

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU110521\  
 Data File : VU045595.D  
 Acq On : 06 Nov 2021 05:57  
 Operator : SY/MD  
 Sample : M4470-02  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 50 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 SP-3

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\_U\Method\82U110521W.M  
 Title : SW846 8260

Signal : TIC: VU045595.D\data.ms

| 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         | 5.292       | 1214          | 1229        | 1243         | rBV      | 119673         | 257354        | 9.31%           | 2.196%        |
| 2         | 5.378       | 1243          | 1256        | 1273         | rVB      | 182489         | 370080        | 13.39%          | 3.157%        |
| 3         | 5.706       | 1343          | 1358        | 1374         | rBV      | 139188         | 278517        | 10.08%          | 2.376%        |
| 4         | 5.912       | 1411          | 1422        | 1435         | rBV      | 15075          | 29284         | 1.06%           | 0.250%        |
| 5         | 6.050       | 1449          | 1465        | 1468         | rBV3     | 21131          | 55303         | 2.00%           | 0.472%        |
| 6         | 6.253       | 1515          | 1528        | 1577         | rVB      | 308310         | 649270        | 23.50%          | 5.539%        |
| 7         | 6.928       | 1716          | 1738        | 1757         | rBV3     | 12193          | 38434         | 1.39%           | 0.328%        |
| 8         | 7.037       | 1758          | 1772        | 1808         | rBV      | 1073825        | 1885715       | 68.24%          | 16.088%       |
| 9         | 7.738       | 1977          | 1990        | 2002         | rBV      | 159246         | 264609        | 9.58%           | 2.257%        |
| 10        | 7.899       | 2026          | 2040        | 2062         | rBV      | 475153         | 826603        | 29.91%          | 7.052%        |
| 11        | 8.160       | 2108          | 2121        | 2137         | rBV2     | 16783          | 28283         | 1.02%           | 0.241%        |
| 12        | 8.465       | 2200          | 2216        | 2233         | rBV      | 39915          | 68228         | 2.47%           | 0.582%        |
| 13        | 8.574       | 2233          | 2250        | 2261         | rVV2     | 104883         | 177292        | 6.42%           | 1.513%        |
| 14        | 8.729       | 2284          | 2298        | 2320         | rVV      | 1766899        | 2763221       | 100.00%         | 23.574%       |
| 15        | 8.835       | 2321          | 2331        | 2352         | rVB      | 184199         | 294950        | 10.67%          | 2.516%        |
| 16        | 9.211       | 2435          | 2448        | 2479         | rBV      | 1066595        | 1636539       | 59.23%          | 13.962%       |
| 17        | 9.420       | 2501          | 2513        | 2531         | rVB      | 453378         | 736410        | 26.65%          | 6.283%        |
| 18        | 10.073      | 2706          | 2716        | 2732         | rBV      | 32661          | 49882         | 1.81%           | 0.426%        |
| 19        | 10.635      | 2877          | 2891        | 2914         | rVB      | 351084         | 553737        | 20.04%          | 4.724%        |
| 20        | 11.812      | 3245          | 3257        | 3273         | rBV      | 492216         | 757865        | 27.43%          | 6.466%        |

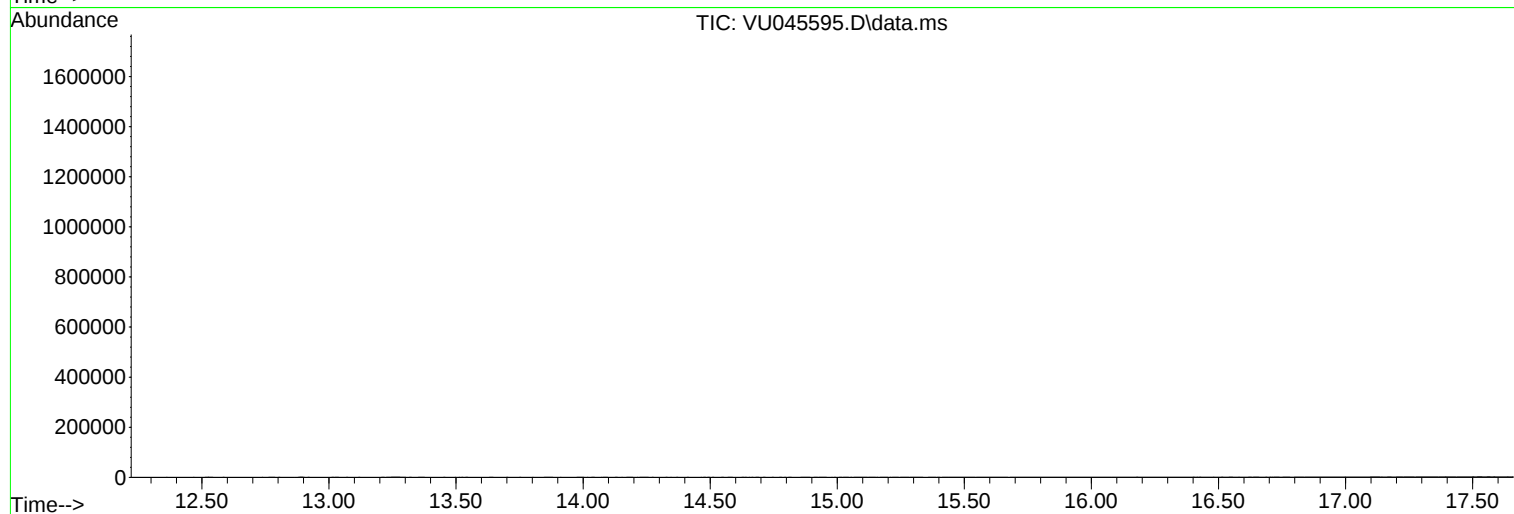
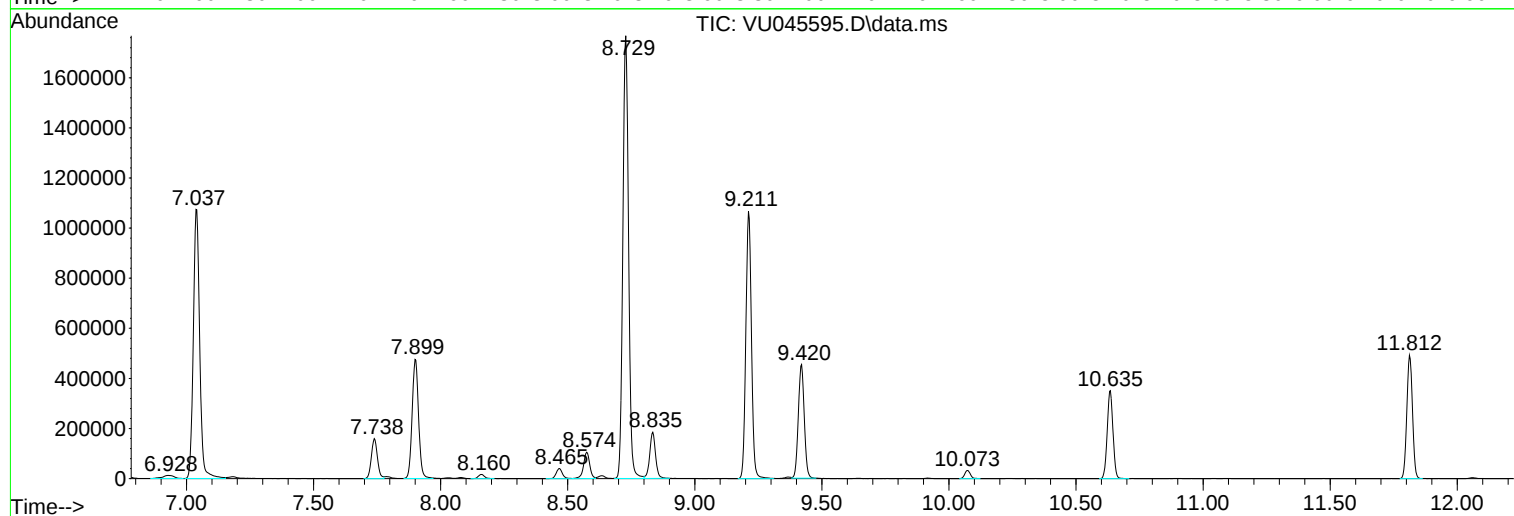
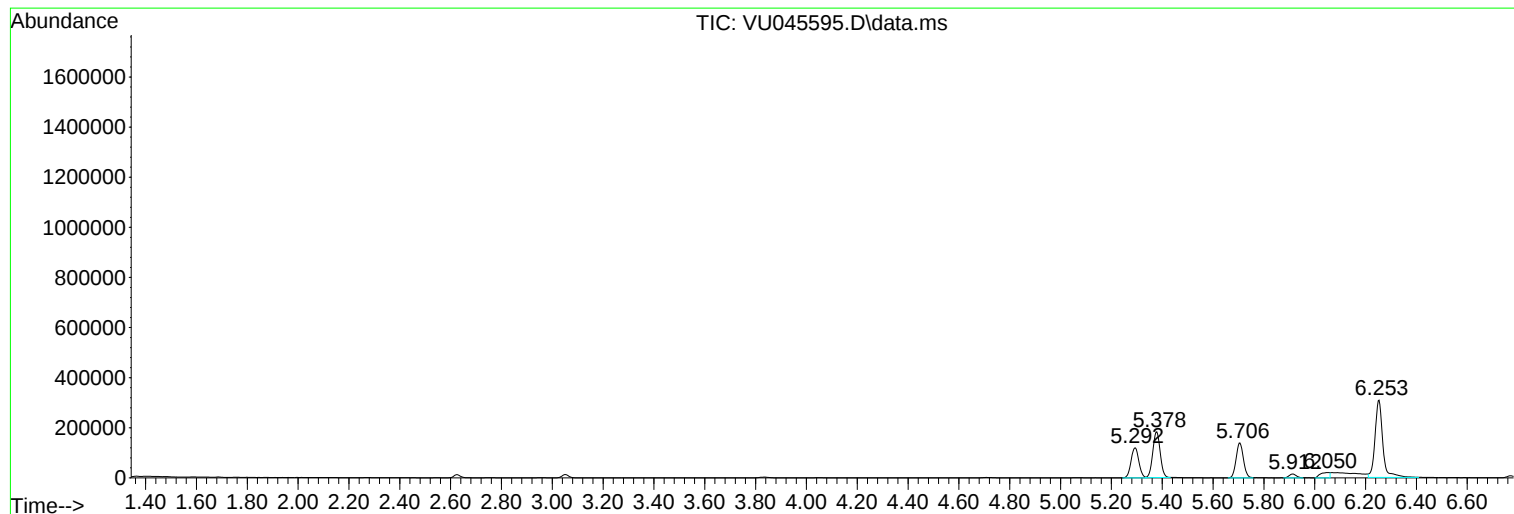
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ALS Vial : 50 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
SP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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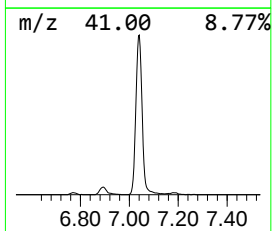
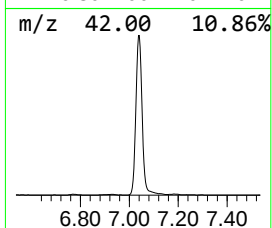
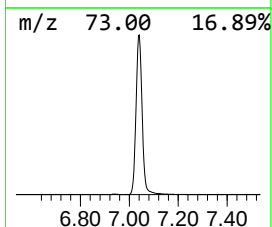
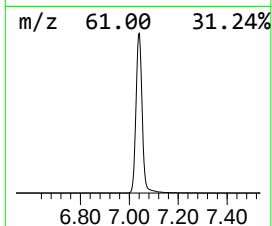
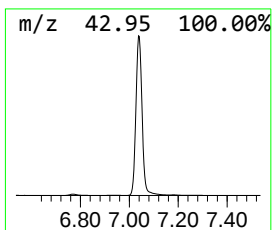
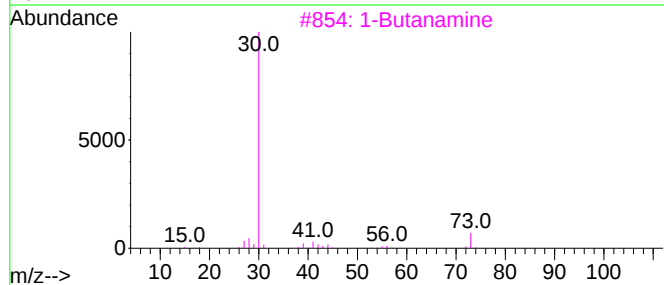
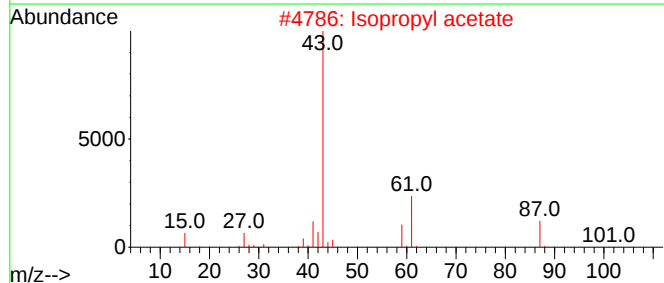
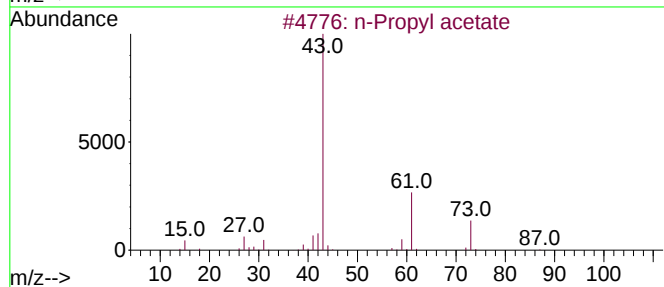
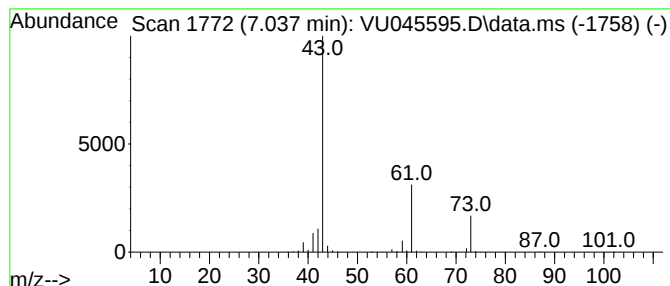
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Propyl acetate Concentration Rank 2

| R.T.  | EstConc     | Area    | Relative to ISTD    | R.T.  |
|-------|-------------|---------|---------------------|-------|
| 7.037 | 145.22 ug/l | 1885720 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | 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    |    |   | Isobutylamine             | 73  | C4H11N  | 000078-81-9 | 4    |
| 5    |    |   | 1,4-Butanediol, diacetate | 174 | C8H14O4 | 000628-67-1 | 4    |



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MSVOA\_U  
ClientSampleId :  
SP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

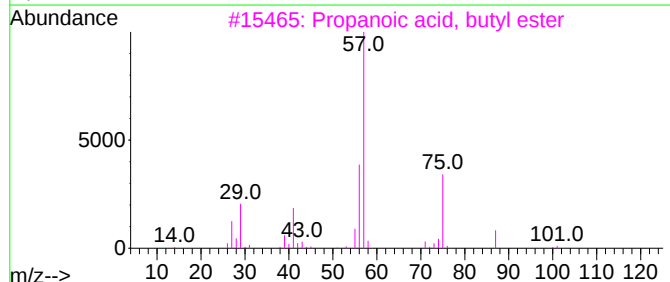
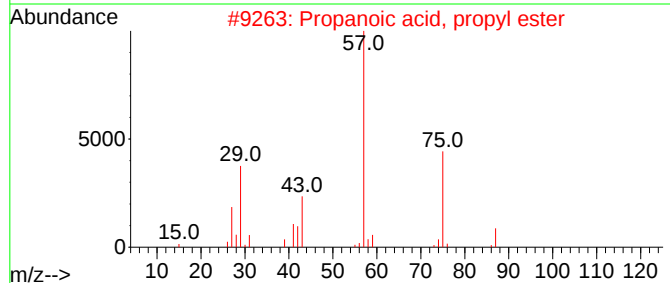
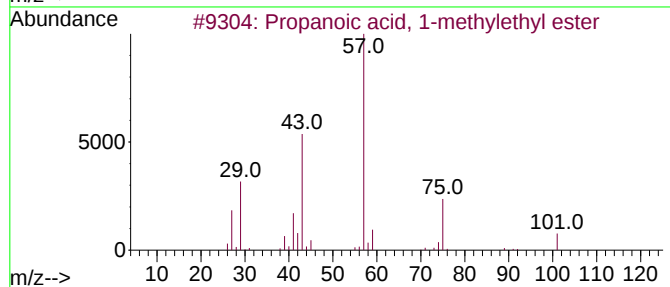
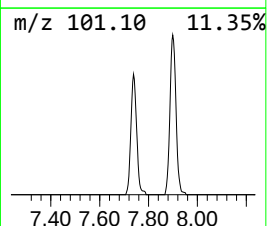
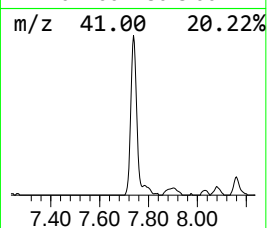
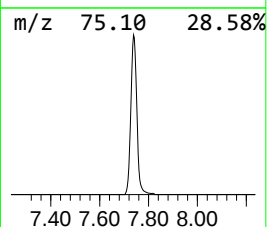
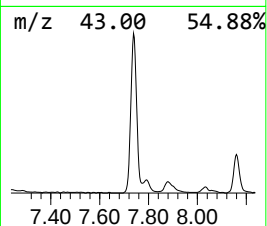
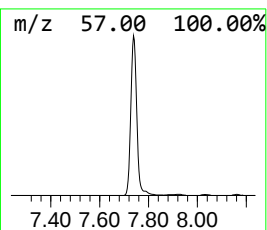
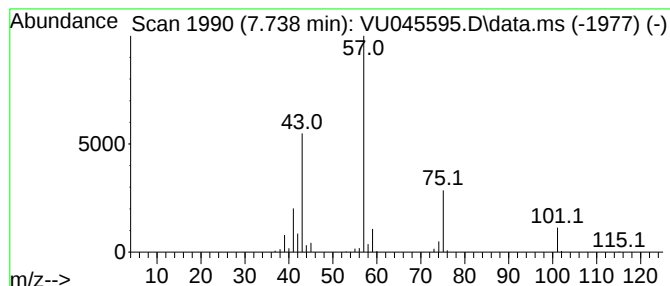
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 7.738 | 20.38 ug/l | 264609 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2 | 000637-78-5 | 90   |
| 2    |    |   | Propanoic acid, propyl ester        | 116 | C6H12O2 | 000106-36-5 | 36   |
| 3    |    |   | Propanoic acid, butyl ester         | 130 | C7H14O2 | 000590-01-2 | 28   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 10   |
| 5    |    |   | N-(n-Propyl)acetamide               | 101 | C5H11NO | 005331-48-6 | 10   |



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MSVOA\_U  
ClientSampleId :  
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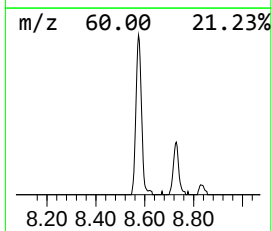
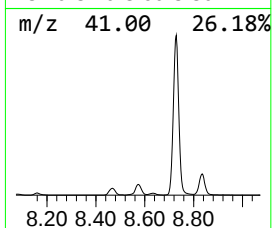
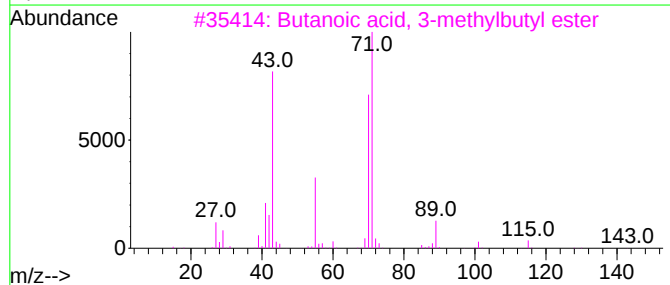
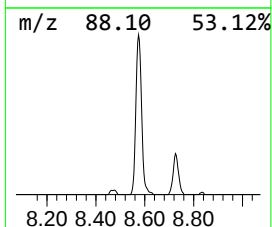
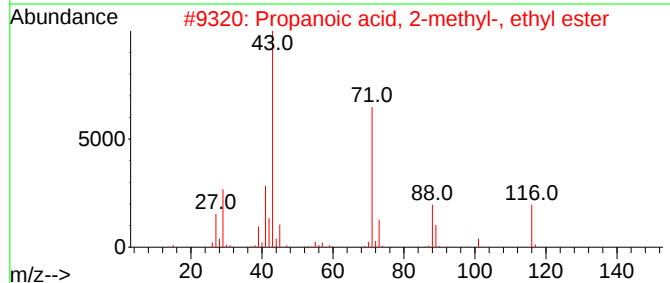
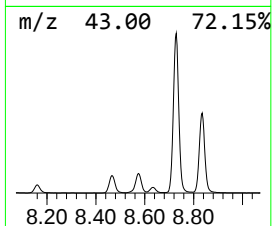
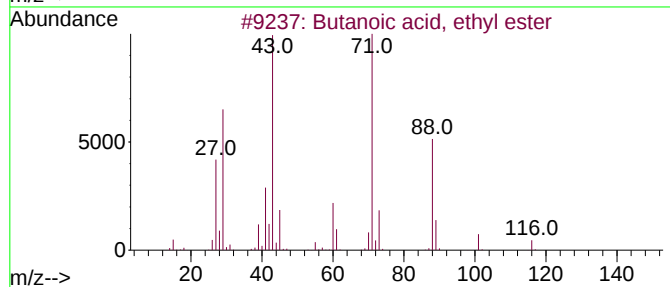
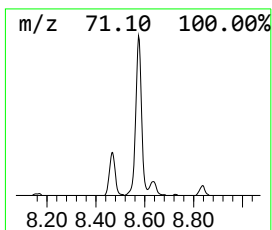
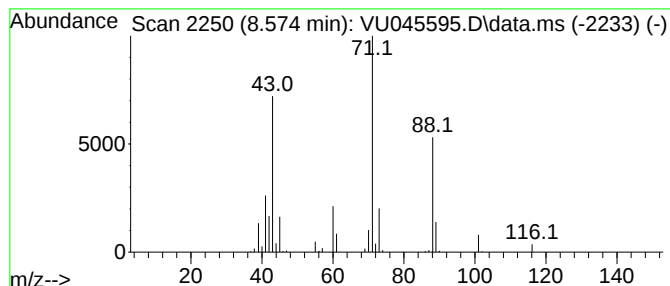
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.574 | 12.04 ug/l | 177292 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Butanoic acid, ethyl ester          | 116 | C6H12O2   | 000105-54-4 | 97   |
| 2    |    |   | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2   | 000097-62-1 | 53   |
| 3    |    |   | Butanoic acid, 3-methylbutyl ester  | 158 | C9H18O2   | 000106-27-4 | 38   |
| 4    |    |   | 3-Mercaptohexyl butanoate           | 204 | C10H20O2S | 136954-21-7 | 37   |
| 5    |    |   | Butanoic acid, anhydride            | 158 | C8H14O3   | 000106-31-0 | 35   |



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Instrument :  
MSVOA\_U  
ClientSampleId :  
SP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

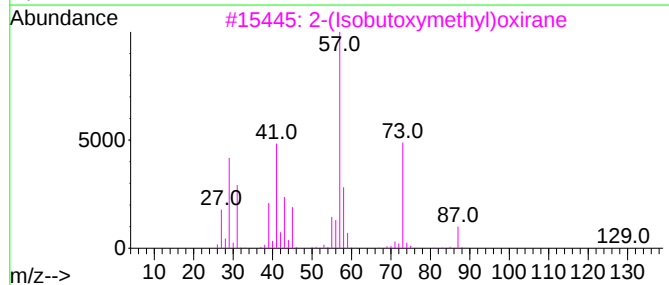
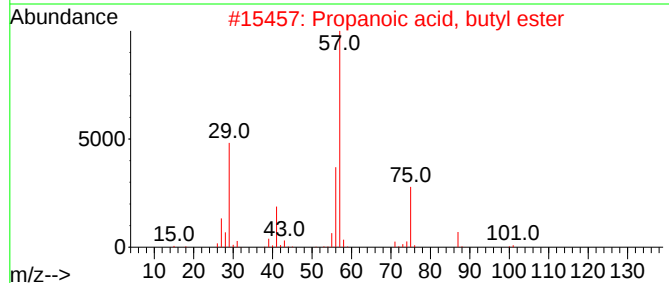
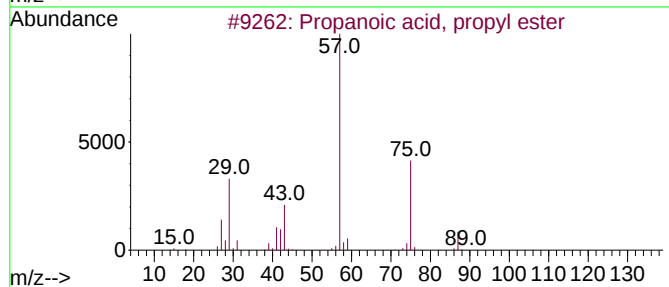
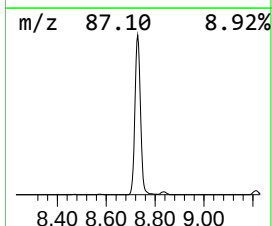
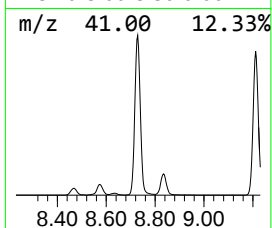
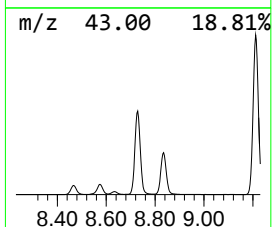
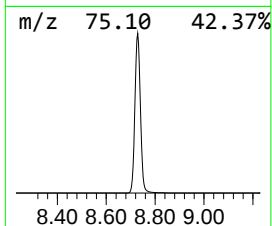
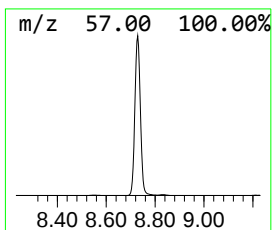
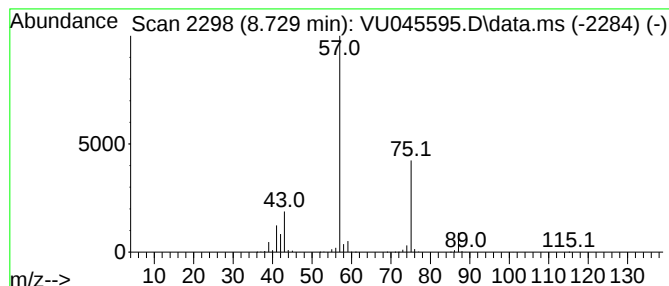
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 8.729 | 187.61 ug/l | 2763220 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm  | CAS#        | Qual |
|------|----|---|------------------------------|-----|----------|-------------|------|
| 1    |    |   | Propanoic acid, propyl ester | 116 | C6H12O2  | 000106-36-5 | 83   |
| 2    |    |   | Propanoic acid, butyl ester  | 130 | C7H14O2  | 000590-01-2 | 28   |
| 3    |    |   | 2-(Isobutoxymethyl)oxirane   | 130 | C7H14O2  | 003814-55-9 | 9    |
| 4    |    |   | di-tert-Butyl dicarbonate    | 218 | C10H18O5 | 024424-99-5 | 9    |
| 5    |    |   | 1-Butanamine, 3-methyl-      | 87  | C5H13N   | 000107-85-7 | 7    |



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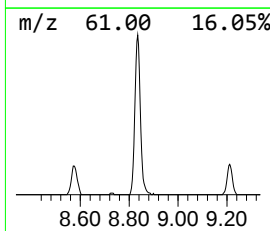
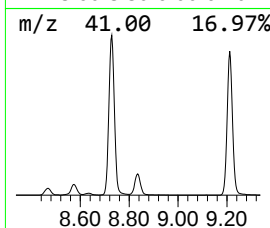
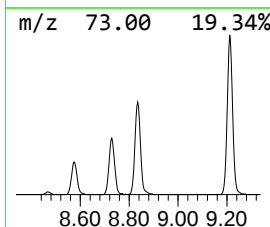
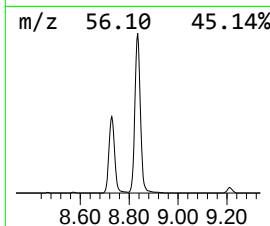
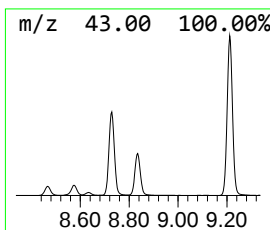
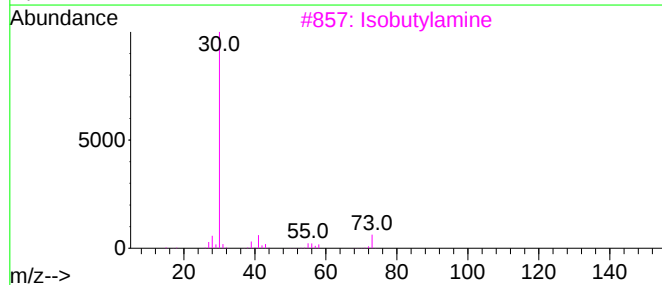
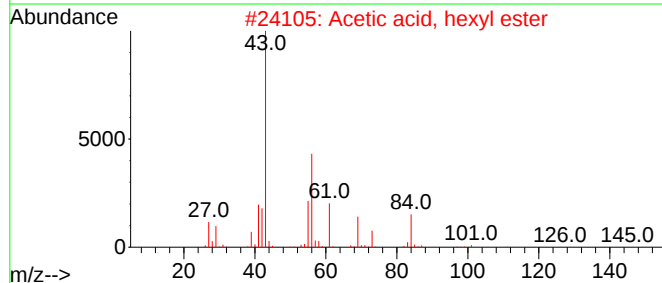
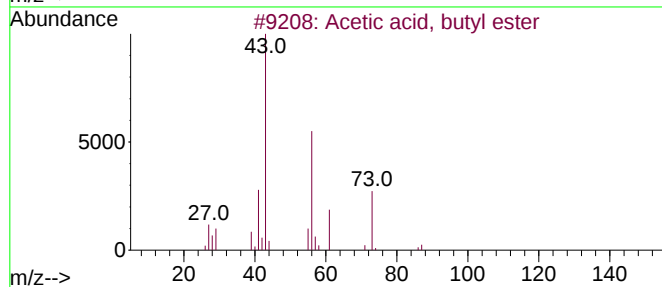
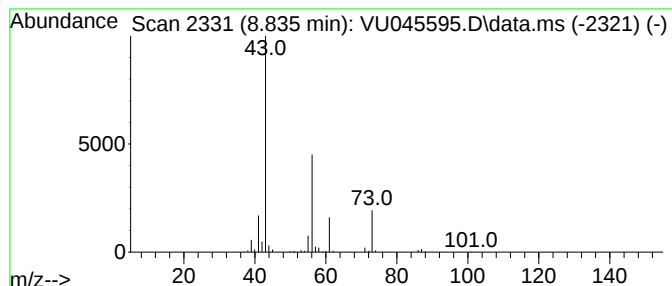
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.835 | 20.03 ug/l | 294950 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Acetic acid, butyl ester      | 116 | C6H12O2   | 000123-86-4 | 78   |
| 2    |    |   | Acetic acid, hexyl ester      | 144 | C8H16O2   | 000142-92-7 | 33   |
| 3    |    |   | Isobutylamine                 | 73  | C4H11N    | 000078-81-9 | 9    |
| 4    |    |   | Ethanol, 2-chloro-, acetate   | 122 | C4H7ClO2  | 000542-58-5 | 9    |
| 5    |    |   | 1-Butanol, 4-chloro-, acetate | 150 | C6H11ClO2 | 006962-92-1 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU110521\  
Data File : VU045595.D  
Acq On : 06 Nov 2021 05:57  
Operator : SY/MD  
Sample : M4470-02  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 50 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
SP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

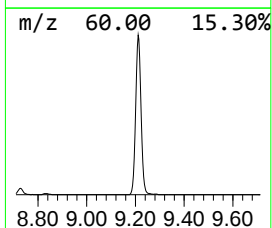
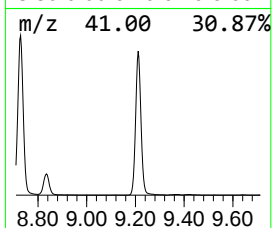
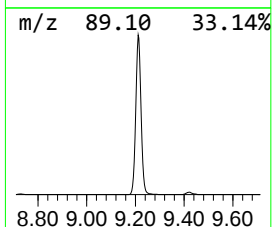
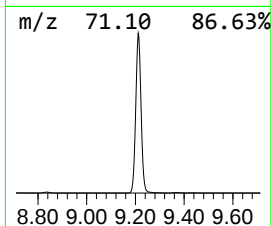
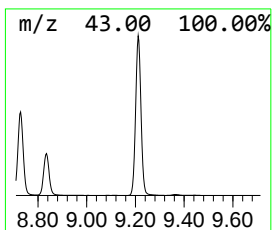
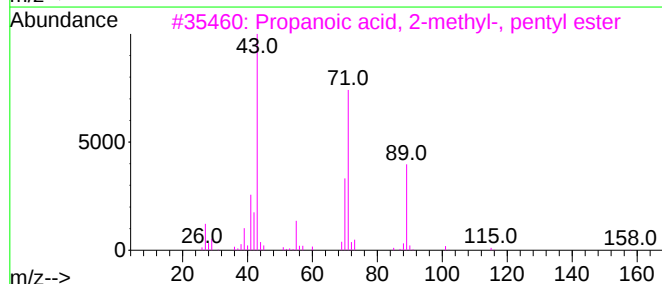
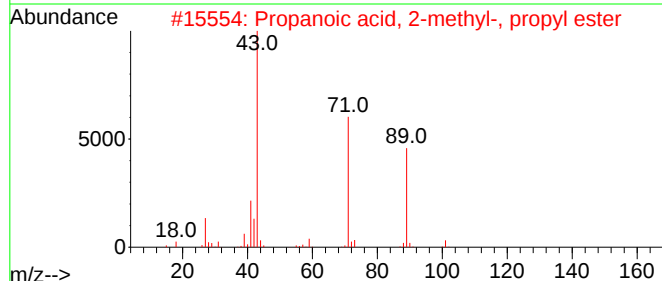
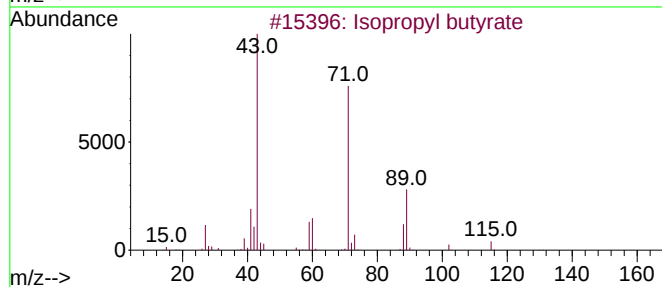
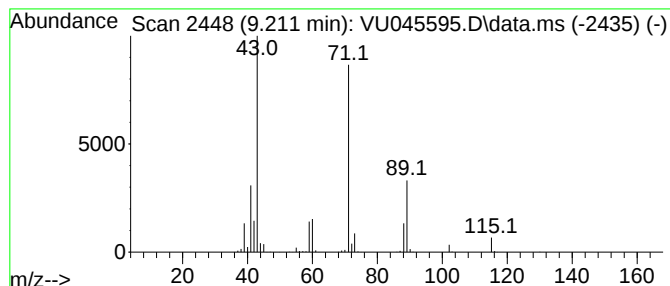
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Isopropyl butyrate Concentration Rank 3

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 9.211 | 111.12 ug/l | 1636540 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                            | MW  | MolForm | CAS#         | Qual |
|------|----|---|-----------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Isopropyl butyrate                      | 130 | C7H14O2 | 000638-11-9  | 95   |
| 2    |    |   | Propanoic acid, 2-methyl-, propyl ester | 130 | C7H14O2 | 000644-49-5  | 72   |
| 3    |    |   | Propanoic acid, 2-methyl-, pentyl ester | 158 | C9H18O2 | 002445-72-9  | 64   |
| 4    |    |   | Ethylene glycol Formate Isobutyrate     | 160 | C7H12O4 | 1000458-48-0 | 64   |
| 5    |    |   | Butanoic acid, propyl ester             | 130 | C7H14O2 | 000105-66-8  | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU110521\  
Data File : VU045595.D  
Acq On : 06 Nov 2021 05:57  
Operator : SY/MD  
Sample : M4470-02  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 50 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
SP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U110521W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| n-Propyl acetate   | 7.037 | 145.2   | ug/l  | 1885720  | 2                     | 6.253 | 649270 | 50.0 |
| Propanoic acid,... | 7.738 | 20.4    | ug/l  | 264609   | 2                     | 6.253 | 649270 | 50.0 |
| Butanoic acid, ... | 8.574 | 12.0    | ug/l  | 177292   | 3                     | 9.420 | 736410 | 50.0 |
| Propanoic acid,... | 8.729 | 187.6   | ug/l  | 2763220  | 3                     | 9.420 | 736410 | 50.0 |
| Acetic acid, bu... | 8.835 | 20.0    | ug/l  | 294950   | 3                     | 9.420 | 736410 | 50.0 |
| Isopropyl butyrate | 9.211 | 111.1   | ug/l  | 1636540  | 3                     | 9.420 | 736410 | 50.0 |