ıs & Research
ı: 12:17:56

ıS Scan For Unknowns

Ended: 4/25/02 12:17 Analyst: DLV

Name	Vial	Result	Qualifier	MDL
ımpounds				
		117		10.0

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\041802\7177.D Vial: 14
Acq On : 18 Apr 2002 7:29 pm Operator: Bohlk
Sample : SAMPLE 7177 3/27/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 24 08:43:17 2002 Quant Results File: 5080402BBC.RES

Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Wed Apr 24 08:08:47 2002
Response via : Initial Calibration
DataAcq Meth : 508SCAN

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.42	152	609683	40.00	ug/L	0.01
10) Naphthalene-d8	12.89	136	2590768	40.00	ug/L	0.00
17) Acenaphthene-d10	17.99	164	1412992	40.00	ug/L	0.00
30) Phenanthrene-d10	22.34	188	1948716	40.00	ug/L	0.00
39) Chrysene-d12	30.14	240	1354789	40.00	ug/L	-0.01
45) Perylene-d12	34.01	264	780392	40.00	ug/L	0.00
System Monitoring Compounds						
28) TCMX (SURR)	19.95	244	26440	4.69	ug/L	0.00
Spiked Amount 4.000			Recovery = 117.25%			
38) 2,4-DDD (SURR)	0.00	235	0	0.00	ug/L	
Spiked Amount 10.000			Recovery = 0.00%			
Target Compounds						Qvalue
2) N-nitroso-dimethyl amine	0.00	74	0	N.D.	d	
3) bis(2-chloroethyl) ether	0.00	93	0	N.D.		
4) 1,3 - Dichlorobenze	0.00	146	0	N.D.		
5) 1,4 - Dichlorobenzene	0.00	146	0	N.D.		
6) 1,2 - Dichlorobenzene	0.00	146	0	N.D.		
7) 2,2 ' - oxybis (1-Chloropr	0.00	45	0	N.D.		
8) N-Nitroso-di-n-propylamine	0.00	70	0	N.D.		
9) Hexachloroethane	0.00	117	0	N.D.		
11) Nitrobenzene	0.00	77	0	N.D.		
12) Isophorone	0.00	82	0	N.D.		
13) bis(2-Chloroethoxy) methan	0.00	93	0	N.D.		
14) 1,2,4-Trichlorobenzene	0.00	180	0	N.D.		
15) Naphthalene	0.00	128	0	N.D.		
16) Hexachlorobutadiene	0.00	225	0	N.D.		
18) Hexachlorocyclopentadiene	0.00	237	0	N.D.		
19) 2-chloronaphthalene	0.00	162	0	N.D.		
20) Dimethylphthalate	0.00	163	0	N.D.		
21) 2,6-Dinitrotoluene	0.00	165	0	N.D.	d	
22) Acenaphthylene	0.00	152	0	N.D.		
23) Acenaphthene	0.00	153	0	N.D.		
24) 2,4-Dinitrotoluene	0.00	165	0	N.D.		
25) Diethylphthalate	0.00	149	0	N.D.		
26) 4-Chlorophenyl-phenyl ethe	0.00	204	0	N.D.		
27) Fluorene	0.00	166	0	N.D.		
29) Azobenzen/ 1,2-Diphenylhyd	0.00	77	0	N.D.		
31) N-Nitrosodiphenylamine	0.00	169	0	N.D.		
32) 4-Bromophenyl-phenyl ether	0.00	248	0	N.D.		
33) Hexachlorobenzene	0.00	284	0	N.D.		
34) Phenanthrene	0.00	178	0	N.D.		
35) Anthracene	0.00	178	0	N.D.		
36) Di-n-butylphthalate	0.00	149	0	N.D.		
37) Fluoranthene	0.00	202	0	N.D.		
40) Pyrene	0.00	202	0	N.D.		
41) Butylbenzylphthalate	0.00	149	0	N.D.		
42) Benzo (a) antracene	0.00	228	0	N.D.	d	
43) Bis (2-ethylhexyl) phthala	30.77	149	115693	3.45	ug/L	93
44) Chrysene	0.00	228	0	N.D.	d	

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

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\041802\7177.D Vial: 14
Acq On : 18 Apr 2002 7:29 pm Operator: Bohlk
Sample : SAMPLE 7177 3/27/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 24 08:43:17 2002 Quant Results File: 5080402BBC.RES

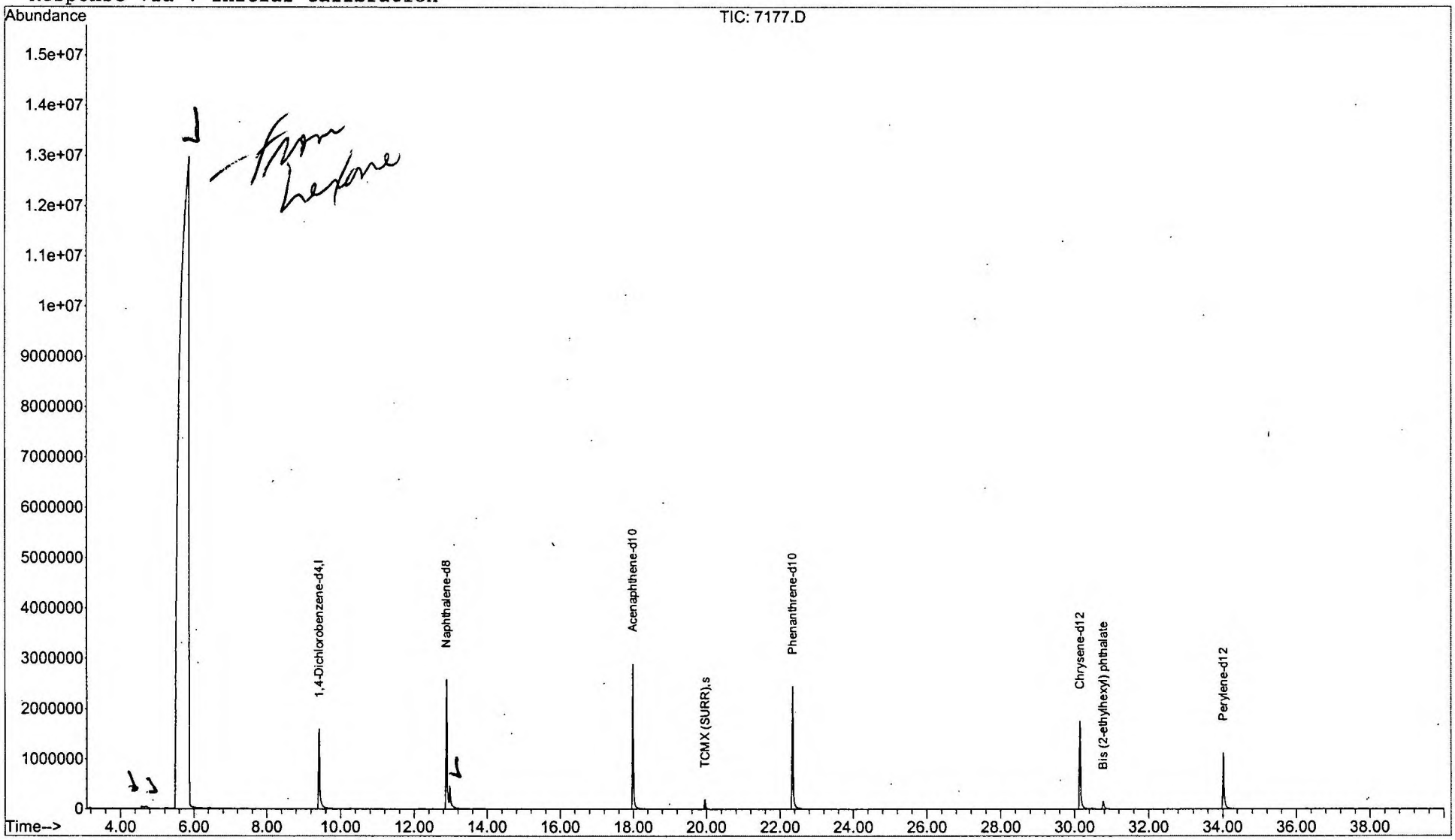
Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Wed Apr 24 08:08:47 2002
Response via : Initial Calibration
DataAcq Meth : 508SCAN

Compound	R.T.	QIon	Response	Conc Unit	Qvalue
46) Di-n-Octylphthalate	0.00	149	0	N.D.	
47) Benzo (b) fluoranthene	0.00	252	0	N.D.	
48) Benzo (k) fluoranthene	0.00	252	0	N.D.	
49) Benzo (a) pyrene	0.00	252	0	N.D.	d
50) Indeno (1,2,3-cd) pyrene	0.00	276	0	N.D.	
51) Dibenz (a,h) anthracene	0.00	278	0	N.D.	
52) Benzo (g,h,i) perylene	0.00	276	0	N.D.	

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

Data File : C:\MSDCHEM\1\DATA\041802\7177.D Vial: 14
Acq On : 18 Apr 2002 7:29 pm Operator: Bohlk
Sample : SAMPLE 7177 3/27/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 24 8:43 2002 Quant Results File: 5080402BBC.RES

Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Wed Apr 24 08:08:47 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\041802\7177.D Vial: 14
Acq On : 18 Apr 2002 7:29 pm Operator: Bohlk
Sample : SAMPLE 7177 3/27/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

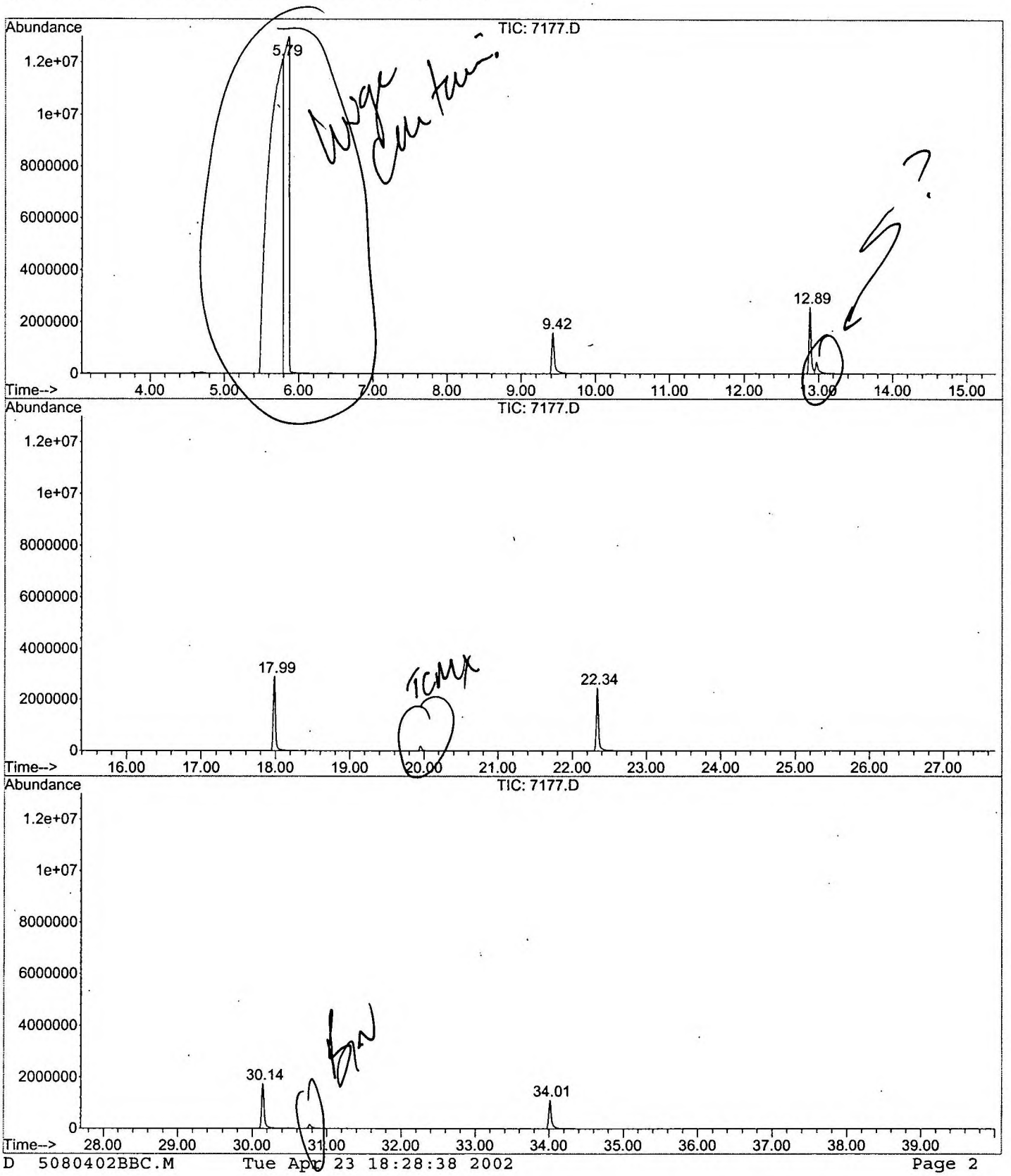
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.788	407	461	462	rBV	12100870	161136963	100.00%	85.207%
2	9.425	1073	1080	1113	rBV	1597096	4023396	2.50%	2.128%
3	12.885	1661	1669	1679	rBV	2586645	5269918	3.27%	2.787%
4	17.991	2529	2538	2559	rBV	2888786	6020999	3.74%	3.184%
5	22.339	3269	3278	3299	rBV2	2447843	5588587	3.47%	2.955%
6	30.142	4597	4606	4630	rBV2	1745682	4258951	2.64%	2.252%
7	34.014	5255	5265	5283	rBV2	1116241	2813801	1.75%	1.488%

Sum of corrected areas: 189112615

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\041802\7177.D
Operator : Bohlk
Acquired : 18 Apr 2002 7:29 pm using AcqMethod 508SCAN
Instrument : Instrumen
Sample Name: SAMPLE 7177 3/27/02
Misc Info :
Vial Number: 14
Quant File :5080402BBC.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\041802\7177.D Vial: 14
Acq On : 18 Apr 2002 7:29 pm Operator: Bohlk
Sample : SAMPLE 7177 3/27/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.P

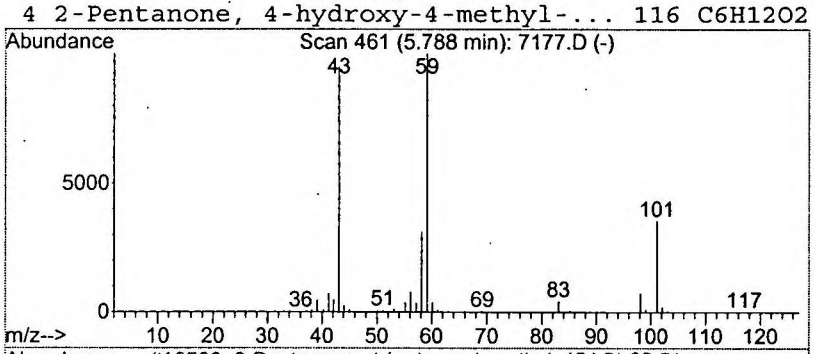
Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Library : C:\DATABASE\WILEY7N.L

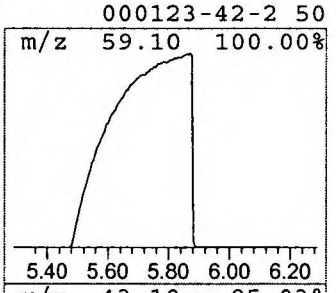
****

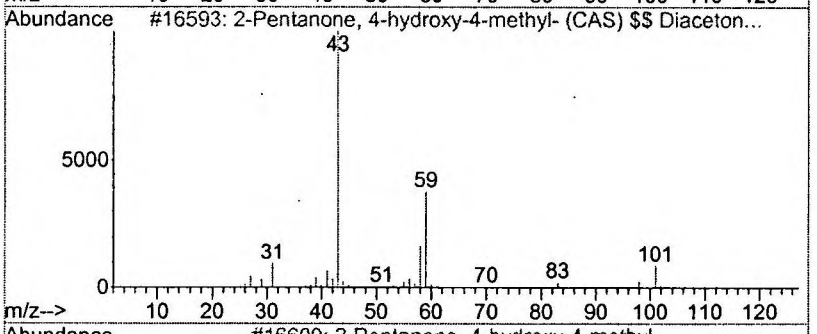
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

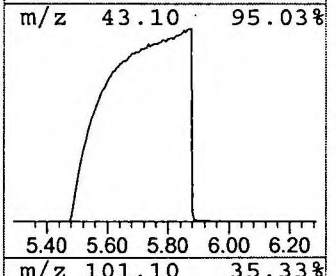
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.79	1602.00 ug/L	161137000	1,4-Dichlorobenzene-d4	9.42

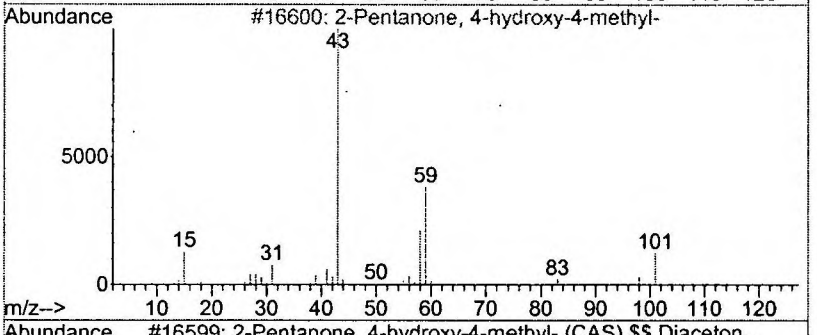
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	78
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	53
4	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	50

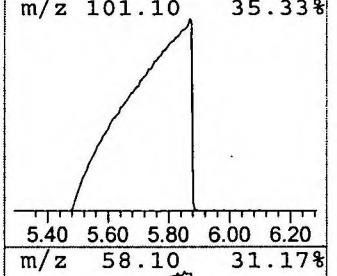


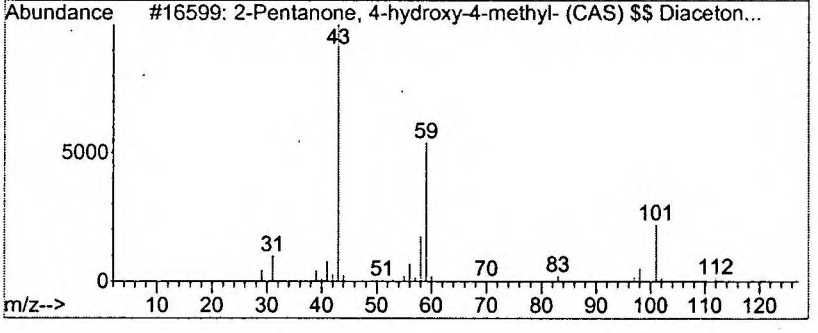


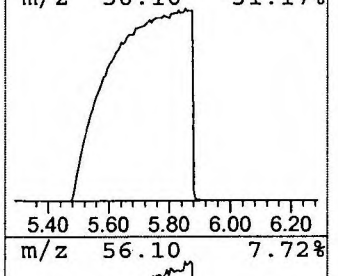


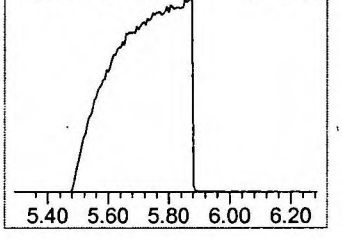












Tentatively Identified Compound (LSC) summary

Operator ID: Bohlk Date Acquired: 18 Apr 2002 7:29 pm
Data File: C:\MSDCHEM\1\DATA\041802\7177.D
Name: SAMPLE 7177 3/27/02
Misc:
Method: C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title: Quantitation For Method 508gcscan
Library Searched: C:\DATABASE\WILEY7N.L

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.79	1602.0	ug/L	161137000	1	9.42	4023400	40.0