

User: Vinci, David L  
Westchester Dept. of Labs & Research  
Date: 03/04/2002 Time: 14:26:10

Sample: AE01506  
Analysis: \$GCMS GCMS Scan For Unknowns  
Units: ug  
Started: 3/4/02 14:25 Ended: 3/4/02 14:25 Analyst: DLV  
Page: 1

|   | Component Name          | Viol | Result | Qualifier | MDL |
|---|-------------------------|------|--------|-----------|-----|
| 1 | Other unknown compounds |      | .      |           |     |
| 2 | Surr_2,4-DDD            |      | 99     |           | 5.0 |

**Comments for Sample AE01506 - Analysis \$GCMS**

Westchester Dept. of Labs & Research

User: Vinci, David L

Date: 03-04-2002 Time: 14:26:30

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recoveries for 22 of the 43 compounds in the LCS Standard were above their acceptance ranges.

## Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D Vial: 3  
Acq On : 21 Feb 2002 12:31 pm Operator:  
Sample : 508 scan Inst : Instrumen  
Misc : February 21, 2002 Multiplr: 1.00  
MS Integration Params: SPLIT.P  
Quant Time: Feb 25 10:49:01 2002 Quant Results File: HP022102.RES

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
Title : 508 scan method  
Last Update : Mon Feb 25 10:47:59 2002  
Response via : Initial Calibration  
DataAcq Meth : HP020702

| Internal Standards        | R.T.  | QIon | Response | Conc  | Units | Dev(Min) |
|---------------------------|-------|------|----------|-------|-------|----------|
| 1) 1,4-Dichlorobenzene-d4 | 9.72  | 152  | 1538690  | 20.00 | ug/L  | 0.00     |
| 10) Naphthalene-d8        | 13.20 | 136  | 6682627  | 20.00 | ug/L  | 0.00     |
| 17) Acenaphthene-d10      | 18.34 | 164  | 3383604  | 20.00 | ug/L  | 0.00     |
| 29) Phenanthrene-d10      | 22.64 | 188  | 6045130  | 20.00 | ug/L  | 0.00     |
| 38) Chrysene-d12          | 30.49 | 240  | 4272904  | 20.00 | ug/L  | -0.03    |
| 44) Perylene-d12          | 34.41 | 264  | 2820465  | 20.00 | ug/L  | -0.04    |

## System Monitoring Compounds

|               |       |     |          |      |        |      |
|---------------|-------|-----|----------|------|--------|------|
| 37) 2,4-DDD   | 27.72 | 235 | 397616   | 4.93 | ug/L   | 0.00 |
| Spiked Amount | 5.000 |     | Recovery | =    | 98.60% |      |

## Target Compounds

|                        |       |     |        |      |      | Qvalue |
|------------------------|-------|-----|--------|------|------|--------|
| 20) Dimethylphthalate  | 18.34 | 163 | 547015 | 2.66 | ug/L | # 58   |
| 21) 2,6-Dinitrotoluene | 18.34 | 165 | 425529 | 8.98 | ug/L | # 27   |

-----  
(#) = qualifier out of range (m) = manual integration

01506.D HP022102.M Mon Feb 25 10:49:03 2002

Page 1

## Quantitation Report

(Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D

Vial: 3

Acq On : 21 Feb 2002 12:31 pm

Operator:

Sample : 508 scan

Inst : Instrumen

Misc : February 21, 2002

Multiplr: 1.00

MS Integration Params: SPLIT.P

Quant Time: Feb 25 10:49 2002

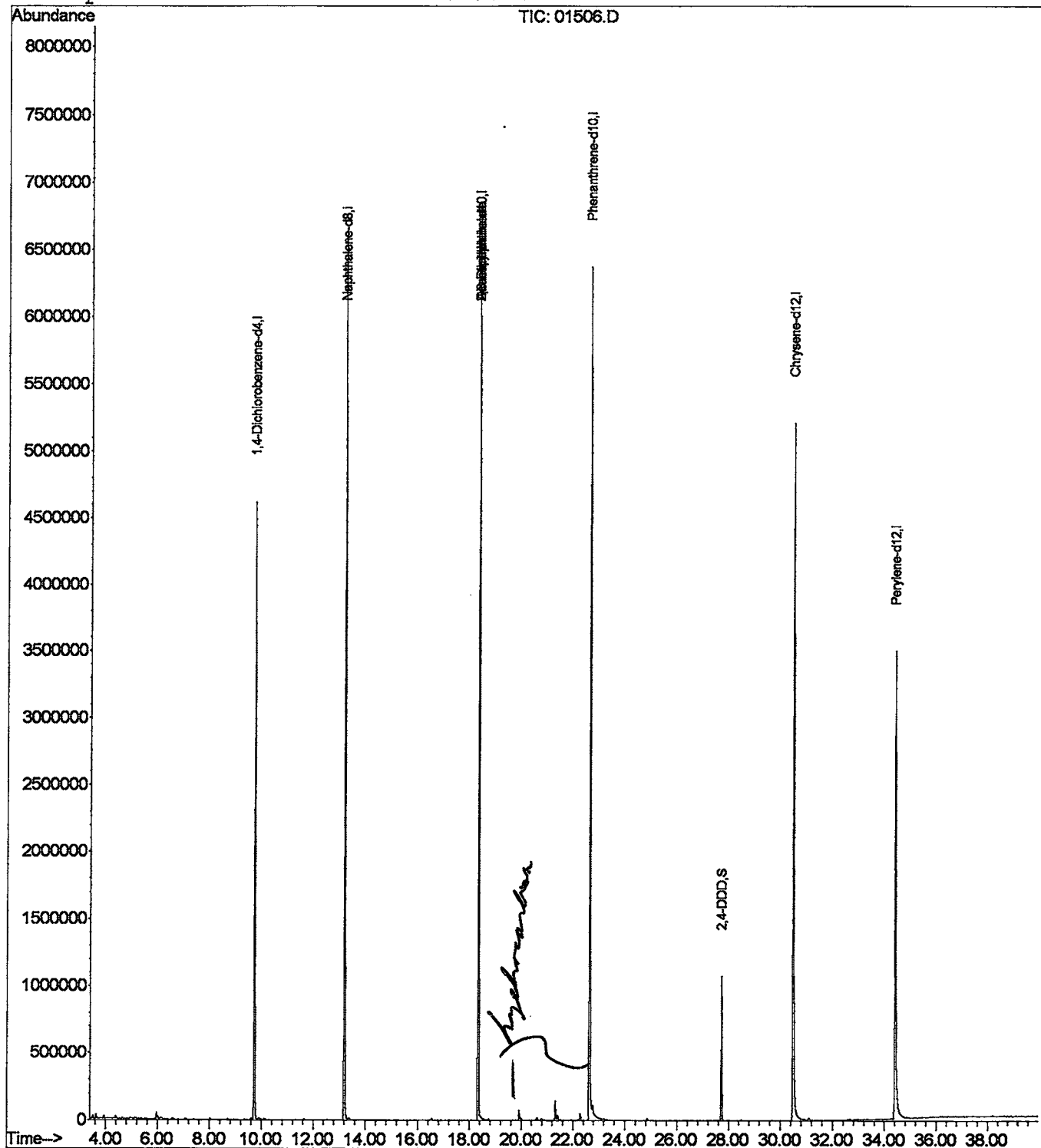
Quant Results File: HP022102.R

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)

Title : 508 scan method

Last Update : Mon Feb 25 10:47:59 2002

Response via : Initial Calibration



## LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Smoothing : OFF  
 Sampling : 2  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 100 Area counts  
 Max Peaks: 20  
 Peak Location: TOP

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

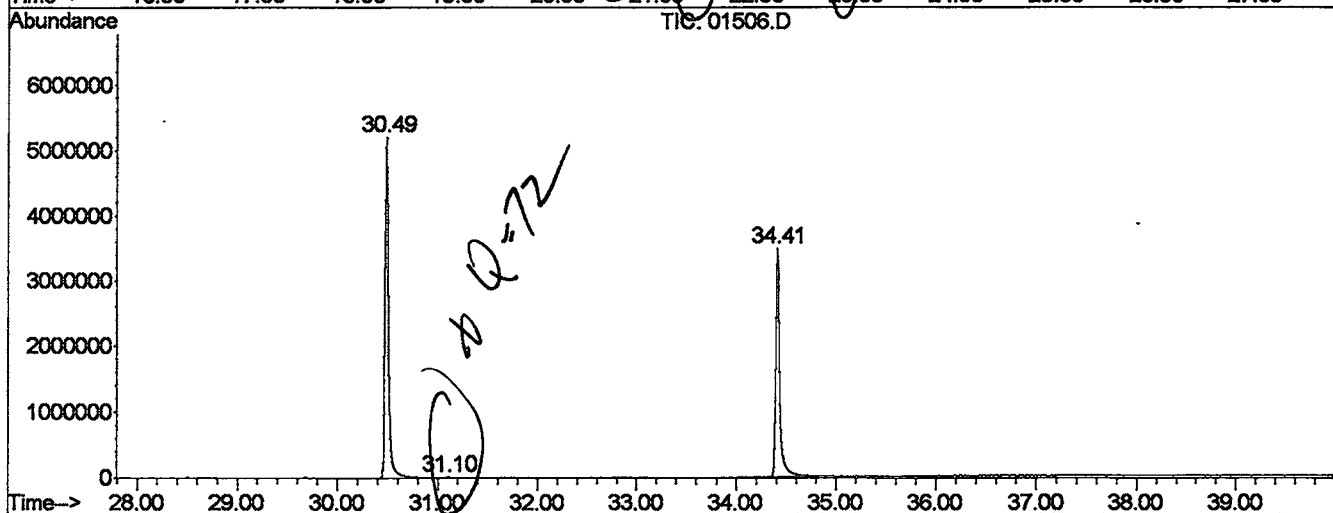
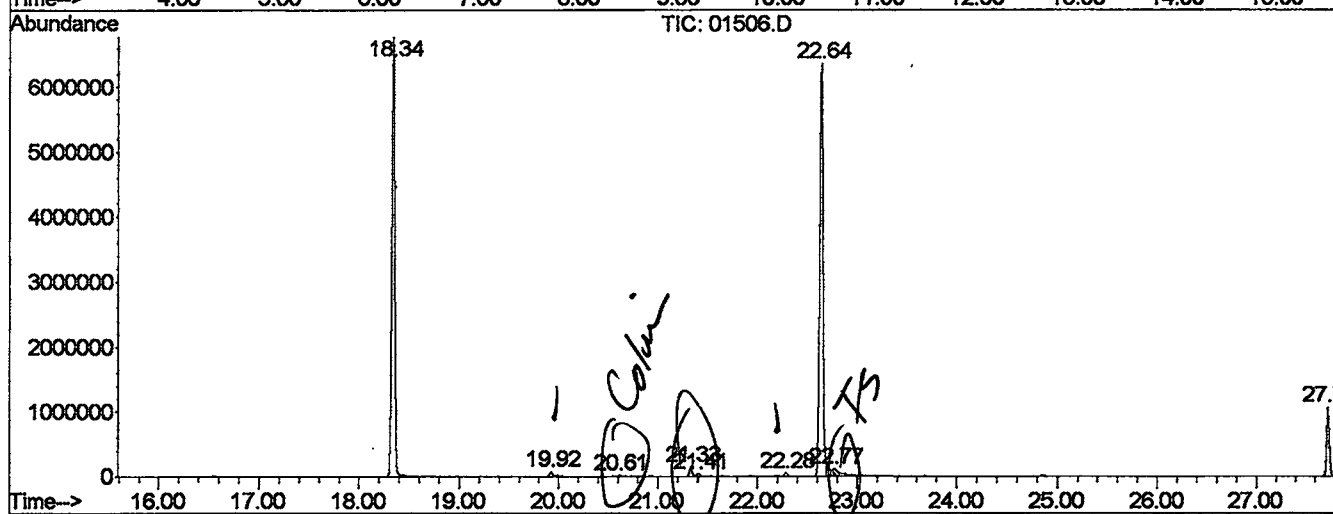
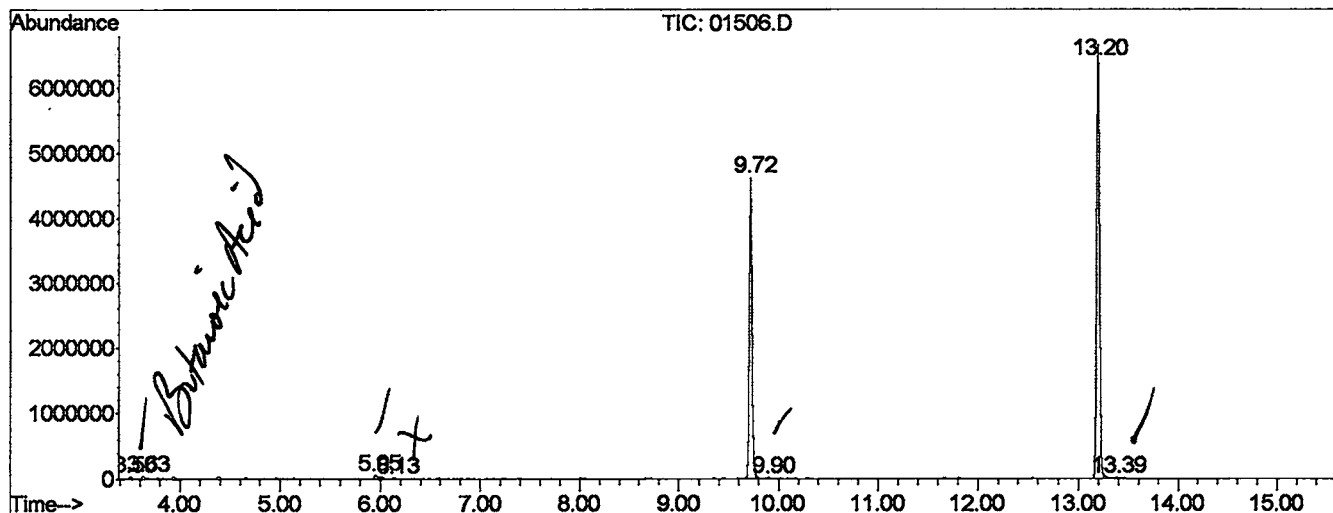
Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 3.498       | 9             | 11          | 19           | rVB2     | 26630          | 49292         | 0.34%           | 0.065%        |
| 2         | 3.634       | 19            | 23          | 27           | rBV      | 38833          | 75106         | 0.51%           | 0.099%        |
| 3         | 5.948       | 225           | 228         | 239          | rBV2     | 52239          | 185010        | 1.26%           | 0.243%        |
| 4         | 6.128       | 241           | 244         | 261          | rVB3     | 14607          | 66692         | 0.45%           | 0.088%        |
| 5         | 9.718       | 557           | 562         | 567          | rBV      | 4614715        | 8496996       | 57.76%          | 11.181%       |
| 6         | 9.899       | 575           | 578         | 593          | rVB      | 13298          | 61543         | 0.42%           | 0.081%        |
| 7         | 13.195      | 865           | 870         | 875          | rBV      | 6634858        | 12615220      | 85.75%          | 16.601%       |
| 8         | 13.387      | 883           | 887         | 899          | rVB2     | 15189          | 48900         | 0.33%           | 0.064%        |
| 9         | 18.343      | 1321          | 1326        | 1331         | rBV      | 6788811        | 13683635      | 93.01%          | 18.007%       |
| 10        | 19.923      | 1463          | 1466        | 1469         | rBV      | 76211          | 134936        | 0.92%           | 0.178%        |
| 11        | 20.612      | 1525          | 1527        | 1535         | rVB      | 20178          | 47922         | 0.33%           | 0.063%        |
| 12        | 21.335      | 1587          | 1591        | 1595         | rBV      | 146256         | 265894        | 1.81%           | 0.350%        |
| 13        | 21.414      | 1595          | 1598        | 1603         | rVB2     | 31114          | 66770         | 0.45%           | 0.088%        |
| 14        | 22.283      | 1671          | 1675        | 1679         | rBV2     | 53207          | 108829        | 0.74%           | 0.143%        |
| 15        | 22.644      | 1701          | 1707        | 1711         | rBV2     | 6368761        | 14711654      | 100.00%         | 19.359%       |
| 16        | 22.768      | 1715          | 1718        | 1753         | rVB      | 108954         | 689309        | 4.69%           | 0.907%        |
| 17        | 27.724      | 2153          | 2157        | 2163         | rBV      | 1072300        | 1961731       | 13.33%          | 2.581%        |
| 18        | 30.490      | 2397          | 2402        | 2437         | rBV2     | 5207038        | 12877224      | 87.53%          | 16.945%       |
| 19        | 31.099      | 2451          | 2456        | 2465         | rVB2     | 18153          | 45806         | 0.31%           | 0.060%        |
| 20        | 34.407      | 2743          | 2749        | 2785         | rBV      | 3488960        | 9799870       | 66.61%          | 12.896%       |

Sum of corrected areas: 75992339

# LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Operator :  
 Acquired : 21 Feb 2002 12:31 pm using AcqMethod HP020702  
 Instrument : Instrumen  
 Sample Name: 508 scan  
 Misc Info : February 21, 2002  
 Vial Number: 3  
 Quant File :HP022102.RES (RTE Integrator)



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

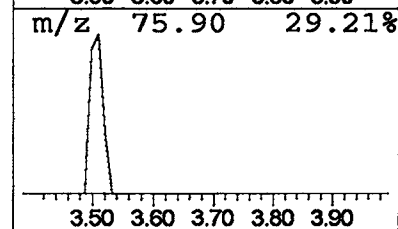
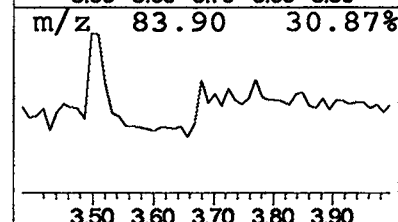
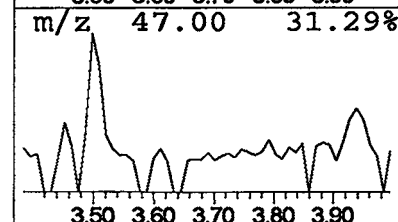
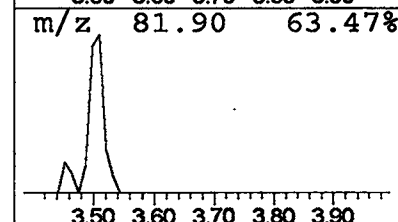
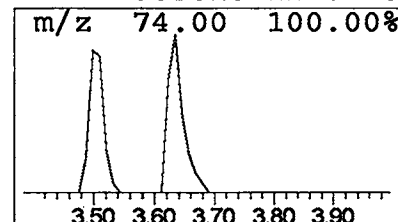
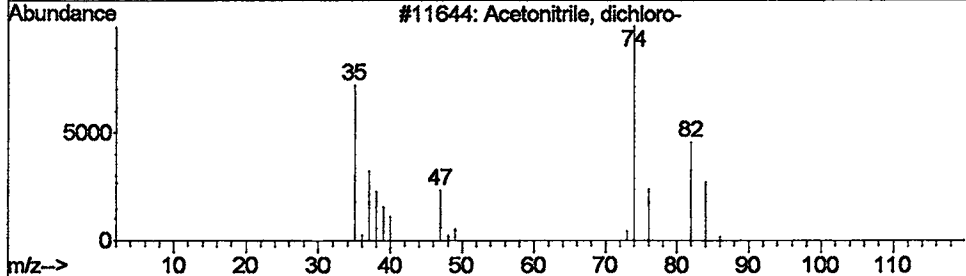
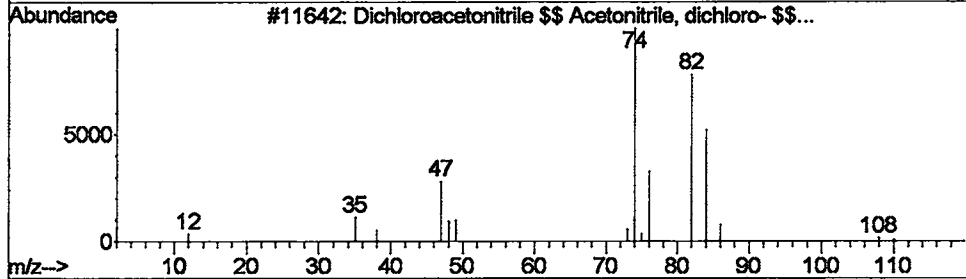
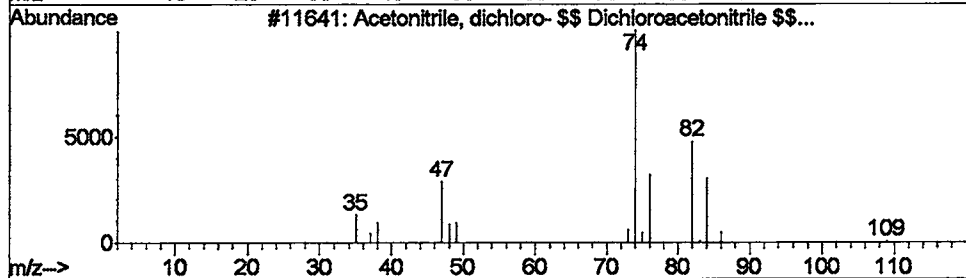
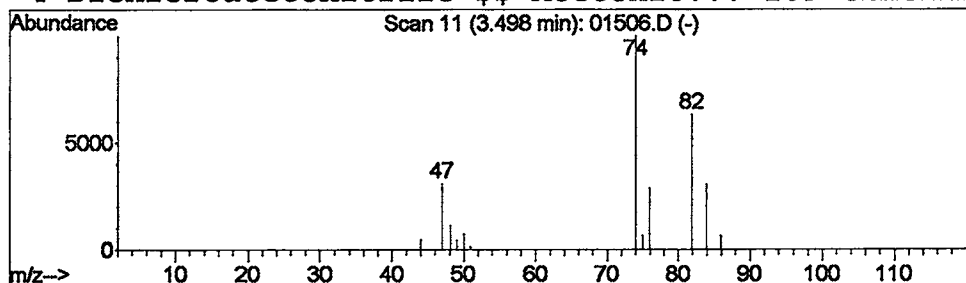
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 1 Acetonitrile, dichloro- \$\$ ... Concentration Rank 9

| R.T. | EstConc   | Area  | Relative to ISTD       | R.T. |
|------|-----------|-------|------------------------|------|
| 3.50 | 0.12 ug/L | 49292 | 1,4-Dichlorobenzene-d4 | 9.72 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Acetonitrile, dichloro- \$\$ Dichl... | 109 | C2HCl2N | 003018-12-0 | 78   |
| 2    |    |   | Dichloroacetonitrile \$\$ Acetonit... | 109 | C2HCl2N | 003018-12-0 | 74   |
| 3    |    |   | Acetonitrile, dichloro-               | 109 | C2HCl2N | 003018-12-0 | 43   |
| 4    |    |   | Dichloroacetonitrile \$\$ Acetonit... | 109 | C2HCl2N | 003018-12-0 | 40   |



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Acq On : 21 Feb 2002 12:31 pm  
Sample : 508 scan  
Misc : February 21, 2002  
MS Integration Params: LSCINT.P

Vial: 3  
Operator:  
Inst : Instrumen  
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)

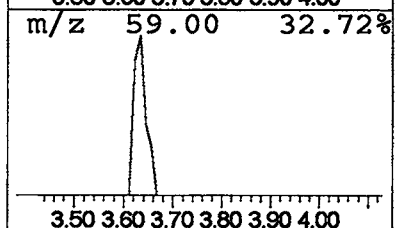
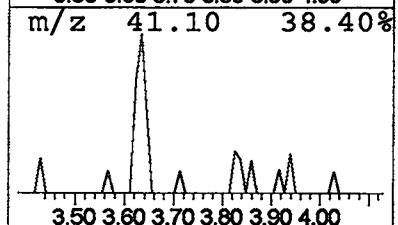
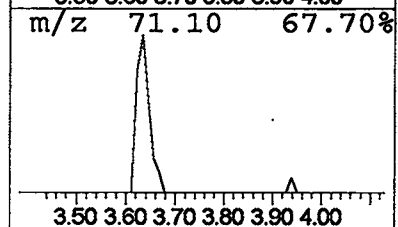
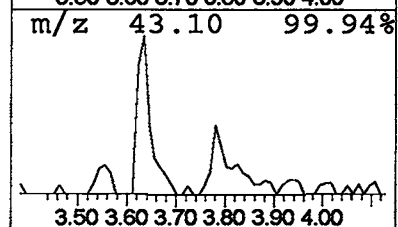
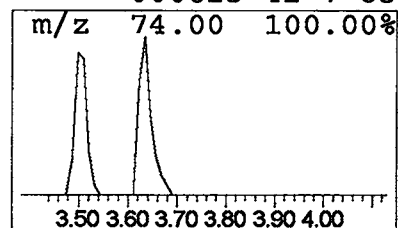
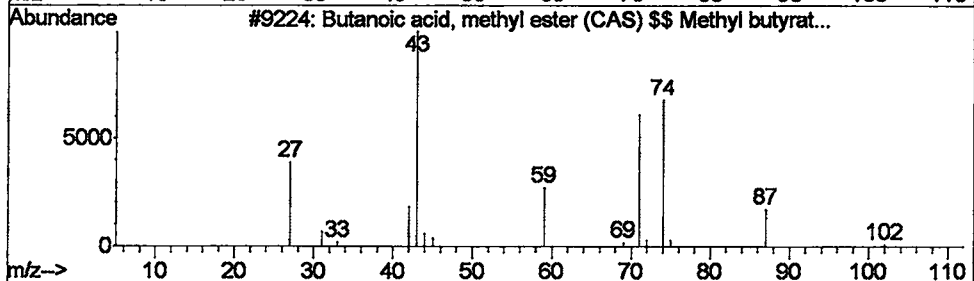
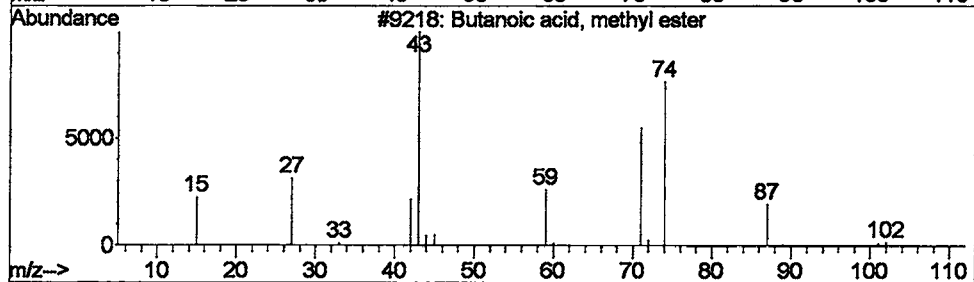
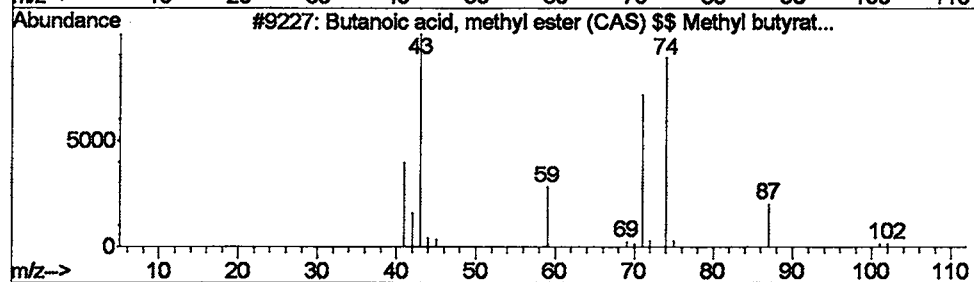
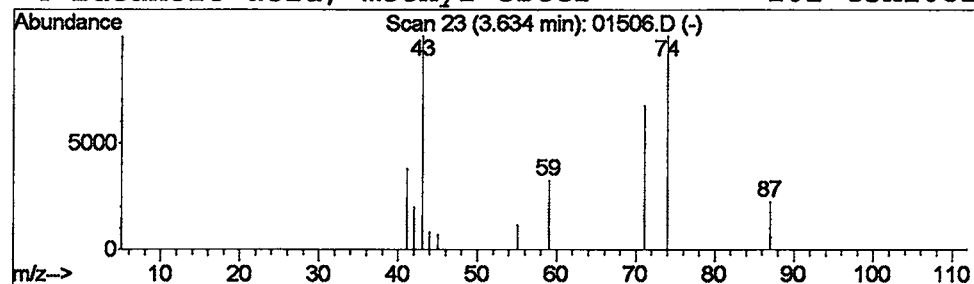
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
Peak Number 2 Butanoic acid, methyl ester... Concentration Rank 5

| R.T. | EstConc   | Area  | Relative to ISTD       | R.T. |
|------|-----------|-------|------------------------|------|
| 3.63 | 0.18 ug/L | 75106 | 1,4-Dichlorobenzene-d4 | 9.72 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Butanoic acid, methyl ester (CAS... | 102 | C5H10O2 | 000623-42-7 | 83   |
| 2    |    |   | Butanoic acid, methyl ester         | 102 | C5H10O2 | 000623-42-7 | 83   |
| 3    |    |   | Butanoic acid, methyl ester (CAS... | 102 | C5H10O2 | 000623-42-7 | 83   |
| 4    |    |   | Butanoic acid, methyl ester         | 102 | C5H10O2 | 000623-42-7 | 83   |



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 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

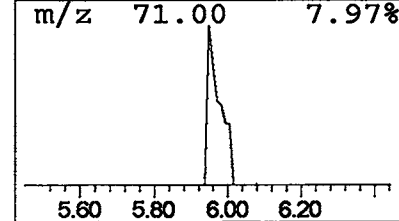
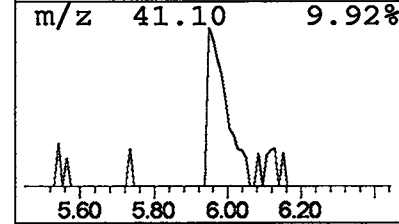
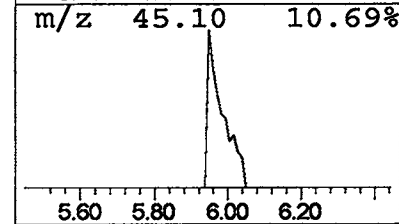
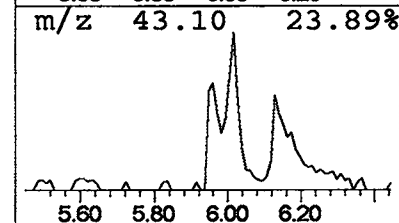
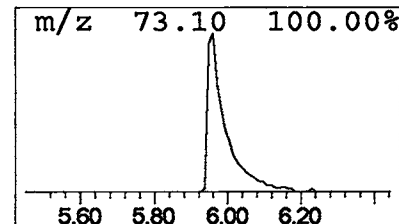
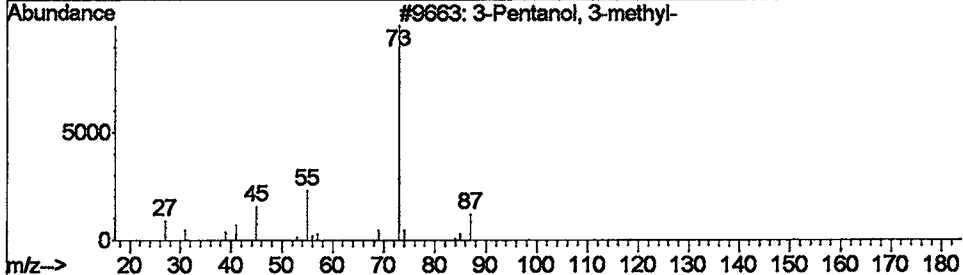
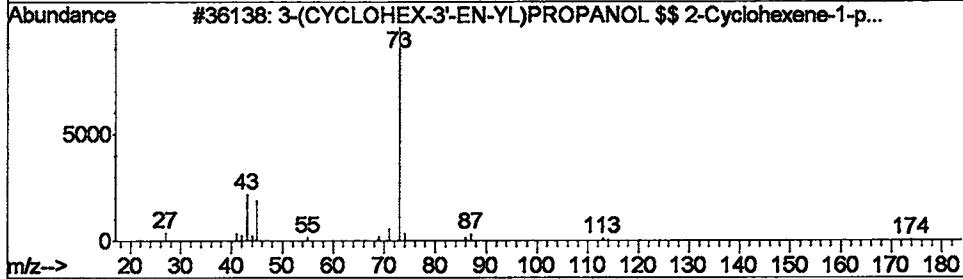
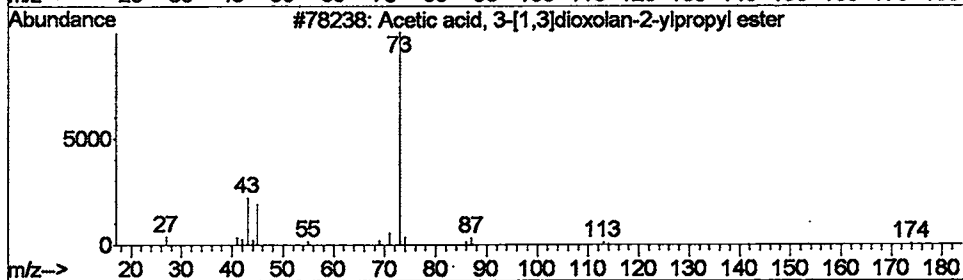
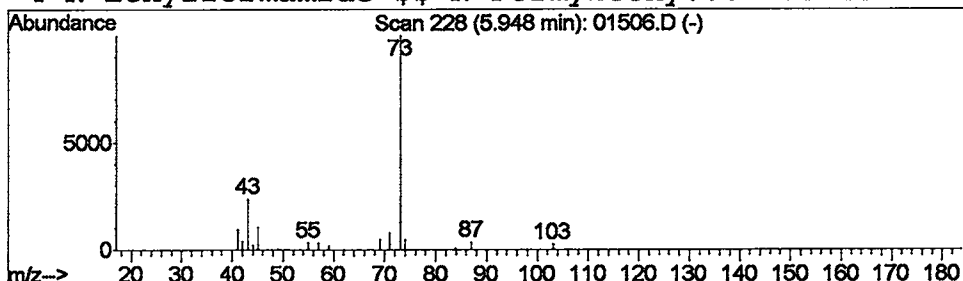
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 3 Acetic acid, 3-[1,3]dioxola... Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD       | R.T. |
|------|-----------|--------|------------------------|------|
| 5.95 | 0.44 ug/L | 185010 | 1,4-Dichlorobenzene-d4 | 9.72 |

| Hit# of | 5 | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|---------|---|---------------------------------------|-----|---------|-------------|------|
| 1       |   | Acetic acid, 3-[1,3]dioxolan-2-y...   | 174 | C8H14O4 | 000000-00-0 | 33   |
| 2       |   | 3-(CYCLOHEX-3'-EN-YL)PROPANOL \$\$... | 174 | C8H14O4 | 015745-87-6 | 33   |
| 3       |   | 3-Pentanol, 3-methyl-                 | 102 | C6H14O  | 000077-74-7 | 28   |
| 4       |   | N-Ethylformamide \$\$ N-Formylethy... | 73  | C3H7NO  | 000627-45-2 | 9    |



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 MS Integration Params: LSCINT.P

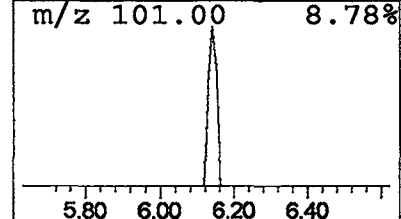
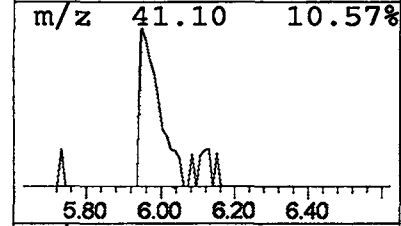
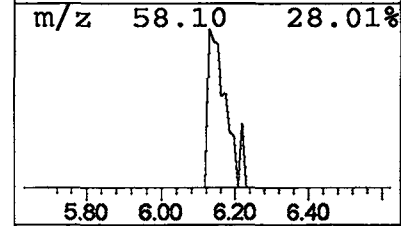
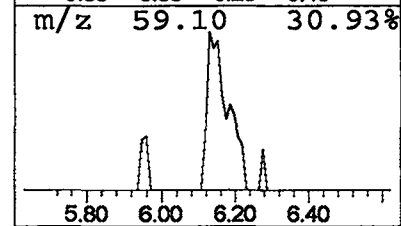
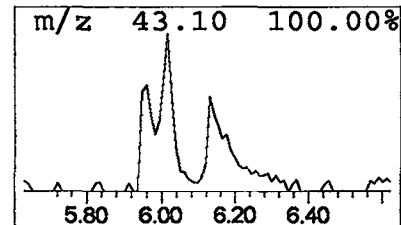
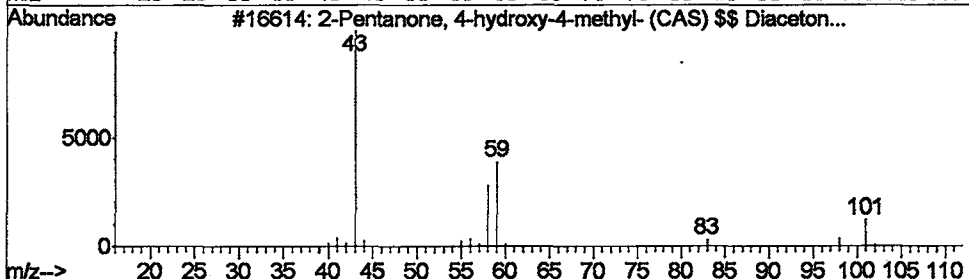
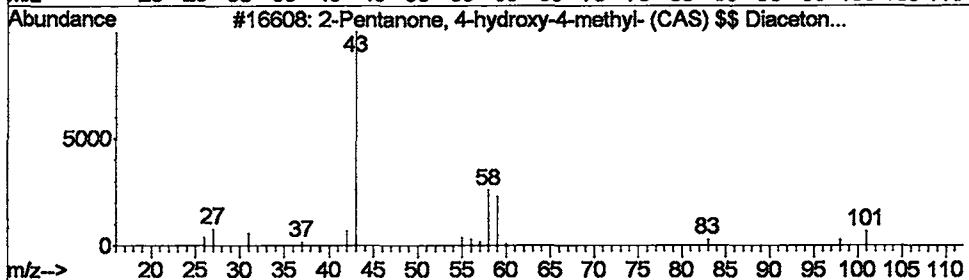
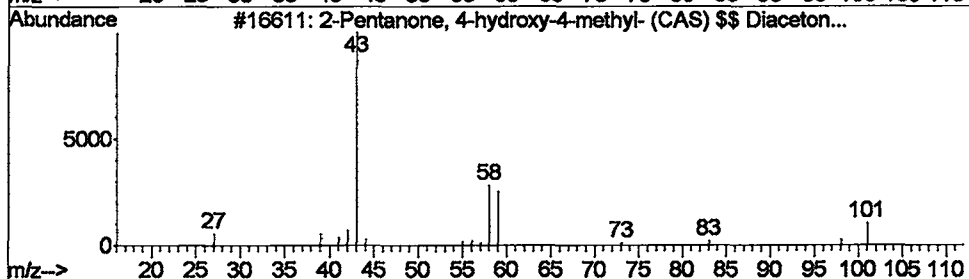
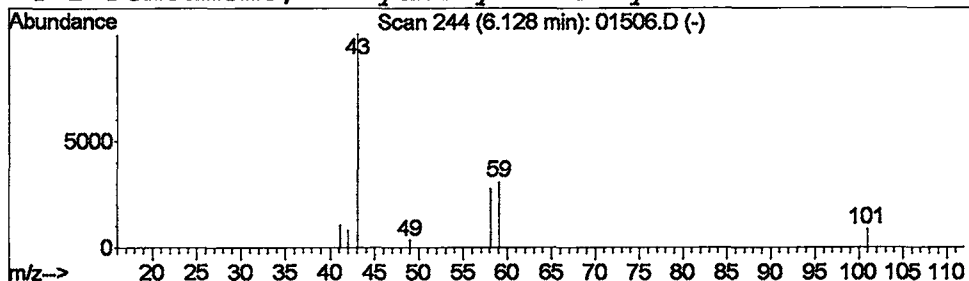
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc   | Area  | Relative to ISTD       | R.T. |
|------|-----------|-------|------------------------|------|
| 6.13 | 0.16 ug/L | 66692 | 1,4-Dichlorobenzene-d4 | 9.72 |

| Hit# of | 5                                   | Tentative ID | MW      | MolForm     | CAS# | Qual |
|---------|-------------------------------------|--------------|---------|-------------|------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-... | 116          | C6H12O2 | 000123-42-2 | 43   |      |
| 2       | 2-Pentanone, 4-hydroxy-4-methyl-... | 116          | C6H12O2 | 000123-42-2 | 9    |      |
| 3       | 2-Pentanone, 4-hydroxy-4-methyl-... | 116          | C6H12O2 | 000123-42-2 | 9    |      |
| 4       | 2-Pentanone, 4-hydroxy-4-methyl-... | 116          | C6H12O2 | 000123-42-2 | 9    |      |



# Library Search Compound Report

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 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

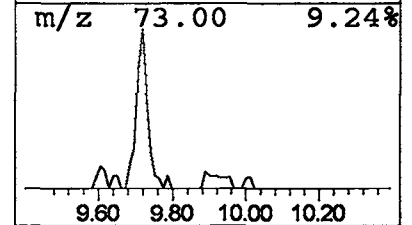
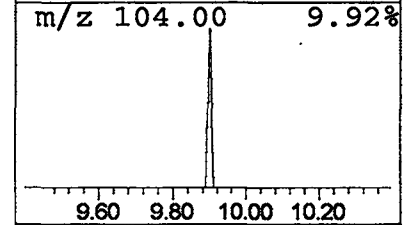
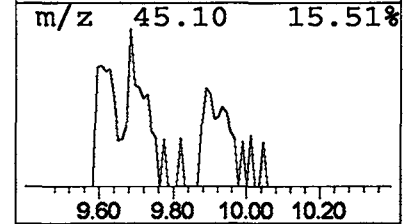
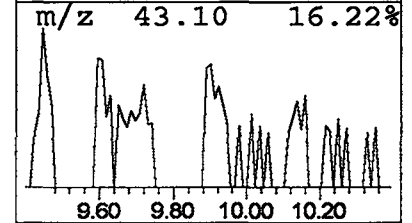
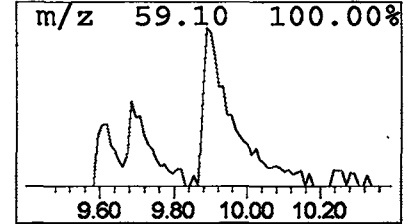
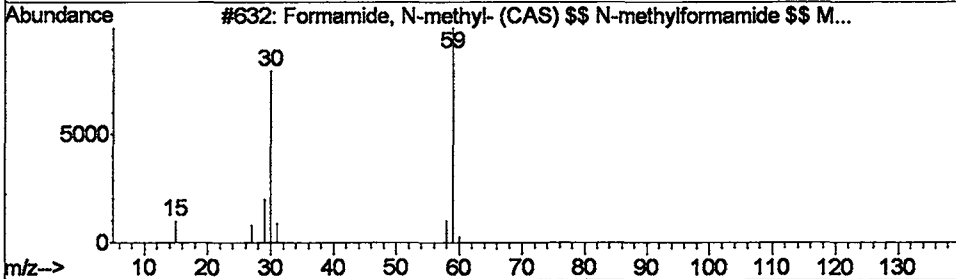
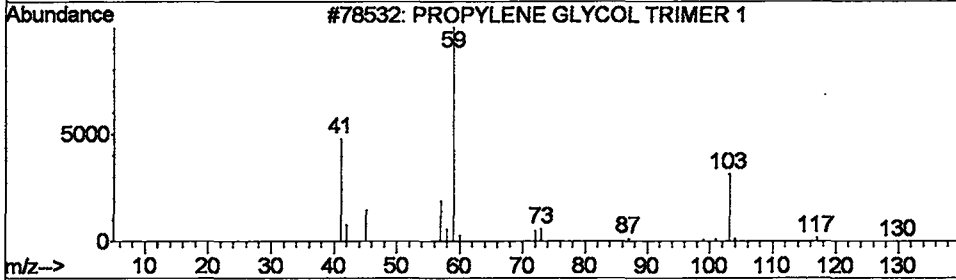
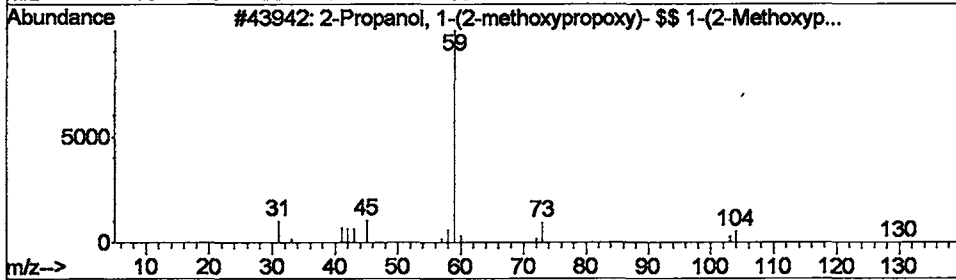
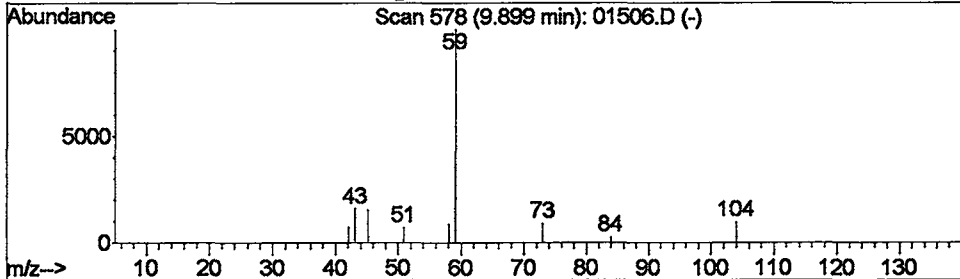
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 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 8

| R.T. | EstConc   | Area  | Relative to ISTD       | R.T. |
|------|-----------|-------|------------------------|------|
| 9.90 | 0.14 ug/L | 61543 | 1,4-Dichlorobenzene-d4 | 9.72 |

| Hit# of | 5 | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|---------|---|---------------------------------------|-----|---------|-------------|------|
| 1       |   | 2-Propanol, 1-(2-methoxypropoxy)...   | 148 | C7H16O3 | 013429-07-7 | 9    |
| 2       |   | PROPYLENE GLYCOL TRIMER 1             | 174 | C9H18O3 | 000000-00-0 | 9    |
| 3       |   | Formamide, N-methyl- (CAS) \$\$ N-... | 59  | C2H5NO  | 000123-39-7 | 4    |
| 4       |   | Formamide, N-methyl- (CAS) \$\$ N-... | 59  | C2H5NO  | 000123-39-7 | 4    |



## Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
Acq On : 21 Feb 2002 12:31 pm  
Sample : 508 scan  
Misc : February 21, 2002  
MS Integration Params: LSCINT.P

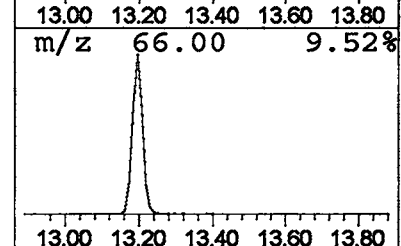
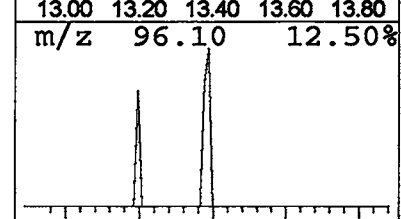
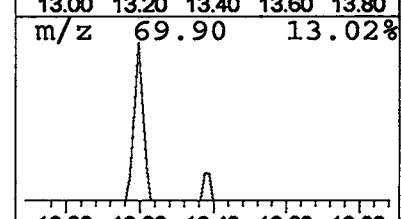
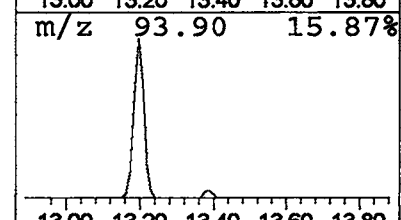
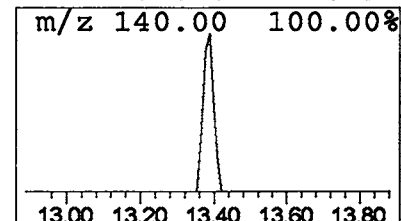
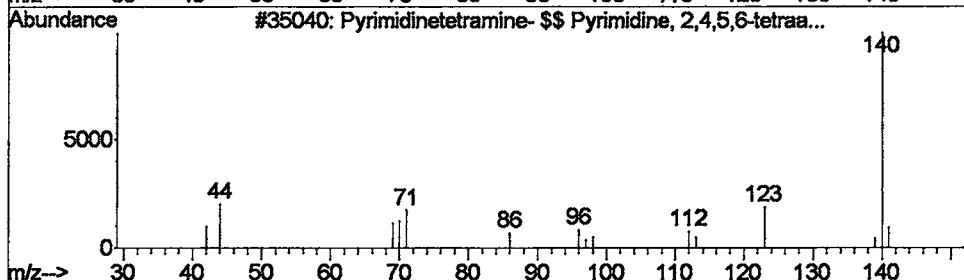
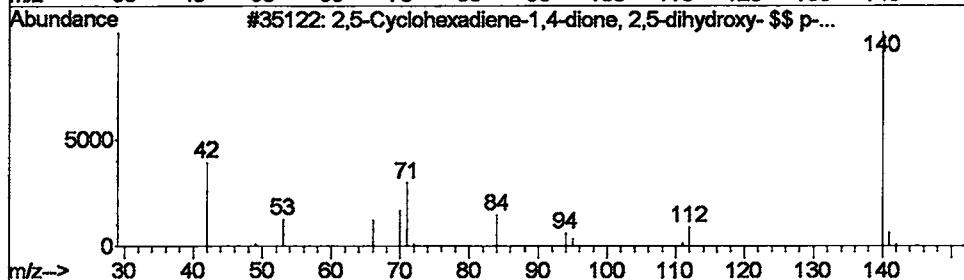
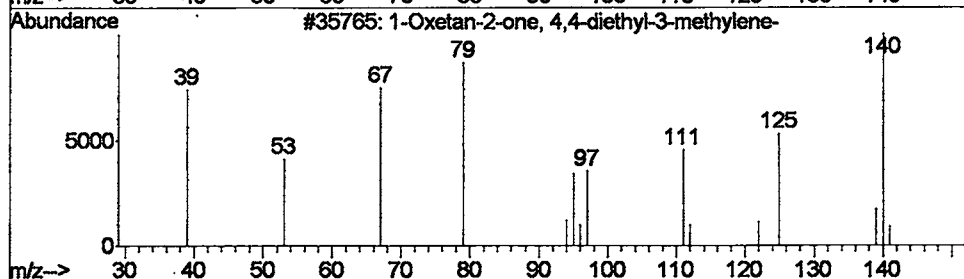
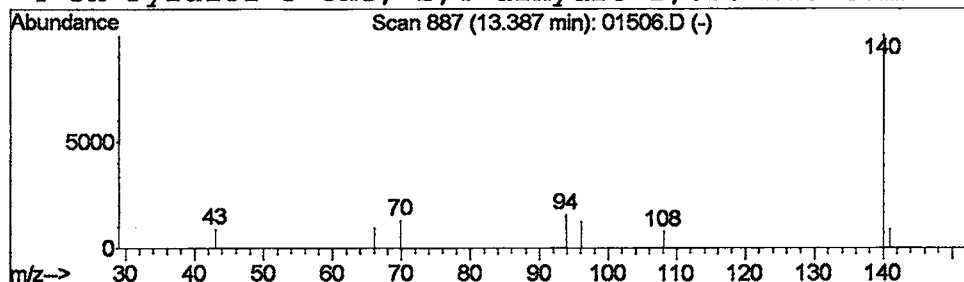
Vial: 3  
Operator:  
Inst : Instrumen  
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
Title : 508 scan method  
Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
Peak Number 6 1-Oxetan-2-one, 4,4-diethyl... Concentration Rank 11

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 13.39 | 0.08 ug/L | 48900 | Naphthalene-d8   | 13.20 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1-Oxetan-2-one, 4,4-diethyl-3-me...   | 140 | C8H12O2  | 000000-00-0 | 64   |
| 2    |    |   | 2,5-Cyclohexadiene-1,4-dione, 2,...   | 140 | C6H4O4   | 000615-94-1 | 56   |
| 3    |    |   | Pyrimidinetetramine- \$\$ Pyrimidi... | 140 | C4H8N6   | 001004-74-6 | 50   |
| 4    |    |   | 3H-Pyrazol-3-one, 2,4-dihydro-2,...   | 140 | C7H12N2O | 003201-25-0 | 9    |



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

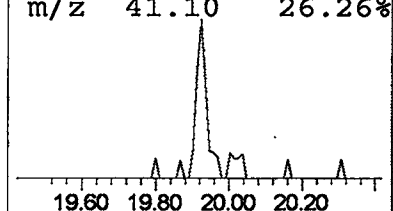
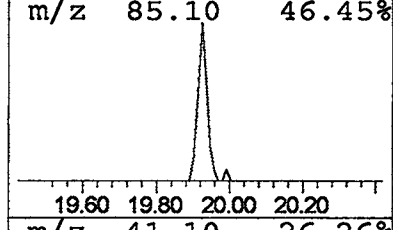
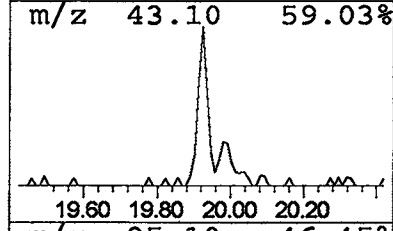
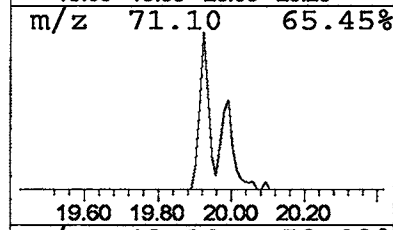
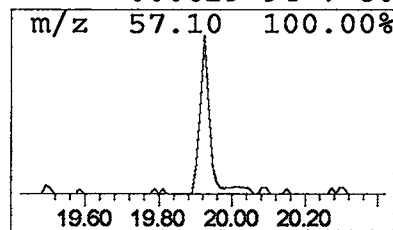
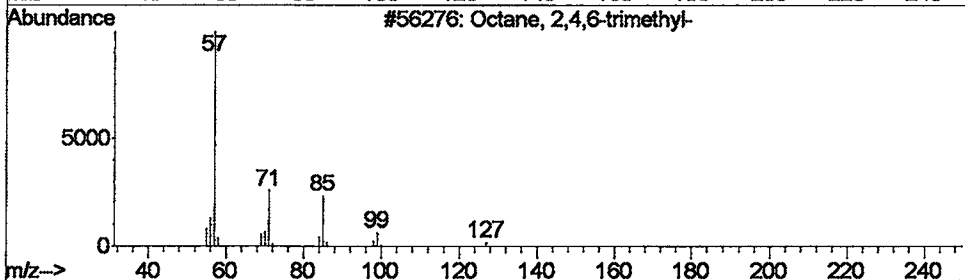
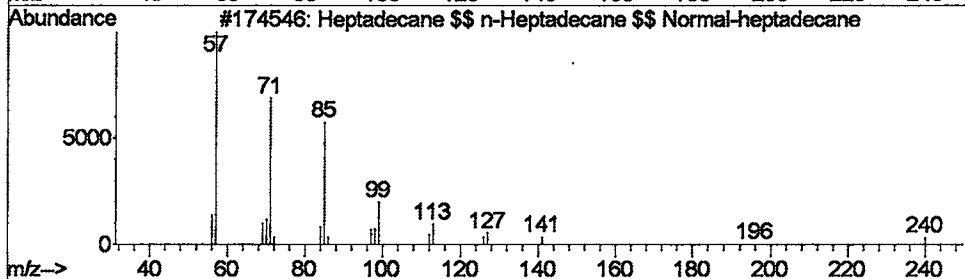
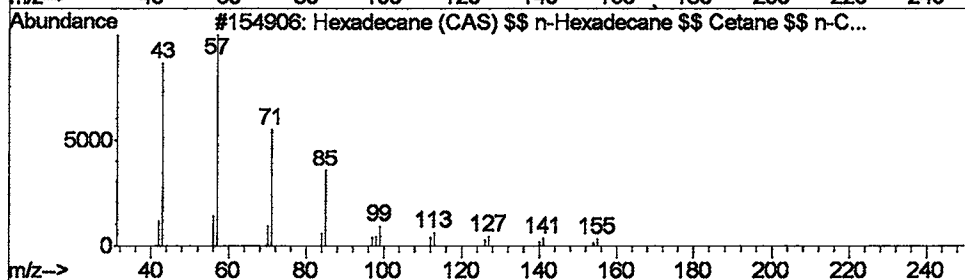
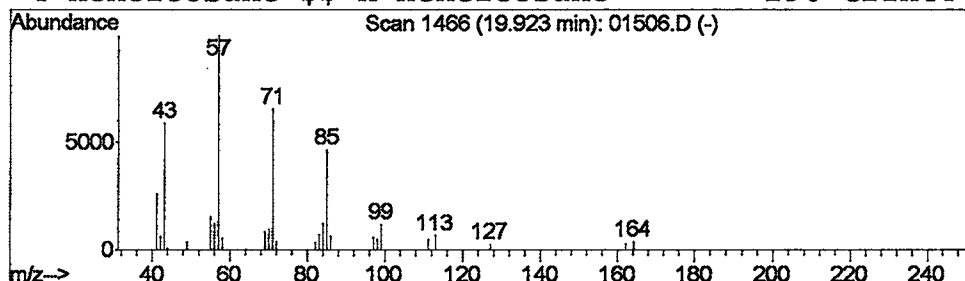
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 7 Hexadecane (CAS) \$\$ n-Hexad... Concentration Rank 4

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 19.92 | 0.20 ug/L | 134936 | Acenaphthene-d10 | 18.34 |

| Hit# of | 5                                       | Tentative ID | MW     | MolForm     | CAS# | Qual |
|---------|-----------------------------------------|--------------|--------|-------------|------|------|
| 1       | Hexadecane (CAS) \$\$ n-Hexadecane...   | 226          | C16H34 | 000544-76-3 | 86   |      |
| 2       | Heptadecane \$\$ n-Heptadecane \$\$ ... | 240          | C17H36 | 000629-78-7 | 86   |      |
| 3       | Octane, 2,4,6-trimethyl-                | 156          | C11H24 | 062016-37-9 | 80   |      |
| 4       | Heneicosane \$\$ n-Heneicosane          | 296          | C21H44 | 000629-94-7 | 80   |      |



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

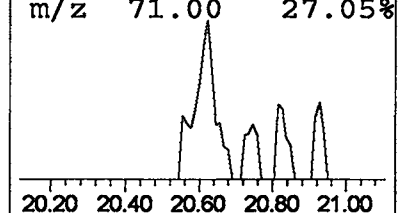
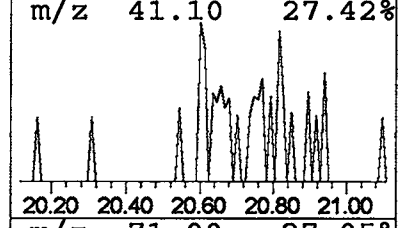
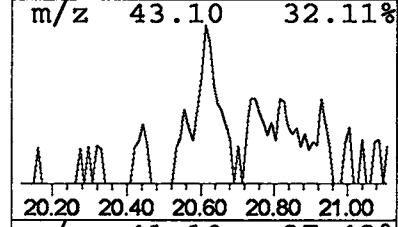
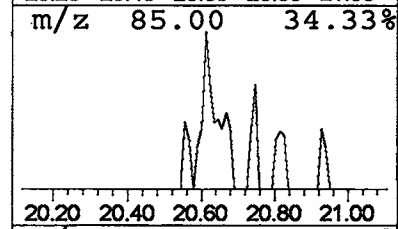
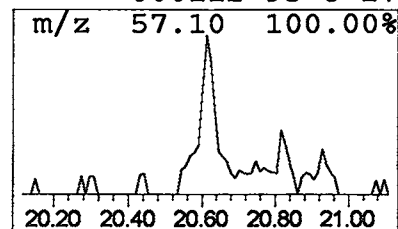
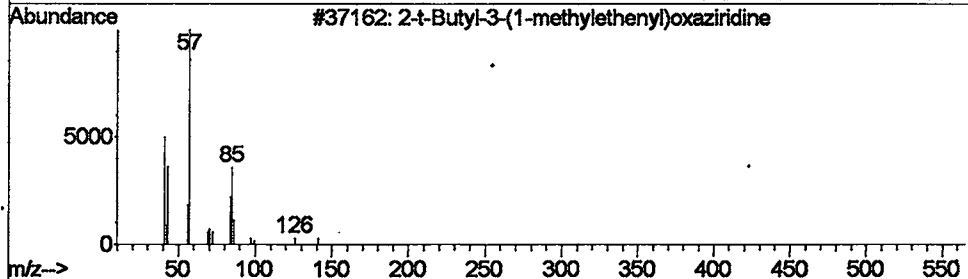
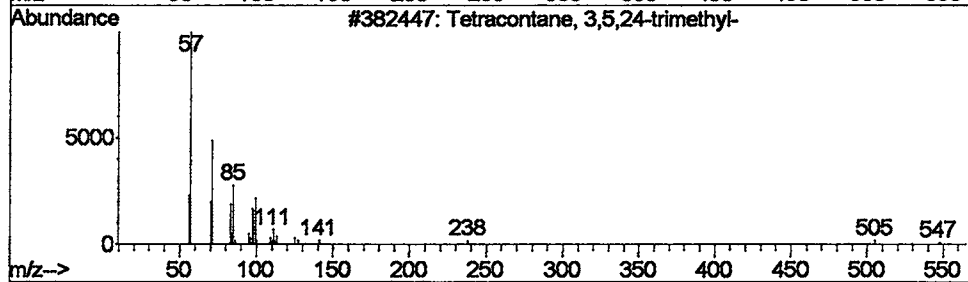
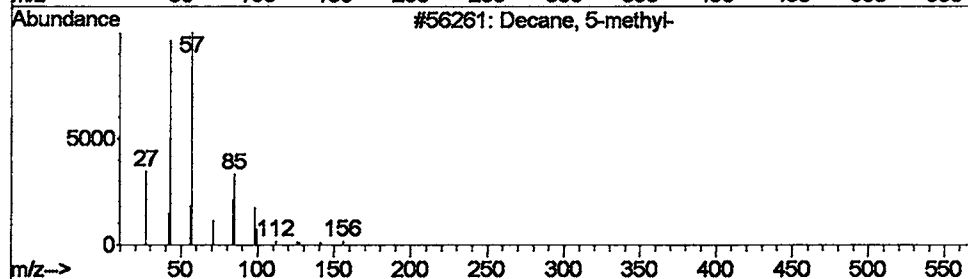
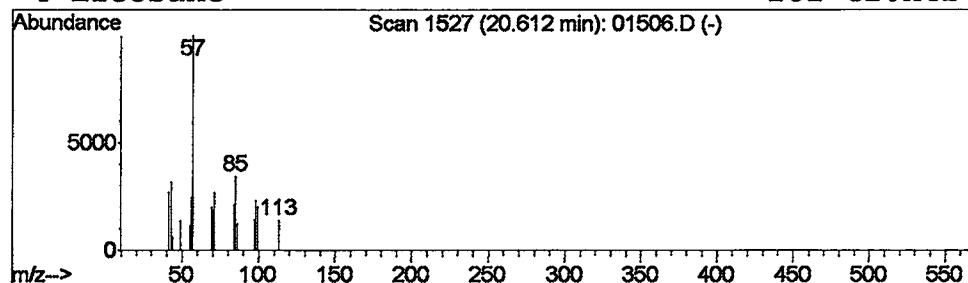
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 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 8 Decane, 5-methyl- Concentration Rank 13

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 20.61 | 0.07 ug/L | 47922 | Phenanthrene-d10 | 22.64 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Decane, 5-methyl-                   | 156 | C11H24  | 013151-35-4 | 38   |
| 2    |    | Tetracontane, 3,5,24-trimethyl-     | 605 | C43H88  | 055162-61-3 | 37   |
| 3    |    | 2-t-Butyl-3-(1-methylethenyl)oxa... | 141 | C8H15NO | 000000-00-0 | 35   |
| 4    |    | Eicosane                            | 282 | C20H42  | 000112-95-8 | 27   |



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
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 Misc : February 21, 2002  
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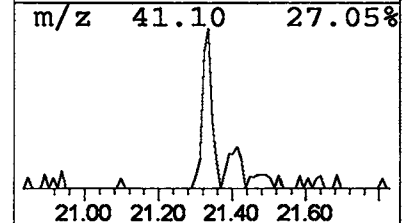
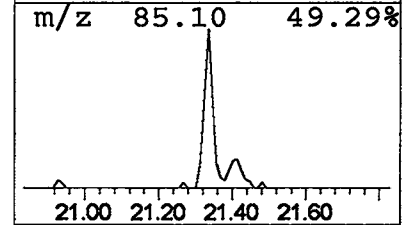
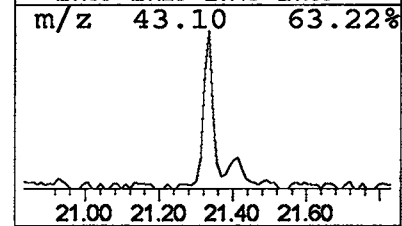
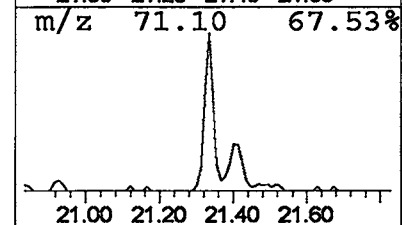
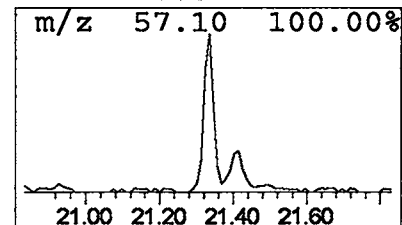
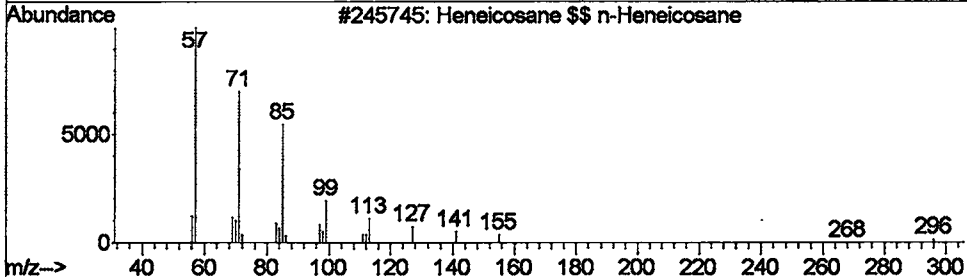
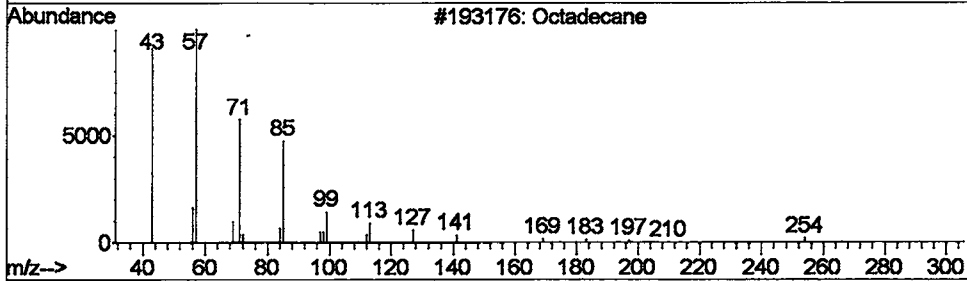
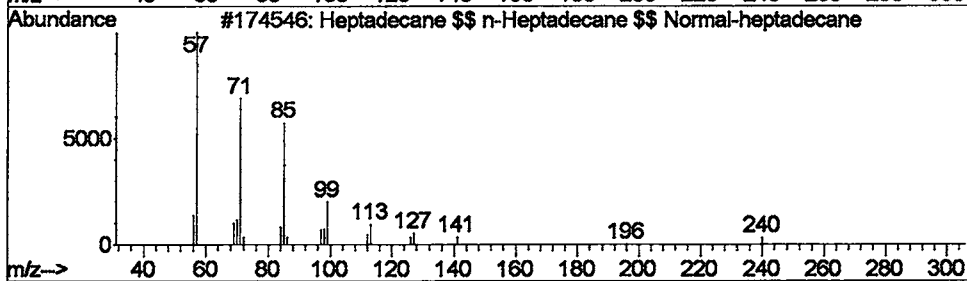
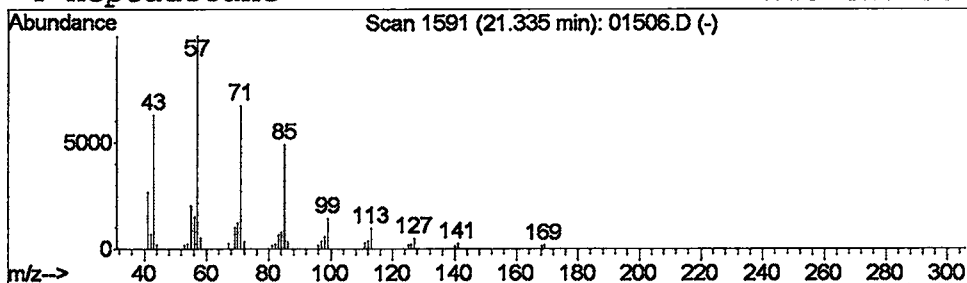
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 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 9 Heptadecane \$\$ n-Heptadecan... Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 21.33 | 0.36 ug/L | 265894 | Phenanthrene-d10 | 22.64 |

| Hit# | of | 5 | Tentative ID                            | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Heptadecane \$\$ n-Heptadecane \$\$ ... | 240 | C17H36  | 000629-78-7 | 91   |
| 2    |    |   | Octadecane                              | 254 | C18H38  | 000593-45-3 | 91   |
| 3    |    |   | Heneicosane \$\$ n-Heneicosane          | 296 | C21H44  | 000629-94-7 | 90   |
| 4    |    |   | Heptadecane                             | 240 | C17H36  | 000629-78-7 | 90   |



## Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
Acq On : 21 Feb 2002 12:31 pm  
Sample : 508 scan  
Misc : February 21, 2002  
MS Integration Params: LSCINT.P

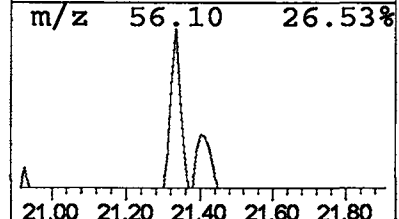
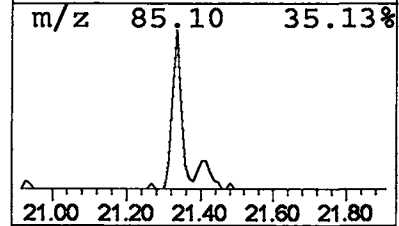
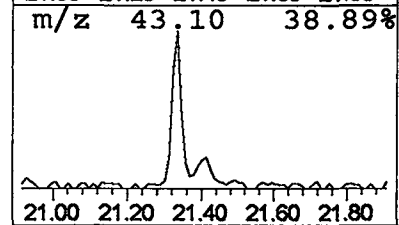
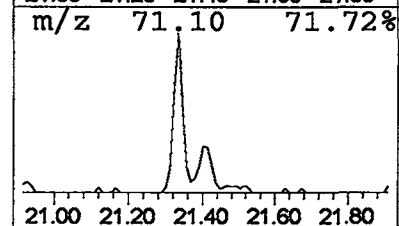
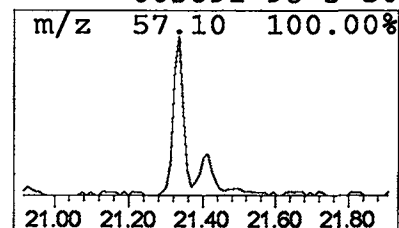
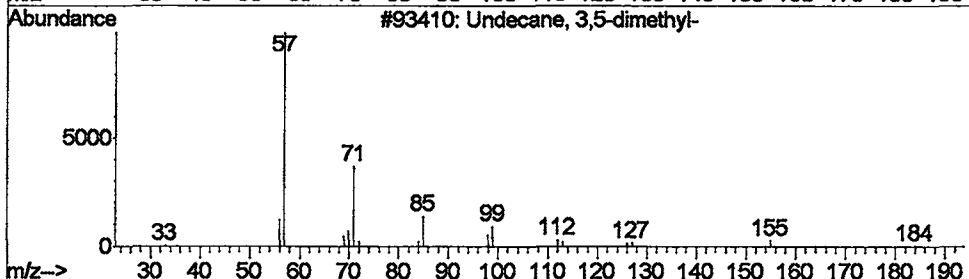
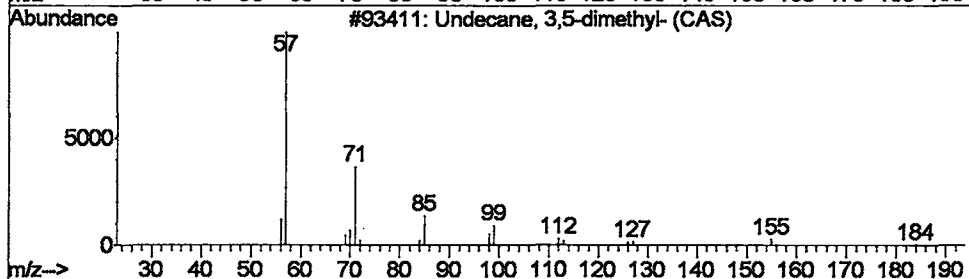
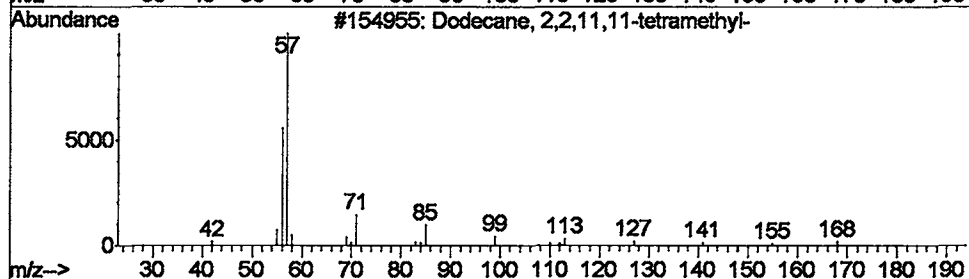
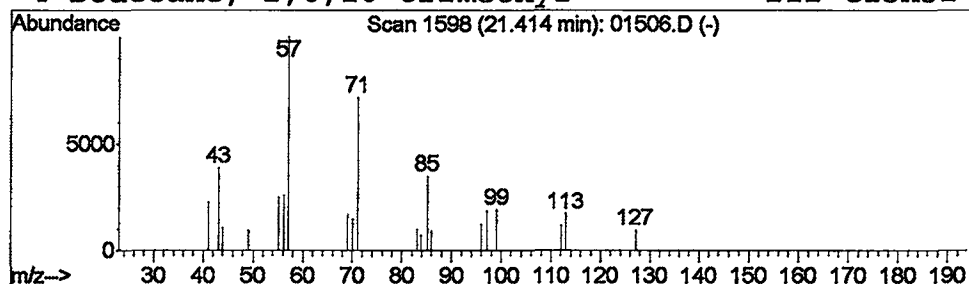
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Operator:  
Inst : Instrumen  
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
Title : 508 scan method  
Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
Peak Number 10 Dodecane, 2,2,11,11-tetrame... Concentration Rank 10

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 21.41 | 0.09 ug/L | 66770 | Phenanthrene-d10 | 22.64 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | Dodecane, 2,2,11,11-tetramethyl- | 226 | C16H34  | 127204-12-0 | 53   |
| 2    |    |   | Undecane, 3,5-dimethyl- (CAS)    | 184 | C13H28  | 017312-81-1 | 50   |
| 3    |    |   | Undecane, 3,5-dimethyl-          | 184 | C13H28  | 017312-81-1 | 50   |
| 4    |    |   | Dodecane, 2,6,10-trimethyl-      | 212 | C15H32  | 003891-98-3 | 50   |



## Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
Acq On : 21 Feb 2002 12:31 pm  
Sample : 508 scan  
Misc : February 21, 2002  
MS Integration Params: LSCINT.P

Vial: 3  
Operator:  
Inst : Instrumen  
Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)

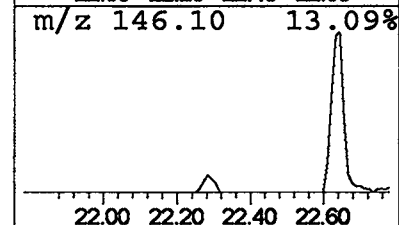
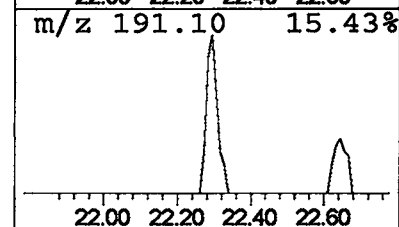
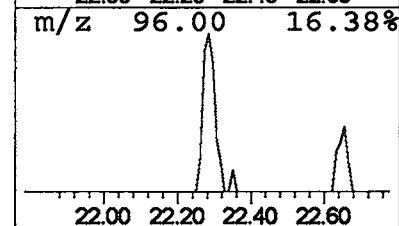
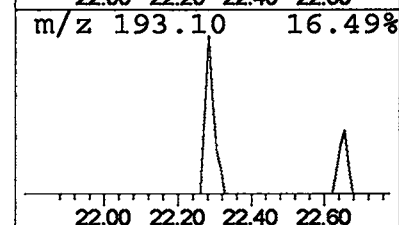
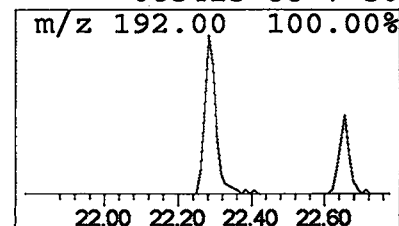
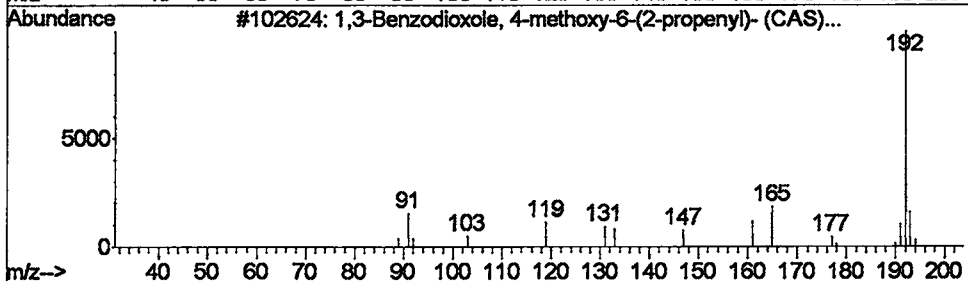
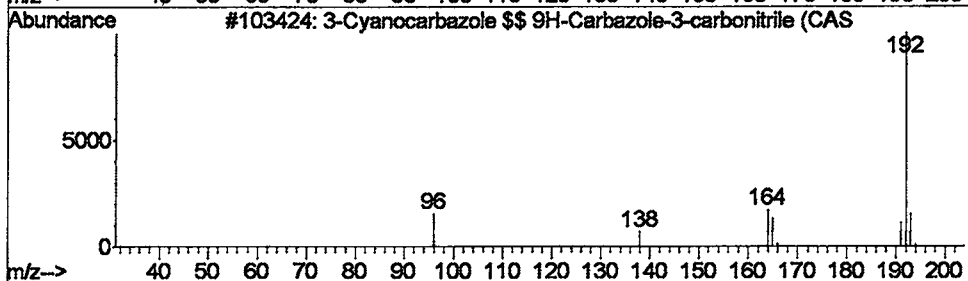
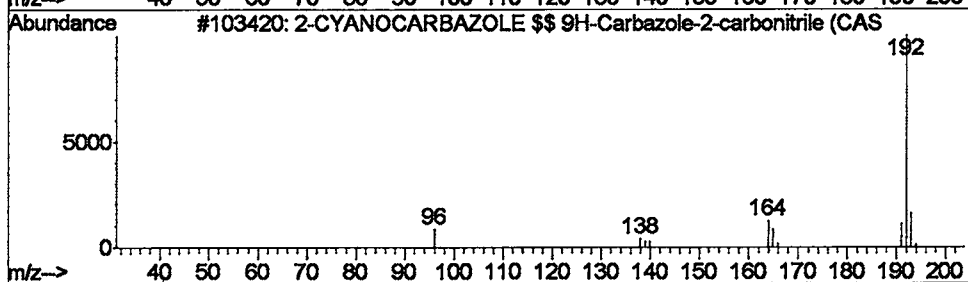
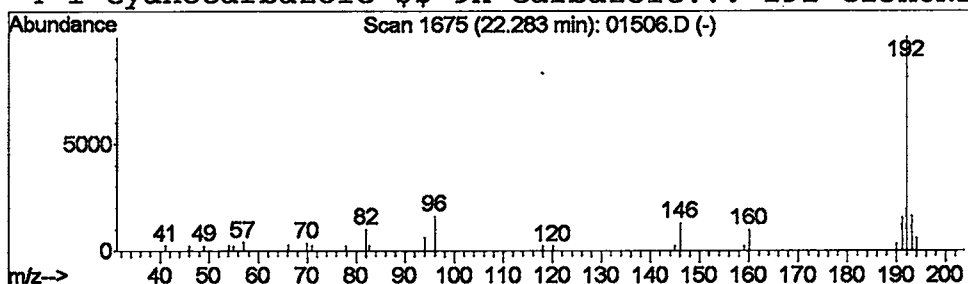
Title : 508 scan method

Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
Peak Number 11 2-CYANOCARBAZOLE \$\$ 9H-Carb... Concentration Rank 7

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 22.28 | 0.15 ug/L | 108829 | Phenanthrene-d10 | 22.64 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-CYANOCARBAZOLE \$\$ 9H-Carbazole... | 192 | C13H8N2  | 057955-18-7 | 72   |
| 2    |    |   | 3-Cyanocarbazole \$\$ 9H-Carbazole... | 192 | C13H8N2  | 057102-93-9 | 72   |
| 3    |    |   | 1,3-Benzodioxole, 4-methoxy-6-(2...   | 192 | C11H12O3 | 000607-91-0 | 53   |
| 4    |    |   | 1-Cyanocarbazole \$\$ 9H-Carbazole... | 192 | C13H8N2  | 083415-88-7 | 50   |



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

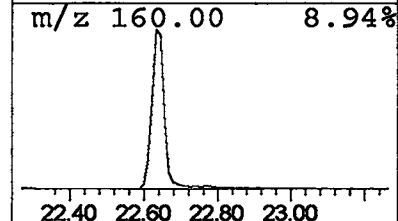
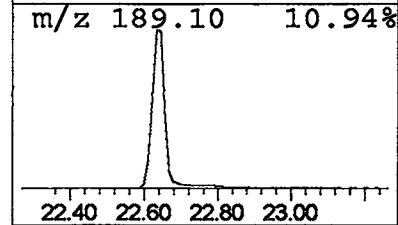
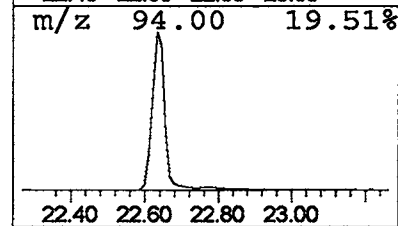
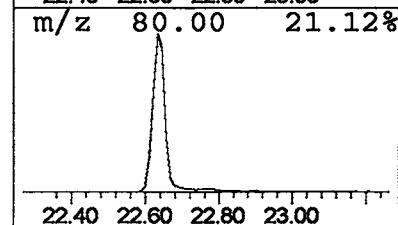
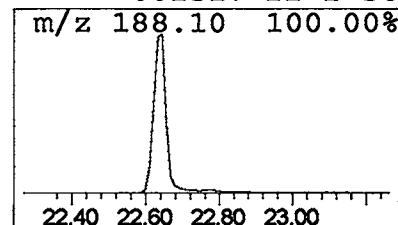
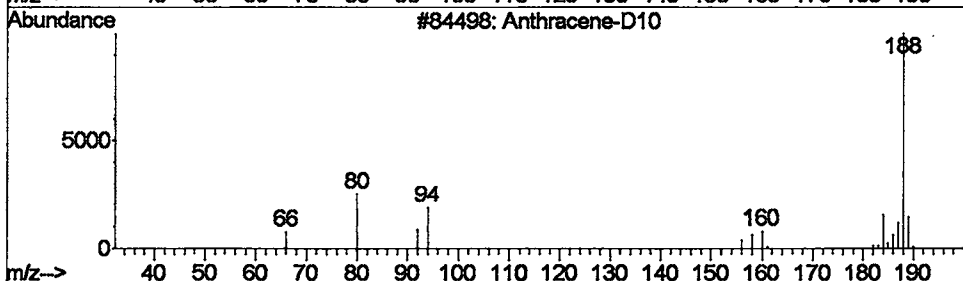
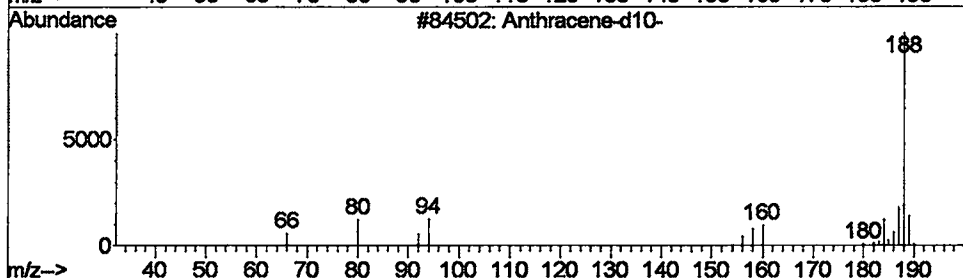
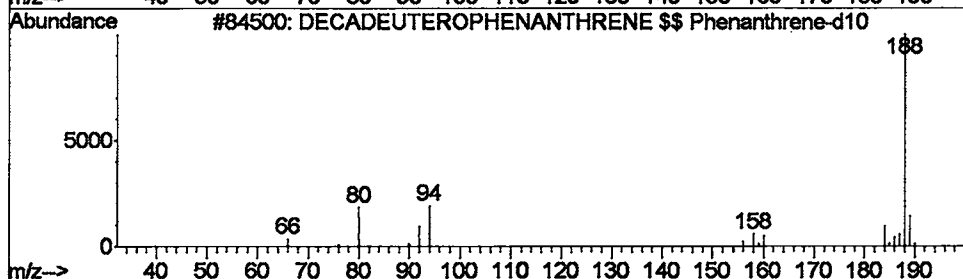
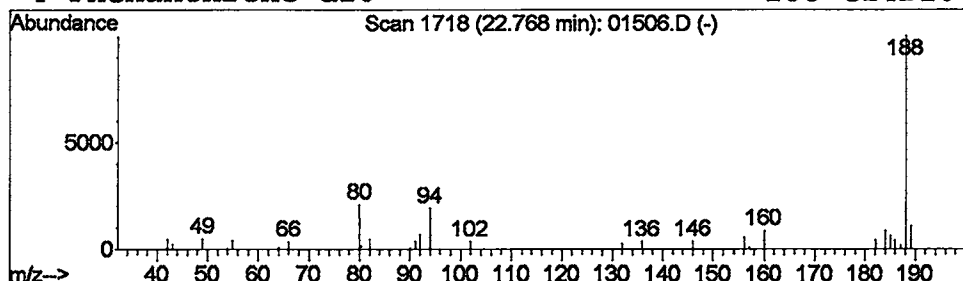
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

\*\*\*\*\*  
 Peak Number 12 DECADEUTEROPHENANTHRENE \$\$ ... Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 22.77 | 0.94 ug/L | 689309 | Phenanthrene-d10 | 22.64 |

| Hit# | of | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------------------------|-----|---------|-------------|------|
| 1    | 5  | DECADEUTEROPHENANTHRENE \$\$ Phena... | 188 | C14D10  | 001517-22-2 | 80   |
| 2    |    | Anthracene-d10-                       | 188 | C14D10  | 001719-06-8 | 64   |
| 3    |    | Anthracene-D10                        | 188 | C14D10  | 000000-00-0 | 56   |
| 4    |    | Phenanthrene-d10                      | 188 | C14D10  | 001517-22-2 | 56   |



# Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Acq On : 21 Feb 2002 12:31 pm  
 Sample : 508 scan  
 Misc : February 21, 2002  
 MS Integration Params: LSCINT.P

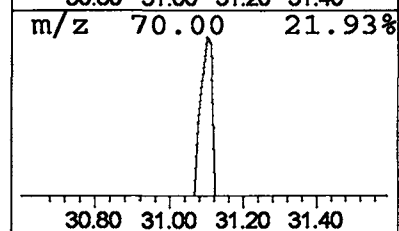
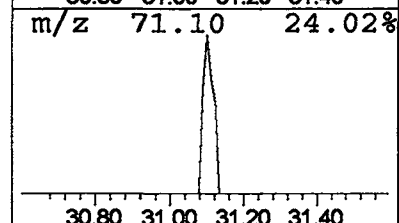
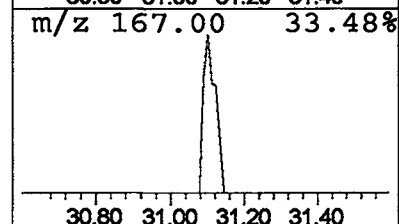
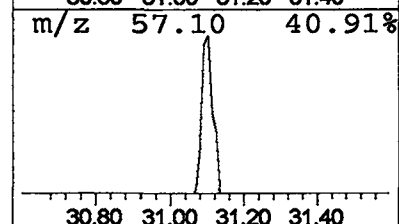
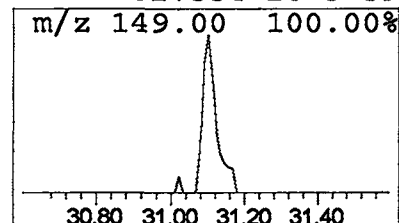
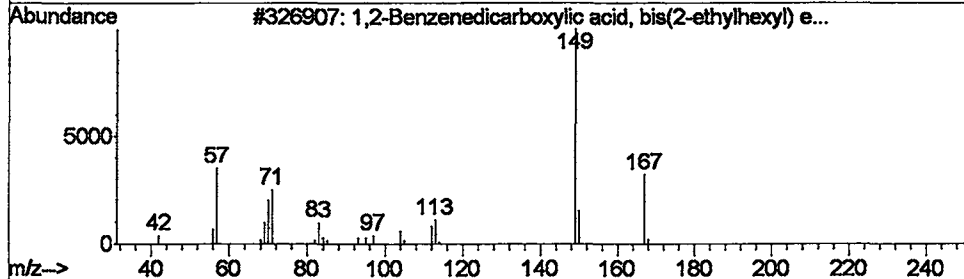
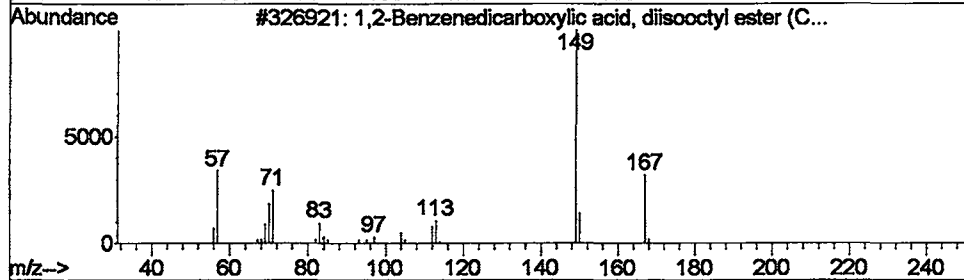
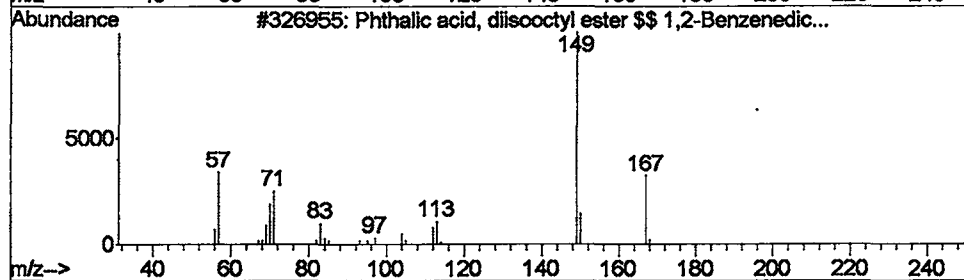
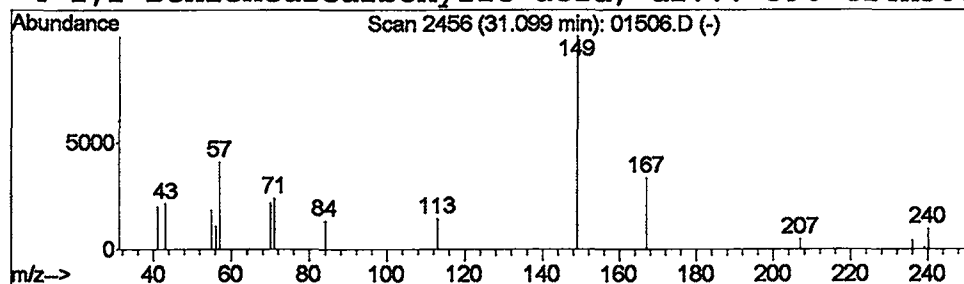
Vial: 3  
 Operator:  
 Inst : Instrumen  
 Multiplr: 1.00

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)  
 Title : 508 scan method  
 Library : C:\DATABASE\WILEY7N.L

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 Peak Number 13 Phthalic acid, diisooctyl e... Concentration Rank 12

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 31.10 | 0.07 ug/L | 45806 | Chrysene-d12     | 30.49 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|---------|---|-------------------------------------|-----|----------|-------------|------|
| 1       |   | Phthalic acid, diisooctyl ester ... | 390 | C24H38O4 | 001330-91-2 | 72   |
| 2       |   | 1,2-Benzenedicarboxylic acid, di... | 390 | C24H38O4 | 027554-26-3 | 72   |
| 3       |   | 1,2-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 000117-81-7 | 72   |
| 4       |   | 1,2-Benzenedicarboxylic acid, di... | 390 | C24H38O4 | 027554-26-3 | 59   |



## .. Tentatively Identified Compound (LSC) summary

Operator ID:                      Date Acquired: 21 Feb 2002 12:31 pm  
 Data File: C:\MSDCHEM\1\5973N\02FEB21\01506.D  
 Name: 508 scan  
 Misc: February 21, 2002  
 Method: C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)  
 Title: 508 scan method  
 Library Searched: C:\DATABASE\WILEY7N.L

| TIC Top Hit name       | RT    | EstConc | Units | Response | --Internal Standard--- |       |          |      |
|------------------------|-------|---------|-------|----------|------------------------|-------|----------|------|
|                        |       |         |       |          | #                      | RT    | Resp     | Conc |
| Acetonitrile, dic...   | 3.50  | 0.1     | ug/L  | 49292    | 1                      | 9.72  | 8497000  | 20.0 |
| Butanoic acid, me...   | 3.63  | 0.2     | ug/L  | 75106    | 1                      | 9.72  | 8497000  | 20.0 |
| Acetic acid, 3-[1...   | 5.95  | 0.4     | ug/L  | 185010   | 1                      | 9.72  | 8497000  | 20.0 |
| 2-Pentanone, 4-hy...   | 6.13  | 0.2     | ug/L  | 66692    | 1                      | 9.72  | 8497000  | 20.0 |
| 2-Propanol, 1-(2-...   | 9.90  | 0.1     | ug/L  | 61543    | 1                      | 9.72  | 8497000  | 20.0 |
| 1-Oxetan-2-one, 4...   | 13.39 | 0.1     | ug/L  | 48900    | 2                      | 13.20 | 12615200 | 20.0 |
| Hexadecane (CAS) ...   | 19.92 | 0.2     | ug/L  | 134936   | 3                      | 18.34 | 13683600 | 20.0 |
| Decane, 5-methyl-      | 20.61 | 0.1     | ug/L  | 47922    | 4                      | 22.64 | 14711700 | 20.0 |
| Heptadecane \$\$ n-... | 21.33 | 0.4     | ug/L  | 265894   | 4                      | 22.64 | 14711700 | 20.0 |
| Dodecane, 2,2,11,...   | 21.41 | 0.1     | ug/L  | 66770    | 4                      | 22.64 | 14711700 | 20.0 |
| 2-CYANOCARBAZOLE ...   | 22.28 | 0.1     | ug/L  | 108829   | 4                      | 22.64 | 14711700 | 20.0 |
| DECADEUTEROPHENAN...   | 22.77 | 0.9     | ug/L  | 689309   | 4                      | 22.64 | 14711700 | 20.0 |
| Phthalic acid, di...   | 31.10 | 0.1     | ug/L  | 45806    | 5                      | 30.49 | 12877200 | 20.0 |