User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 03/05/2002 Time: 12:16:55

Sample: AE02718
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 3/5/02 12:16 Ended: 3/5/02 12:16 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		97		5.0

Comments for Sample AE02718 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 03-05-2002 Time: 12:17:05

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recoveries for 14 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Mar 01 09:02:57 2002 Quant Results File: HP022102.RES

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Last Update : Mon Feb 25 10:47:59 2002
Response via : Initial Calibration
DataAcq Meth : HP020702

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.72	152	1378279	20.00	ug/L	0.00
10) Naphthalene-d8	13.20	136	5973201	20.00	ug/L	0.00
17) Acenaphthene-d10	18.34	164	2971117	20.00	ug/L	0.00
29) Phenanthrene-d10	22.63	188	5193287	20.00	ug/L	-0.01
38) Chrysene-d12	30.49	240	3868162	20.00	ug/L	-0.03
44) Perylene-d12	34.41	264	2499584	20.00	ug/L	-0.04
System Monitoring Compounds						
37) 2,4-DDD	27.72	235	335699	4.85	ug/L	0.00
Spiked Amount 5.000			Recovery = 97.00%			
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	475920	2.64	ug/L	# 57
21) 2,6-Dinitrotoluene	18.33	165	378401	9.09	ug/L	# 27

(#) = qualifier out of range (m) = manual integration

Quantitation Report (Not Reviewed)

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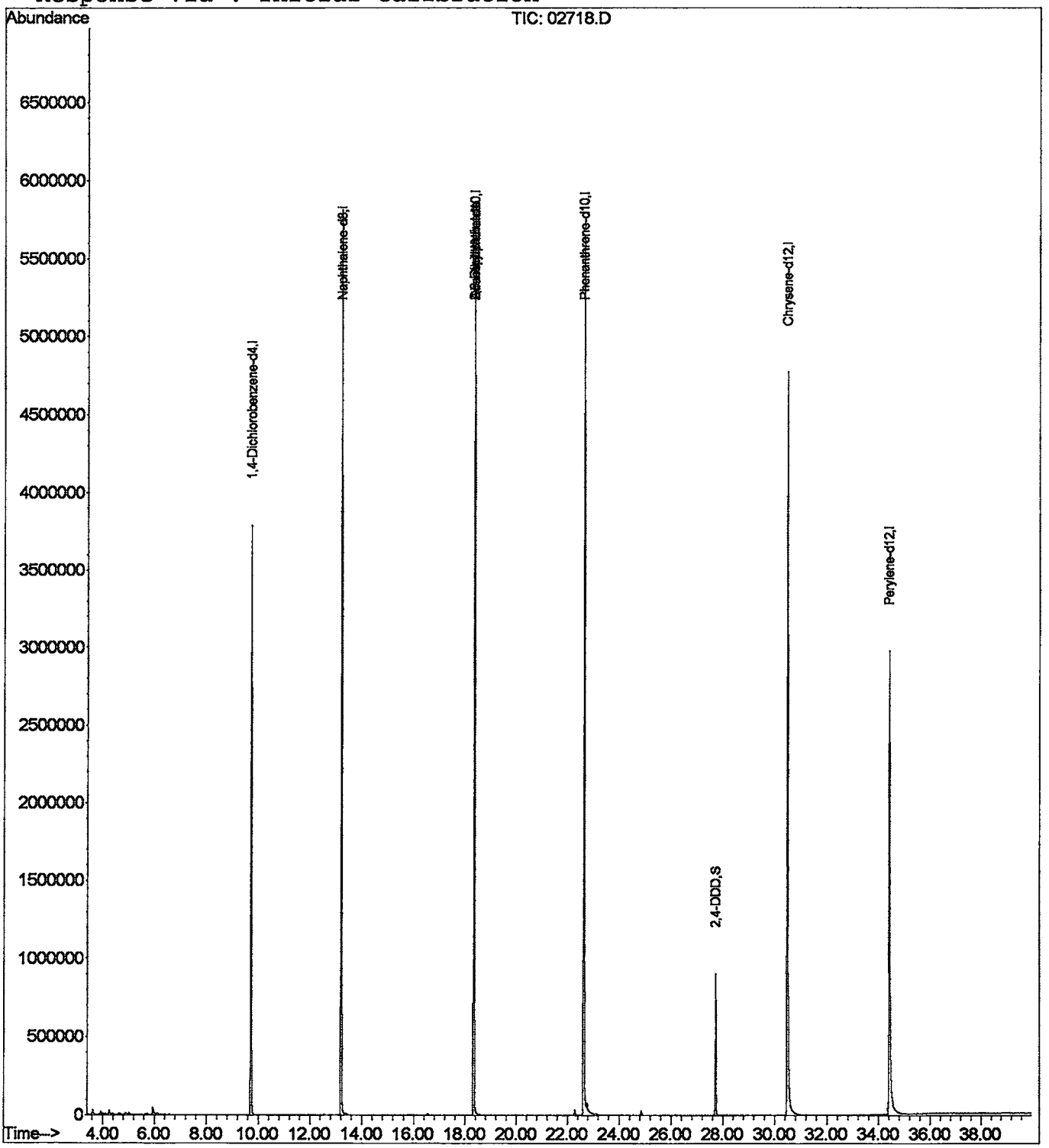
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Mar 1 9:02 2002 Quant Results File: HP022102.R

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)
Title : 508 scan method
Last Update : Mon Feb 25 10:47:59 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.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

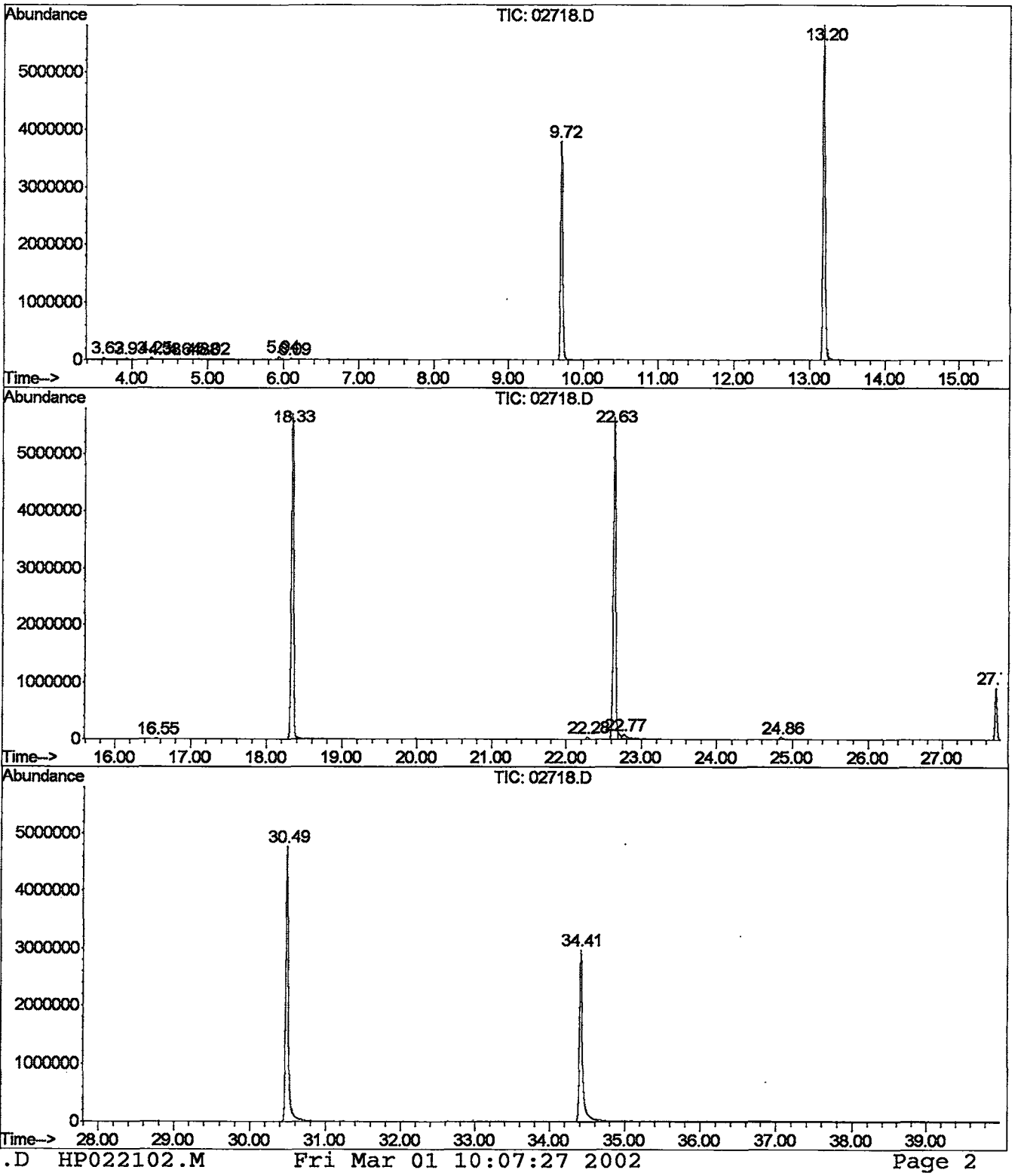
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.622	19	22	25	rBV	33825	55421	0.43%	0.084%
2	3.927	47	49	55	rBV	21167	31835	0.25%	0.048%
3	4.254	73	78	85	rVV3	28825	62658	0.49%	0.095%
4	4.378	85	89	99	rVB3	7272	22285	0.17%	0.034%
5	4.638	107	112	119	rBV5	9305	22267	0.17%	0.034%
6	4.875	131	133	143	rBV2	10501	30173	0.24%	0.046%
7	5.022	143	146	155	rVB	13142	25247	0.20%	0.038%
8	5.936	223	227	239	rBV	45655	119908	0.94%	0.181%
9	6.094	239	241	249	rVV2	11357	38674	0.30%	0.058%
10	9.718	557	562	567	rBV	3792184	7695783	60.19%	11.615%
11	13.195	865	870	875	rBV	5812328	11253753	88.01%	16.985%
12	16.548	1161	1167	1171	rBV2	10195	20957	0.16%	0.032%
13	18.332	1319	1325	1331	rBV	5706831	12089075	94.54%	18.246%
14	22.283	1671	1675	1679	rBV	37895	70950	0.55%	0.107%
15	22.633	1701	1706	1711	rBV2	5643704	12786872	100.00%	19.299%
16	22.768	1715	1718	1737	rVB	68134	278511	2.18%	0.420%
17	24.857	1899	1903	1911	rVV	31351	69414	0.54%	0.105%
18	27.724	2153	2157	2163	rBV	906267	1607803	12.57%	2.427%
19	30.490	2397	2402	2439	rBV	4771958	11416722	89.28%	17.231%
20	34.407	2743	2749	2789	rBV	2971690	8556814	66.92%	12.915%

Sum of corrected areas: 66255122

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02FEB28\02718.D
Operator :
Acquired : 28 Feb 2002 4:20 pm using AcqMethod HP020702
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : February 28, 2002
Vial Number: 3
Quant File :HP022102.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

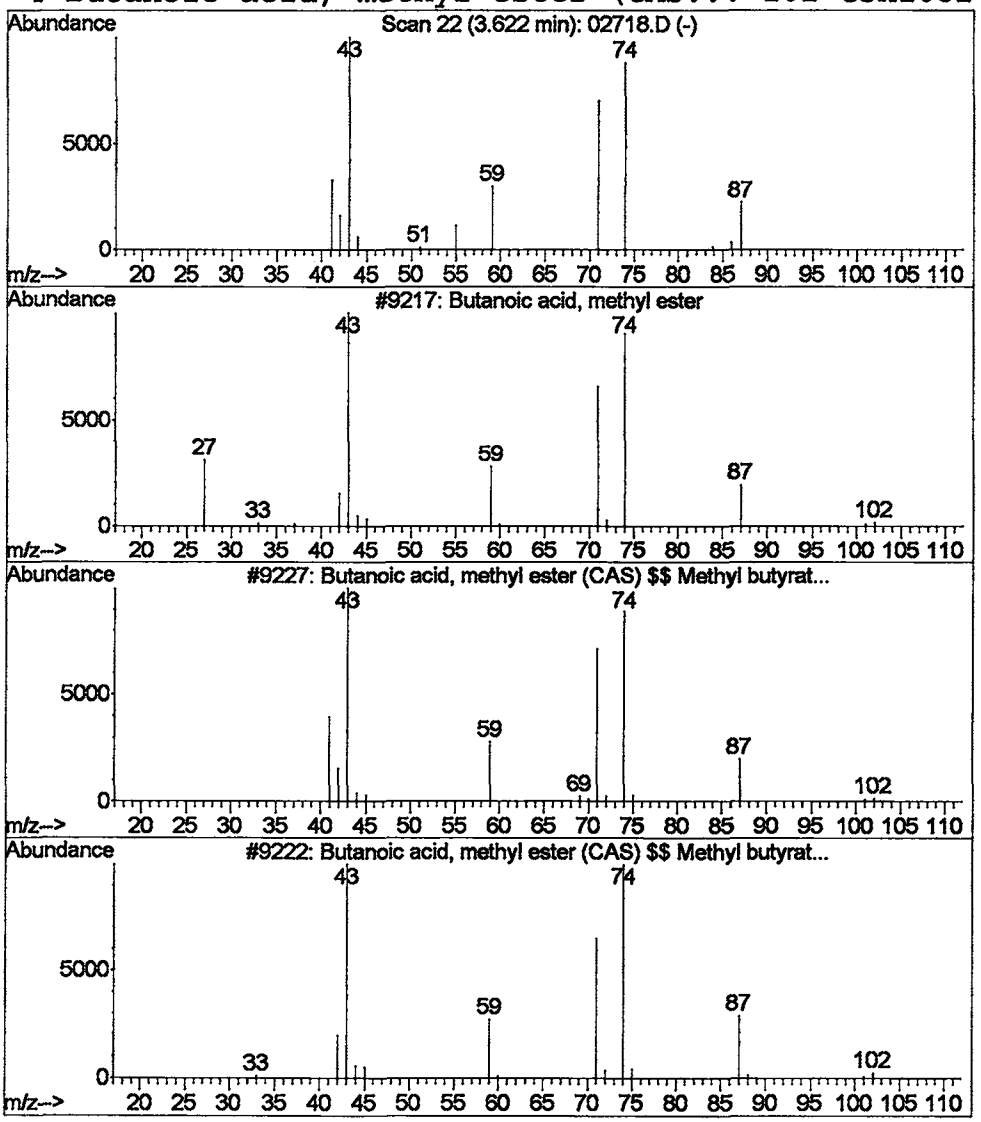
Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

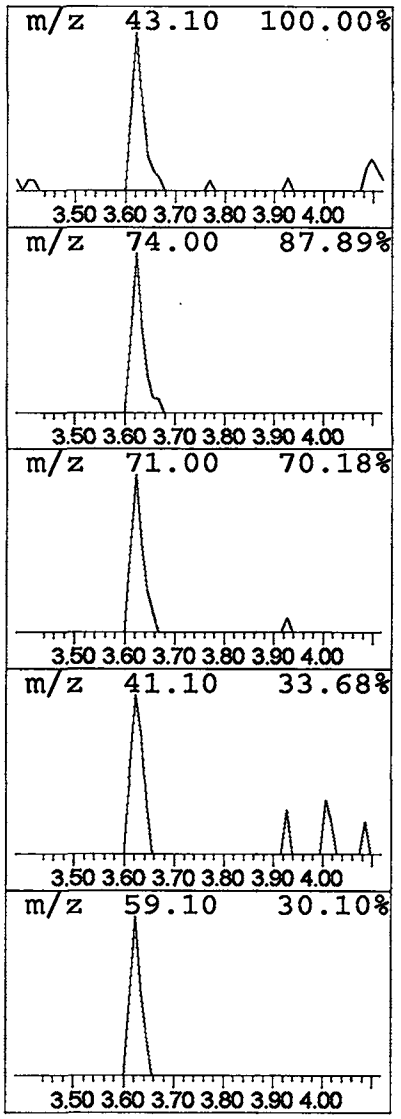
****

Peak Number 1 Butanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	0.14 ug/L	55421	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
2	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
3	Butanoic acid, methyl ester (CAS...	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\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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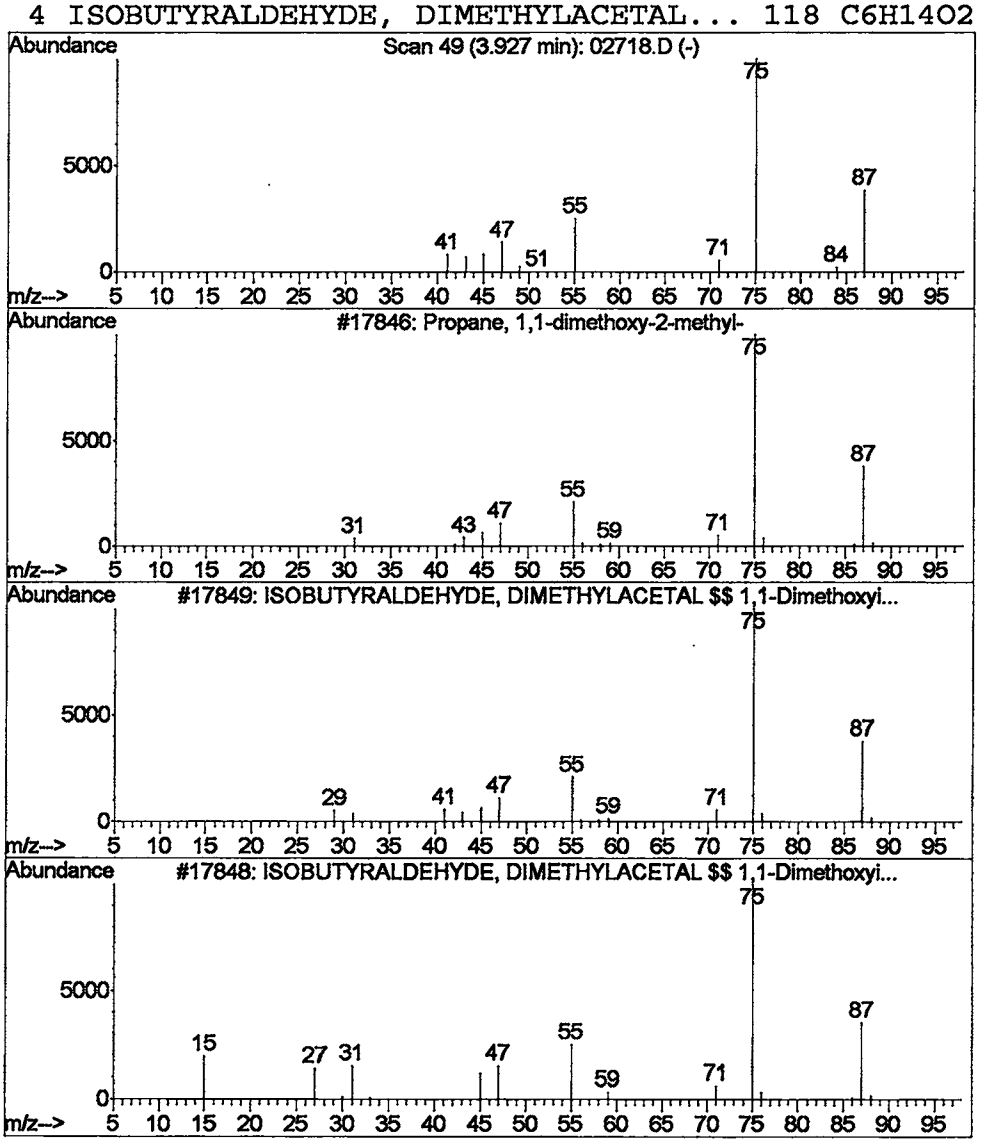
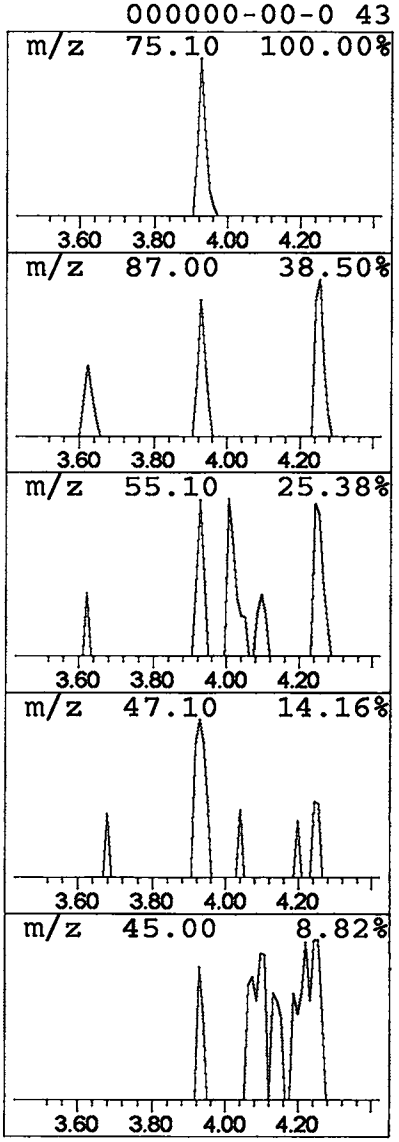
Peak Number 2 Propane, 1,1-dimethoxy-2-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	0.08 ug/L	31835	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	83
2	ISOBUTYRALDEHYDE, DIMETHYLACETAL...	118	C6H14O2	000000-00-0	74
3	ISOBUTYRALDEHYDE, DIMETHYLACETAL...	118	C6H14O2	000000-00-0	74
4	ISOBUTYRALDEHYDE, DIMETHYLACETAL...	118	C6H14O2	000000-00-0	43





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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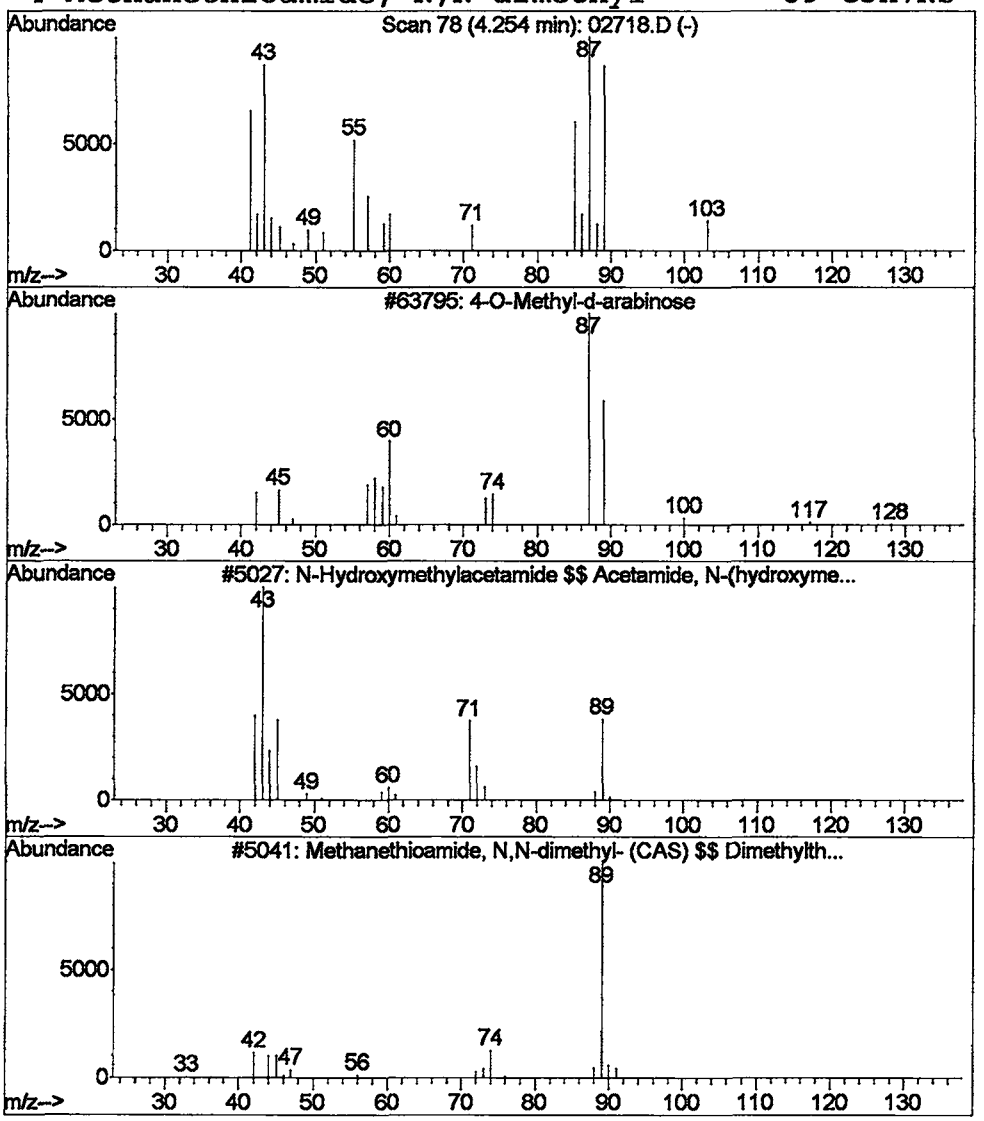
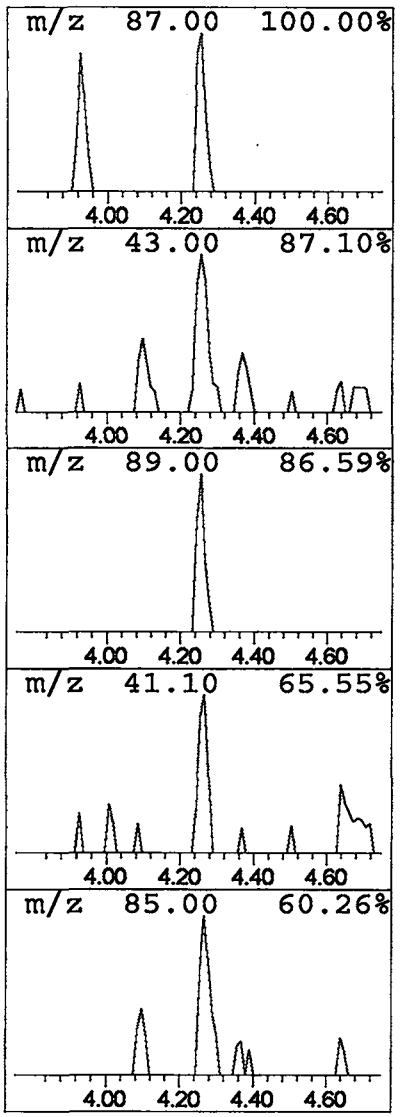
Peak Number 3 4-O-Methyl-d-arabinose Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	0.16 ug/L	62658	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-O-Methyl-d-arabinose	164	C6H12O5	000000-00-0	64
2	N-Hydroxymethylacetamide $$ Acet...	89	C3H7NO2	000625-51-4	53
3	Methanethioamide, N,N-dimethyl- ...	89	C3H7NS	000758-16-7	47
4	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

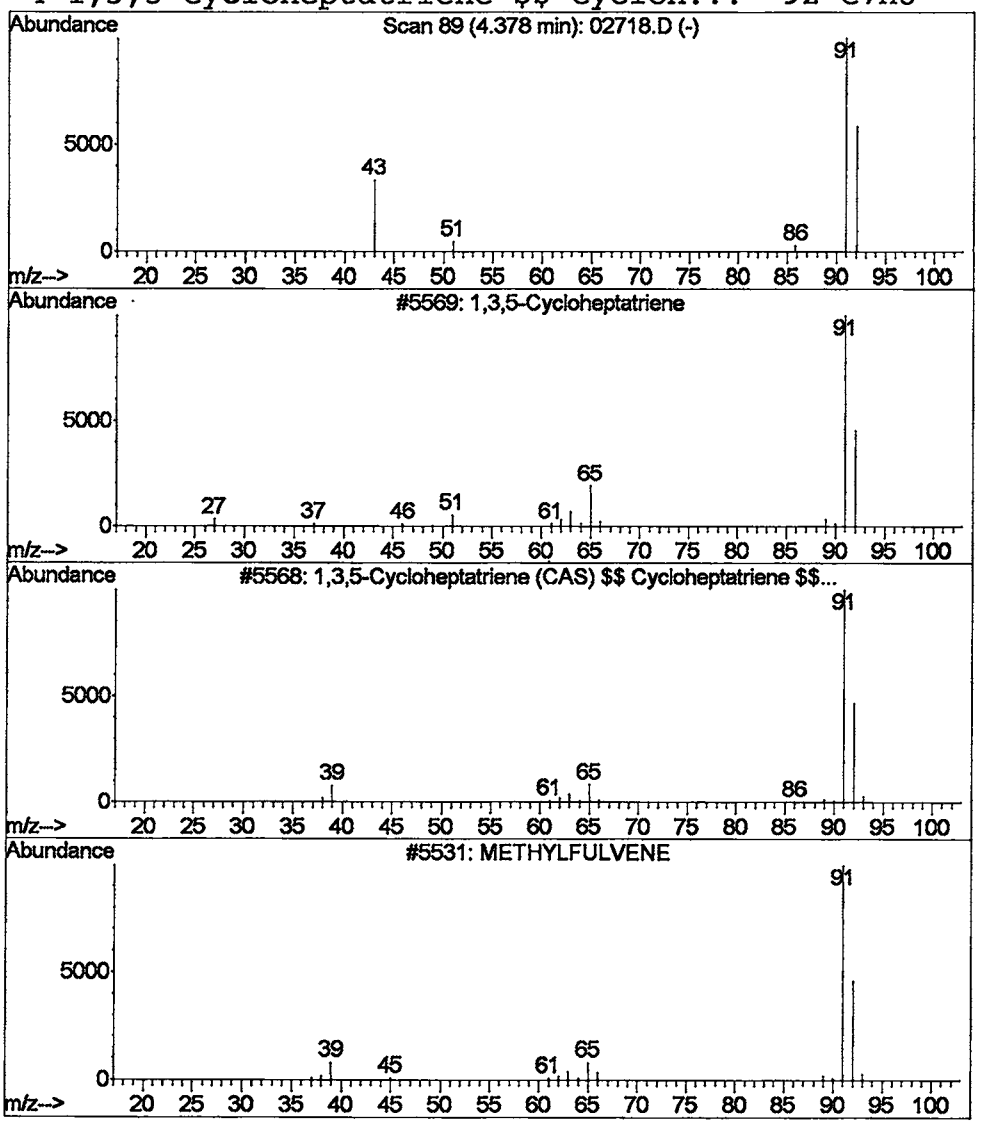
Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

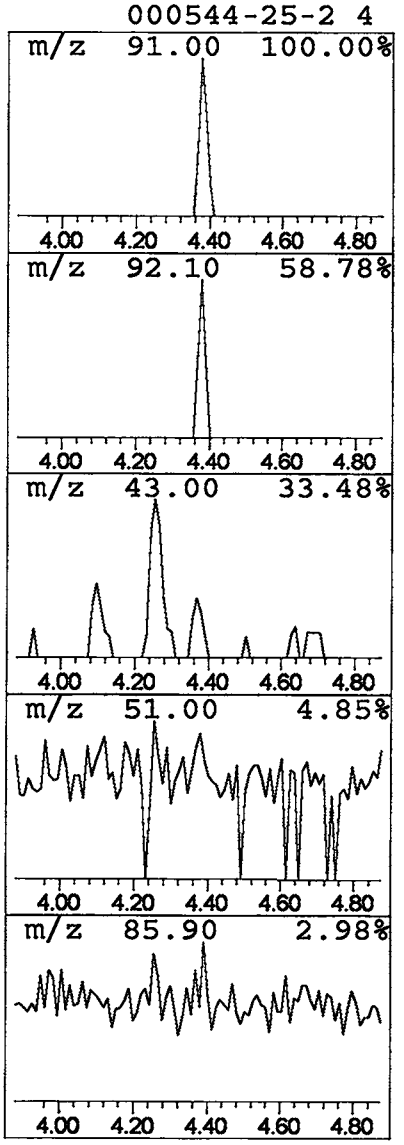
****

Peak Number 4 1,3,5-Cycloheptatriene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	0.06 ug/L	22285	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	7
2	1,3,5-Cycloheptatriene (CAS) $$ ...	92	C7H8	000544-25-2	4
3	METHYLFULVENE	92	C7H8	000000-00-0	4
4	1,3,5-Cycloheptatriene $$ Cycloh...	92	C7H8	000544-25-2	4





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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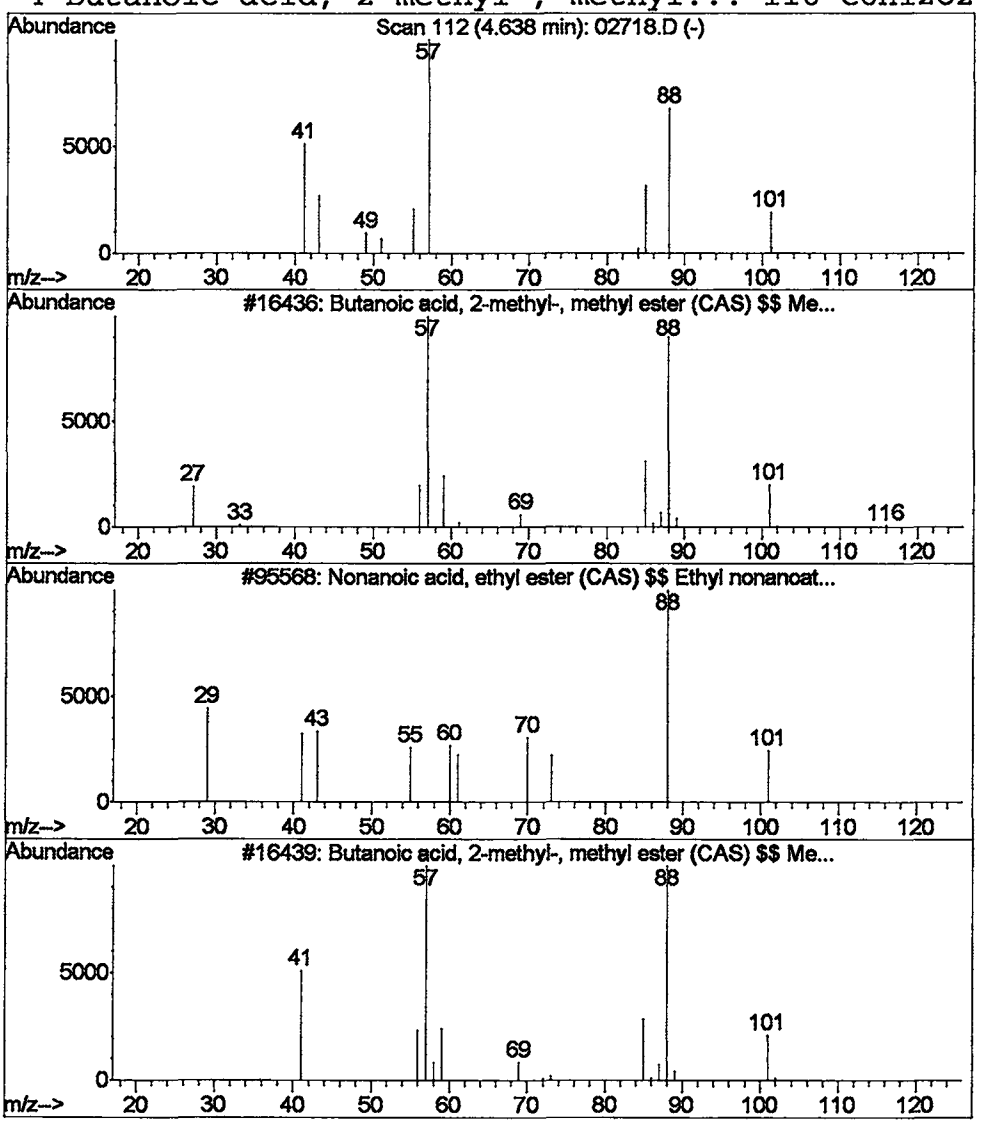
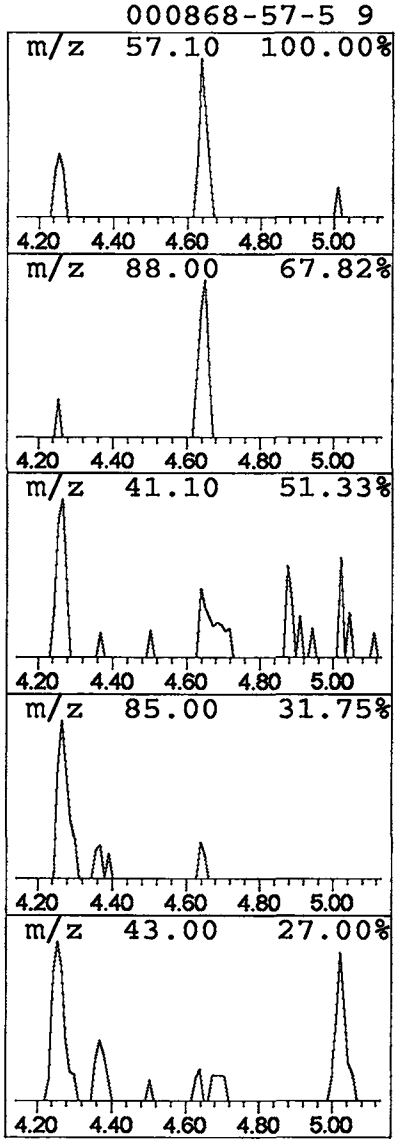
Peak Number 5 Butanoic acid, 2-methyl-, m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	0.06 ug/L	22267	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	40
2	Nonanoic acid, ethyl ester (CAS)...	186	C11H22O2	000123-29-5	9
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	9
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	9





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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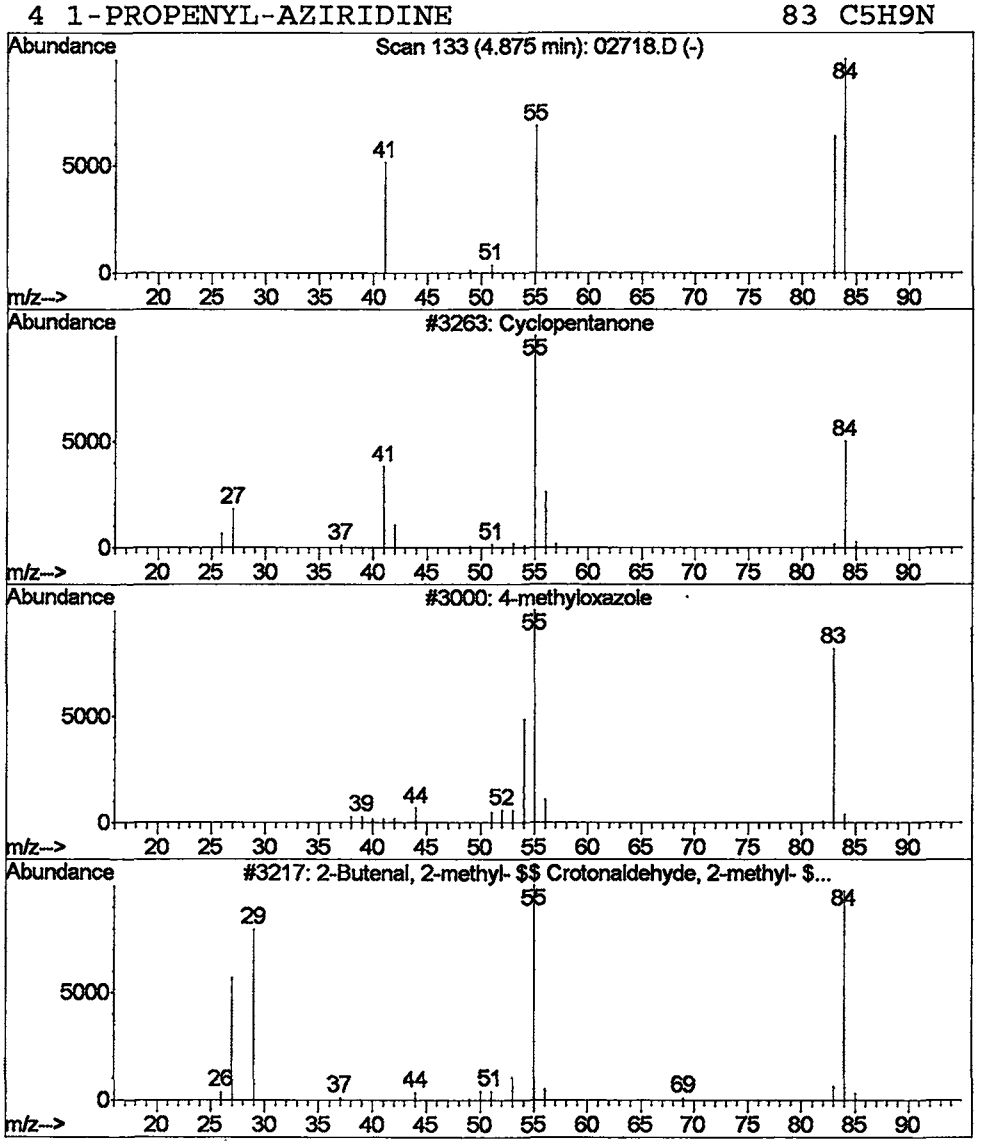
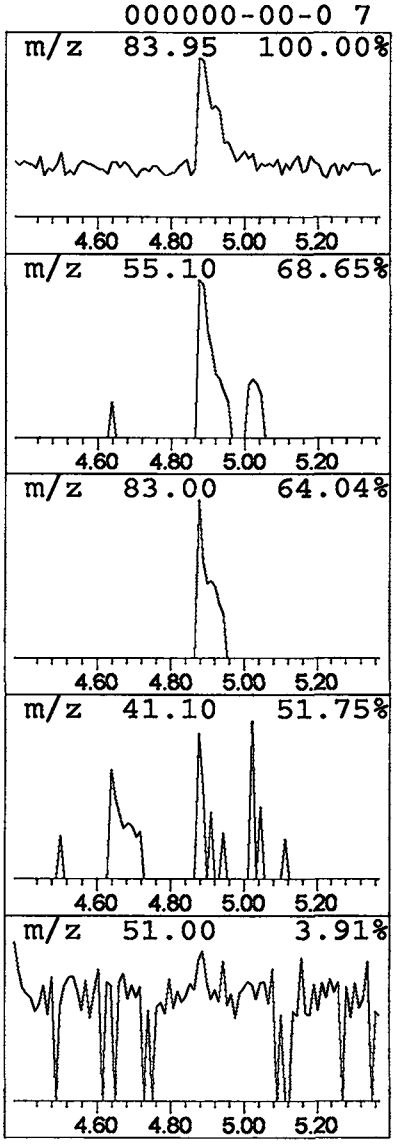
Peak Number 6 Cyclopentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	0.08 ug/L	30173	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	7
2	4-methyloxazole	83	C4H5NO	000000-00-0	7
3	2-Butenal, 2-methyl- $$ Crotonal...	84	C5H8O	001115-11-3	7
4	1-PROPENYL-AZIRIDINE	83	C5H9N	000000-00-0	7





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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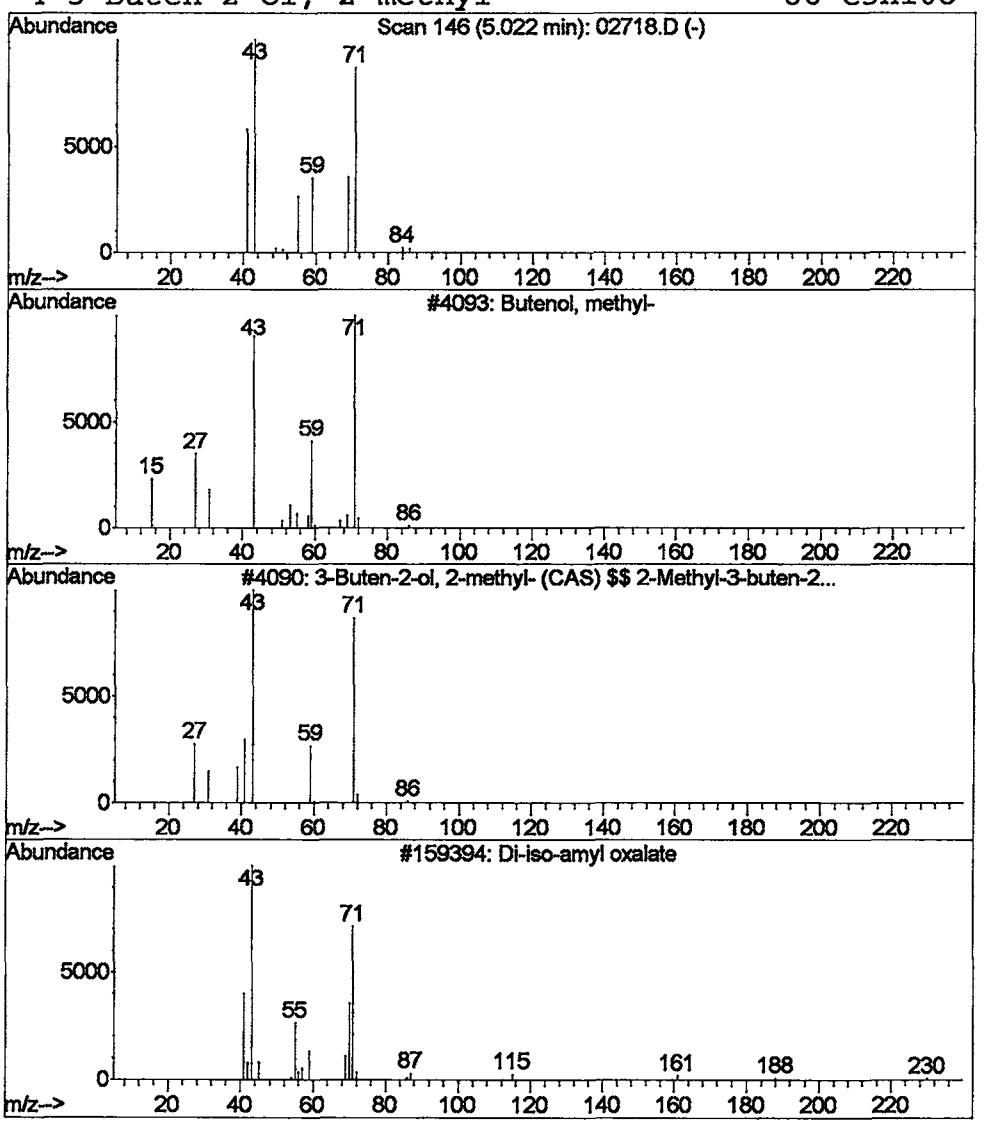
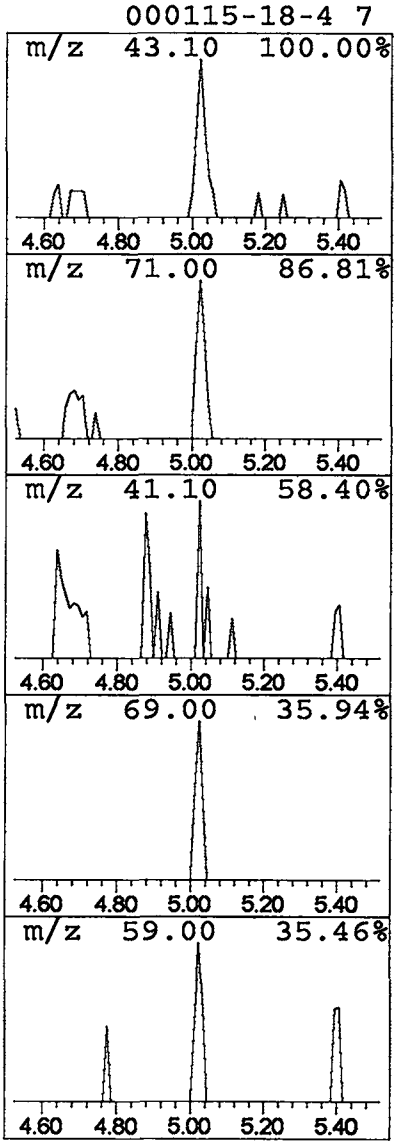
Peak Number 7 Butenol, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	0.07 ug/L	25247	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butenol, methyl-	86	C5H10O	060766-00-9	74
2	3-Buten-2-ol, 2-methyl- (CAS) $$...	86	C5H10O	000115-18-4	9
3	Di-iso-amyl oxalate	230	C12H22O4	000000-00-0	9
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	7





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
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Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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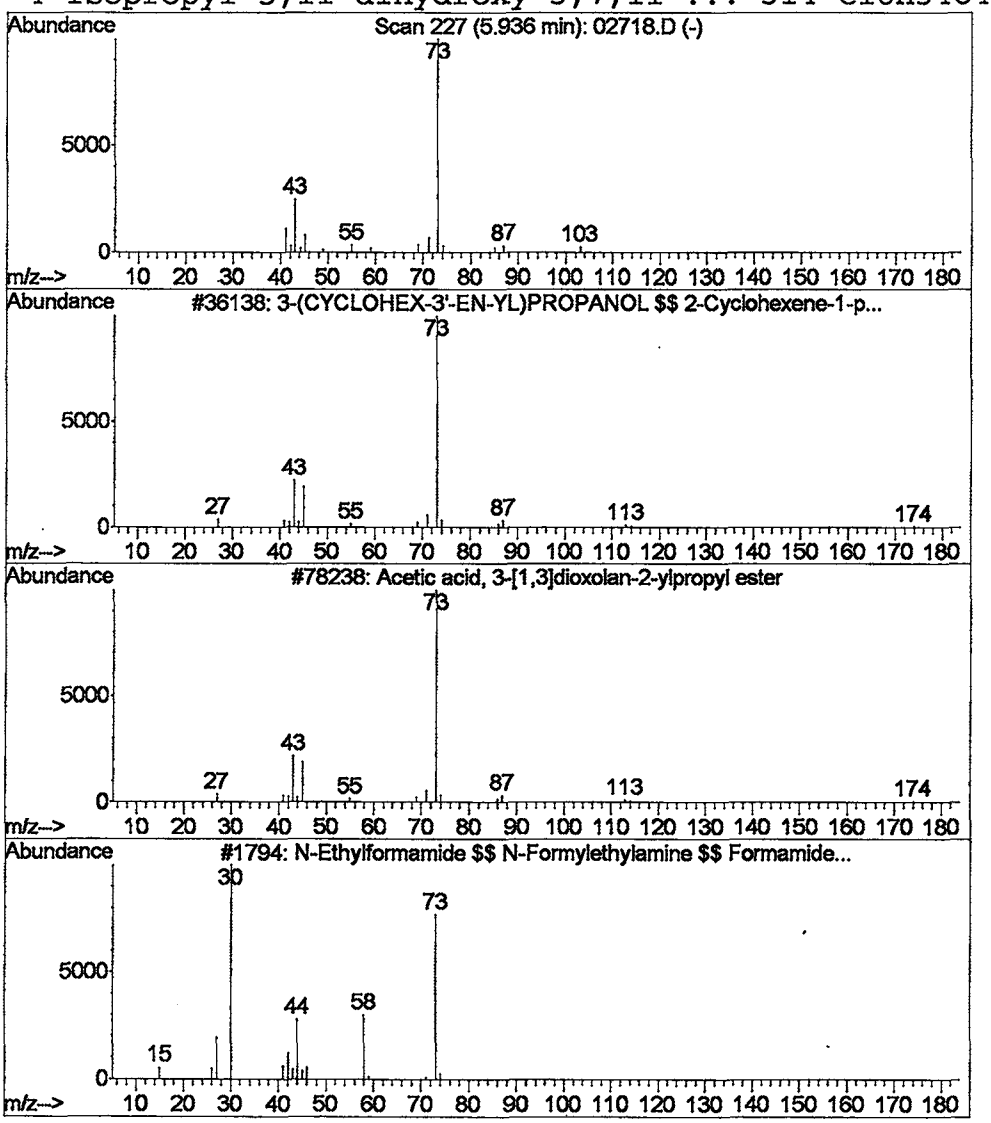
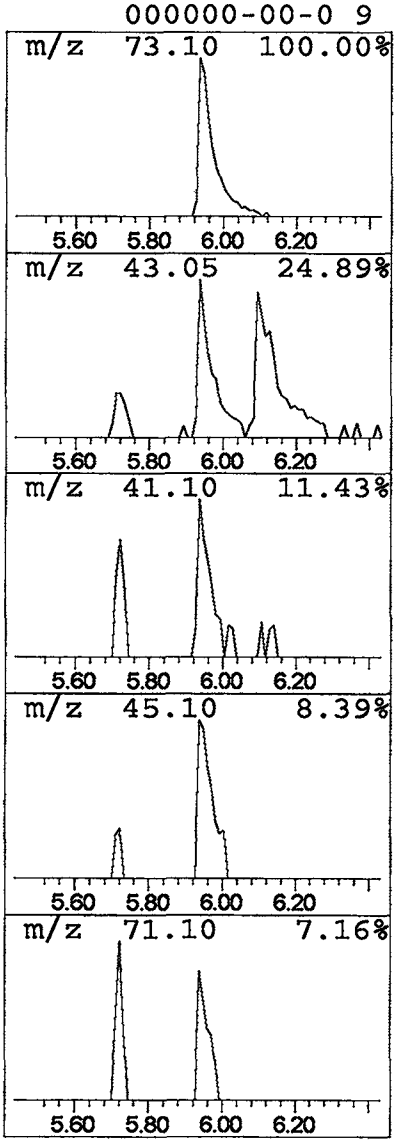
Peak Number 8 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.94	0.31 ug/L	119908	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33
2	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
3	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4	Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	000000-00-0	9





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Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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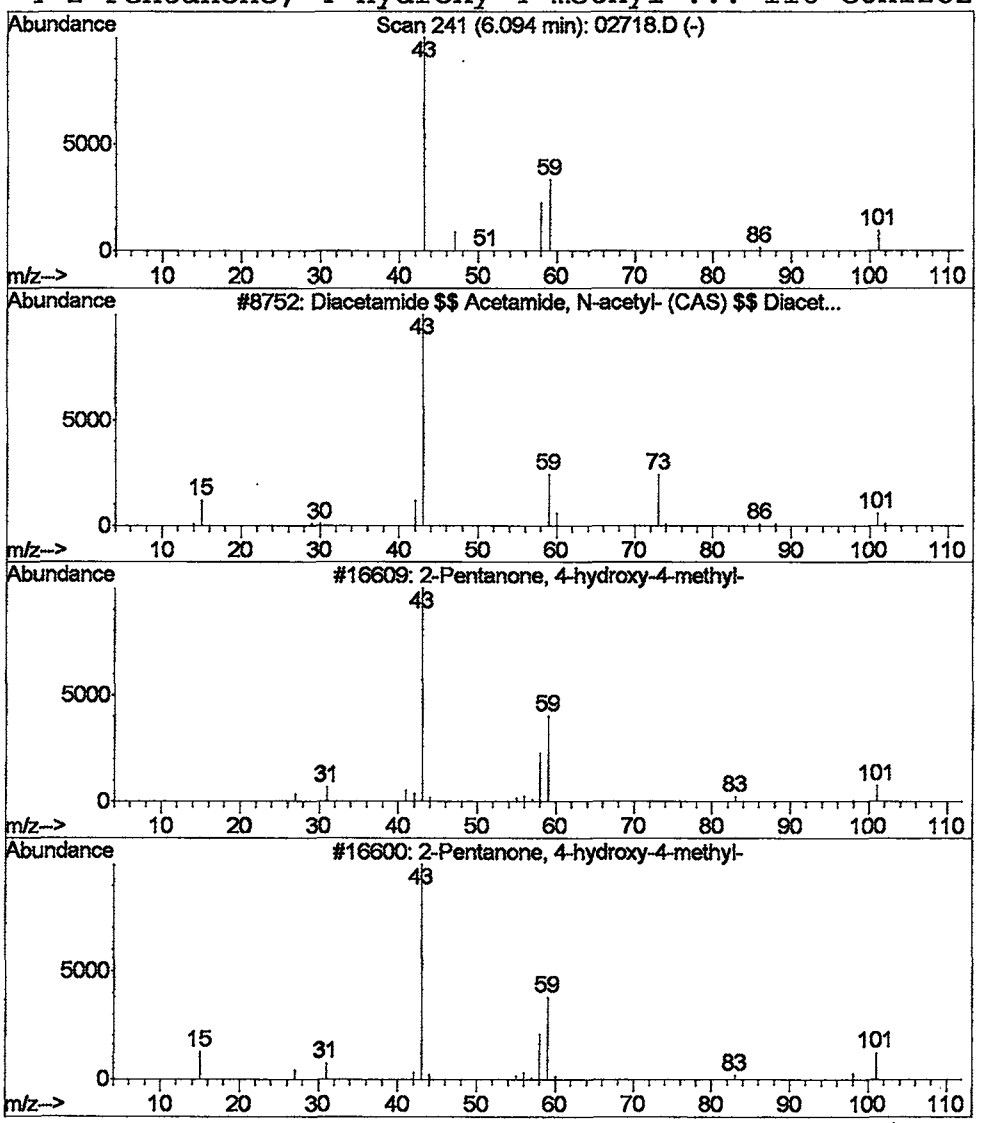
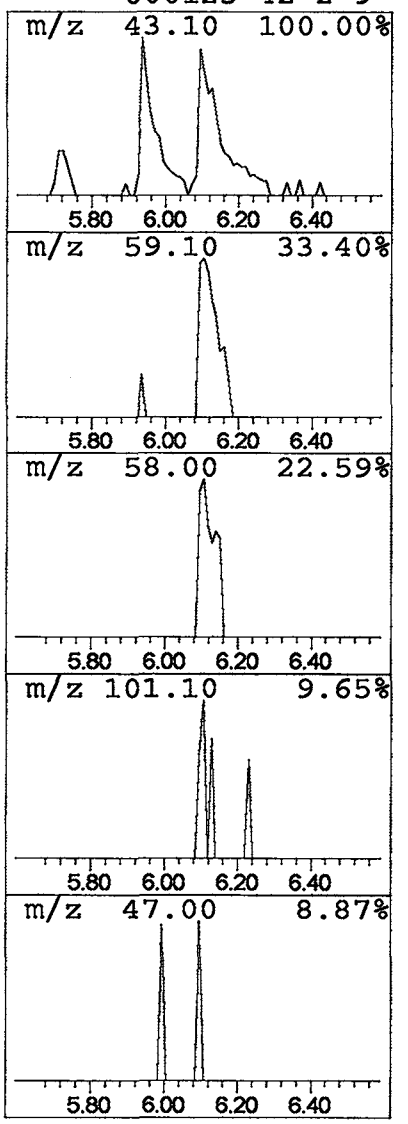
Peak Number 9 Diacetamide $$ Acetamide, N... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.09	0.10 ug/L	38674	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide $$ Acetamide, N-acet...	101	C4H7NO2	000625-77-4	9
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	9





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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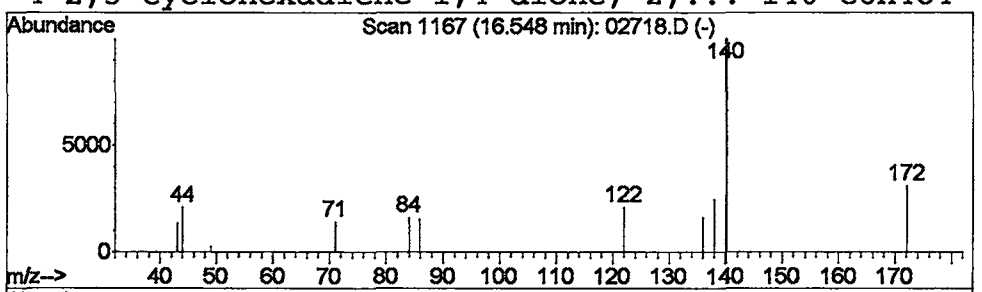
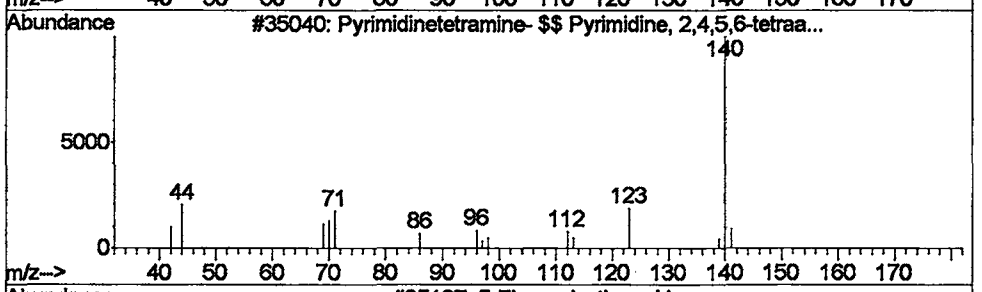
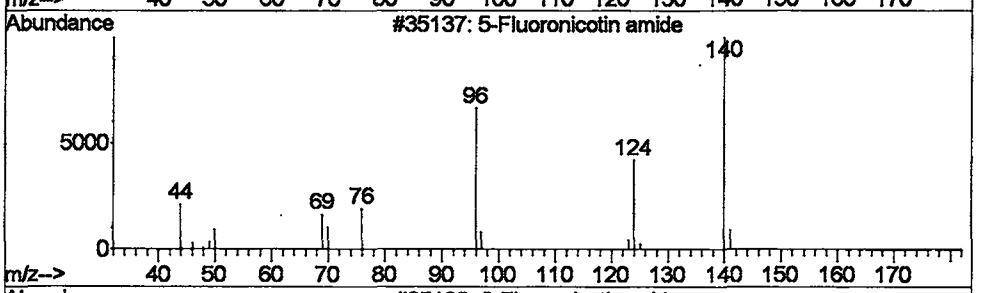
Peak Number 10 Pyrimidinetetramine- $$ Pyr... Concentration Rank 13

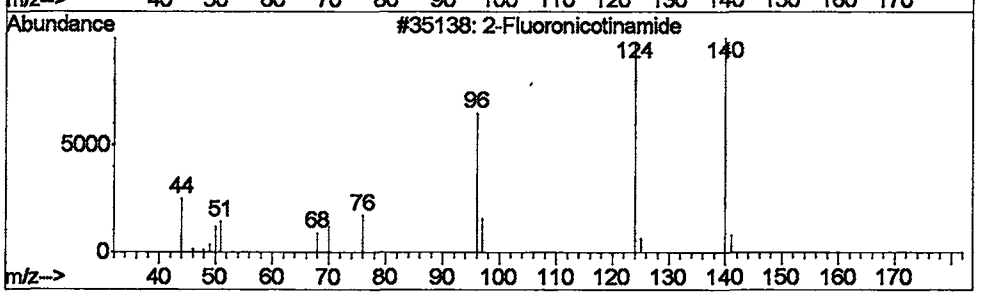
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	0.03 ug/L	20957	Acenaphthene-d10	18.34

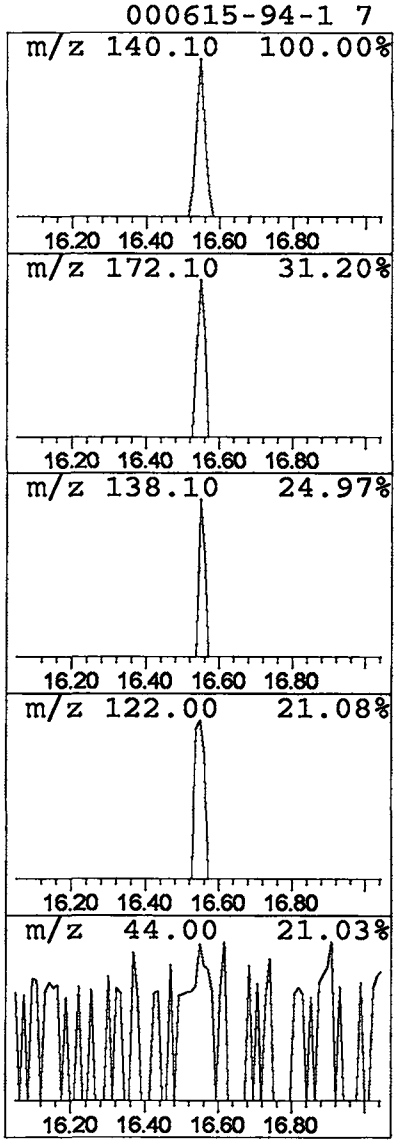
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidinetetramine- $$ Pyrimidi...	140	C4H8N6	001004-74-6	9
2	5-Fluoronicotin amide	140	C6H5FN2O	000000-00-0	9
3	2-Fluoronicotinamide	140	C6H5FN2O	000364-22-7	9
4	2,5-Cyclohexadiene-1,4-dione, 2,...	140	C6H4O4	000615-94-1	7











Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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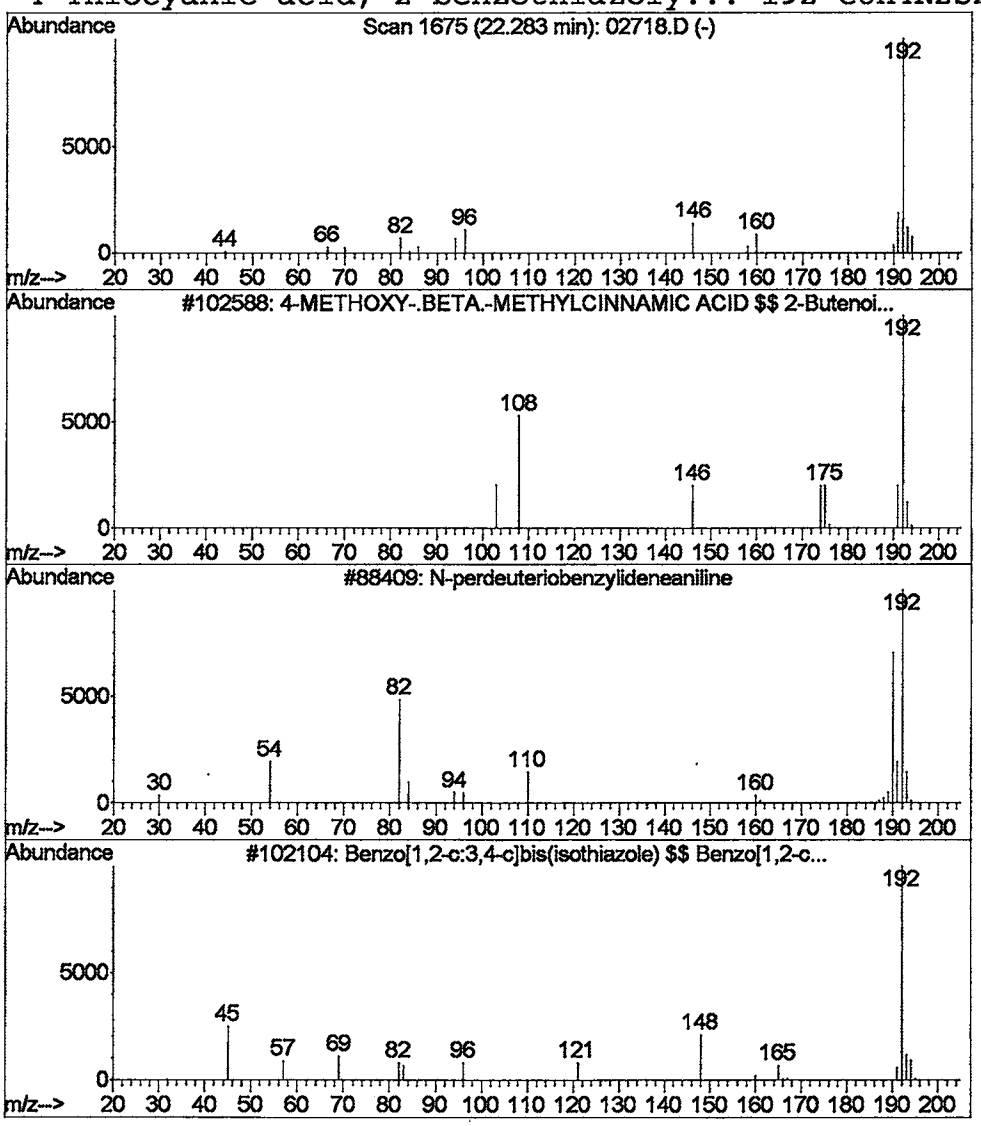
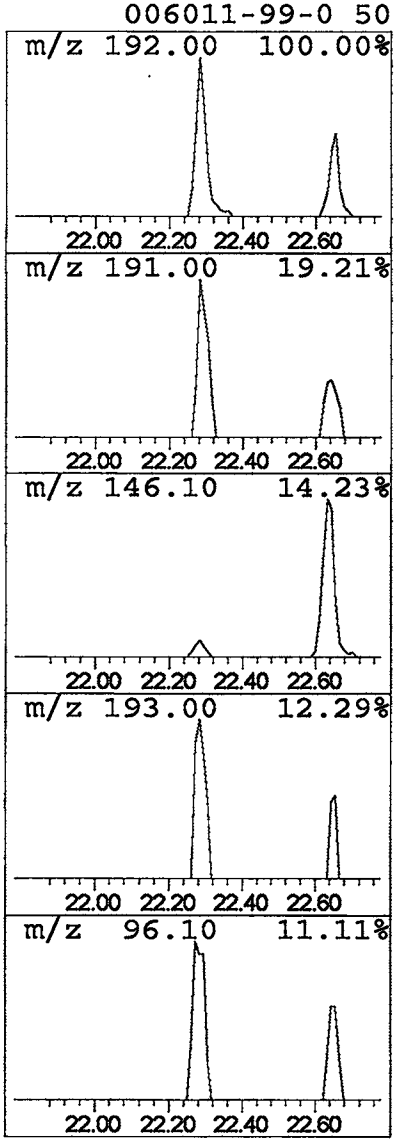
Peak Number 11 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.11 ug/L	70950	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
2	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	64
3	Benzo[1,2-c:3,4-c]bis(isothiazol...	192	C8H4N2S2	074960-05-7	53
4	Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	50





Library Search Compound Report

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Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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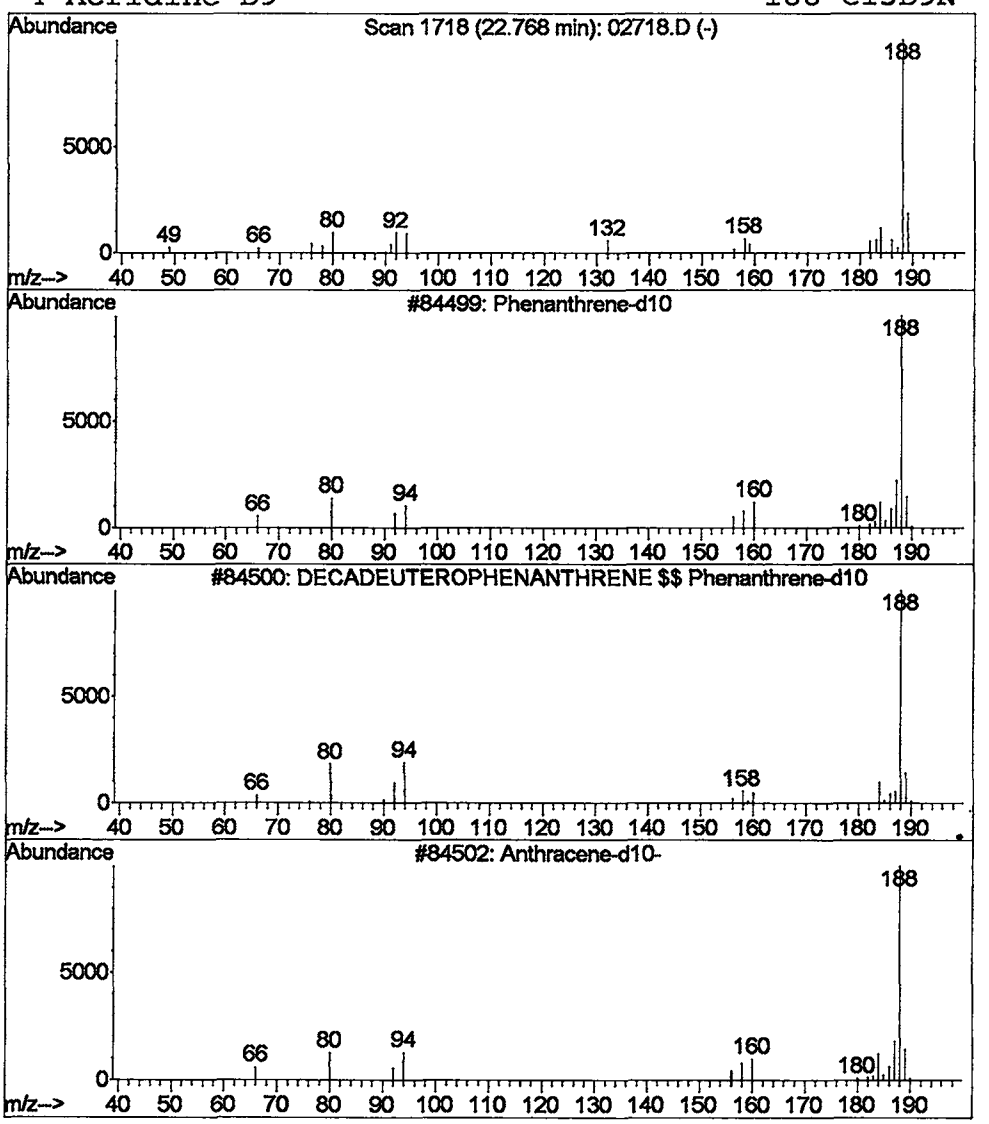
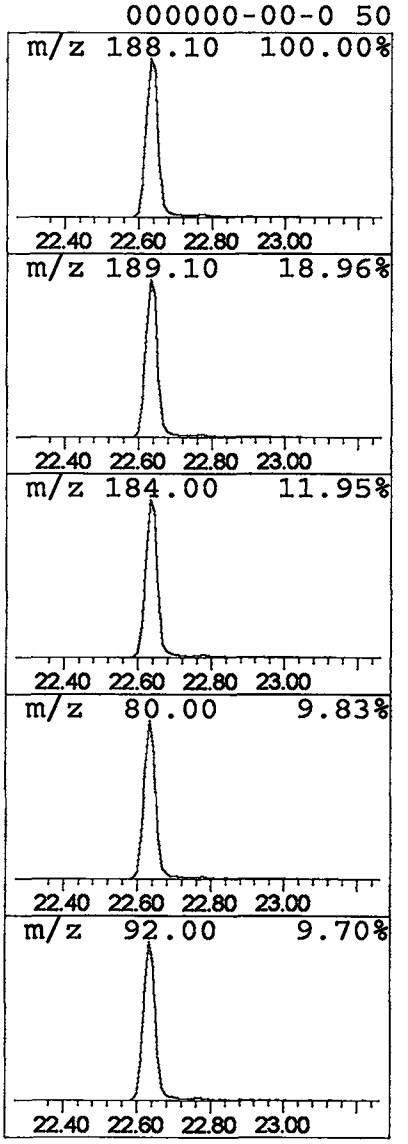
Peak Number 12 Phenanthrene-d10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.44 ug/L	278511	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene-d10	188	C14D10	001517-22-2	86
2	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	86
3	Anthracene-d10-	188	C14D10	001719-06-8	78
4	Acridine-D9	188	C13D9N	000000-00-0	50





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB28\02718.D Vial: 3
Acq On : 28 Feb 2002 4:20 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 28, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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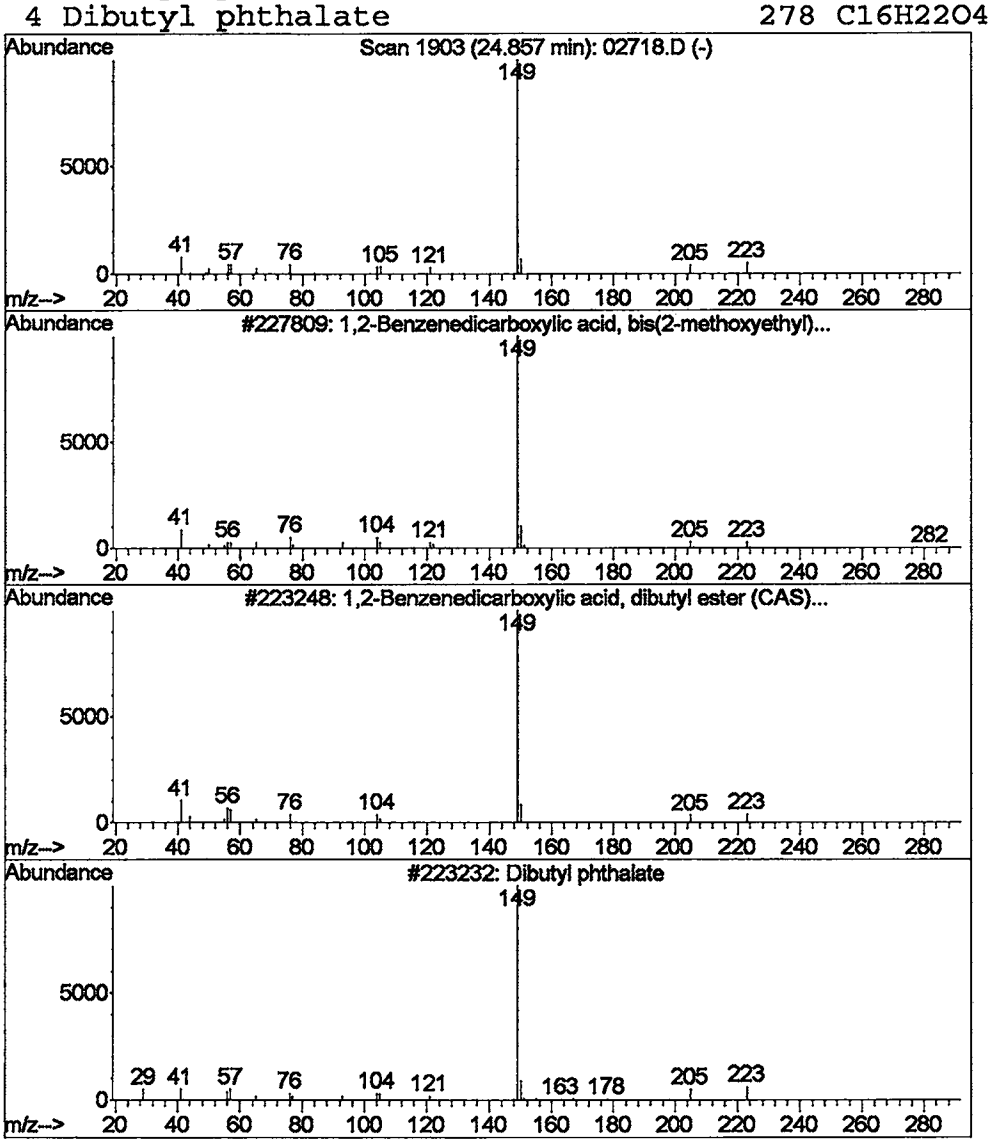
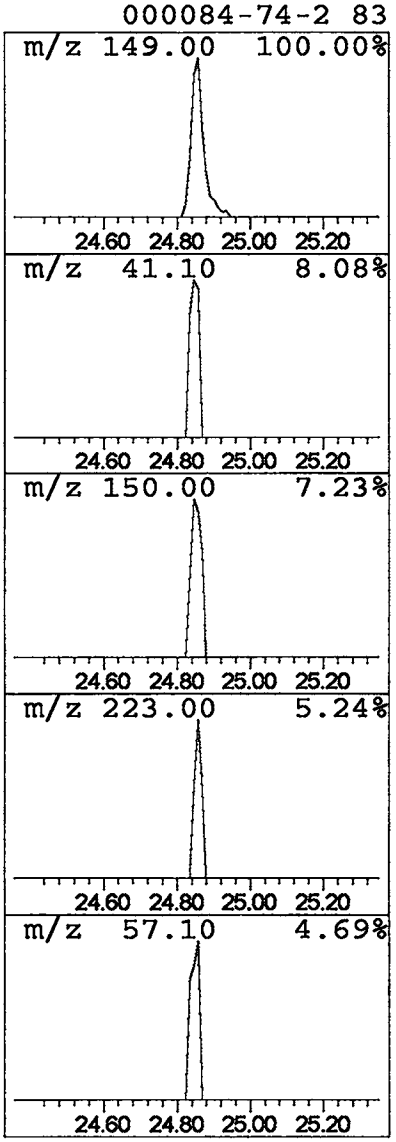
Peak Number 13 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.86	0.11 ug/L	69414	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	282	C14H18O6	000117-82-8	83
2	1,2-Benzenedicarboxylic acid, di...	278	C16H22O4	000084-74-2	83
3	Dibutyl phthalate	278	C16H22O4	000084-74-2	83
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	83





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 28 Feb 2002 4:20 pm
Data File: C:\MSDCHEM\1\5973N\02FEB28\02718.D
Name: 508 scan
Misc: February 28, 2002
Method: C:\MSDCHEM\1\METHODS\METHODS\HP022102.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...	3.62	0.1	ug/L	55421	1	9.72	7695780	20.0
Propane, 1,1-dime...	3.93	0.1	ug/L	31835	1	9.72	7695780	20.0
4-O-Methyl-d-arab...	4.25	0.2	ug/L	62658	1	9.72	7695780	20.0
1,3,5-Cycloheptat...	4.38	0.1	ug/L	22285	1	9.72	7695780	20.0
Butanoic acid, 2-...	4.64	0.1	ug/L	22267	1	9.72	7695780	20.0
Cyclopentanone	4.88	0.1	ug/L	30173	1	9.72	7695780	20.0
Butenol, methyl-	5.02	0.1	ug/L	25247	1	9.72	7695780	20.0
3-(CYCLOHEX-3'-EN...	5.94	0.3	ug/L	119908	1	9.72	7695780	20.0
Diacetamide $$ Ac...	6.09	0.1	ug/L	38674	1	9.72	7695780	20.0
Pyrimidinetetrami...	16.55	0.0	ug/L	20957	3	18.34	12089100	20.0
4-METHOXY-.BETA.-...	22.28	0.1	ug/L	70950	4	22.63	12786900	20.0
Phenanthrene-d10	22.77	0.4	ug/L	278511	4	22.63	12786900	20.0
1,2-Benzenedicarb...	24.86	0.1	ug/L	69414	4	22.63	12786900	20.0