

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040422\  
 Data File : VX027968.D  
 Acq On : 04 Apr 2022 19:17  
 Operator : JC/MD  
 Sample : PB143824ZHE#05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 PB143824ZHE#05

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\_X\Method\82X032922W.M  
 Title : SW846 8260

Signal : TIC: VX027968.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         | 1.246       | 22            | 26          | 32           | rBV      | 15168          | 21467         | 1.56%           | 0.328%        |
| 2         | 2.788       | 271           | 279         | 292          | rBV      | 153131         | 277810        | 20.20%          | 4.249%        |
| 3         | 3.574       | 400           | 408         | 419          | rBV2     | 6835           | 15158         | 1.10%           | 0.232%        |
| 4         | 5.391       | 695           | 706         | 722          | rBV      | 55414          | 161706        | 11.76%          | 2.473%        |
| 5         | 5.556       | 722           | 733         | 748          | rVB      | 97944          | 275494        | 20.03%          | 4.213%        |
| 6         | 5.958       | 789           | 799         | 813          | rBV2     | 55083          | 150325        | 10.93%          | 2.299%        |
| 7         | 6.342       | 855           | 862         | 879          | rVB3     | 5914           | 15914         | 1.16%           | 0.243%        |
| 8         | 6.702       | 915           | 921         | 923          | rBV2     | 6814           | 14554         | 1.06%           | 0.223%        |
| 9         | 6.763       | 923           | 931         | 945          | rVB      | 150005         | 372129        | 27.06%          | 5.691%        |
| 10        | 7.799       | 1093          | 1101        | 1118         | rBV      | 576467         | 977986        | 71.11%          | 14.957%       |
| 11        | 8.549       | 1217          | 1224        | 1234         | rBV      | 89062          | 141498        | 10.29%          | 2.164%        |
| 12        | 8.653       | 1234          | 1241        | 1251         | rBV      | 295620         | 472577        | 34.36%          | 7.228%        |
| 13        | 8.958       | 1286          | 1291        | 1298         | rVB      | 10019          | 15041         | 1.09%           | 0.230%        |
| 14        | 9.244       | 1333          | 1338        | 1344         | rBV      | 24233          | 35404         | 2.57%           | 0.541%        |
| 15        | 9.348       | 1350          | 1355        | 1359         | rBV      | 62425          | 84360         | 6.13%           | 1.290%        |
| 16        | 9.488       | 1371          | 1378        | 1384         | rBV      | 1019534        | 1375222       | 100.00%         | 21.033%       |
| 17        | 9.579       | 1388          | 1393        | 1403         | rVB      | 120347         | 156364        | 11.37%          | 2.391%        |
| 18        | 9.915       | 1442          | 1448        | 1463         | rBV      | 666787         | 822429        | 59.80%          | 12.578%       |
| 19        | 10.055      | 1465          | 1471        | 1478         | rBV      | 318792         | 419426        | 30.50%          | 6.415%        |
| 20        | 10.640      | 1562          | 1567        | 1577         | rBV      | 25574          | 30895         | 2.25%           | 0.473%        |
| 21        | 11.085      | 1634          | 1640        | 1649         | rBV      | 267340         | 345548        | 25.13%          | 5.285%        |
| 22        | 12.024      | 1788          | 1794        | 1806         | rBV      | 288187         | 357211        | 25.97%          | 5.463%        |

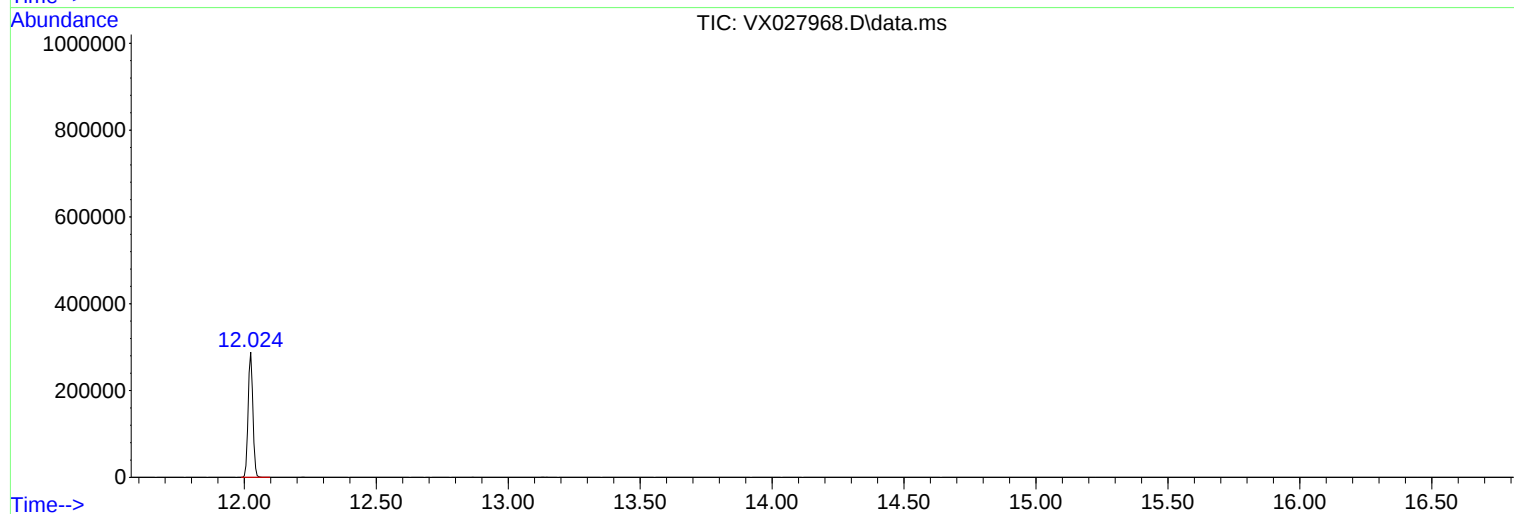
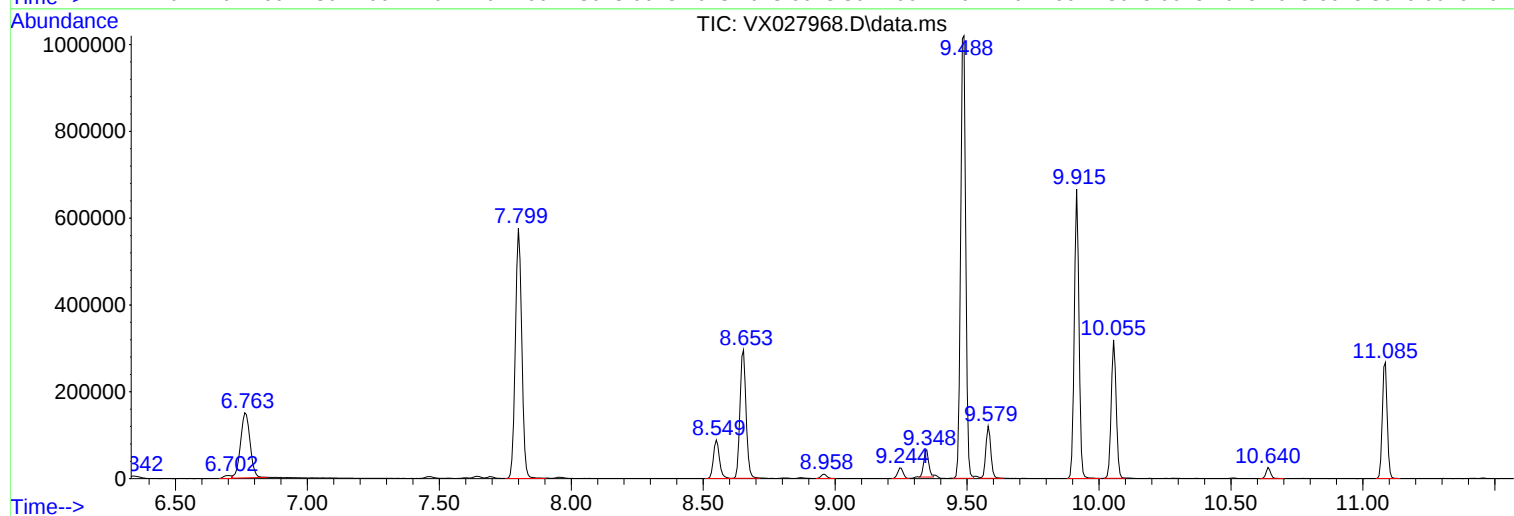
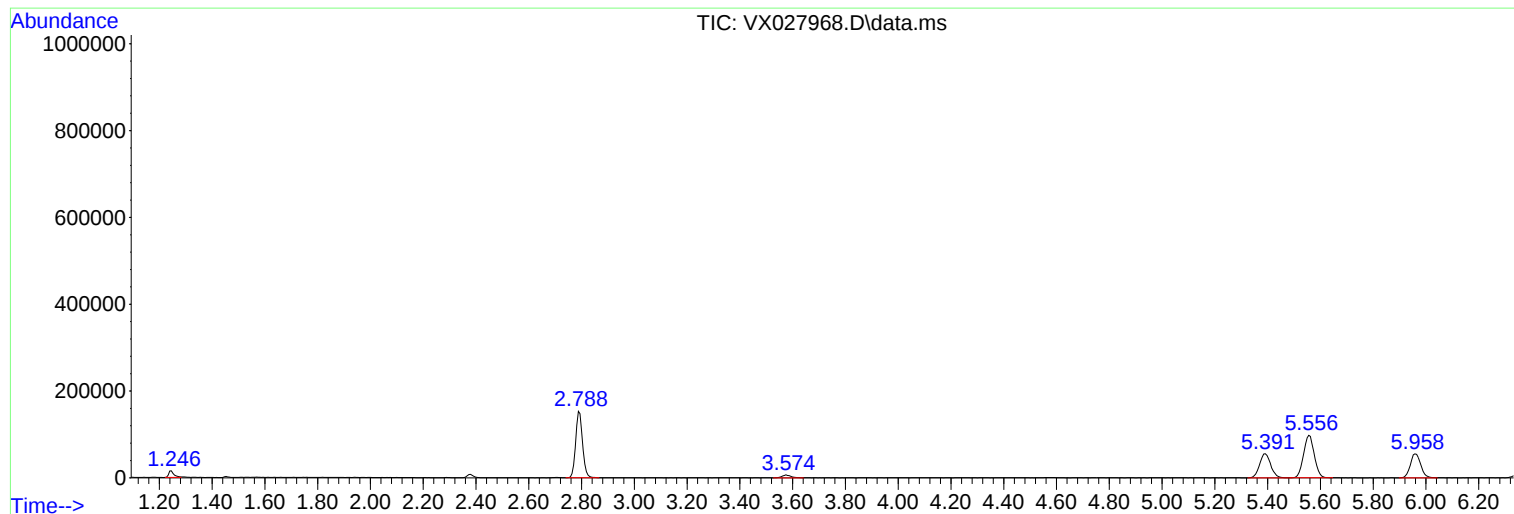
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ClientSampleId :  
PB143824ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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



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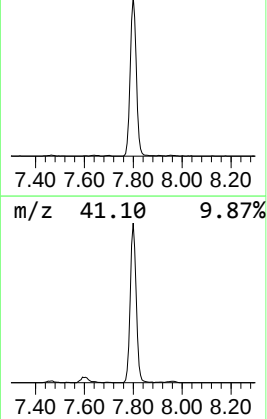
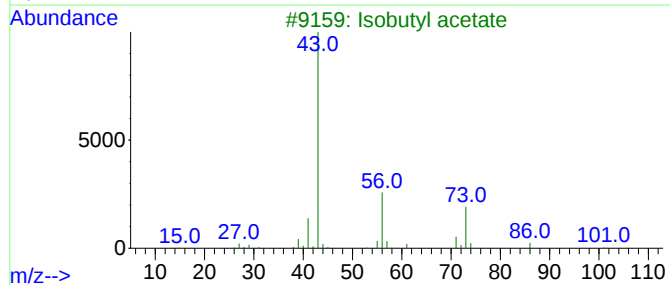
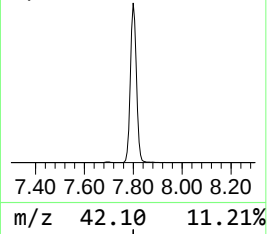
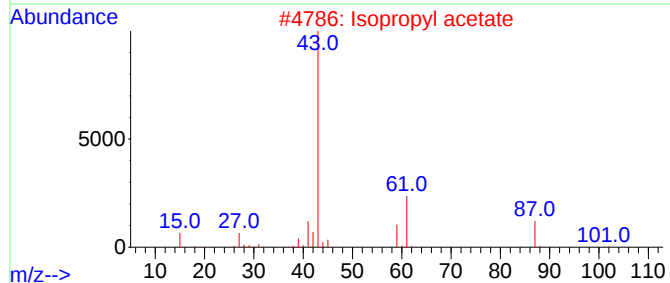
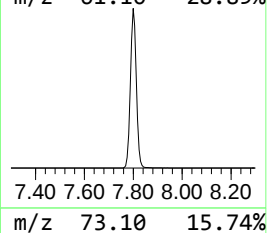
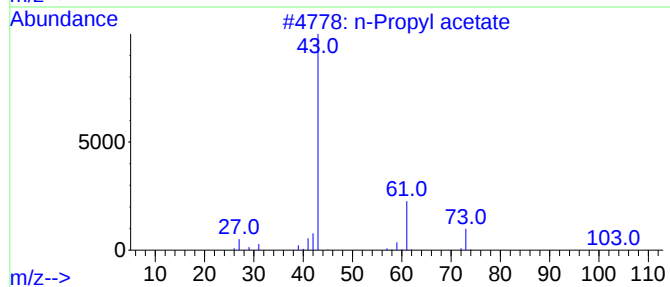
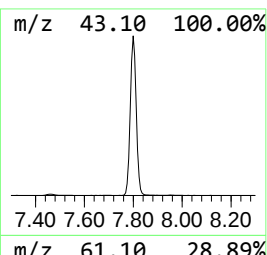
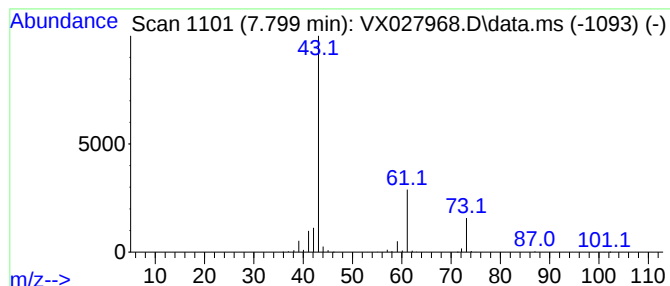
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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.  |
|-------|-------------|--------|---------------------|-------|
| 7.799 | 131.40 ug/l | 977986 | 1,4-Difluorobenzene | 6.763 |

| 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    |      | 1-Butanamine      | 73  | C4H11N  | 000109-73-9 | 5    |
| 5    |      | Isobutylamine     | 73  | C4H11N  | 000078-81-9 | 5    |



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MSVOA\_X  
ClientSampleId :  
PB143824ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

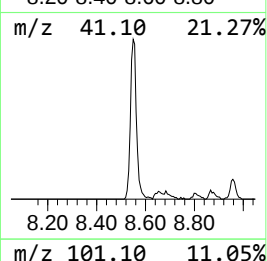
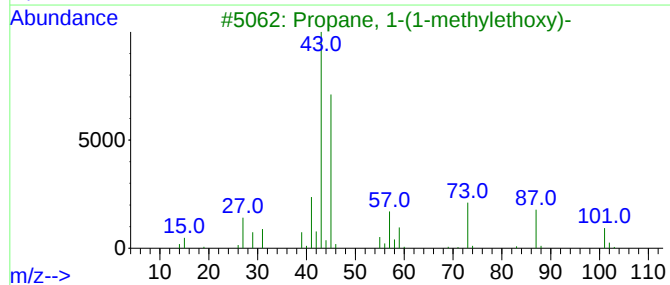
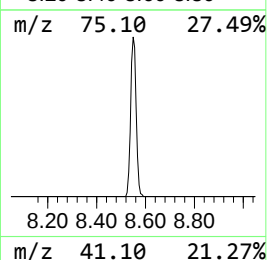
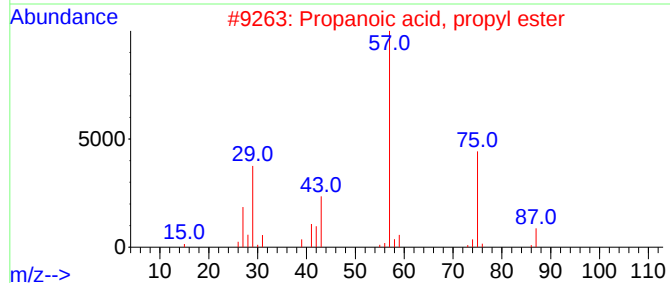
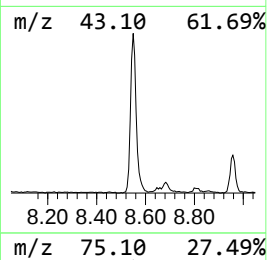
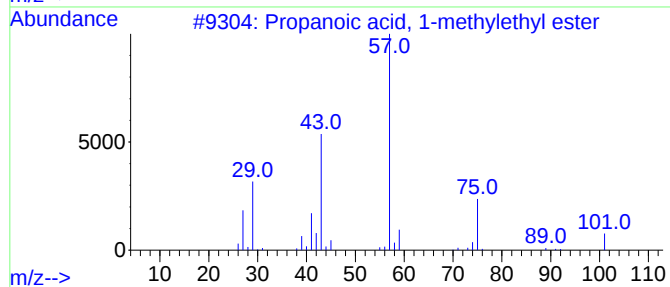
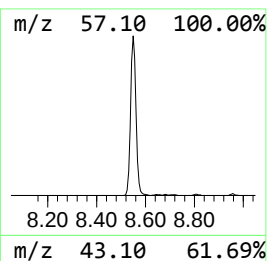
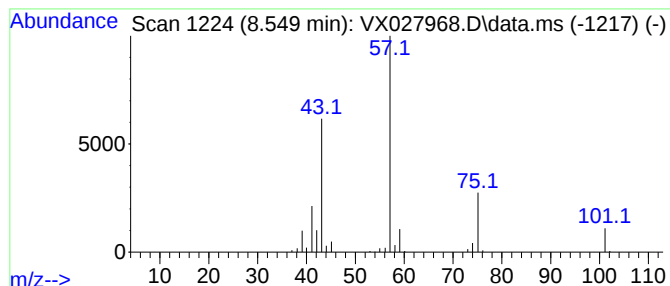
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.   |
|-------|------------|--------|------------------|--------|
| 8.549 | 16.87 ug/l | 141498 | Chlorobenzene-d5 | 10.055 |

| 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    |    |   | Propane, 1-(1-methylethoxy)-        | 102 | C6H14O  | 000627-08-7 | 23   |
| 4    |    |   | Azetidine                           | 57  | C3H7N   | 000503-29-7 | 12   |
| 5    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO | 000109-02-4 | 9    |



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ALS Vial : 23 Sample Multiplier: 1

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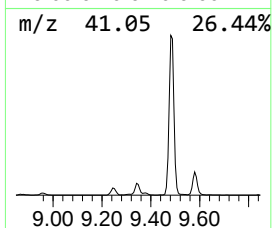
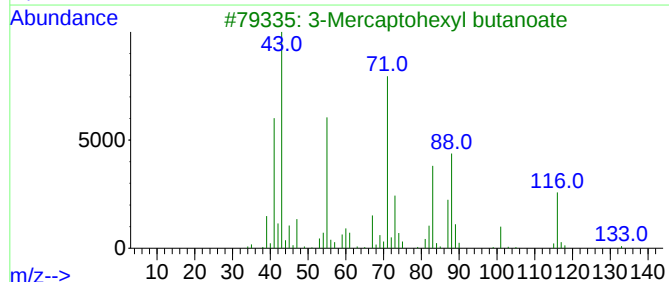
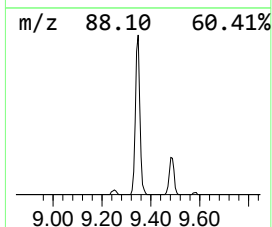
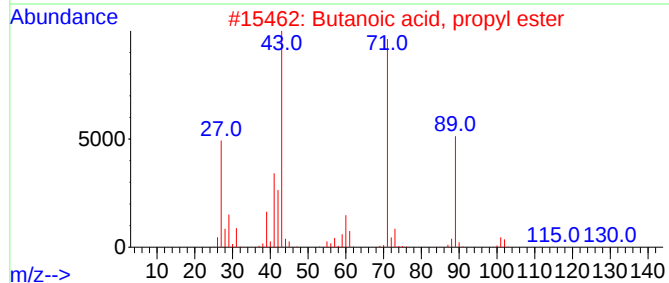
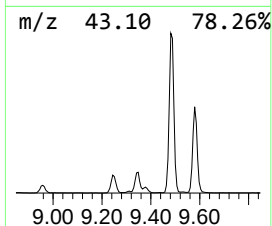
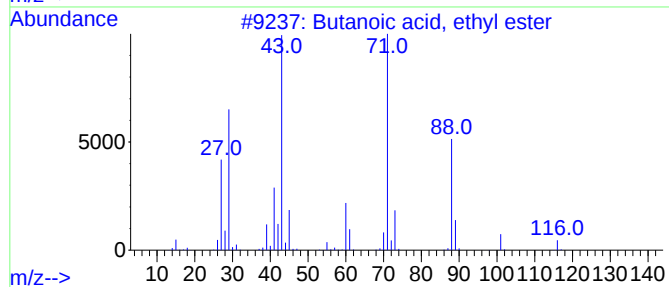
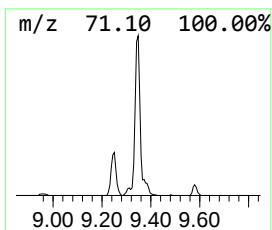
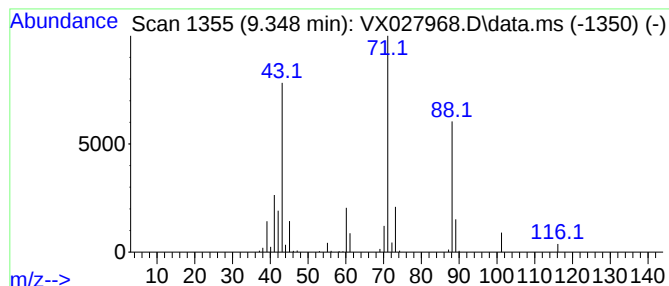
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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.   |
|-------|------------|-------|------------------|--------|
| 9.348 | 10.06 ug/l | 84360 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Butanoic acid, ethyl ester          | 116 | C6H12O2   | 000105-54-4 | 94   |
| 2    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2   | 000105-66-8 | 50   |
| 3    |    |   | 3-Mercaptohexyl butanoate           | 204 | C10H20O2S | 136954-21-7 | 42   |
| 4    |    |   | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2   | 000097-62-1 | 42   |
| 5    |    |   | 4-Butoxy-2-butanone                 | 144 | C8H16O2   | 030536-44-8 | 38   |



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ALS Vial : 23 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
PB143824ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

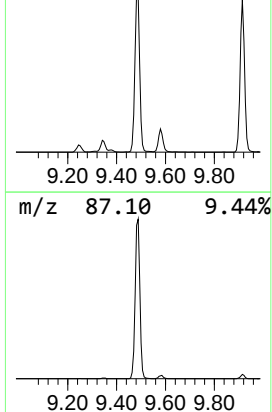
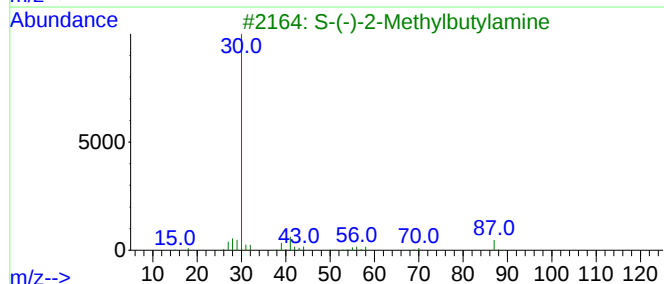
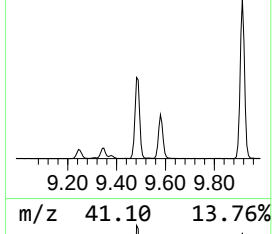
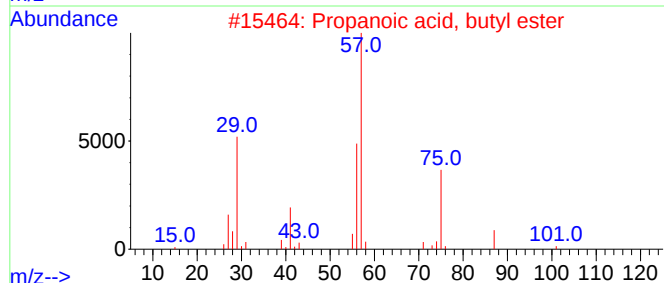
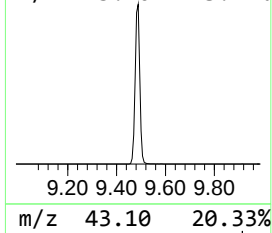
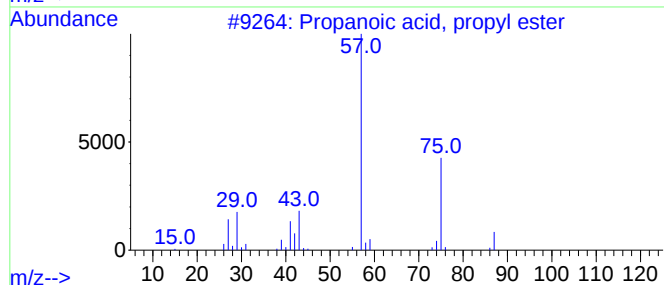
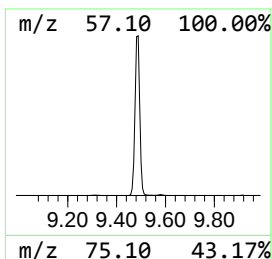
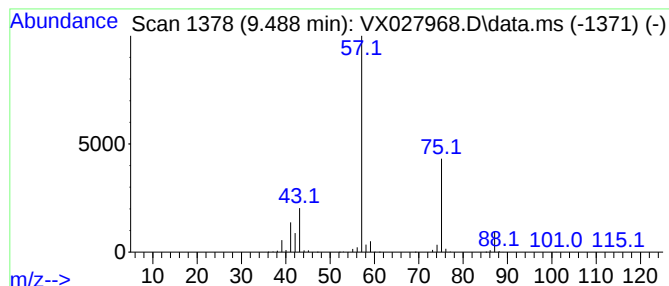
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.   |
|-------|-------------|---------|------------------|--------|
| 9.488 | 163.94 ug/l | 1375220 | Chlorobenzene-d5 | 10.055 |

| 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 | 40   |
| 3    |    |   | S-(-)-2-Methylbutylamine     | 87  | C5H13N  | 020626-52-2 | 9    |
| 4    |    |   | 2-(Isobutoxymethyl)oxirane   | 130 | C7H14O2 | 003814-55-9 | 9    |
| 5    |    |   | 1-Butanamine, 3-methyl-      | 87  | C5H13N  | 000107-85-7 | 7    |



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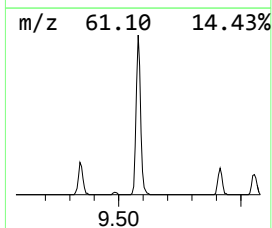
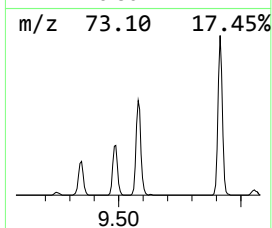
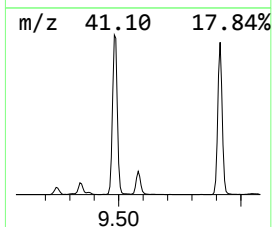
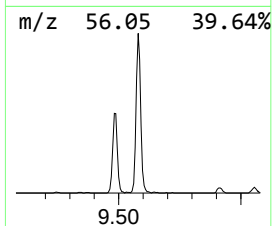
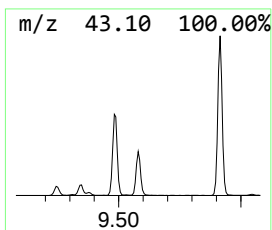
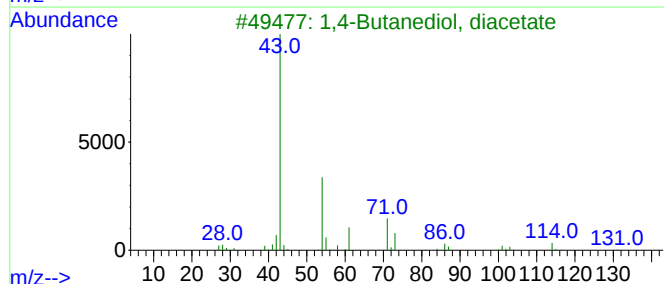
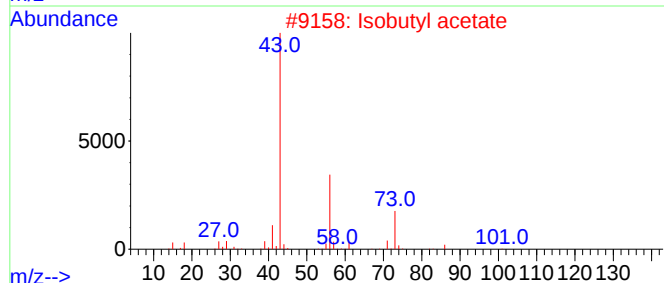
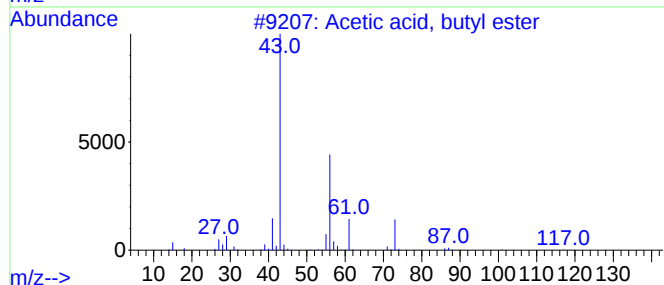
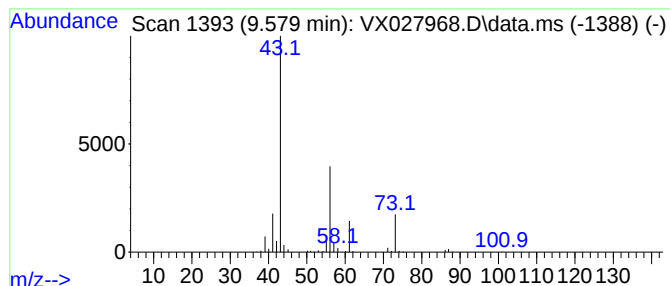
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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

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Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.   |
|-------|------------|--------|------------------|--------|
| 9.579 | 18.64 ug/l | 156364 | Chlorobenzene-d5 | 10.055 |

| 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 | 17   |
| 4    |    |   | Isobutylamine             | 73  | C4H11N  | 000078-81-9 | 9    |
| 5    |    |   | Pentanoic acid, 4-oxo-    | 116 | C5H8O3  | 000123-76-2 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VO040422\  
Data File : VX027968.D  
Acq On : 04 Apr 2022 19:17  
Operator : JC/MD  
Sample : PB143824ZHE#05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#05

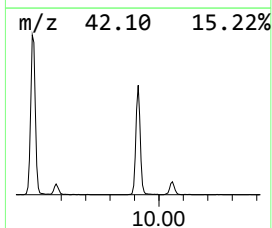
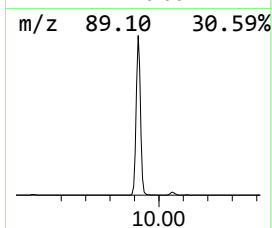
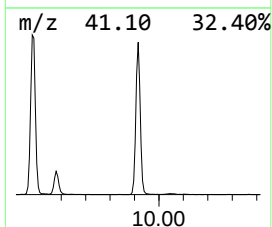
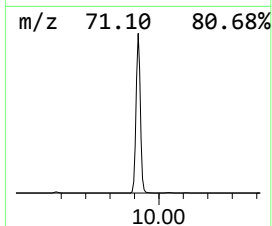
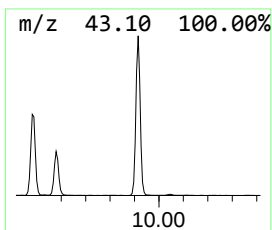
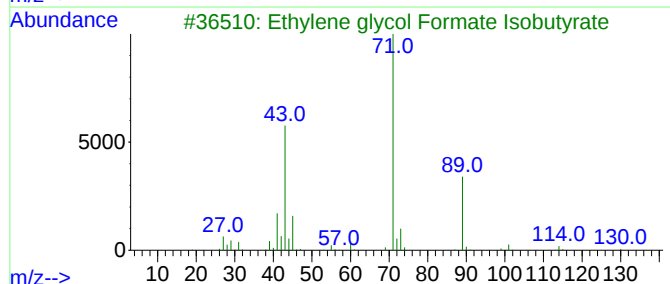
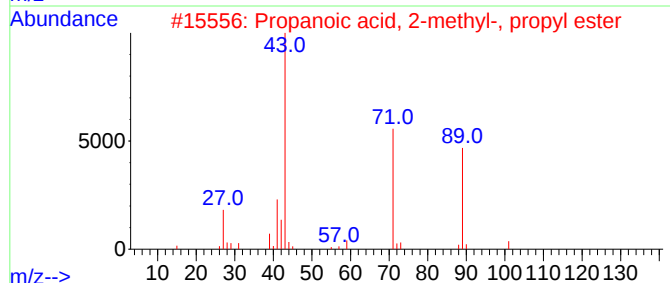
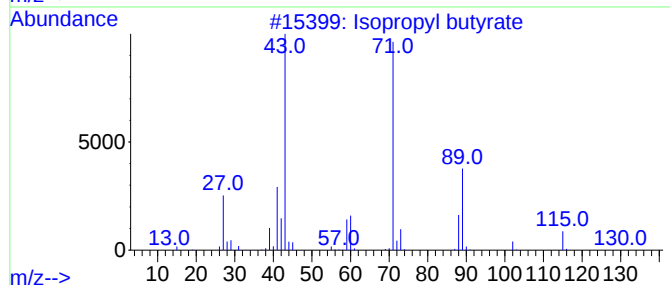
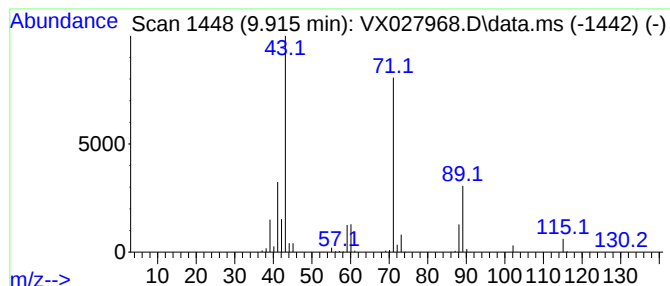
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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.   |
|-------|------------|--------|------------------|--------|
| 9.915 | 98.04 ug/l | 822429 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Isopropyl butyrate                  | 130 | C7H14O2 | 000638-11-9  | 91   |
| 2    |    |   | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5  | 72   |
| 3    |    |   | Ethylene glycol Formate Isobutyrate | 160 | C7H12O4 | 1000458-48-0 | 64   |
| 4    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2 | 000105-66-8  | 64   |
| 5    |    |   | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5  | 64   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040422\  
Data File : VX027968.D  
Acq On : 04 Apr 2022 19:17  
Operator : JC/MD  
Sample : PB143824ZHE#05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.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   | 7.799 | 131.4   | ug/l  | 977986   | 2                     | 6.763  | 372129 | 50.0 |
| Propanoic acid,... | 8.549 | 16.9    | ug/l  | 141498   | 3                     | 10.055 | 419426 | 50.0 |
| Butanoic acid, ... | 9.348 | 10.1    | ug/l  | 84360    | 3                     | 10.055 | 419426 | 50.0 |
| Propanoic acid,... | 9.488 | 163.9   | ug/l  | 1375220  | 3                     | 10.055 | 419426 | 50.0 |
| Acetic acid, bu... | 9.579 | 18.6    | ug/l  | 156364   | 3                     | 10.055 | 419426 | 50.0 |
| Isopropyl butyrate | 9.915 | 98.0    | ug/l  | 822429   | 3                     | 10.055 | 419426 | 50.0 |