User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/18/2002 Time: 09:33:59

Sample: AE00327
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/18/02 09:32 Ended: 1/18/02 09:32 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		100		5.0

87/100 ,26 mg/L

1/6/02
4 AC out
3
FB 329 - closed

CAS ?

general perfume antiseptic

Comments for Sample AE00327 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-18-2002 Time: 09:42:21

The GCMS scan, from 35 to 550 amu, reveals the possible presence of alpha-Terpineol at an estimated level of 0.26 ug/L, and with a fit of 87 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\00327.D Vial: 3
Acq On : 10 Jan 2002 2:00 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 10:13:43 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

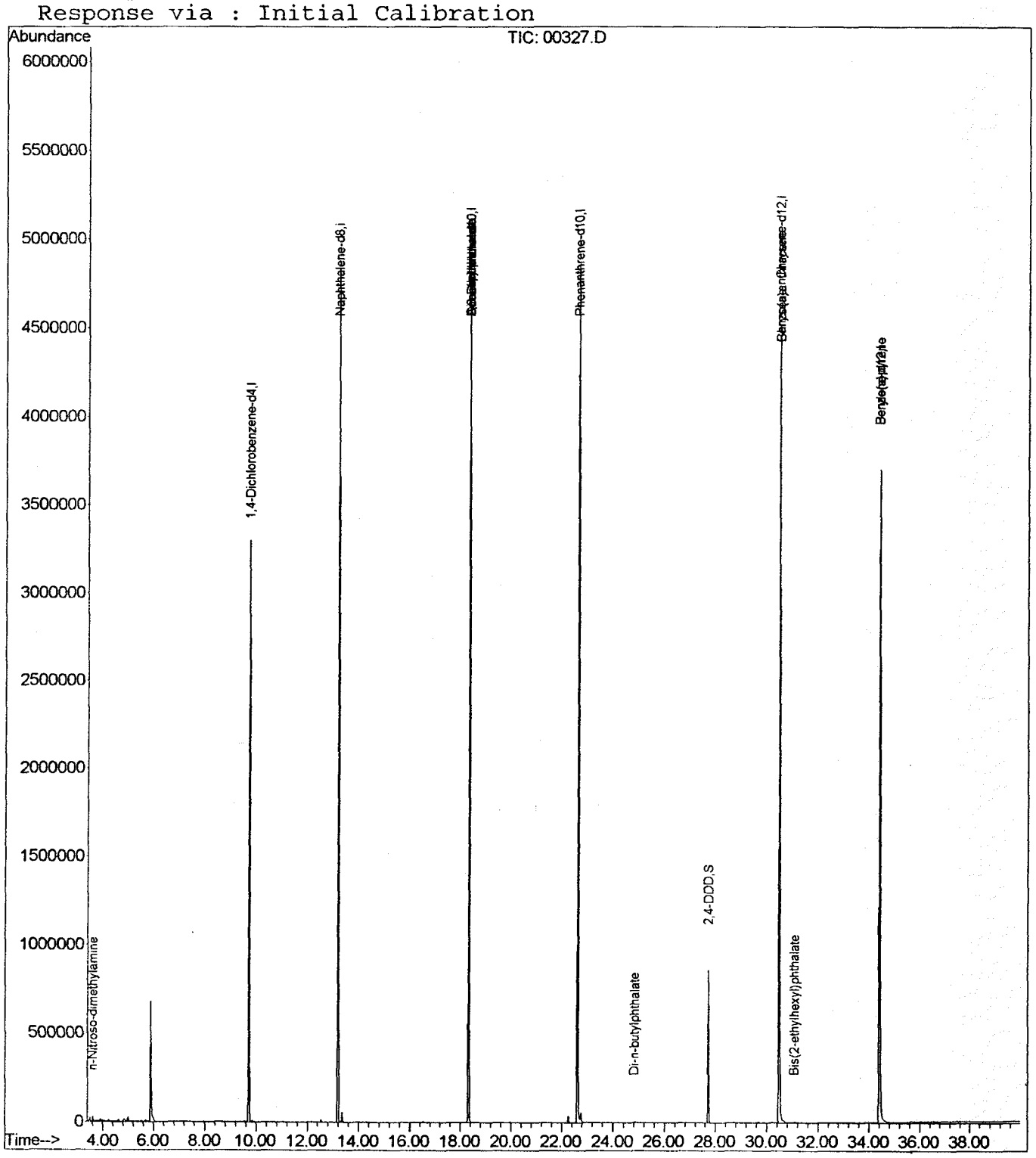
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.72	152	1133419	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4714864	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2417708	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	4040255	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3699150	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2768086	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	319609	5.00	ug/L	0.00
Spiked Amount 5.000			Recovery = 100.00%			
Target Compounds						Qvalue
2) n-Nitroso-dimethylamine	3.61	74	10676	0.22	ug/L #	13
20) Dimethylphthalate	18.34	163	389565	2.44	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	311156	9.99	ug/L #	17
35) Di-n-butylphthalate	24.85	149	8572	0.03	ug/L #	76
41) Benzo(a)anthracene	30.50	228	10288	0.05	ug/L #	55
42) Bis(2-ethylhexyl)phthalate	31.11	149	6725	0.58	ug/L	100
43) Chrysene	30.50	228	10288	0.05	ug/L #	52
48) Benzo(a)pyrene	34.42	252	9991	0.06	ug/L #	1

(#) = qualifier out of range (m) = manual integration
00327.D SCAN508.M Fri Jan 11 10:18:03 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN10\00327.D Vial: 3
Acq On : 10 Jan 2002 2:00 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 10:13 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\00327.D Vial: 3
Acq On : 10 Jan 2002 2:00 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

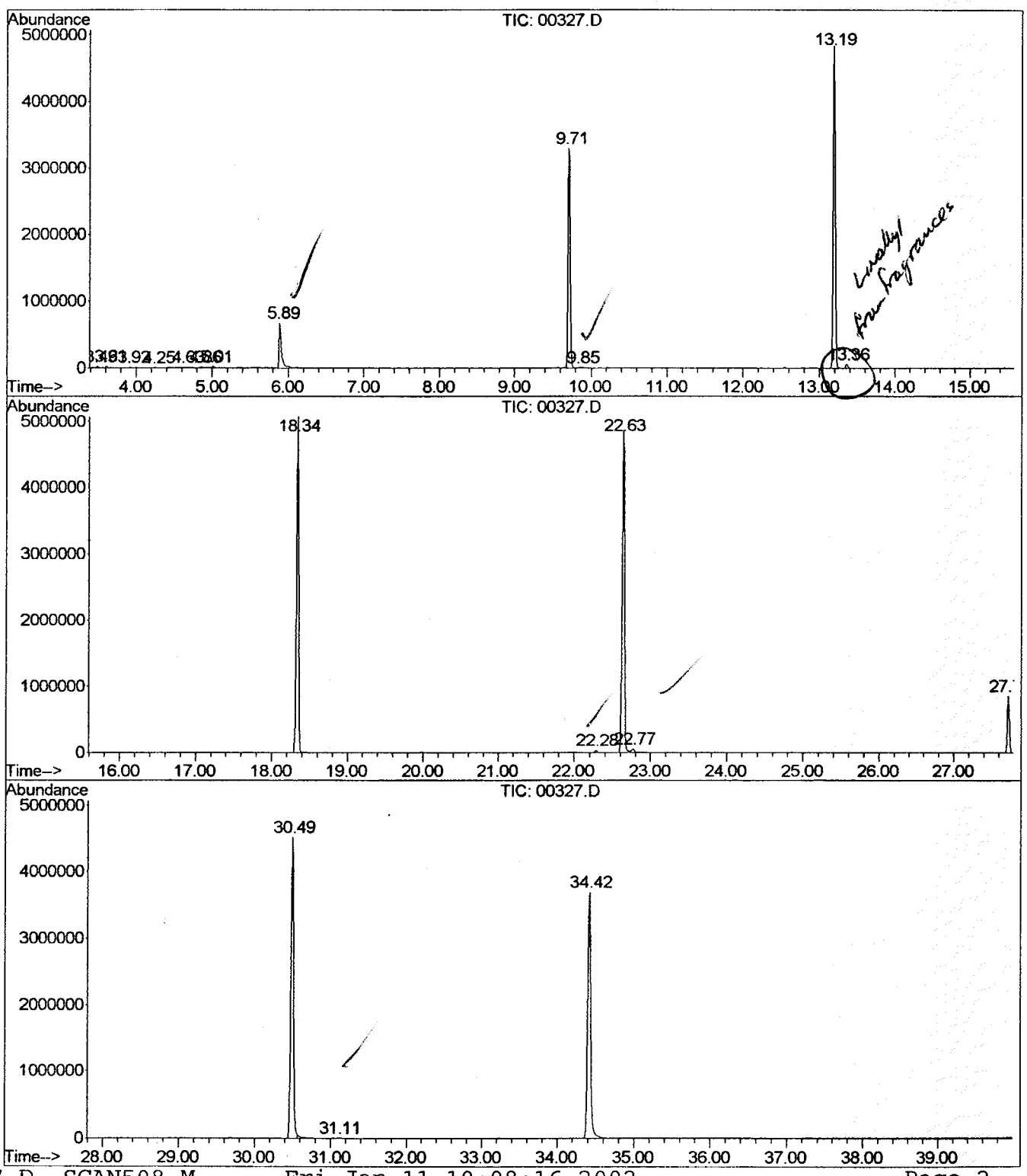
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.488	7	10	13	rBV	22180	35136	0.32%	0.059%
2	3.614	19	21	25	rBV	26656	45803	0.42%	0.076%
3	3.922	45	48	53	rVB	10918	21411	0.20%	0.036%
4	4.253	71	77	83	rVB6	8996	23612	0.22%	0.039%
5	4.630	107	110	123	rVB5	13184	38009	0.35%	0.063%
6	4.858	123	130	137	rBV3	12923	48568	0.45%	0.081%
7	5.006	141	143	151	rVB	25201	42608	0.39%	0.071%
8	5.886	217	220	243	rVB	676077	1402255	12.94%	2.341%
9	9.710	551	555	561	rVV	3295182	6468147	59.68%	10.800%
10	9.847	561	567	585	rVB6	9159	44552	0.41%	0.074%
11	13.192	855	860	865	rBV	4830066	9101922	83.99%	15.197%
12	13.364	869	875	881	rVB2	58805	118941	1.10%	0.199%
13	18.341	1305	1311	1315	rBV	5068758	9820142	90.61%	16.396%
14	22.280	1651	1656	1661	rBV	39044	76133	0.70%	0.127%
15	22.634	1681	1687	1693	rBV2	4858849	10637784	98.16%	17.761%
16	22.771	1695	1699	1713	rVB	57128	160863	1.48%	0.269%
17	27.726	2127	2133	2139	rVV	860467	1544322	14.25%	2.578%
18	30.489	2369	2375	2381	rBV2	4520485	10837343	100.00%	18.095%
19	31.105	2425	2429	2435	rVB4	8849	27009	0.25%	0.045%
20	34.416	2713	2719	2751	rBV	3694969	9398263	86.72%	15.692%

Sum of corrected areas: 59892823

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN10\00327.D
Operator :
Acquired : 10 Jan 2002 2:00 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan ext 1/8
Misc Info : January 10, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00327.D Vial: 3
Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

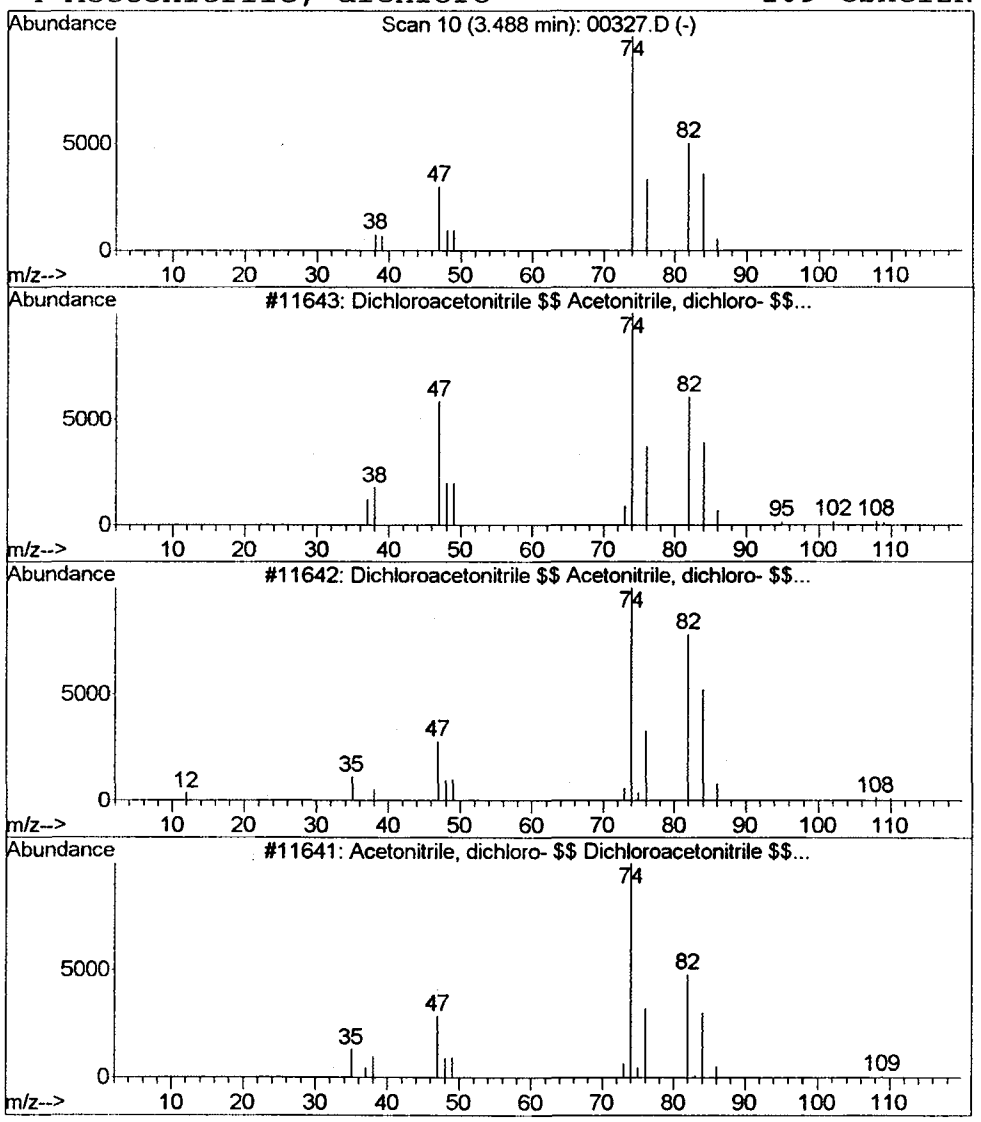
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

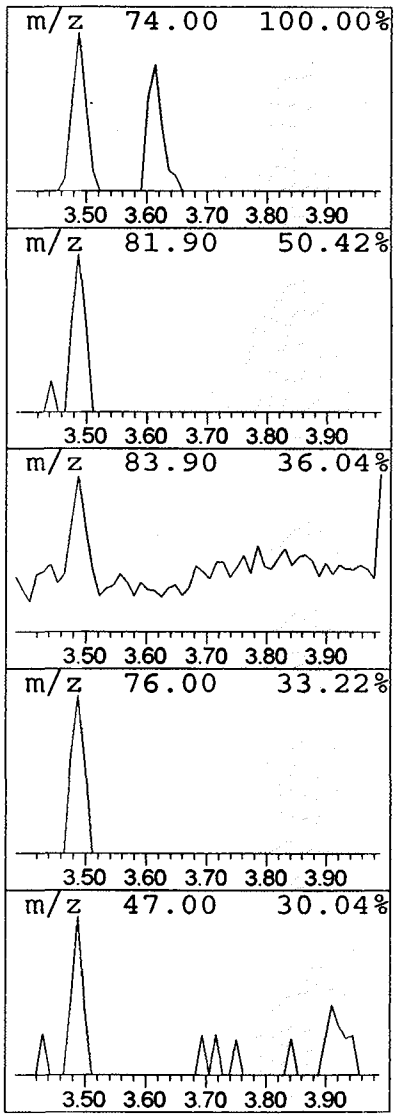
****

Peak Number 1 Dichloroacetonitrile $$ Ace... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	0.11 ug/L	35136	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetonitrile $$ Acetonit...	109	C2HCl2N	003018-12-0	83
2	Dichloroacetonitrile $$ Acetonit...	109	C2HCl2N	003018-12-0	83
3	Acetonitrile, dichloro- $$ Dichl...	109	C2HCl2N	003018-12-0	83
4	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	56





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

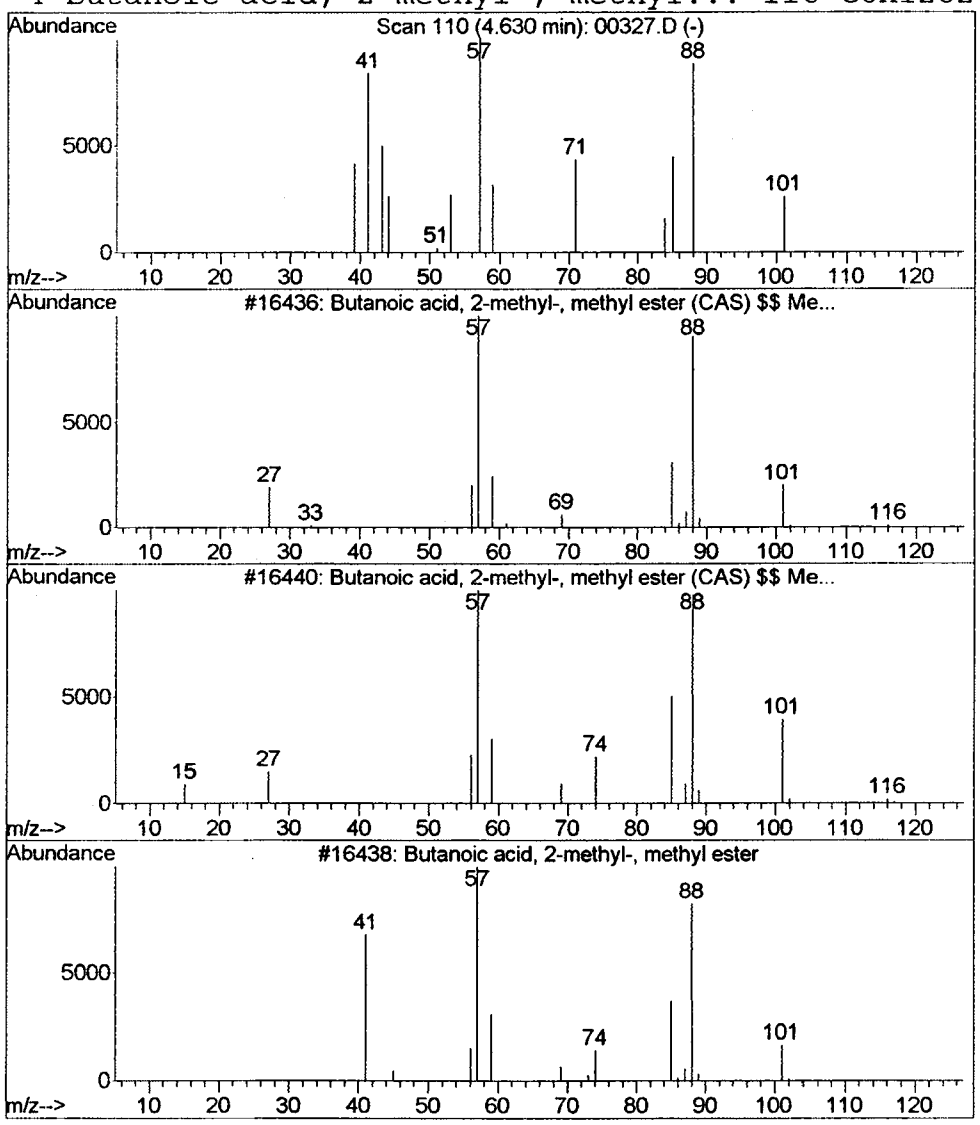
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

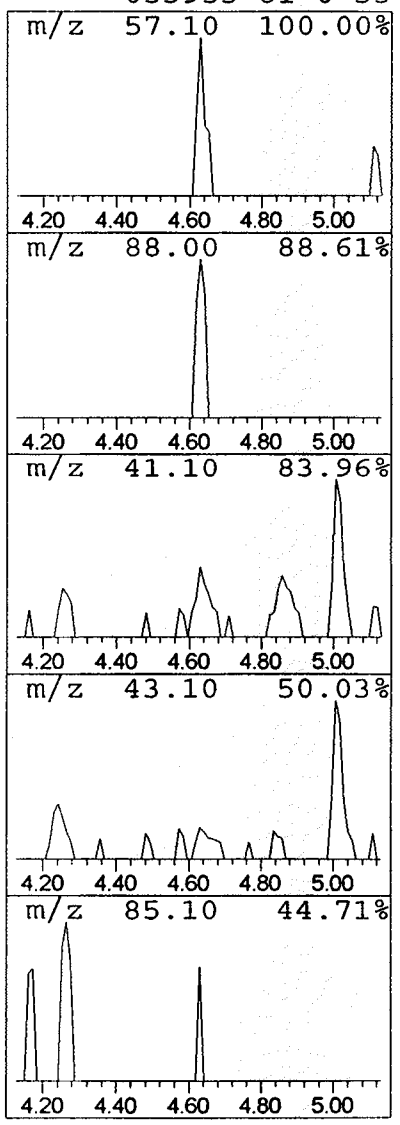
****

Peak Number 2 Butanoic acid, 2-methyl-, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	0.12 ug/L	38009	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	53
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	53
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	42
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	053955-81-0	33





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 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

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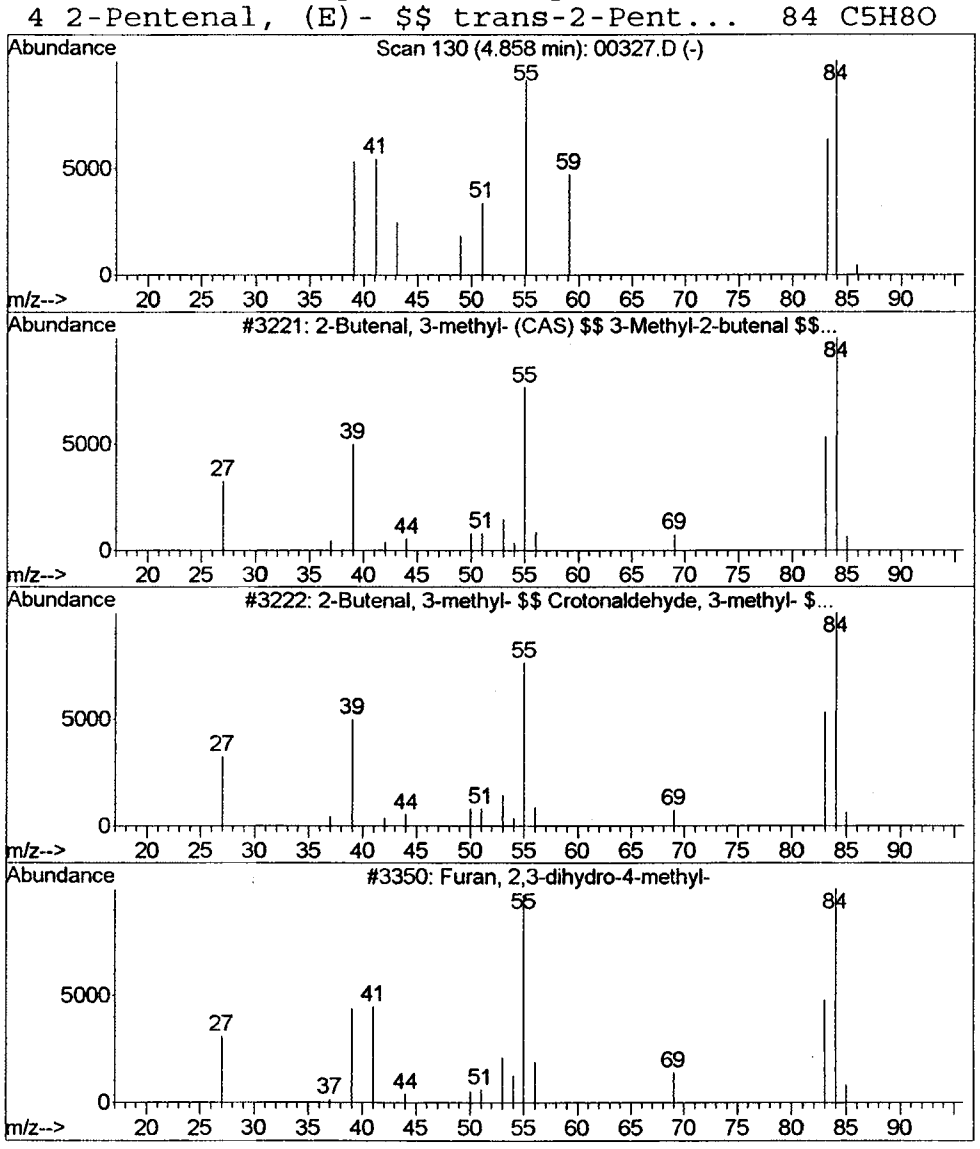
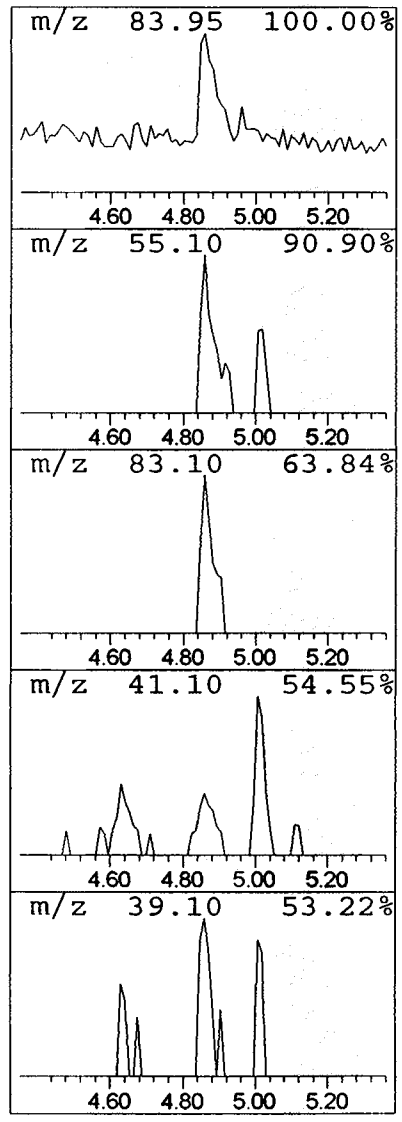
Peak Number 3 2-Butenal, 3-methyl- (CAS) ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	0.15 ug/L	48568	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl- (CAS) $$ 3-...	84	C5H8O	000107-86-8	58
2	2-Butenal, 3-methyl- $$ Crotonal...	84	C5H8O	000107-86-8	58
3	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	53
4	2-Pentenal, (E)- $$ trans-2-Pent...	84	C5H8O	001576-87-0	53





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

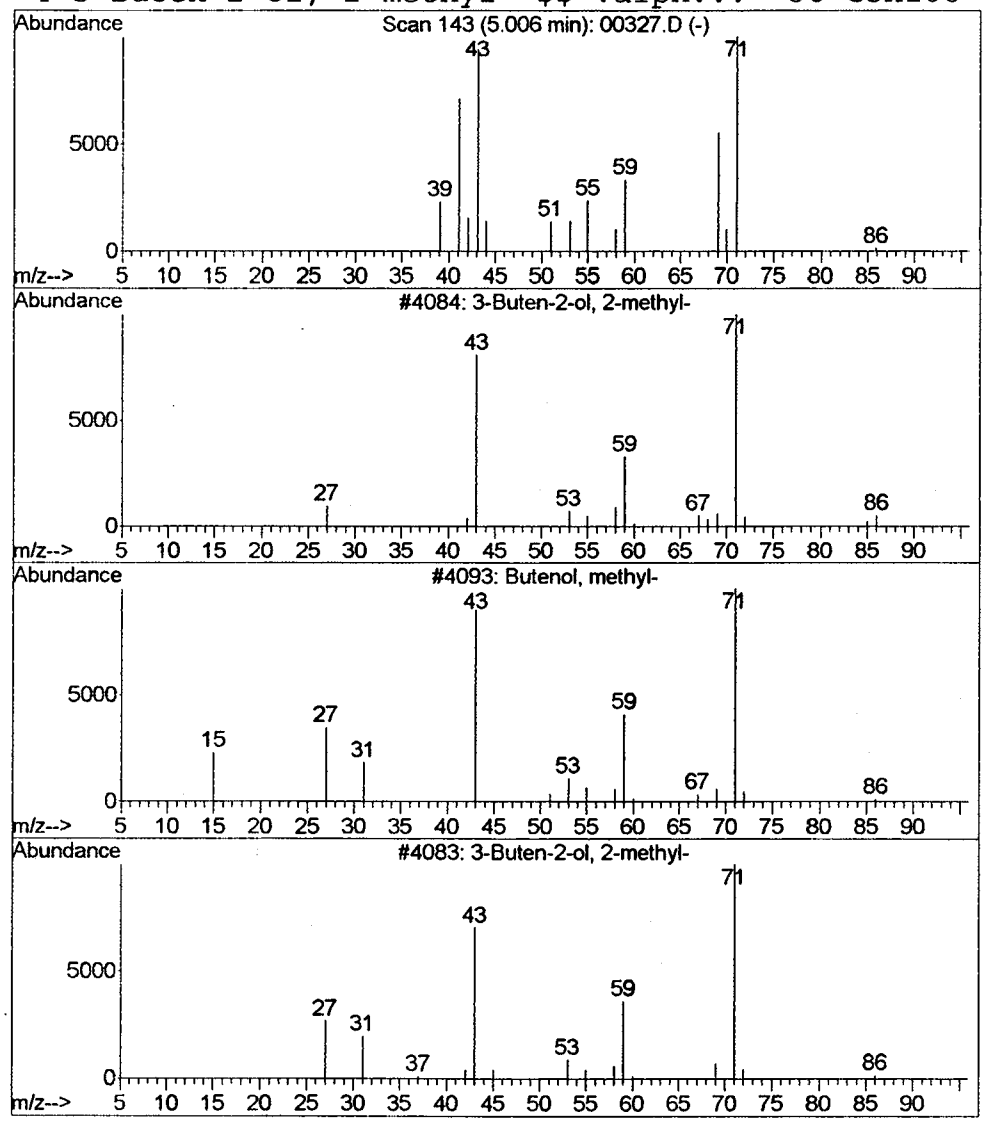
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

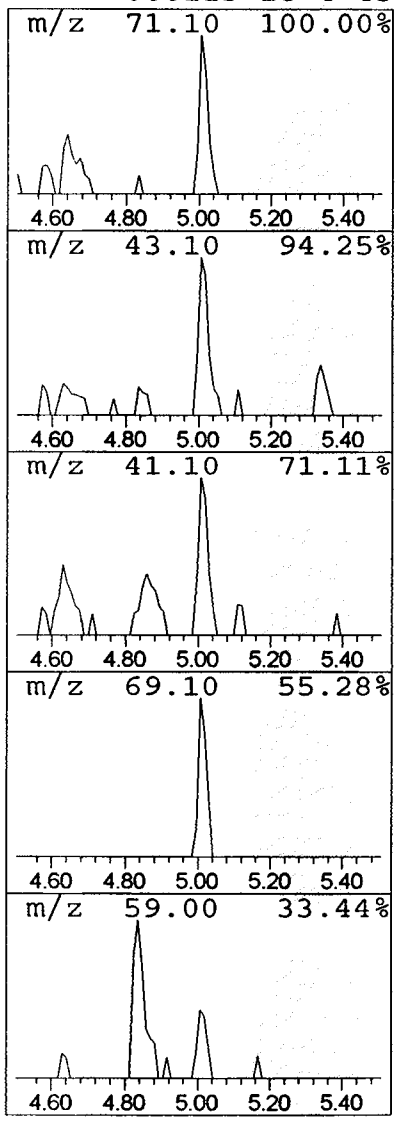
****

Peak Number 4 3-Buten-2-ol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.13 ug/L	42608	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2	Butenol, methyl-	86	C5H10O	060766-00-9	64
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
4	3-Buten-2-ol, 2-methyl- $$ .alph...	86	C5H10O	000115-18-4	45





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

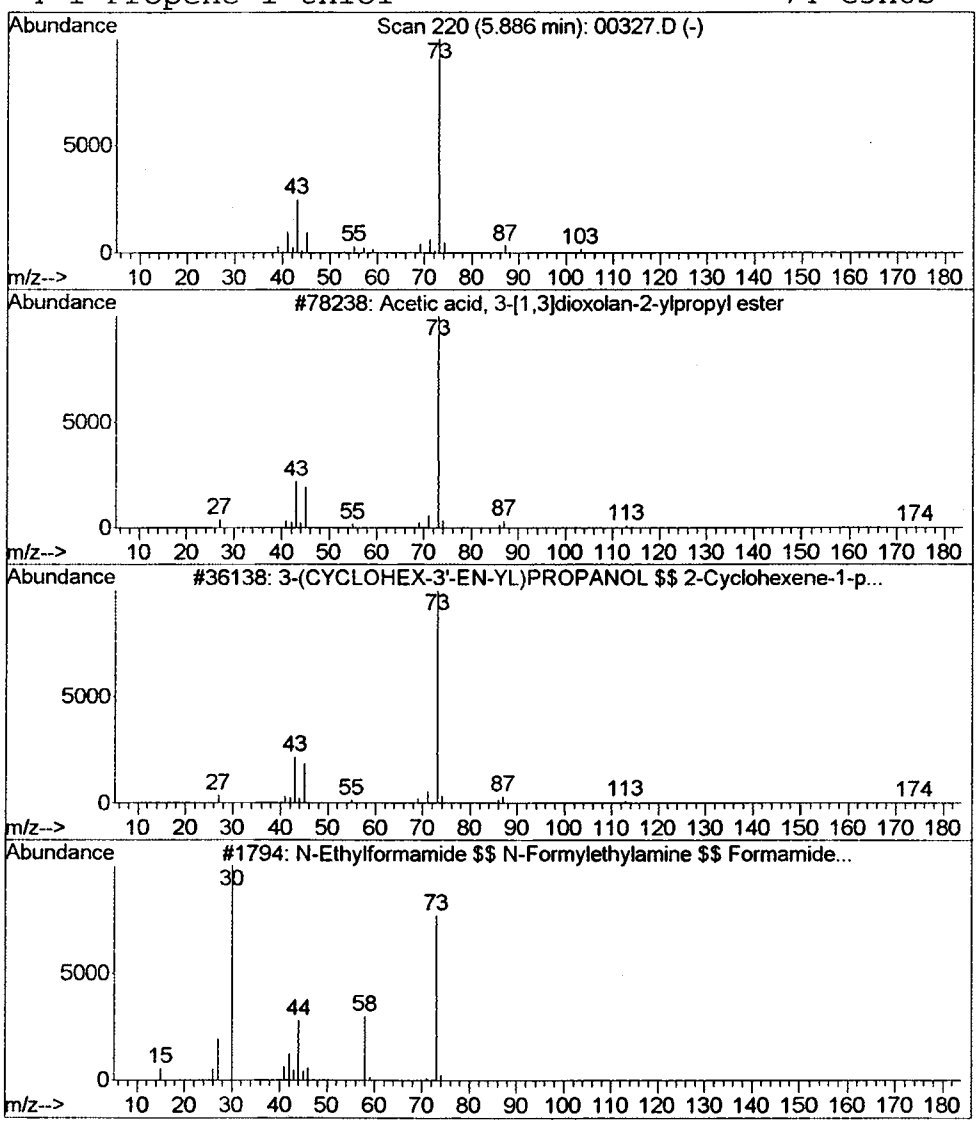
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

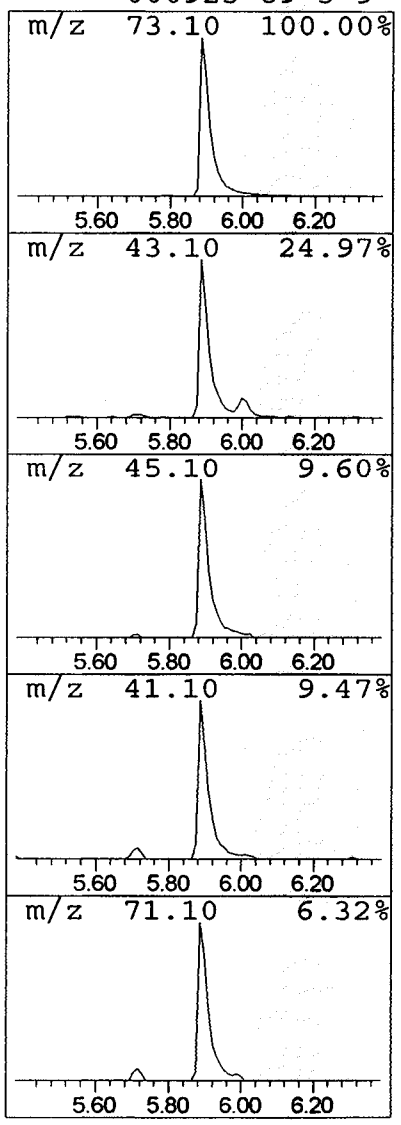
****

Peak Number 5 Acetic acid, 3-[1,3]dioxola... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.34 ug/L	1402260	1,4-Dichlorobenzene-d4	9.72

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	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN10\00327.D Vial: 3
Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

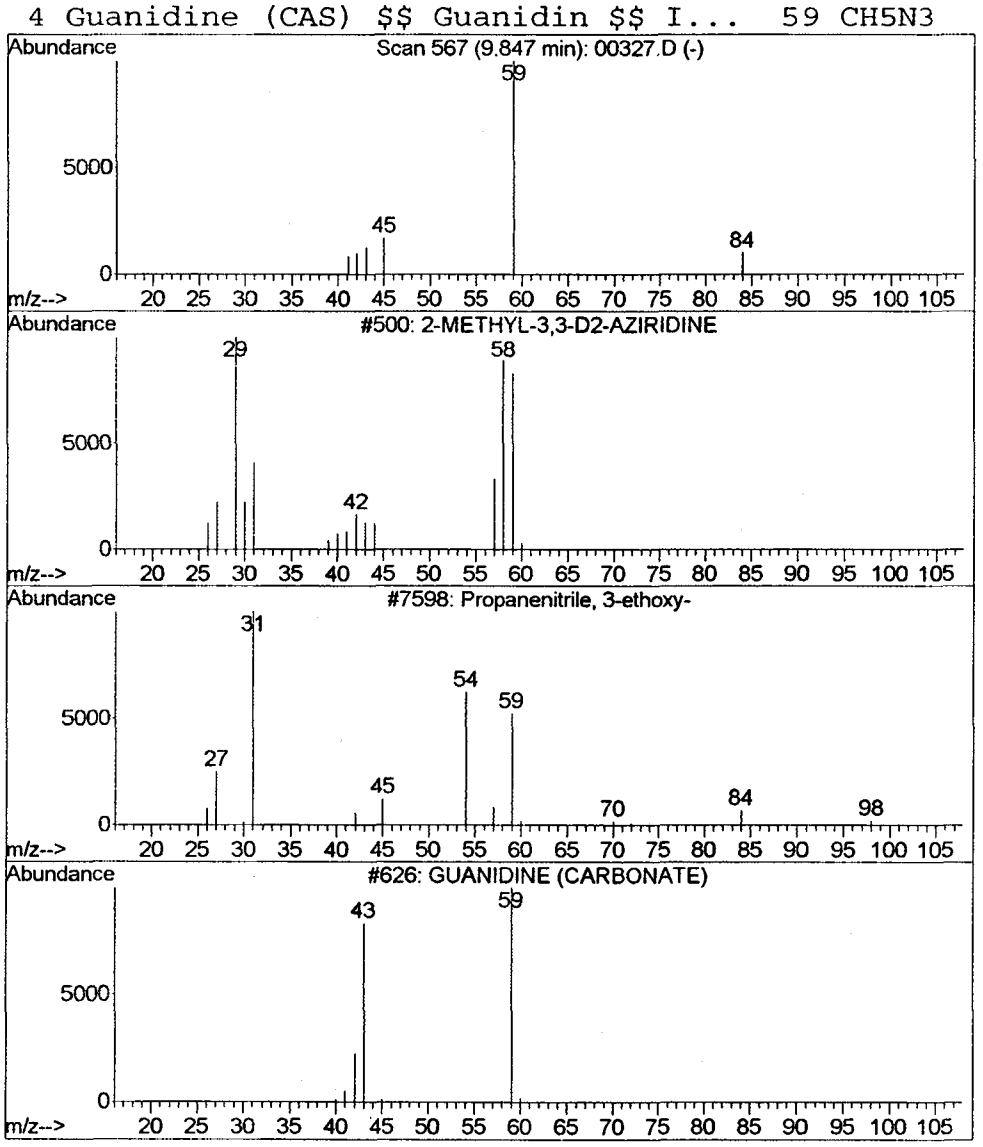
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

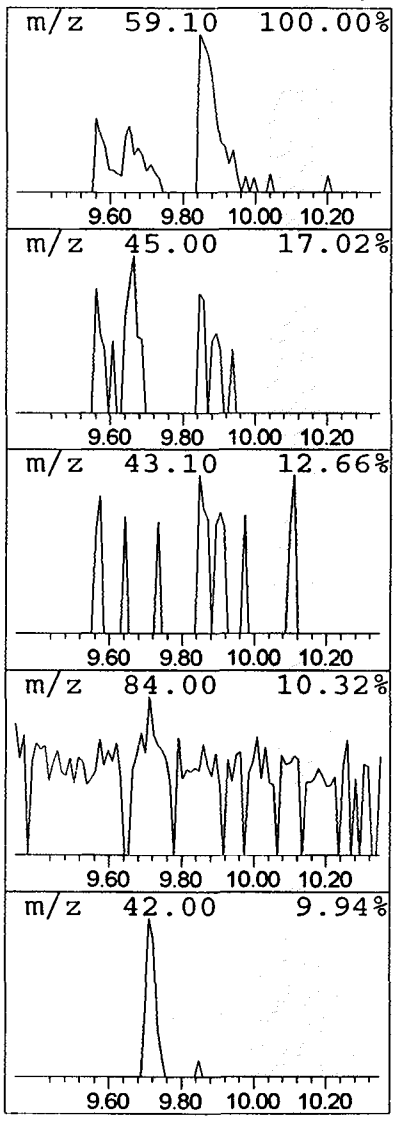
****

Peak Number 6 2-METHYL-3,3-D2-AZIRIDINE Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	0.14 ug/L	44552	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-METHYL-3,3-D2-AZIRIDINE	59	C3H5D2N	030691-55-5	4
2	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	4
3	GUANIDINE (CARBONATE)	59	CH5N3	000000-00-0	3
4	Guanidine (CAS) $$ Guanidin $$ I...	59	CH5N3	000113-00-8	3





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

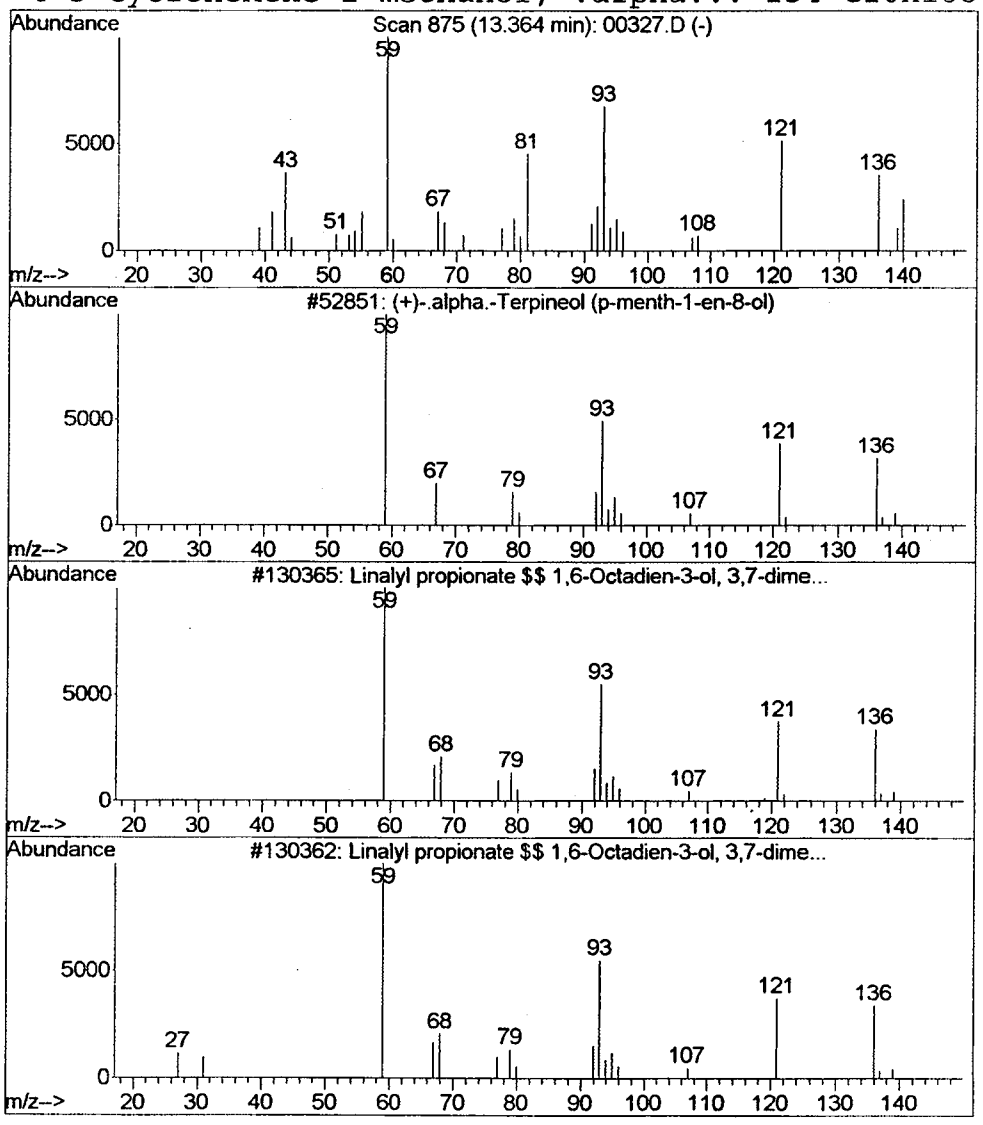
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

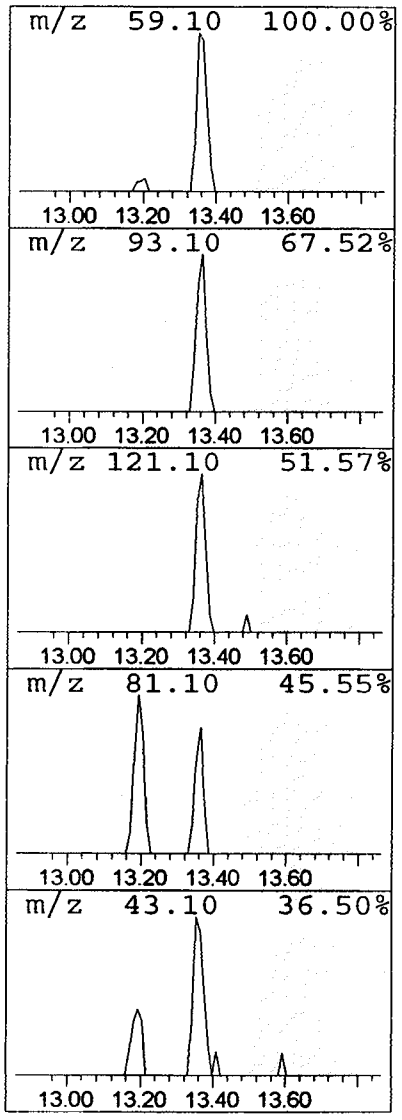
****

Peak Number 7 (+)-.alpha.-Terpineol (p-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	0.26 ug/L	118941	Naphthalene-d8	13.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-.alpha.-Terpineol (p-menth-1...	154	C10H18O	000000-00-0	87
2	Linalyl propionate $$ 1,6-Octadi...	210	C13H22O2	000144-39-8	87
3	Linalyl propionate $$ 1,6-Octadi...	210	C13H22O2	000144-39-8	87
4	3-Cyclohexene-1-methanol, .alpha...	154	C10H18O	010482-56-1	86





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
Sample : 508 scan ext 1/8 Inst : Instrumen
Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

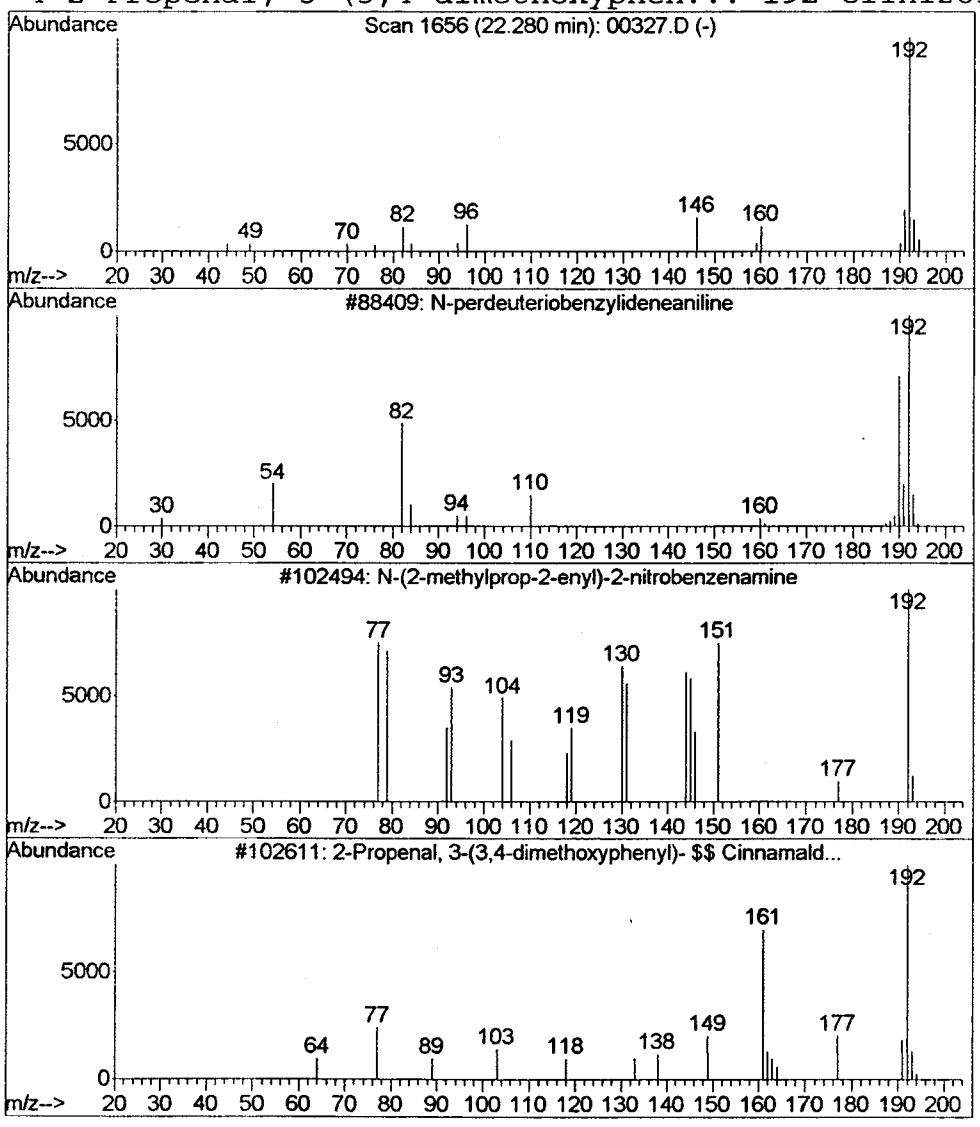
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

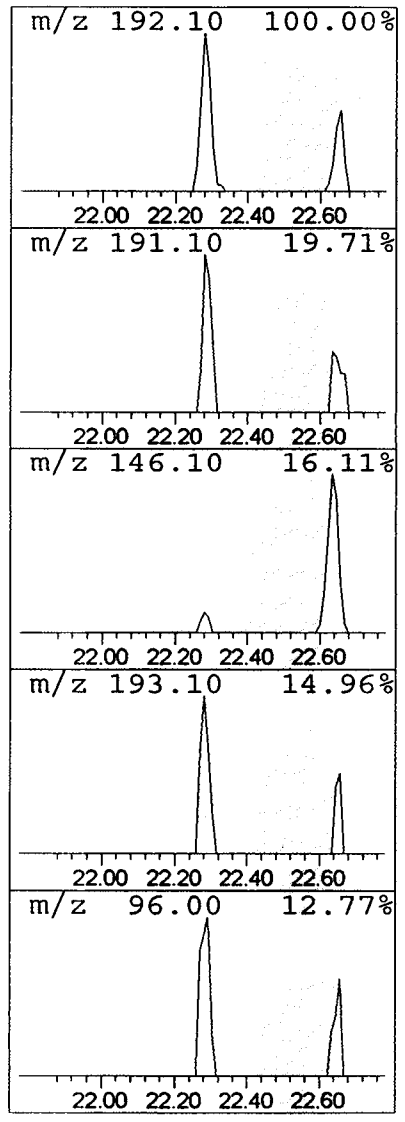
****

Peak Number 8 N-perdeuteriobenzylideneani... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.14 ug/L	76133	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	53
2	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	46
3	2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	45
4	2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	45





Library Search Compound Report

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Acq On : 10 Jan 2002 2:00 pm Operator:
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Misc : January 10, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

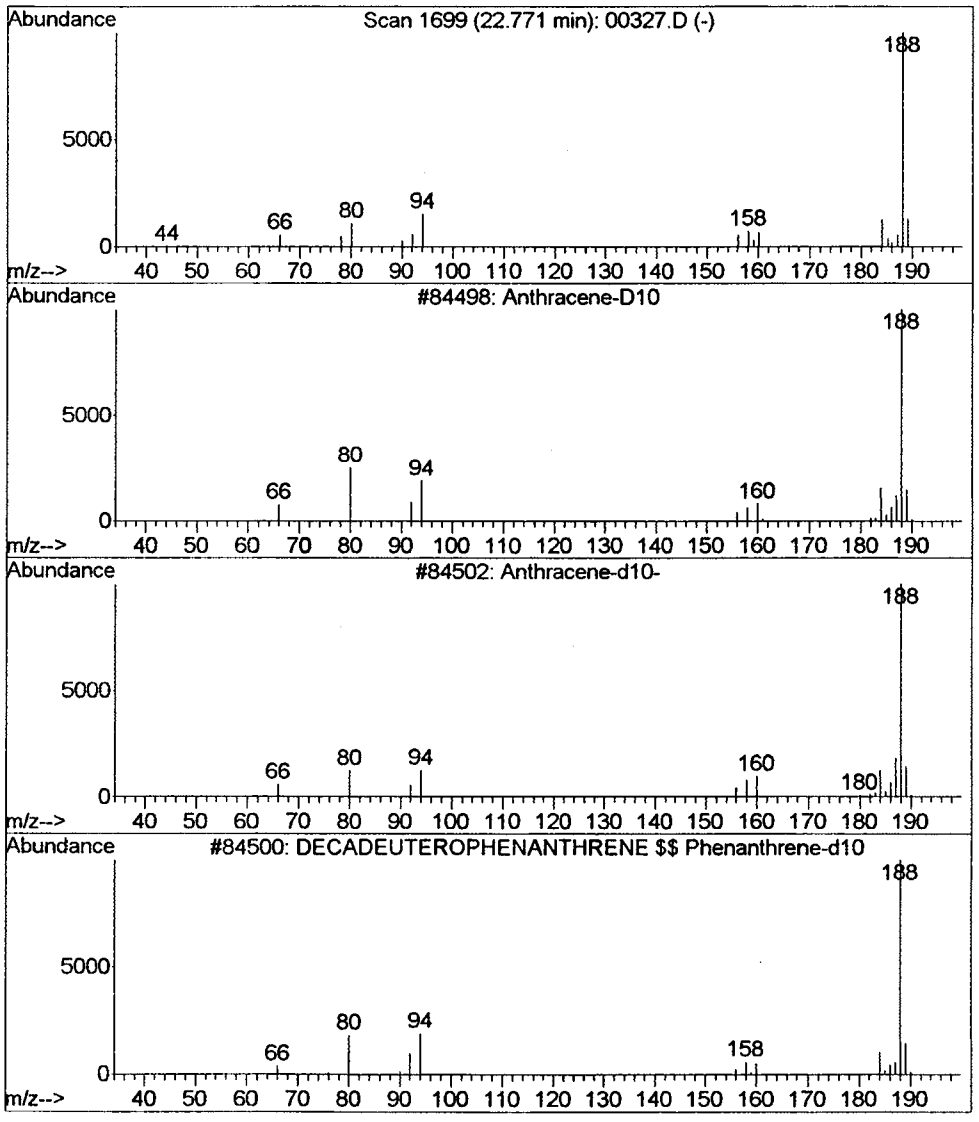
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

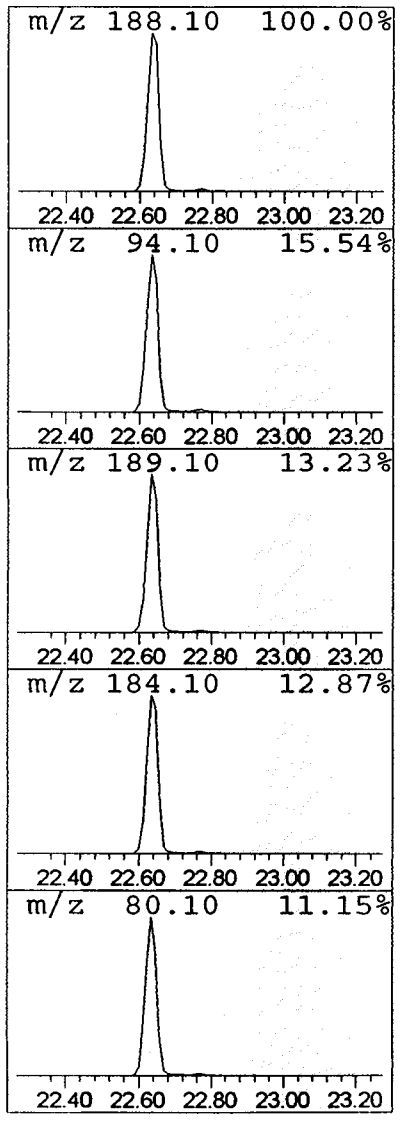
****

Peak Number 9 Anthracene-D10 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.30 ug/L	160863	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene-D10	188	C14D10	000000-00-0	91
2	Anthracene-d10-	188	C14D10	001719-06-8	90
3	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	90
4	Phenanthrene-d10	188	C14D10	001517-22-2	86





Tentatively Identified Compound (LSC) summary

)perator ID: Date Acquired: 10 Jan 2002 2:00 pm
)ata File: C:\MSDCHEM\1\5973N\02JAN10\00327.D
lame: 508 scan ext 1/8
lisc: January 10, 2002
lethod: C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
:itle: 508 scan method
.ibrary Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--- #	RT	Resp	Conc
~~)ichloroacetonitr...~~	3.49	0.1	ug/L	35136	1	9.72	6468150	20.0
~~)utanoic acid, 2-...~~	4.63	0.1	ug/L	38009	1	9.72	6468150	20.0
~~:-Butenal, 3-meth...~~	4.86	0.2	ug/L	48568	1	9.72	6468150	20.0
~~:-Buten-2-ol, 2-m...~~	5.01	0.1	ug/L	42608	1	9.72	6468150	20.0
~~xcetic acid, 3-[1...~~	5.89	4.3	ug/L	1402260	1	9.72	6468150	20.0
~~:-METHYL-3,3-D2-A...~~	9.85	0.1	ug/L	44552	1	9.72	6468150	20.0
(+)-.alpha.-Terpi...	13.36	0.3	ug/L	118941	2	13.19	9101920	20.0
~~D-perdeuteriobenz...~~	22.28	0.1	ug/L	76133	4	22.63	10637800	20.0
~~anthracene-D10~~	22.77	0.3	ug/L	160863	4	22.63	10637800	20.0

possible