

User: Vinci, David L
 Westchester Dept. of Labs & Research
 Date: 05/28/2002 Time: 11:59:08

Sample: AE11304
 Analysis: \$GCMS GCMS Scan For Unknowns
 Units: ug
 Started: 5/28/02 11:58 Ended: 5/28/02 11:58 Analyst: DLV
 Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		91		10.0

Comments for Sample AE11304 - Analysis \$GCMS

Westchester Dept. of Labs & Research

User: Vinci, David L.

Date: 05-28-2002 Time: 11:59:51

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\020516\11304.D
Acq On : 16 May 2002 11:11 pm
Sample : sample
Misc :
MS Integration Params: rteint.e
Quant Time: May 17 13:10:00 2002

Vial: 15
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

Quant Results File: SCAN020507.RE

Quant Method : C:\MSDCHEM\1\METHODS\SCAN020507.M (RTE Integrator)
Title : Method 508 GC/MS Scan
Last Update : Thu May 16 14:49:15 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	328543	40.00	ug/l	-0.01
10) Naphthalene-d8	16.53	136	1223635	40.00	ug/l	-0.04
17) Acenaphthene-d10	24.45	164	659107	40.00	ug/l	-0.02
30) Phenanthrene-d10	31.72	188	1118932	40.00	ug/l	-0.02
38) Chrysene-d12	39.93	240	880364	40.00	ug/l	-0.05
44) Perylene-d12	43.15	264	508754	40.00	ug/l	-0.03

System Monitoring Compounds

27) TCMX	27.56	207	191892	36.45	ug/l	-0.02
Spiked Amount	40.000		Recovery	=	91.13%	

Target Compounds

43) Bis(2-ethylhexyl)phthalate	40.52	149	45262	2.40	ug/l	Qvalue 96
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(#) = qualifier out of range (m) = manual integration (+) = signals summed
11304.D SCAN020507.M Fri May 17 13:11:05 2002 Page 1

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\020516\11304.D

Vial: 15

Acq On : 16 May 2002 11:11 pm

Operator: Nefliu

Sample : sample

Inst : Instrumen

Misc :

Multiplr: 1.00

MS Integration Params: rteint.e

Quant Time: May 17 13:11 2002

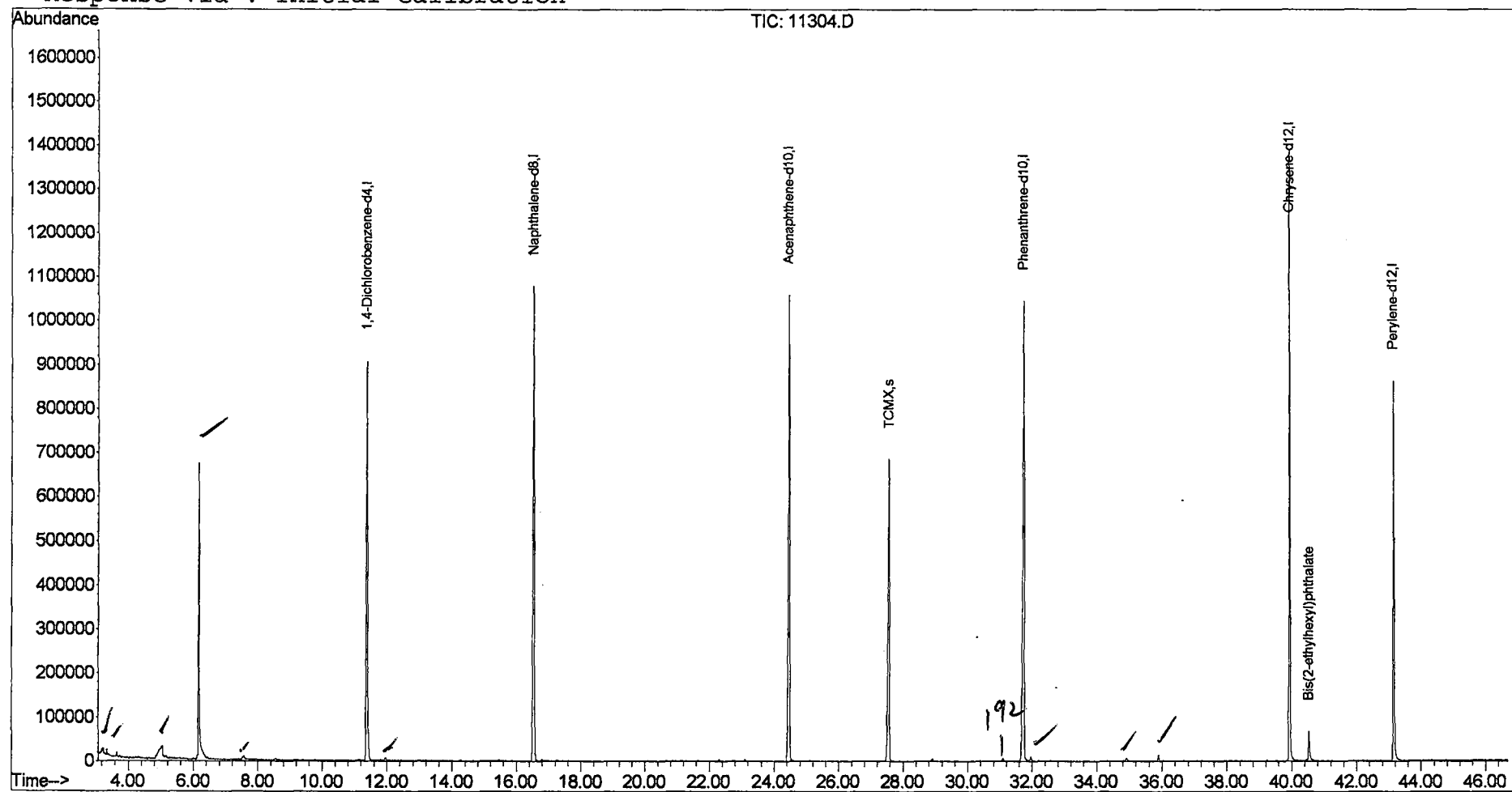
Quant Results File: SCAN020507.RES

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

Title : Method 508 GC/MS Scan

Last Update : Thu May 16 14:49:15 2002

Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D
 Acq On : 16 May 2002 11:11 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

Vial: 15
 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

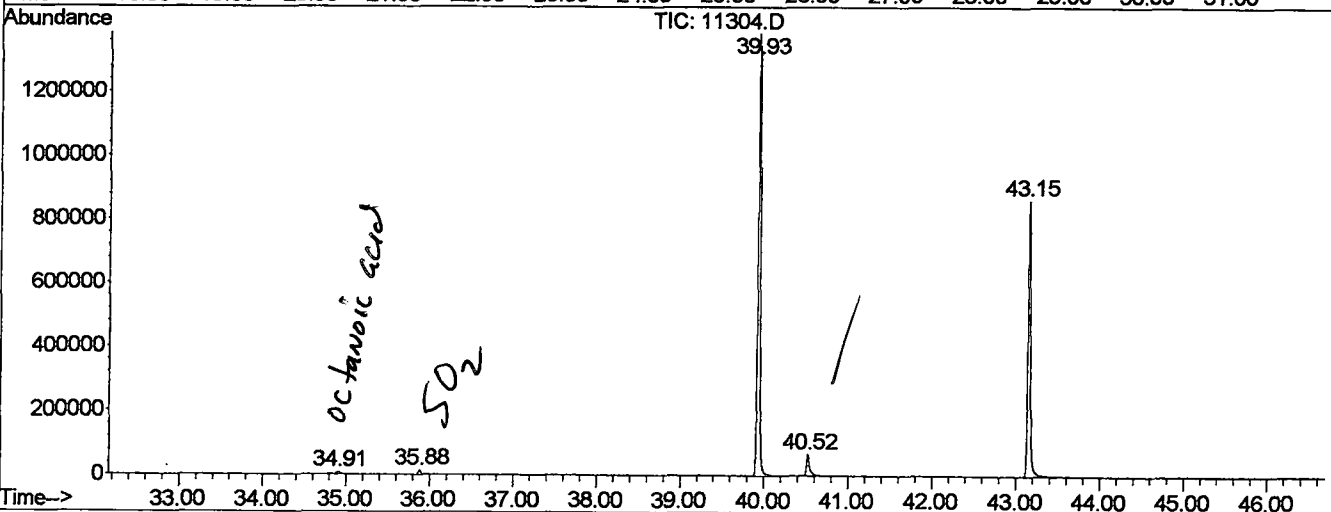
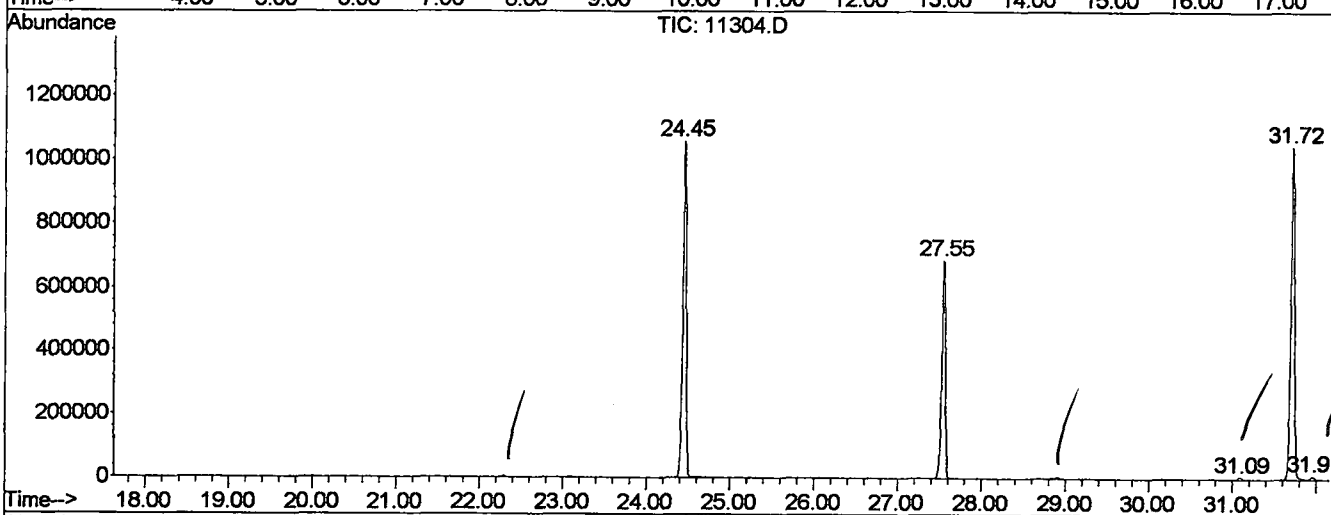
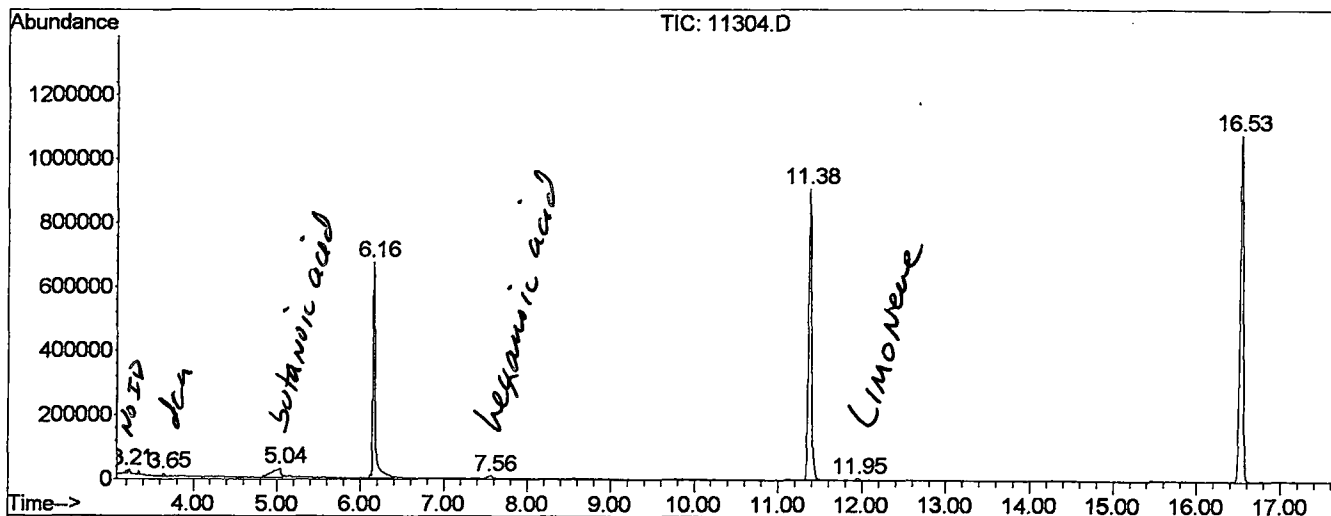
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.214	17	23	24	rBV6	10455	17640	0.56%	0.090%
2	3.649	94	97	106	rVB4	10817	16729	0.53%	0.085%
3	5.042	295	334	339	rBV3	30052	232612	7.39%	1.187%
4	6.158	512	524	566	rBV	672829	1332893	42.36%	6.803%
5	7.556	748	762	776	rBV5	9119	42746	1.36%	0.218%
6	11.375	1397	1412	1439	rBV	907230	2284596	72.61%	11.661%
7	11.945	1499	1509	1521	rBV8	6370	18718	0.59%	0.096%
8	16.534	2274	2290	2310	rBV	1080053	2827180	89.85%	14.430%
9	24.455	3622	3638	3651	rBV	1058934	2954660	93.90%	15.081%
10	27.551	4144	4165	4176	rBV3	686759	1986339	63.13%	10.138%
11	31.088	4758	4767	4781	rVB3	7219	19287	0.61%	0.098%
12	31.717	4855	4874	4900	rBV3	1045983	3146581	100.00%	16.060%
13	31.952	4906	4914	4924	rVB5	10046	25995	0.83%	0.133%
14	34.907	5408	5417	5429	rBV6	7529	22126	0.70%	0.113%
15	35.883	5576	5583	5594	rBV2	13597	28033	0.89%	0.143%
16	39.931	6260	6272	6303	rBV2	1383875	2685509	85.35%	13.707%
17	40.518	6364	6372	6394	rBV	66605	174092	5.53%	0.889%
18	43.151	6806	6820	6843	rBV2	863659	1776509	56.46%	9.067%

Sum of corrected areas: 19592245

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\020516\11304.D
 Operator : Nefliu
 Acquired : 16 May 2002 11:11 pm using AcqMethod 508SCAN1
 Instrument : Instrumen
 Sample Name: sample
 Misc Info :
 Vial Number: 15
 Quant File :SCAN020507.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D
 Acq On : 16 May 2002 11:11 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

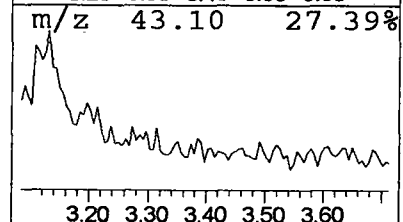
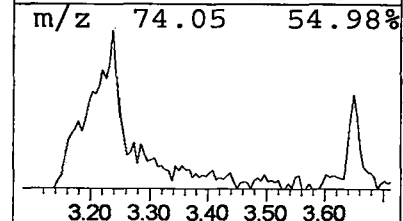
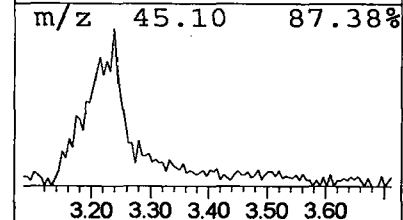
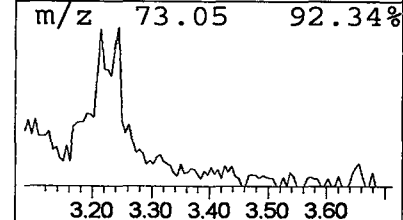
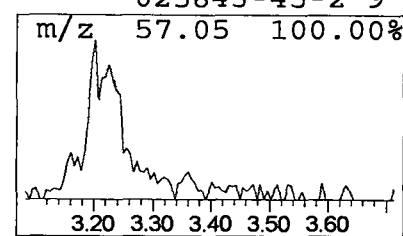
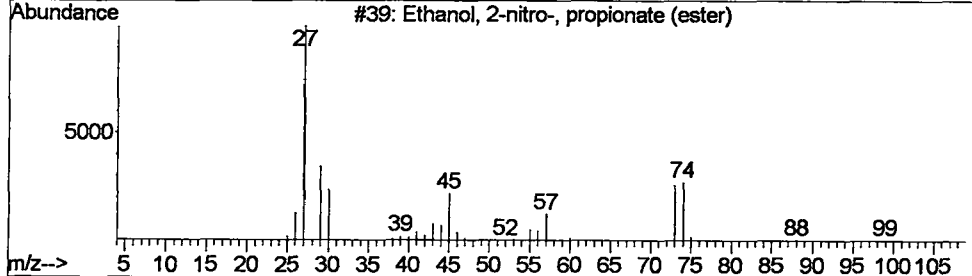
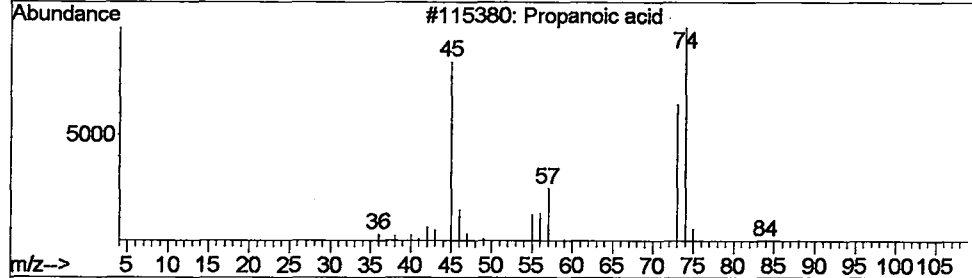
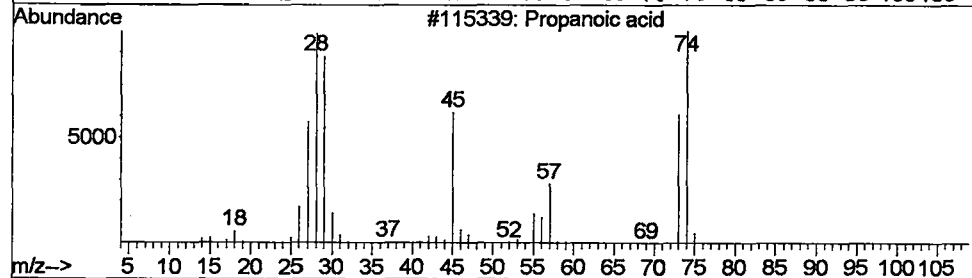
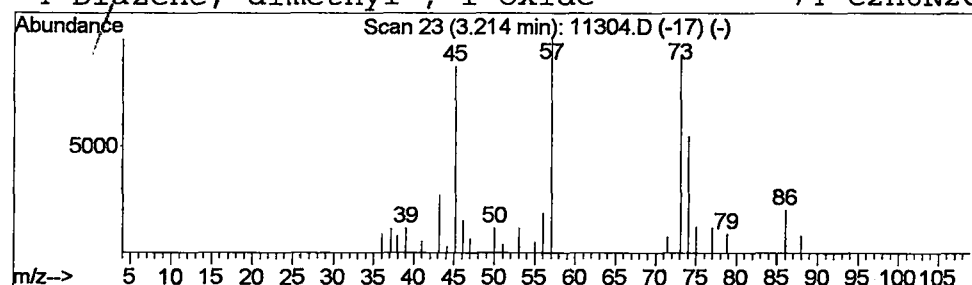
Vial: 15
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 1 Propanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	0.31 ug/l	17640	1,4-Dichlorobenzene-d4	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid	74	C3H6O2	000079-09-4	47
2		Propanoic acid	74	C3H6O2	000079-09-4	47
3		Ethanol, 2-nitro-, propionate (e...	147	C5H9NO4	005390-28-3	47
4		Diazene, dimethyl-, 1-oxide	74	C2H6N2O	025843-45-2	9



Library Search Compound Report

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Acq On : 16 May 2002 11:11 pm
Sample : sample
Misc :
MS Integration Params: rteint.e

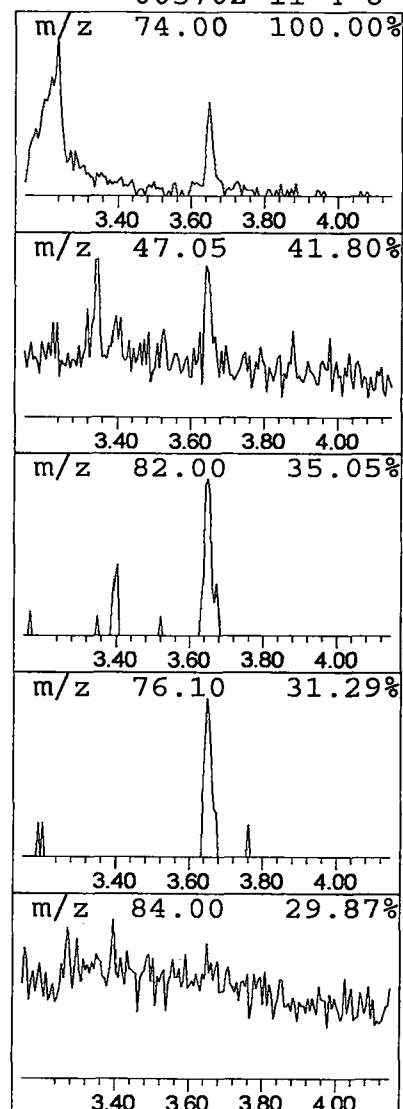
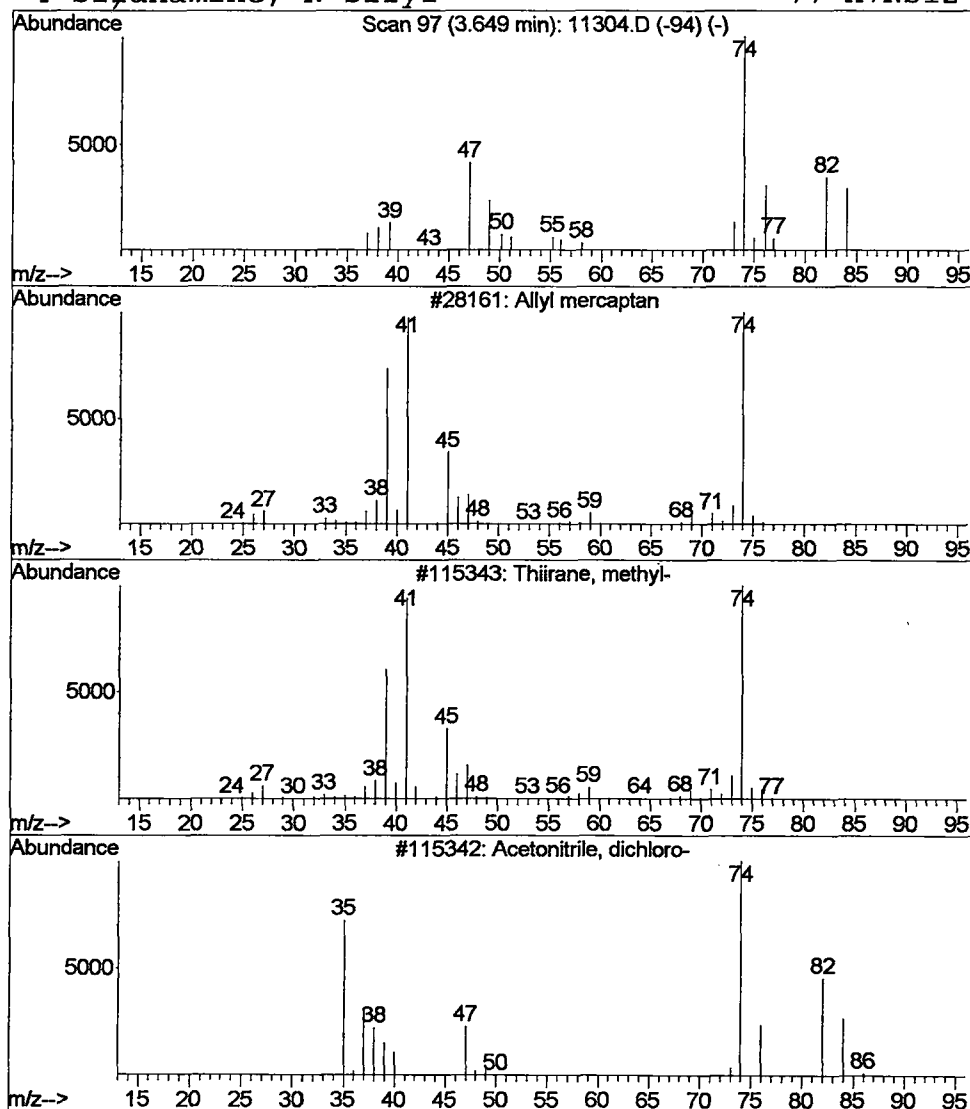
Vial: 15
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 2 Allyl mercaptan Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.65	0.29 ug/l	16729	1,4-Dichlorobenzene-d4	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl mercaptan		74	C3H6S	000870-23-5	25
2	Thiirane, methyl-		74	C3H6S	001072-43-1	9
3	Acetonitrile, dichloro-		109	C2HCl2N	003018-12-0	9
4	Sil'anamine, N-silyl-		77	H7NSi2	005702-11-4	8



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D
 Acq On : 16 May 2002 11:11 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

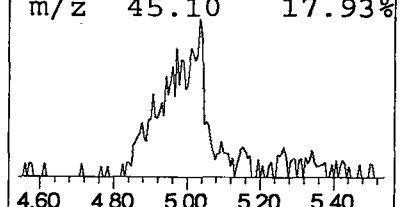
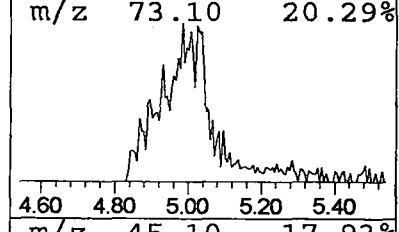
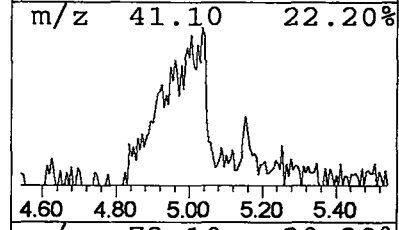
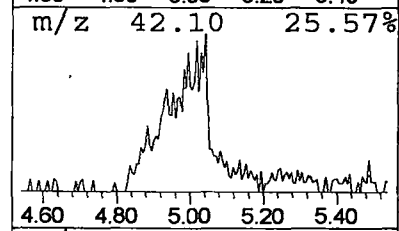
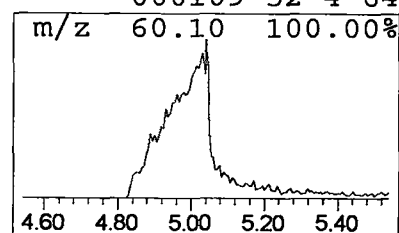
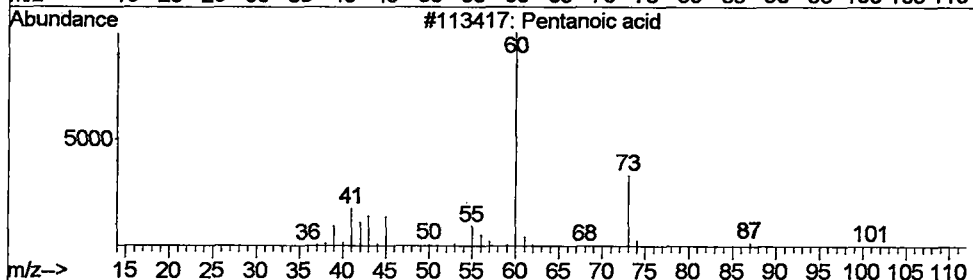
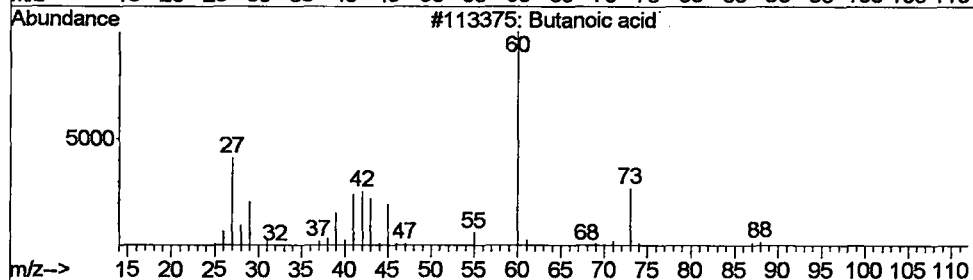
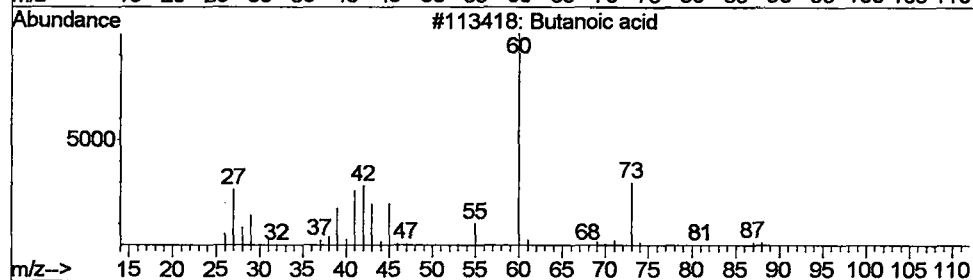
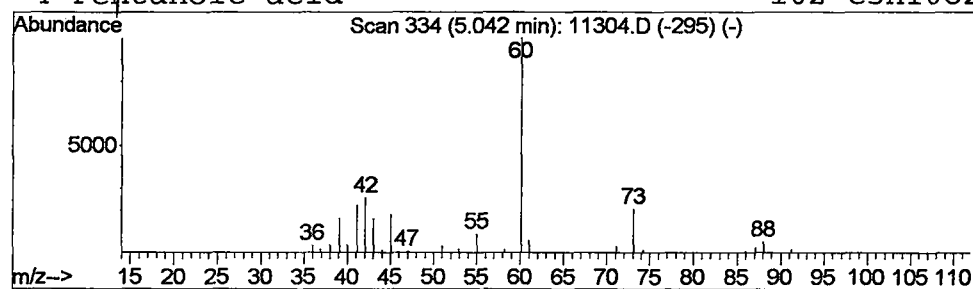
Vial: 15
 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 3 Butanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.07 ug/l	232612	1,4-Dichlorobenzene-d4	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	78	
2	Butanoic acid	88	C4H8O2	000107-92-6	78	
3	Pentanoic acid	102	C5H10O2	000109-52-4	72	
4	Pentanoic acid	102	C5H10O2	000109-52-4	64	



Library Search Compound Report

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Acq On : 16 May 2002 11:11 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 15

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

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

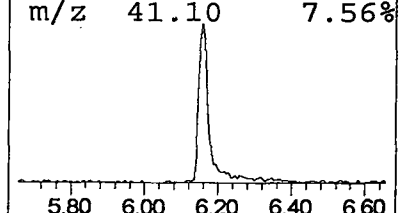
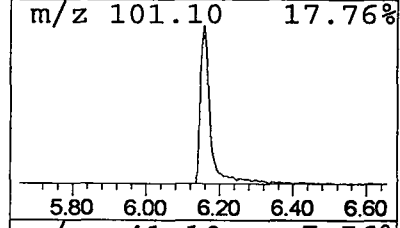
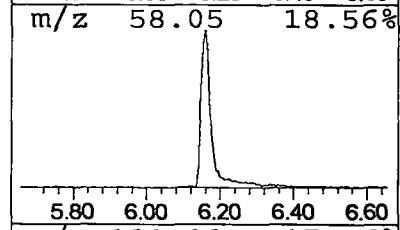
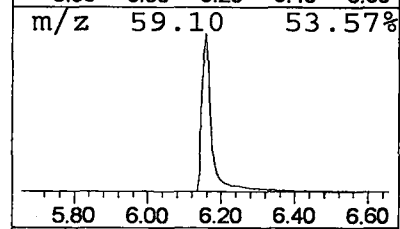
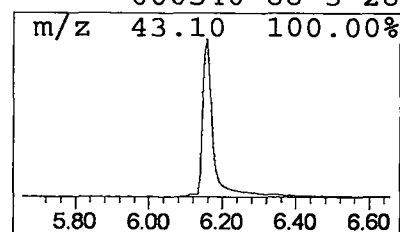
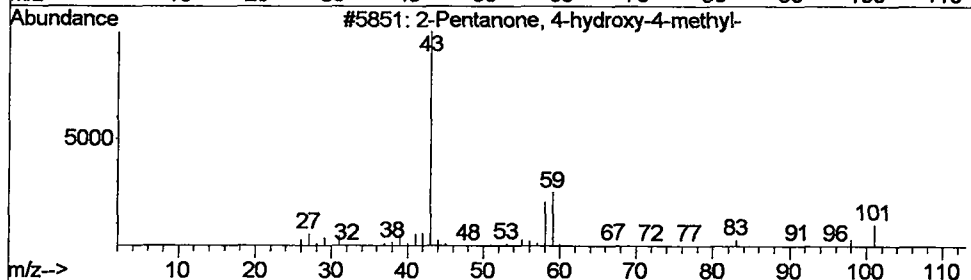
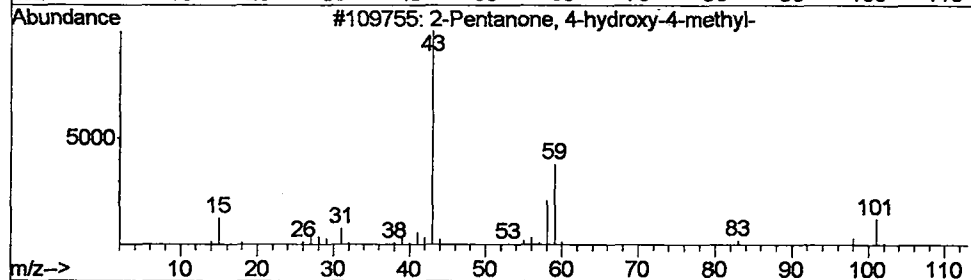
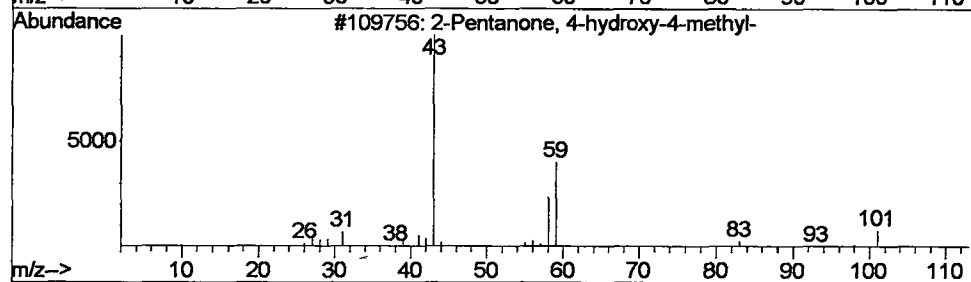
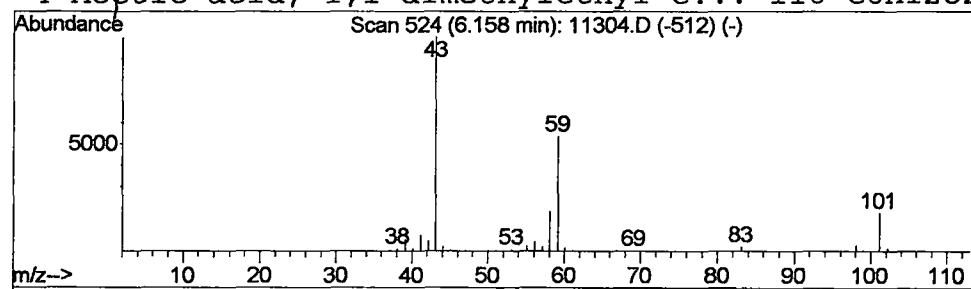
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\nist98.l

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	23.34 ug/l	1332890	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	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	39		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		



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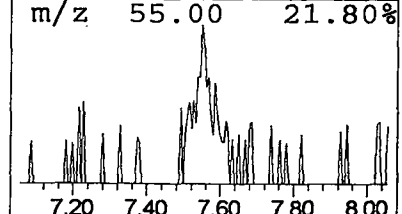
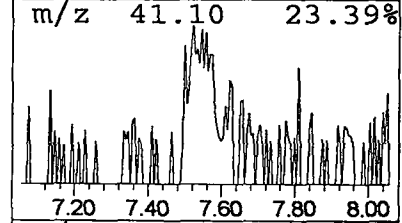
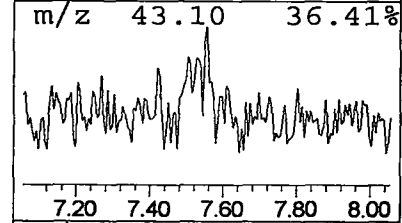
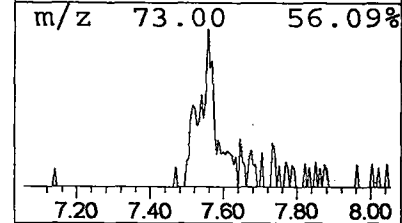
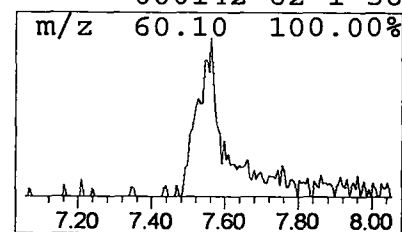
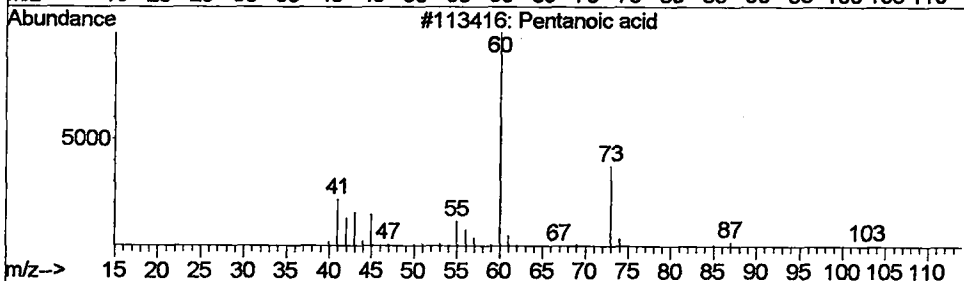
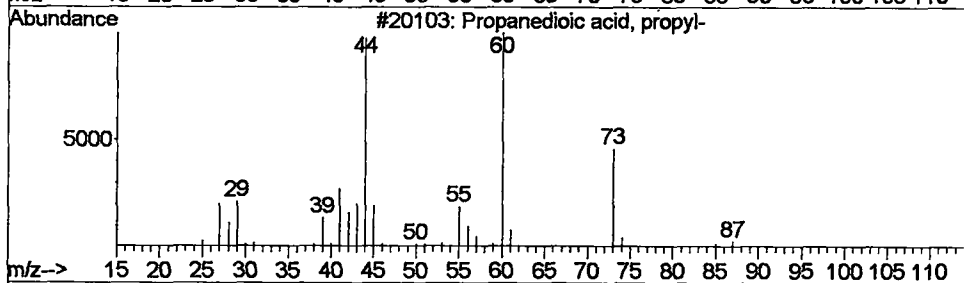
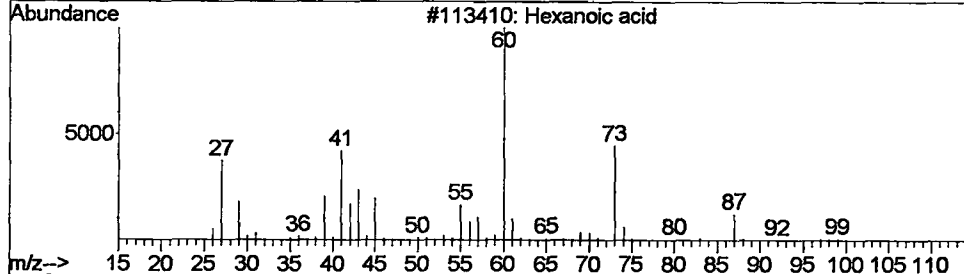
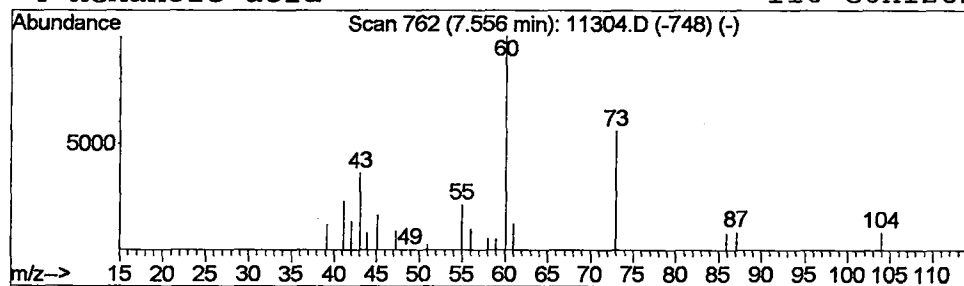
Vial: 15
 Operator: Nefliu
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 Multiplr: 1.00

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

 Peak Number 5 Hexanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	0.75 ug/l	42746	1,4-Dichlorobenzene-d4	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	64	
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	59	
3	Pentanoic acid	102	C5H10O2	000109-52-4	59	
4	Hexanoic acid	116	C6H12O2	000142-62-1	56	



Library Search Compound Report

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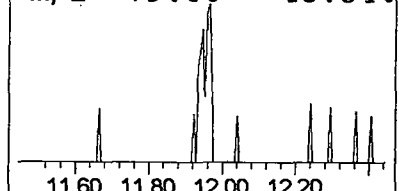
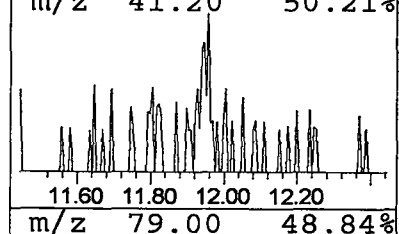
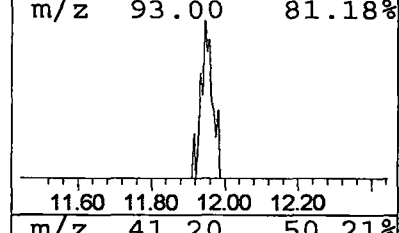
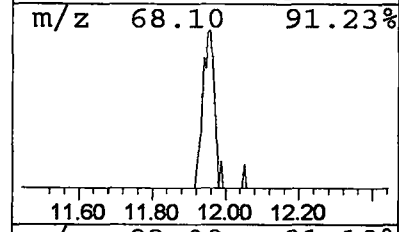
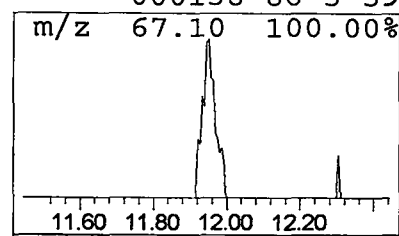
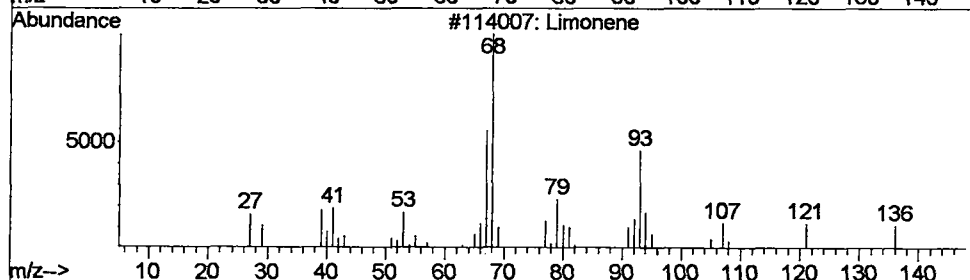
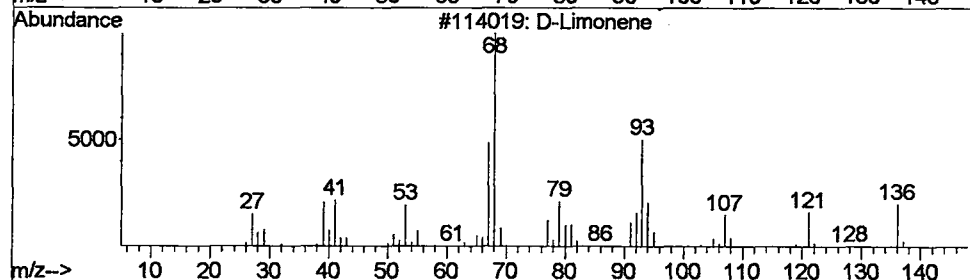
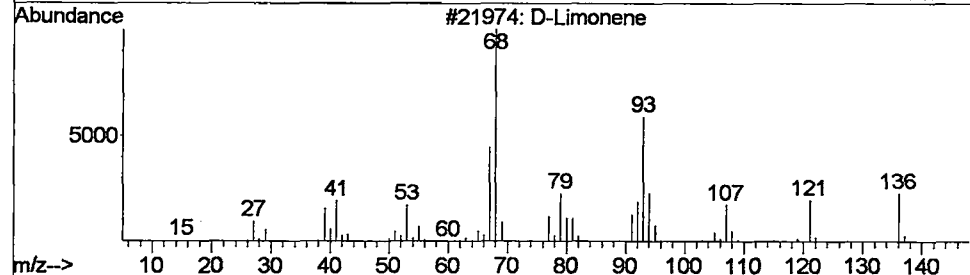
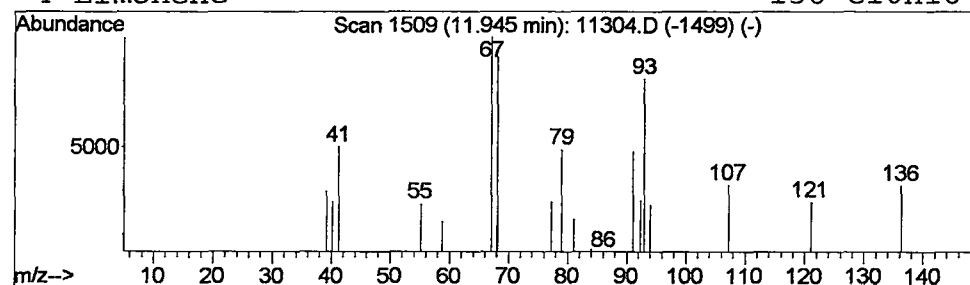
Vial: 15
Operator: Nefliu
Inst : Instrumen
Multiplr: 1.00

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

Peak Number 6 D-Limonene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	0.33 ug/l	18718	1,4-Dichlorobenzene-d4	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
✓ 1			D-Limonene	136	C10H16	005989-27-5	64
2			D-Limonene	136	C10H16	005989-27-5	64
3			Limonene	136	C10H16	000138-86-3	59
4			Limonene	136	C10H16	000138-86-3	59



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D
 Acq On : 16 May 2002 11:11 pm
 Sample : sample
 Misc :
 MS Integration Params: rteint.e

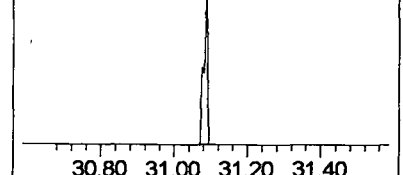
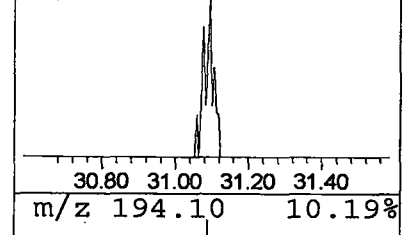
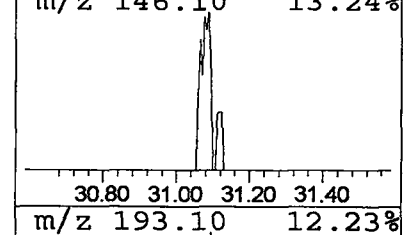
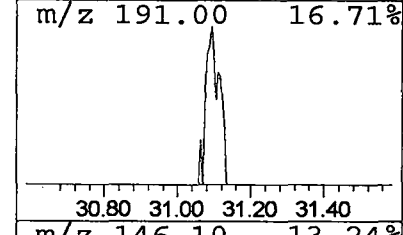
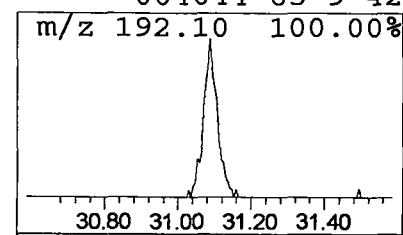
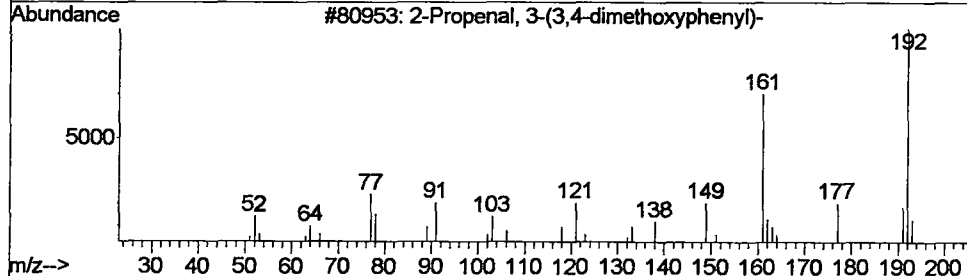
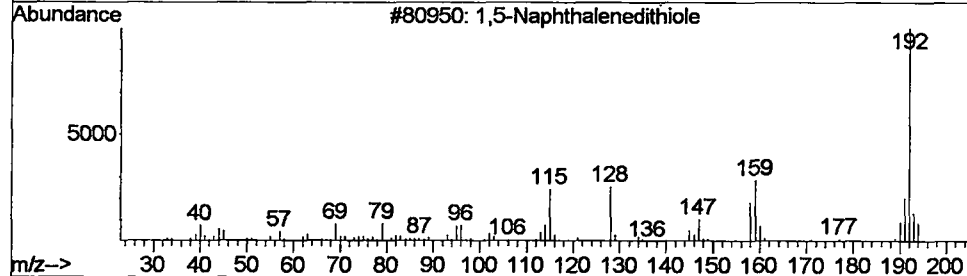
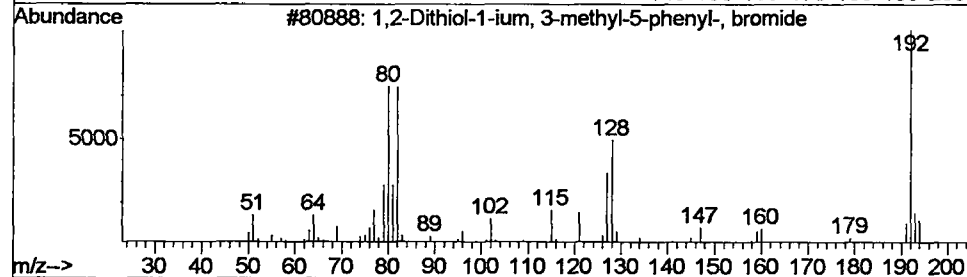
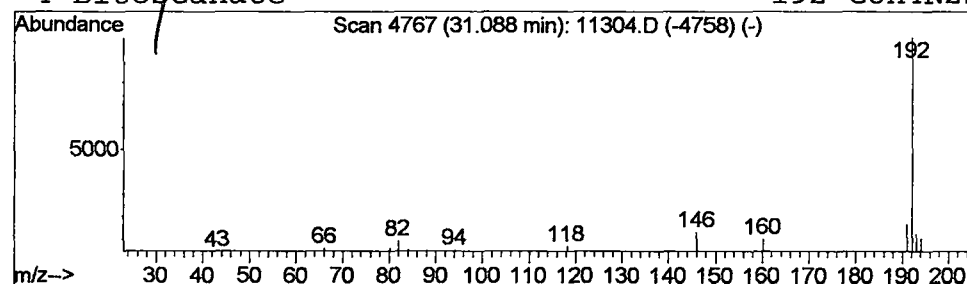
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 Operator: Nefliu
 Inst : Instrumen
 Multiplr: 1.00

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

 Peak Number 7 1,2-Dithiol-1-ium, 3-methyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.09	0.25 ug/l	19287	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dithiol-1-ium, 3-methyl-5-ph...	272	C10H9BrS2	055836-87-8	59
2			1,5-Naphthalenedithiole	192	C10H8S2	1000223-69-5	50
3			2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	42
4			Bitoscanate	192	C8H4N2S2	004044-65-9	42



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D

Acq On : 16 May 2002 11:11 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 15

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

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

Title : Method 508 GC/MS Scan

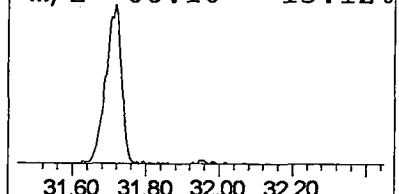
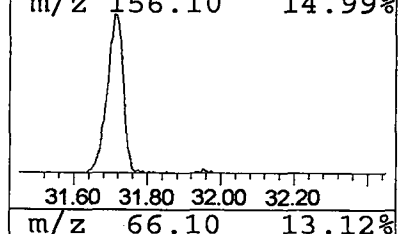
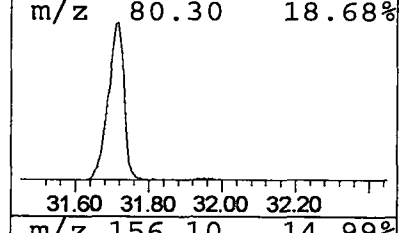
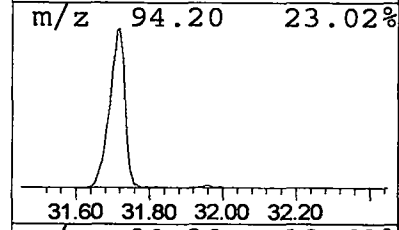
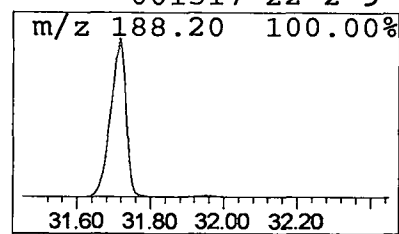
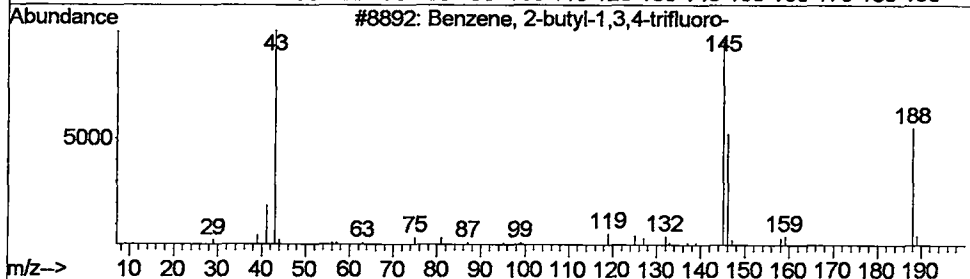
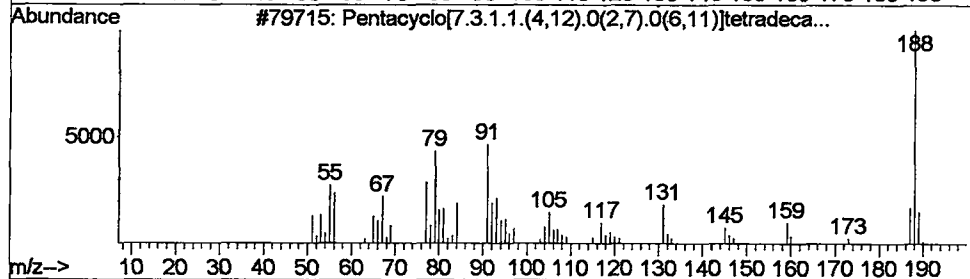
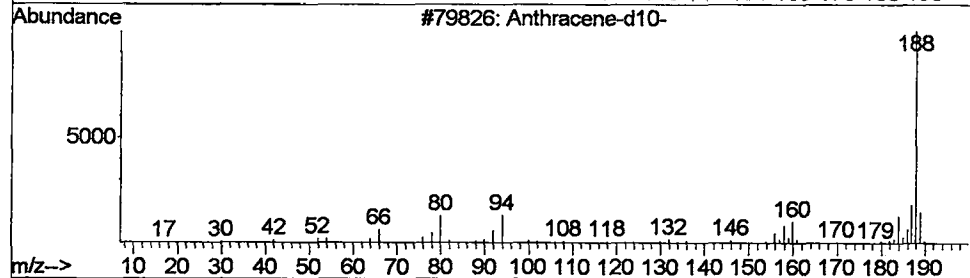
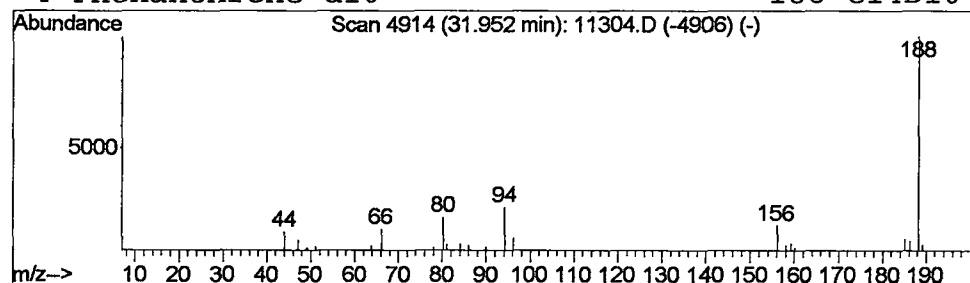
Library : C:\DATABASE\mist98.1

Peak Number 8 Anthracene-d10-

Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.95	0.33 ug/l	25995	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
✓ 1			Anthracene-d10-	188	C14D10	001719-06-8	50
2			Pentacyclo[7.3.1.1.(4,12).0(2,7)...]	188	C14H20	1000215-61-8	36
3			Benzene, 2-butyl-1,3,4-trifluoro-	188	C10H11F3	022872-43-1	9
4			Phenanthrene-d10	188	C14D10	001517-22-2	9



Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D

Acq On : 16 May 2002 11:11 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 15

Operator: Nefliu

Inst : Instrumen

Multiplr: 1.00

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

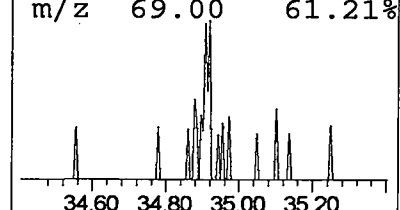
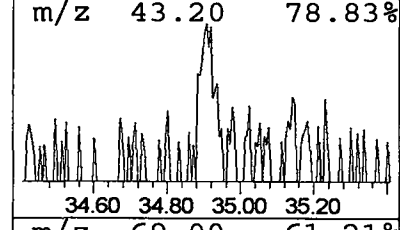
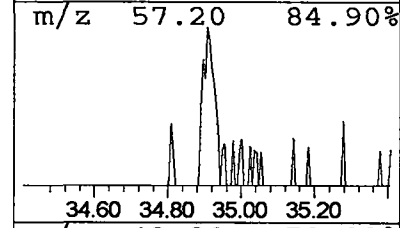
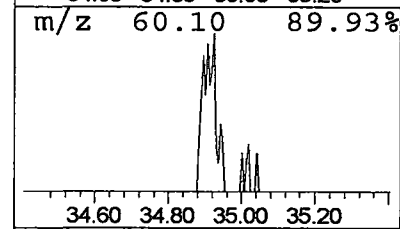
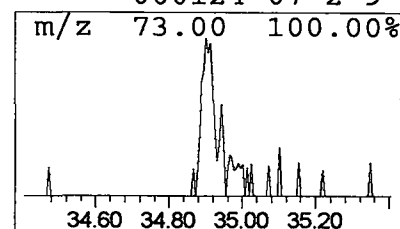
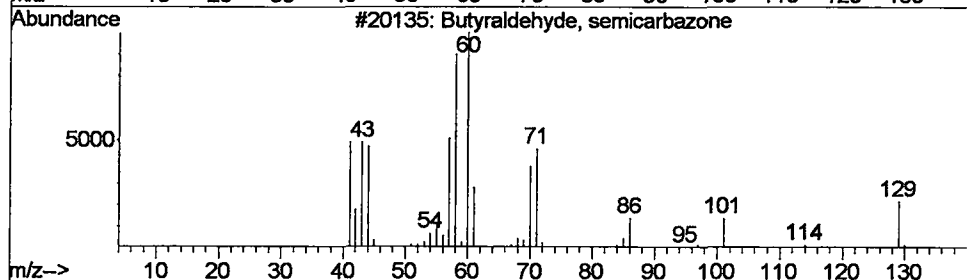
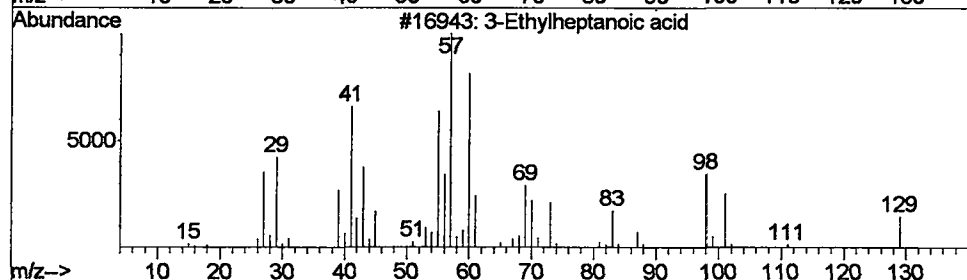
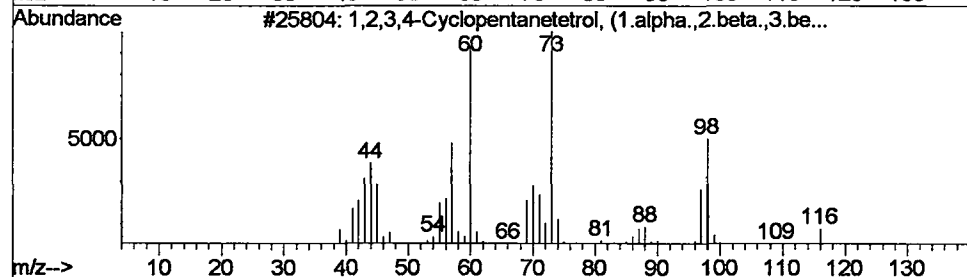
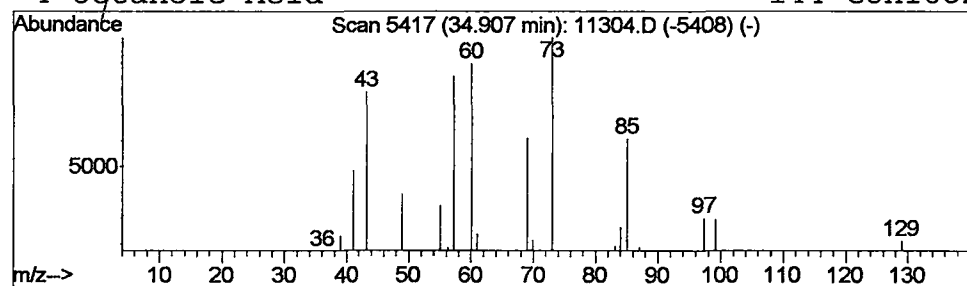
Title : Method 508 GC/MS Scan

Library : C:\DATABASE\NIST98.1

Peak Number 9 1,2,3,4-Cyclopentanetetrol,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
34.91	0.28 ug/l	22126	Phenanthrene-d10	31.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	10
2			3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	10
3			Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	9
4			Octanoic Acid	144	C8H16O2	000124-07-2	9



tentatively identified Compound (LSC) summary

Operator ID: Nefliu Date Acquired: 16 May 2002 11:11 pm
 Data File: C:\MSDCHEM\1\DATA\020516\11304.D
 Name: sample
 Misc:
 Method: C:\MSDCHEM\1\METHODS\SCAN020507.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
Propanoic acid	3.21	0.3	ug/l	17640	1	11.38	2284600	40.0
Allyl mercaptan <i>for quibit</i>	3.65	0.3	ug/l	16729	1	11.38	2284600	40.0
Butanoic acid <i>did not</i>	5.04	4.1	ug/l	232612	1	11.38	2284600	40.0
2-Pentanone, 4-hy...	6.16	23.3	ug/l	1332890	1	11.38	2284600	40.0
Hexanoic acid	7.56	0.7	ug/l	42746	1	11.38	2284600	40.0
D-Limonene	11.95	0.3	ug/l	18718	1	11.38	2284600	40.0
1,2-Dithiol-1-ium...	31.09	0.2	ug/l	19287	4	31.72	3146580	40.0
Anthracene-d10-	31.95	0.3	ug/l	25995	4	31.72	3146580	40.0
1,2/3,4-Cyclopent...	34.91	0.3	ug/l	22126	4	31.72	3146580	40.0
Sulfur dioxide	35.88	0.4	ug/l	28033	5	39.93	2685510	40.0

Library Search Compound Report

Data File : C:\MSDCHEM\1\DATA\020516\11304.D

Acq On : 16 May 2002 11:11 pm

Sample : sample

Misc :

MS Integration Params: rteint.e

Vial: 15

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 10 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
35.88	0.42 ug/l	28033	Chrysene-d12	39.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	7
2			Sulfur dioxide	64	O2S	007446-09-5	4
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	4
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4

