

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040422\  
 Data File : VX027965.D  
 Acq On : 04 Apr 2022 18:07  
 Operator : JC/MD  
 Sample : PB143824ZHE#02  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 PB143824ZHE#02

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: VX027965.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         | 1.240       | 22            | 25          | 38           | rBV      | 25066          | 34142         | 2.64%           | 0.553%        |
| 2         | 2.788       | 272           | 279         | 289          | rBV      | 83808          | 153577        | 11.86%          | 2.490%        |
| 3         | 5.391       | 695           | 706         | 718          | rBV2     | 54710          | 157317        | 12.15%          | 2.550%        |
| 4         | 5.556       | 722           | 733         | 751          | rVB      | 98547          | 277864        | 21.46%          | 4.505%        |
| 5         | 5.958       | 790           | 799         | 812          | rBV      | 57398          | 152280        | 11.76%          | 2.469%        |
| 6         | 6.342       | 852           | 862         | 875          | rBV2     | 5222           | 14245         | 1.10%           | 0.231%        |
| 7         | 6.696       | 915           | 920         | 923          | rBV3     | 6584           | 14264         | 1.10%           | 0.231%        |
| 8         | 6.763       | 923           | 931         | 944          | rVB      | 146629         | 355273        | 27.43%          | 5.759%        |
| 9         | 7.799       | 1093          | 1101        | 1114         | rBV      | 552412         | 921855        | 71.18%          | 14.944%       |
| 10        | 8.549       | 1217          | 1224        | 1233         | rBV      | 85320          | 131487        | 10.15%          | 2.132%        |
| 11        | 8.653       | 1234          | 1241        | 1250         | rBV      | 297953         | 464597        | 35.88%          | 7.532%        |
| 12        | 8.958       | 1285          | 1291        | 1296         | rBV      | 9255           | 13733         | 1.06%           | 0.223%        |
| 13        | 9.244       | 1332          | 1338        | 1345         | rBV      | 22717          | 33877         | 2.62%           | 0.549%        |
| 14        | 9.342       | 1350          | 1354        | 1358         | rVV      | 60263          | 86336         | 6.67%           | 1.400%        |
| 15        | 9.482       | 1372          | 1377        | 1384         | rBV      | 970096         | 1295032       | 100.00%         | 20.994%       |
| 16        | 9.580       | 1388          | 1393        | 1404         | rVB      | 114489         | 145930        | 11.27%          | 2.366%        |
| 17        | 9.915       | 1442          | 1448        | 1459         | rBV      | 610736         | 776701        | 59.98%          | 12.591%       |
| 18        | 10.055      | 1465          | 1471        | 1478         | rBV      | 308349         | 409358        | 31.61%          | 6.636%        |
| 19        | 10.640      | 1562          | 1567        | 1572         | rBV      | 24008          | 29140         | 2.25%           | 0.472%        |
| 20        | 11.079      | 1634          | 1639        | 1654         | rVB      | 257733         | 341454        | 26.37%          | 5.535%        |
| 21        | 12.024      | 1789          | 1794        | 1805         | rVB      | 297742         | 360078        | 27.80%          | 5.837%        |

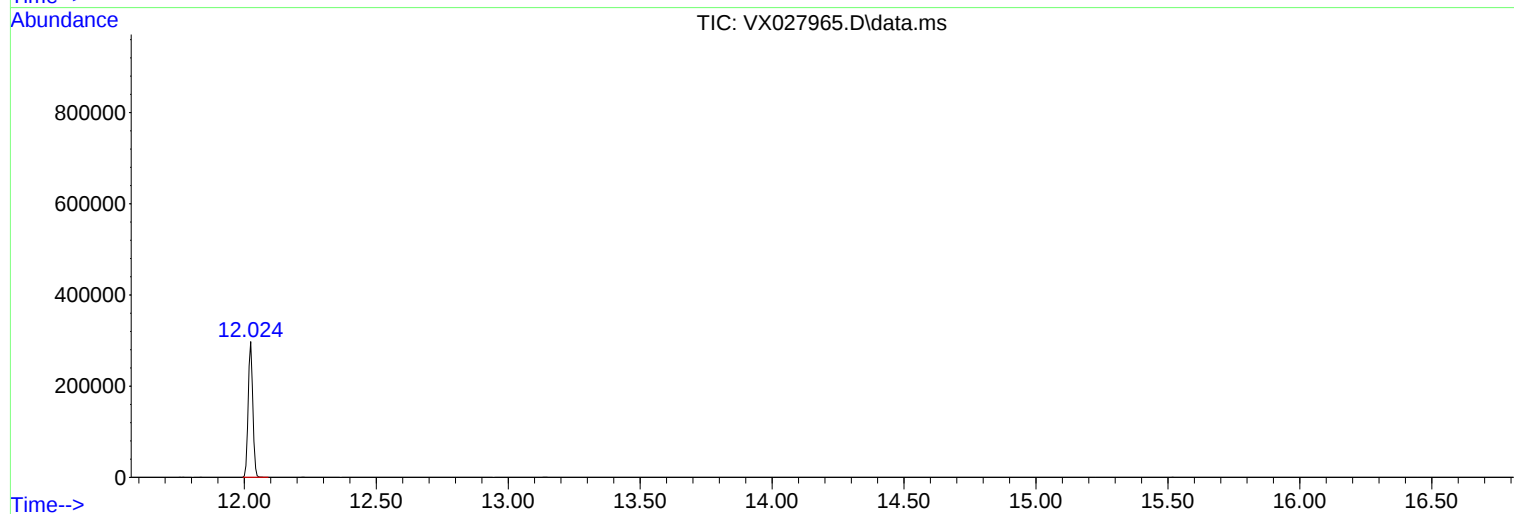
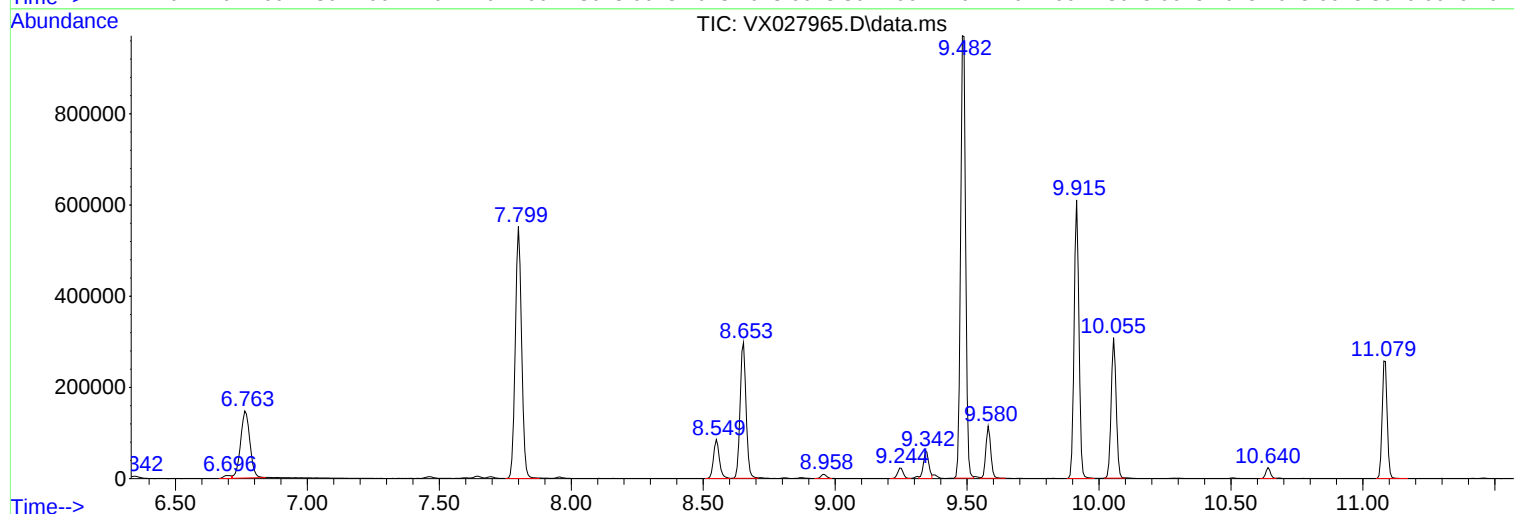
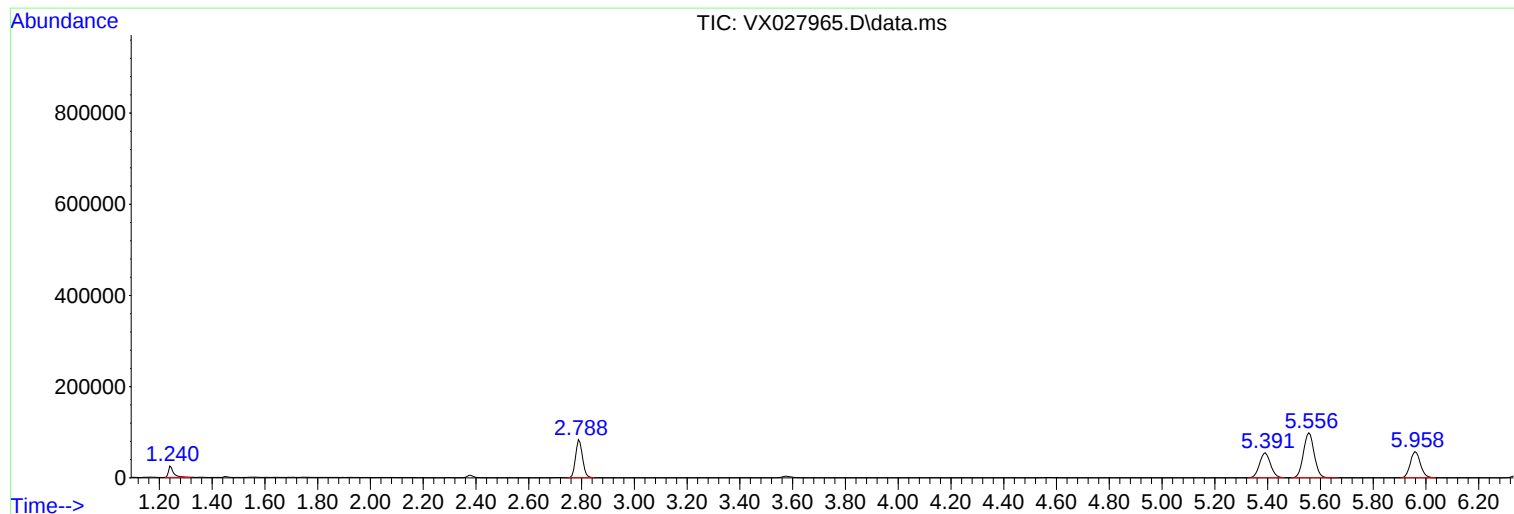
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Sample : PB143824ZHE#02  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#02

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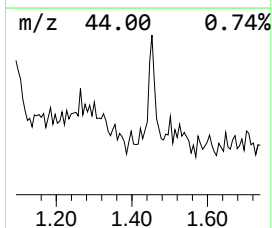
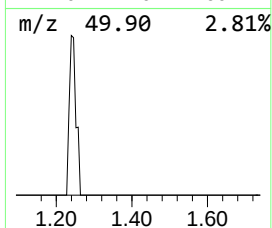
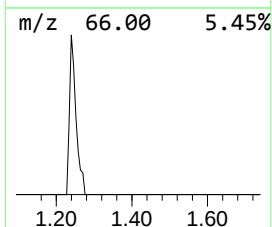
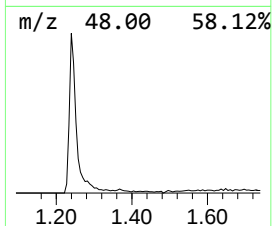
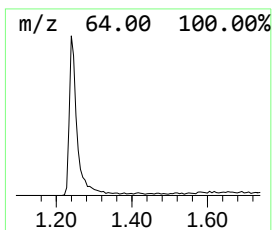
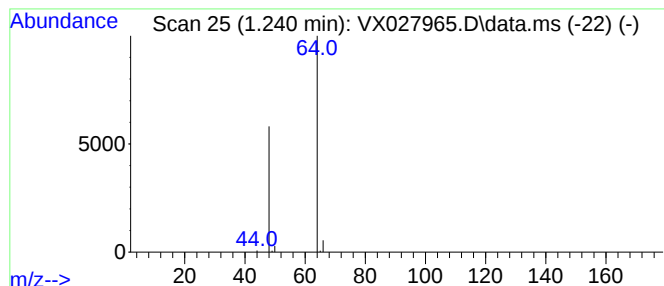
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Sulfur dioxide Concentration Rank 7

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.240 | 6.14 ug/l | 34142 | Pentafluorobenzene | 5.562 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |
| 5    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 3    |



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PB143824ZHE#02

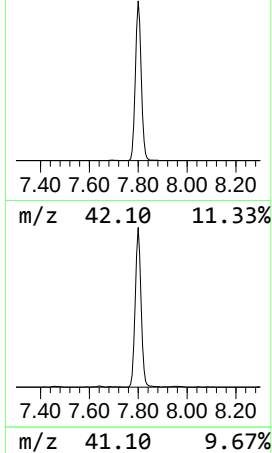
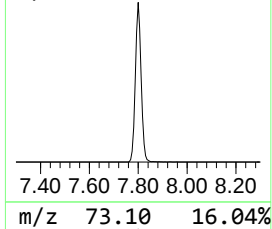
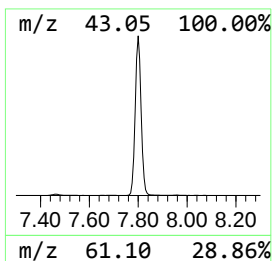
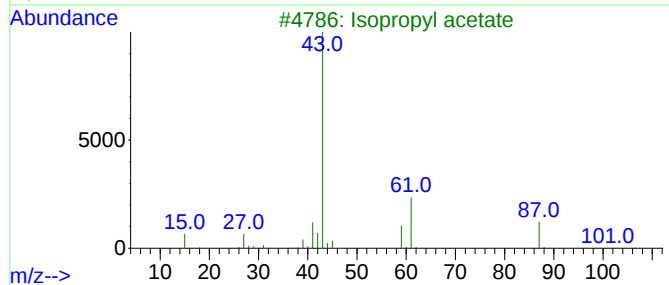
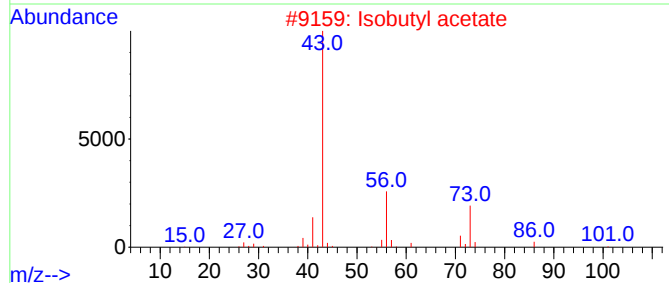
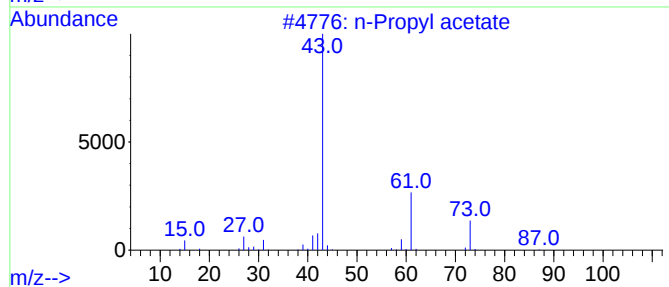
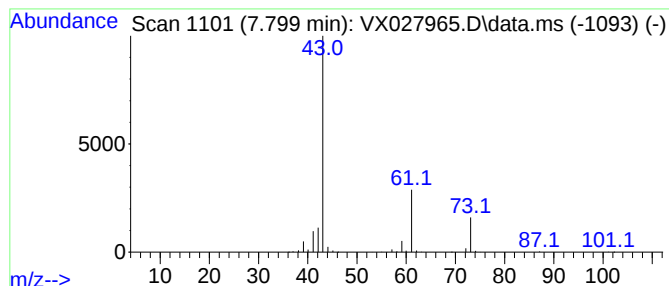
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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

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Peak Number 2 n-Propyl acetate Concentration Rank 2

| R.T.  | EstConc     | Area   | Relative to ISTD    | R.T.  |
|-------|-------------|--------|---------------------|-------|
| 7.799 | 129.74 ug/l | 921855 | 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    |    |   | Isobutyl acetate  | 116 | C6H12O2 | 000110-19-0 | 9    |
| 3    |    |   | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 9    |
| 4    |    |   | Isobutylamine     | 73  | C4H11N  | 000078-81-9 | 7    |
| 5    |    |   | 1-Butanamine      | 73  | C4H11N  | 000109-73-9 | 5    |



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ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#02

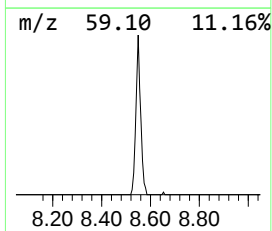
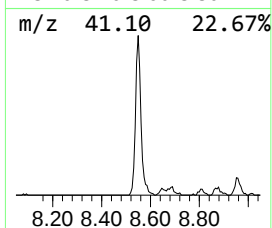
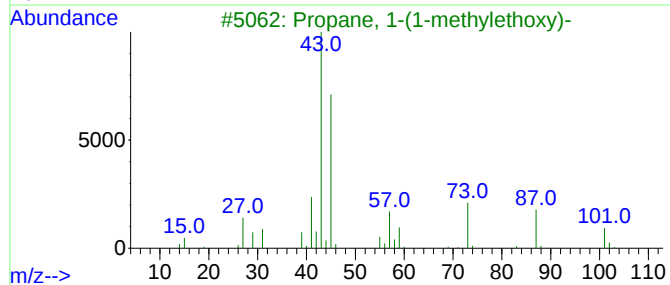
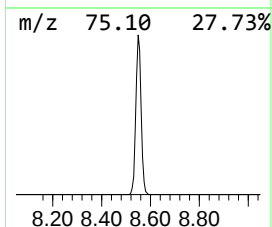
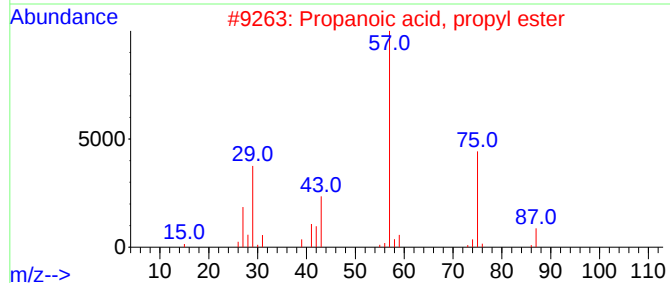
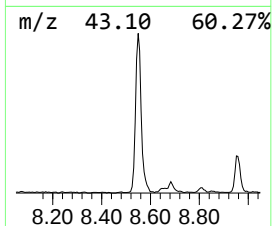
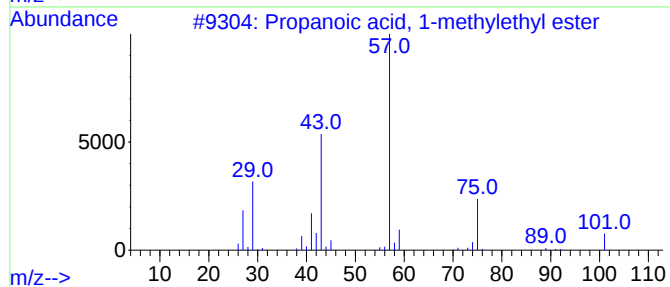
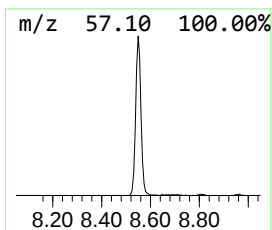
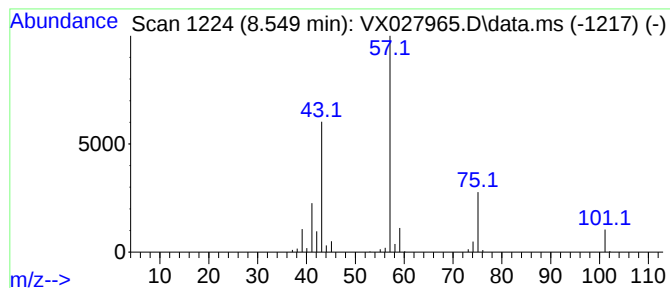
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.   |
|-------|------------|--------|------------------|--------|
| 8.549 | 16.06 ug/l | 131487 | 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 | 45   |
| 3    |    |   | Propane, 1-(1-methylethoxy)-        | 102 | C6H14O  | 000627-08-7 | 25   |
| 4    |    |   | Propanoic acid, butyl ester         | 130 | C7H14O2 | 000590-01-2 | 23   |
| 5    |    |   | Azetidine                           | 57  | C3H7N   | 000503-29-7 | 12   |



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ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#02

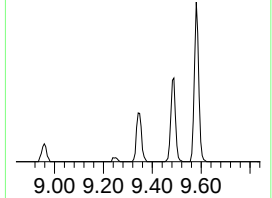
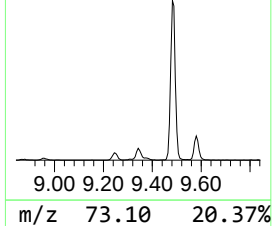
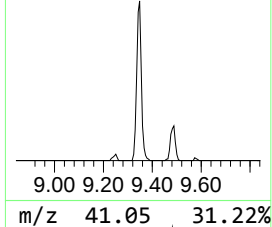
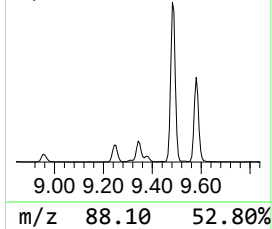
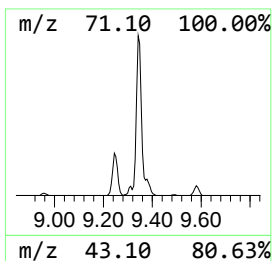
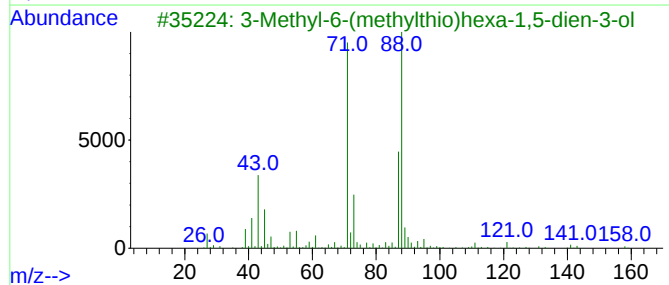
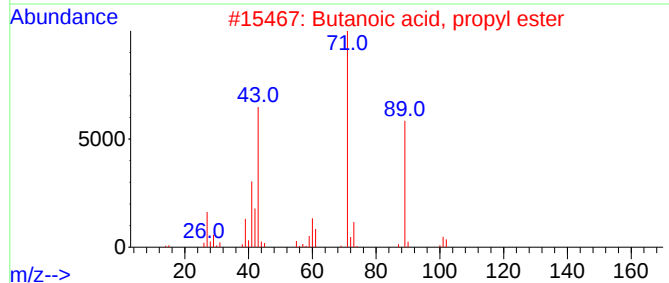
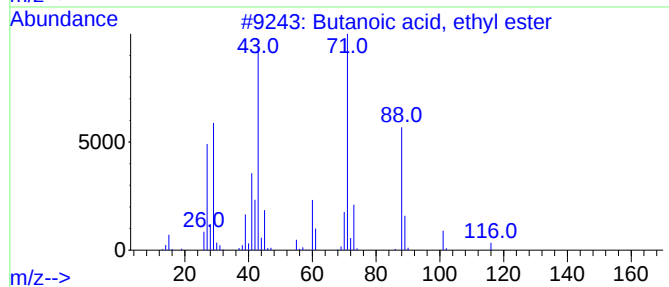
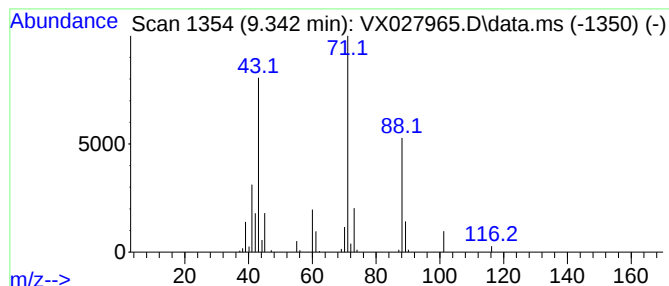
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

| R.T.  | EstConc    | Area  | Relative to ISTD | R.T.   |
|-------|------------|-------|------------------|--------|
| 9.342 | 10.55 ug/l | 86336 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Butanoic acid, ethyl ester          | 116 | C6H12O2 | 000105-54-4  | 95   |
| 2    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2 | 000105-66-8  | 47   |
| 3    |    |   | 3-Methyl-6-(methylthio)hexa-1,5-... | 158 | C8H14OS | 1000191-74-2 | 45   |
| 4    |    |   | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2 | 000097-62-1  | 42   |
| 5    |    |   | 4-Butoxy-2-butanone                 | 144 | C8H16O2 | 030536-44-8  | 40   |



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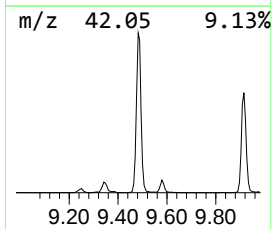
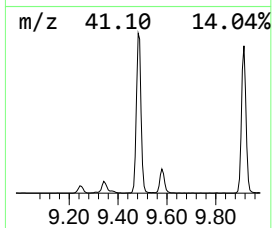
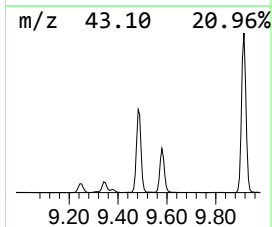
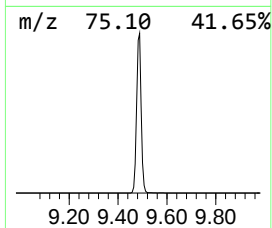
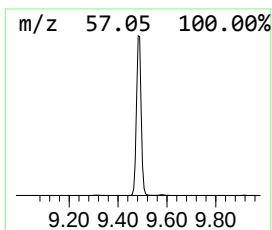
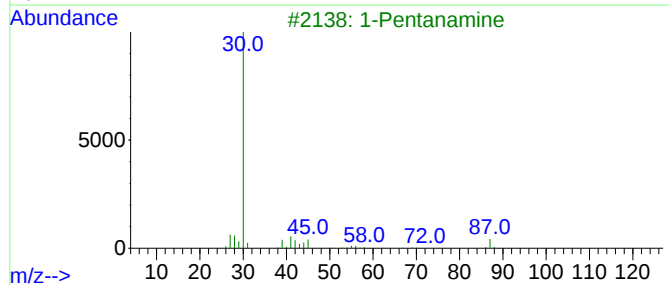
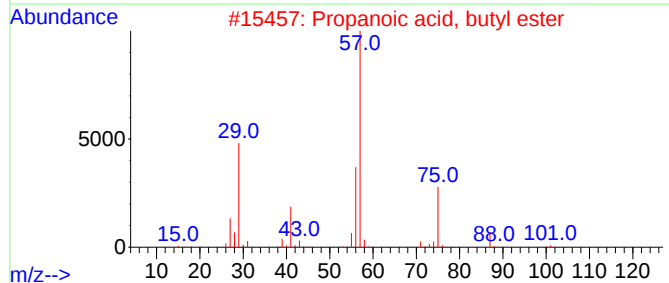
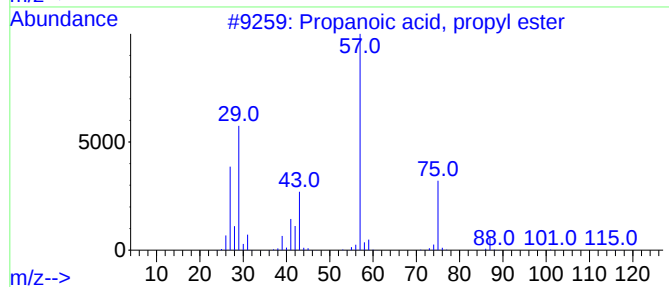
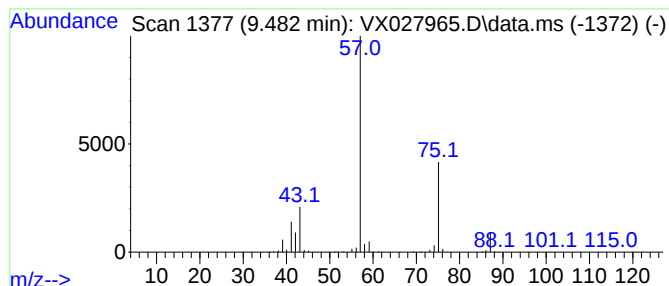
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD | R.T.   |
|-------|-------------|---------|------------------|--------|
| 9.482 | 158.18 ug/l | 1295030 | 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 | 28   |
| 3    |    |   | 1-Pentanamine                | 87  | C5H13N  | 000110-58-7 | 10   |
| 4    |    |   | Azetidine                    | 57  | C3H7N   | 000503-29-7 | 9    |
| 5    |    |   | Isobutyl ether               | 130 | C8H18O  | 000628-55-7 | 9    |



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ClientSampleId :  
PB143824ZHE#02

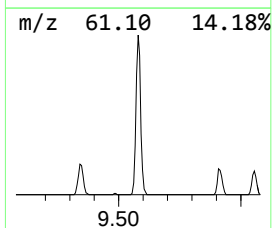
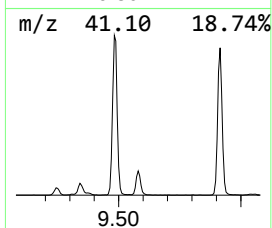
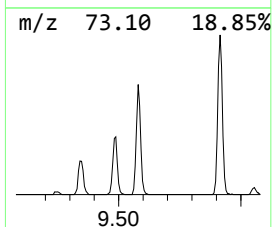
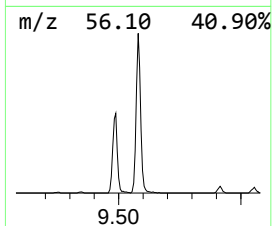
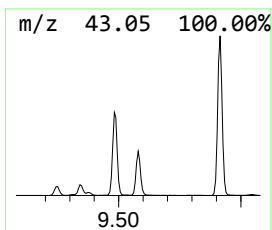
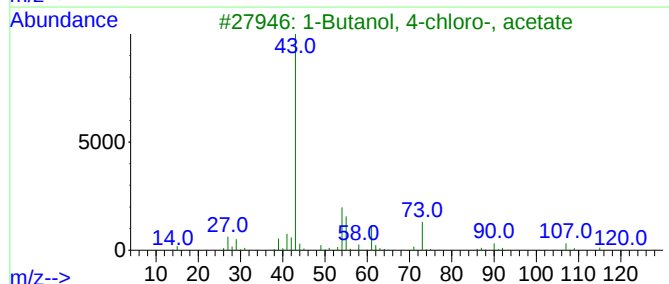
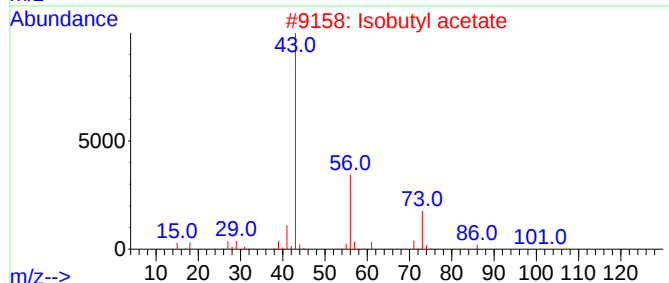
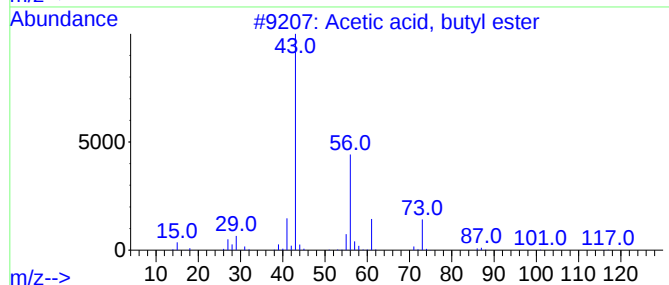
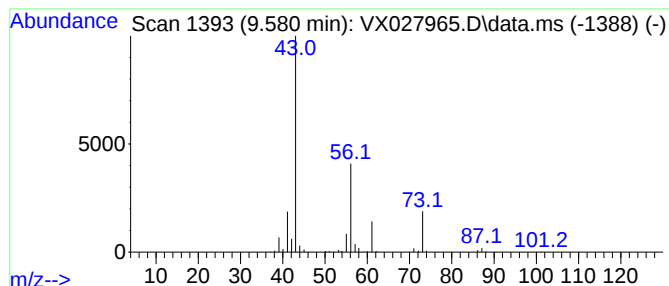
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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

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Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.   |
|-------|------------|--------|------------------|--------|
| 9.580 | 17.82 ug/l | 145930 | 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-Butanol, 4-chloro-, acetate | 150 | C6H11ClO2 | 006962-92-1 | 17   |
| 4    |    |   | Isobutylamine                 | 73  | C4H11N    | 000078-81-9 | 9    |
| 5    |    |   | Isopropyl acetate             | 102 | C5H10O2   | 000108-21-4 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040422\  
Data File : VX027965.D  
Acq On : 04 Apr 2022 18:07  
Operator : JC/MD  
Sample : PB143824ZHE#02  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#02

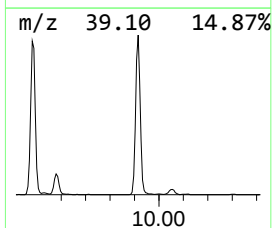
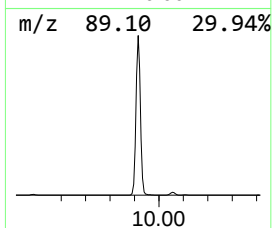
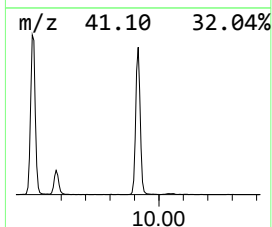
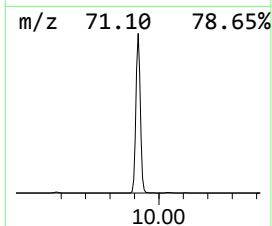
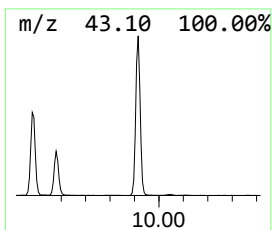
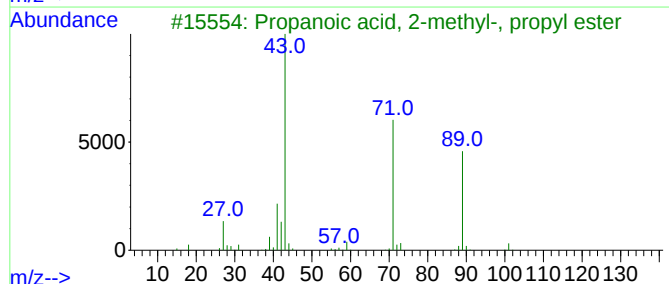
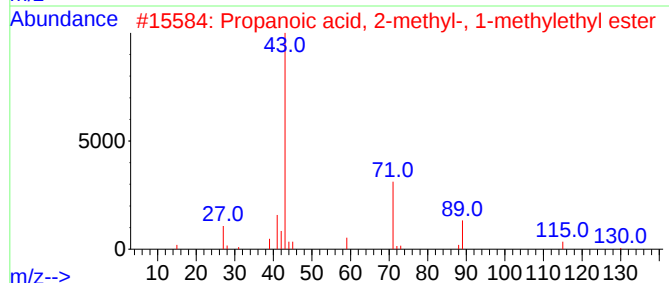
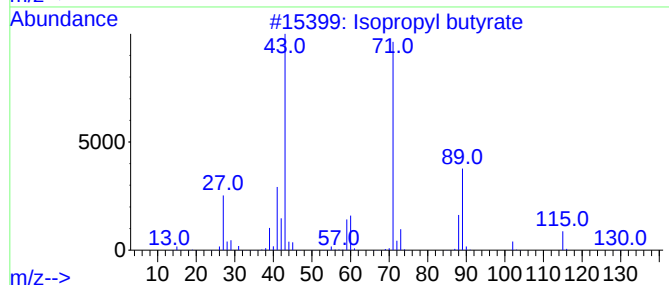
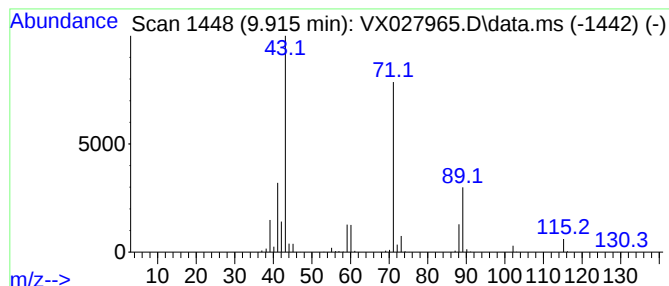
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X032922W.M  
Quant Title : SW846 8260

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

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Peak Number 7 Isopropyl butyrate Concentration Rank 3

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.   |
|-------|------------|--------|------------------|--------|
| 9.915 | 94.87 ug/l | 776701 | 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-, 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  | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040422\  
Data File : VX027965.D  
Acq On : 04 Apr 2022 18:07  
Operator : JC/MD  
Sample : PB143824ZHE#02  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
PB143824ZHE#02

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 |
| Sulfur dioxide     | 1.240 | 6.1     | ug/l  | 34142    | 1                     | 5.562  | 277864 | 50.0 |
| n-Propyl acetate   | 7.799 | 129.7   | ug/l  | 921855   | 2                     | 6.763  | 355273 | 50.0 |
| Propanoic acid,... | 8.549 | 16.1    | ug/l  | 131487   | 3                     | 10.055 | 409358 | 50.0 |
| Butanoic acid, ... | 9.342 | 10.5    | ug/l  | 86336    | 3                     | 10.055 | 409358 | 50.0 |
| Propanoic acid,... | 9.482 | 158.2   | ug/l  | 1295030  | 3                     | 10.055 | 409358 | 50.0 |
| Acetic acid, bu... | 9.580 | 17.8    | ug/l  | 145930   | 3                     | 10.055 | 409358 | 50.0 |
| Isopropyl butyrate | 9.915 | 94.9    | ug/l  | 776701   | 3                     | 10.055 | 409358 | 50.0 |