

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 05/06/2002 Time: 14:01:12

Sample: AE08429
Analysis: \$GCMS GCMS Scan For Unknowns
Units: ug
Started: 5/6/02 13:58 Ended: 5/6/02 13:58 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		72		10.0

Comments for Sample AE08429 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 05-06-2002 Time: 14:01:45

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\08429.D
 Acq On : 19 Apr 2002 10:54 pm
 Sample : sample
 Misc :
 MS Integration Params: EVENTS.E
 Quant Time: Apr 26 14:51:19 2002

Vial: 16
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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	10815323	40.00	ug/l	-0.05
10) Naphthalene-d8	16.54	136	41607140	40.00	ug/l	-0.07
17) Acenaphthene-d10	24.46	164	22893968	40.00	ug/l	-0.06
30) Phenanthrene-d10	31.72	188	34289348	40.00	ug/l	-0.06
38) Chrysene-d12	39.94	240	26336914	40.00	ug/l	-0.07
44) Perylene-d12	43.16	264	18921223	40.00	ug/l	-0.04
System Monitoring Compounds						
27) TCMX	27.54	207	823333	5.79	ug/l	-0.07
Spiked Amount	10.000 8.0		Recovery	=	57.90% 72.4	
Target Compounds						
35) Di-n-butylphthalate	34.81	149	101442	0.08	ug/l	97
36) Fluoranthene	36.05	202	127792	0.13	ug/l	80
39) Pyrene	36.66	202	86325	0.08	ug/l	81

 (#) = qualifier out of range (m) = manual integration (+) = signals summed
 08429.D SCAN020418.M Fri Apr 26 15:04:00 2002 Page 1

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020419\08429.D

Vial: 16

Acq On : 19 Apr 2002 10:54 pm

Operator: Nefliu

Sample : sample

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: EVENTS.E

Quant Time: Apr 26 15:03 2002

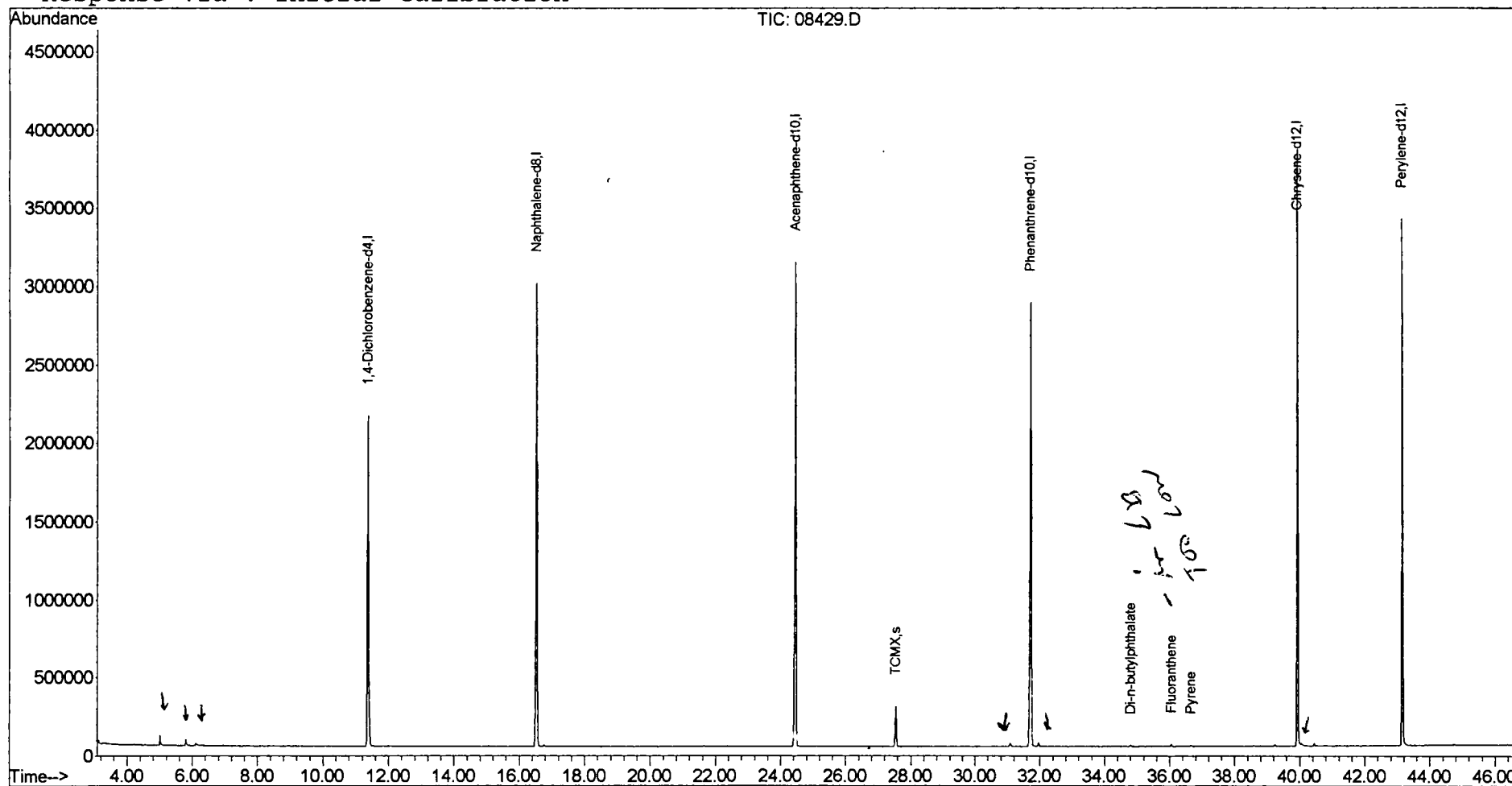
Quant Results File: SCAN020418.RES

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



08429.D SCAN020418.M

Fri Apr 26 15:04:01 2002

Page 2

LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
 Acq On : 19 Apr 2002 10:54 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

Vial: 16
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\SCAN020418.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0.01

Filtering: 5
 Min Area: 5 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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

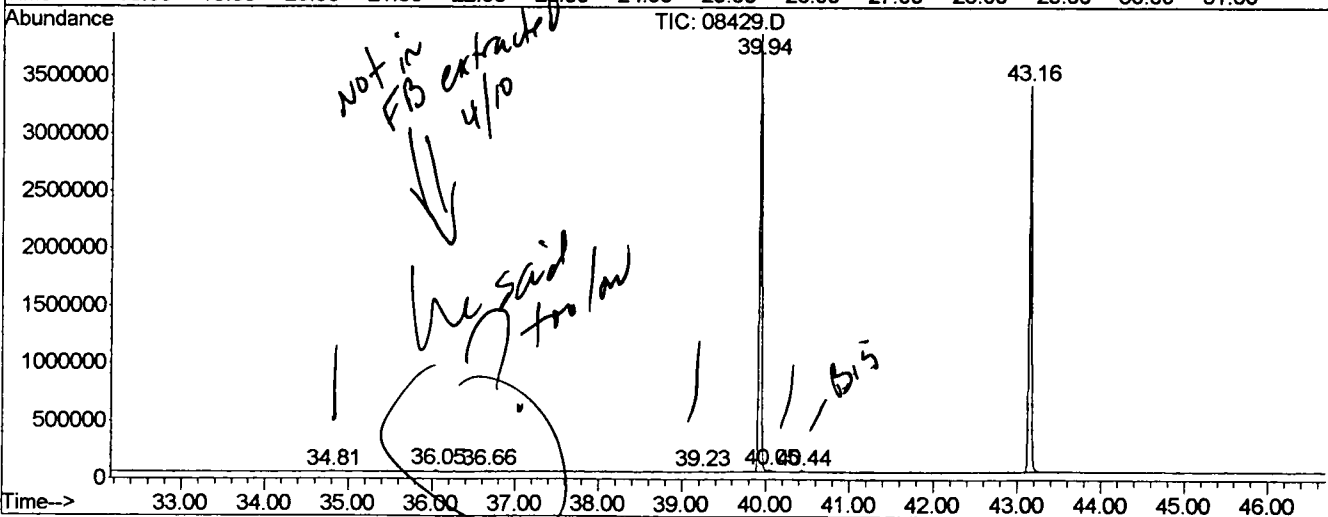
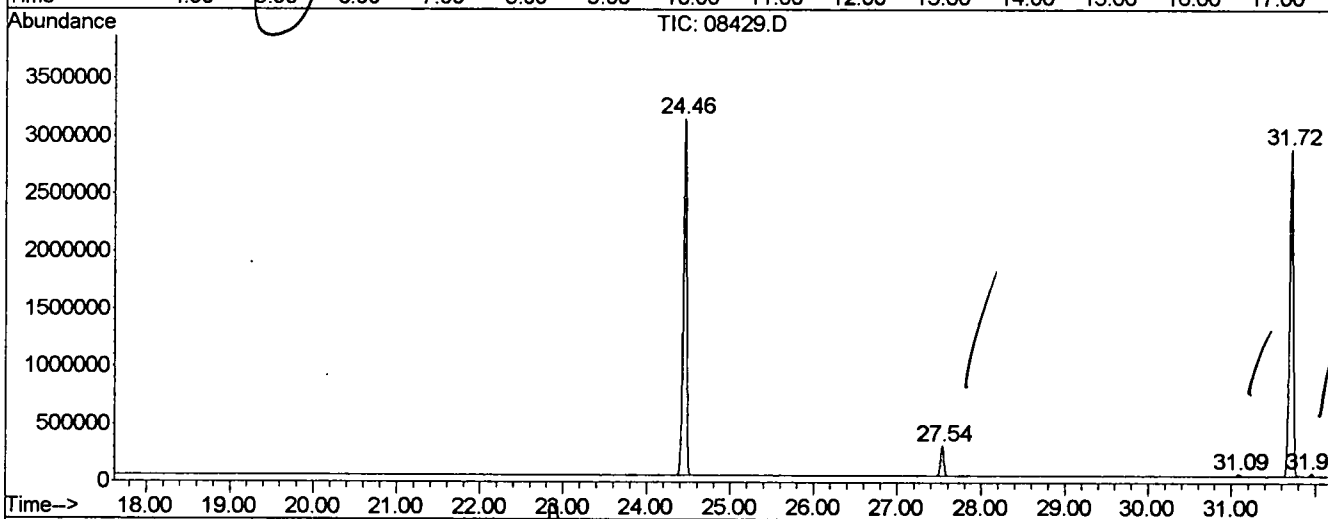
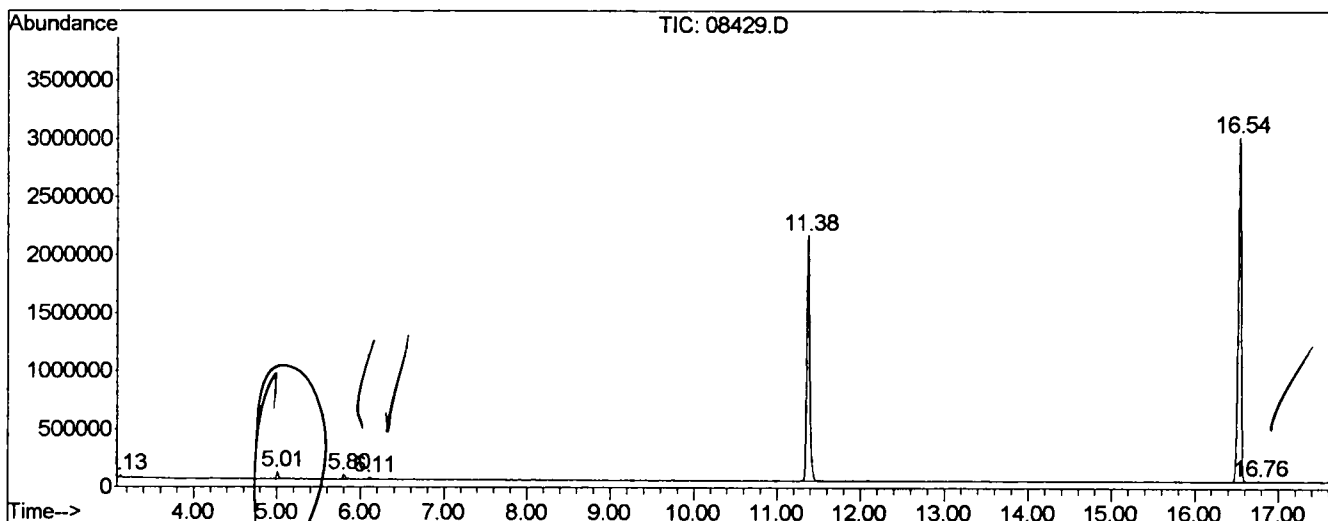
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	3	9	14	BV	4	21348	249477	0.054%
2	5.006	321	328	336	VV	3	63034	1108360	0.242%
3	5.799	456	463	473	PV	2	42527	888412	0.194%
4	6.111	512	516	535	PV	3	17923	528838	0.115%
5	11.375	1397	1412	1441	PV		2095624	54544882	63.47%
6	16.540	2276	2291	2306	PV		2967568	75761339	88.16%
7	16.763	2321	2329	2340	VV	2	8045	224370	0.26%
8	24.460	3617	3639	3655	VV		3077260	85931608	100.00%
9	27.539	4149	4163	4179	PV	2	259419	7141468	8.31%
10	31.088	4756	4767	4778	VV	4	20754	630738	0.73%
11	31.722	4855	4875	4888	PV	3	2823406	85361587	99.34%
12	31.951	4908	4914	4922	VV	2	24939	605214	0.70%
13	34.807	5384	5400	5409	VV	2	9854	287513	0.33%
14	36.047	5604	5611	5619	PV	4	16012	348829	0.41%
15	36.658	5706	5715	5726	PV	2	9227	200092	0.23%
16	39.225	6139	6152	6161	VV	3	11729	291959	0.34%
17	39.936	6260	6273	6286	PV	2	3812534	77444568	90.12%
18	40.048	6286	6292	6304	VV	4	19934	754779	0.88%
19	40.436	6353	6358	6365	PV	4	15952	331317	0.39%
20	43.156	6809	6821	6841	PV		3275303	65557158	76.29%

Sum of corrected areas: 458192508

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020419\08429.D
 Operator : Nefliu
 Acquired : 19 Apr 2002 10:54 pm using AcqMethod 508SCAN1
 Instrument : Instrumen
 Sample Name: sample
 Misc Info :
 Vial Number: 16
 Quant File : SCAN020418.RES (Chemstation Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

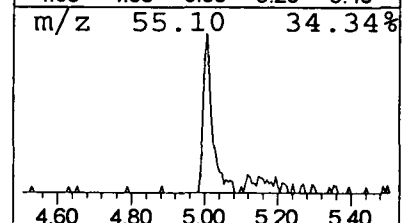
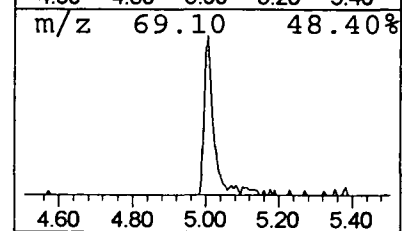
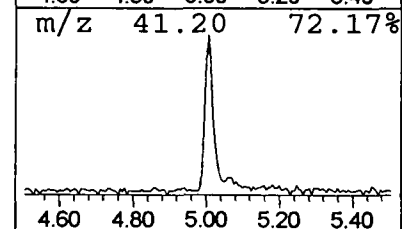
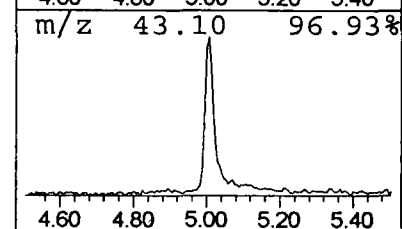
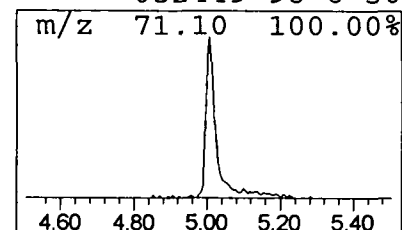
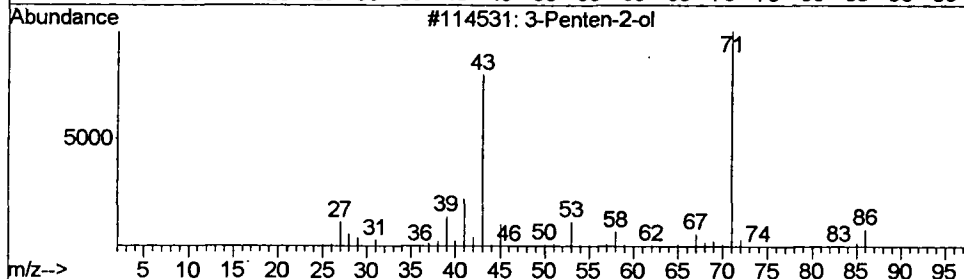
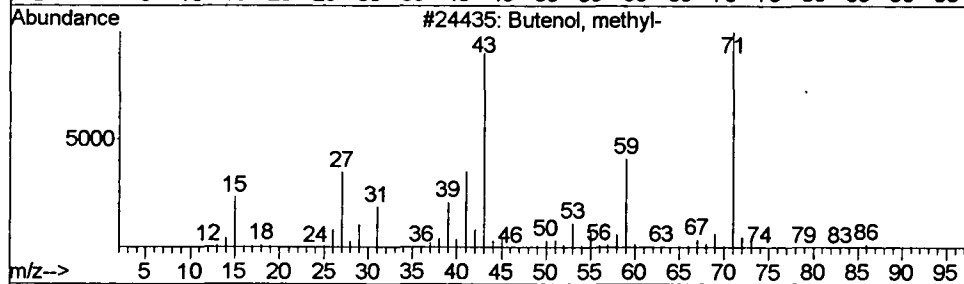
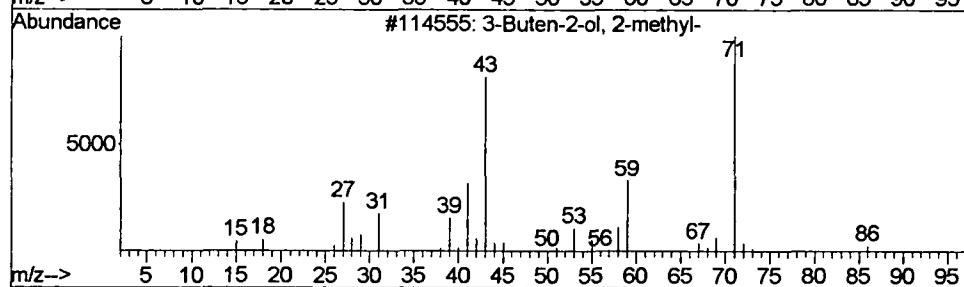
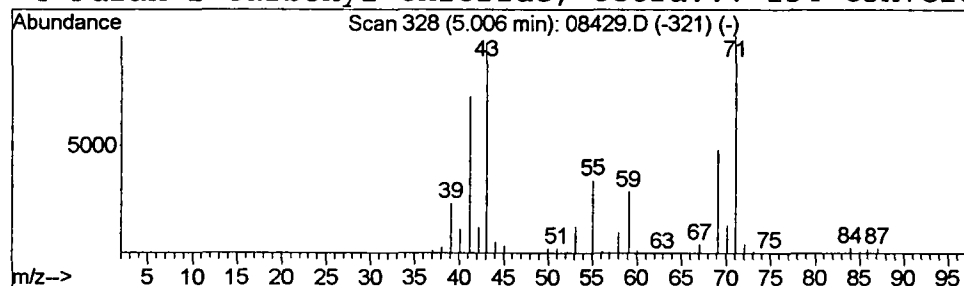
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	0.81 ug/l	1108360	1,4-Dichlorobenzene-d4	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	81
2		Butenol, methyl-	86	C5H10O	060766-00-9	53
3		3-Penten-2-ol	86	C5H10O	001569-50-2	53
4		Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

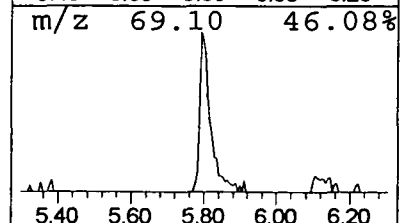
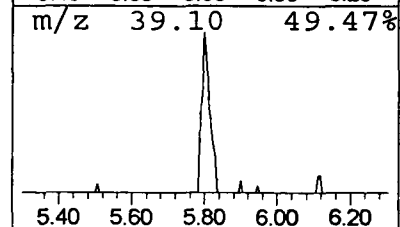
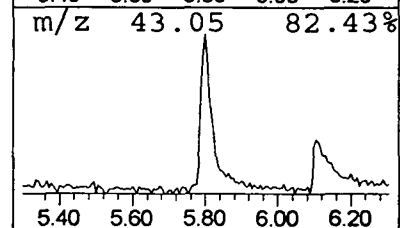
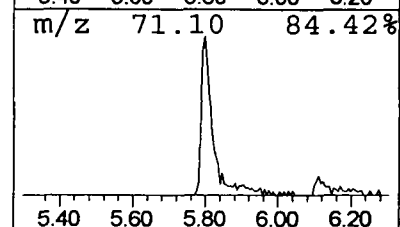
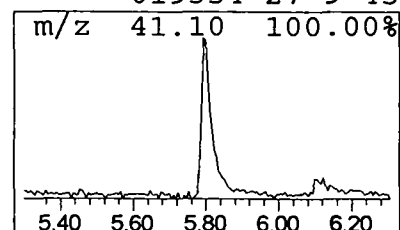
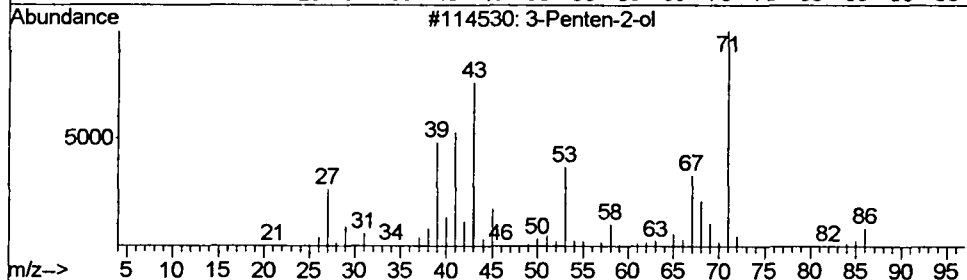
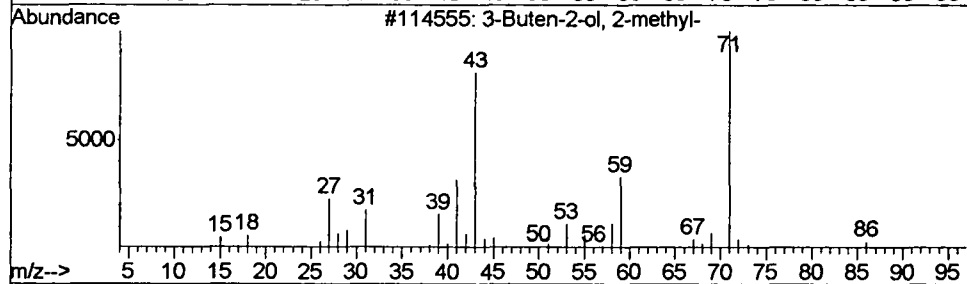
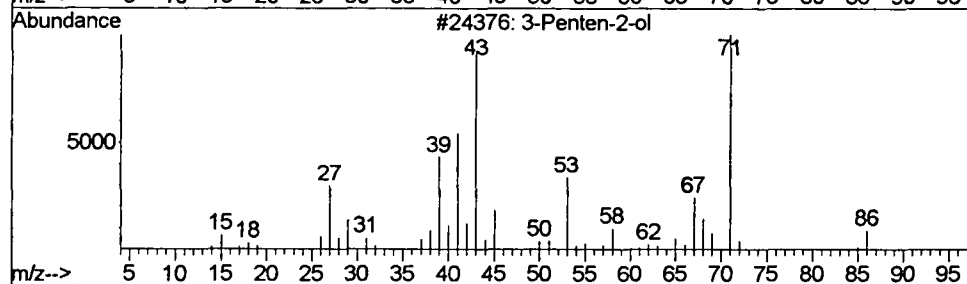
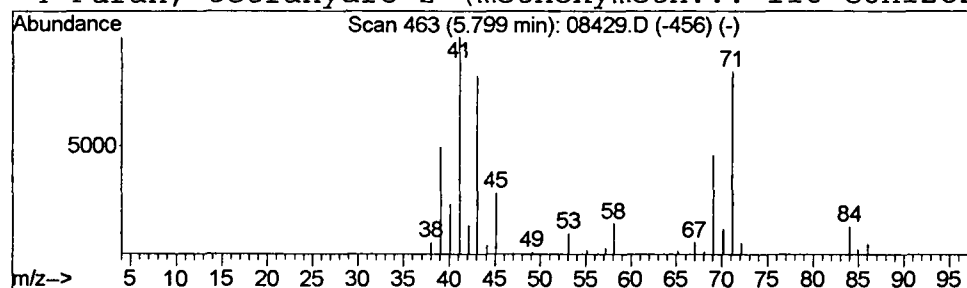
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	0.65 ug/l	888412	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	59
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	49
3			3-Penten-2-ol	86	C5H10O	001569-50-2	45
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	45



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

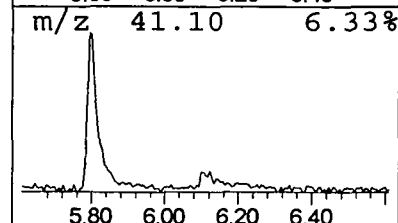
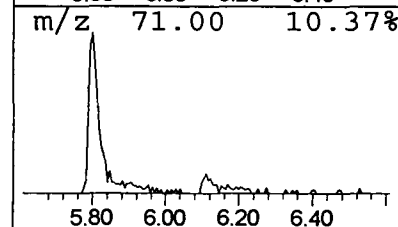
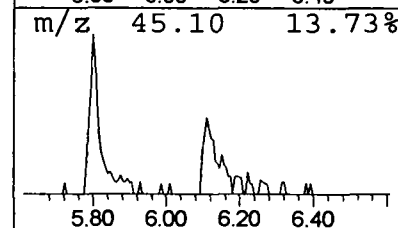
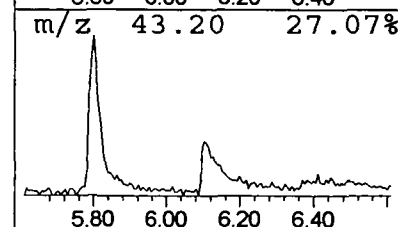
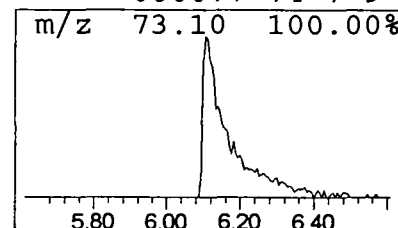
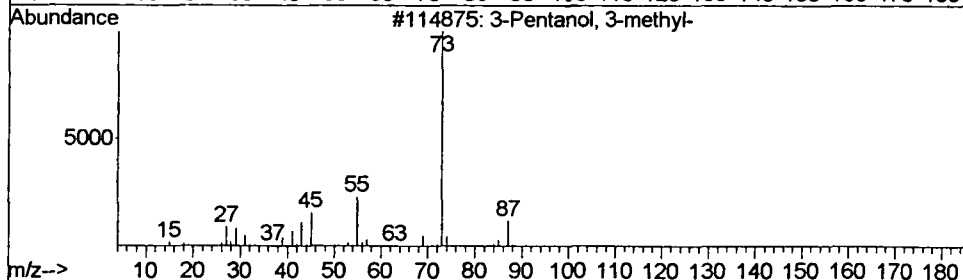
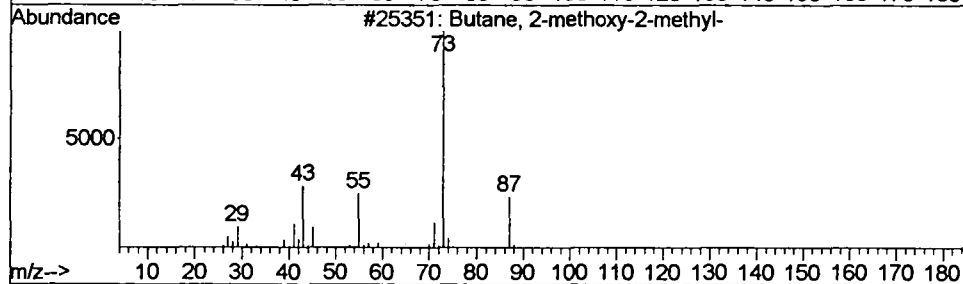
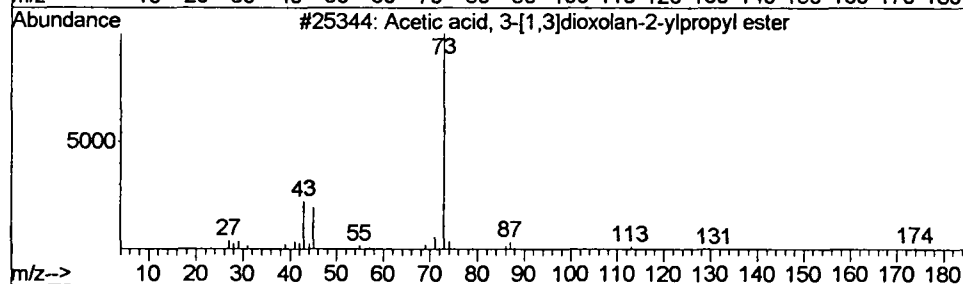
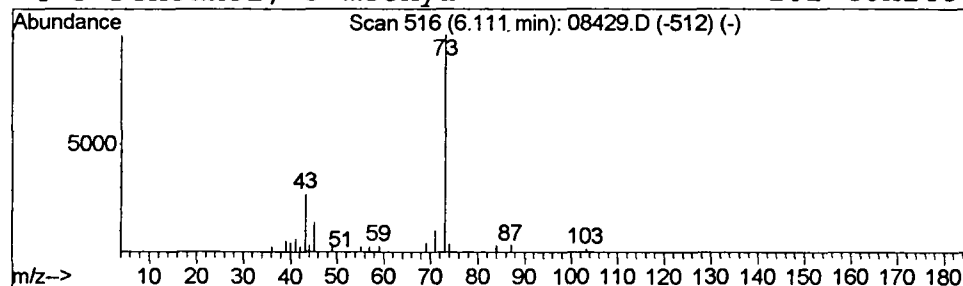
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.11	0.39 ug/l	528838	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	50
2			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	38
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

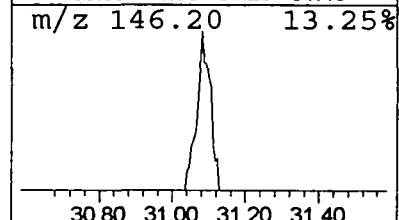
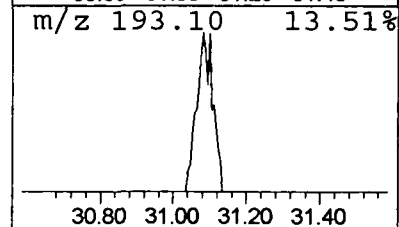
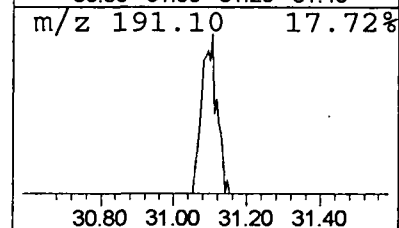
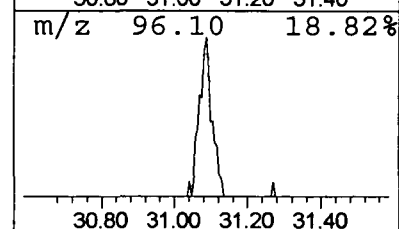
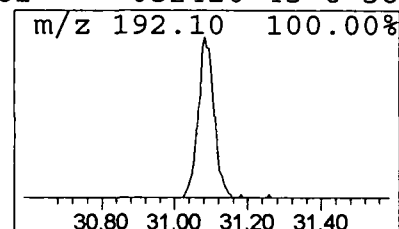
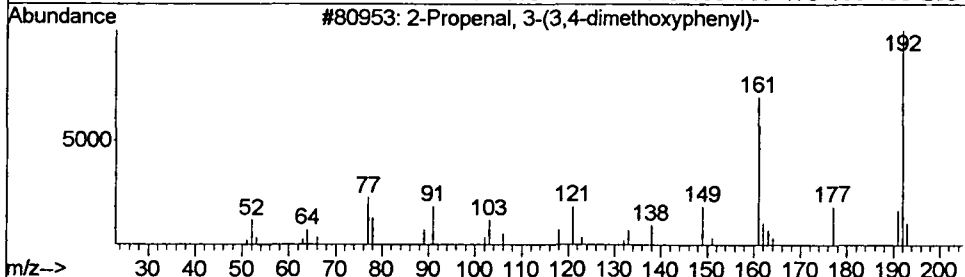
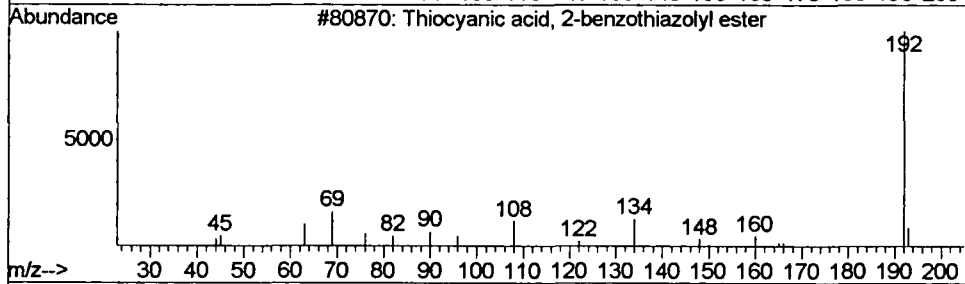
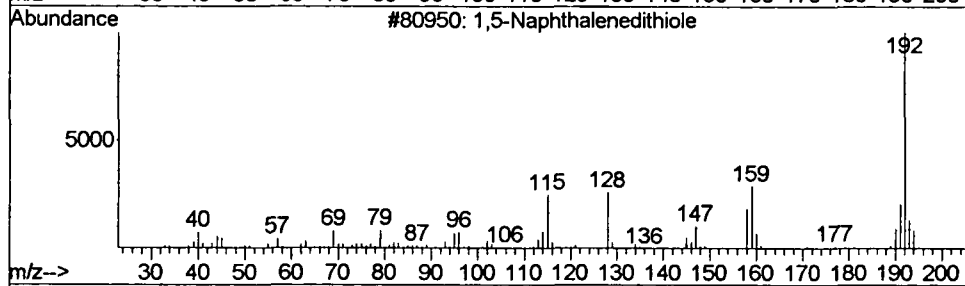
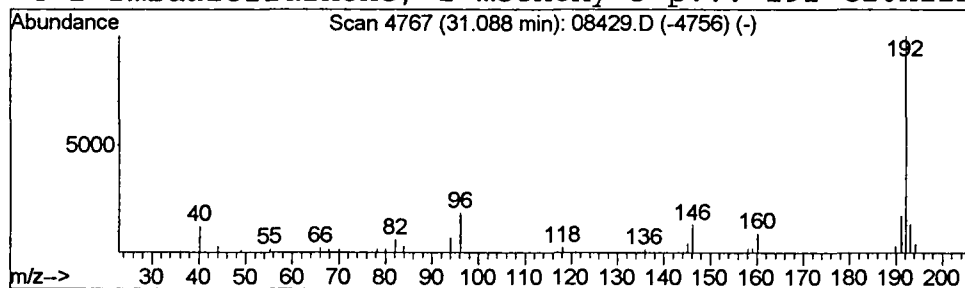
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 4 1,5-Naphthalenedithiole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.09	0.30 ug/l	630738	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5-Naphthalenedithiole	192	C10H8S2	1000223-69-5	45
2		Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	42
3		2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	42
4		2-Imidazolidinone, 1-methoxy-3-p...	192	C10H12N2O2	052420-43-6	38



Library Search Compound Report

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Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

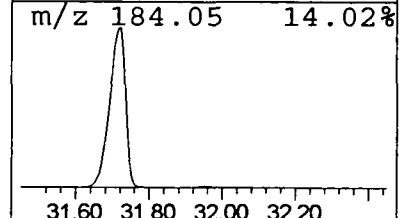
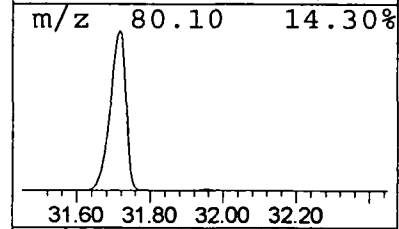
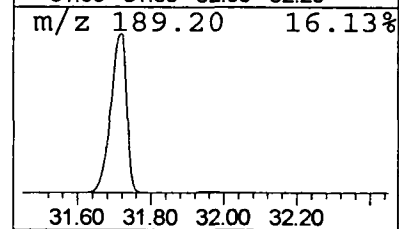
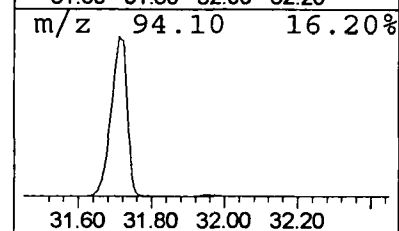
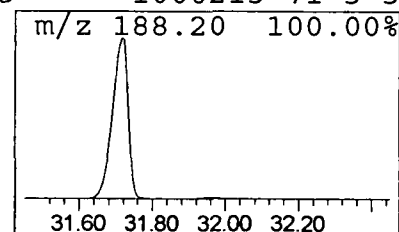
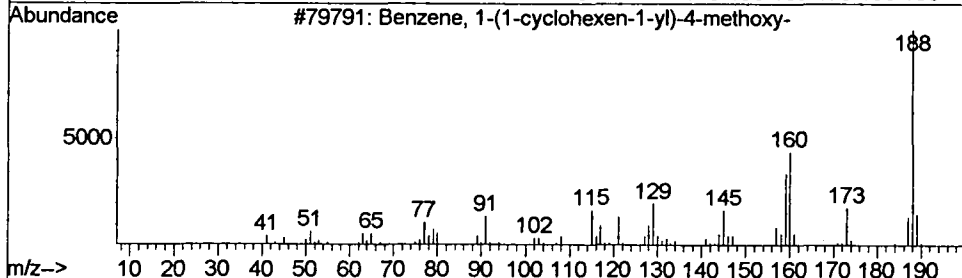
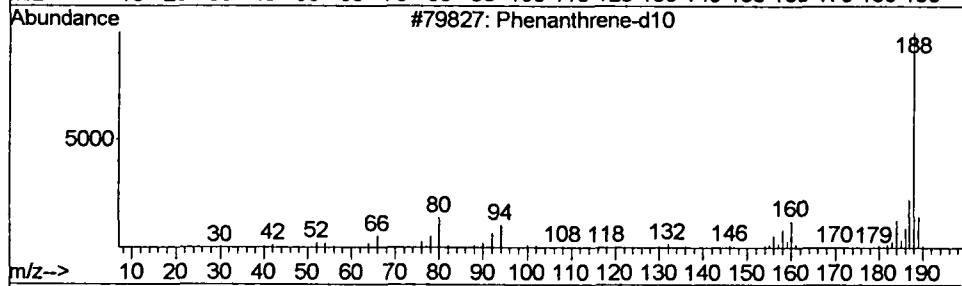
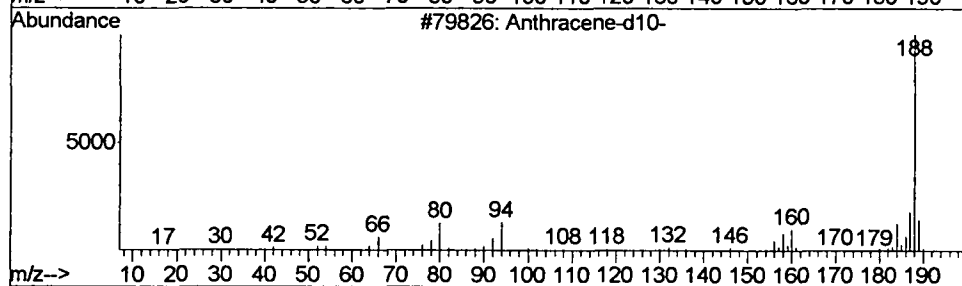
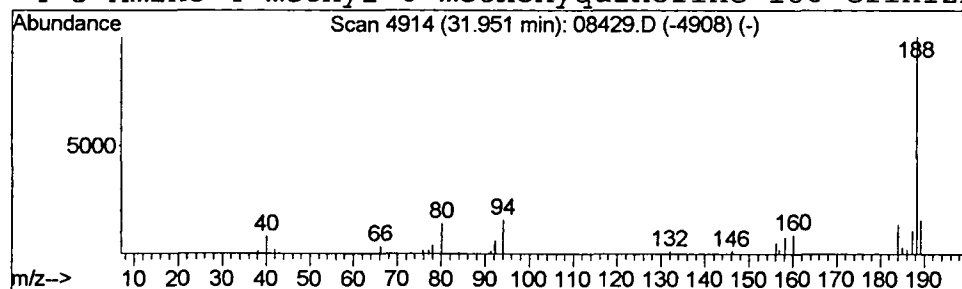
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 5 Anthracene-d10- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.95	0.28 ug/l	605214	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene-d10-	188	C14D10	001719-06-8	87
2		Phenanthrene-d10	188	C14D10	001517-22-2	83
3		Benzene, 1-(1-cyclohexen-1-yl)-4...	188	C13H16O	020758-60-5	42
4		3-Amino-4-methyl-6-methoxyquinoline	188	C11H12N2O	1000213-71-3	36



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020419\08429.D
Acq On : 19 Apr 2002 10:54 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

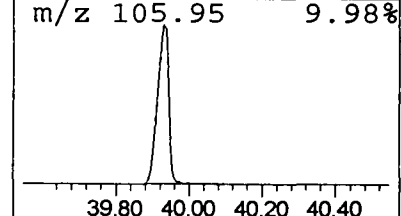
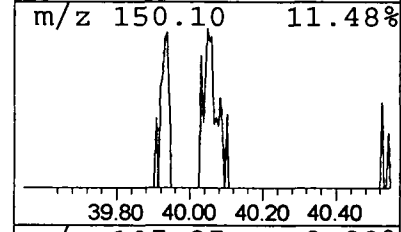
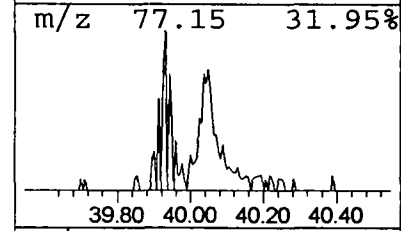
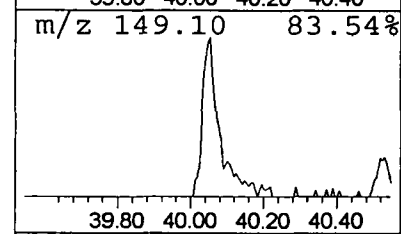
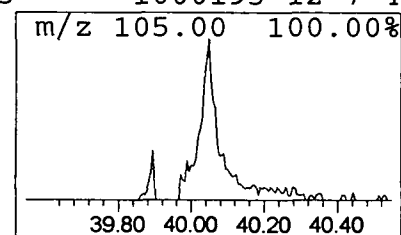
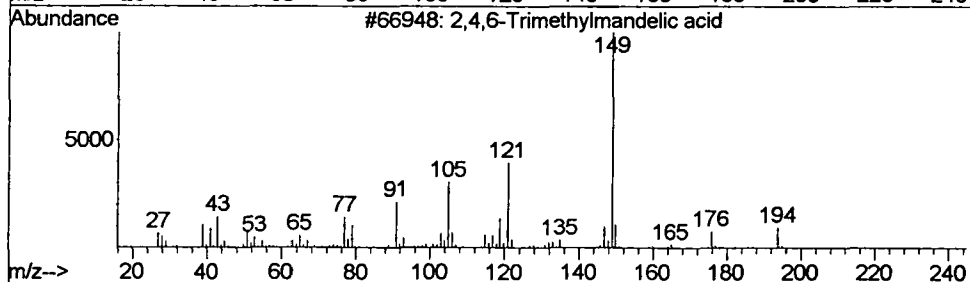
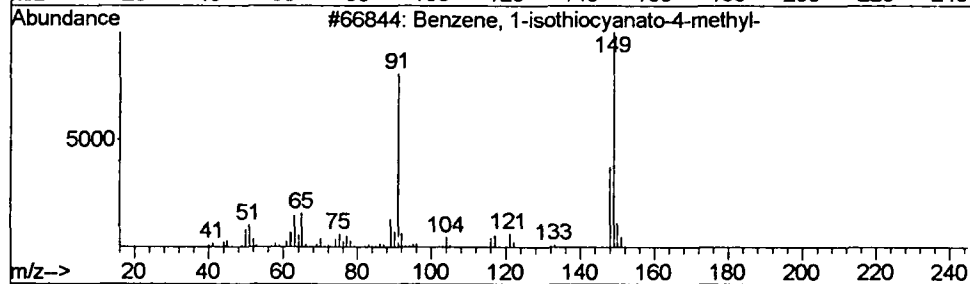
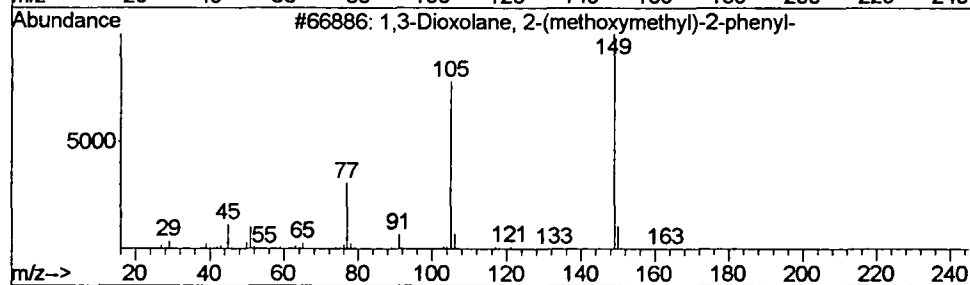
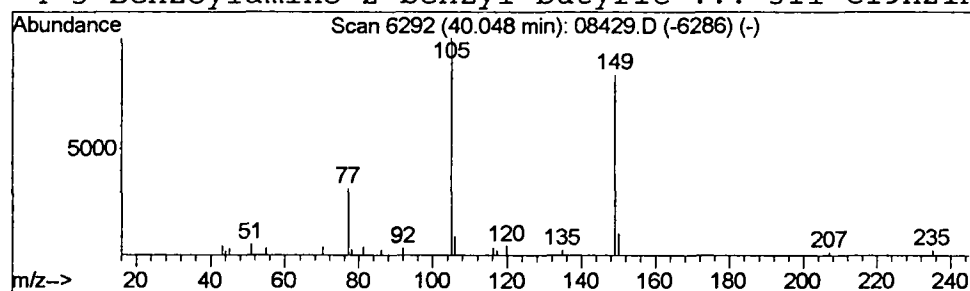
Vial: 16
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
40.05	0.39 ug/l	754779	Chrysene-d12	39.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	56
2		Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	47
3		2,4,6-Trimethylmandelic acid	194	C11H14O3	020797-56-2	40
4		3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	40



Tentatively Identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 19 Apr 2002 10:54 pm
 Data File: C:\MSDCHEM\1\DATA\020419\08429.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
✓ 3-Buten-2-ol, 2-m...	5.01	0.8	ug/l	1108360	1	11.38	54544900	40.0
3-Penten-2-ol	5.80	0.7	ug/l	888412	1	11.38	54544900	40.0
Acetic acid, 3-[1...	6.11	0.4	ug/l	528838	1	11.38	54544900	40.0
1,5-Naphthalenedi...	31.09	0.3	ug/l	630738	4	31.72	85361600	40.0
Anthracene-d10-	31.95	0.3	ug/l	605214	4	31.72	85361600	40.0
1,3-Dioxolane, 2-...	40.05	0.4	ug/l	754779	5	39.94	77444600	40.0
→ Phenanthrene-d10								