

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/28/2002 Time: 15:34:48

Sample: AD31672

Analysis: \$GCMS GCMS Scan For Unknowns

Units: ug

Started: 1/28/02 15:34 Ended: 1/28/02 15:34 Analyst: DLV

Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		83		5.0

Comments for Sample AD31672 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-28-2002 Time: 15:34:51

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\31672.D

Vial: 7

Acq On : 17 Jan 2002 7:49 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 17, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 08:30:18 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	1187715	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4997587	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2596215	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4370403	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3847777	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2809225	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	285611	4.13	ug/L	0.00
Spiked Amount	5.000		Recovery	=	82.60%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	412364	2.41	ug/L	# 56
21) 2,6-Dinitrotoluene	18.34	165	329660	9.86	ug/L	# 17
35) Di-n-butylphthalate	24.85	149	99450	0.35	ug/L	99
42) Bis(2-ethylhexyl)phthalate	31.11	149	6493	0.58	ug/L	91

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

31672.D SCAN508.M

Tue Jan 22 08:30:19 2002

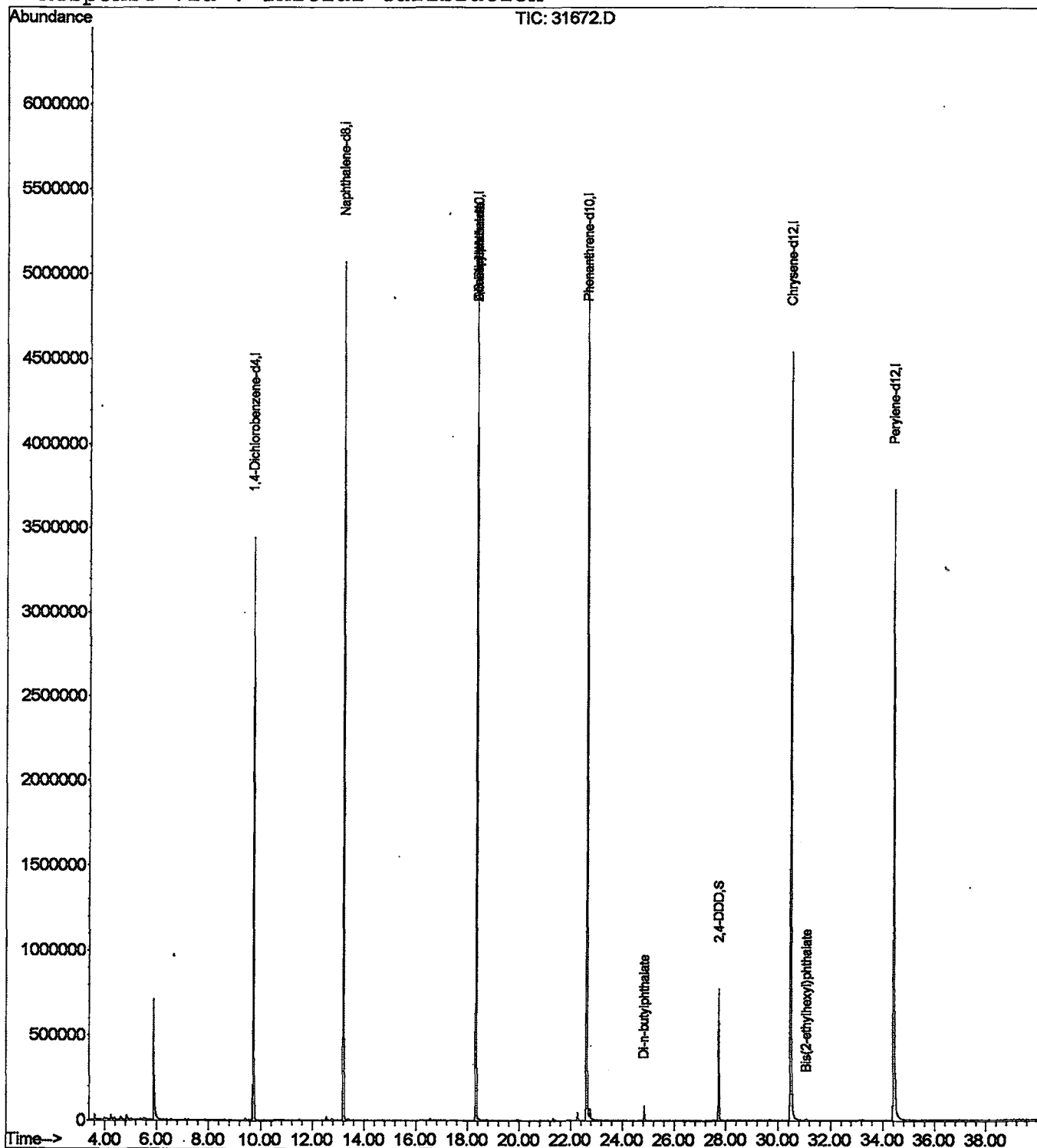
Page 1

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D
 Acq On : 17 Jan 2002 7:49 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 22 8:30 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



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D

Vial: 7

Acq On : 17 Jan 2002 7:49 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

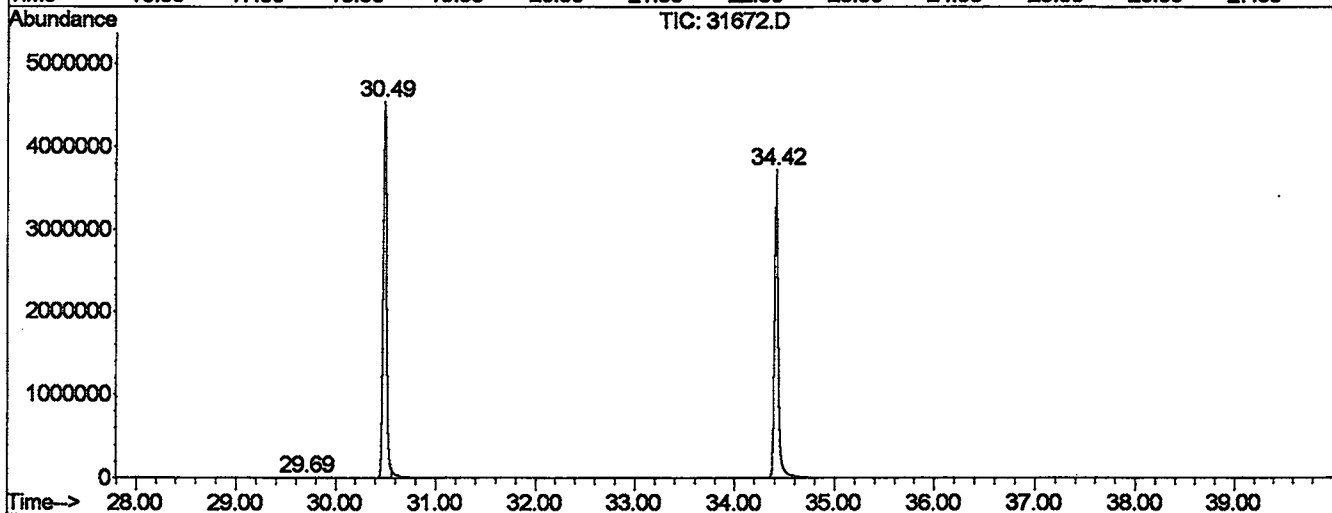
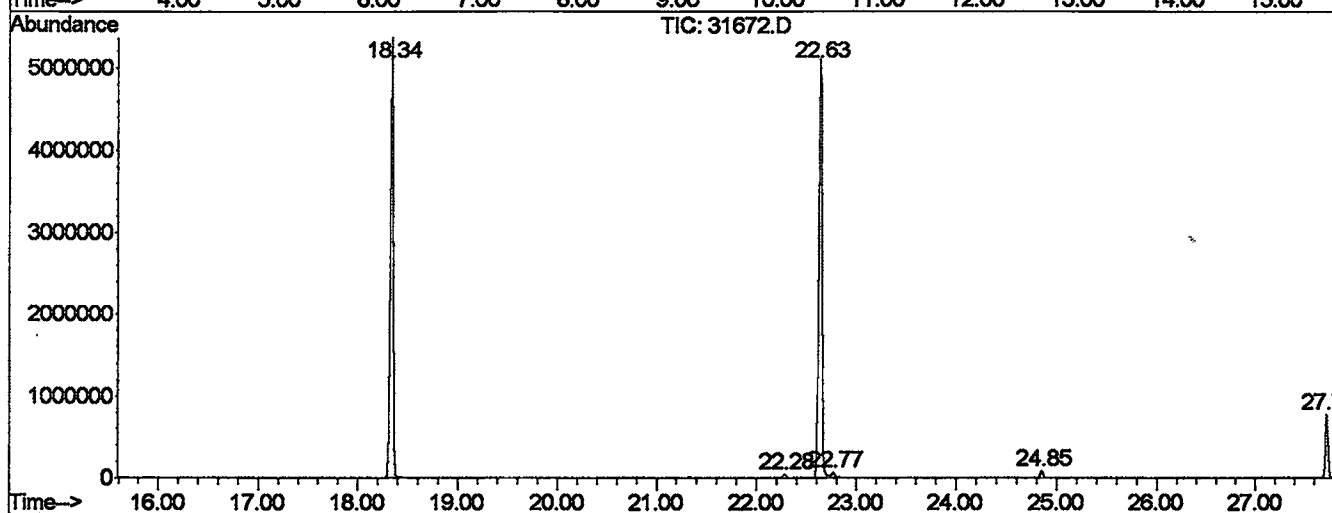
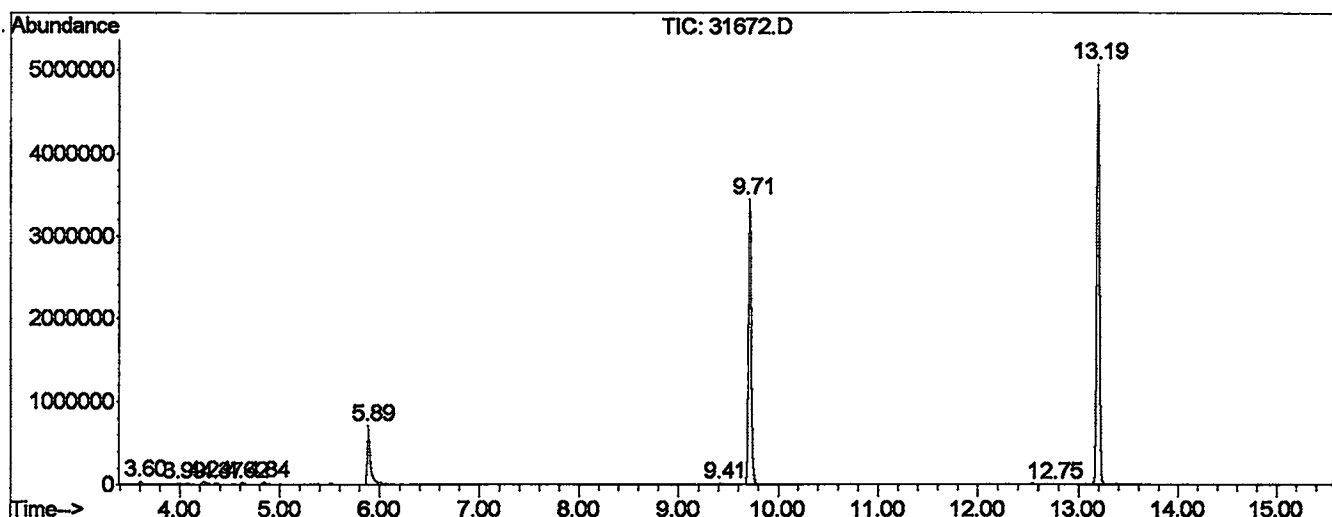
Signal : TIC

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	rBV	34380	52169	0.45%	0.083%
2	3.990	51	54	59	rVV	11845	25109	0.22%	0.040%
3	4.241	71	76	83	rBV4	30044	70054	0.61%	0.112%
4	4.367	83	87	91	rBV2	13361	26009	0.23%	0.042%
5	4.618	107	109	117	rVB	18060	39139	0.34%	0.062%
6	4.835	125	128	139	rBV3	27967	71081	0.62%	0.113%
7	5.885	217	220	247	rVB	707629	1492977	12.98%	2.383%
8	9.413	525	529	535	rBV3	11313	30731	0.27%	0.049%
9	9.710	551	555	561	rBV	3438188	6691739	58.18%	10.683%
10	12.747	815	821	831	rBV3	8505	33724	0.29%	0.054%
11	13.192	855	860	865	rBV	5065660	9581385	83.30%	15.296%
12	18.341	1305	1311	1315	rBV	5367348	10515269	91.42%	16.787%
13	22.280	1653	1656	1661	rVB	47876	86693	0.75%	0.138%
14	22.634	1681	1687	1693	rBV2	5106354	11502493	100.00%	18.363%
15	22.771	1695	1699	1711	rVB	66097	188124	1.64%	0.300%
16	24.849	1877	1881	1887	rBV	87749	163975	1.43%	0.262%
17	27.726	2129	2133	2139	rVV	773062	1363624	11.86%	2.177%
18	29.690	2299	2305	2313	rVB5	6752	27713	0.24%	0.044%
19	30.489	2369	2375	2381	rBV2	4537835	11133118	96.79%	17.773%
20	34.416	2713	2719	2747	rBV	3722687	9545205	82.98%	15.238%

Sum of corrected areas: 62640331

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31672.D
 Operator :
 Acquired : 17 Jan 2002 7:49 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 17, 2002
 Vial Number: 7
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D

Acq On : 17 Jan 2002 7:49 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 7

Operator:

Inst : Instrumen

Multiplr: 1.00

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

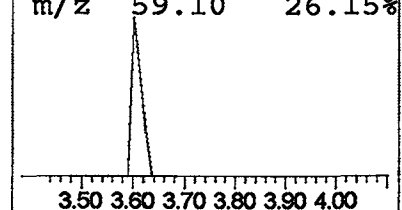
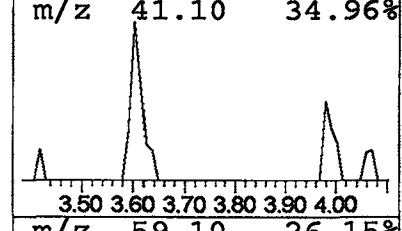
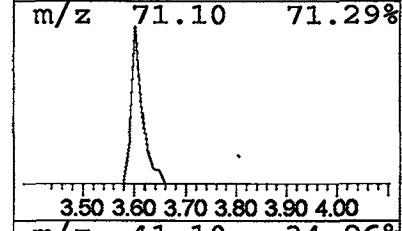
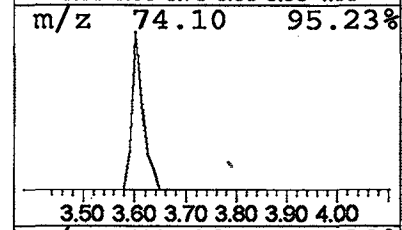
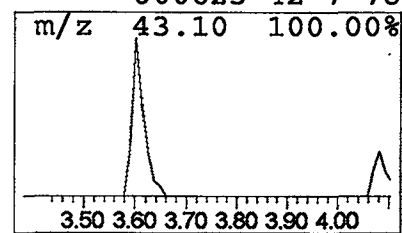
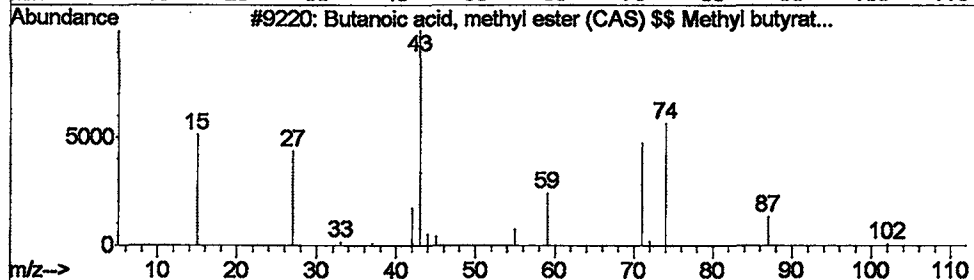
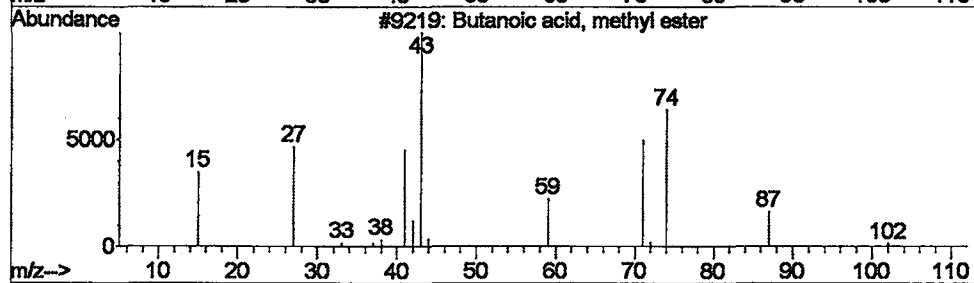
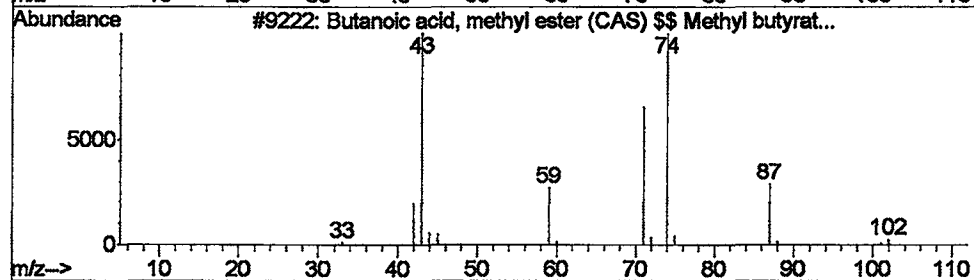
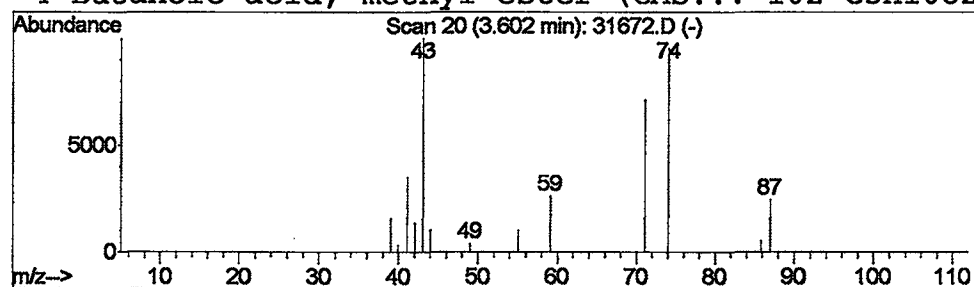
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.16 ug/L	52169	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78
3			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
4			Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D
 Acq On : 17 Jan 2002 7:49 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: LSCINT.P

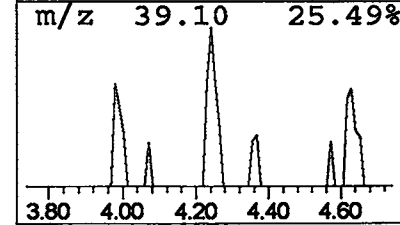
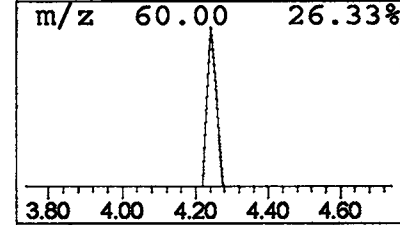
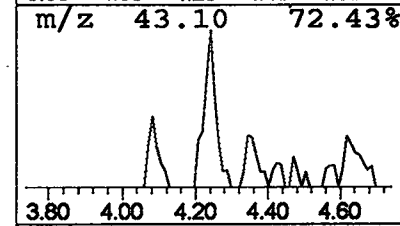
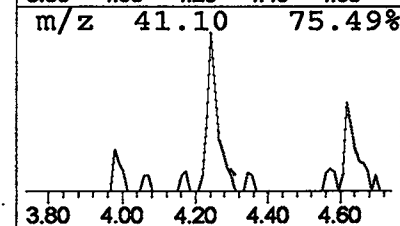
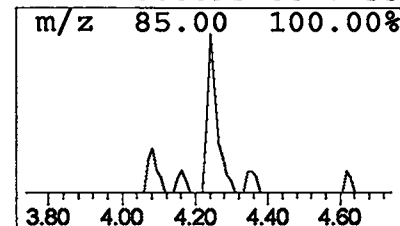
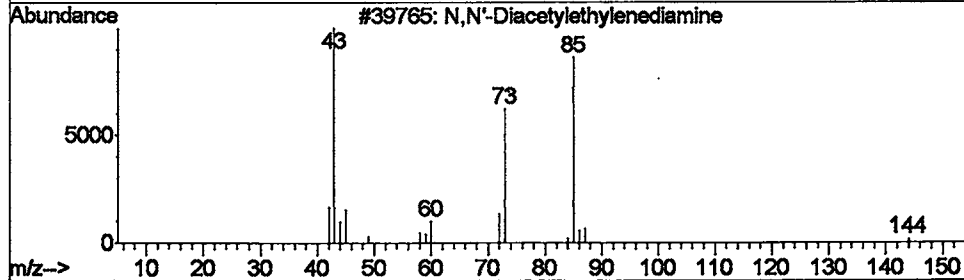
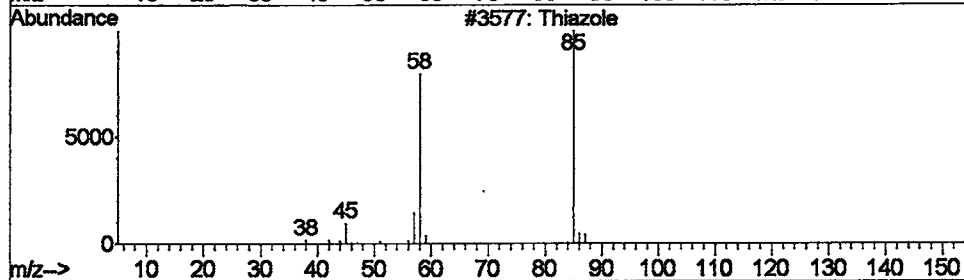
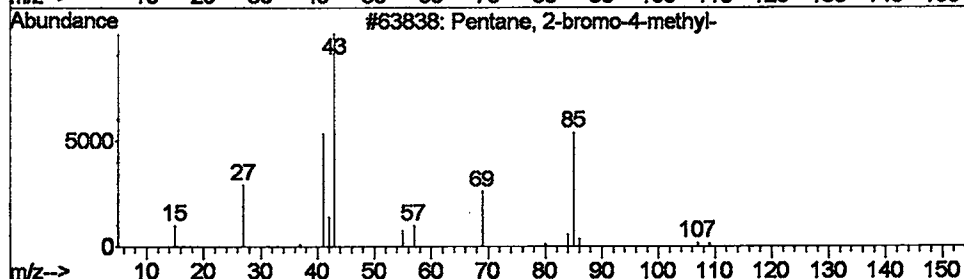
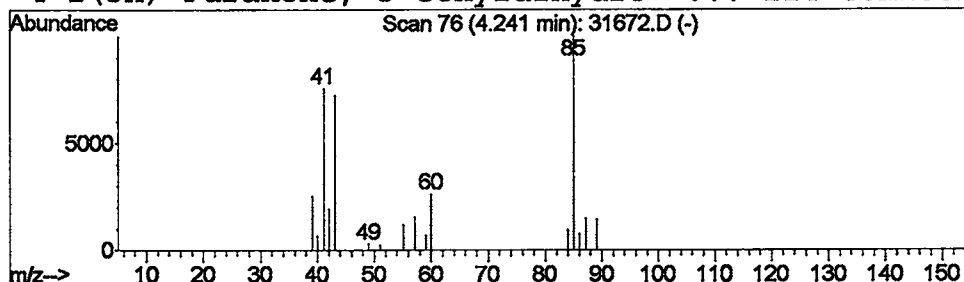
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 2 Pentane, 2-bromo-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.21 ug/L	70054	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-bromo-4-methyl-	164	C6H13Br	030310-22-6	42
2			Thiazole	85	C3H3NS	000288-47-1	38
3			N,N'-Diacetylenediamine	144	C6H12N2O2	000871-78-3	38
4			2(3H)-Furanone, 5-ethylidihydro- ...	114	C6H10O2	000695-06-7	33



Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D

Acq On : 17 Jan 2002 7:49 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 7

Operator:

Inst : Instrumen

Multiplr: 1.00

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

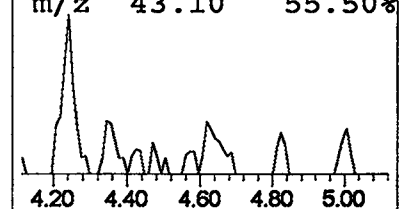
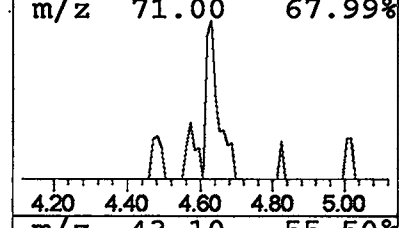
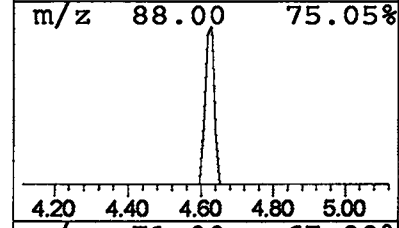
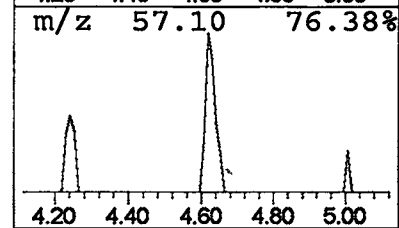
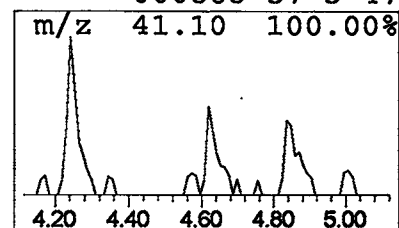
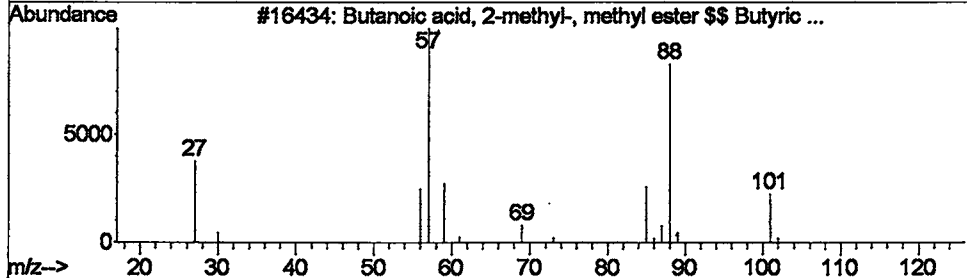
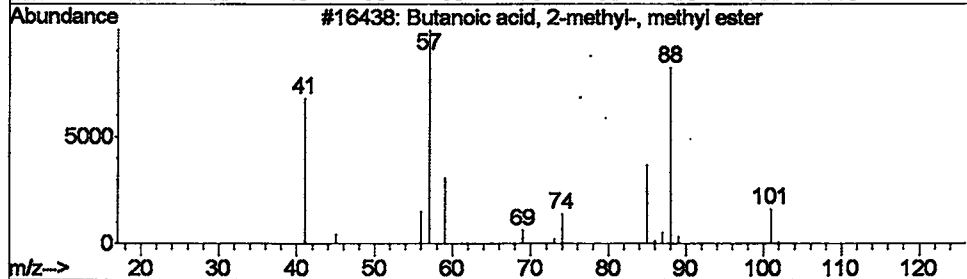
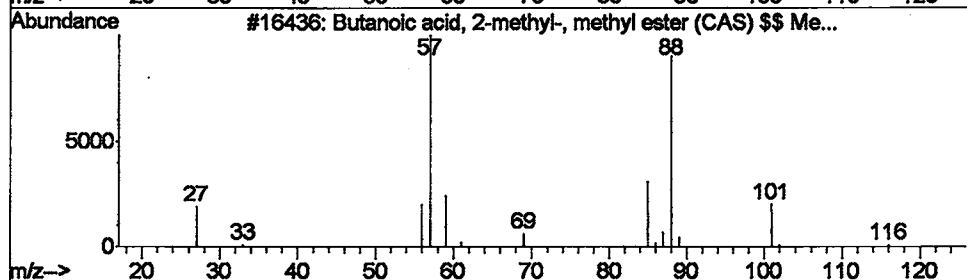
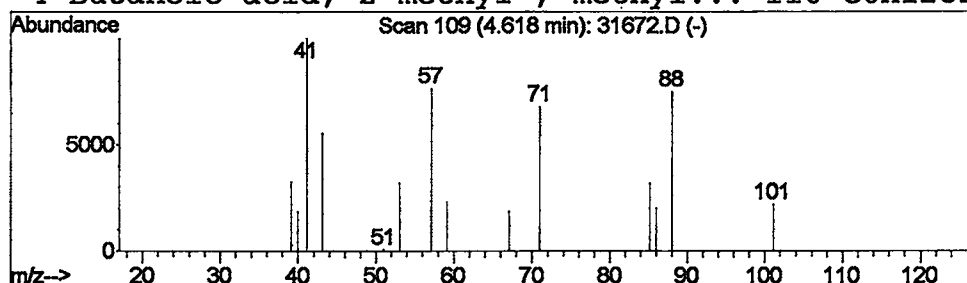
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 3 Butanoic acid, 2-methyl-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	0.12 ug/L	39139	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	50
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47



LIBRARY SEARCH COMPOUND REPORT

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D

Acq On : 17 Jan 2002 7:49 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 7

Operator:

Inst : Instrumen

Multiplr: 1.00

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

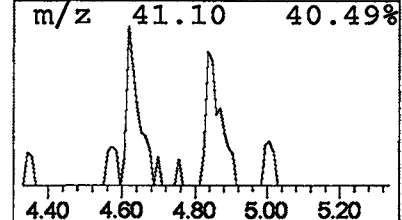
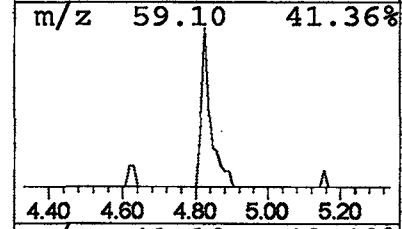
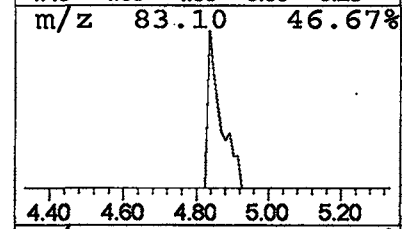
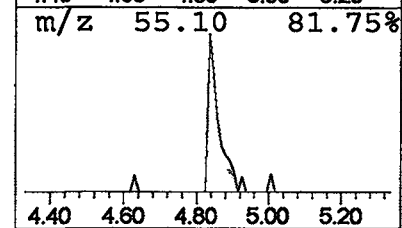
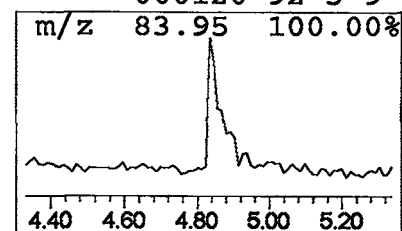
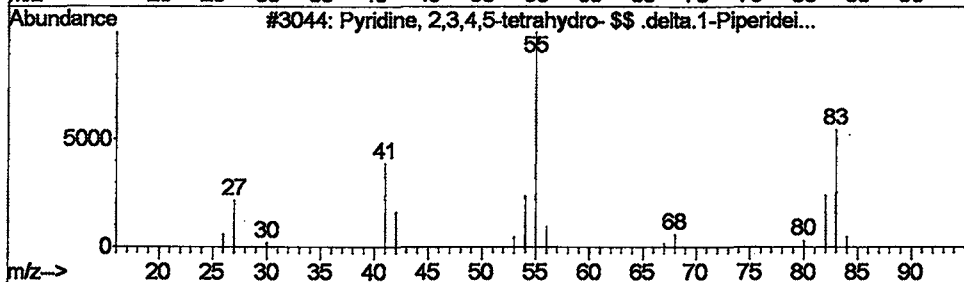
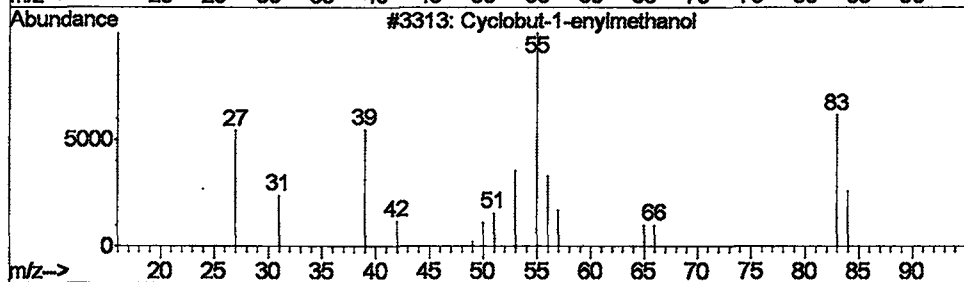
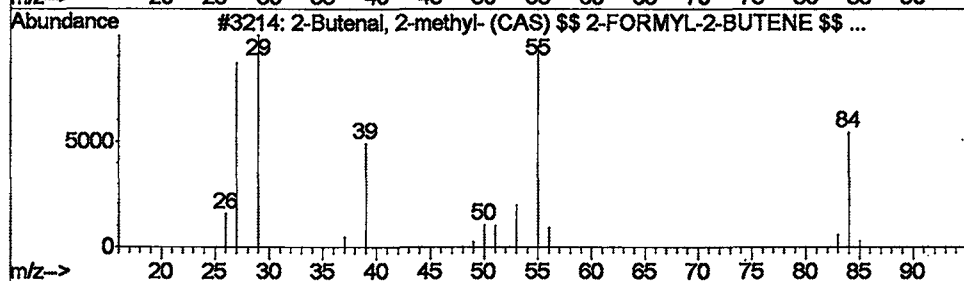
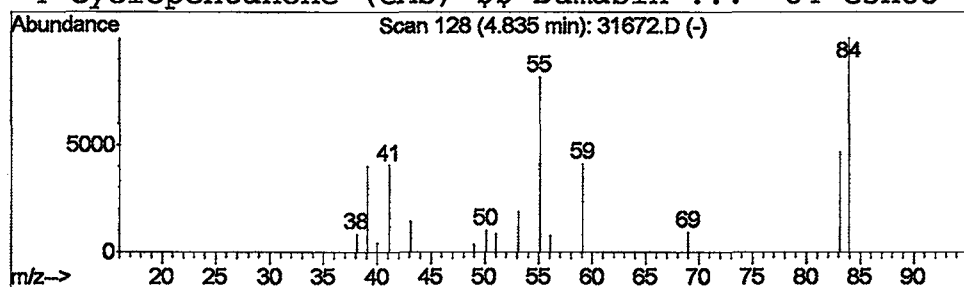
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 4 2-Butenal, 2-methyl- (CAS) ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.21 ug/L	71081	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 2-methyl- (CAS) \$\$ 2-...	84	C5H8O	001115-11-3	38
2			Cyclobut-1-enylmethanol	84	C5H8O	000000-00-0	17
3			Pyridine, 2,3,4,5-tetrahydro- \$\$...	83	C5H9N	000505-18-0	9
4			Cyclopentanone (CAS) \$\$ Dumasine ...	84	C5H8O	000120-92-3	9



LIBRARY SEARCH COMPOUND REPORT

Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D
 Acq On : 17 Jan 2002 7:49 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: LSCINT.P

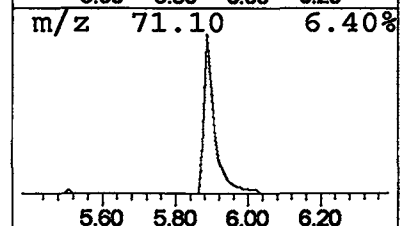
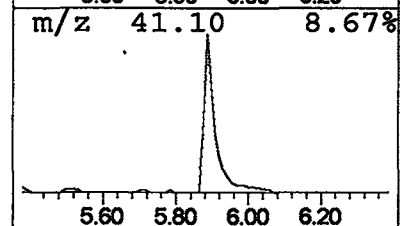
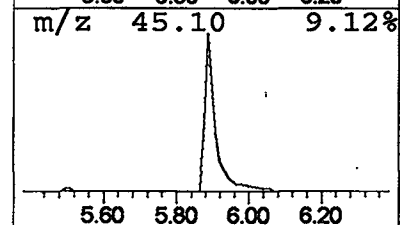
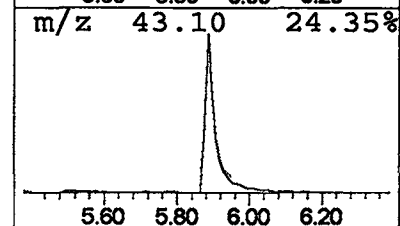
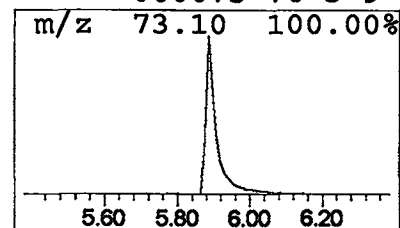
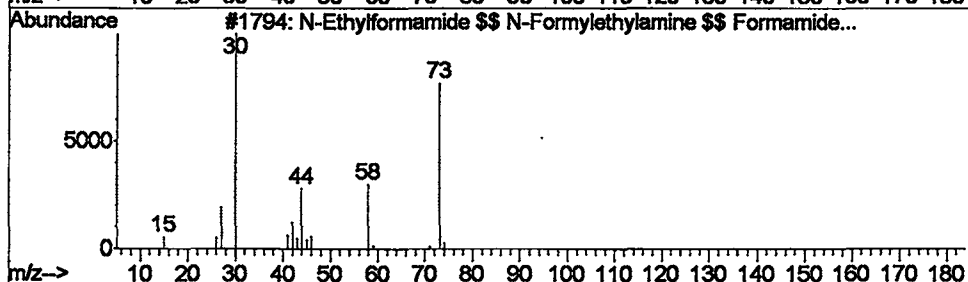
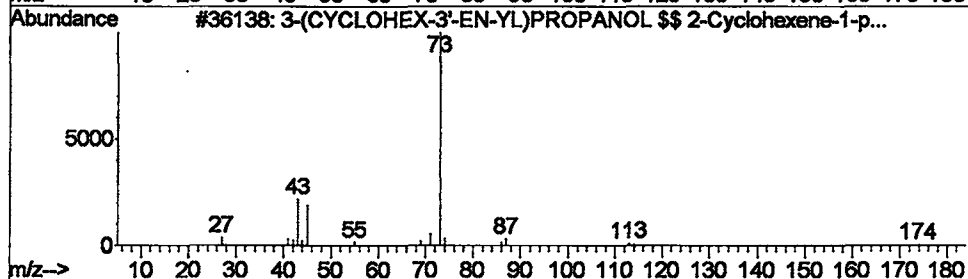
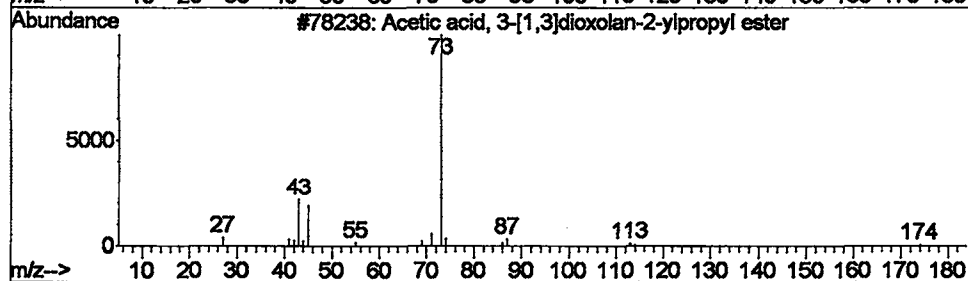
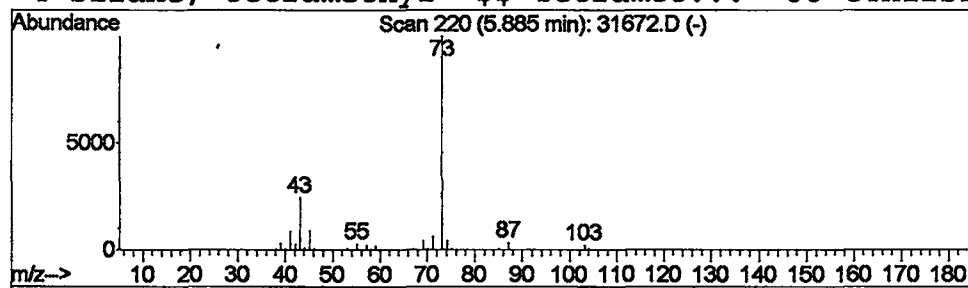
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.46 ug/L	1492980	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		N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4		Silane, tetramethyl- \$\$ Tetramet...	88	C4H12Si	000075-76-3	9



Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D
 Acq On : 17 Jan 2002 7:49 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: LSCINT.P

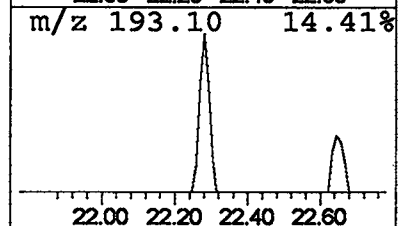
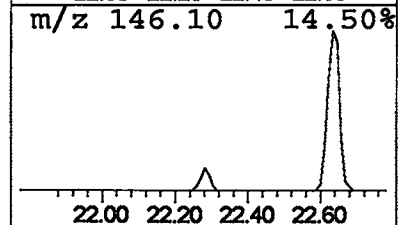
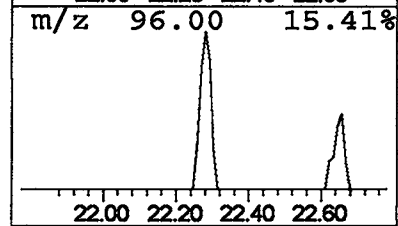
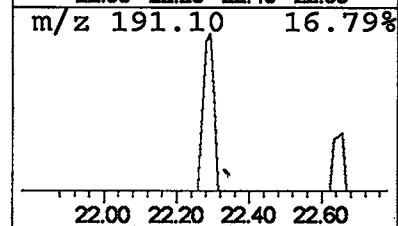
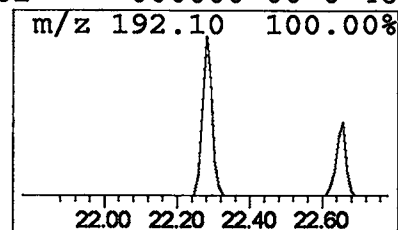
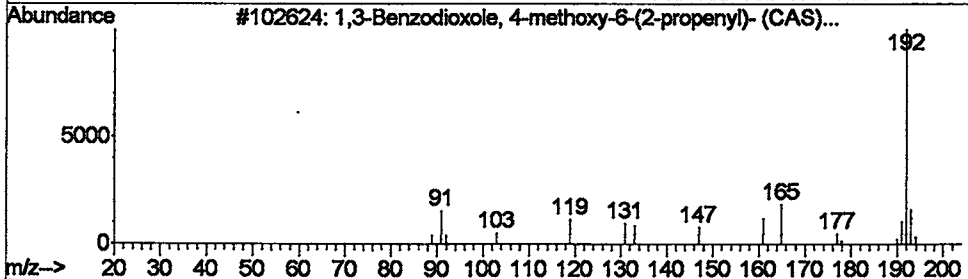
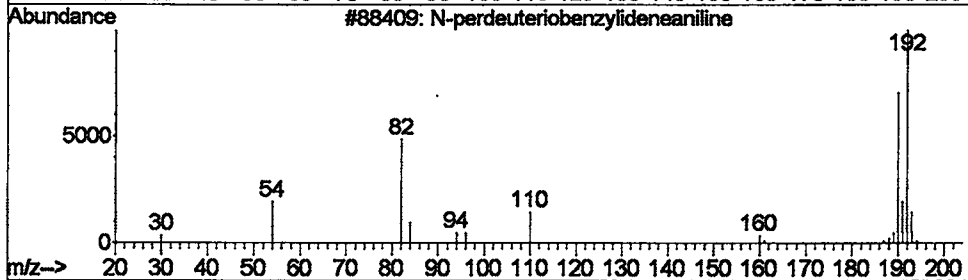
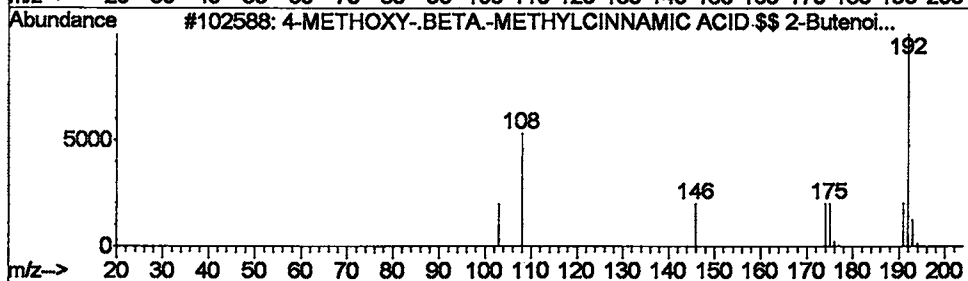
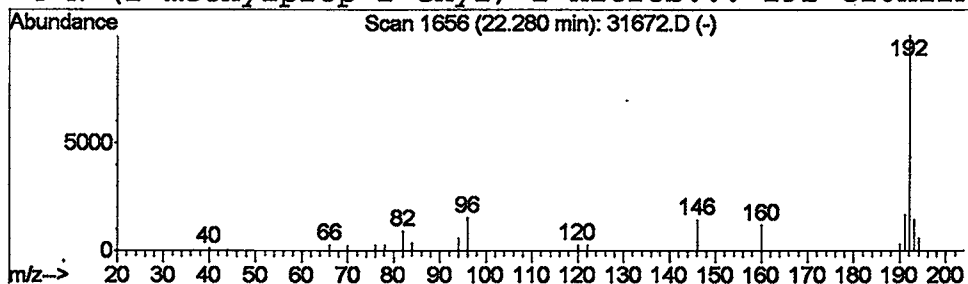
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 6 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	86693	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
2		N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	64
3		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	52
4		N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	46



Data File : C:\MSDCHEM\1\5973N\02JAN17\31672.D

Acq On : 17 Jan 2002 7:49 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 7

Operator:

Inst : Instrumen

Multiplr: 1.00

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

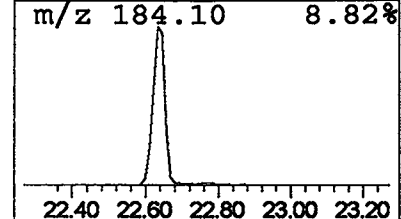
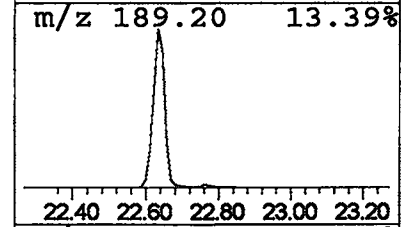
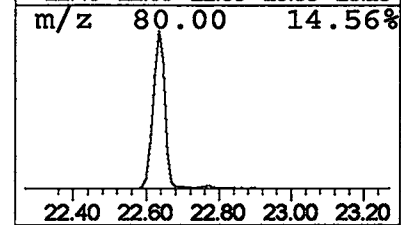
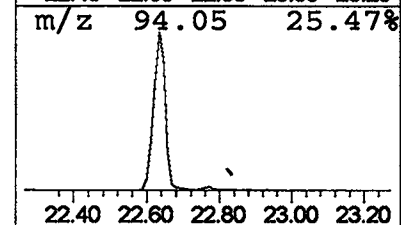
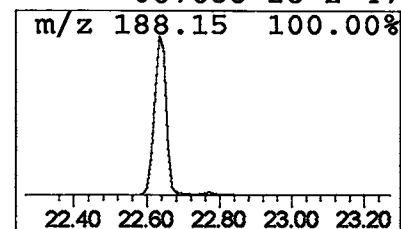
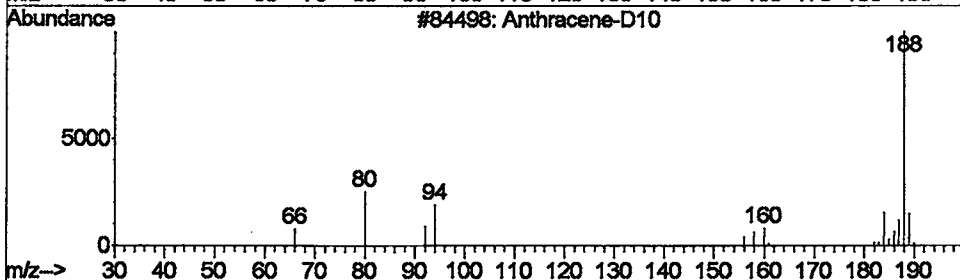
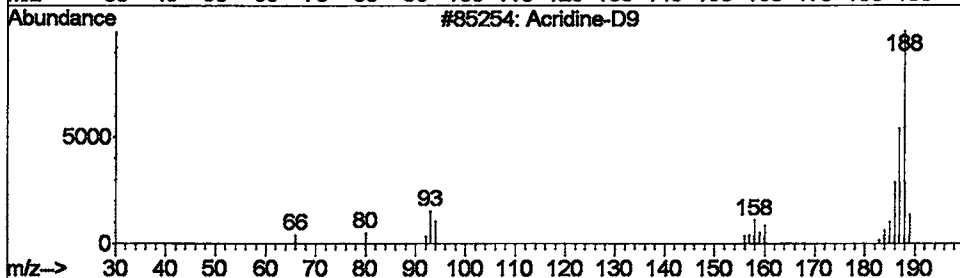
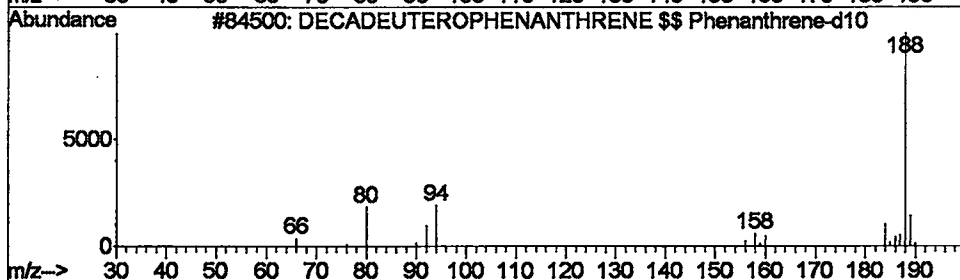
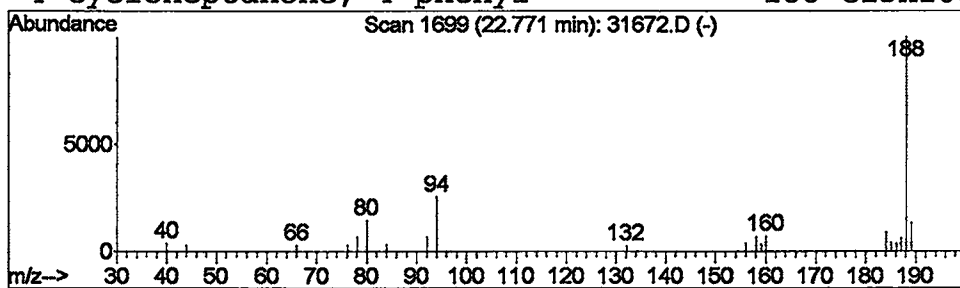
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 7 DECADEUTEROPHENANTHRENE \$\$... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.33 ug/L	188124	Phenanthrene-d10	22.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	90
2			Acridine-D9	188	C13D9N	000000-00-0	59
3			Anthracene-D10	188	C14D10	000000-00-0	50
4			Cycloheptanone, 4-phenyl-	188	C13H16O	067688-28-2	47



tentatively identified compound (LSC) summary

Operator ID: Date Acquired: 17 Jan 2002 7:49 pm
Data File: C:\MSDCHEM\1\5973N\02JAN17\31672.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	0.2	ug/L	52169	1	9.71	6691740	20.0
Pentane, 2-bromo-...	4.24	0.2	ug/L	70054	1	9.71	6691740	20.0
Butanoic acid, 2-...	4.62	0.1	ug/L	39139	1	9.71	6691740	20.0
2-Butenal, 2-meth...	4.84	0.2	ug/L	71081	1	9.71	6691740	20.0
Acetic acid, 3-[1...	5.89	4.5	ug/L	1492980	1	9.71	6691740	20.0
4-METHOXY-.BETA.-...	22.28	0.2	ug/L	86693	4	22.63	11502500	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	188124	4	22.63	11502500	20.0