User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 02/08/2002 Time: 13:03:55

Sample: AD28860
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 12/16/01 12:25 Ended: 12/16/01 12:25 Analyst: DLV
Result source: manual entry
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		95		5.0

Comments for Sample AD28860 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 02-08-2002 Time: 13:05:41

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.
The recovery for the Surrogate Standard in this sample was below its acceptance range. This sample will be re-extracted and re-analyzed. Re-analysis was performed with a Surrogate Standard recovery of 95%. Also, the pH of this sample when received was less than 2.

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 04 08:34:12 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

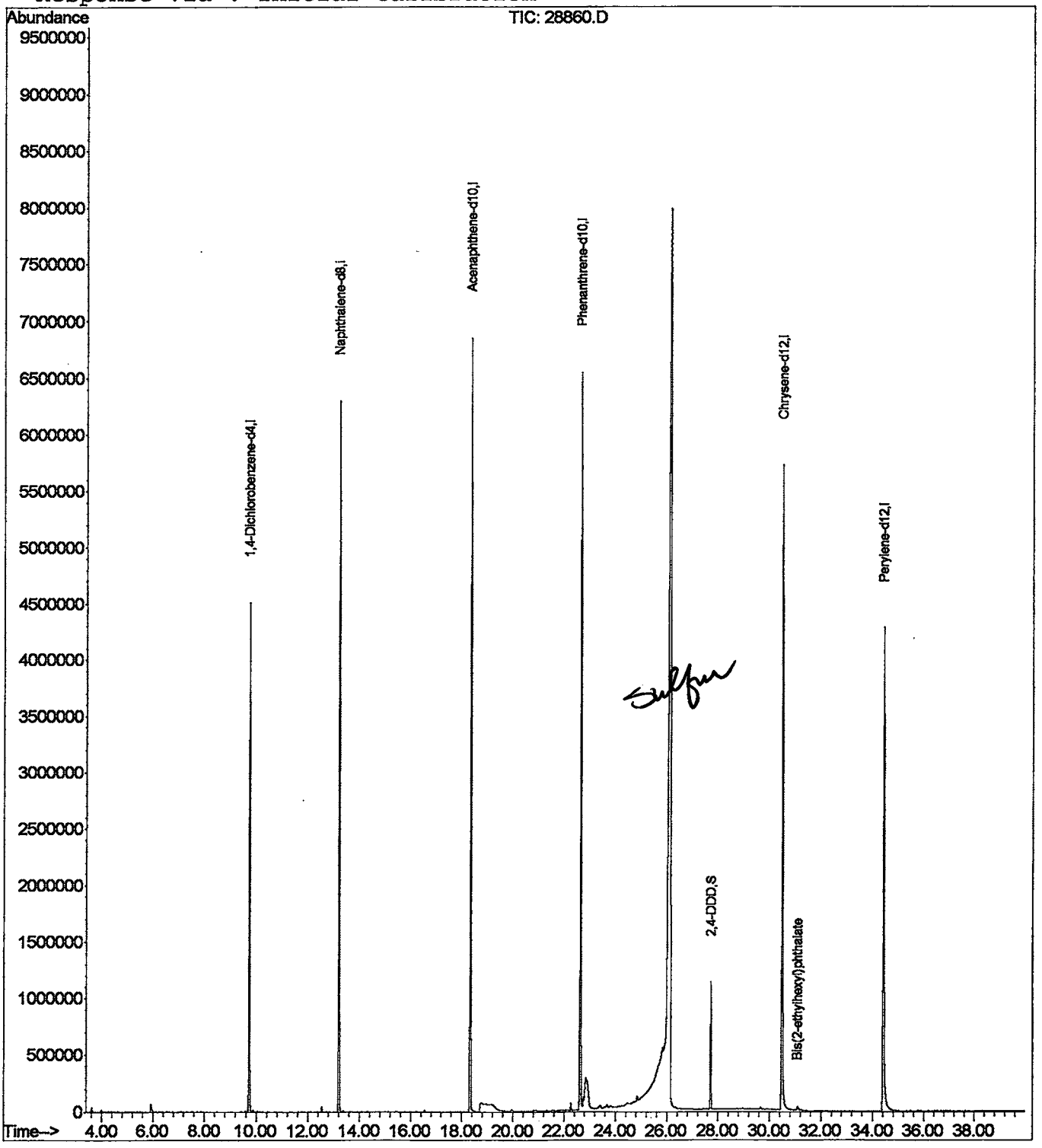
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1533032	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	6548713	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	3373103	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	5516415	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	4824350	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3504572	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	414928	4.76	ug/L	0.00
Spiked Amount 5.000			Recovery =	95.20%		
Target Compounds						Qvalue
42) Bis(2-ethylhexyl)phthalate	31.11	149	39118	0.71	ug/L	88

(#) = qualifier out of range (m) = manual integration
28860.D SCAN508.M Mon Feb 04 09:31:45 2002 Page 1

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 4 9:31 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\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

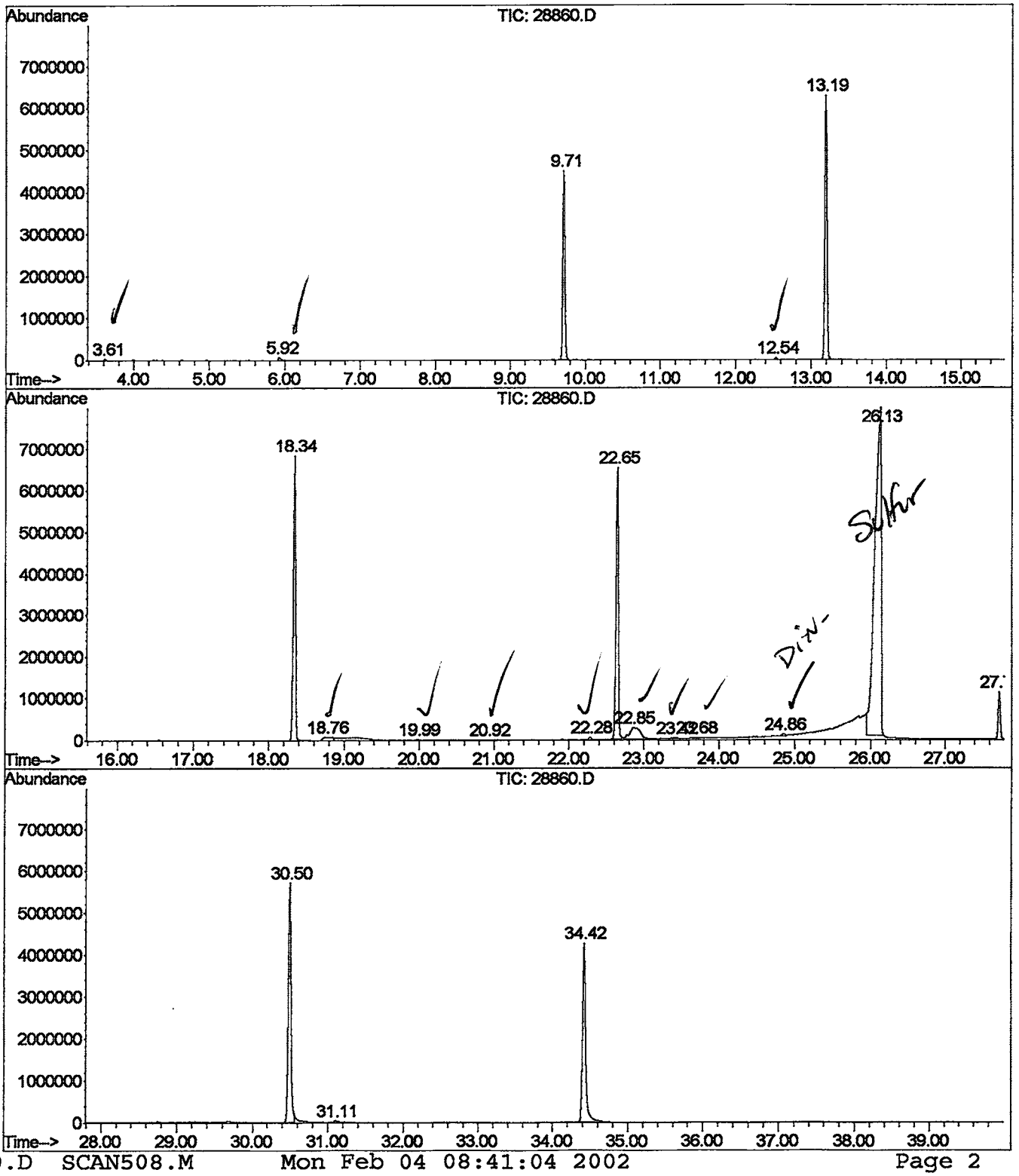
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.613	19	21	25	rVV	41067	60266	0.13%	0.046%
2	5.920	221	223	233	rBV	72309	167506	0.35%	0.129%
3	9.710	551	555	561	rBV	4505960	8697828	18.30%	6.703%
4	12.541	797	803	807	rBV	46403	78493	0.17%	0.060%
5	13.192	855	860	865	rBV	6300914	12558919	26.43%	9.679%
6	18.341	1305	1311	1315	rBV	6852410	13660262	28.75%	10.528%
7	18.764	1339	1348	1357	rBV4	79797	701629	1.48%	0.541%
8	19.985	1447	1455	1461	rBV4	16143	47525	0.10%	0.037%
9	20.921	1529	1537	1539	rVV5	9168	47316	0.10%	0.036%
10	22.280	1651	1656	1661	rBV2	67137	126724	0.27%	0.098%
11	22.645	1681	1688	1693	rBV	6532821	14668919	30.87%	11.305%
12	22.851	1695	1706	1735	rVB4	275535	2733009	5.75%	2.106%
13	23.422	1747	1756	1761	rBV3	22708	101158	0.21%	0.078%
14	23.684	1765	1779	1783	rBV5	30618	168363	0.35%	0.130%
15	24.860	1877	1882	1885	rBV	46410	106452	0.22%	0.082%
16	26.128	1977	1993	1997	rVB	7886823	47518742	100.00%	36.621%
17	27.726	2127	2133	2139	rBV	1122548	2094362	4.41%	1.614%
18	30.500	2369	2376	2381	rBV	5709267	14063664	29.60%	10.838%
19	31.105	2419	2429	2447	rVB2	34337	183680	0.39%	0.142%
20	34.416	2713	2719	2755	rBV	4277831	11972651	25.20%	9.227%

Sum of corrected areas: 129757468

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02FEB01\28860.D
Operator :
Acquired : 1 Feb 2002 12:14 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : February 1, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

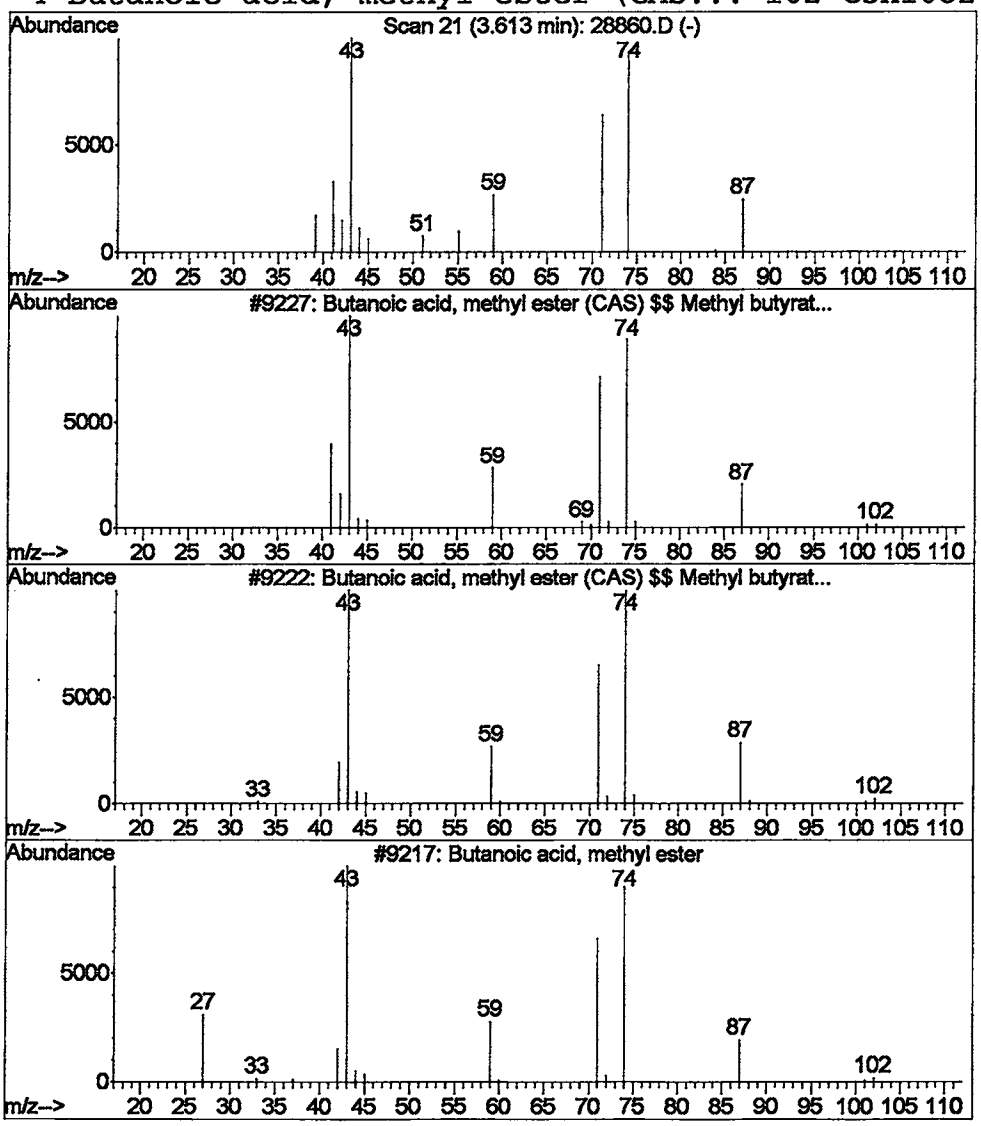
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

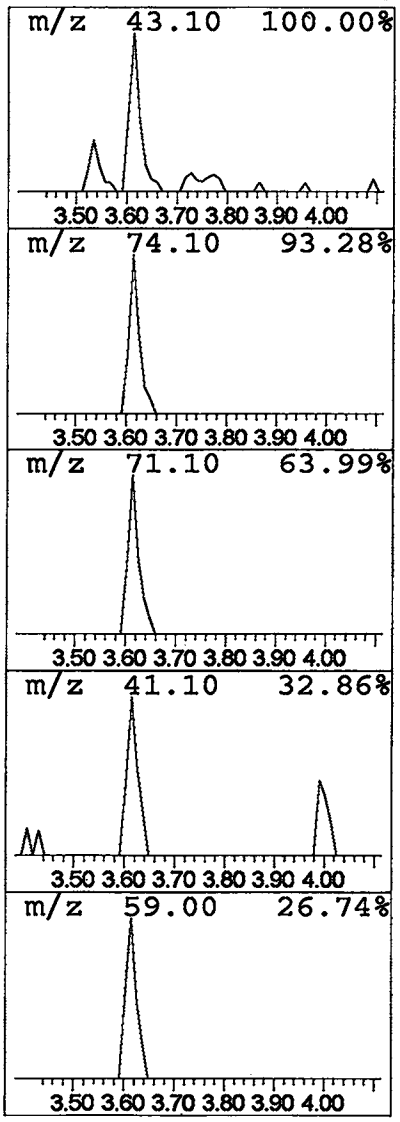
****

Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	0.14 ug/L	60266	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	83
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
4	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

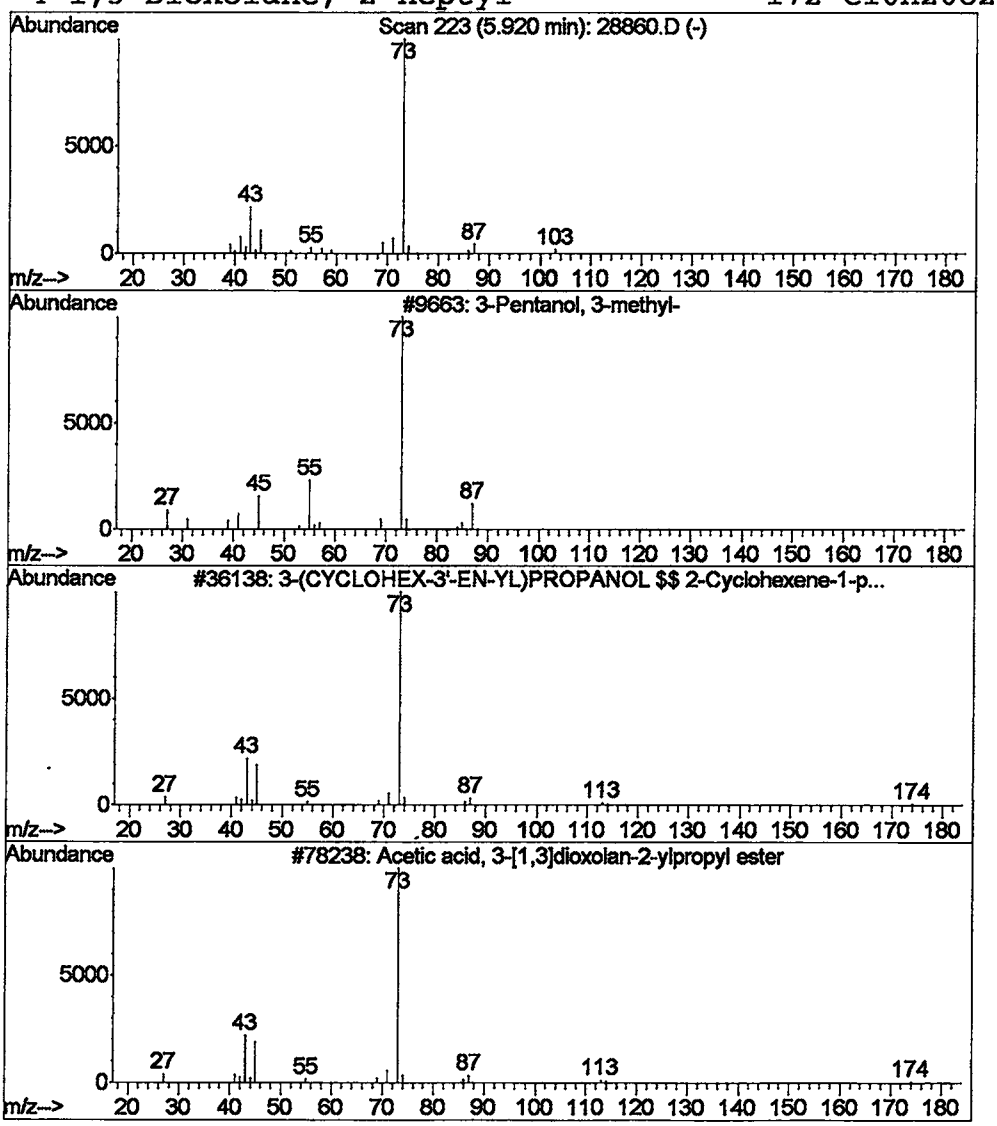
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

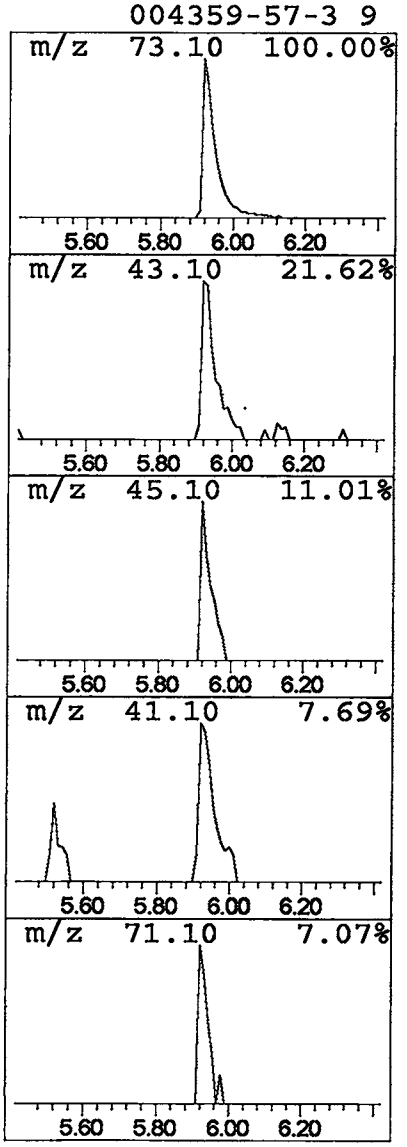
****

Peak Number 2 3-Pentanol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	0.39 ug/L	167506	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	36
2	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33
3	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
4	1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

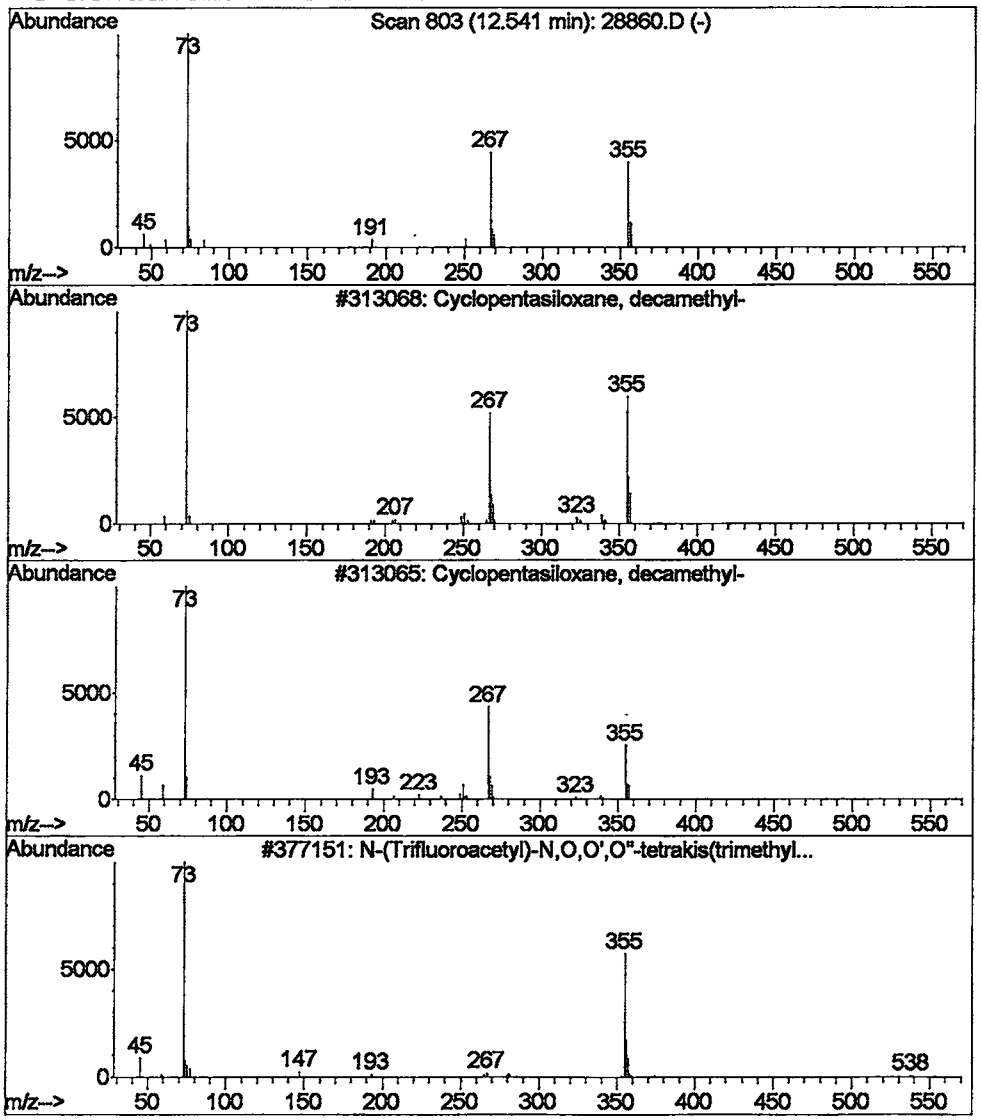
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

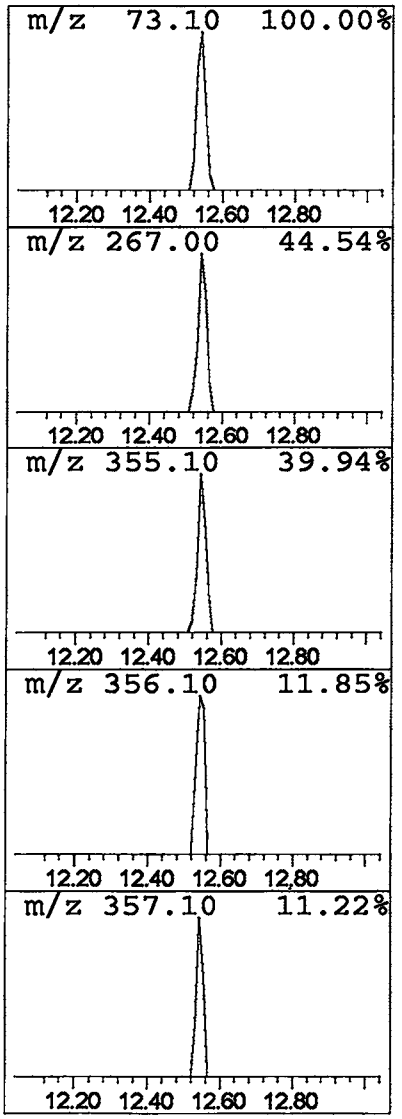
****

Peak Number 3 Cyclopentasiloxane, decamet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	0.13 ug/L	78493	Naphthalene-d8	13.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	53
2	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	42
3	N-(Trifluoroacetyl)-N,O,O',O''-t...	553	C22H42F3NO4Si4	000000-00-0	37
4	Noradrenaline tetraTMS	457	C20H43NO3Si4	068595-65-3	37





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

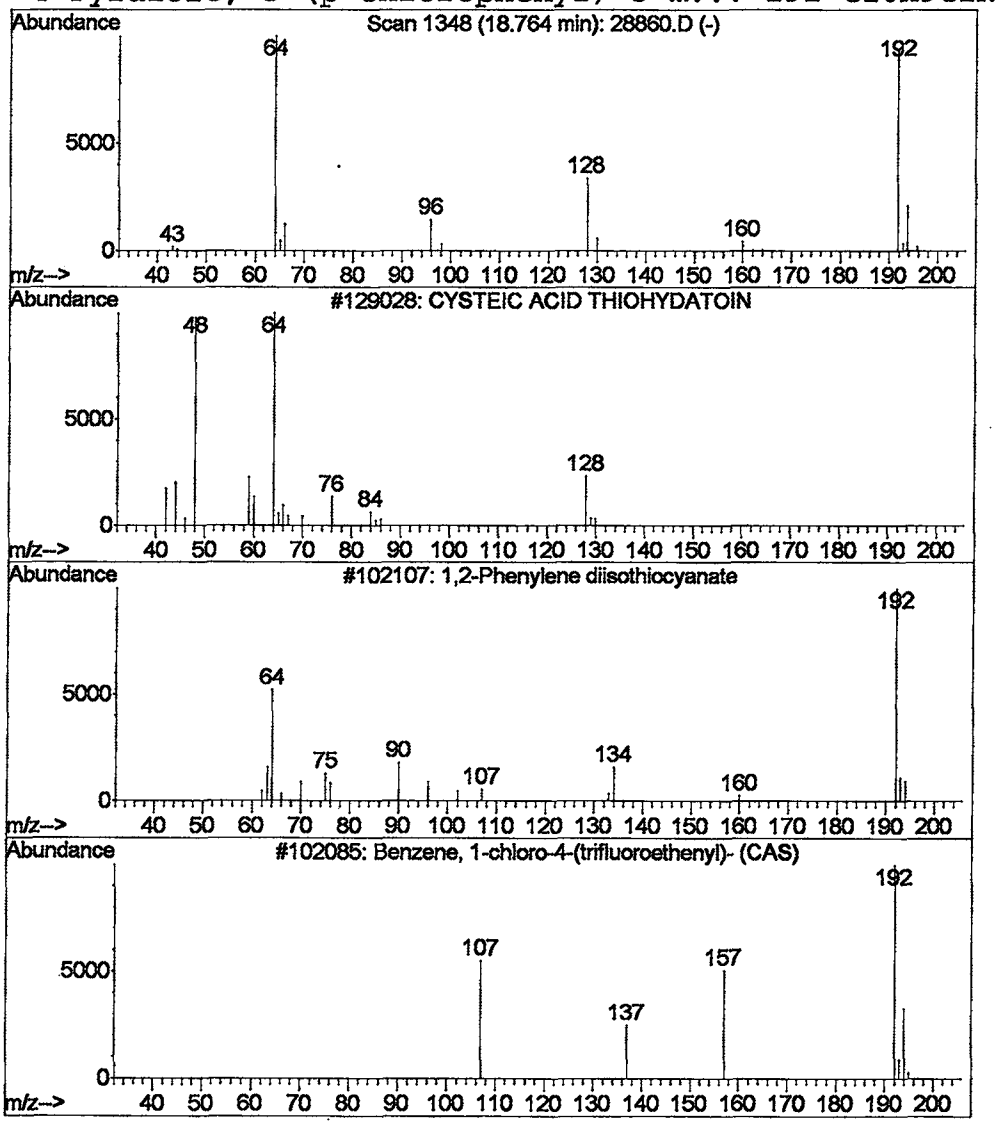
****

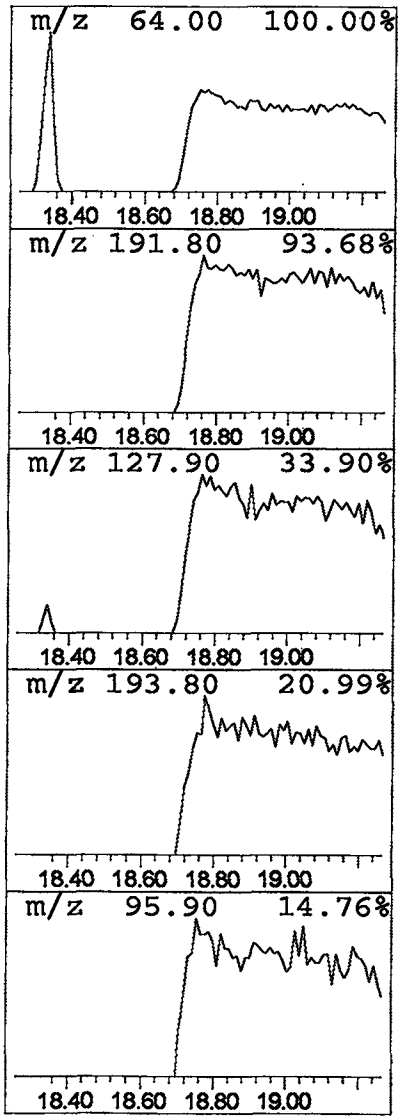
Peak Number 4 CYSTEIC ACID THIOHYDATOIN Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	1.03 ug/L	701629	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	CYSTEIC ACID THIOHYDATOIN	210	C4H6N2O4S2	000000-00-0	38
2	1,2-Phenylene diisothiocyanate	192	C8H4N2S2	071105-17-4	9
3	Benzene, 1-chloro-4-(trifluoroet...	192	C8H4ClF3	082907-01-5	5
4	Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	5

NO GOOD MATCH





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

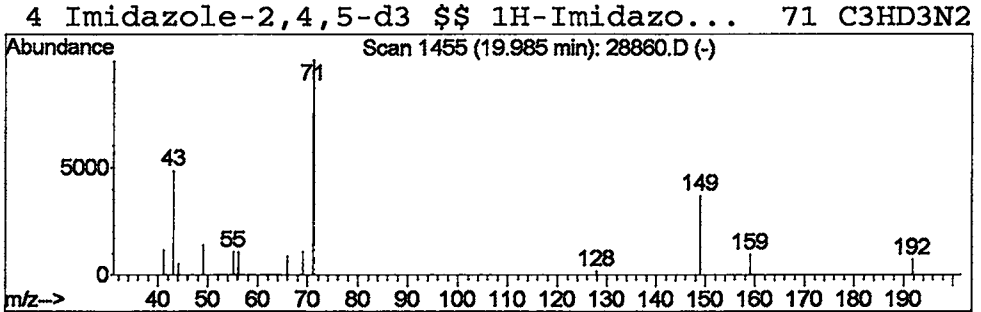
****

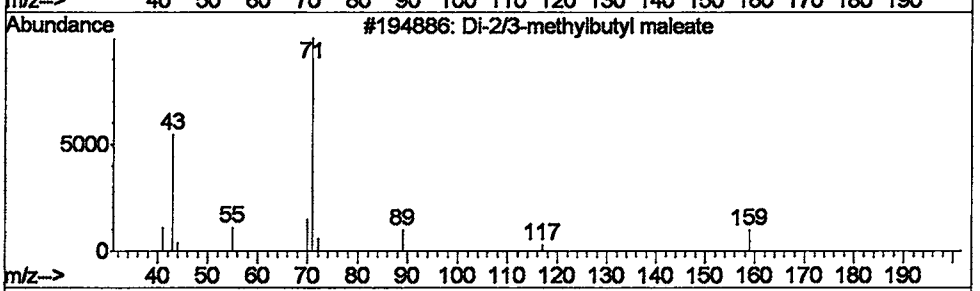
Peak Number 5 Di-2/3-methylbutyl maleate Concentration Rank 11

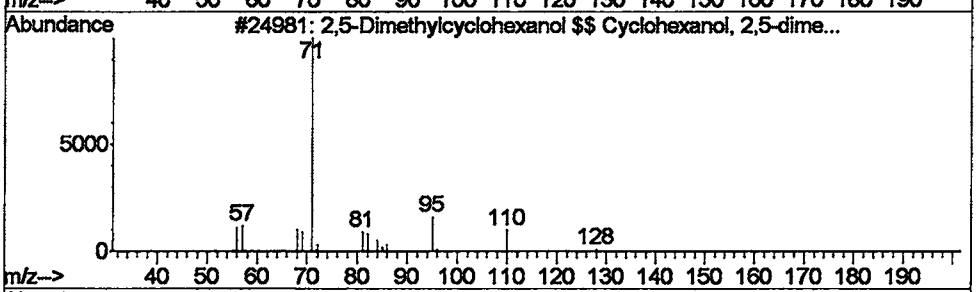
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.99	0.07 ug/L	47525	Acenaphthene-d10	18.34

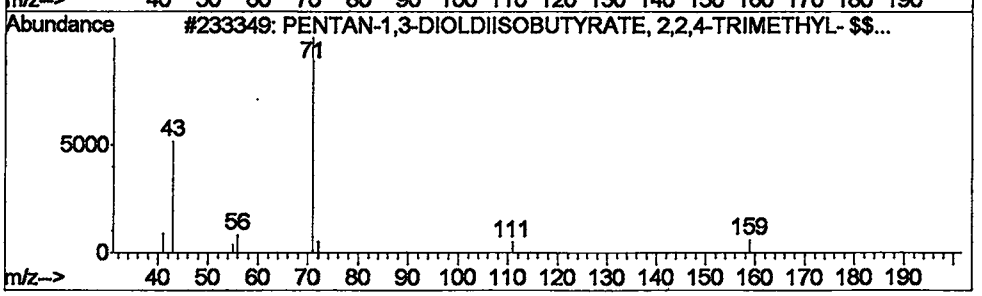
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-2/3-methylbutyl maleate	256	C14H24O4	000000-00-0	28
2	2,5-Dimethylcyclohexanol $$ Cycl...	128	C8H16O	003809-32-3	9
3	PENTAN-1,3-DIOLDIISOBUTYRATE, 2,...	286	C16H30O4	006846-50-0	9
4	Imidazole-2,4,5-d3 $$ 1H-Imidazo...	71	C3HD3N2	006745-43-3	7

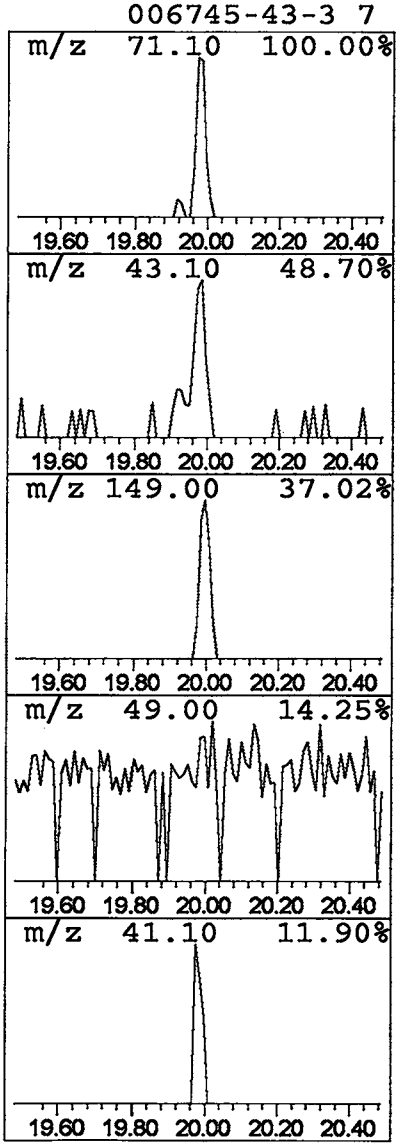
NO GOOD MATCH











Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

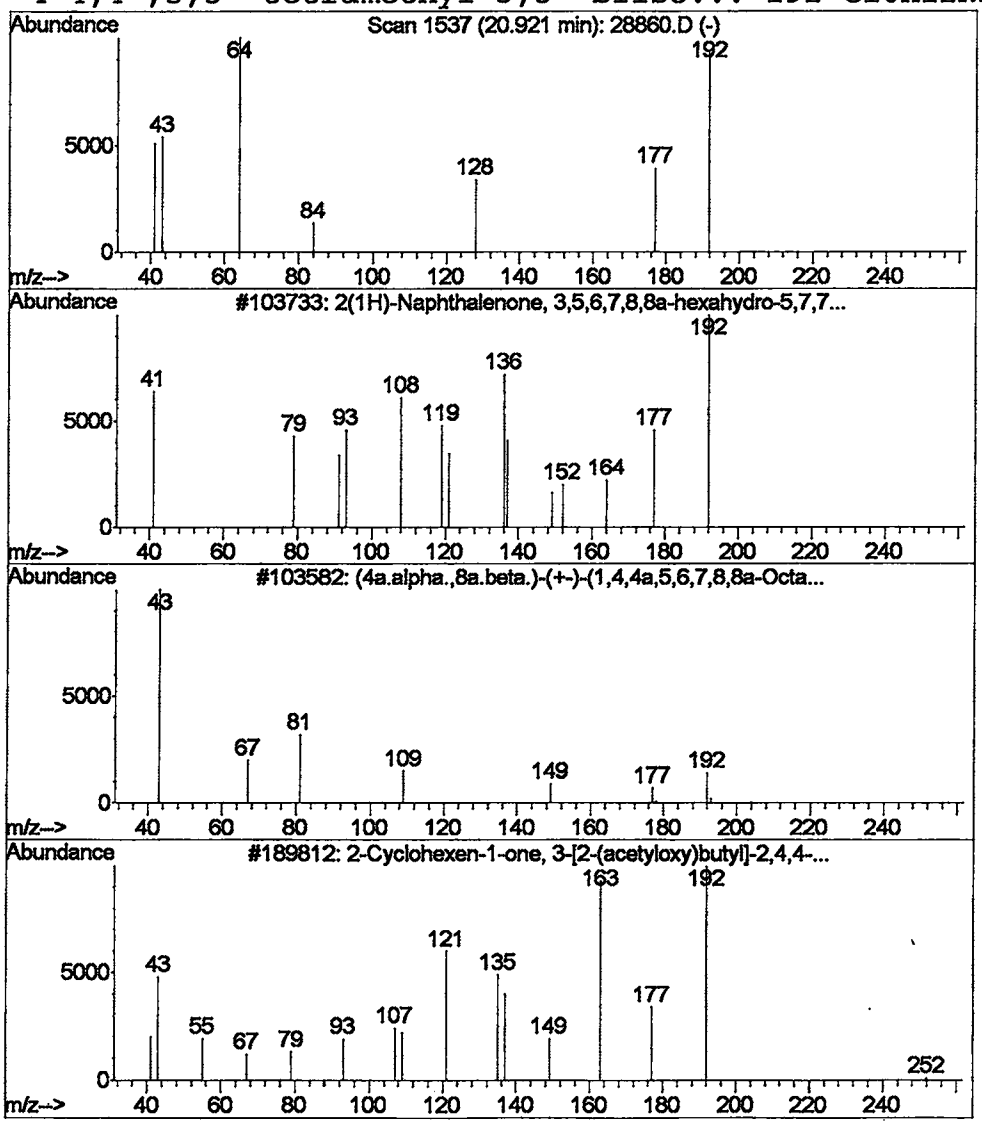
****

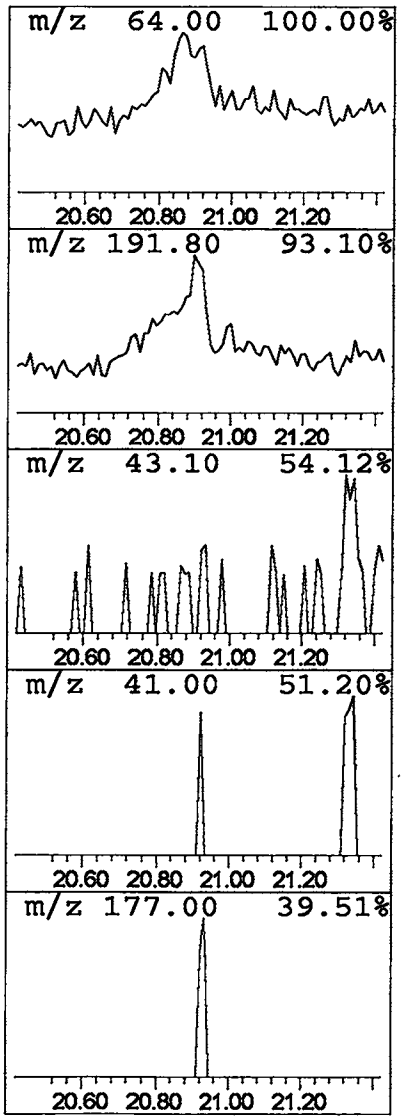
Peak Number 6 2(1H)-Naphthalenone, 3,5,6,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	0.06 ug/L	47316	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, 3,5,6,7,8,8...	192	C13H20O	075314-20-4	9
2	(4a.alpha.,8a.beta.)-(+-)-(1,4,4...	192	C13H20O	000000-00-0	4
3	2-Cyclohexen-1-one, 3-[2-(acetyl...	252	C15H24O3	075332-27-3	4
4	4,4',5,5'-tetramethyl-3,3'-biiso...	192	C10H12N2O2	111080-79-6	4

NO GOOD MATCH





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

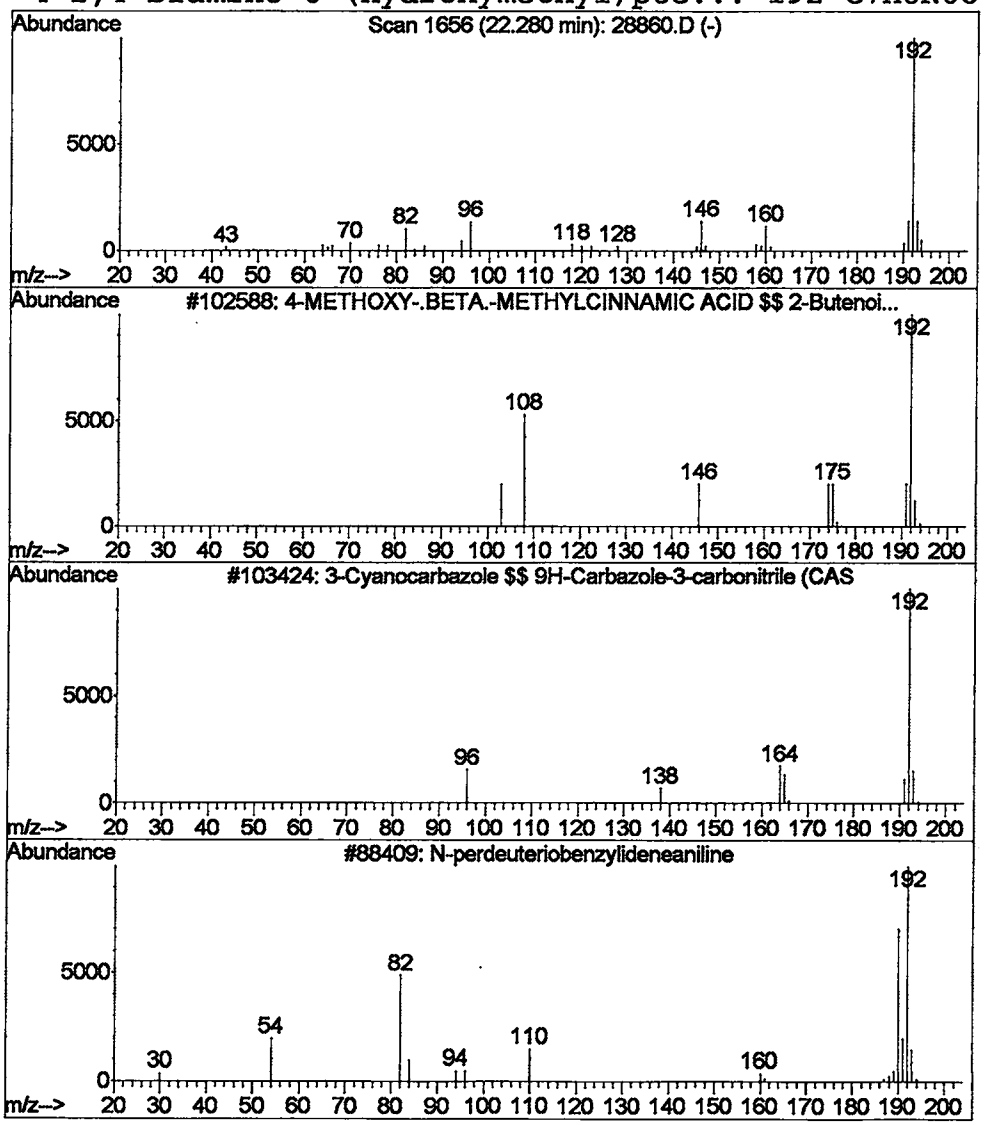
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

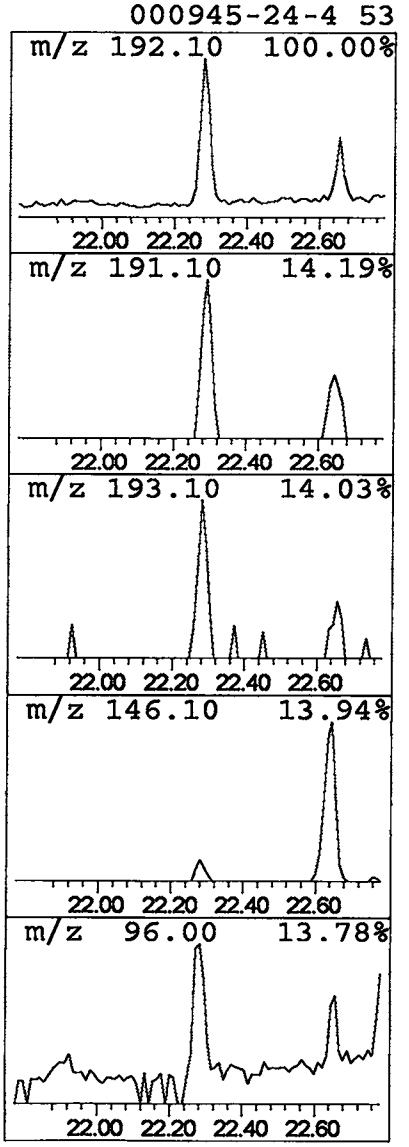
****

Peak Number 7 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.17 ug/L	126724	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
2	3-Cyanocarbazole $$ 9H-Carbazole...	192	C13H8N2	057102-93-9	59
3	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	53
4	2,4-Diamino-6-(hydroxymethyl)pte...	192	C7H8N6O	000945-24-4	53





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

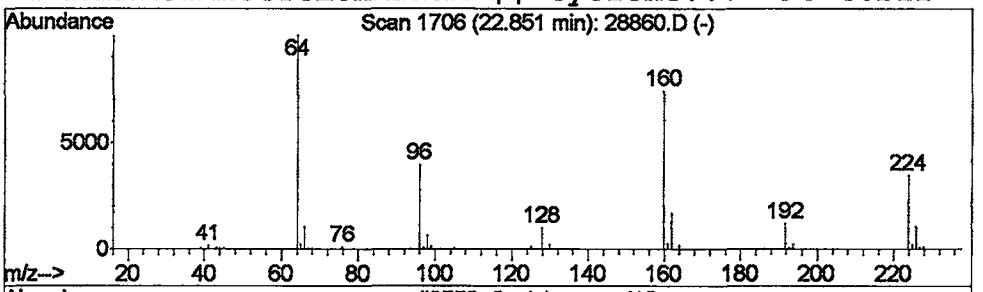
****

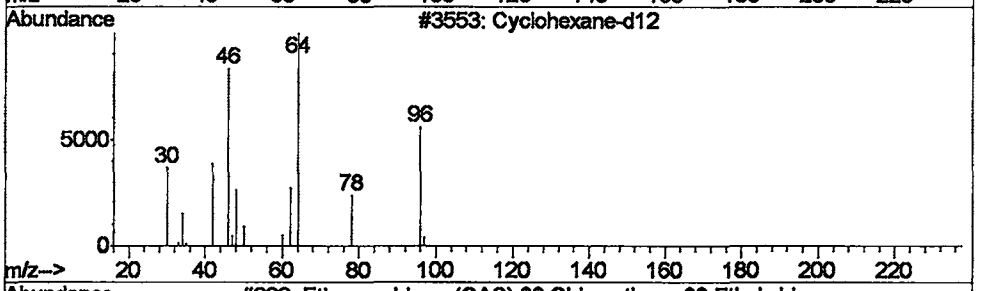
Peak Number 8 Cyclohexane-d12 Concentration Rank 2

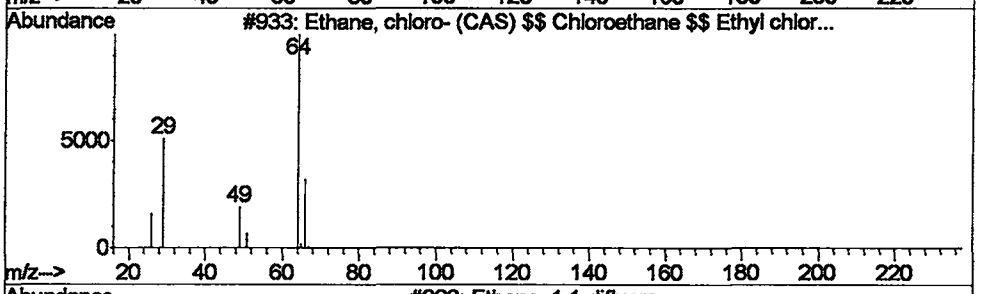
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.85	3.73 ug/L	2733010	Phenanthrene-d10	22.65

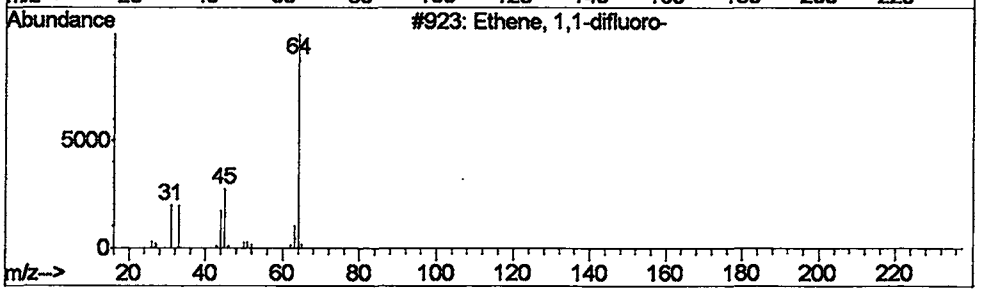
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane-d12	96	C6D12	001735-17-7	7
2	Ethane, chloro- (CAS) $$ Chloroe...	64	C2H5Cl	000075-00-3	5
3	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
4	PERDEUTEROCYCLOHEXANE $$ Cyclohe...	96	C6D12	001735-17-7	5

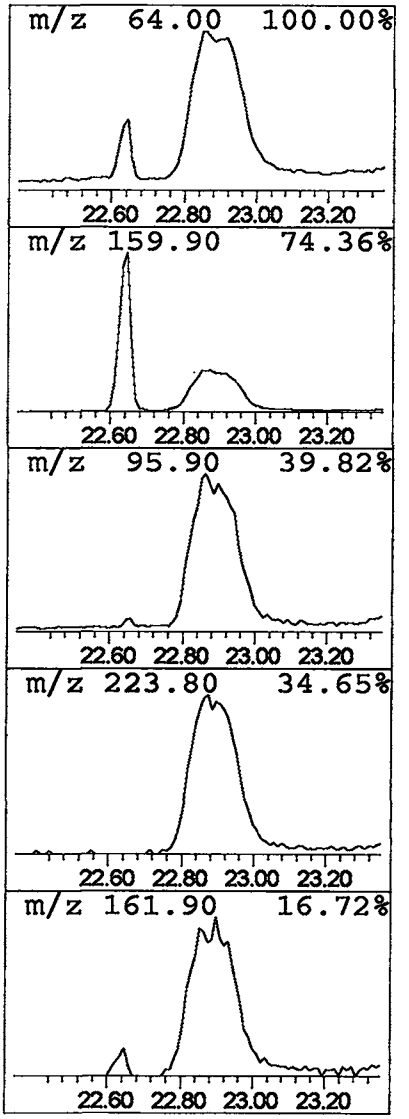
NO GOOD MATCH











Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

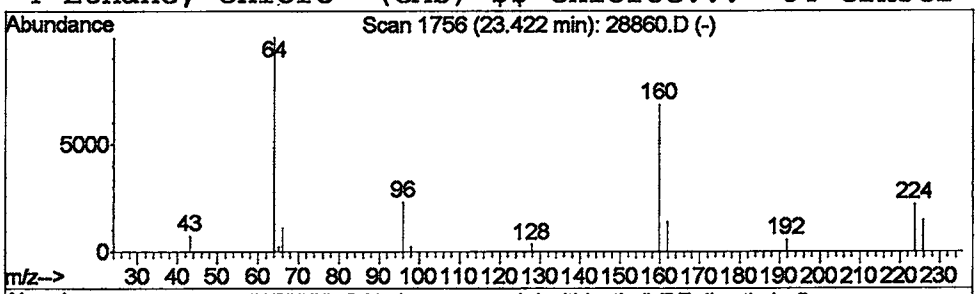
****

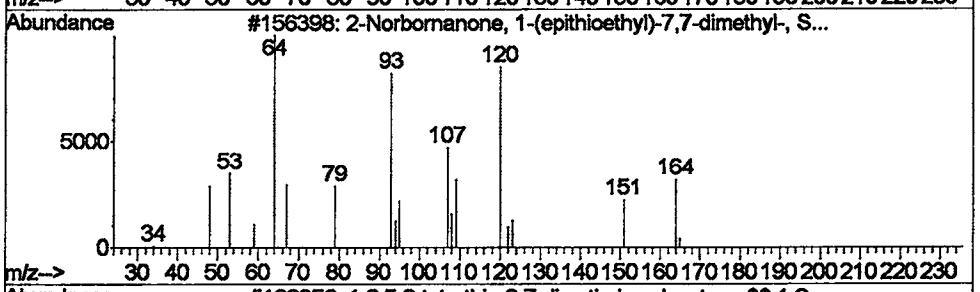
Peak Number 9 2-Norbornanone, 1-(epithioe... Concentration Rank 9

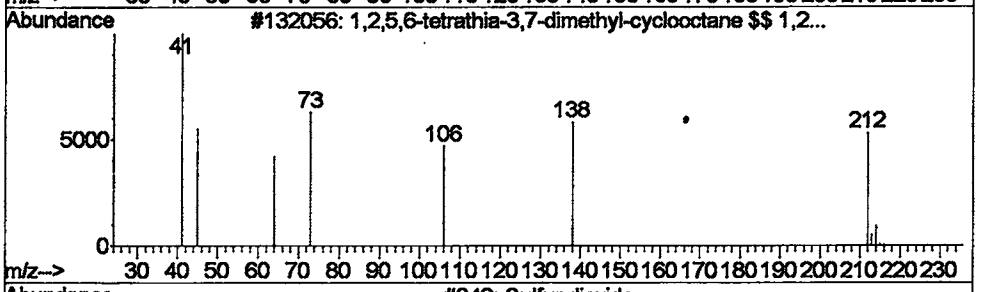
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.42	0.14 ug/L	101158	Phenanthrene-d10	22.65

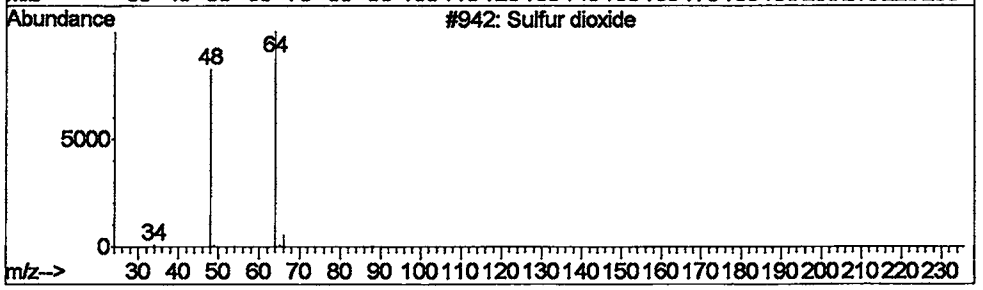
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	36
2	1,2,5,6-tetrathia-3,7-dimethyl-c...	212	C6H12S4	116664-31-4	7
3	Sulfur dioxide	64	O2S	007446-09-5	4
4	Ethane, chloro- (CAS) $$ Chloroe...	64	C2H5Cl	000075-00-3	4

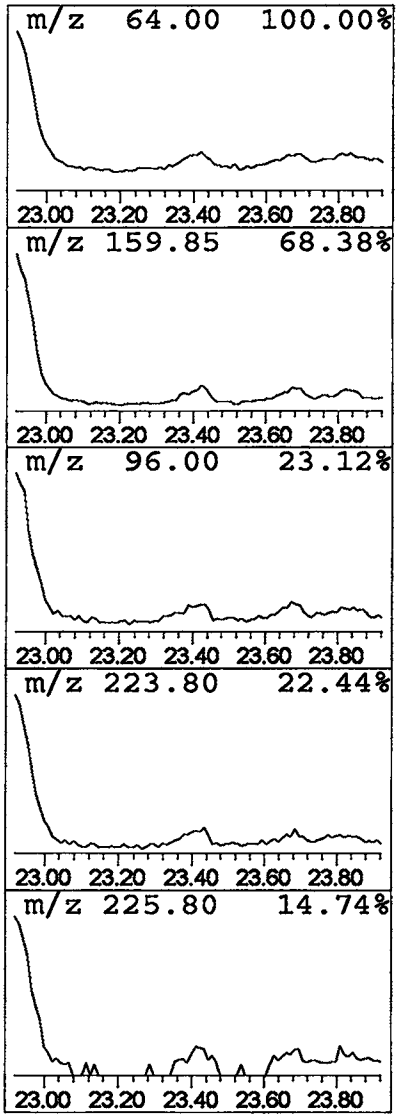
NO GOOD MATCH











Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 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

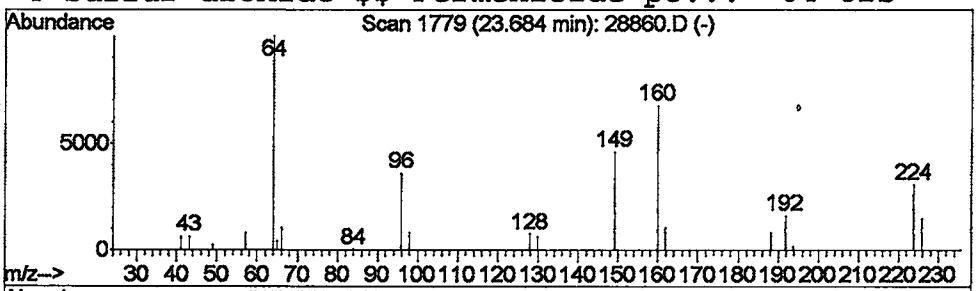
****

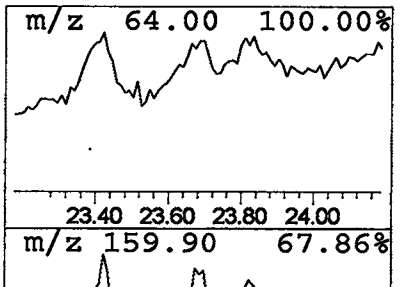
Peak Number 10 2-Norbornanone, 1-(epithioe... Concentration Rank 5

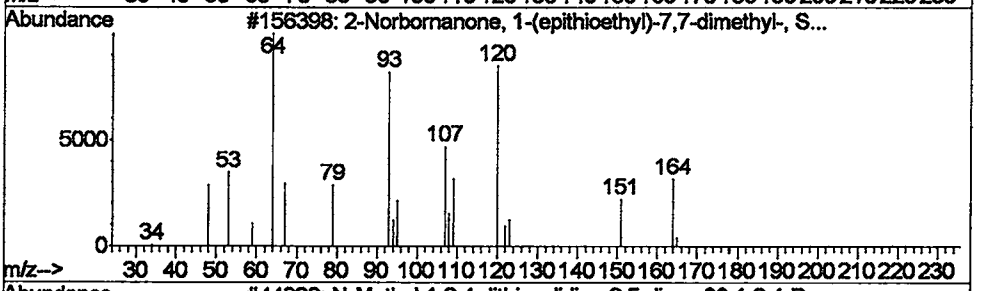
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.68	0.23 ug/L	168363	Phenanthrene-d10	22.65

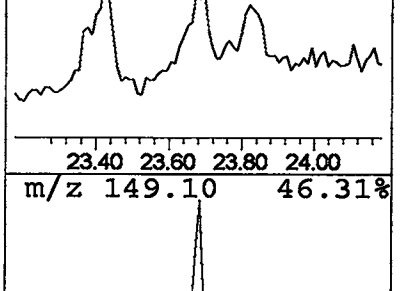
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	33
2	N-Methyl-1,2,4-dithiazolidine-3,...	149	C3H3NO2S2	018137-43-4	9
3	8-Oxo-8H-indeno[1,2-d]-1,2,3-thi...	188	C9H4N2OS	000000-00-0	4
4	Sulfur dioxide $$ Fermenicide po...	64	O2S	007446-09-5	4

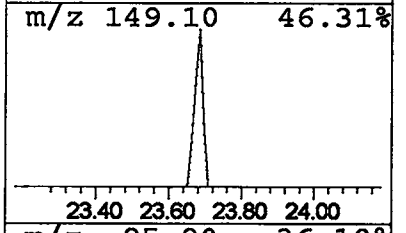
NO GOOD MATCH

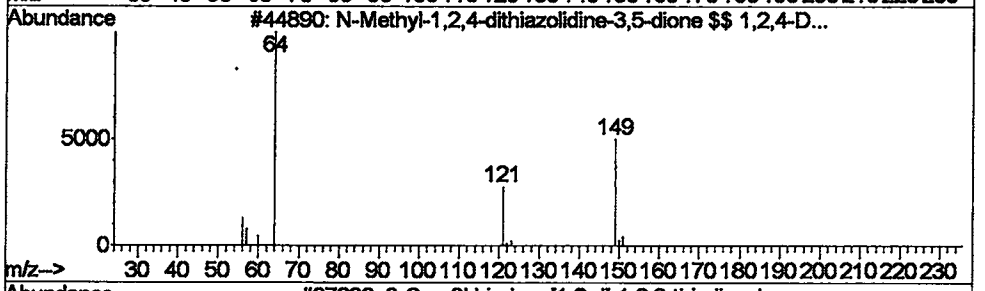


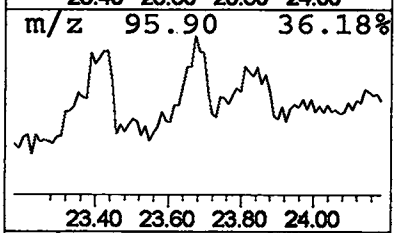


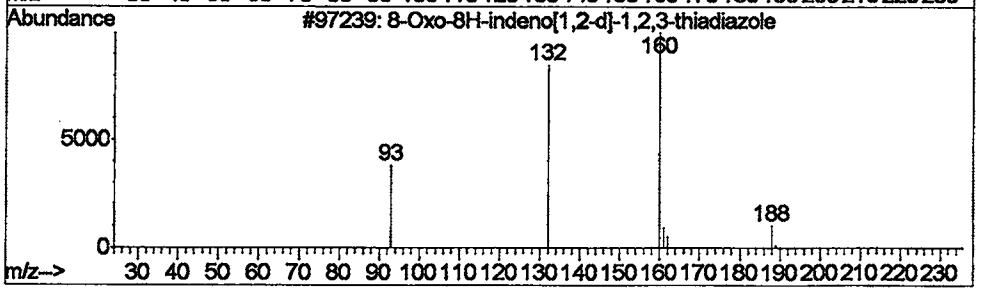


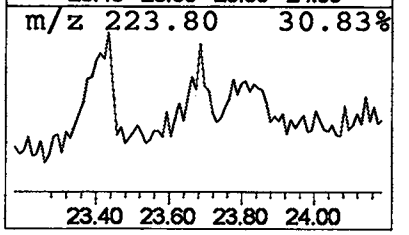












Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

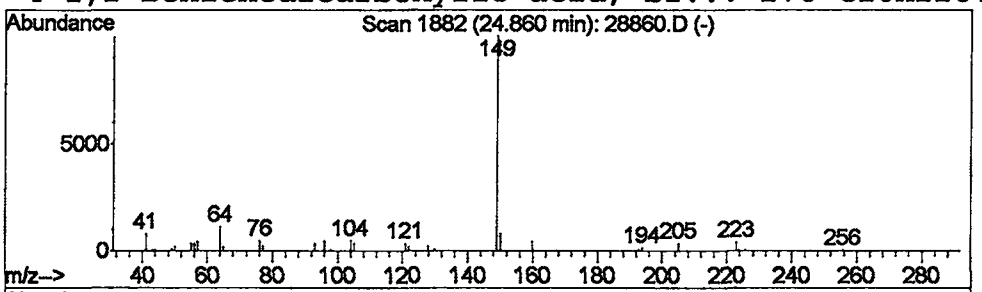
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

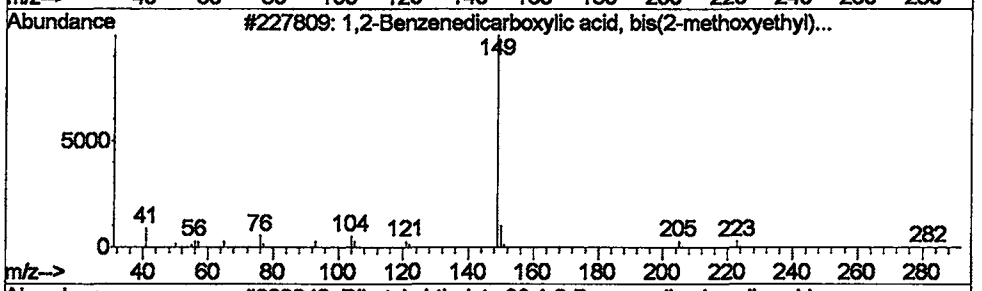
****

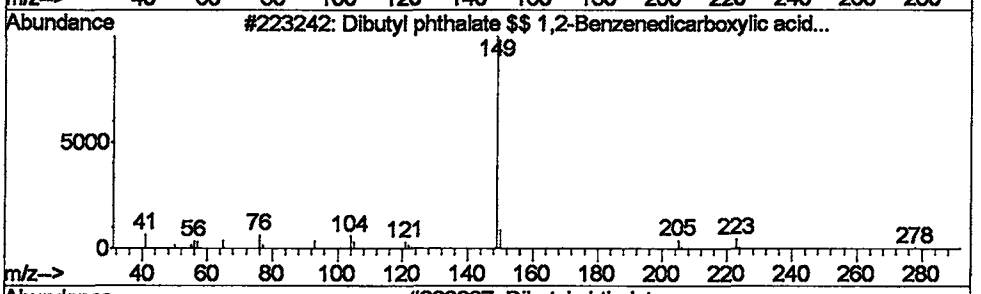
Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 7

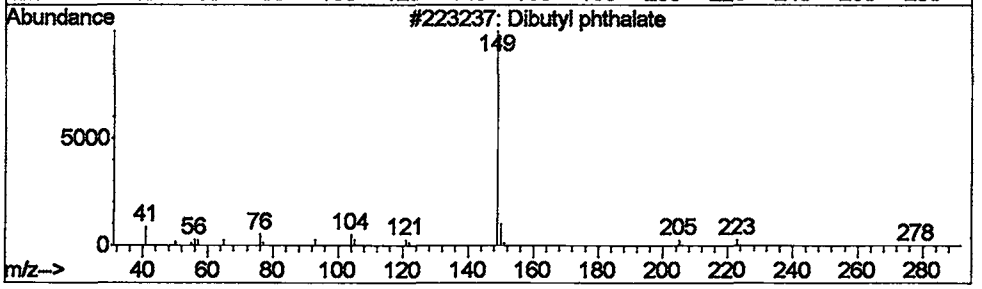
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.86	0.15 ug/L	106452	Phenanthrene-d10	22.65

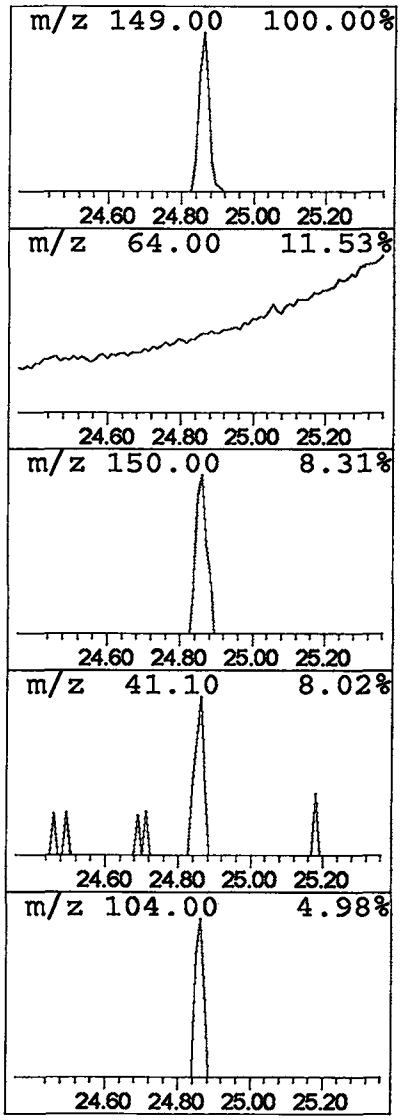
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	282	C14H18O6	000117-82-8	72
2	Dibutyl phthalate $$ 1,2-Benzene...	278	C16H22O4	000084-74-2	72
3	Dibutyl phthalate	278	C16H22O4	000084-74-2	72
4	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	64











Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB01\28860.D Vial: 3
Acq On : 1 Feb 2002 12:14 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 1, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

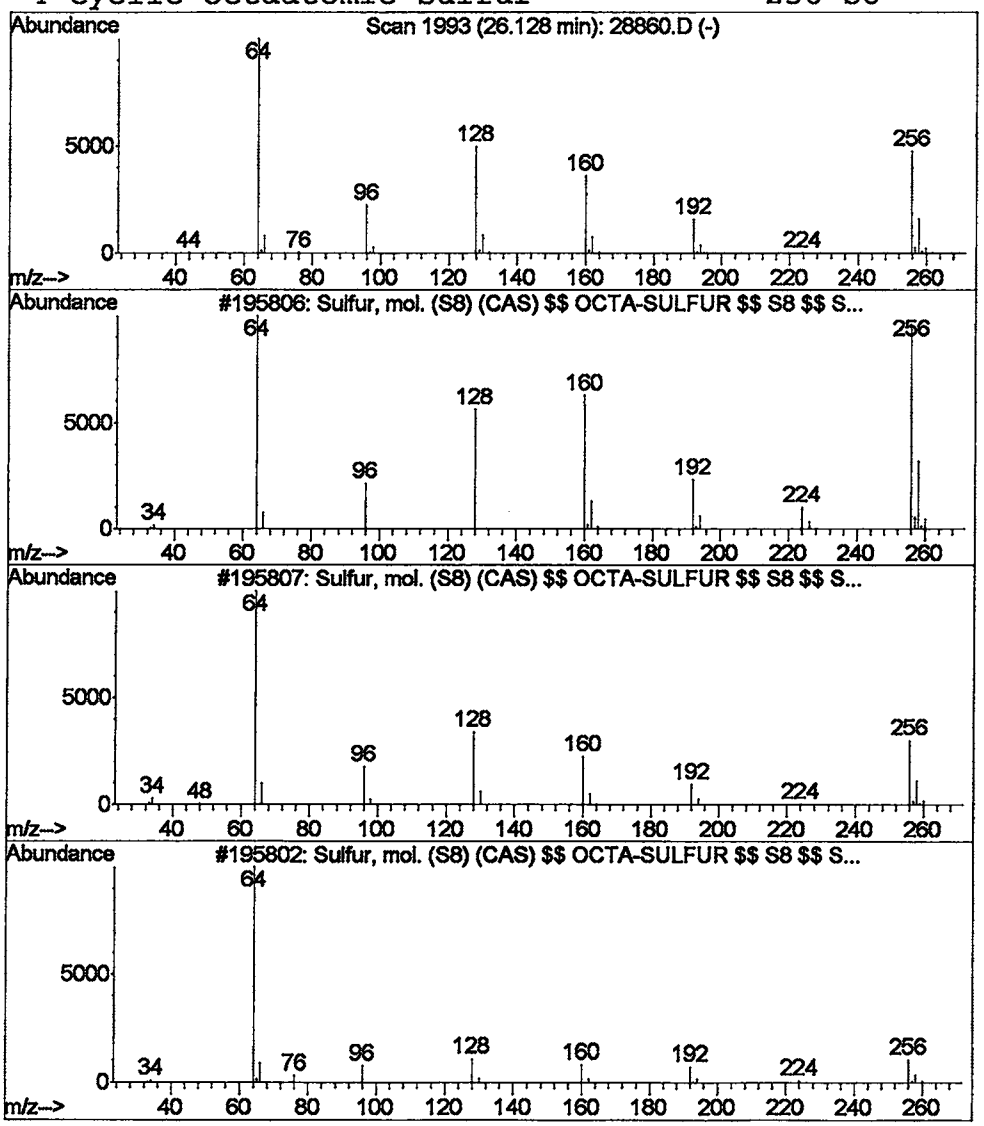
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

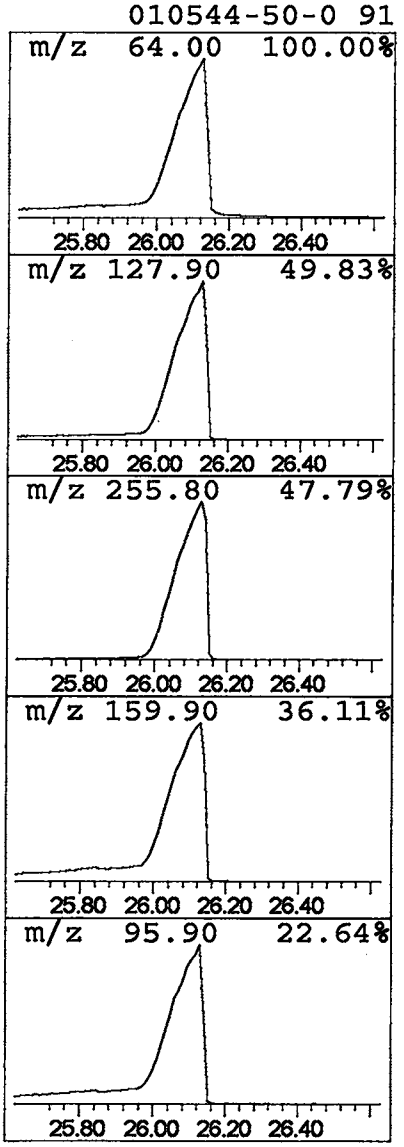
****

Peak Number 12 Sulfur, mol. (S8) (CAS) $$ ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.13	64.79 ug/L	47518700	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	94
3	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	91
4	Cyclic octaatomic sulfur	256	S8	010544-50-0	91





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 1 Feb 2002 12:14 pm
Data File: C:\MSDCHEM\1\5973N\02FEB01\28860.D
Name: 508 scan
Misc: February 1, 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...	3.61	0.1	ug/L	60266	1	9.71	8697830	20.0
3-Pentanol, 3-met...	5.92	0.4	ug/L	167506	1	9.71	8697830	20.0
Cyclopentasiloxan...	12.54	0.1	ug/L	78493	2	13.19	12558900	20.0
CYSTEIC ACID THIO...	18.76	1.0	ug/L	701629	3	18.34	13660300	20.0
Di-2/3-methylbuty...	19.99	0.1	ug/L	47525	3	18.34	13660300	20.0
2(1H)-Naphthaleno...	20.92	0.1	ug/L	47316	4	22.65	14668900	20.0
4-METHOXY-.BETA.-...	22.28	0.2	ug/L	126724	4	22.65	14668900	20.0
Cyclohexane-d12	22.85	3.7	ug/L	2733010	4	22.65	14668900	20.0
2-Norbornanone, 1...	23.42	0.1	ug/L	101158	4	22.65	14668900	20.0
2-Norbornanone, 1...	23.68	0.2	ug/L	168363	4	22.65	14668900	20.0
1,2-Benzenedicarb...	24.86	0.1	ug/L	106452	4	22.65	14668900	20.0
Sulfur, mol. (S8)...	26.13	64.8	ug/L	47518700	4	22.65	14668900	20.0