

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
 Data File : VU045017.D  
 Acq On : 30 Sep 2021 01:29  
 Operator : SY/MD  
 Sample : PB139450TB  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 36 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 PB139450TB

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82U092821W.M  
 Title : SW846 8260

Signal : TIC: VU045017.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         | 2.629       | 390           | 401         | 424          | rBV      | 44810          | 75863         | 1.72%           | 0.412%        |
| 2         | 3.047       | 520           | 531         | 547          | rBV      | 27449          | 51606         | 1.17%           | 0.281%        |
| 3         | 5.292       | 1213          | 1229        | 1242         | rBV      | 180984         | 380538        | 8.61%           | 2.069%        |
| 4         | 5.375       | 1242          | 1255        | 1278         | rVB      | 318661         | 655845        | 14.84%          | 3.566%        |
| 5         | 5.706       | 1342          | 1358        | 1377         | rBV      | 220155         | 446211        | 10.10%          | 2.426%        |
| 6         | 5.915       | 1410          | 1423        | 1438         | rBV2     | 24013          | 48133         | 1.09%           | 0.262%        |
| 7         | 6.253       | 1514          | 1528        | 1565         | rVB      | 487453         | 946095        | 21.41%          | 5.144%        |
| 8         | 6.931       | 1717          | 1739        | 1759         | rBV3     | 21944          | 68878         | 1.56%           | 0.375%        |
| 9         | 7.041       | 1759          | 1773        | 1804         | rBV      | 1711178        | 2947806       | 66.69%          | 16.028%       |
| 10        | 7.742       | 1976          | 1991        | 2002         | rBV      | 252717         | 411587        | 9.31%           | 2.238%        |
| 11        | 7.902       | 2025          | 2041        | 2070         | rVV      | 750619         | 1304657       | 29.52%          | 7.094%        |
| 12        | 8.163       | 2109          | 2122        | 2134         | rBV      | 27634          | 44955         | 1.02%           | 0.244%        |
| 13        | 8.468       | 2206          | 2217        | 2230         | rBV      | 65757          | 104089        | 2.35%           | 0.566%        |
| 14        | 8.578       | 2232          | 2251        | 2262         | rVV      | 182271         | 299431        | 6.77%           | 1.628%        |
| 15        | 8.732       | 2279          | 2299        | 2318         | rVV      | 2861292        | 4419948       | 100.00%         | 24.033%       |
| 16        | 8.838       | 2321          | 2332        | 2355         | rVB      | 302851         | 489825        | 11.08%          | 2.663%        |
| 17        | 9.214       | 2434          | 2449        | 2484         | rBV      | 1663473        | 2533860       | 57.33%          | 13.777%       |
| 18        | 9.420       | 2502          | 2513        | 2535         | rVB      | 695514         | 1129608       | 25.56%          | 6.142%        |
| 19        | 10.076      | 2705          | 2717        | 2741         | rBV      | 59207          | 96792         | 2.19%           | 0.526%        |
| 20        | 10.635      | 2878          | 2891        | 2913         | rBV      | 546883         | 858087        | 19.41%          | 4.666%        |
| 21        | 11.815      | 3245          | 3258        | 3276         | rBV      | 684470         | 1077487       | 24.38%          | 5.859%        |

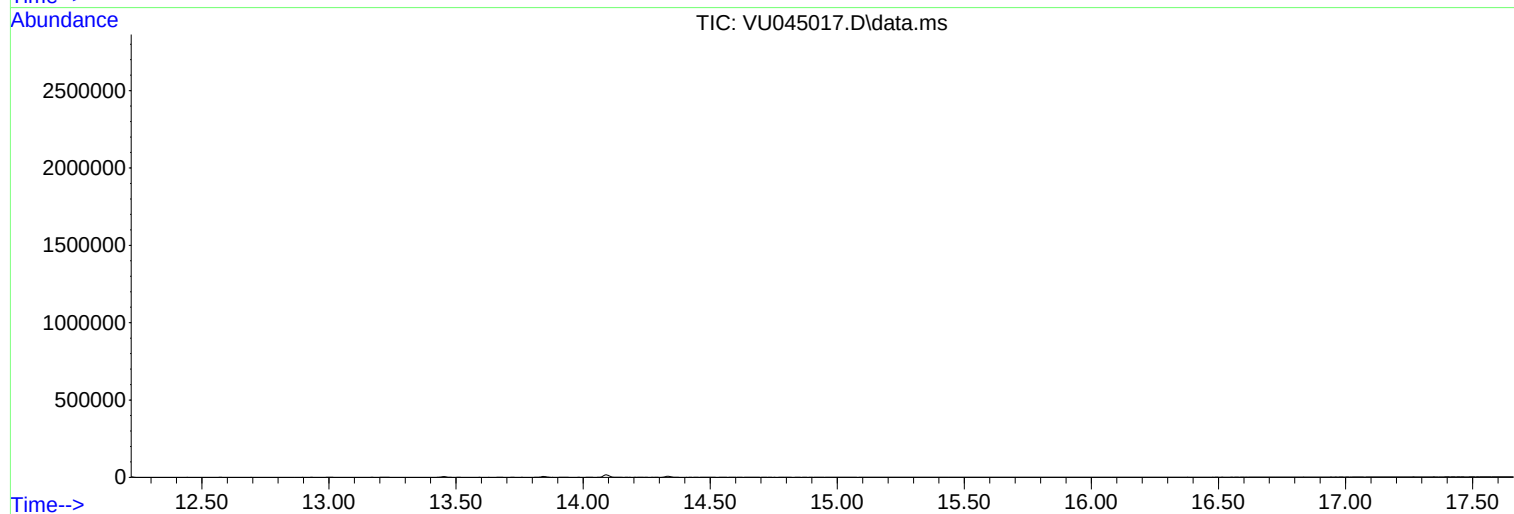
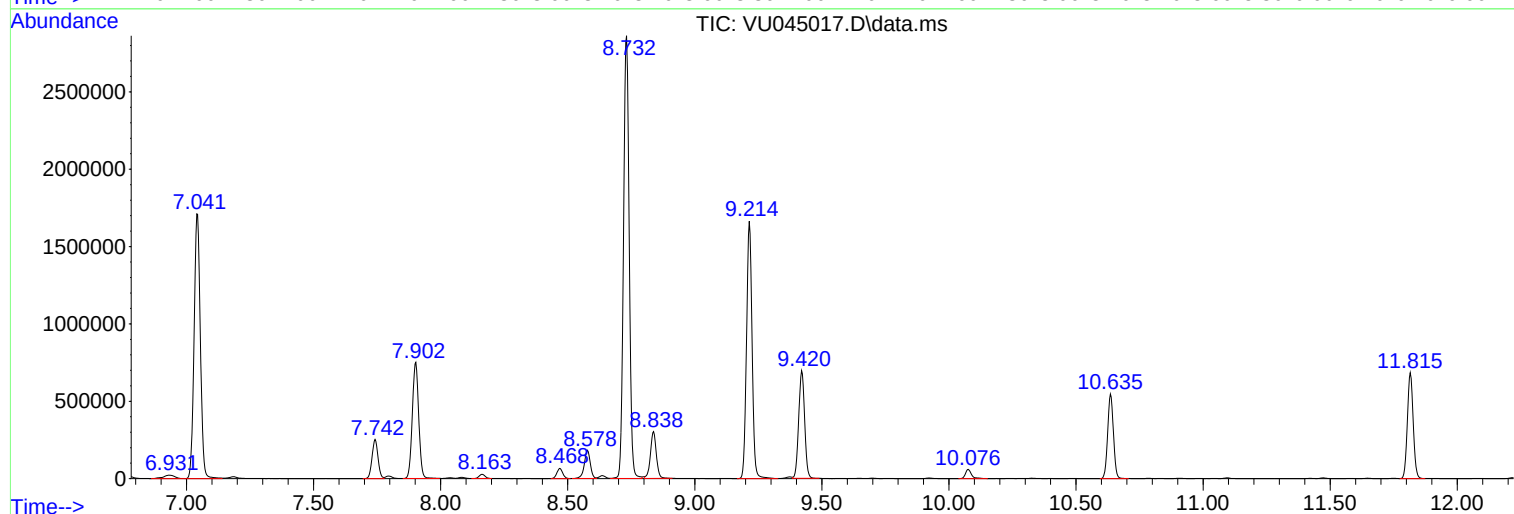
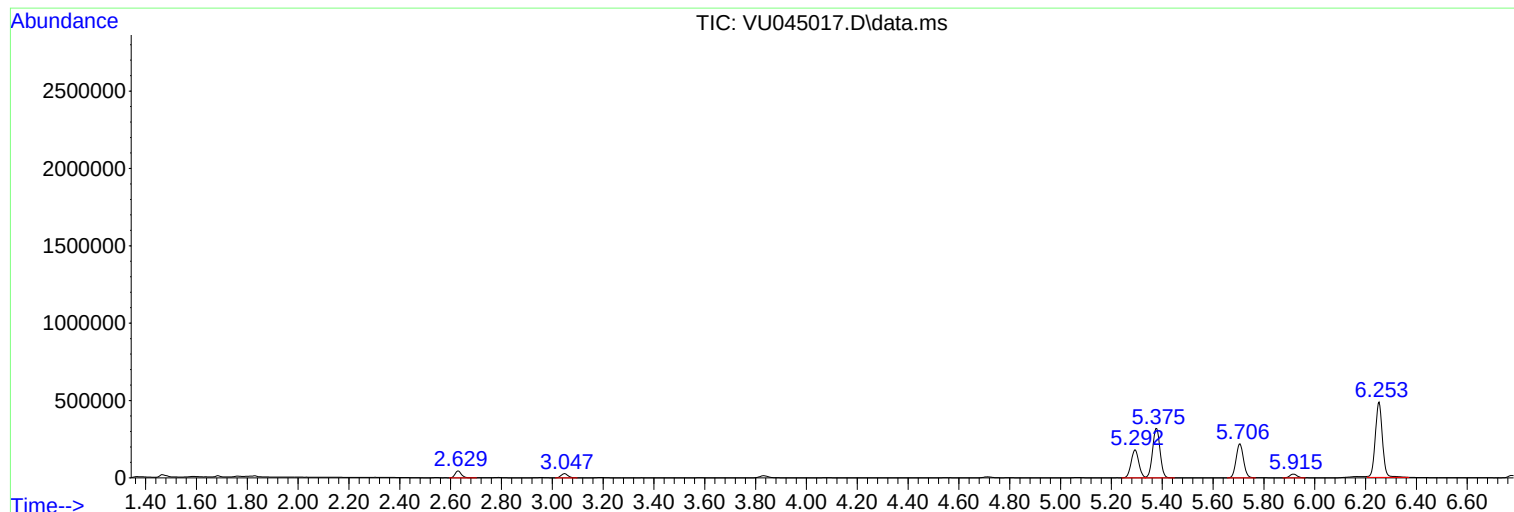
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ALS Vial : 36 Sample Multiplier: 1

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ClientSampleId :  
PB139450TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

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



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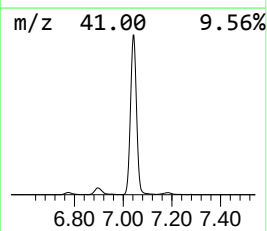
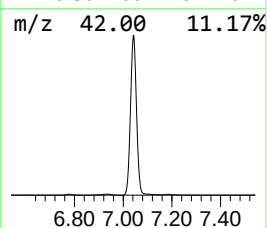
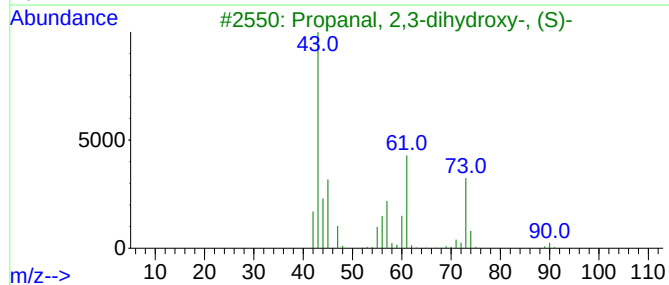
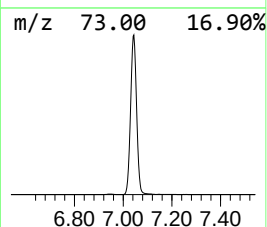
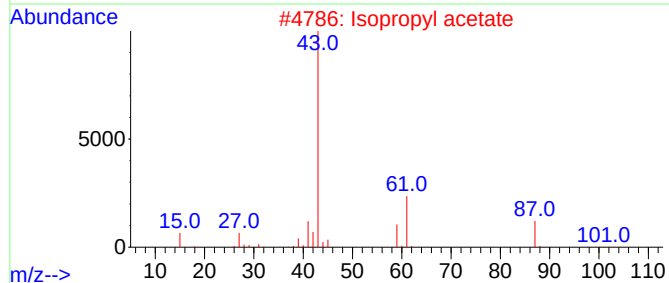
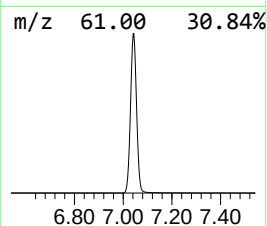
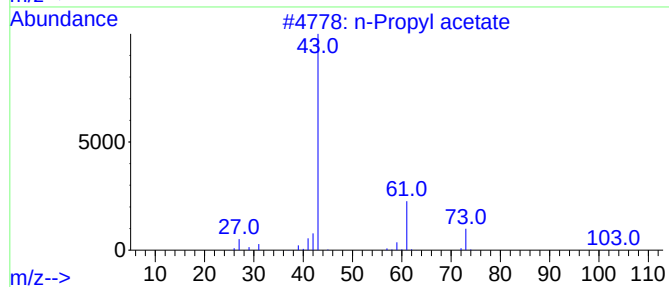
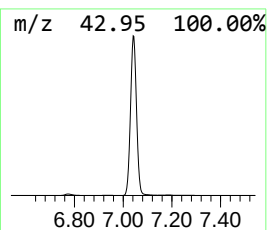
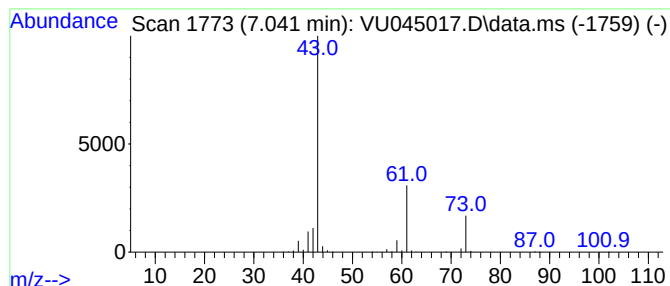
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

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.  |
|-------|-------------|---------|---------------------|-------|
| 7.041 | 155.79 ug/l | 2947810 | 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    |    |   | Propanal, 2,3-dihydroxy-, (S)- | 90  | C3H6O3  | 000497-09-6 | 9    |
| 4    |    |   | Isobutyl acetate               | 116 | C6H12O2 | 000110-19-0 | 9    |
| 5    |    |   | 1-Butanamine                   | 73  | C4H11N  | 000109-73-9 | 7    |



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MSVOA\_U  
ClientSampleId :  
PB139450TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

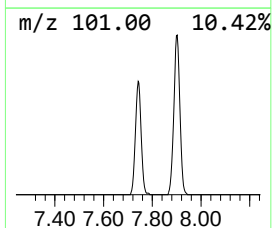
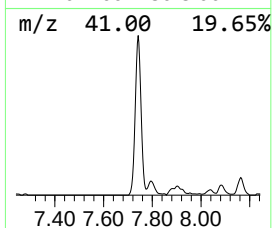
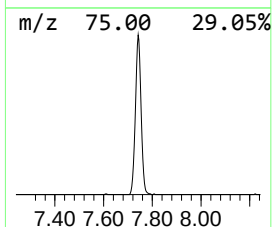
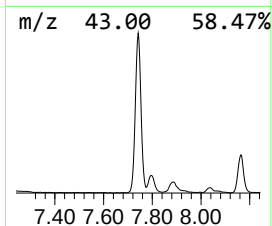
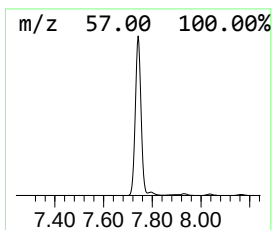
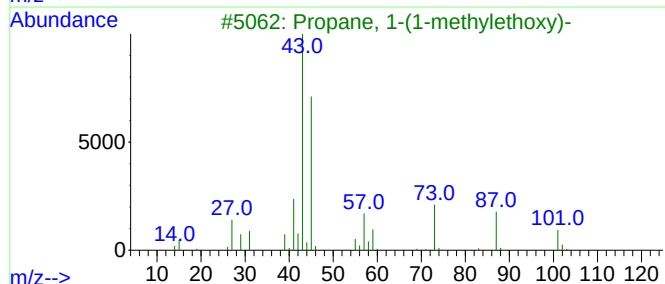
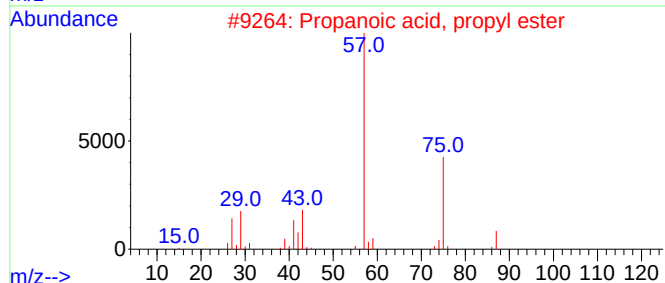
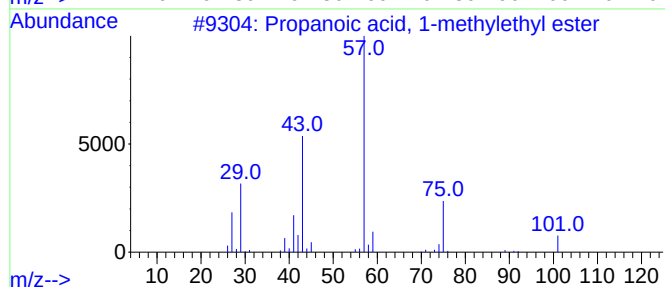
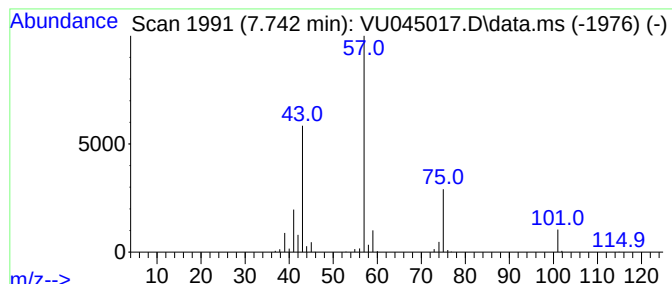
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 7.742 | 21.75 ug/l | 411587 | 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 | 47   |
| 3         | Propane, 1-(1-methylethoxy)-        | 102 | C6H14O  | 000627-08-7 | 23   |
| 4         | Propanoic acid, butyl ester         | 130 | C7H14O2 | 000590-01-2 | 23   |
| 5         | Butanoic acid, methyl ester         | 102 | C5H10O2 | 000623-42-7 | 10   |



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ClientSampleId :  
PB139450TB

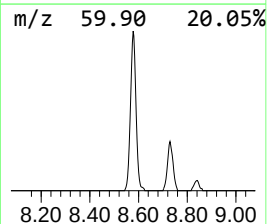
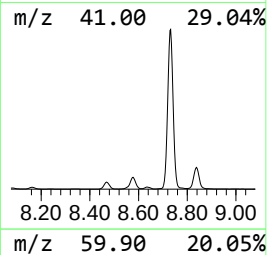
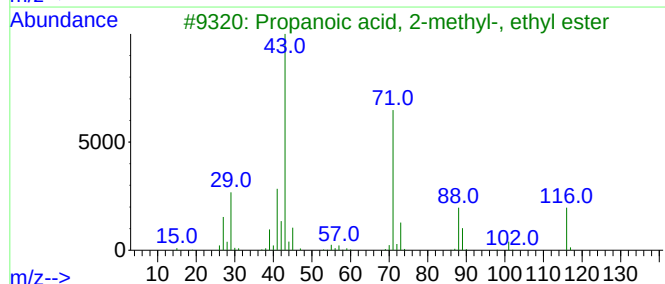
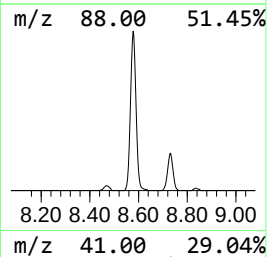
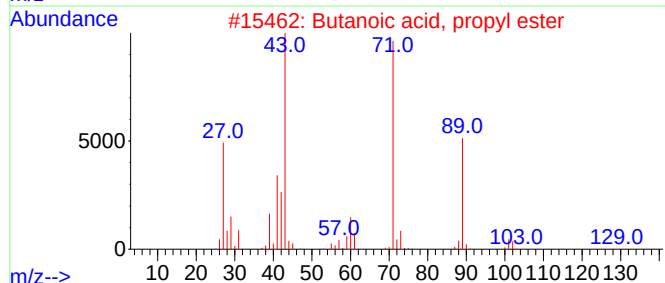
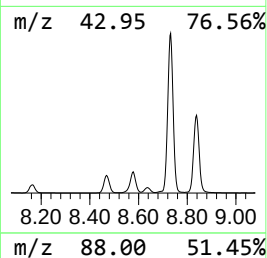
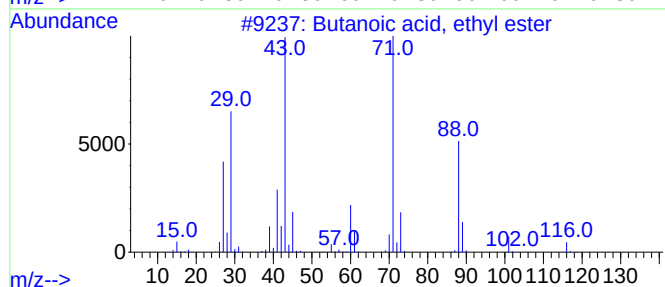
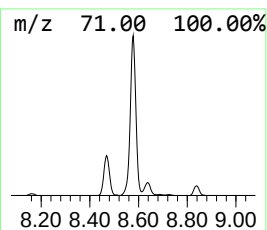
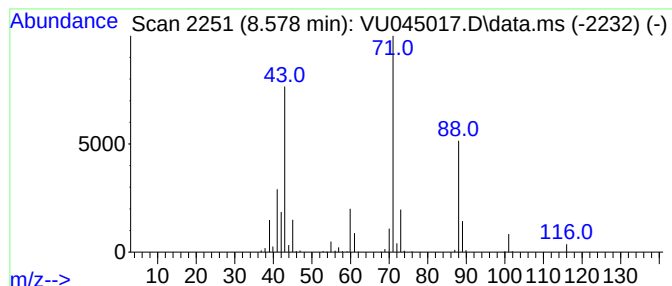
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

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.  |
|-------|------------|--------|------------------|-------|
| 8.578 | 13.25 ug/l | 299431 | 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    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2 | 000105-66-8 | 43   |
| 3    |    |   | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2 | 000097-62-1 | 42   |
| 4    |    |   | 4-Butoxy-2-butanone                 | 144 | C8H16O2 | 030536-44-8 | 40   |
| 5    |    |   | Butanoic acid, 3-methylbutyl ester  | 158 | C9H18O2 | 000106-27-4 | 38   |



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ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

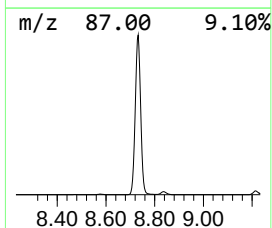
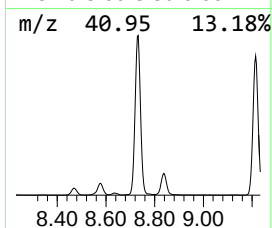
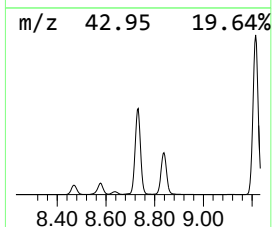
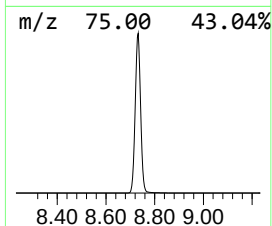
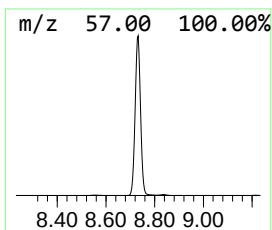
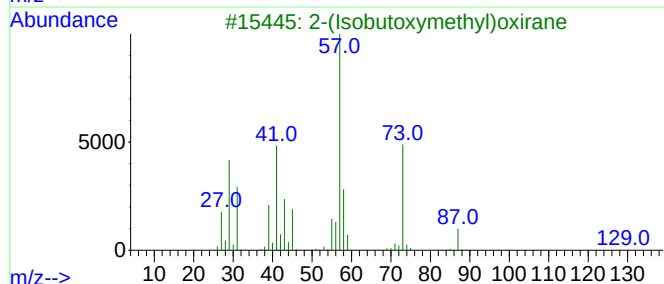
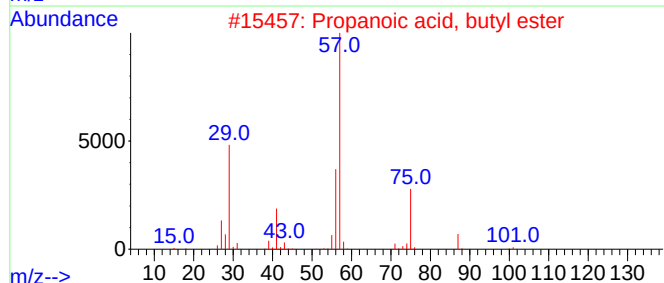
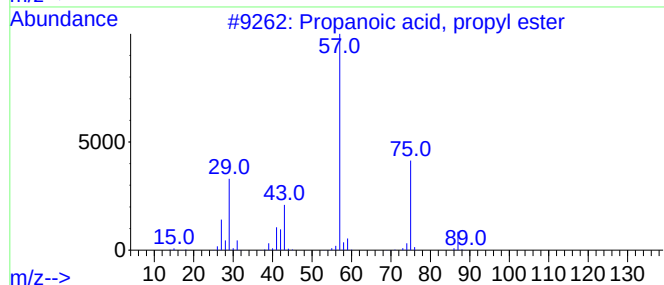
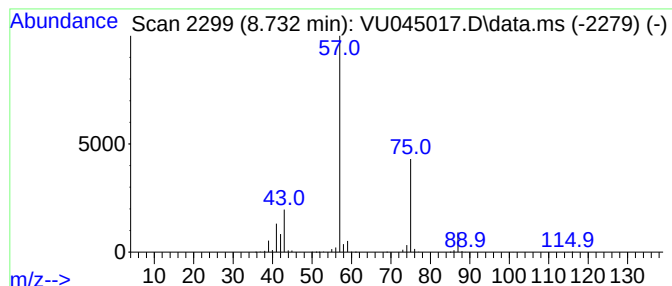
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 8.732 | 195.64 ug/l | 4419950 | 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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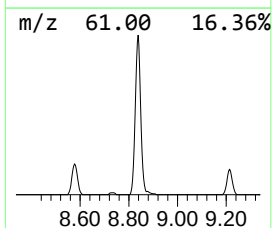
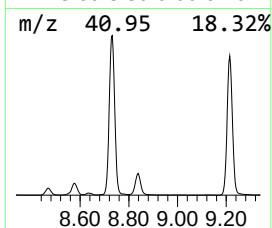
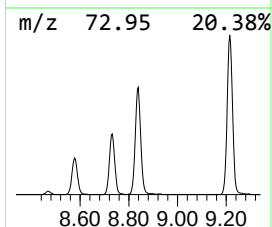
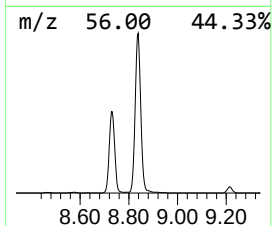
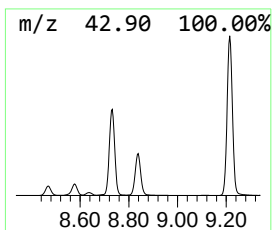
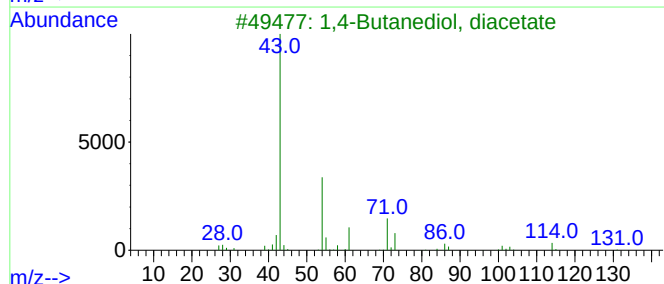
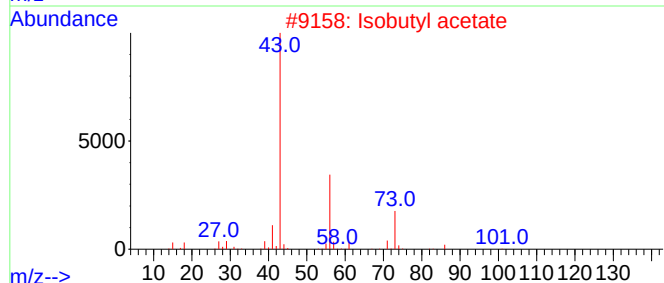
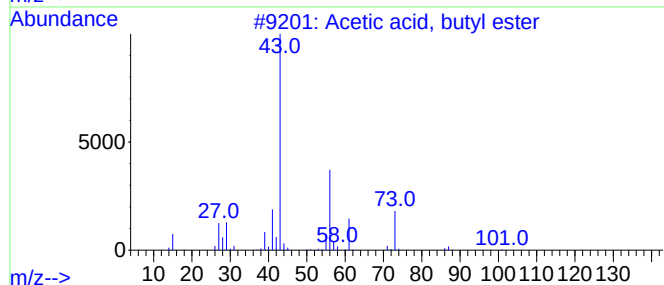
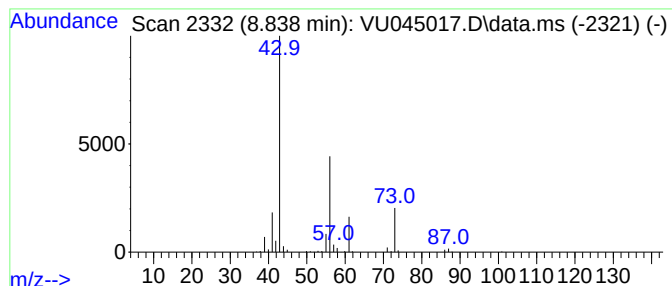
TIC Library : C:\Database\NIST20.L  
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Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.838 | 21.68 ug/l | 489825 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Acetic acid, butyl ester       | 116 | C6H12O2 | 000123-86-4 | 83   |
| 2    |    |   | Isobutyl acetate               | 116 | C6H12O2 | 000110-19-0 | 40   |
| 3    |    |   | 1,4-Butanediol, diacetate      | 174 | C8H14O4 | 000628-67-1 | 12   |
| 4    |    |   | Isobutylamine                  | 73  | C4H11N  | 000078-81-9 | 9    |
| 5    |    |   | 3,3-Dimethyl-2,4-pentane dione | 128 | C7H12O2 | 003142-58-3 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045017.D  
Acq On : 30 Sep 2021 01:29  
Operator : SY/MD  
Sample : PB139450TB  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

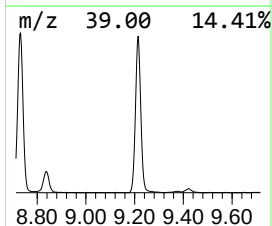
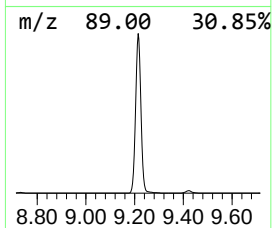
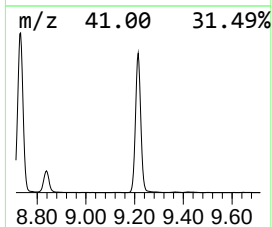
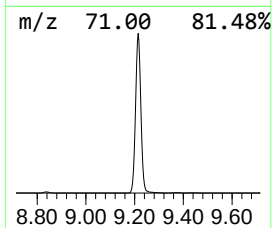
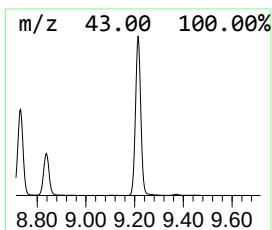
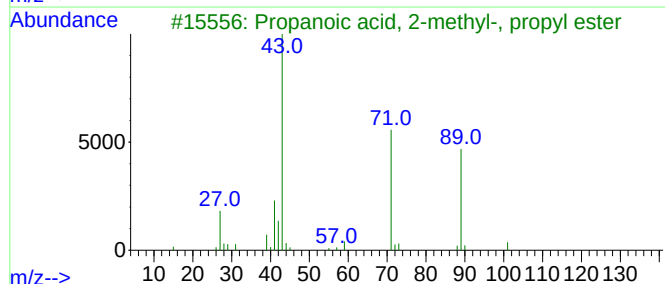
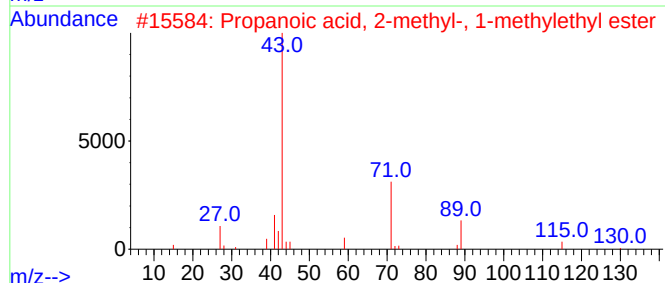
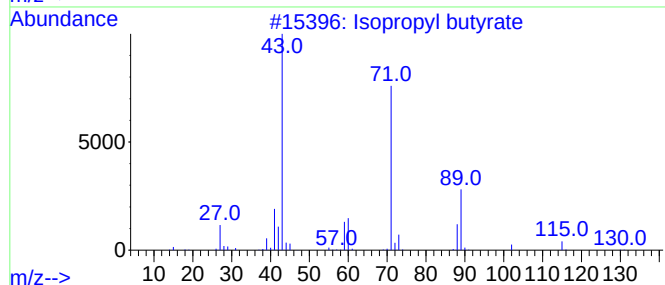
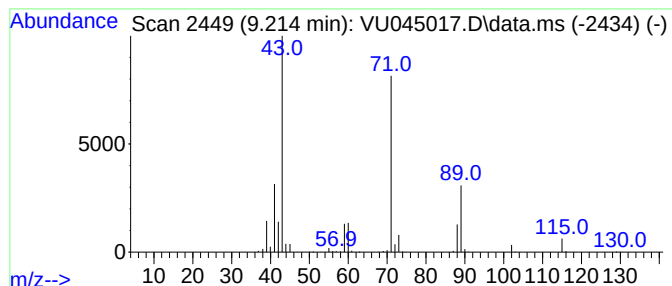
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 6 Isopropyl butyrate Concentration Rank 3

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 9.214 | 112.16 ug/l | 2533860 | Chlorobenzene-d5 | 9.420 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Isopropyl butyrate                  | 130 | C7H14O2 | 000638-11-9  | 91   |
| 2    |    |   | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5  | 78   |
| 3    |    |   | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5  | 72   |
| 4    |    |   | Ethylene glycol Formate Isobutyrate | 160 | C7H12O4 | 1000458-48-0 | 64   |
| 5    |    |   | Butanoic acid, pentyl ester         | 158 | C9H18O2 | 000540-18-1  | 64   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045017.D  
Acq On : 30 Sep 2021 01:29  
Operator : SY/MD  
Sample : PB139450TB  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                    |       |         |       |          | #                     | RT    | Resp    | Conc |
| n-Propyl acetate   | 7.041 | 155.8   | ug/l  | 2947810  | 2                     | 6.253 | 946095  | 50.0 |
| Propanoic acid,... | 7.742 | 21.8    | ug/l  | 411587   | 2                     | 6.253 | 946095  | 50.0 |
| Butanoic acid, ... | 8.578 | 13.3    | ug/l  | 299431   | 3                     | 9.420 | 1129610 | 50.0 |
| Propanoic acid,... | 8.732 | 195.6   | ug/l  | 4419950  | 3                     | 9.420 | 1129610 | 50.0 |
| Acetic acid, bu... | 8.838 | 21.7    | ug/l  | 489825   | 3                     | 9.420 | 1129610 | 50.0 |
| Isopropyl butyrate | 9.214 | 112.2   | ug/l  | 2533860  | 3                     | 9.420 | 1129610 | 50.0 |