

Comments for Sample AE11480 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 05-29-2002 Time: 14:08:14

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

User: Vinci, David L
 Westchester Dept. of Labs & Research
 Date: 05/29/2002 Time: 14:07:27

Sample: AE11480
 Analysis: \$GCMS GCMS Scan For Unknowns
 Units: ug
 Started: 5/29/02 14:07 Ended: 5/29/02 14:07 Analyst: DLV
 Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		85		10.0

Data File : C:\MSDCHEM\1\DATA\020521\11480.D

Vial: 14

Acq On : 21 May 2002 9:12 pm

Operator: Nefliu

Sample : sample

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: rteint.e

Quant Time: May 24 09:30:41 2002

Quant Results File: SCAN020521.RE

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)

Title : Method 508 GC/MS Scan

Last Update : Fri May 24 09:17:56 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	411228	40.00	ug/l	-0.01
10) Naphthalene-d8	16.53	136	1551963	40.00	ug/l	-0.04
17) Acenaphthene-d10	24.45	164	834370	40.00	ug/l	-0.03
30) Phenanthrene-d10	31.72	188	1417831	40.00	ug/l	-0.02
38) Chrysene-d12	39.93	240	1133452	40.00	ug/l	-0.05
44) Perylene-d12	43.15	264	632643	40.00	ug/l	-0.03

System Monitoring Compounds

27) TCMX	27.55	207	227725	34.03	ug/l	-0.04
Spiked Amount	40.000		Recovery	=	85.08%	

Target Compounds

35) Di-n-butylphthalate	34.81	149	11412	0.25	ug/l	Qvalue 88
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(#) = qualifier out of range (m) = manual integration (+) = signals summed
11480.D SCAN020521.M Fri May 24 09:32:11 2002 Page 1

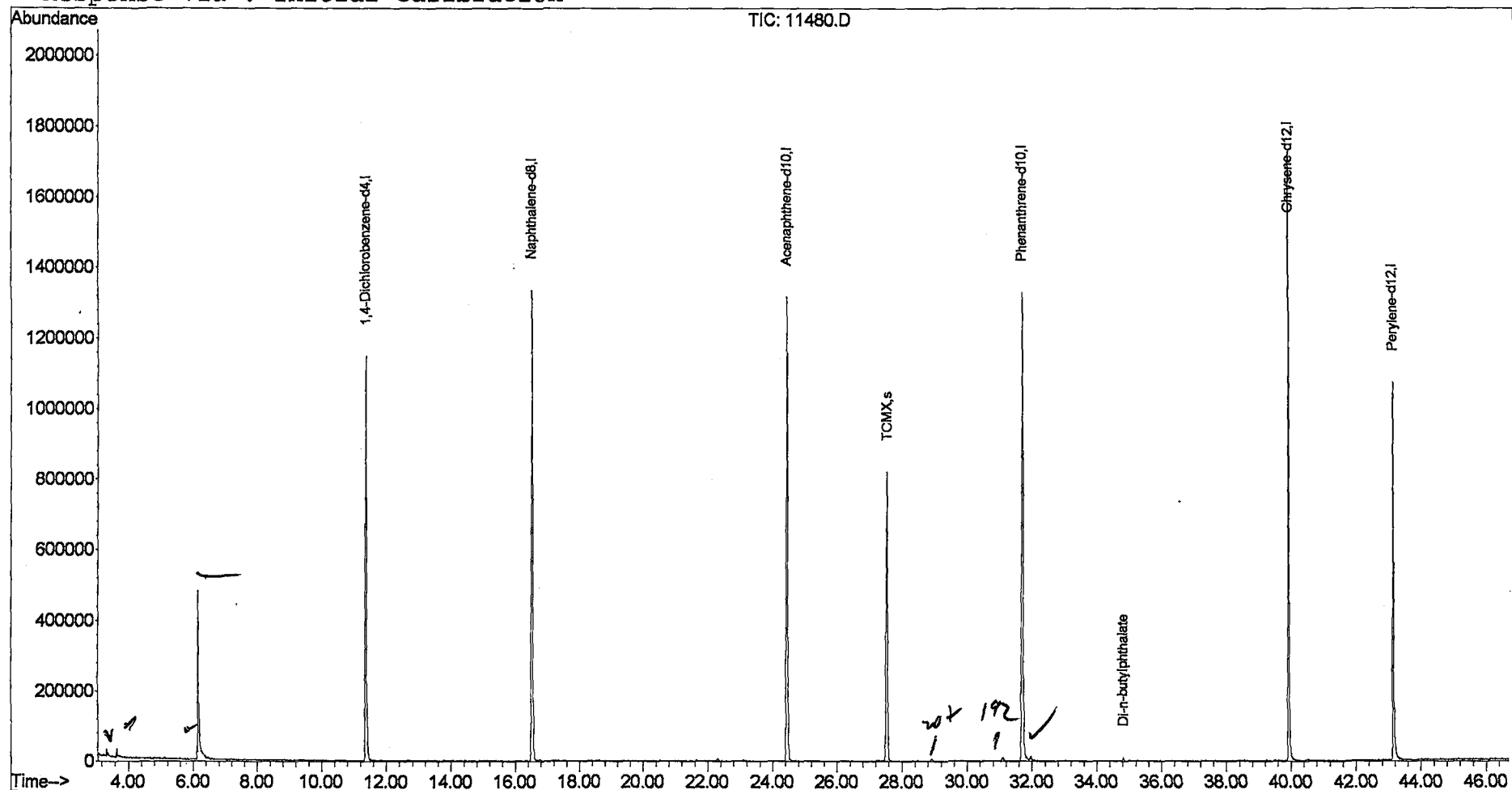
Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020521\11480.D
 Acq On : 21 May 2002 9:12 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e
 Quant Time: May 24 9:32 2002

Vial: 14
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Results File: SCAN020521.RES

Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Last Update : Fri May 24 09:17:56 2002
 Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\020521\11480.D

Acq On : 21 May 2002 9:12 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 14

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)

Title : Method 508 GC/MS Scan

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 0.5 % 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

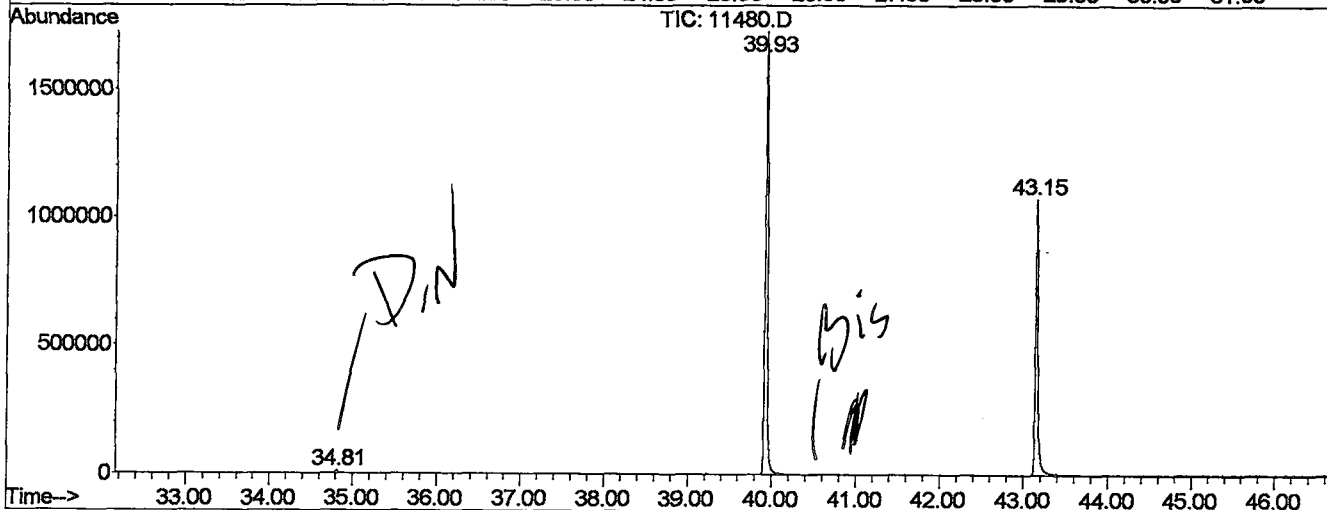
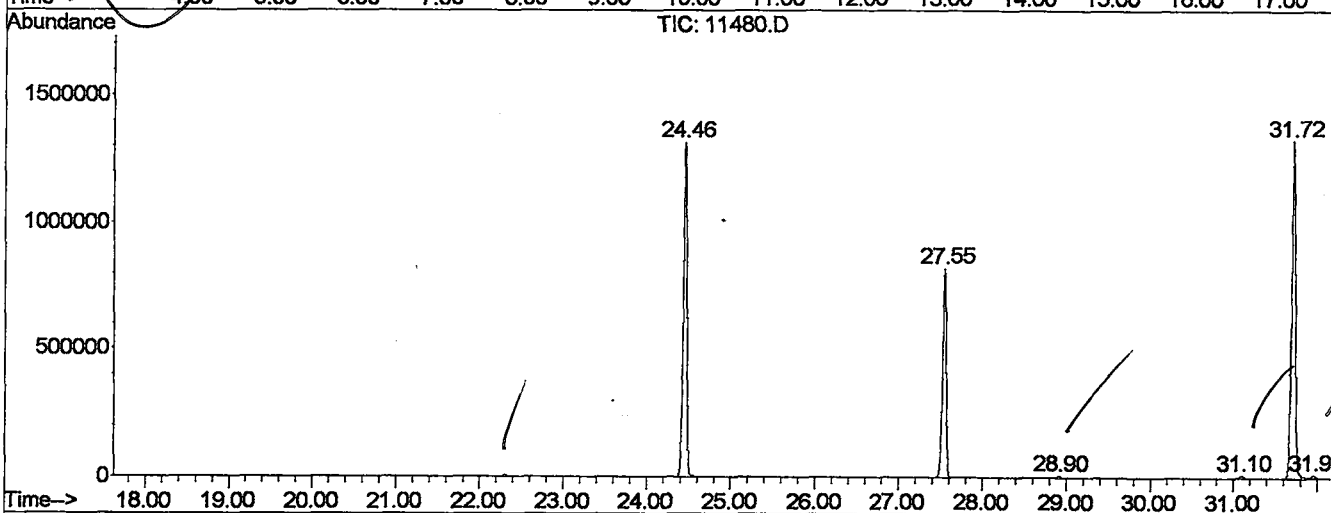
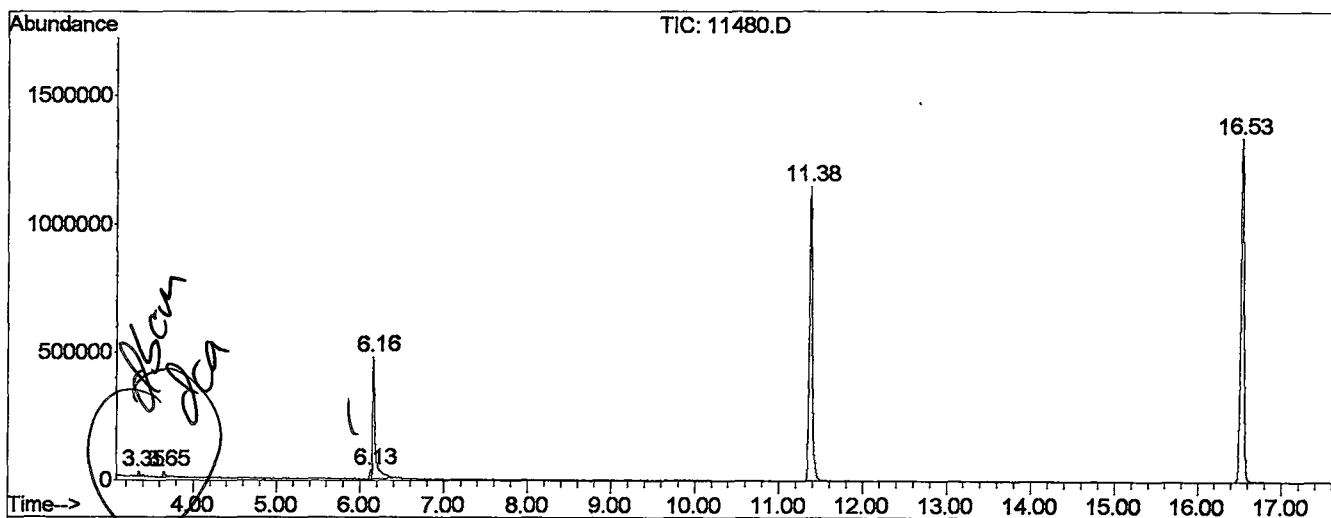
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.349	43	46	52	rBV	18733	24823	0.62%	0.106%
2	3.655	94	98	107	rVB2	23096	35516	0.89%	0.151%
3	6.128	512	519	521	rBV	38121	55598	1.39%	0.237%
4	6.158	521	524	565	rVB	477337	965746	24.17%	4.110%
5	11.375	1401	1412	1433	rBV	1147008	2885266	72.22%	12.280%
6	16.534	2275	2290	2311	rBV	1333982	3592045	89.91%	15.288%
7	24.460	3620	3639	3664	rBV	1315738	3760621	94.13%	16.005%
8	27.551	4145	4165	4178	rBV2	821593	2413711	60.41%	10.273%
9	28.902	4388	4395	4406	rVB6	6657	20576	0.52%	0.088%
10	31.099	4759	4769	4774	rBV5	9790	24827	0.62%	0.106%
11	31.716	4855	4874	4890	rBV2	1326408	3995315	100.00%	17.004%
12	31.957	4907	4915	4929	rVB4	12467	36159	0.91%	0.154%
13	34.813	5394	5401	5412	rVB2	10783	22811	0.57%	0.097%
14	39.930	6261	6272	6292	rBV2	1726026	3437615	86.04%	14.631%
15	43.150	6806	6820	6850	rBV	1072365	2225581	55.70%	9.472%

Sum of corrected areas: 23496210

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020521\11480.D
Operator : Nefliu
Acquired : 21 May 2002 9:12 pm using AcqMethod 508SCAN1
Instrument : Instrumen
Sample Name: sample
Misc Info :
Vial Number: 14
Quant File :SCAN020521.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020521\11480.D

Acq On : 21 May 2002 9:12 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 14

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)

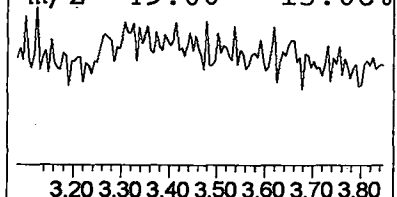
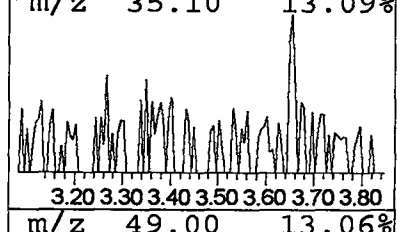
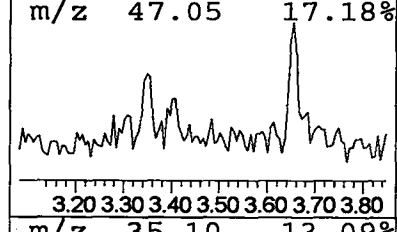
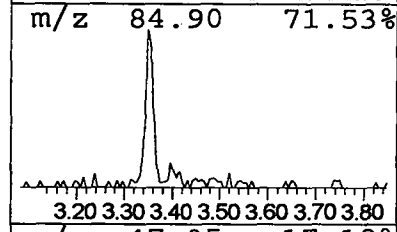
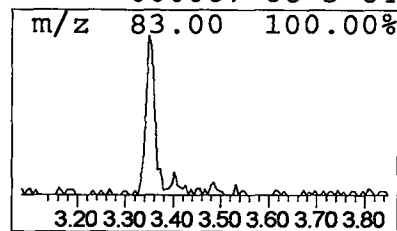
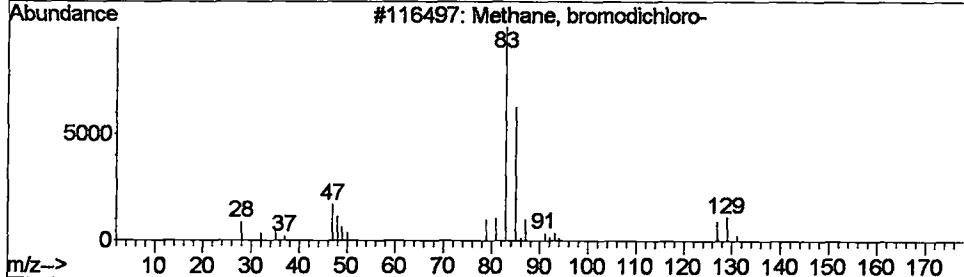
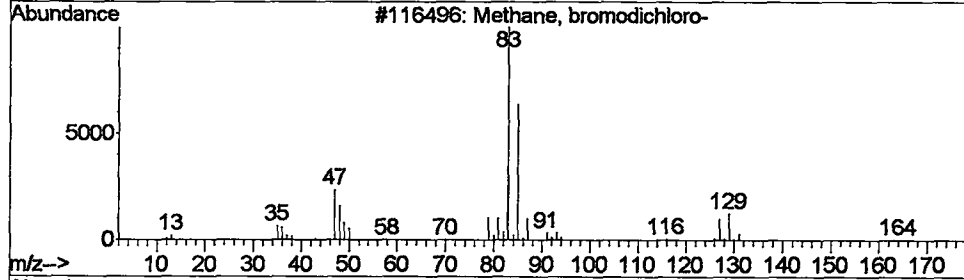
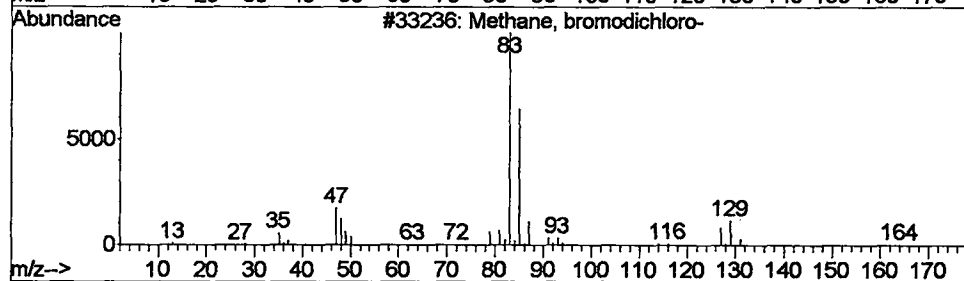
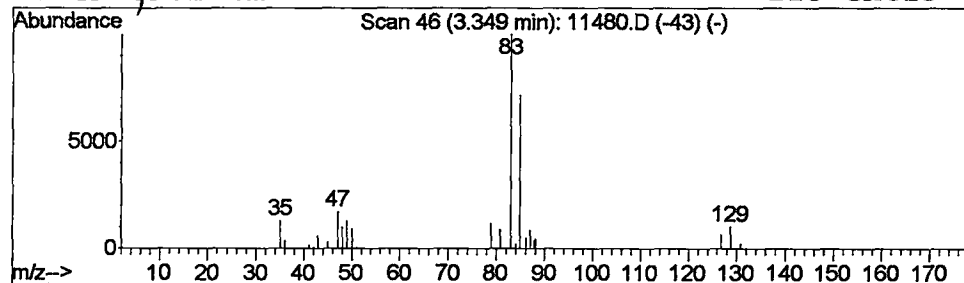
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\nist98.1

Peak Number 1 Methane, bromodichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.35	0.34 ug/l	24823	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, bromodichloro-	162	CHBrCl2	000075-27-4	78
2			Methane, bromodichloro-	162	CHBrCl2	000075-27-4	78
3			Methane, bromodichloro-	162	CHBrCl2	000075-27-4	78
4			Chloroform	118	CHCl3	000067-66-3	64



Library Search Compound Report

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Acq On : 21 May 2002 9:12 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 14

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)

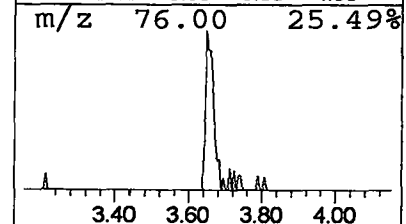
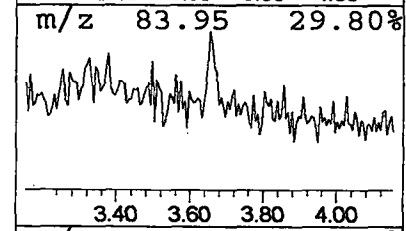
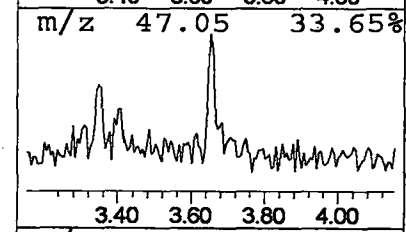
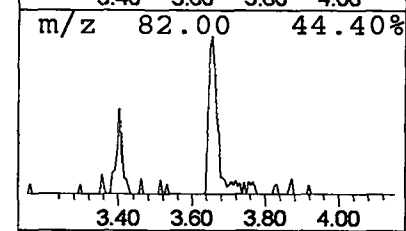
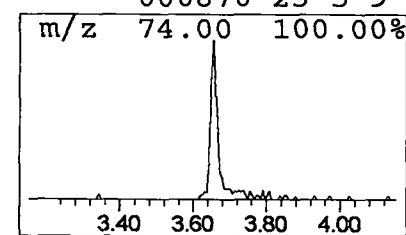
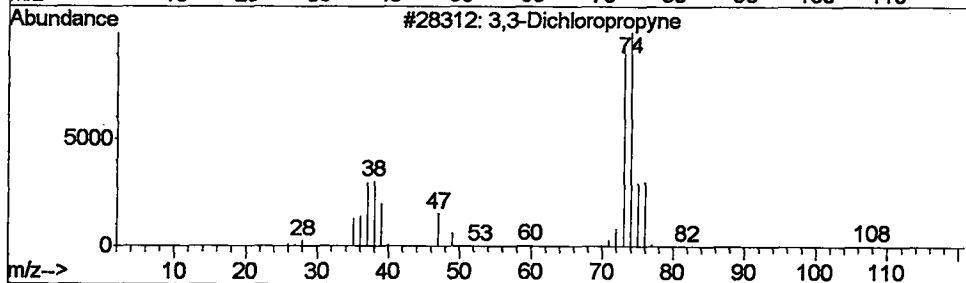
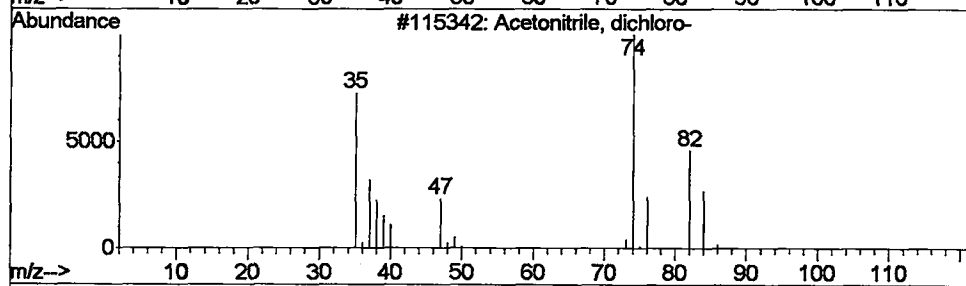
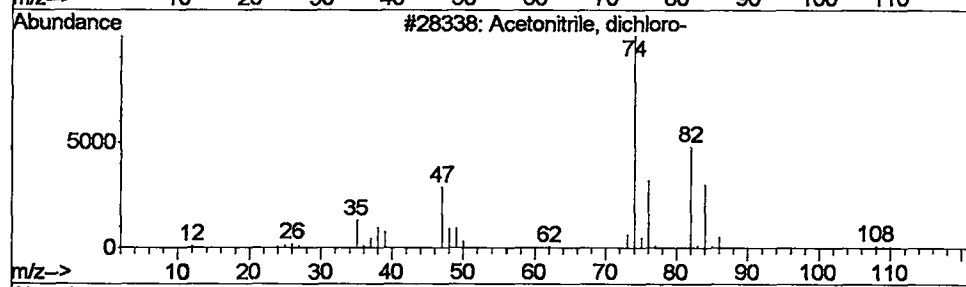
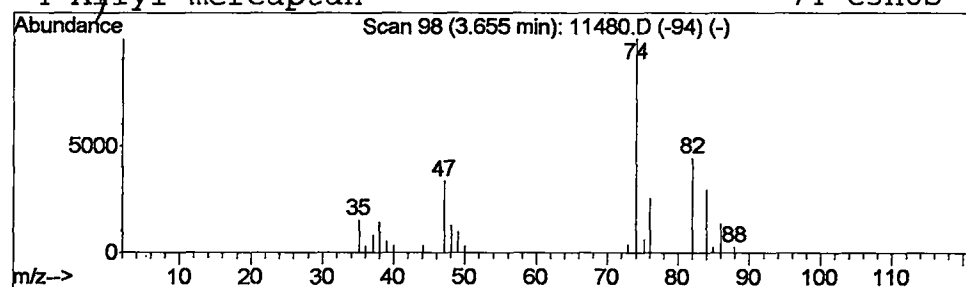
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\nist98.1

Peak Number 2 Acetonitrile, dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.65	0.49 ug/l	35516	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	53
2			Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	40
3			3,3-Dichloropropyne	108	C3H2Cl2	1000222-23-9	25
4			Allyl mercaptan	74	C3H6S	000870-23-5	9



Library Search Compound Report

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Acq On : 21 May 2002 9:12 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 14

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)

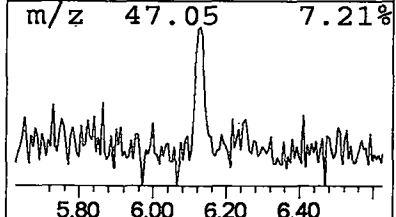
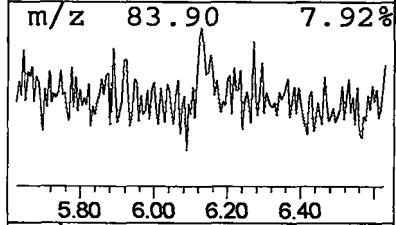
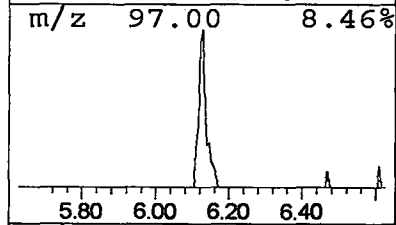
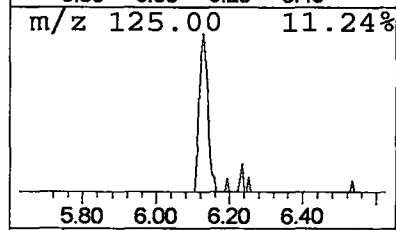
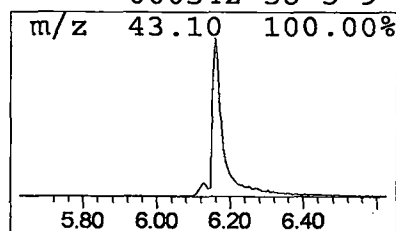
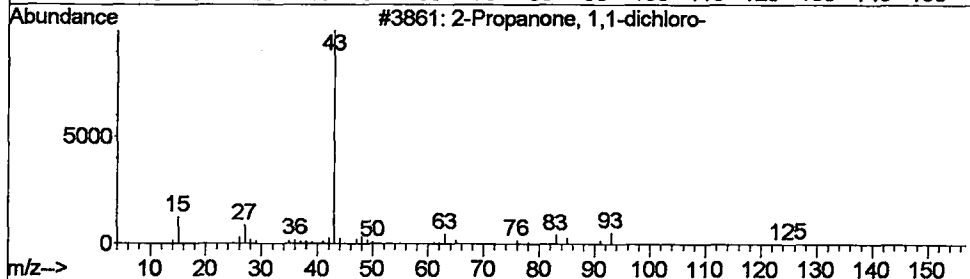
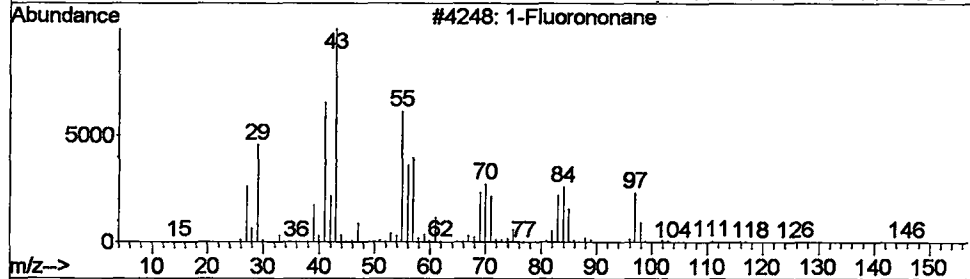
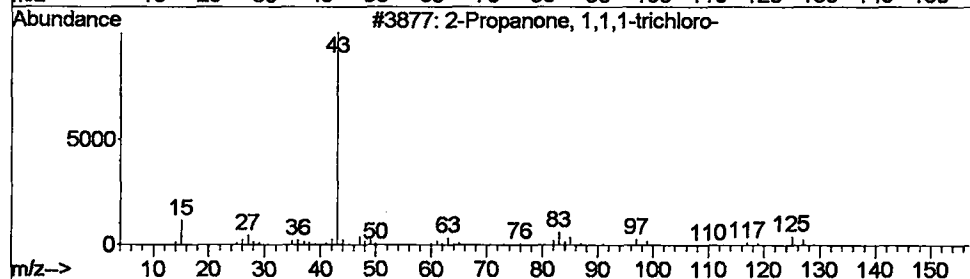
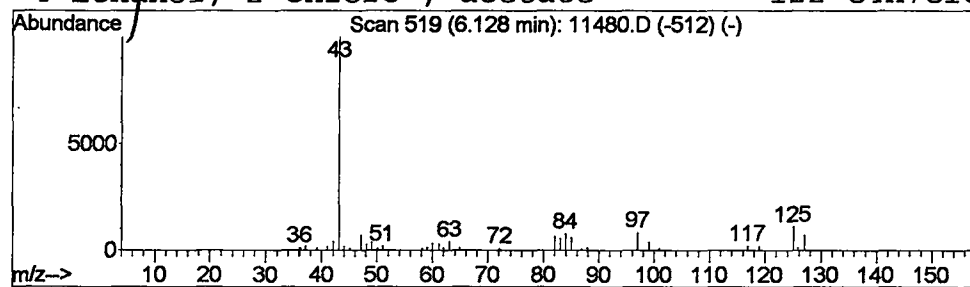
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\nist98.1

Peak Number 3 2-Propanone, 1,1,1-trichloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	0.77 ug/l	55598	1,4-Dichlorobenzene-d4	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanone, 1,1,1-trichloro-	160	C3H3Cl3O	000918-00-3	56
2		1-Fluorononane	146	C9H19F	000463-18-3	9
3		2-Propanone, 1,1-dichloro-	126	C3H4Cl2O	000513-88-2	9
4		Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9



Library Search Compound Report

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 Sample : sample
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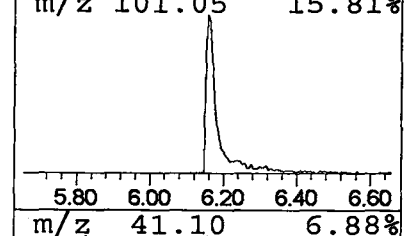
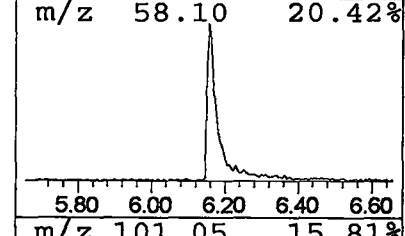
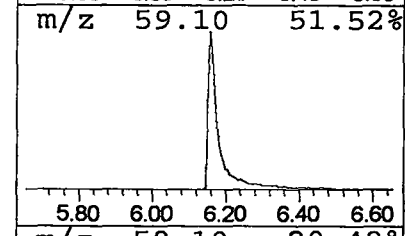
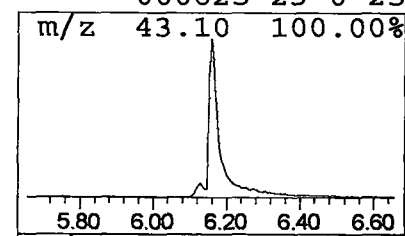
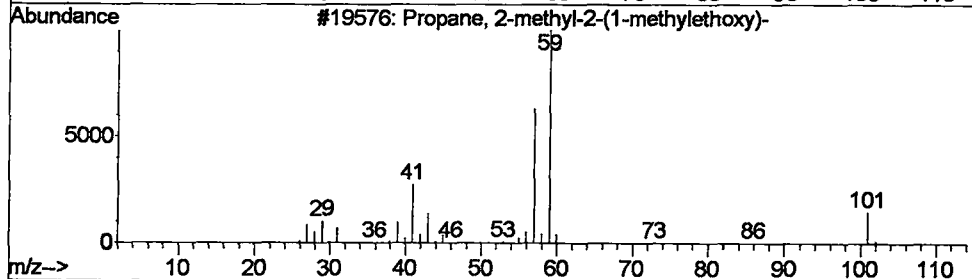
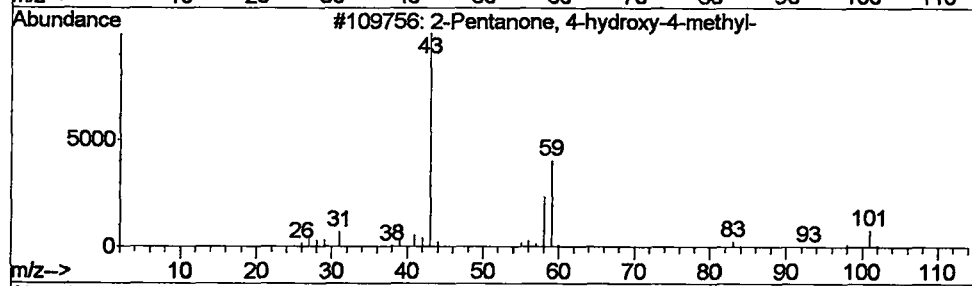
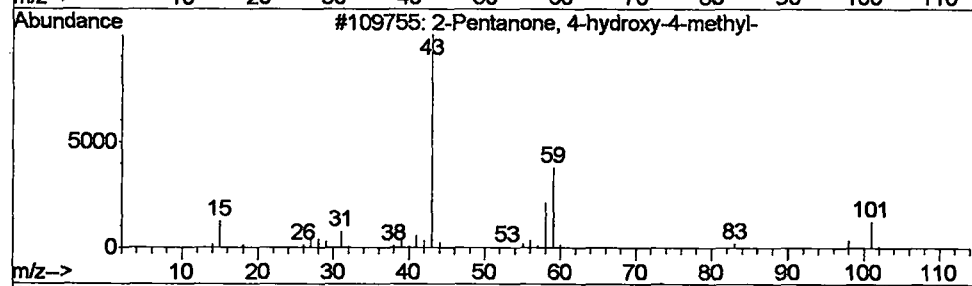
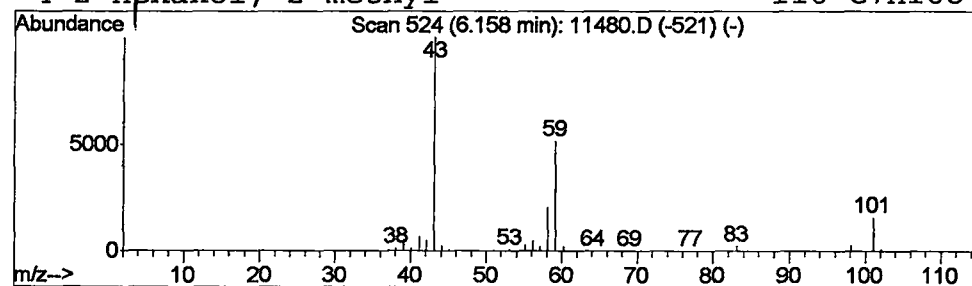
Vial: 14
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	13.39 ug/l	965746	1,4-Dichlorobenzene-d4	11.38

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	56
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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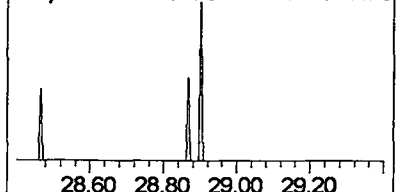
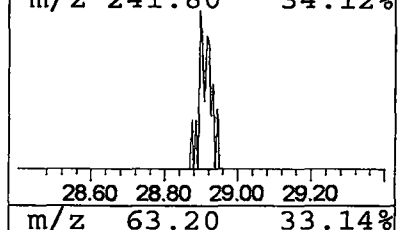
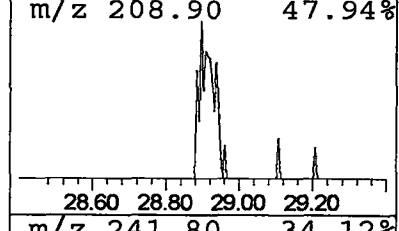
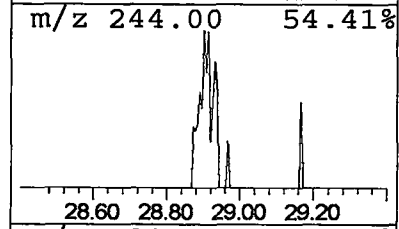
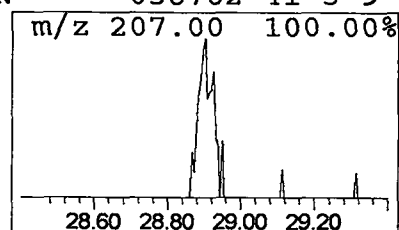
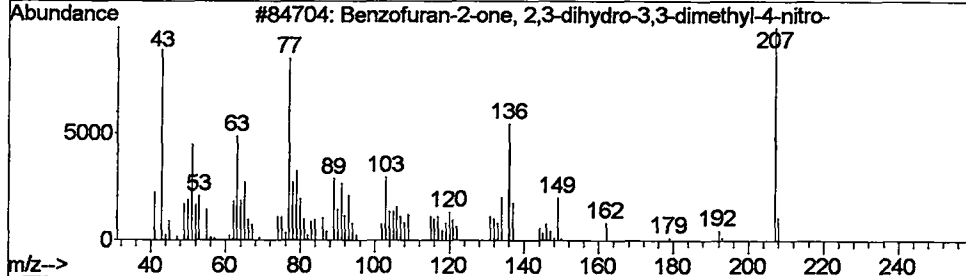
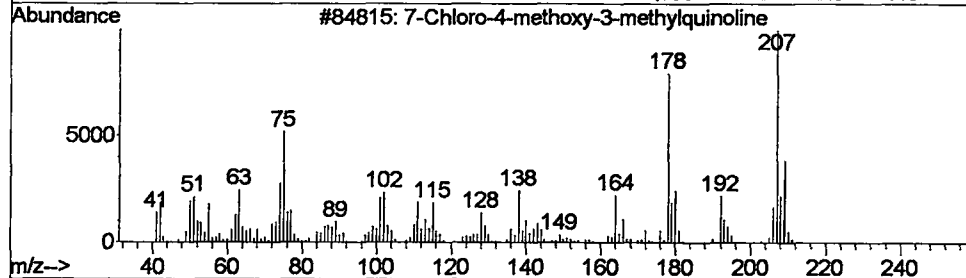
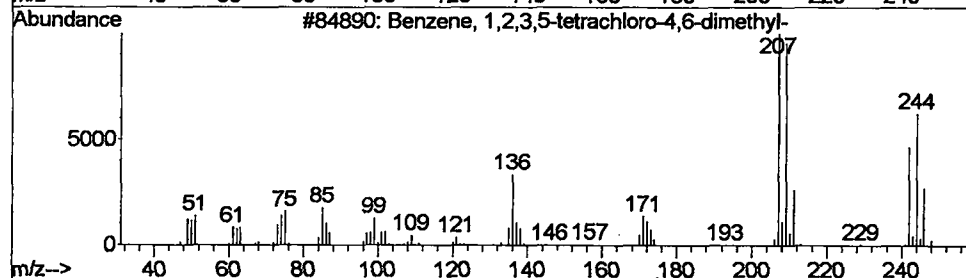
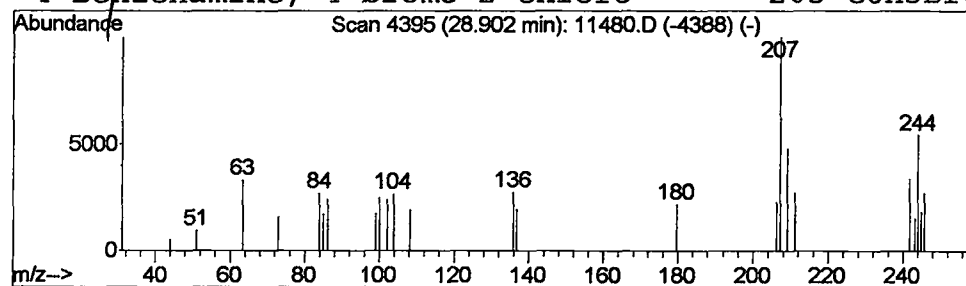
Vial: 14
 Operator: Nefliu
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Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.l

 Peak Number 5 Benzene, 1,2,3,5-tetrachlor... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.90	0.21 ug/l	20576	Phenanthrene-d10	31.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,5-tetrachloro-4,6...	242	C8H6Cl4	000877-09-8	37
2		7-Chloro-4-methoxy-3-methylquino...	207	C11H10ClNO	1000213-52-2	35
3		Benzofuran-2-one, 2,3-dihydro-3,...	207	C10H9NO4	1000129-53-4	10
4		Benzenamine, 4-bromo-2-chloro-	205	C6H5BrClN	038762-41-3	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020521\11480.D
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 Sample : sample
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 MS Integration Params: rteint.e

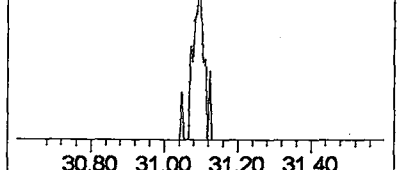
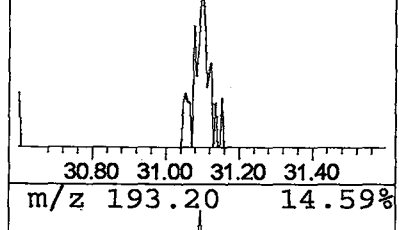
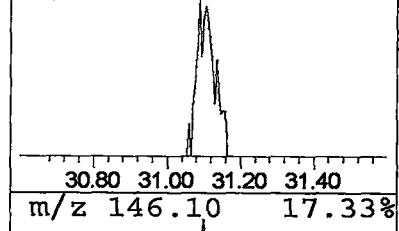
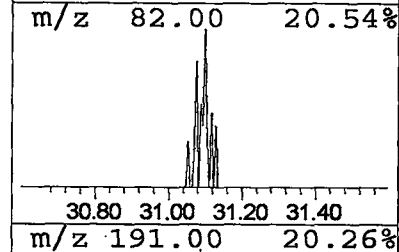
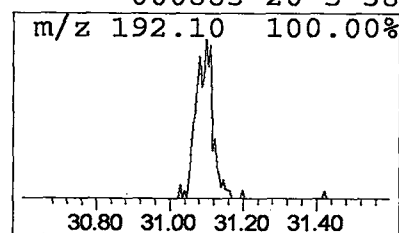
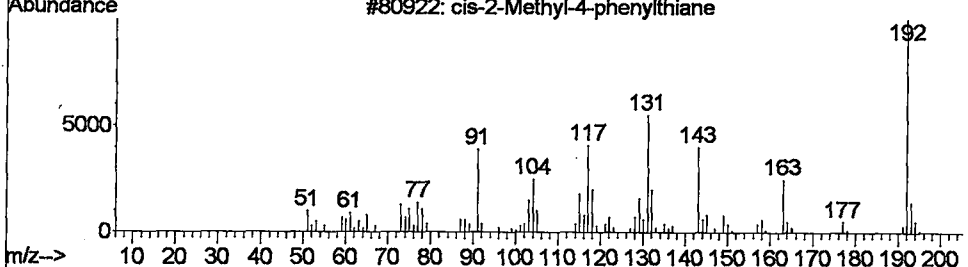
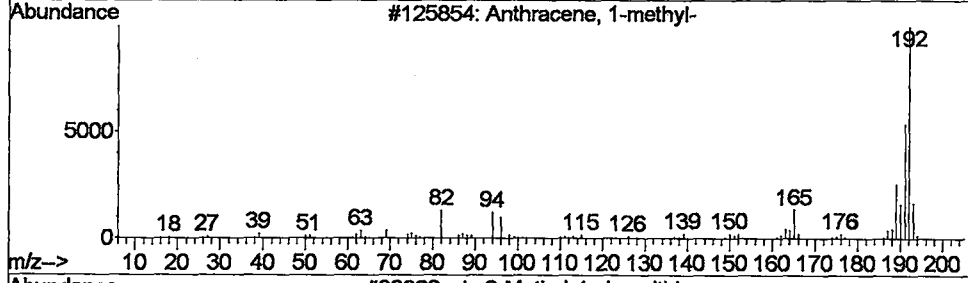
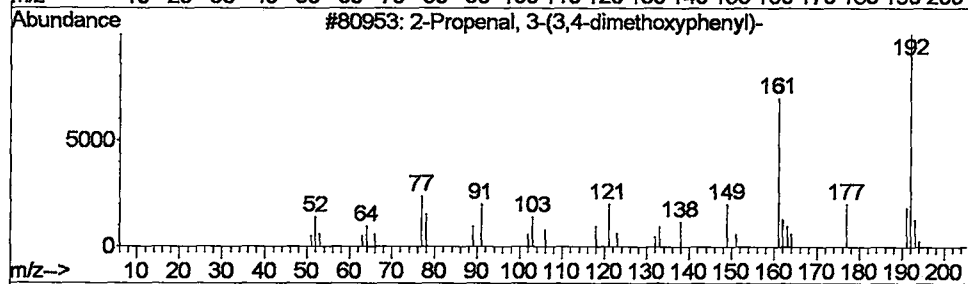
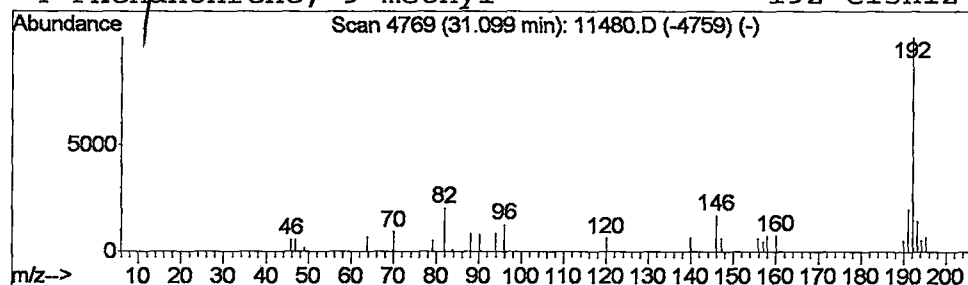
Vial: 14
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 6 2-Propenal, 3-(3,4-dimethox... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.10	0.25 ug/l	24827	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	58
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
3		cis-2-Methyl-4-phenylthiane	192	C12H16S	076097-69-3	38
4		Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	38



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020521\11480.D
 Acq On : 21 May 2002 9:12 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

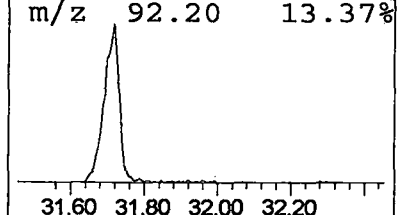
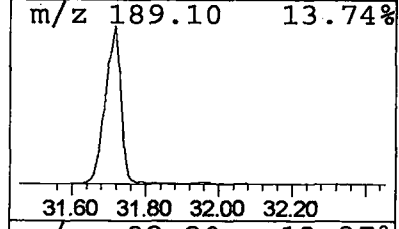
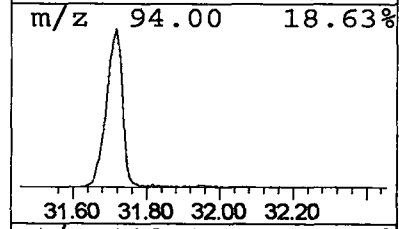
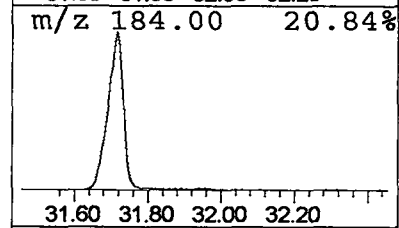
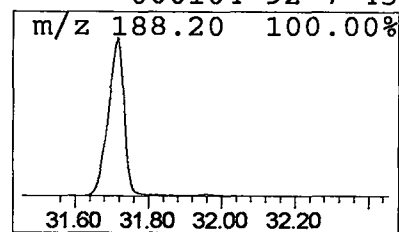
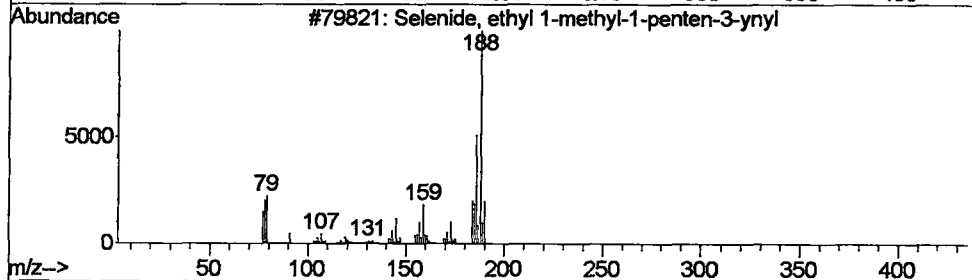
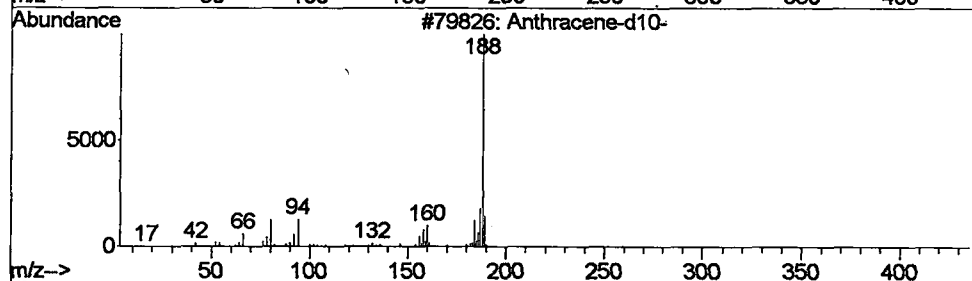
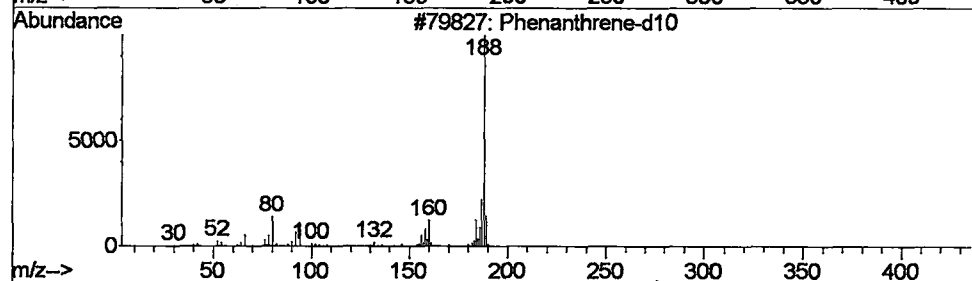
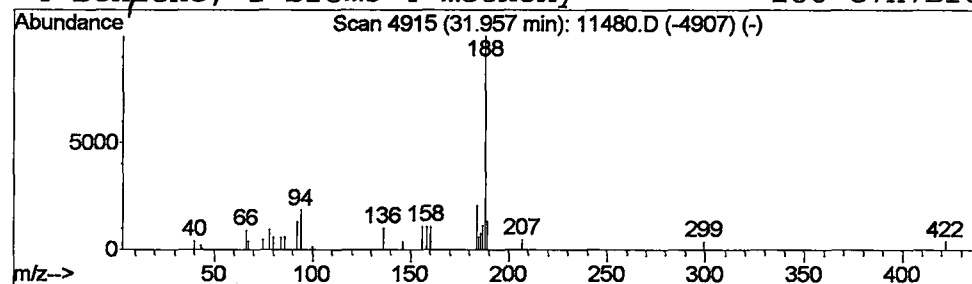
Vial: 14
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 7 Phenanthrene-d10 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.96	0.36 ug/l	36159	Phenanthrene-d10	31.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene-d10	188	C14D10	001517-22-2	64
2		Anthracene-d10-	188	C14D10	001719-06-8	59
3		Selenide, ethyl 1-methyl-1-pente...	188	C8H12Se	025128-48-7	53
4		Benzene, 1-bromo-4-methoxy-	186	C7H7BrO	000104-92-7	43



tentatively identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 21 May 2002 9:12 pm
Data File: C:\MSDCHEM\1\DATA\020521\11480.D
Name: sample
Misc:
Method: C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE 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
✓ Methane, bromodic...	3.35	0.3	ug/l	24823	1	11.38	2885270	40.0
✓ Acetonitrile, dic...	3.65	0.5	ug/l	35516	1	11.38	2885270	40.0
✓ 2-Propanone, 1,1,...	6.13	0.8	ug/l	55598	1	11.38	2885270	40.0
2-Pentanone, 4-hy...	6.16	13.4	ug/l	965746	1	11.38	2885270	40.0
Benzene, 1,2,3,5-...	28.90	0.2	ug/l	20576	4	31.72	3995320	40.0
2-Propenal, 3-(3,...	31.10	0.2	ug/l	24827	4	31.72	3995320	40.0
Phenanthrene d10 <i>Anthracene-d10</i>	31.96	0.4	ug/l	36159	4	31.72	3995320	40.0