User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/18/2002 Time: 12:28:33

Sample: AE00466
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/18/02 12:28 Ended: 1/18/02 12:28 Analyst: DLV
Page: 1

	Component Name	Vial	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		102		5.0

4.20 MJ/L
28/100
CAS 1782-93-0
CR6 CAT
1/6/02 by Sutton
FB 329 dbw

Comments for Sample AE00466 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-18-2002 Time: 12:30:51

The GCMS scan, from 35 to 550 amu, reveals the presence of 1-(epithioethyl)-2-Norbornanone at an estimated level of 4.2 ug/L and with a fit of 28 out of 100. The recovery for 1 of the 43 compounds in the LCS Standard was above its acceptance range.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 11 10:18:53 2002 Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Thu Jan 10 11:01:02 2002
Response via : Initial Calibration
DataAcq Meth : SCAN508

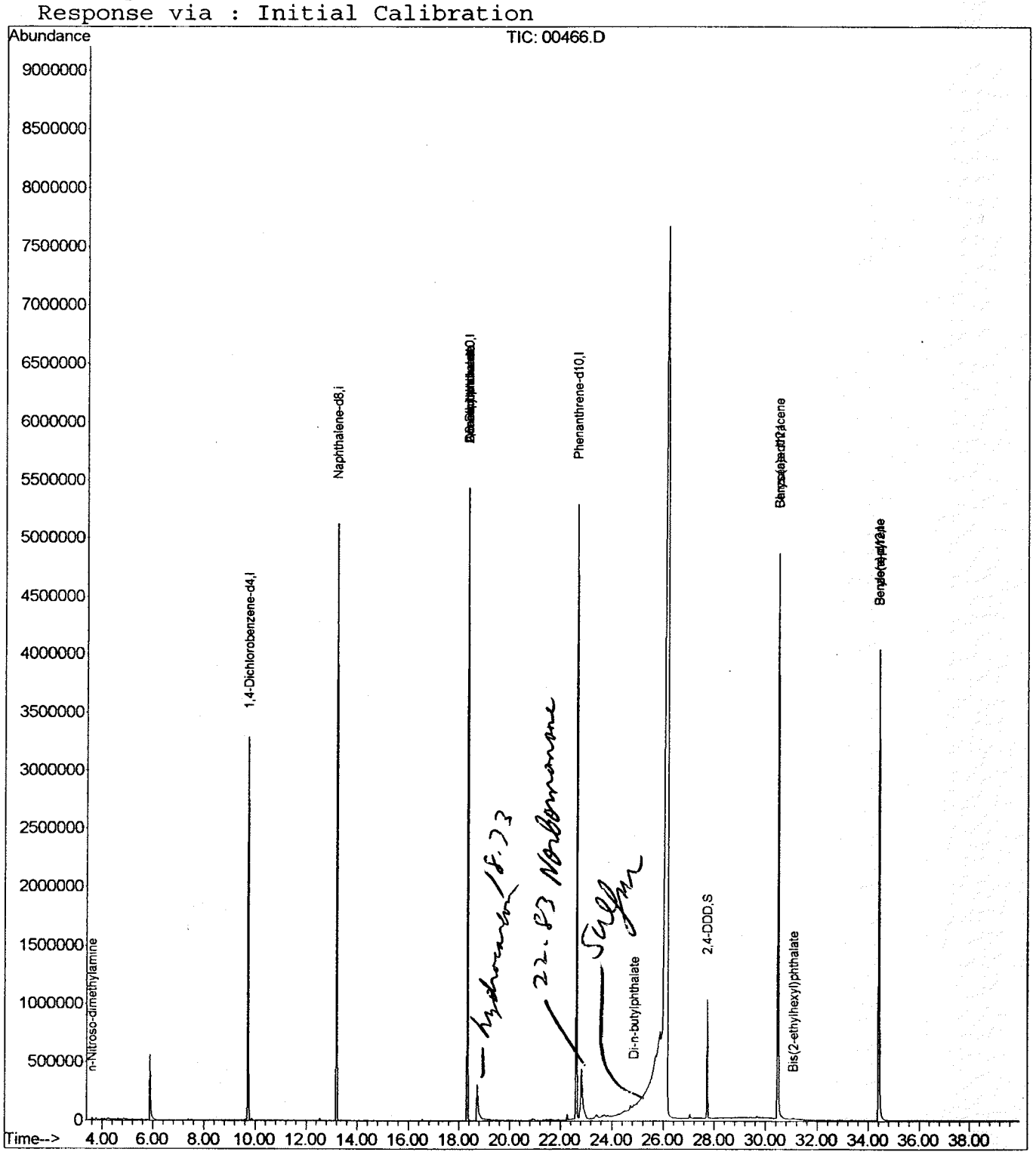
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.72	152	1179617	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4996144	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2601840	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4374156	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	4038958	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3047097	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	352943	5.10	ug/L	0.00
Spiked Amount 5.000			Recovery = 102.00%			
Target Compounds						Qvalue
2) n-Nitroso-dimethylamine	3.61	74	8701	0.17	ug/L #	16
20) Dimethylphthalate	18.34	163	418340	2.43	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	330066	9.85	ug/L #	17
35) Di-n-butylphthalate	24.86	149	20395	0.07	ug/L	95
41) Benzo(a)anthracene	30.50	228	11652	0.05	ug/L #	55
42) Bis(2-ethylhexyl)phthalate	31.11	149	10417	0.60	ug/L	92
43) Chrysene	30.50	228	11652	0.05	ug/L #	52
48) Benzo(a)pyrene	34.42	252	10648	0.05	ug/L #	1

(#) = qualifier out of range (m) = manual integration
00466.D SCAN508.M Fri Jan 11 10:18:54 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 11 10:18 2002 Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Thu Jan 10 11:01:02 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 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

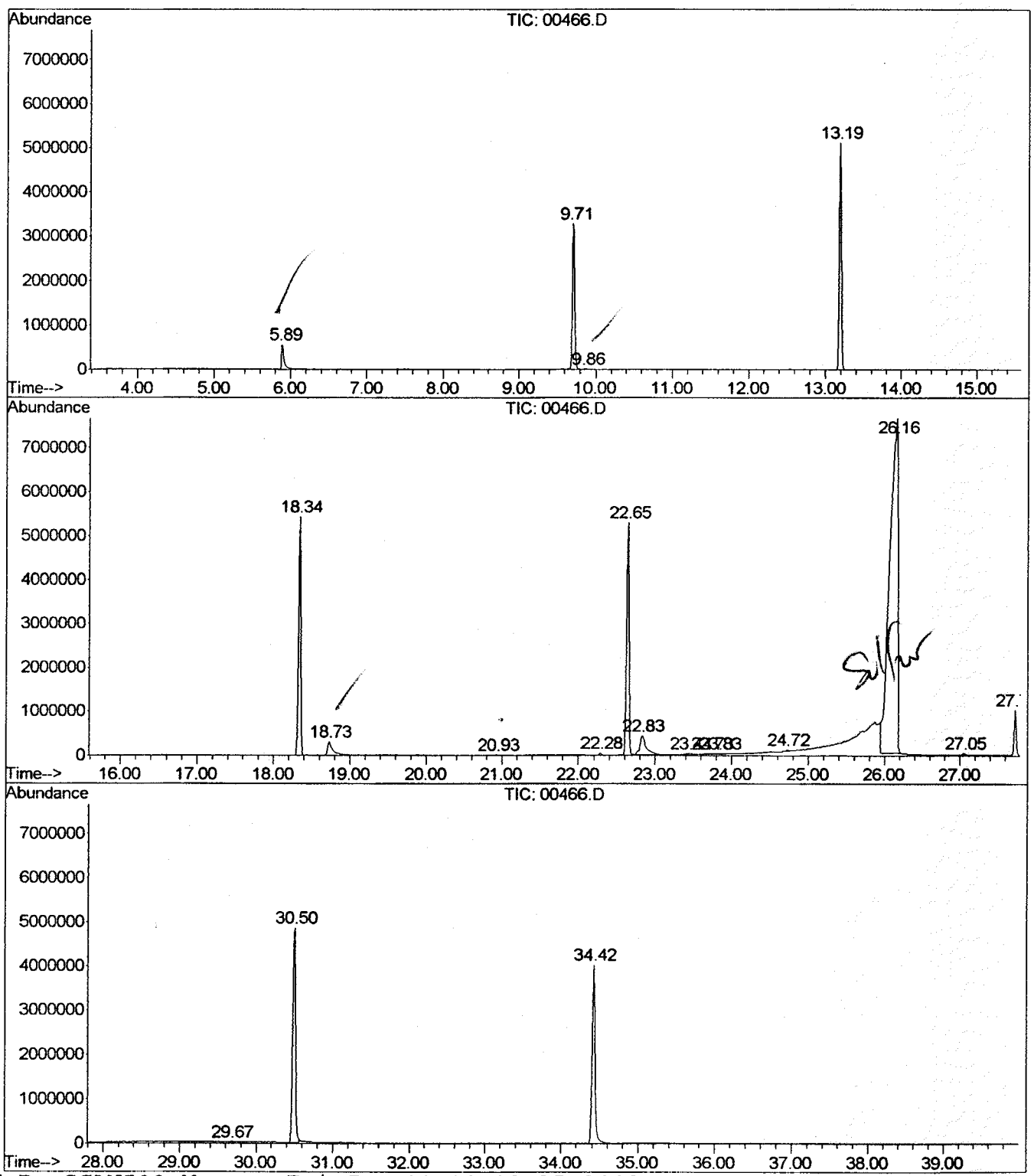
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.885	217	220	249	rVB	559909	1309964	2.25%	1.030%
2	9.710	551	555	561	rVV	3284420	6675235	11.44%	5.249%
3	9.858	561	568	577	rVV2	17333	57059	0.10%	0.045%
4	13.192	855	860	865	rBV	5121052	9608239	16.47%	7.556%
5	18.341	1305	1311	1315	rBV	5434866	10596875	18.16%	8.333%
6	18.729	1339	1345	1371	rBV	307879	1526223	2.62%	1.200%
7	20.933	1533	1538	1547	rVB6	16875	71353	0.12%	0.056%
8	22.280	1651	1656	1661	rBV	52199	107450	0.18%	0.084%
9	22.645	1681	1688	1693	rVV2	5280271	11583949	19.86%	9.109%
10	22.828	1695	1704	1731	rVB2	421607	2434752	4.17%	1.915%
11	23.445	1745	1758	1767	rBV3	30990	196468	0.34%	0.154%
12	23.730	1769	1783	1789	rBV4	24743	175777	0.30%	0.138%
13	23.833	1789	1792	1801	rVB5	8862	47005	0.08%	0.037%
14	24.723	1865	1870	1873	rBV3	43309	114686	0.20%	0.090%
15	26.162	1977	1996	2001	rVB	7609435	58342543	100.00%	45.879%
16	27.052	2069	2074	2083	rBV7	34525	87168	0.15%	0.069%
17	27.726	2129	2133	2139	rVV	1011099	1793640	3.07%	1.410%
18	29.667	2299	2303	2315	rVB2	14281	52278	0.09%	0.041%
19	30.500	2369	2376	2381	rBV	4847484	11930667	20.45%	9.382%
20	34.416	2713	2719	2747	rBV	4033125	10455429	17.92%	8.222%

Sum of corrected areas: 127166760

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN10\00466.D
Operator :
Acquired : 10 Jan 2002 5:18 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan ext 1/8
Misc Info : January 10, 2002
Vial Number: 4
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

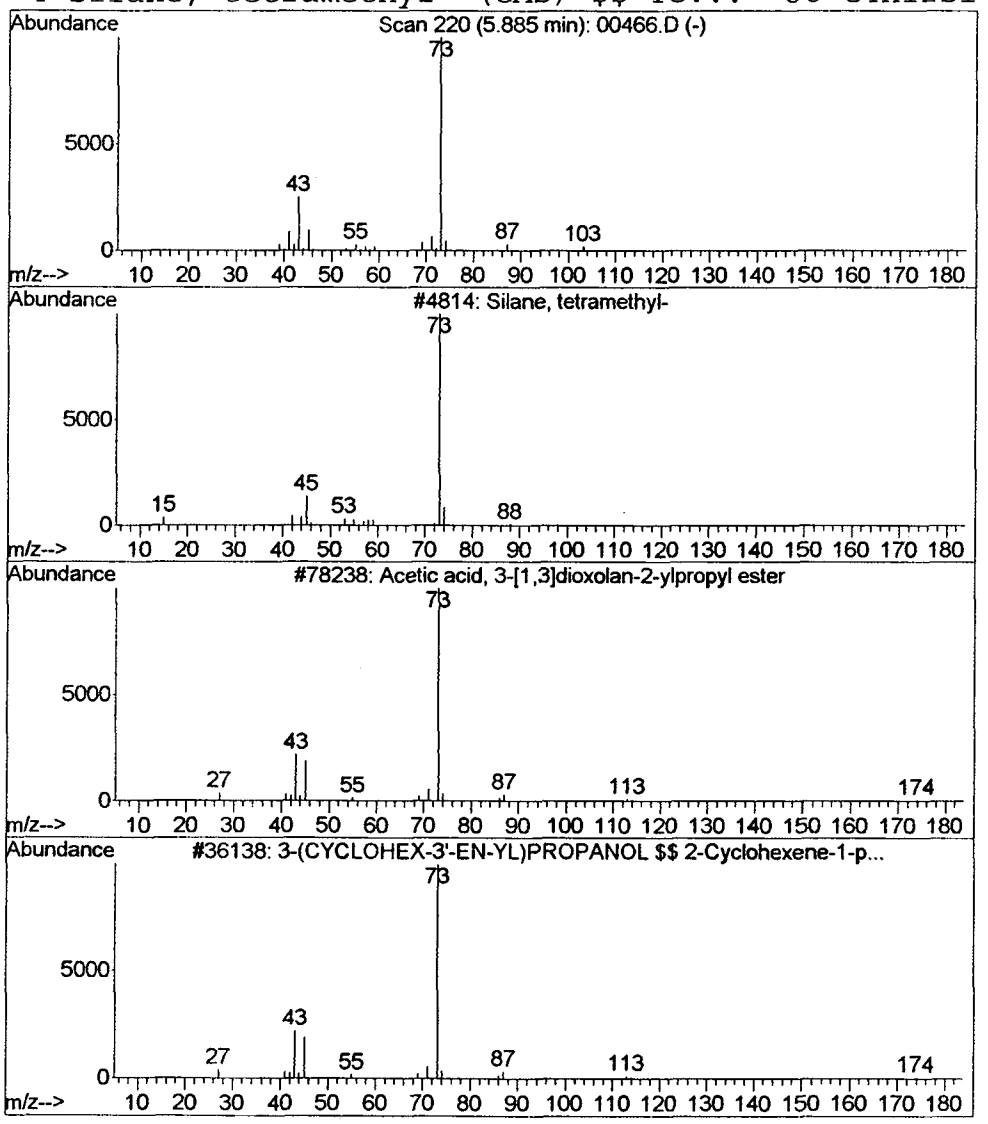
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

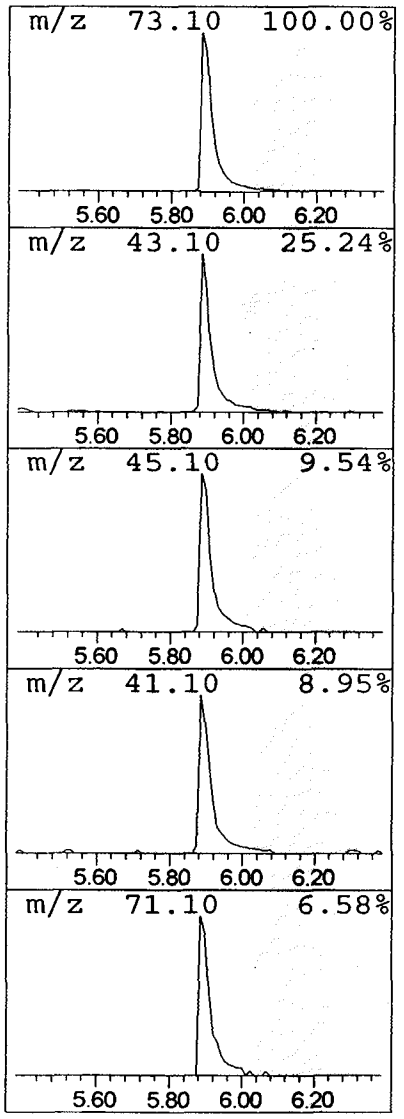
****

Peak Number 1 Silane, tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	3.92 ug/L	1309960	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, tetramethyl-	88	C4H12Si	000075-76-3	37
2	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
3	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33
4	Silane, tetramethyl- (CAS) $$ Te...	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

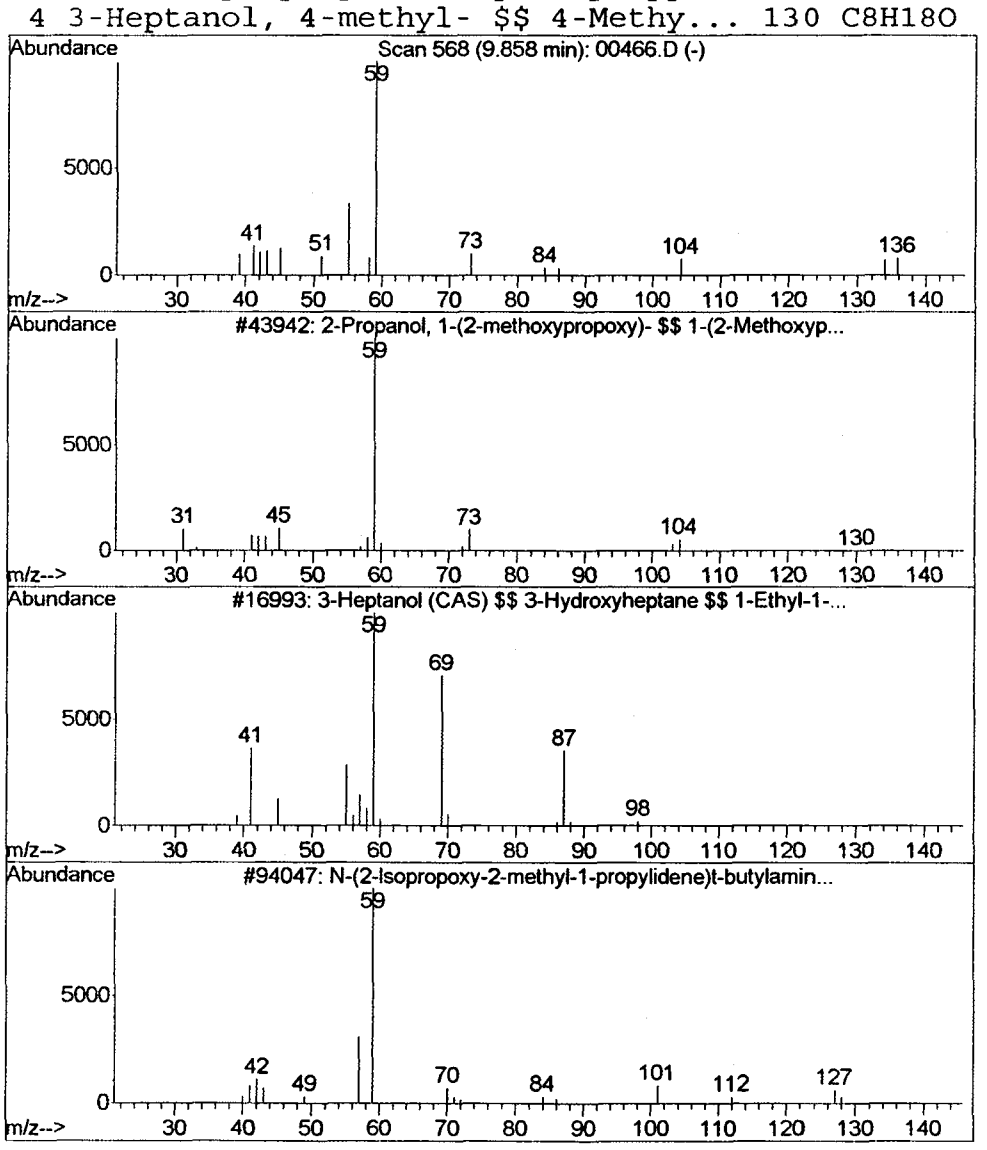
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

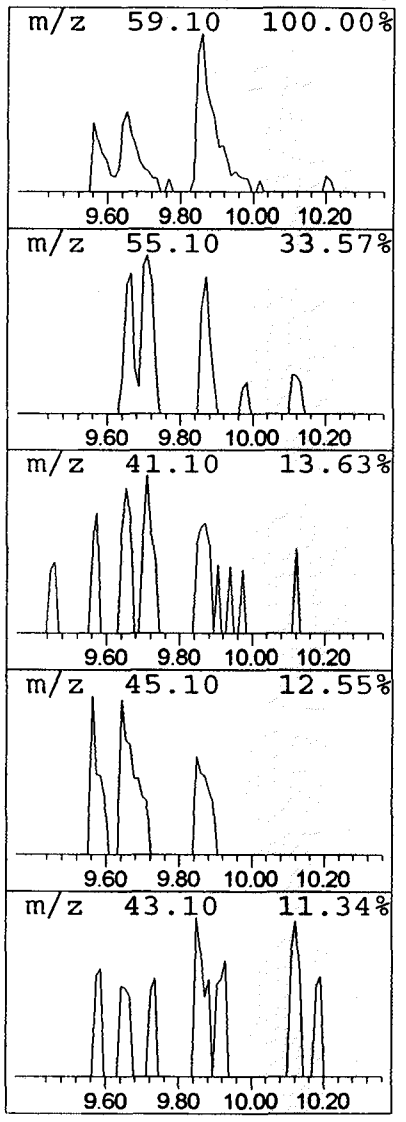
****

Peak Number 2 2-Propanol, 1-(2-methoxypro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	0.17 ug/L	57059	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	64
2	3-Heptanol (CAS) $$ 3-Hydroxyhep...	116	C7H16O	000589-82-2	33
3	N-(2-Isopropoxy-2-methyl-1-propy...	185	C11H23NO	132555-83-0	33
4	3-Heptanol, 4-methyl- $$ 4-Methy...	130	C8H18O	014979-39-6	33





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 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

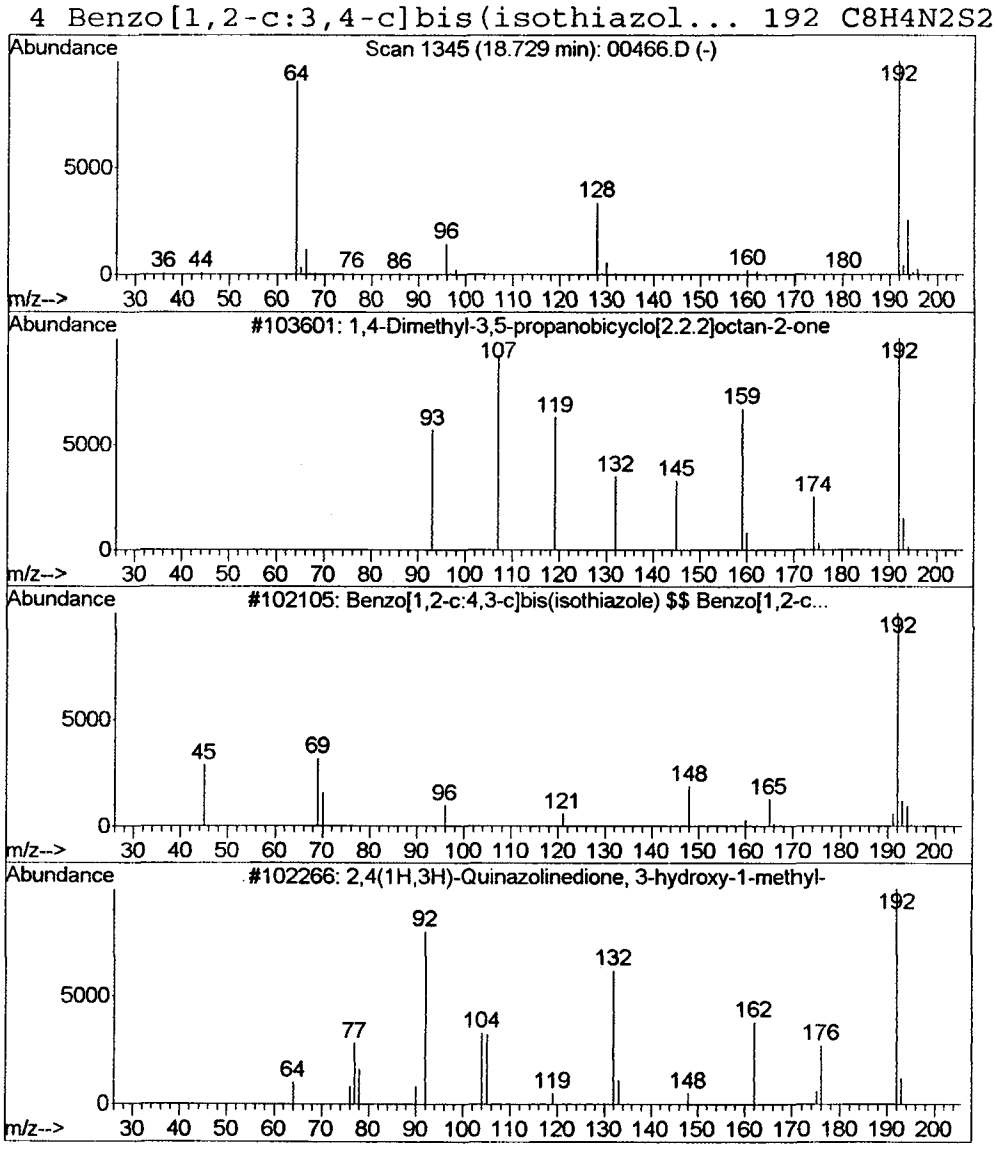
NOT A GOOD MATCH

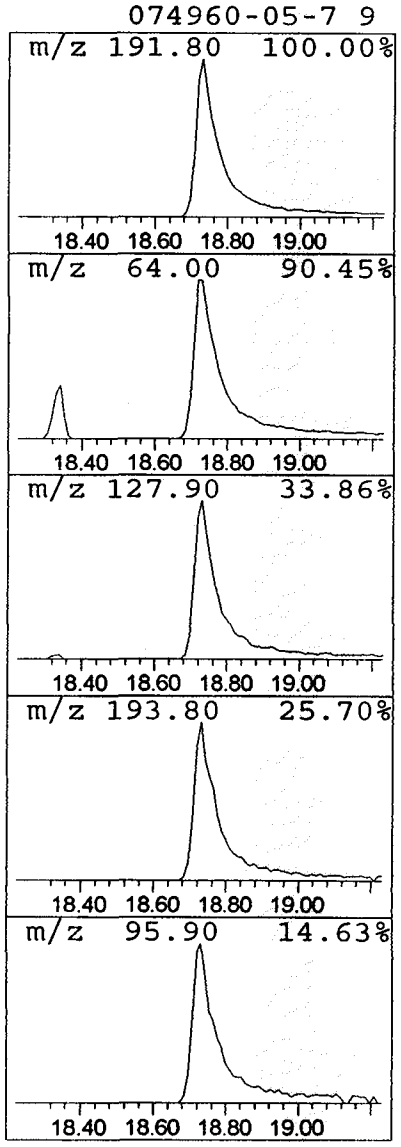
****

Peak Number 3 1,4-Dimethyl-3,5-propanobic... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	2.88 ug/L	1526220	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-3,5-propanobicyclo[...	192	C13H20O	000000-00-0	37
2	Benzo[1,2-c:4,3-c]bis(isothiazol...	192	C8H4N2S2	074960-06-8	9
3	2,4(1H,3H)-Quinazolinedione, 3-h...	192	C9H8N2O3	037833-99-1	9
4	Benzo[1,2-c:3,4-c]bis(isothiazol...	192	C8H4N2S2	074960-05-7	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 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

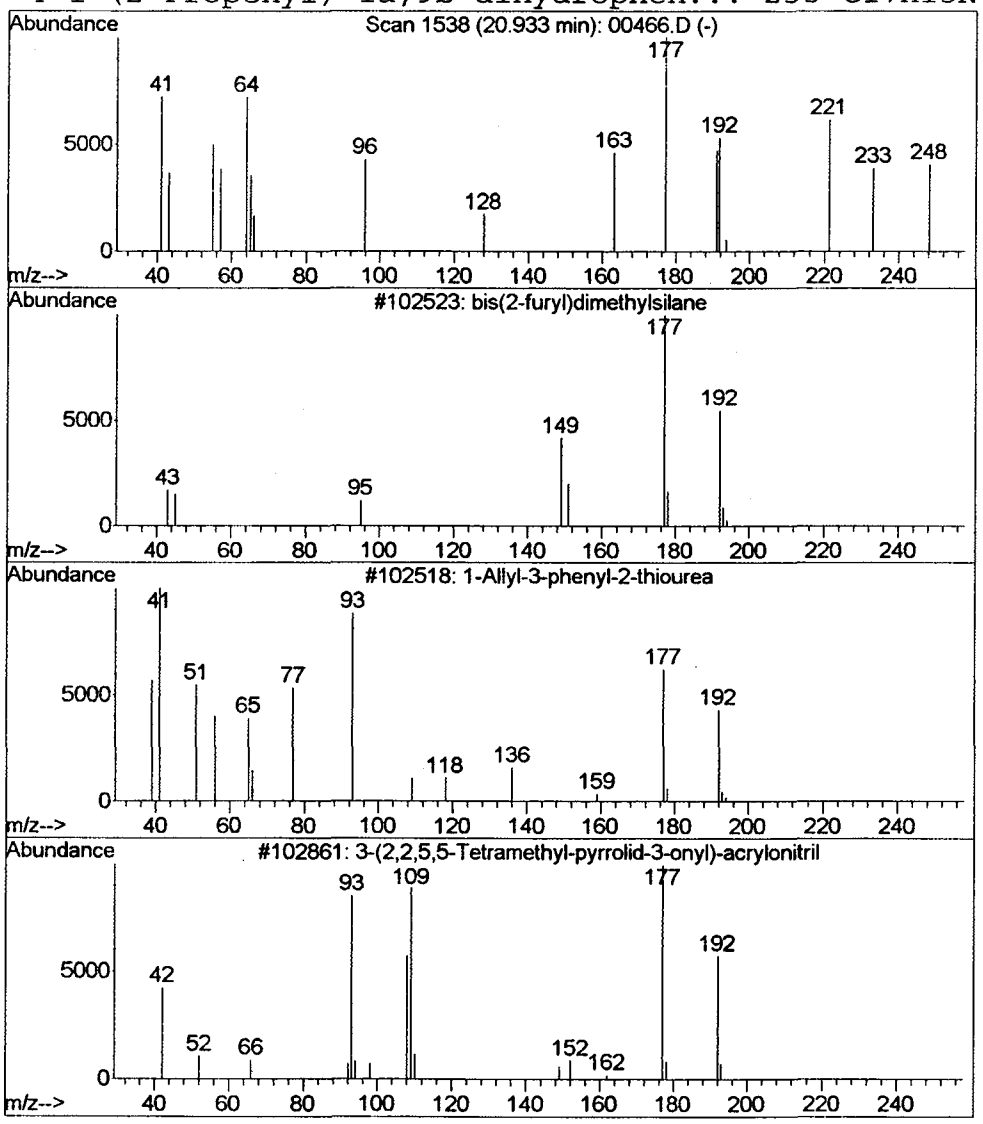
****

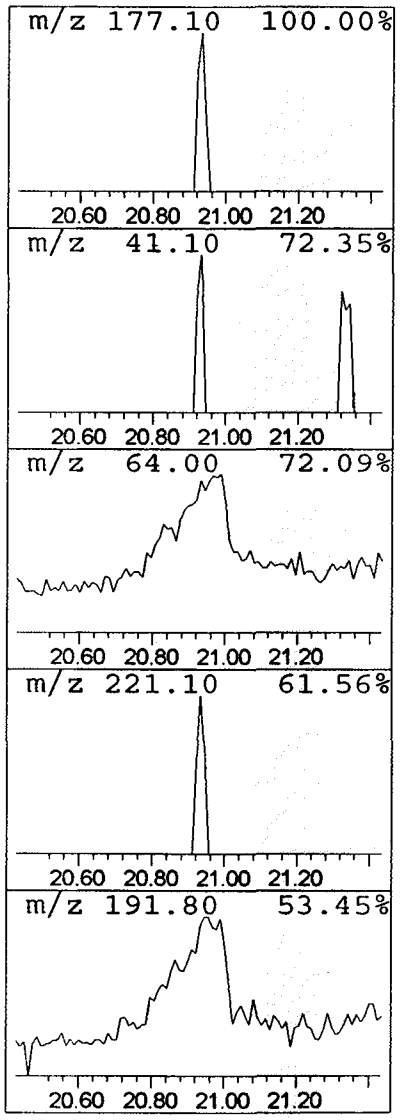
Peak Number 4 bis(2-furyl)dimethylsilane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	0.12 ug/L	71353	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	bis(2-furyl)dimethylsilane	192	C10H12O2Si	000000-00-0	9
2	1-Allyl-3-phenyl-2-thiourea	192	C10H12N2S	000000-00-0	9
3	3-(2,2,5,5-Tetramethyl-pyrrolid-...	192	C11H16N2O	000000-00-0	9
4	1-(2-Propenyl)-1a,9b-dihydrophen...	233	C17H15N	091540-30-6	9

NOT A GOOD MATCH





Library Search Compound Report

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Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

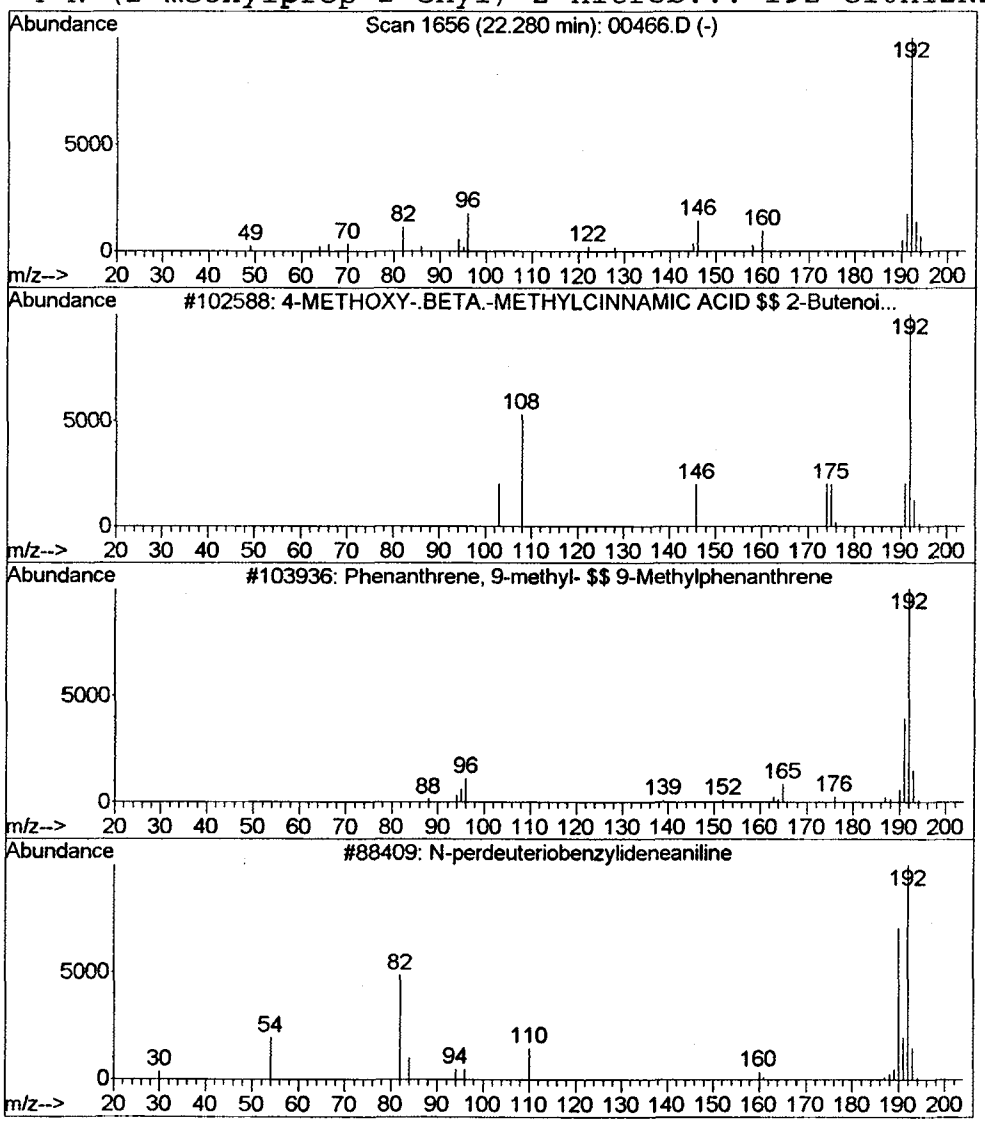
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

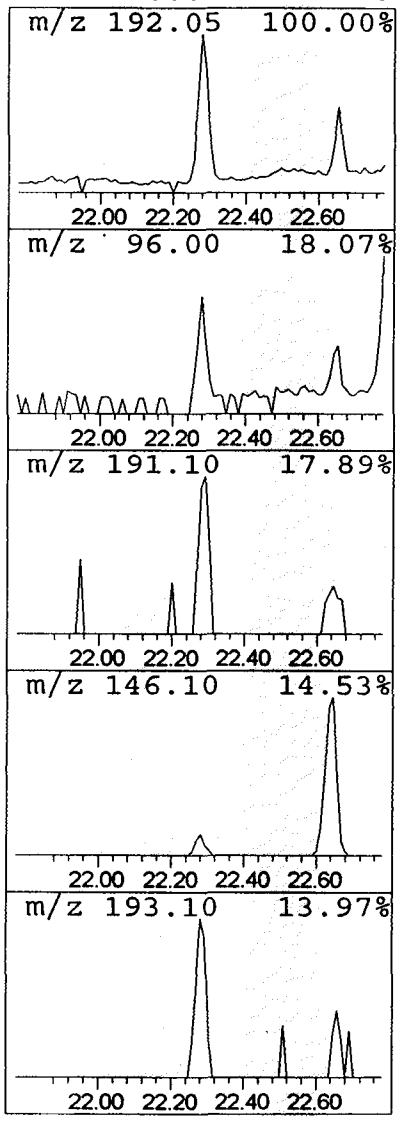
****

Peak Number 5 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.19 ug/L	107450	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	64
2	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	59
3	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	49





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

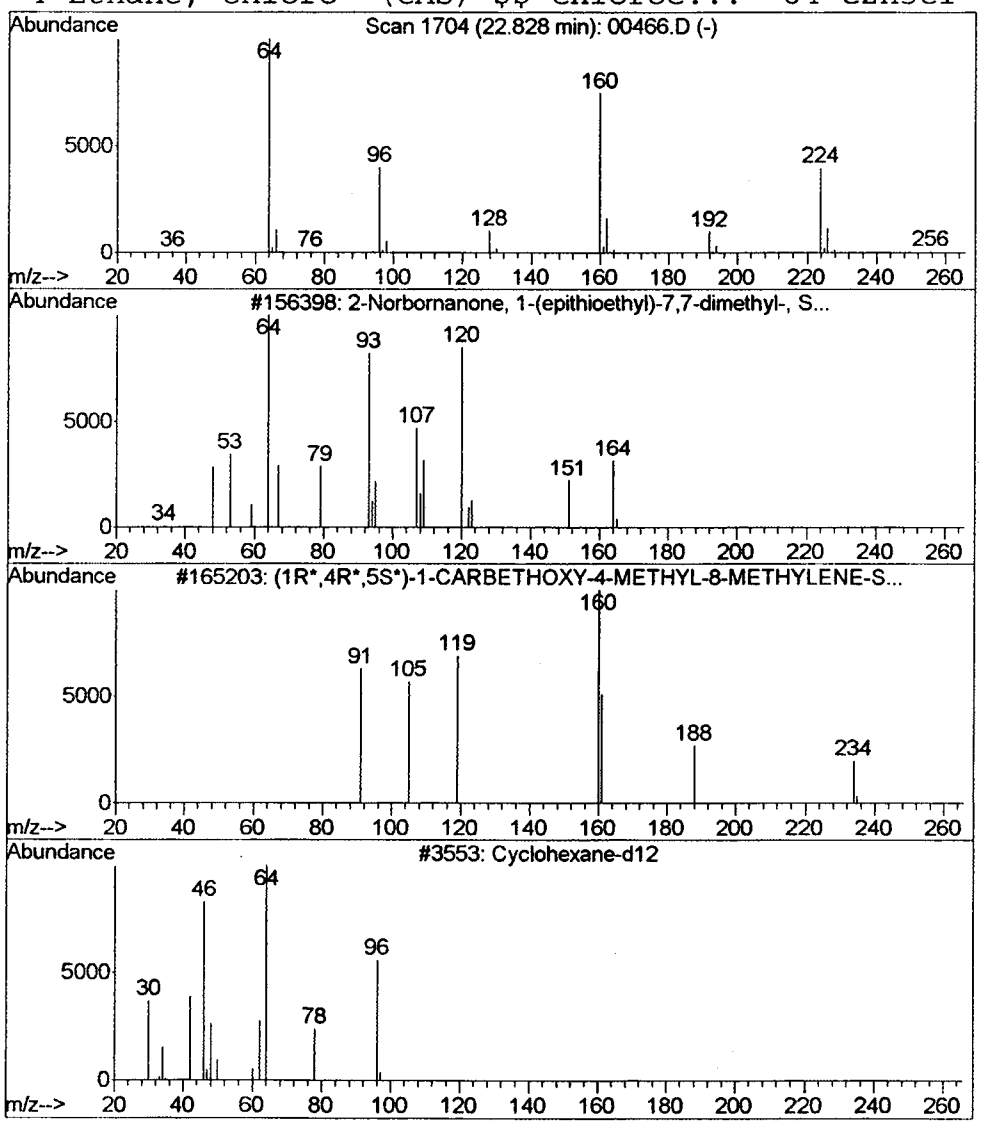
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

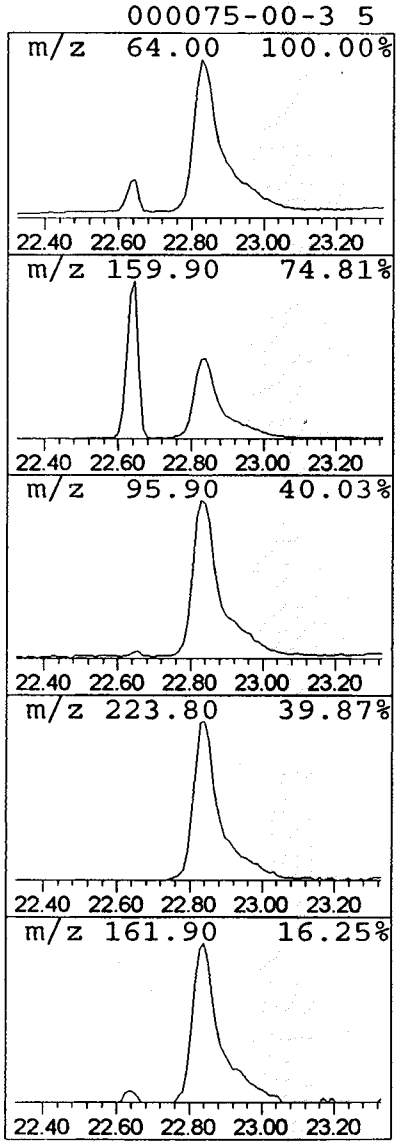
****

Peak Number 6 2-Norbornanone, 1-(epithioe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.83	4.20 ug/L	2434750	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	28
2	(1R*,4R*,5S*)-1-CARBETHOXY-4-MET...	234	C15H22O2	043219-76-7	9
3	Cyclohexane-d12	96	C6D12	001735-17-7	7
4	Ethane, chloro- (CAS) $$ Chloroe...	64	C2H5Cl	000075-00-3	5





Library Search Compound Report

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Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

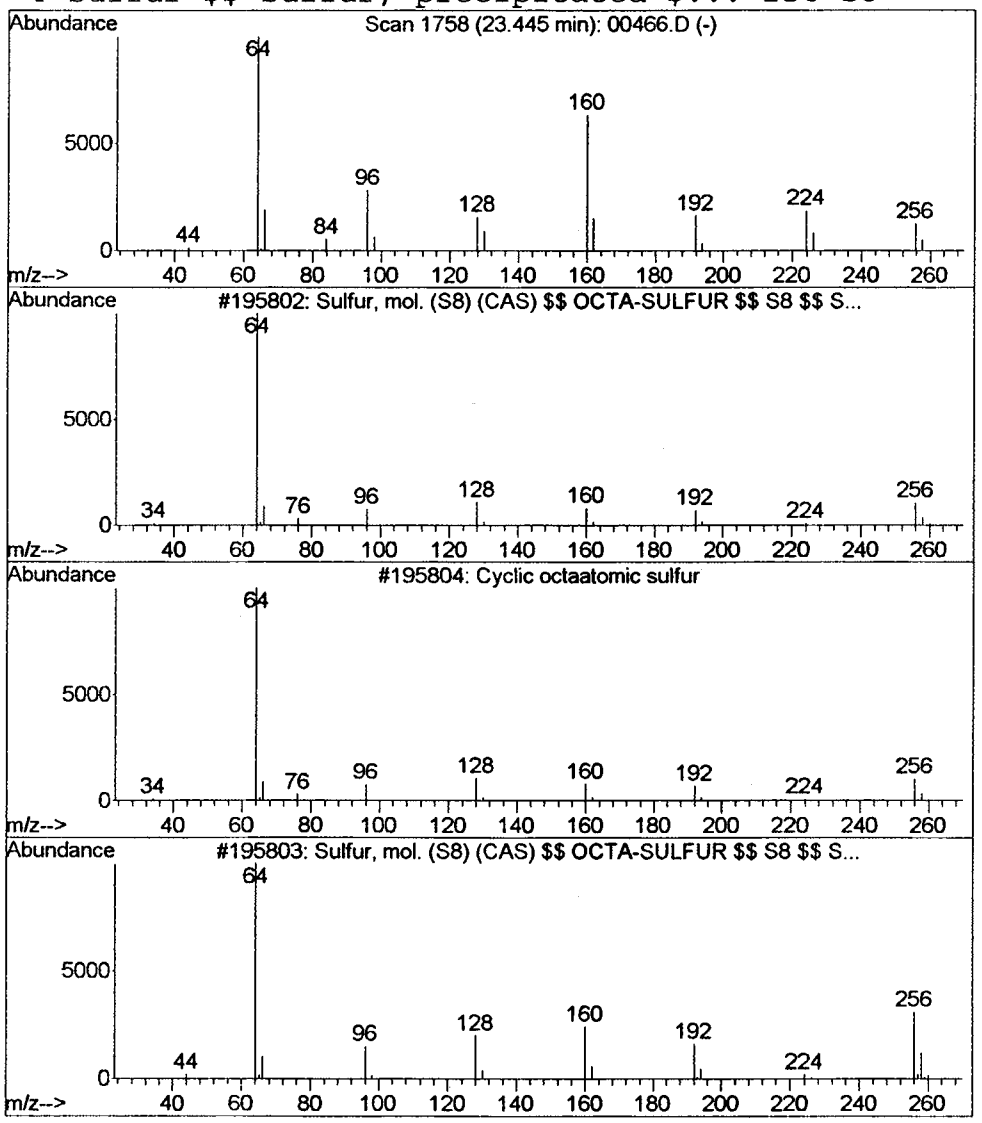
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

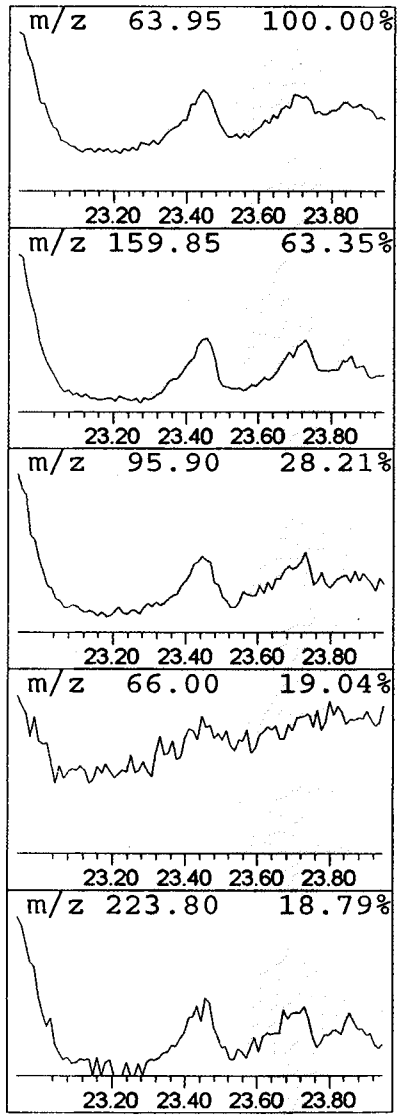
****

Peak Number 7 Sulfur, mol. (S8) (CAS) $$ ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.44	0.34 ug/L	196468	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	80
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	80
3	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	72
4	Sulfur $$ Sulfur, precipitated $...	256	S8	007704-34-9	59





Library Search Compound Report

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Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 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

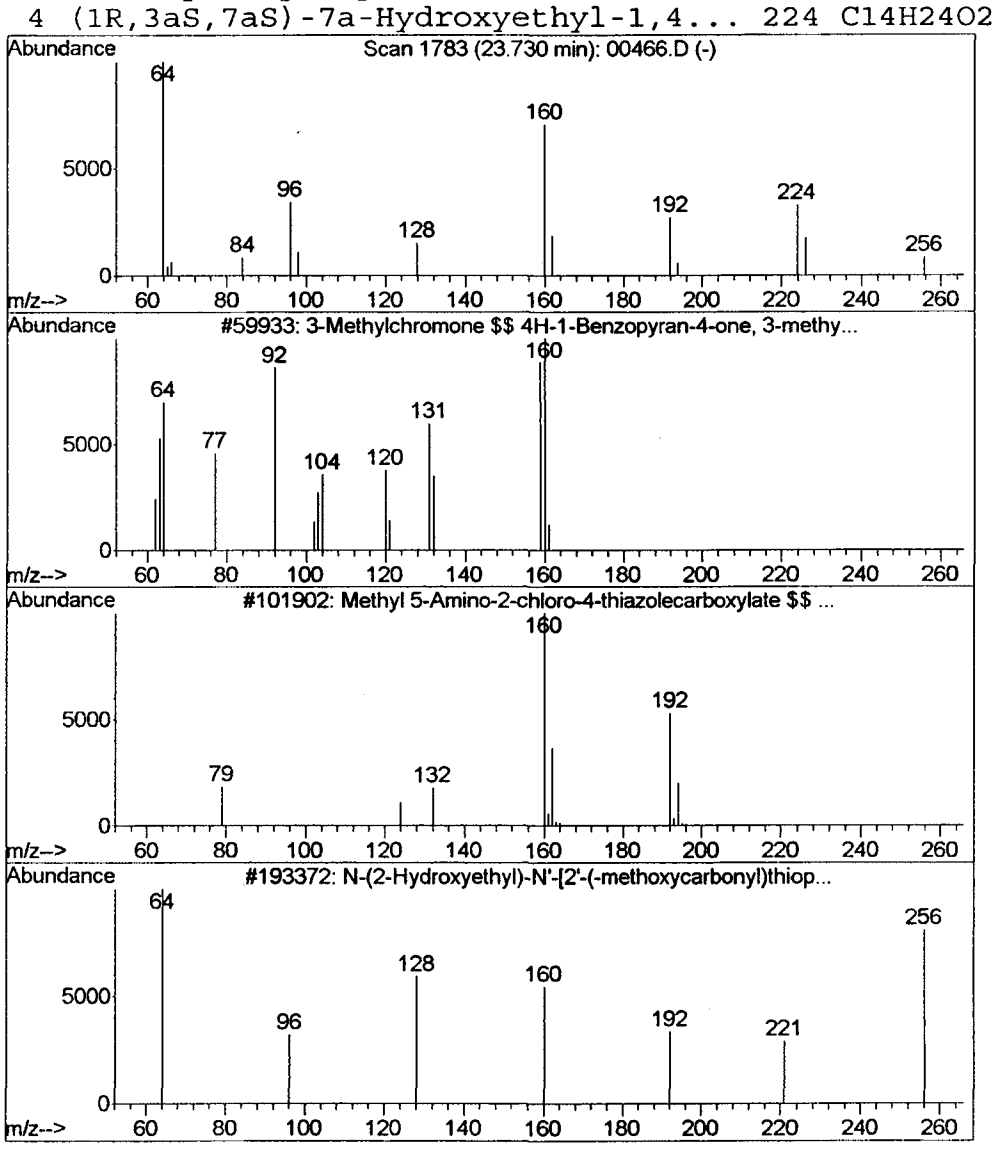
****

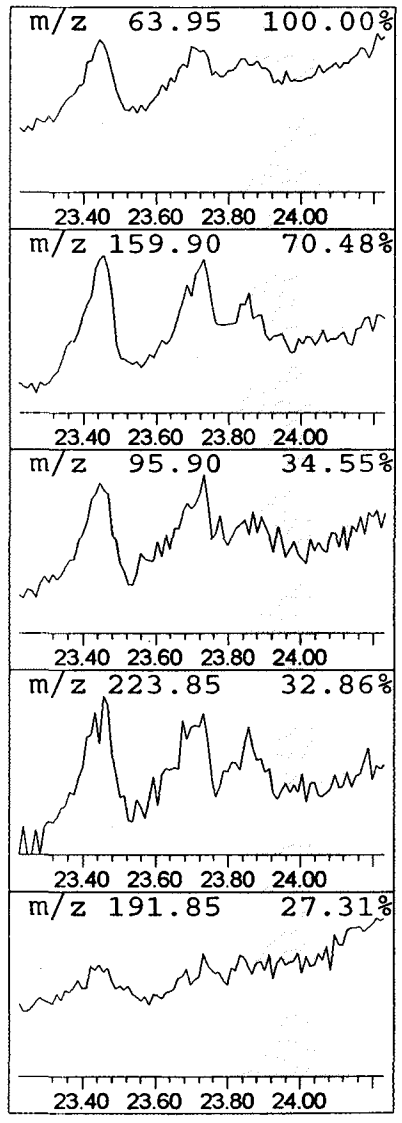
Peak Number 8 3-Methylchromone $$ 4H-1-Be... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.73	0.30 ug/L	175777	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylchromone $$ 4H-1-Benzopy...	160	C10H8O2	000085-90-5	50
2	Methyl 5-Amino-2-chloro-4-thiazo...	192	C5H5ClN2O2S	000000-00-0	23
3	N-(2-Hydroxyethyl)-N'-[2'-(-meth...	255	C10H13N3O3S	000000-00-0	9
4	(1R,3aS,7aS)-7a-Hydroxyethyl-1,4...	224	C14H24O2	128790-34-1	9

ND GOOD MATCH





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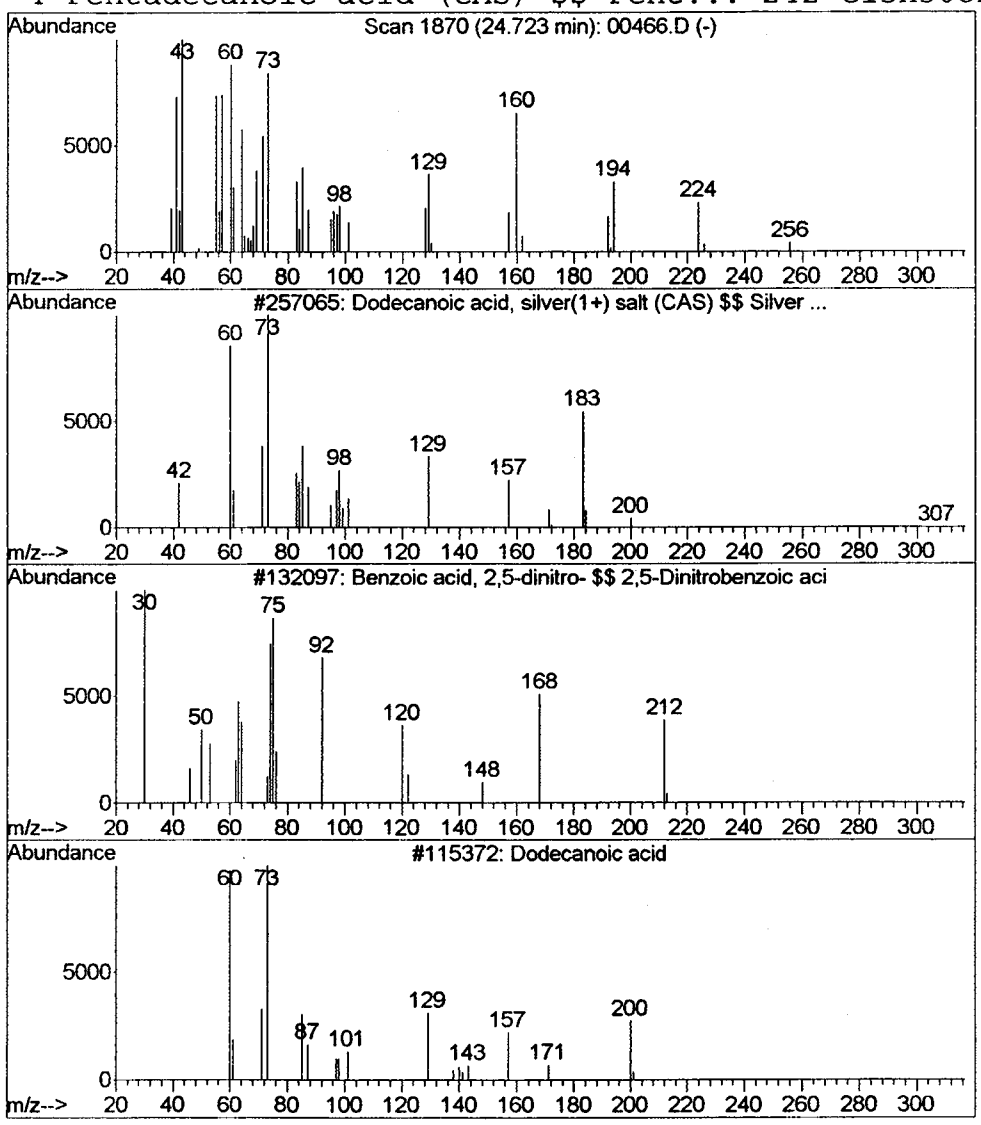
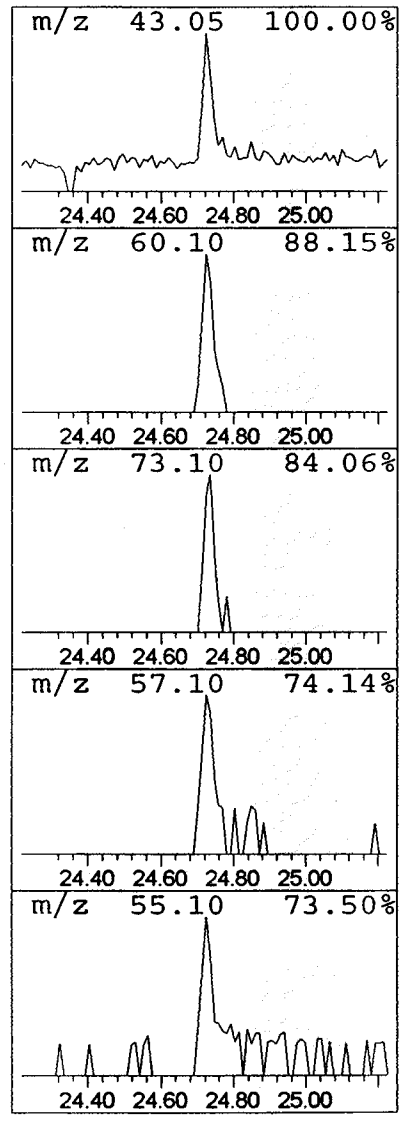
****

Peak Number 9 Dodecanoic acid, silver(1+)... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.72	0.20 ug/L	114686	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, silver(1+) salt...	307	C12H24AgO2	018268-45-6	30
2	Benzoic acid, 2,5-dinitro- $$ 2,...	212	C7H4N2O6	000610-28-6	25
3	Dodecanoic acid	200	C12H24O2	000143-07-7	14
4	Pentadecanoic acid (CAS) $$ Pent...	242	C15H30O2	001002-84-2	14





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

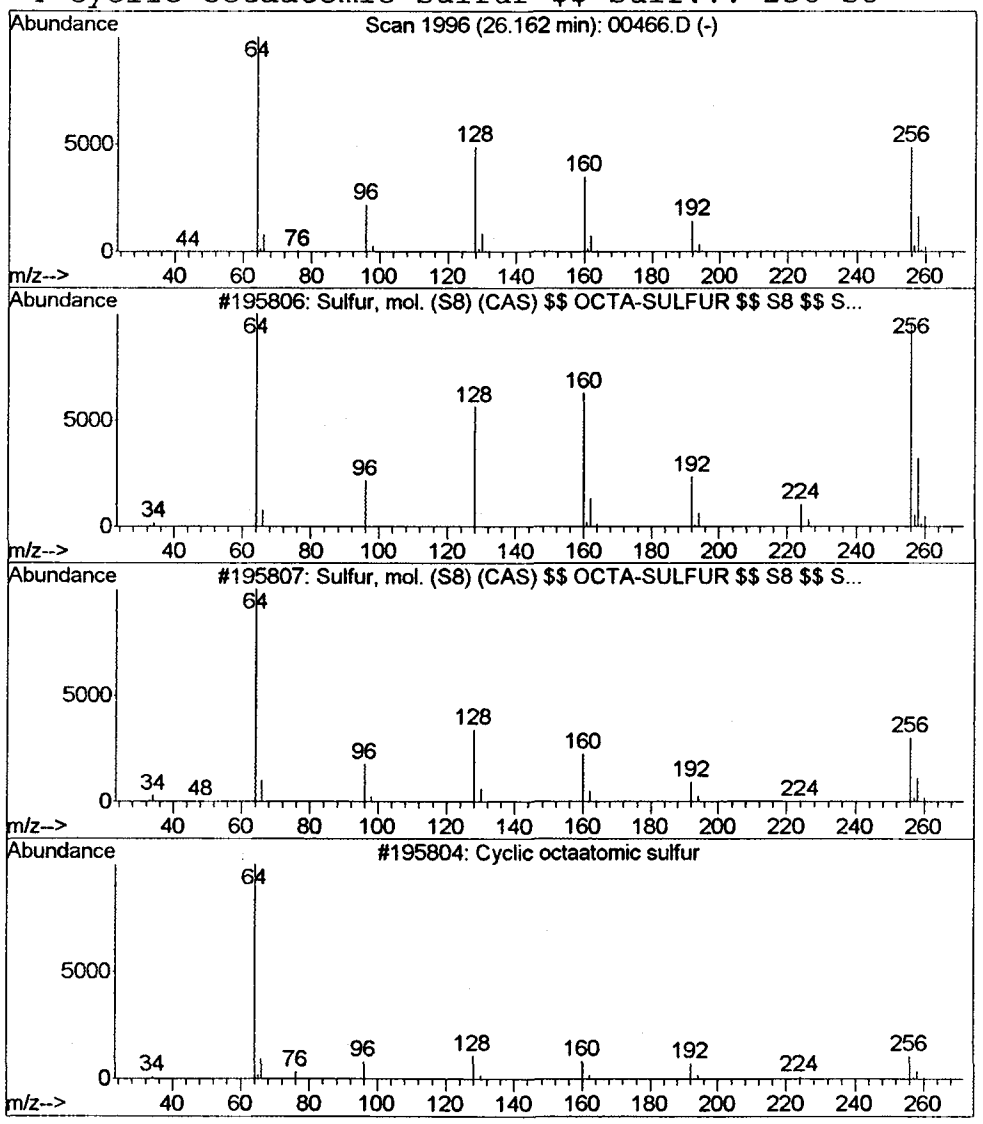
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

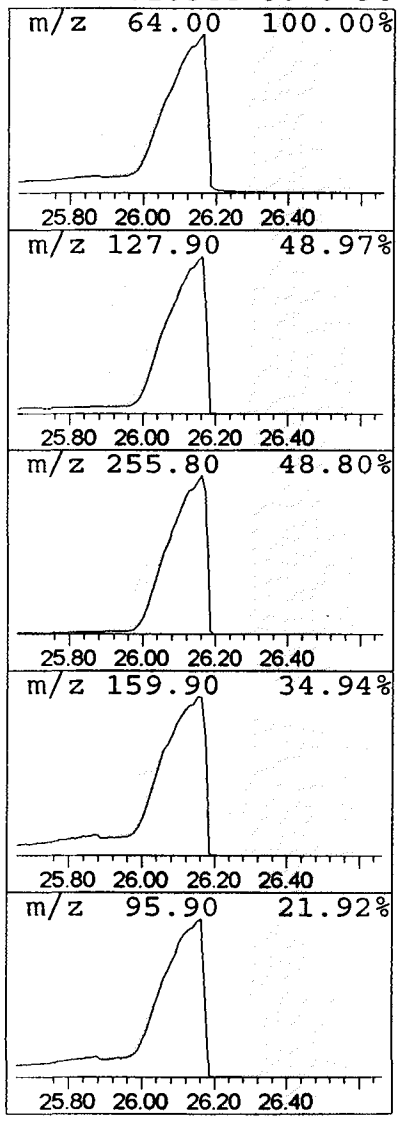
****

Peak Number 10 Sulfur, mol. (S8) (CAS) $$ ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.16	100.73 ug/L	58342500	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	97
2	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	97
3	Cyclic octaatomic sulfur	256	S8	010544-50-0	91
4	Cyclic octaatomic sulfur $$ Sulf...	256	S8	010544-50-0	90





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00466.D Vial: 4
Acq On : 10 Jan 2002 5:18 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

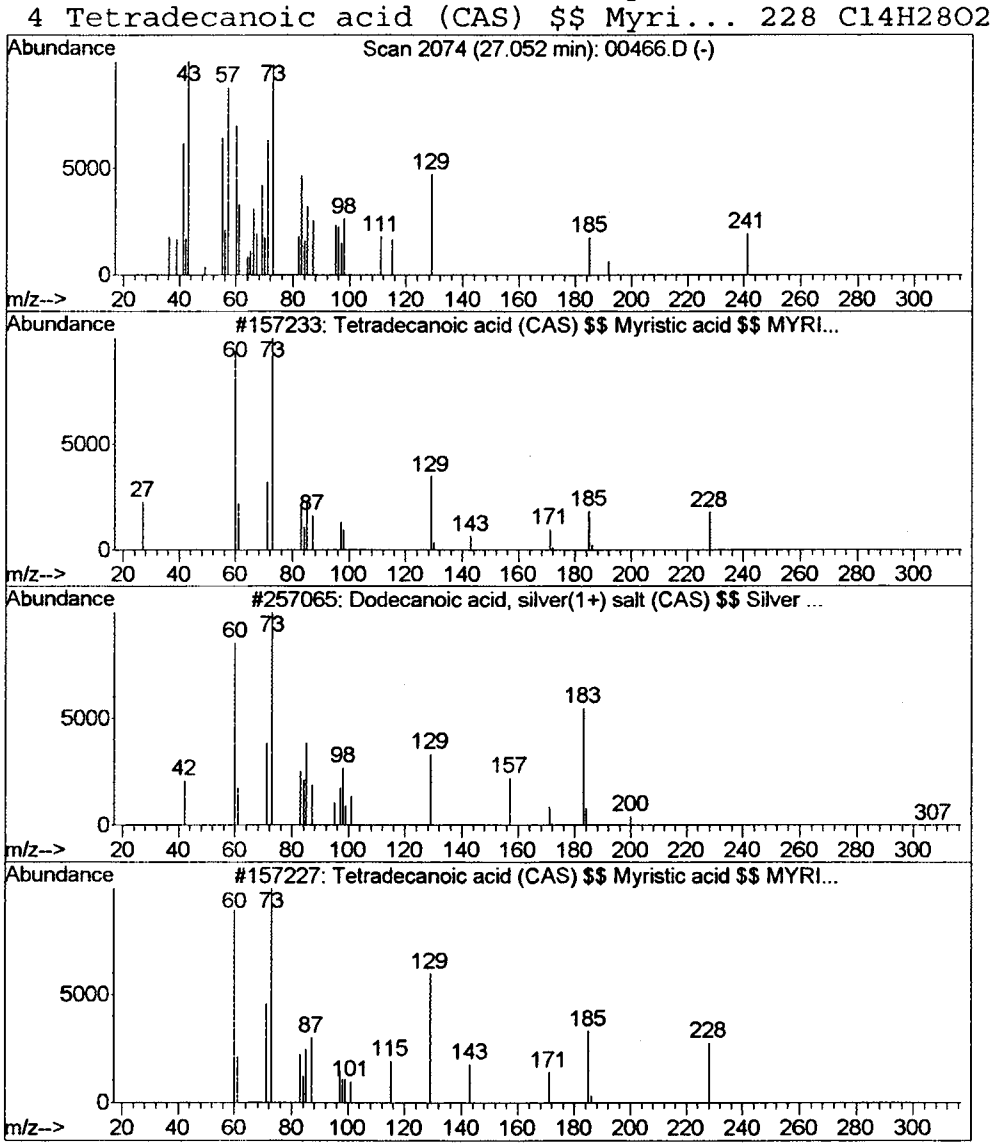
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

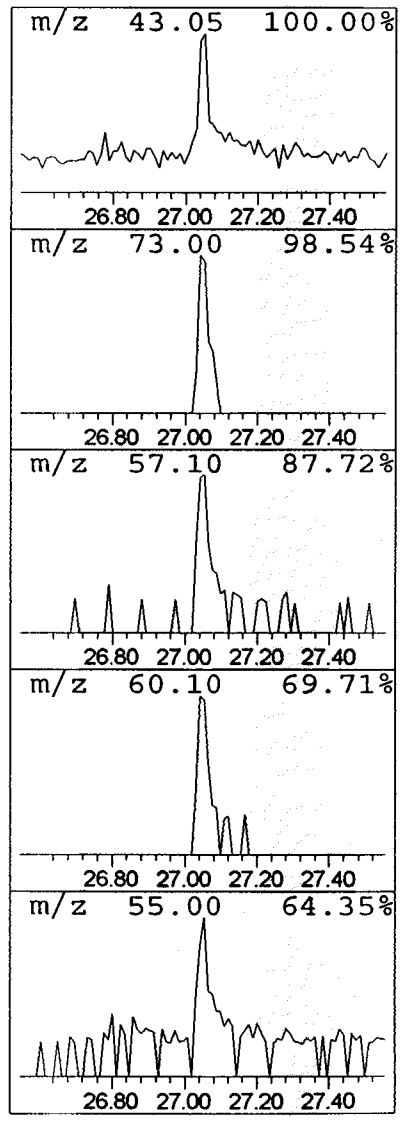
****

Peak Number 11 Tetradecanoic acid (CAS) $$... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.05	0.15 ug/L	87168	Chrysene-d12	30.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid (CAS) $$ Myri...	228	C14H28O2	000544-63-8	35
2	Dodecanoic acid, silver(1+) salt...	307	C12H24AgO2	018268-45-6	27
3	Tetradecanoic acid (CAS) $$ Myri...	228	C14H28O2	000544-63-8	27
4	Tetradecanoic acid (CAS) $$ Myri...	228	C14H28O2	000544-63-8	22





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 10 Jan 2002 5:18 pm
Data File: C:\MSDCHEM\1\5973N\02JAN10\00466.D
Name: 508 scan ext 1/8
Misc: January 10, 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
Silane, tetramethyl-	5.89	3.9	ug/L	1309960	1	9.72	6675240	20.0
2-Propanol, 1-(2-...	9.86	0.2	ug/L	57059	1	9.72	6675240	20.0
1,4-Dimethyl-3,5-...	18.73	2.9	ug/L	1526220	3	18.34	10596900	20.0
bis(2-furyl)dimet...	20.93	0.1	ug/L	71353	4	22.65	11583900	20.0
4-METHOXY-.BETA.-...	22.28	0.2	ug/L	107450	4	22.65	11583900	20.0
2-Norbornanone, 1-...	22.83	4.2	ug/L	2434750	4	22.65	11583900	20.0
Sulfur, mol. (S8)...	23.44	0.3	ug/L	196468	4	22.65	11583900	20.0
3-Methylchromone ...	23.73	0.3	ug/L	175777	4	22.65	11583900	20.0
Dodecanoic acid, ...	24.72	0.2	ug/L	114686	4	22.65	11583900	20.0
Sulfur, mol. (S8)...	26.16	100.7	ug/L	58342500	4	22.65	11583900	20.0
Tetradecanoic aci...	27.05	0.1	ug/L	87168	5	30.50	11930700	20.0