User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/29/2002 Time: 09:52:26

Sample: AE00701
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/29/02 09:52 Ended: 1/29/02 09:52 Analyst: DLV
Page: 1

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

d-Limonene 98/100 1.7 ng/L CAS 5989-27-5

commercial & flavor use
Secret to why NYC water testers so good!

24350 / 00787
Brown 1/8/2

FB —
616,562

Comments for Sample AE00701 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-29-2002 Time: 09:56:04

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds, except for d-Limonene at an estimated level of 1.7 ug/L and with a fit of 98 out of 100. The recoveries for 15 of the 43 compounds in the LCS Standard were outside of their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 17 08:12:18 2002 Quant Results File: SCAN508.RES

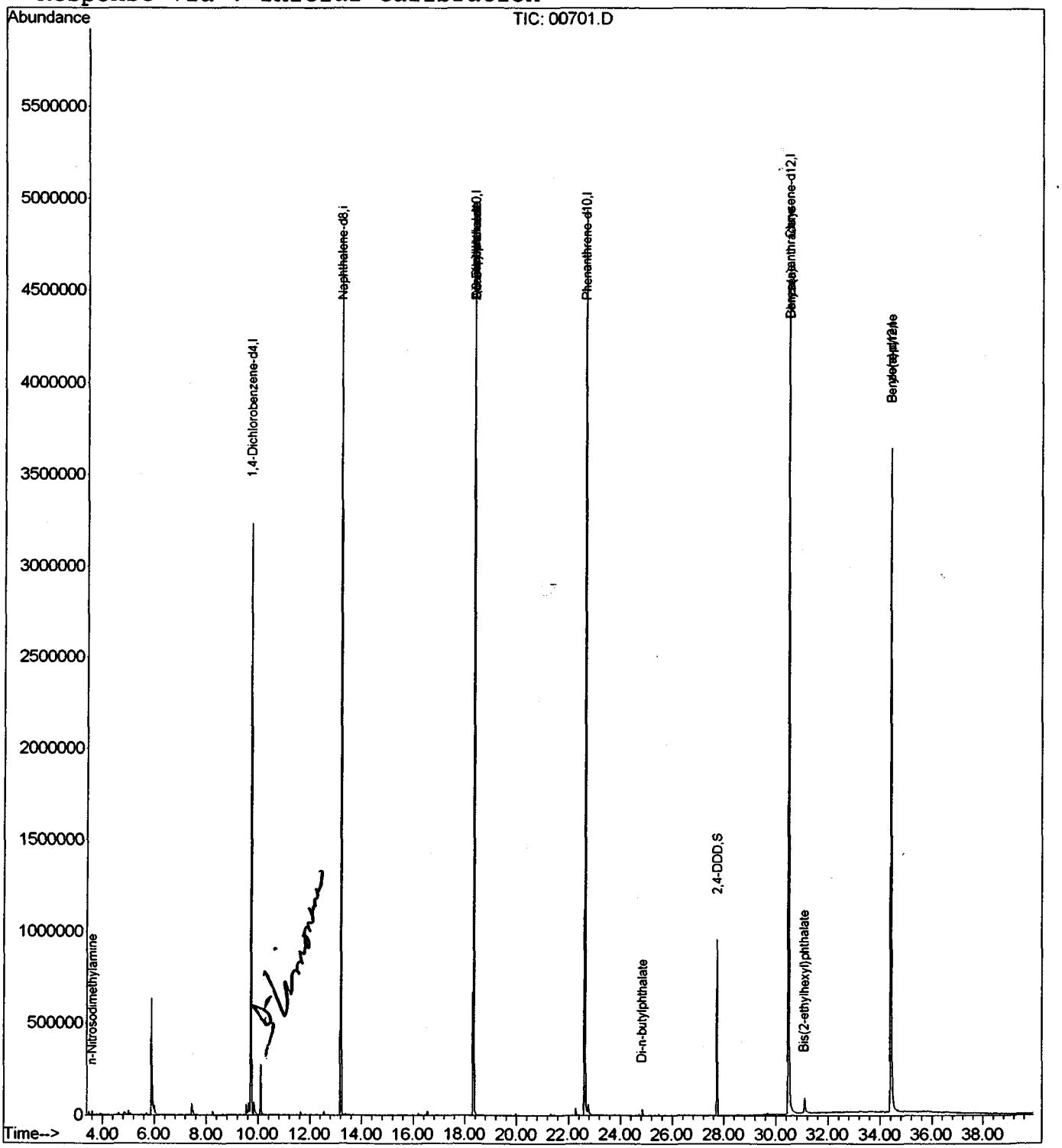
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration
DataAcq Meth : SCAN508

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1093872	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	4622818	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2421298	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4100961	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3715484	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2786372	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	362952	5.60	ug/L	0.00
Spiked Amount 5.000			Recovery = 112.00%			
Target Compounds						Qvalue
2) n-Nitrosodimethylamine	3.60	74	8567	0.18	ug/L #	17
20) Dimethylphthalate	18.34	163	390914	2.44	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	304348	9.76	ug/L #	17
35) Di-n-butylphthalate	24.85	149	39705	0.15	ug/L	97
41) Benzo(a)anthracene	30.50	228	8685	0.04	ug/L #	56
42) Bis(2-ethylhexyl)phthalate	31.11	149	86763	1.02	ug/L	98
43) Chrysene	30.50	228	8684	0.04	ug/L #	53
48) Benzo(a)pyrene	34.42	252	10162	0.06	ug/L #	1

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

Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 17 8:12 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



Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 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

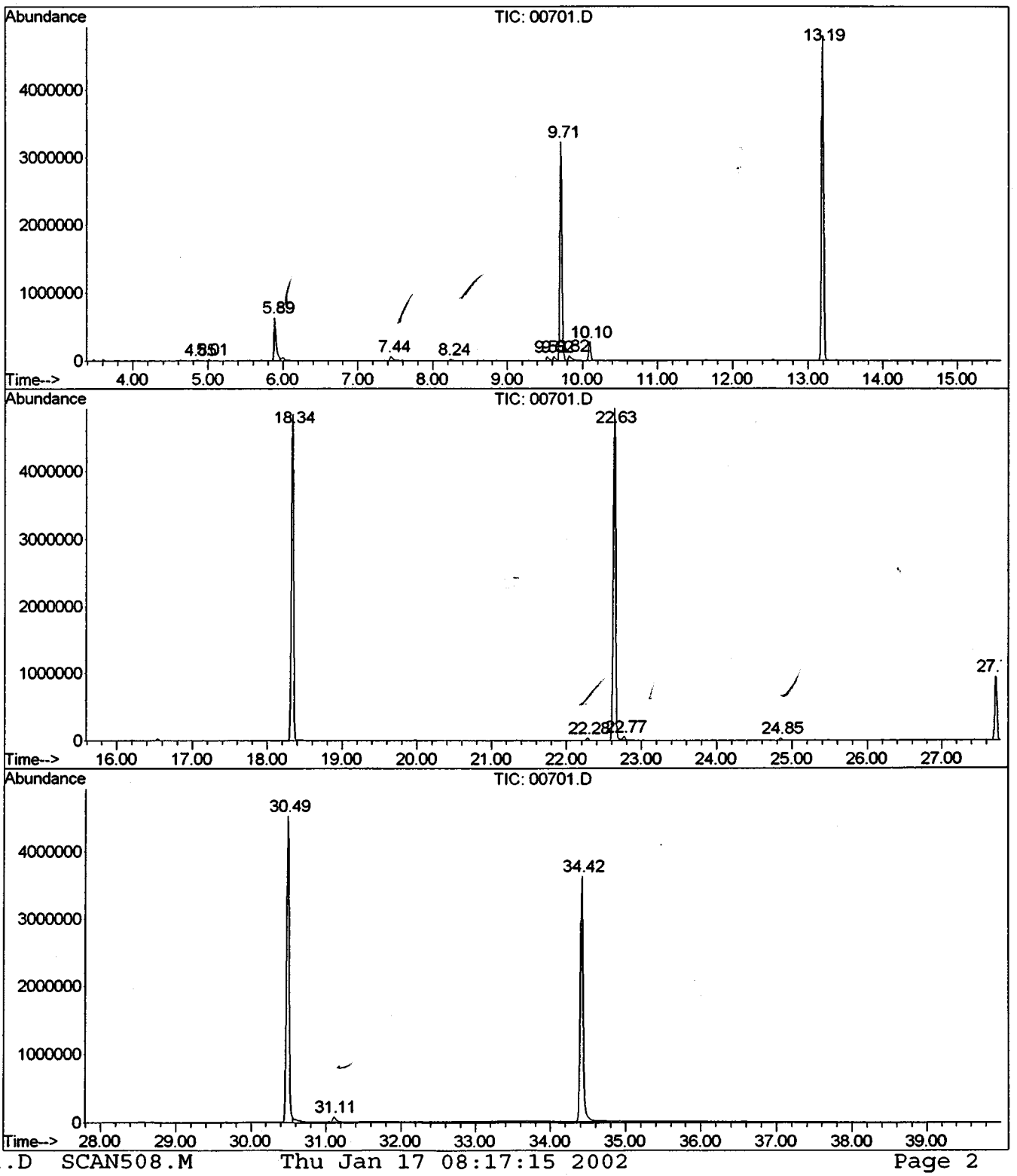
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.846	119	129	139	rBV6	15552	61092	0.56%	0.100%
2	5.006	139	143	149	rVB	26257	47352	0.43%	0.077%
3	5.885	215	220	227	rBV	634380	1244781	11.35%	2.037%
4	7.438	353	356	367	rBV	63807	174390	1.59%	0.285%
5	8.237	423	426	433	rVB	23150	54177	0.49%	0.089%
6	9.527	535	539	545	rBV	55575	133163	1.21%	0.218%
7	9.619	545	547	551	rVV	59428	122446	1.12%	0.200%
8	9.710	551	555	561	rVV	3230375	6179918	56.37%	10.113%
9	9.824	561	565	583	rVB	70769	215217	1.96%	0.352%
10	10.098	583	589	593	rBV	272002	516996	4.72%	0.846%
11	13.192	855	860	865	rBV	4793700	8843758	80.67%	14.472%
12	18.341	1305	1311	1315	rBV	4851962	9830359	89.67%	16.087%
13	22.280	1653	1656	1661	rVB2	40984	77034	0.70%	0.126%
14	22.634	1681	1687	1693	rBV2	4936151	10871735	99.17%	17.791%
15	22.771	1693	1699	1703	rVB	53285	135502	1.24%	0.222%
16	24.849	1877	1881	1887	rVB	35458	64603	0.59%	0.106%
17	27.726	2127	2133	2139	rVB	956172	1752429	15.99%	2.868%
18	30.489	2369	2375	2381	rBV2	4522259	10962790	100.00%	17.940%
19	31.105	2425	2429	2441	rVV	80393	255732	2.33%	0.418%
20	34.416	2713	2719	2751	rBV	3623282	9565833	87.26%	15.654%

Sum of corrected areas: 61109307

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN16\00701.D
Operator :
Acquired : 16 Jan 2002 3:07 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508scan
Misc Info : January 16, 2002
Vial Number: 1
Quant File :SCAN508.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

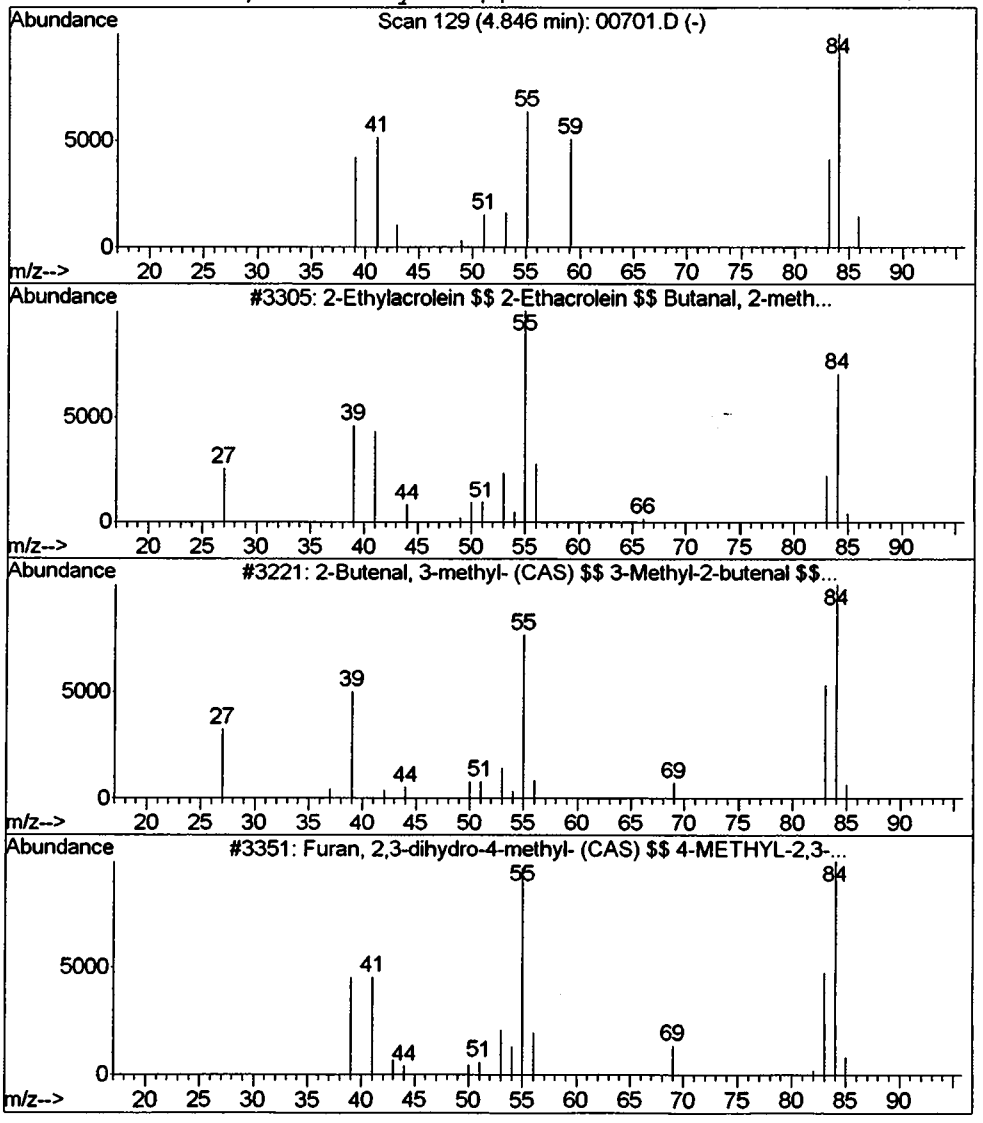
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

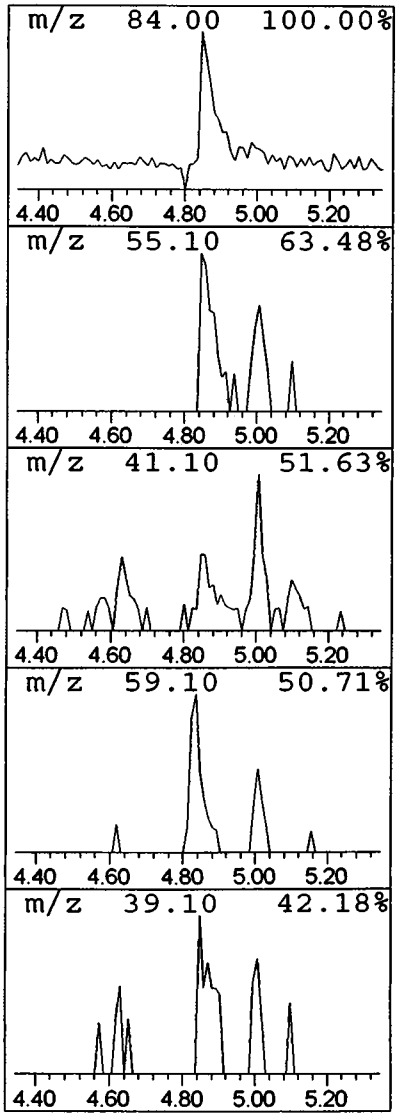
****

Peak Number 1 2-Ethylacrolein $$ 2-Ethacr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	0.20 ug/L	61092	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylacrolein $$ 2-Ethacrolein...	84	C5H8O	000922-63-4	64
2	2-Butenal, 3-methyl- (CAS) $$ 3-...	84	C5H8O	000107-86-8	59
3	Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	59
4	2-Butenal, 3-methyl- $$ Crotonal...	84	C5H8O	000107-86-8	59





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

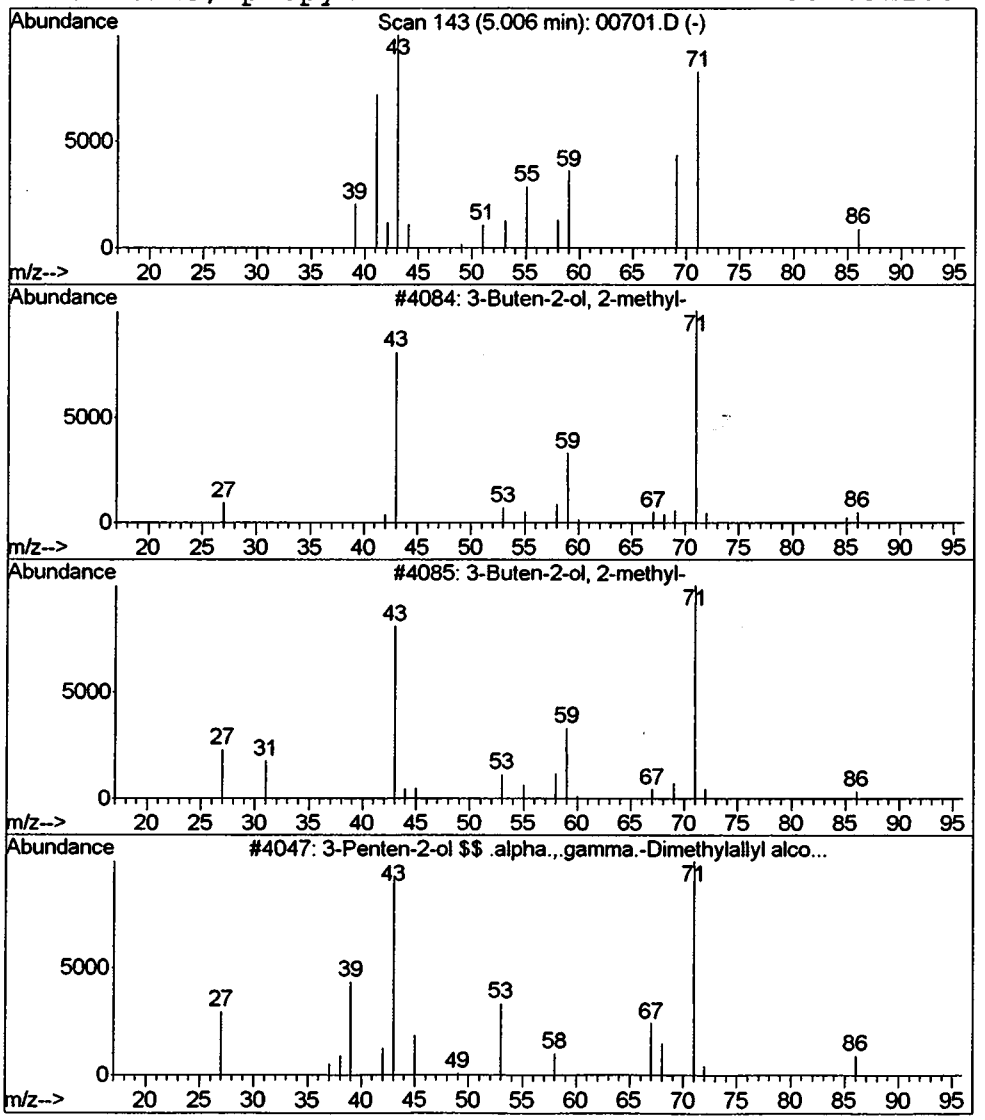
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

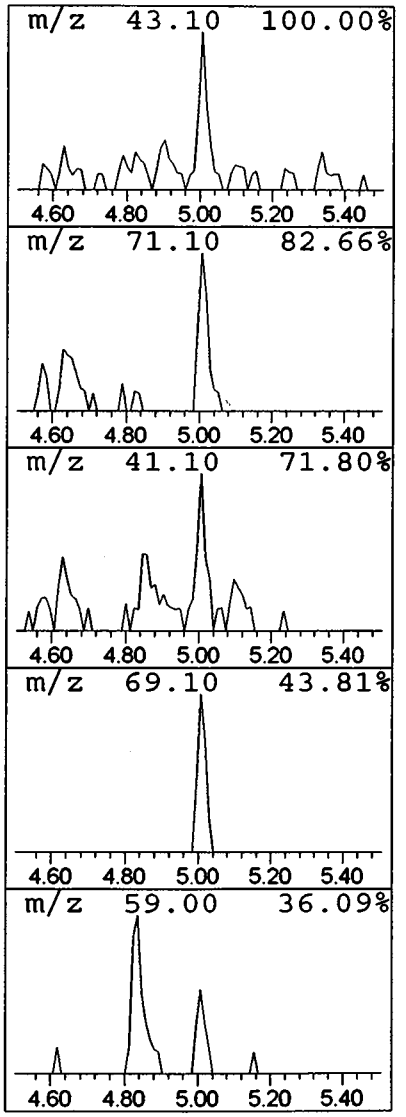
****

Peak Number 2 3-Buten-2-ol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.15 ug/L	47352	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	39
3	3-Penten-2-ol $$ .alpha.,.gamma....	86	C5H10O	001569-50-2	38
4	Oxirane, propyl-	86	C5H10O	001003-14-1	38





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

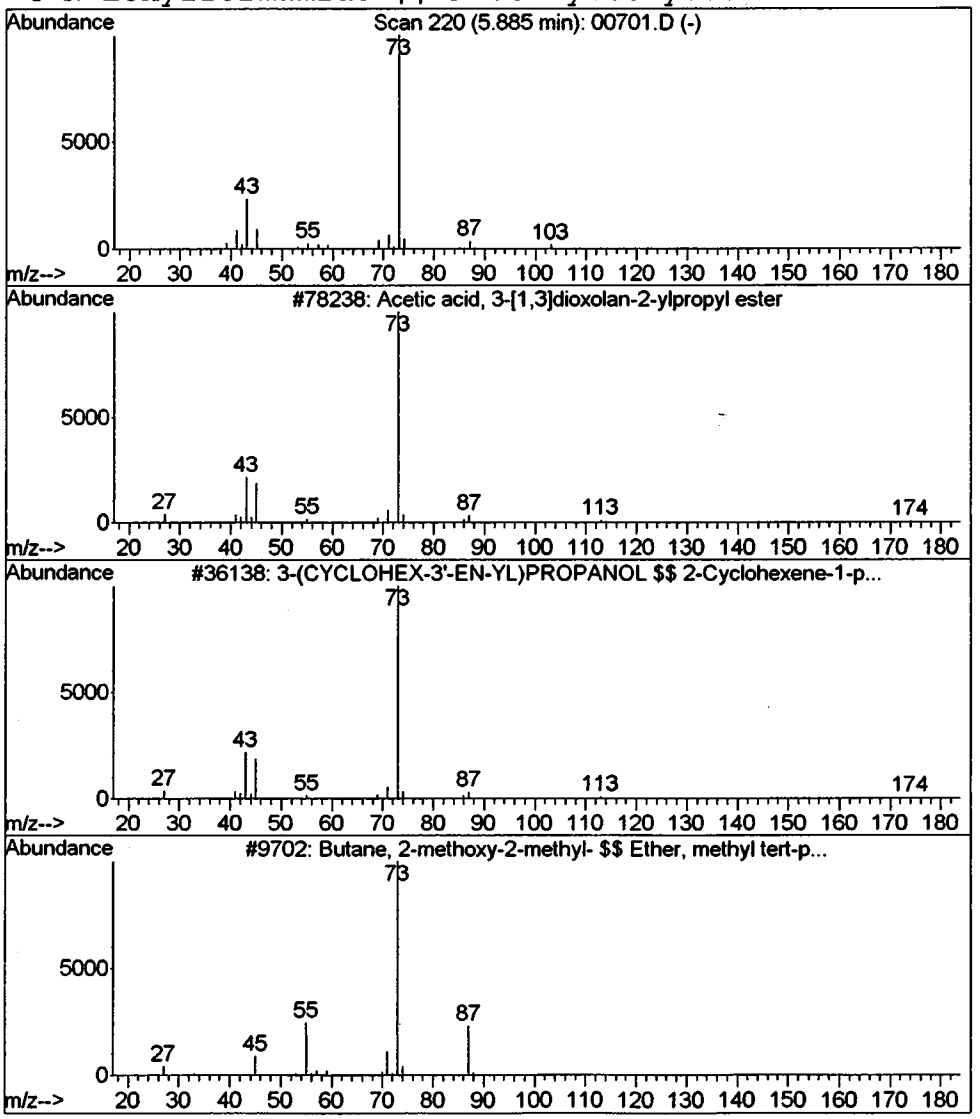
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

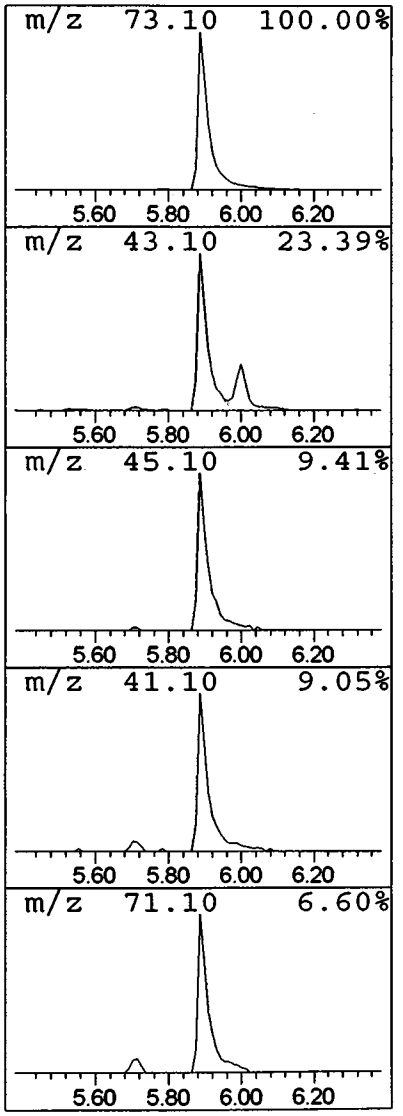
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.03 ug/L	1244780	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 $$...	174	C8H14O4	015745-87-6	33
3	Butane, 2-methoxy-2-methyl- $$ E...	102	C6H14O	000994-05-8	33
4	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

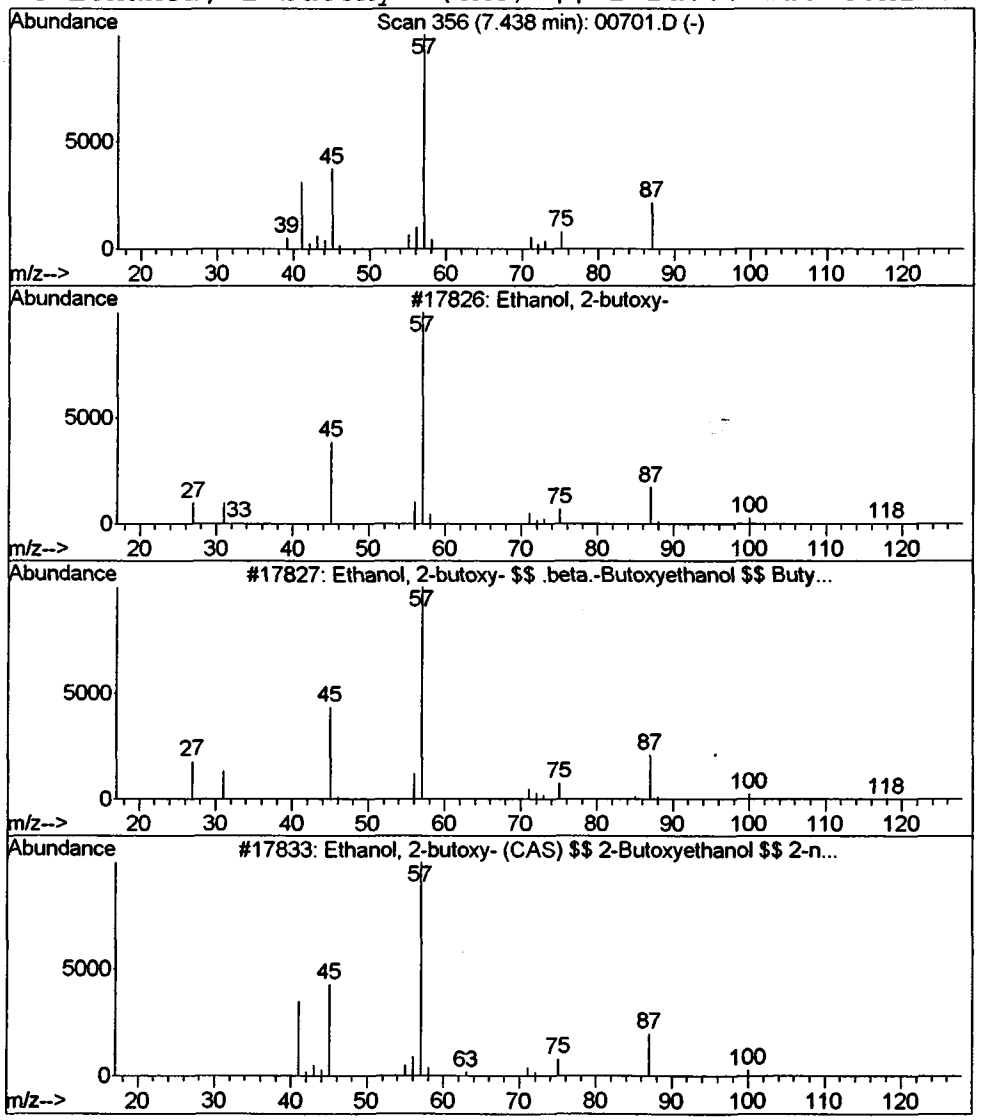
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

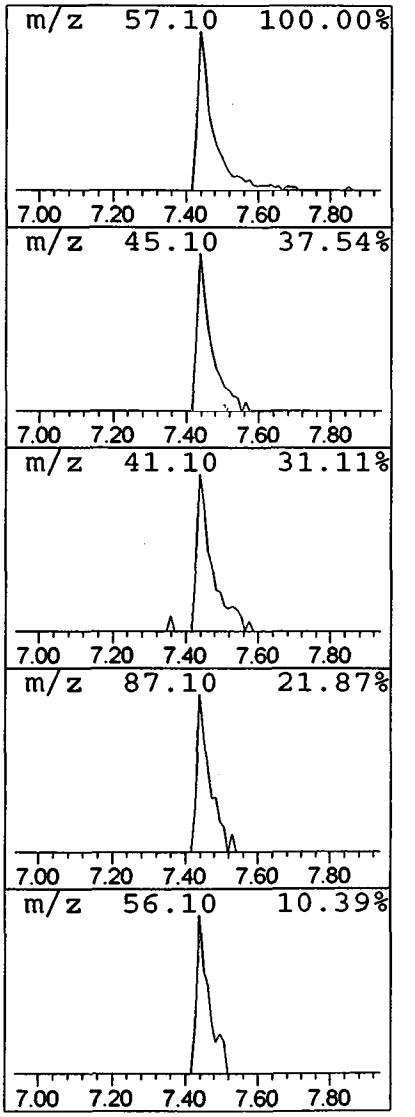
****

Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	0.56 ug/L	174390	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- $$ .beta.-But...	118	C6H14O2	000111-76-2	83
3	Ethanol, 2-butoxy- (CAS) $$ 2-Bu...	118	C6H14O2	000111-76-2	78
4	Ethanol, 2-butoxy- (CAS) $$ 2-Bu...	118	C6H14O2	000111-76-2	78





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

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

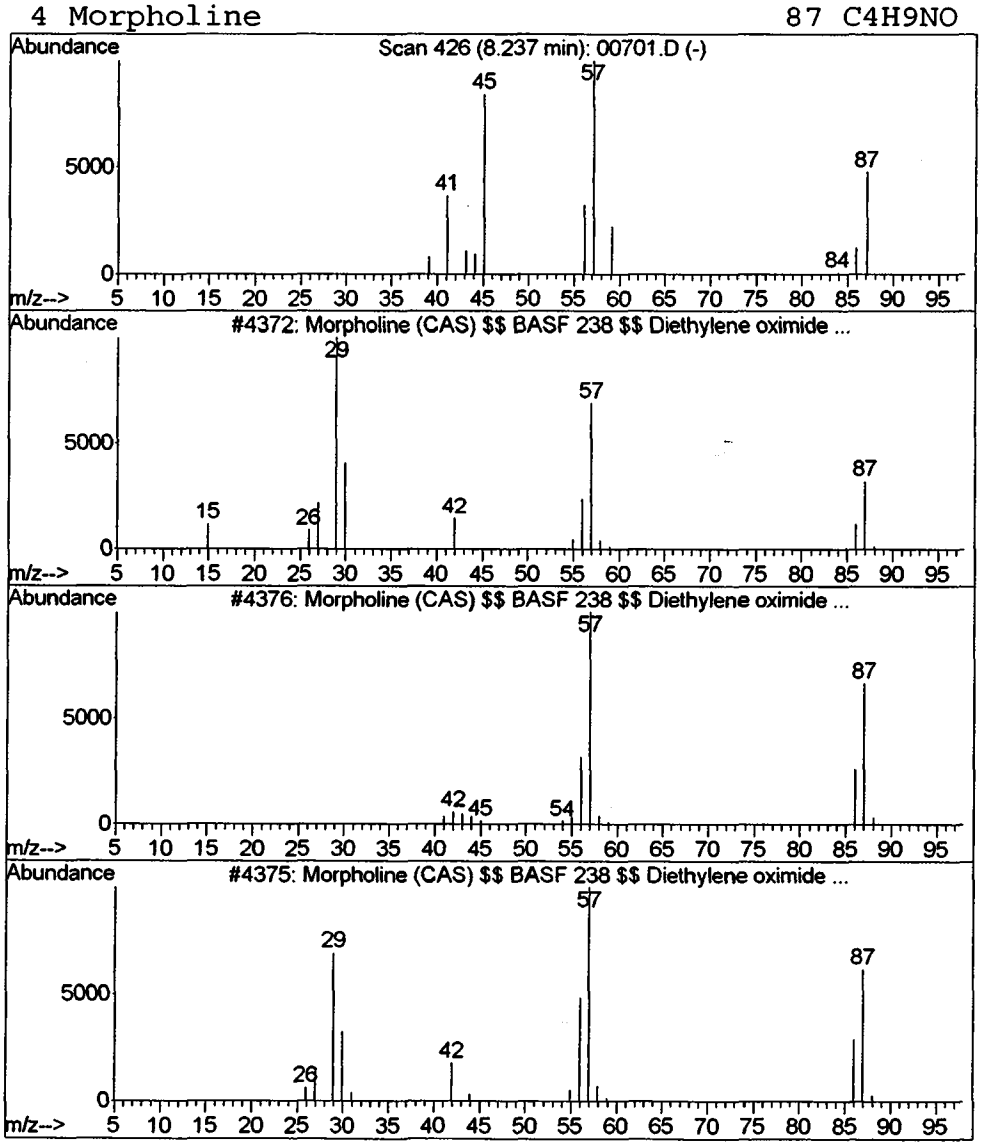
****

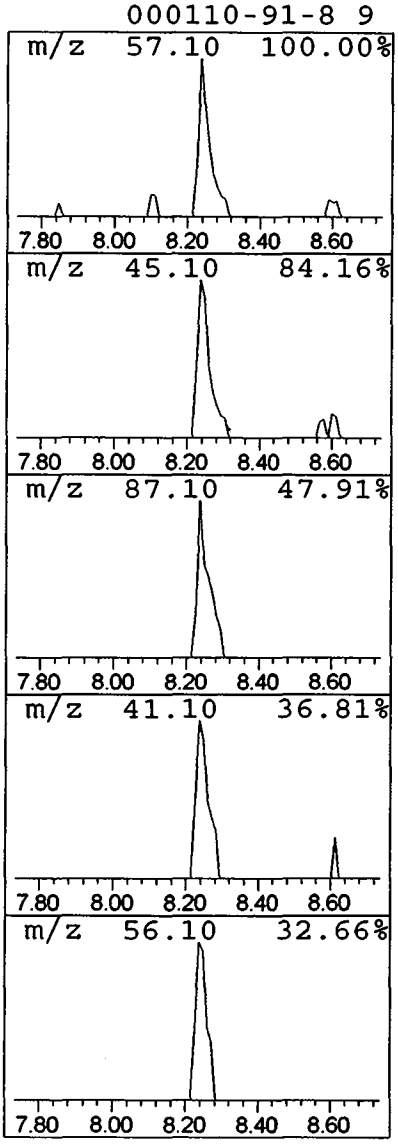
Peak Number 5 Morpholine (CAS) $$ BASF 23... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	0.18 ug/L	54177	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine (CAS) $$ BASF 238 $$ ...	87	C4H9NO	000110-91-8	25
2	Morpholine (CAS) $$ BASF 238 $$ ...	87	C4H9NO	000110-91-8	9
3	Morpholine (CAS) $$ BASF 238 $$ ...	87	C4H9NO	000110-91-8	9
4	Morpholine	87	C4H9NO	000110-91-8	9

NO GOOD MATCH





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

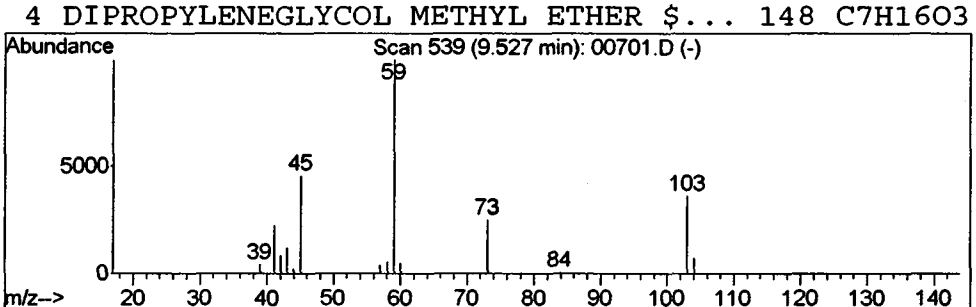
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

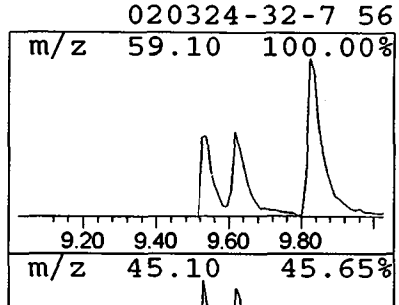
****

Peak Number 6 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	0.43 ug/L	133163	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	64
3	BIS(1-METHYL-2-HYDROXYETHYL)ETHER	134	C6H14O3	000000-00-0	64
4	DIPROPYLENEGLYCOL METHYL ETHER $...	148	C7H16O3	020324-32-7	56





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

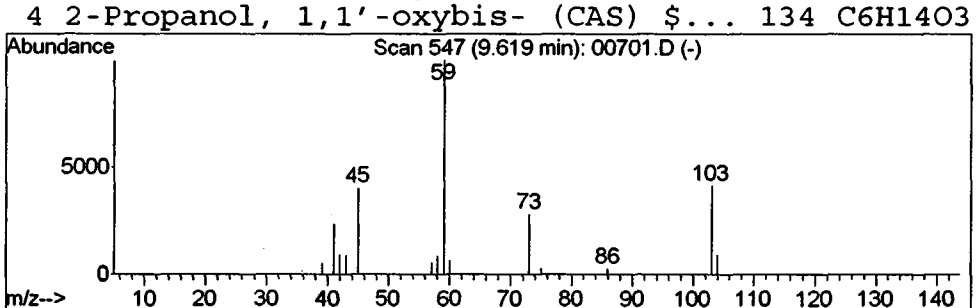
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

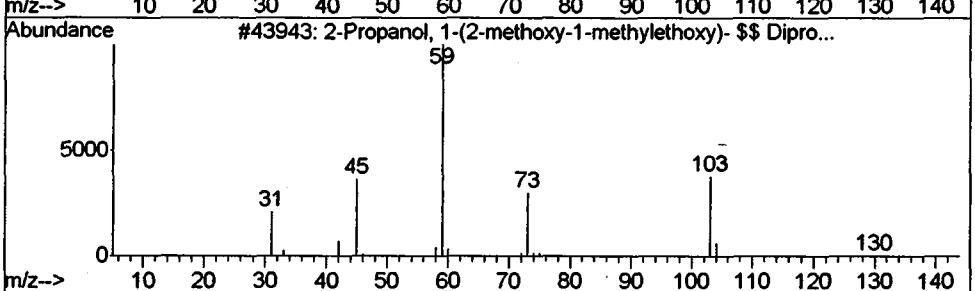
****

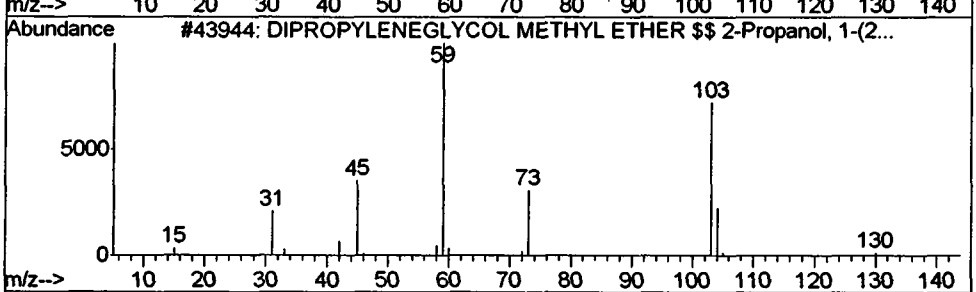
Peak Number 7 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

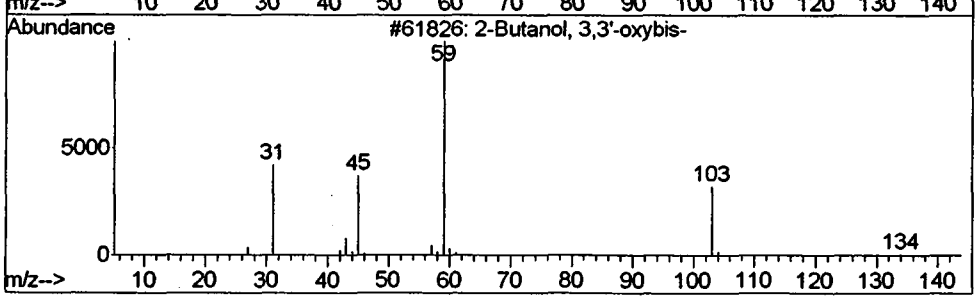
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	0.40 ug/L	122446	1,4-Dichlorobenzene-d4	9.71

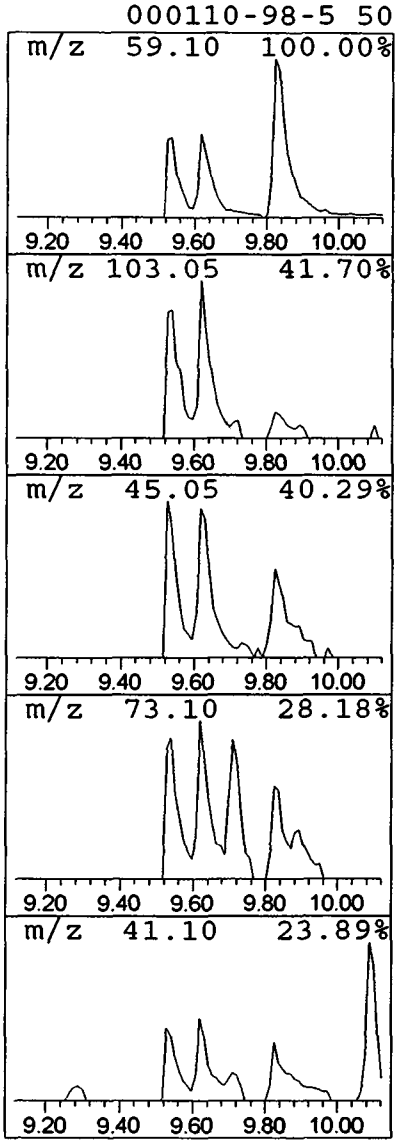
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	DIPROPYLENEGLYCOL METHYL ETHER $...	148	C7H16O3	020324-32-7	72
3	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	50
4	2-Propanol, 1,1'-oxybis- (CAS) $...	134	C6H14O3	000110-98-5	50











Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

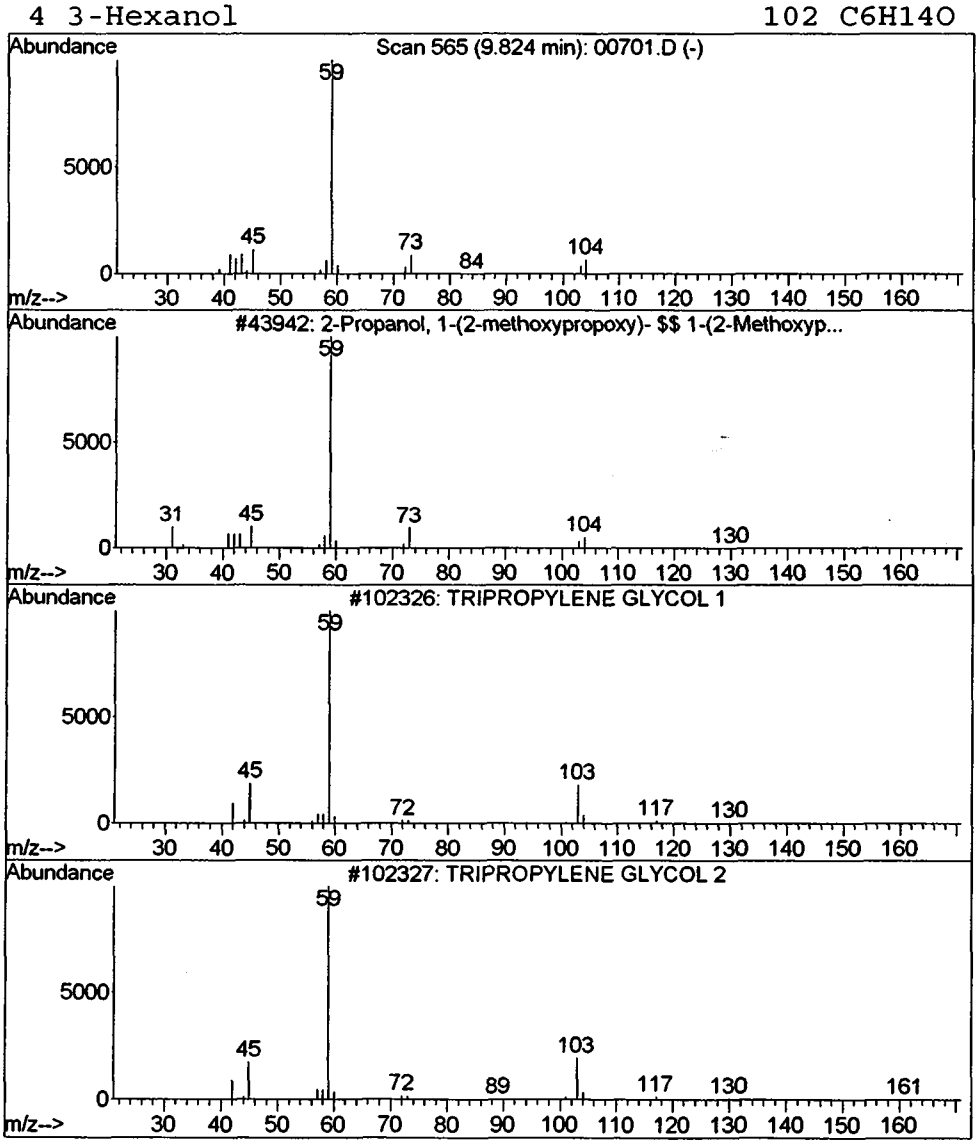
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

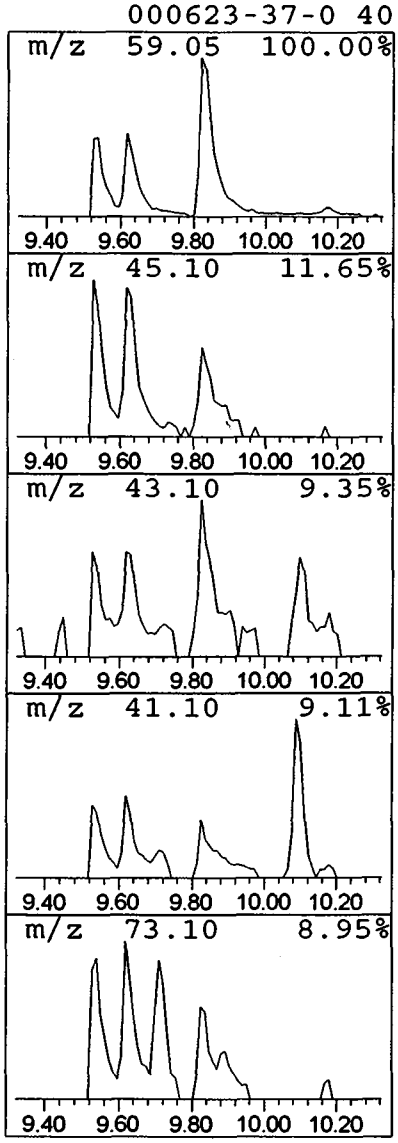
****

Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	0.70 ug/L	215217	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	78
2	TRIPROPYLENE GLYCOL 1	192	C9H20O4	000000-00-0	64
3	TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	56
4	3-Hexanol	102	C6H14O	000623-37-0	40





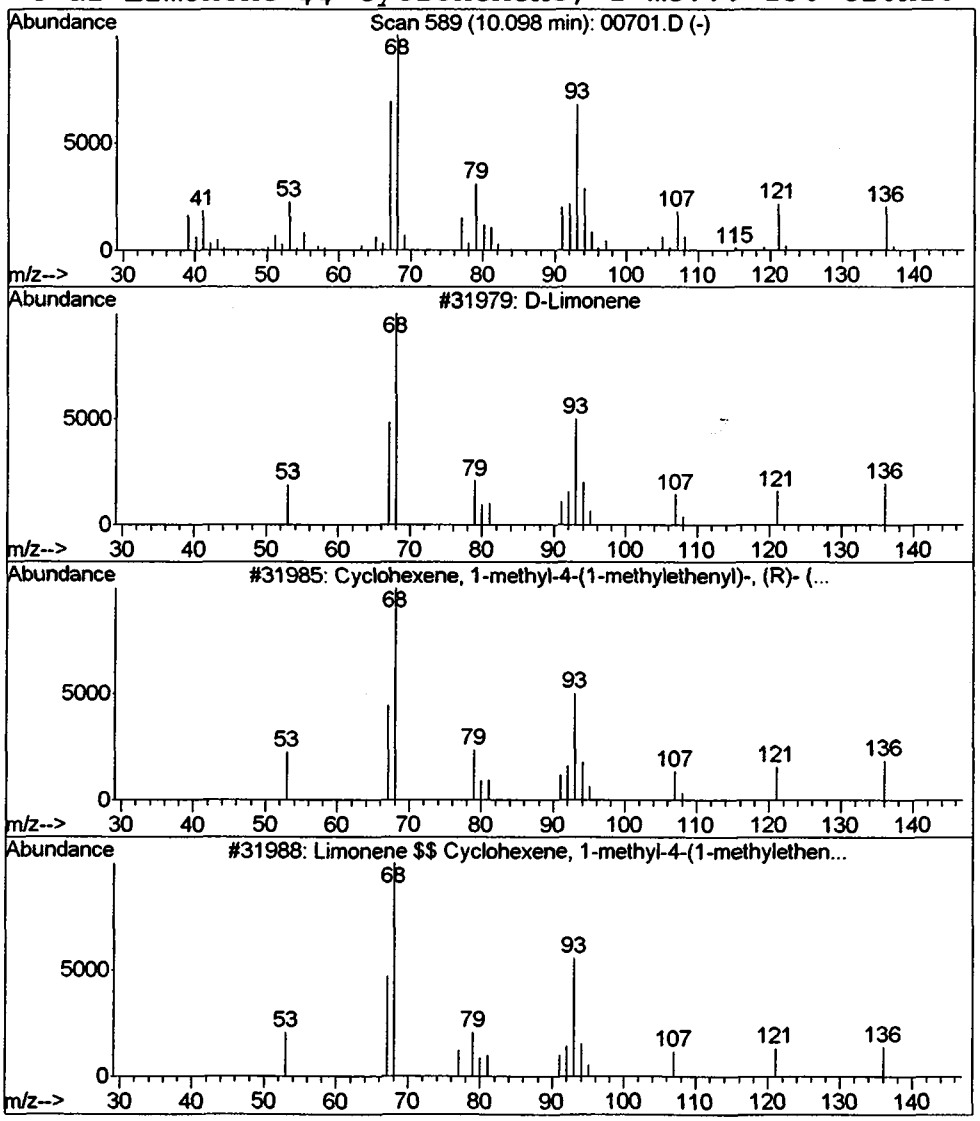
```
Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D          Vial: 1
Acq On    : 16 Jan 2002    3:07 pm                    Operator:
Sample    : 508scan                                   Inst    : Instrumen
Misc      : January 16, 2002                          Multiplr: 1.00
MS Integration Params: LSCINT.P

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

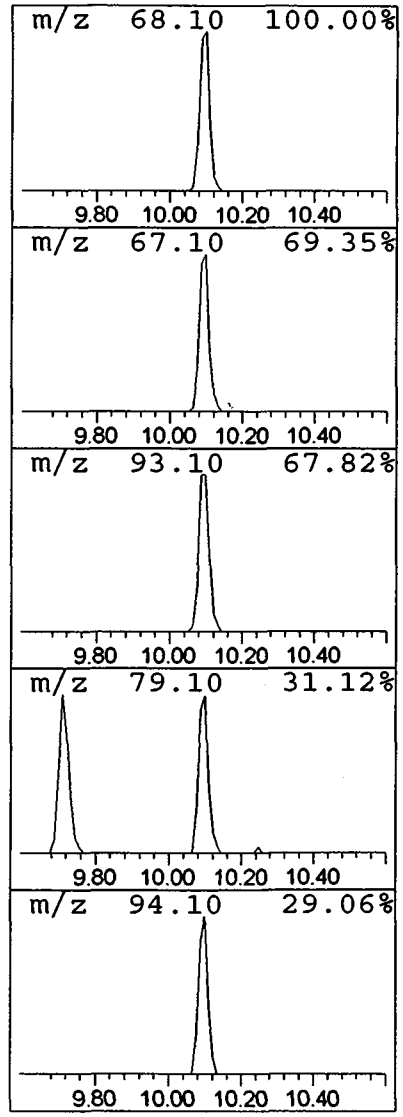
****

Peak Number 9 D-Limonene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	1.67 ug/L	516996	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-27-5	97
3	Limonene $$ Cyclohexene, 1-methy...	136	C10H16	000138-86-3	97
4	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	97





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

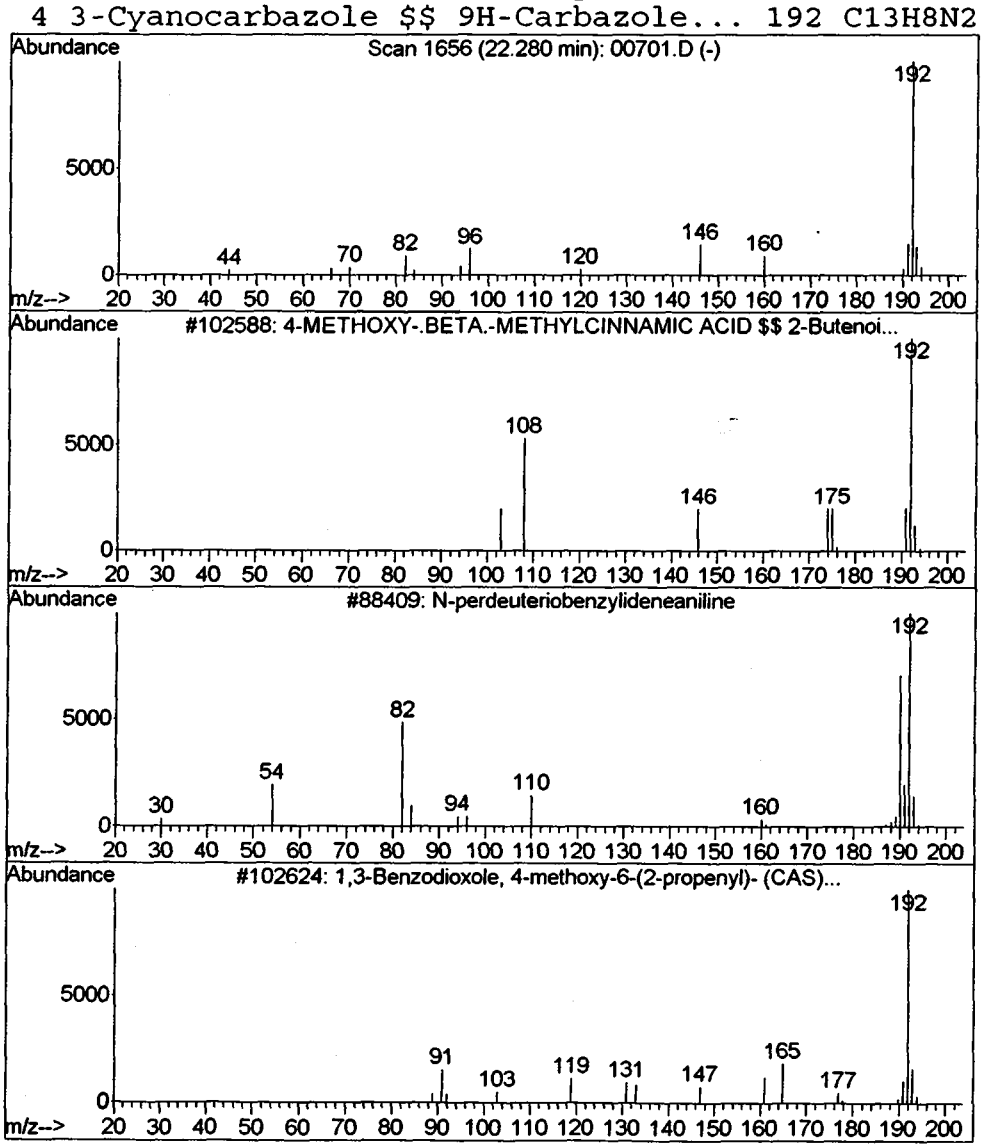
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

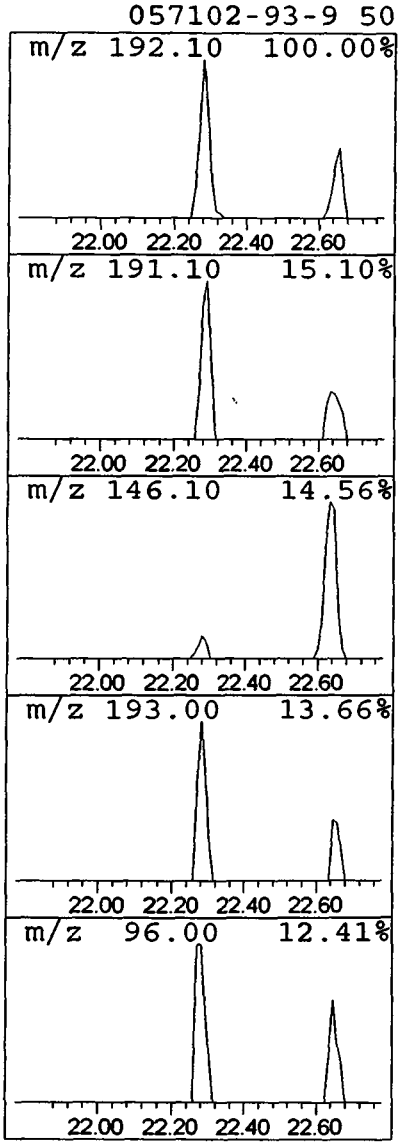
****

Peak Number 10 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.14 ug/L	77034	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	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	64
3	1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	58
4	3-Cyanocarbazole $$ 9H-Carbazole...	192	C13H8N2	057102-93-9	50





Data File : C:\MSDCHEM\1\5973N\02JAN16\00701.D Vial: 1
Acq On : 16 Jan 2002 3:07 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

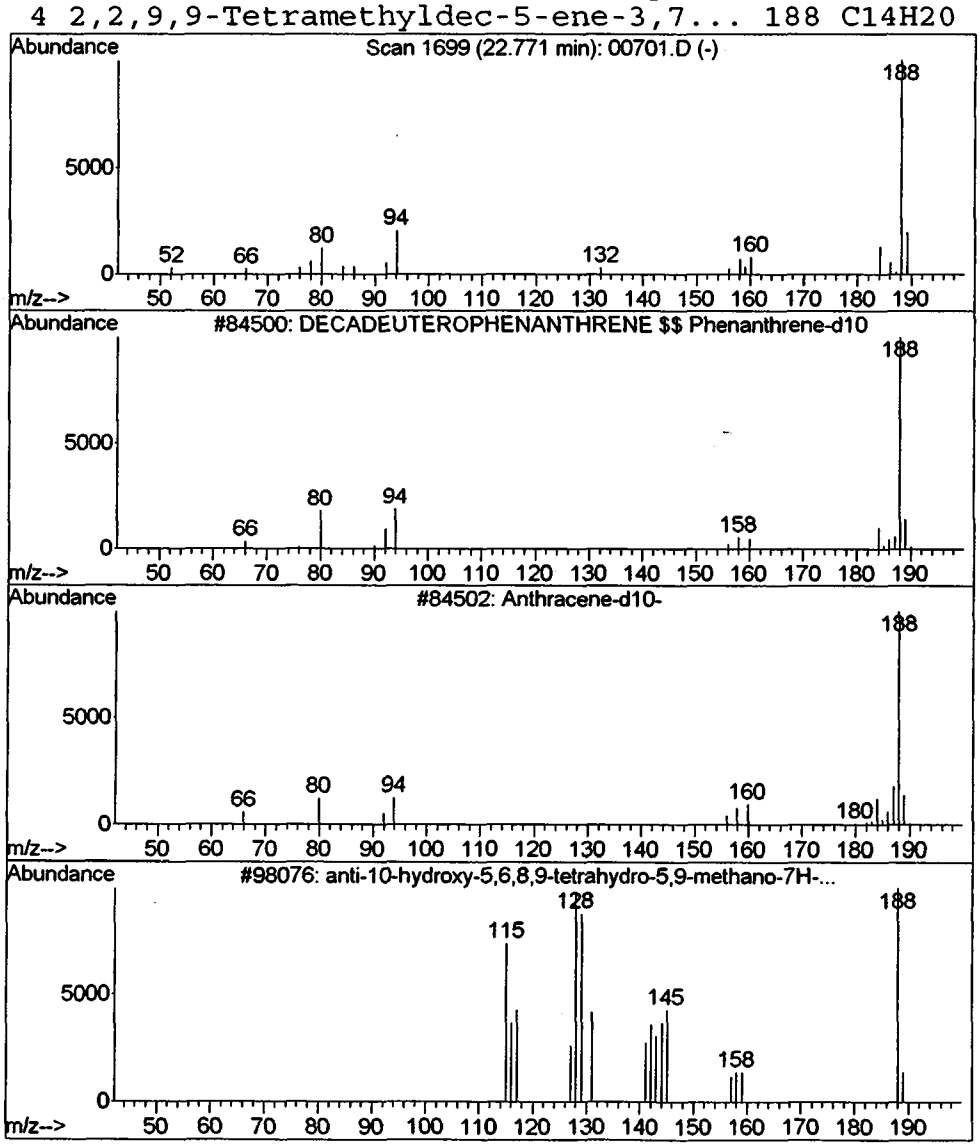
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

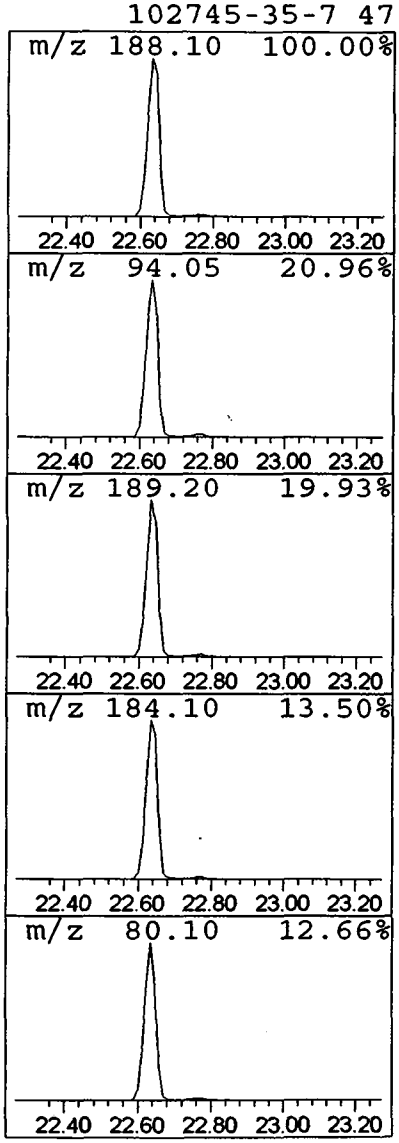
****

Peak Number 11 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.25 ug/L	135502	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	72
3	anti-10-hydroxy-5,6,8,9-tetrahyd...	188	C12H12O2	055139-53-2	50
4	2,2,9,9-Tetramethyldec-5-ene-3,7...	188	C14H20	102745-35-7	47





Operator ID: Date Acquired: 16 Jan 2002 3:07 pm
Data File: C:\MSDCHEM\1\5973N\02JAN16\00701.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-Ethylacrolein $...	4.85	0.2	ug/L	61092	1	9.71	6179920	20.0
3-Buten-2-ol, 2-m...	5.01	0.2	ug/L	47352	1	9.71	6179920	20.0
Acetic acid, 3-[1...	5.89	4.0	ug/L	1244780	1	9.71	6179920	20.0
Ethanol, 2-butoxy-	7.44	0.6	ug/L	174390	1	9.71	6179920	20.0
Morpholine (CAS) ...	8.24	0.2	ug/L	54177	1	9.71	6179920	20.0
2-Propanol, 1-(2-...	9.53	0.4	ug/L	133163	1	9.71	6179920	20.0
2-Propanol, 1-(2-...	9.62	0.4	ug/L	122446	1	9.71	6179920	20.0
2-Propanol, 1-(2-...	9.82	0.7	ug/L	215217	1	9.71	6179920	20.0
D-Limonene	10.10	1.7	ug/L	516996	1	9.71	6179920	20.0
4-METHOXY-,BETA.-...	22.28	0.1	ug/L	77034	4	22.63	10871700	20.0
DECADEUTEROPHENAN...	22.77	0.2	ug/L	135502	4	22.63	10871700	20.0