

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
 Data File : VU045021.D  
 Acq On : 30 Sep 2021 03:04  
 Operator : SY/MD  
 Sample : PB139450ZHE#04  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 40 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 PB139450ZHE#04

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: VU045021.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       | 389           | 401         | 415          | rBV      | 45805          | 77222         | 1.70%           | 0.412%        |
| 2         | 3.047       | 519           | 531         | 546          | rVB      | 27998          | 52965         | 1.17%           | 0.283%        |
| 3         | 5.292       | 1213          | 1229        | 1242         | rBV      | 176735         | 374573        | 8.27%           | 2.000%        |
| 4         | 5.375       | 1242          | 1255        | 1284         | rVB      | 311292         | 643440        | 14.20%          | 3.436%        |
| 5         | 5.703       | 1342          | 1357        | 1376         | rBV      | 219269         | 441717        | 9.75%           | 2.359%        |
| 6         | 5.915       | 1409          | 1423        | 1438         | rBV      | 24594          | 48839         | 1.08%           | 0.261%        |
| 7         | 6.253       | 1515          | 1528        | 1580         | rVB      | 494003         | 1039945       | 22.95%          | 5.554%        |
| 8         | 6.931       | 1717          | 1739        | 1757         | rBV3     | 22614          | 68808         | 1.52%           | 0.367%        |
| 9         | 7.044       | 1759          | 1774        | 1807         | rBV      | 1756070        | 3023378       | 66.73%          | 16.146%       |
| 10        | 7.742       | 1977          | 1991        | 2002         | rBV      | 255059         | 419216        | 9.25%           | 2.239%        |
| 11        | 7.902       | 2025          | 2041        | 2057         | rBV      | 741276         | 1286268       | 28.39%          | 6.869%        |
| 12        | 8.163       | 2111          | 2122        | 2135         | rBV2     | 28140          | 45911         | 1.01%           | 0.245%        |
| 13        | 8.468       | 2206          | 2217        | 2232         | rBV      | 67526          | 109494        | 2.42%           | 0.585%        |
| 14        | 8.578       | 2232          | 2251        | 2262         | rVV      | 184973         | 305839        | 6.75%           | 1.633%        |
| 15        | 8.732       | 2282          | 2299        | 2317         | rVV      | 2975998        | 4530444       | 100.00%         | 24.194%       |
| 16        | 8.838       | 2321          | 2332        | 2362         | rVB      | 312345         | 505698        | 11.16%          | 2.701%        |
| 17        | 9.214       | 2433          | 2449        | 2481         | rBV      | 1710246        | 2609266       | 57.59%          | 13.934%       |
| 18        | 9.420       | 2502          | 2513        | 2537         | rVB      | 703016         | 1130124       | 24.95%          | 6.035%        |
| 19        | 10.076      | 2706          | 2717        | 2731         | rBV      | 61491          | 95495         | 2.11%           | 0.510%        |
| 20        | 10.635      | 2879          | 2891        | 2913         | rBV      | 552954         | 852768        | 18.82%          | 4.554%        |
| 21        | 11.815      | 3245          | 3258        | 3280         | rBV      | 684078         | 1064349       | 23.49%          | 5.684%        |

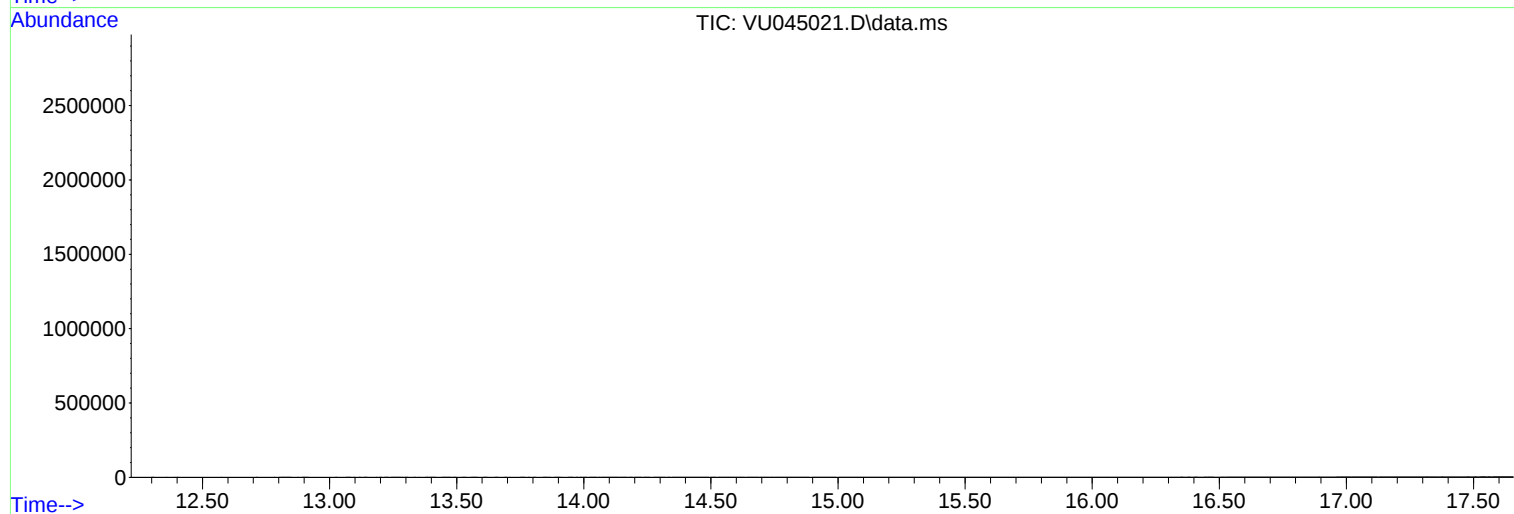
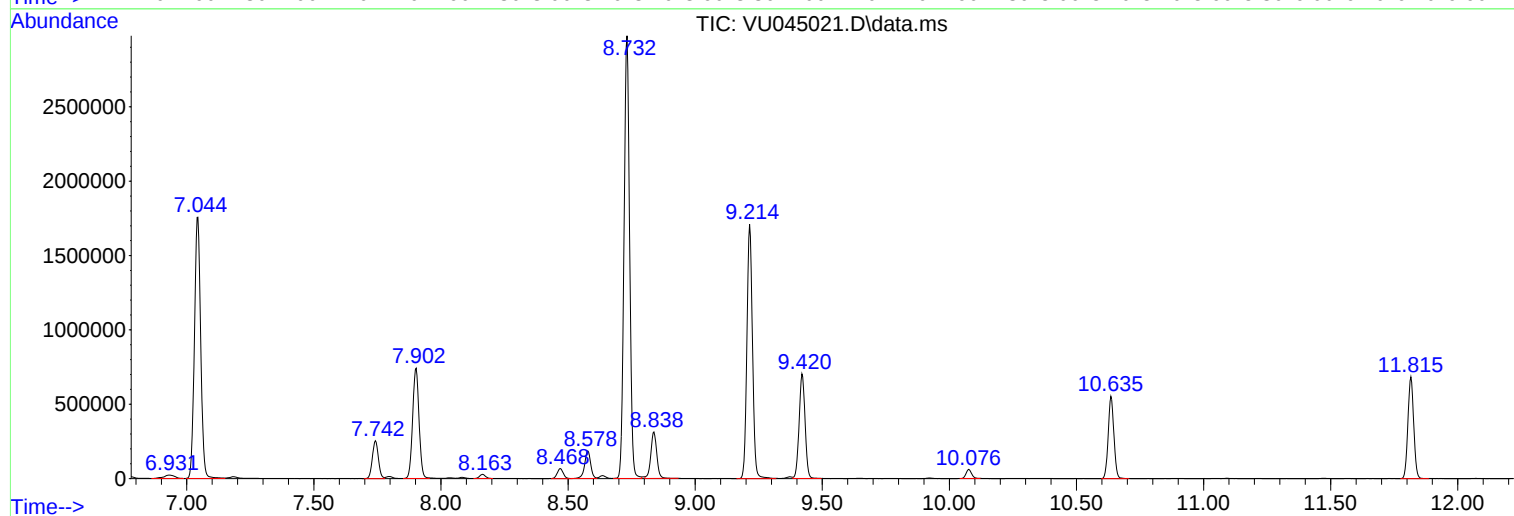
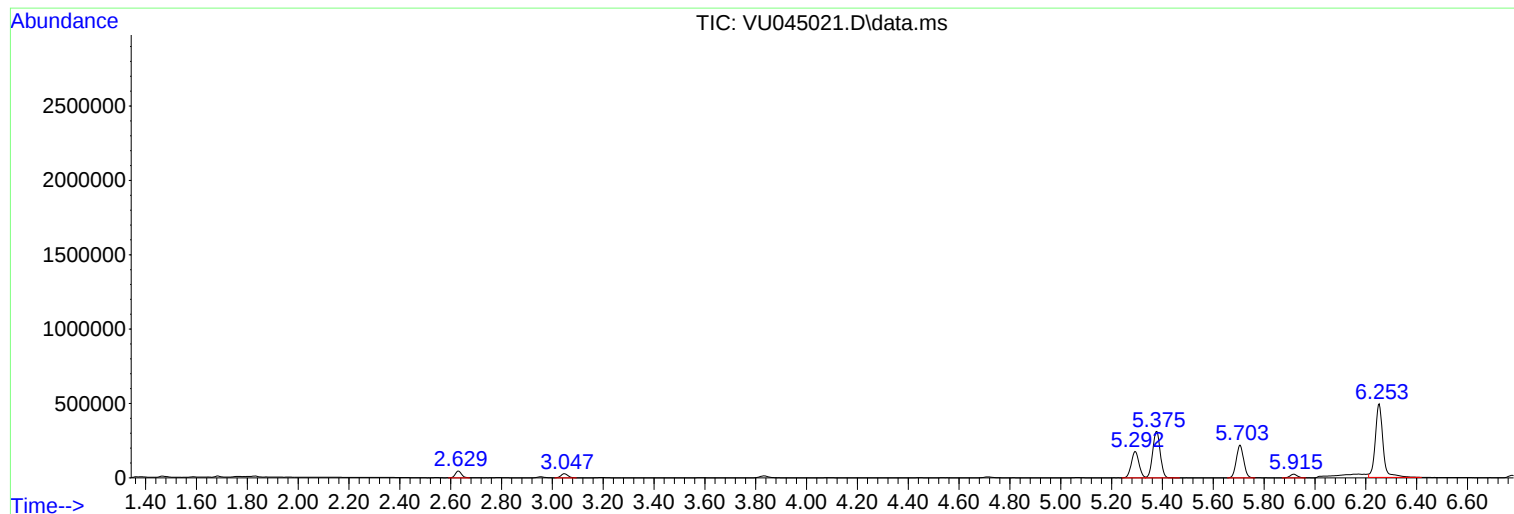
Sum of corrected areas: 18725759

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

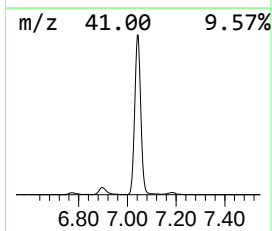
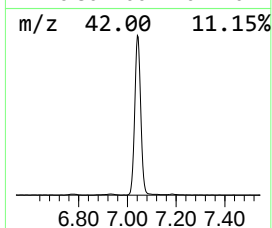
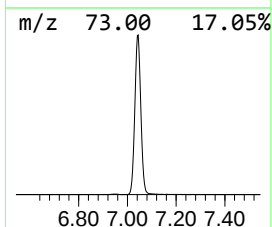
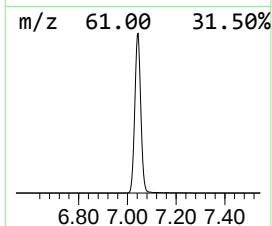
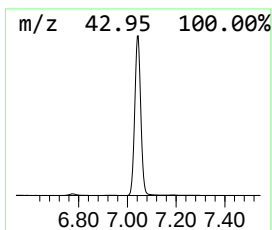
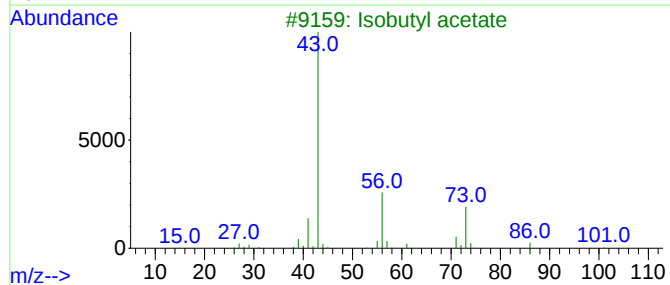
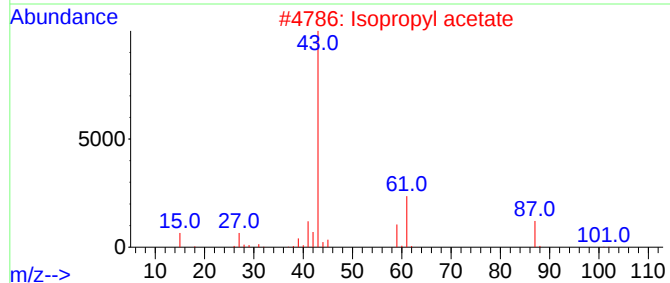
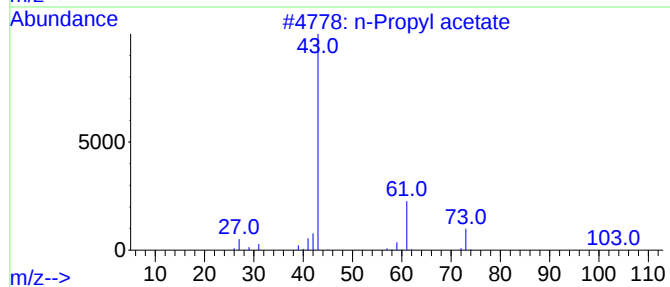
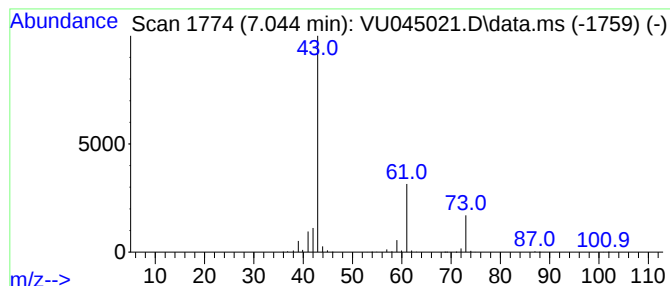
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 n-Propyl acetate Concentration Rank 2

| R.T.  | EstConc     | Area    | Relative to ISTD    | R.T.  |
|-------|-------------|---------|---------------------|-------|
| 7.044 | 145.36 ug/l | 3023380 | 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    |    |   | Isobutyl acetate               | 116 | C6H12O2 | 000110-19-0 | 9    |
| 4    |    |   | Propanal, 2,3-dihydroxy-, (S)- | 90  | C3H6O3  | 000497-09-6 | 9    |
| 5    |    |   | 1-Butanamine                   | 73  | C4H11N  | 000109-73-9 | 7    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

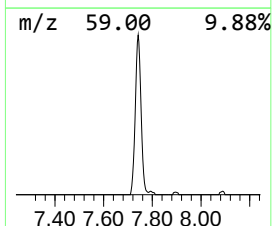
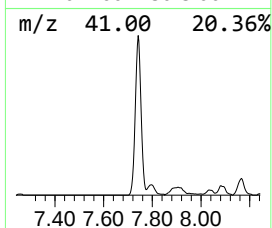
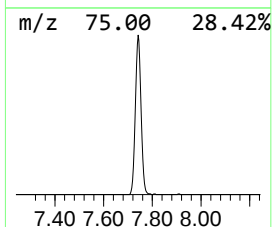
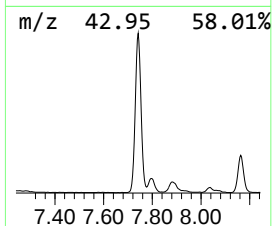
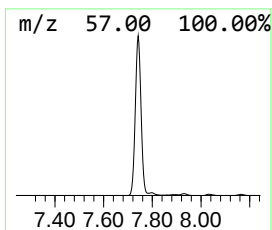
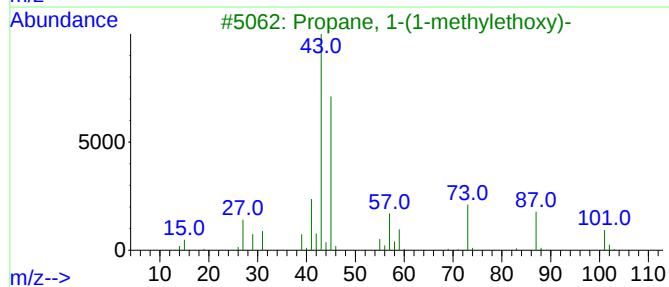
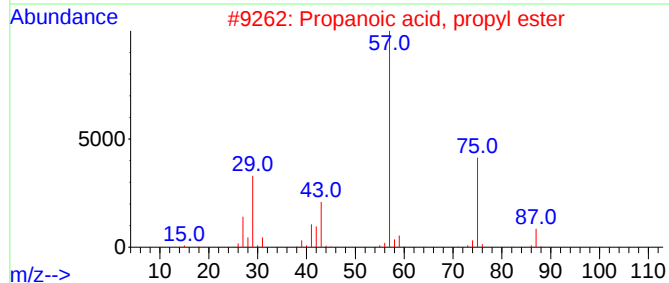
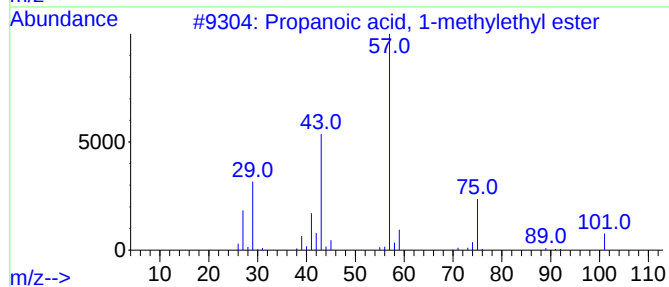
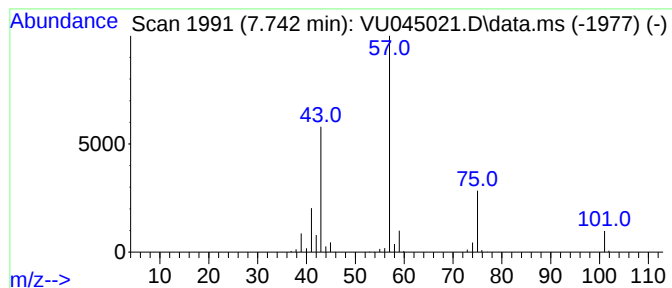
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 7.742 | 20.16 ug/l | 419216 | 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  | 40   |
| 3    |    |   | Propane, 1-(1-methylethoxy)-        | 102 | C6H14O  | 000627-08-7  | 25   |
| 4    |    |   | o-Isopropylhydroxylamine            | 75  | C3H9NO  | 1000322-42-6 | 9    |
| 5    |    |   | Butanoic acid, methyl ester         | 102 | C5H10O2 | 000623-42-7  | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

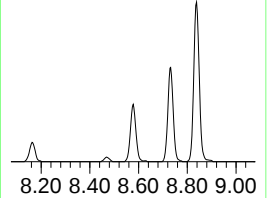
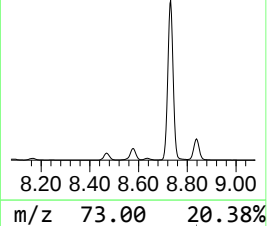
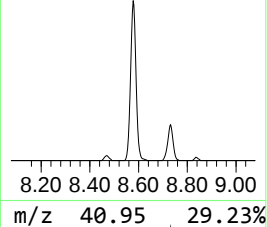
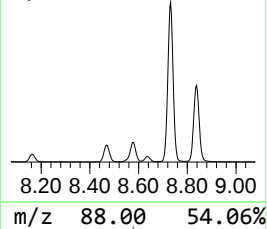
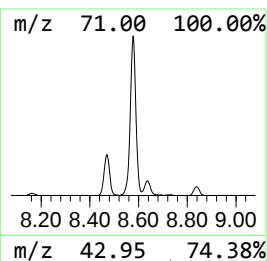
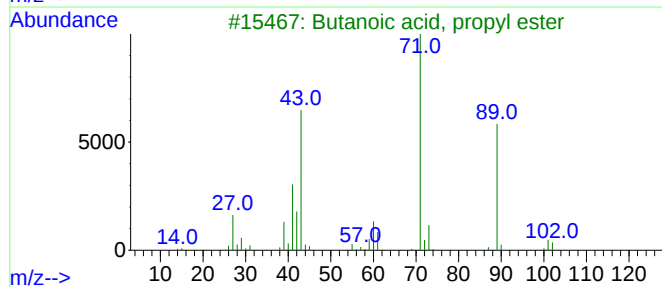
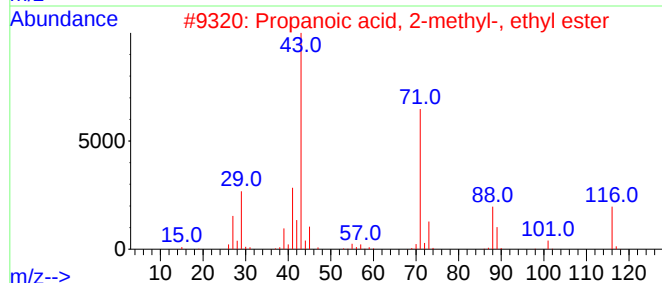
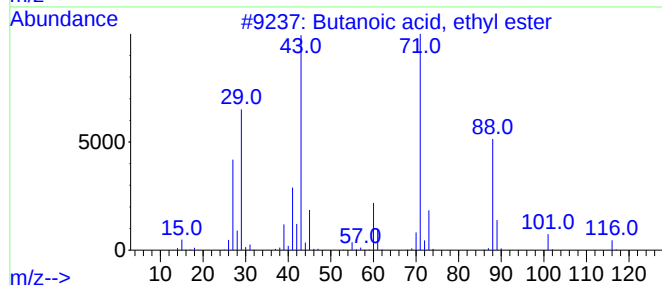
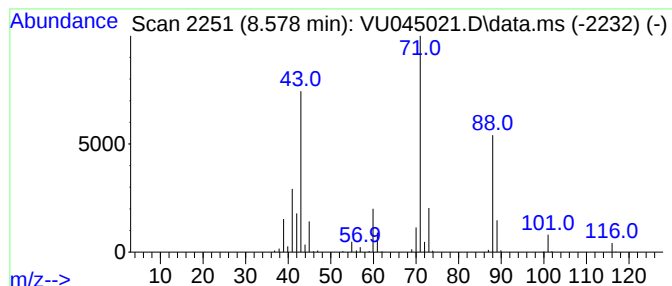
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.578 | 13.53 ug/l | 305839 | 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 | 50   |
| 3    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2   | 000105-66-8 | 47   |
| 4    |    |   | 3-Mercaptohexyl butanoate           | 204 | C10H20O2S | 136954-21-7 | 45   |
| 5    |    |   | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2   | 000097-85-8 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

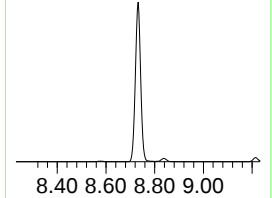
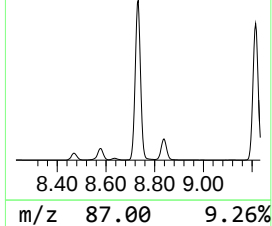
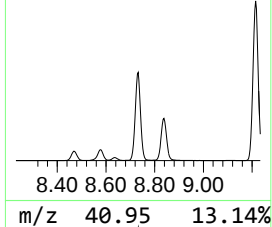
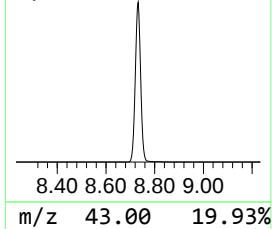
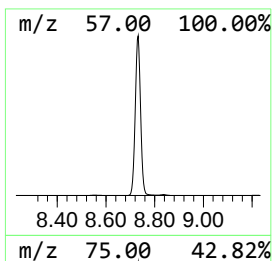
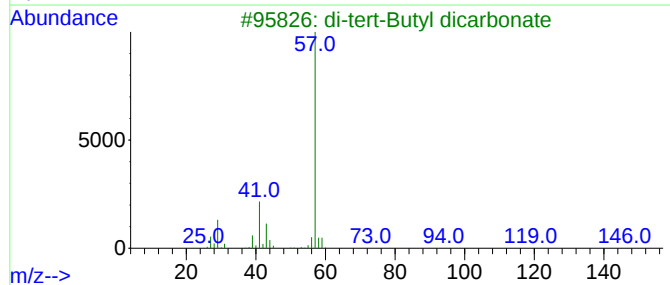
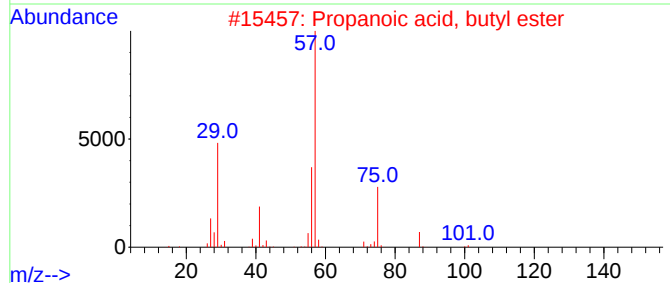
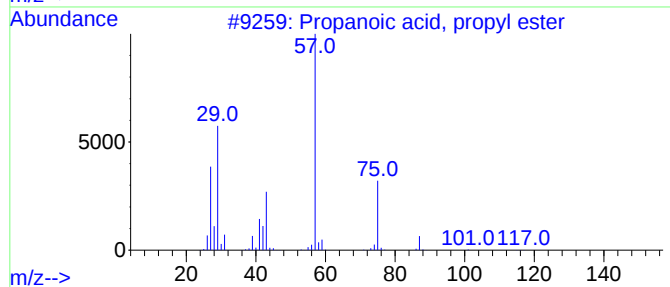
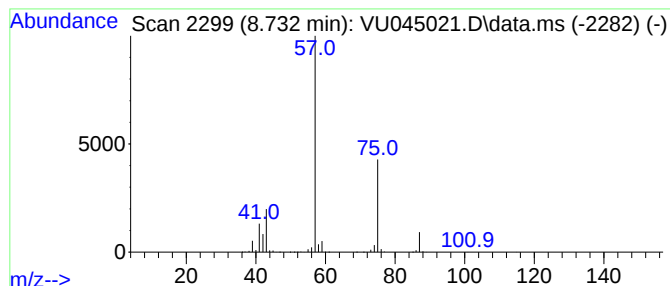
\*\*\*\*\*

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 8.732 | 200.44 ug/l | 4530440 | 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    |    |   | di-tert-Butyl dicarbonate    | 218 | C10H18O5 | 024424-99-5 | 9    |
| 4    |    |   | 2-(Isobutoxymethyl)oxirane   | 130 | C7H14O2  | 003814-55-9 | 9    |
| 5    |    |   | 1-Butanamine, 3-methyl-      | 87  | C5H13N   | 000107-85-7 | 7    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

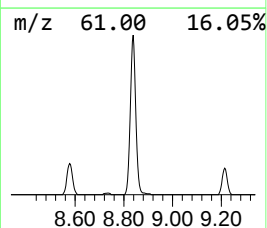
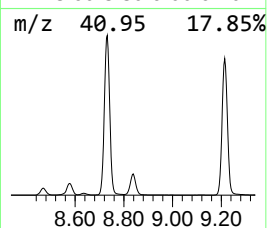
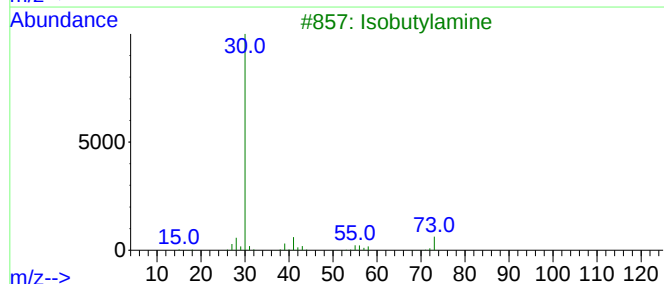
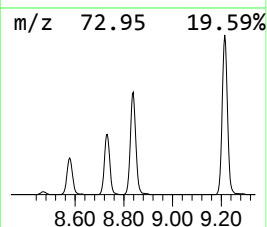
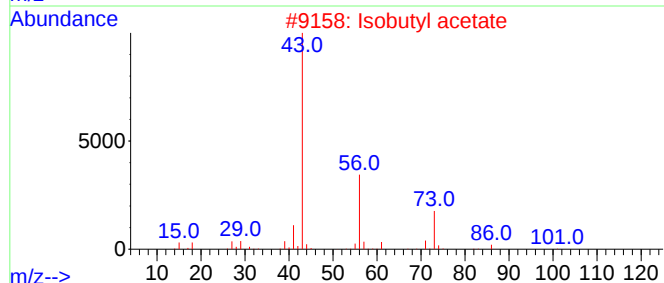
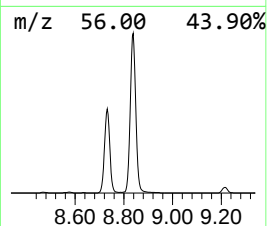
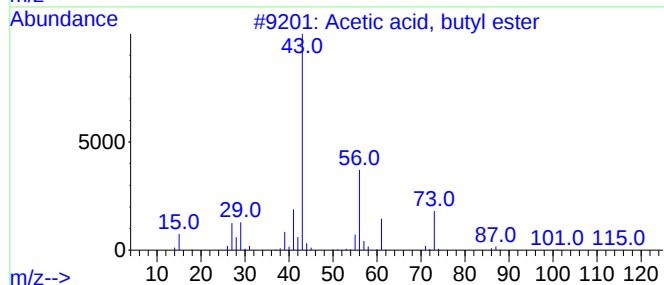
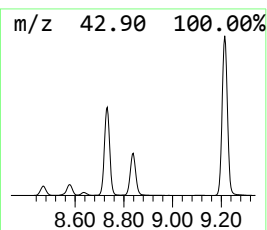
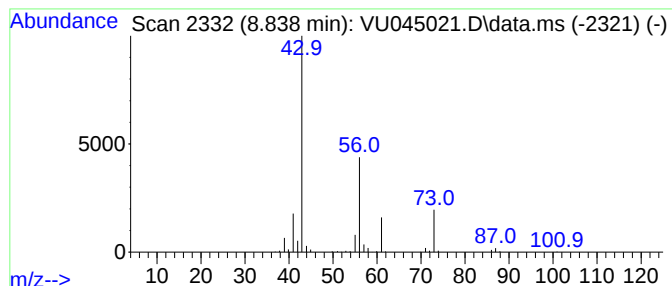
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 8.838 | 22.37 ug/l | 505698 | 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         | Isobutylamine            | 73  | C4H11N  | 000078-81-9 | 9    |
| 4         | n-Propyl acetate         | 102 | C5H10O2 | 000109-60-4 | 9    |
| 5         | 2-Butanone, 3-methyl-    | 86  | C5H10O  | 000563-80-4 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

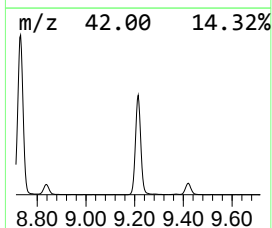
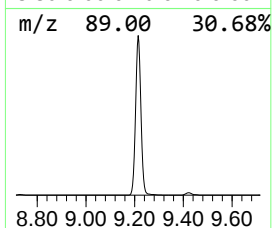
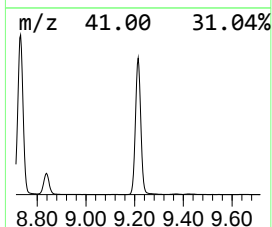
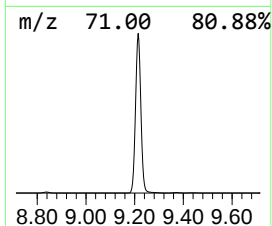
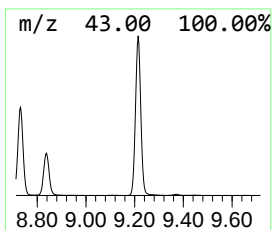
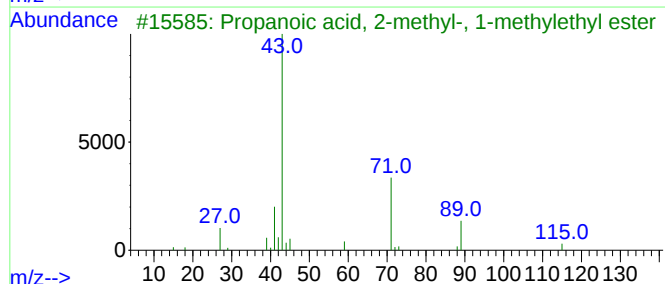
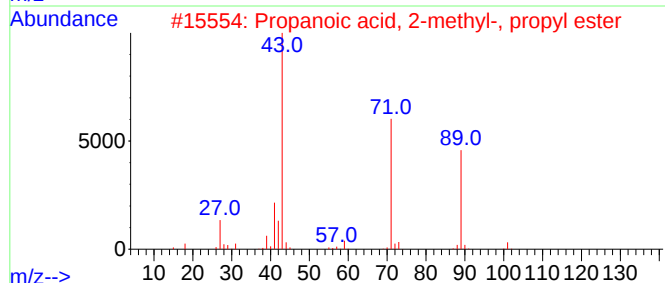
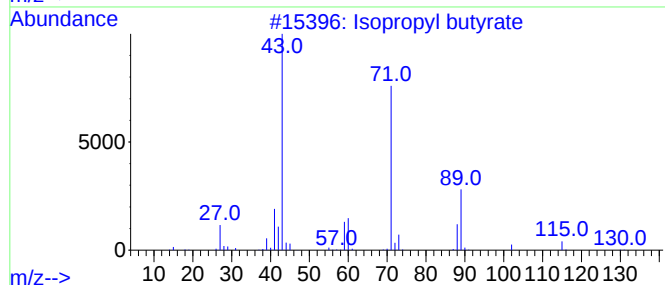
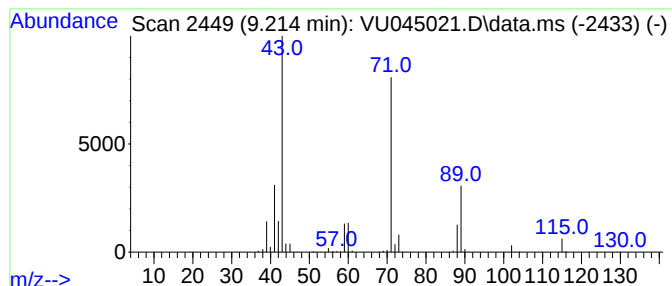
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 6 Isopropyl butyrate Concentration Rank 3

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.  |
|-------|-------------|---------|------------------|-------|
| 9.214 | 115.44 ug/l | 2609270 | 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... | 130 | C7H14O2 | 000644-49-5  | 72   |
| 3    |    |   | Propanoic acid, 2-methyl-, 1-met...  | 130 | C7H14O2 | 000617-50-5  | 64   |
| 4    |    |   | Ethylene glycol Formate Isobutyrate  | 160 | C7H12O4 | 1000458-48-0 | 64   |
| 5    |    |   | Butanoic acid, pentyl ester          | 158 | C9H18O2 | 000540-18-1  | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092921\  
Data File : VU045021.D  
Acq On : 30 Sep 2021 03:04  
Operator : SY/MD  
Sample : PB139450ZHE#04  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 40 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PB139450ZHE#04

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

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                    |       |         |       |          | #                     | RT    | Resp    | Conc |
| n-Propyl acetate   | 7.044 | 145.4   | ug/l  | 3023380  | 2                     | 6.253 | 1039950 | 50.0 |
| Propanoic acid,... | 7.742 | 20.2    | ug/l  | 419216   | 2                     | 6.253 | 1039950 | 50.0 |
| Butanoic acid, ... | 8.578 | 13.5    | ug/l  | 305839   | 3                     | 9.420 | 1130120 | 50.0 |
| Propanoic acid,... | 8.732 | 200.4   | ug/l  | 4530440  | 3                     | 9.420 | 1130120 | 50.0 |
| Acetic acid, bu... | 8.838 | 22.4    | ug/l  | 505698   | 3                     | 9.420 | 1130120 | 50.0 |
| Isopropyl butyrate | 9.214 | 115.4   | ug/l  | 2609270  | 3                     | 9.420 | 1130120 | 50.0 |