

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
 Data File : VU045018.D  
 Acq On : 30 Sep 2021 01:53  
 Operator : SY/MD  
 Sample : PB139450ZHE#01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 37 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 PB139450ZHE#01

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: VU045018.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       | 388           | 401         | 421          | rBV      | 43018          | 74669         | 1.63%           | 0.400%        |
| 2         | 3.044       | 517           | 530         | 548          | rVB      | 26377          | 50130         | 1.09%           | 0.268%        |
| 3         | 5.292       | 1213          | 1229        | 1242         | rBV      | 172175         | 361497        | 7.88%           | 1.935%        |
| 4         | 5.375       | 1242          | 1255        | 1279         | rVB      | 305054         | 620940        | 13.54%          | 3.324%        |
| 5         | 5.703       | 1339          | 1357        | 1376         | rBV      | 210173         | 424144        | 9.25%           | 2.271%        |
| 6         | 5.915       | 1411          | 1423        | 1443         | rBV      | 24178          | 48484         | 1.06%           | 0.260%        |
| 7         | 6.253       | 1515          | 1528        | 1572         | rVB      | 470858         | 962320        | 20.99%          | 5.152%        |
| 8         | 6.931       | 1719          | 1739        | 1758         | rVB3     | 22654          | 68638         | 1.50%           | 0.367%        |
| 9         | 7.044       | 1759          | 1774        | 1805         | rBV      | 1722276        | 2972374       | 64.83%          | 15.914%       |
| 10        | 7.742       | 1977          | 1991        | 2002         | rBV      | 252956         | 421548        | 9.19%           | 2.257%        |
| 11        | 7.902       | 2022          | 2041        | 2058         | rBV      | 727207         | 1258897       | 27.46%          | 6.740%        |
| 12        | 8.163       | 2112          | 2122        | 2136         | rBV      | 27512          | 45945         | 1.00%           | 0.246%        |
| 13        | 8.472       | 2206          | 2218        | 2233         | rBV      | 67064          | 109404        | 2.39%           | 0.586%        |
| 14        | 8.578       | 2233          | 2251        | 2262         | rVV      | 185829         | 310661        | 6.78%           | 1.663%        |
| 15        | 8.732       | 2280          | 2299        | 2318         | rVV      | 2991712        | 4584971       | 100.00%         | 24.548%       |
| 16        | 8.838       | 2321          | 2332        | 2359         | rVB      | 317476         | 509199        | 11.11%          | 2.726%        |
| 17        | 9.214       | 2434          | 2449        | 2482         | rBV      | 1722190        | 2659607       | 58.01%          | 14.239%       |
| 18        | 9.420       | 2502          | 2513        | 2534         | rVB      | 693593         | 1132604       | 24.70%          | 6.064%        |
| 19        | 10.076      | 2707          | 2717        | 2736         | rBV      | 62940          | 100659        | 2.20%           | 0.539%        |
| 20        | 10.635      | 2879          | 2891        | 2917         | rVB      | 546249         | 870589        | 18.99%          | 4.661%        |
| 21        | 11.815      | 3245          | 3258        | 3281         | rBV      | 679887         | 1090522       | 23.78%          | 5.839%        |

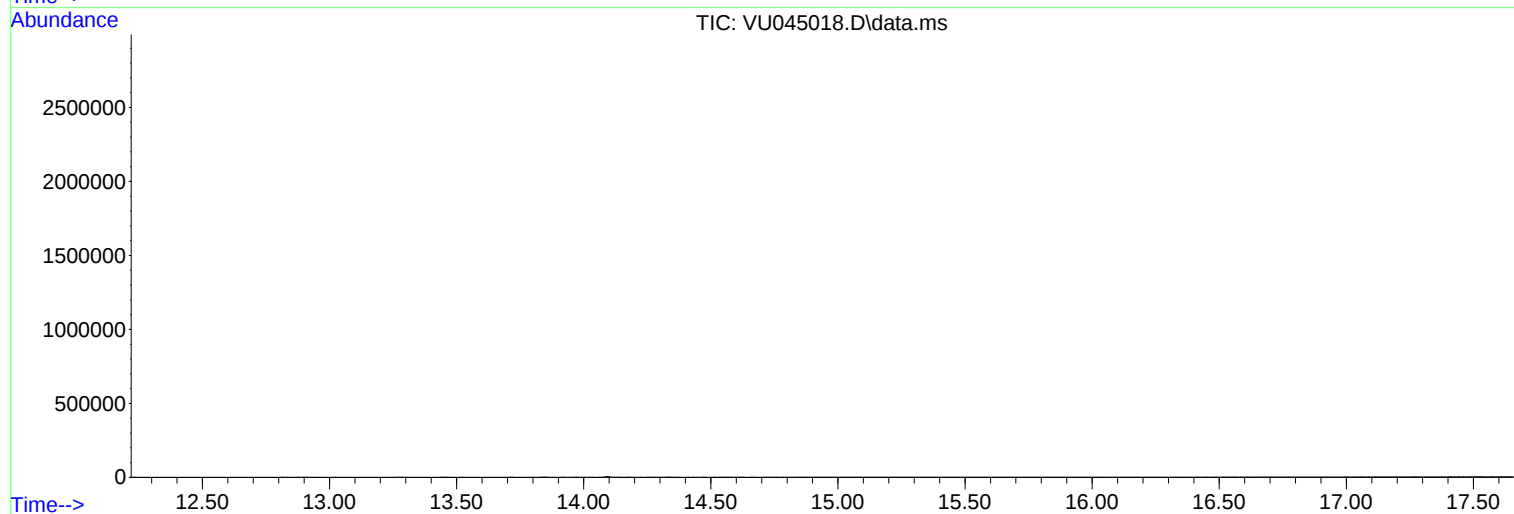
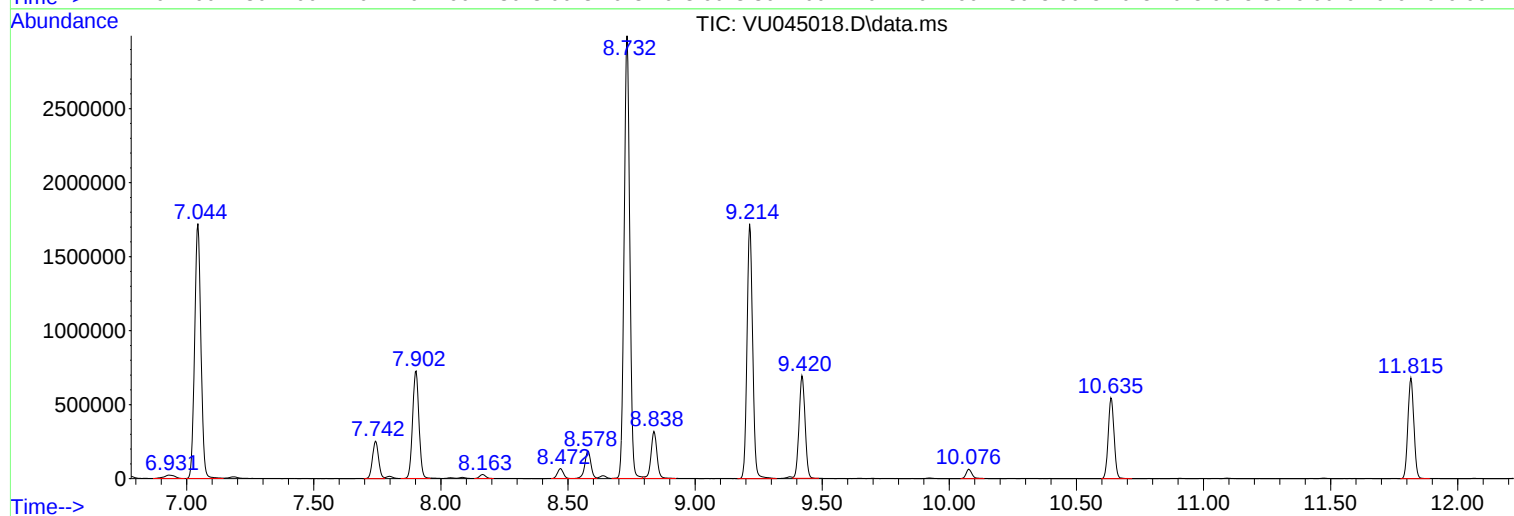
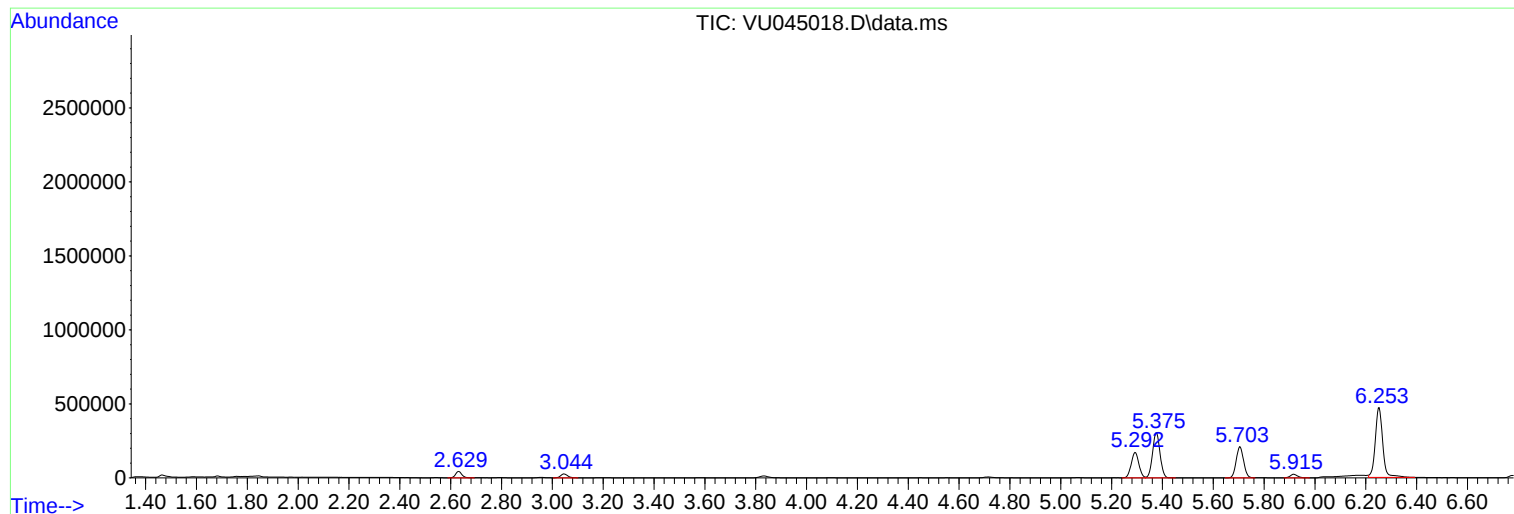
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

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



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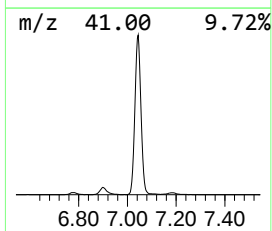
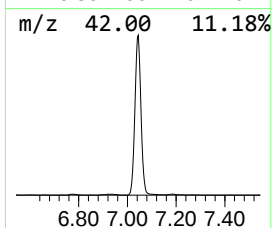
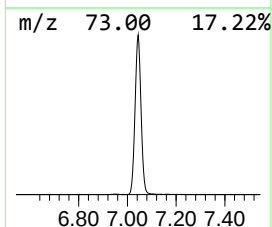
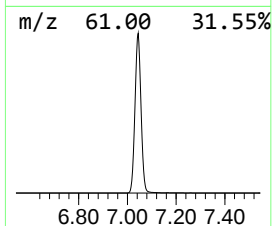
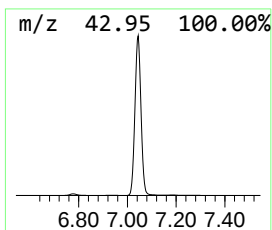
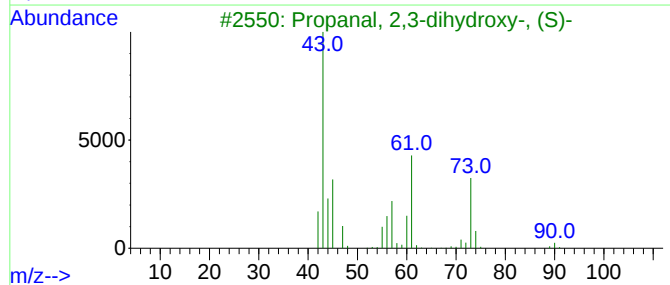
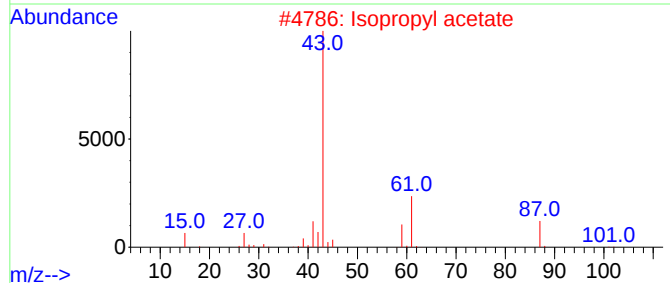
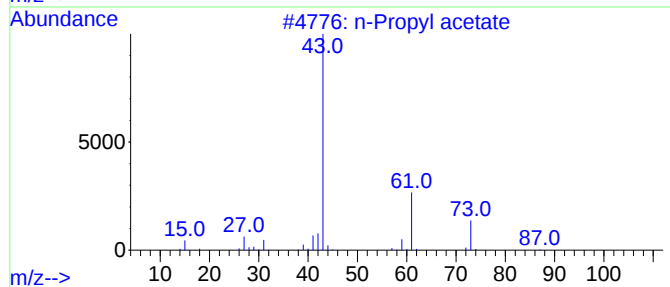
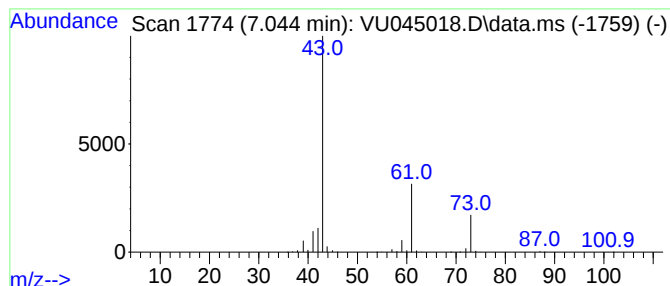
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\82U092821W.M  
Quant Title : SW846 8260

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.  |
|-------|-------------|---------|---------------------|-------|
| 7.044 | 154.44 ug/l | 2972370 | 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 | 5    |



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Instrument :  
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ClientSampleId :  
PB139450ZHE#01

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

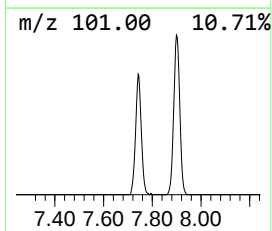
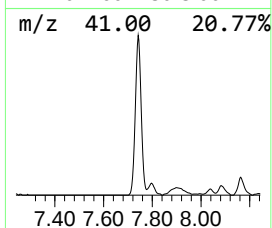
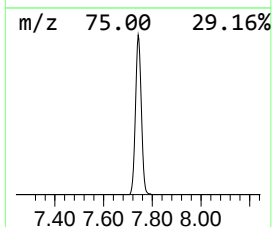
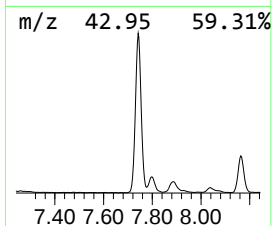
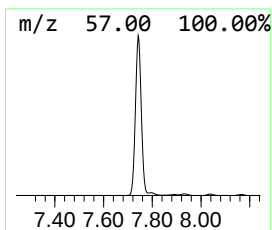
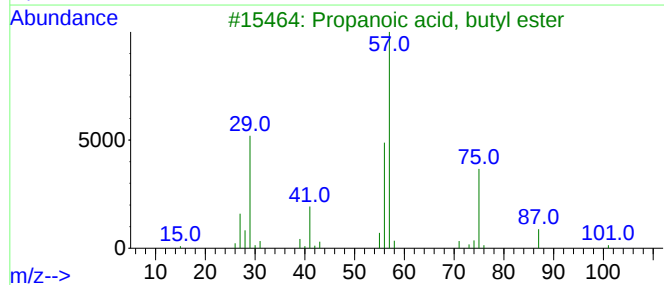
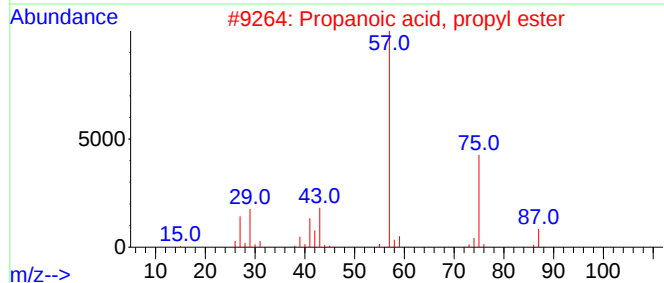
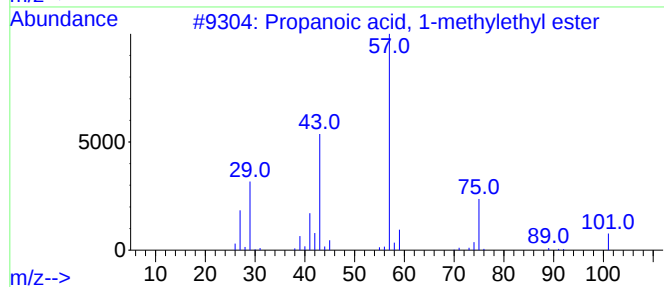
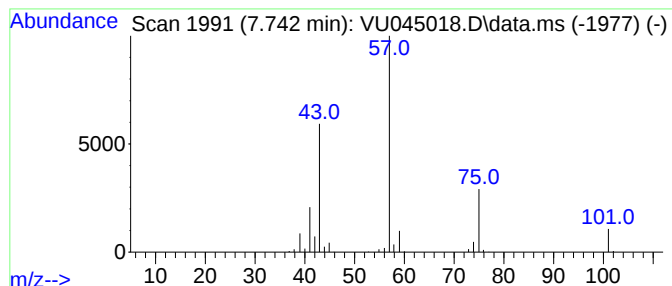
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 7.742 | 21.90 ug/l | 421548 | 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  | 50   |
| 3    |    |   | Propanoic acid, butyl ester         | 130 | C7H14O2 | 000590-01-2  | 28   |
| 4    |    |   | Propane, 1-(1-methylethoxy)-        | 102 | C6H14O  | 000627-08-7  | 23   |
| 5    |    |   | o-Isopropylhydroxylamine            | 75  | C3H9NO  | 1000322-42-6 | 9    |



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ALS Vial : 37 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
PB139450ZHE#01

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Quant Title : SW846 8260

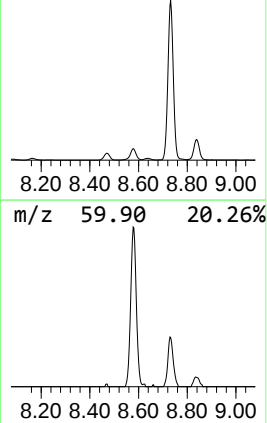
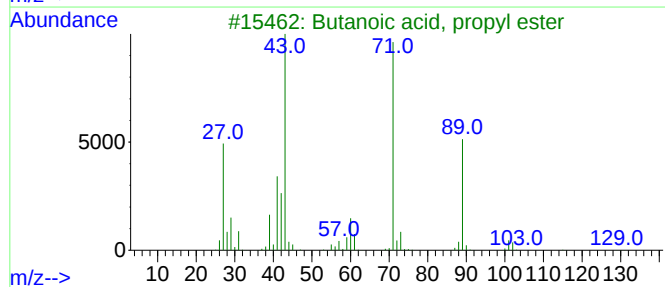
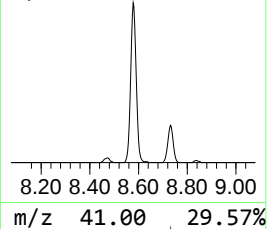
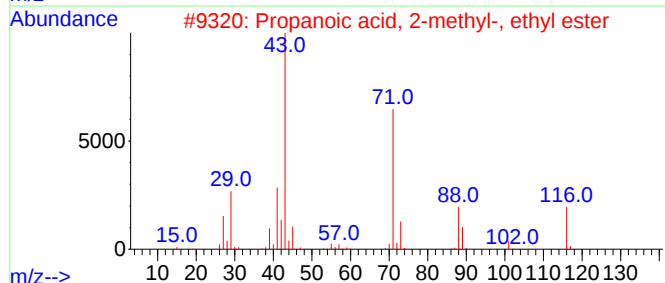
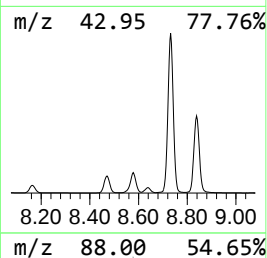
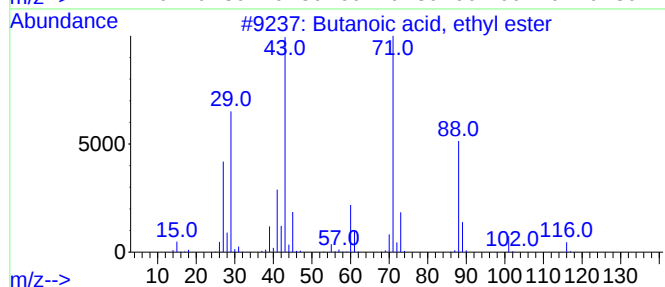
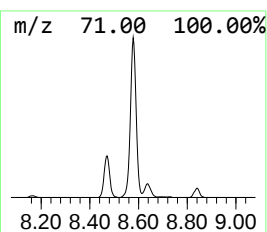
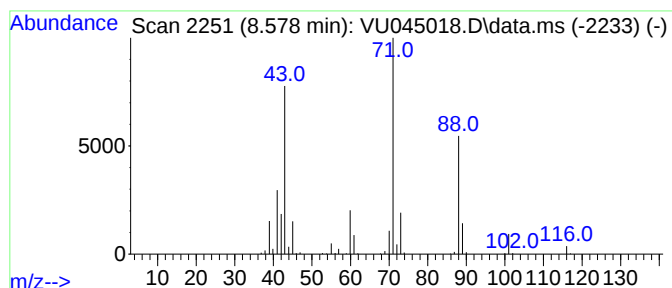
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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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 | 13.71 ug/l | 310661 | 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, propyl ester         | 130 | C7H14O2 | 000105-66-8 | 47   |
| 4    |    |   | Butanoic acid, 3-methylbutyl ester  | 158 | C9H18O2 | 000106-27-4 | 38   |
| 5    |    |   | Butanoic acid, anhydride            | 158 | C8H14O3 | 000106-31-0 | 35   |



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ALS Vial : 37 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#01

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

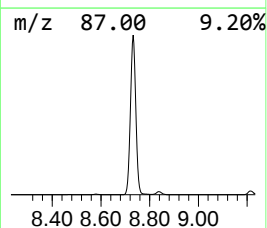
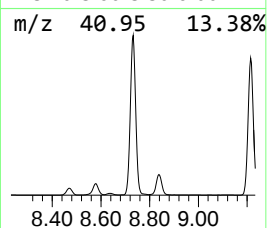
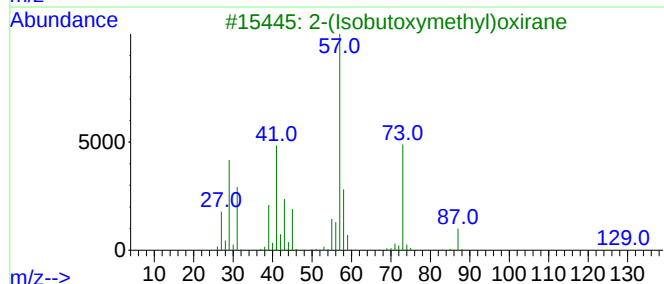
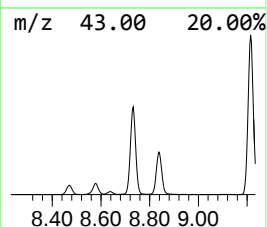
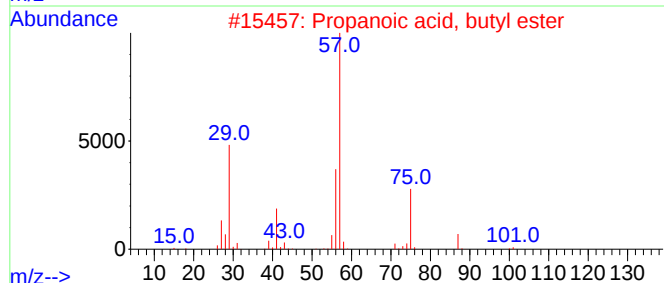
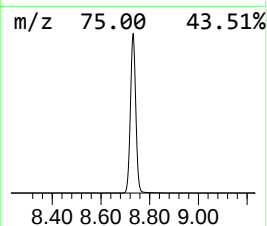
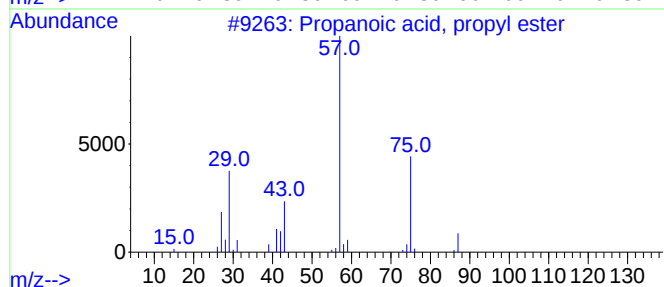
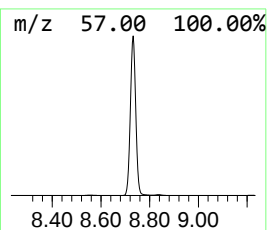
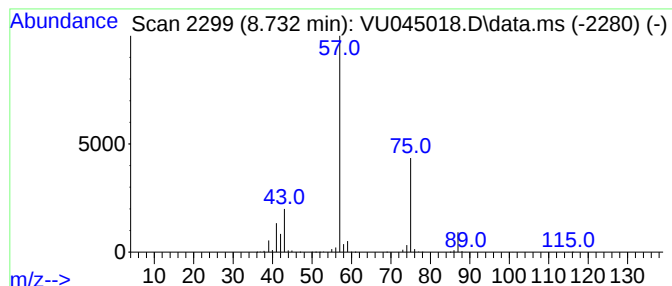
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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 8.732 | 202.41 ug/l | 4584970 | 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, 2-methyl-      | 87  | C5H13N   | 000096-15-1 | 7    |



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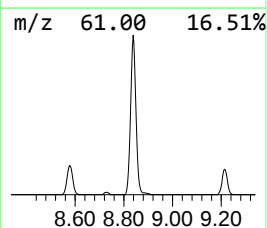
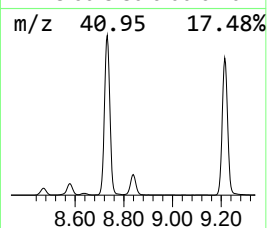
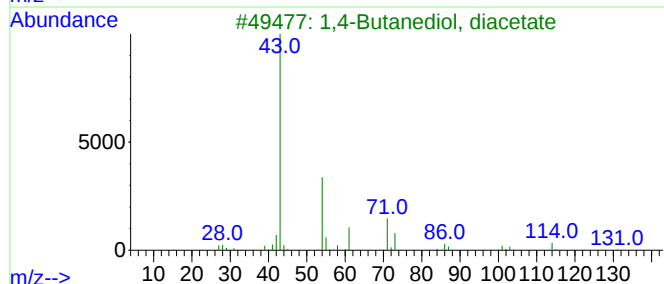
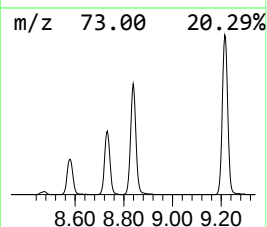
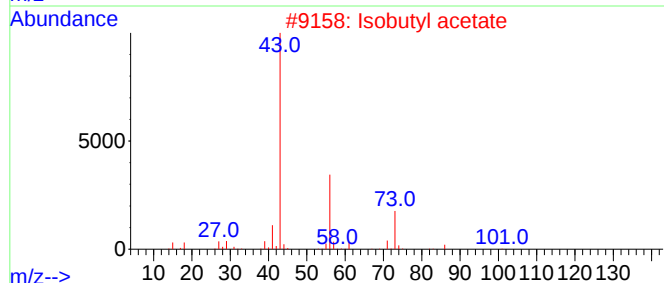
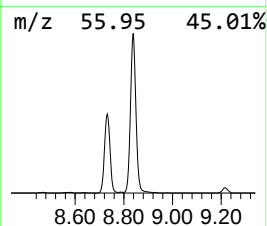
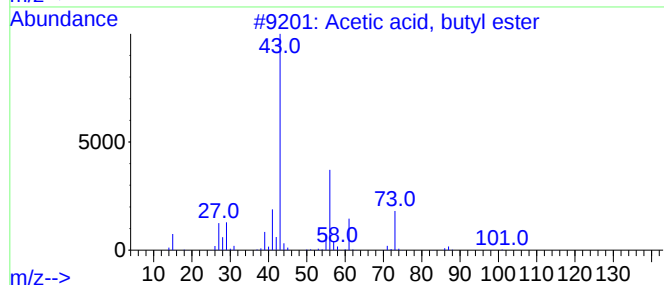
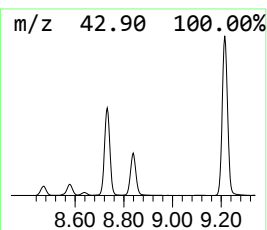
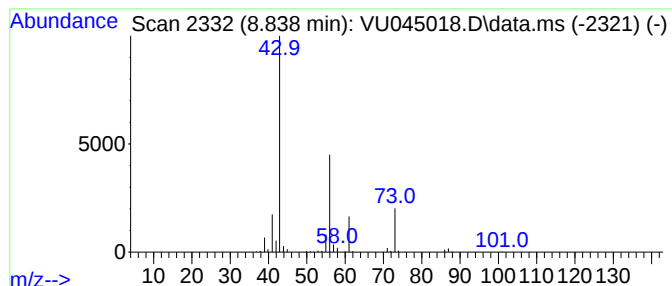
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Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.838 | 22.48 ug/l | 509199 | 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    |    |   | Ethanol, 2-chloro-, acetate | 122 | C4H7ClO2 | 000542-58-5 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045018.D  
Acq On : 30 Sep 2021 01:53  
Operator : SY/MD  
Sample : PB139450ZHE#01  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 37 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#01

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

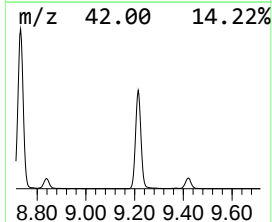
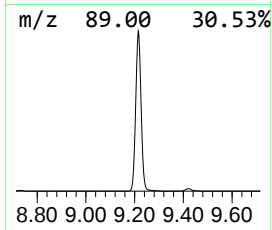
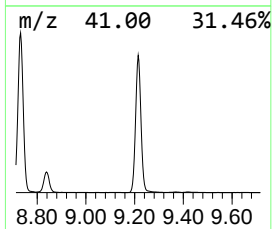
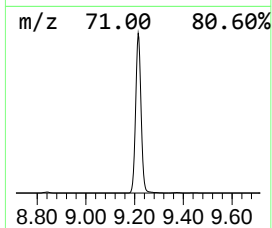
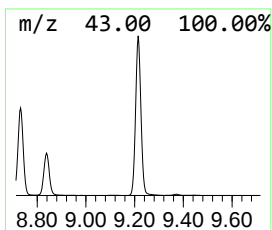
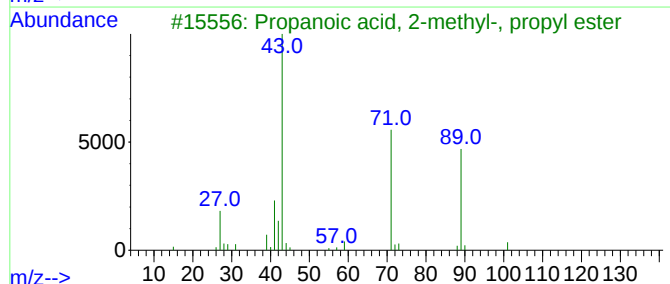
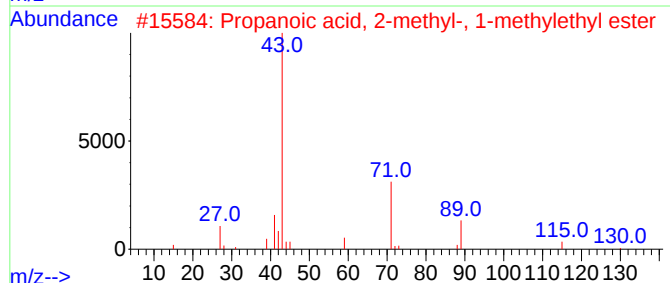
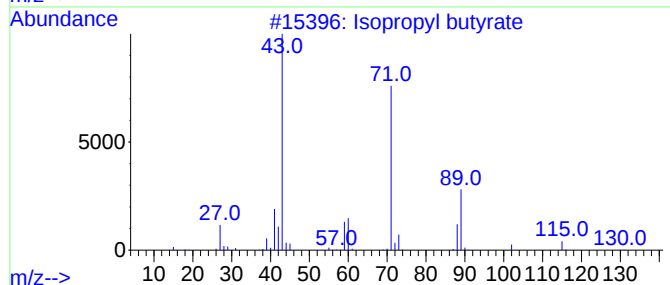
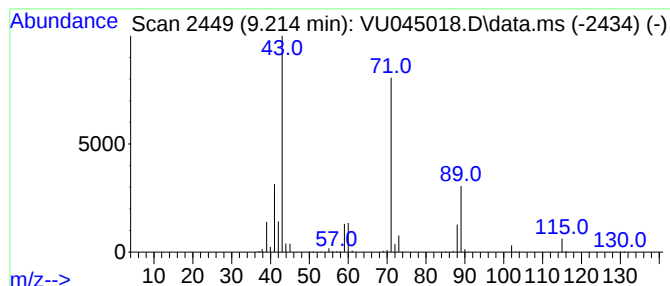
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Isopropyl butyrate Concentration Rank 3

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 9.214 | 117.41 ug/l | 2659610 | 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 : VU045018.D  
Acq On : 30 Sep 2021 01:53  
Operator : SY/MD  
Sample : PB139450ZHE#01  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 37 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#01

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   | 7.044 | 154.4   | ug/l  | 2972370  | 2                     | 6.253 | 962320  | 50.0 |
| Propanoic acid,... | 7.742 | 21.9    | ug/l  | 421548   | 2                     | 6.253 | 962320  | 50.0 |
| Butanoic acid, ... | 8.578 | 13.7    | ug/l  | 310661   | 3                     | 9.420 | 1132600 | 50.0 |
| Propanoic acid,... | 8.732 | 202.4   | ug/l  | 4584970  | 3                     | 9.420 | 1132600 | 50.0 |
| Acetic acid, bu... | 8.838 | 22.5    | ug/l  | 509199   | 3                     | 9.420 | 1132600 | 50.0 |
| Isopropyl butyrate | 9.214 | 117.4   | ug/l  | 2659610  | 3                     | 9.420 | 1132600 | 50.0 |