User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 01/28/2002 Time: 15:23:58

Sample: AD31585
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 1/28/02 15:23 Ended: 1/28/02 15:23 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		87		5.0

Comments for Sample AD31585 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 01-28-2002 Time: 15:24:41

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\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 22 08:30:04 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

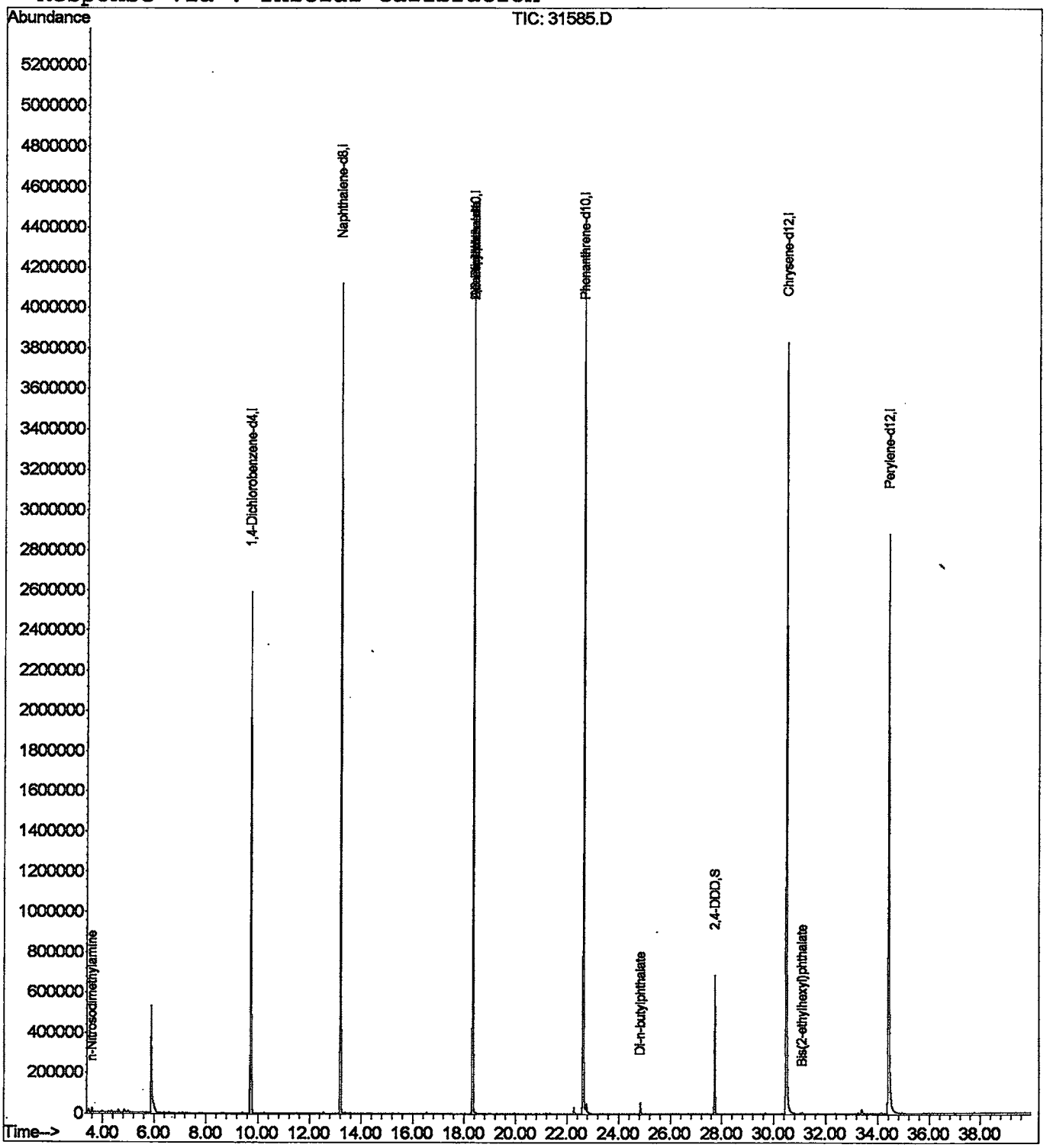
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	961624	20.00	ug/L	-0.01
10) Naphthalene-d8	13.19	136	4011334	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2113183	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.63	188	3582329	20.00	ug/L	-0.03
38) Chrysene-d12	30.49	240	3070253	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	2166696	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	245744	4.34	ug/L	0.00
Spiked Amount 5.000			Recovery = 86.80%			
Target Compounds						Qvalue
2) n-Nitrosodimethylamine	3.59	74	10959	0.27	ug/L #	14
20) Dimethylphthalate	18.34	163	341718	2.45	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	263509	9.68	ug/L #	17
35) Di-n-butylphthalate	24.85	149	70419	0.30	ug/L	94
42) Bis(2-ethylhexyl)phthalate	31.09	149	5516	0.58	ug/L	92

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

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 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\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 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

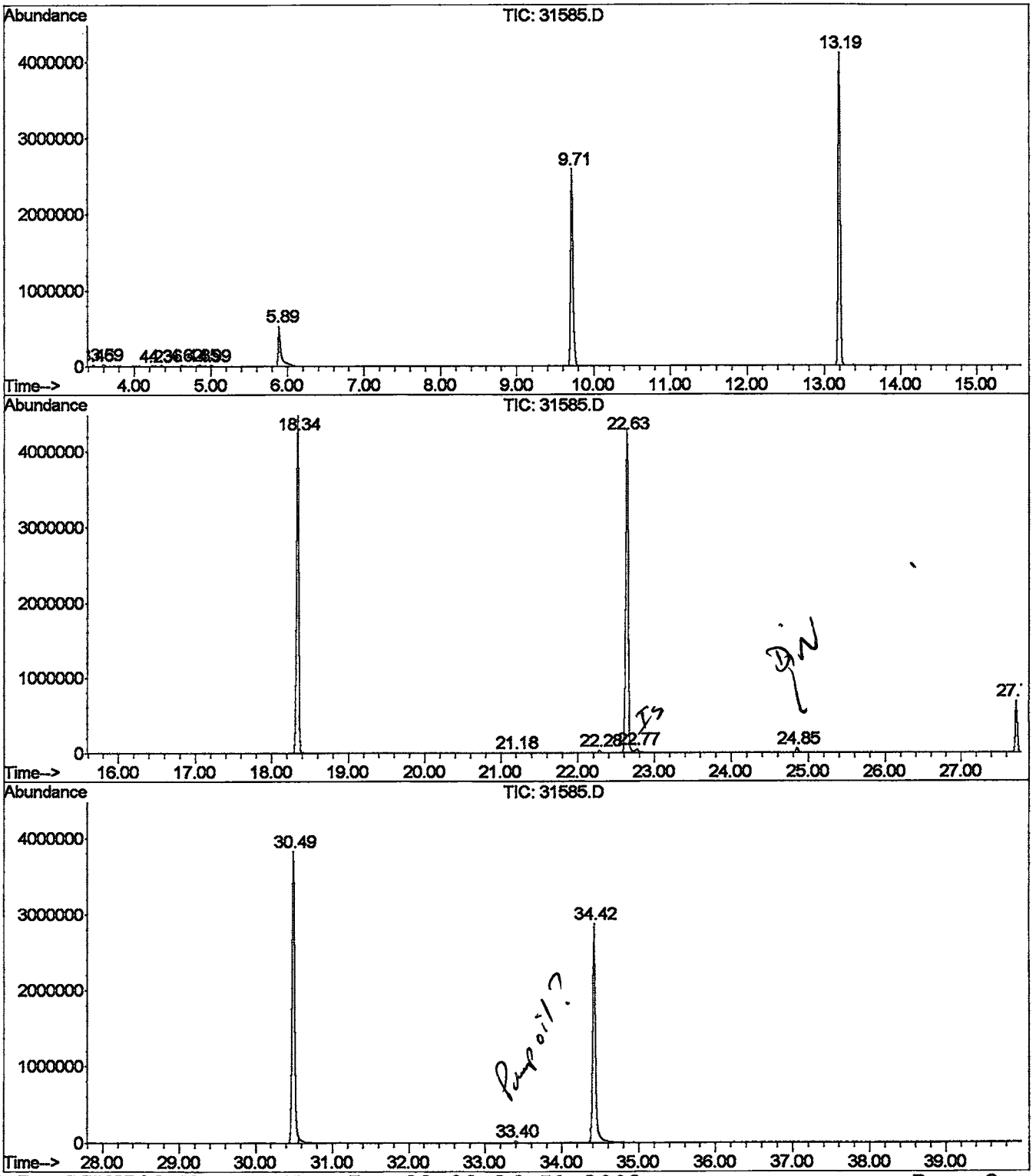
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.465	5	8	11	rVB	17186	25377	0.27%	0.050%
2	3.590	17	19	25	rBV	22722	42132	0.44%	0.083%
3	4.230	71	75	83	rVV3	5351	18774	0.20%	0.037%
4	4.355	83	86	91	rVB	11300	19050	0.20%	0.038%
5	4.618	107	109	117	rVB3	13944	30530	0.32%	0.060%
6	4.846	125	129	139	rBV6	14891	50415	0.53%	0.100%
7	4.995	139	142	149	rVB3	10503	28209	0.30%	0.056%
8	5.885	215	220	251	rVB	529435	1356041	14.28%	2.682%
9	9.710	551	555	563	rBV	2588541	5457493	57.47%	10.795%
10	13.192	855	860	865	rBV	4115782	7697049	81.05%	15.226%
11	18.341	1305	1311	1315	rBV	4482886	8555786	90.09%	16.924%
12	21.184	1553	1560	1571	rVV4	4516	19988	0.21%	0.040%
13	22.280	1653	1656	1661	rBV2	33996	63179	0.67%	0.125%
14	22.634	1681	1687	1693	rBV2	4285624	9496447	100.00%	18.785%
15	22.771	1695	1699	1703	rVB	45976	107417	1.13%	0.212%
16	24.849	1877	1881	1887	rVB	60936	108888	1.15%	0.215%
17	27.726	2127	2133	2139	rVV	685497	1205415	12.69%	2.384%
18	30.489	2369	2375	2381	rBV2	3825405	8866040	93.36%	17.538%
19	33.400	2625	2630	2635	rBV2	21988	47753	0.50%	0.094%
20	34.416	2713	2719	2751	rBV	2876202	7357536	77.48%	14.554%

Sum of corrected areas: 50553519

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN17\31585.D
Operator :
Acquired : 17 Jan 2002 2:50 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 17, 2002
Vial Number: 1
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

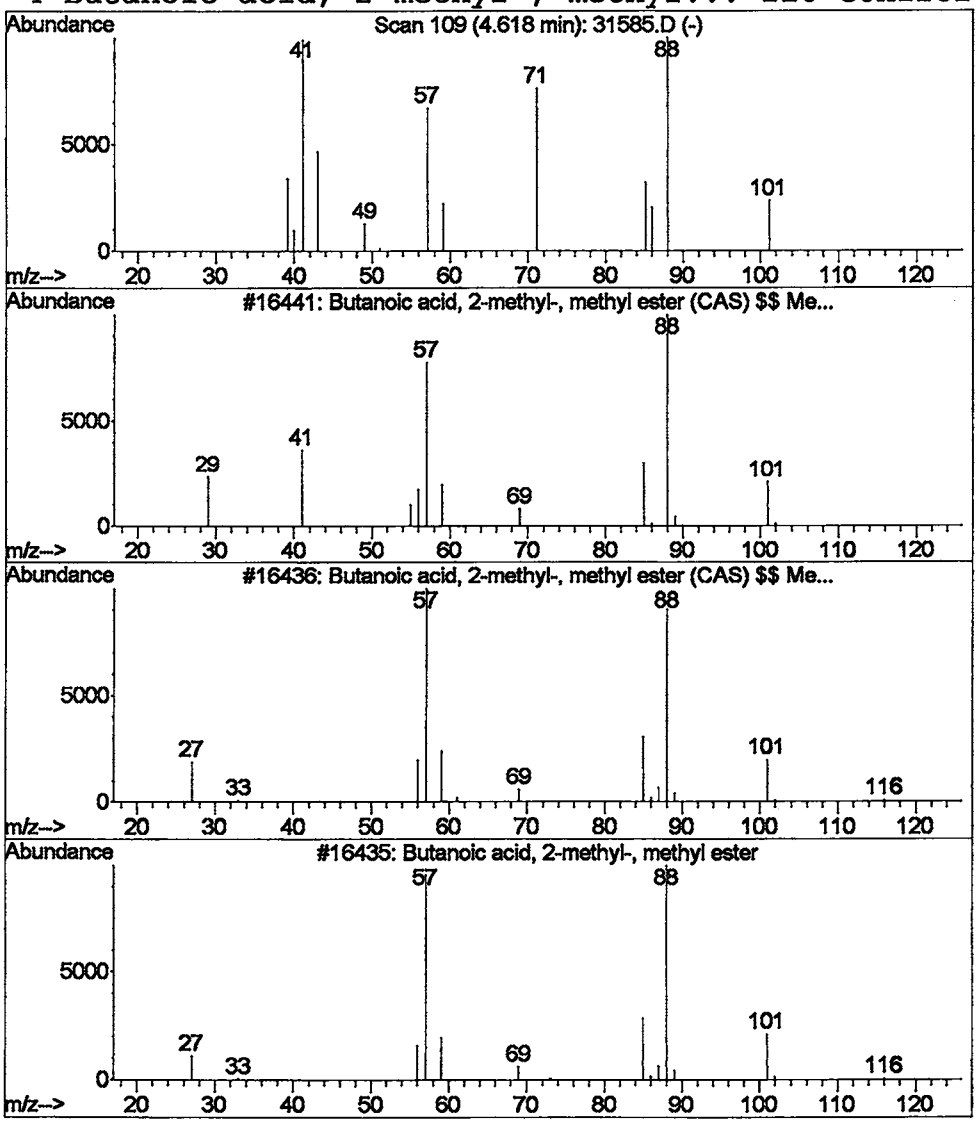
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

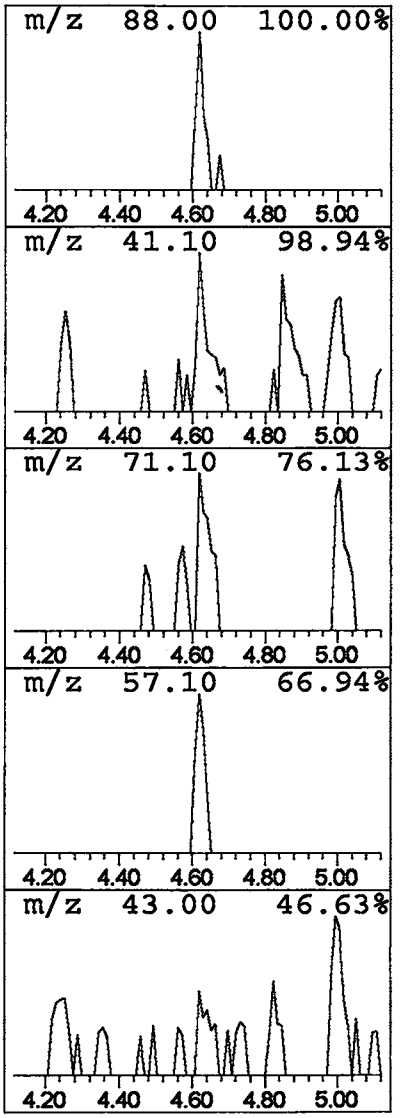
****

Peak Number 1 Butanoic acid, 2-methyl-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	0.11 ug/L	30530	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	43
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	25
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	25
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	25





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

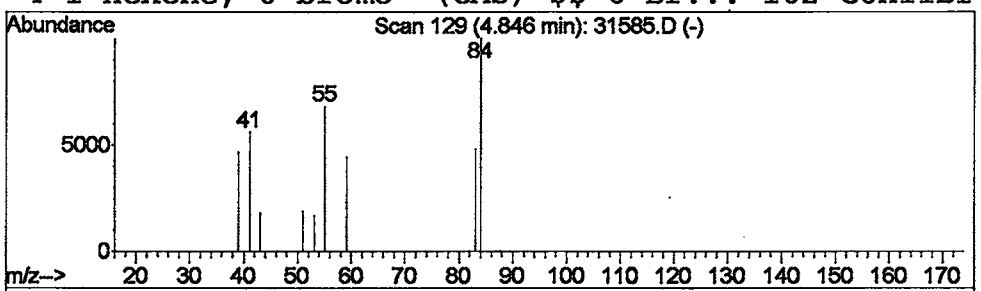
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

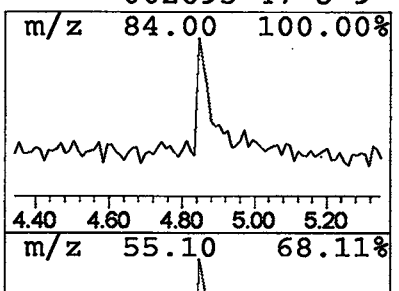
****

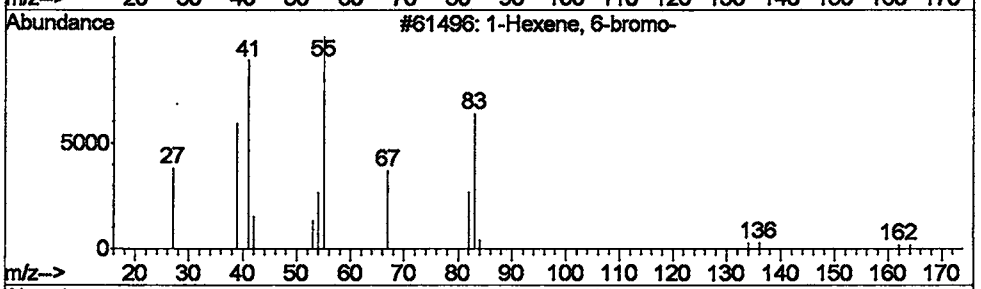
Peak Number 2 1-Hexene, 6-bromo- Concentration Rank 3

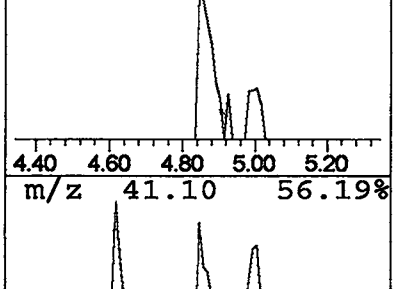
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	0.18 ug/L	50415	1,4-Dichlorobenzene-d4	9.71

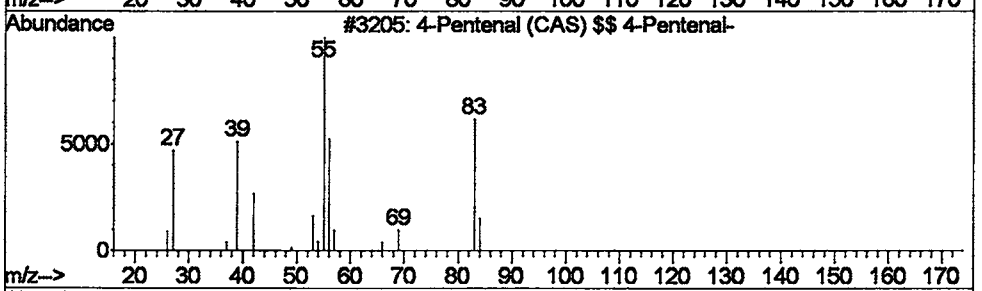
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	12
2	4-Pentenal (CAS) $$ 4-Pentenal-	84	C5H8O	002100-17-6	9
3	1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	9
4	1-Hexene, 6-bromo- (CAS) $$ 6-Br...	162	C6H11Br	002695-47-8	9

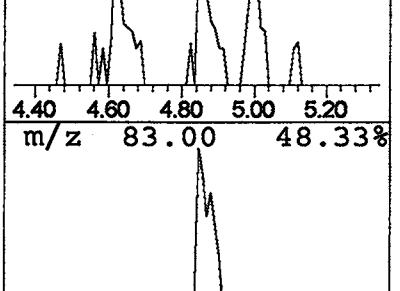


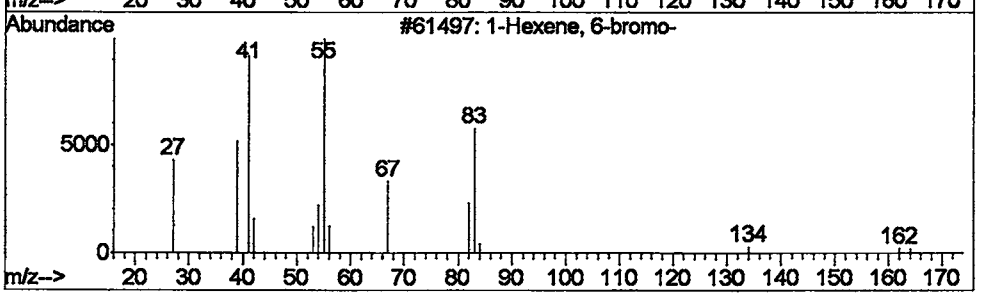


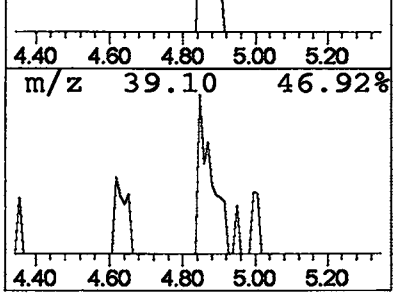












Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

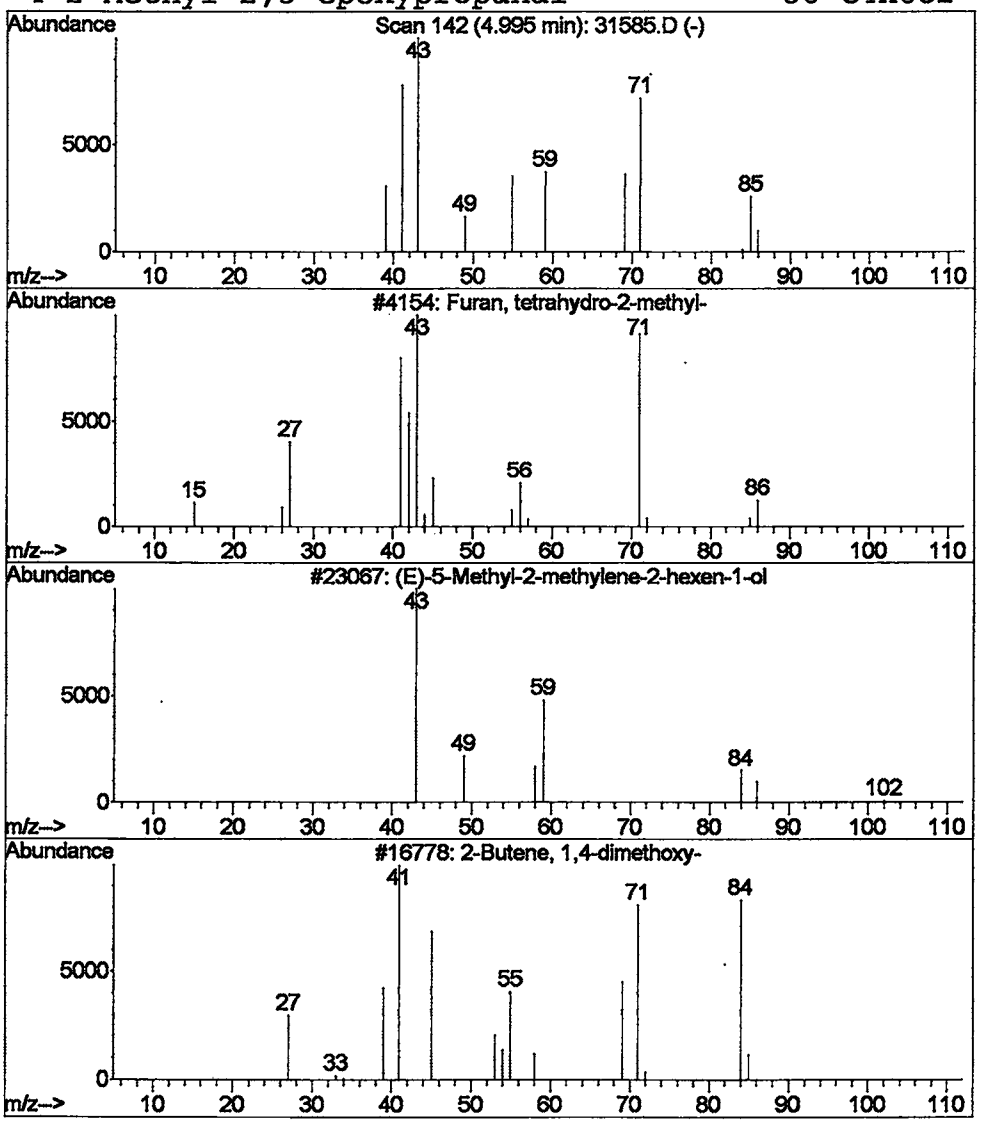
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

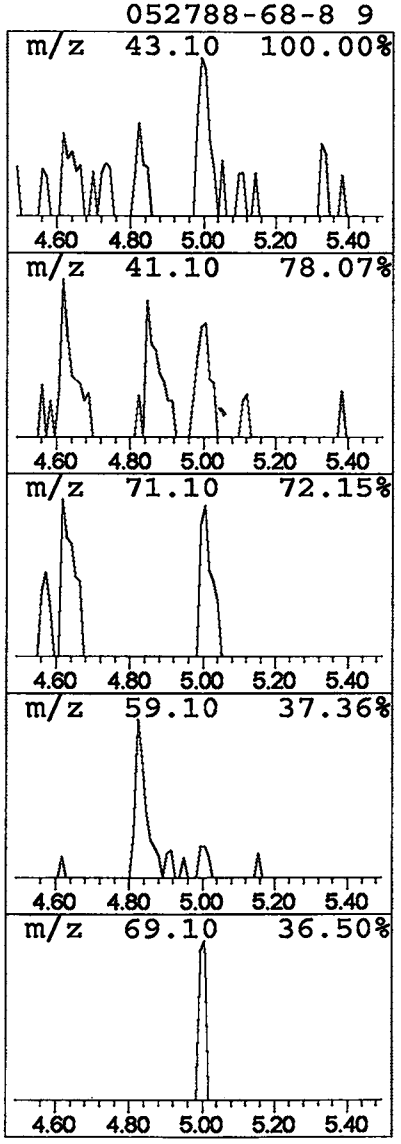
****

Peak Number 3 Furan, tetrahydro-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	0.10 ug/L	28209	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	40
2	(E)-5-Methyl-2-methylene-2-hexen...	126	C8H14O	000000-00-0	23
3	2-Butene, 1,4-dimethoxy-	116	C6H12O2	026649-86-5	17
4	2-Methyl-2,3-epoxypropanal	86	C4H6O2	052788-68-8	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

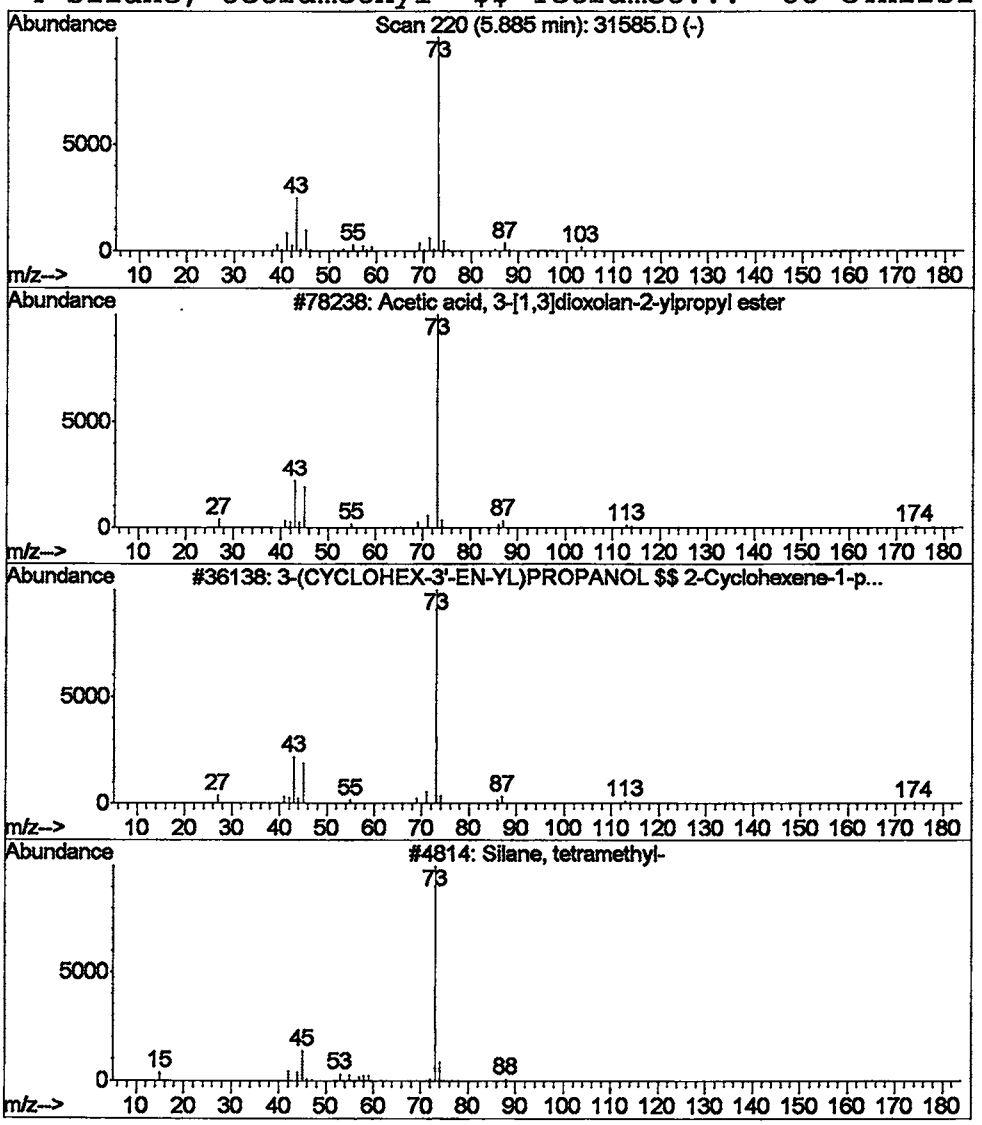
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

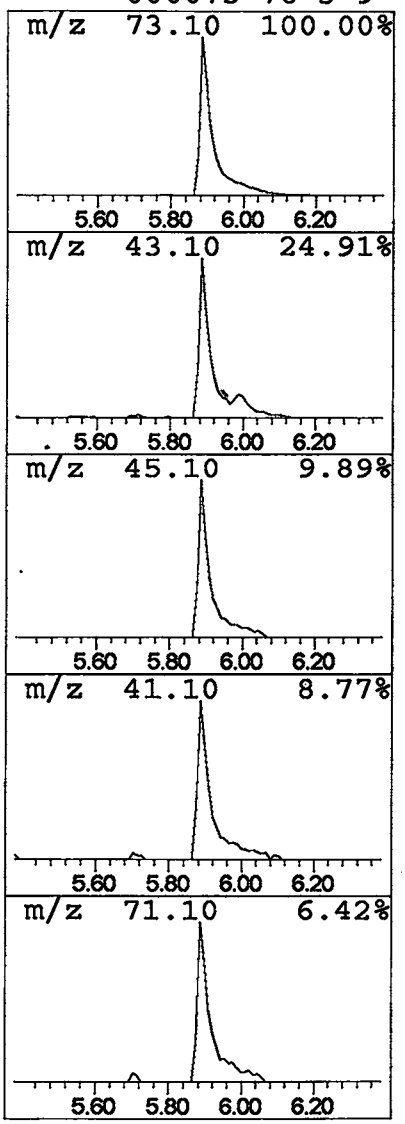
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.97 ug/L	1356040	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 $$...	174	C8H14O4	015745-87-6	33
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	Silane, tetramethyl- $$ Tetramet...	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

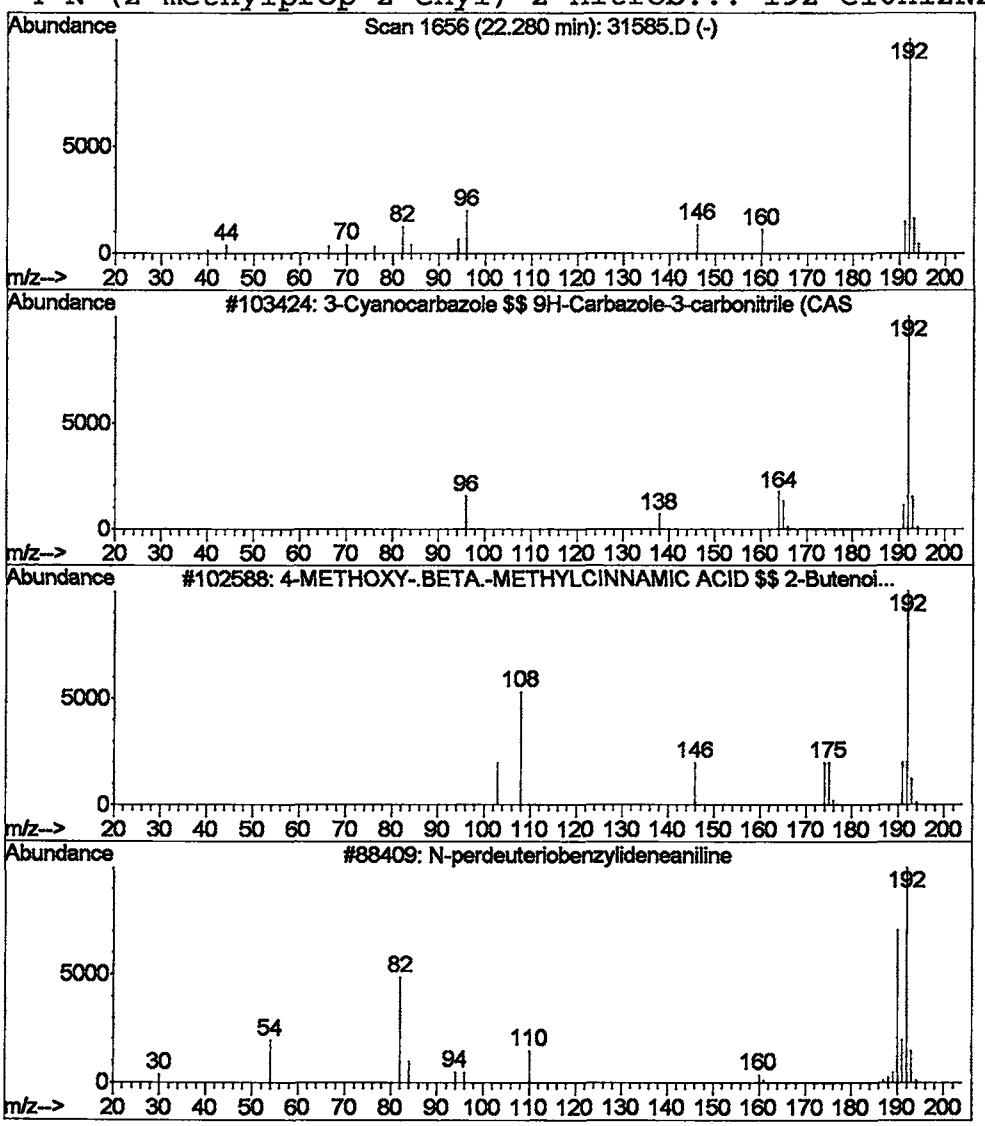
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

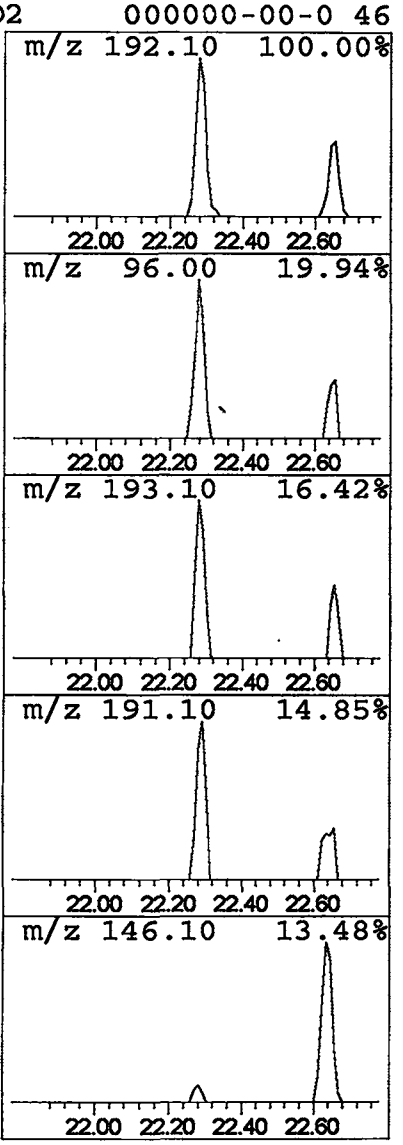
****

Peak Number 5 3-Cyanocarbazole $$ 9H-Carb... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.13 ug/L	63179	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyanocarbazole $$ 9H-Carbazole...	192	C13H8N2	057102-93-9	80
2	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
3	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	46





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 17, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

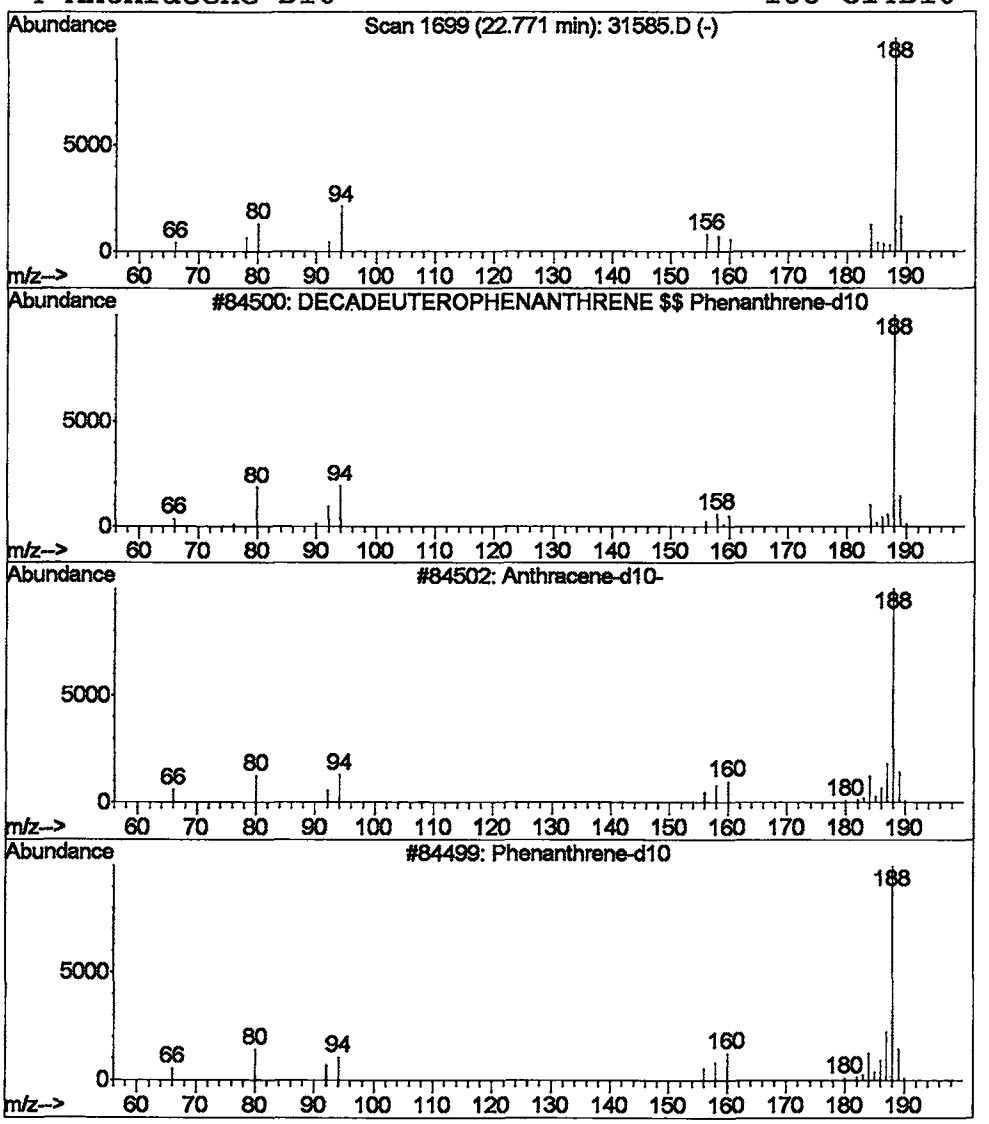
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

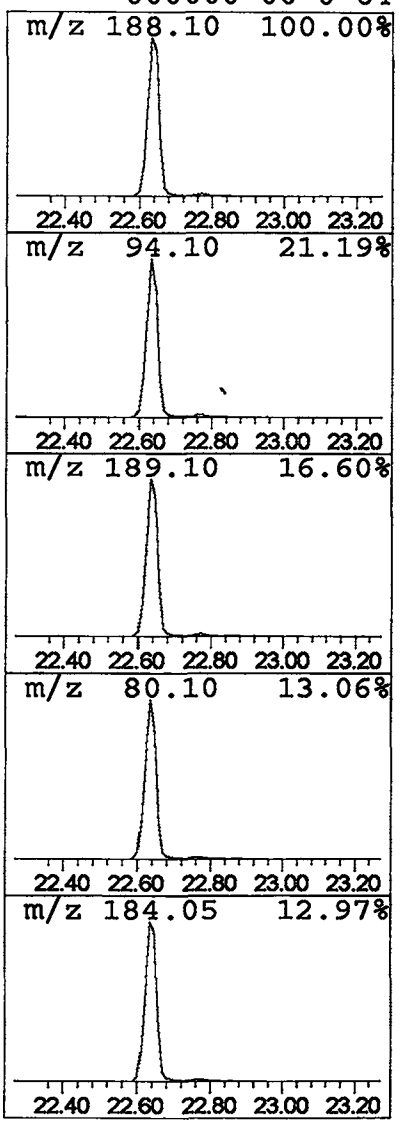
****

Peak Number 6 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.23 ug/L	107417	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	80
2	Anthracene-d10-	188	C14D10	001719-06-8	80
3	Phenanthrene-d10	188	C14D10	001517-22-2	80
4	Anthracene-D10	188	C14D10	000000-00-0	64





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN17\31585.D Vial: 1
Acq On : 17 Jan 2002 2:50 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

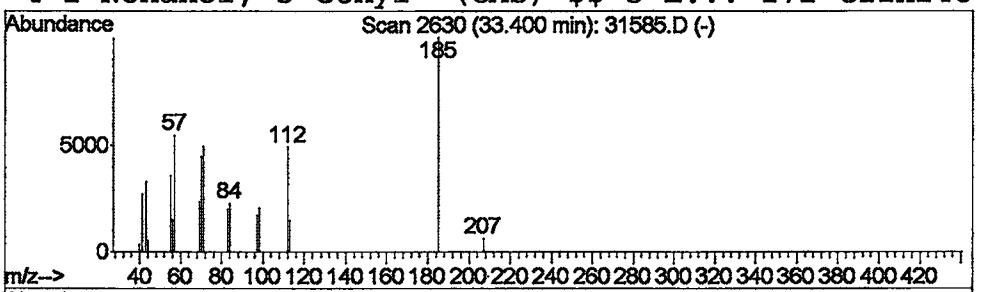
****

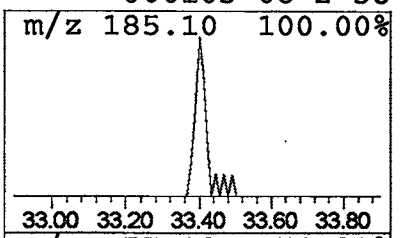
Peak Number 7 8-Benzenesulphonyloxyquinoline Concentration Rank 5

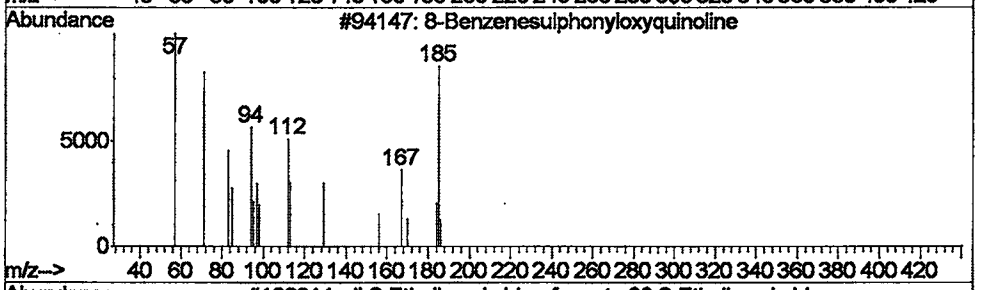
R.T.	EstConc	Area	Relative to ISTD	R.T.
33.40	0.13 ug/L	47753	Perylene-d12	34.42

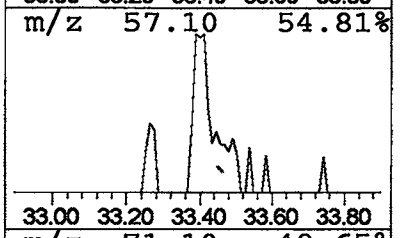
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Benzenesulphonyloxyquinoline	185	C12H11NO	000000-00-0	47
2	dl-2-Ethylhexyl chloroformate $$...	192	C9H17ClO2	024468-13-1	43
3	Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	42
4	2-Nonanol, 5-ethyl- (CAS) $$ 5-E...	172	C11H24O	000103-08-2	38

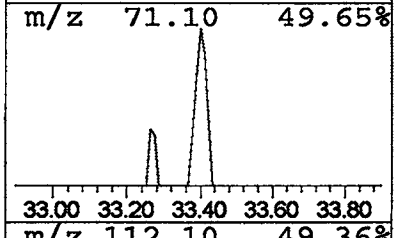
NO GOOD MATCH

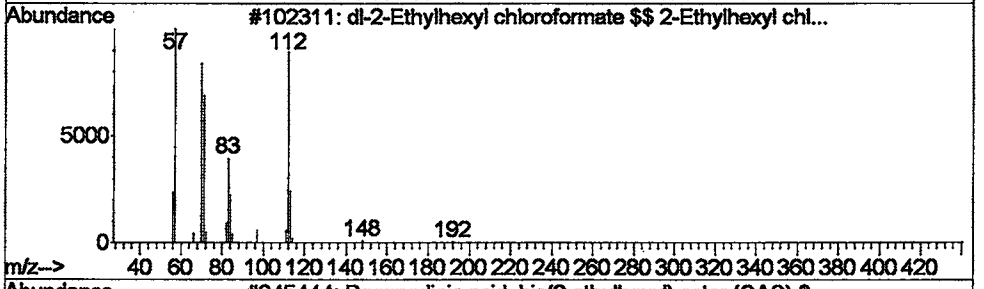


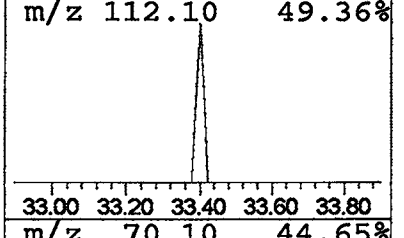


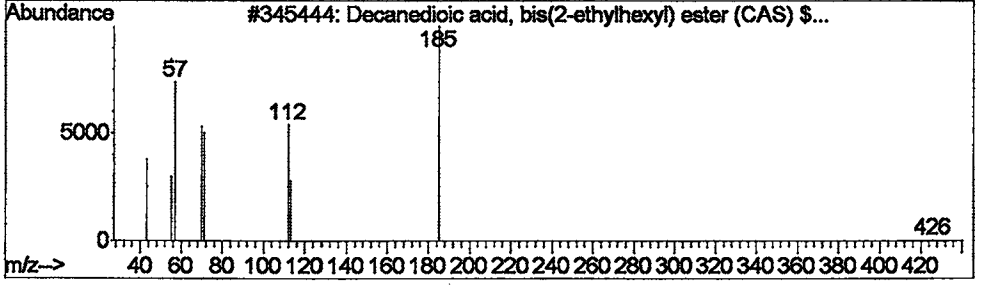


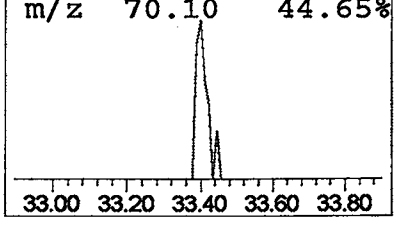












Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 17 Jan 2002 2:50 pm
Data File: C:\MSDCHEM\1\5973N\02JAN17\31585.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, 2-...	4.62	0.1	ug/L	30530	1	9.71	5457490	20.0
1-Hexene, 6-bromo-	4.85	0.2	ug/L	50415	1	9.71	5457490	20.0
Furan, tetrahydro...	4.99	0.1	ug/L	28209	1	9.71	5457490	20.0
Acetic acid, 3-[1...	5.89	5.0	ug/L	1356040	1	9.71	5457490	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	63179	4	22.63	9496450	20.0
DECADEUTEROPHENAN...	22.77	0.2	ug/L	107417	4	22.63	9496450	20.0
8-Benzenesulphony...	33.40	0.1	ug/L	47753	6	34.42	7357540	20.0