User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/28/2002 Time: 15:25:44

Sample: AD31631
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/28/02 15:25 Ended: 1/28/02 15:25 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		89		5.0

Comments for Sample AD31631 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-28-2002 Time: 15:26:05

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.
The recoveries for 2 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 22 08:30:05 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

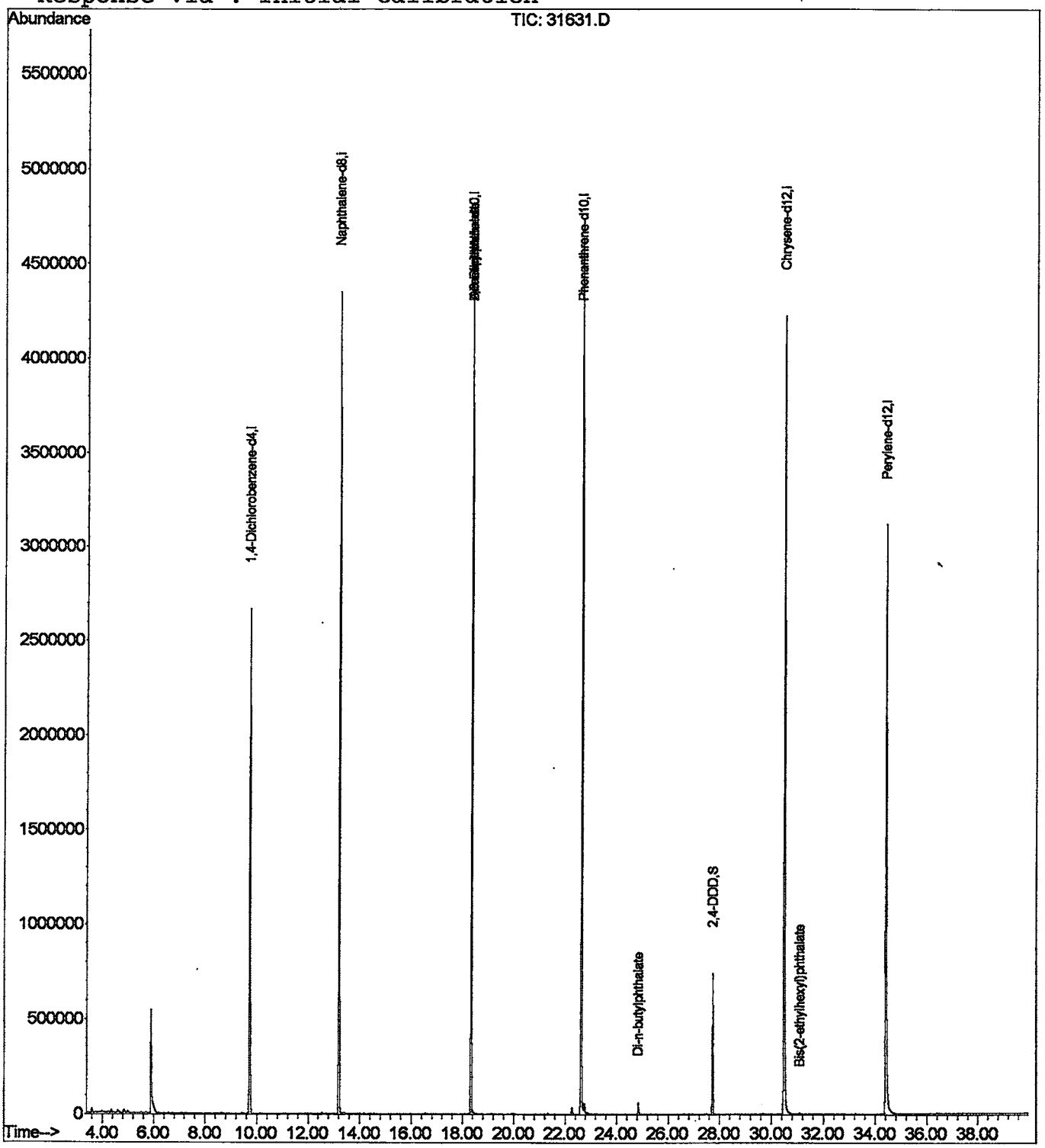
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1037895	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	4397164	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2286382	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	3839331	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3363452	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2362774	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	269458	4.44	ug/L	0.00
Spiked Amount 5.000			Recovery =	88.80%		
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	366955	2.43	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	292958	9.95	ug/L #	17
35) Di-n-butylphthalate	24.85	149	69236	0.28	ug/L	98
42) Bis(2-ethylhexyl)phthalate	31.11	149	5368	0.58	ug/L	94

(#) = qualifier out of range (m) = manual integration
31631.D SCAN508.M Tue Jan 22 08:30:06 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 22 8:30 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\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 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

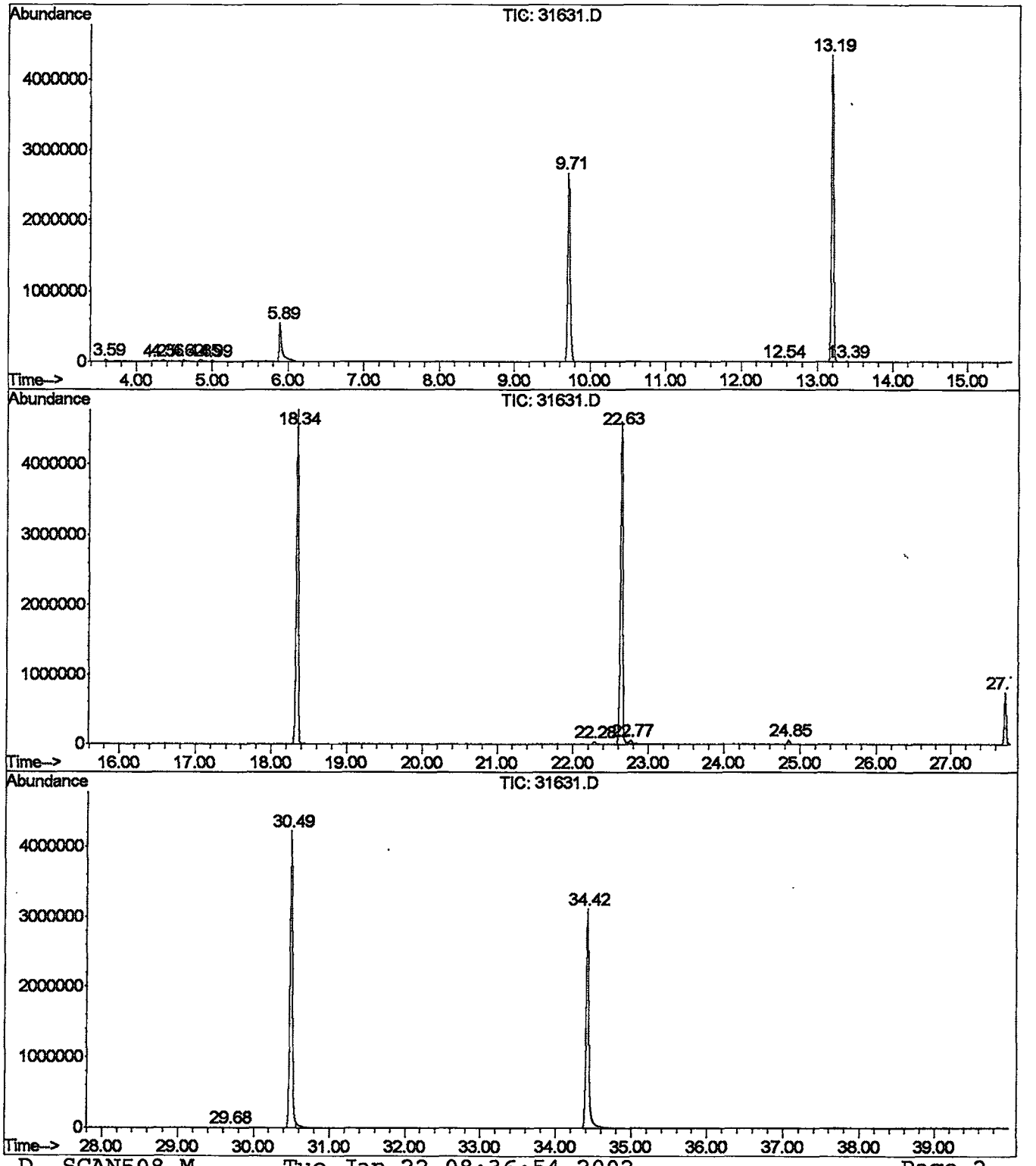
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.591	15	19	25	rBV	24532	42895	0.42%	0.078%
2	4.253	73	77	81	rBV3	5297	17295	0.17%	0.032%
3	4.356	81	86	91	rVB	13804	25703	0.25%	0.047%
4	4.618	107	109	113	rVV3	11776	22595	0.22%	0.041%
5	4.846	125	129	139	rBV4	15954	55646	0.55%	0.102%
6	4.995	139	142	151	rVB4	11385	31458	0.31%	0.058%
7	5.885	217	220	243	rBV	545341	1378700	13.58%	2.521%
8	9.710	551	555	563	rBV	2665454	5853841	57.66%	10.704%
9	12.541	799	803	809	rBV	7820	18223	0.18%	0.033%
10	13.192	855	860	865	rBV	4348535	8424022	82.98%	15.403%
11	13.386	873	877	893	rVB3	7493	27491	0.27%	0.050%
12	18.341	1305	1311	1315	rBV	4775684	9260214	91.22%	16.932%
13	22.280	1651	1656	1661	rBV	34669	66901	0.66%	0.122%
14	22.634	1681	1687	1693	rBV2	4604849	10151494	100.00%	18.562%
15	22.771	1695	1699	1707	rVB	50986	136519	1.34%	0.250%
16	24.849	1877	1881	1889	rVV	61804	108881	1.07%	0.199%
17	27.726	2127	2133	2139	rVV	742095	1307438	12.88%	2.391%
18	29.678	2301	2304	2311	rBV4	5733	16579	0.16%	0.030%
19	30.489	2369	2375	2381	rBV2	4221479	9730484	95.85%	17.792%
20	34.416	2713	2719	2745	rBV	3114576	8013283	78.94%	14.652%

Sum of corrected areas: 54689662

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31631.D
Operator :
Acquired : 17 Jan 2002 11:52 am using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 17, 2002
Vial Number: 3
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

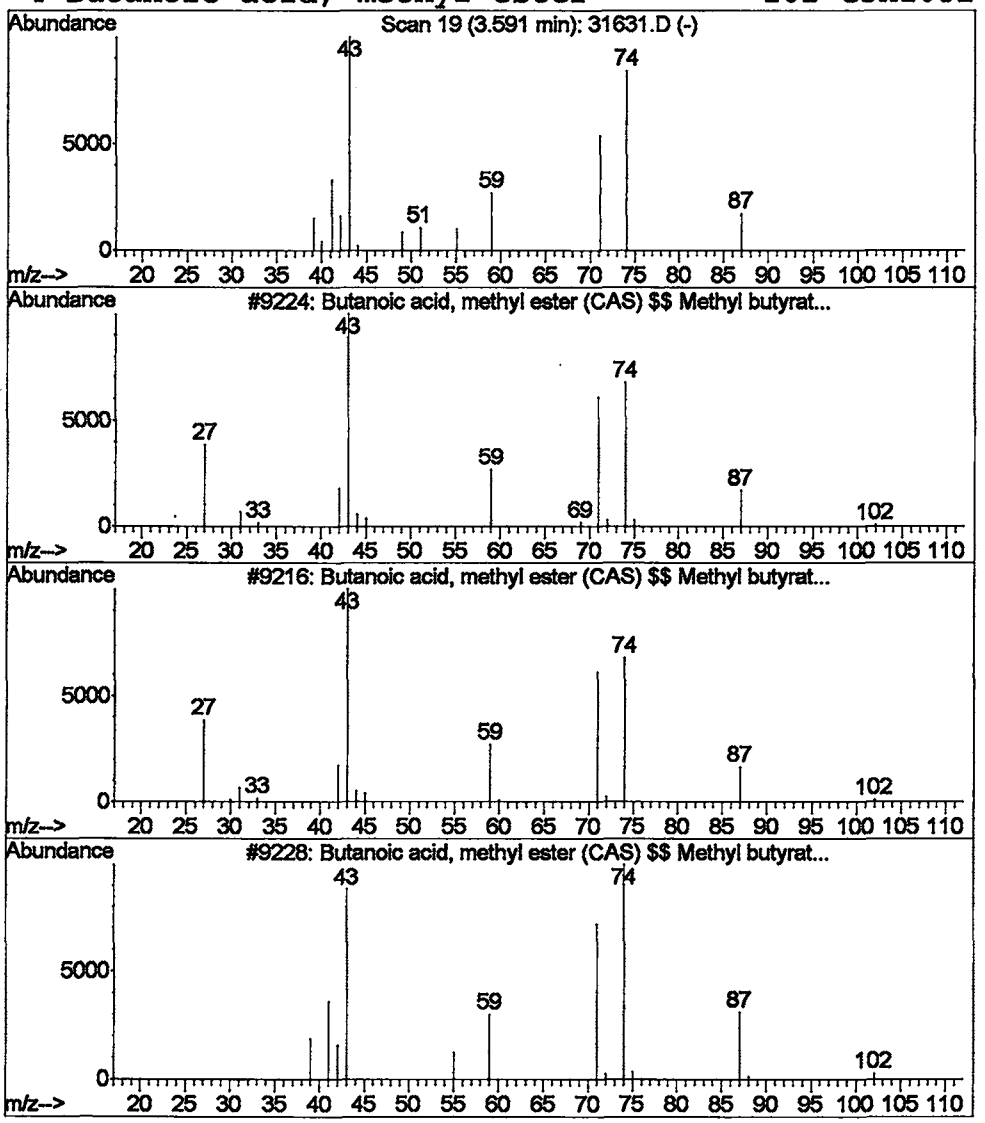
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

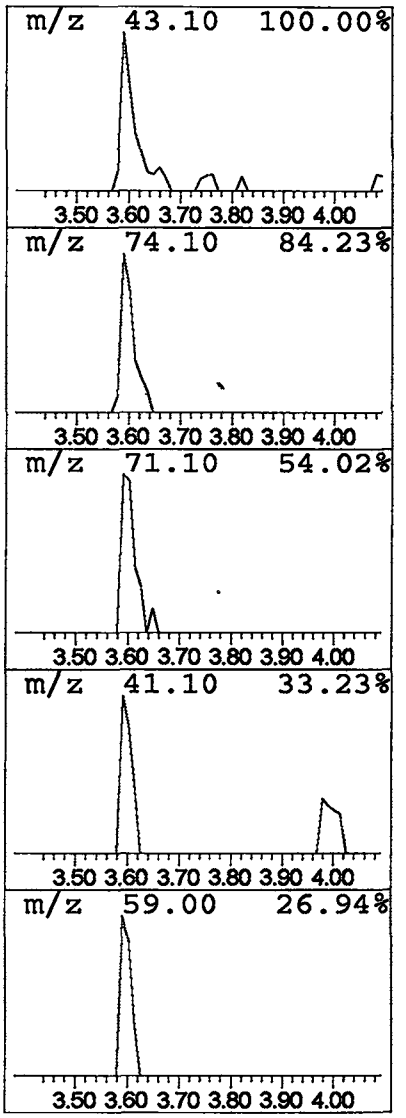
****

Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	0.15 ug/L	42895	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	78
2	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
3	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	78
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	64





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

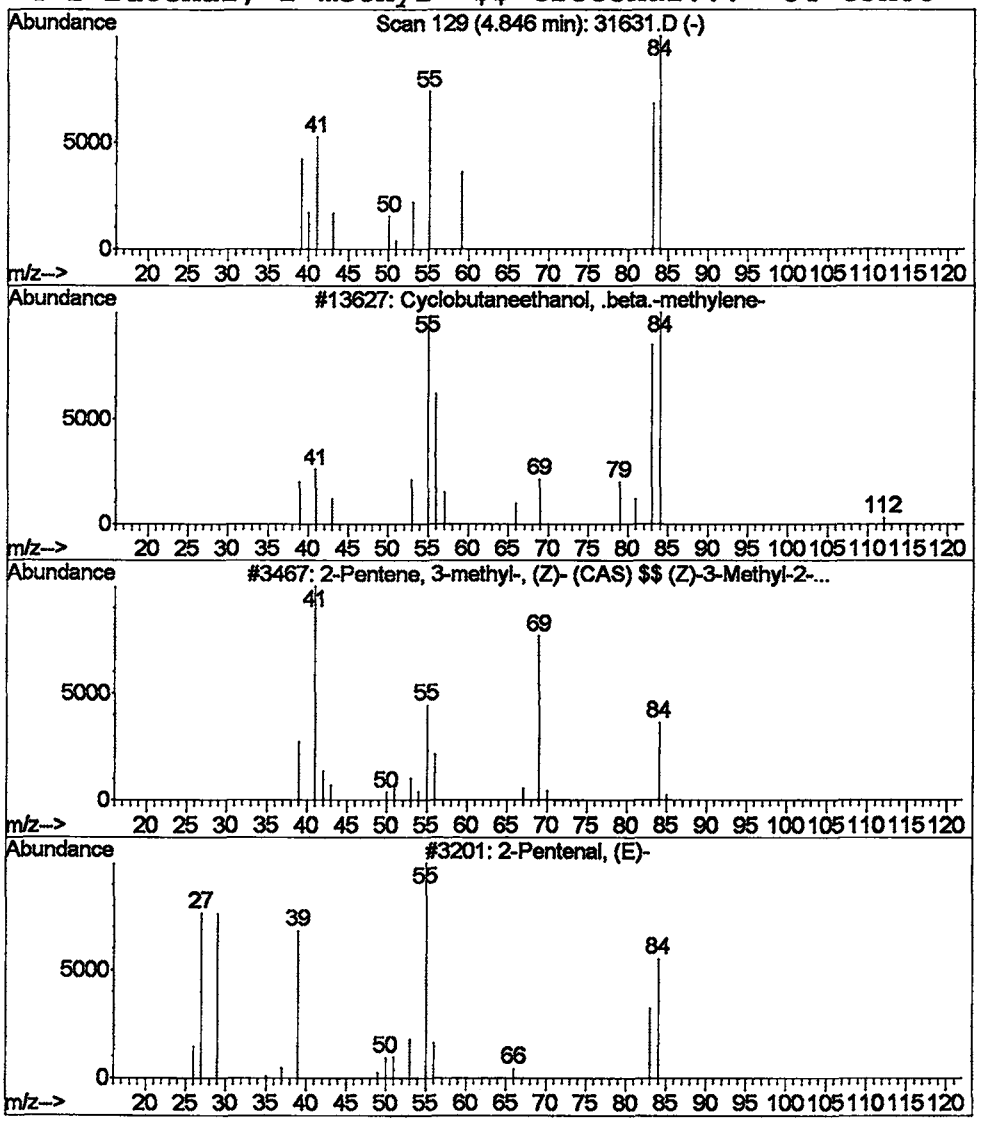
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

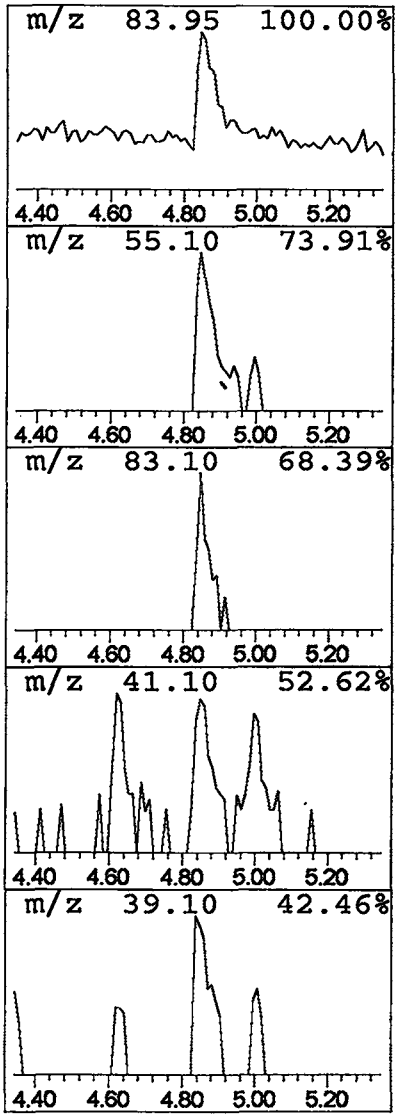
****

Peak Number 2 Cyclobutaneethanol, .beta.-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	0.19 ug/L	55646	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutaneethanol, .beta.-methy...	112	C7H12O	116203-80-6	36
2	2-Pentene, 3-methyl-, (Z)- (CAS)...	84	C6H12	000922-62-3	9
3	2-Pentenal, (E)-	84	C5H8O	001576-87-0	7
4	2-Butenal, 2-methyl- $$ Crotonal...	84	C5H8O	001115-11-3	7





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

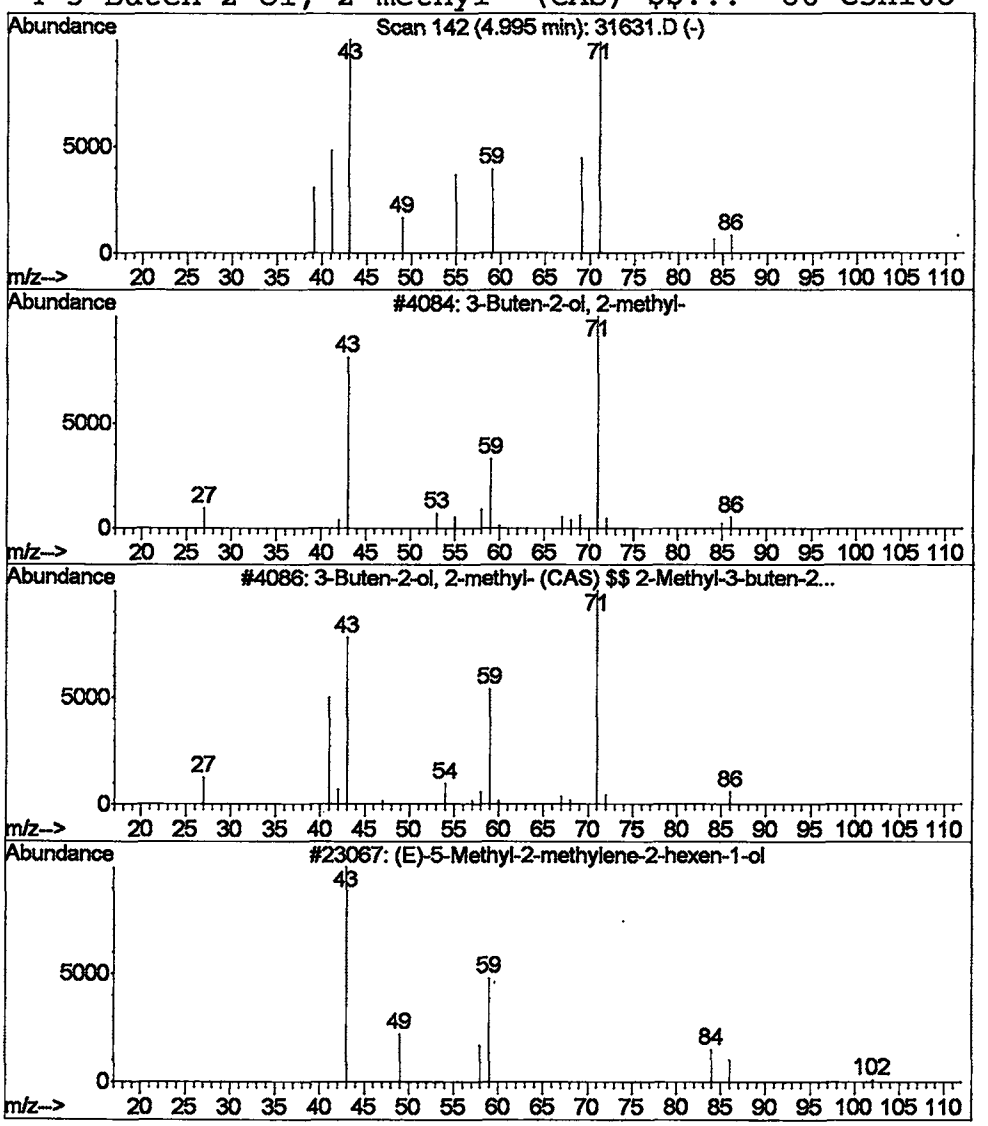
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

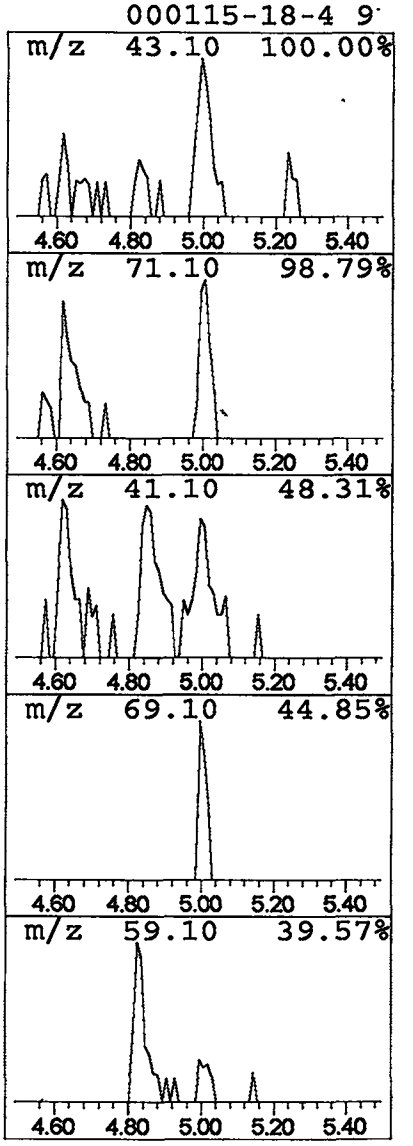
****

Peak Number 3 3-Buten-2-ol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	0.11 ug/L	31458	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	56
2	3-Buten-2-ol, 2-methyl- (CAS) $$...	86	C5H10O	000115-18-4	50
3	(E)-5-Methyl-2-methylene-2-hexen...	126	C8H14O	000000-00-0	10
4	3-Buten-2-ol, 2-methyl- (CAS) $$...	86	C5H10O	000115-18-4	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

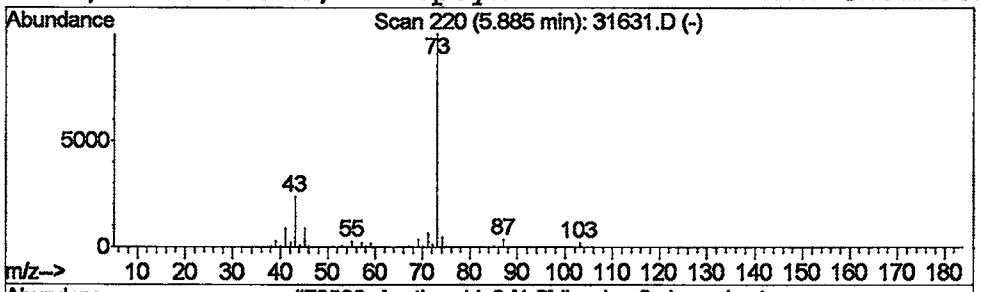
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

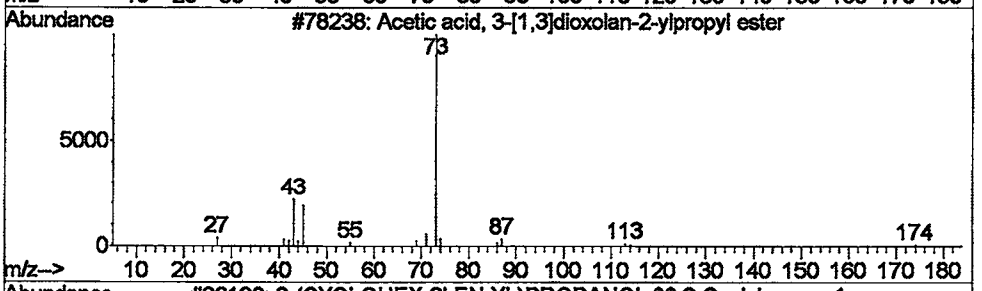
****

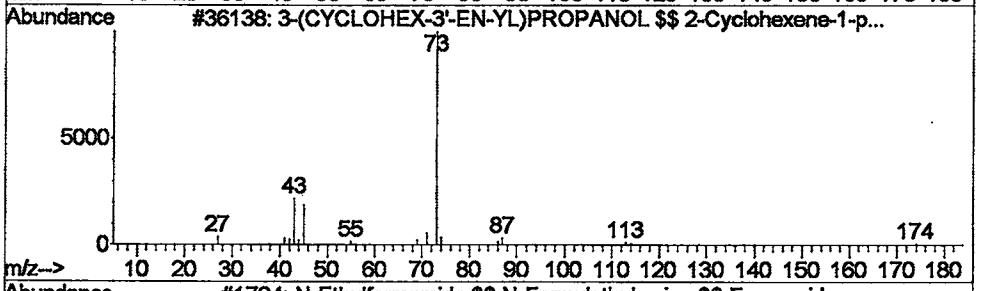
Peak Number 4 Acetic acid, 3-[1,3]dioxola... Concentration Rank 1

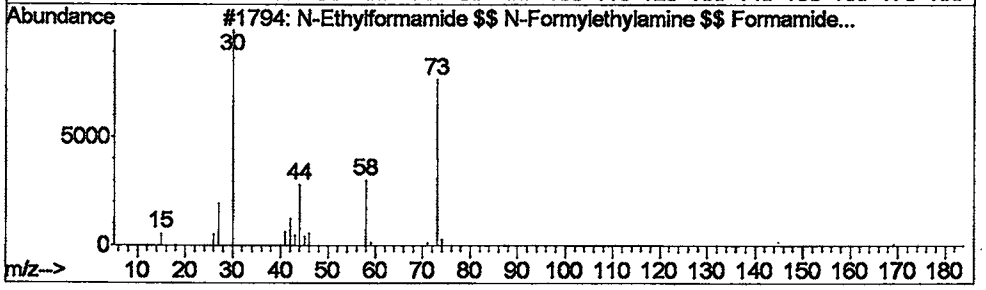
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.71 ug/L	1378700	1,4-Dichlorobenzene-d4	9.71

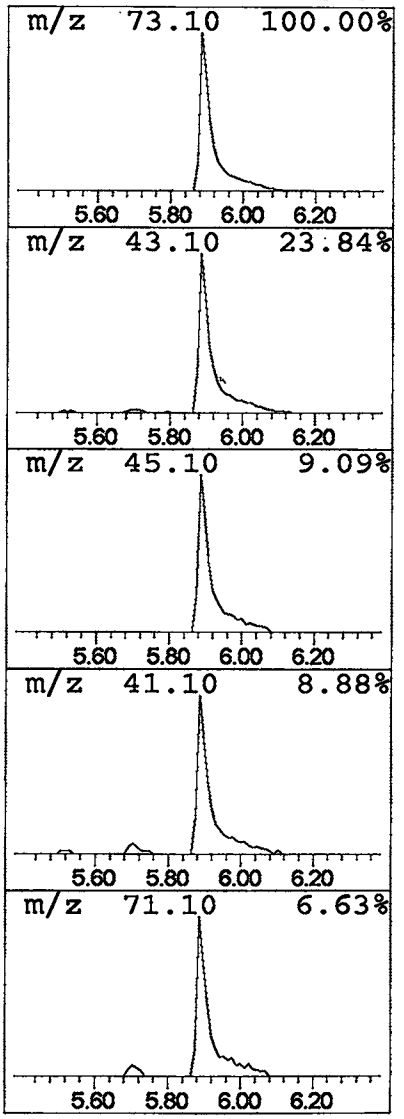
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	33
2	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33
3	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4	1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9











Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

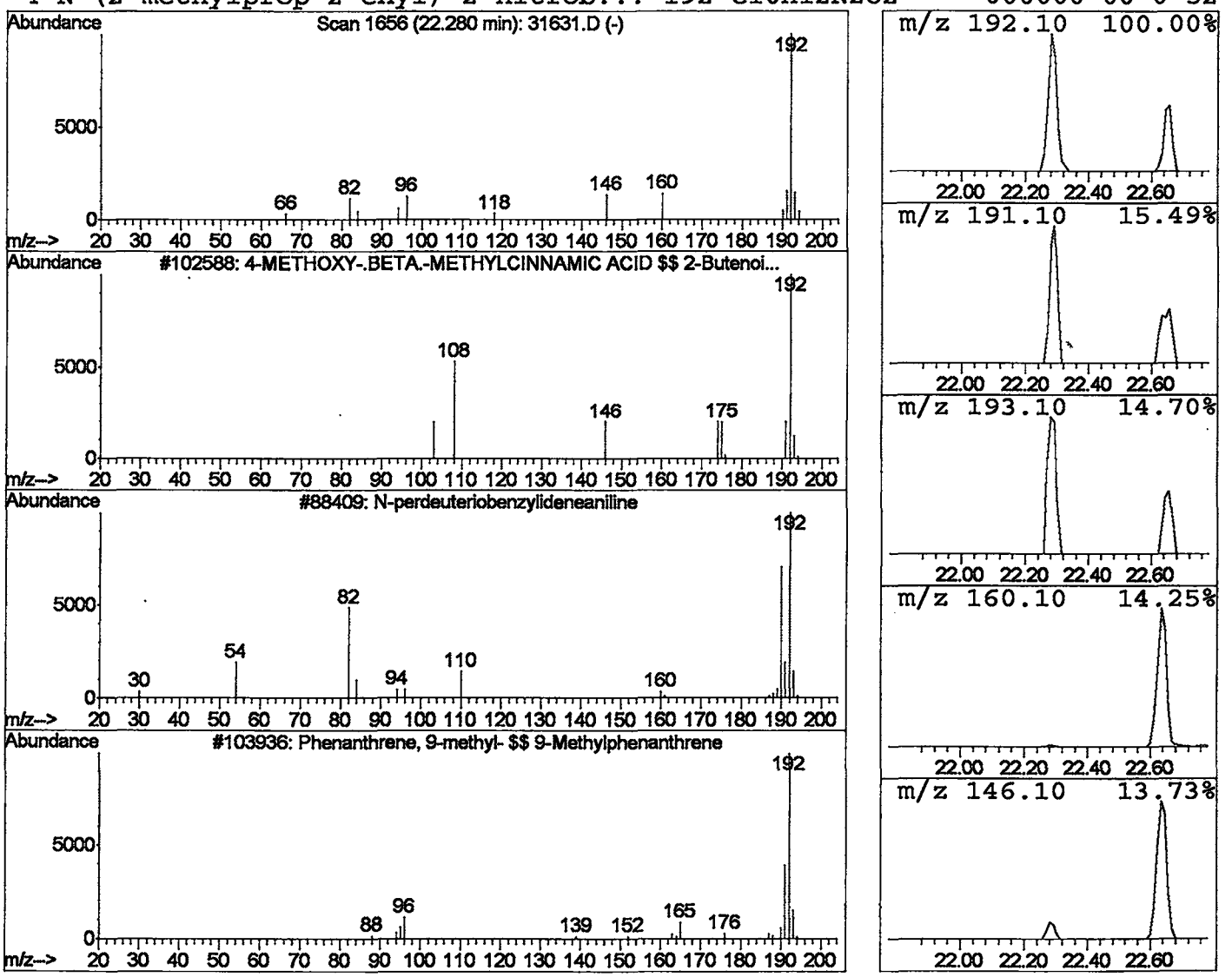
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.13 ug/L	66901	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	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	59
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	52



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31631.D Vial: 3
Acq On : 17 Jan 2002 11:52 am Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

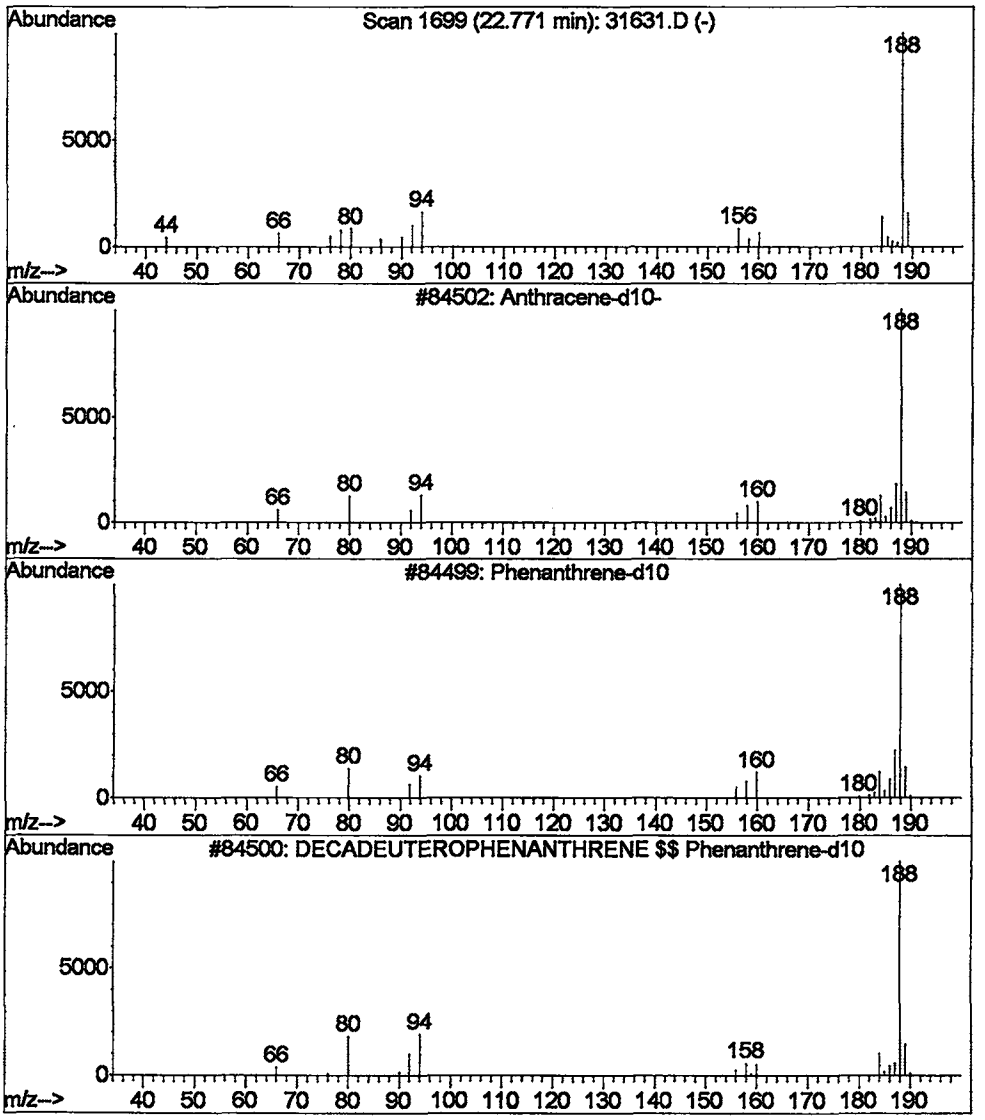
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

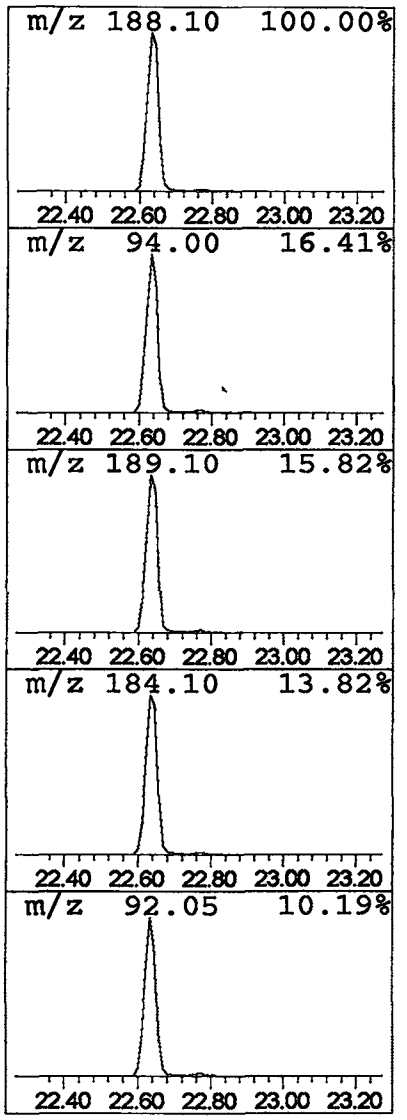
****

Peak Number 6 Anthracene-d10- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.27 ug/L	136519	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene-d10-	188	C14D10	001719-06-8	87
2	Phenanthrene-d10	188	C14D10	001517-22-2	78
3	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	72
4	Acridine-D9	188	C13D9N	000000-00-0	64





Tentatively Identified Compound (TIC) Summary

Operator ID: Date Acquired: 17 Jan 2002 11:52 am
Data File: C:\MSDCHEM\1\5973N\02JAN17\31631.D
Name: 508 scan
Misc: January 17, 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...	3.59	0.1	ug/L	42895	1	9.71	5853840	20.0
Cyclobutaneethano...	4.85	0.2	ug/L	55646	1	9.71	5853840	20.0
3-Buten-2-ol, 2-m...	4.99	0.1	ug/L	31458	1	9.71	5853840	20.0
Acetic acid, 3-[1...	5.89	4.7	ug/L	1378700	1	9.71	5853840	20.0
4-METHOXY-.BETA.-...	22.28	0.1	ug/L	66901	4	22.63	10151500	20.0
Anthracene-d10-	22.77	0.3	ug/L	136519	4	22.63	10151500	20.0