

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN122023\  
 Data File : VN080545.D  
 Acq On : 20 Dec 2023 14:32  
 Operator : JC\MD  
 Sample : 05886-01 50X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 AUD-1295

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\_N\methods\82N121223W.M

Title : SW846 8260

Signal : TIC: VN080545.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         | 2.665       | 114           | 121         | 130          | rBV      | 67187          | 125610        | 2.20%           | 0.609%        |
| 2         | 4.283       | 384           | 396         | 412          | rBV      | 2004903        | 5716991       | 100.00%         | 27.730%       |
| 3         | 4.424       | 413           | 420         | 435          | rVB2     | 42045          | 143392        | 2.51%           | 0.696%        |
| 4         | 4.700       | 457           | 467         | 482          | rBV      | 29618          | 94475         | 1.65%           | 0.458%        |
| 5         | 6.718       | 797           | 810         | 833          | rBV      | 556665         | 1680771       | 29.40%          | 8.153%        |
| 6         | 8.165       | 1044          | 1056        | 1061         | rBV      | 201026         | 487073        | 8.52%           | 2.363%        |
| 7         | 8.224       | 1061          | 1066        | 1080         | rVB2     | 318481         | 700610        | 12.25%          | 3.398%        |
| 8         | 8.577       | 1117          | 1126        | 1137         | rVB      | 190772         | 415701        | 7.27%           | 2.016%        |
| 9         | 9.100       | 1207          | 1215        | 1229         | rBV      | 505170         | 1037459       | 18.15%          | 5.032%        |
| 10        | 10.565      | 1456          | 1464        | 1474         | rBV      | 716709         | 1340699       | 23.45%          | 6.503%        |
| 11        | 10.800      | 1496          | 1504        | 1517         | rBV      | 2577912        | 4427196       | 77.44%          | 21.474%       |
| 12        | 10.947      | 1521          | 1529        | 1542         | rVB      | 526185         | 897740        | 15.70%          | 4.355%        |
| 13        | 11.865      | 1679          | 1685        | 1699         | rVB      | 784069         | 1382517       | 24.18%          | 6.706%        |
| 14        | 12.847      | 1846          | 1852        | 1861         | rVB      | 578989         | 979370        | 17.13%          | 4.750%        |
| 15        | 13.794      | 2005          | 2013        | 2021         | rBV      | 711587         | 1186653       | 20.76%          | 5.756%        |

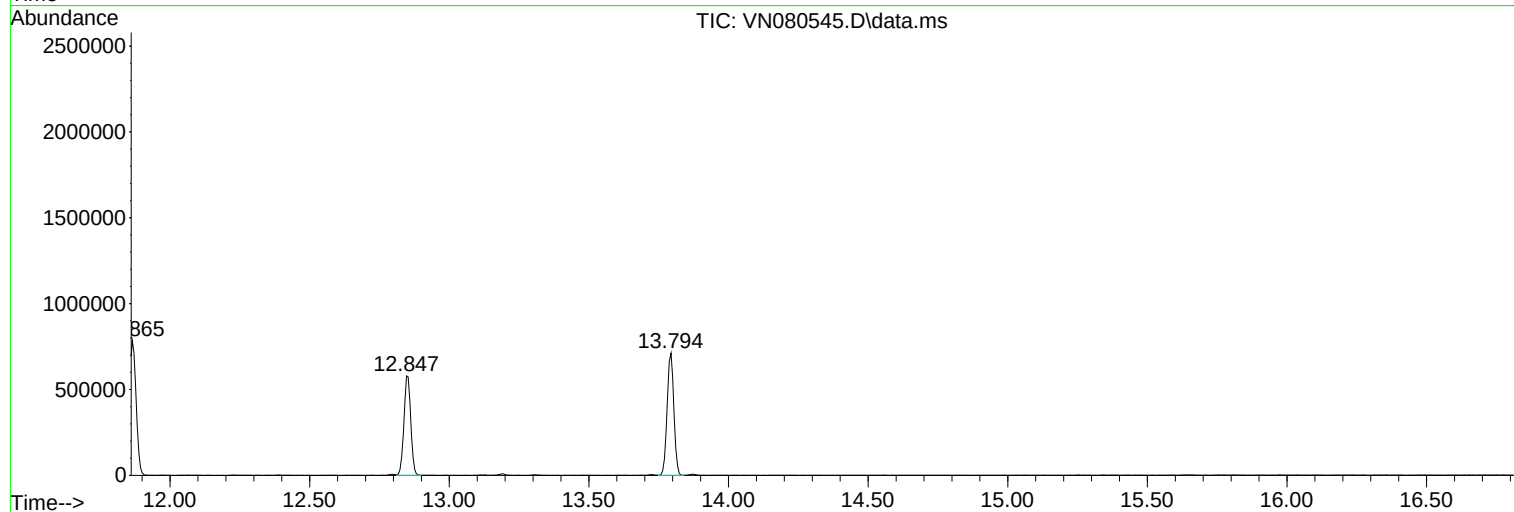
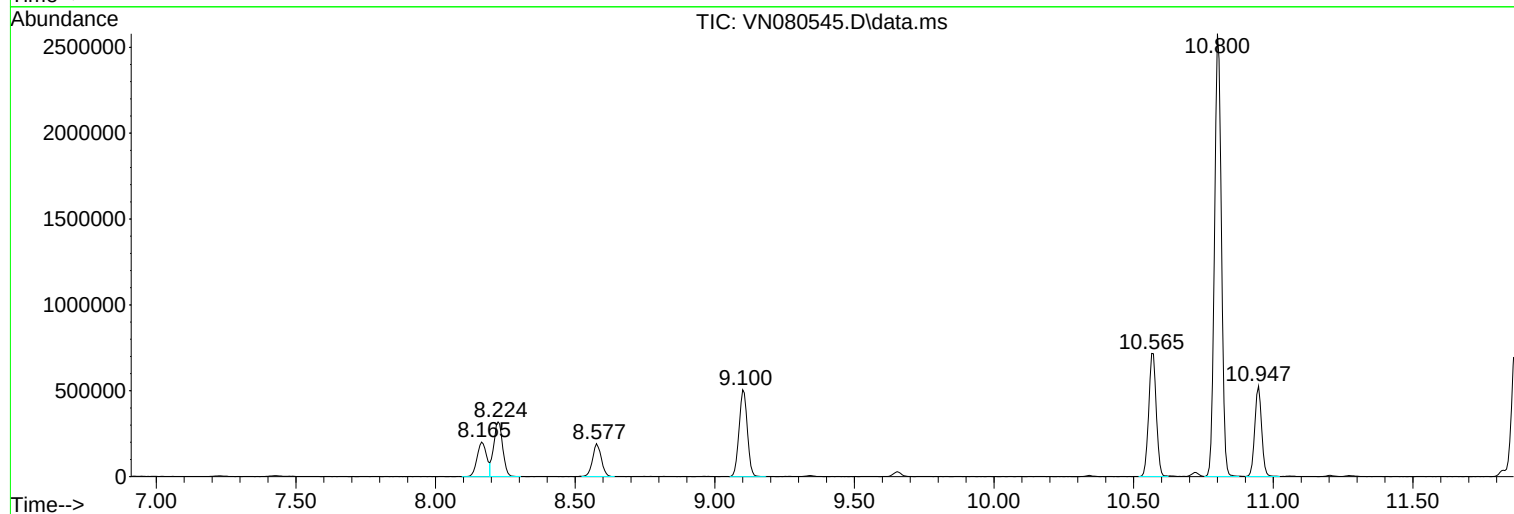
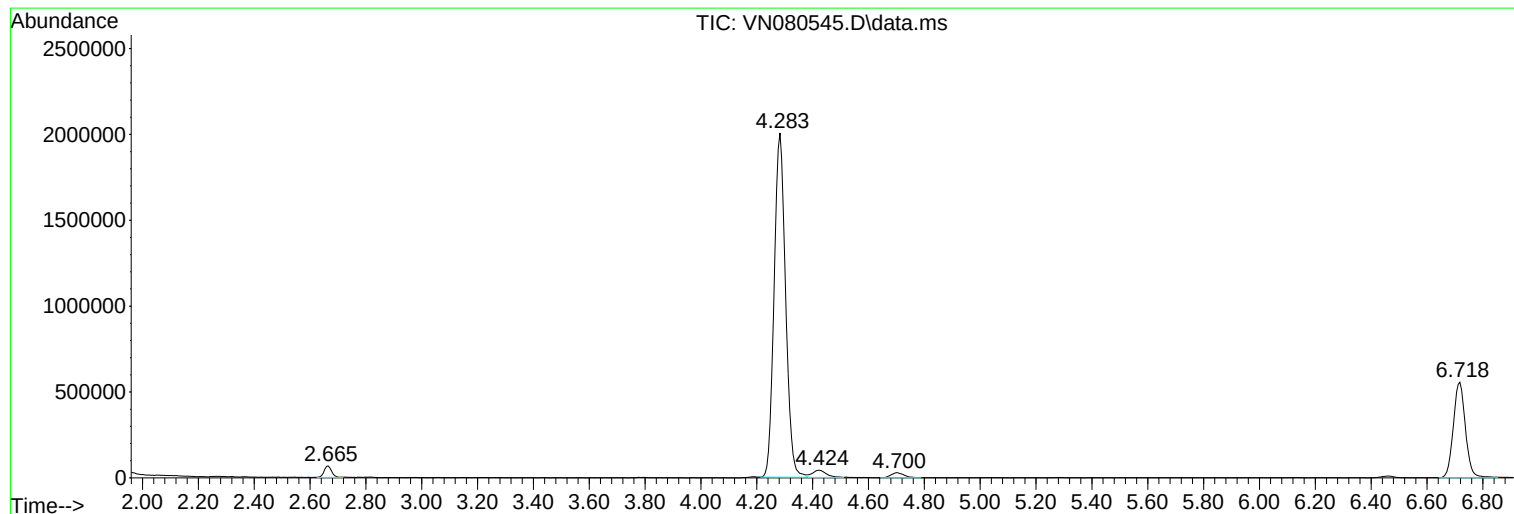
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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.M  
Quant Title : SW846 8260

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



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Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.M  
Quant Title : SW846 8260

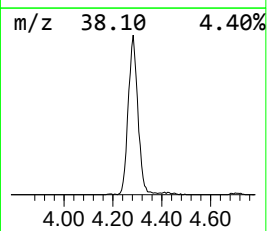
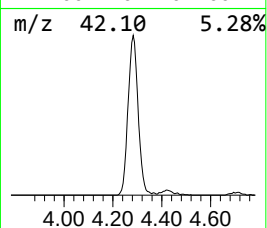
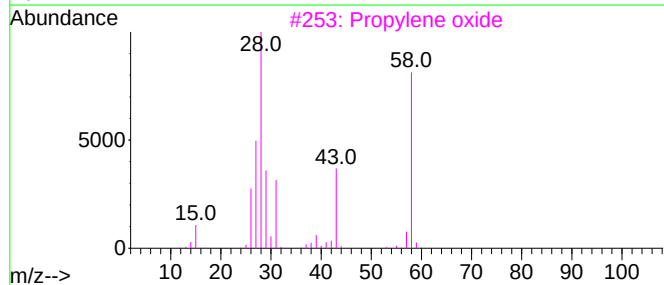
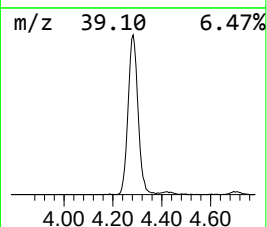
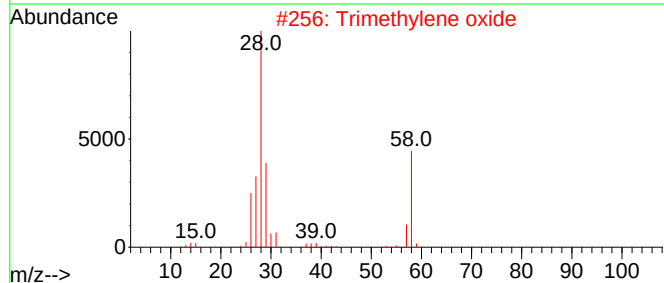
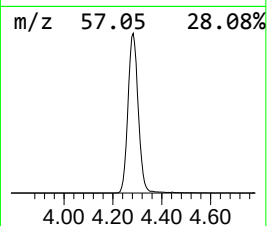
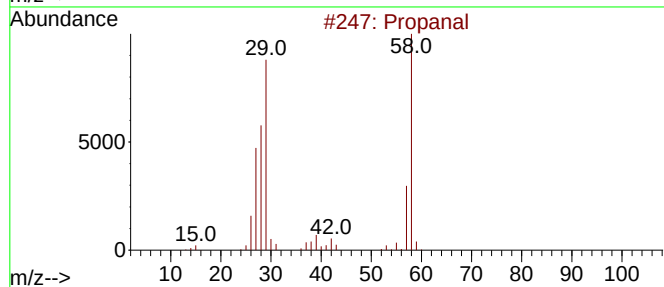
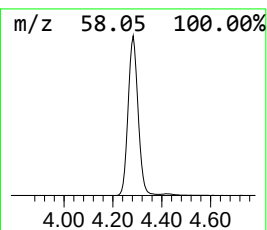
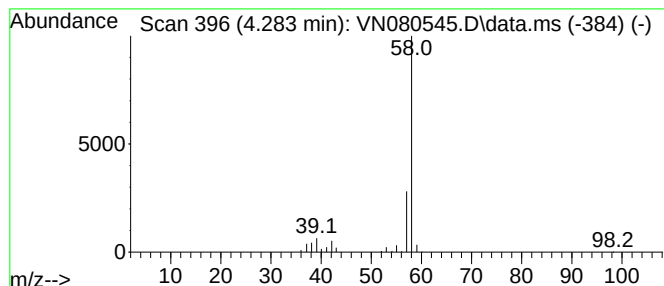
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Propanal Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 4.283 | 408.00 ug/l | 5716990 | Pentafluorobenzene | 8.224 |

| Hit# | of | 5 | Tentative ID                | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|----|---------|-------------|------|
| 1    |    |   | Propanal                    | 58 | C3H6O   | 000123-38-6 | 78   |
| 2    |    |   | Trimethylene oxide          | 58 | C3H6O   | 000503-30-0 | 9    |
| 3    |    |   | Propylene oxide             | 58 | C3H6O   | 000075-56-9 | 7    |
| 4    |    |   | Oxirane, methyl-, (S)-      | 58 | C3H6O   | 016088-62-3 | 5    |
| 5    |    |   | 1,2-Ethanediamine, N-ethyl- | 88 | C4H12N2 | 000110-72-5 | 4    |



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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

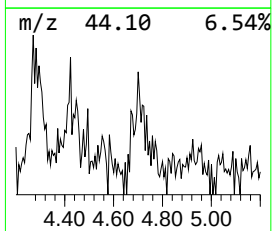
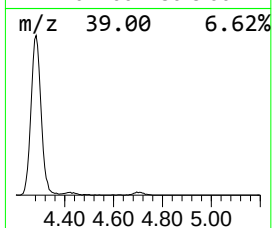
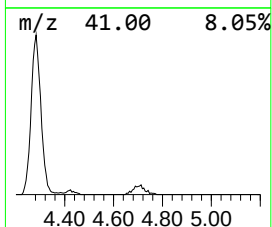
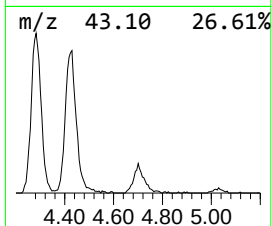
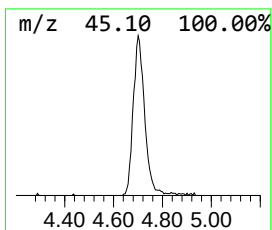
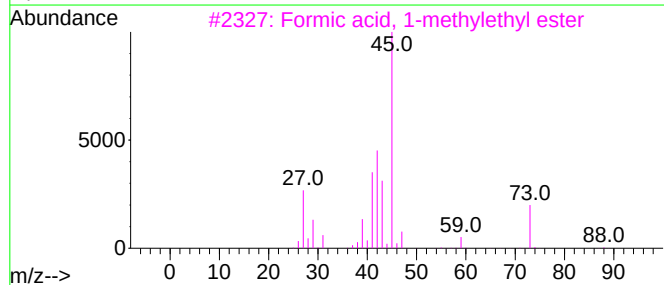
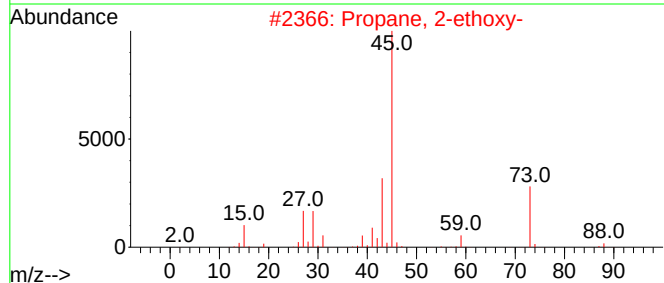
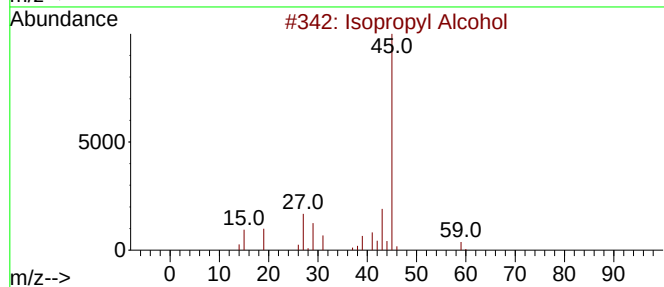
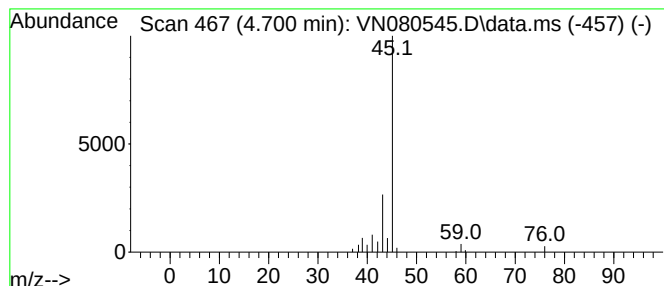
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Isopropyl Alcohol Concentration Rank 6

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 4.700 | 6.74 ug/l | 94475 | Pentafluorobenzene | 8.224 |

| Hit# | of | 5 | Tentative ID                     | MW | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|----|---------|-------------|------|
| 1    |    |   | Isopropyl Alcohol                | 60 | C3H8O   | 000067-63-0 | 83   |
| 2    |    |   | Propane, 2-ethoxy-               | 88 | C5H12O  | 000625-54-7 | 43   |
| 3    |    |   | Formic acid, 1-methylethyl ester | 88 | C4H8O2  | 000625-55-8 | 40   |
| 4    |    |   | (R)-(-)-2-Pentanol               | 88 | C5H12O  | 031087-44-2 | 9    |
| 5    |    |   | 2-Pentanol                       | 88 | C5H12O  | 006032-29-7 | 9    |



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Sample : 05886-01 50X  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

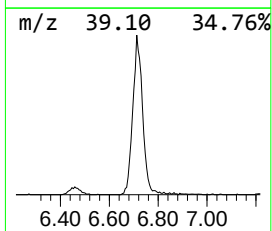
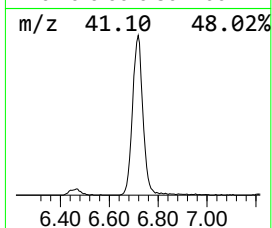
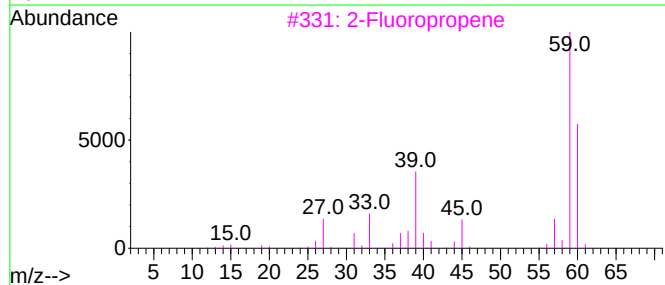
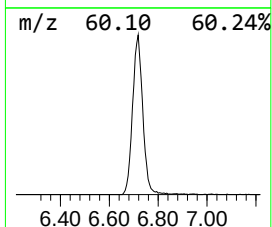
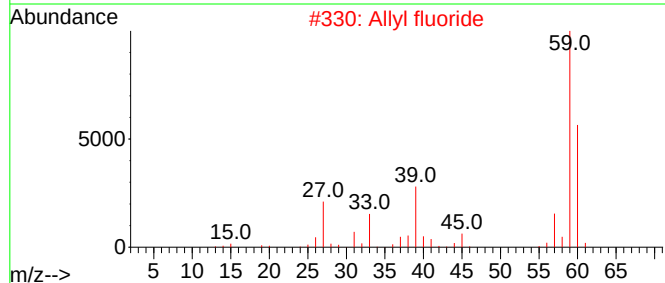
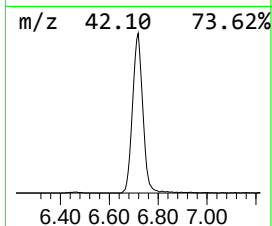
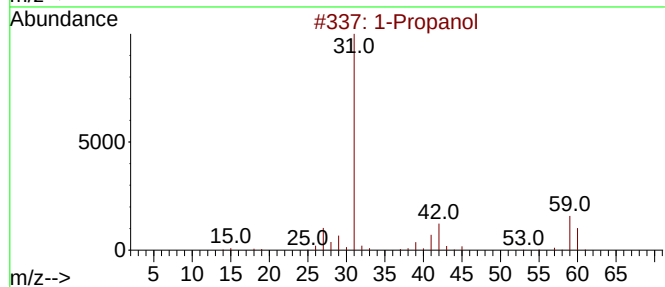
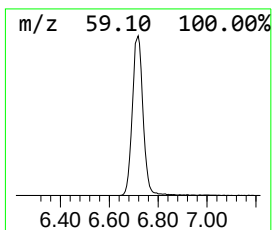
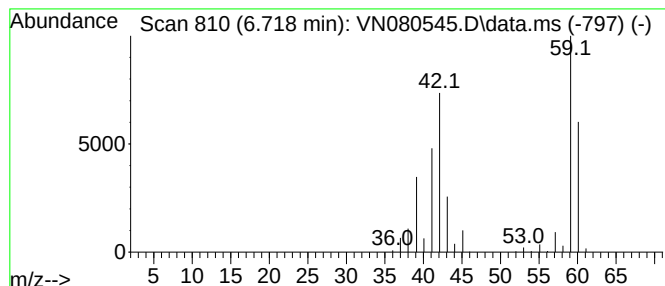
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.M  
Quant Title : SW846 8260

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

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Peak Number 4 1-Propanol Concentration Rank 3

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 6.718 | 119.95 ug/l | 1680770 | Pentafluorobenzene | 8.224 |

| Hit# | of                               | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|----------------------------------|---|--------------|----|---------|-------------|------|
| 1    | 1-Propanol                       |   |              | 60 | C3H8O   | 000071-23-8 | 78   |
| 2    | Allyl fluoride                   |   |              | 60 | C3H5F   | 000818-92-8 | 47   |
| 3    | 2-Fluoropropene                  |   |              | 60 | C3H5F   | 001184-60-7 | 38   |
| 4    | Cyclopropane                     |   |              | 42 | C3H6    | 000075-19-4 | 12   |
| 5    | Methanamine, N-hydroxy-N-methyl- |   |              | 61 | C2H7NO  | 005725-96-2 | 9    |



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Sample : 05886-01 50X  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

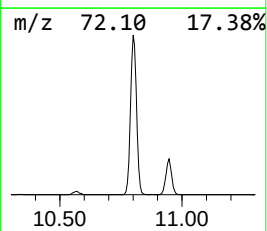
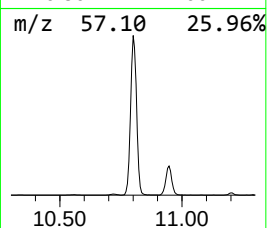
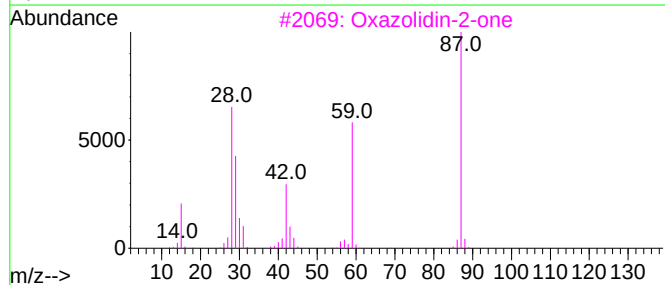
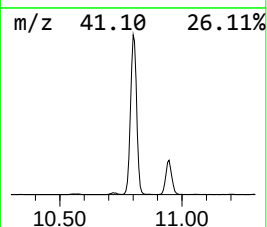
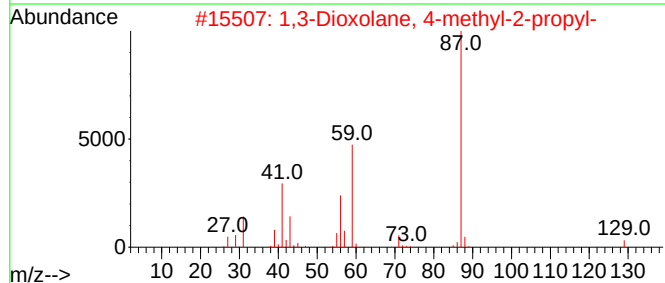
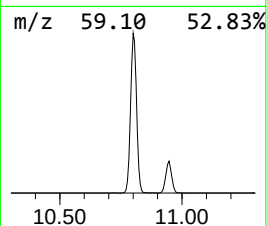
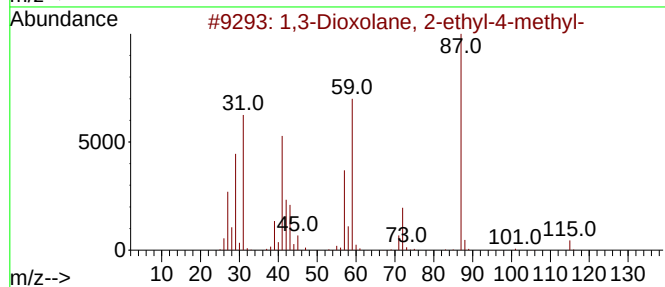
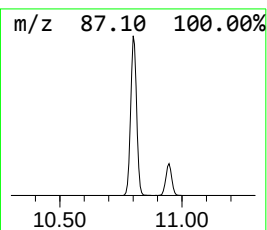
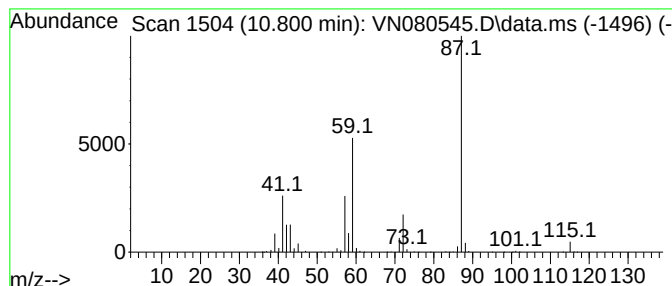
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

| R.T.      | EstConc                           | Area    | Relative to ISTD |         |             | R.T.   |
|-----------|-----------------------------------|---------|------------------|---------|-------------|--------|
| 10.800    | 160.11 ug/l                       | 4427200 | Chlorobenzene-d5 |         |             | 11.865 |
| Hit# of 5 | Tentative ID                      |         | MW               | MolForm | CAS#        | Qual   |
| 1         | 1,3-Dioxolane, 2-ethyl-4-methyl-  |         | 116              | C6H12O2 | 004359-46-0 | 91     |
| 2         | 1,3-Dioxolane, 4-methyl-2-propyl- |         | 130              | C7H14O2 | 004352-99-2 | 72     |
| 3         | Oxazolidin-2-one                  |         | 87               | C3H5NO2 | 000497-25-6 | 72     |
| 4         | 2-Propanone, O-methyloxime        |         | 87               | C4H9NO  | 003376-35-0 | 52     |
| 5         | Acetamide, N-ethyl-               |         | 87               | C4H9NO  | 000625-50-3 | 50     |



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MSVOA\_N  
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AUD-1295

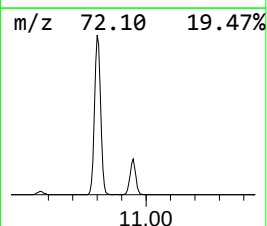
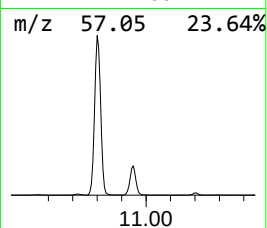
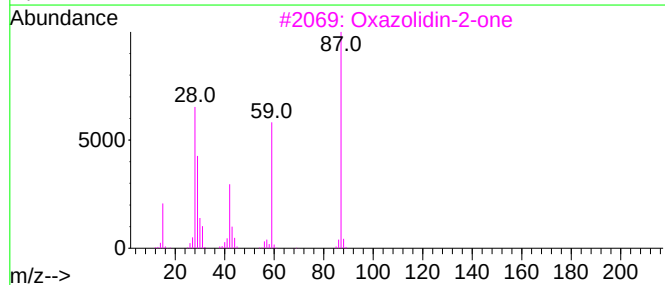
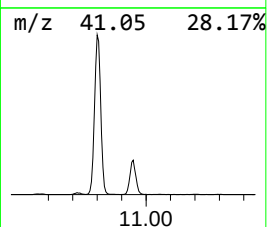
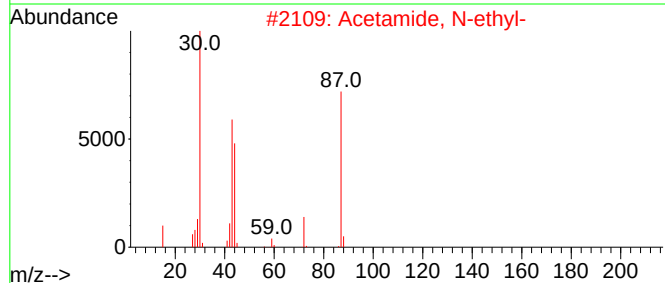
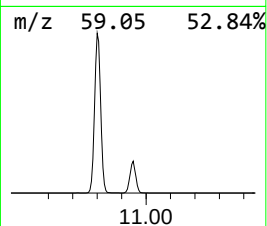
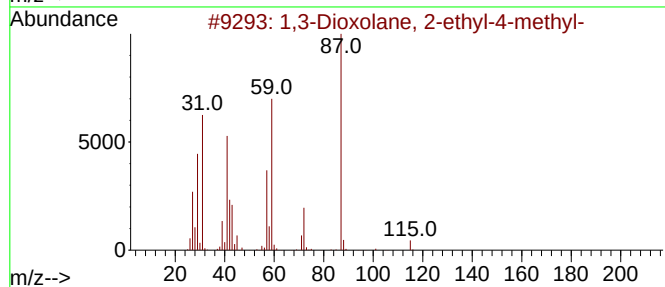
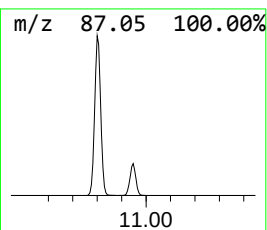
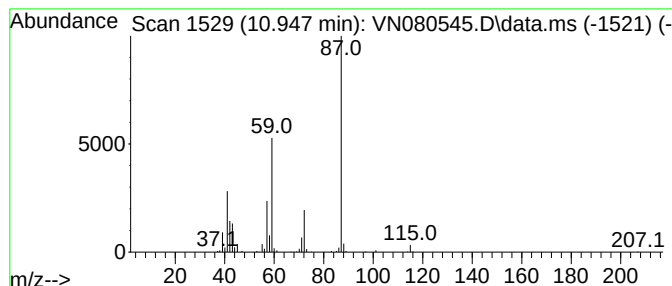
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.M  
Quant Title : SW846 8260

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

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Peak Number 6 Acetamide, N-ethyl- Concentration Rank 4

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 10.947 | 32.47 ug/l | 897740 | Chlorobenzene-d5 | 11.865 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | 1,3-Dioxolane, 2-ethyl-4-methyl- | 116 | C6H12O2 | 004359-46-0 | 91   |
| 2    |    |   | Acetamide, N-ethyl-              | 87  | C4H9NO  | 000625-50-3 | 53   |
| 3    |    |   | Oxazolidin-2-one                 | 87  | C3H5NO2 | 000497-25-6 | 50   |
| 4    |    |   | 2-Propanone, O-methyloxime       | 87  | C4H9NO  | 003376-35-0 | 47   |
| 5    |    |   | 1,3-Dioxolane, 2-butyl-4-methyl- | 144 | C8H16O2 | 074094-60-3 | 39   |



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Sample : 05886-01 50X  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
AUD-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121223W.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 |
| Propanal           | 4.283  | 408.0   | ug/l  | 5716990  | 1                     | 8.224  | 700610  | 50.0 |
| Isopropyl Alcohol  | 4.700  | 6.7     | ug/l  | 94475    | 1                     | 8.224  | 700610  | 50.0 |
| 1-Propanol         | 6.718  | 120.0   | ug/l  | 1680770  | 1                     | 8.224  | 700610  | 50.0 |
| 1,3-Dioxolane, ... | 10.800 | 160.1   | ug/l  | 4427200  | 3                     | 11.865 | 1382520 | 50.0 |
| Acetamide, N-et... | 10.947 | 32.5    | ug/l  | 897740   | 3                     | 11.865 | 1382520 | 50.0 |