User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/25/2002 Time: 16:46:25

Sample: AE00100
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/25/02 16:46 Ended: 1/25/02 16:46 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 AE00100 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-25-2002 Time: 17:11:10

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.
The recoveries for 9 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN23\00100.D Vial: 3
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 24 09:46:35 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	1269197	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	5384166	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2770769	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4551516	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	3911161	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	2831367	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	298868	4.15	ug/L	0.00
Spiked Amount 5.000			Recovery = 83.00%			
Target Compounds						Qvalue
2) n-Nitrosodimethylamine	3.60	74	14146	0.26	ug/L #	11
20) Dimethylphthalate	18.34	163	443535	2.42	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	356302	9.98	ug/L #	17
35) Di-n-butylphthalate	24.85	149	107662	0.37	ug/L	96
42) Bis(2-ethylhexyl)phthalate	31.11	149	11072	0.61	ug/L	94

(#) = qualifier out of range (m) = manual integration
00100.D SCAN508.M Thu Jan 24 09:46:35 2002 Page 1

Quantitation Report (Not Reviewed)

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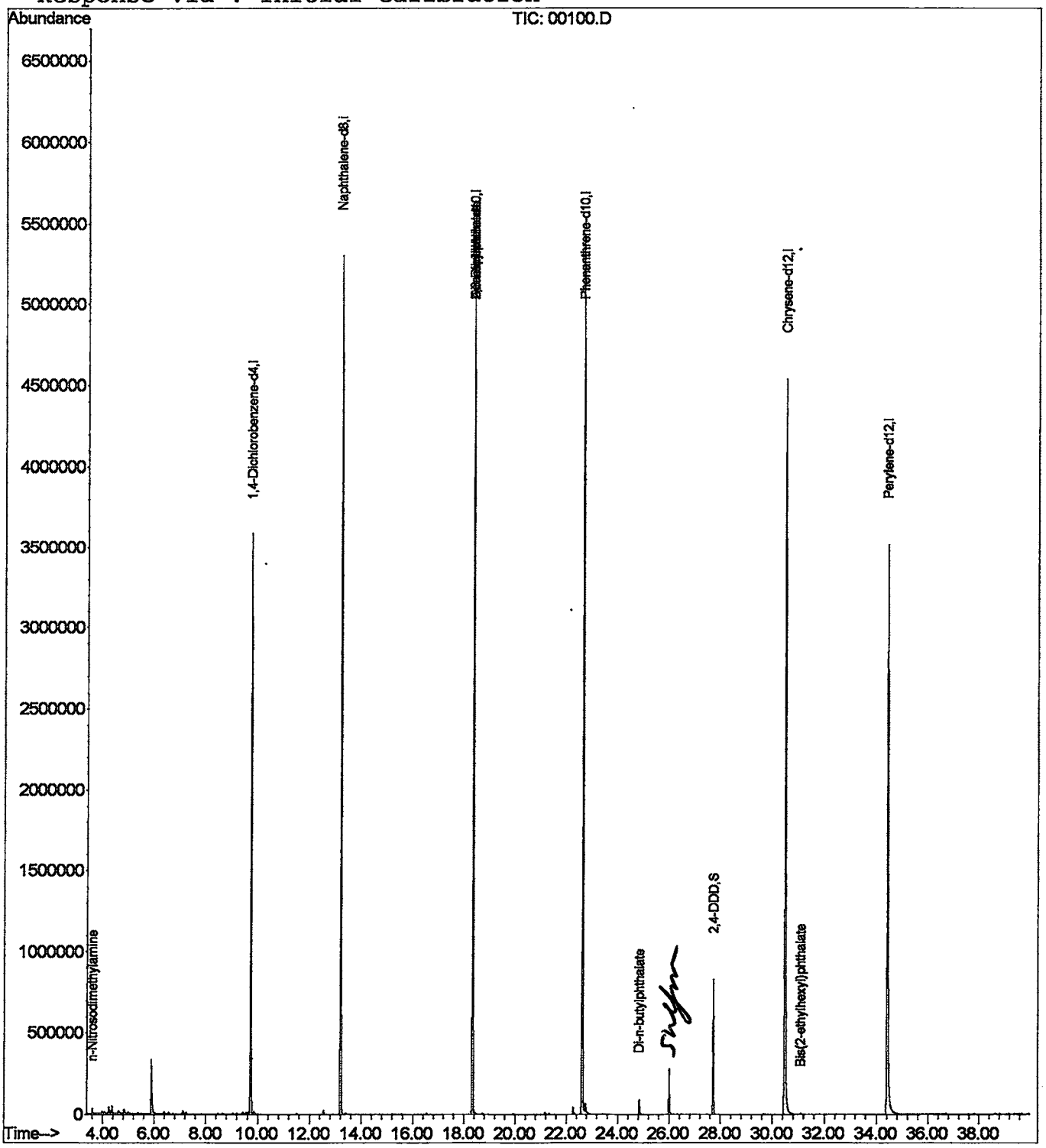
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 24 9:46 2002 Quant Results File: SCAN508.RE

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\02JAN23\00100.D Vial: 3
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 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

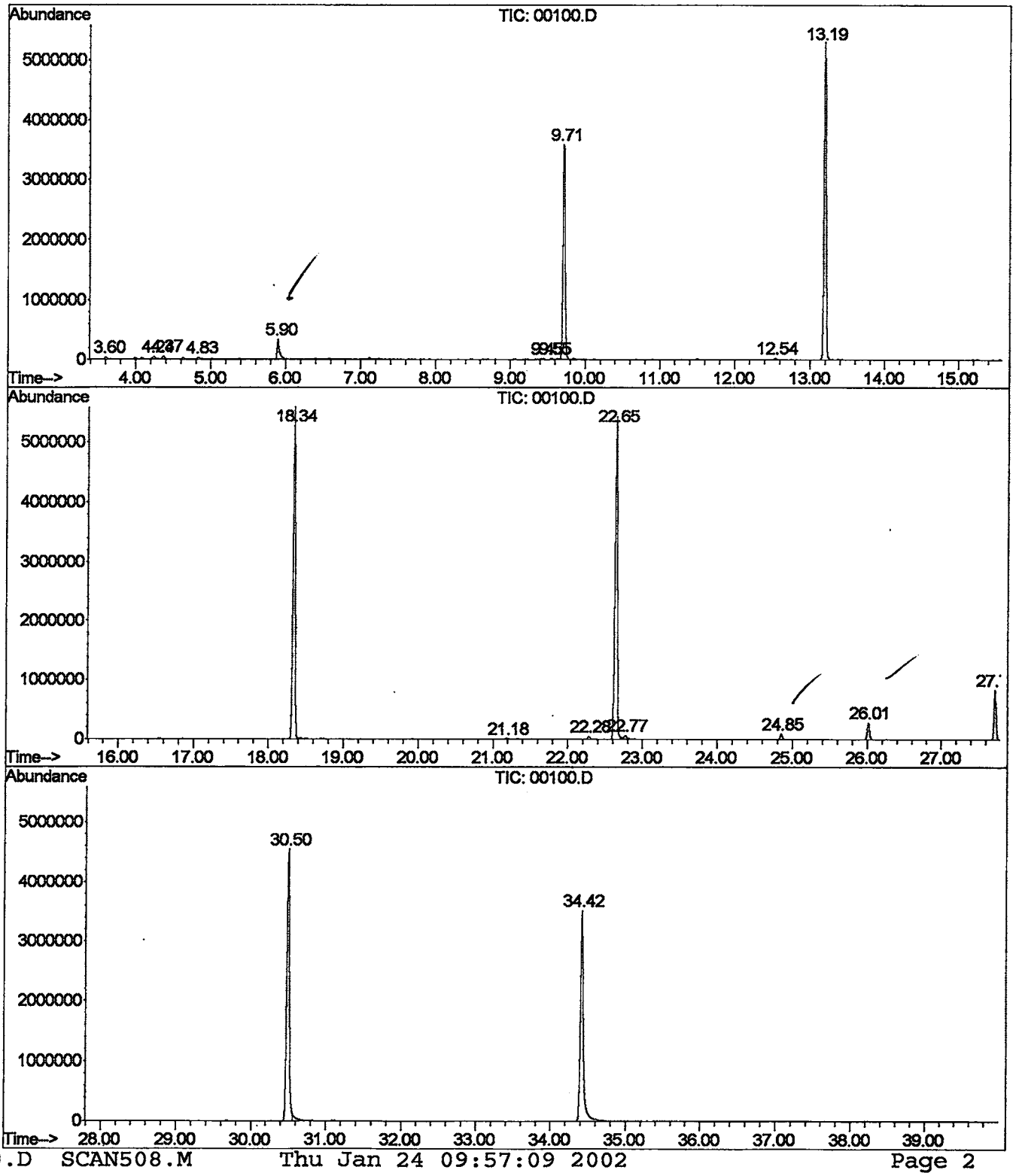
Signal : TIC

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	40338	60506	0.50%	0.092%
2	4.241	71	76	83	rVV3	42851	89259	0.74%	0.136%
3	4.367	83	87	91	rVB2	46500	83755	0.69%	0.128%
4	4.835	123	128	139	rBV	29000	75799	0.63%	0.116%
5	5.897	217	221	243	rVB	331740	736773	6.08%	1.123%
6	9.447	527	532	539	rVB2	16204	50302	0.41%	0.077%
7	9.550	539	541	545	rBV	16287	41950	0.35%	0.064%
8	9.710	551	555	561	rVV	3584519	7300588	60.21%	11.125%
9	12.541	799	803	807	rVB	27944	43050	0.36%	0.066%
10	13.192	855	860	865	rBV	5300288	10436237	86.07%	15.903%
11	18.341	1305	1311	1315	rBV	5587897	11322365	93.38%	17.254%
12	21.184	1557	1560	1569	rVV2	15857	43113	0.36%	0.066%
13	22.280	1651	1656	1661	rBV	49277	91894	0.76%	0.140%
14	22.645	1681	1688	1693	rBV	5431377	12125684	100.00%	18.478%
15	22.771	1695	1699	1707	rVB	61761	158720	1.31%	0.242%
16	24.849	1877	1881	1887	rVV	94791	171549	1.41%	0.261%
17	26.013	1977	1983	1989	rVV	280783	549206	4.53%	0.837%
18	27.726	2127	2133	2139	rVV	831573	1470451	12.13%	2.241%
19	30.500	2369	2376	2381	rBV	4540001	11253738	92.81%	17.149%
20	34.416	2713	2719	2749	rBV	3520752	9518572	78.50%	14.505%

Sum of corrected areas: 65623511

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN23\00100.D
Operator :
Acquired : 23 Jan 2002 4:36 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 22, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\00100.D Vial: 3
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

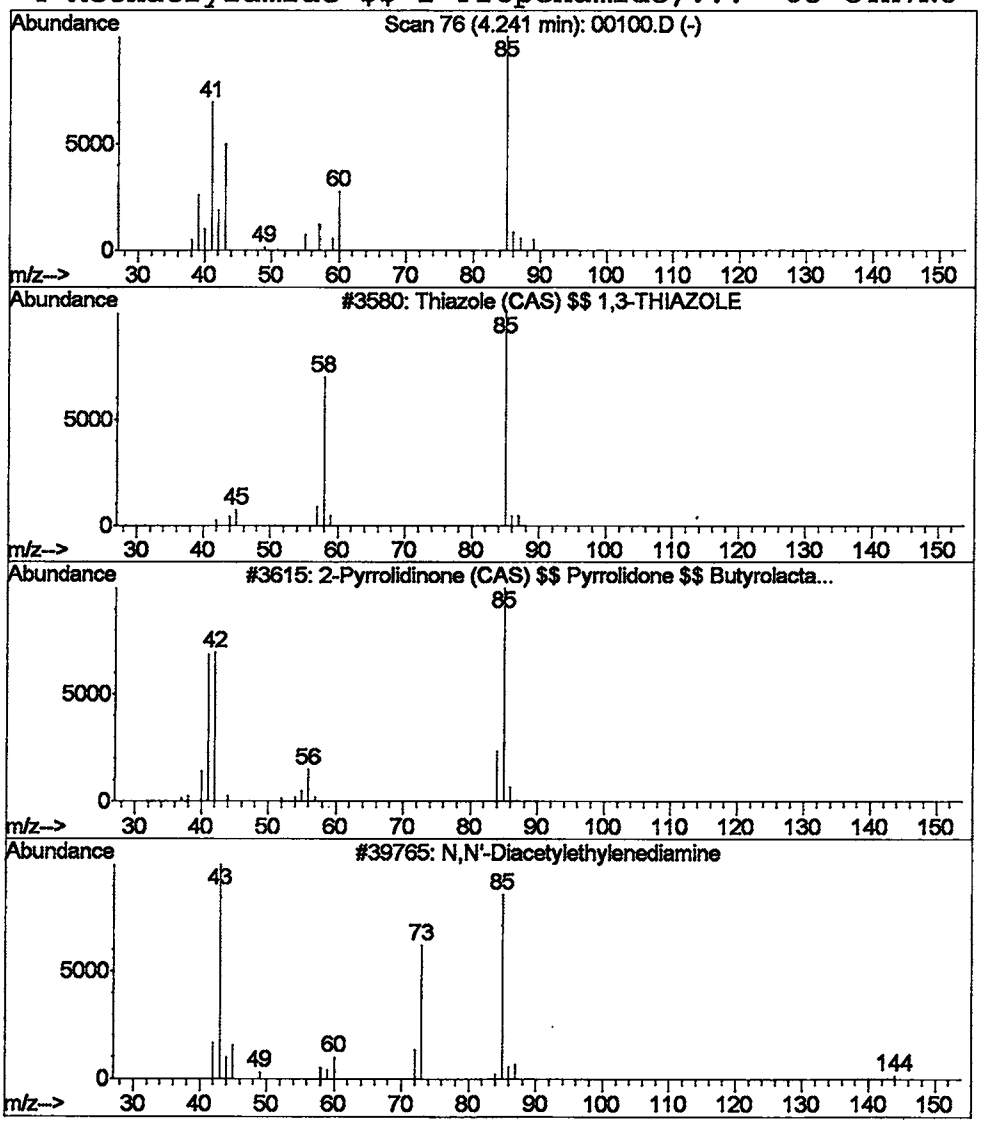
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

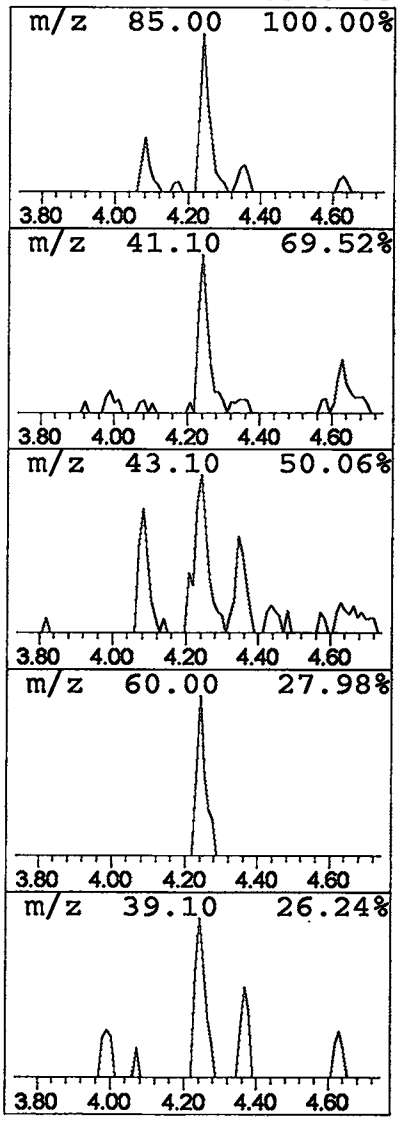
****

Peak Number 1 Thiazole (CAS) $$ 1,3-THIAZOLE Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.24 ug/L	89259	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole (CAS) $$ 1,3-THIAZOLE	85	C3H3NS	000288-47-1	53
2	2-Pyrrolidinone (CAS) $$ Pyrroli...	85	C4H7NO	000616-45-5	38
3	N,N'-Diacetylethylenediamine	144	C6H12N2O2	000871-78-3	38
4	Methacrylamide $$ 2-Propenamide,...	85	C4H7NO	000079-39-0	33





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Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 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

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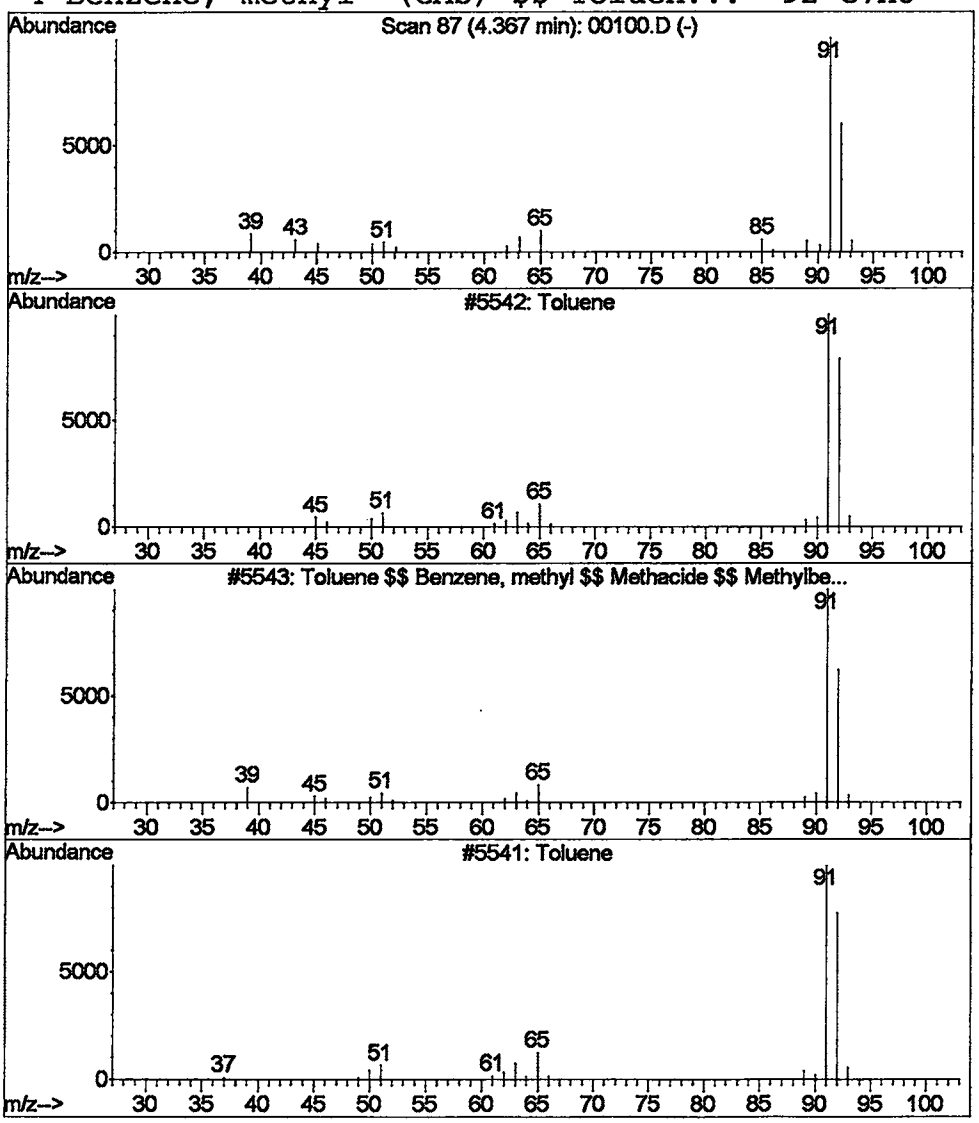
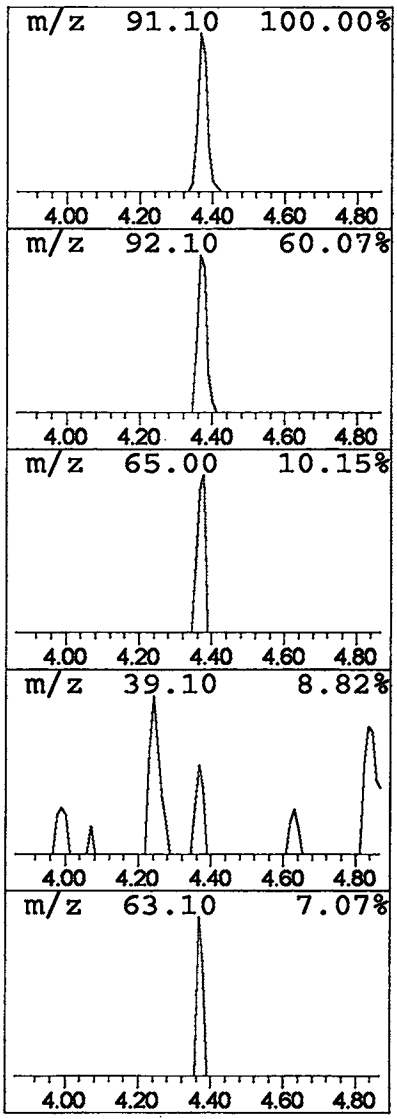
Peak Number 2 Toluene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	0.23 ug/L	83755	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	90
2	Toluene $$ Benzene, methyl $$ Me...	92	C7H8	000108-88-3	87
3	Toluene	92	C7H8	000108-88-3	87
4	Benzene, methyl- (CAS) $$ Toluen...	92	C7H8	000108-88-3	87





Library Search Compound Report

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Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

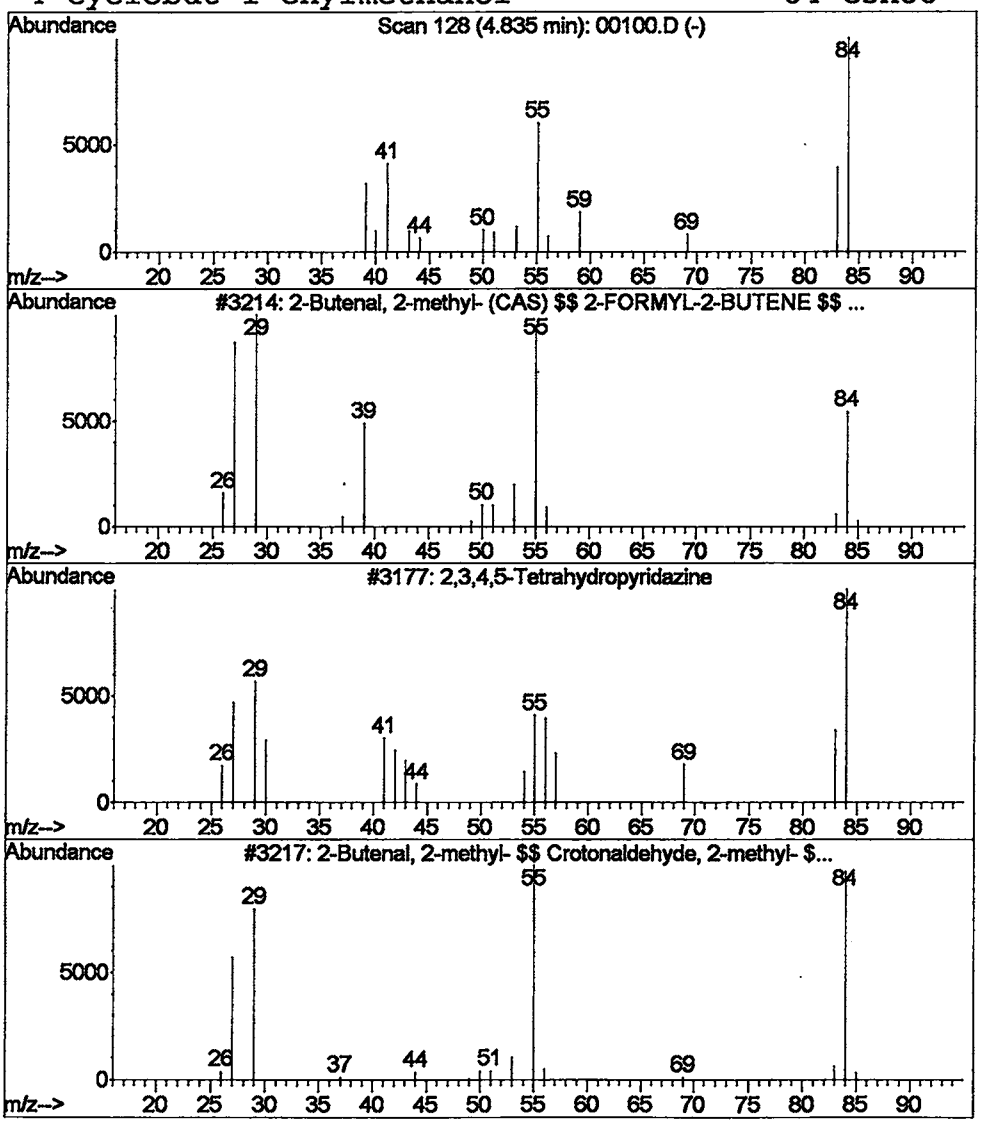
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

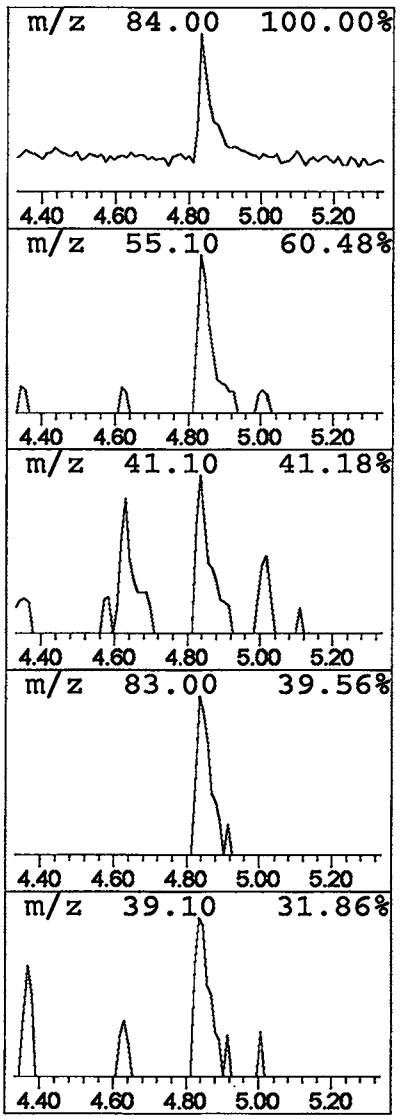
****

Peak Number 3 2-Butenal, 2-methyl- (CAS) ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.21 ug/L	75799	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl- (CAS) $$ 2-...	84	C5H8O	001115-11-3	59
2	2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	42
3	2-Butenal, 2-methyl- $$ Crotonal...	84	C5H8O	001115-11-3	33
4	Cyclobut-1-enylmethanol	84	C5H8O	000000-00-0	17





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Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

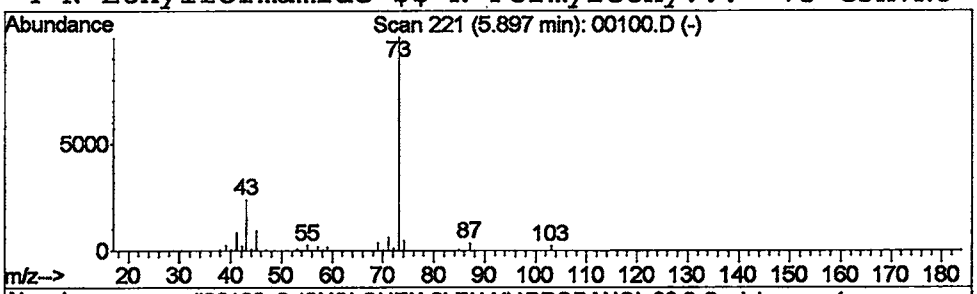
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

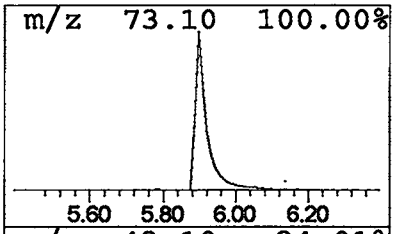
****

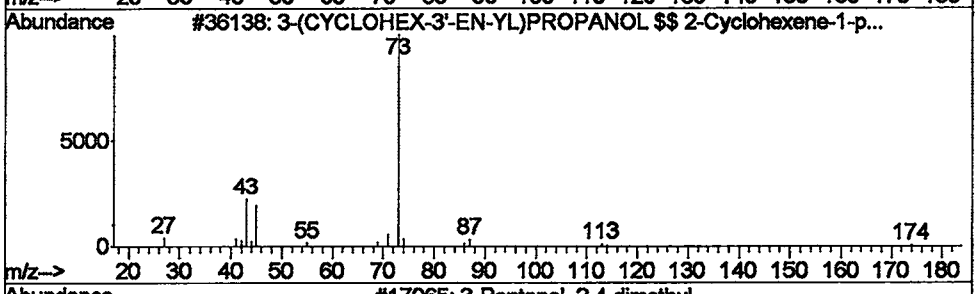
Peak Number 4 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 1

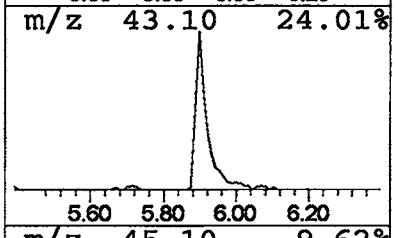
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.02 ug/L	736773	1,4-Dichlorobenzene-d4	9.72

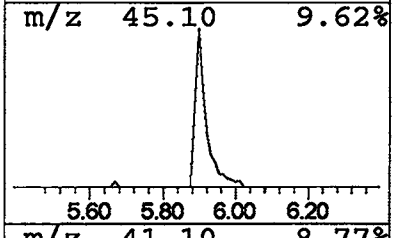
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	33
3	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
4	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9

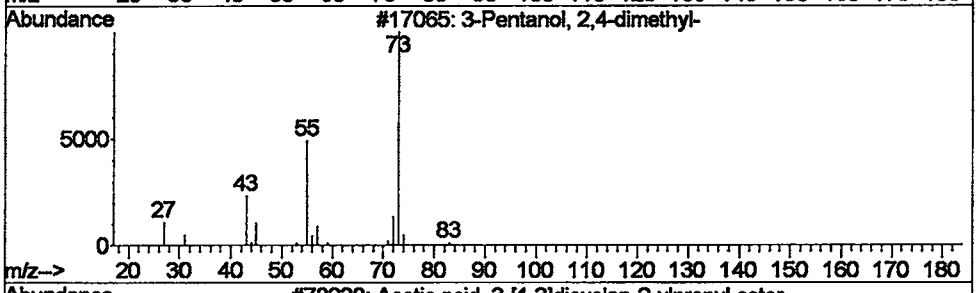


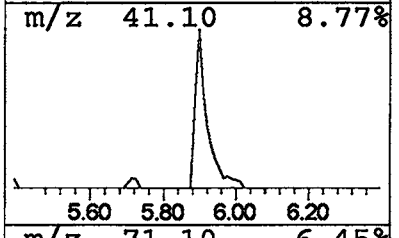


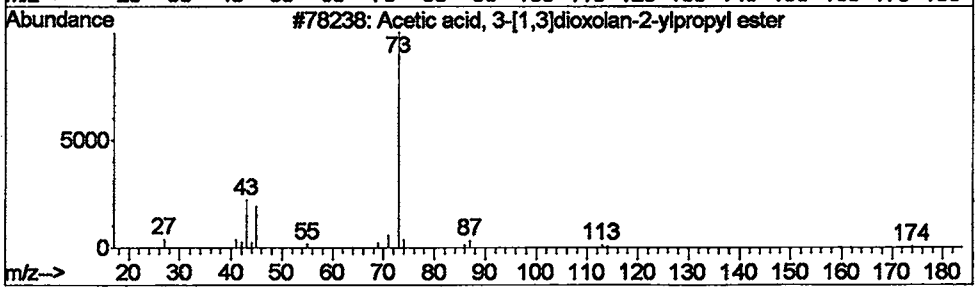


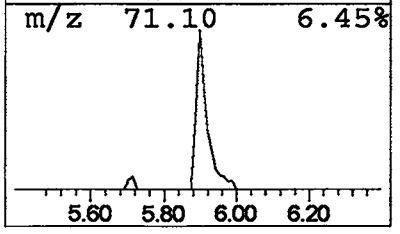












Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\00100.D Vial: 3
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

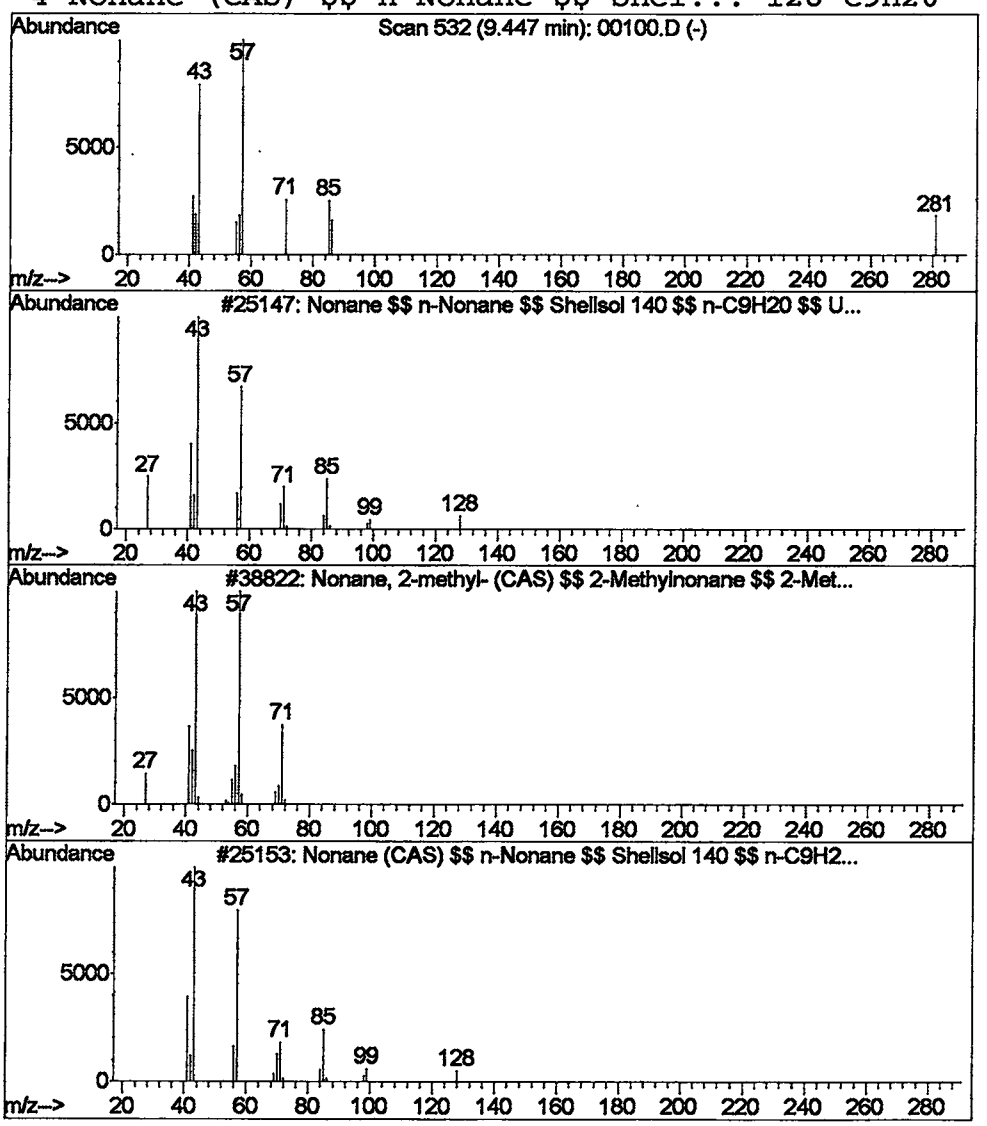
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

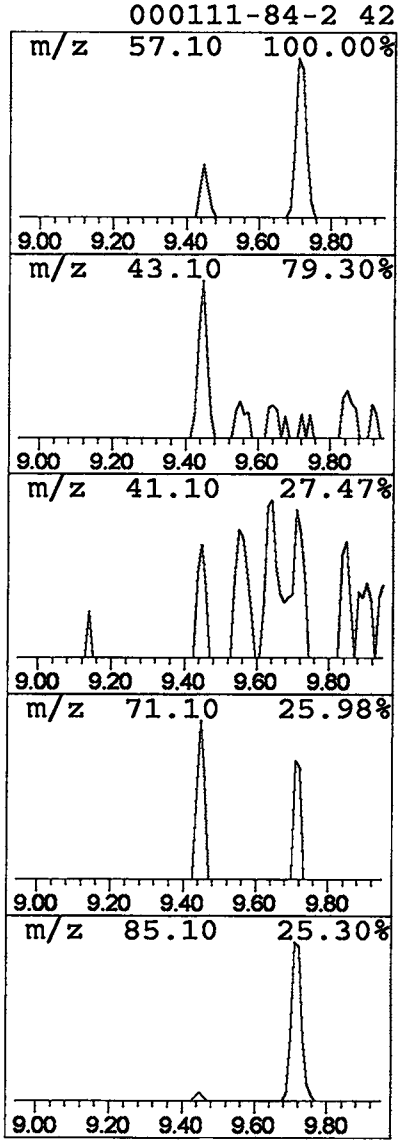
****

Peak Number 5 Nonane $$ n-Nonane $$ Shell... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	0.14 ug/L	50302	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane $$ n-Nonane $$ Shellsol 1...	128	C9H20	000111-84-2	53
2	Nonane, 2-methyl- (CAS) $$ 2-Met...	142	C10H22	000871-83-0	47
3	Nonane (CAS) $$ n-Nonane $$ Shel...	128	C9H20	000111-84-2	42
4	Nonane (CAS) $$ n-Nonane $$ Shel...	128	C9H20	000111-84-2	42





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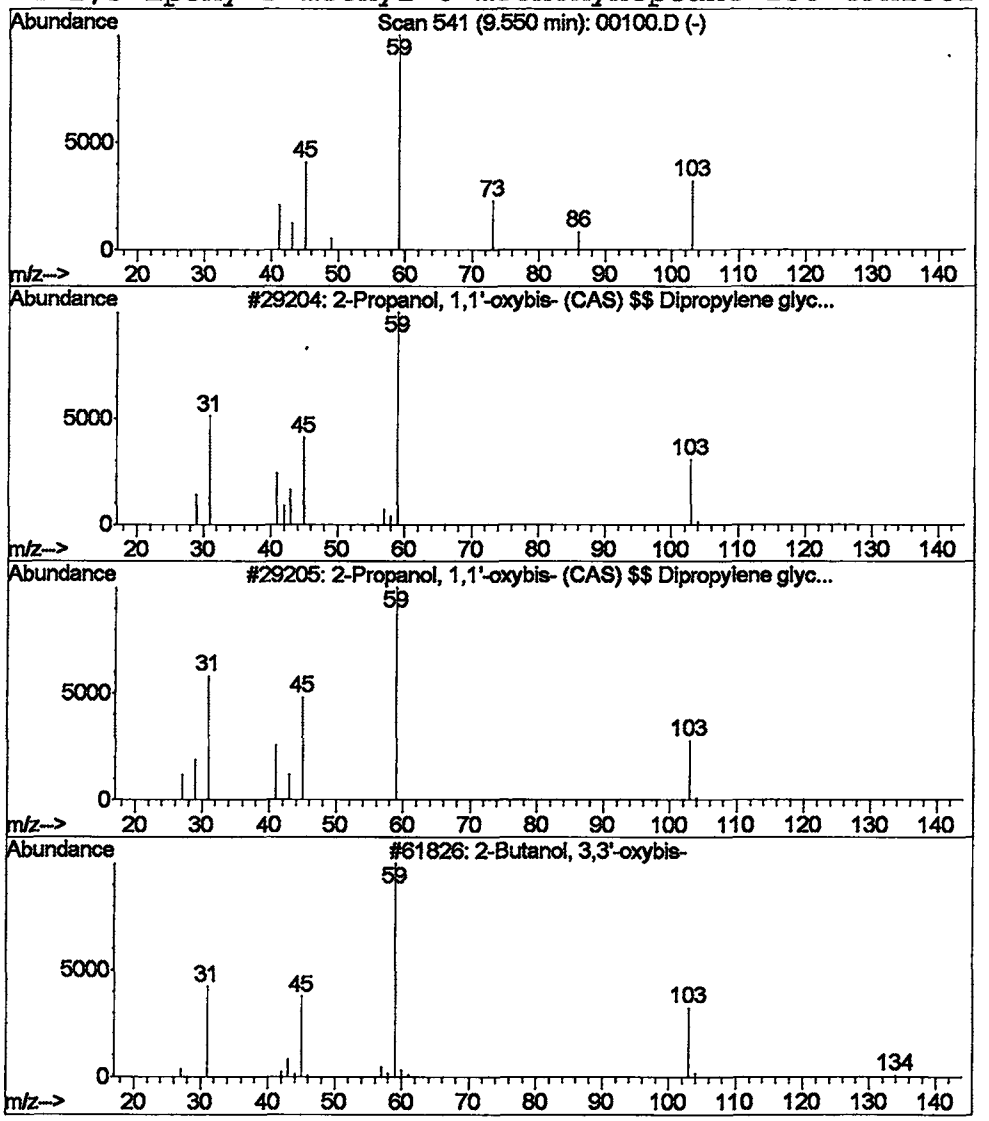
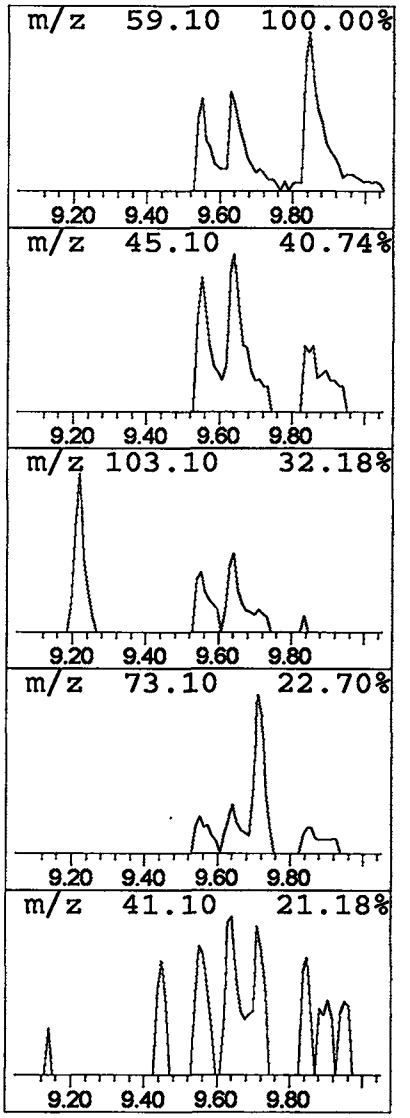
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	0.11 ug/L	41950	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,1'-oxybis- (CAS) $...	134	C6H14O3	000110-98-5	40
2	2-Propanol, 1,1'-oxybis- (CAS) $...	134	C6H14O3	000110-98-5	40
3	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	9
4	2,3-Epoxy-3-methyl-6-methoxyheptane	158	C9H18O2	088083-53-8	9





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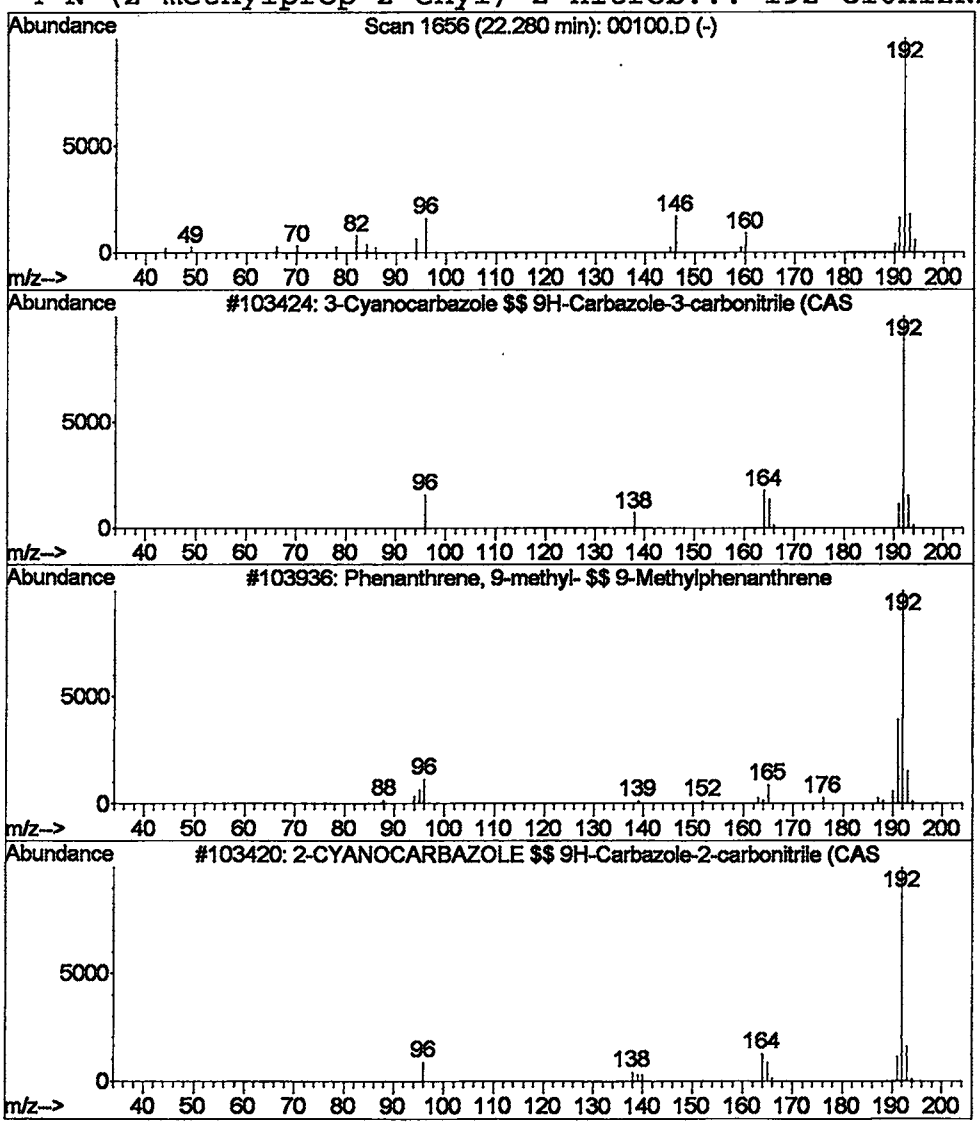
Library : C:\DATABASE\WILEY7N.L

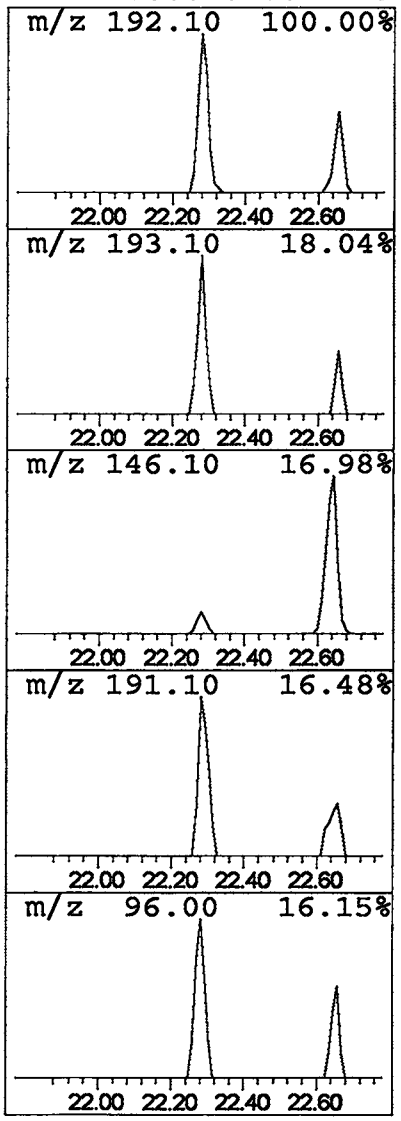
****

Peak Number 7 3-Cyanocarbazole $$ 9H-Carb... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	91894	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyanocarbazole $$ 9H-Carbazole...	192	C13H8N2	057102-93-9	64
2	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	59
3	2-CYANOCARBAZOLE $$ 9H-Carbazole...	192	C13H8N2	057955-18-7	50
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	49





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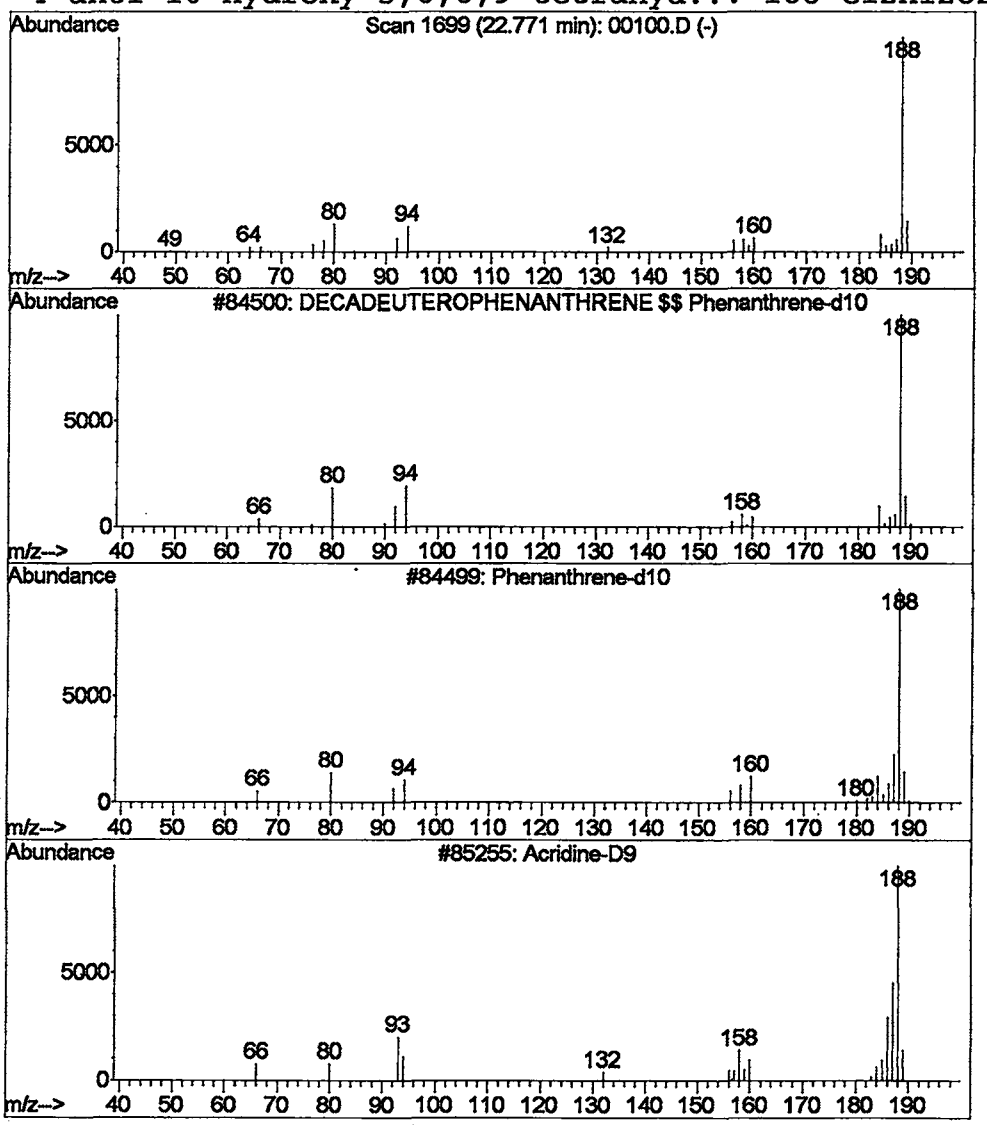
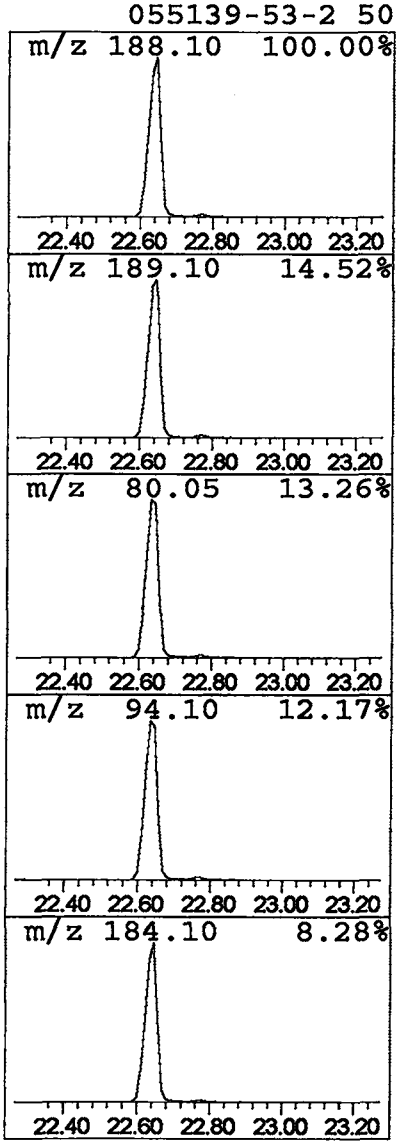
****

Peak Number 8 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.26 ug/L	158720	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	91
2	Phenanthrene-d10	188	C14D10	001517-22-2	87
3	Acridine-D9	188	C13D9N	000000-00-0	56
4	anti-10-hydroxy-5,6,8,9-tetrahyd...	188	C12H12O2	055139-53-2	50





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN23\00100.D Vial: 3
Acq On : 23 Jan 2002 4:36 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 22, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

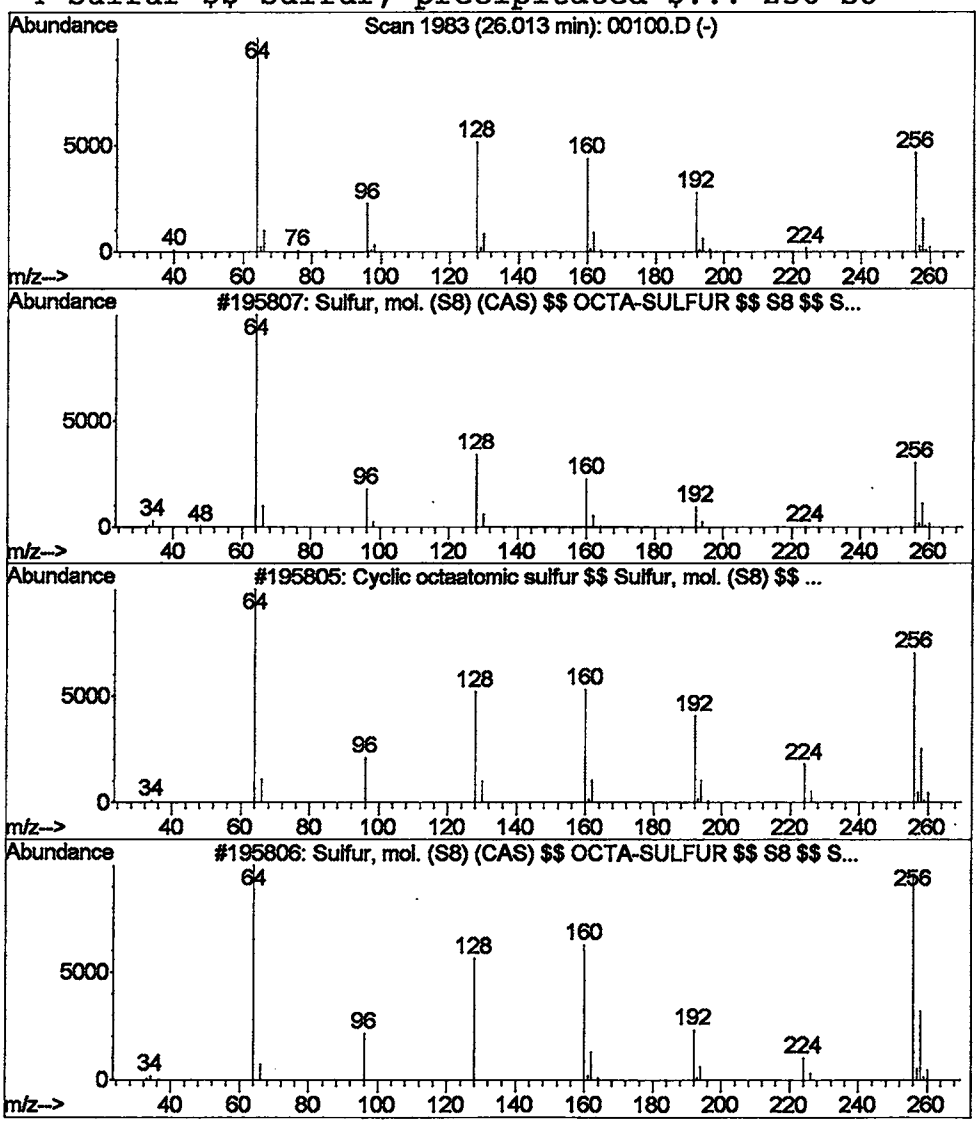
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

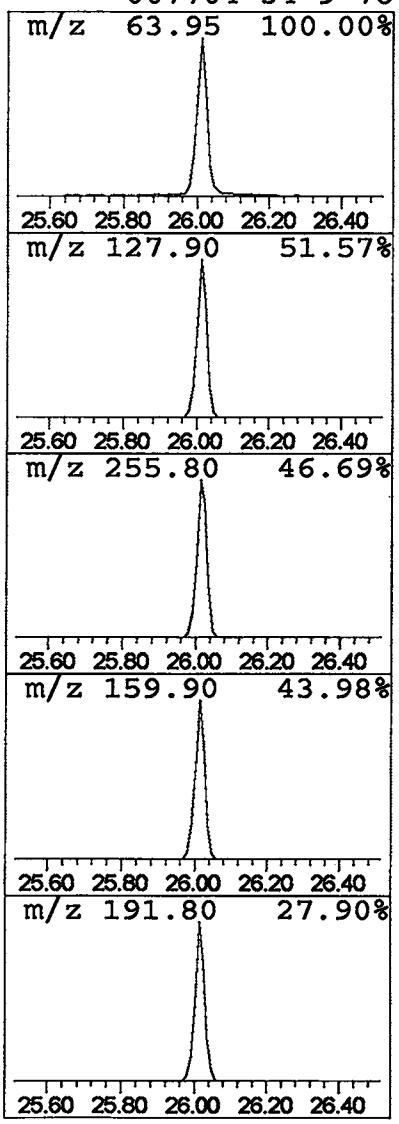
****

Peak Number 9 Sulfur, mol. (S8) (CAS) $$ ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.01	0.91 ug/L	549206	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	97
2	Cyclic octaatomic sulfur $$ Sulf...	256	S8	010544-50-0	95
3	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	94
4	Sulfur $$ Sulfur, precipitated $...	256	S8	007704-34-9	78





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 23 Jan 2002 4:36 pm
Data File: C:\MSDCHEM\1\5973N\02JAN23\00100.D
Name: 508 scan
Misc: January 22, 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
Thiazole (CAS) $$...	4.24	0.2	ug/L	89259	1	9.72	7300590	20.0
Toluene	4.37	0.2	ug/L	83755	1	9.72	7300590	20.0
2-Butenal, 2-meth...	4.83	0.2	ug/L	75799	1	9.72	7300590	20.0
3-(CYCLOHEX-3'-EN...	5.90	2.0	ug/L	736773	1	9.72	7300590	20.0
Nonane $$ n-Nonan...	9.45	0.1	ug/L	50302	1	9.72	7300590	20.0
2-Propanol, 1,1'-...	9.55	0.1	ug/L	41950	1	9.72	7300590	20.0
3-Cyanocarbazole ...	22.28	0.2	ug/L	91894	4	22.65	12125700	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	158720	4	22.65	12125700	20.0
Sulfur, mol. (S8)...	26.01	0.9	ug/L	549206	4	22.65	12125700	20.0