

Quantitation Report (NOT Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN10\00472.D
 Acq On : 10 Jan 2002 7:46 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: SPLIT.P
 Quant Time: Jan 11 10:18:58 2002

Vial: 7
 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 : Thu Jan 10 11:01:02 2002
 Response via : Initial Calibration
 DataAcq Meth : SCAN508

to be re-ext

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1212224	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	5109867	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2674787	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4484432	20.00	ug/L	-0.03
38) Chrysene-d12	30.50	240	4108440	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3066558	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	228134	3.22	ug/L	0.00
Spiked Amount	5.000		Recovery	=	64.40%	
Target Compounds						
2) n-Nitroso-dimethylamine	3.61	74	11236	0.22	ug/L #	11
20) Dimethylphthalate	18.34	163	429748	2.43	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	338826	9.83	ug/L #	17
35) Di-n-butylphthalate	24.85	149	10717	0.04	ug/L #	76
41) Benzo(a)anthracene	30.50	228	9356	0.04	ug/L #	69
42) Bis(2-ethylhexyl)phthalate	31.11	149	8713	0.59	ug/L	91
43) Chrysene	30.50	228	9356	0.04	ug/L #	67
48) Benzo(a)pyrene	34.42	252	10326	0.05	ug/L #	1

 (#) = qualifier out of range (m) = manual integration
 00472.D SCAN508.M Fri Jan 11 10:18:59 2002

Page 1

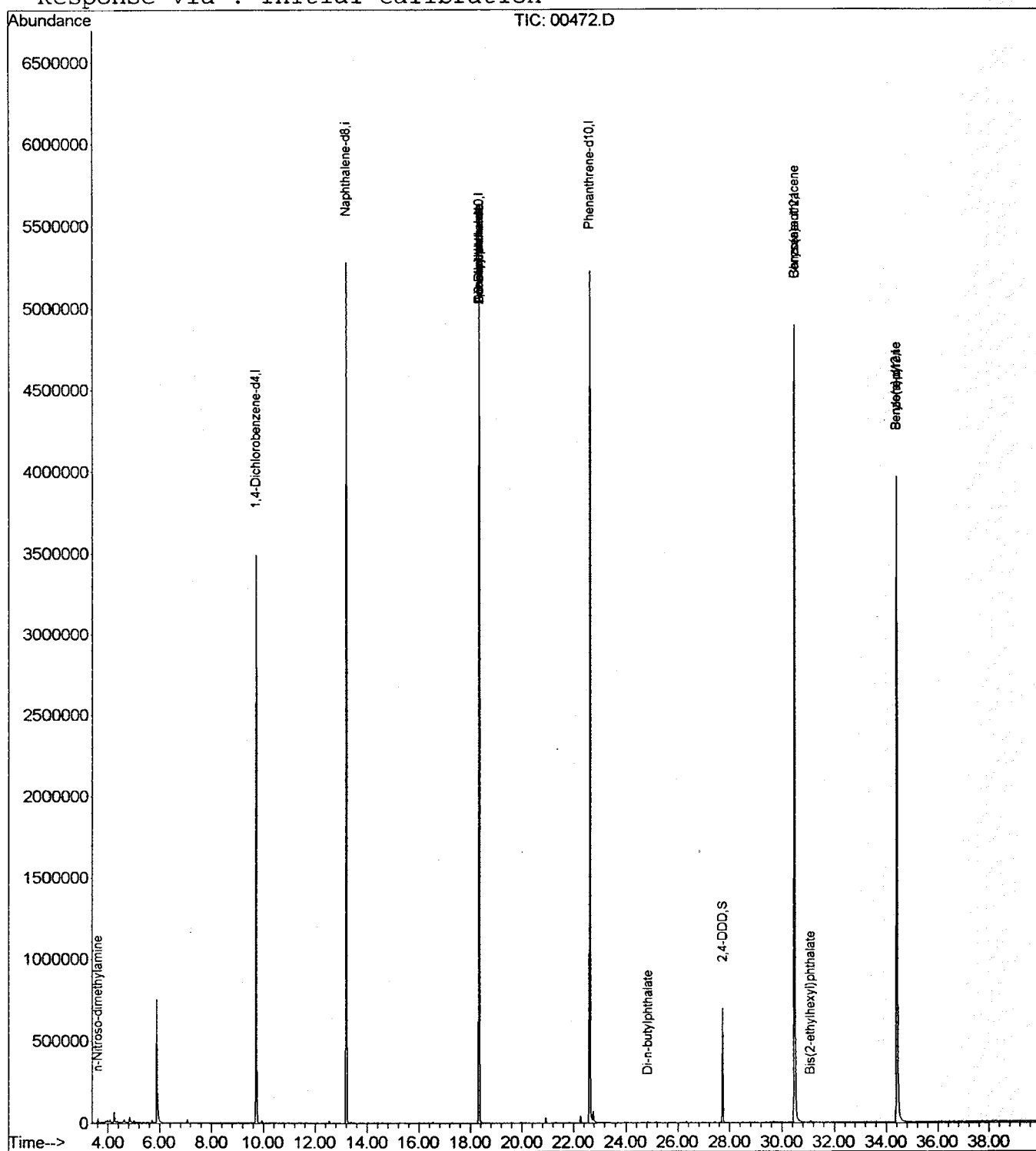
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Acq On : 10 Jan 2002 7:46 pm
Sample : 508 scan ext 1/8
Misc : January 10, 2002
MS Integration Params: SPLIT.P
Quant Time: Jan 11 10:18 2002

Vial: 7
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 : Thu Jan 10 11:01:02 2002
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00472.D SCAN508.M

Fri Jan 11 10:18:59 2002

Page 2

LSC Area Percent Report

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 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

Vial: 7
 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

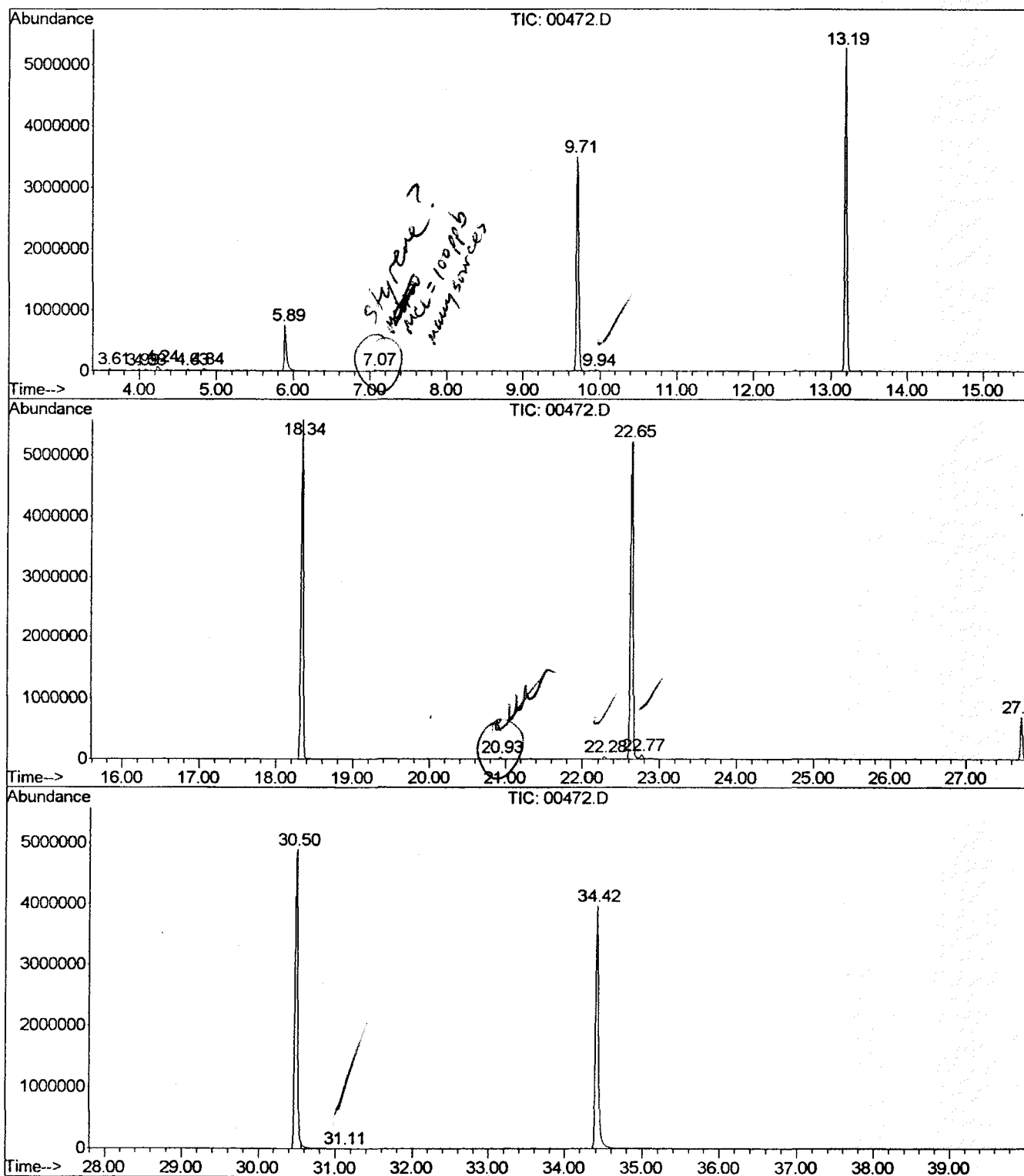
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.613	17	21	25	rBV	27842	48351	0.40%	0.074%
2	3.990	51	54	59	rVV2	16990	32850	0.27%	0.050%
3	4.082	59	62	67	rVV2	17995	35339	0.29%	0.054%
4	4.241	71	76	83	rVV2	67277	148086	1.23%	0.226%
5	4.630	101	110	117	rVB2	18961	54275	0.45%	0.083%
6	4.835	125	128	141	rVB2	34480	89634	0.75%	0.137%
7	5.885	217	220	241	rBV	750785	1504369	12.51%	2.296%
8	7.073	321	324	329	rBV	25252	43784	0.36%	0.067%
9	9.710	551	555	561	rBV	3490463	6836155	56.85%	10.433%
10	9.938	573	575	587	rVB3	21372	43523	0.36%	0.066%
11	13.192	855	860	865	rBV	5278749	9846745	81.89%	15.028%
12	18.341	1305	1311	1315	rBV	5582907	10911807	90.74%	16.653%
13	20.933	1533	1538	1543	rVV	33456	56499	0.47%	0.086%
14	22.280	1653	1656	1661	rBV2	44980	86530	0.72%	0.132%
15	22.645	1681	1688	1693	rBV2	5226300	11862759	98.65%	18.105%
16	22.771	1695	1699	1709	rVB	66722	168318	1.40%	0.257%
17	27.726	2129	2133	2139	rBV	697596	1260658	10.48%	1.924%
18	30.500	2369	2376	2381	rBV	4894349	12024796	100.00%	18.352%
19	31.105	2425	2429	2443	rVB4	9229	39807	0.33%	0.061%
20	34.416	2713	2719	2745	rBV	3962713	10428372	86.72%	15.916%

Sum of corrected areas: 65522657

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN10\00472.D.
 Operator :
 Acquired : 10 Jan 2002 7:46 pm using AcqMethod SCAN508
 Instrument : Instrumen
 Sample Name: 508 scan ext 1/8
 Misc Info : January 10, 2002
 Vial Number: 7
 Quant File :SCAN508.RES (RTE Integrator)



00472.D SCAN508.M

Fri Jan 11 10:08:54 2002

Page 2

Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00472.D
 Acq On : 10 Jan 2002 7:46 pm
 Sample : 508 scan ext 1/8
 Misc : January 10, 2002
 MS Integration Params: LSCINT.P

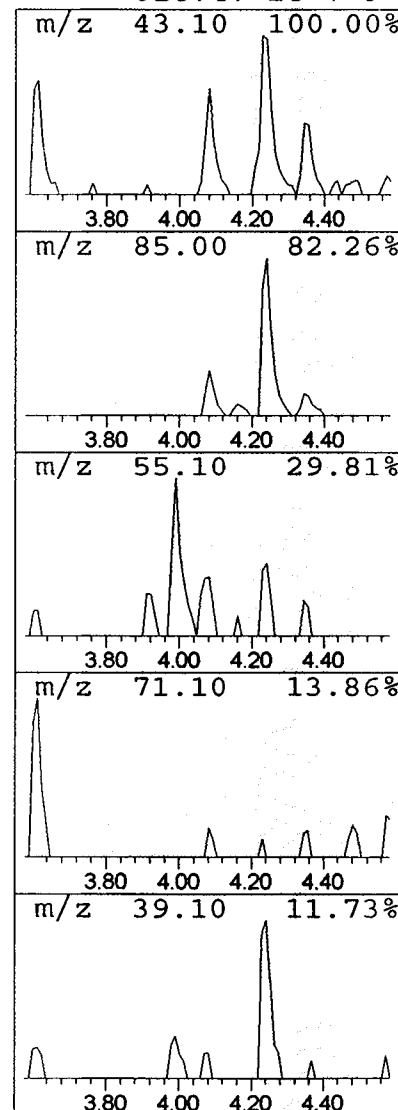
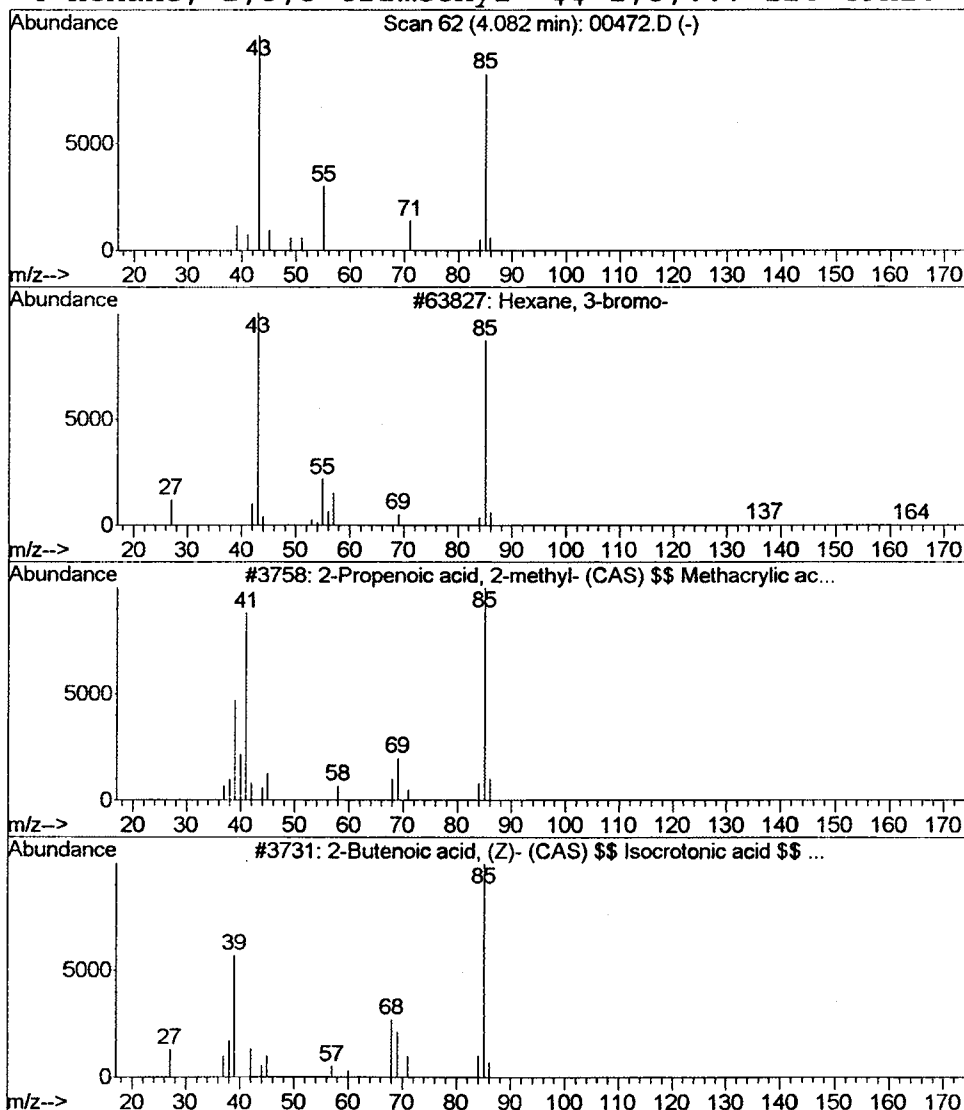
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 Hexane, 3-bromo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	0.10 ug/L	35339	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-bromo-	164	C6H13Br	003377-87-5	39
2			2-Propenoic acid, 2-methyl- (CAS...	86	C4H6O2	000079-41-4	9
3			2-Butenoic acid, (Z)- (CAS) \$\$ I...	86	C4H6O2	000503-64-0	9
4			Hexane, 2,3,3-trimethyl- \$\$ 2,3,...	128	C9H20	016747-28-7	9



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Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

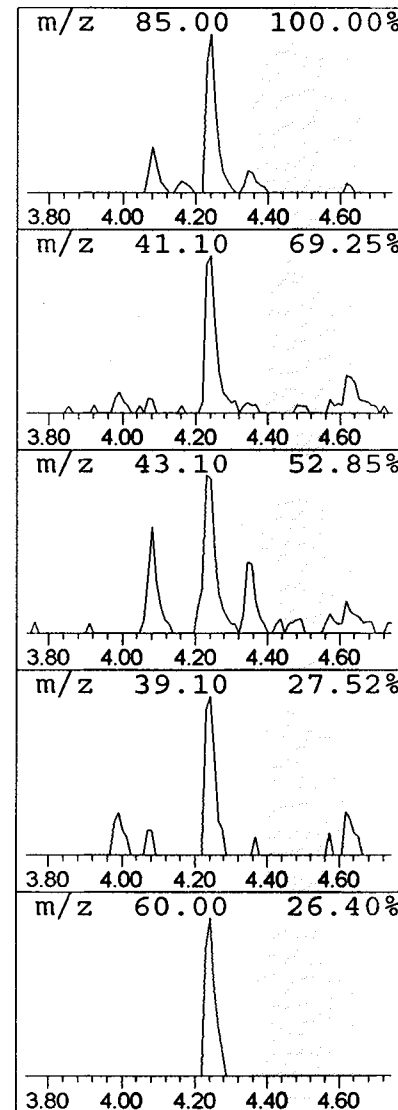
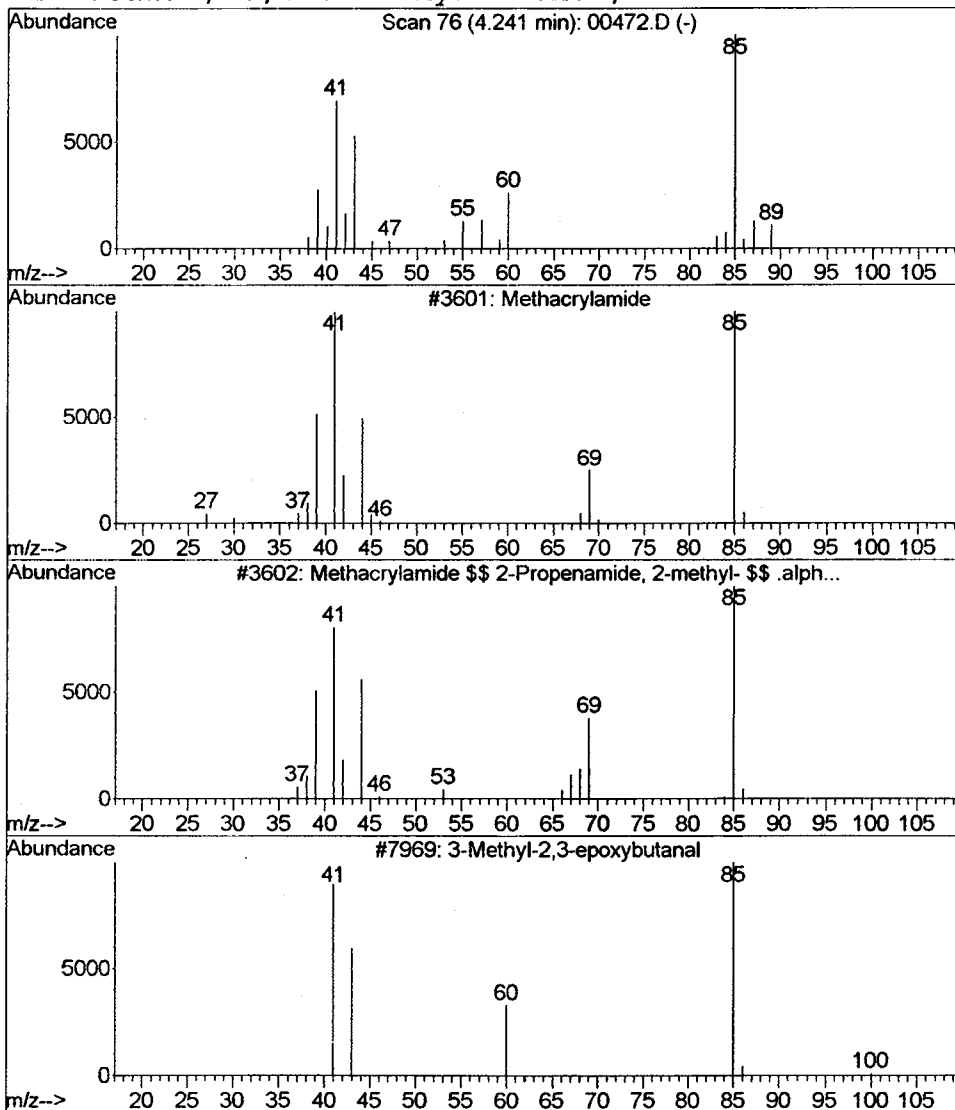
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 2 Methacrylamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.43 ug/L	148086	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methacrylamide	85	C4H7NO	000079-39-0	38
2			Methacrylamide \$\$ 2-Propenamide,...	85	C4H7NO	000079-39-0	38
3			3-Methyl-2,3-epoxybutanal	100	C5H8O2	000000-00-0	33
4			Butanal, 3,3-dimethyl-2-oxo-, he...	114	C6H10O2	077572-68-0	28

NO
 GOOD
 MATCH



Library Search Compound Report

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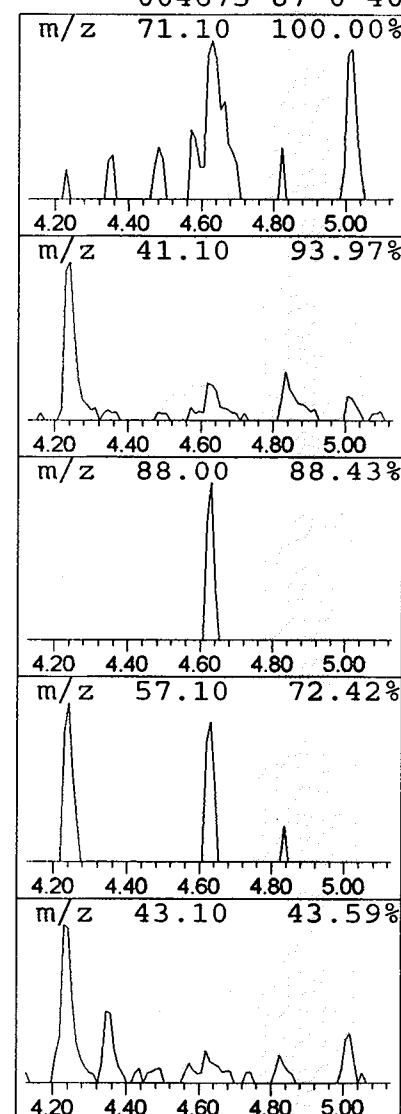
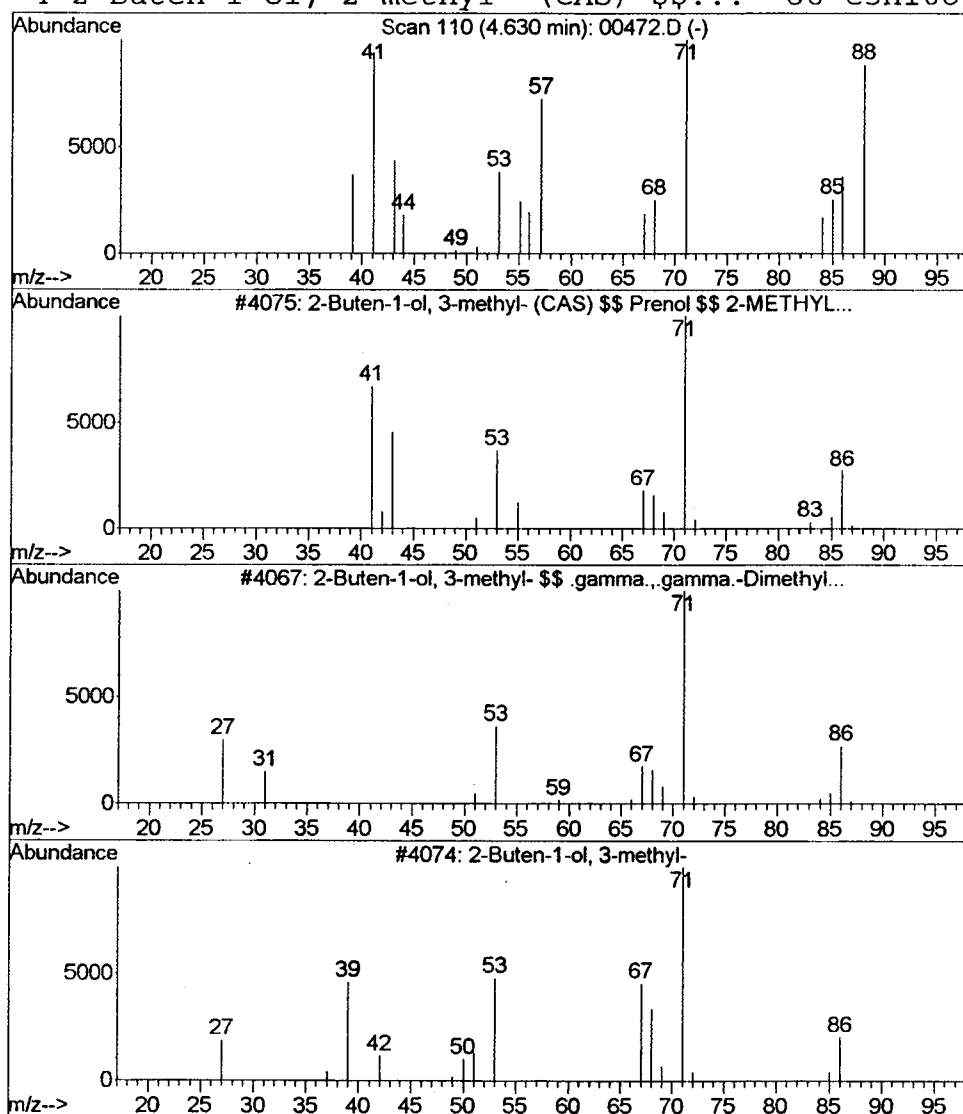
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 2-Buten-1-ol, 3-methyl- (CA... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	0.16 ug/L	54275	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol, 3-methyl- (CAS) \$\$...	86	C5H10O	000556-82-1	52		
2	2-Buten-1-ol, 3-methyl- \$\$.gamm...	86	C5H10O	000556-82-1	52		
3	2-Buten-1-ol, 3-methyl-	86	C5H10O	000556-82-1	47		
4	2-Buten-1-ol, 2-methyl- (CAS) \$\$...	86	C5H10O	004675-87-0	40		



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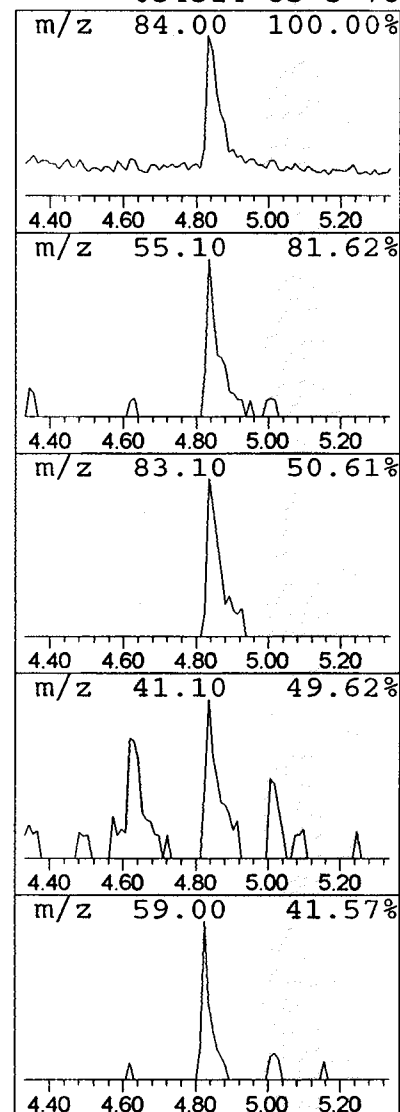
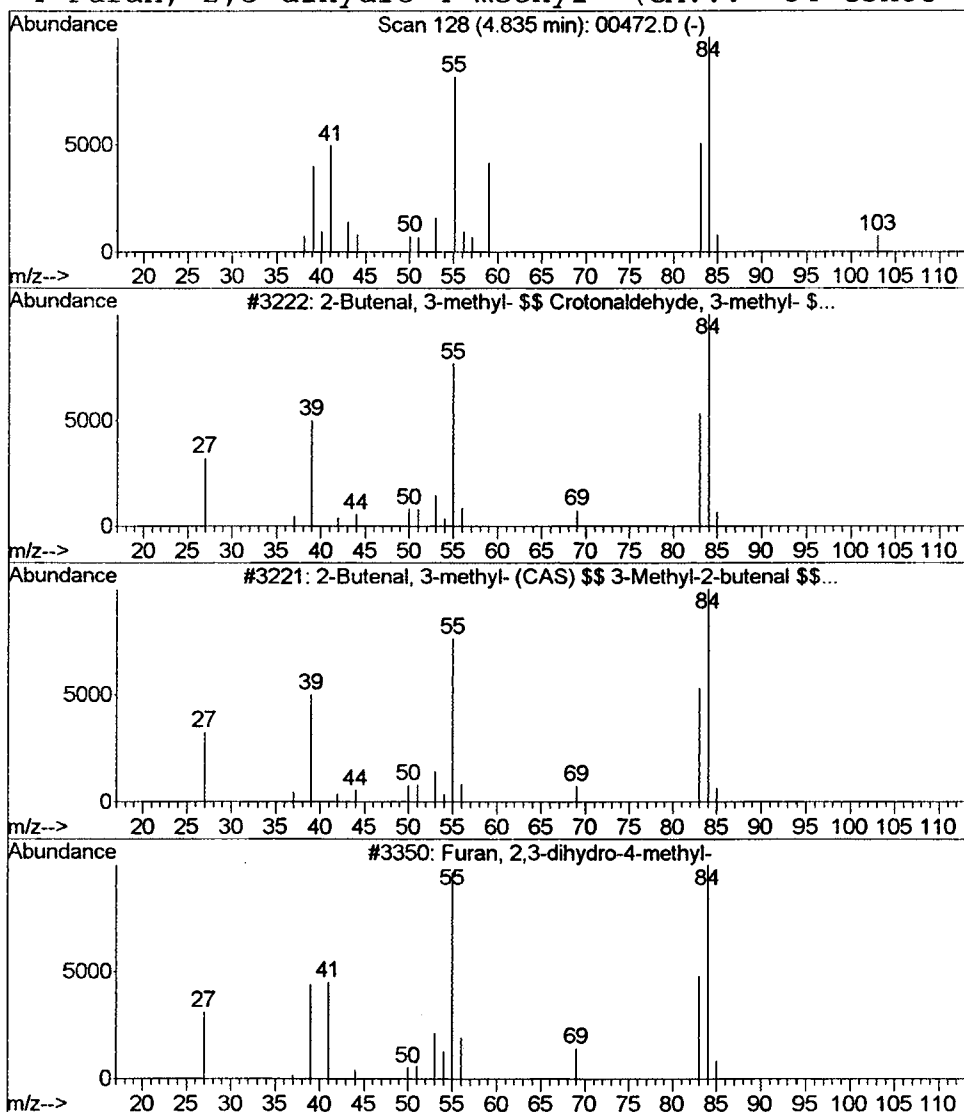
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 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 4 2-Butenal, 3-methyl- \$\$ Cro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.26 ug/L	89634	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl- \$\$ Crotonal...	84	C5H8O	000107-86-8	81
2			2-Butenal, 3-methyl- (CAS) \$\$ 3-...	84	C5H8O	000107-86-8	81
3			Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	76
4			Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	76



Too blank

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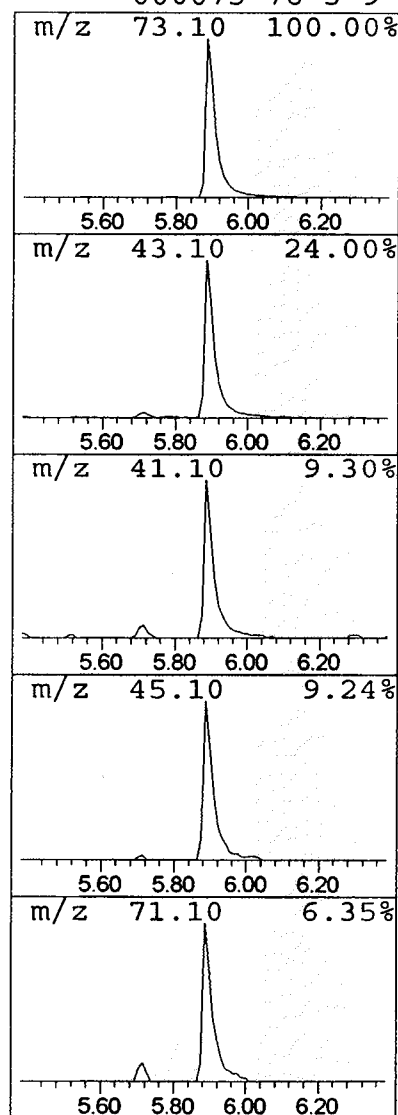
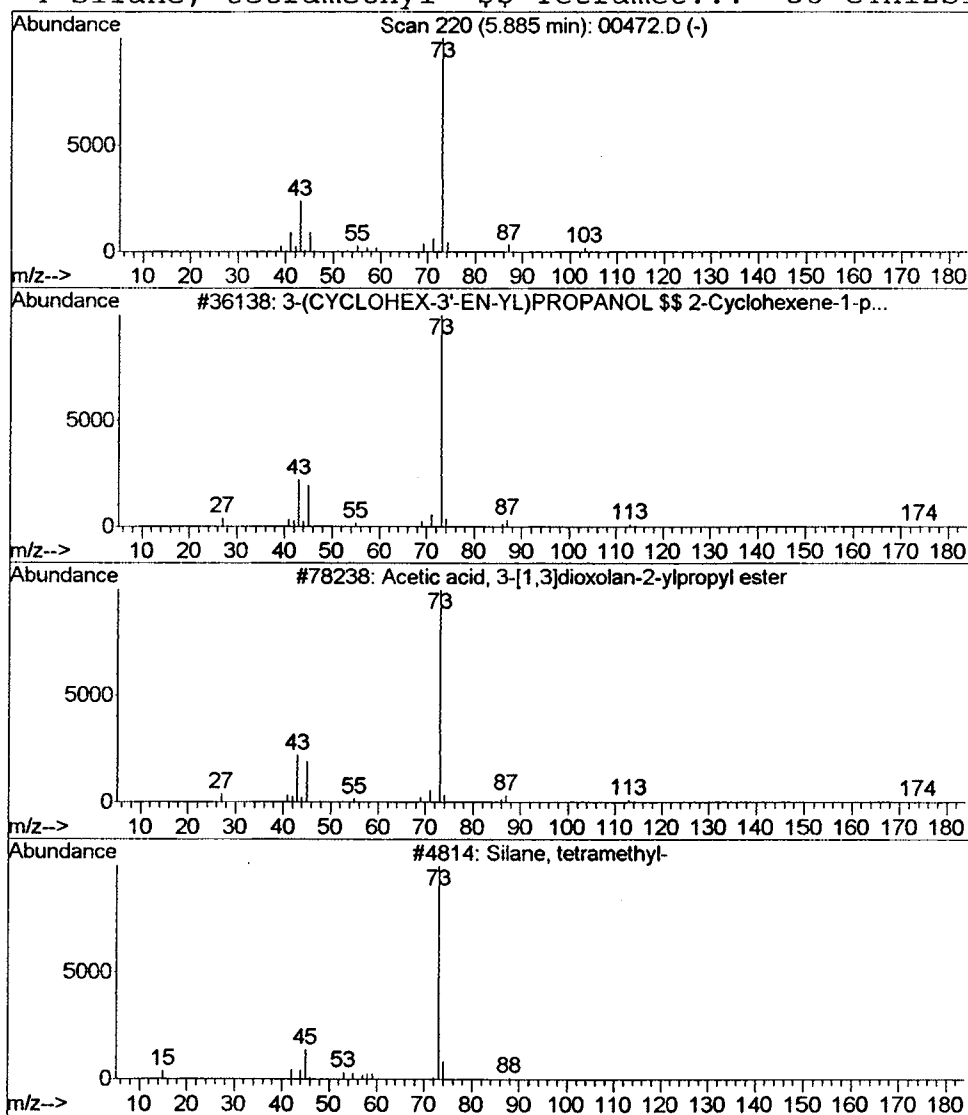
Vial: 7
 Operator:
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 5 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.40 ug/L	1504370	1,4-Dichlorobenzene-d4	9.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$...	174	C8H14O4	015745-87-6	33
2		Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4		Silane, tetramethyl- \$\$ Tetramet...	88	C4H12Si	000075-76-3	9



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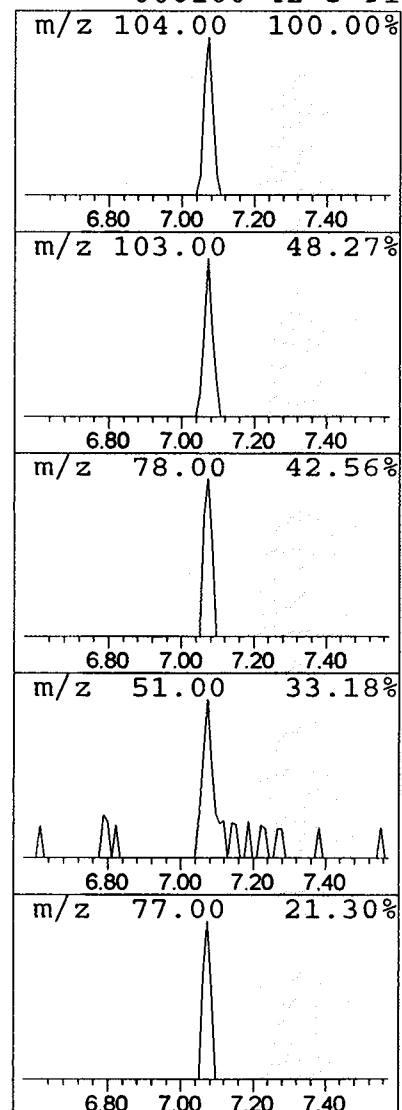
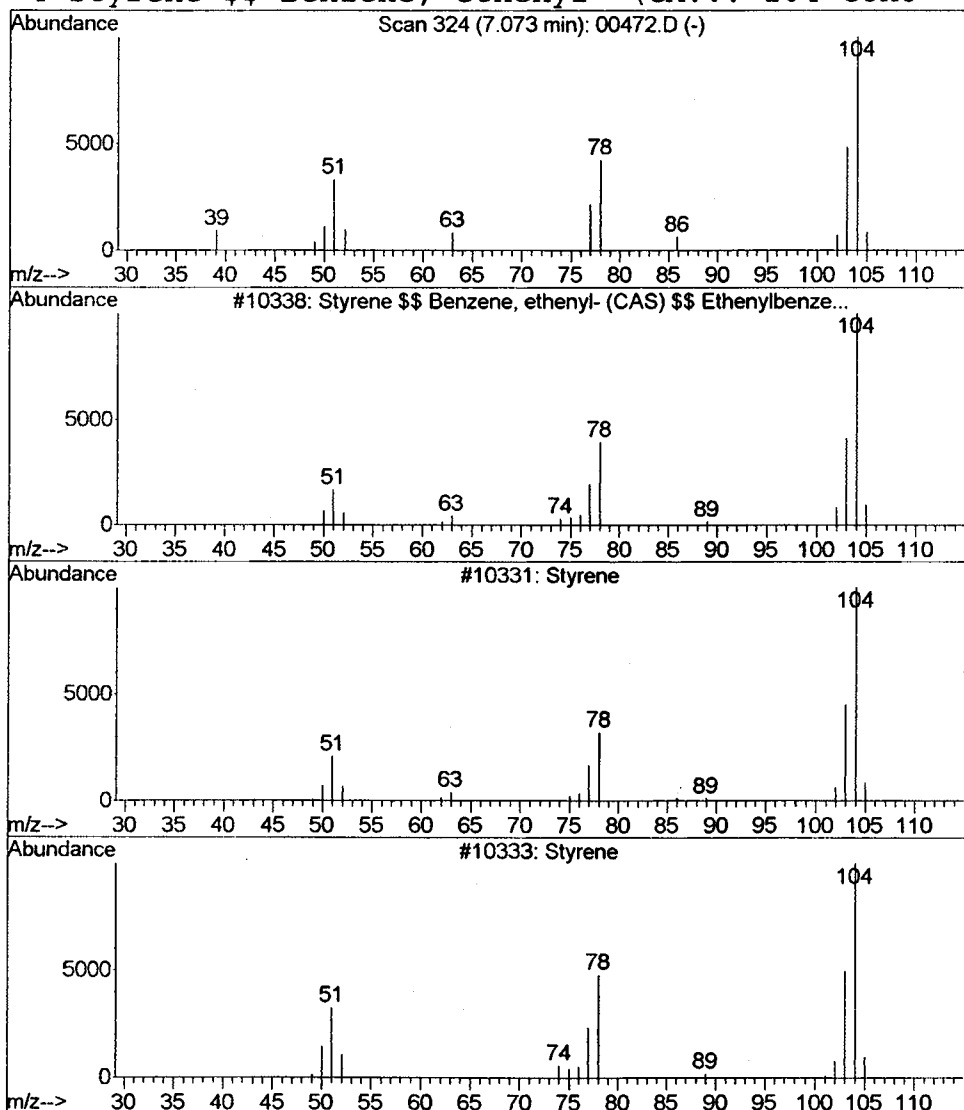
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 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
 Title : 508 scan method
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 Peak Number 6 Styrene \$\$ Benzene, ethenyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	0.13 ug/L	43784	1,4-Dichlorobenzene-d4	9.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Styrene \$\$ Benzene, ethenyl-	(CA...	104	C8H8	000100-42-5	91
2	Styrene		104	C8H8	000100-42-5	91
3	Styrene		104	C8H8	000100-42-5	91
4	Styrene \$\$ Benzene, ethenyl-	(CA...	104	C8H8	000100-42-5	91



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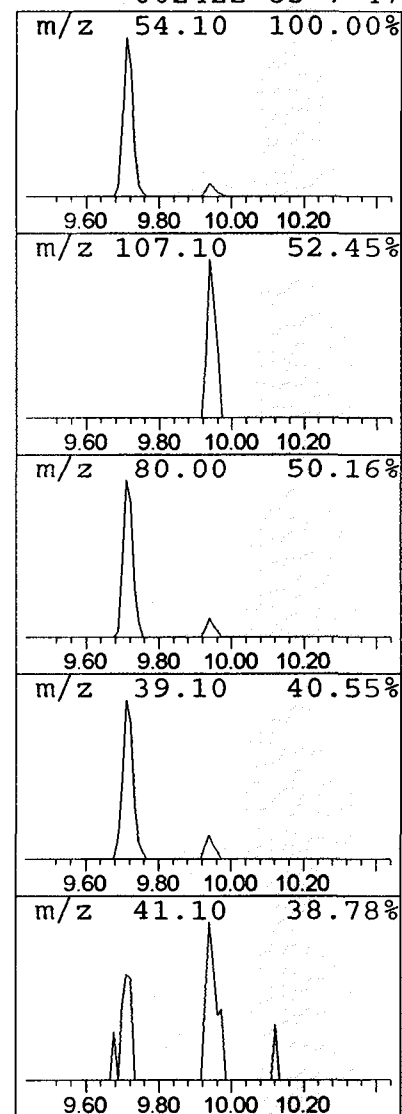
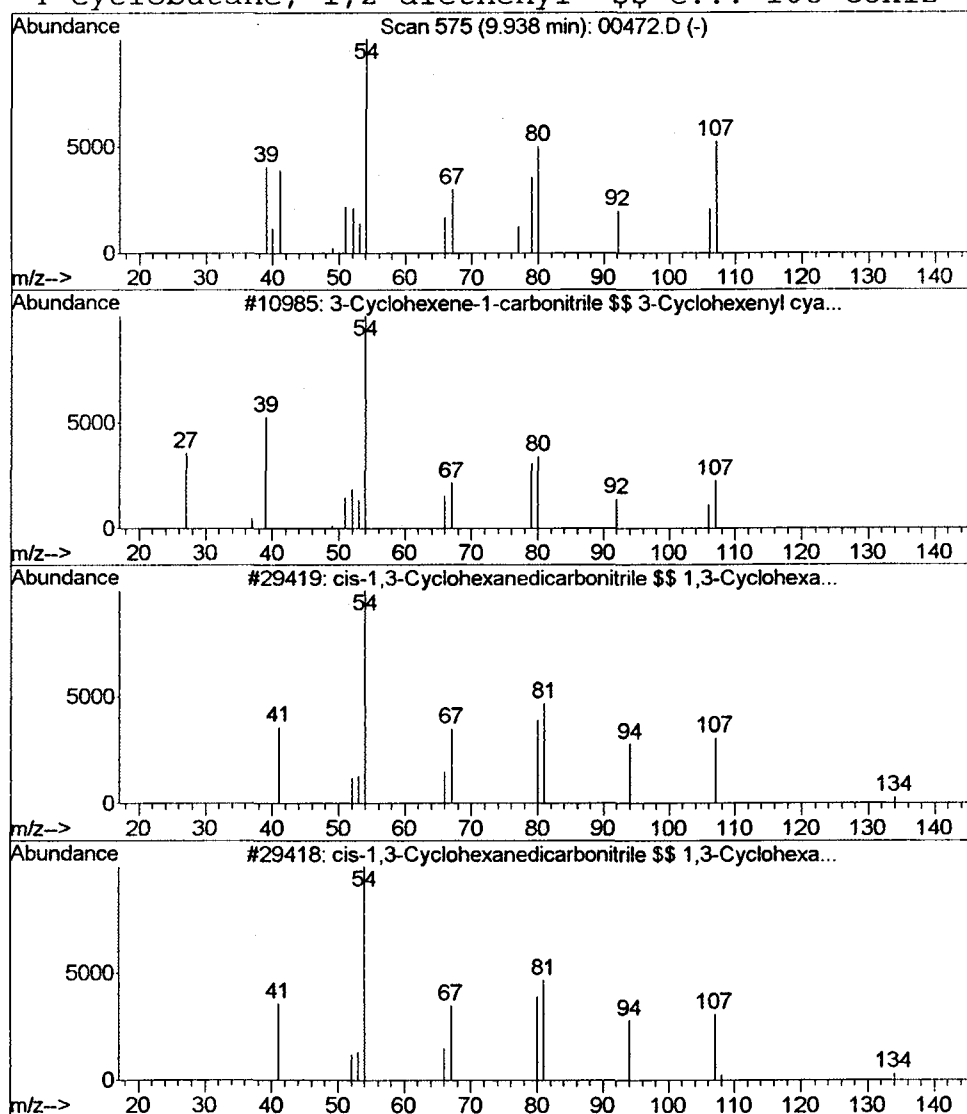
Vial: 7
Operator:
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Multiplr: 1.00

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

Peak Number 7 3-Cyclohexene-1-carbonitril... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	0.13 ug/L	43523	1,4-Dichlorobenzene-d4	9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Cyclohexene-1-carbonitrile \$\$...	107	C7H9N	000100-45-8	83
2			cis-1,3-Cyclohexanedicarbonitril...	134	C8H10N2	010340-01-9	53
3			cis-1,3-Cyclohexanedicarbonitril...	134	C8H10N2	010340-01-9	53
4			Cyclobutane, 1,2-diethenyl- \$\$ C...	108	C8H12	002422-85-7	47



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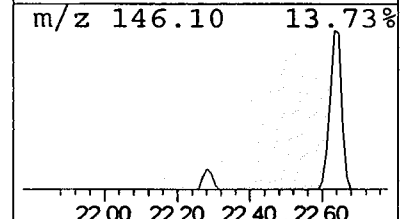
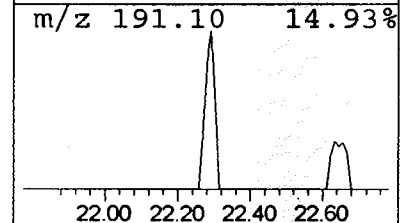
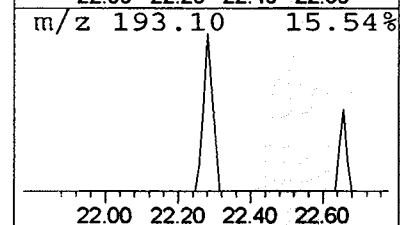
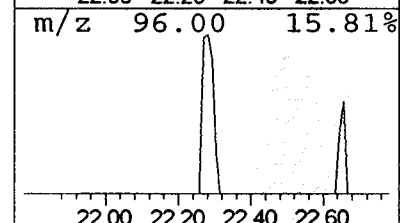
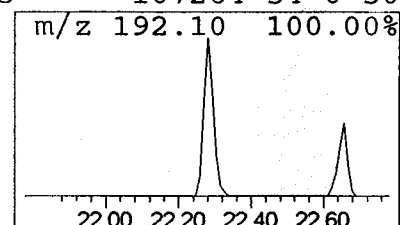
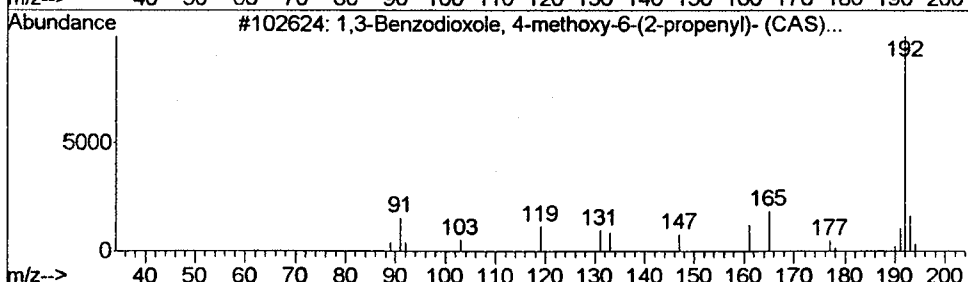
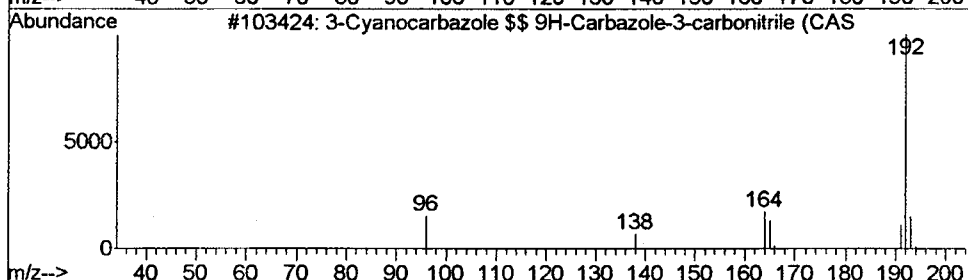
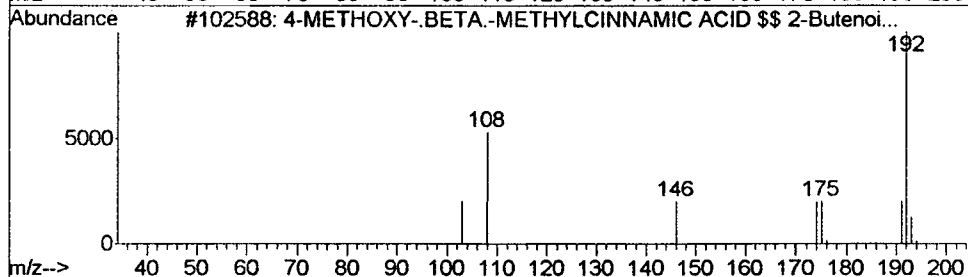
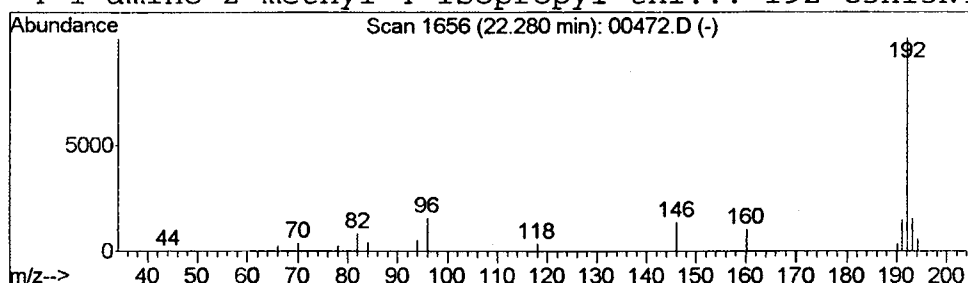
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 Peak Number 8 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	86530	Phenanthrene-d10	22.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	64
2			3-Cyanocarbazole \$\$ 9H-Carbazole...	192	C13H8N2	057102-93-9	64
3			1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	53
4			1-amino-2-methyl-4-isopropyl-thi...	192	C5H13N4PS	107264-54-0	50



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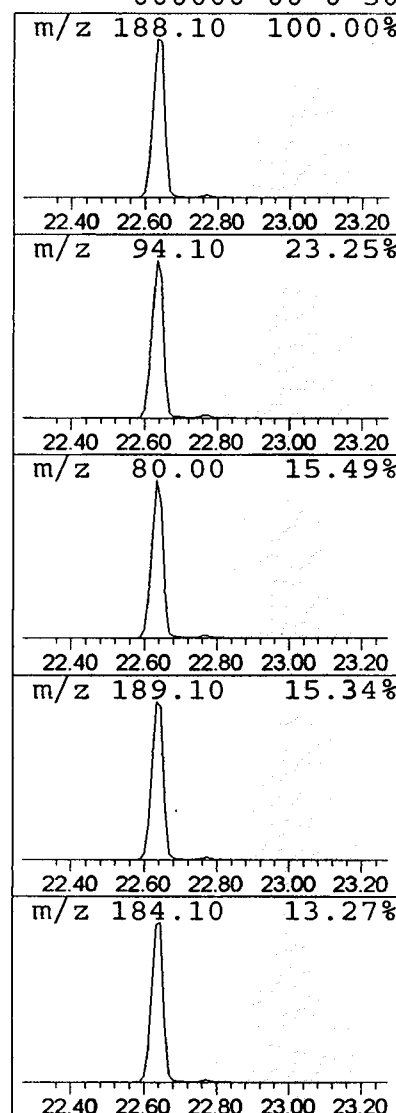
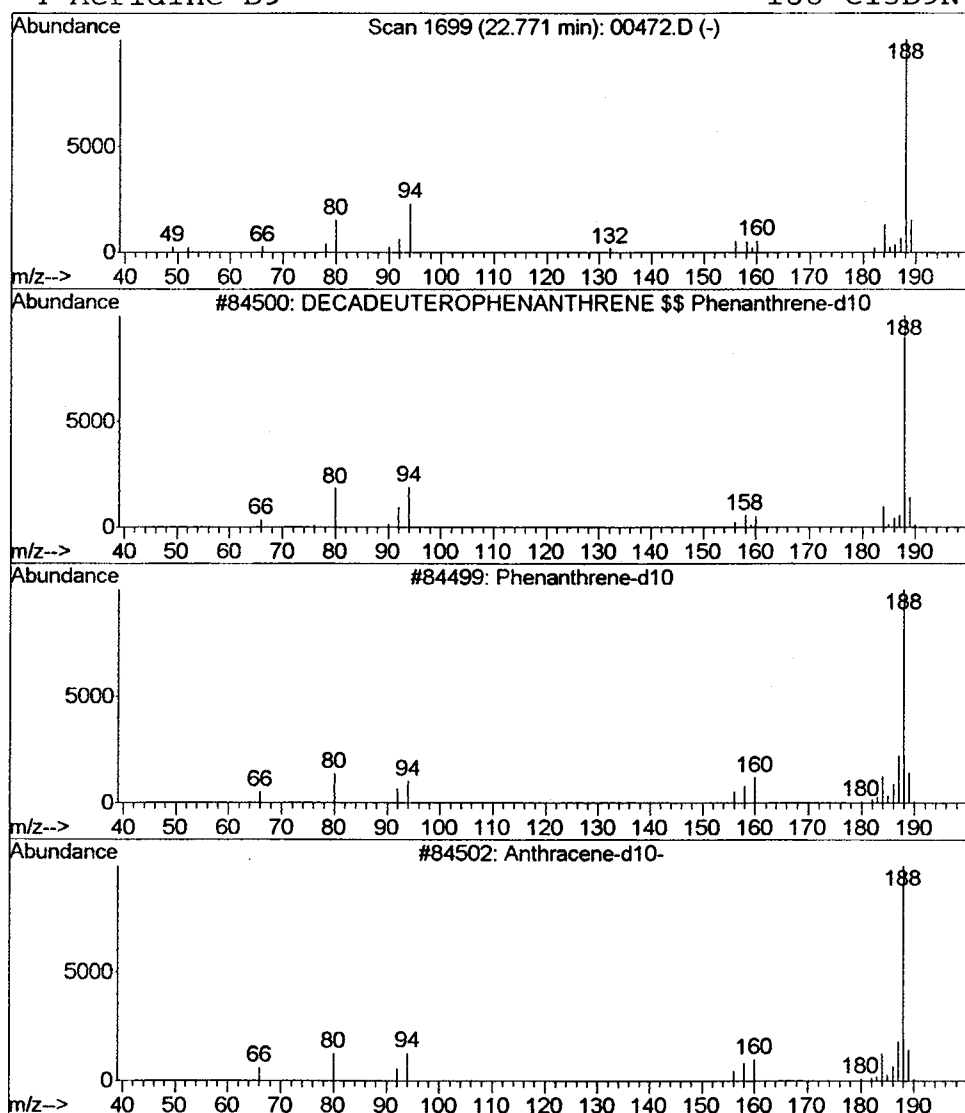
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 Peak Number 9 DECADEUTEROPHENANTHRENE \$\$... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.28 ug/L	168318	Phenanthrene-d10	22.63

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	72
3			Anthracene-d10-	188	C14D10	001719-06-8	64
4			Acridine-D9	188	C13D9N	000000-00-0	50



Tentatively Identified Compound (LSC) summary

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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
Hexane, 3-Bromo-	4.08	0.1	ug/L	35339	1	9.71	6836160	20.0
Methacrylamide	4.24	0.4	ug/L	148086	1	9.71	6836160	20.0
2-Buten-1-ol, 3-m...	4.63	0.2	ug/L	54275	1	9.71	6836160	20.0
2-Butenal, 3-meth	4.84	0.3	ug/L	89634	1	9.71	6836160	20.0
3-(CYCLOHEX-3'-EN...	5.89	4.4	ug/L	1504370	1	9.71	6836160	20.0
Styrene \$\$ Benzen...	7.07	0.1	ug/L	43784	1	9.71	6836160	20.0
3-Cyclohexene-1-c...	9.94	0.1	ug/L	43523	1	9.71	6836160	20.0
4-METHOXY-.BETA.-...	22.28	0.1	ug/L	86530	4	22.63	11862800	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	168318	4	22.63	11862800	20.0