

User: Vinci, David L
 Westchester Dept. of Labs & Research
 Date: 01/28/2002 Time: 15:35:43

Sample: AD31673
 Analysis: \$GCMS GCMS Scan For Unknowns
 Units: ug
 Started: 1/28/02 15:35 Ended: 1/28/02 15:35 Analyst: DLV
 Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		91		5.0

Comments for Sample AD31673 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-28-2002 Time: 15:35:45

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\31673.D

Vial: 8

Acq On : 17 Jan 2002 8:39 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : January 17, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Jan 22 08:30:20 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	1160576	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4953557	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2615115	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4307518	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	3749211	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	2785342	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-DDD	27.73	235	310447	4.56	ug/L	0.00
Spiked Amount	5.000		Recovery	=	91.20%	

Target Compounds

						Qvalue
20) Dimethylphthalate	18.34	163	417175	2.42	ug/L	# 56
21) 2,6-Dinitrotoluene	18.34	165	336105	9.98	ug/L	# 17
35) Di-n-butylphthalate	24.85	149	100680	0.36	ug/L	99
42) Bis(2-ethylhexyl)phthalate	31.11	149	20723	0.66	ug/L	95

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

31673.D SCAN508.M Tue Jan 22 08:30:21 2002

Page 1

Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31673.D

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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

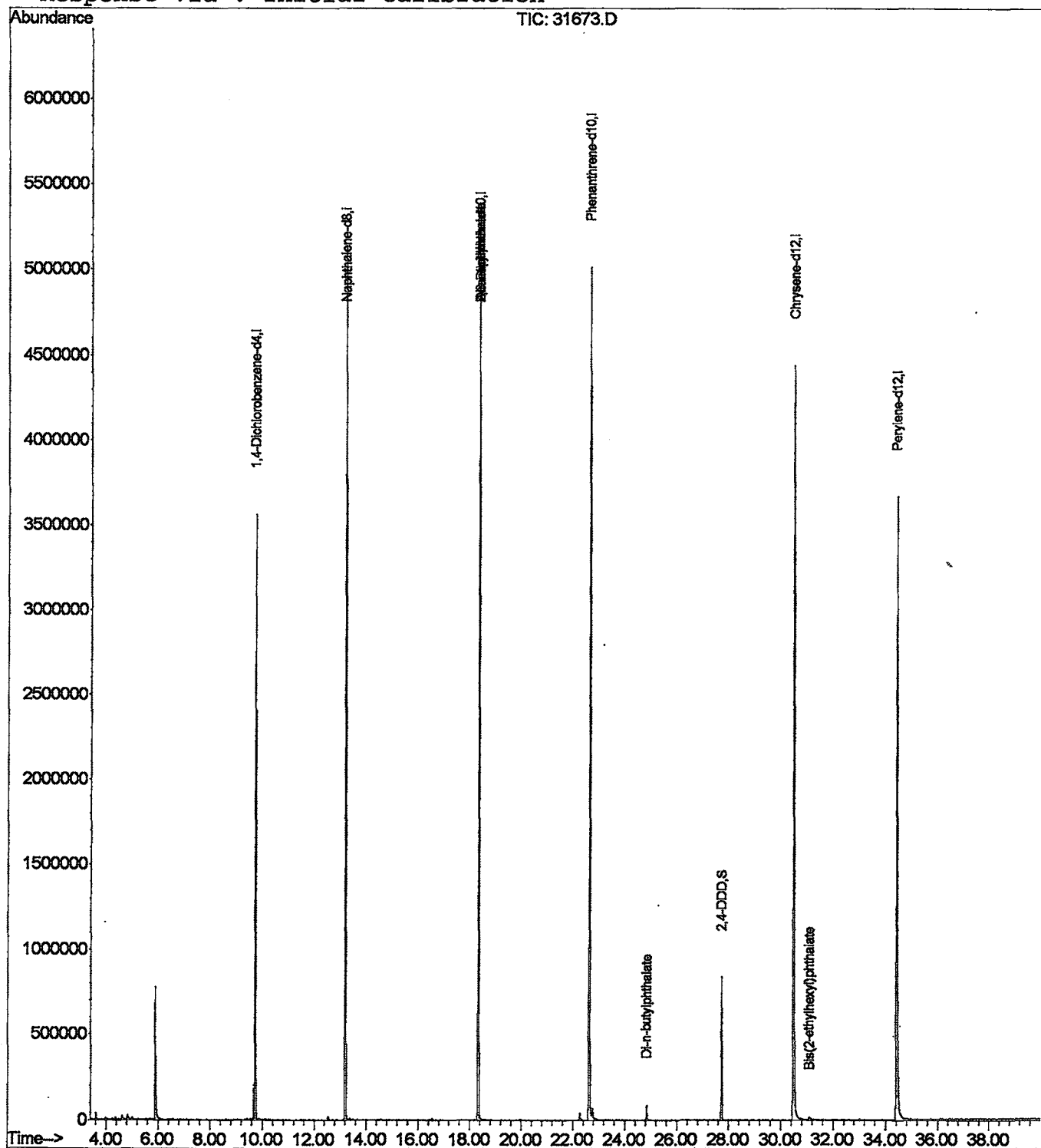
Quant Results File: SCAN508.RE

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\31673.D

Vial: 8

Acq On : 17 Jan 2002 8:39 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

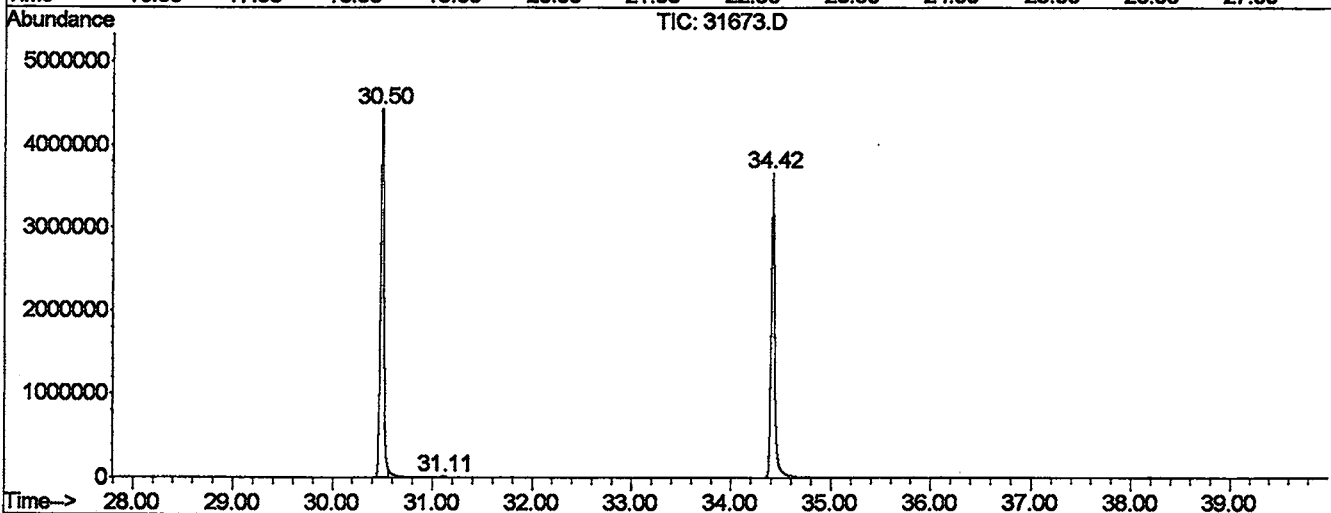
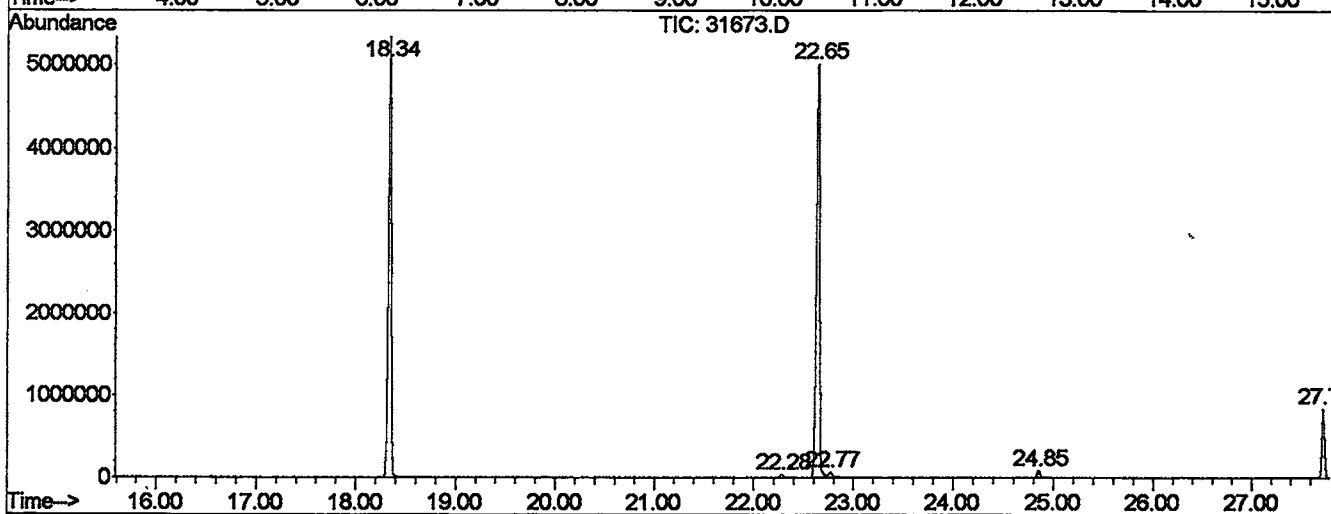
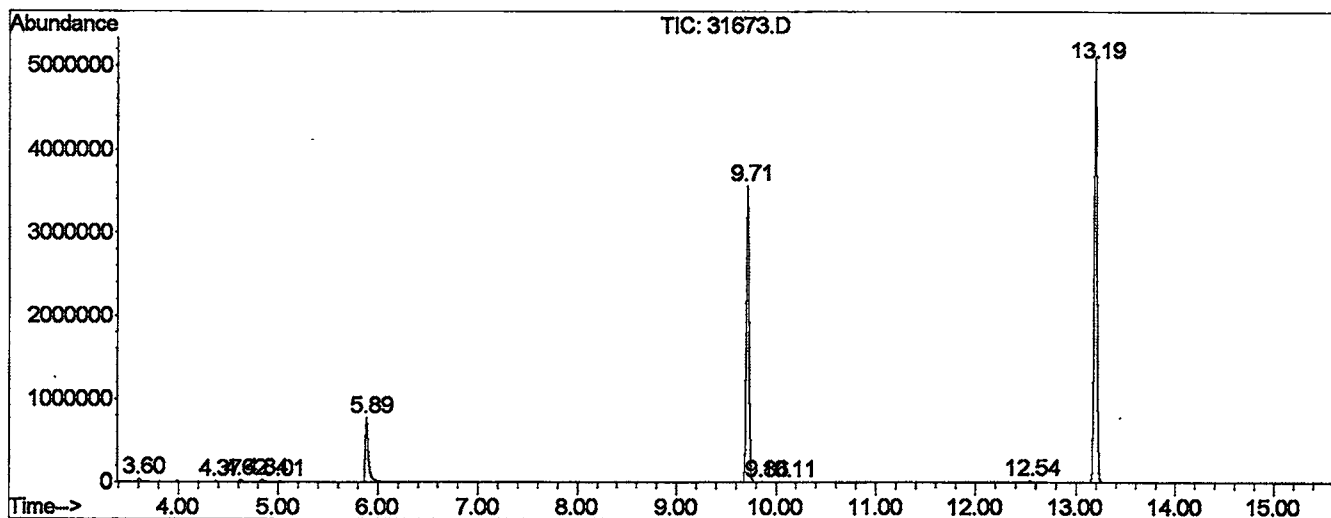
Signal : TIC

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	39329	56405	0.49%	0.091%
2	4.367	85	87	95	rVB	13895	25133	0.22%	0.040%
3	4.618	107	109	117	rVB2	21116	36545	0.32%	0.059%
4	4.835	125	128	137	rBV2	26522	68683	0.60%	0.110%
5	5.006	139	143	149	rVB2	13855	26055	0.23%	0.042%
6	5.885	217	220	245	rBV	772347	1627691	14.28%	2.615%
7	9.710	551	555	561	rVV	3560069	6594197	57.83%	10.595%
8	9.858	561	568	577	rVV2	7951	30131	0.26%	0.048%
9	10.110	585	590	595	rVB3	7690	20146	0.18%	0.032%
10	12.541	799	803	807	rVB	19615	35913	0.31%	0.058%
11	13.192	855	860	865	rBV	5101035	9523863	83.53%	15.302%
12	18.341	1305	1311	1315	rBV	5335576	10589412	92.87%	17.014%
13	22.280	1653	1656	1661	rBV2	39828	73843	0.65%	0.119%
14	22.645	1681	1688	1693	rBV2	5007657	11401817	100.00%	18.320%
15	22.771	1695	1699	1713	rVB	62183	181159	1.59%	0.291%
16	24.849	1877	1881	1891	rBV	85436	157025	1.38%	0.252%
17	27.726	2127	2133	2139	rBV	835458	1475559	12.94%	2.371%
18	30.500	2369	2376	2381	rBV	4433448	10827209	94.96%	17.396%
19	31.105	2419	2429	2437	rBV4	16484	62488	0.55%	0.100%
20	34.416	2713	2719	2765	rBV	3662055	9424706	82.66%	15.143%

Sum of corrected areas: 62237980

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31673.D
 Operator :
 Acquired : 17 Jan 2002 8:39 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan
 Misc Info : January 17, 2002
 Vial Number: 8
 Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31673.D
 Acq On : 17 Jan 2002 8:39 pm
 Sample : 508 scan
 Misc : January 17, 2002
 MS Integration Params: LSCINT.P

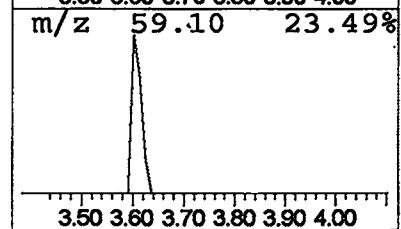
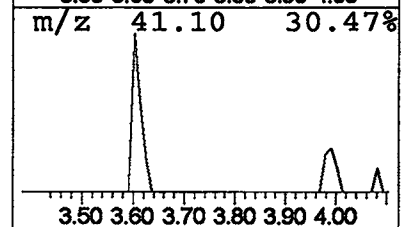
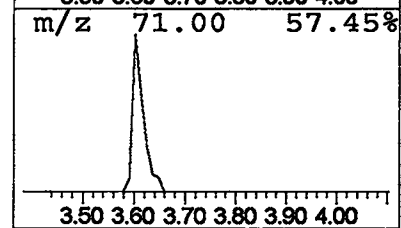
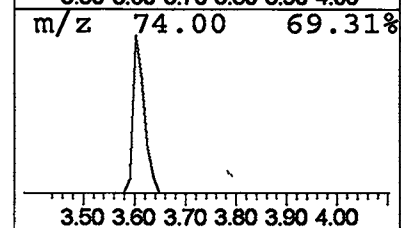
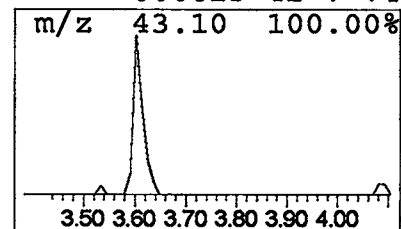
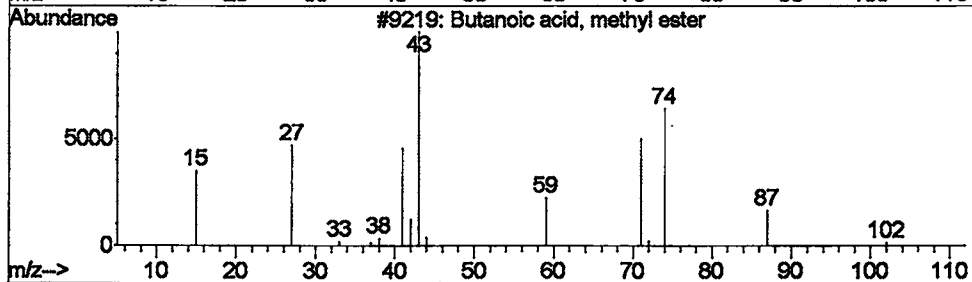
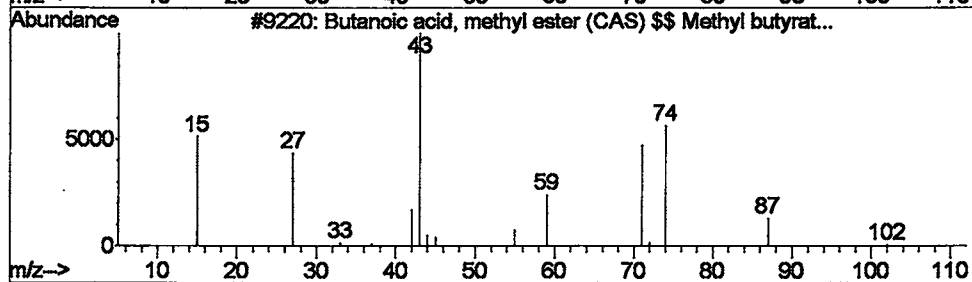
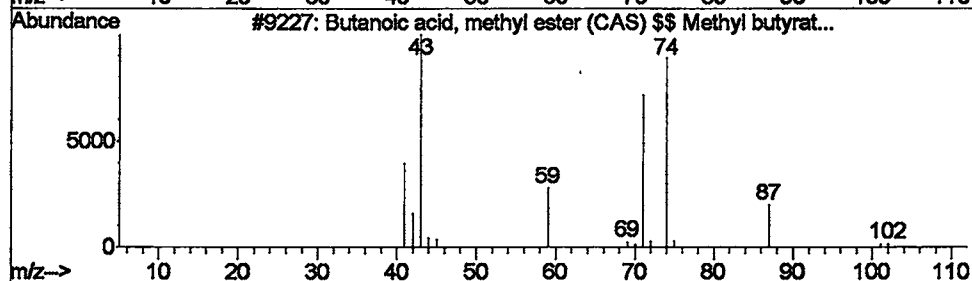
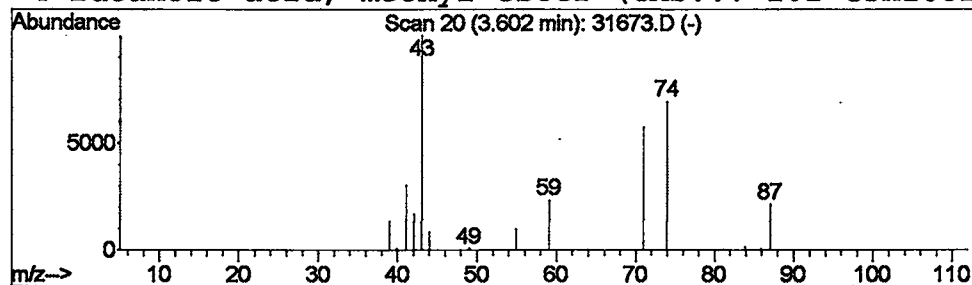
Vial: 8
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.17 ug/L	56405	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 (CAS...	102	C5H10O2	000623-42-7	78
3		Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78
4		Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	74



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31673.D

Acq On : 17 Jan 2002 8:39 pm

Sample : 508 scan

Misc : January 17, 2002

MS Integration Params: LSCINT.P

Vial: 8

Operator:

Inst : Instrumen

Multiplr: 1.00

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

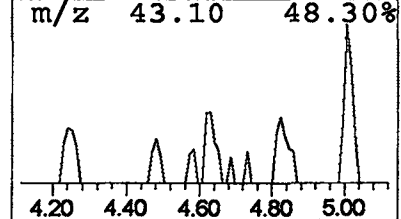
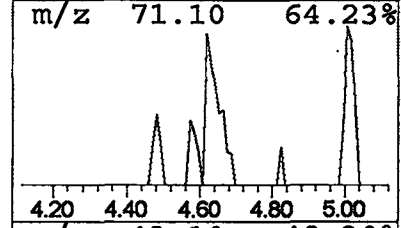
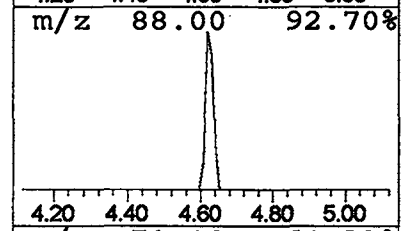
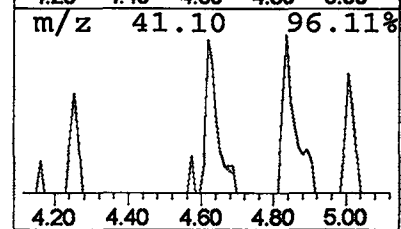
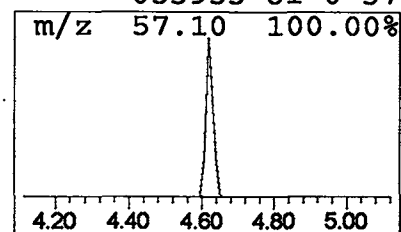
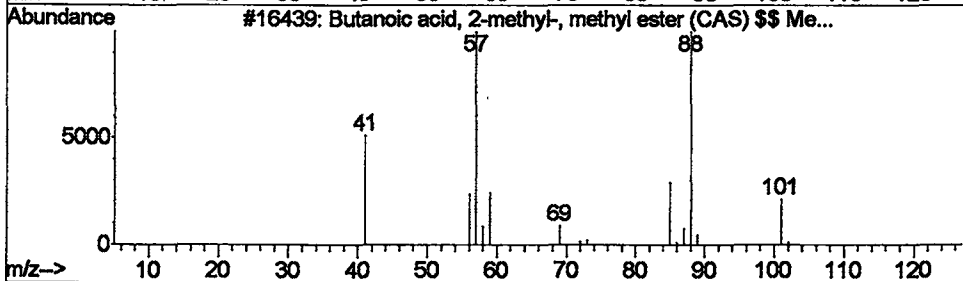
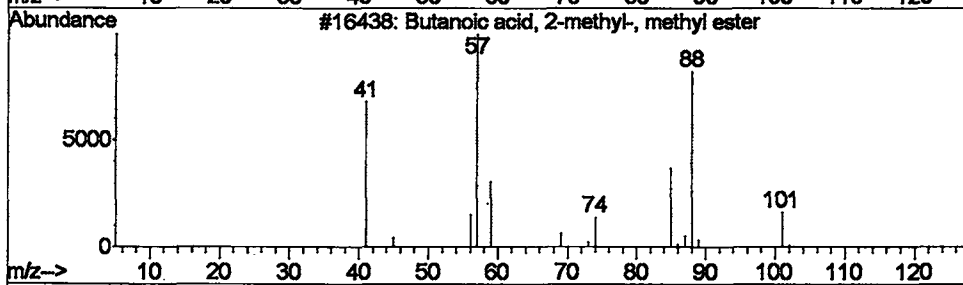
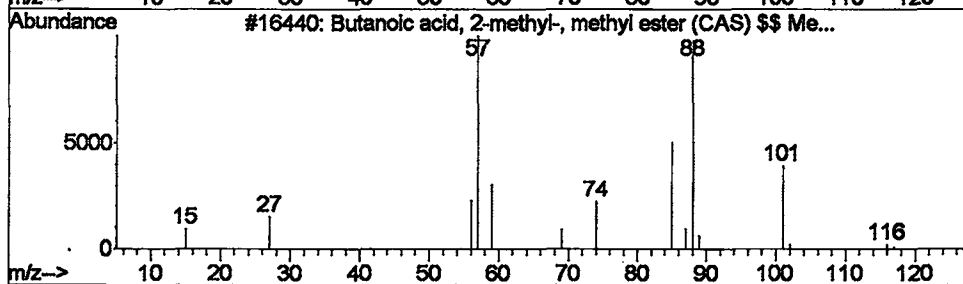
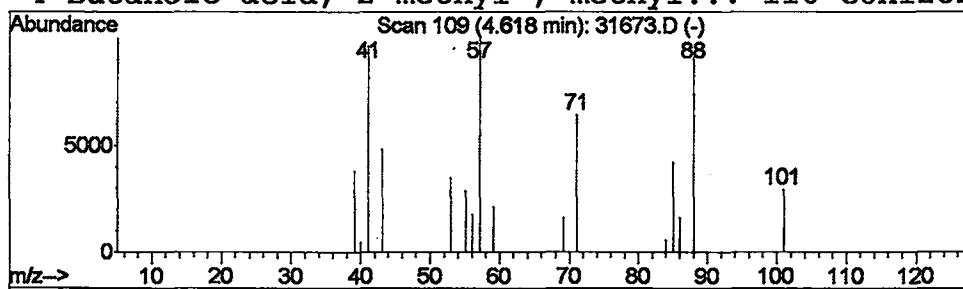
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 2 Butanoic acid, 2-methyl-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	0.11 ug/L	36545	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	47
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	053955-81-0	37



Library Search Compound Report

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Acq On : 17 Jan 2002 8:39 pm
Sample : 508 scan
Misc : January 17, 2002
MS Integration Params: LSCINT.P

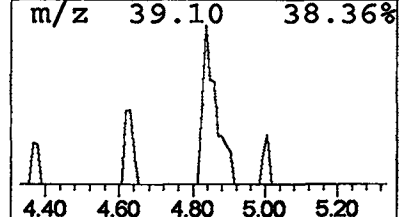
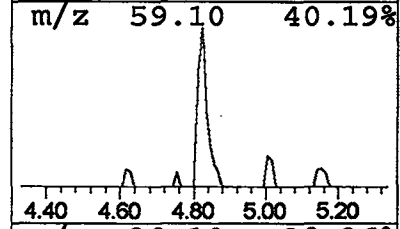
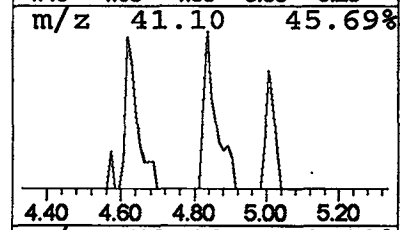
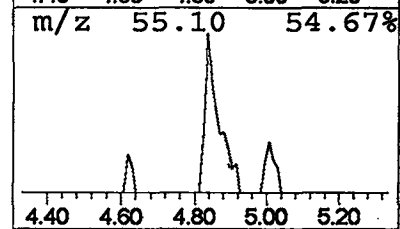
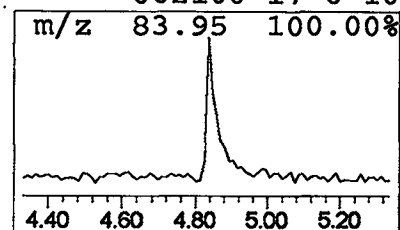
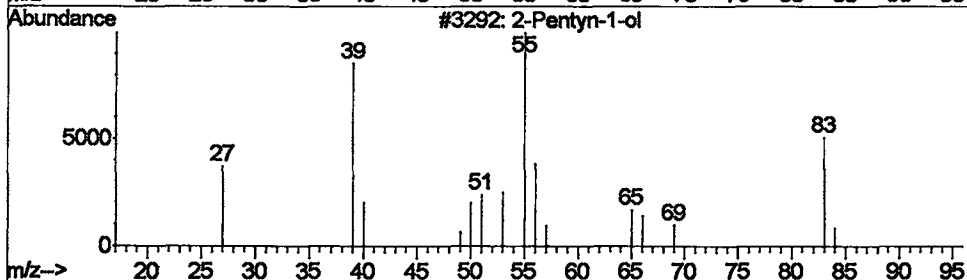
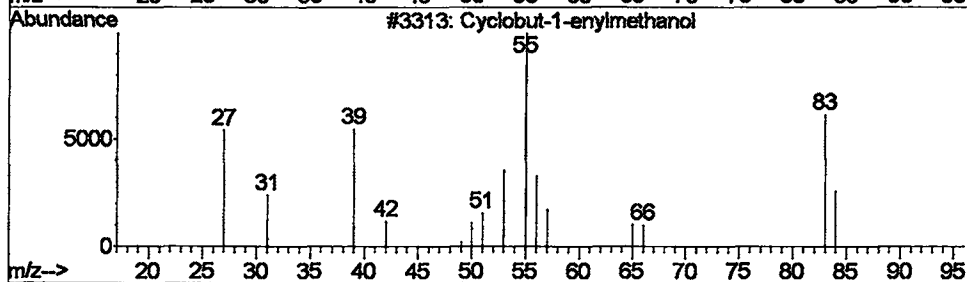
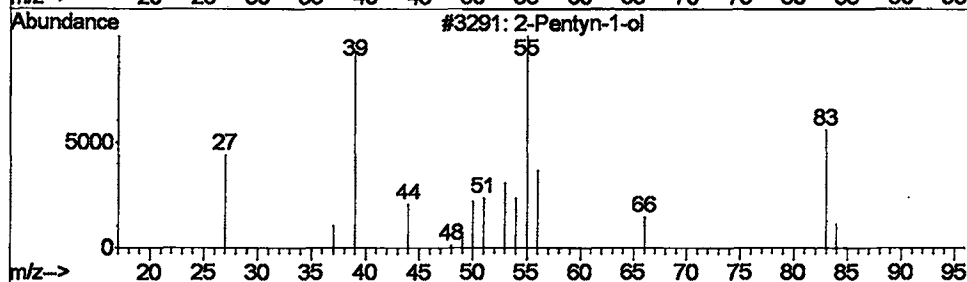
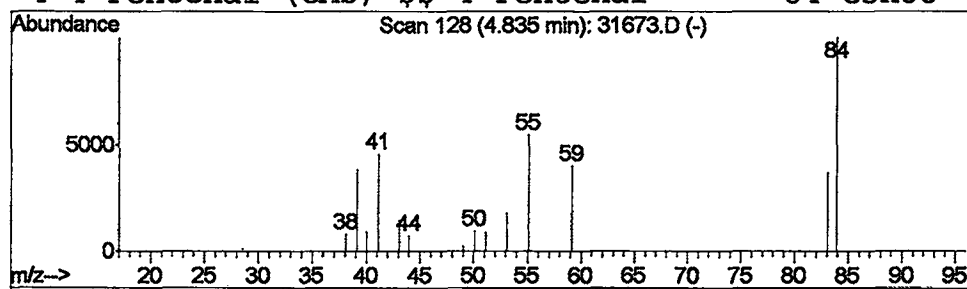
Vial: 8
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 3 2-Pentyn-1-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.21 ug/L	68683	1,4-Dichlorobenzene-d4	9.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentyn-1-ol		84	C5H8O	006261-22-9	32
2	Cyclobut-1-enylmethanol		84	C5H8O	000000-00-0	32
3	2-Pentyn-1-ol		84	C5H8O	006261-22-9	25
4	4-Pentenal (CAS) \$\$ 4-Pentenal-		84	C5H8O	002100-17-6	10



Library Search Compound Report

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MS Integration Params: LSCINT.P

Vial: 8

Operator:

Inst : Instrumen

Multiplr: 1.00

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

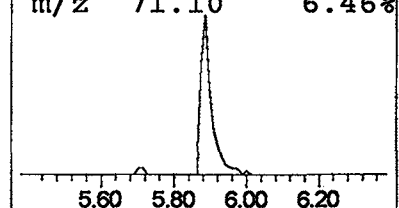
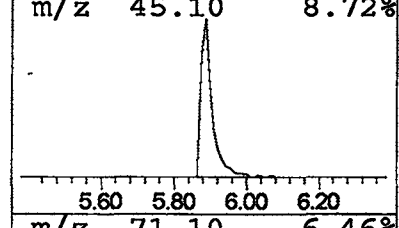
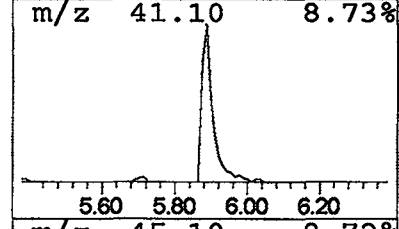
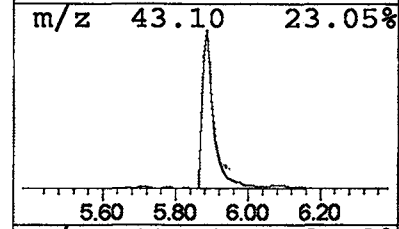
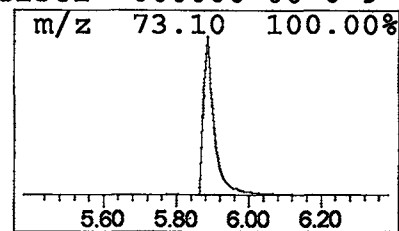
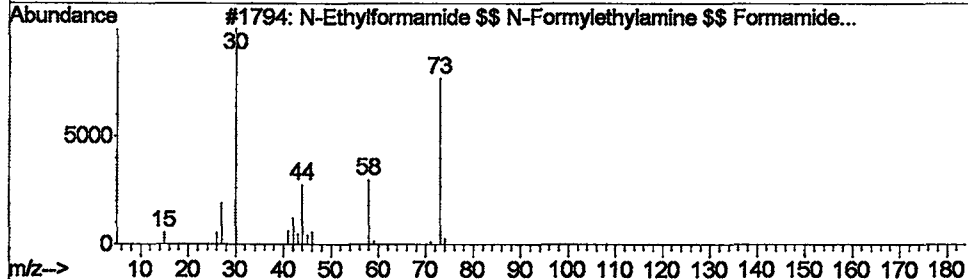
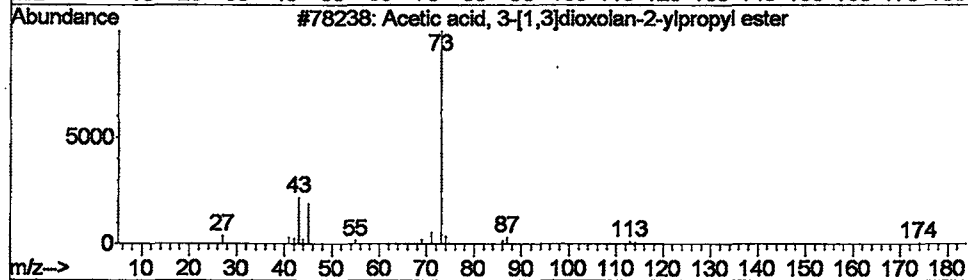
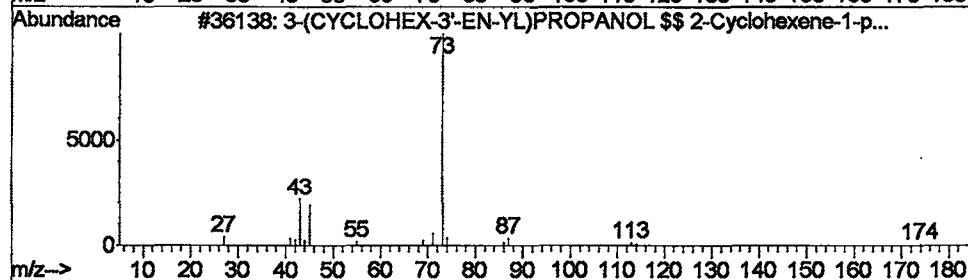
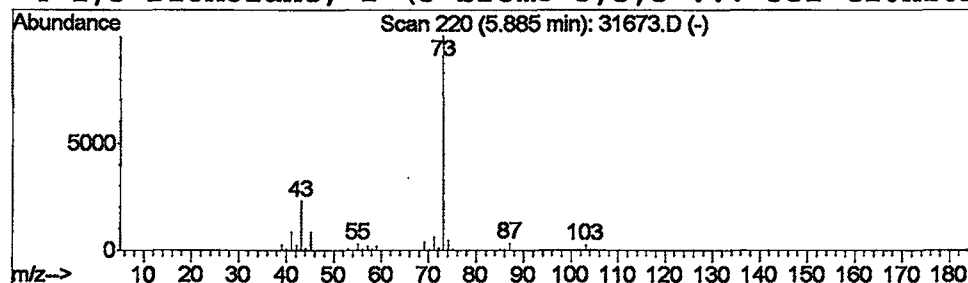
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

Peak Number 4 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.94 ug/L	1627690	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	36
2			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	36
3			N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	000000-00-0	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31673.D
Acq On : 17 Jan 2002 8:39 pm
Sample : 508 scan
Misc : January 17, 2002
MS Integration Params: LSCINT.P

Vial: 8
Operator:
Inst : Instrumen
Multiplr: 1.00

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

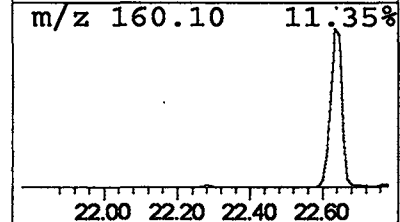
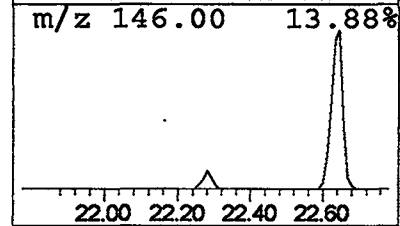
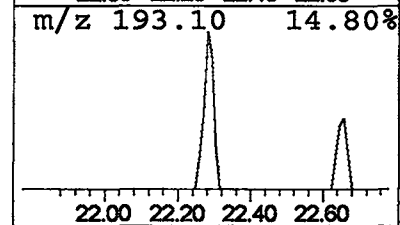
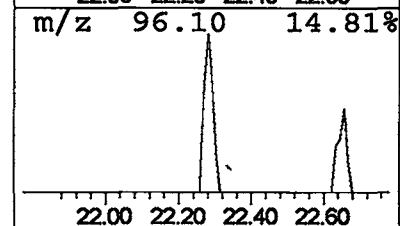
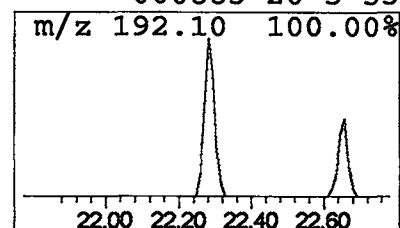
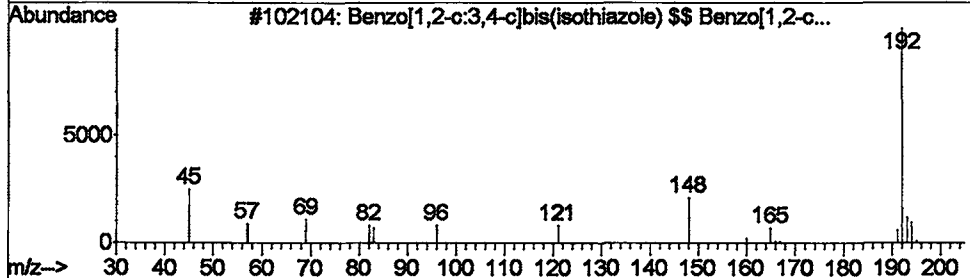
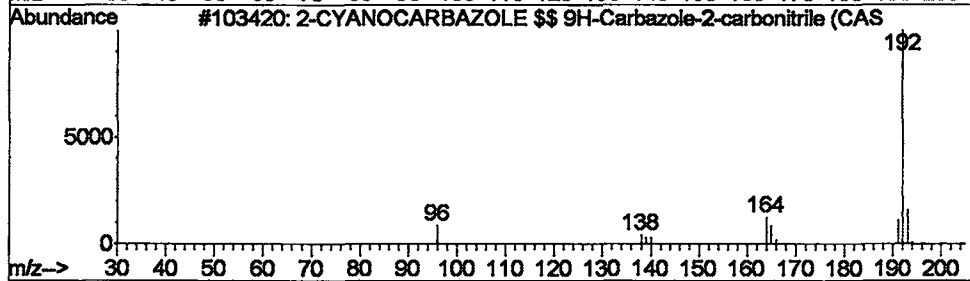
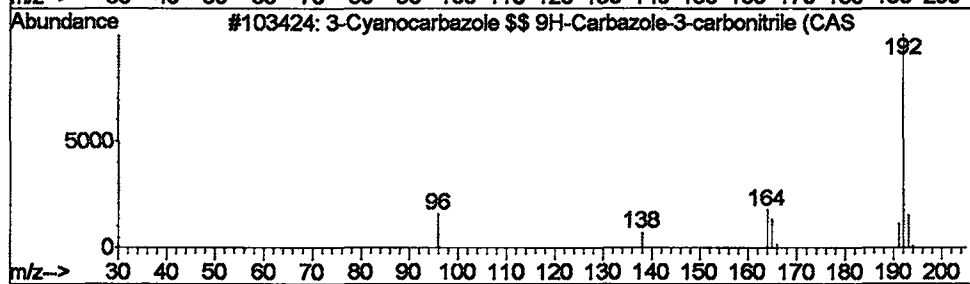
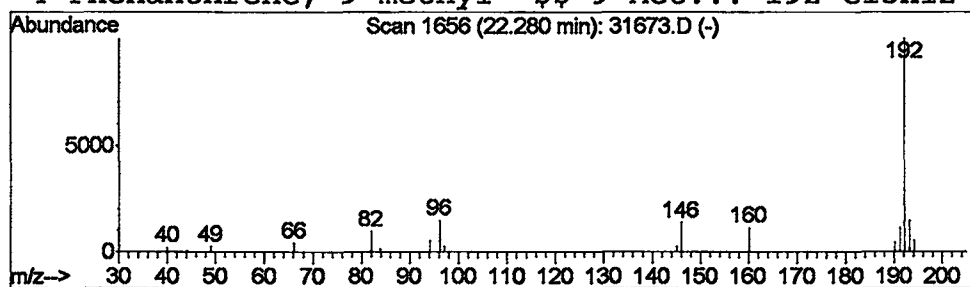
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.13 ug/L	73843	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	72
2	2-CYANOCARBAZOLE \$\$ 9H-Carbazole...	192	C13H8N2	057955-18-7	72
3	Benzo[1,2-c:3,4-c]bis(isothiazol...	192	C8H4N2S2	074960-05-7	64
4	Phenanthrene, 9-methyl- \$\$ 9-Met...	192	C15H12	000883-20-5	53



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31673.D
Acq On : 17 Jan 2002 8:39 pm
Sample : 508 scan
Misc : January 17, 2002
MS Integration Params: LSCINT.P

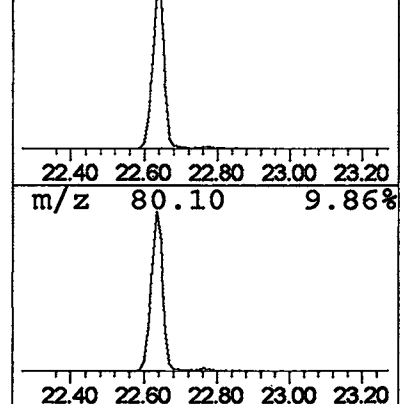
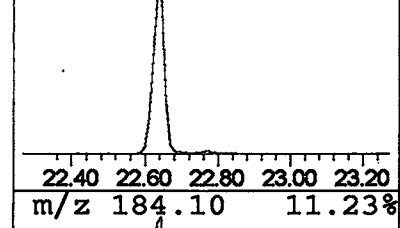
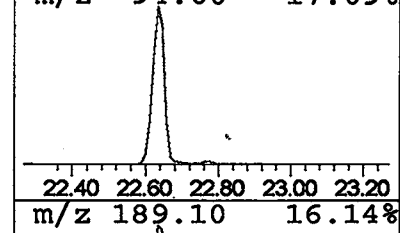
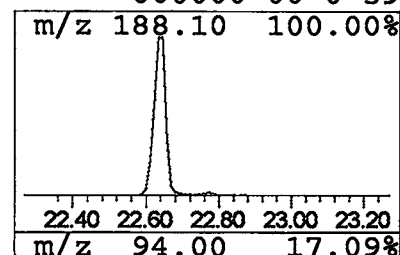
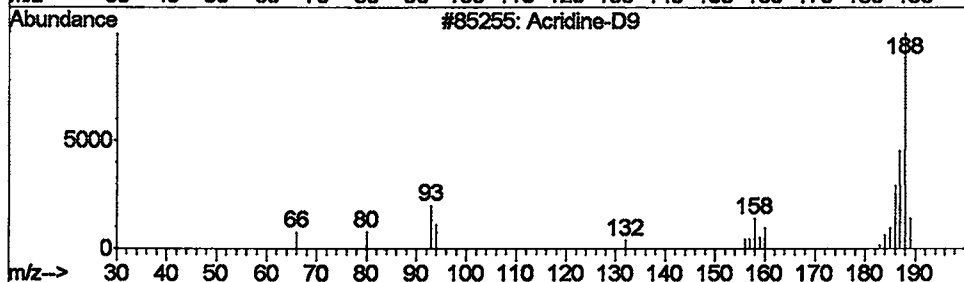
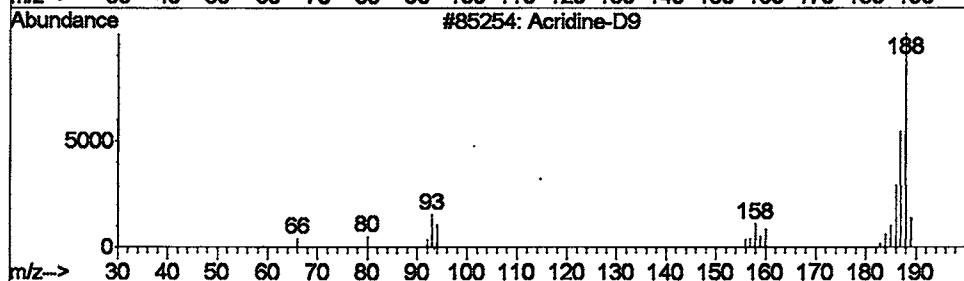
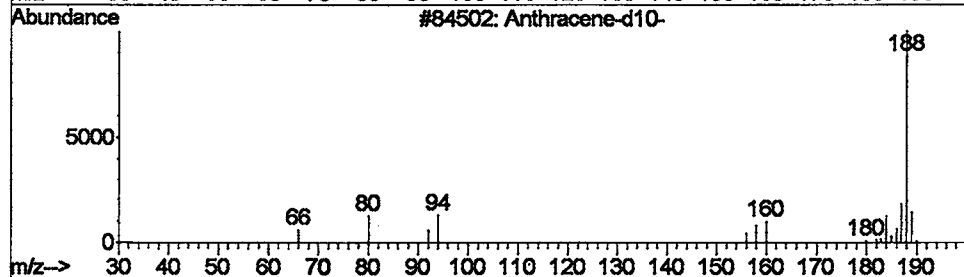
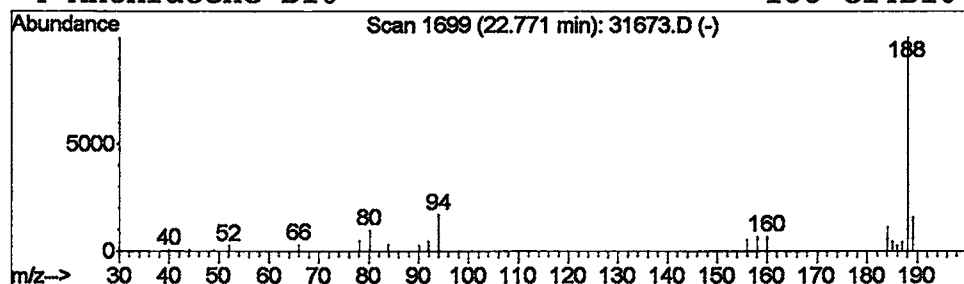
Vial: 8
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 6 Anthracene-d10- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.32 ug/L	181159	Phenanthrene-d10	22.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene-d10-	188	C14D10	001719-06-8	86
2			Acridine-D9	188	C13D9N	000000-00-0	72
3			Acridine-D9	188	C13D9N	000000-00-0	72
4			Anthracene-D10	188	C14D10	000000-00-0	59



Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 17 Jan 2002 8:39 pm
 Data File: C:\MSDCHEM\1\5973N\02JAN17\31673.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	56405	1	9.71	6594200	20.0
Butanoic acid, 2-...	4.62	0.1	ug/L	36545	1	9.71	6594200	20.0
2-Pentyn-1-ol	4.84	0.2	ug/L	68683	1	9.71	6594200	20.0
3-(CYCLOHEX-3'-EN...	5.89	4.9	ug/L	1627690	1	9.71	6594200	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	73843	4	22.65	11401800	20.0
Anthracene-d10-	22.77	0.3	ug/L	181159	4	22.65	11401800	20.0