

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 05/06/2002 Time: 13:47:58

Sample: AE08431
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 5/6/02 13:47 Ended: 5/6/02 13:47 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		76		10.0

Comments for Sample AE08431 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 05-06-2002 Time: 13:48:59

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.

Quantitation Report

(QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020419\08431.D

Vial: 18

Acq On : 20 Apr 2002 12:52 am

Operator: Nefliu

Sample : sample

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: EVENTS.E

Quant Time: Apr 26 15:00:41 2002

Quant Results File: SCAN020418.RE

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)

Title : Method 508 GC/MS Scan

Last Update : Mon Apr 22 08:00:39 2002

Response via : Initial Calibration

DataAcq Meth : 508SCAN1

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	11.38	152	11228858	40.00	ug/l	-0.05
10) Naphthalene-d8	16.54	136	42977621	40.00	ug/l	-0.07
17) Acenaphthene-d10	24.46	164	23435601	40.00	ug/l	-0.06
30) Phenanthrene-d10	31.72	188	34636268	40.00	ug/l	-0.05
38) Chrysene-d12	39.93	240	24756855	40.00	ug/l	-0.08
44) Perylene-d12	43.16	264	17975292	40.00	ug/l	-0.04
System Monitoring Compounds						
27) TCMX	27.54	207	882345	6.06	ug/l	-0.08
Spiked Amount	10.000 8.0		Recovery	=	60.60% 75.8	
Target Compounds						
35) Di-n-butylphthalate	34.81	149	120465	0.10	ug/l	99
43) Bis(2-ethylhexyl)phthalate	40.53	149	75316	0.12	ug/l	90

Qvalue

 (#) = qualifier out of range (m) = manual integration (+) = signals summed
 08431.D SCAN020418.M Fri Apr 26 15:03:19 2002 Page 1

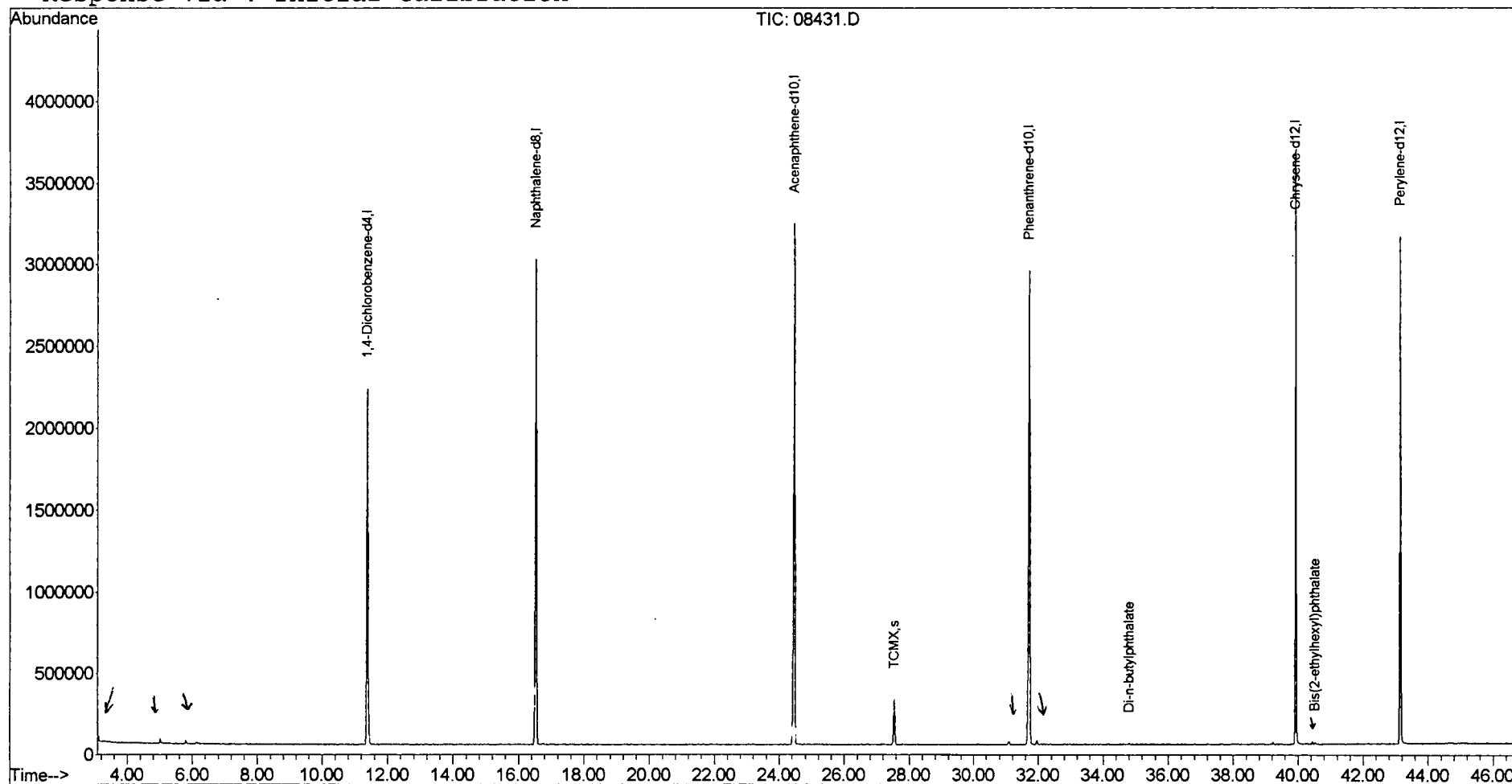
Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
 Acq On : 20 Apr 2002 12:52 am
 Sample : sample
 Misc :
 MS Integration Params: EVENTS.E
 Quant Time: Apr 26 15:03 2002

Vial: 18
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Results File: SCAN020418.RES

Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
 Title : Method 508 GC/MS Scan
 Last Update : Mon Apr 22 08:00:39 2002
 Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
 Acq On : 20 Apr 2002 12:52 am
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

Vial: 18
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 5 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0.01 Peak Location: TOP

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

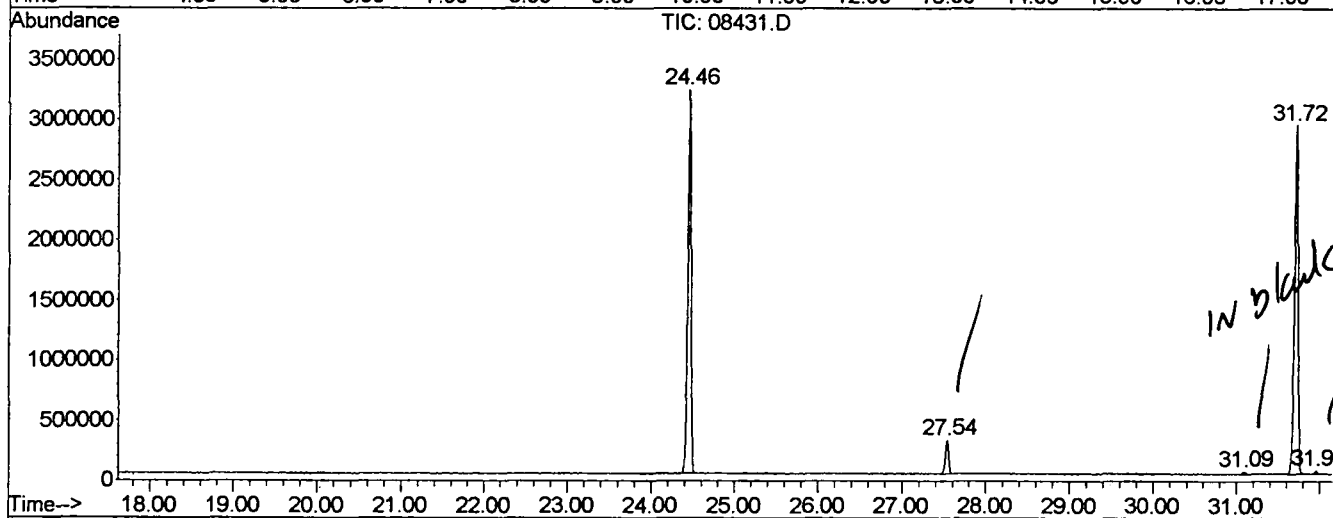
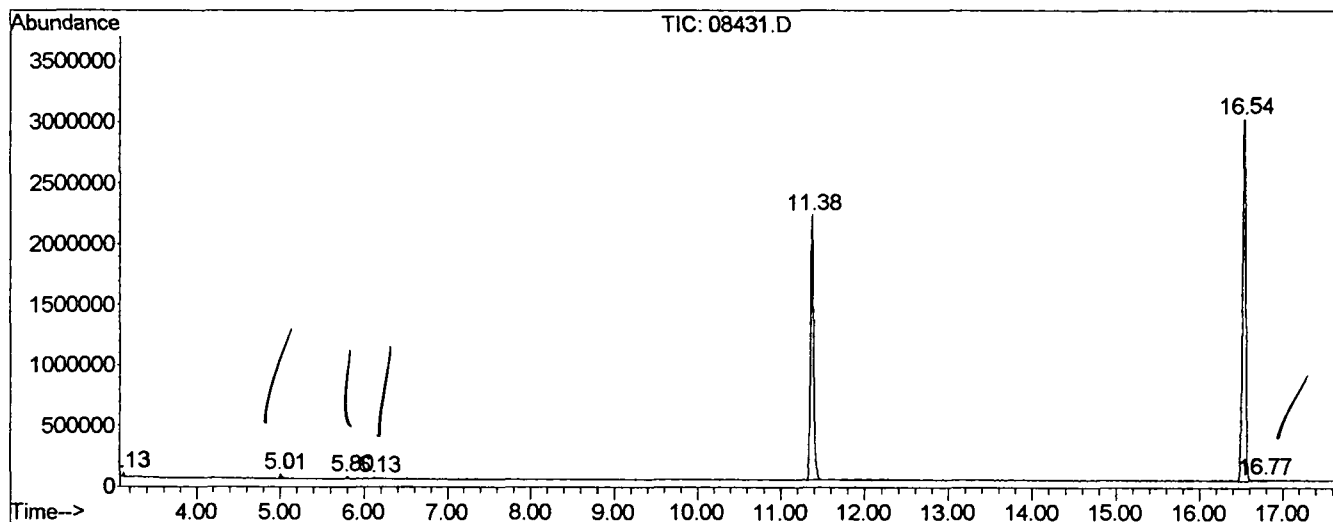
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.126	3	8	17	BV	32069	357694	0.41%	0.078%
2	5.006	321	328	343	PV	2 33719	681179	0.77%	0.149%
3	5.799	459	463	473	VV	2 22818	429712	0.49%	0.094%
4	6.128	514	519	530	PV	2 8158	247503	0.28%	0.054%
5	11.375	1398	1412	1435	PV	2176886	56683712	64.31%	12.390%
6	16.540	2275	2291	2309	PV	2994224	78461784	89.02%	17.150%
7	16.769	2316	2330	2339	VV	10466	305567	0.35%	0.067%
8	24.466	3617	3640	3658	PV	3171048	88139227	100.00%	19.266%
9	27.539	4149	4163	4178	PV	2 277311	7627673	8.65%	1.667%
10	31.088	4757	4767	4780	VV	5 21575	755897	0.86%	0.165%
11	31.722	4855	4875	4893	VV	2 2881072	86544954	98.19%	18.917%
12	31.957	4905	4915	4923	PV	3 28699	725655	0.82%	0.159%
13	34.813	5393	5401	5405	PV	2 8942	184453	0.21%	0.040%
14	39.226	6147	6152	6161	VV	2 14983	307044	0.35%	0.067%
15	39.936	6260	6273	6292	VV	2 3599549	72752281	82.54%	15.902%
16	40.436	6353	6358	6368	VV	3 17706	408946	0.46%	0.089%
17	40.524	6368	6373	6380	VV	2 12147	308507	0.35%	0.067%
18	43.156	6799	6821	6837	PV	3110967	62432601	70.83%	13.647%
19	43.262	6837	6839	6846	VV	7252	137369	0.16%	0.030%

Sum of corrected areas: 457491759

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020419\08431.D
 Operator : Nefliu
 Acquired : 20 Apr 2002 12:52 am using AcqMethod 508SCAN1
 Instrument : Instrumen
 Sample Name: sample
 Misc Info :
 Vial Number: 18
 Quant File :SCAN020418.RES (Chemstation Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
Acq On : 20 Apr 2002 12:52 am
Sample : sample
Misc :
MS Integration Params: rteint.e

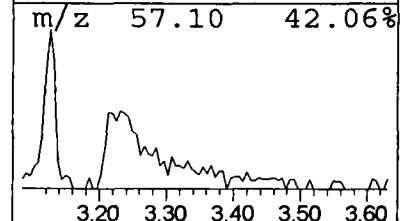
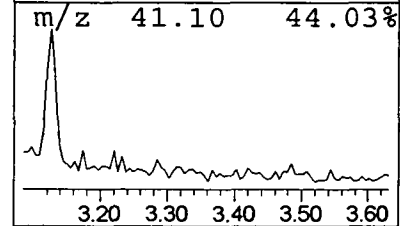
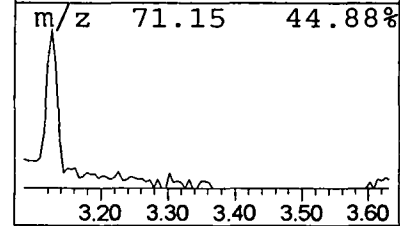
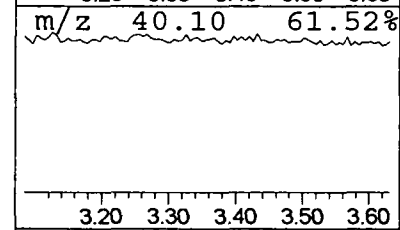
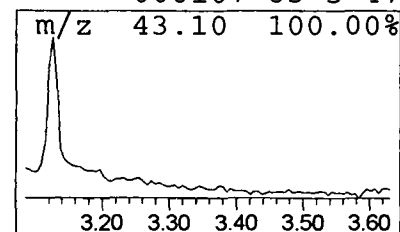
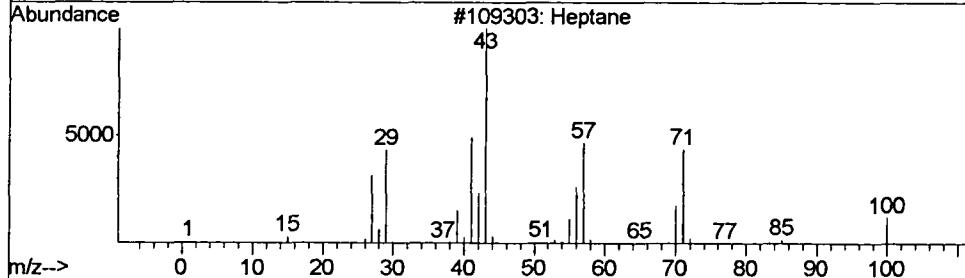
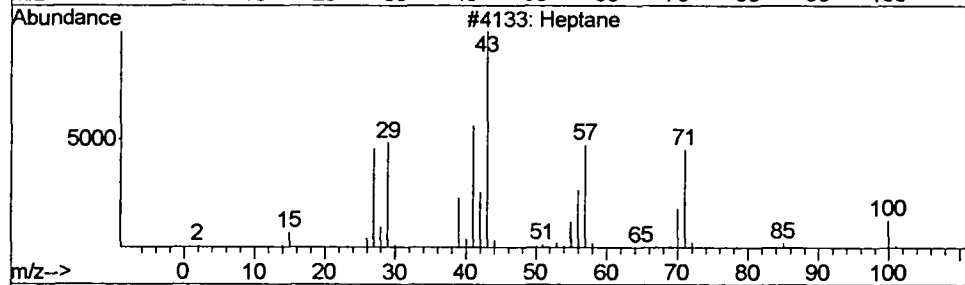
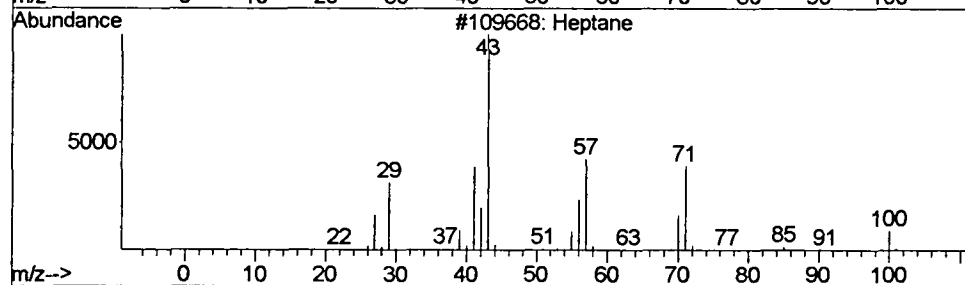
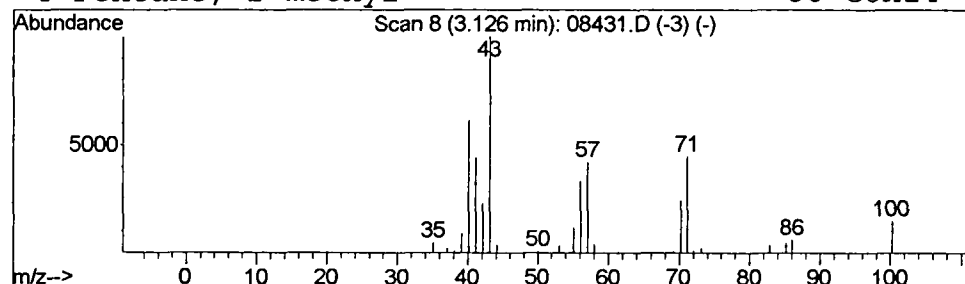
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Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
Title : Method 508 GC/MS Scan
Library : C:\DATABASE\nist98.1

Peak Number 1 Heptane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	0.25 ug/l	357694	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane			100	C7H16	000142-82-5	90
2	Heptane			100	C7H16	000142-82-5	80
3	Heptane			100	C7H16	000142-82-5	80
4	Pentane, 2-methyl-			86	C6H14	000107-83-5	47



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
Acq On : 20 Apr 2002 12:52 am
Sample : sample
Misc :
MS Integration Params: rteint.e

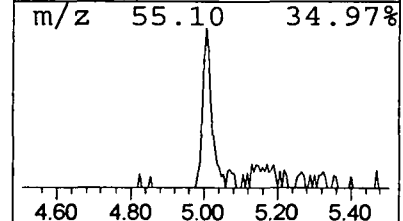
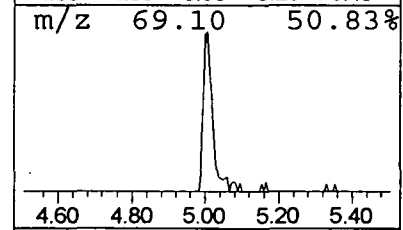
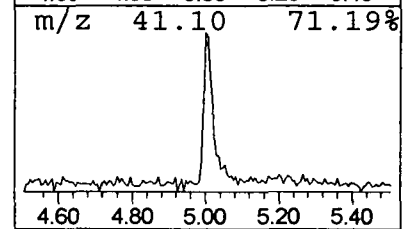
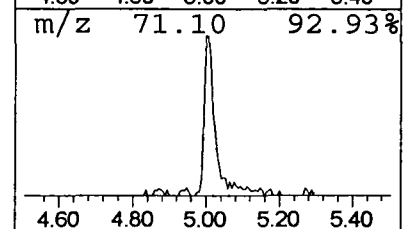
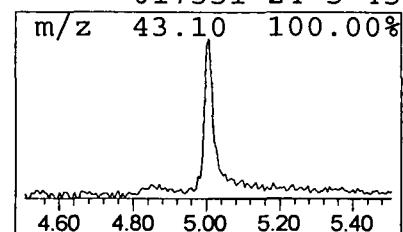
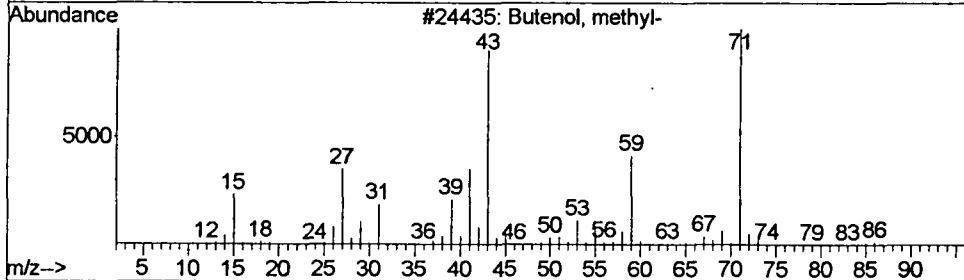
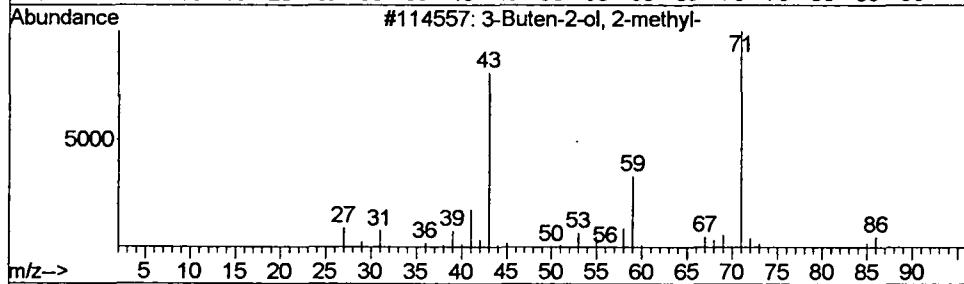
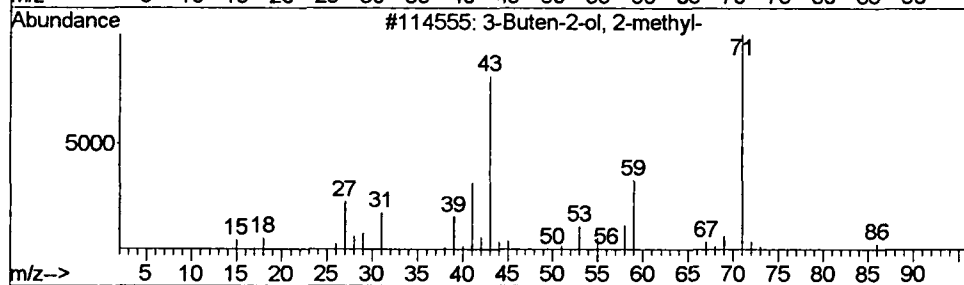
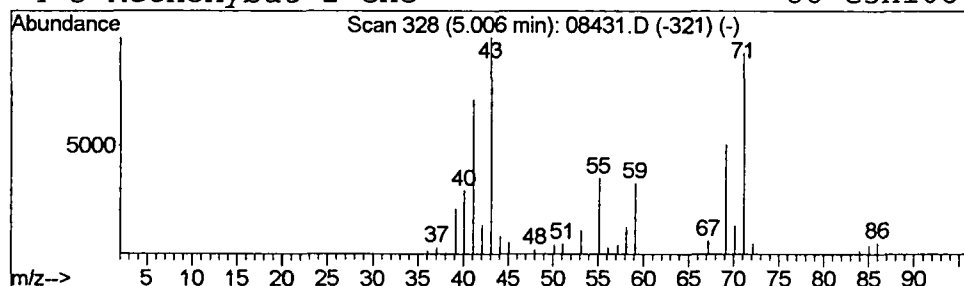
Vial: 18
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
Title : Method 508 GC/MS Scan
Library : C:\DATABASE\nist98.l

Peak Number 2 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.48 ug/l	681179	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	87
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	80
3			Butenol, methyl-	86	C5H10O	060766-00-9	64
4			3-Methoxybut-1-ene	86	C5H10O	017351-24-5	45



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
 Acq On : 20 Apr 2002 12:52 am
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

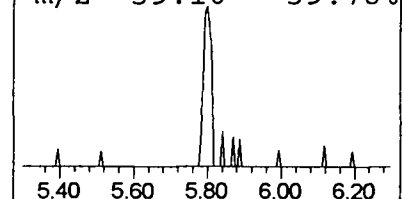
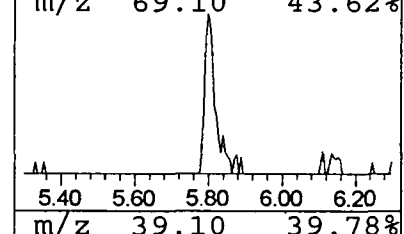
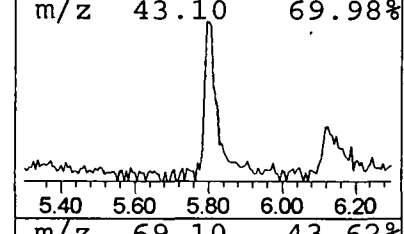
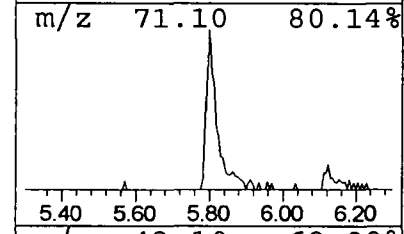
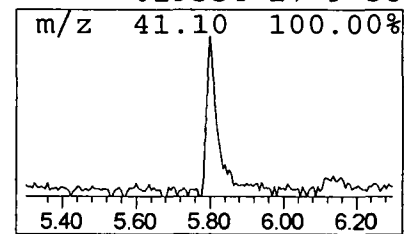
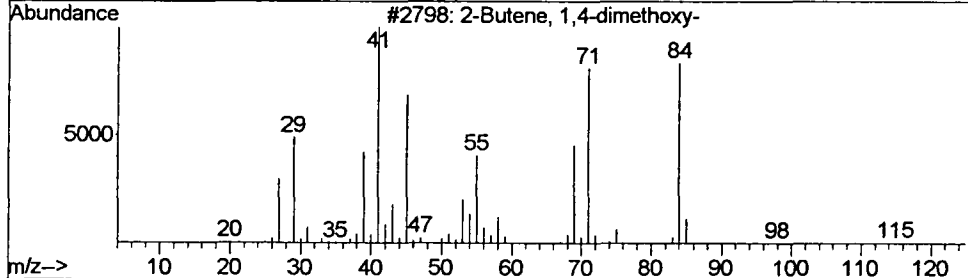
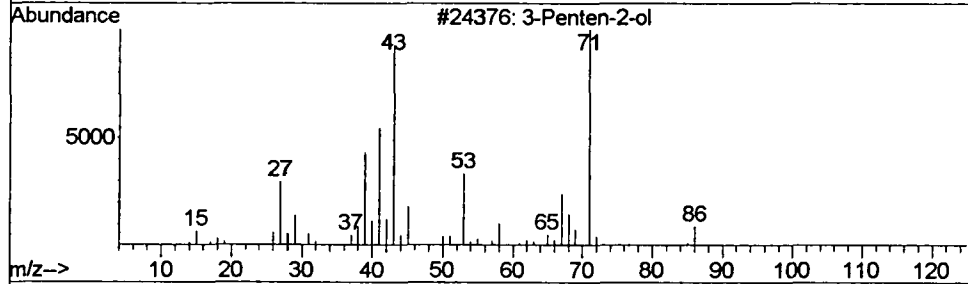
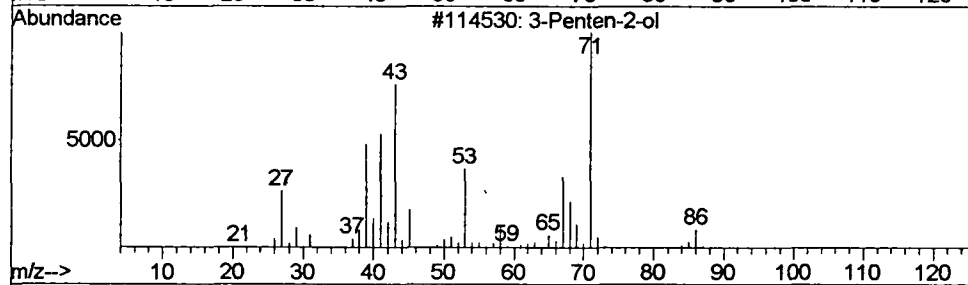
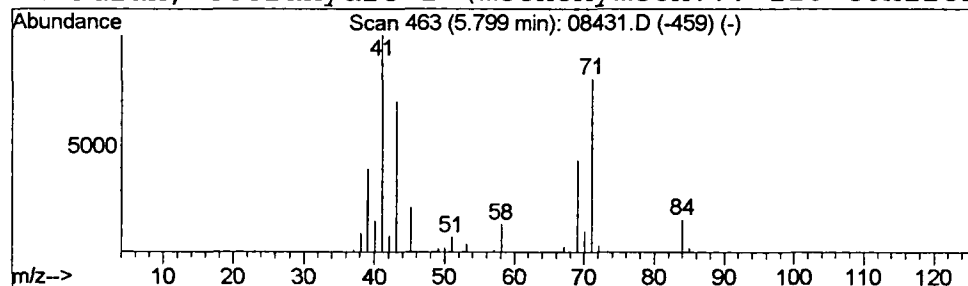
Vial: 18
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 3 3-Penten-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	0.30 ug/l	429712	1,4-Dichlorobenzene-d4	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-ol	86	C5H10O	001569-50-2	45
2		3-Penten-2-ol	86	C5H10O	001569-50-2	45
3		2-Butene, 1,4-dimethoxy-	116	C6H12O2	026649-86-5	45
4		Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	38



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
 Acq On : 20 Apr 2002 12:52 am
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

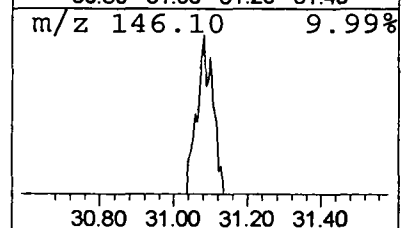
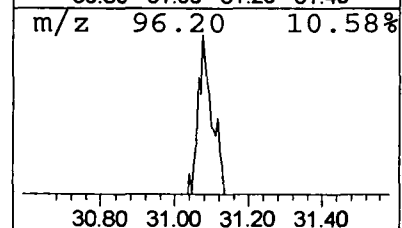
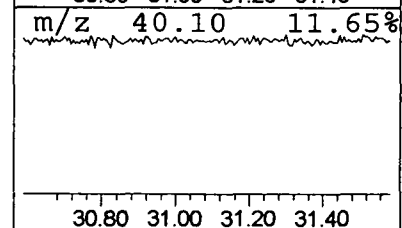
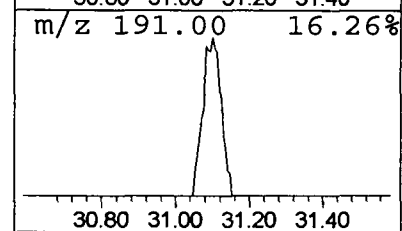
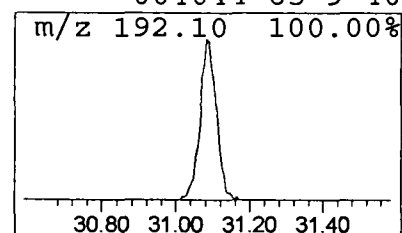
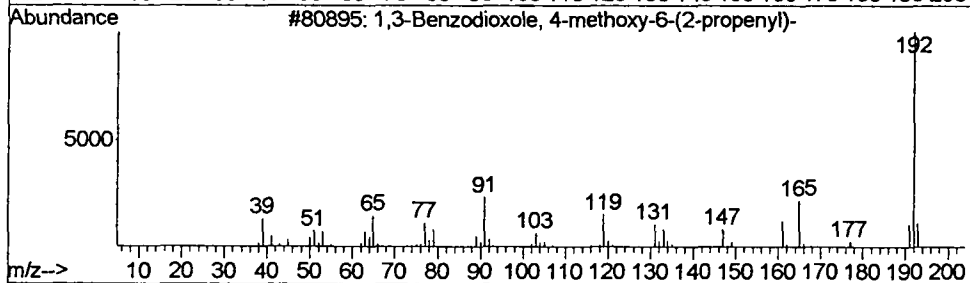
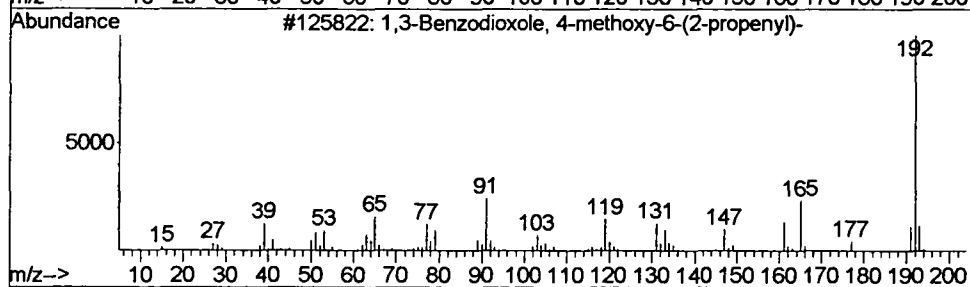
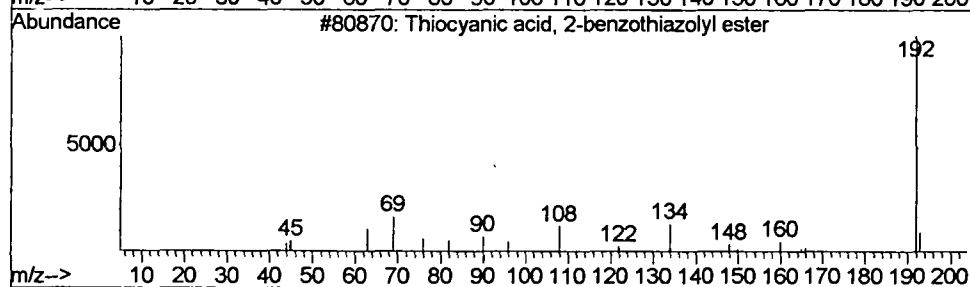
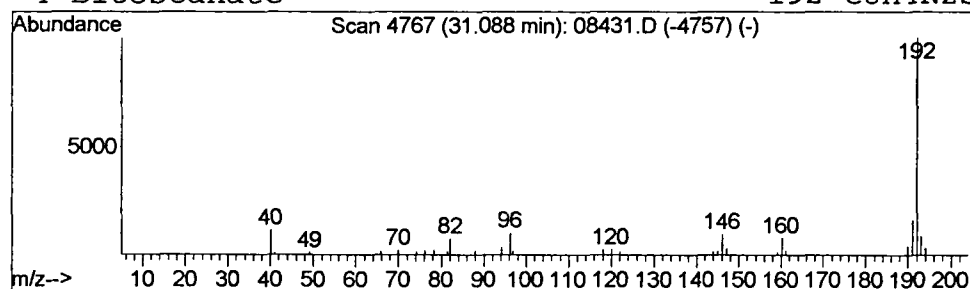
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 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 4 Thiocyanic acid, 2-benzothi... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.09	0.35 ug/l	755897	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	53
2		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	42
3		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	42
4		Bitoscanate	192	C8H4N2S2	004044-65-9	40



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08431.D
Acq On : 20 Apr 2002 12:52 am
Sample : sample
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MS Integration Params: rteint.e

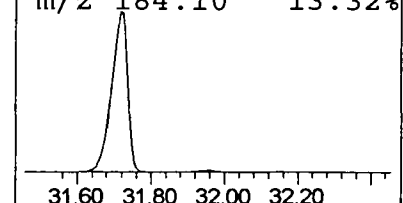
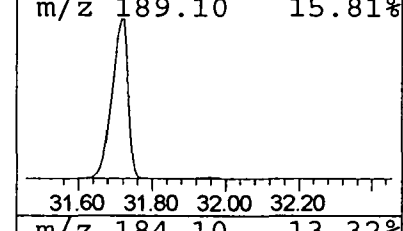
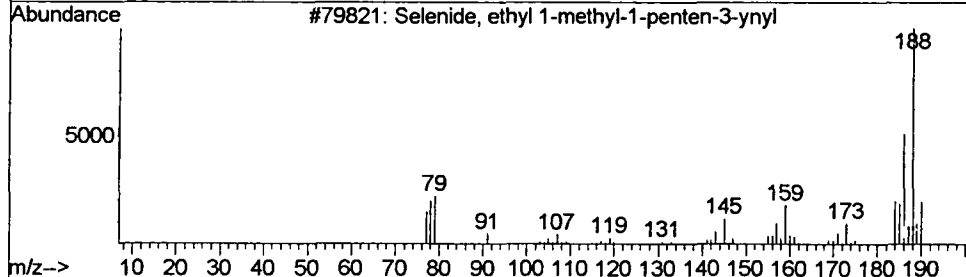
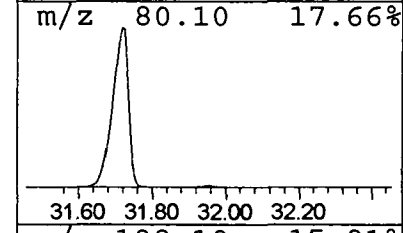
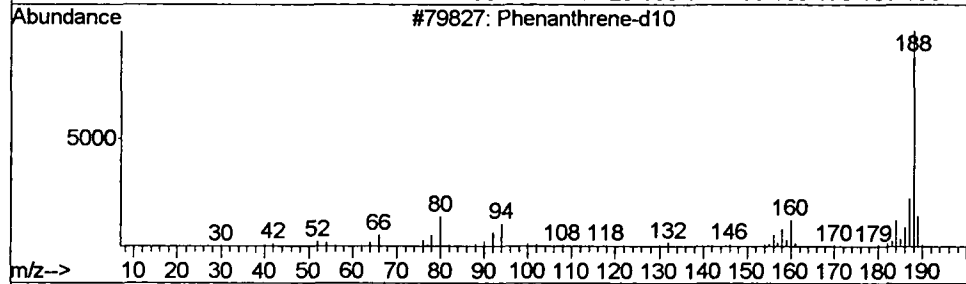
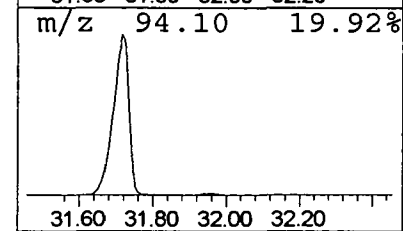
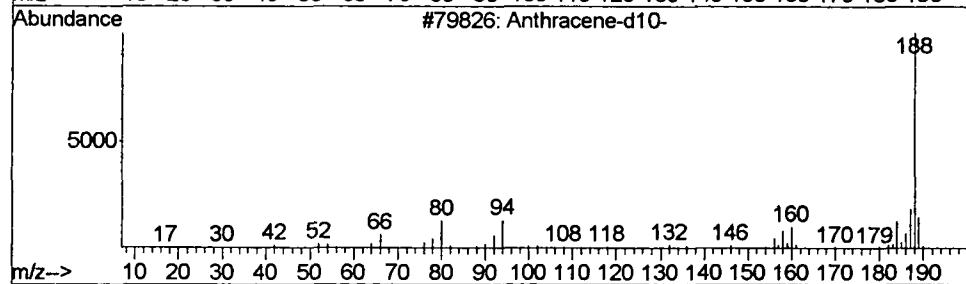
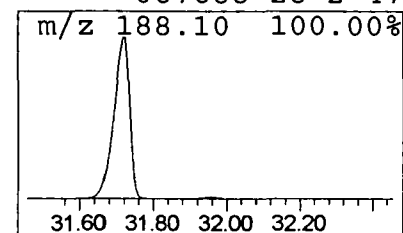
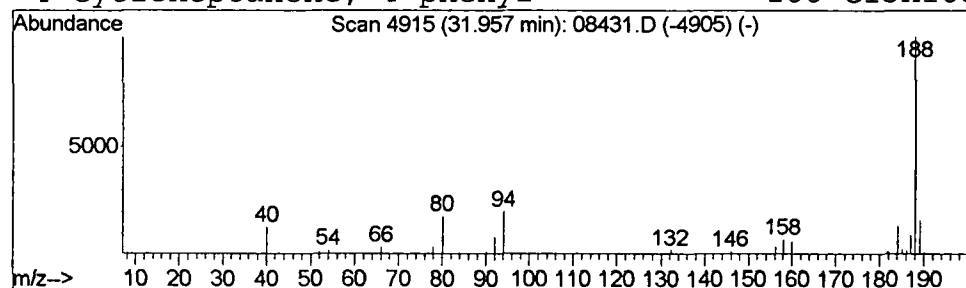
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Operator: Nefliu
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Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
Title : Method 508 GC/MS Scan
Library : C:\DATABASE\nist98.1

Peak Number 5 Anthracene-d10- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.96	0.34 ug/l	725655	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene-d10-	188	C14D10	001719-06-8	72
2			Phenanthrene-d10	188	C14D10	001517-22-2	64
3			Selenide, ethyl 1-methyl-1-pente...	188	C8H12Se	025128-48-7	53
4			Cycloheptanone, 4-phenyl-	188	C13H16O	067688-28-2	47



Library Search Compound Report

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 Sample : sample
 Misc :
 MS Integration Params: rteint.e

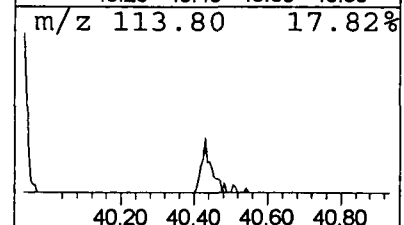
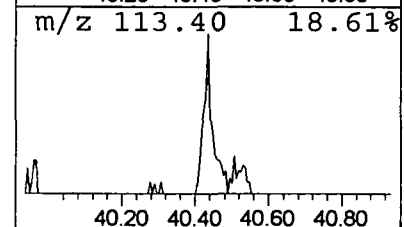
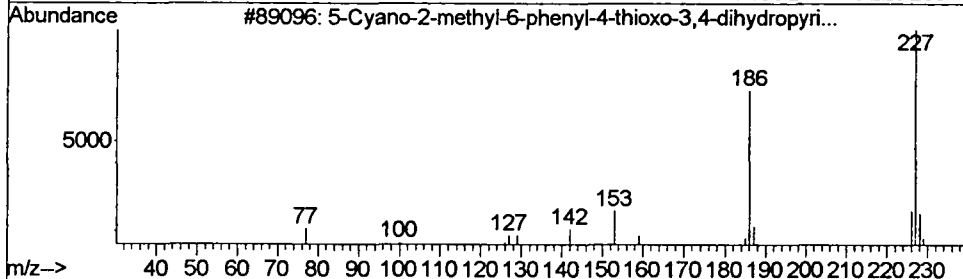
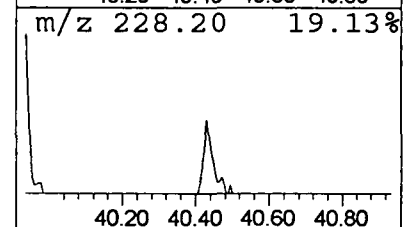
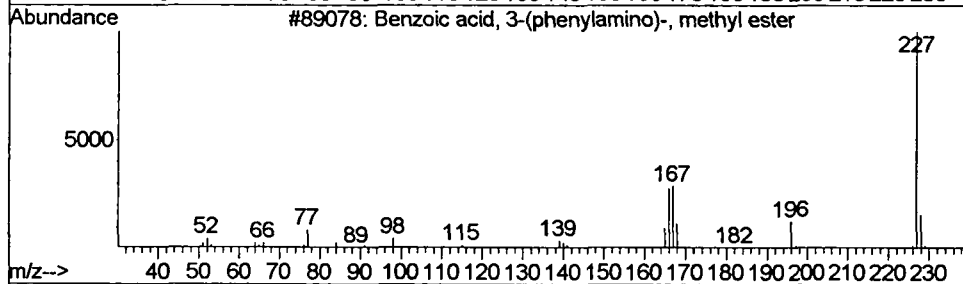
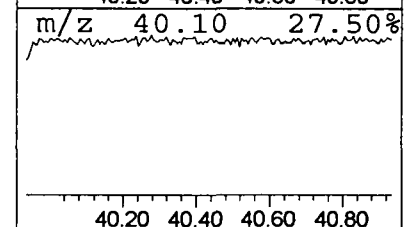
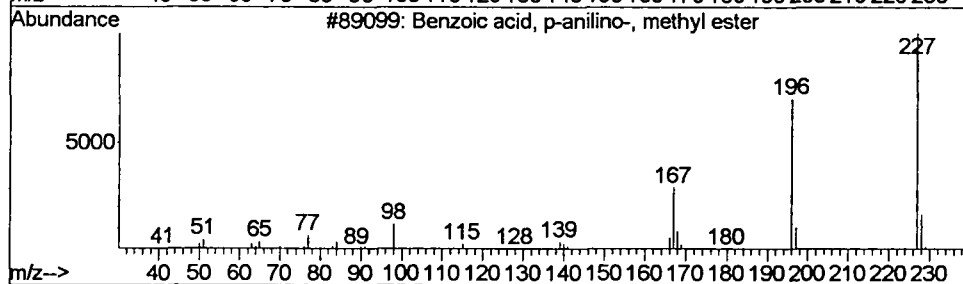
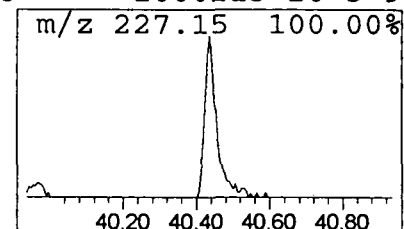
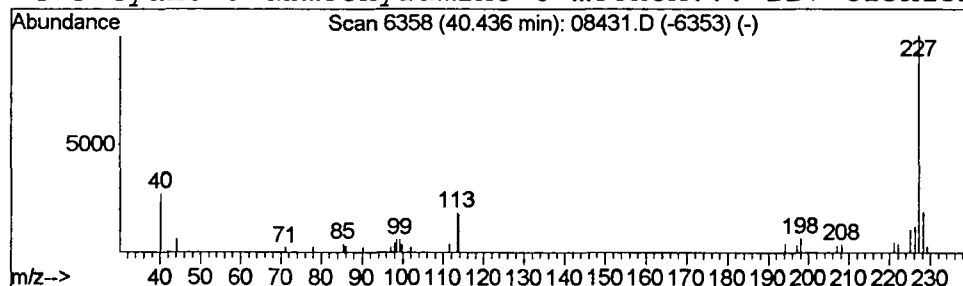
Vial: 18
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 6 Benzoic acid, p-anilino-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
40.44	0.22 ug/l	408946	Chrysene-d12	39.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, p-anilino-, methyl...	227	C14H13NO2	004058-18-8	47
2		Benzoic acid, 3-(phenylamino)-, ...	227	C14H13NO2	055622-43-0	40
3		5-Cyano-2-methyl-6-phenyl-4-thio...	227	C12H9N3S	013996-07-1	33
4		5-Cyano-8-dimethylamino-6-methox...	227	C13H13N3O	1000213-20-5	9



Tentatively Identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 20 Apr 2002 12:52 am
Data File: C:\MSDCHEM\1\DATA\020419\08431.D
Name: sample
Misc:
Method: C:\MSDCHEM\1\METHODS\SCAN020418.M (Chemstation Integrator)
Title: Method 508 GC/MS Scan
Library Searched: C:\DATABASE\nist98.1

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
✓ Heptane	3.13	0.3	ug/l	357694	1	11.38	56683700	40.0
✓ 3-Buten-2-ol, 2-m...	5.01	0.5	ug/l	681179	1	11.38	56683700	40.0
3-Penten-2-ol	5.80	0.3	ug/l	429712	1	11.38	56683700	40.0
Thiocyanic acid, ...	31.09	0.3	ug/l	755897	4	31.72	86545000	40.0
Anthracene-d10-	31.96	0.3	ug/l	725655	4	31.72	86545000	40.0
Benzoic acid, p-a...	40.44	0.2	ug/l	408946	5	39.93	72752300	40.0
→ Phenanthrene-d10								