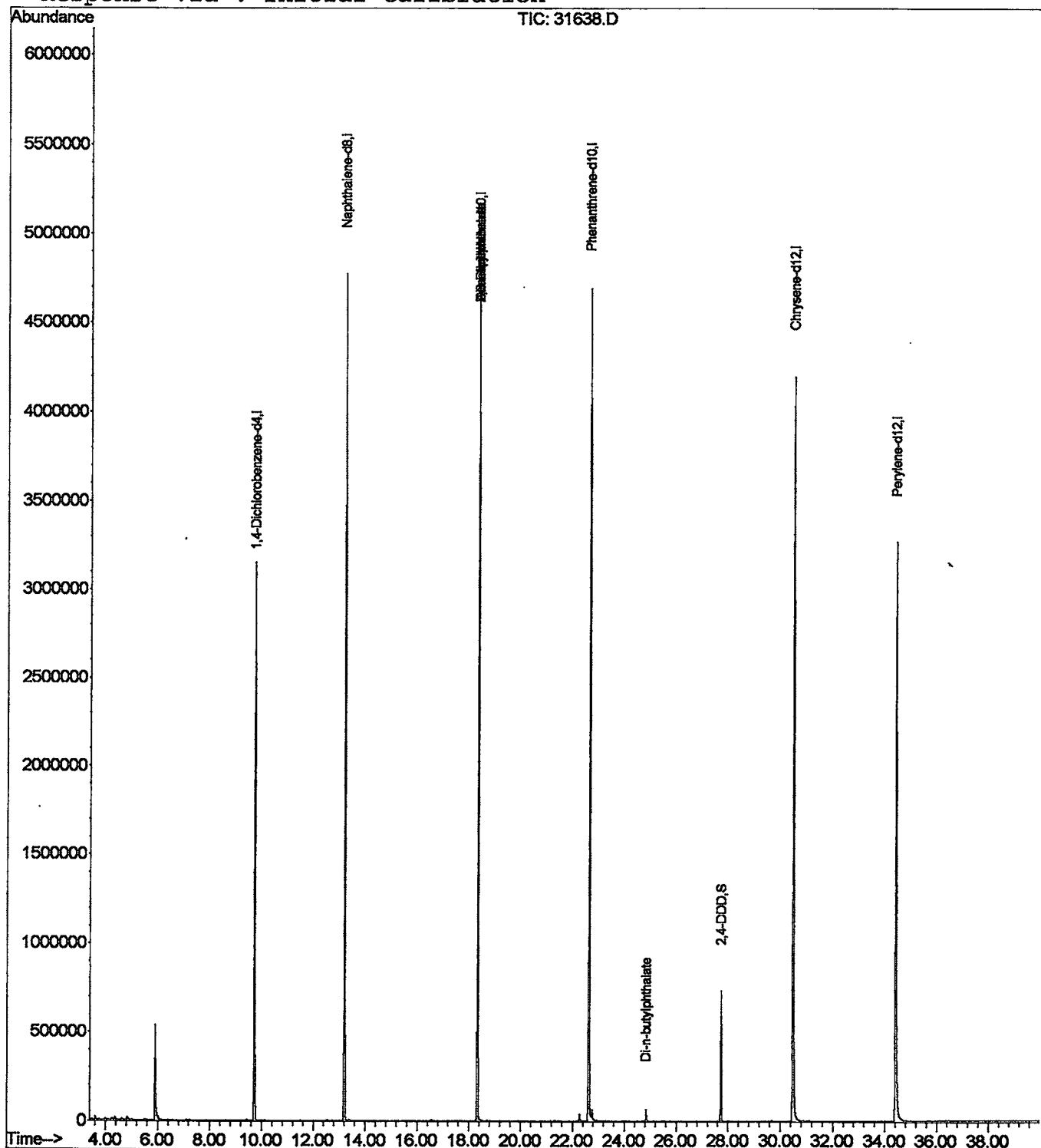
Quant Results File: SCAN508.RE

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\02JAN17\31638.D

Vial: 5

Acq On : 17 Jan 2002 1:32 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 17, 2002

Multiplr: 1.00

MS Integration Params: LSCINT.P

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

Title : 508 scan method

Smoothing : OFF

Filtering: 5

Sampling : 2

Min Area: 100 Area counts

Start Thrs: 0.2

Max Peaks: 20

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

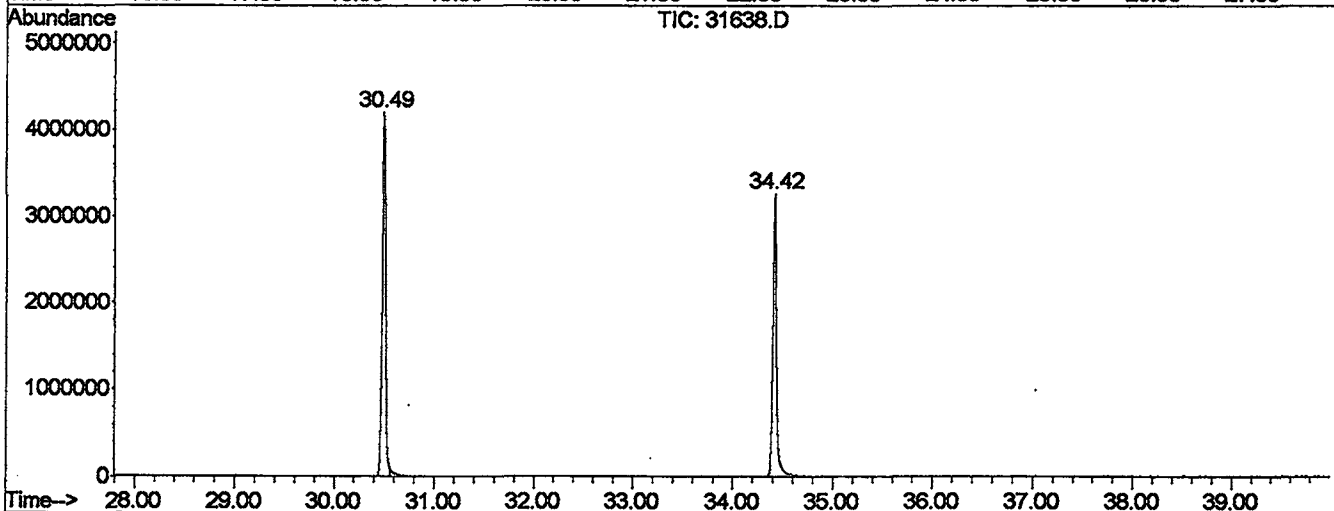
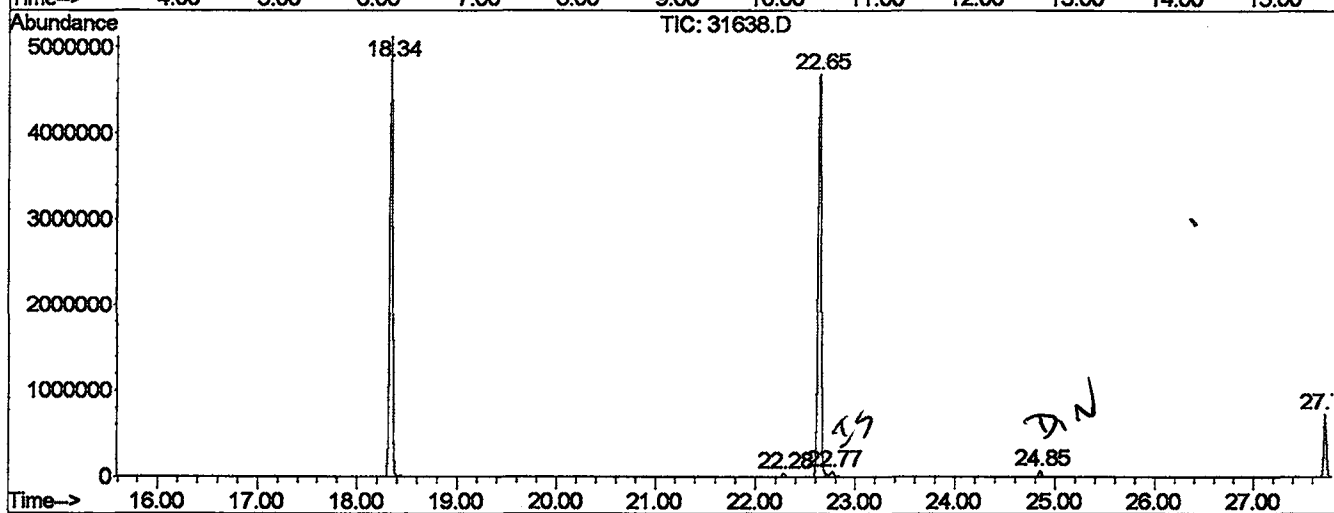
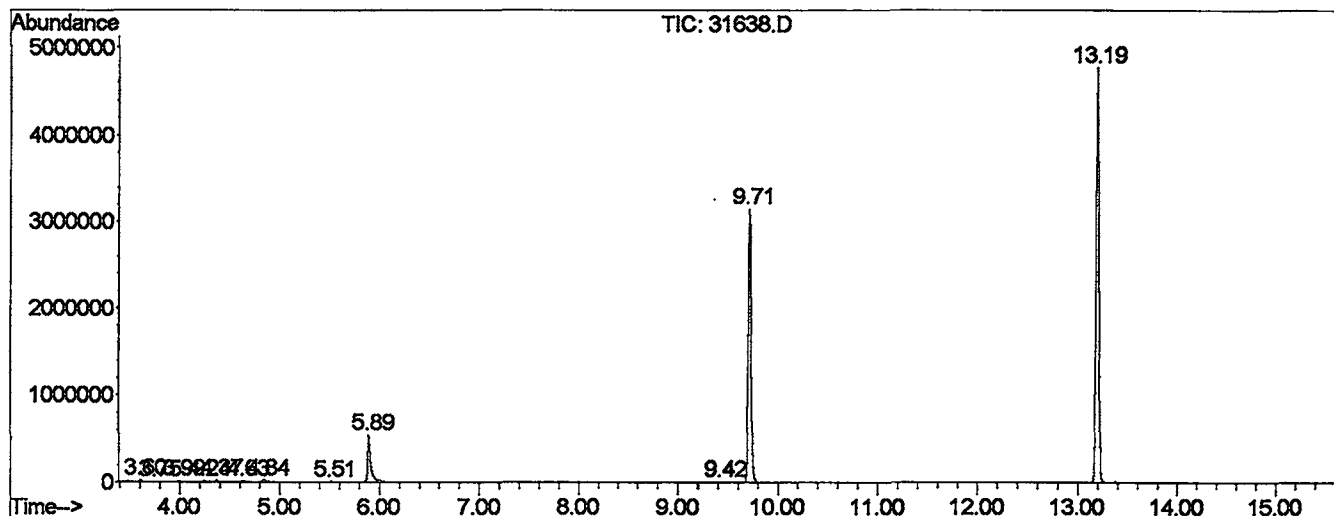
Signal : TIC

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	22912	32295	0.30%	0.056%
2	3.750	31	33	45	rVV4	4287	17603	0.16%	0.031%
3	3.990	49	54	59	rVV4	8284	18289	0.17%	0.032%
4	4.241	73	76	79	rBV2	9987	18683	0.17%	0.032%
5	4.367	83	87	91	rVB	17464	30022	0.28%	0.052%
6	4.630	107	110	117	rVB3	10393	24043	0.22%	0.042%
7	4.835	123	128	139	rBV5	19794	56273	0.52%	0.098%
8	5.509	183	187	203	rVB6	7255	35093	0.33%	0.061%
9	5.885	217	220	247	rVB	537856	1167899	10.86%	2.031%
10	9.425	527	530	537	rBV2	6155	16929	0.16%	0.029%
11	9.710	551	555	561	rBV	3147755	6319513	58.76%	10.988%
12	13.192	855	860	865	rBV	4768928	9040847	84.06%	15.720%
13	18.341	1305	1311	1315	rBV	5121843	9965298	92.65%	17.327%
14	22.280	1653	1656	1661	rVV2	40641	76442	0.71%	0.133%
15	22.645	1681	1688	1693	rVV2	4688645	10755702	100.00%	18.701%
16	22.771	1695	1699	1721	rVV	63141	210091	1.95%	0.365%
17	24.849	1877	1881	1887	rBV	71528	127765	1.19%	0.222%
18	27.726	2127	2133	2139	rBV	730357	1257471	11.69%	2.186%
19	30.489	2369	2375	2381	rBV2	4194047	10059035	93.52%	17.490%
20	34.416	2713	2719	2747	rBV	3262216	8284203	77.02%	14.404%

Sum of corrected areas: 57513496

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31638.D
 Operator :
 Acquired : 17 Jan 2002 1:32 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 17, 2002
 Vial Number: 5
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31638.D

Acq On : 17 Jan 2002 1:32 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 5

Operator:

Inst : Instrumen

Multiplr: 1.00

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

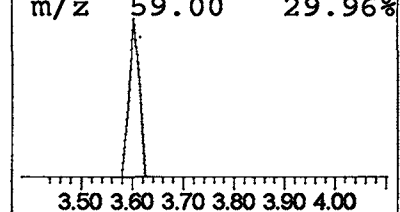
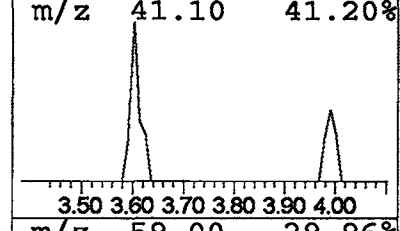
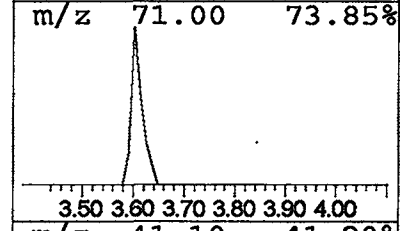
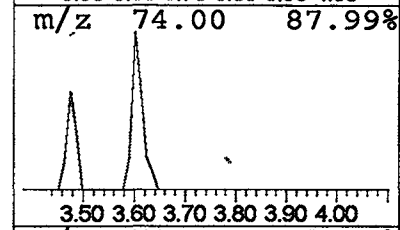
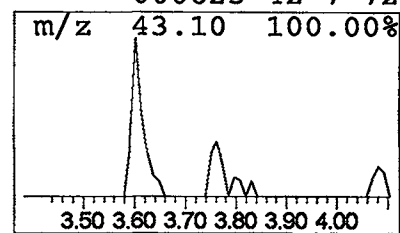
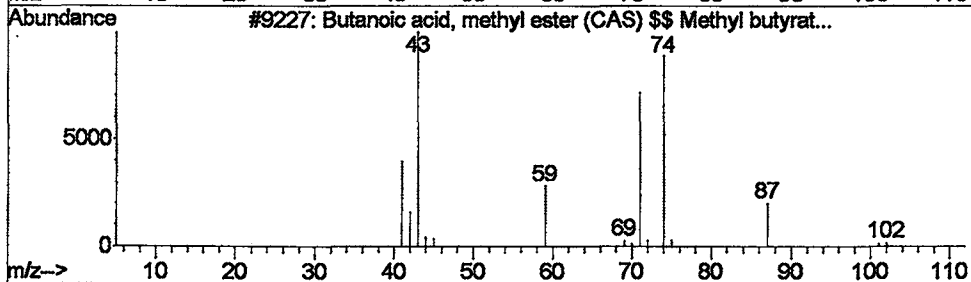
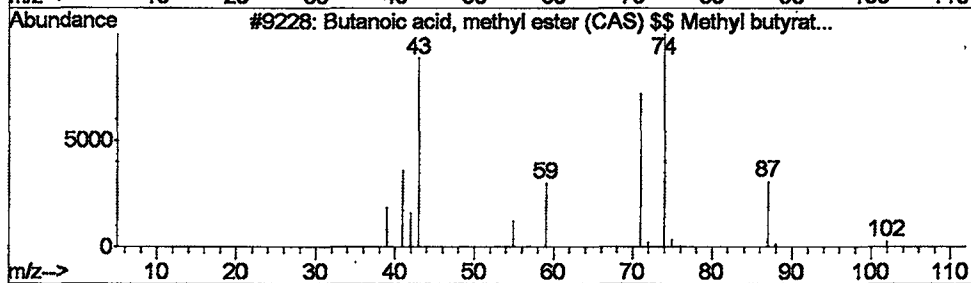
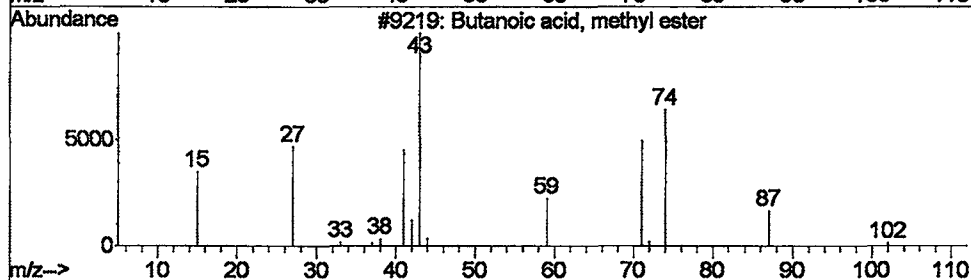
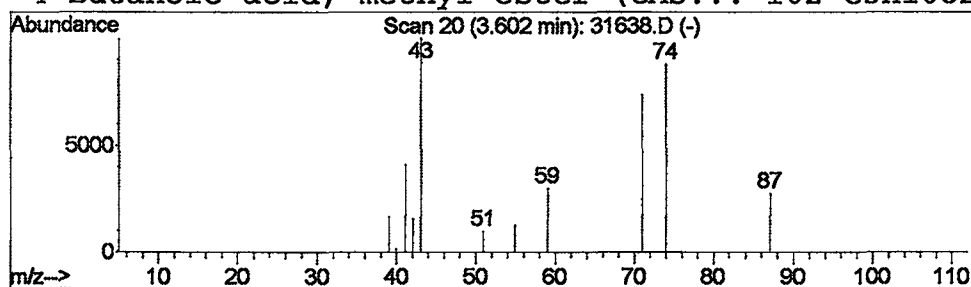
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Butanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.10 ug/L	32295	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
2			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
3			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
4			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	72



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31638.D

Acq On : 17 Jan 2002 1:32 pm

Sample : 508 scan

Misc : January 17, 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

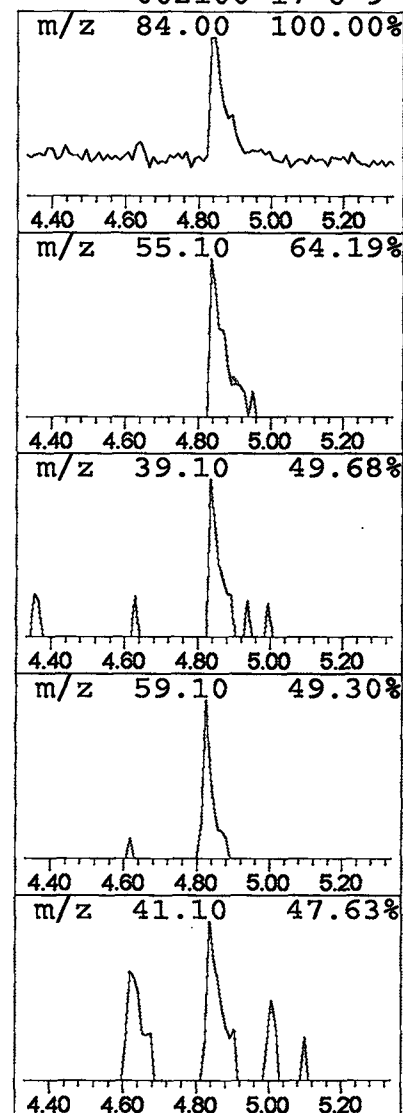
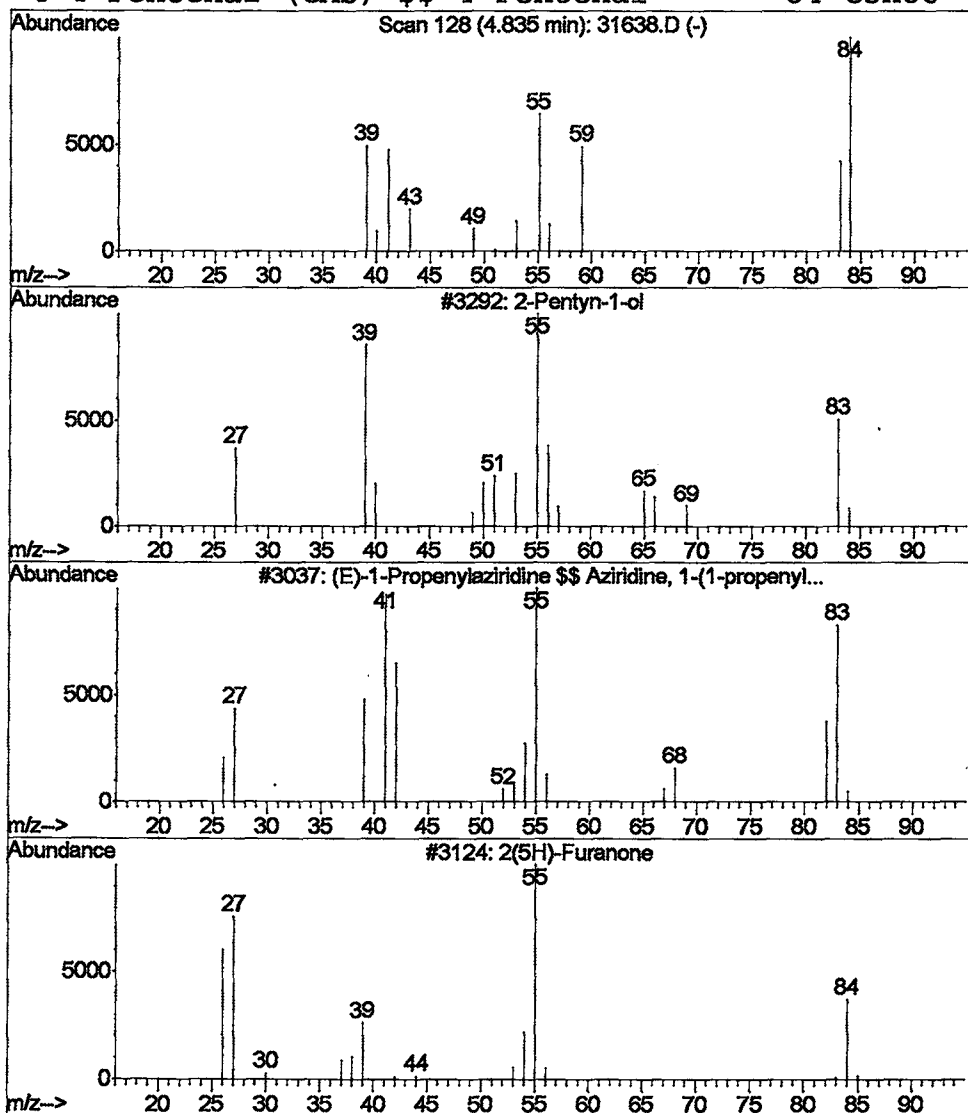
Library : C:\DATABASE\WILEY7N.L

Peak Number 2 2-Pentyn-1-ol

Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.18 ug/L	56273	1,4-Dichlorobenzene-d4	9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentyn-1-ol	84	C5H8O	006261-22-9	17
2			(E)-1-Propenylaziridine \$\$ Aziri...	83	C5H9N	080839-91-4	9
3			2(5H)-Furanone	84	C4H4O2	000497-23-4	9
4			4-Pentenal (CAS) \$\$ 4-Pentenal-	84	C5H8O	002100-17-6	9



Library Search Compound Report

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 Acq On : 17 Jan 2002 1:32 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: LSCINT.P

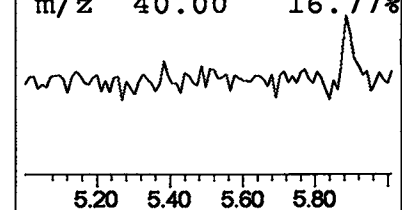
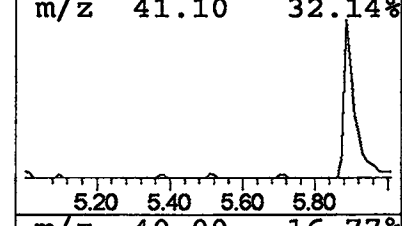
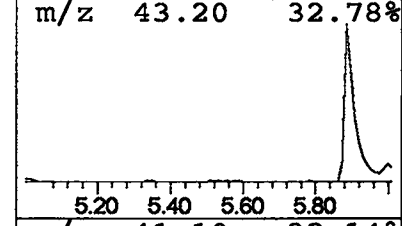
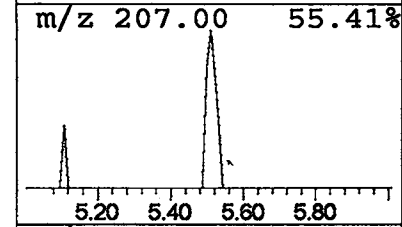
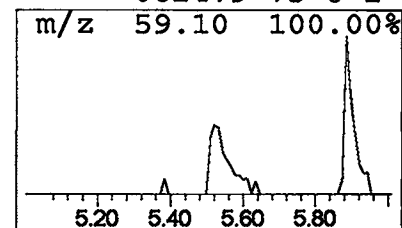
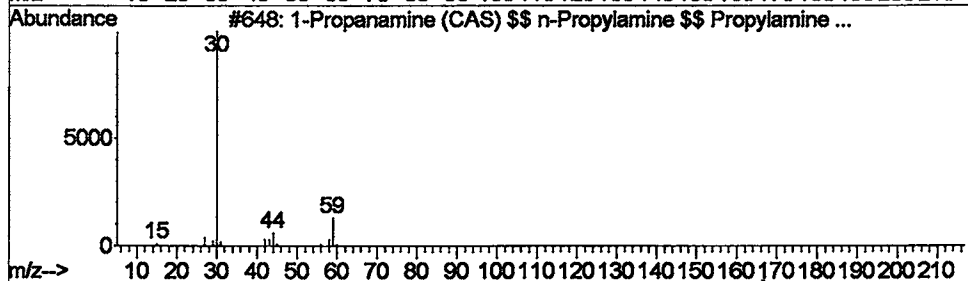
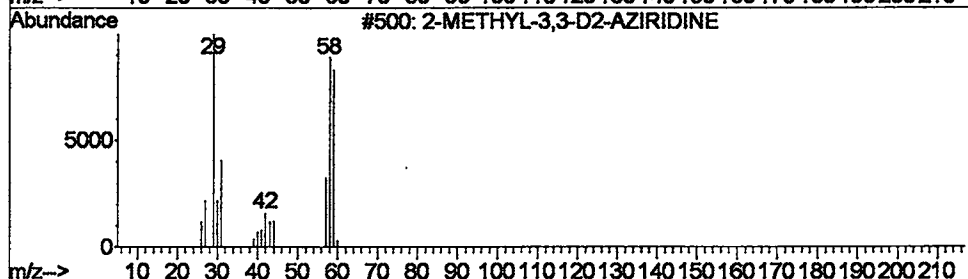
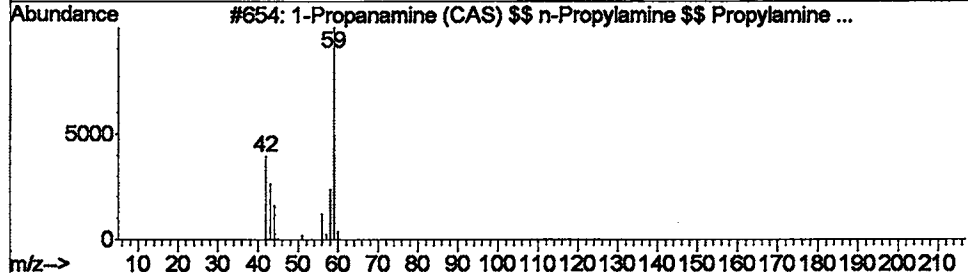
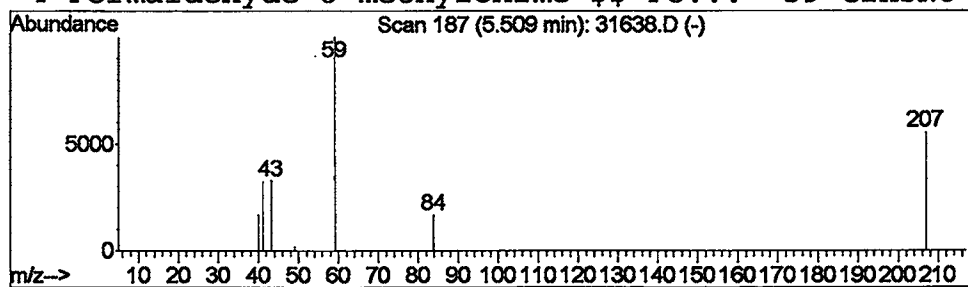
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 1-Propanamine (CAS) \$\$ n-Pr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	0.11 ug/L	35093	1,4-Dichlorobenzene-d4	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanamine (CAS) \$\$ n-Propyla...	59	C3H9N	000107-10-8	4
2		2-METHYL-3,3-D2-AZIRIDINE	59	C3H5D2N	030691-55-5	3
3		1-Propanamine (CAS) \$\$ n-Propyla...	59	C3H9N	000107-10-8	3
4		Formaldehyde O-methyloxime \$\$ Fo...	59	C2H5NO	062479-73-6	2



Library Search Compound Report

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Sample : 508 scan
Misc : January 17, 2002
MS Integration Params: LSCINT.P

Vial: 5
Operator:
Inst : Instrumen
Multiplr: 1.00

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

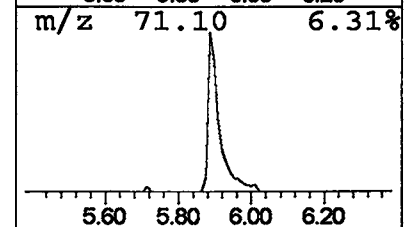
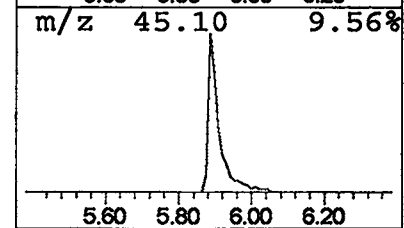
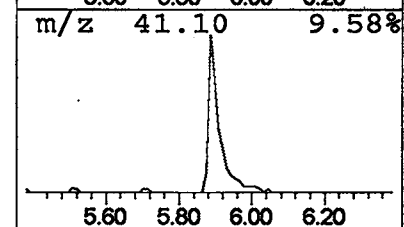
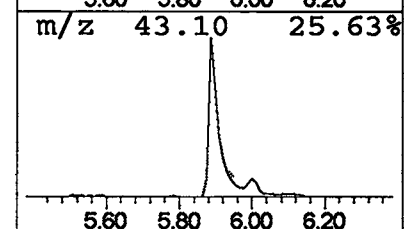
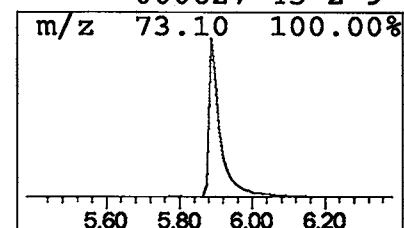
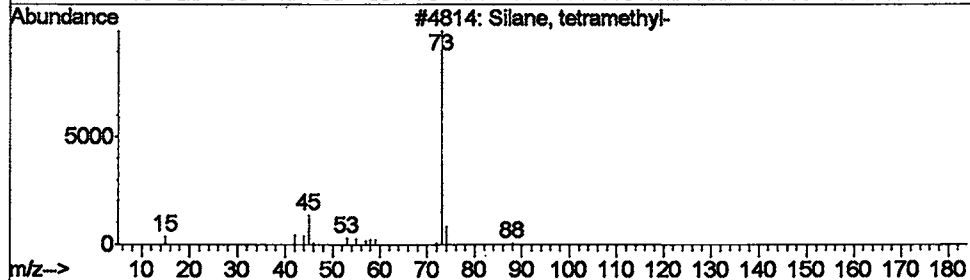
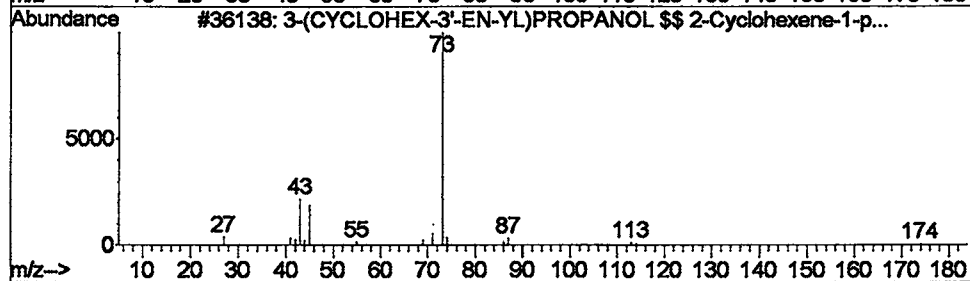
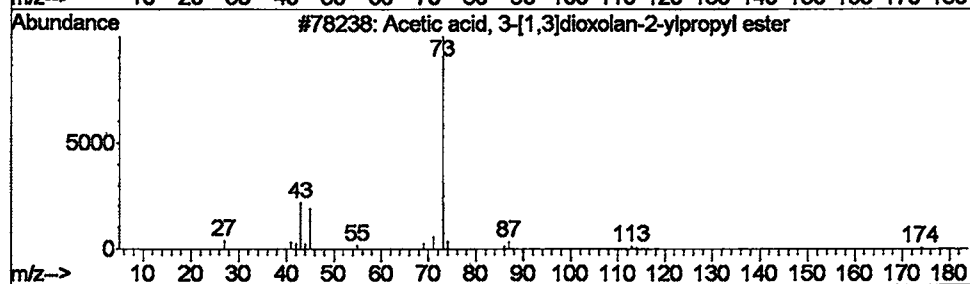
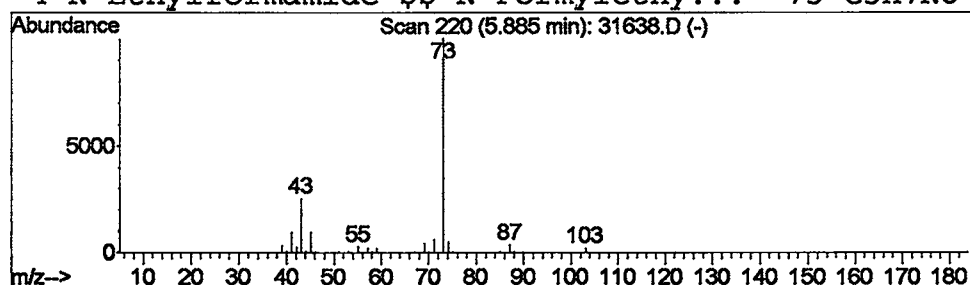
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 4 Acetic acid, 3-[1,3]dioxola... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	3.70 ug/L	1167900	1,4-Dichlorobenzene-d4	9.72

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	9
4			N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9



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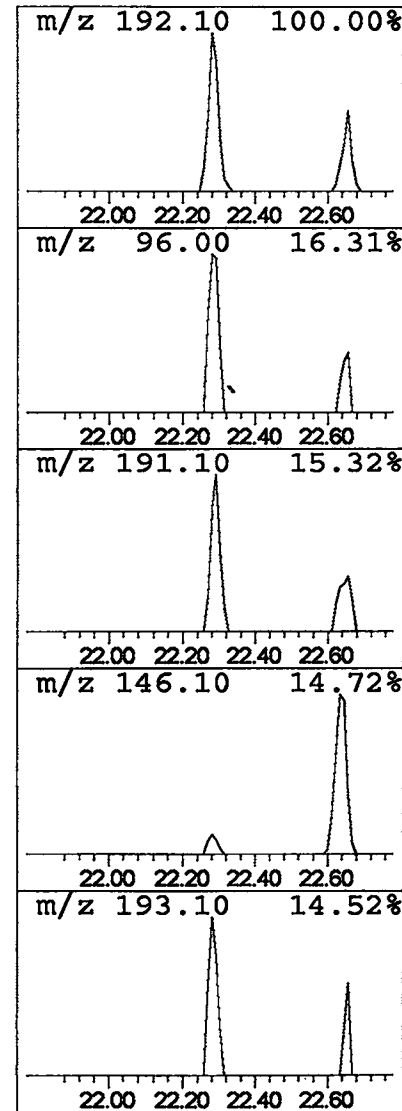
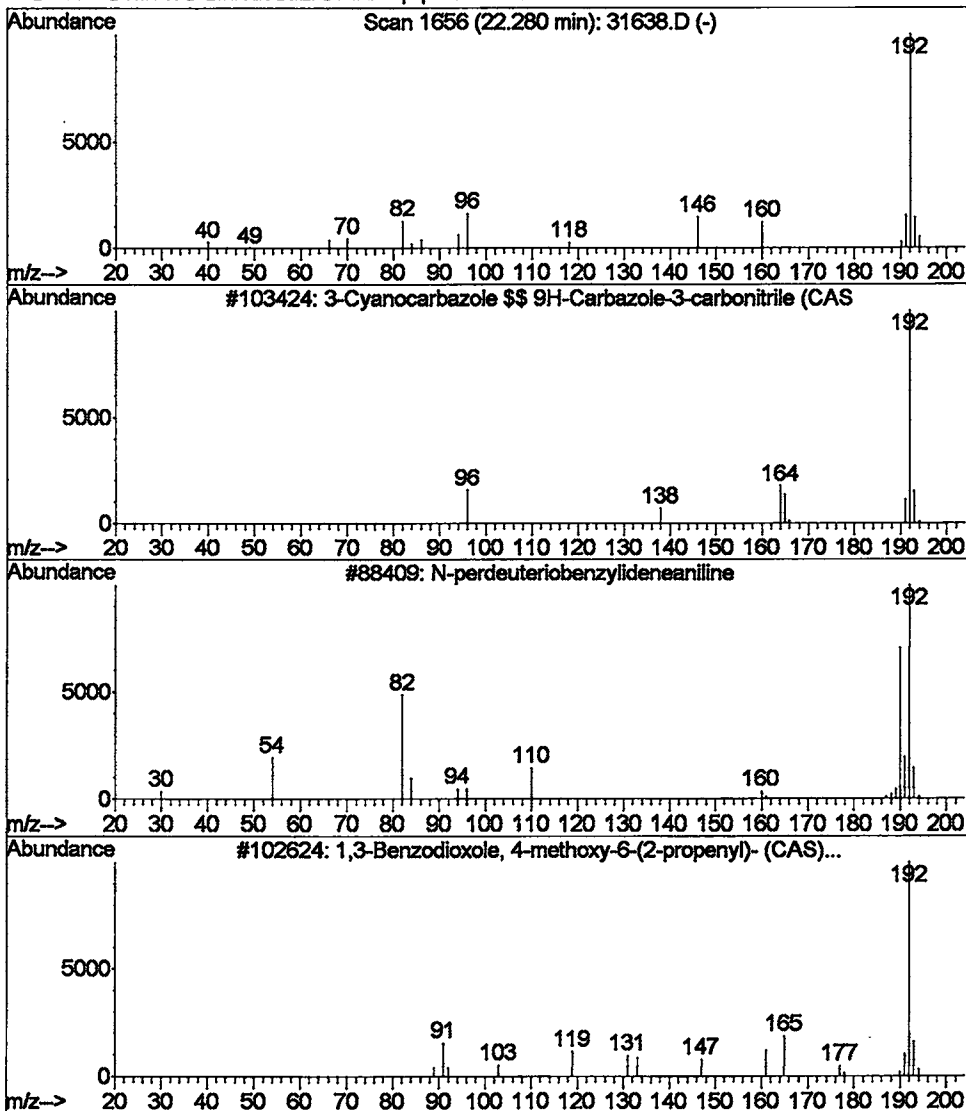
Vial: 5
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 5 3-Cyanocarbazole \$\$ 9H-Carb... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.14 ug/L	76442	Phenanthrene-d10	22.63

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	59
3		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	52
4		2-CYANOCARBAZOLE \$\$ 9H-Carbazole...	192	C13H8N2	057955-18-7	50



Library Search Compound Report

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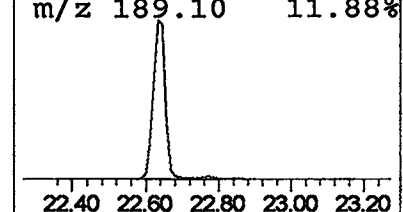
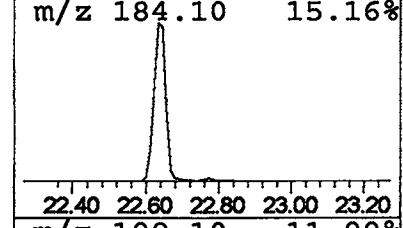
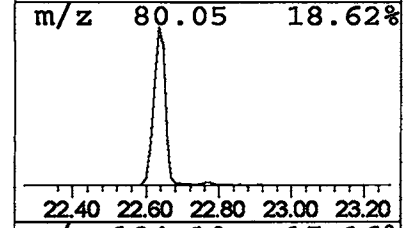
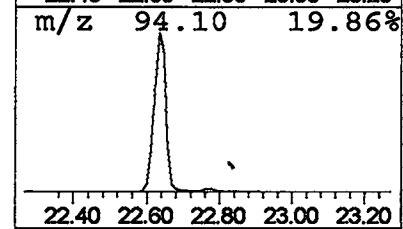
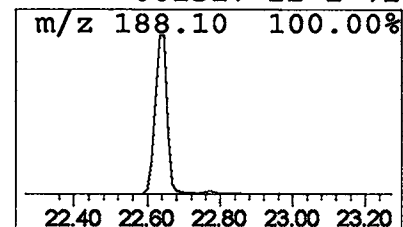
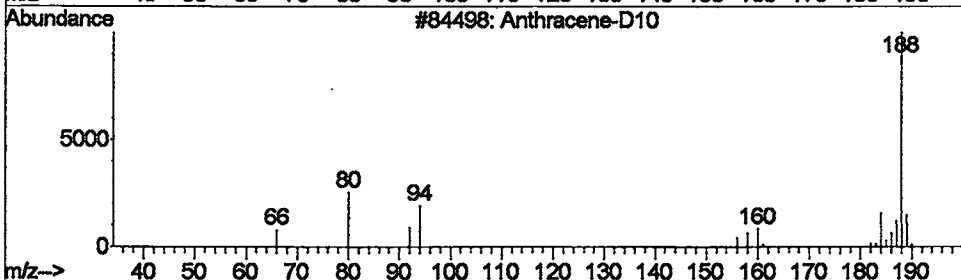
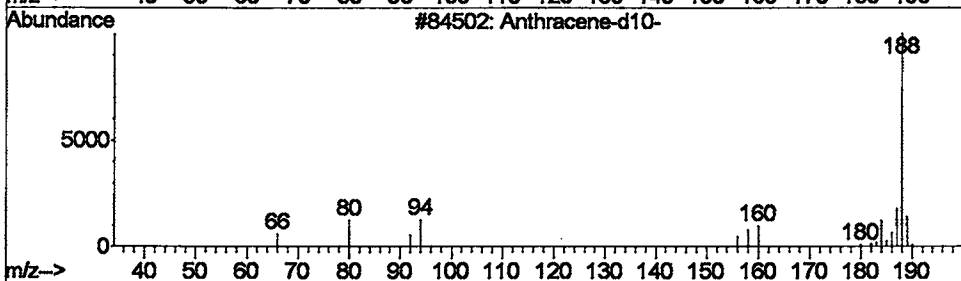
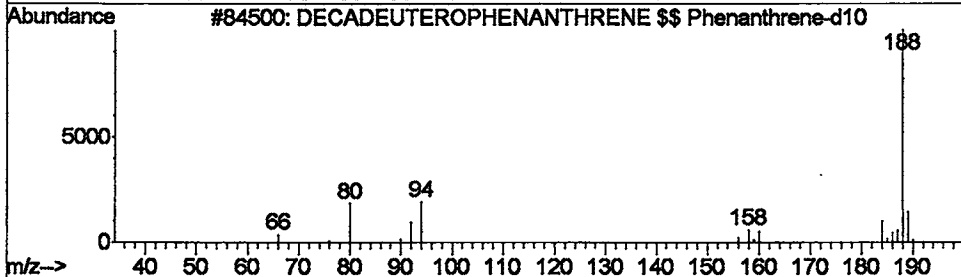
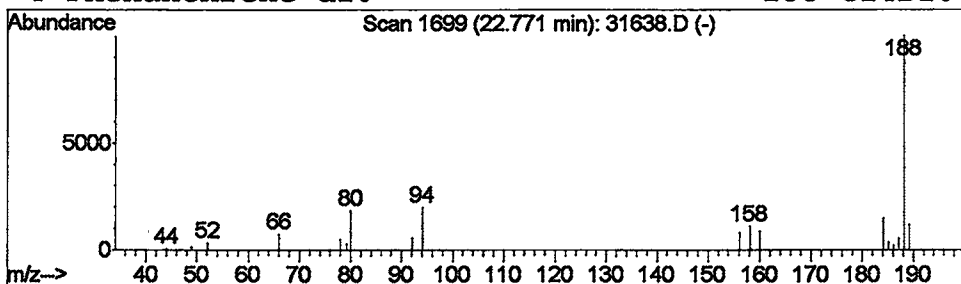
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Multiplr: 1.00

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

Peak Number 6 DECADEUTEROPHENANTHRENE \$\$... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.39 ug/L	210091	Phenanthrene-d10	22.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	86
2			Anthracene-d10-	188	C14D10	001719-06-8	83
3			Anthracene-D10	188	C14D10	000000-00-0	80
4			Phenanthrene-d10	188	C14D10	001517-22-2	72



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 17 Jan 2002 1:32 pm
Data File: C:\MSDCHEM\1\5973N\02JAN17\31638.D
Name: 508 scan
Misc: January 17, 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, me...	3.60	0.1	ug/L	32295	1	9.72	6319510	20.0
2-Pentyn-1-ol	4.84	0.2	ug/L	56273	1	9.72	6319510	20.0
1-Propanamine (CA...	5.51	0.1	ug/L	35093	1	9.72	6319510	20.0
Acetic acid, 3-[1...	5.89	3.7	ug/L	1167900	1	9.72	6319510	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	76442	4	22.63	10755700	20.0
DECADEUTEROPHENAN...	22.77	0.4	ug/L	210091	4	22.63	10755700	20.0