

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121118\  
 Data File : VX006433.D  
 Acq On : 11 Dec 2018 20:51  
 Operator : JC/MD  
 Sample : J6331-36  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 TP-6

## Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
 Title : SW846 8260

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         | 1.611       | 65            | 75          | 79           | rBV2     | 39003          | 84189         | 1.86%           | 0.265%        |
| 2         | 2.782       | 261           | 267         | 273          | rBV      | 24458          | 45882         | 1.02%           | 0.144%        |
| 3         | 2.861       | 273           | 280         | 287          | rBV      | 107890         | 204587        | 4.53%           | 0.644%        |
| 4         | 5.507       | 702           | 714         | 729          | rBV      | 418723         | 1214691       | 26.91%          | 3.825%        |
| 5         | 5.665       | 729           | 740         | 756          | rVB2     | 733623         | 2070290       | 45.86%          | 6.520%        |
| 6         | 6.068       | 795           | 806         | 823          | rVB      | 426339         | 1088155       | 24.10%          | 3.427%        |
| 7         | 6.464       | 861           | 871         | 883          | rBV      | 35563          | 93445         | 2.07%           | 0.294%        |
| 8         | 6.860       | 925           | 936         | 951          | rBV      | 1073122        | 2576071       | 57.06%          | 8.113%        |
| 9         | 7.634       | 1057          | 1063        | 1069         | rBV2     | 43426          | 105210        | 2.33%           | 0.331%        |
| 10        | 7.884       | 1095          | 1104        | 1124         | rBV      | 2573945        | 4514500       | 100.00%         | 14.217%       |
| 11        | 8.616       | 1218          | 1224        | 1233         | rBV      | 529324         | 794809        | 17.61%          | 2.503%        |
| 12        | 8.713       | 1233          | 1240        | 1249         | rVV      | 2216366        | 3495005       | 77.42%          | 11.007%       |
| 13        | 9.018       | 1286          | 1290        | 1298         | rVB      | 60867          | 95421         | 2.11%           | 0.301%        |
| 14        | 9.305       | 1332          | 1337        | 1344         | rBV      | 305331         | 449714        | 9.96%           | 1.416%        |
| 15        | 9.372       | 1344          | 1348        | 1350         | rVV2     | 46379          | 62770         | 1.39%           | 0.198%        |
| 16        | 9.402       | 1350          | 1353        | 1357         | rVV      | 137027         | 195916        | 4.34%           | 0.617%        |
| 17        | 9.439       | 1357          | 1359        | 1365         | rVB      | 38632          | 48873         | 1.08%           | 0.154%        |
| 18        | 9.543       | 1371          | 1376        | 1388         | rVV      | 2309635        | 2959348       | 65.55%          | 9.320%        |
| 19        | 9.640       | 1388          | 1392        | 1399         | rVB      | 178178         | 225855        | 5.00%           | 0.711%        |
| 20        | 9.969       | 1441          | 1446        | 1460         | rVB      | 1720525        | 2192746       | 48.57%          | 6.906%        |
| 21        | 10.110      | 1463          | 1469        | 1477         | rBV      | 2174519        | 3009311       | 66.66%          | 9.477%        |
| 22        | 10.360      | 1505          | 1510        | 1518         | rVB      | 32764          | 49663         | 1.10%           | 0.156%        |
| 23        | 10.695      | 1561          | 1565        | 1569         | rBV2     | 119134         | 142791        | 3.16%           | 0.450%        |
| 24        | 10.738      | 1569          | 1572        | 1580         | rVB      | 37266          | 48821         | 1.08%           | 0.154%        |
| 25        | 11.140      | 1632          | 1638        | 1645         | rBV      | 1819669        | 2397868       | 53.11%          | 7.552%        |
| 26        | 11.804      | 1742          | 1747        | 1753         | rBV      | 72177          | 99249         | 2.20%           | 0.313%        |
| 27        | 12.079      | 1786          | 1792        | 1799         | rBV      | 2346822        | 2937944       | 65.08%          | 9.252%        |
| 28        | 12.298      | 1824          | 1828        | 1835         | rVB3     | 27174          | 47472         | 1.05%           | 0.150%        |
| 29        | 13.347      | 1996          | 2000        | 2006         | rVB2     | 54383          | 77274         | 1.71%           | 0.243%        |
| 30        | 13.719      | 2054          | 2061        | 2069         | rVB2     | 27418          | 57956         | 1.28%           | 0.183%        |
| 31        | 13.835      | 2073          | 2080        | 2088         | rBV      | 114343         | 152715        | 3.38%           | 0.481%        |
| 32        | 14.280      | 2146          | 2153        | 2162         | rBV3     | 26340          | 59480         | 1.32%           | 0.187%        |
| 33        | 14.694      | 2213          | 2221        | 2225         | rBV      | 61386          | 96890         | 2.15%           | 0.305%        |
| 34        | 14.840      | 2241          | 2245        | 2249         | rBV      | 45985          | 58613         | 1.30%           | 0.185%        |

## LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121118\  
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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
TP-6

Integration Parameters: RTEINT.P  
Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 Max Peaks: 100  
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Title : SW846 8260

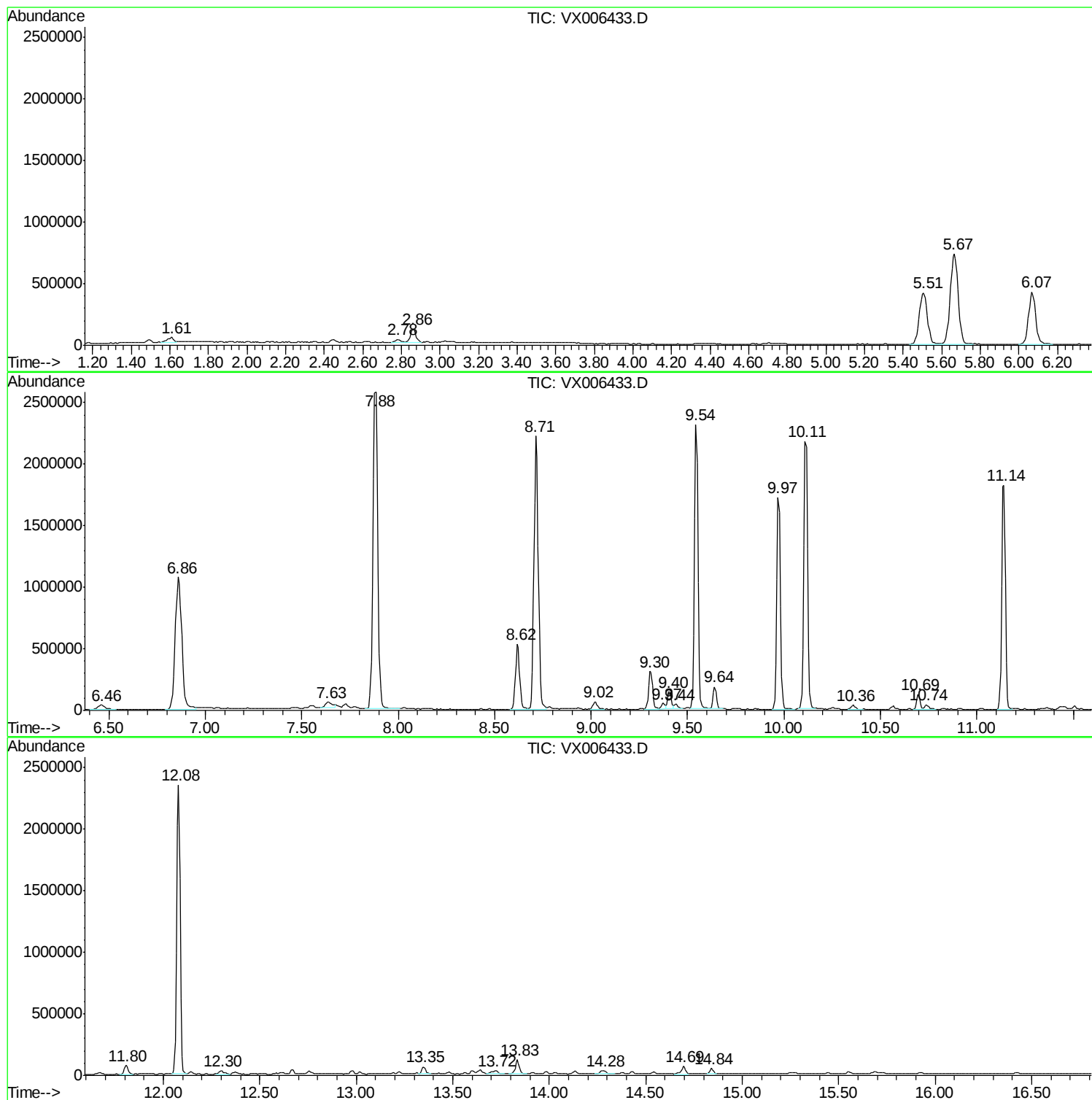
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Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\  
Data File : VX006433.D  
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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampled :  
TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Sample : J6331-36  
Misc : 5.0mL/MSVOA X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

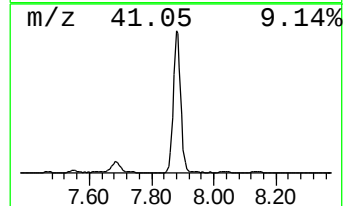
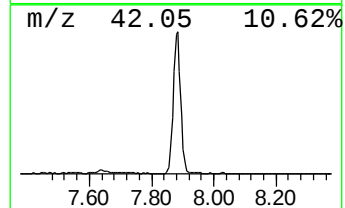
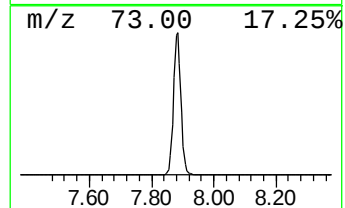
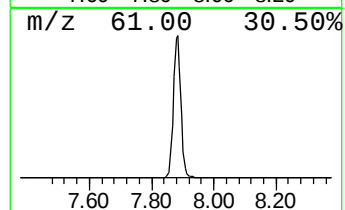
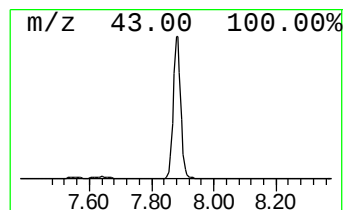
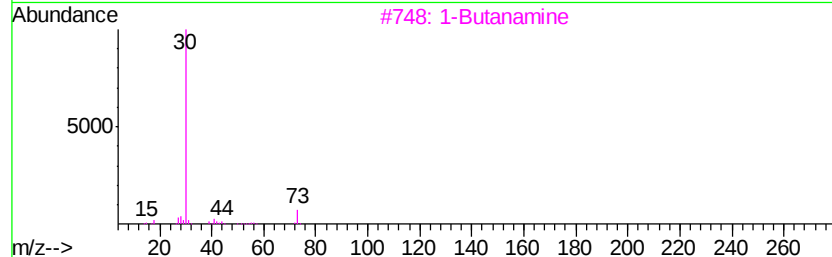
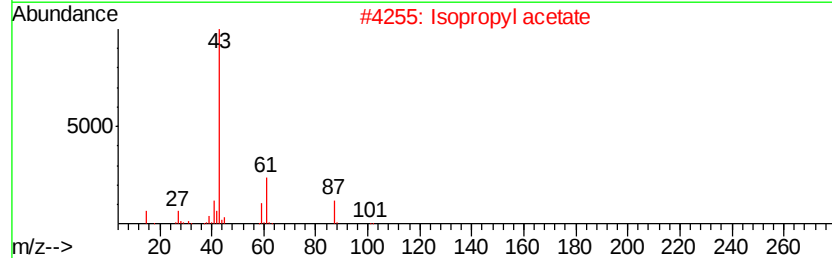
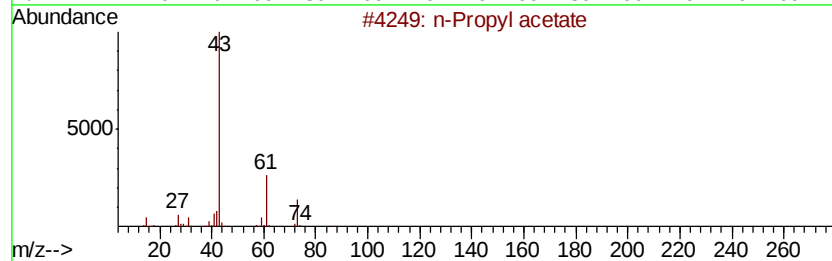
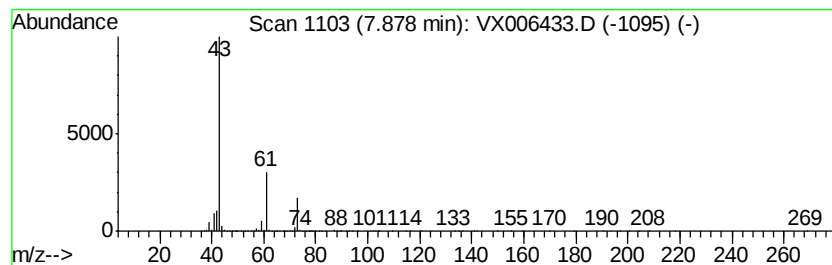
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Propyl acetate Concentration Rank 1

| R.T. | EstConc    | Area    | Relative to ISTD    | R.T. |
|------|------------|---------|---------------------|------|
| 7.88 | 87.62 ug/l | 4514500 | 1,4-Difluorobenzene | 6.86 |

| Hit# | of | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------|-----|---------|-------------|------|
| 1    | 5  | n-Propyl acetate  | 102 | C5H10O2 | 000109-60-4 | 83   |
| 2    |    | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 36   |
| 3    |    | 1-Butanamine      | 73  | C4H11N  | 000109-73-9 | 7    |
| 4    |    | Butane, 2-methyl- | 72  | C5H12   | 000078-78-4 | 4    |
| 5    |    | Isobutylamine     | 73  | C4H11N  | 000078-81-9 | 4    |



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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

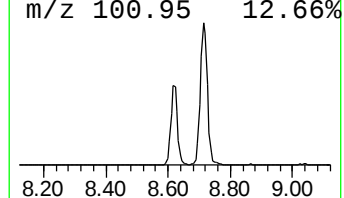
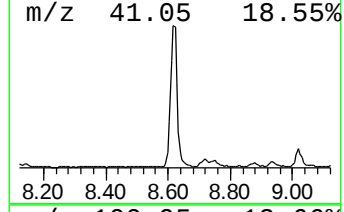
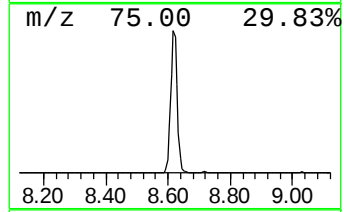
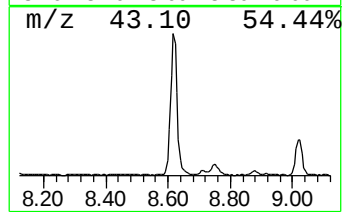
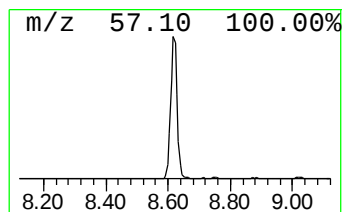
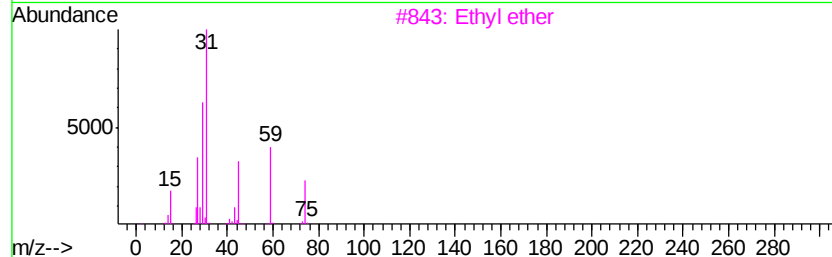
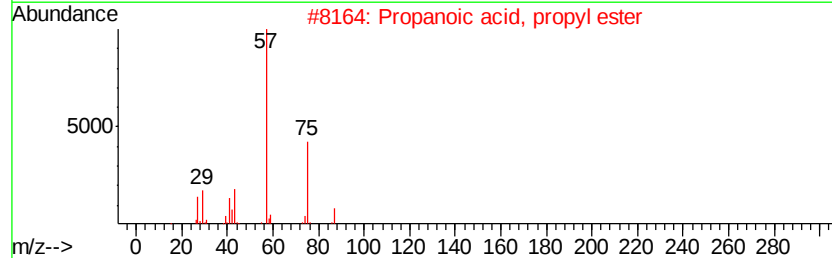
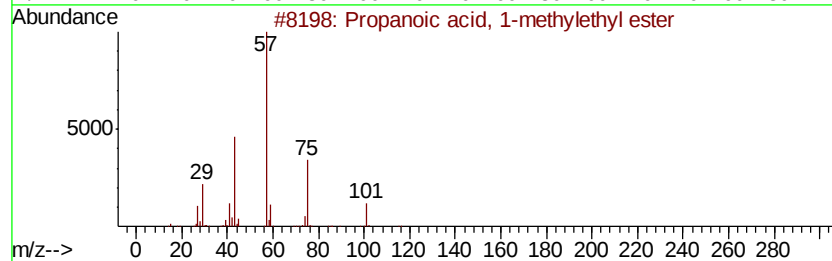
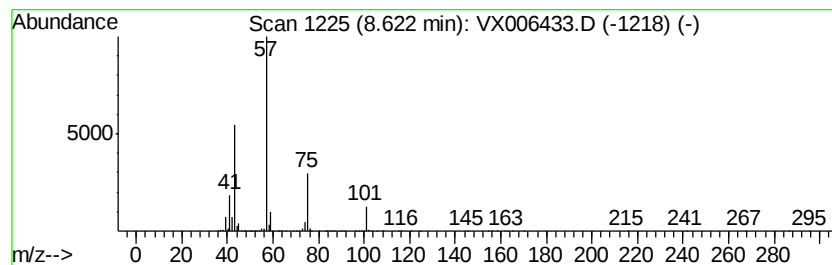
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

| R.T. | EstConc    | Area   | Relative to ISTD | R.T.  |
|------|------------|--------|------------------|-------|
| 8.62 | 13.21 ug/l | 794809 | Chlorobenzene-d5 | 10.12 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2 | 000637-78-5  | 78   |
| 2    |    | Propanoic acid, propyl ester        | 116 | C6H12O2 | 000106-36-5  | 53   |
| 3    |    | Ethyl ether                         | 74  | C4H10O  | 000060-29-7  | 9    |
| 4    |    | o-Isopropylhydroxylamine            | 75  | C3H9NO  | 1000322-42-6 | 9    |
| 5    |    | Propanoic acid, butyl ester         | 130 | C7H14O2 | 000590-01-2  | 9    |



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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

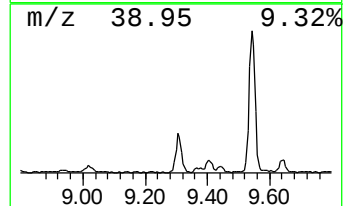
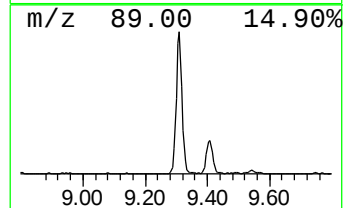
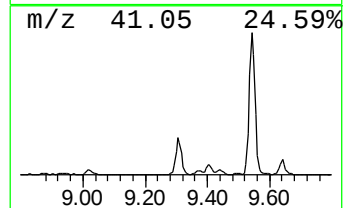
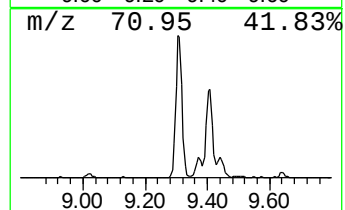
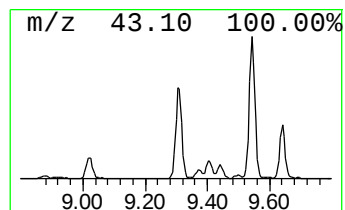
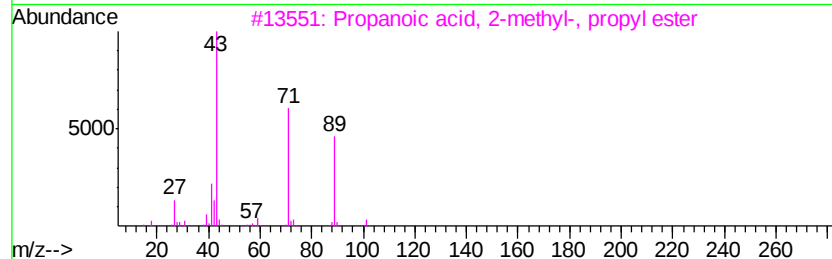
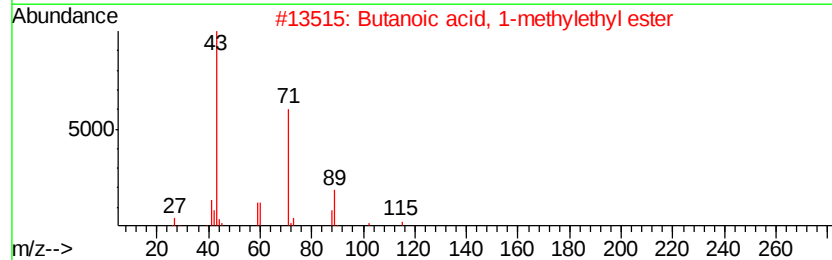
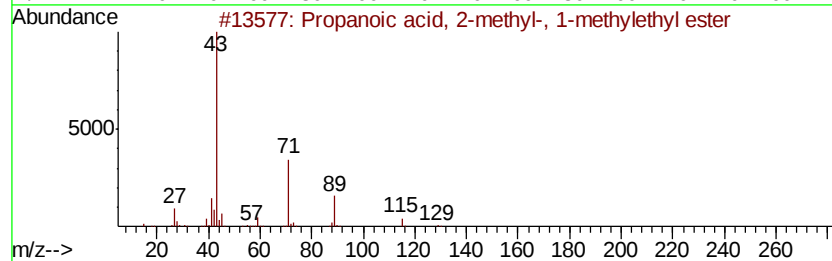
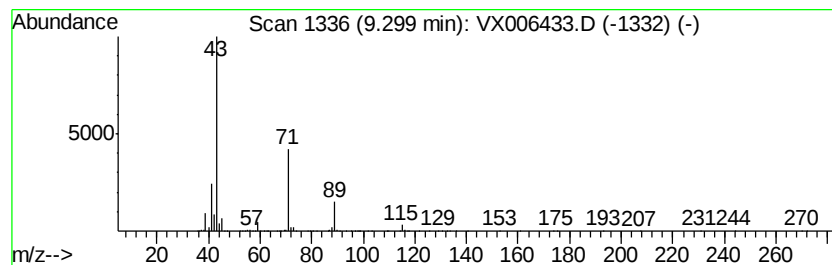
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

| R.T. | EstConc   | Area   | Relative to ISTD | R.T.  |
|------|-----------|--------|------------------|-------|
| 9.30 | 7.47 ug/l | 449714 | Chlorobenzene-d5 | 10.12 |

| Hit# | of | Tentative ID                         | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propanoic acid, 2-methyl-, 1-met...  | 130 | C7H14O2 | 000617-50-5 | 83   |
| 2    |    | Butanoic acid, 1-methylethyl ester   | 130 | C7H14O2 | 000638-11-9 | 56   |
| 3    |    | Propanoic acid, 2-methyl-, propyl... | 130 | C7H14O2 | 000644-49-5 | 53   |
| 4    |    | Butanoic acid, propyl ester          | 130 | C7H14O2 | 000105-66-8 | 40   |
| 5    |    | 2-Oxo-n-valeric acid                 | 116 | C5H8O3  | 001821-02-9 | 38   |



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TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

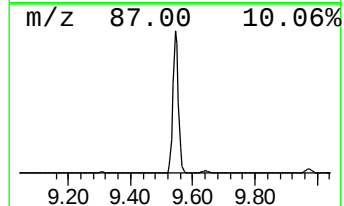
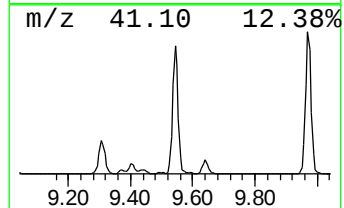
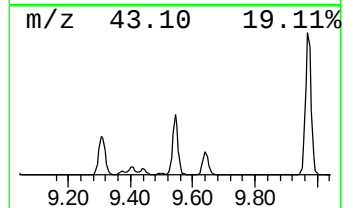
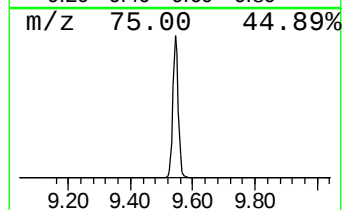
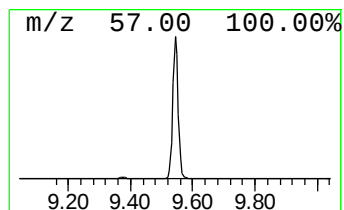
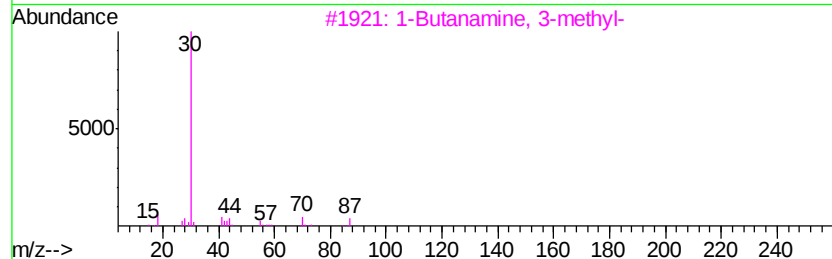
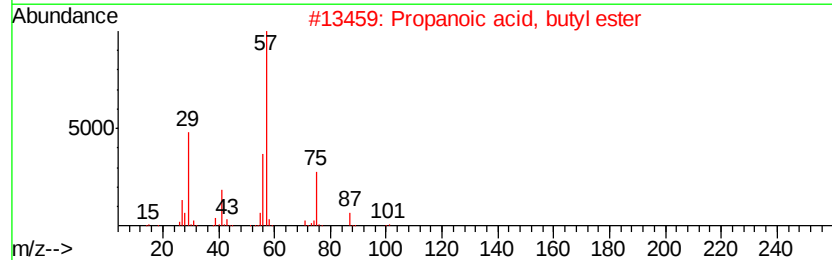
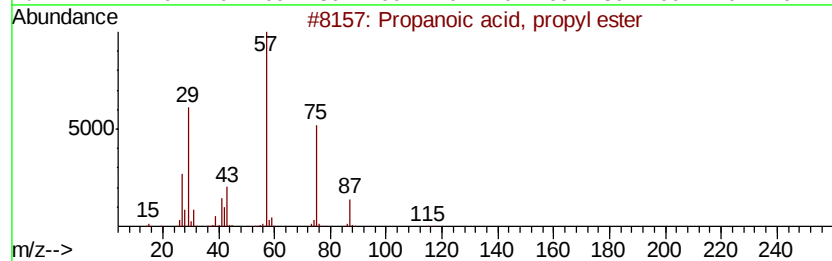
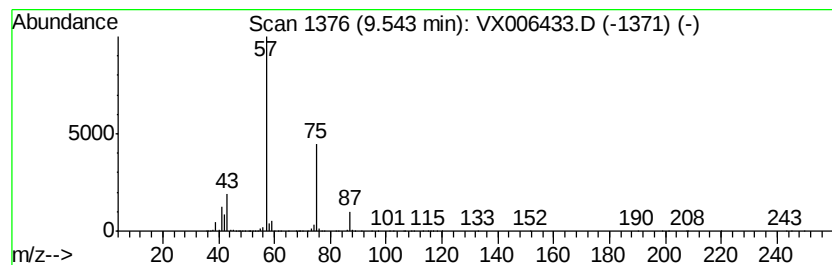
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

| R.T. | EstConc    | Area    | Relative to ISTD | R.T.  |
|------|------------|---------|------------------|-------|
| 9.54 | 49.17 ug/l | 2959350 | Chlorobenzene-d5 | 10.12 |

| Hit# | of | Tentative ID                 | MW  | MolForm  | CAS#         | Qual |
|------|----|------------------------------|-----|----------|--------------|------|
| 1    | 5  | Propanoic acid, propyl ester | 116 | C6H12O2  | 000106-36-5  | 83   |
| 2    |    | Propanoic acid, butyl ester  | 130 | C7H14O2  | 000590-01-2  | 28   |
| 3    |    | 1-Butanamine, 3-methyl-      | 87  | C5H13N   | 000107-85-7  | 9    |
| 4    |    | di-tert-Butyl dicarbonate    | 218 | C10H18O5 | 024424-99-5  | 9    |
| 5    |    | Acetaldehyde, O-ethyloxime-  | 87  | C4H9NO   | 1000288-34-6 | 7    |



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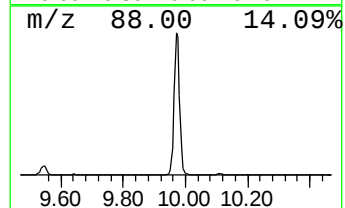
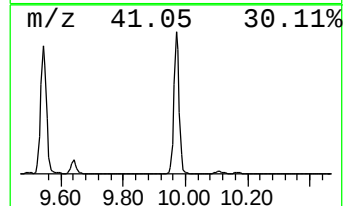
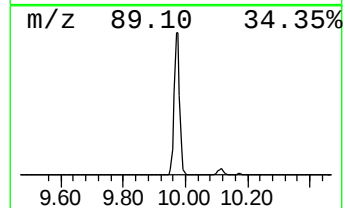
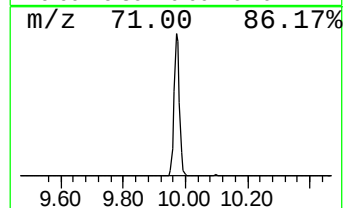
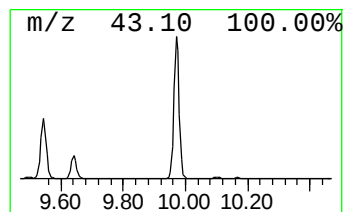
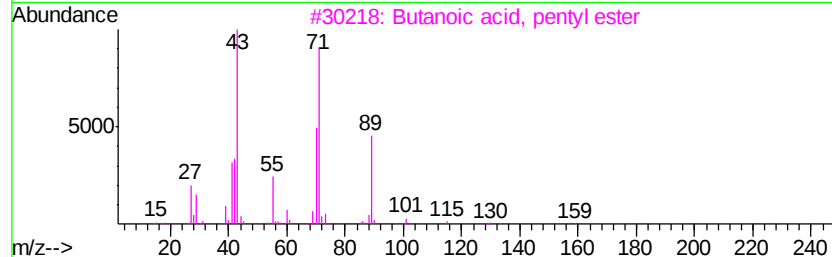
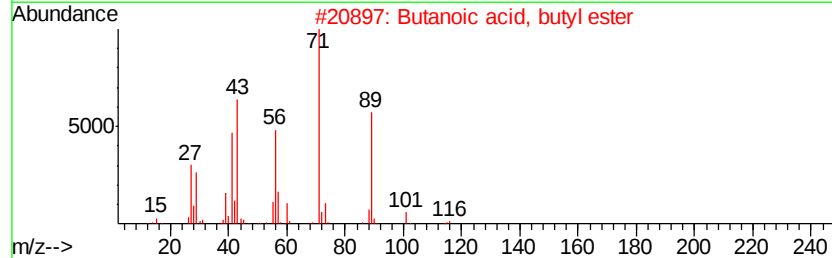
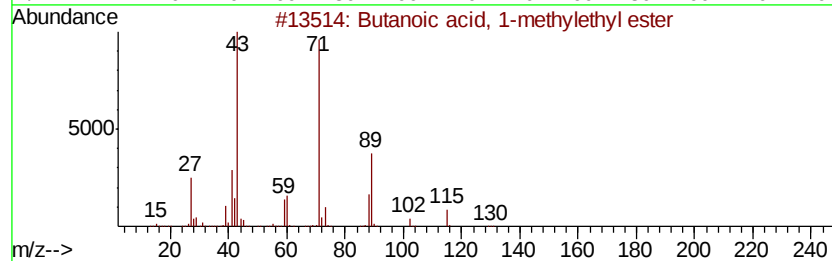
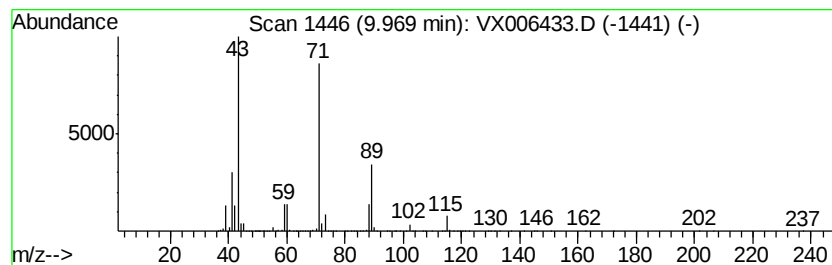
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

| R.T. | EstConc    | Area    | Relative to ISTD | R.T.  |
|------|------------|---------|------------------|-------|
| 9.97 | 36.43 ug/l | 2192750 | Chlorobenzene-d5 | 10.12 |

| Hit# of | 5 | Tentative ID                         | MW  | MolForm | CAS#        | Qual |
|---------|---|--------------------------------------|-----|---------|-------------|------|
| 1       |   | Butanoic acid, 1-methylethyl ester   | 130 | C7H14O2 | 000638-11-9 | 91   |
| 2       |   | Butanoic acid, butyl ester           | 144 | C8H16O2 | 000109-21-7 | 64   |
| 3       |   | Butanoic acid, pentyl ester          | 158 | C9H18O2 | 000540-18-1 | 64   |
| 4       |   | Propanoic acid, 2-methyl-, propyl... | 130 | C7H14O2 | 000644-49-5 | 56   |
| 5       |   | Propanoic acid, 2-methyl-, 1-met...  | 130 | C7H14O2 | 000617-50-5 | 56   |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_X\DATA\VX121118\  
Data File : VX006433.D  
Acq On : 11 Dec 2018 20:51  
Operator : JC/MD  
Sample : J6331-36  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
TP-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X112918W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |      |         |       |          | #                     | RT    | Resp    | Conc |
| n-Propyl acetate     | 7.88 | 87.6    | ug/l  | 4514500  | 2                     | 6.86  | 2576070 | 50.0 |
| Propanoic acid, 1... | 8.62 | 13.2    | ug/l  | 794809   | 3                     | 10.12 | 3009310 | 50.0 |
| Propanoic acid, 2... | 9.30 | 7.5     | ug/l  | 449714   | 3                     | 10.12 | 3009310 | 50.0 |
| Propanoic acid, p... | 9.54 | 49.2    | ug/l  | 2959350  | 3                     | 10.12 | 3009310 | 50.0 |
| Butanoic acid, 1-... | 9.97 | 36.4    | ug/l  | 2192750  | 3                     | 10.12 | 3009310 | 50.0 |