User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/29/2002 Time: 11:23:22

Sample: AE00704
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/29/02 11:22 Ended: 1/29/02 11:22 Analyst: DLV
Page: 1

	Component Name	Vial	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		103		5.0

Comments for Sample AE00704 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-29-2002 Time: 11:25:32

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds, except for the presence of bis(2-Ethylhexyl)phthalate at 5.45 ug/L. Its presence could be due to collection and laboratory contamination. The recoveries for 15 of the 43 compounds in the LCS Standard were outside of their acceptance ranges.

Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 17 08:12:22 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

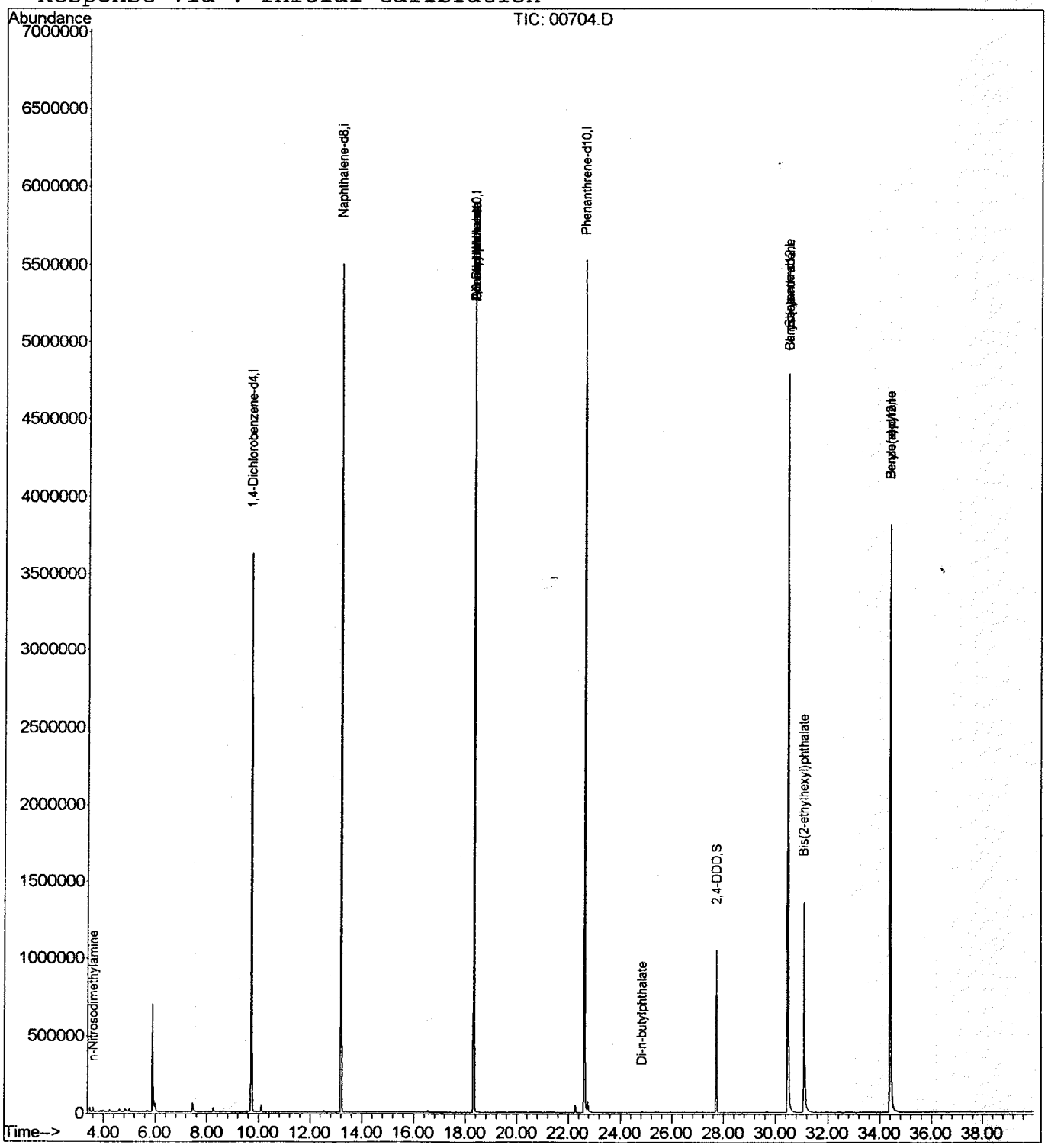
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1260434	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	5358364	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2836706	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4793095	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	4073812	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2904961	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	388494	5.13	ug/L	0.00
Spiked Amount 5.000			Recovery = 102.60%			
Target Compounds						Qvalue
2) n-Nitrosodimethylamine	3.60	74	10102	0.19	ug/L #	15
20) Dimethylphthalate	18.34	163	462445	2.47	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	360444	9.86	ug/L #	17
35) Di-n-butylphthalate	24.85	149	14726	0.05	ug/L	96
41) Benzo(a)anthracene	30.50	228	12488	0.05	ug/L #	60
42) Bis(2-ethylhexyl)phthalate	31.11	149	986254	5.45	ug/L	95
43) Chrysene	30.50	228	12488	0.05	ug/L #	58
48) Benzo(a)pyrene	34.42	252	9781	0.05	ug/L #	1

(#) = qualifier out of range (m) = manual integration
00704.D SCAN508.M Thu Jan 17 08:12:22 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 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



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 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

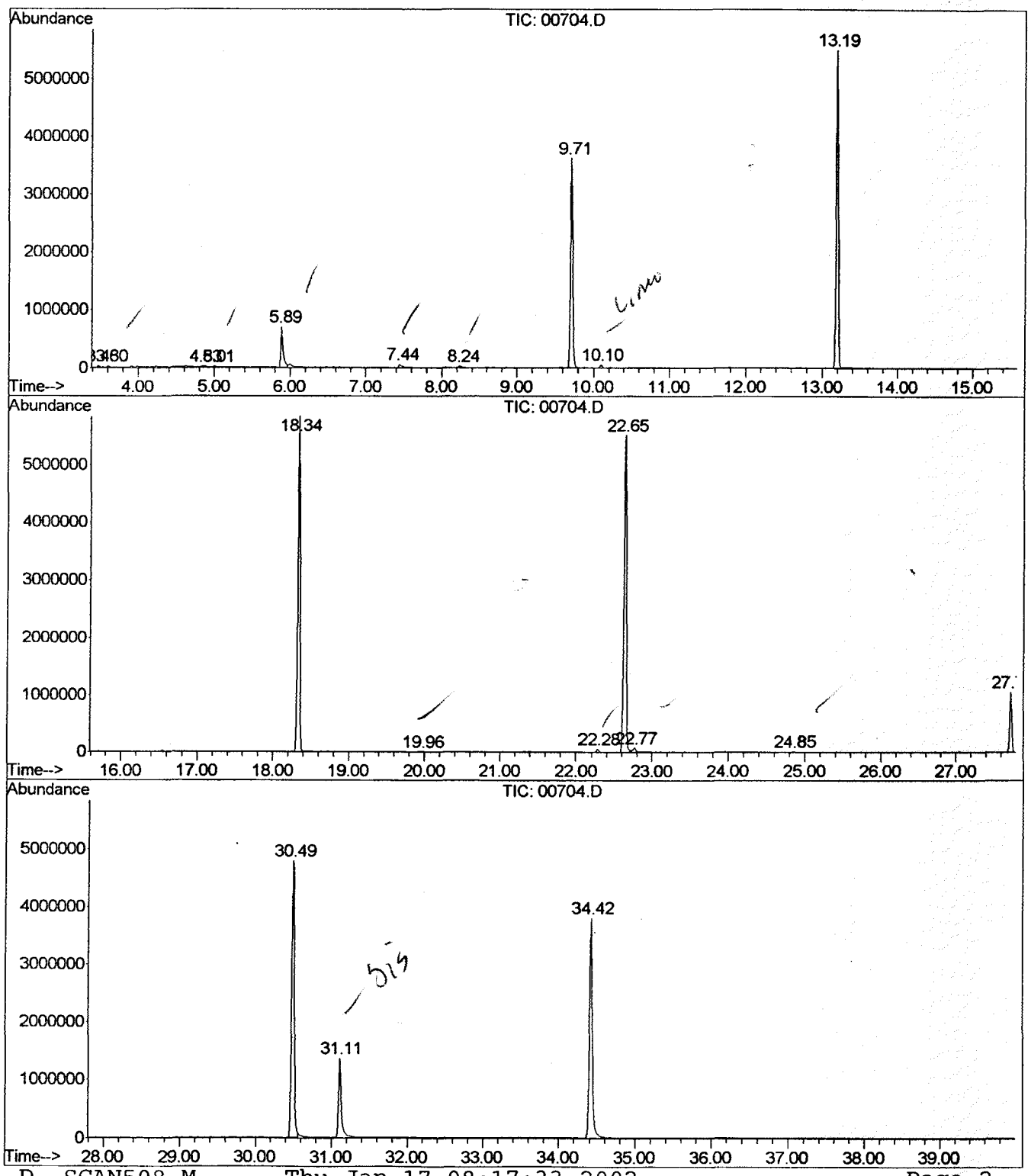
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.476	7	9	13	rVB	29332	42154	0.33%	0.060%
2	3.602	17	20	25	rVB	29610	48358	0.38%	0.068%
3	4.835	123	128	139	rVB5	20100	75353	0.59%	0.106%
4	5.006	139	143	149	rVB	20833	41944	0.33%	0.059%
5	5.885	215	220	227	rBV	693852	1386796	10.93%	1.959%
6	7.438	353	356	367	rBV	57467	150118	1.18%	0.212%
7	8.237	421	426	441	rBV2	28011	72142	0.57%	0.102%
8	9.710	551	555	561	rBV	3617623	7072115	55.72%	9.992%
9	10.098	585	589	593	rBV2	48670	90650	0.71%	0.128%
10	13.192	855	860	865	rBV	5491773	10265335	80.88%	14.504%
11	18.341	1305	1311	1315	rBV	5837470	11544974	90.96%	16.312%
12	19.962	1447	1453	1461	rVB4	6606	30597	0.24%	0.043%
13	22.280	1653	1656	1661	rVV2	50799	88294	0.70%	0.125%
14	22.645	1681	1688	1693	rBV2	5518615	12692312	100.00%	17.933%
15	22.771	1695	1699	1713	rVB	69568	205634	1.62%	0.291%
16	24.849	1875	1881	1887	rBV	9986	32747	0.26%	0.046%
17	27.726	2129	2133	2137	rBV	1048683	1882596	14.83%	2.660%
18	30.489	2369	2375	2381	rBV2	4782874	11865594	93.49%	16.765%
19	31.105	2425	2429	2463	rVV	1358722	3382846	26.65%	4.780%
20	34.416	2713	2719	2749	rVV	3804674	9803991	77.24%	13.852%

Sum of corrected areas: 70774550

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN16\00704.D
Operator :
Acquired : 16 Jan 2002 5:37 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508scan
Misc Info : January 16, 2002
Vial Number: 4
Quant File :SCAN508.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

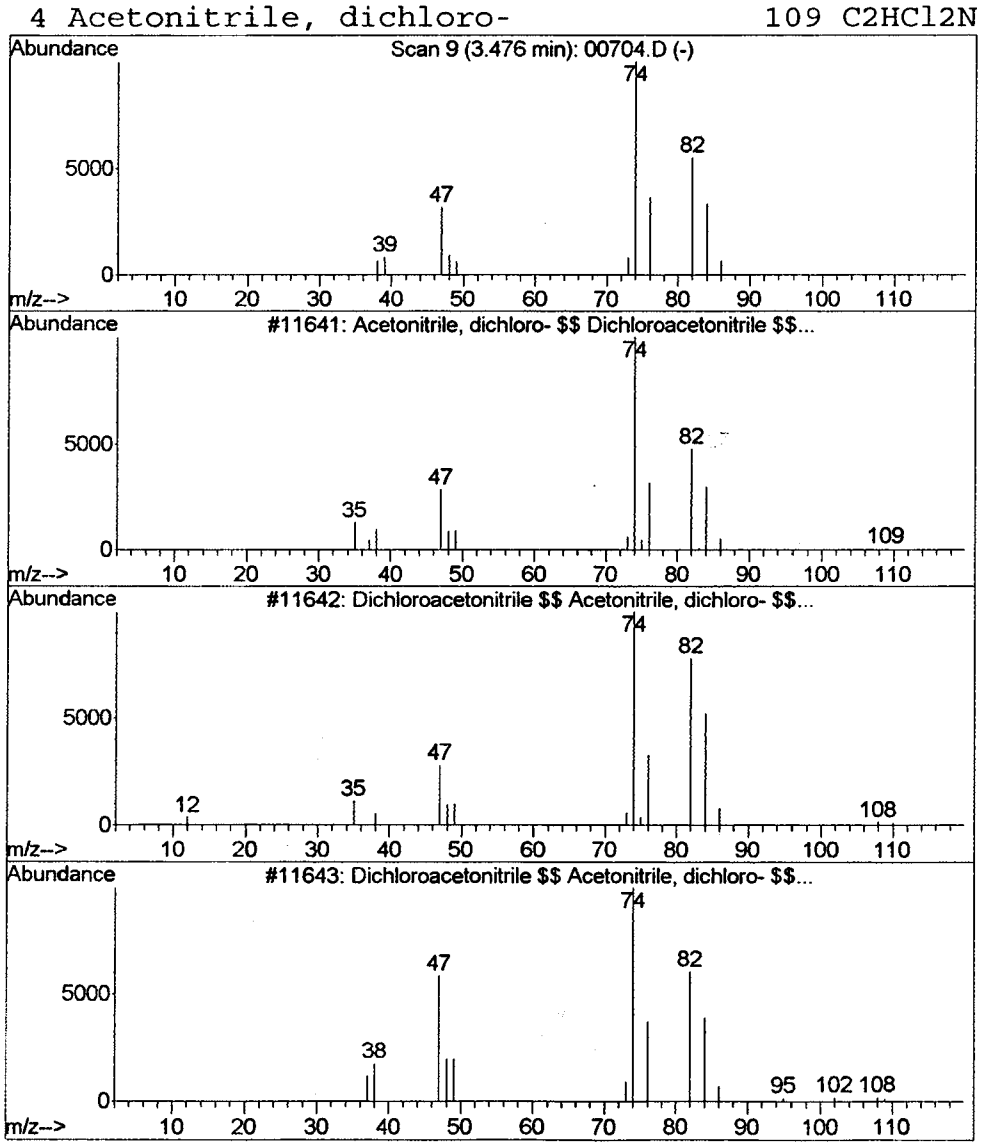
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

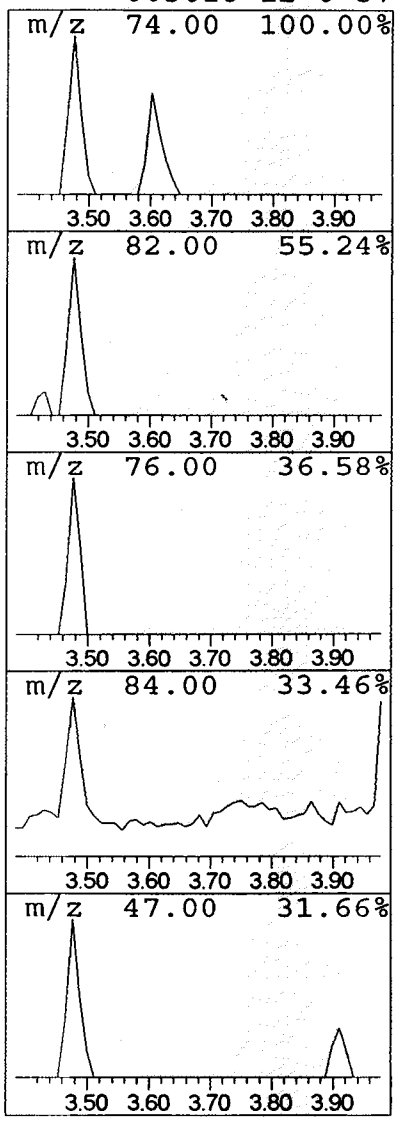
****

Peak Number 1 Acetonitrile, dichloro- $$ ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.48	0.12 ug/L	42154	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, dichloro- $$ Dichl...	109	C2HCl2N	003018-12-0	74
2	Dichloroacetonitrile $$ Acetonit...	109	C2HCl2N	003018-12-0	59
3	Dichloroacetonitrile $$ Acetonit...	109	C2HCl2N	003018-12-0	50
4	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	37





Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

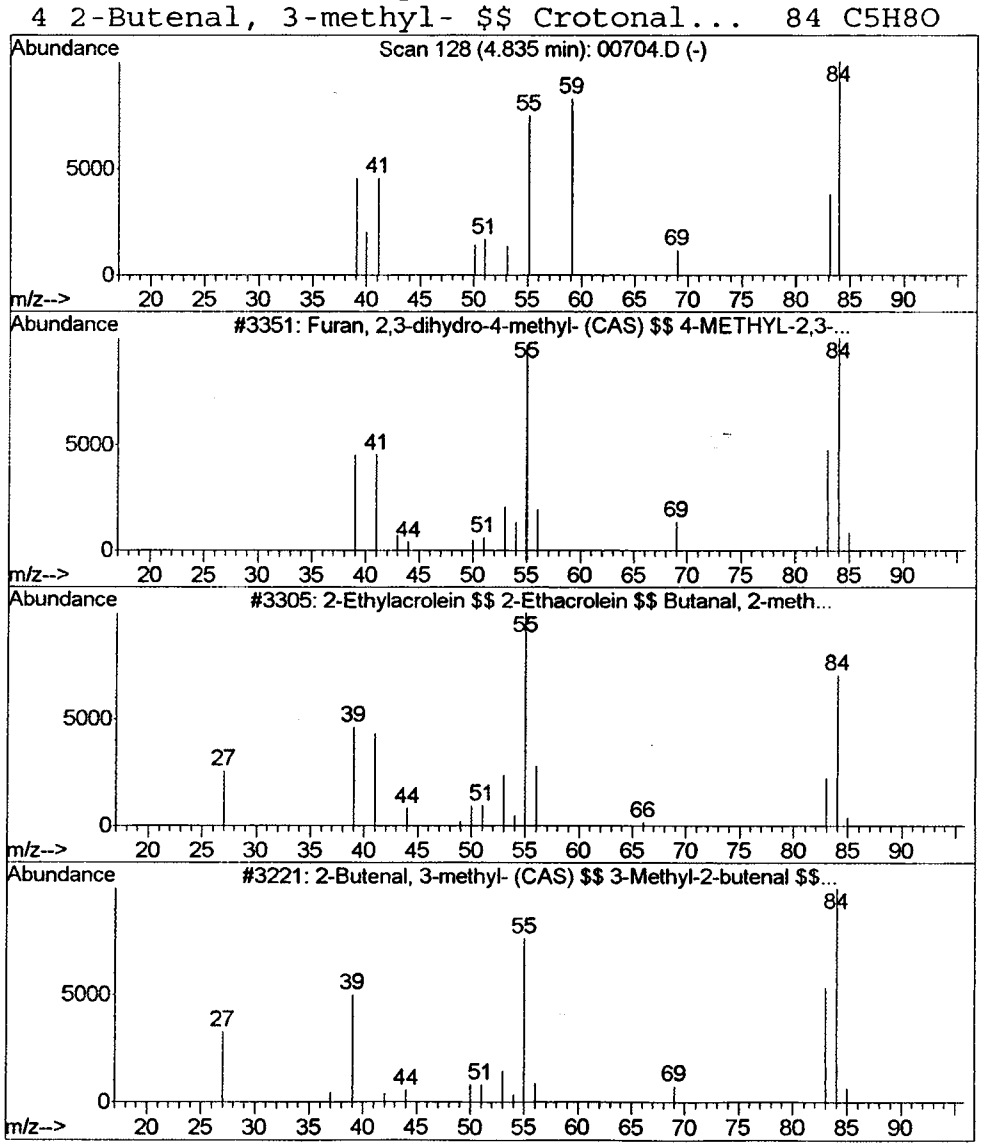
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

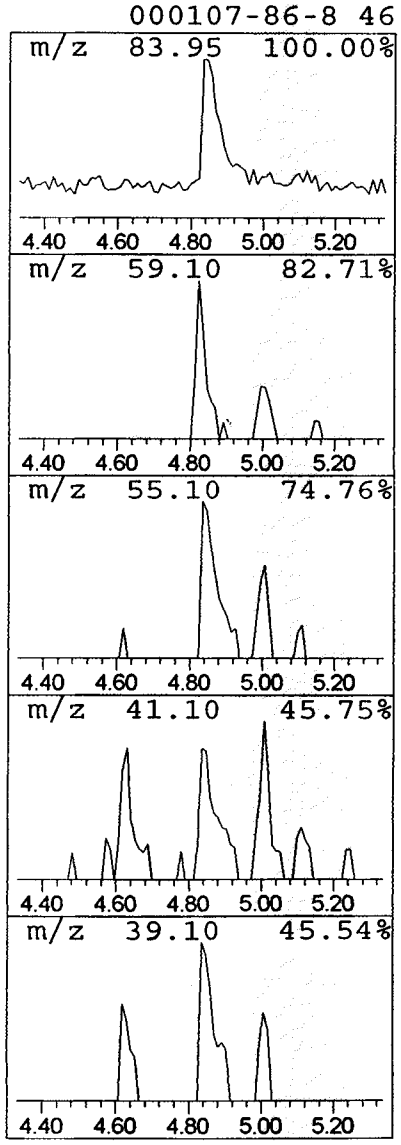
****

Peak Number 2 Furan, 2,3-dihydro-4-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.21 ug/L	75353	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	53
2	2-Ethylacrolein $$ 2-Ethacrolein...	84	C5H8O	000922-63-4	47
3	2-Butenal, 3-methyl- (CAS) $$ 3-...	84	C5H8O	000107-86-8	46
4	2-Butenal, 3-methyl- $$ Crotonal...	84	C5H8O	000107-86-8	46





Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 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

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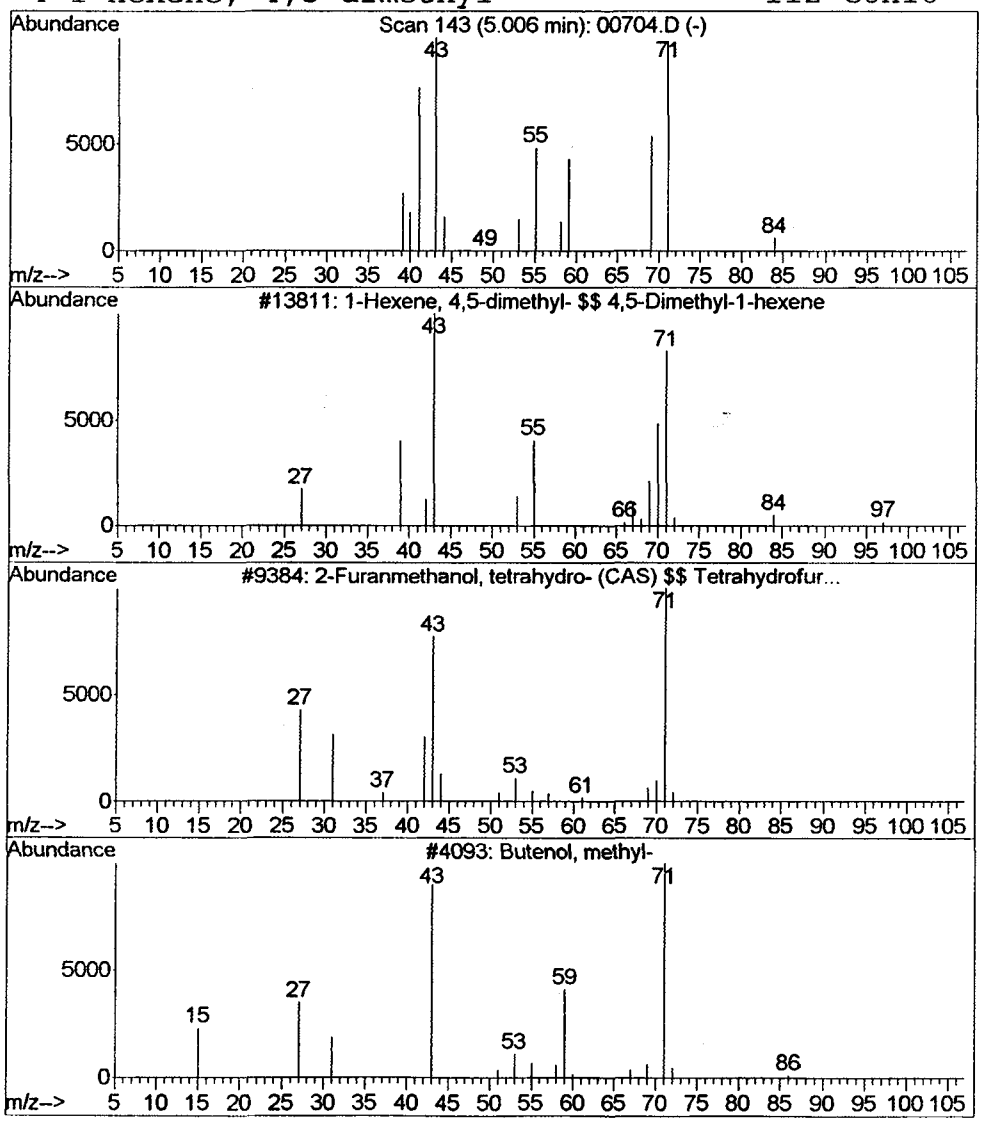
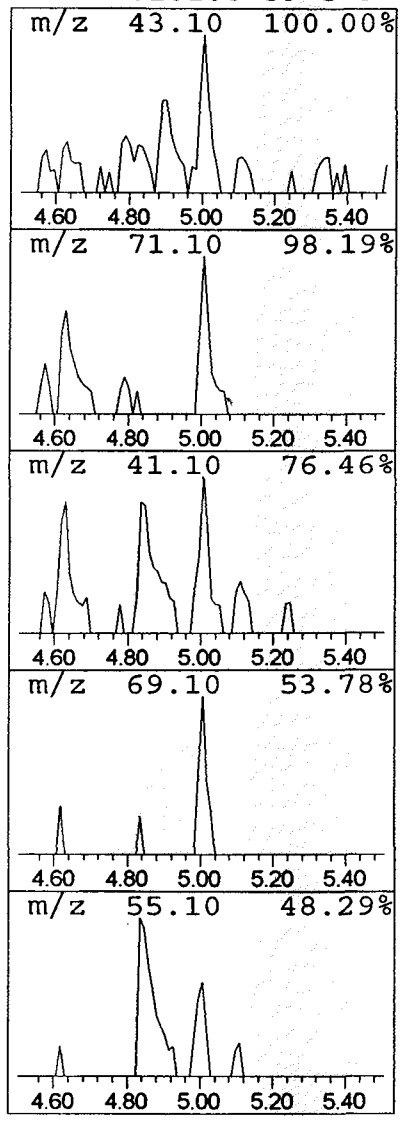
Peak Number 3 1-Hexene, 4,5-dimethyl- $$ ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.12 ug/L	41944	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 4,5-dimethyl- $$ 4,5-D...	112	C8H16	016106-59-5	33
2	2-Furanmethanol, tetrahydro- (CA...	102	C5H10O2	000097-99-4	9
3	Butenol, methyl-	86	C5H10O	060766-00-9	9
4	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	9





Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

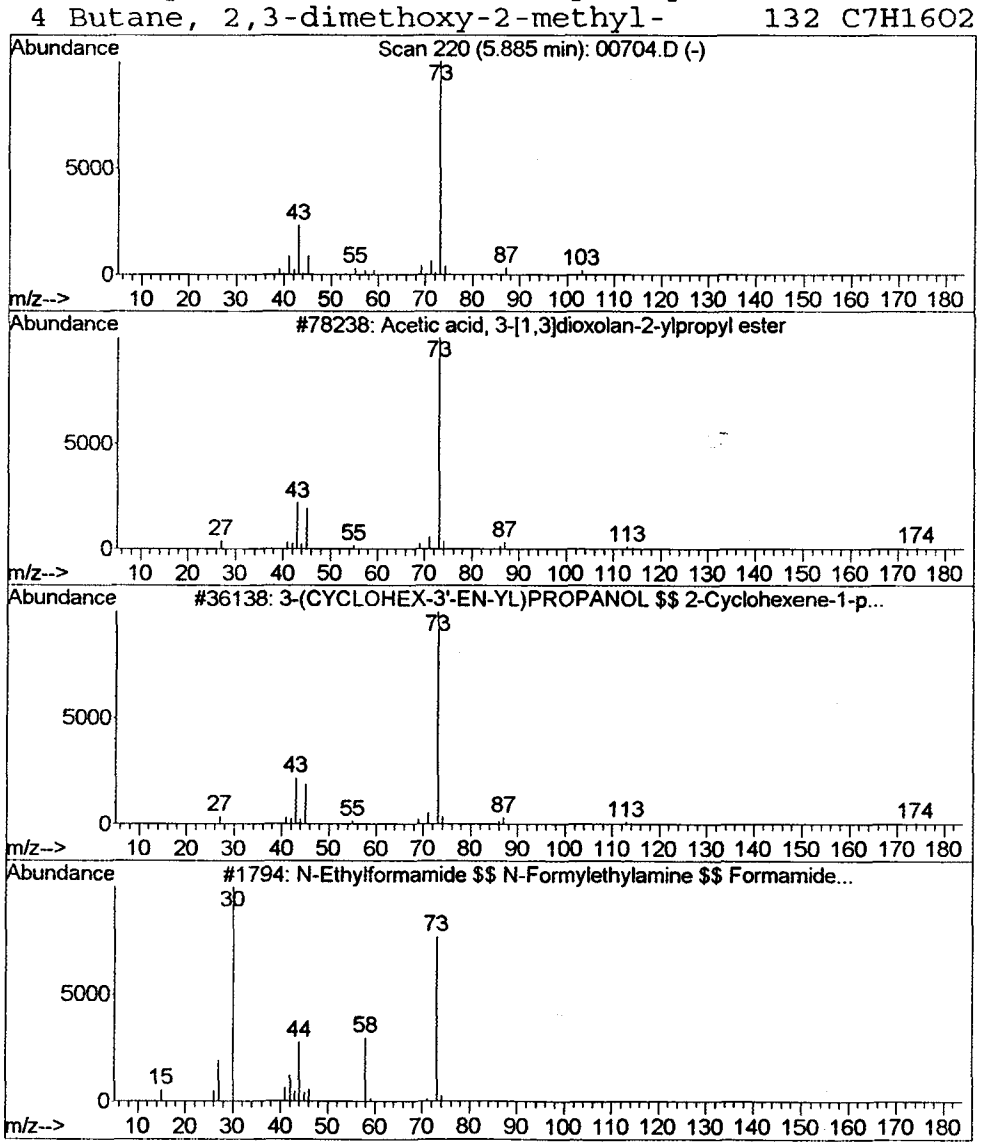
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

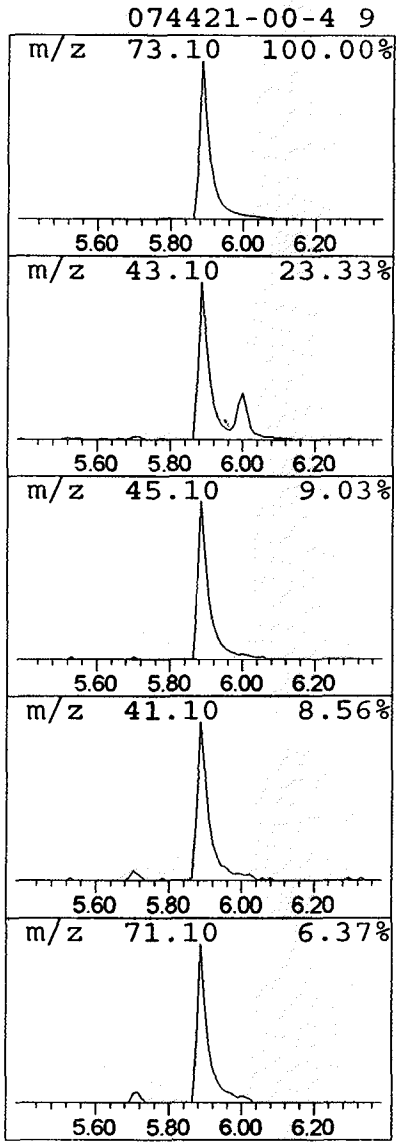
****

Peak Number 4 Acetic acid, 3-[1,3]dioxola... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	3.92 ug/L	1386800	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 $$...	174	C8H14O4	015745-87-6	33
3	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4	Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	9





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Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

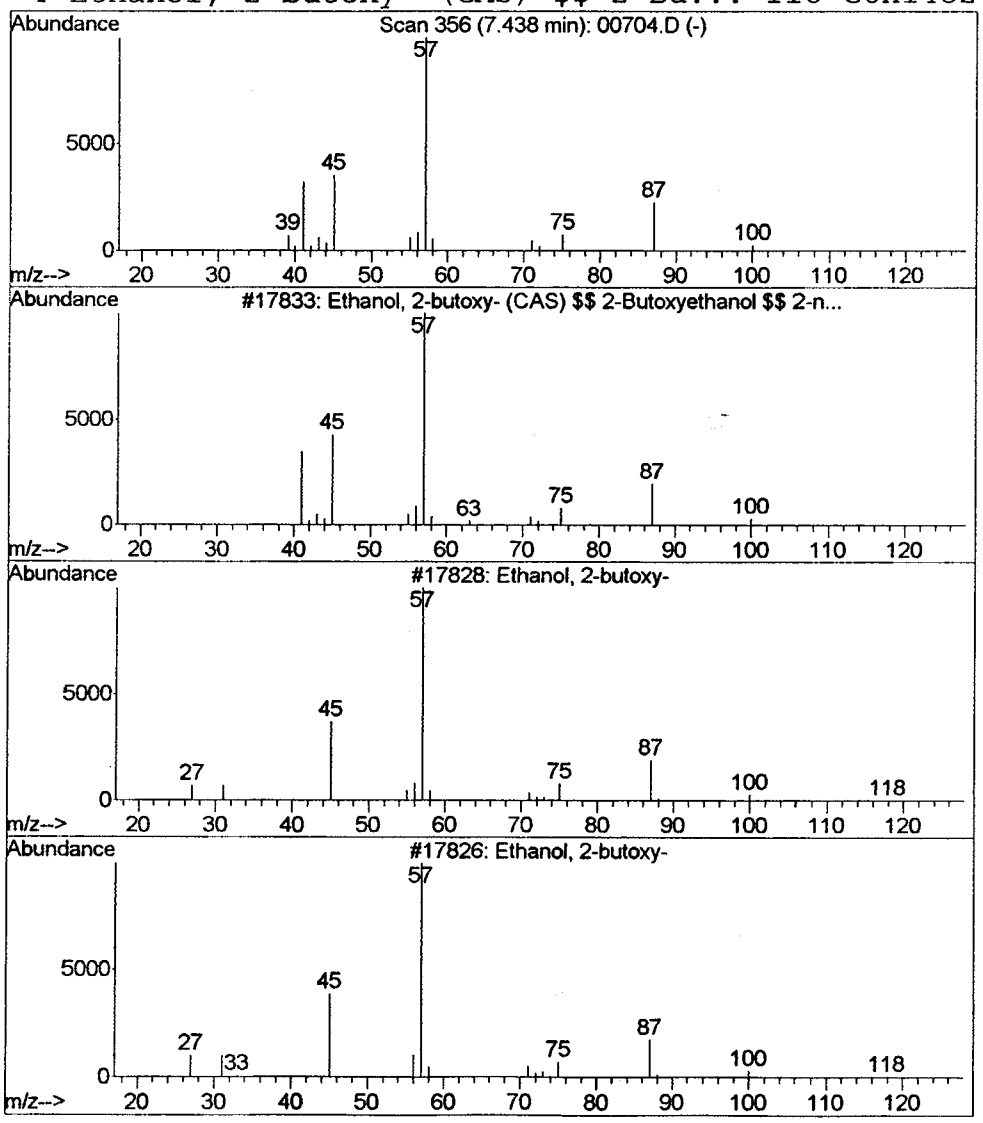
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

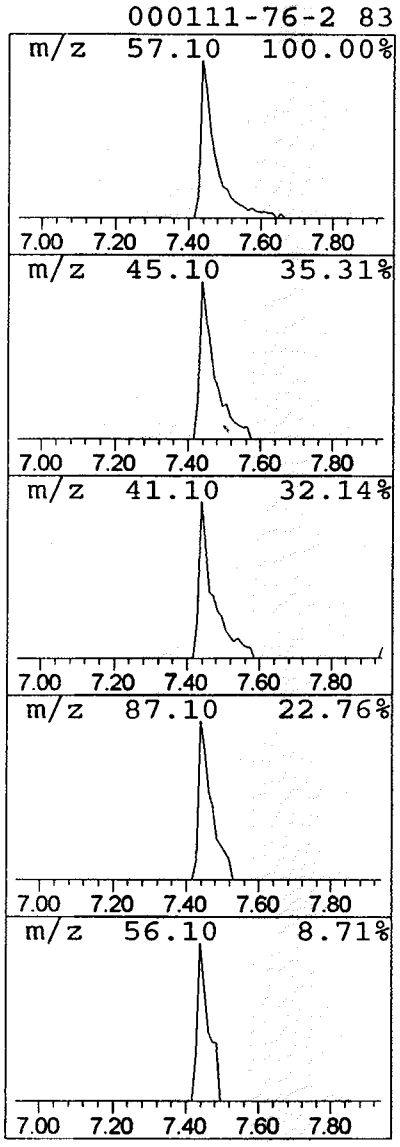
****

Peak Number 5 Ethanol, 2-butoxy- (CAS) $$... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	0.42 ug/L	150118	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy- (CAS) $$ 2-Bu...	118	C6H14O2	000111-76-2	90
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
4	Ethanol, 2-butoxy- (CAS) $$ 2-Bu...	118	C6H14O2	000111-76-2	83





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

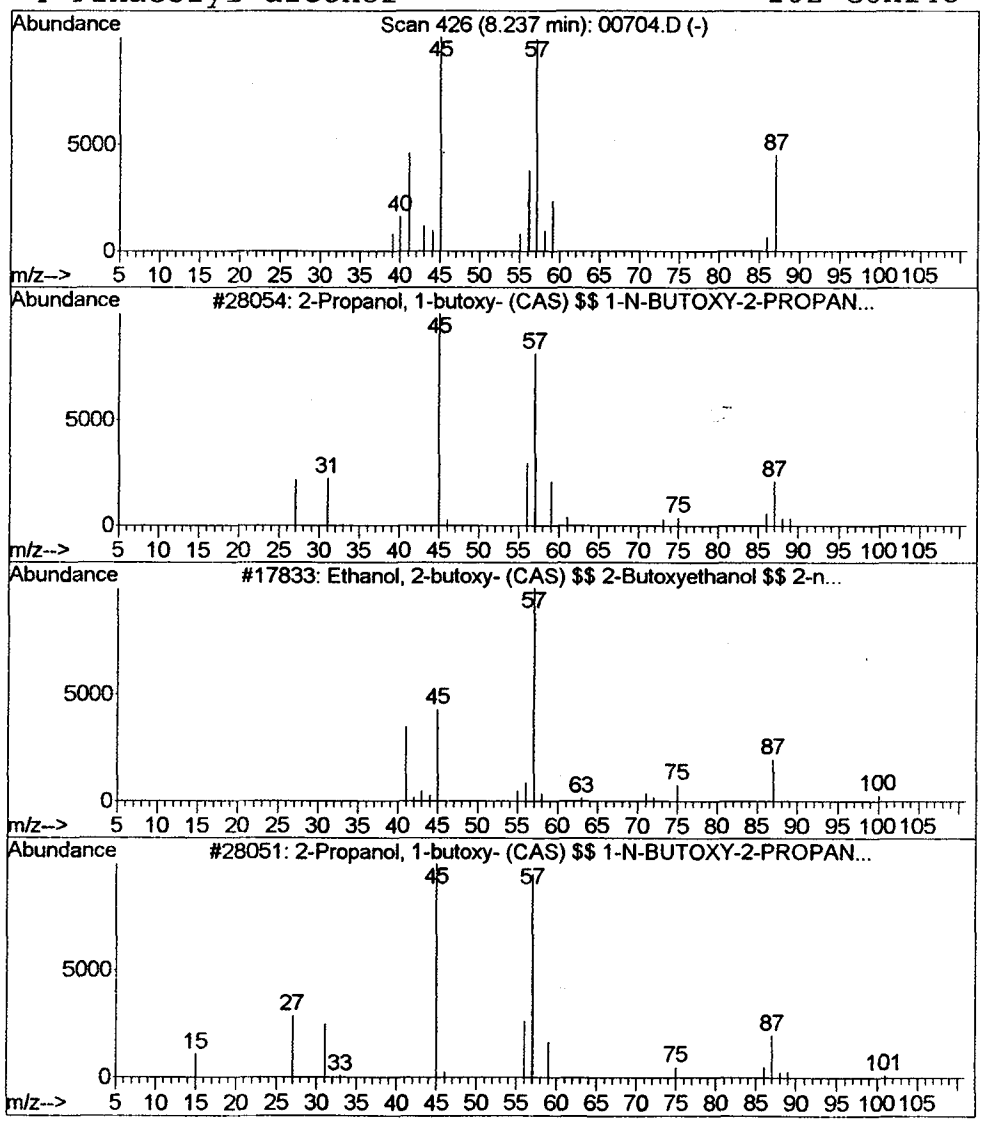
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

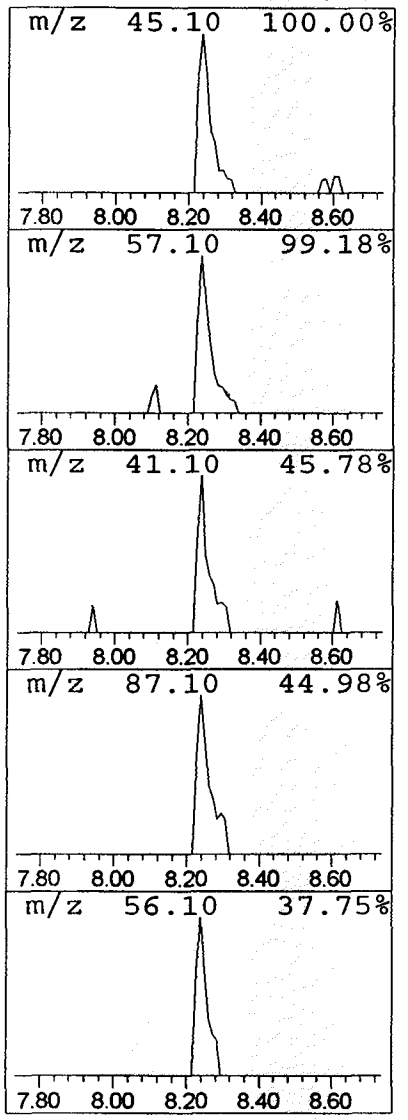
****

Peak Number 6 2-Propanol, 1-butoxy- (CAS)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	0.20 ug/L	72142	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy- (CAS) $$ 1...	132	C7H16O2	005131-66-8	50
2	Ethanol, 2-butoxy- (CAS) $$ 2-Bu...	118	C6H14O2	000111-76-2	50
3	2-Propanol, 1-butoxy- (CAS) $$ 1...	132	C7H16O2	005131-66-8	39
4	Pinacolyl alcohol	102	C6H14O	000464-07-3	38





Library Search Compound Report

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MS Integration Params: LSCINT.P

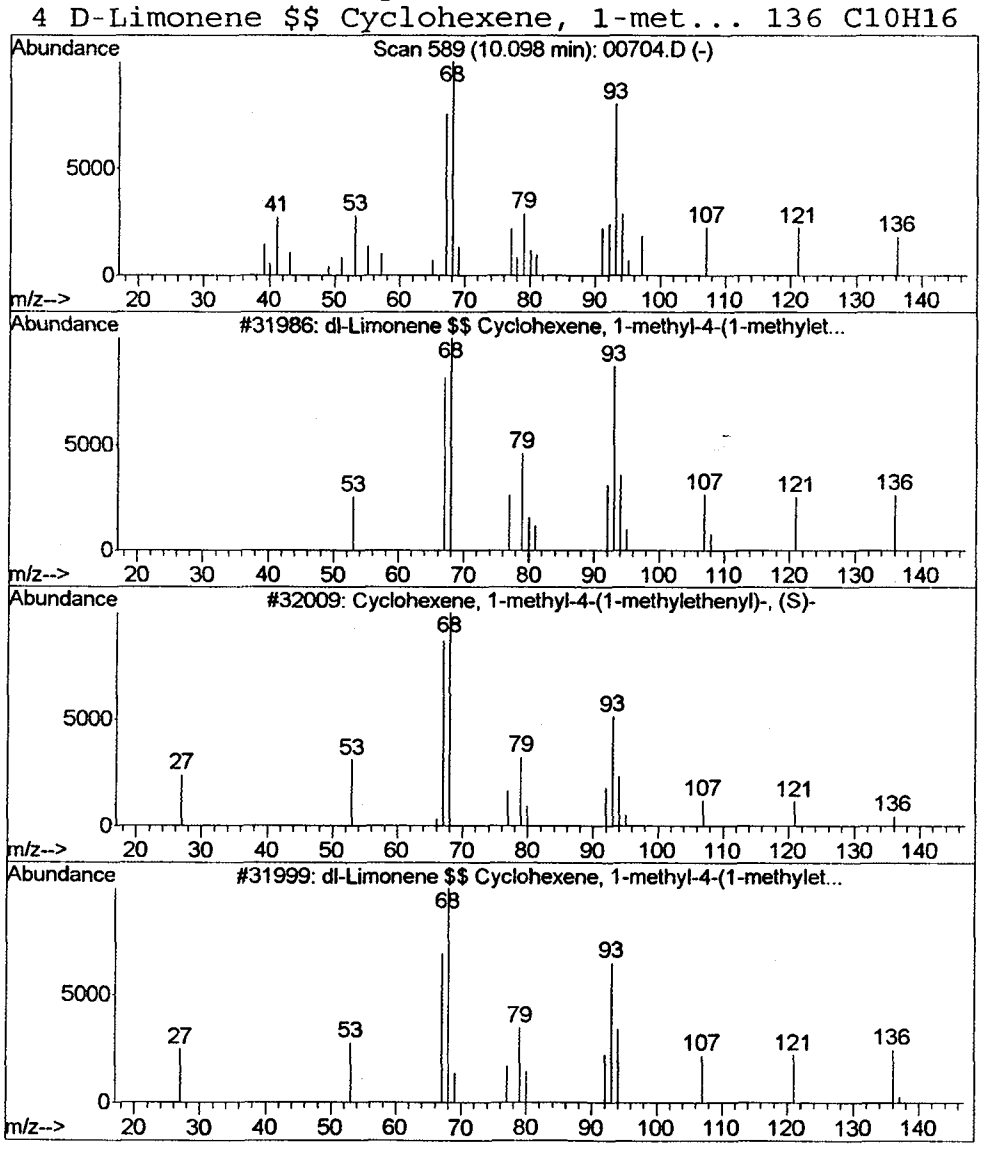
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

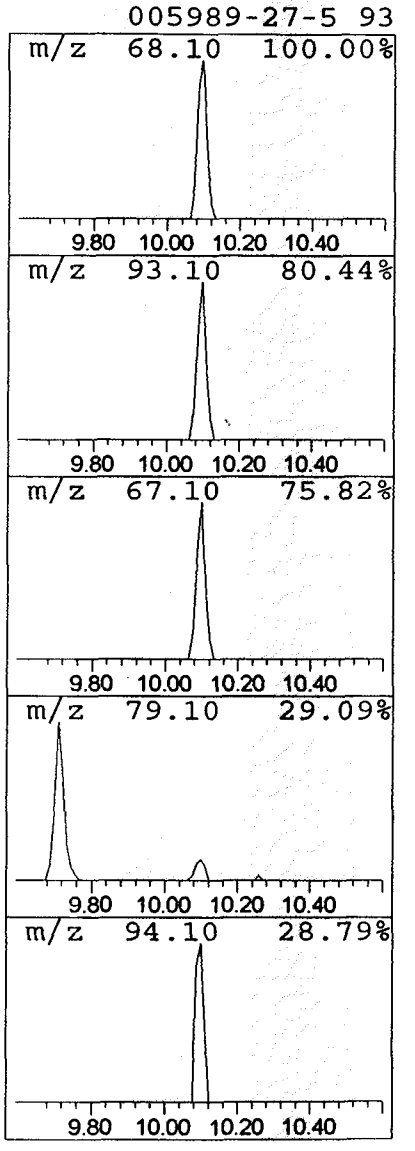
****

Peak Number 7 dl-Limonene $$ Cyclohexene,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	0.26 ug/L	90650	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	96
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	95
3	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	95
4	D-Limonene $$ Cyclohexene, 1-met...	136	C10H16	005989-27-5	93





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00704.D Vial: 4
Acq On : 16 Jan 2002 5:37 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

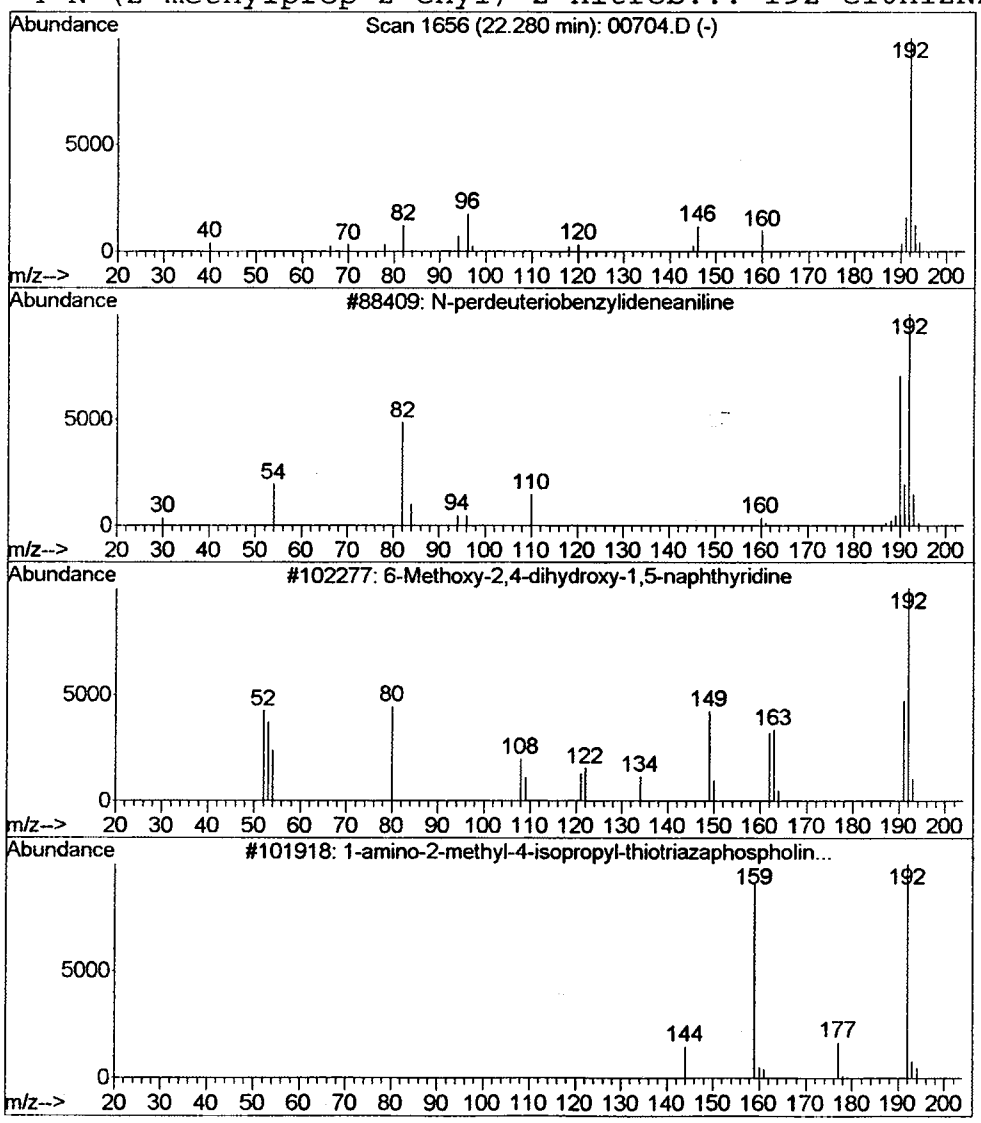
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

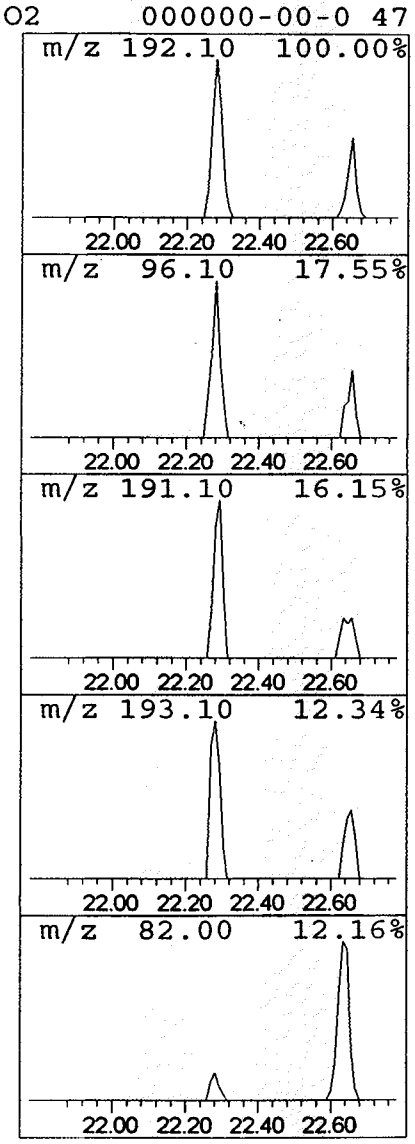
****

Peak Number 8 N-perdeuteriobenzylideneani... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.14 ug/L	88294	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58
2	6-Methoxy-2,4-dihydroxy-1,5-naph...	192	C9H8N2O3	000000-00-0	50
3	1-amino-2-methyl-4-isopropyl-thi...	192	C5H13N4PS	107264-54-0	50
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	47





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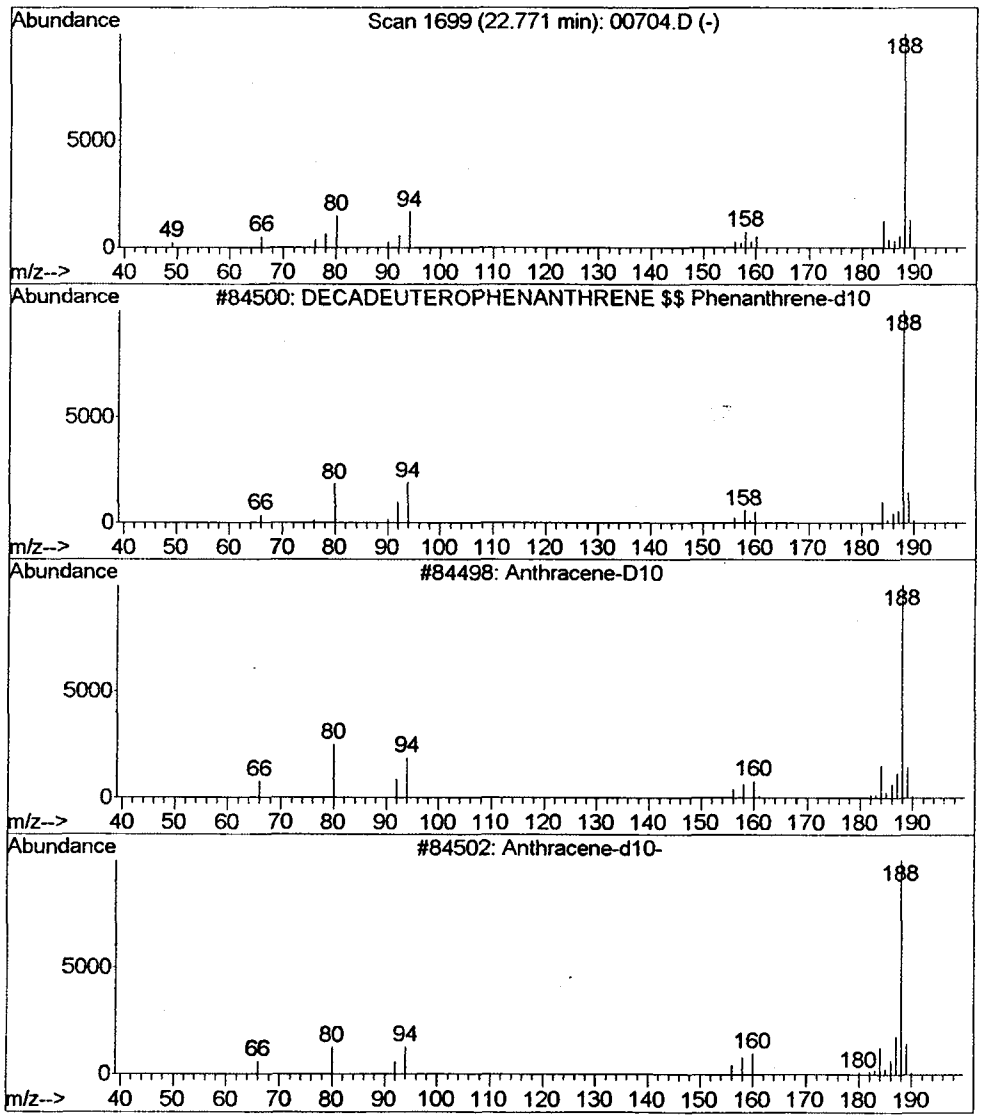
Library : C:\DATABASE\WILEY7N.L

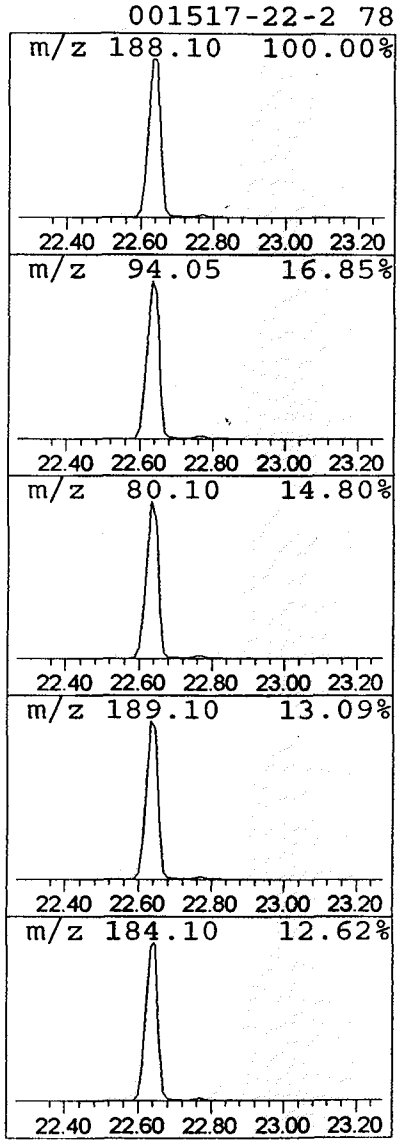
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.32 ug/L	205634	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	91
2	Anthracene-D10	188	C14D10	000000-00-0	87
3	Anthracene-d10-	188	C14D10	001719-06-8	86
4	Phenanthrene-d10	188	C14D10	001517-22-2	78





Tentatively Identified Compound (ESC) Summary

Operator ID: Date Acquired: 16 Jan 2002 5:37 pm
Data File: C:\MSDCHEM\1\5973N\02JAN16\00704.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
Acetonitrile, dic...	3.48	0.1	ug/L	42154	1	9.71	7072120	20.0
Furan, 2,3-dihydr...	4.83	0.2	ug/L	75353	1	9.71	7072120	20.0
1-Hexene, 4,5-dim...	5.01	0.1	ug/L	41944	1	9.71	7072120	20.0
Acetic acid, 3-[1...	5.89	3.9	ug/L	1386800	1	9.71	7072120	20.0
Ethanol, 2-butoxy...	7.44	0.4	ug/L	150118	1	9.71	7072120	20.0
2-Propanol, 1-but...	8.24	0.2	ug/L	72142	1	9.71	7072120	20.0
dl-Limonene $$ Cy...	10.10	0.3	ug/L	90650	1	9.71	7072120	20.0
N-perdeuteriobenz...	22.28	0.1	ug/L	88294	4	22.63	12692300	20.0
DECADEUTEROPHENAN...	22.77	0.3	ug/L	205634	4	22.63	12692300	20.0