User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/28/2002 Time: 15:31:29

Sample: AD31644
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/28/02 15:31 Ended: 1/28/02 15:31 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		91		5.0

Comments for Sample AD31644 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-28-2002 Time: 15:31:32

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\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 22 08:30:13 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

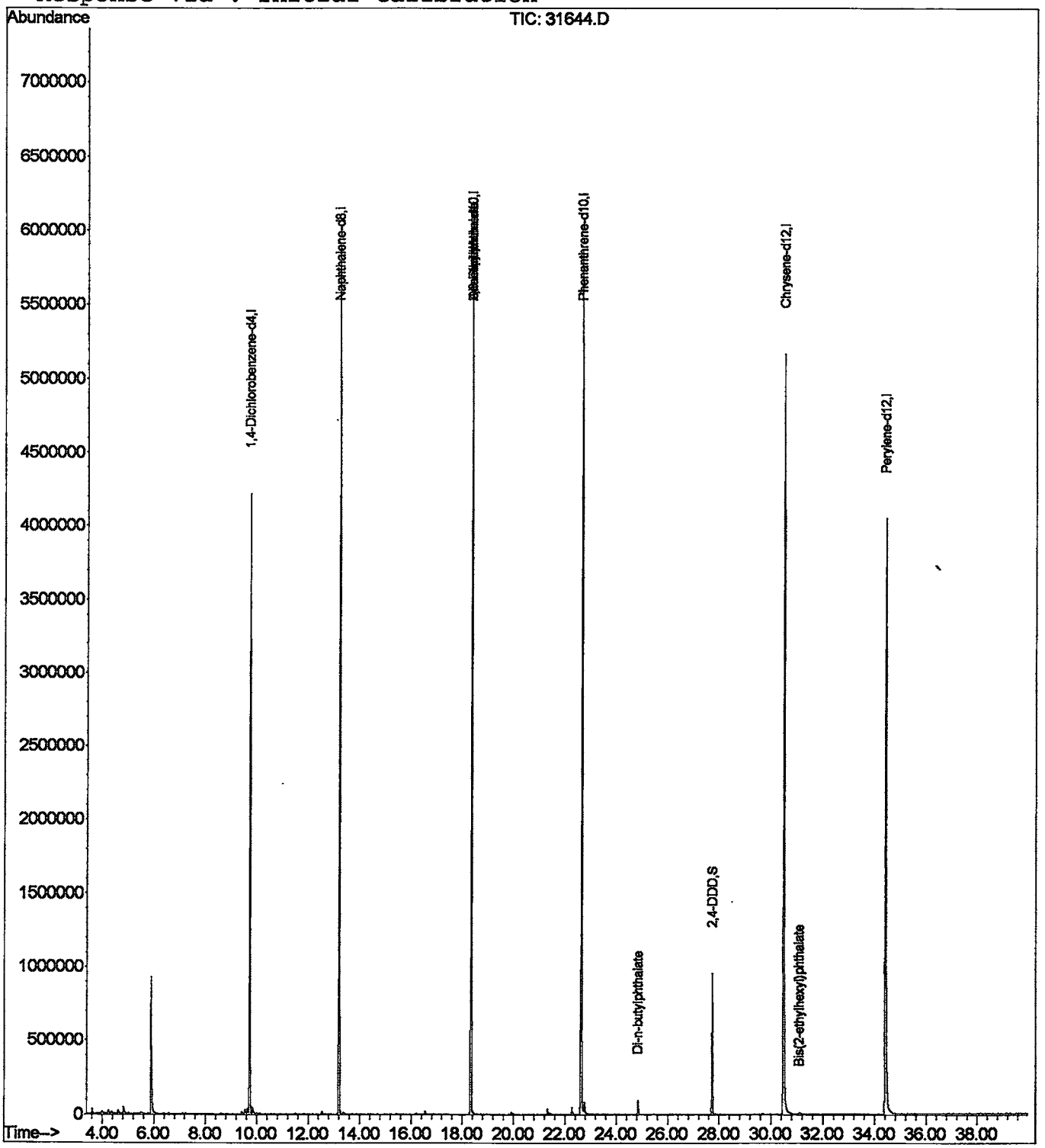
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1408100	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	5932711	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2995197	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4831524	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	4314827	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3126965	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	348663	4.57	ug/L	0.00
Spiked Amount 5.000			Recovery = 91.40%			
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	489831	2.48	ug/L #	55
21) 2,6-Dinitrotoluene	18.34	165	380407	9.86	ug/L #	17
35) Di-n-butylphthalate	24.85	149	108064	0.35	ug/L	97
42) Bis(2-ethylhexyl)phthalate	31.11	149	9717	0.59	ug/L	96

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

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

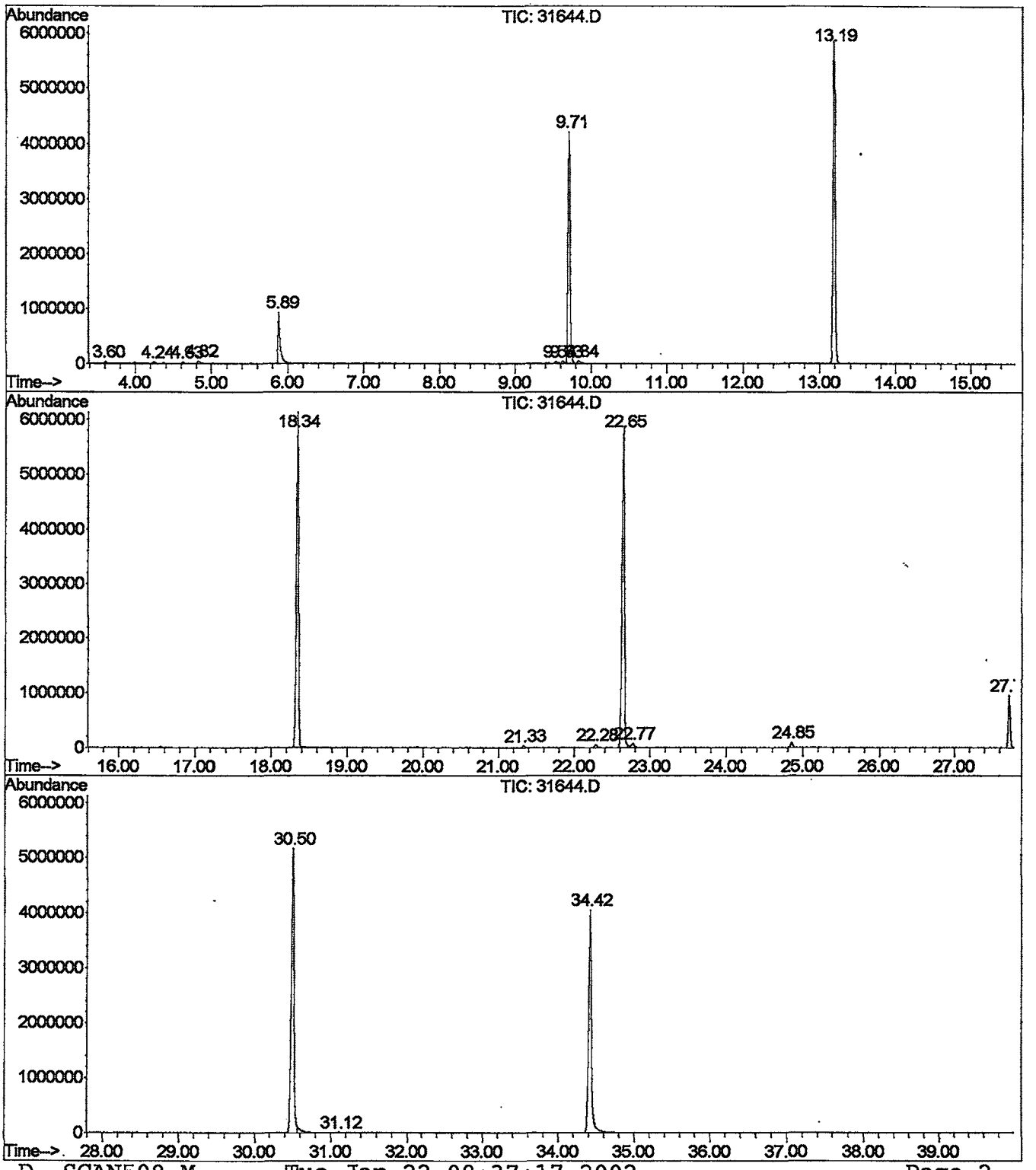
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.602	19	20	25	rBV	34079	59574	0.46%	0.082%
2	4.241	71	76	83	rVV3	22683	53655	0.42%	0.074%
3	4.629	107	110	125	rVB4	21550	53910	0.42%	0.075%
4	4.824	125	127	141	rBV2	45881	107924	0.84%	0.149%
5	5.885	215	220	241	rBV	925799	1819742	14.10%	2.518%
6	9.539	535	540	545	rBV	32703	73633	0.57%	0.102%
7	9.630	545	548	551	rVV	36809	84006	0.65%	0.116%
8	9.710	551	555	561	rVV	4214615	8072346	62.53%	11.168%
9	9.836	561	566	575	rVV	44391	132973	1.03%	0.184%
10	13.192	855	860	865	rBV	5861888	11433959	88.57%	15.819%
11	18.341	1305	1311	1315	rBV	6129764	12199414	94.50%	16.878%
12	21.332	1569	1573	1577	rBV	39798	66045	0.51%	0.091%
13	22.280	1651	1656	1661	rBV2	51959	99241	0.77%	0.137%
14	22.645	1681	1688	1693	rBV	5858908	12909387	100.00%	17.860%
15	22.771	1695	1699	1713	rVB	78016	213554	1.65%	0.295%
16	24.849	1877	1881	1887	rBV	93202	165128	1.28%	0.228%
17	27.726	2129	2133	2139	rVV	956092	1680953	13.02%	2.326%
18	30.500	2369	2376	2381	rBV	5162503	12415338	96.17%	17.177%
19	31.117	2419	2430	2437	rBV7	9539	43022	0.33%	0.060%
20	34.416	2713	2719	2749	rBV	4041740	10596026	82.08%	14.660%

Sum of corrected areas: 72279830

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31644.D
Operator :
Acquired : 17 Jan 2002 5:19 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 17, 2002
Vial Number: 4
Quant File :SCAN508.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

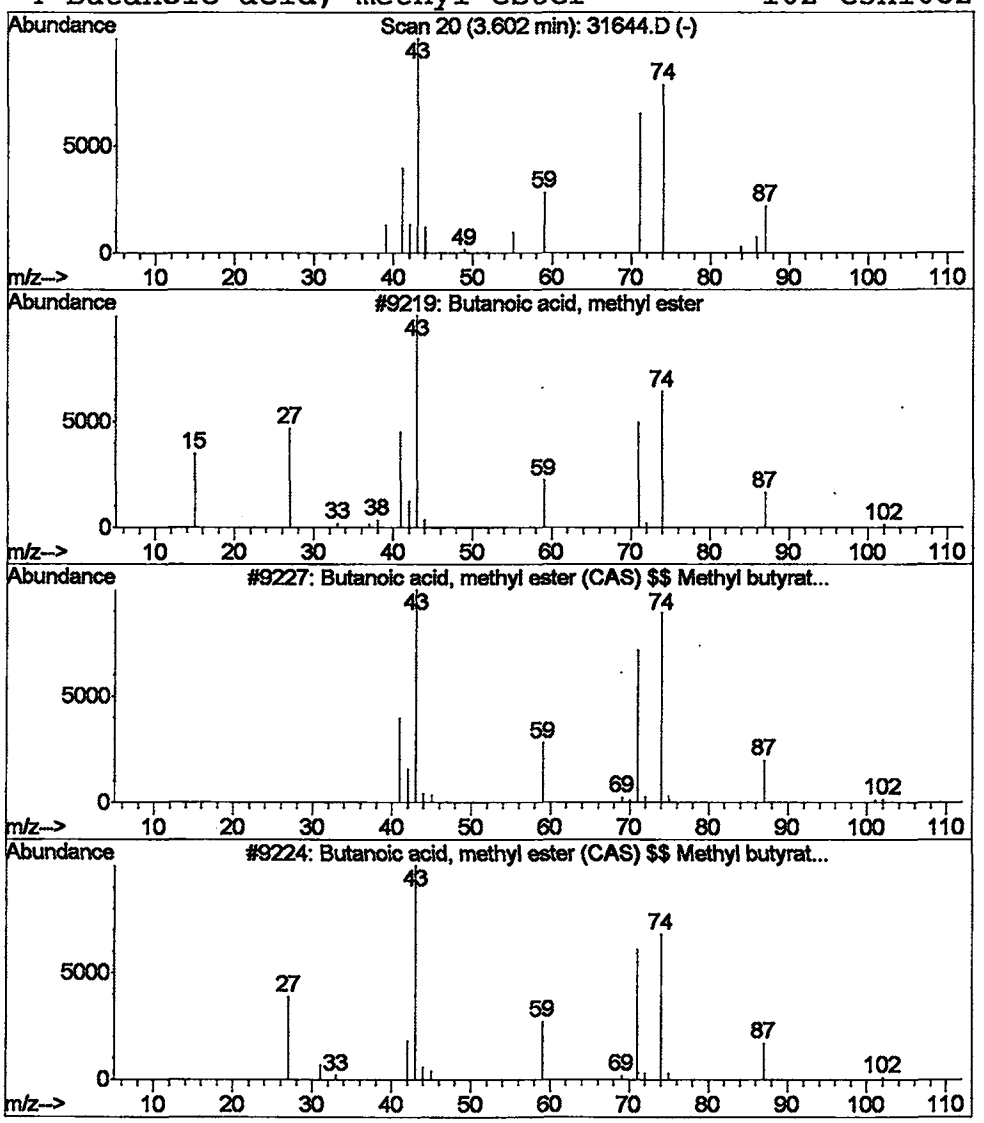
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

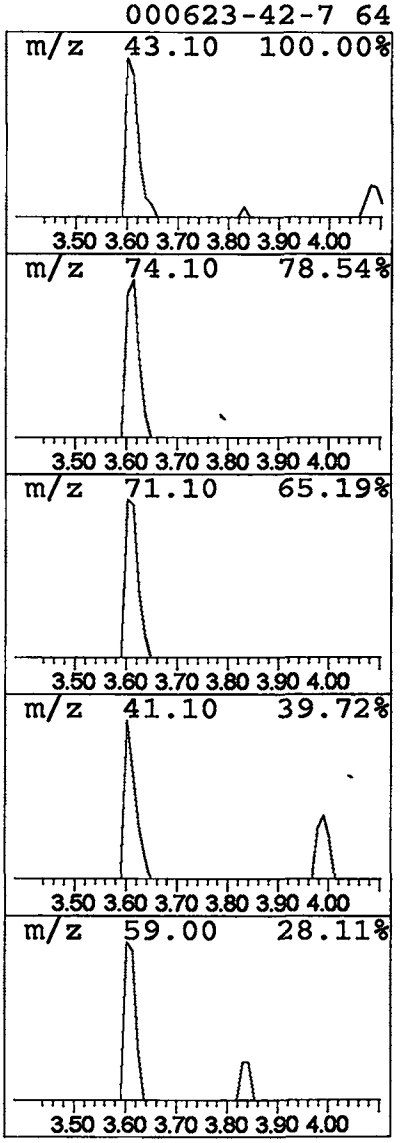
****

Peak Number 1 Butanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.15 ug/L	59574	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	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	72
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	64





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

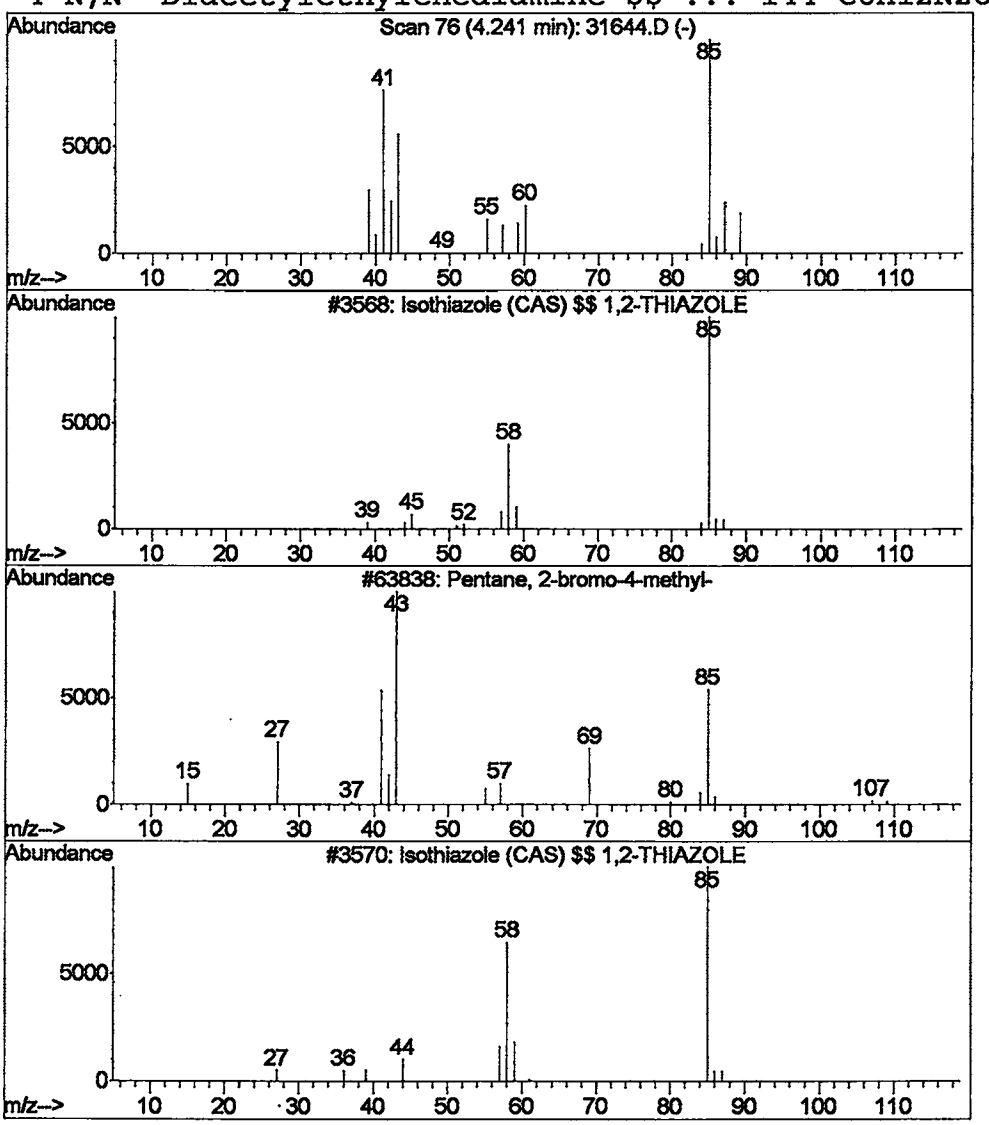
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

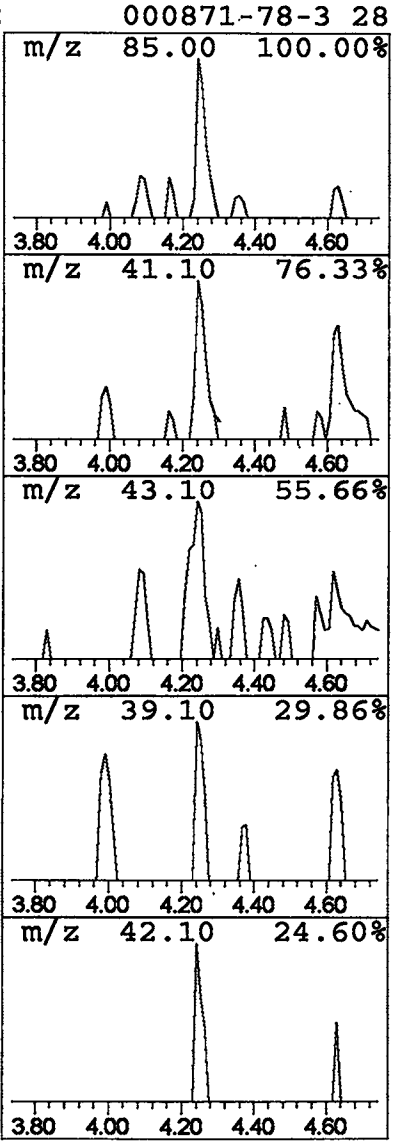
****

Peak Number 2 Isothiazole (CAS) $$ 1,2-TH... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	0.13 ug/L	53655	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isothiazole (CAS) $$ 1,2-THIAZOLE	85	C3H3NS	000288-16-4	37
2	Pentane, 2-bromo-4-methyl-	164	C6H13Br	030310-22-6	33
3	Isothiazole (CAS) $$ 1,2-THIAZOLE	85	C3H3NS	000288-16-4	32
4	N,N'-Diacetylethylenediamine $$ ...	144	C6H12N2O2	000871-78-3	28





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

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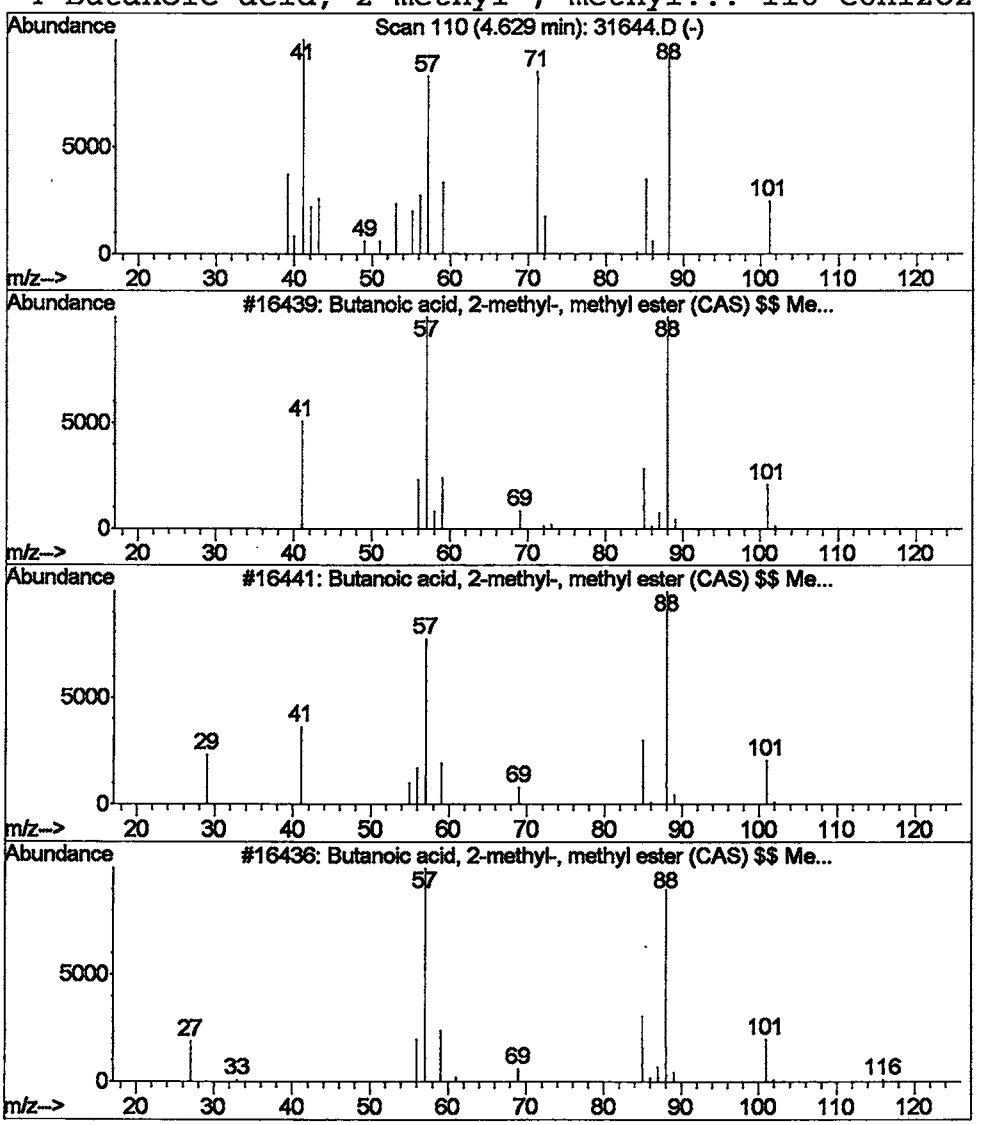
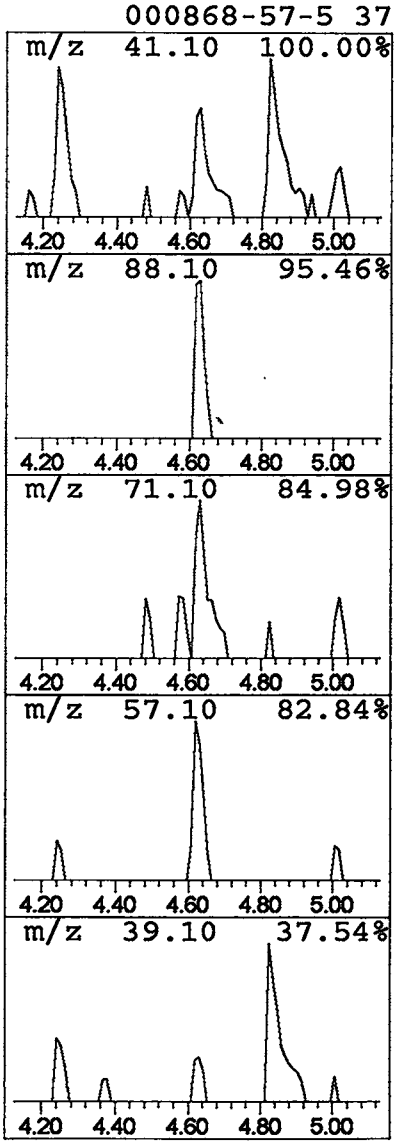
Peak Number 3 Butanoic acid, 2-methyl-, m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	0.13 ug/L	53910	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	37
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	37
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	37





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

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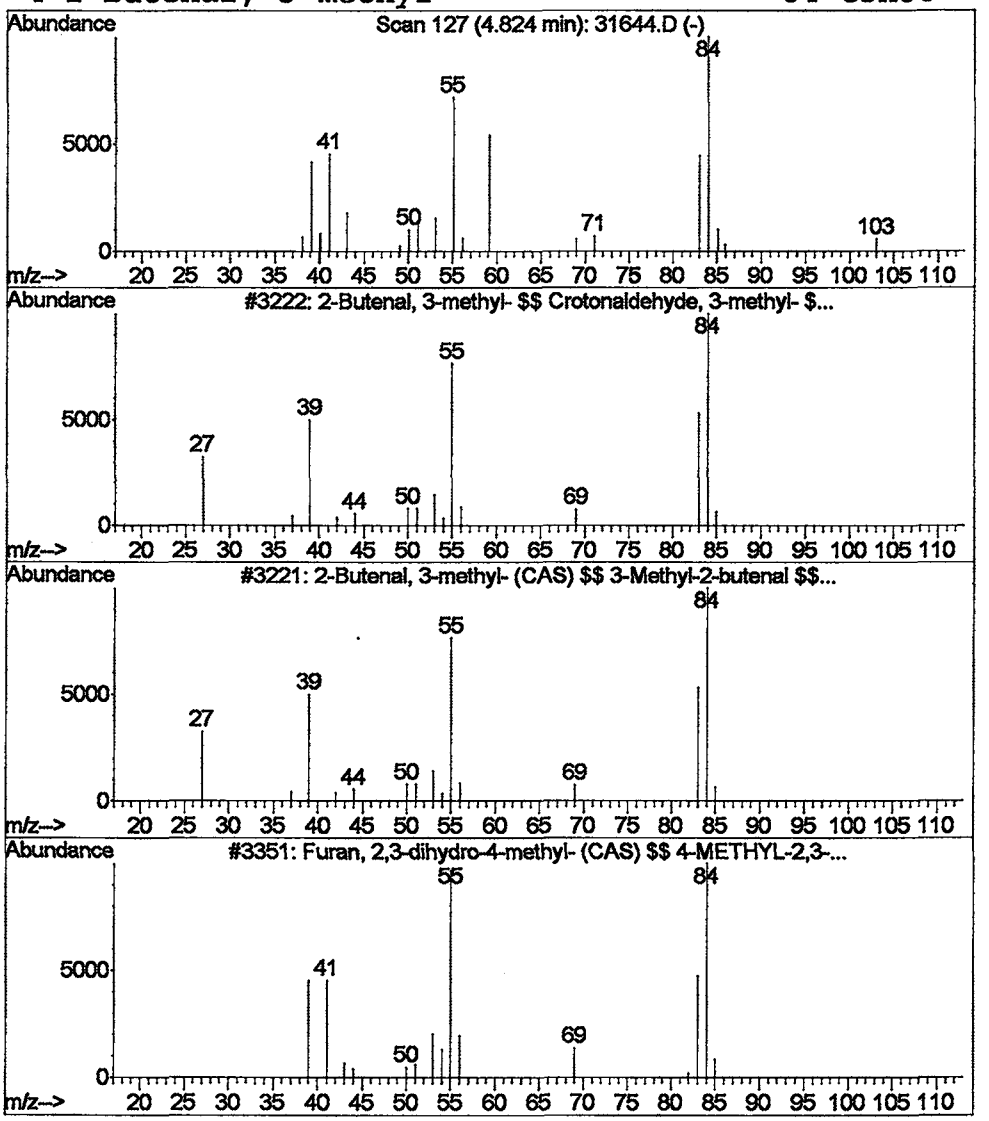
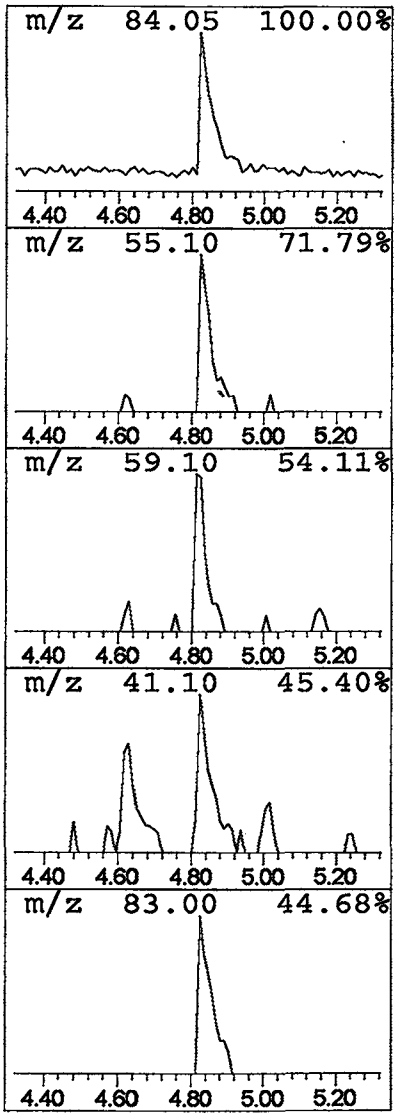
Peak Number 4 2-Butenal, 3-methyl- $$ Cro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	0.27 ug/L	107924	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl- $$ Crotonal...	84	C5H8O	000107-86-8	74
2	2-Butenal, 3-methyl- (CAS) $$ 3-...	84	C5H8O	000107-86-8	74
3	Furan, 2,3-dihydro-4-methyl- (CA...	84	C5H8O	034314-83-5	64
4	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	64





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

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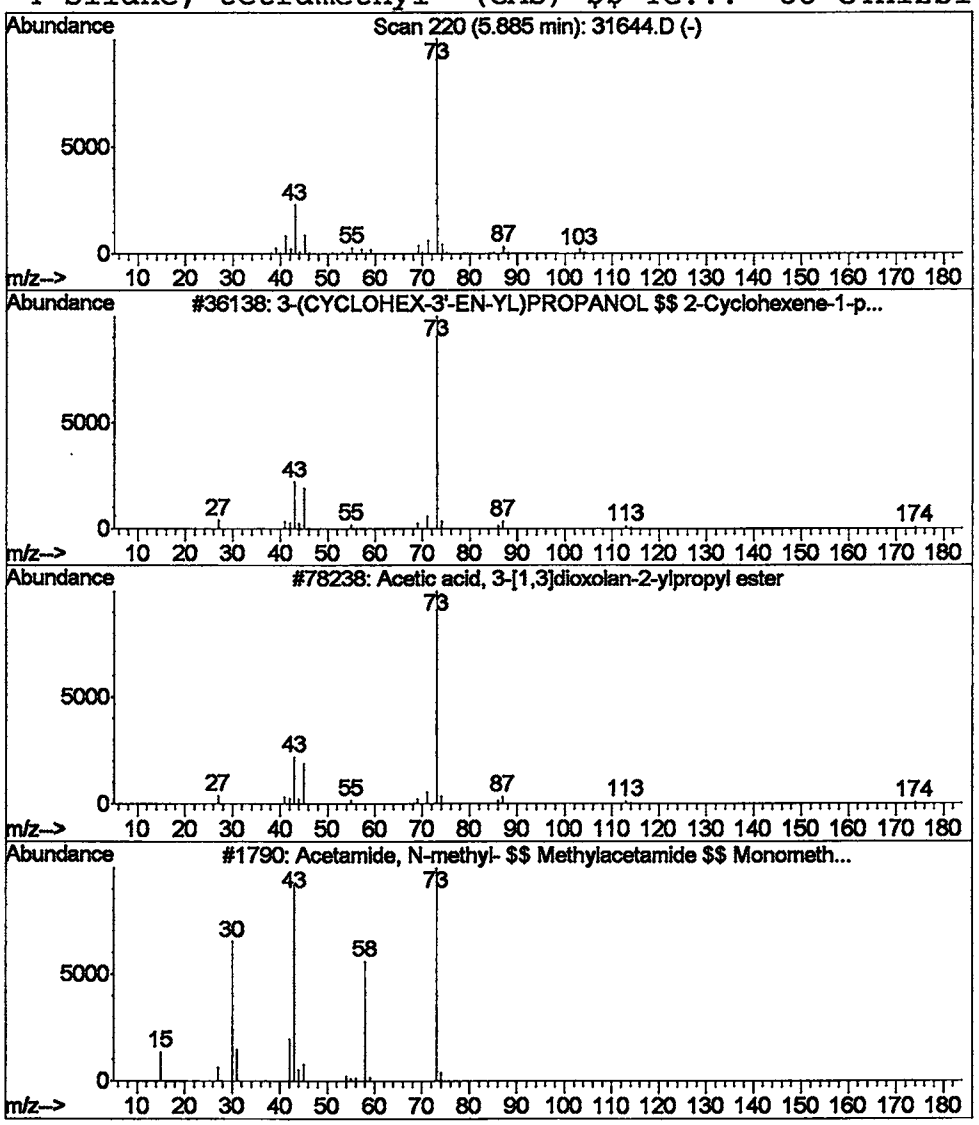
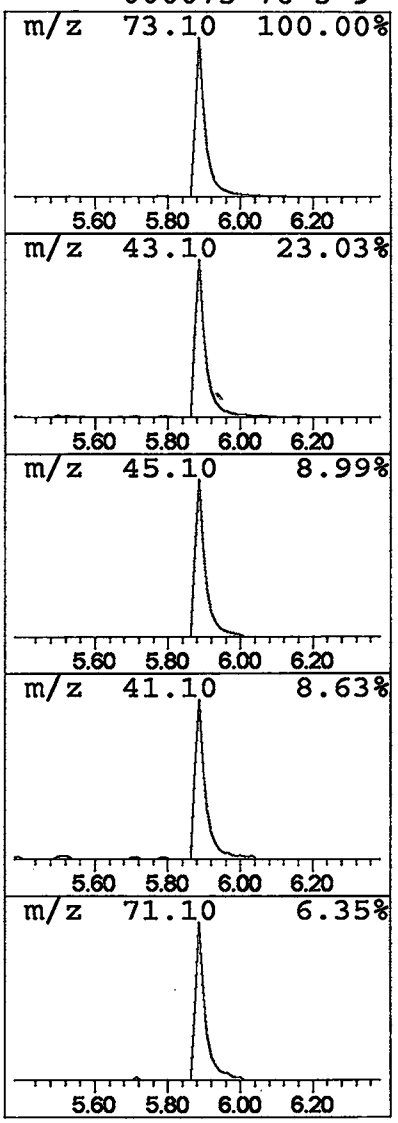
Peak Number 5 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.51 ug/L	1819740	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	36
2	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	36
3	Acetamide, N-methyl- $$ Methylac...	73	C3H7NO	000079-16-3	9
4	Silane, tetramethyl- (CAS) $$ Te...	88	C4H12Si	000075-76-3	9





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

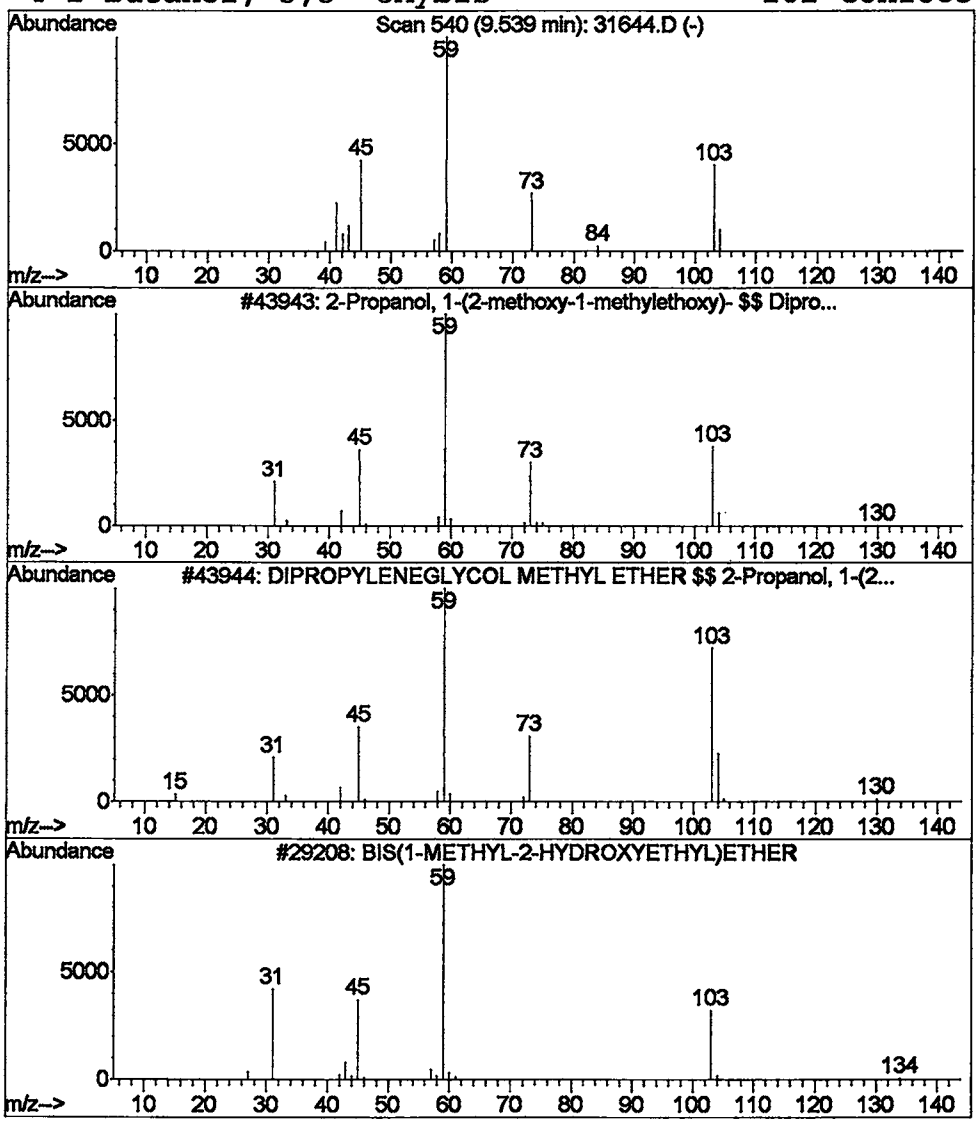
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

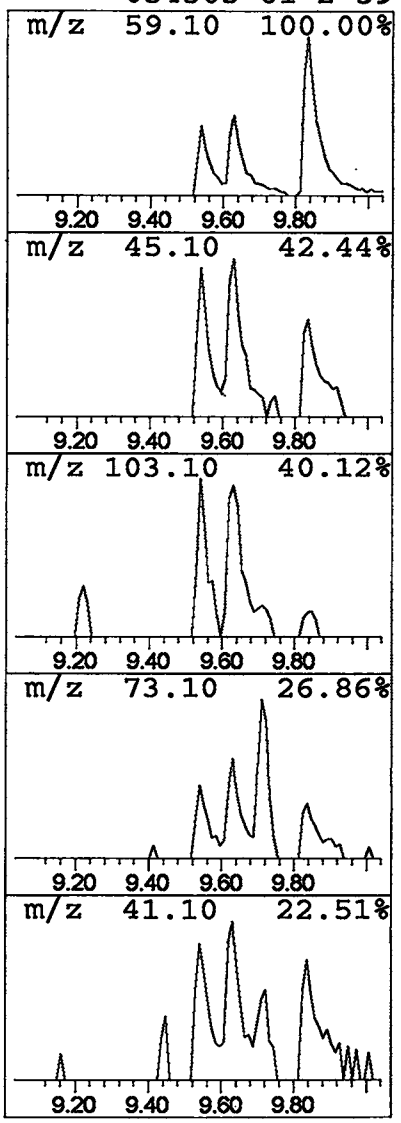
****

Peak Number 6 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	0.18 ug/L	73633	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
2	DIPROPYLENEGLYCOL METHYL ETHER $...	148	C7H16O3	020324-32-7	72
3	BIS(1-METHYL-2-HYDROXYETHYL)ETHER	134	C6H14O3	000000-00-0	39
4	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	39





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

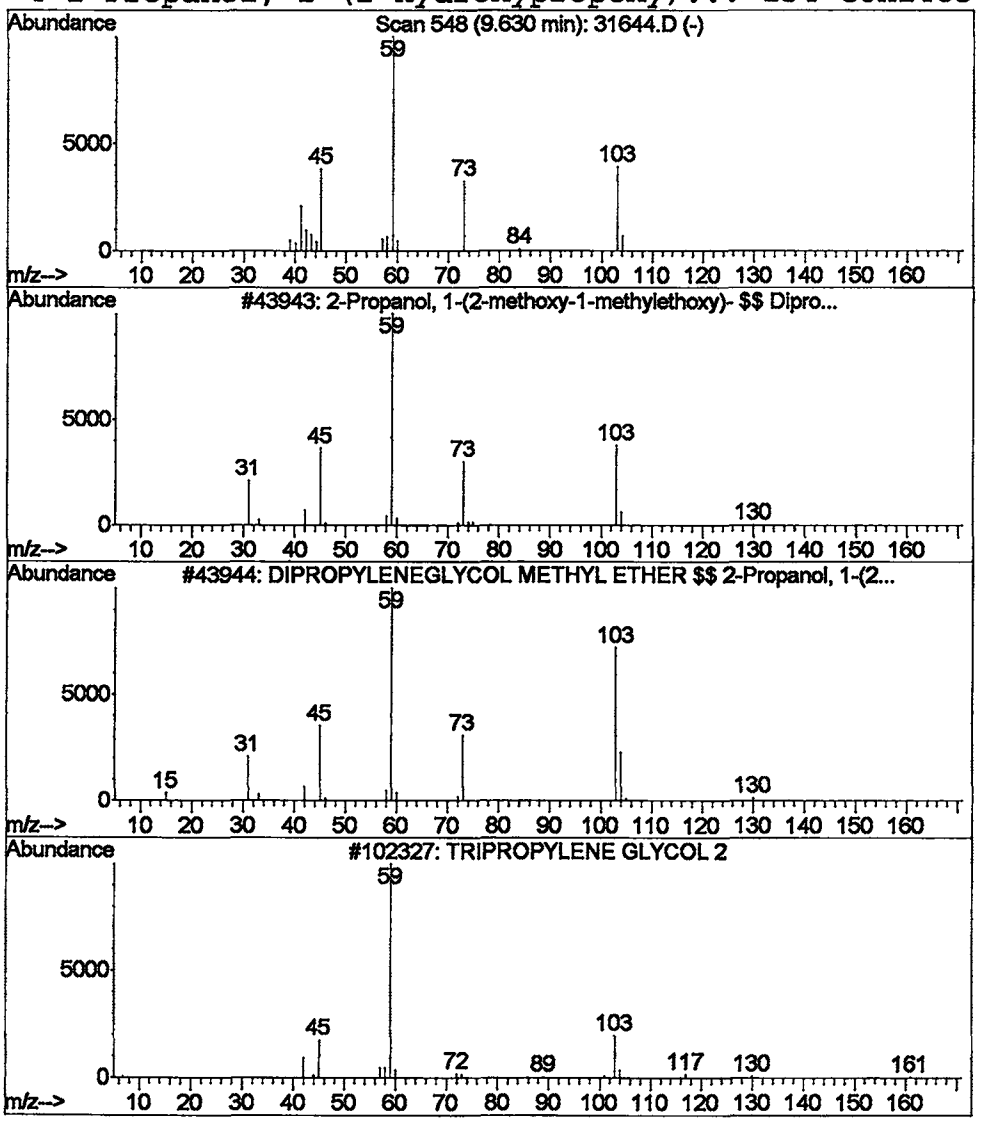
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

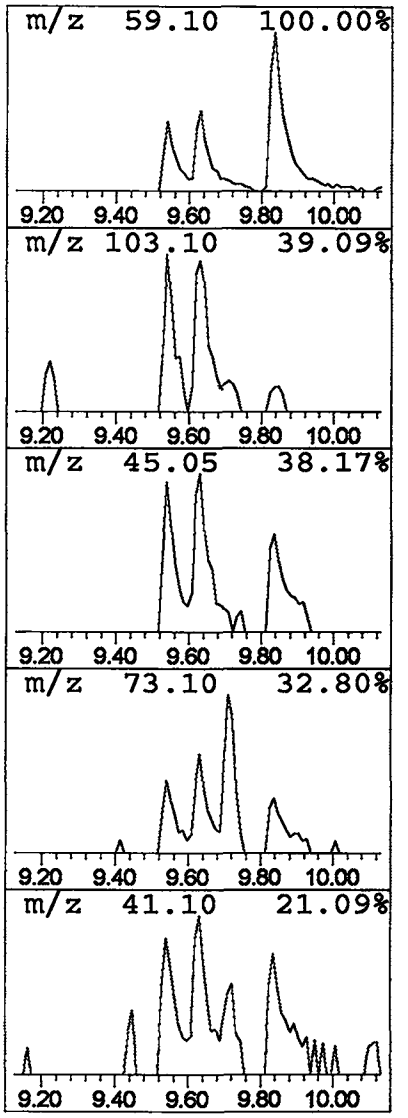
****

Peak Number 7 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	0.21 ug/L	84006	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	DIPROPYLENEGLYCOL METHYL ETHER $...	148	C7H16O3	020324-32-7	74
3	TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	56
4	1-Propanol, 2-(2-hydroxypropoxy)...	134	C6H14O3	000106-62-7	56





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

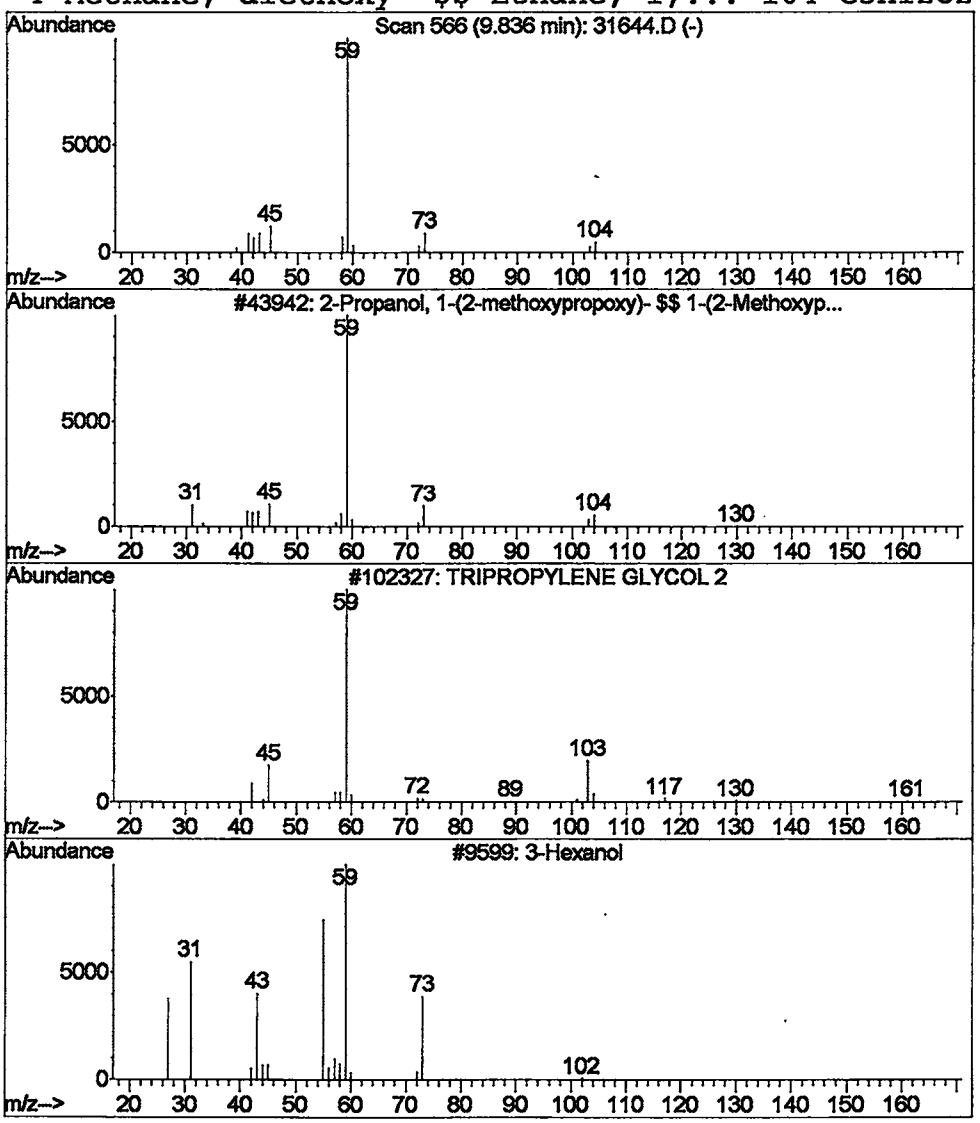
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

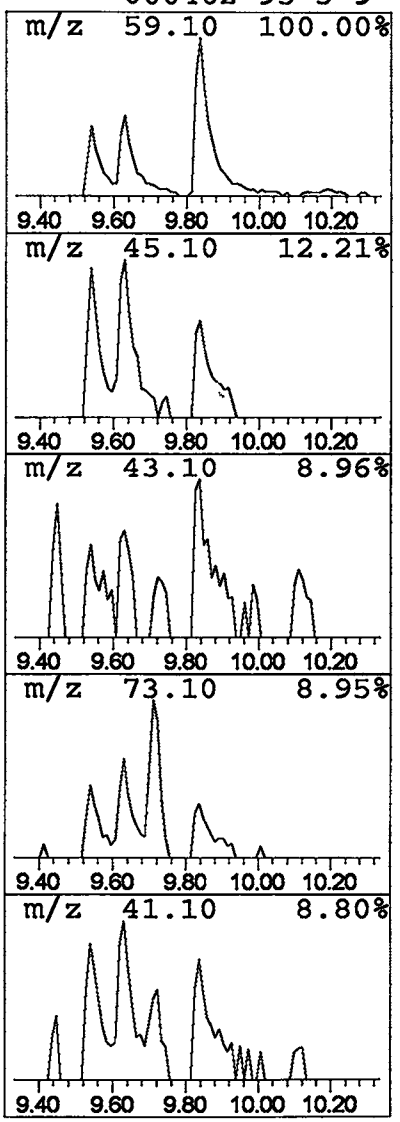
****

Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	0.33 ug/L	132973	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	83
2	TRIPROPYLENE GLYCOL 2	192	C9H20O4	000000-00-0	43
3	3-Hexanol	102	C6H14O	000623-37-0	40
4	Methane, diethoxy- $$ Ethane, 1,...	104	C5H12O2	000462-95-3	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

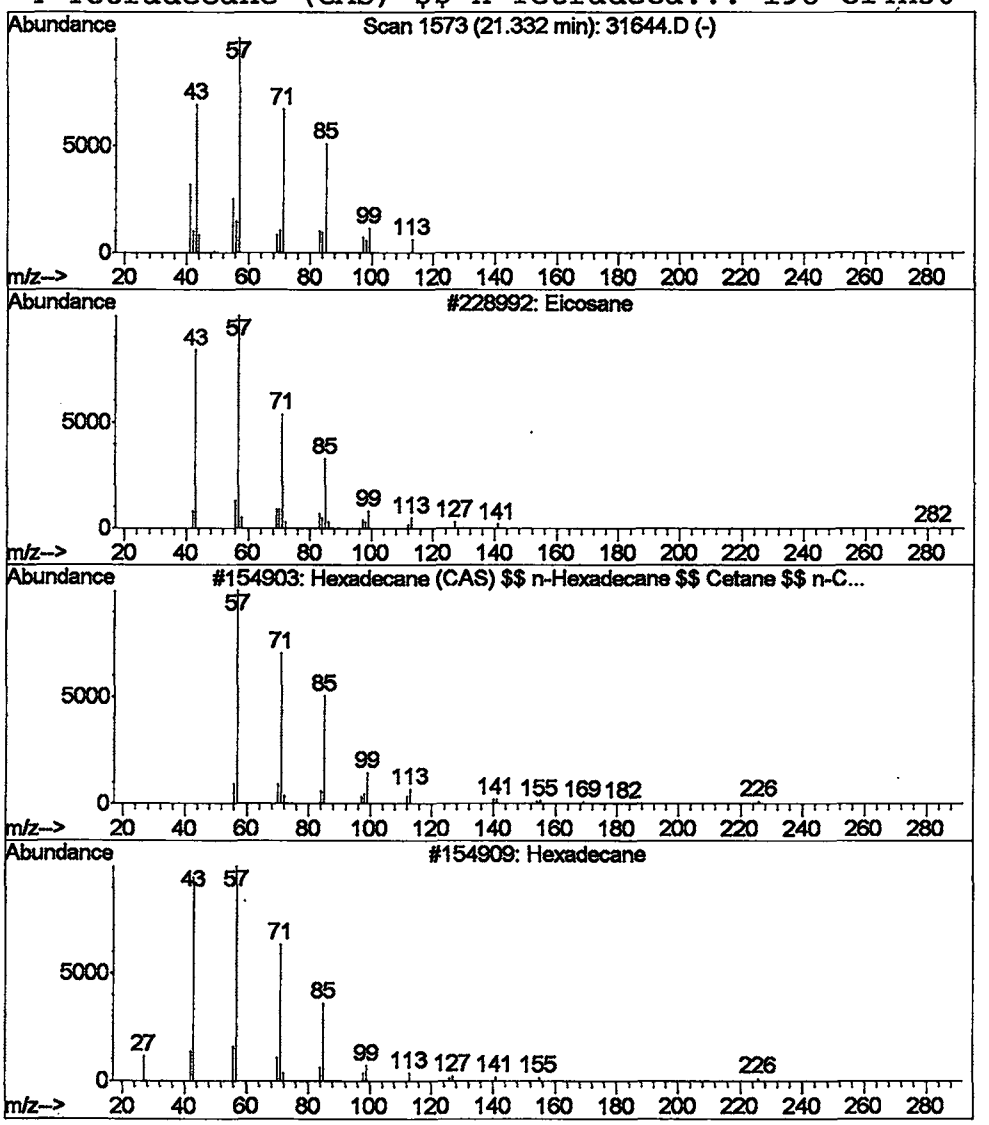
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

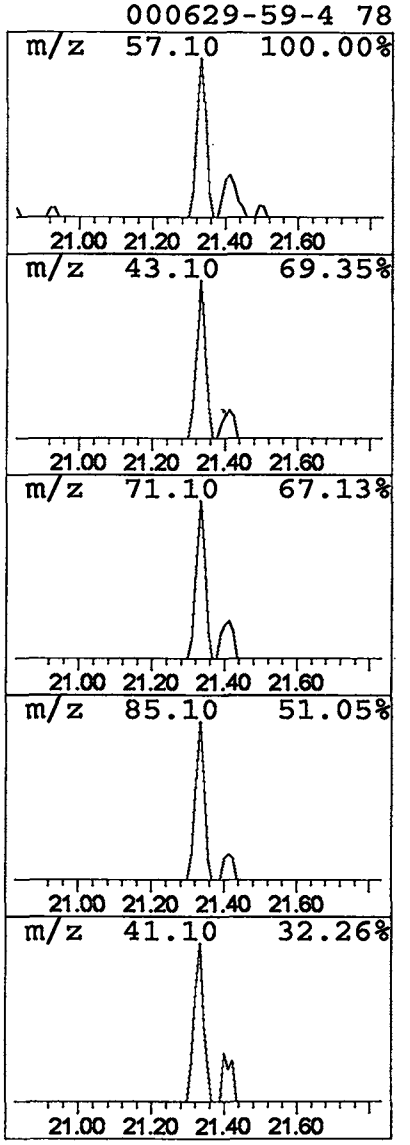
****

Peak Number 9 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	0.10 ug/L	66045	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Hexadecane (CAS) $$ n-Hexadecane...	226	C16H34	000544-76-3	78
3	Hexadecane	226	C16H34	000544-76-3	78
4	Tetradecane (CAS) $$ n-Tetradeca...	198	C14H30	000629-59-4	78





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

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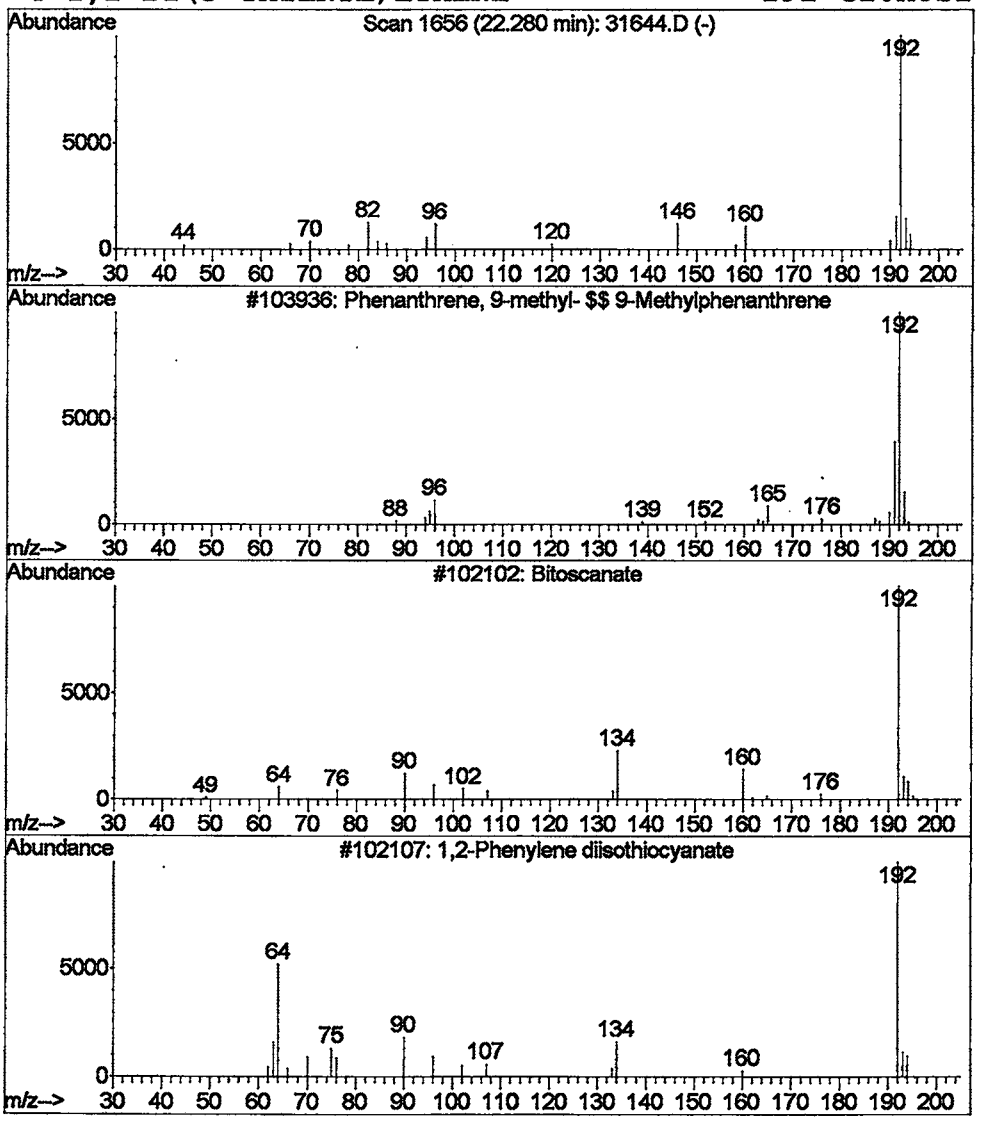
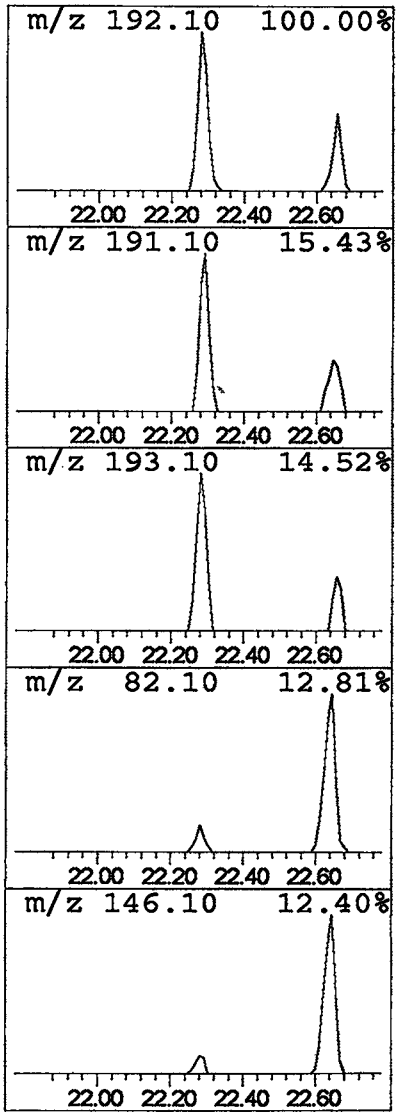
Peak Number 10 Phenanthrene, 9-methyl- $$ ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.15 ug/L	99241	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	59
2	Bitoscanate	192	C8H4N2S2	004044-65-9	59
3	1,2-Phenylene diisothiocyanate	192	C8H4N2S2	071105-17-4	53
4	1,2-DI(3-THIENYL)ETHENE	192	C10H8S2	013640-84-1	53





Data File : C:\MSDCHEM\1\5973N\02JAN17\31644.D Vial: 4
Acq On : 17 Jan 2002 5:19 pm 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

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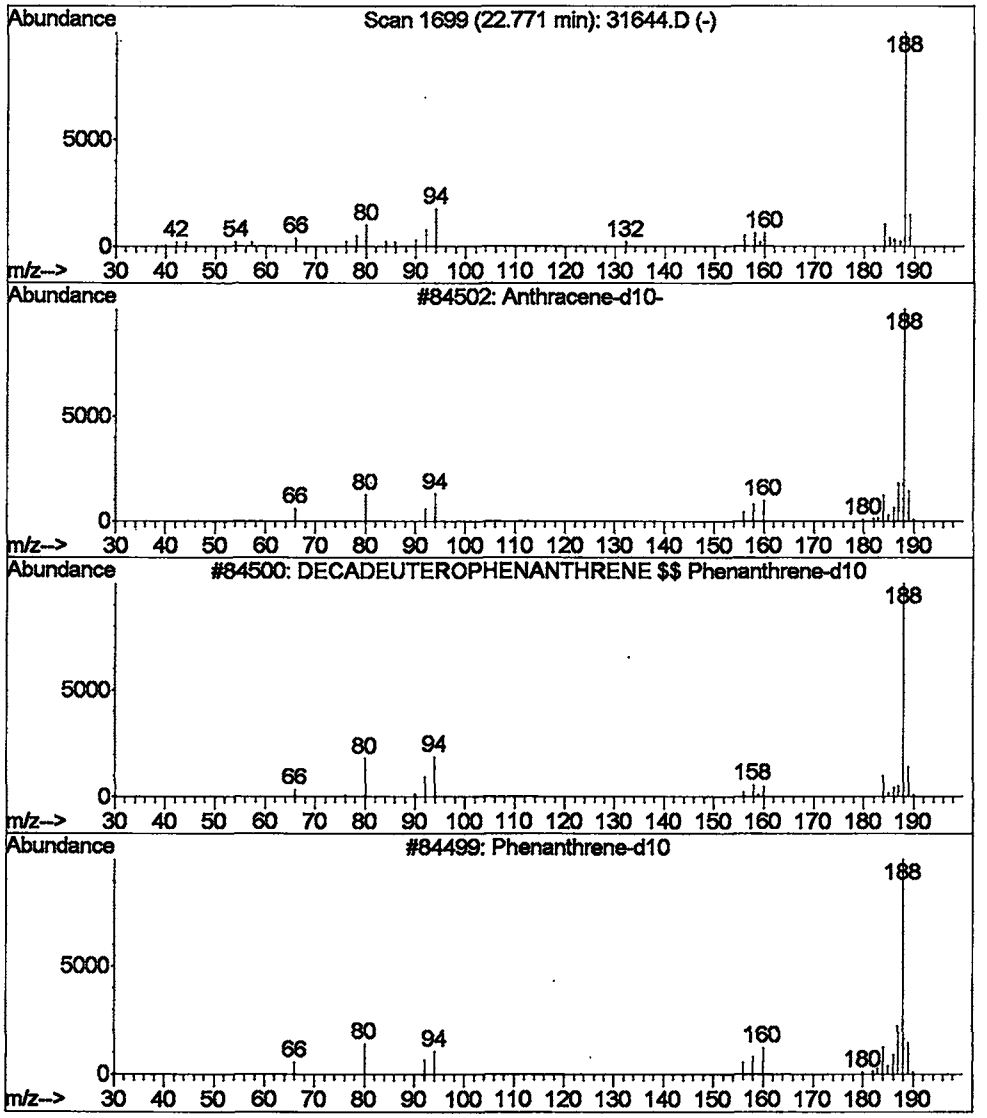
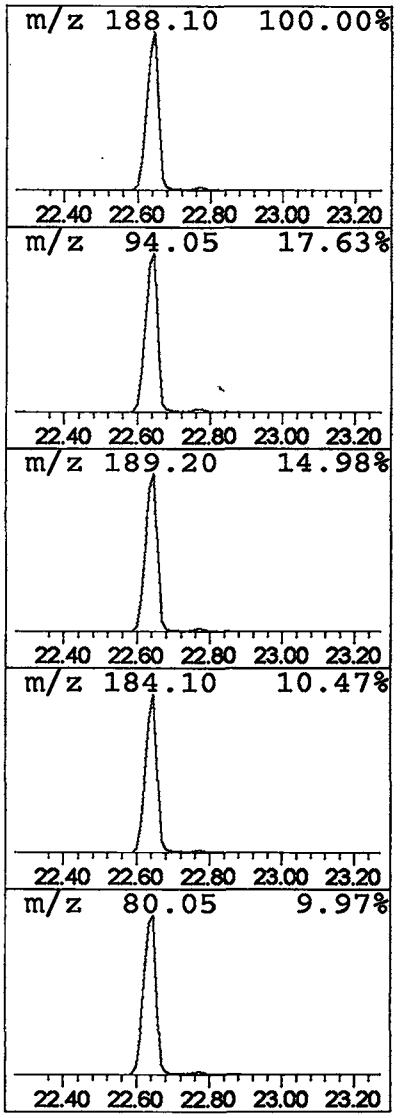
Peak Number 11 Anthracene-d10- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.33 ug/L	213554	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene-d10-	188	C14D10	001719-06-8	90
2	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	87
3	Phenanthrene-d10	188	C14D10	001517-22-2	86
4	Anthracene-D10	188	C14D10	000000-00-0	72





Tentatively Identified Compound (LSC) Summary

Operator ID: Date Acquired: 17 Jan 2002 5:19 pm
Data File: C:\MSDCHEM\1\5973N\02JAN17\31644.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...	3.60	0.1	ug/L	59574	1	9.71	8072350	20.0
Isothiazole (CAS)...	4.24	0.1	ug/L	53655	1	9.71	8072350	20.0
Butanoic acid, 2-...	4.63	0.1	ug/L	53910	1	9.71	8072350	20.0
2-Butenal, 3-meth...	4.82	0.3	ug/L	107924	1	9.71	8072350	20.0
3-(CYCLOHEX-3'-EN...	5.89	4.5	ug/L	1819740	1	9.71	8072350	20.0
2-Propanol, 1-(2-...	9.54	0.2	ug/L	73633	1	9.71	8072350	20.0
2-Propanol, 1-(2-...	9.63	0.2	ug/L	84006	1	9.71	8072350	20.0
2-Propanol, 1-(2-...	9.84	0.3	ug/L	132973	1	9.71	8072350	20.0
Eicosane	21.33	0.1	ug/L	66045	4	22.65	12909400	20.0
Phenanthrene, 9-m...	22.28	0.2	ug/L	99241	4	22.65	12909400	20.0
Anthracene-d10-	22.77	0.3	ug/L	213554	4	22.65	12909400	20.0