

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/29/2002 Time: 09:47:25

Sample: AE00697
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/29/02 09:47 Ended: 1/29/02 09:47 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		112		5.0

Comments for Sample AE00697 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 01-29-2002 Time: 09:49:04

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.

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
 Acq On : 16 Jan 2002 12:31 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 16 14:05:04 2002

Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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	1136790	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4801548	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2527095	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4241949	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3830389	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2745994	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	375325	5.60	ug/L	0.00
Spiked Amount	5.000		Recovery	=	112.00%	
Target Compounds						
2) n-Nitrosodimethylamine	3.60	74	9028	0.19	ug/L #	15
20) Dimethylphthalate	18.34	163	408030	2.44	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	321579	9.88	ug/L #	17
35) Di-n-butylphthalate	24.85	149	10554	0.04	ug/L	88
41) Benzo(a)anthracene	30.50	228	10070	0.04	ug/L #	54
42) Bis(2-ethylhexyl)phthalate	31.11	149	24398	0.68	ug/L	96
43) Chrysene	30.50	228	10070	0.05	ug/L #	51
48) Benzo(a)pyrene	34.42	252	9083	0.05	ug/L #	1

(#) = qualifier out of range (m) = manual integration
 00697.D SCAN508.M Wed Jan 16 14:05:05 2002

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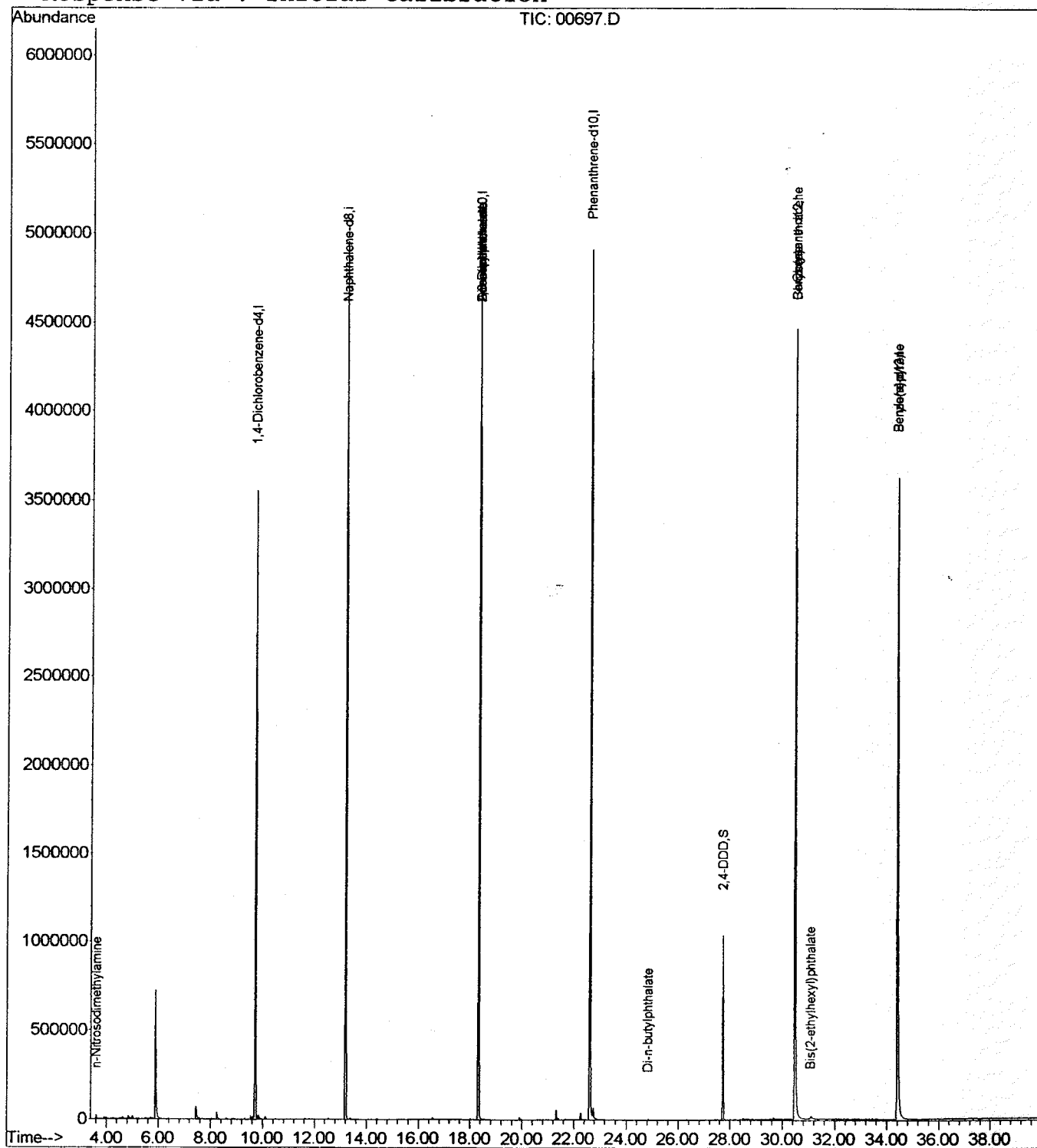
Quantification Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
Acq On : 16 Jan 2002 12:31 pm
Sample : 508scan
Misc : January 16, 2002
MS Integration Params: SPLIT.P
Quant Time: Jan 16 14:05 2002

Vial: 3
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



00697.D SCAN508.M

Wed Jan 16 14:05:05 2002

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Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
 Acq On : 16 Jan 2002 12:31 pm
 Sample : 508scan
 Misc : January 16, 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

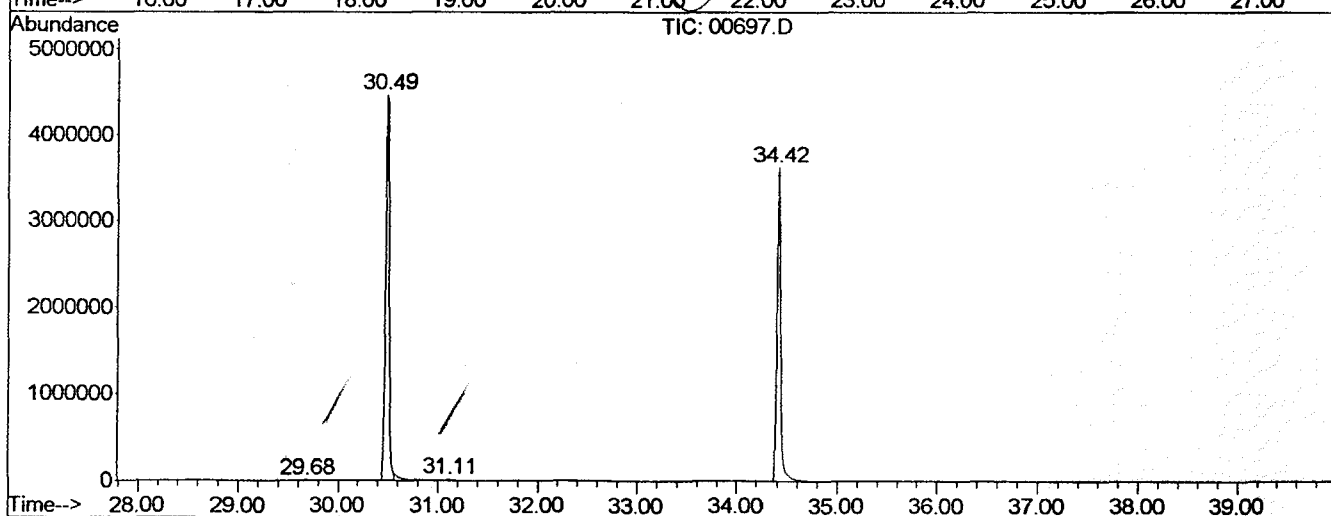
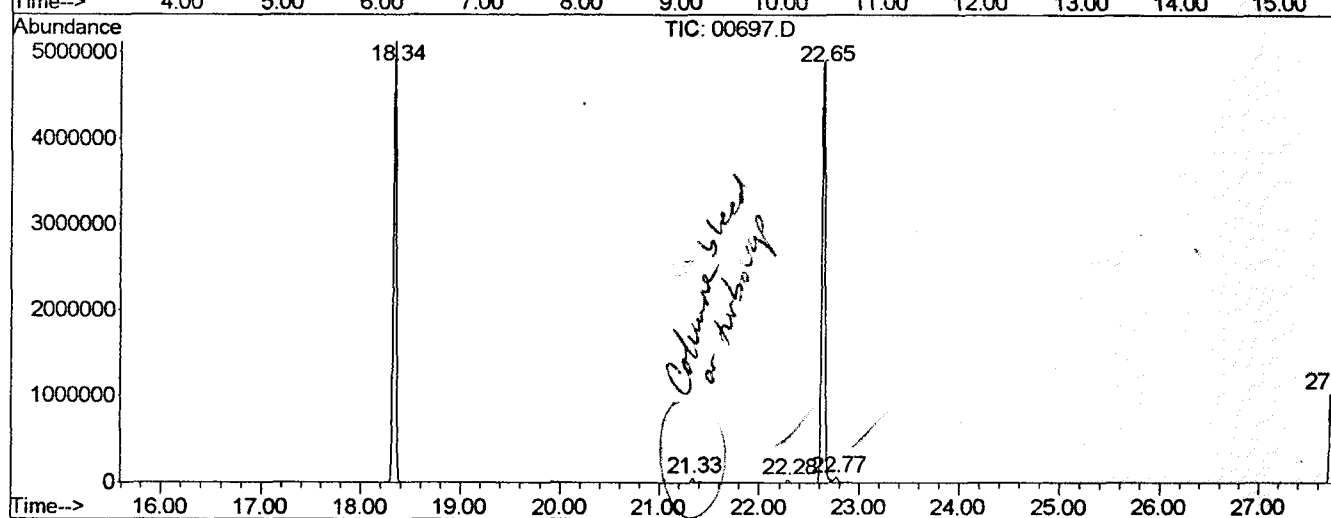
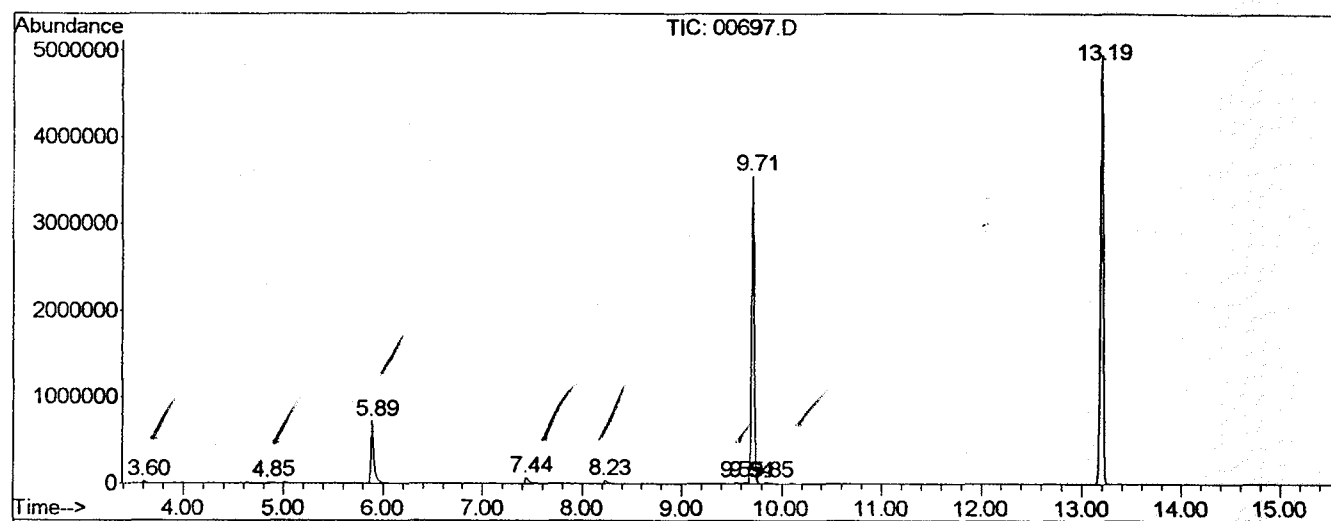
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.602	19	20	25	rVB	24323	40972	0.36%	0.066%
2	4.846	123	129	141	rBV3	16293	58411	0.52%	0.094%
3	5.885	215	220	239	rBV	723756	1414591	12.55%	2.283%
4	7.438	351	356	373	rBV	68445	194761	1.73%	0.314%
5	8.226	423	425	437	rBV	37833	80592	0.72%	0.130%
6	9.550	539	541	545	rVV	17143	40163	0.36%	0.065%
7	9.642	545	549	551	rVV	17980	43232	0.38%	0.070%
8	9.710	551	555	561	rVV	3552538	6459925	57.32%	10.426%
9	9.847	561	567	575	rVV	20225	65372	0.58%	0.106%
10	13.192	855	860	865	rBV	4953006	9218565	81.80%	14.878%
11	18.341	1305	1311	1315	rBV	5126229	10267029	91.10%	16.570%
12	21.332	1569	1573	1577	rVB	53481	84665	0.75%	0.137%
13	22.280	1651	1656	1661	rVB2	40608	76551	0.68%	0.124%
14	22.645	1681	1688	1693	rBV2	4909512	11269449	100.00%	18.188%
15	22.771	1695	1699	1717	rVB	62879	182479	1.62%	0.295%
16	27.726	2127	2133	2139	rVB	1037435	1838337	16.31%	2.967%
17	29.678	2299	2304	2309	rVB3	10157	35667	0.32%	0.058%
18	30.489	2369	2375	2381	rBV2	4464693	11186849	99.27%	18.054%
19	31.105	2425	2429	2445	rVB3	19464	98433	0.87%	0.159%
20	34.416	2713	2719	2747	rBV	3621281	9305695	82.57%	15.018%

Sum of corrected areas: 61961738

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
Operator :
Acquired : 16 Jan 2002 12:31 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508scan
Misc Info : January 16, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



00697.D SCAN508.M

Thu Jan 17 08:16:54 2002

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Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D

Acq On : 16 Jan 2002 12:31 pm

Sample : 508scan

Misc : January 16, 2002

MS Integration Params: LSCINT.P

Vial: 3

Operator:

Inst : Instrumen

Multiplr: 1.00

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

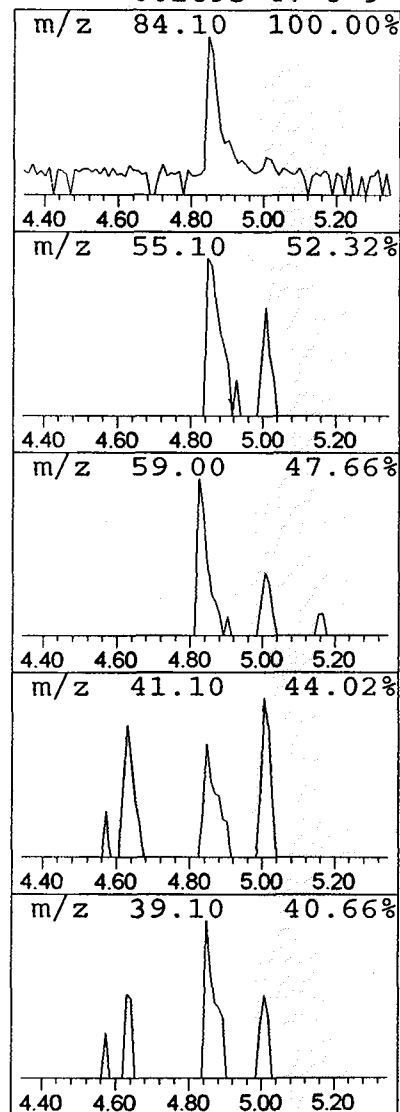
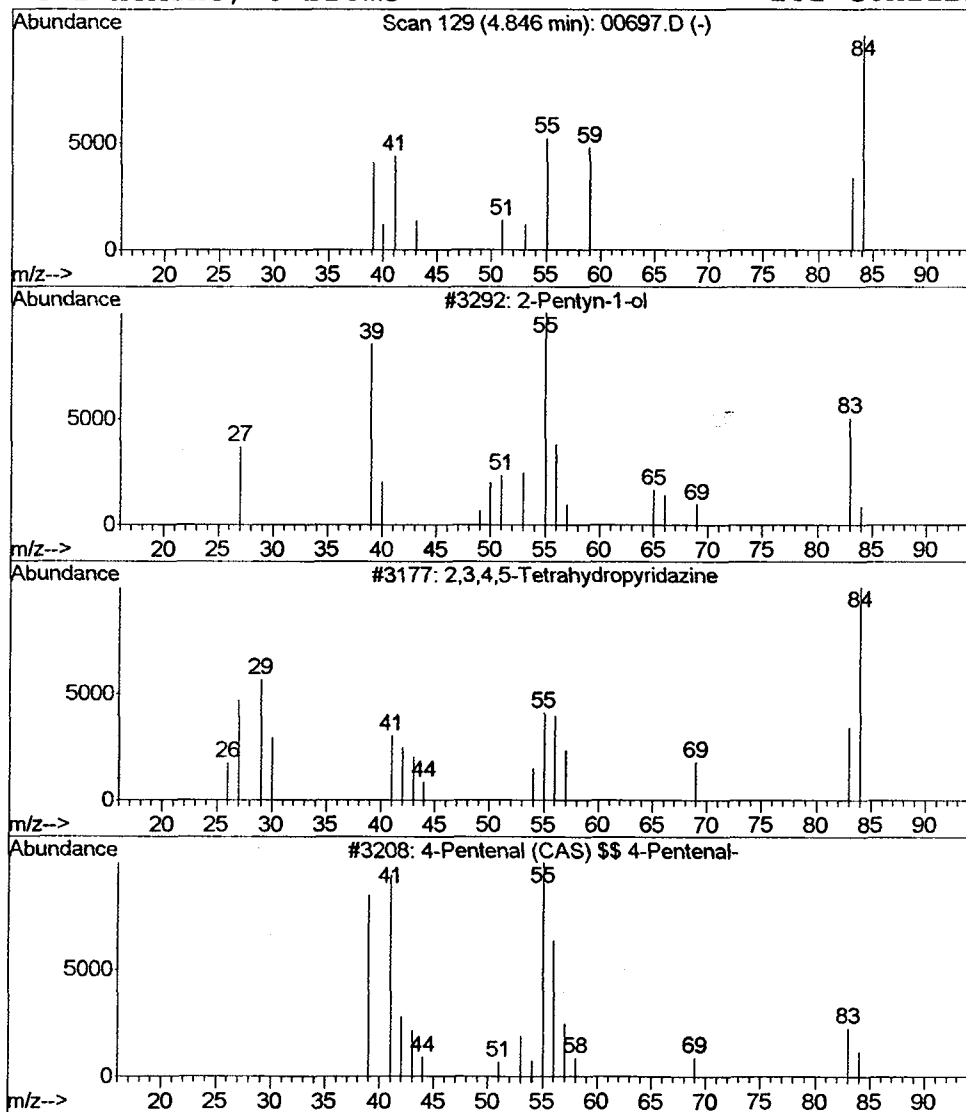
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

 Peak Number 1 2-Pentyn-1-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	0.18 ug/L	58411	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentyn-1-ol	84	C5H8O	006261-22-9	35
2		2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	32
3		4-Pentenal (CAS) \$\$ 4-Pentenal-	84	C5H8O	002100-17-6	9
4		1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	9



-----, Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
 Acq On : 16 Jan 2002 12:31 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

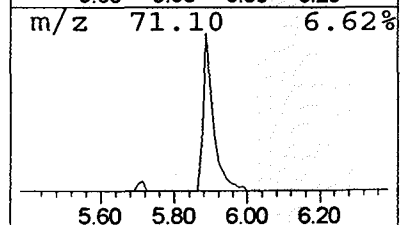
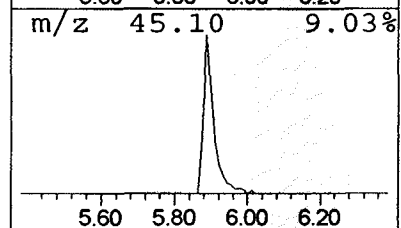
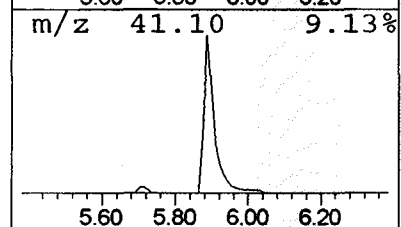
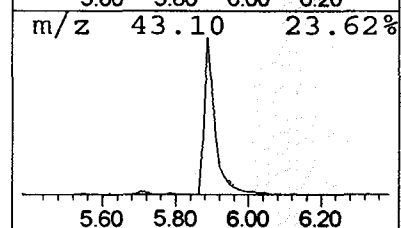
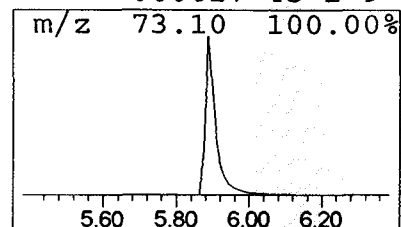
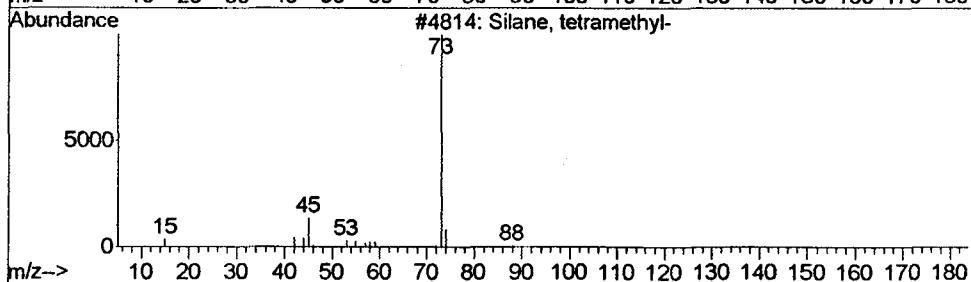
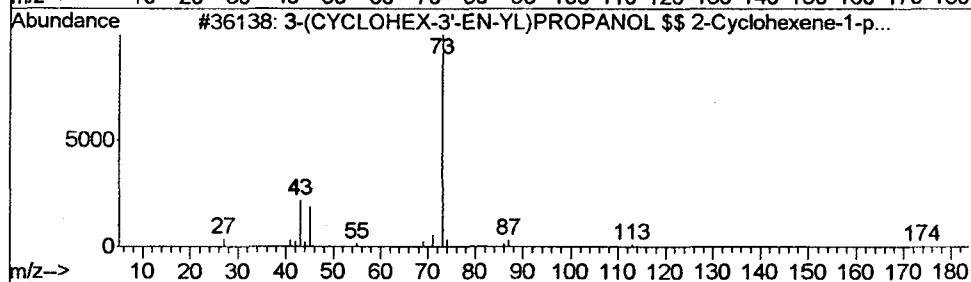
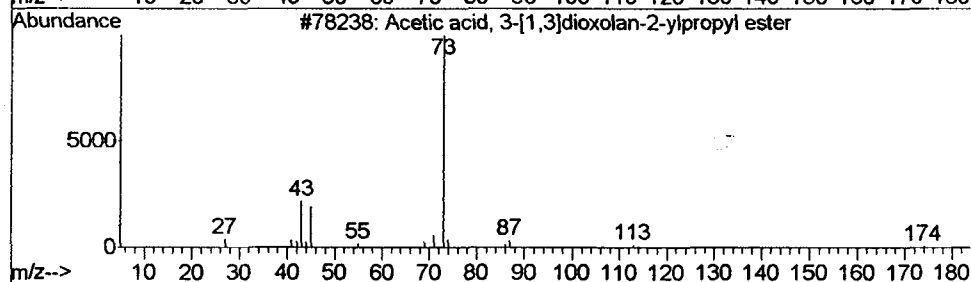
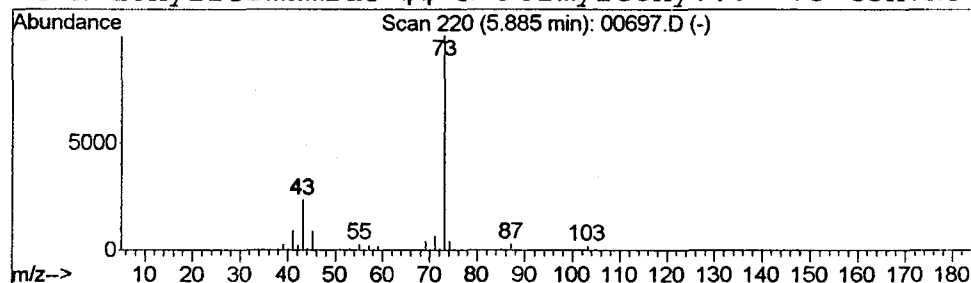
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.38 ug/L	1414590	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	33
2		3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	33
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4		N-Ethylformamide \$\$ N-Formylethy...	73	C3H7NO	000627-45-2	9



Library Search Compound Report

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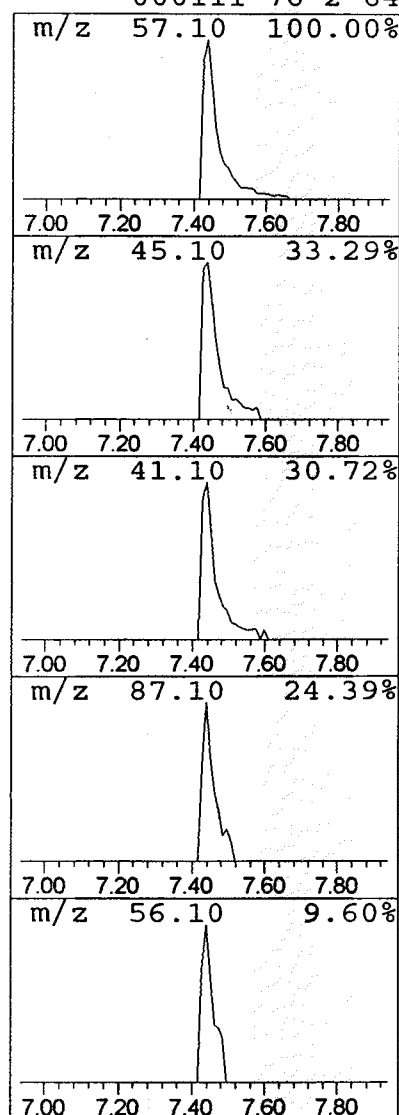
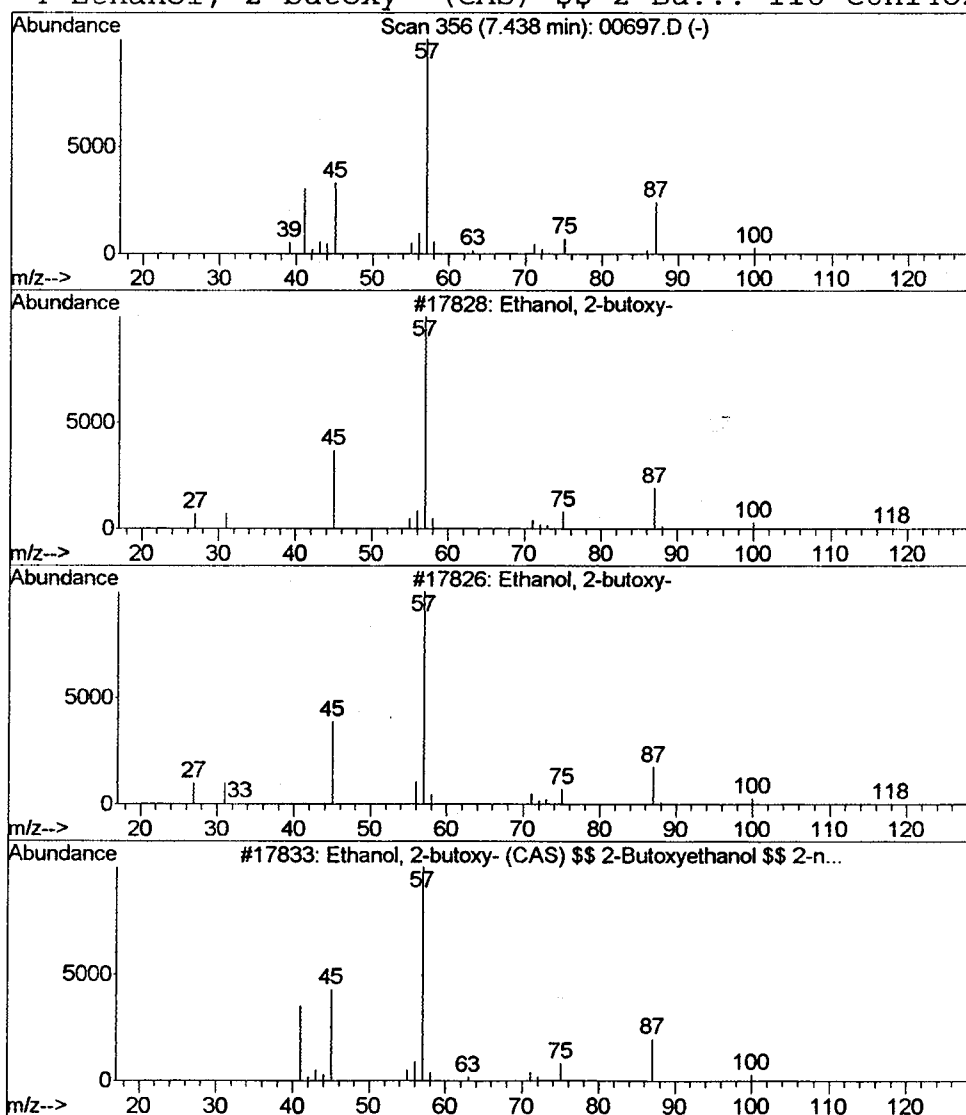
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	0.60 ug/L	194761	1,4-Dichlorobenzene-d4	9.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
3		Ethanol, 2-butoxy- (CAS) \$\$ 2-Bu...	118	C6H14O2	000111-76-2	72
4		Ethanol, 2-butoxy- (CAS) \$\$ 2-Bu...	118	C6H14O2	000111-76-2	64



Library Search Compound Report

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Acq On : 16 Jan 2002 12:31 pm
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Misc : January 16, 2002
MS Integration Params: LSCINT.P

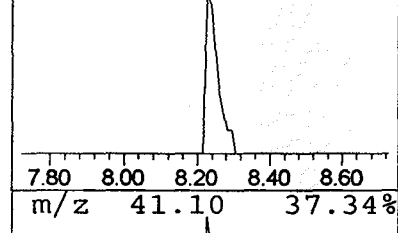
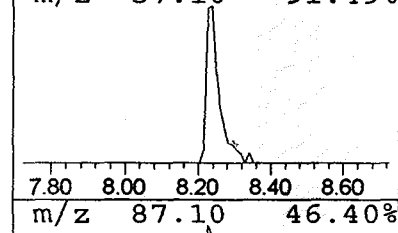
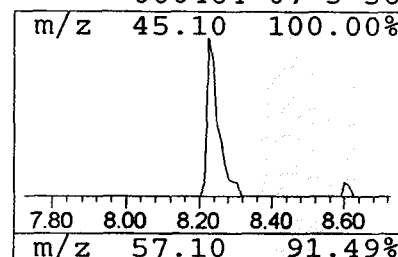
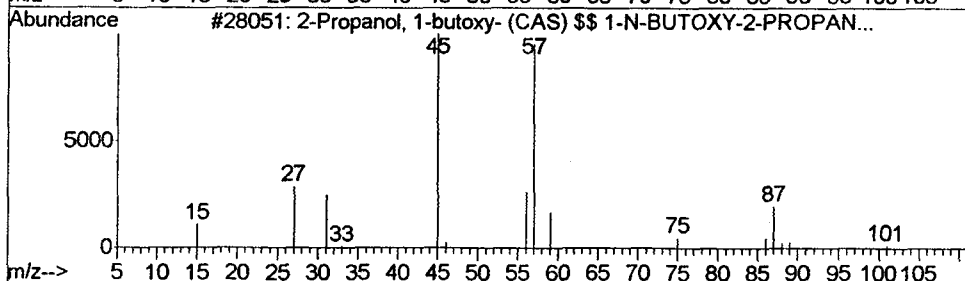
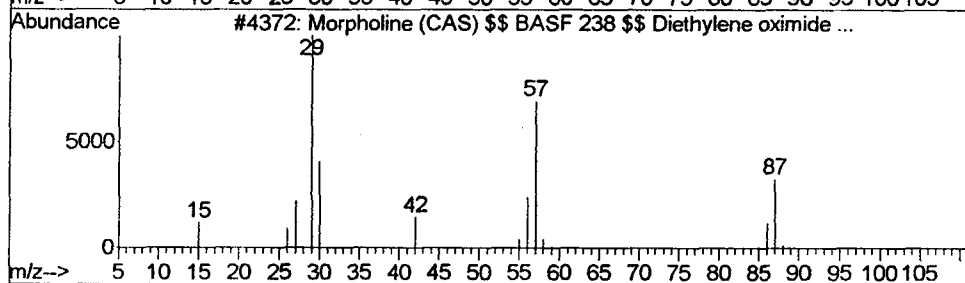
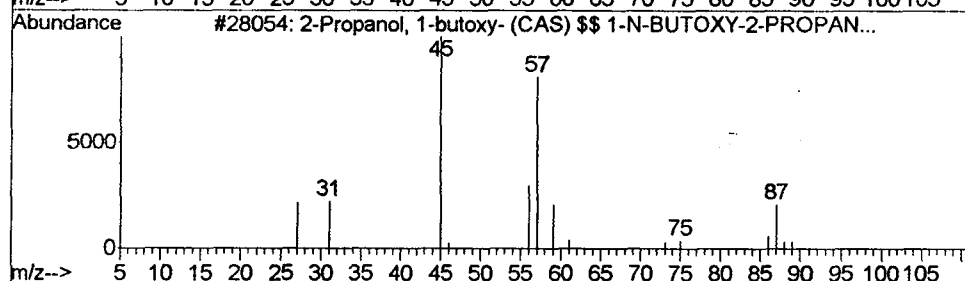
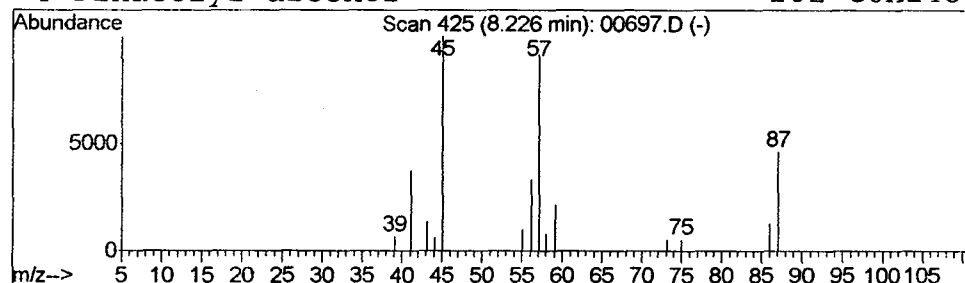
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 2-Propanol, 1-butoxy- (CAS)... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	0.25 ug/L	80592	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-butoxy- (CAS) \$\$ 1...	132	C7H16O2	005131-66-8	74
2			Morpholine (CAS) \$\$ BASF 238 \$\$...	87	C4H9NO	000110-91-8	38
3			2-Propanol, 1-butoxy- (CAS) \$\$ 1...	132	C7H16O2	005131-66-8	38
4			Pinacolyl alcohol	102	C6H14O	000464-07-3	36



Sample Search Compound Report

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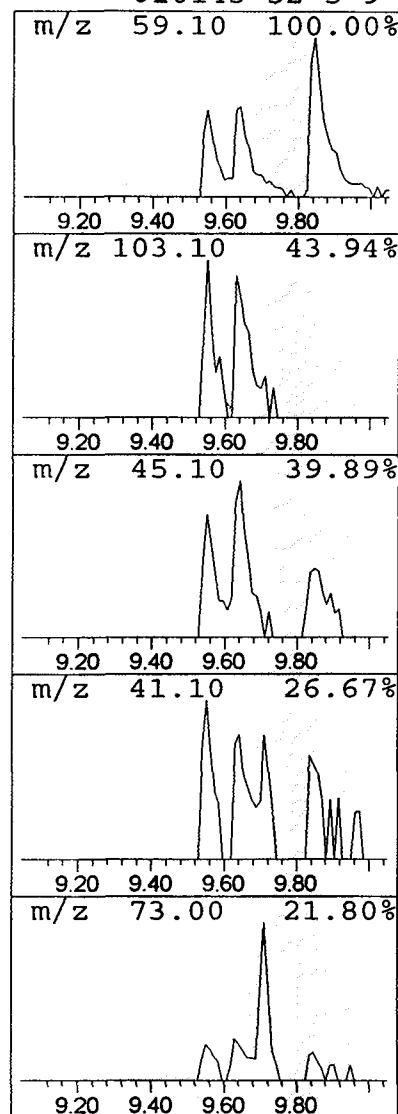
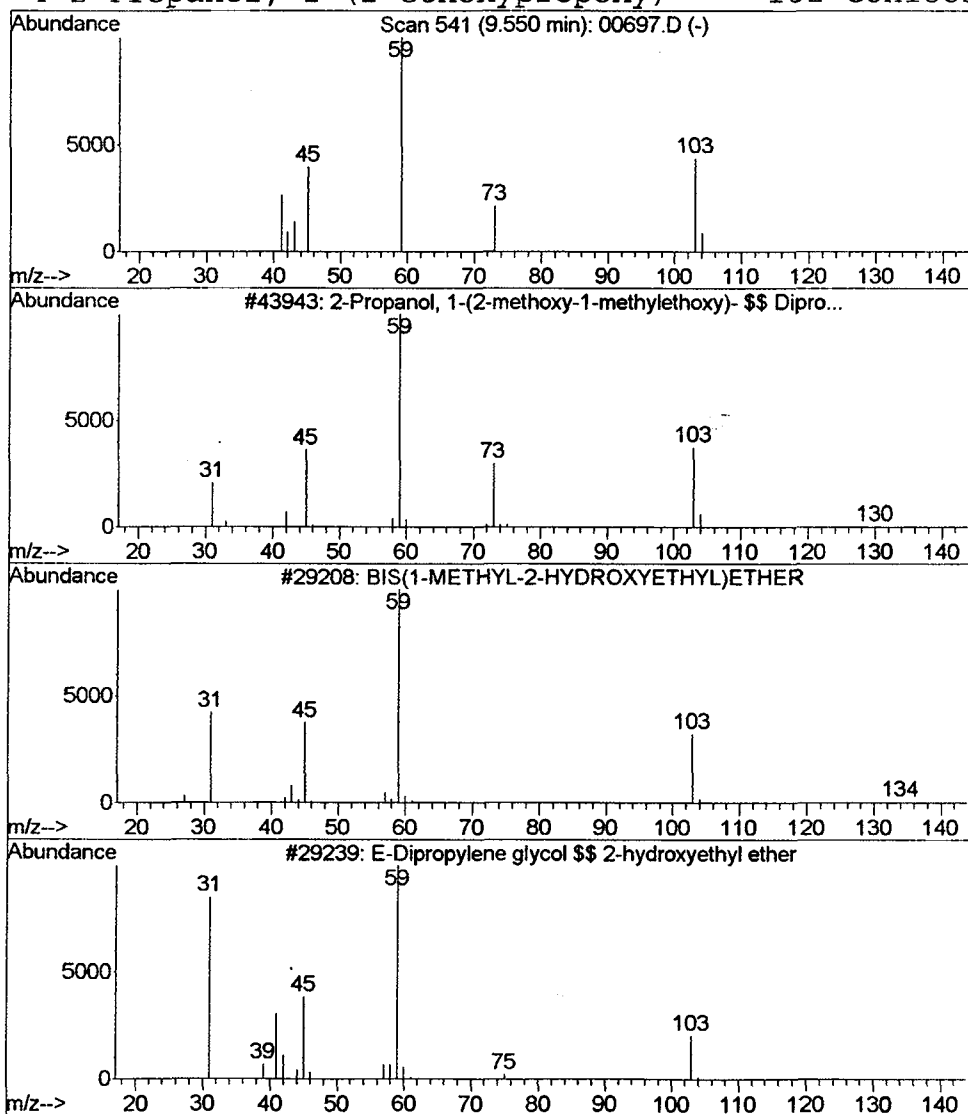
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 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 5 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	0.12 ug/L	40163	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	43
2		BIS(1-METHYL-2-HYDROXYETHYL)ETHER	134	C6H14O3	000000-00-0	9
3		E-Dipropylene glycol \$\$ 2-hydrox...	134	C6H14O3	000000-00-0	9
4		2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	9



Library Search Compound Report

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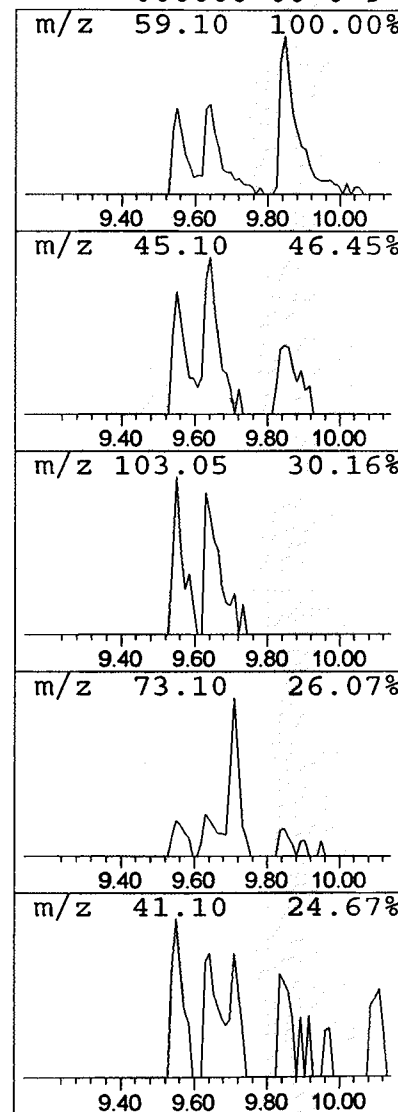
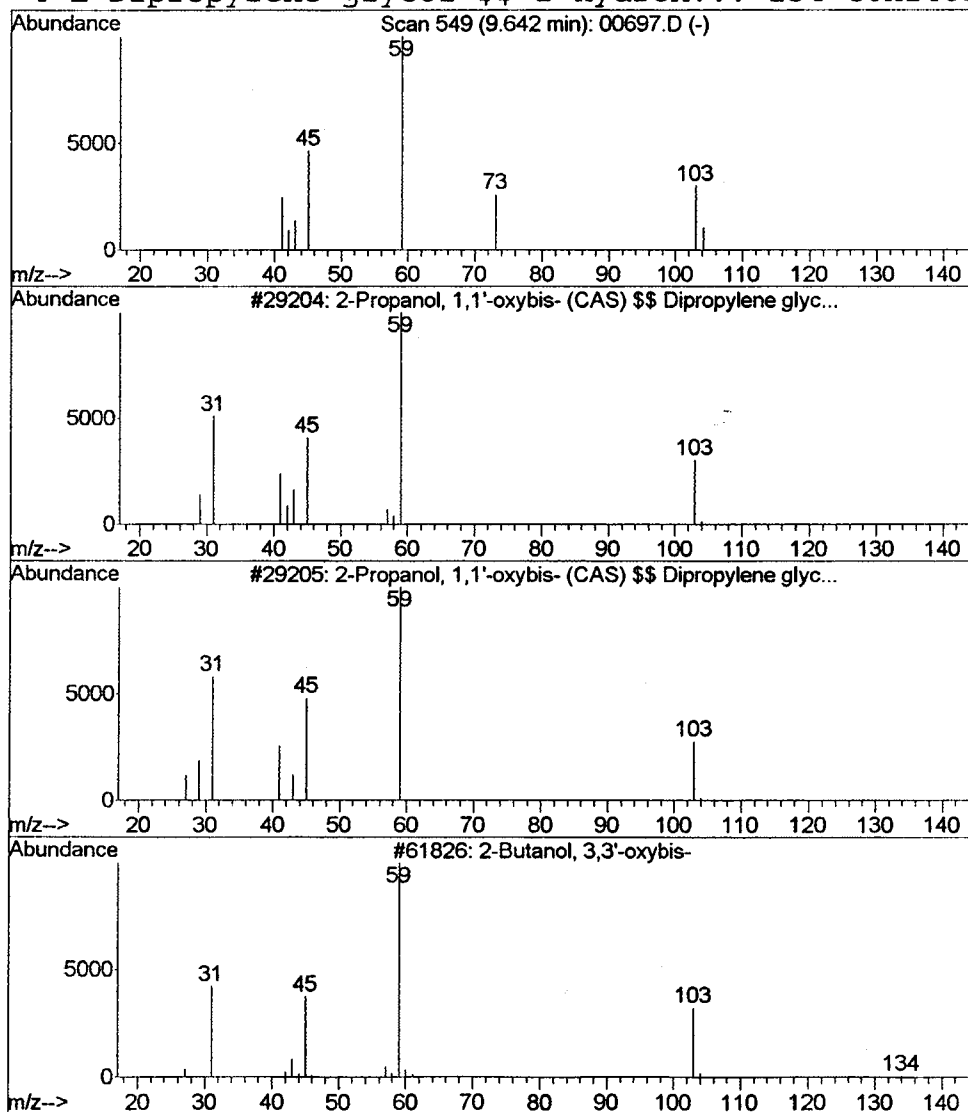
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 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 6 2-Propanol, 1,1'-oxybis- (C... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.64	0.13 ug/L	43232	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1,1'-oxybis- (CAS) \$...	134	C6H14O3	000110-98-5	50
2		2-Propanol, 1,1'-oxybis- (CAS) \$...	134	C6H14O3	000110-98-5	39
3		2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	9
4		E-Dipropylene glycol \$\$ 2-hydrox...	134	C6H14O3	000000-00-0	9



Library Search Compound Report

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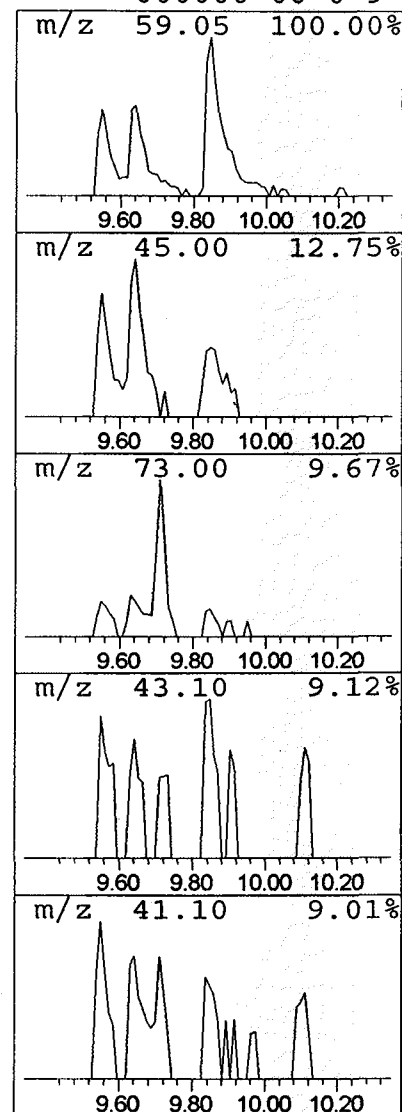
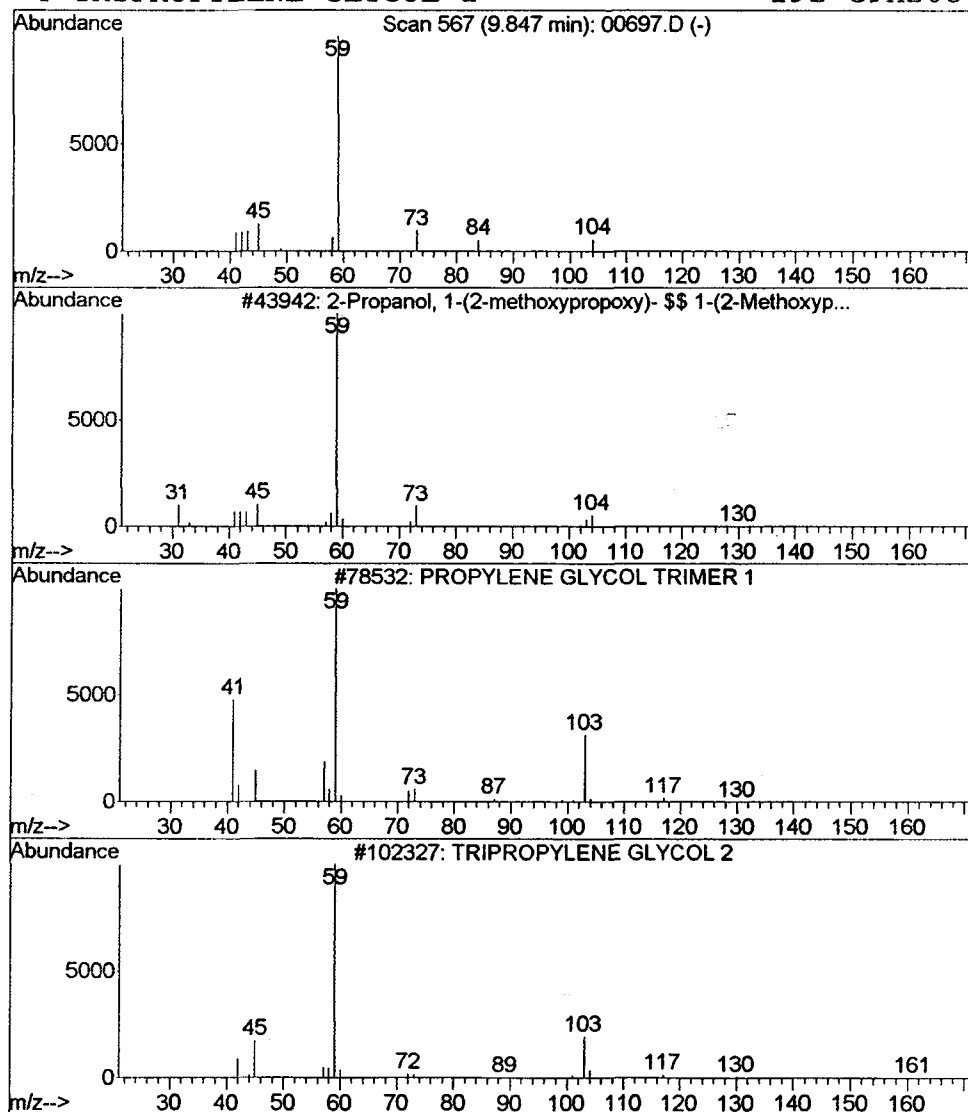
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	0.20 ug/L	65372	1,4-Dichlorobenzene-d4	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	78
2		PROPYLENE GLYCOL TRIMER 1	174	C9H18O3	000000-00-0	9
3		TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	9
4		TRIPROPYLENE GLYCOL 1	192	C9H20O4	000000-00-0	9



Library Search Compound Report

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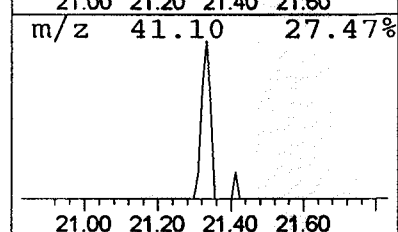
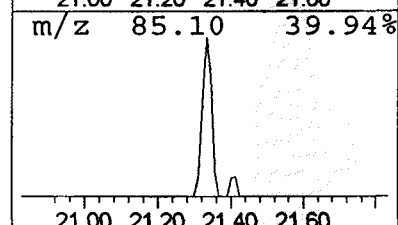
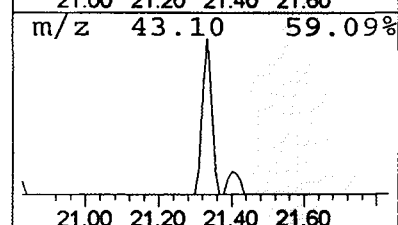
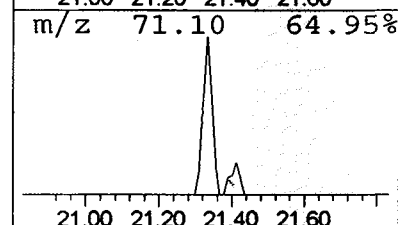
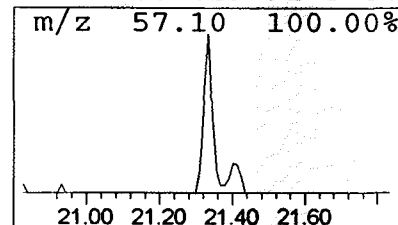
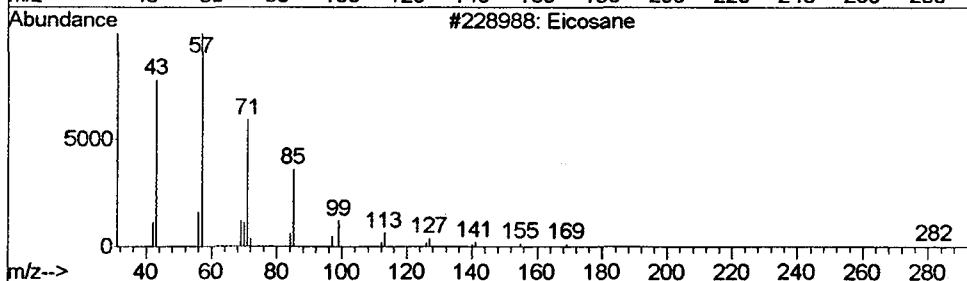
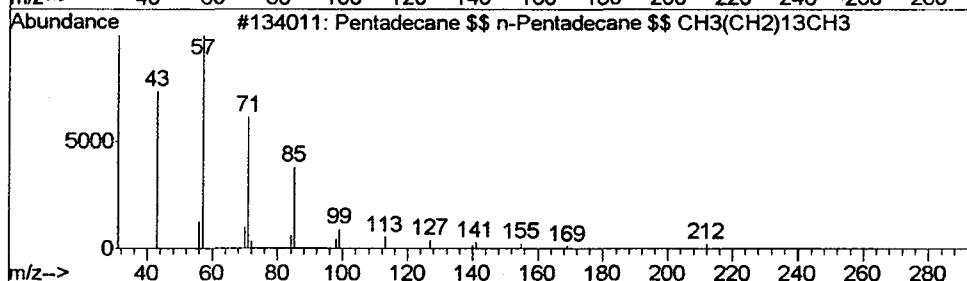
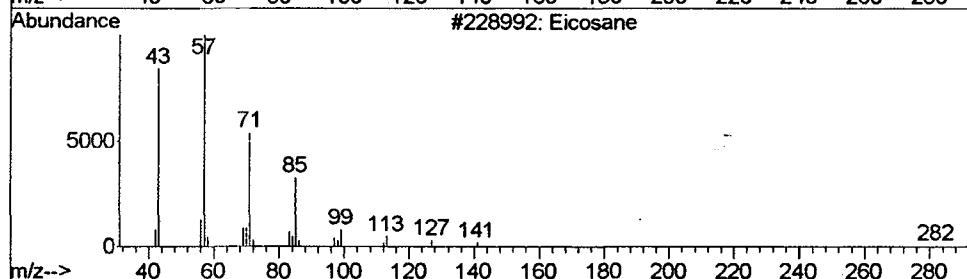
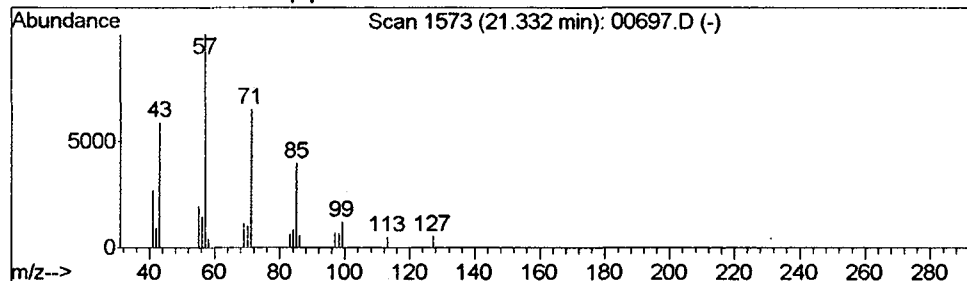
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	0.15 ug/L	84665	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Pentadecane \$\$ n-Pentadecane \$\$...	212	C15H32	000629-62-9	86
3		Eicosane	282	C20H42	000112-95-8	86
4		Nonadecane \$\$ n-Nonadecane	268	C19H40	000629-92-5	86



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
Acq On : 16 Jan 2002 12:31 pm
Sample : 508scan
Misc : January 16, 2002
MS Integration Params: LSCINT.P

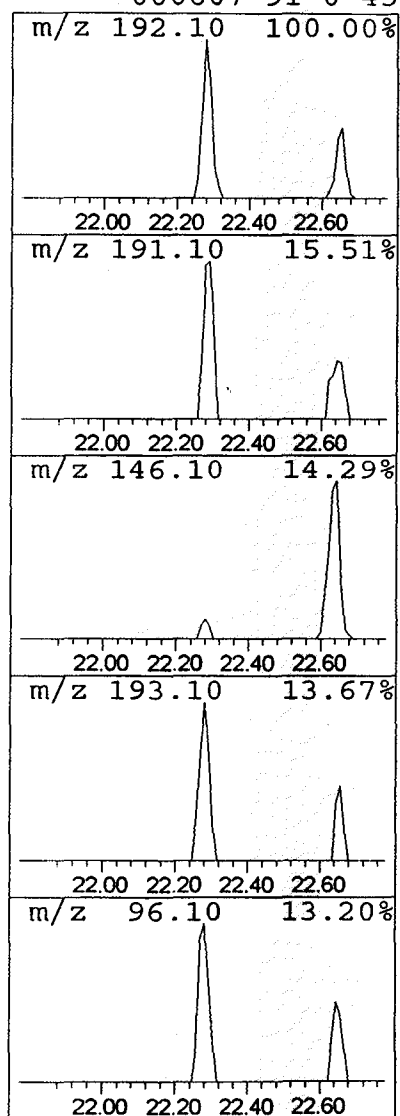
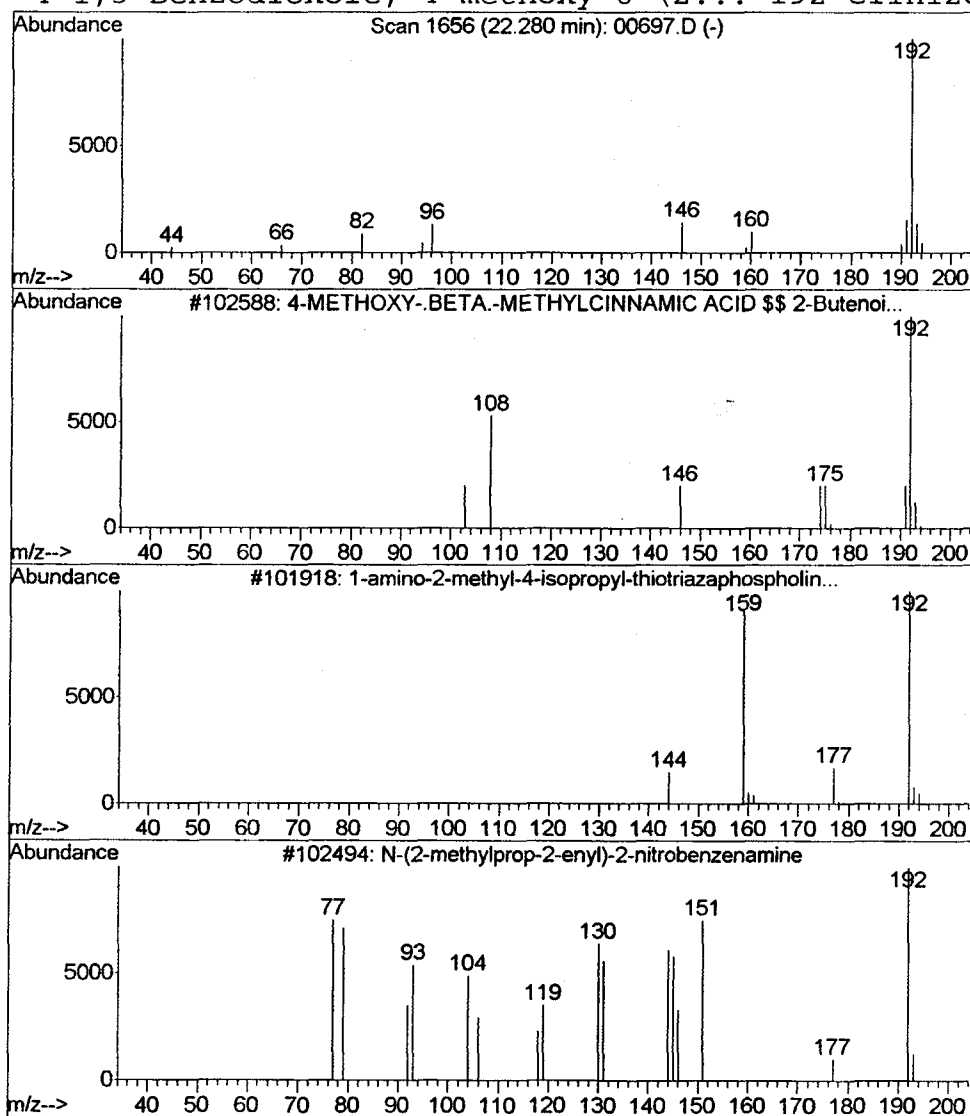
Vial: 3
Operator:
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 9 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.14 ug/L	76551	Phenanthrene-d10	22.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
2			1-amino-2-methyl-4-isopropyl-thi...	192	C5H13N4PS	107264-54-0	50
3			N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	47
4			1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	45



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00697.D
 Acq On : 16 Jan 2002 12:31 pm
 Sample : 508scan
 Misc : January 16, 2002
 MS Integration Params: LSCINT.P

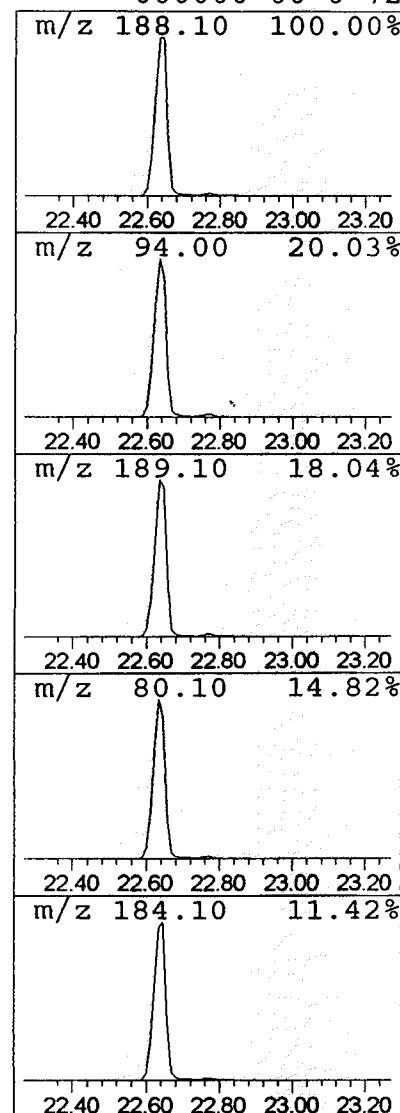
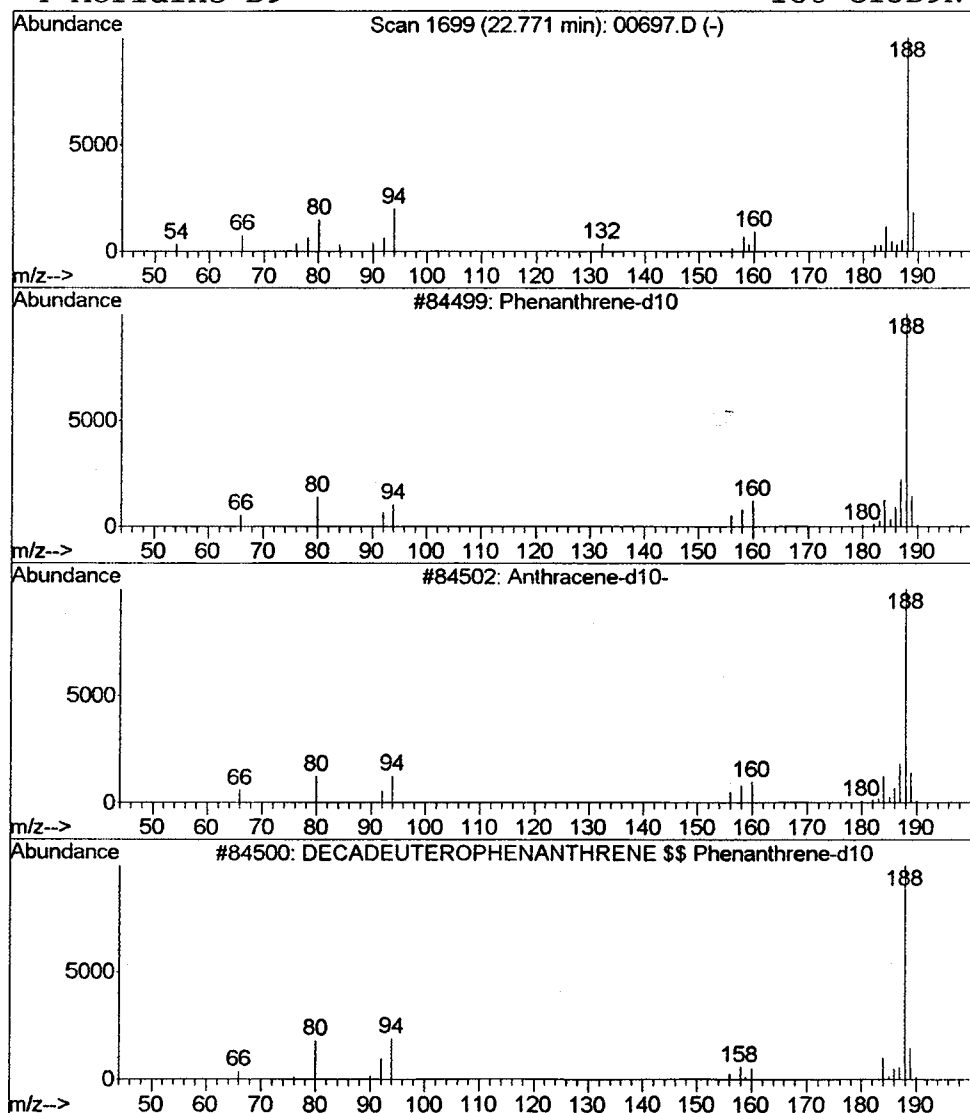
Vial: 3
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 10 Phenanthrene-d10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.32 ug/L	182479	Phenanthrene-d10	22.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene-d10	188	C14D10	001517-22-2	87
2		Anthracene-d10-	188	C14D10	001719-06-8	83
3		DECADEUTEROPHENANTHRENE \$\$ Phena...	188	C14D10	001517-22-2	78
4		Acridine-D9	188	C13D9N	000000-00-0	72



Identification, Identified Compound (200, Summary)

Operator ID: Date Acquired: 16 Jan 2002 12:31 pm
Data File: C:\MSDCHEM\1\5973N\02JAN16\00697.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-Pentyn-1-ol	4.85	0.2	ug/L	58411	1	9.71	6459930	20.0
Acetic acid, 3-[1...	5.89	4.4	ug/L	1414590	1	9.71	6459930	20.0
Ethanol, 2-butoxy	7.44	0.6	ug/L	194761	1	9.71	6459930	20.0
2-Propanol, 1-but...	8.23	0.2	ug/L	80592	1	9.71	6459930	20.0
2-Propanol, 1-(2-...	9.55	0.1	ug/L	40163	1	9.71	6459930	20.0
2-Propanol, 1,1'-...	9.64	0.1	ug/L	43232	1	9.71	6459930	20.0
2-Propanol, 1-(2-...	9.85	0.2	ug/L	65372	1	9.71	6459930	20.0
Eicosane	21.33	0.2	ug/L	84665	4	22.63	11269400	20.0
4-METHOXY-.BETA.-...	22.28	0.1	ug/L	76551	4	22.63	11269400	20.0
Phenanthrene-d10	22.77	0.3	ug/L	182479	4	22.63	11269400	20.0