

Data File : C:\MSDCHEM\1\DATA\020515\11154.D

Vial: 20

Acq On : 16 May 2002 6:34 am

Operator: Nefliu

Sample : sample

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: rteint.e

Quant Time: May 16 08:41:38 2002

Quant Results File: SCAN020507.RE

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)

Title : Method 508 GC/MS Scan

Last Update : Wed May 15 15:22:39 2002

Response via : Initial Calibration

DataAcq Meth : 508SCAN1

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	11.37	152	430425	40.00	ug/l	-0.02
10) Naphthalene-d8	16.53	136	1604812	40.00	ug/l	-0.04
17) Acenaphthene-d10	24.45	164	860670	40.00	ug/l	-0.02
30) Phenanthrene-d10	31.72	188	1480009	40.00	ug/l	-0.02
38) Chrysene-d12	39.93	240	1198518	40.00	ug/l	-0.05
44) Perylene-d12	43.15	264	717082	40.00	ug/l	-0.03
System Monitoring Compounds						
27) TCMX	27.55	207	226626	32.96	ug/l	-0.02
Spiked Amount	40.000		Recovery	=	82.40%	
Target Compounds						
35) Di-n-butylphthalate	34.80	149	9027	0.19	ug/l	95
43) Bis(2-ethylhexyl)phthalate	40.52	149	155316	6.05	ug/l	99

 (#) = qualifier out of range (m) = manual integration (+) = signals summed
 11154.D SCAN020507.M Thu May 16 09:33:16 2002 Page 1

Data File : C:\MSDCHEM\1\DATA\020515\11154.D

Acq On : 16 May 2002 6:34 am

Sample : sample

Misc :

MS Integration Params: rteint.e

Quant Time: May 16 9:33 2002

Vial: 20

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

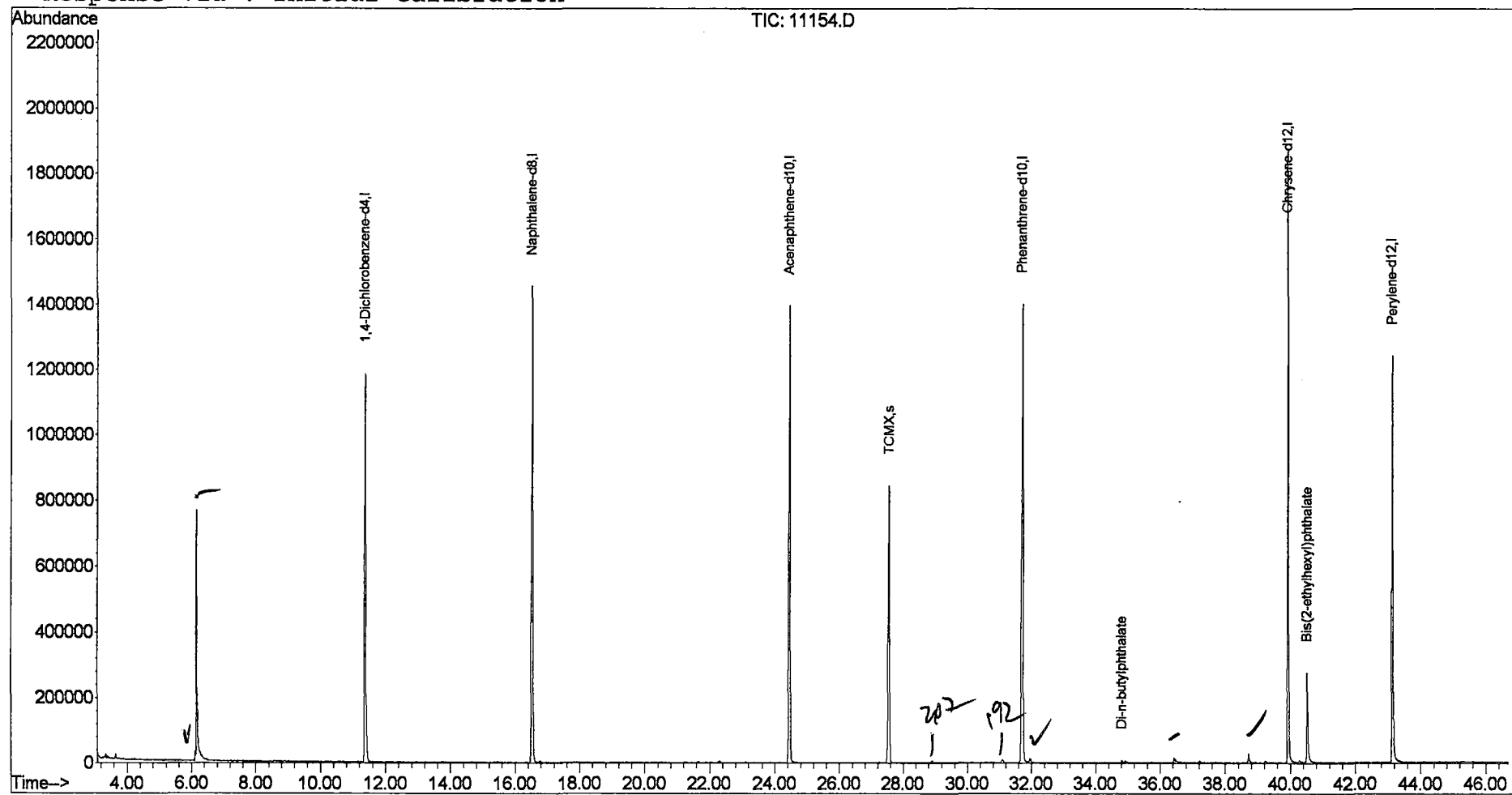
Quant Results File: SCAN020507.RES

Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)

Title : Method 508 GC/MS Scan

Last Update : Wed May 15 15:22:39 2002

Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\020515\11154.D

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Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 20

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)

Title : Method 508 GC/MS Scan

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.5 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

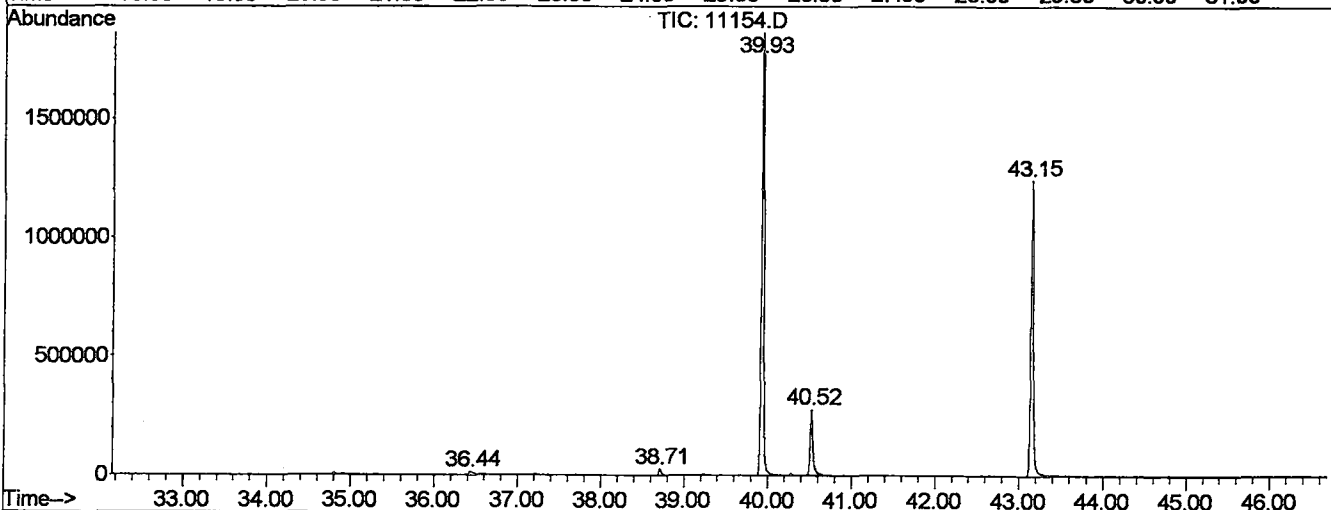
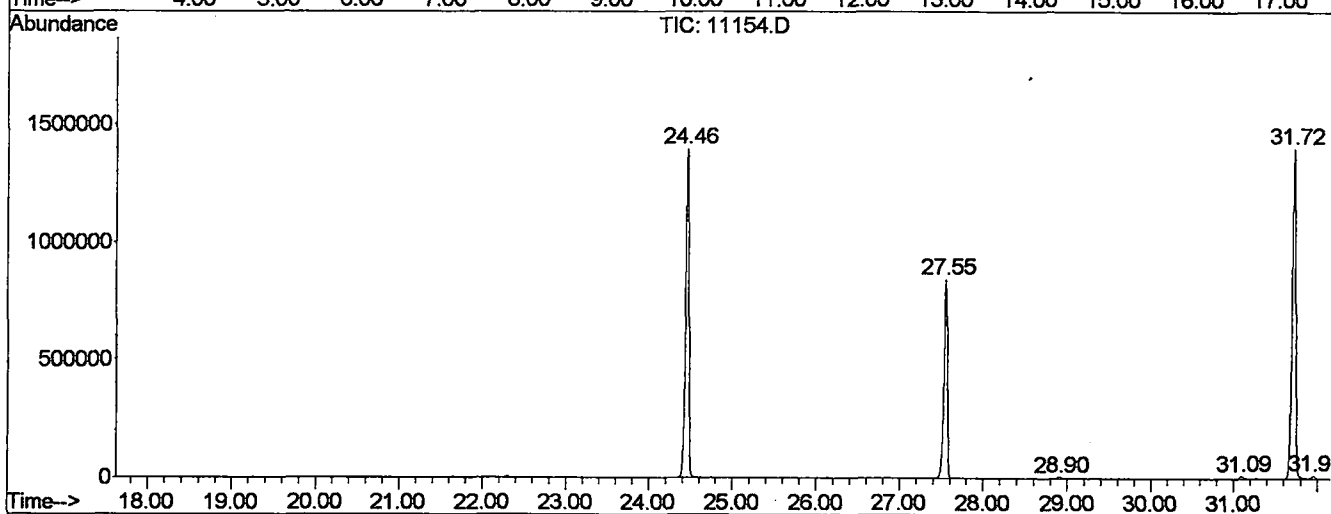
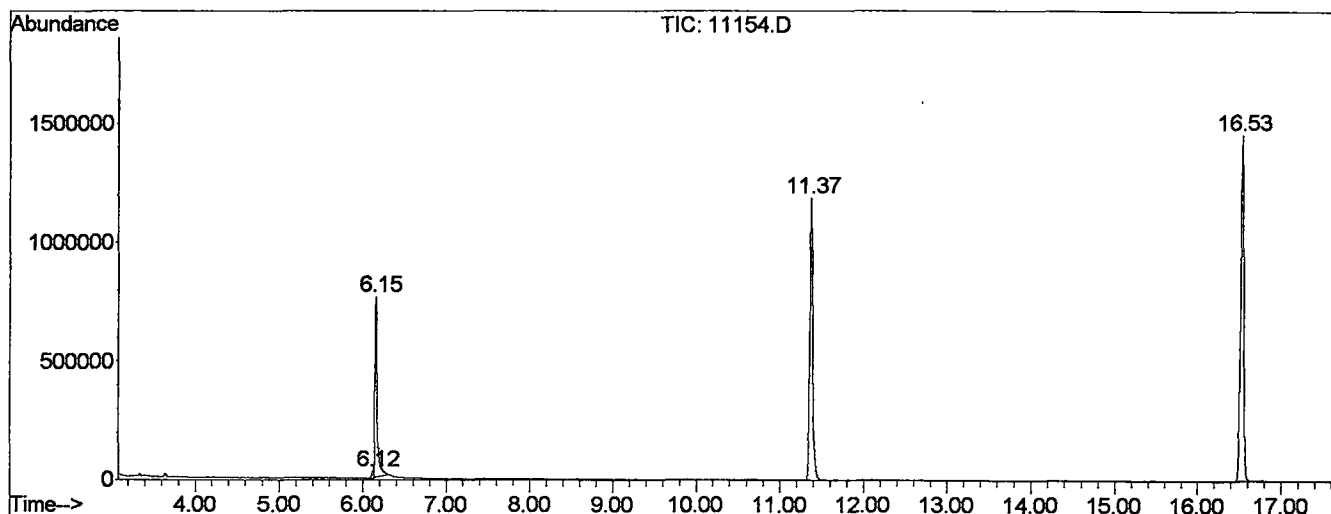
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.117	508	517	519	rBV	30811	45029	1.08%	0.176%
2	6.152	519	523	548	rVB	757270	1393759	33.58%	5.454%
3	11.370	1400	1411	1431	rBV	1185778	2971058	71.59%	11.627%
4	16.534	2274	2290	2308	rBV	1456304	3718817	89.60%	14.553%
5	24.461	3622	3639	3655	rBV2	1397664	3851166	92.79%	15.071%
6	27.551	4146	4165	4180	rBV3	845371	2373197	57.18%	9.287%
7	28.902	4387	4395	4407	rVB8	6735	20783	0.50%	0.081%
8	31.094	4755	4768	4779	rVB4	11194	34884	0.84%	0.137%
9	31.717	4857	4874	4900	rBV2	1401935	4150356	100.00%	16.242%
10	31.946	4906	4913	4925	rBV4	11780	33335	0.80%	0.130%
11	36.441	5667	5678	5692	rBV8	14424	60628	1.46%	0.237%
12	38.715	6056	6065	6080	rBV2	27612	71889	1.73%	0.281%
13	39.931	6258	6272	6295	rBV2	1864817	3652731	88.01%	14.295%
14	40.518	6363	6372	6401	rVB	273560	637845	15.37%	2.496%
15	43.151	6809	6820	6844	rBV	1241864	2537580	61.14%	9.931%

Sum of corrected areas: 25553057

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020515\11154.D
 Operator : Nefliu
 Acquired : 16 May 2002 6:34 am using AcqMethod 508SCAN1
 Instrument : Instrumen
 Sample Name: sample
 Misc Info :
 Vial Number: 20
 Quant File :SCAN020507.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020515\11154.D
 Acq On : 16 May 2002 6:34 am
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

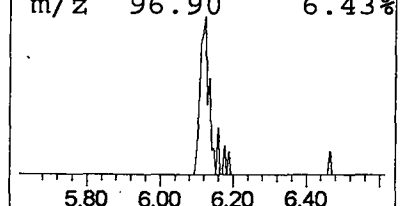
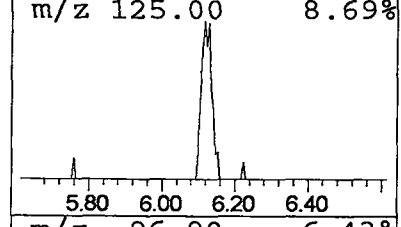
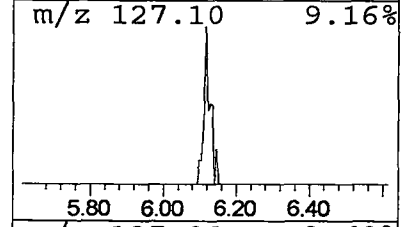
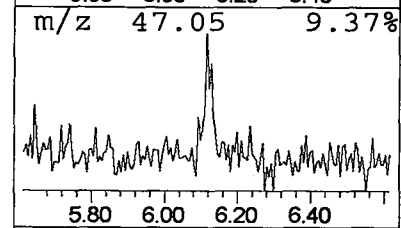
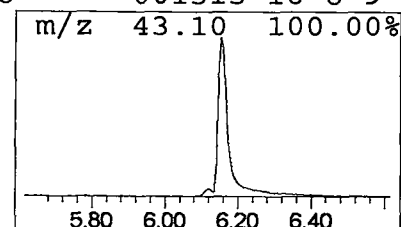
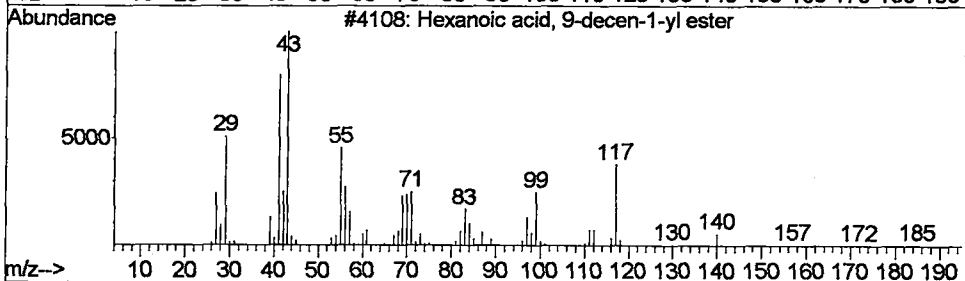
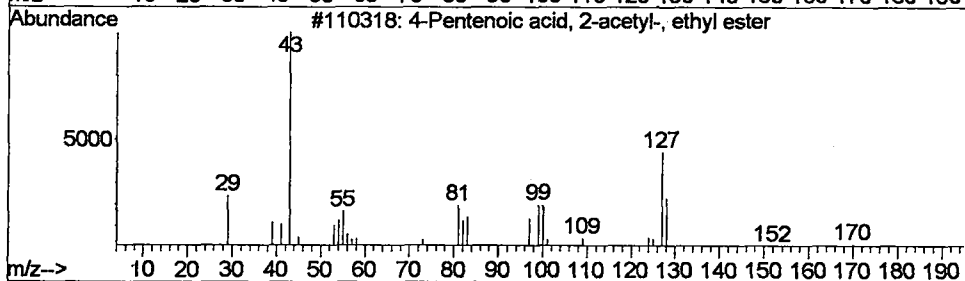
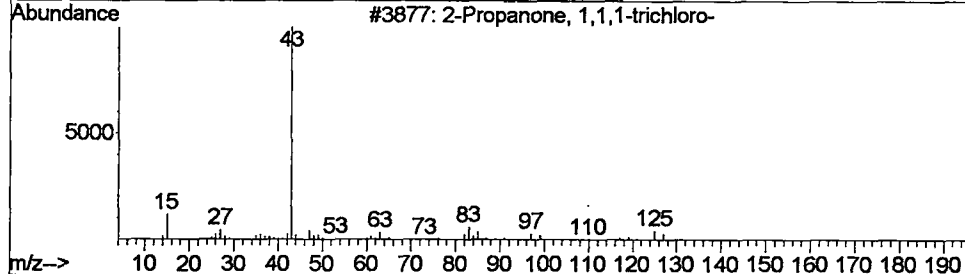
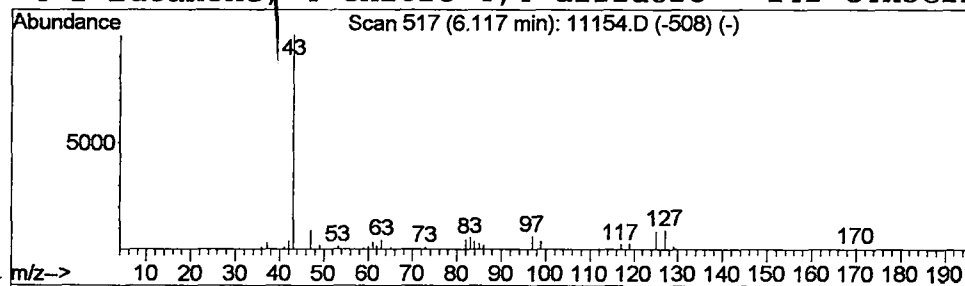
Vial: 20
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.l

 Peak Number 1 2-Propanone, 1,1,1-trichloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	0.61 ug/l	45029	1,4-Dichlorobenzene-d4	11.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
✓ 1			2-Propanone, 1,1,1-trichloro-	160	C3H3Cl3O	000918-00-3	50
2			4-Pentenoid acid, 2-acetyl-, eth...	170	C9H14O3	000610-89-9	9
3			Hexanoic acid, 9-decen-1-yl ester	254	C16H30O2	1000160-13-5	9
4			2-Butanone, 4-chloro-4,4-difluoro-	142	C4H5ClF2O	001515-16-8	9



Library Search Compound Report

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

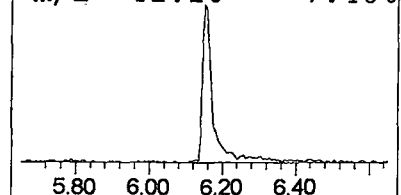
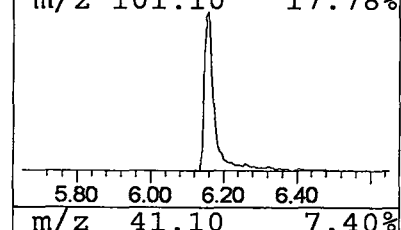
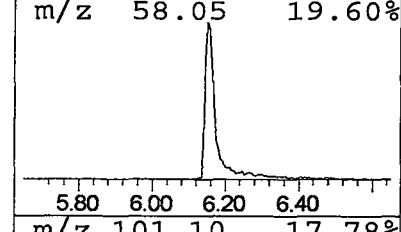
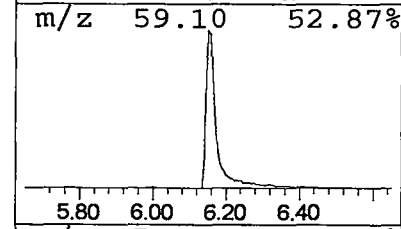
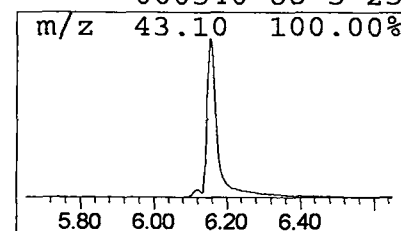
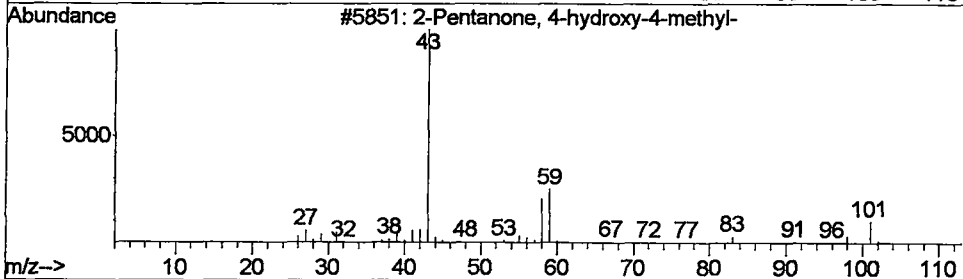
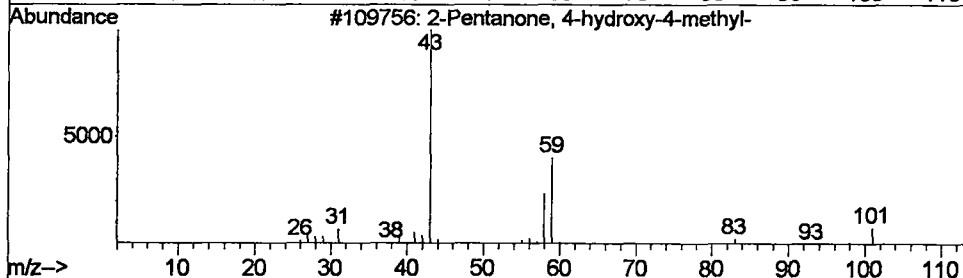
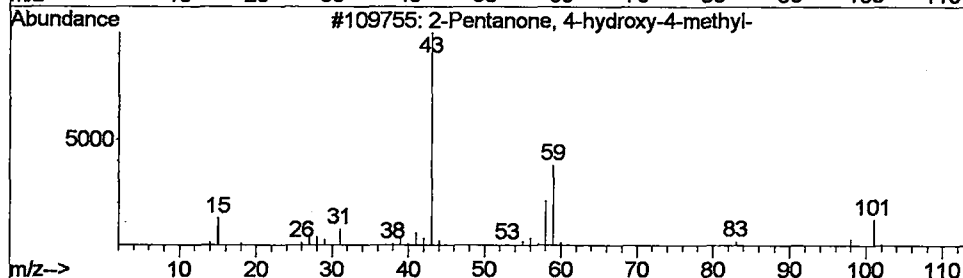
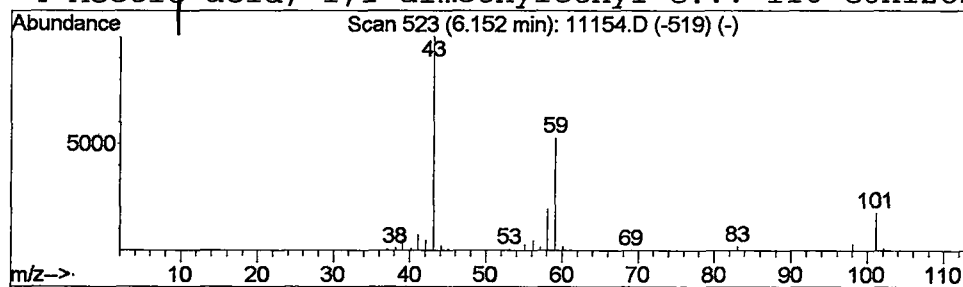
Vial: 20
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.15	18.76 ug/l	1393760	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	64
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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Sample : sample

Misc :

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Vial: 20

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)

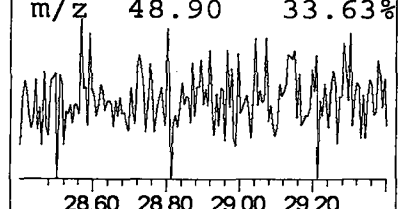
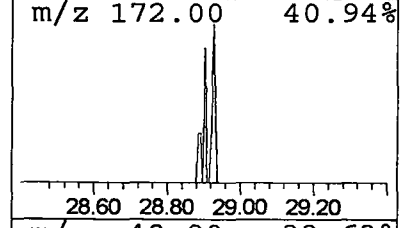
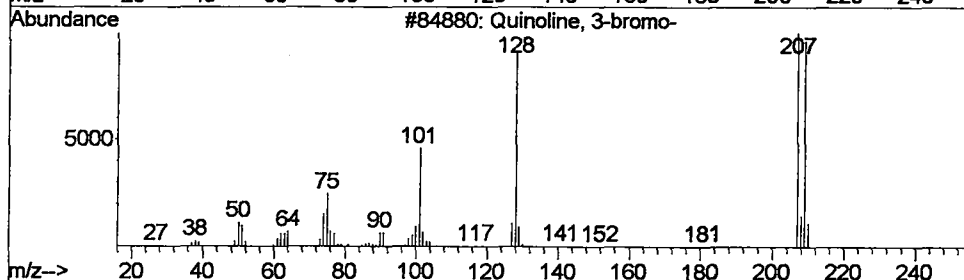
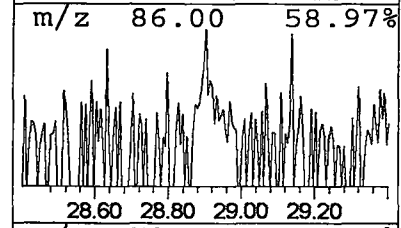
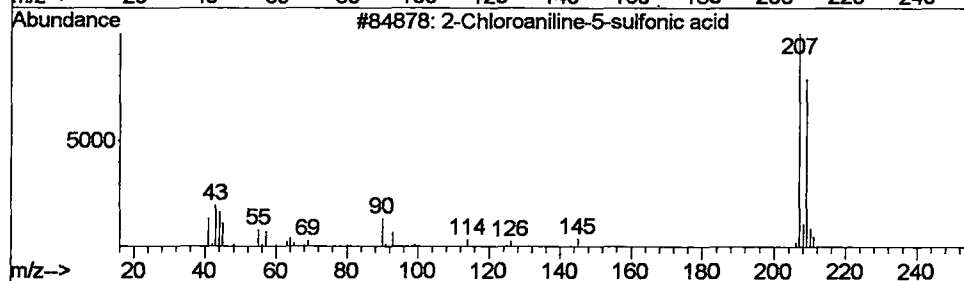
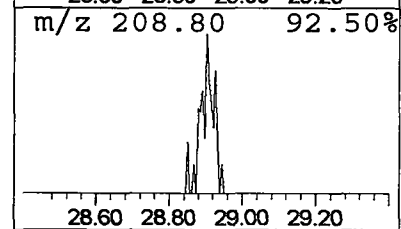
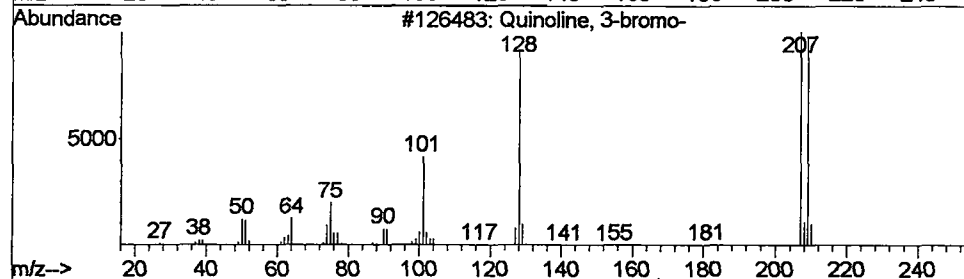
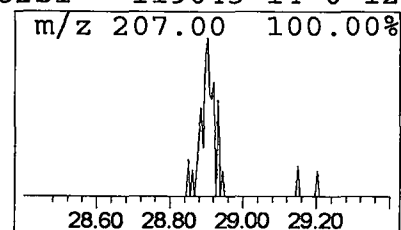
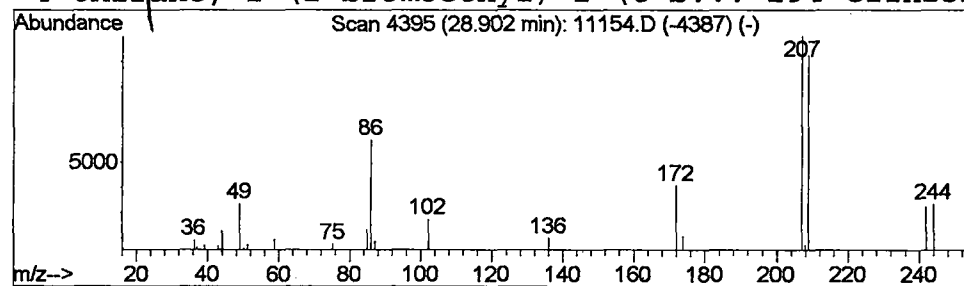
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\nist98.l

Peak Number 3 Quinoline, 3-bromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.90	0.20 ug/l	20783	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinoline, 3-bromo-	207	C9H6BrN	005332-24-1	27
2			2-Chloroaniline-5-sulfonic acid	207	C6H6ClNO3S	000098-36-2	27
3			Quinoline, 3-bromo-	207	C9H6BrN	005332-24-1	27
4			Oxirane, 2-(2-bromoethyl)-2-(t-b...	294	C11H23BrO2Si	119043-14-0	12



Library Search Compound Report

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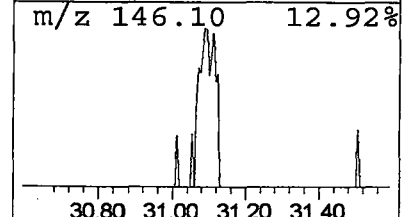
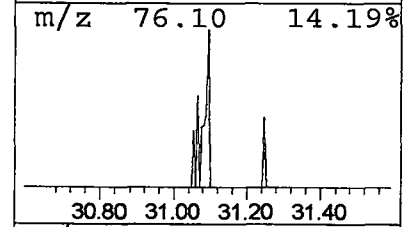
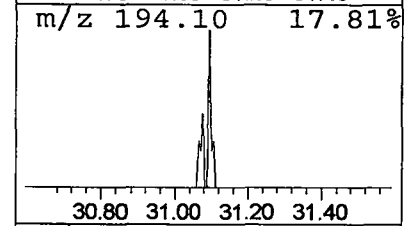
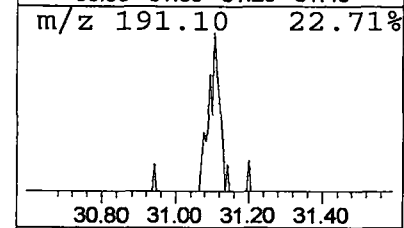
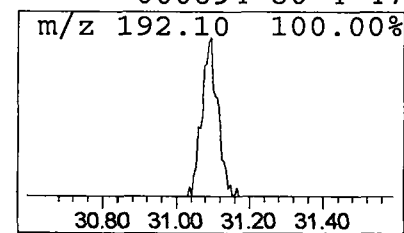
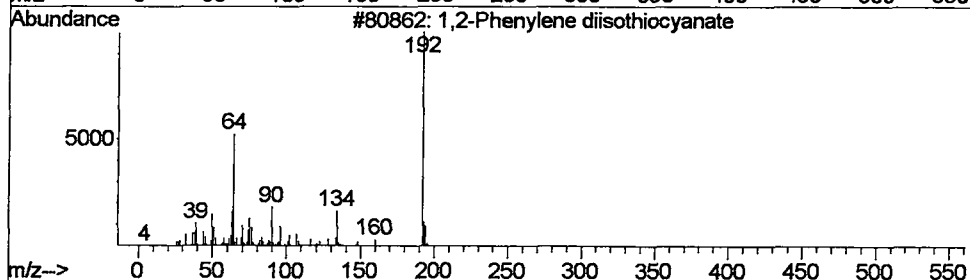
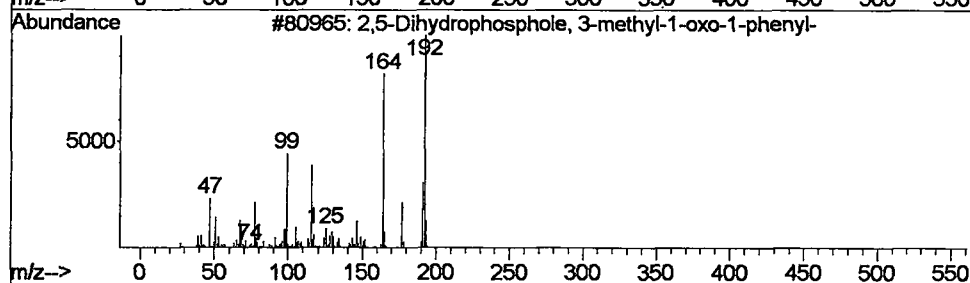
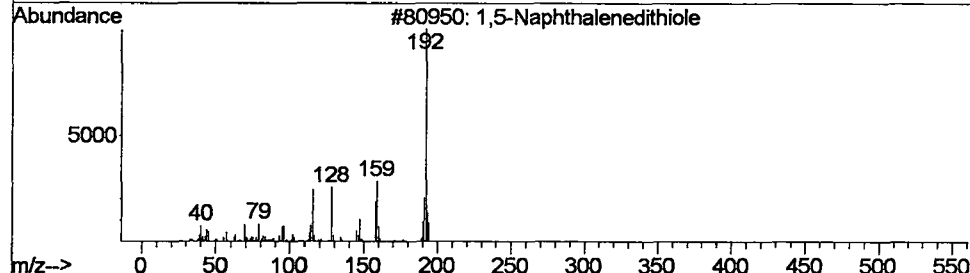
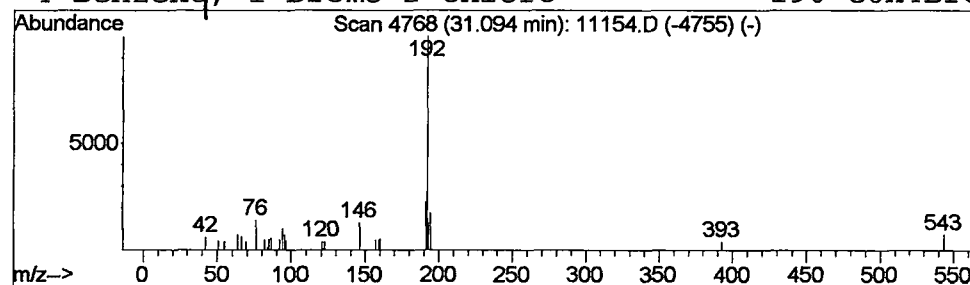
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Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
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 Library : C:\DATABASE\nist98.1

 Peak Number 4 1,5-Naphthalenedithiole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.09	0.34 ug/l	34884	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5-Naphthalenedithiole	192	C10H8S2	1000223-69-5	53
2		2,5-Dihydrophosphole, 3-methyl-1...	192	C11H13OP	1000196-97-5	53
3		1,2-Phenylene diisothiocyanate	192	C8H4N2S2	071105-17-4	50
4		Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	47



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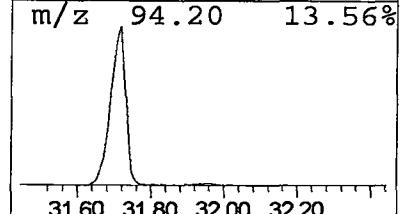
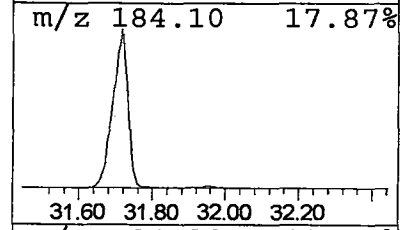
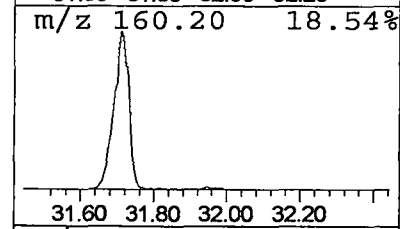
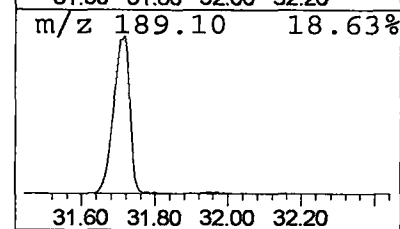
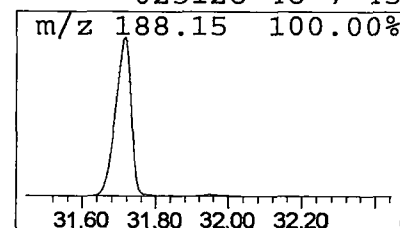
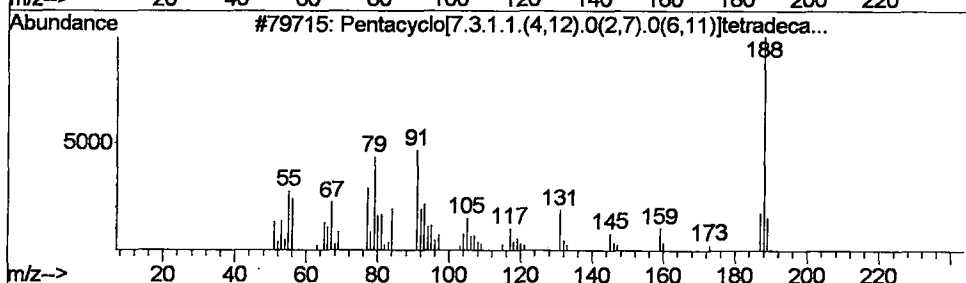
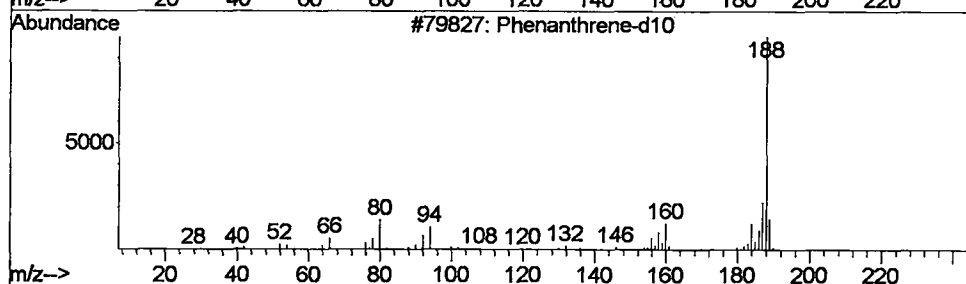
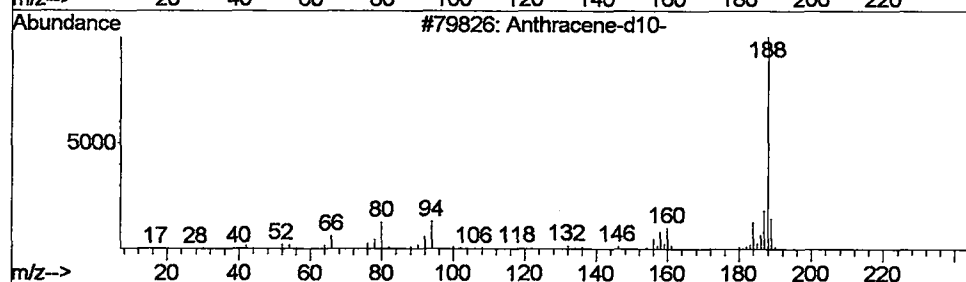
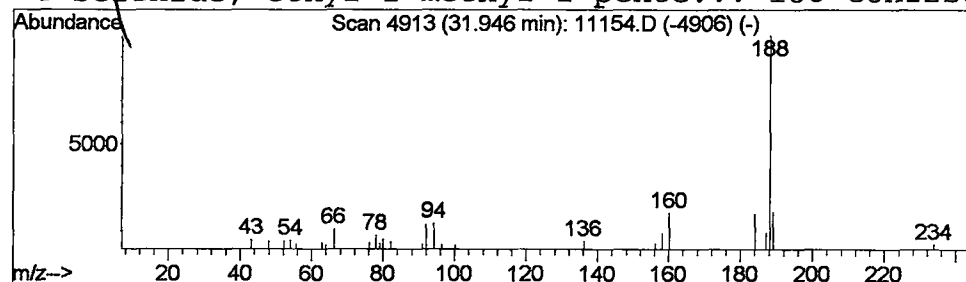
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 Operator: Nefliu
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Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 5 Anthracene-d10- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.95	0.32 ug/l	33335	Phenanthrene-d10	31.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene-d10-	188	C14D10	001719-06-8	72
2		Phenanthrene-d10	188	C14D10	001517-22-2	72
3		Pentacyclo[7.3.1.1.(4,12).0(2,7)...]	188	C14H20	1000215-61-8	53
4		Selenide, ethyl 1-methyl-1-pente...	188	C8H12Se	025128-48-7	45



Library Search Compound Report

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MS Integration Params: rteint.e

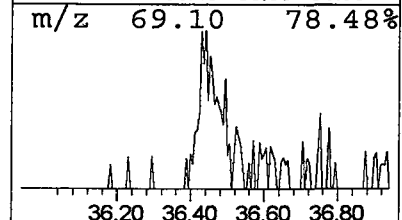
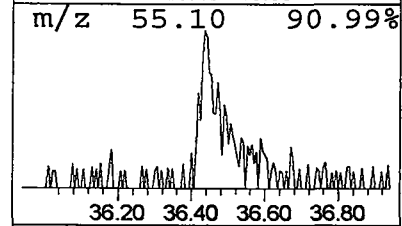
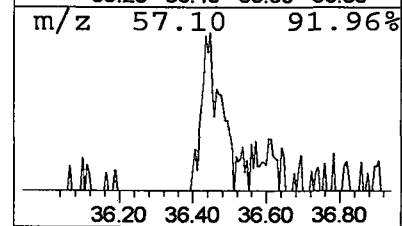
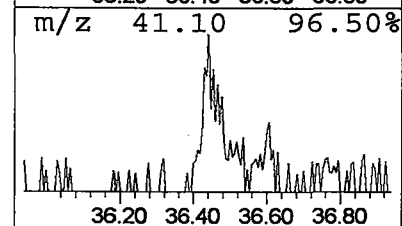
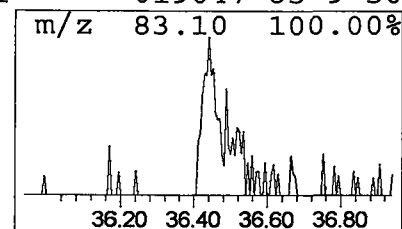
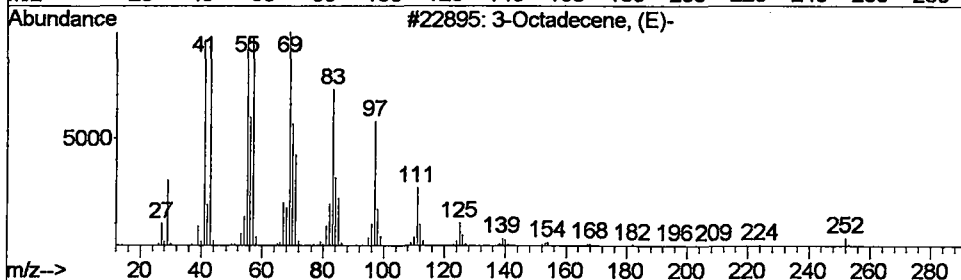
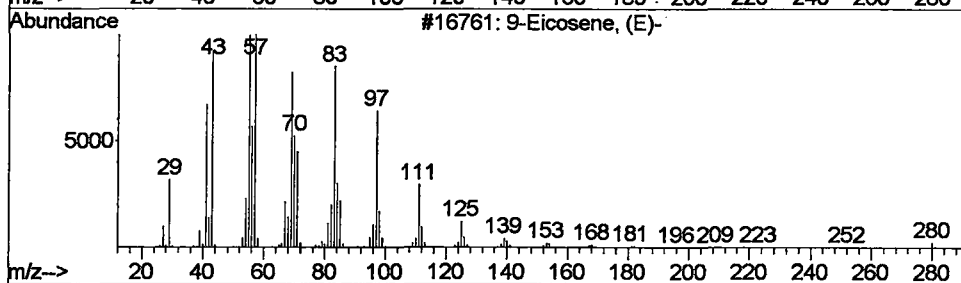
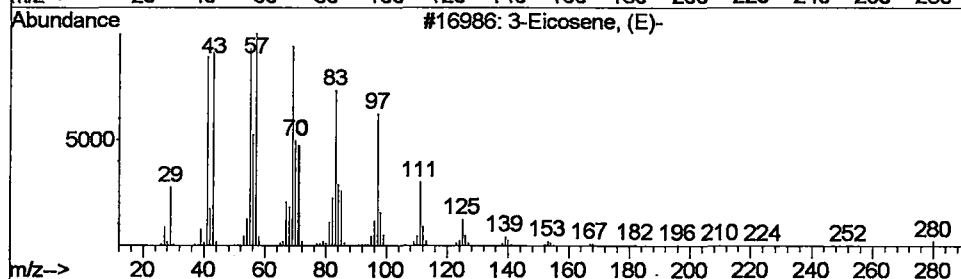
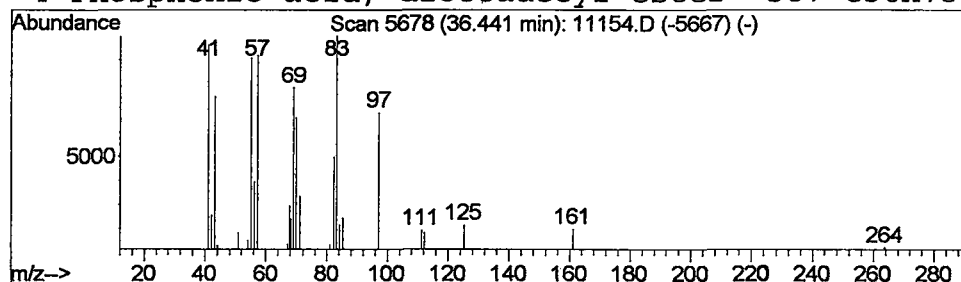
Vial: 20
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
Title : Method 508 GC/MS Scan
Library : C:\DATABASE\nist98.1

Peak Number 6 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
36.44	0.66 ug/l	60628	Chrysene-d12	39.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	52
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	52
3			3-Octadecene, (E)-	252	C18H36	007206-19-1	52
4			Phosphonic acid, dioctadecyl ester	587	C36H75O3P	019047-85-9	50



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020515\11154.D
 Acq On : 16 May 2002 6:34 am
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

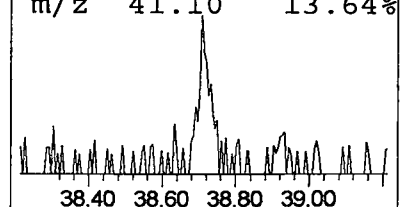
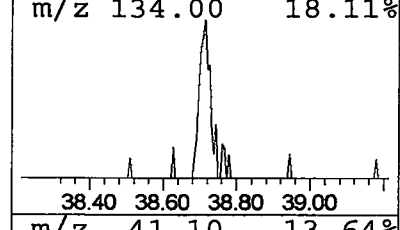
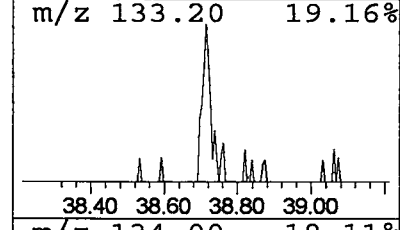
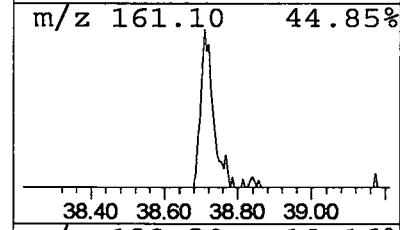
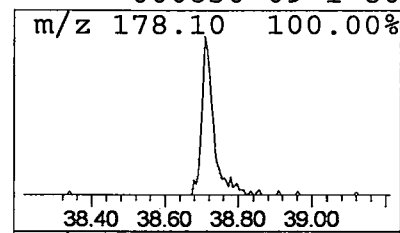
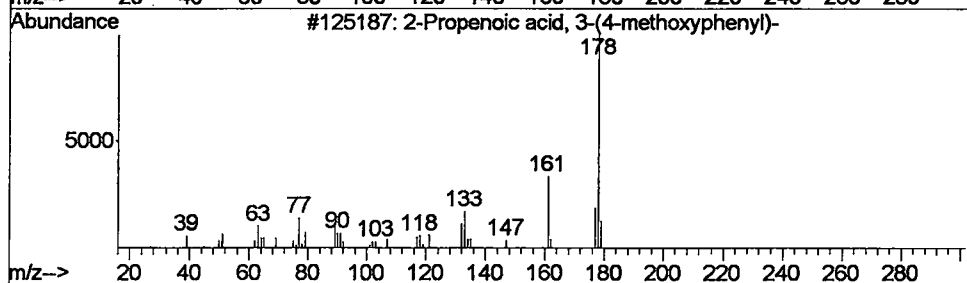
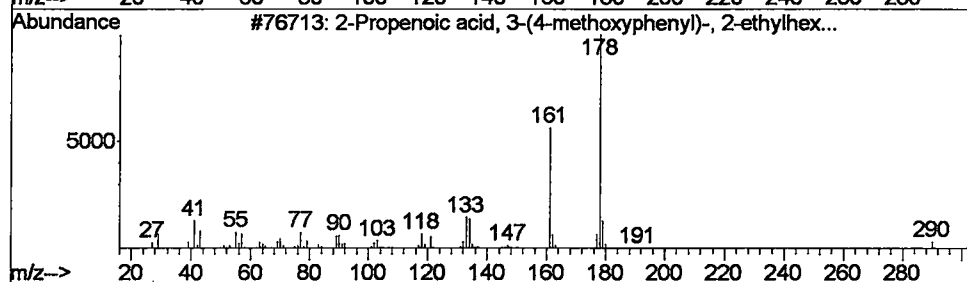
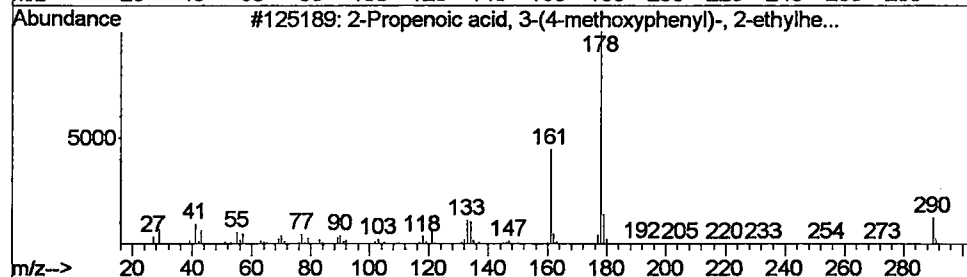
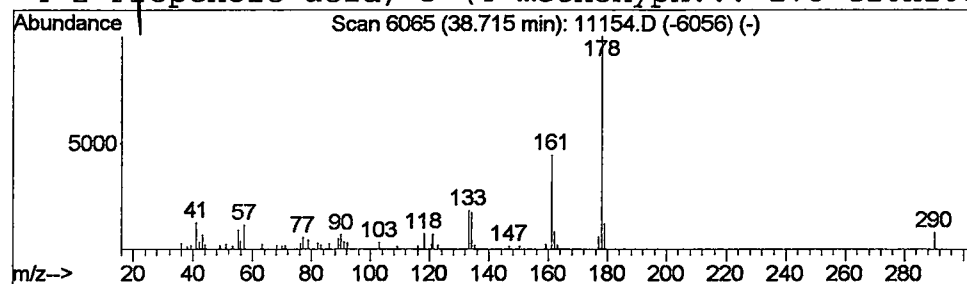
Vial: 20
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
 Title : Method 508 GC/MS Scan
 Library : C:\DATABASE\nist98.1

 Peak Number 7 2-Propenoic acid, 3-(4-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
38.71	0.79 ug/l	71889	Chrysene-d12	39.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
✓1	5	2-Propenoic acid, 3-(4-methoxyph...	290	C18H26O3	005466-77-3	95
2		2-Propenoic acid, 3-(4-methoxyph...	290	C18H26O3	005466-77-3	91
3		2-Propenoic acid, 3-(4-methoxyph...	178	C10H10O3	000830-09-1	86
4		2-Propenoic acid, 3-(4-methoxyph...	178	C10H10O3	000830-09-1	80



Tentatively Identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 16 May 2002 6:34 am
Data File: C:\MSDCHEM\1\DATA\020515\11154.D
Name: sample
Misc:
Method: C:\MSDCHEM\1\METHODS\SCAN020507.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
2-Propanone, 1,1,...	6.12	0.6	ug/l	45029	1	11.37	2971060	40.0
2-Pentanone, 4-hy...	6.15	18.8	ug/l	1393760	1	11.37	2971060	40.0
Quinoline, 3-bromo-	28.90	0.2	ug/l	20783	4	31.72	4150360	40.0
1,5-Naphthalenedi...	31.09	0.3	ug/l	34884	4	31.72	4150360	40.0
Anthracene-d10-	31.95	0.3	ug/l	33335	4	31.72	4150360	40.0
3-Eicosene, (E) -	36.44	0.7	ug/l	60628	5	39.93	3652730	40.0
2-Propenoic acid,...	38.71	0.8	ug/l	71889	5	39.93	3652730	40.0