

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081020\  
 Data File : VX017850.D  
 Acq On : 10 Aug 2020 15:14  
 Operator : JC/SP  
 Sample : L3675-07  
 Misc : 25.0mL/MSVOA X/WATER  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 GAYA3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR080720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.160       | 9             | 12          | 18           | rVB2     | 50166          | 55489         | 4.69%           | 0.764%        |
| 2         | 1.282       | 28            | 32          | 35           | rBV2     | 22262          | 24490         | 2.07%           | 0.337%        |
| 3         | 1.386       | 45            | 49          | 55           | rBV      | 109095         | 111994        | 9.47%           | 1.542%        |
| 4         | 1.471       | 61            | 63          | 71           | rVB      | 20012          | 21342         | 1.80%           | 0.294%        |
| 5         | 1.581       | 75            | 81          | 86           | rBV9     | 17065          | 38868         | 3.28%           | 0.535%        |
| 6         | 1.691       | 95            | 99          | 106          | rVB      | 64082          | 83194         | 7.03%           | 1.145%        |
| 7         | 2.099       | 160           | 166         | 170          | rBV5     | 8226           | 15562         | 1.32%           | 0.214%        |
| 8         | 2.343       | 200           | 206         | 215          | rVB      | 128097         | 247696        | 20.93%          | 3.410%        |
| 9         | 2.422       | 215           | 219         | 228          | rVB      | 31162          | 53258         | 4.50%           | 0.733%        |
| 10        | 2.587       | 241           | 246         | 252          | rVB      | 33986          | 58101         | 4.91%           | 0.800%        |
| 11        | 2.831       | 279           | 286         | 291          | rBV      | 19956          | 40407         | 3.42%           | 0.556%        |
| 12        | 3.501       | 390           | 396         | 404          | rVB10    | 8426           | 21555         | 1.82%           | 0.297%        |
| 13        | 4.532       | 555           | 565         | 577          | rBV      | 187899         | 542367        | 45.84%          | 7.466%        |
| 14        | 4.660       | 578           | 586         | 598          | rVV2     | 64656          | 228476        | 19.31%          | 3.145%        |
| 15        | 4.800       | 601           | 609         | 618          | rVB2     | 43656          | 121488        | 10.27%          | 1.672%        |
| 16        | 5.141       | 652           | 665         | 677          | rBV2     | 97848          | 324436        | 27.42%          | 4.466%        |
| 17        | 6.044       | 798           | 813         | 832          | rBV2     | 237012         | 734518        | 62.08%          | 10.111%       |
| 18        | 6.830       | 934           | 942         | 951          | rBV      | 176677         | 424197        | 35.85%          | 5.839%        |
| 19        | 7.171       | 993           | 998         | 1000         | rBV6     | 8904           | 16763         | 1.42%           | 0.231%        |
| 20        | 7.373       | 1022          | 1031        | 1040         | rBV      | 151078         | 325598        | 27.52%          | 4.482%        |
| 21        | 8.372       | 1189          | 1195        | 1205         | rBV      | 90681          | 158215        | 13.37%          | 2.178%        |
| 22        | 8.695       | 1242          | 1248        | 1256         | rBV      | 303983         | 466749        | 39.45%          | 6.425%        |
| 23        | 8.769       | 1256          | 1260        | 1264         | rVB      | 21973          | 30303         | 2.56%           | 0.417%        |
| 24        | 8.994       | 1291          | 1297        | 1307         | rBV2     | 68554          | 108734        | 9.19%           | 1.497%        |
| 25        | 9.317       | 1345          | 1350        | 1355         | rBV6     | 7650           | 14264         | 1.21%           | 0.196%        |
| 26        | 9.427       | 1362          | 1368        | 1378         | rBV      | 859321         | 1183214       | 100.00%         | 16.287%       |
| 27        | 10.098      | 1472          | 1478        | 1488         | rBV      | 364560         | 497100        | 42.01%          | 6.843%        |
| 28        | 10.348      | 1512          | 1519        | 1526         | rVB8     | 7556           | 14934         | 1.26%           | 0.206%        |
| 29        | 11.232      | 1656          | 1664        | 1671         | rBV      | 208925         | 267300        | 22.59%          | 3.679%        |
| 30        | 11.799      | 1752          | 1757        | 1761         | rBV5     | 9178           | 12479         | 1.05%           | 0.172%        |
| 31        | 12.061      | 1795          | 1800        | 1806         | rVB      | 339192         | 439103        | 37.11%          | 6.044%        |
| 32        | 12.262      | 1829          | 1833        | 1837         | rBV5     | 8727           | 15853         | 1.34%           | 0.218%        |
| 33        | 12.359      | 1844          | 1849        | 1856         | rVB      | 373084         | 474710        | 40.12%          | 6.534%        |
| 34        | 12.890      | 1933          | 1936        | 1942         | rVB7     | 16988          | 22577         | 1.91%           | 0.311%        |

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ALS Vial : 12 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
GAYA3

Integration Parameters: rteint.p  
Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.1 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\SOMXTR080720WMA.M  
Title : TRACE VOA SOM01.0

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 35 | 13.628 | 2051 | 2057 | 2062 | rVB9 | 13083 | 21572 | 1.82% | 0.297% |
| 36 | 13.719 | 2069 | 2072 | 2077 | rBV5 | 9778  | 17950 | 1.52% | 0.247% |
| 37 | 14.499 | 2194 | 2200 | 2204 | rBV9 | 7424  | 13758 | 1.16% | 0.189% |
| 38 | 14.676 | 2221 | 2229 | 2235 | rBV9 | 6779  | 16261 | 1.37% | 0.224% |

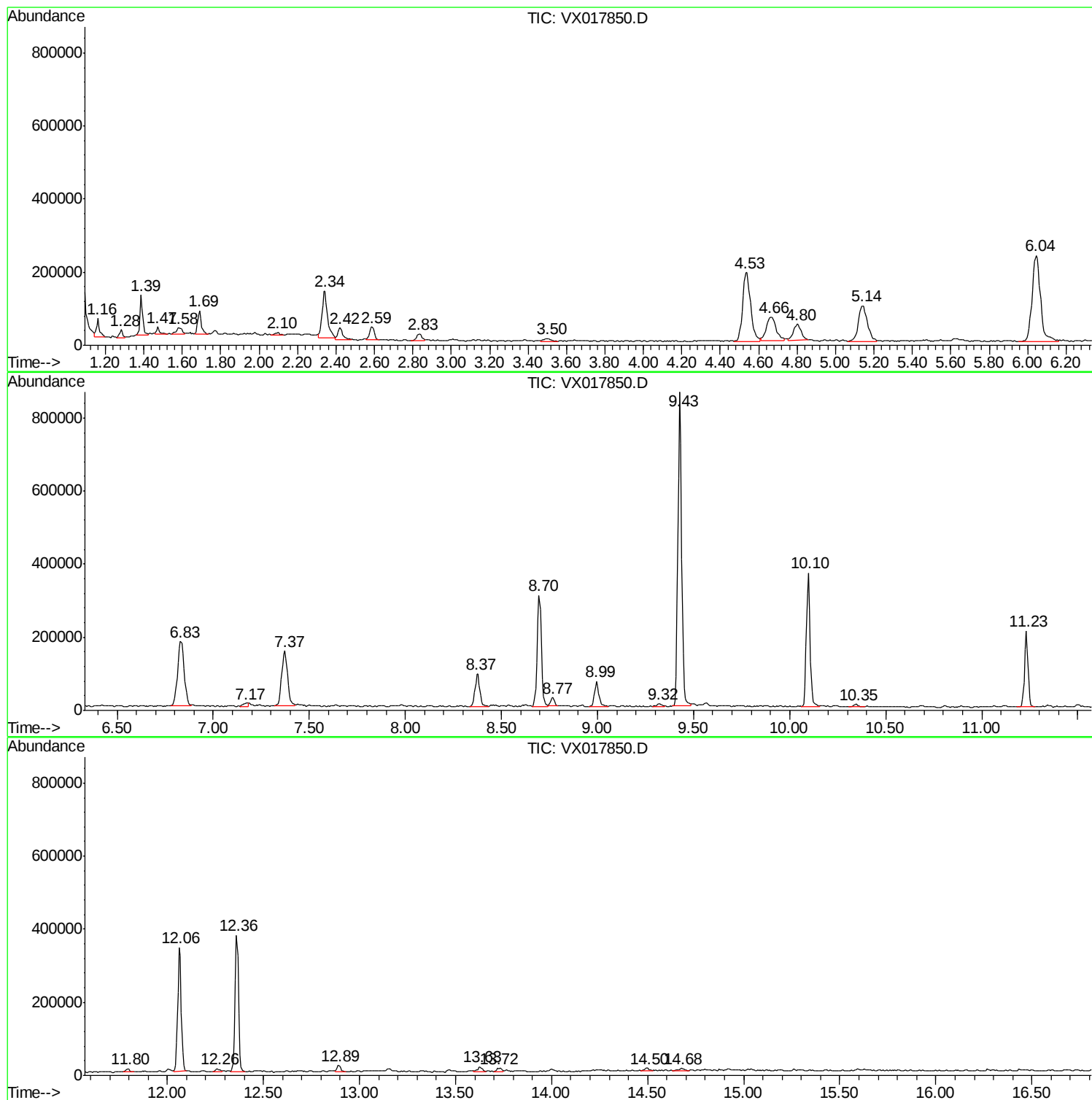
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR080720WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR080720WMA.M  
Quant Title : TRACE VOA SOM01.0

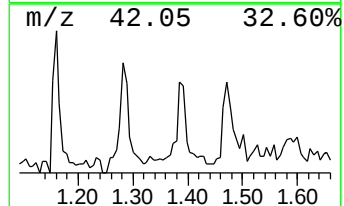
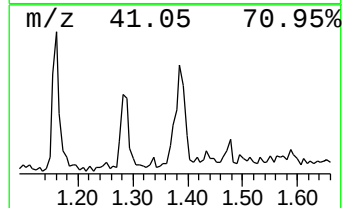
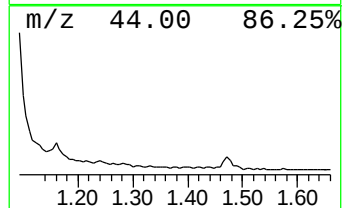
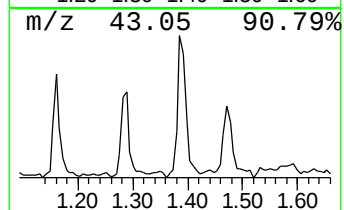
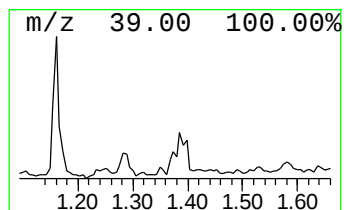
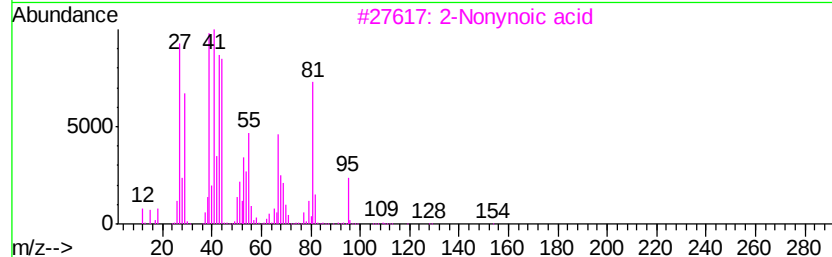
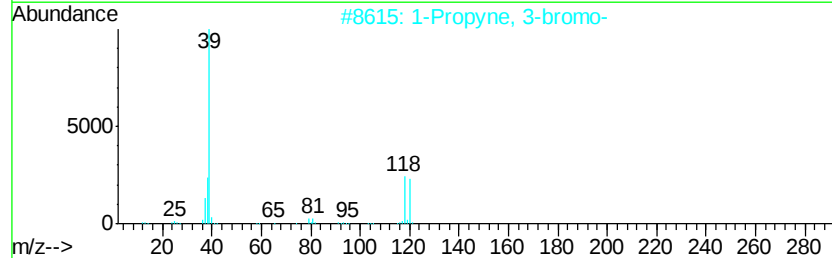
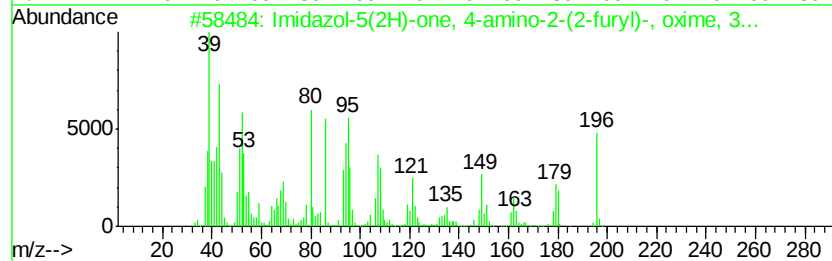
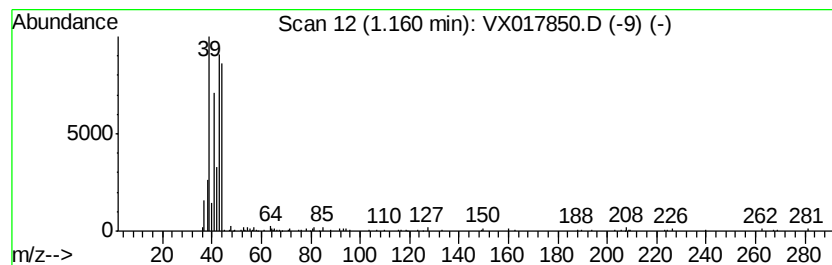
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Imidazol-5(2H)-one, 4-amino... Concentration Rank 3

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 1.16 | 0.65 ug/L | 55489 | 1,4-Difluorobenzene | 6.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Imidazol-5(2H)-one, 4-amino-2-(2... | 196 | C7H8N4O3 | 318259-17-5 | 50   |
| 2    |    | 1-Propyne, 3-bromo-                 | 118 | C3H3Br   | 000106-96-7 | 45   |
| 3    |    | 2-Nonynoic acid                     | 154 | C9H14O2  | 001846-70-4 | 45   |
| 4    |    | 1-Propyne, 3-chloro-                | 74  | C3H3Cl   | 000624-65-7 | 39   |
| 5    |    | Furan                               | 68  | C4H4O    | 000110-00-9 | 39   |



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ALS Vial : 12 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
GAYA3

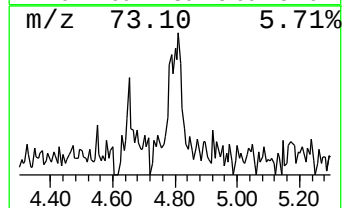
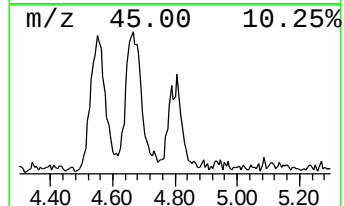
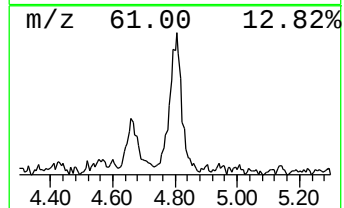
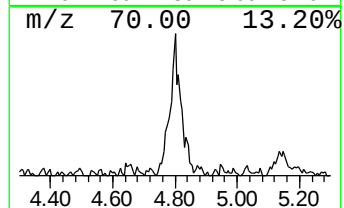
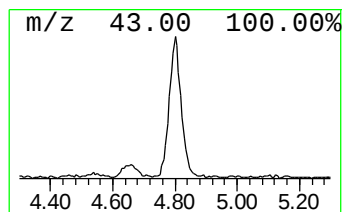
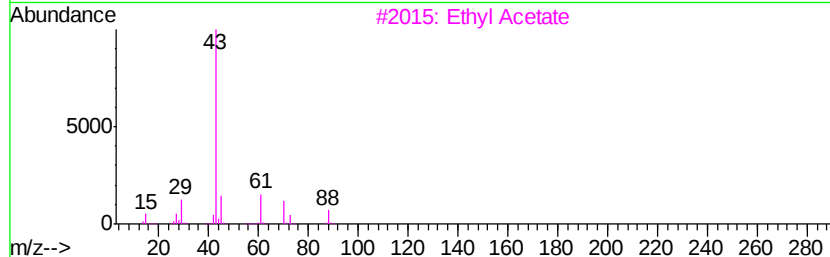
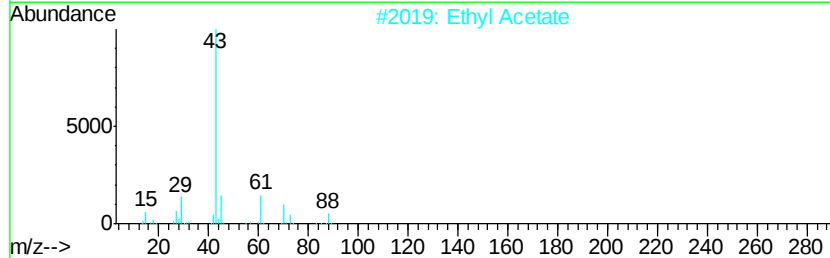
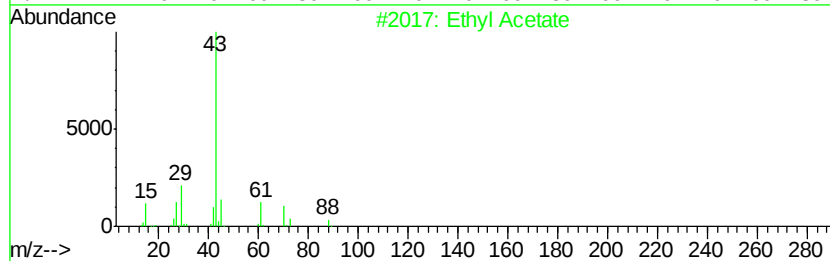
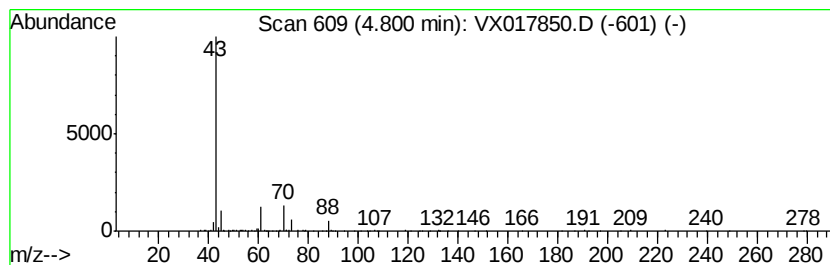
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR080720WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Ethyl Acetate Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 4.80 | 1.43 ug/L | 121488 | 1,4-Difluorobenzene | 6.83 |

| Hit# | of | 5 | Tentative ID    | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------|----|---------|-------------|------|
| 1    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 59   |
| 2    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 58   |
| 3    |    |   | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 58   |
| 4    |    |   | CH3C(O)CH2CH2OH | 88 | C4H8O2  | 000590-90-9 | 50   |
| 5    |    |   | CH3C(O)CH2CH2OH | 88 | C4H8O2  | 000590-90-9 | 50   |



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Sample : L3675-07  
Misc : 25.0mL/MSVOA X/WATER  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
GAYA3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR080720WMA.M  
Quant Title : TRACE VOA SOM01.0

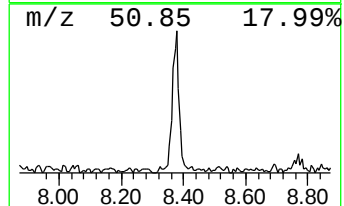
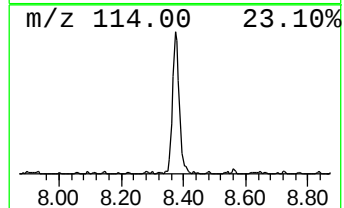
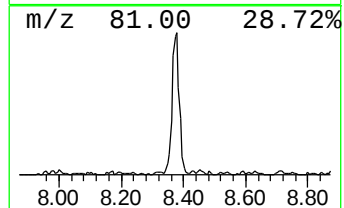
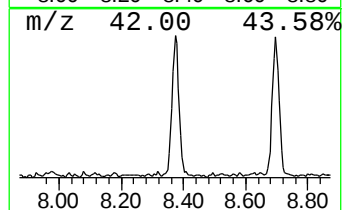
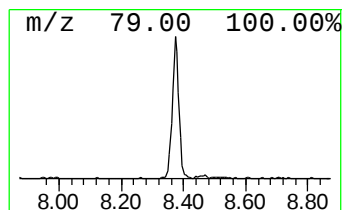
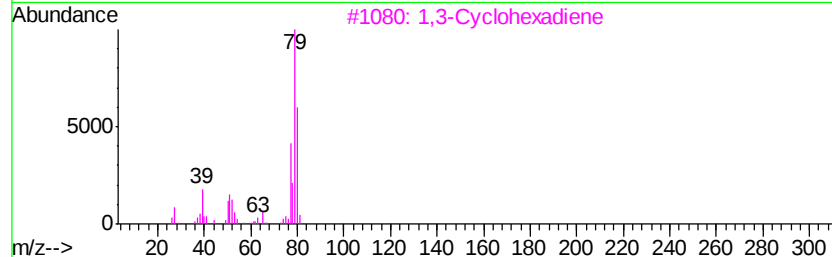
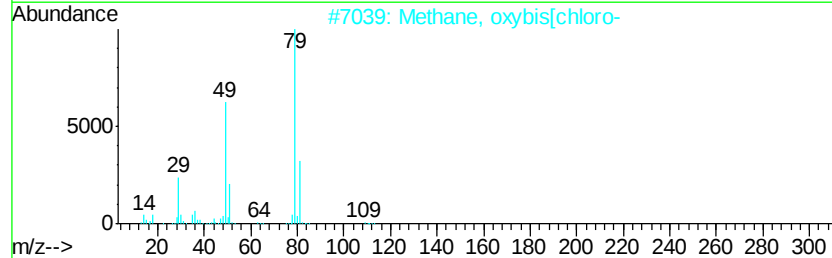
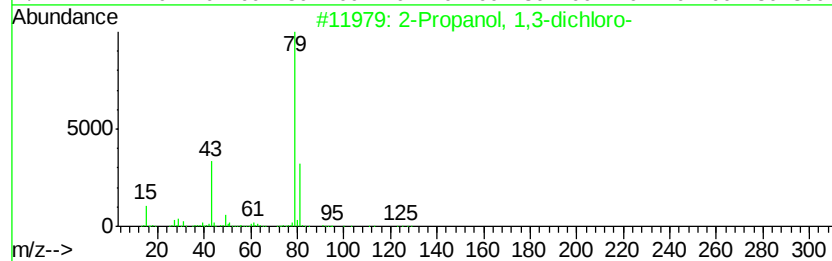
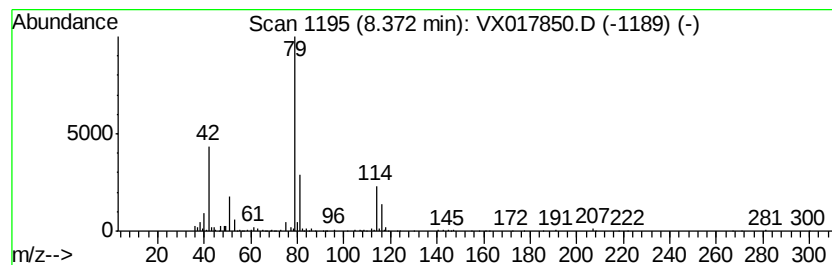
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown-01 Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 8.37 | 1.86 ug/L | 158215 | 1,4-Difluorobenzene | 6.83 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Propanol, 1,3-dichloro-           | 128 | C3H6Cl2O | 000096-23-1  | 38   |
| 2    |    |   | Methane, oxybis[chloro-             | 114 | C2H4Cl2O | 000542-88-1  | 37   |
| 3    |    |   | 1,3-Cyclohexadiene                  | 80  | C6H8     | 000592-57-4  | 32   |
| 4    |    |   | 3-Thiatricyclo[3.1.1.0(2,4)]heptane | 112 | C6H8S    | 1000221-37-0 | 32   |
| 5    |    |   | 2-Propanol, 1,3-dichloro-           | 128 | C3H6Cl2O | 000096-23-1  | 25   |



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Misc : 25.0mL/MSVOA\_X/WATER  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
GAYA3

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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Imidazol-5(2H)-on... | 1.16 | 0.7     | ug/L  | 55489    | 1                     | 6.83 | 424197 | 5.0  |
| Ethyl Acetate        | 4.80 | 1.4     | ug/L  | 121488   | 1                     | 6.83 | 424197 | 5.0  |
| unknown-01           | 8.37 | 1.9     | ug/L  | 158215   | 1                     | 6.83 | 424197 | 5.0  |