

Comments for Sample AE10519 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 05-29-2002 Time: 14:22:16

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. This sample will be extracted again because of the low Surrogate Standard recovery. Re-analysis yielded a Surrogate Standard recovery of 86%.

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020521\10519.D
 Acq On : 21 May 2002 4:17 pm
 Sample : sample
 Misc :

Vial: 9
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

MS Integration Params: rteint.e
 Quant Time: May 24 09:19:19 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

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Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	11.37	152	465567	40.00	ug/l	-0.02
10) Naphthalene-d8	16.53	136	1742438	40.00	ug/l	-0.04
17) Acenaphthene-d10	24.45	164	938761	40.00	ug/l	-0.03
30) Phenanthrene-d10	31.72	188	1588970	40.00	ug/l	-0.02
38) Chrysene-d12	39.93	240	1178155	40.00	ug/l	-0.05
44) Perylene-d12	43.15	264	677647	40.00	ug/l	-0.03

System Monitoring Compounds

27) TCMX 27.55 207 259172 34.42 ug/l -0.04
 Spiked Amount 40.000 Recovery = 86.05%

Target Compounds

Qvalue

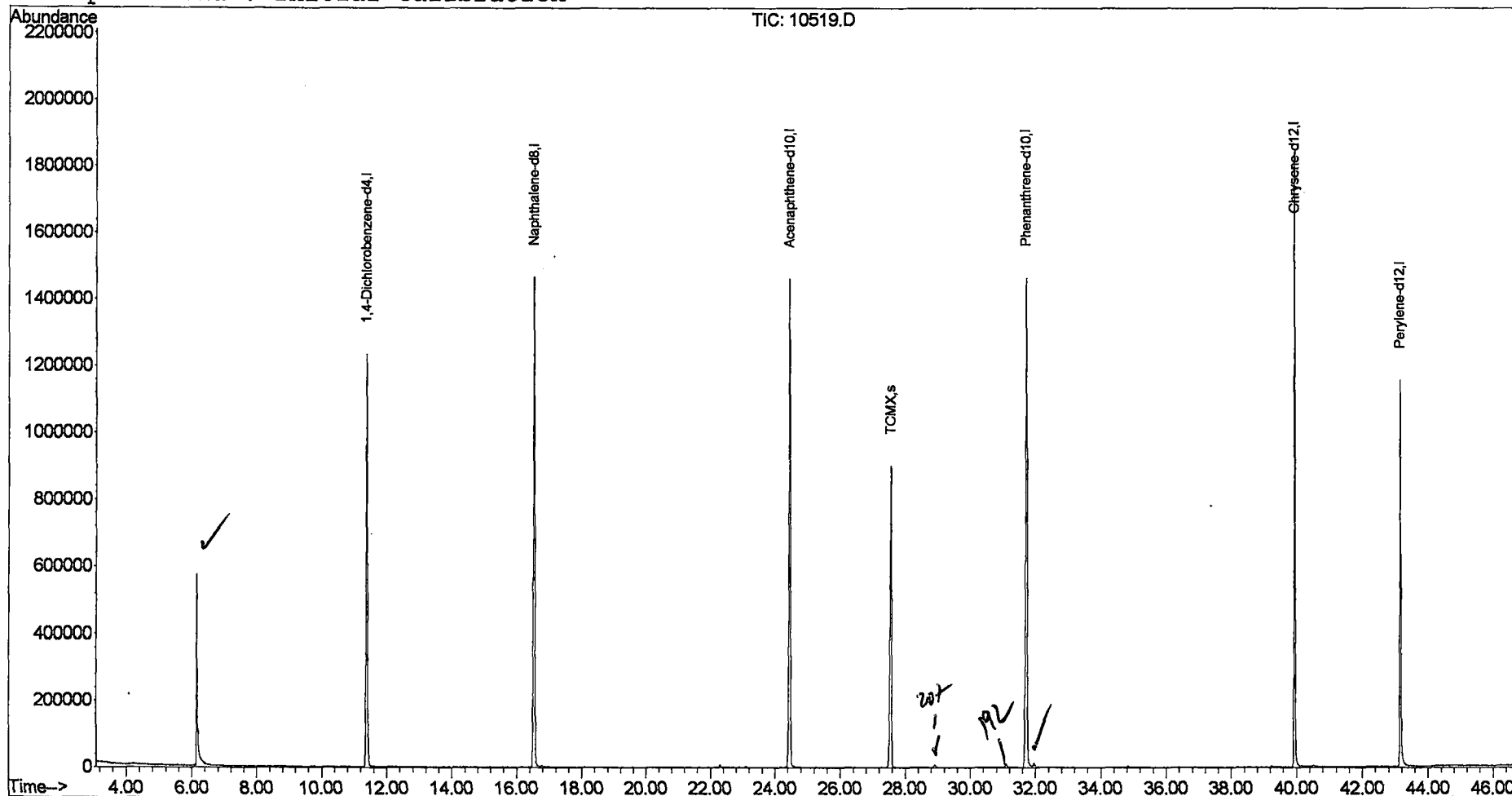
Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020521\10519.D
Acq On : 21 May 2002 4:17 pm
Sample : sample
Misc :
MS Integration Params: rteint.e
Quant Time: May 24 9:20 2002

Vial: 9
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\10519.D

Acq On : 21 May 2002 4:17 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 9

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

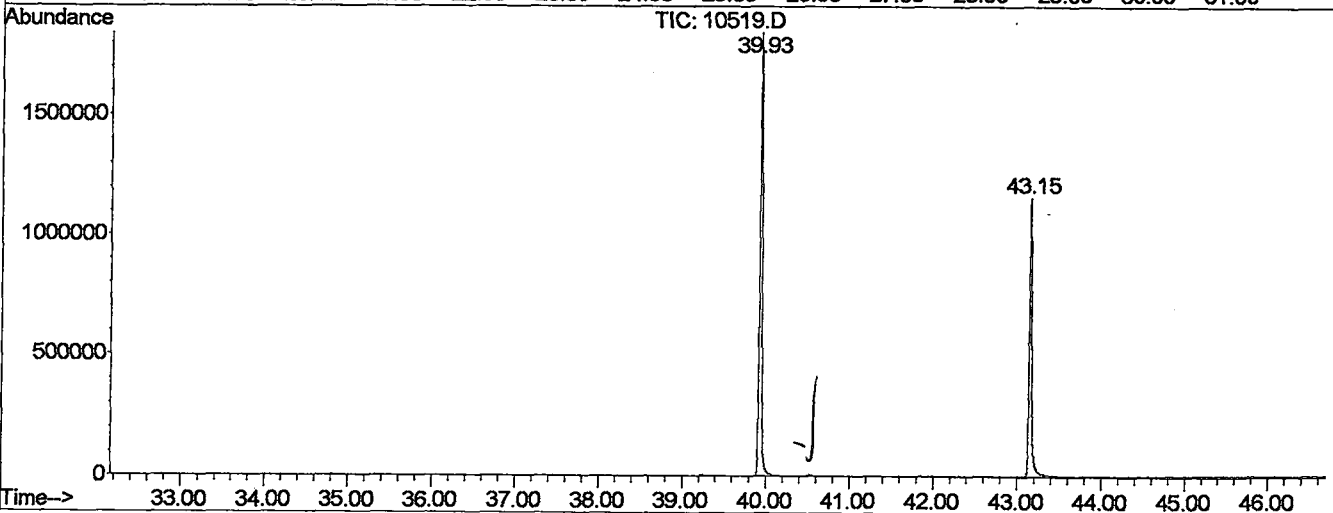
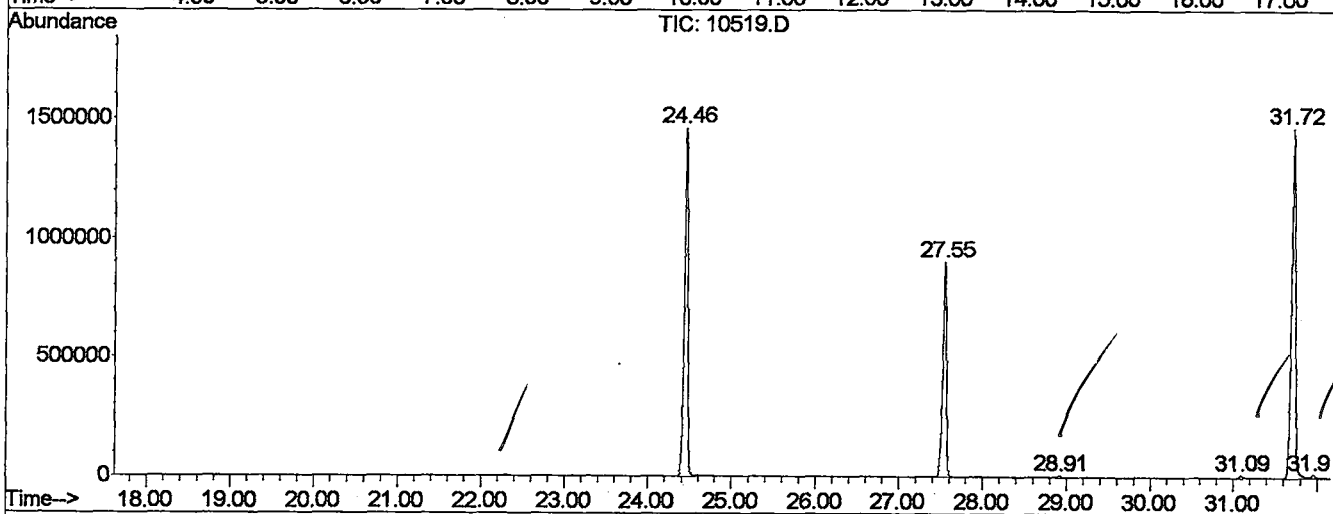
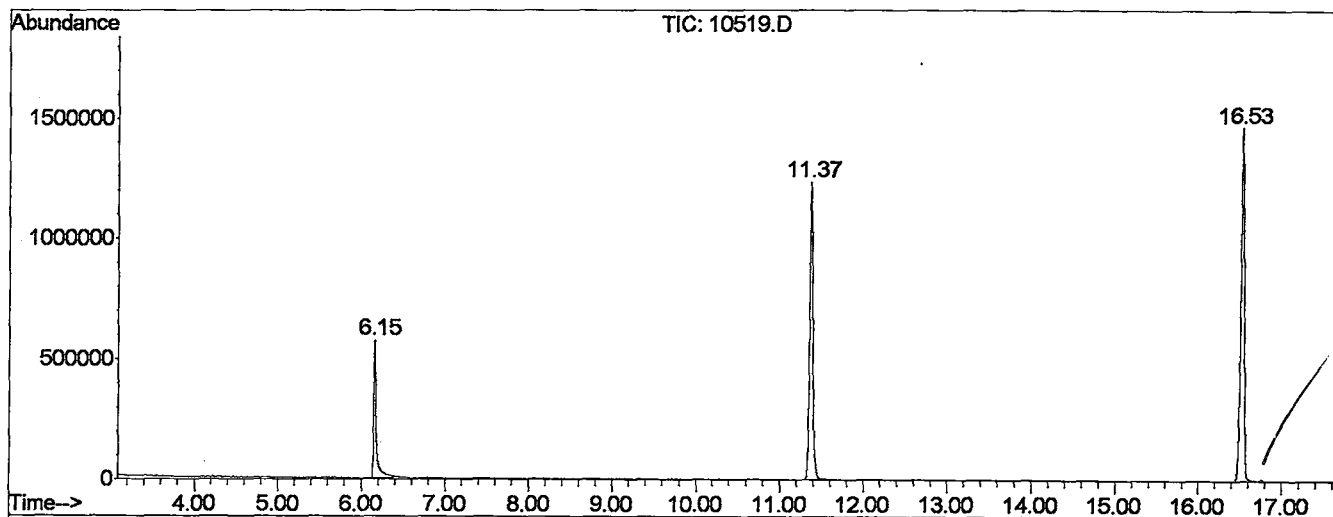
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.152	518	523	561	rBV	572002	1179737	26.26%	4.542%
2	11.370	1400	1411	1434	rBV	1233298	3231396	71.94%	12.442%
3	16.534	2272	2290	2309	rBV	1467155	4035529	89.84%	15.538%
4	24.460	3618	3639	3654	rBV	1461705	4212643	93.78%	16.220%
5	27.551	4144	4165	4182	rBV2	903317	2676800	59.59%	10.307%
6	28.908	4386	4396	4404	rVB5	8210	24672	0.55%	0.095%
7	31.088	4759	4767	4780	rBV3	11288	32064	0.71%	0.123%
8	31.717	4852	4874	4904	rBV2	1466214	4491876	100.00%	17.295%
9	31.952	4906	4914	4925	rVB5	12221	38001	0.85%	0.146%
10	39.931	6262	6272	6301	rBV2	1841316	3642789	81.10%	14.026%
11	43.151	6809	6820	6849	rBV2	1156144	2405946	53.56%	9.264%

Sum of corrected areas: 25971453

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020521\10519.D
 Operator : Nefliu
 Acquired : 21 May 2002 4:17 pm using AcqMethod 508SCAN1
 Instrument : Instrumen
 Sample Name: sample
 Misc Info :
 Vial Number: 9
 Quant File :SCAN020521.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020521\10519.D
 Acq On : 21 May 2002 4:17 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

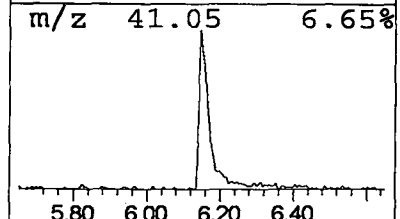
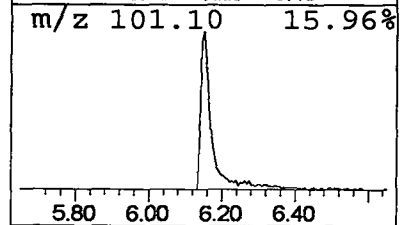
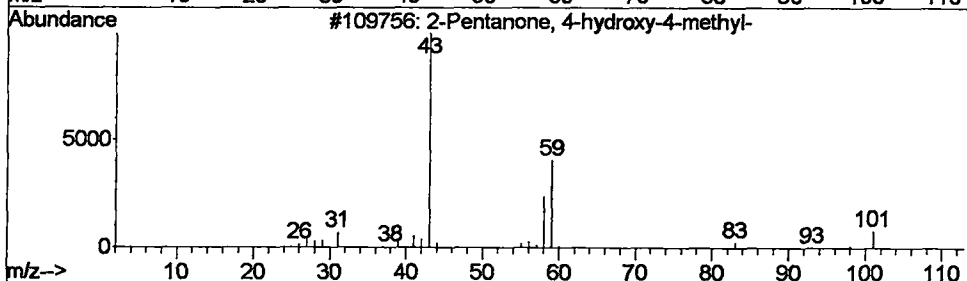
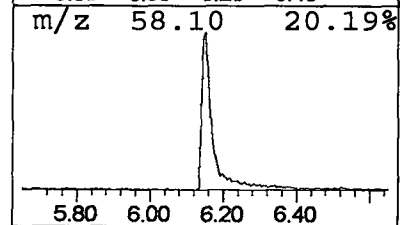
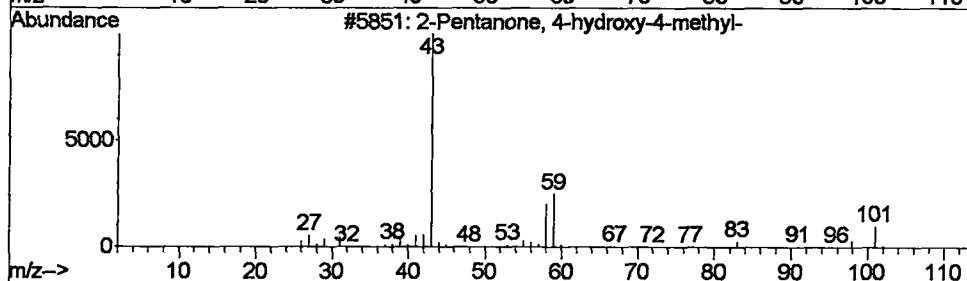
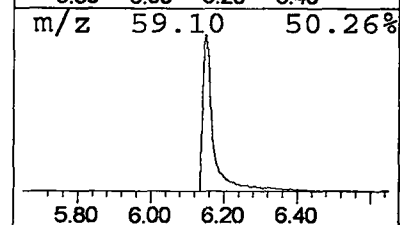
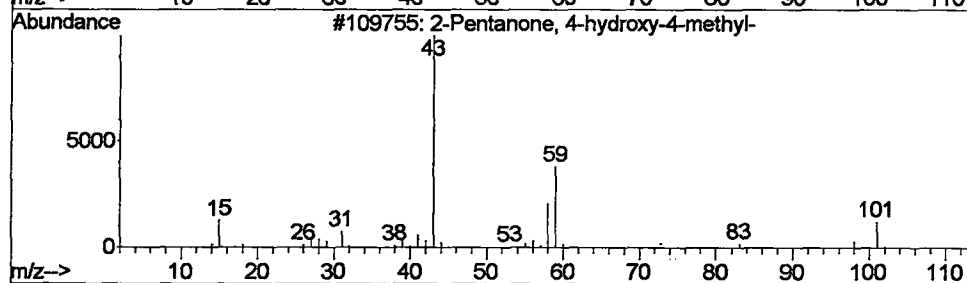
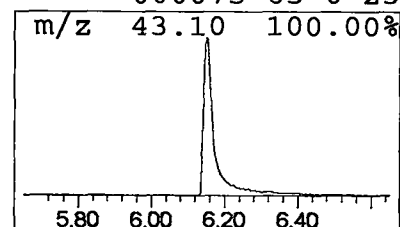
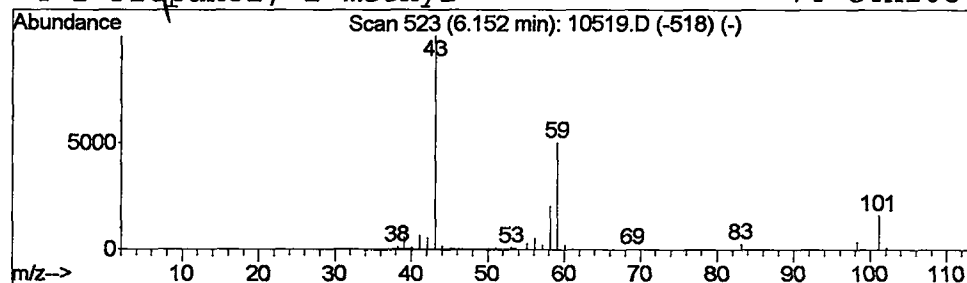
Vial: 9
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

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

R.T.	EstConc	Area	Relative to. ISTD	R.T.
6.15	14.60 ug/l	1179740	1,4-Dichlorobenzene-d4	11.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	23



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MS Integration Params: rteint.e

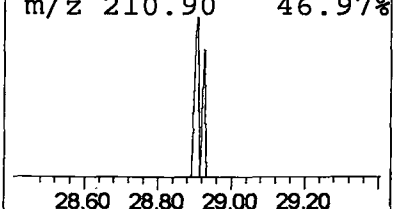
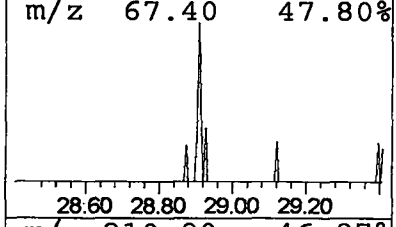
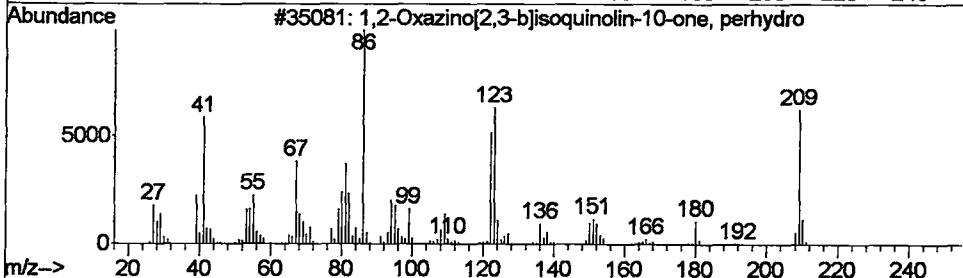
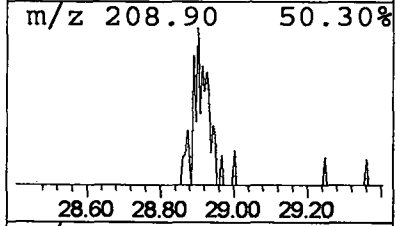
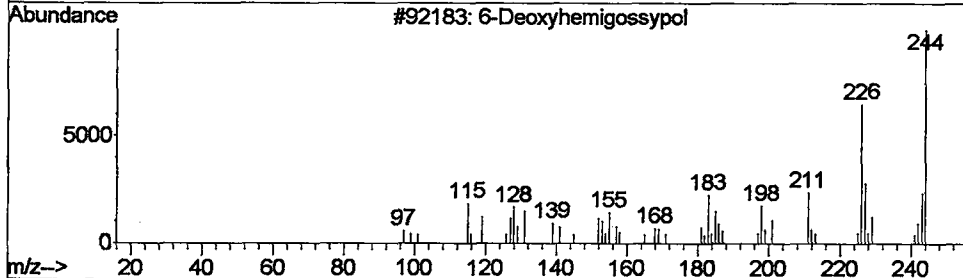
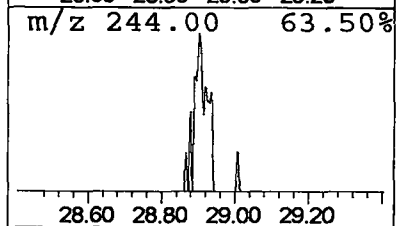
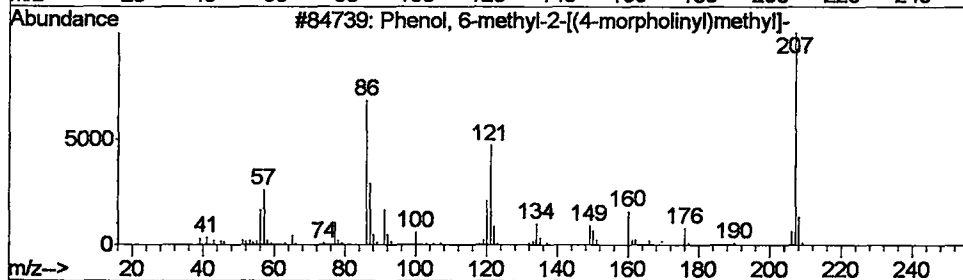
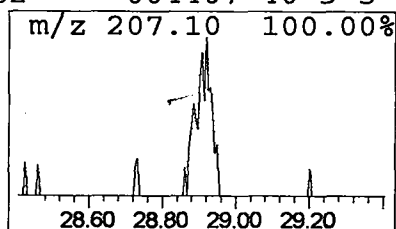
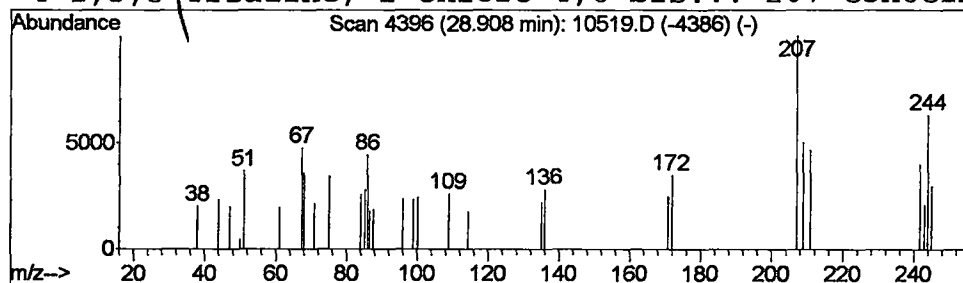
Vial: 9
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 2 Phenol, 6-methyl-2-[(4-morp... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.91	0.22 ug/l	24672	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 6-methyl-2-[(4-morpholin...	207	C12H17NO2	060460-71-1	5
2		6-Deoxyhemigossypol	244	C15H16O3	055824-28-7	5
3		1,2-Oxazino[2,3-b]isoquinolin-10...	209	C12H19NO2	1000196-76-2	5
4		1,3,5-Triazine, 2-chloro-4,6-bis...	207	C5H6ClN3S2	004407-40-3	5



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 Sample : sample
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 MS Integration Params: rteint.e

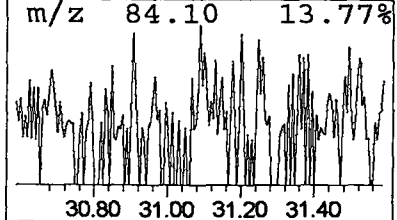
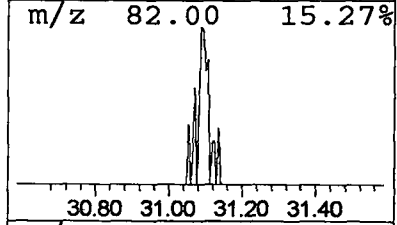
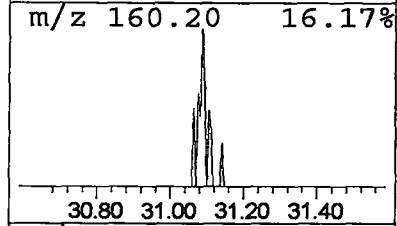
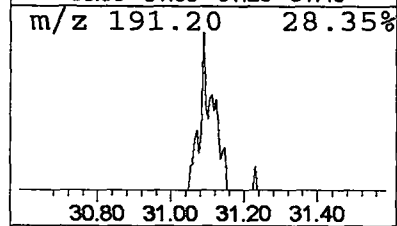
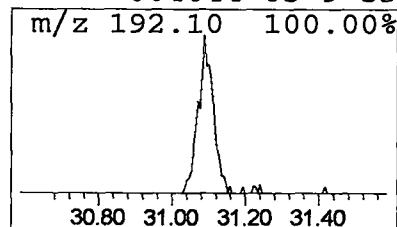
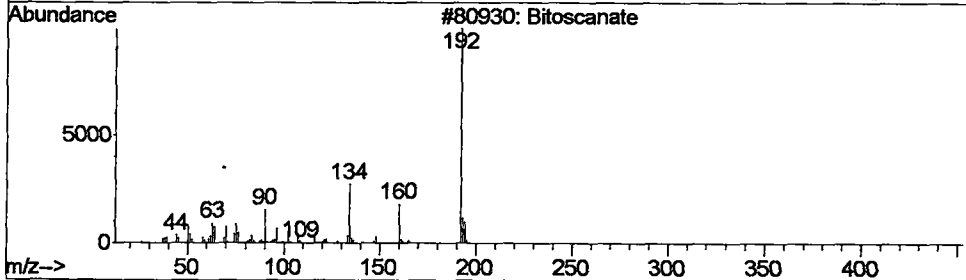
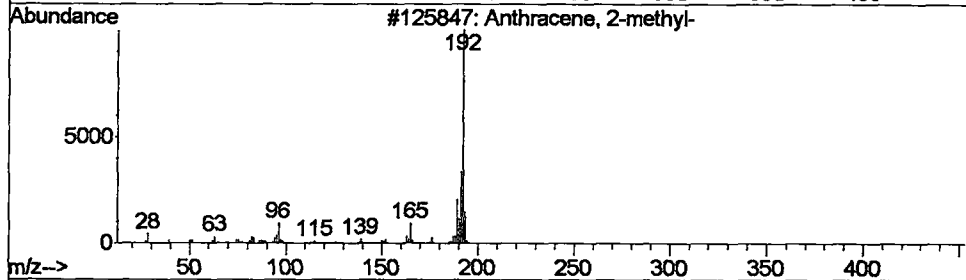
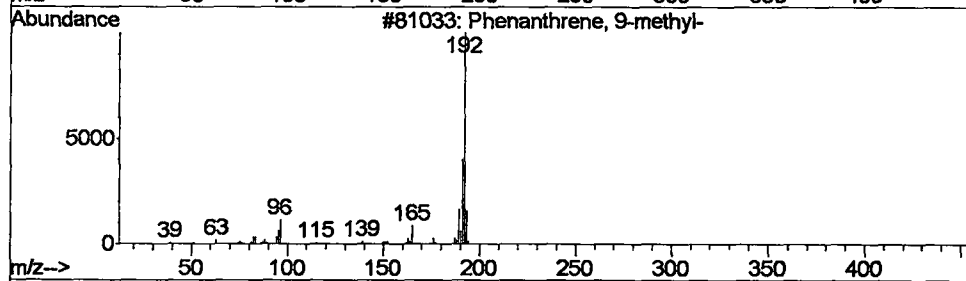
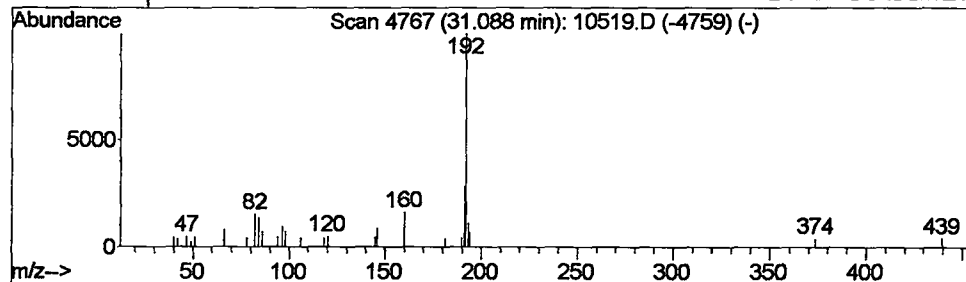
Vial: 9
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 Phenanthrene, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.09	0.29 ug/l	32064	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	64
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	59
3			Bitoscanate	192	C8H4N2S2	004044-65-9	53
4			Bitoscanate	192	C8H4N2S2	004044-65-9	53



Library Search Compound Report

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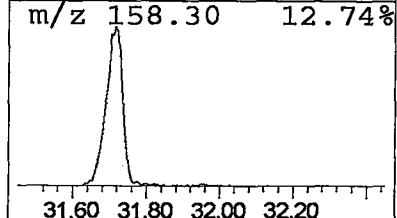
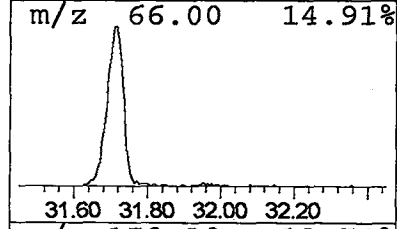
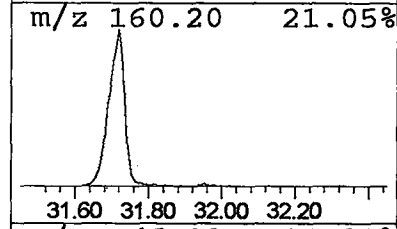
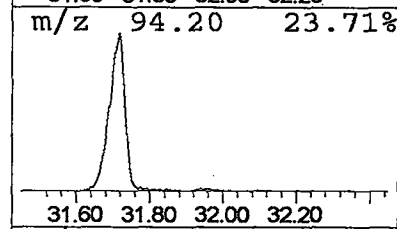
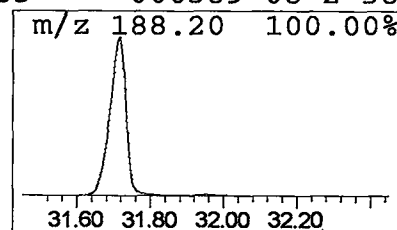
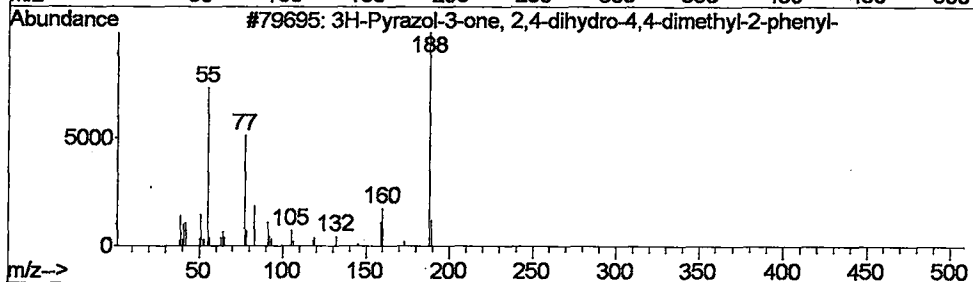
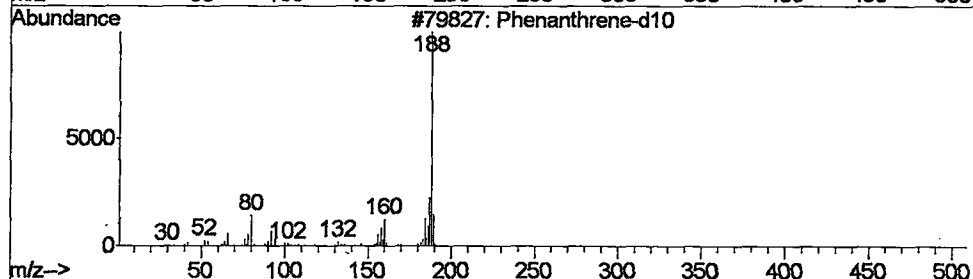
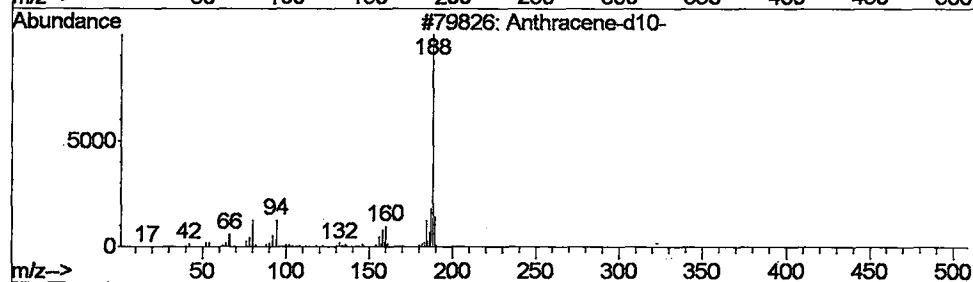
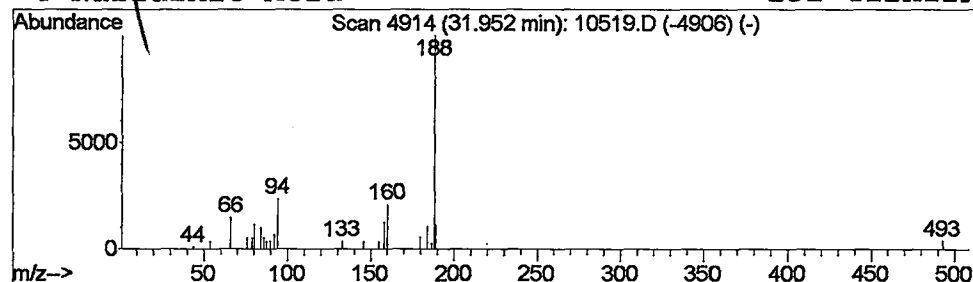
Vial: 9
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 4 Anthracene-d10- Concentration Rank 2

R.T.	EstConc	Area	Relative to. ISTD	R.T.
31.95	0.34 ug/l	38001	Phenanthrene-d10	31.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene-d10-	188	C14D10	001719-06-8	59	
2	Phenanthrene-d10	188	C14D10	001517-22-2	59	
3	3H-Pyrazol-3-one, 2,4-dihydro-4,...	188	C11H12N2O	017694-06-3	38	
4	Nalidixic Acid	232	C12H12N2O3	000389-08-2	38	



Tentatively Identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 21 May 2002 4:17 pm
Data File: C:\MSDCHEM\1\DATA\020521\10519.D
Name: sample
Misc:
Method: C:\MSDCHEM\1\METHODS\SCAN020521.M (RTE Integrator)
Title: Method 508 GC/MS Scan
Library Searched: C:\DATABASE\nist98.l

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	6.15	14.6	ug/l	1179740	1	11.37	3231400	40.0
Phenol, 6-methyl-...	28.91	0.2	ug/l	24672	4	31.72	4491880	40.0
Phenanthrene, 9-m...	31.09	0.3	ug/l	32064	4	31.72	4491880	40.0
Anthracene-d10-	31.95	0.3	ug/l	38001	4	31.72	4491880	40.0