

User: Vinci, David L
 Westchester Dept. of Labs & Research
 Date: 03/29/2002 Time: 10:49:04

Sample: AE03736
 Analysis: \$GCMS GCMS Scan For Unknowns
 Units: ug
 Started: 3/29/02 10:48 Ended: 3/29/02 10:48 Analyst: DLV
 Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds				
2	Surr 24-DDD	USPEC	133		5.0

Vassiler
 2/14/02

05079

FD Chem
 Data, MS

Comments for Sample AE03736 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 03-29-2002 Time: 10:51:35

The GCMS scan, from 35 to 550 amu, reveals the presence of n-Octylester Lauric acid at an estimated level of 0.88 ug/l and with a fit of 64 out of 100. The recoveries for 5 of the 43 compounds in the LCS Standard were outside of their acceptance limits. New limits will be calculated.

Quantitation Report

(QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\031202\3736.D

Vial: 61

Acq On : 13 Mar 2002 7:08 am

Operator: McLean

Sample : SAMPLE 3736 2/19/02

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: BENZO.P

Quant Time: Mar 15 14:17:05 2002

Quant Results File: 5080302.RES

Quant Method : C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)

Title : Quantitation For Method 508gcscan

Last Update : Thu Mar 14 13:02:27 2002

Response via : Initial Calibration

DataAcq Meth : 508SCAN

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.55	150	1609628	20.00	ug/L	0.00
10) Naphthalene-d8	13.03	136	4391404	20.00	ug/L	0.00
17) Acenaphthene-d10	18.14	164	2423562	20.00	ug/L	0.00
29) Phenanthrene-d10	22.50	188	3823728	20.00	ug/L	0.00
38) Chrysene-d12	30.31	240	3638940	20.00	ug/L	0.00
44) Perylene-d12	34.19	264	2176745	20.00	ug/L	0.00

System Monitoring Compounds

37) 2,4-ddd surr	27.43	235	304189	6.67	ug/L	0.00
Spiked Amount	5.000		Recovery	=	133.40%	

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.		
28) Azobenzen/ 1,2-Diphenylhyd	0.00	77	0	N.D.		
30) N-Nitrosodiphenylamine	0.00	169	0	N.D.		
31) 4-Bromophenyl-phenyl ether	0.00	248	0	N.D.		
32) Hexachlorobenzene	0.00	284	0	N.D.		
33) Phenanthrene	0.00	178	0	N.D.		
34) Anthracene	0.00	178	0	N.D.		
35) Di-n-butylphthalate	0.00	149	0	N.D.	d	
36) Fluoranthene	0.00	202	0	N.D.		
39) Pyrene	0.00	202	0	N.D.		
40) Butylbenzylphthalate	0.00	149	0	N.D.		
41) Benzo (a) anthracene	0.00	228	0	N.D.	d	
42) Bis (2-ethylhexyl) phthala	30.91	149	86840	0.61	ug/L	97
43) Chrysene	0.00	228	0	N.D.	d	
45) Di-n-Octylphthalate	0.00	149	0	N.D.		
46) Benzo (b) fluoranthene	0.00	252	0	N.D.		

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

3736.D 5080302.M Fri Mar 15 14:18:07 2002

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\031202\3736.D Vial: 61
 Acq On : 13 Mar 2002 7:08 am Operator: McLean
 Sample : SAMPLE 3736 2/19/02 Inst : Instrumen
 Misc : Multiplr: 1.00
 MS Integration Params: BENZO.P
 Quant Time: Mar 15 14:17:05 2002 Quant Results File: 5080302.RES

Quant Method : C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)
 Title : Quantitation For Method 508gcscan
 Last Update : Thu Mar 14 13:02:27 2002
 Response via : Initial Calibration
 DataAcq Meth : 508SCAN

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

 (#) = qualifier out of range (m) = manual integration
 3736.D 5080302.M Fri Mar 15 14:18:08 2002

Data File : C:\MSDCHEM\1\DATA\031202\3736.D

Vial: 61

Acq On : 13 Mar 2002 7:08 am

Operator: McLean

Sample : SAMPLE 3736 2/19/02

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: BENZO.P

Quant Time: Mar 15 14:17 2002

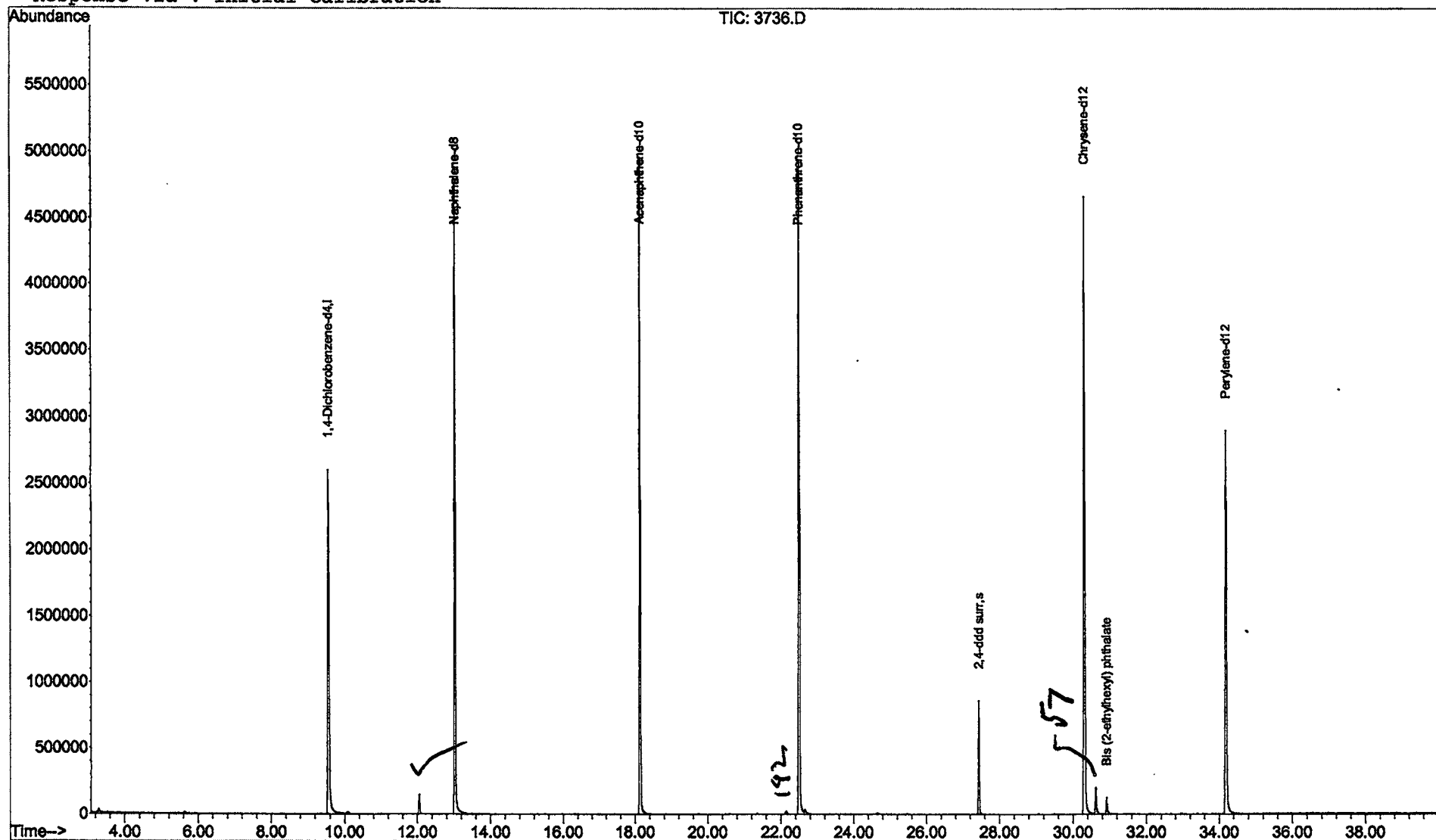
Quant Results File: 5080302.RES

Method : C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)

Title : Quantitation For Method 508gcscan

Last Update : Thu Mar 14 13:02:27 2002

Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\031202\3736.D

Acq On : 13 Mar 2002 7:08 am

Sample : SAMPLE 3736 2/19/02

Misc :

MS Integration Params: LSCINT.P

Vial: 61

Operator: McLean

Inst : Instrumen

Multiplr: 1.00

Method : C:\MSDCHEM\1\5973N\5080302.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

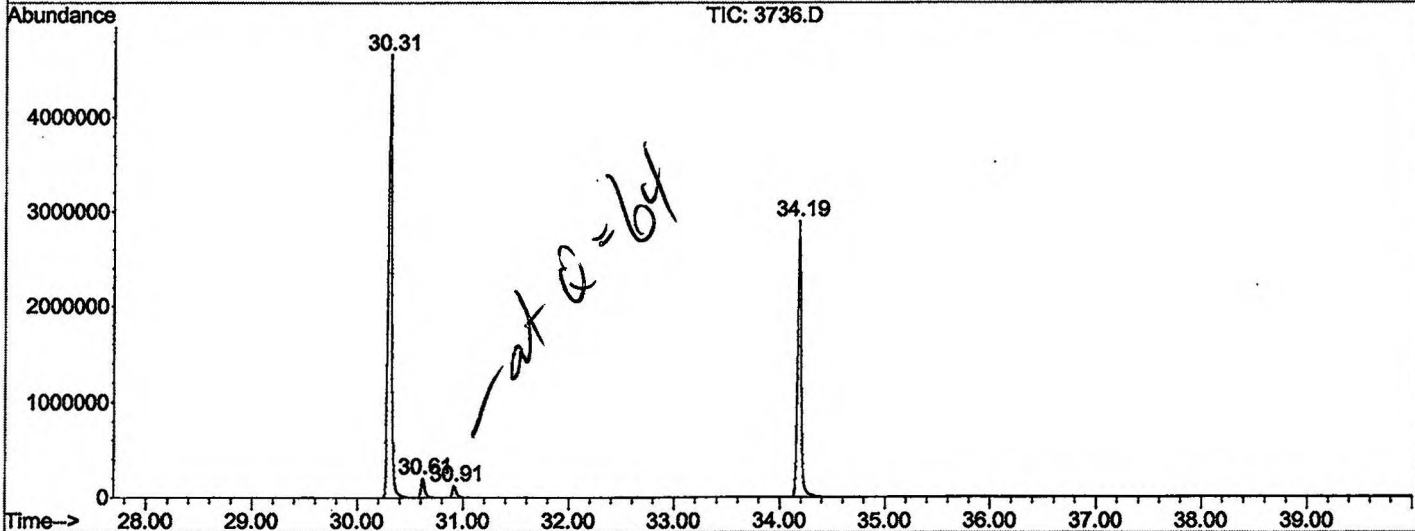
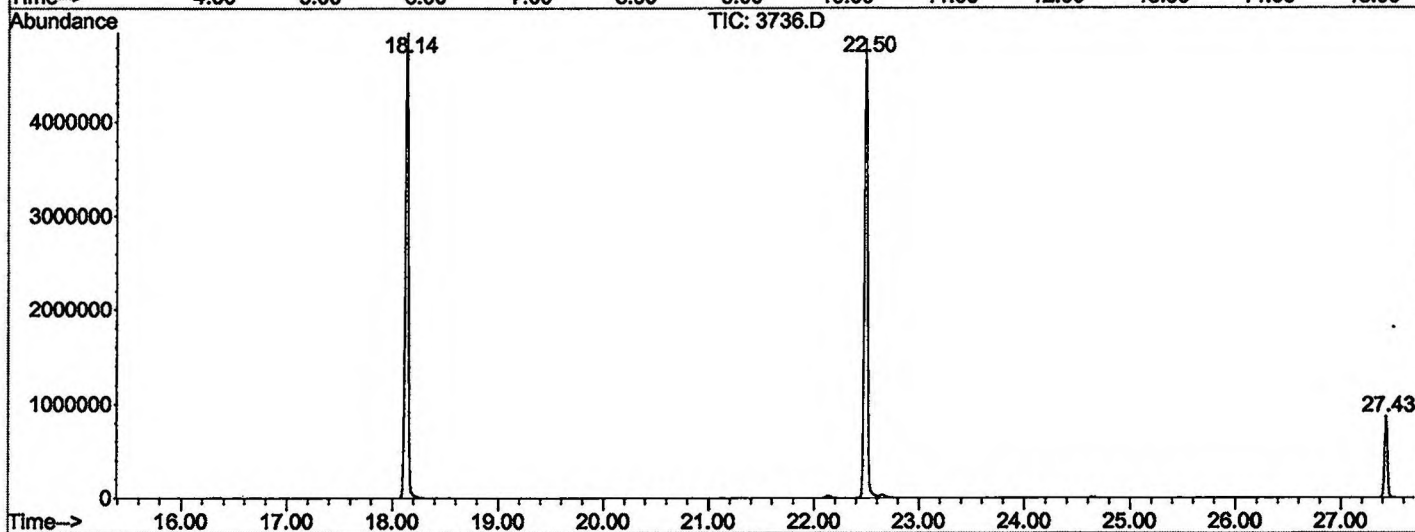
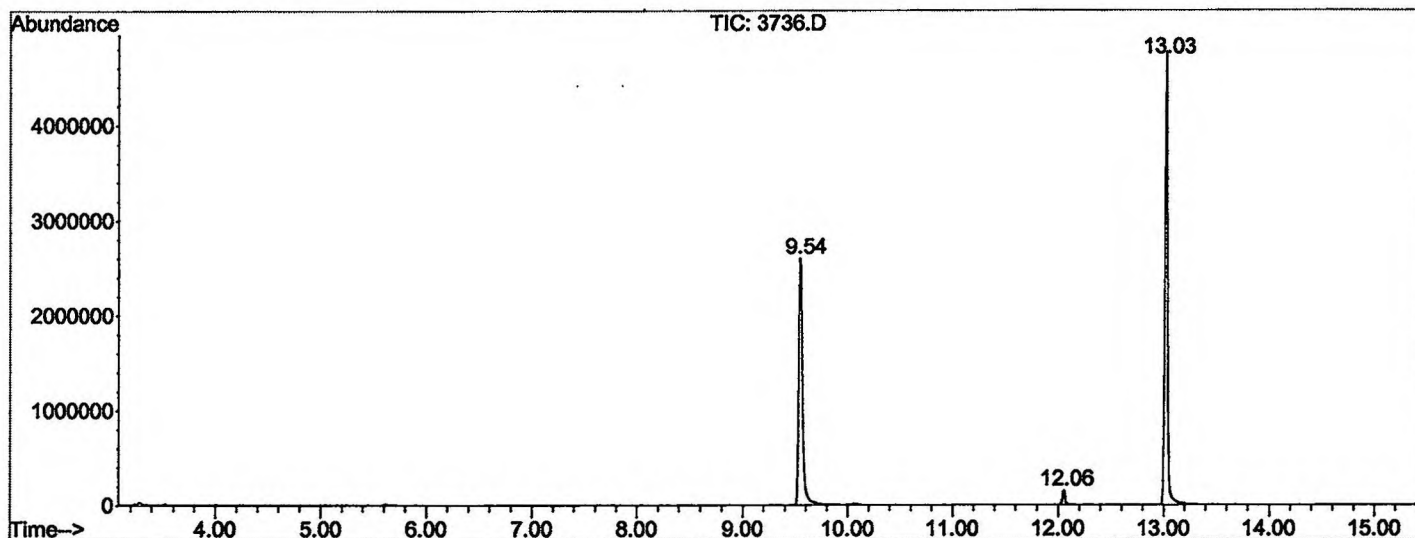
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.543	709	713	737	rBV	2598889	6727579	63.25%	11.757%
2	12.055	985	990	995	rVB	148008	256159	2.41%	0.448%
3	13.026	1091	1097	1112	rBV	4769654	9378217	88.17%	16.390%
4	18.142	1654	1661	1675	rBV	4951427	10130594	95.24%	17.705%
5	22.495	2135	2141	2155	rBV2	4884168	10499215	98.71%	18.349%
6	27.430	2680	2685	2693	rBV	860965	1605073	15.09%	2.805%
7	30.314	2995	3003	3025	rBV2	4663726	10636527	100.00%	18.589%
8	30.613	3031	3036	3045	rBV	200552	469439	4.41%	0.820%
9	30.913	3064	3069	3081	rBV	124075	303466	2.85%	0.530%
10	34.187	3422	3430	3449	rBV2	2898228	7213655	67.82%	12.607%

Sum of corrected areas: 57219924

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\031202\3736.D
 Operator : McLean
 Acquired : 13 Mar 2002 7:08 am using AcqMethod 508SCAN
 Instrument : Instrumen
 Sample Name: SAMPLE 3736 2/19/02
 Misc Info :
 Vial Number: 61
 Quant File :5080302.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\031202\3736.D
Acq On : 13 Mar 2002 7:08 am
Sample : SAMPLE 3736 2/19/02
Misc :
MS Integration Params: LSCINT.P

Vial: 61
Operator: McLean
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)

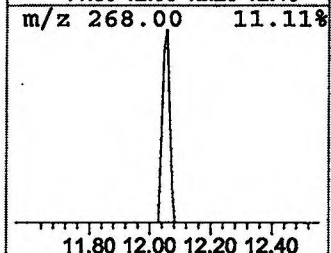
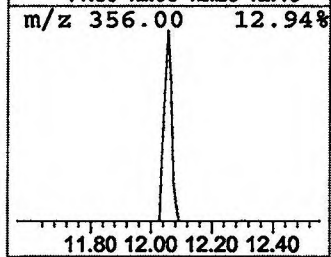
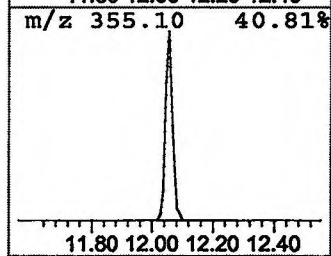
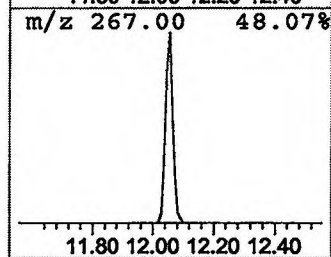
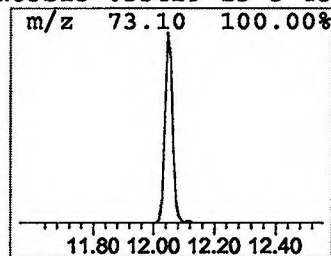
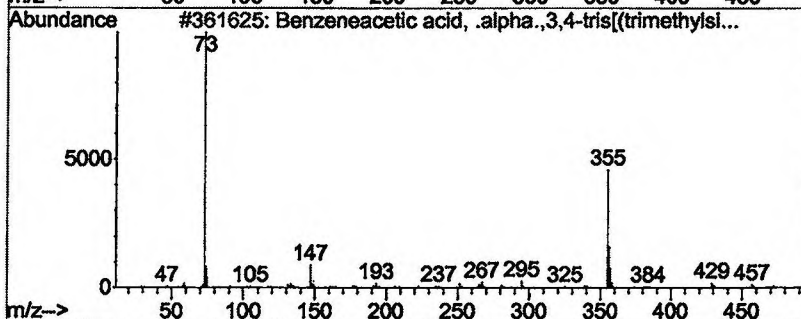
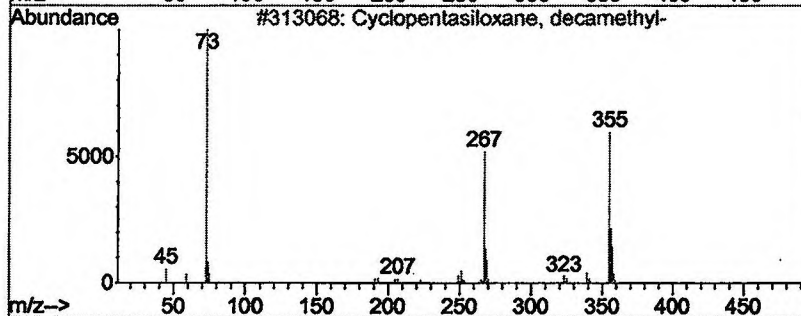
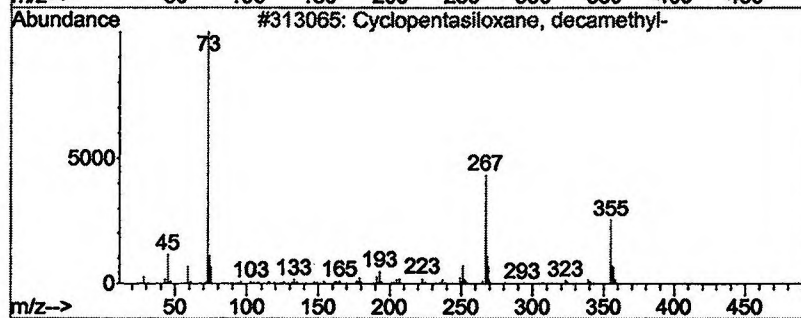
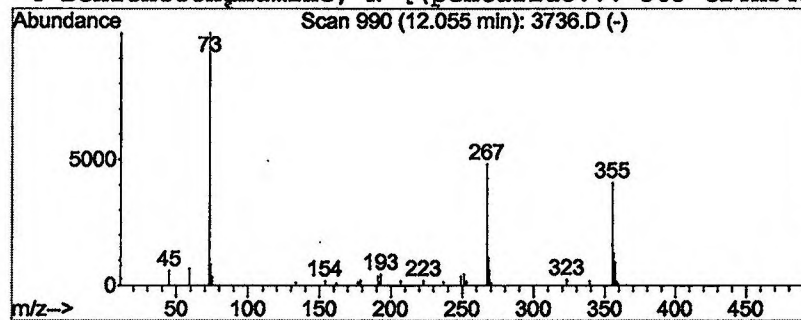
Title : Quantitation For Method 508gcscan

Library : C:\DATABASE\WILEY7N.L

Peak Number 1 Cyclopentasiloxane, decamet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	0.55 ug/L	256159	Naphthalene-d8	13.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	68
2			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	47
3			Benzeneacetic acid, .alpha.,3,4-...	472	C20H40O5Si4	037148-65-5	47
4			Benzeneethanamine, N-[(pentafluo...	563	C24H34F5NO3Si3	055429-13-5	43



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\031202\3736.D
 Acq On : 13 Mar 2002 7:08 am
 Sample : SAMPLE 3736 2/19/02
 Misc :
 MS Integration Params: LSCINT.P

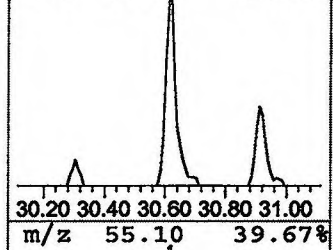
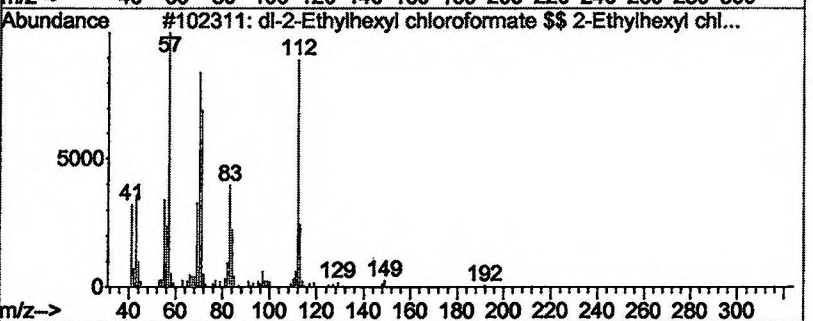
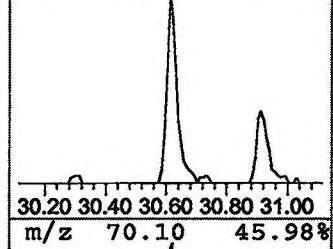
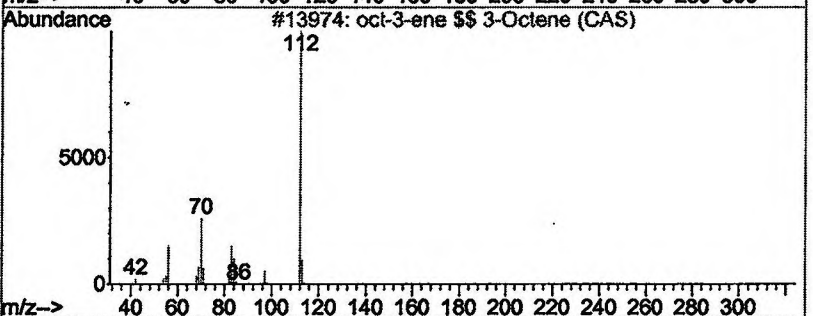
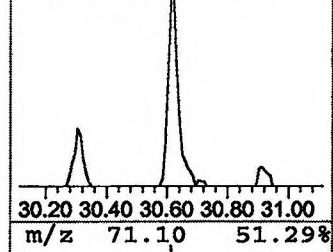
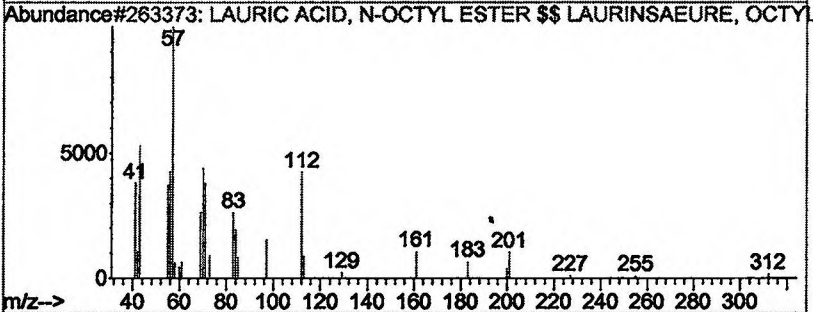
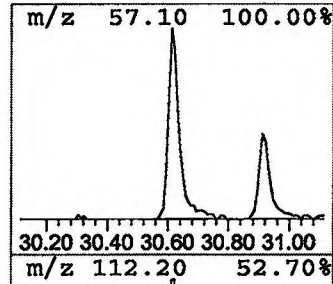
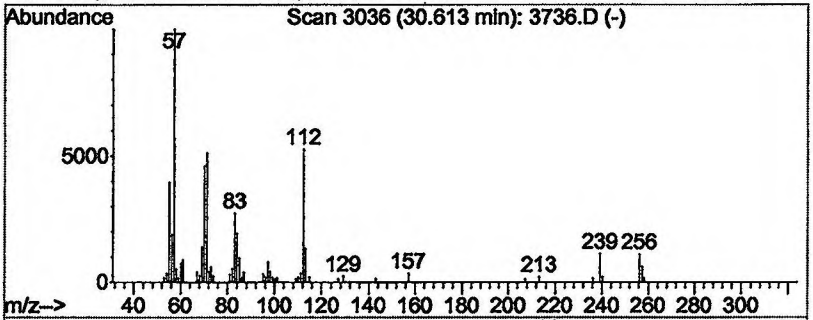
Vial: 61
 Operator: McLean
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)
 Title : Quantitation For Method 508gcscan
 Library : C:\DATABASE\WILEY7N.L

 Peak Number 2 LAURIC ACID, N-OCTYL ESTER ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.61	0.88 ug/L	469439	Chrysene-d12	30.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		LAURIC ACID, N-OCTYL ESTER \$\$ LA...	312	C20H40O2	000000-00-0	64
2		oct-3-ene \$\$ 3-Octene (CAS)	112	C8H16	000592-98-3	60
3		dl-2-Ethylhexyl chloroformate \$\$...	192	C9H17ClO2	024468-13-1	59
4		DI(2-ETHYLHEXYL) MALONATE	328	C19H36O4	000000-00-0	47



Tentatively Identified Compound (LSC) summary

Operator ID: McLean Date Acquired: 13 Mar 2002 7:08 am
 Data File: C:\MSDCHEM\1\DATA\031202\3736.D
 Name: SAMPLE 3736 2/19/02
 Misc:
 Method: C:\MSDCHEM\1\5973N\5080302.M (RTE Integrator)
 Title: Quantitation For Method 508gcscan
 Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentasiloxan...	12.06	0.5 ug/L		256159	2	13.03	9378220	20.0
LAURIC ACID, N-OC...	30.61	0.9 ug/L		469439	5	30.31	10636500	20.0