

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061820\  
 Data File : VU038970.D  
 Acq On : 18 Jun 2020 15:18  
 Operator : SY/MD  
 Sample : L3058-04  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F9L31

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\_U\METHOD\SOMUTR061720WMA.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         | 1.623       | 78            | 88          | 102          | rVB      | 118477         | 148452        | 10.74%          | 1.411%        |
| 2         | 1.758       | 123           | 130         | 143          | rVB2     | 21634          | 29560         | 2.14%           | 0.281%        |
| 3         | 1.944       | 179           | 188         | 201          | rBV      | 103062         | 132131        | 9.56%           | 1.256%        |
| 4         | 2.179       | 235           | 261         | 267          | rBV4     | 26023          | 104992        | 7.59%           | 0.998%        |
| 5         | 2.597       | 379           | 391         | 413          | rVB      | 264943         | 428858        | 31.02%          | 4.075%        |
| 6         | 3.536       | 673           | 683         | 686          | rBV4     | 36364          | 66466         | 4.81%           | 0.632%        |
| 7         | 4.523       | 976           | 990         | 991          | rBV3     | 10471          | 14239         | 1.03%           | 0.135%        |
| 8         | 4.780       | 1041          | 1070        | 1109         | rBV3     | 117004         | 553764        | 40.05%          | 5.262%        |
| 9         | 5.124       | 1160          | 1177        | 1193         | rVB      | 203794         | 440914        | 31.89%          | 4.190%        |
| 10        | 5.777       | 1361          | 1380        | 1402         | rBV2     | 433349         | 1010157       | 73.06%          | 9.599%        |
| 11        | 6.298       | 1526          | 1542        | 1557         | rVB      | 341418         | 621983        | 44.98%          | 5.911%        |
| 12        | 6.684       | 1650          | 1662        | 1666         | rBV5     | 8789           | 15087         | 1.09%           | 0.143%        |
| 13        | 6.738       | 1666          | 1679        | 1701         | rVB      | 246863         | 482553        | 34.90%          | 4.586%        |
| 14        | 7.221       | 1818          | 1829        | 1845         | rVB      | 41322          | 79701         | 5.76%           | 0.757%        |
| 15        | 7.603       | 1935          | 1948        | 1961         | rBV      | 115950         | 204937        | 14.82%          | 1.947%        |
| 16        | 7.841       | 2008          | 2022        | 2026         | rBV3     | 15968          | 26713         | 1.93%           | 0.254%        |
| 17        | 7.883       | 2027          | 2035        | 2039         | rVV2     | 35425          | 61318         | 4.43%           | 0.583%        |
| 18        | 7.928       | 2039          | 2049        | 2066         | rVB      | 455640         | 778473        | 56.30%          | 7.398%        |
| 19        | 8.211       | 2125          | 2137        | 2153         | rVB2     | 77298          | 128004        | 9.26%           | 1.216%        |
| 20        | 8.526       | 2218          | 2235        | 2244         | rBV7     | 6232           | 15118         | 1.09%           | 0.144%        |
| 21        | 8.671       | 2265          | 2280        | 2303         | rBV      | 744158         | 1382667       | 100.00%         | 13.139%       |
| 22        | 8.816       | 2319          | 2325        | 2337         | rVB6     | 9034           | 15567         | 1.13%           | 0.148%        |
| 23        | 9.439       | 2507          | 2519        | 2537         | rBV      | 501550         | 811472        | 58.69%          | 7.711%        |
| 24        | 9.658       | 2578          | 2587        | 2600         | rVB      | 36543          | 55799         | 4.04%           | 0.530%        |
| 25        | 9.787       | 2616          | 2627        | 2640         | rBV4     | 18158          | 35269         | 2.55%           | 0.335%        |
| 26        | 10.774      | 2922          | 2934        | 2950         | rBV      | 213001         | 345863        | 25.01%          | 3.287%        |
| 27        | 11.372      | 3110          | 3120        | 3126         | rBV2     | 13119          | 18785         | 1.36%           | 0.179%        |
| 28        | 11.825      | 3248          | 3261        | 3275         | rVB      | 498688         | 783848        | 56.69%          | 7.449%        |
| 29        | 12.076      | 3327          | 3339        | 3361         | rBV2     | 29917          | 68076         | 4.92%           | 0.647%        |
| 30        | 12.204      | 3367          | 3379        | 3394         | rVB      | 489773         | 771473        | 55.80%          | 7.331%        |
| 31        | 14.227      | 3997          | 4008        | 4021         | rVB2     | 45795          | 71366         | 5.16%           | 0.678%        |
| 32        | 14.870      | 4197          | 4208        | 4216         | rBV5     | 14296          | 27397         | 1.98%           | 0.260%        |
| 33        | 15.745      | 4470          | 4480        | 4491         | rBV7     | 29395          | 48574         | 3.51%           | 0.462%        |
| 34        | 16.191      | 4613          | 4619        | 4628         | rVB6     | 12694          | 20466         | 1.48%           | 0.194%        |

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Sample : L3058-04  
Misc : 25.0mL/MSVOA U/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

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\_U\METHOD\SOMUTR061720WMA.M  
Title : TRACE VOA SOM01.0

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 16.838 | 4809 | 4820 | 4832 | rBV2 | 74807  | 125587 | 9.08%  | 1.193% |
| 36 | 16.963 | 4847 | 4859 | 4874 | rBV  | 361165 | 597577 | 43.22% | 5.679% |

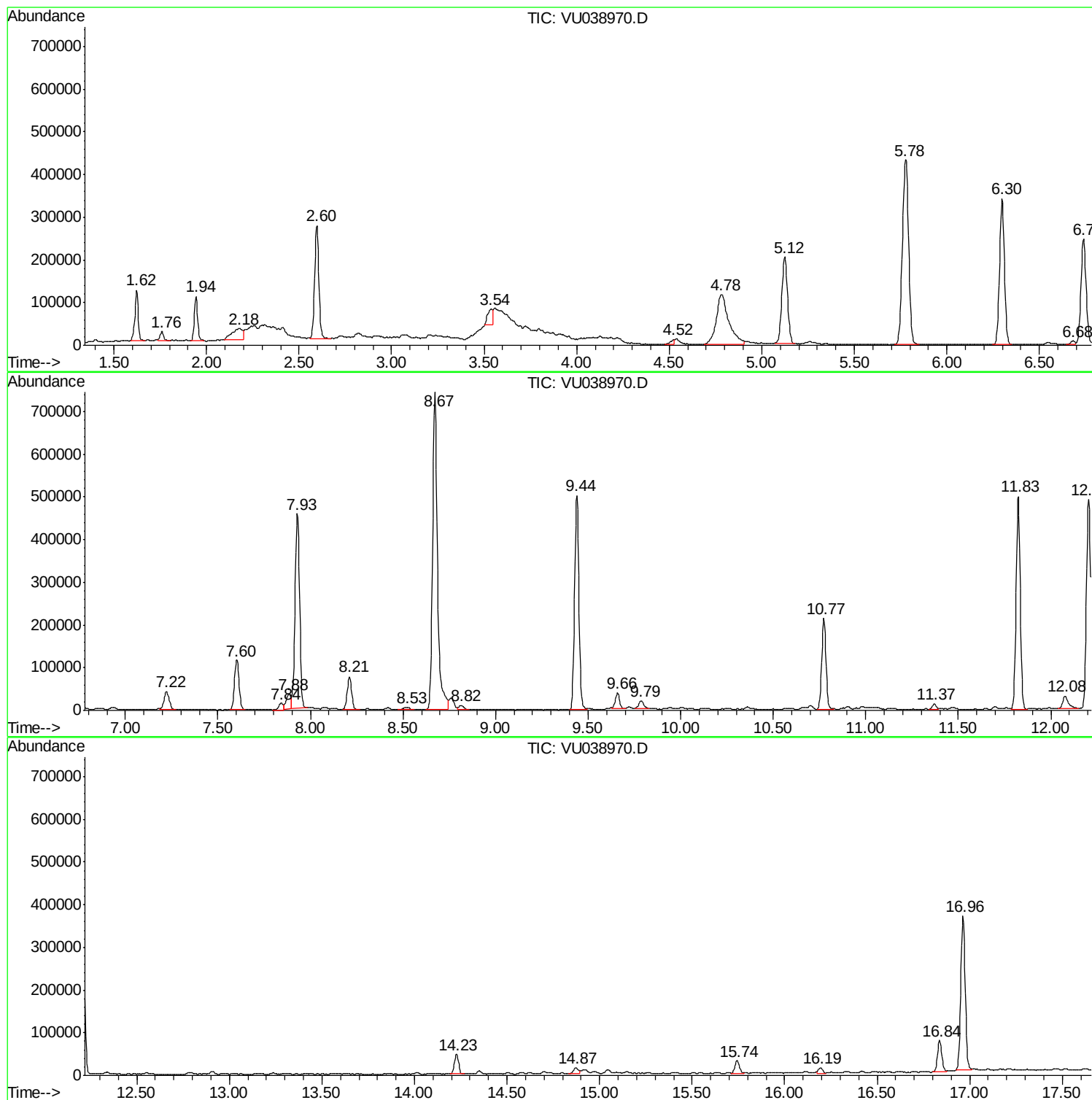
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Instrument :  
MSVOA\_U  
ClientSampled :  
F9L31

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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Sample : L3058-04  
Misc : 25.0mL/MSVOA U/WATER  
ALS Vial : 1 Sample Multiplier: 1

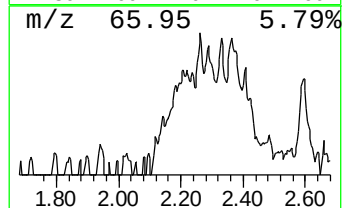
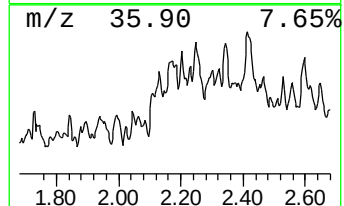
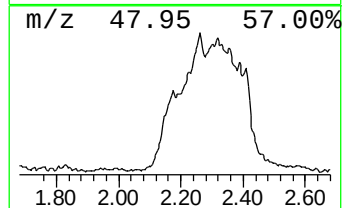
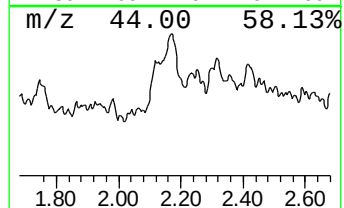
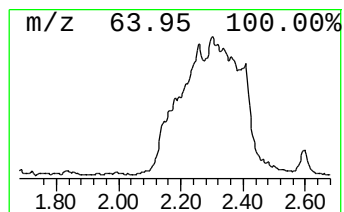
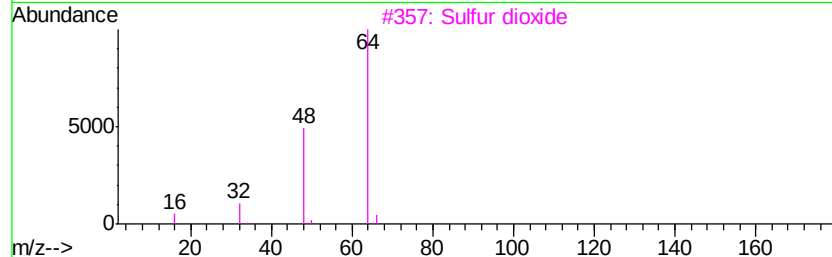
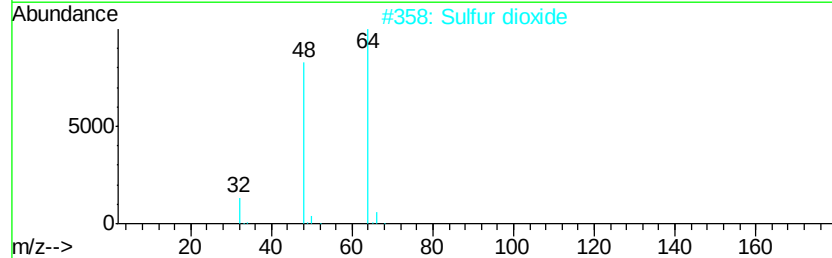
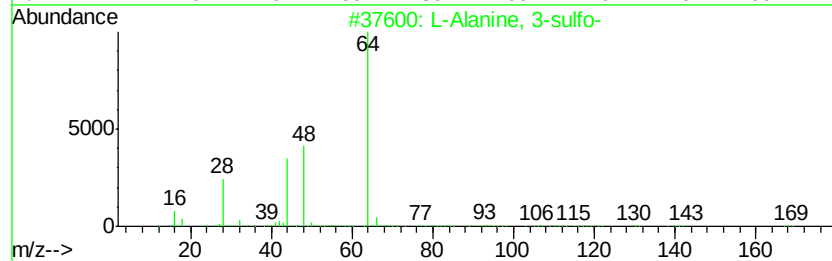
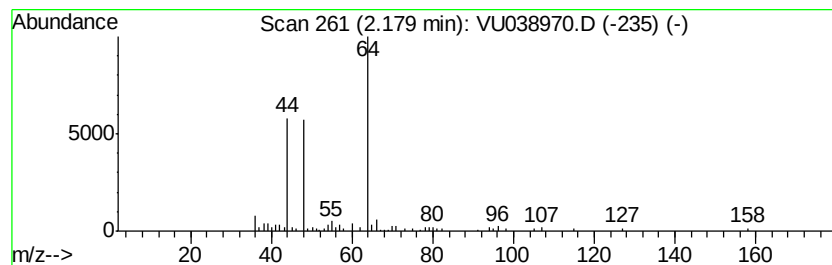
Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.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 L-Alanine, 3-sulfo- Concentration Rank 3

| R.T.    | EstConc   | Area                                | Relative to ISTD    | R.T.       |             |      |
|---------|-----------|-------------------------------------|---------------------|------------|-------------|------|
| 2.18    | 0.84 ug/L | 104992                              | 1,4-Difluorobenzene | 6.30       |             |      |
| Hit# of | 5         | Tentative ID                        | MW                  | MolForm    | CAS#        | Qual |
| 1       |           | L-Alanine, 3-sulfo-                 | 169                 | C3H7N05S   | 000498-40-8 | 74   |
| 2       |           | Sulfur dioxide                      | 64                  | O2S        | 007446-09-5 | 56   |
| 3       |           | Sulfur dioxide                      | 64                  | O2S        | 007446-09-5 | 56   |
| 4       |           | Ethene, 1,1-difluoro-               | 64                  | C2H2F2     | 000075-38-7 | 45   |
| 5       |           | (N-(-2-Acetamido))-2-aminoethane... | 182                 | C4H10N2O4S | 007365-82-4 | 40   |



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ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
Quant Title : TRACE VOA SOM01.0

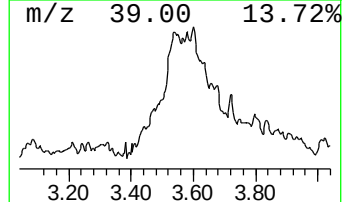
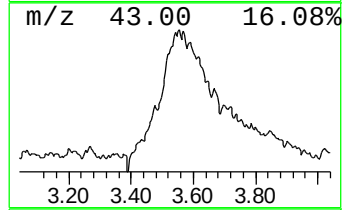
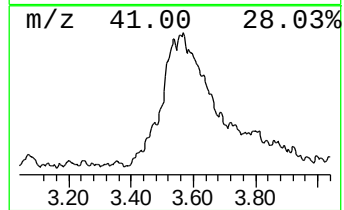
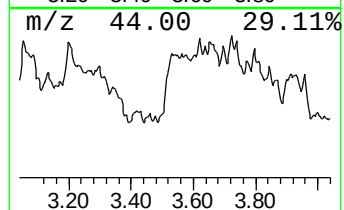
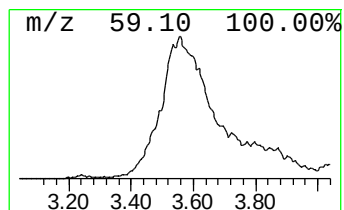
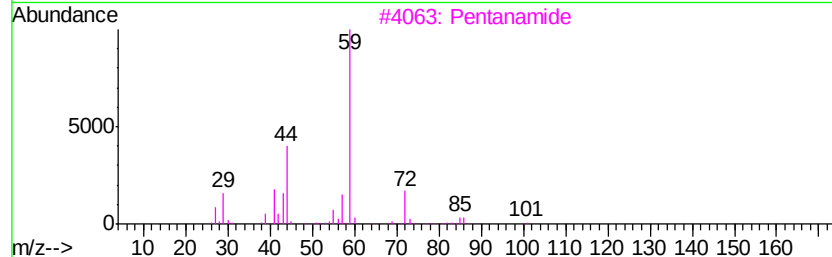
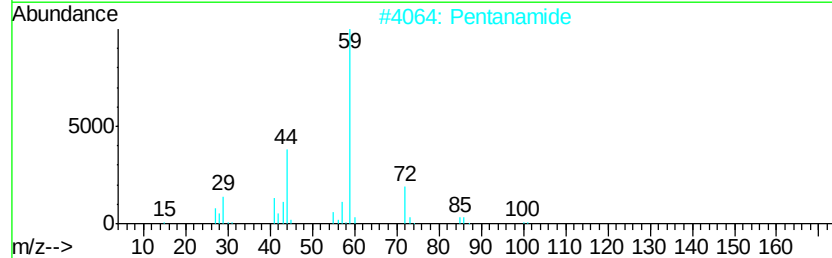
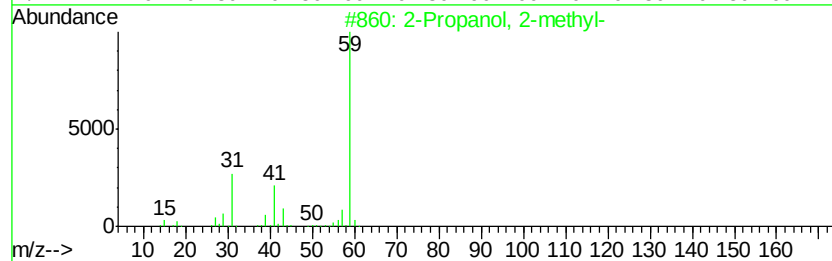
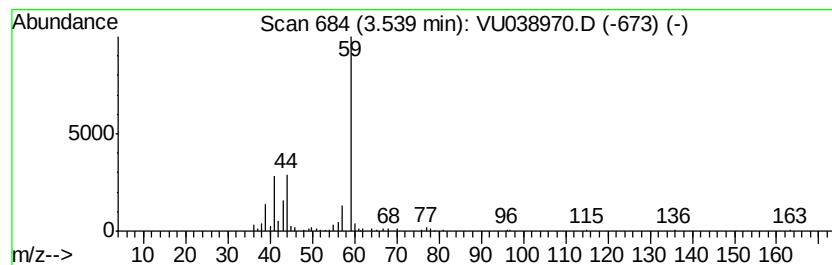
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown-01 Concentration Rank 6

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 3.54 | 0.53 ug/L | 66466 | 1,4-Difluorobenzene | 6.30 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Propanol, 2-methyl-               | 74  | C4H10O  | 000075-65-0 | 45   |
| 2    |    | Pentanamide                         | 101 | C5H11NO | 000626-97-1 | 40   |
| 3    |    | Pentanamide                         | 101 | C5H11NO | 000626-97-1 | 40   |
| 4    |    | Butanamide, 3-methyl-               | 101 | C5H11NO | 000541-46-8 | 40   |
| 5    |    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O  | 017348-59-3 | 40   |



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Misc : 25.0mL/MSVOA U/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
Quant Title : TRACE VOA SOM01.0

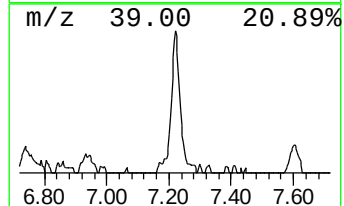
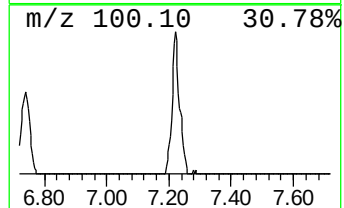
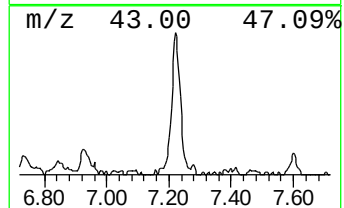
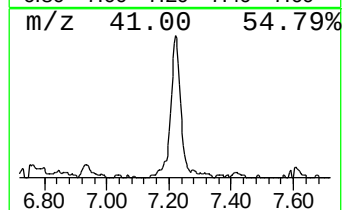
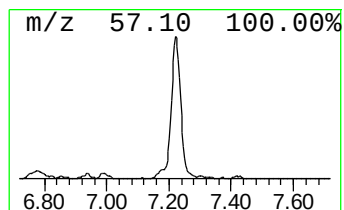
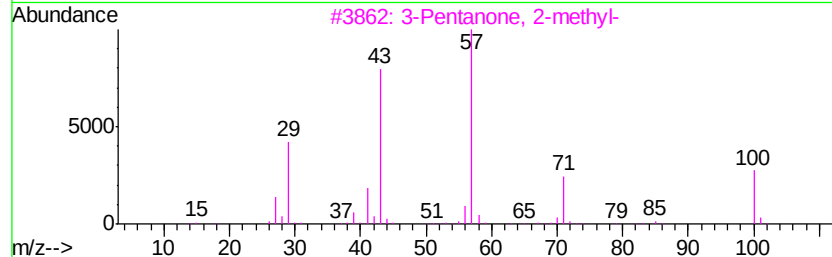
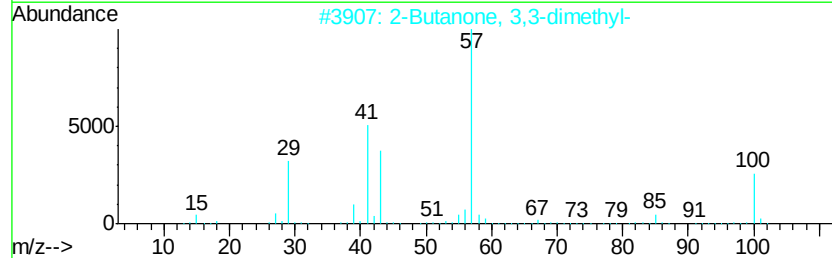
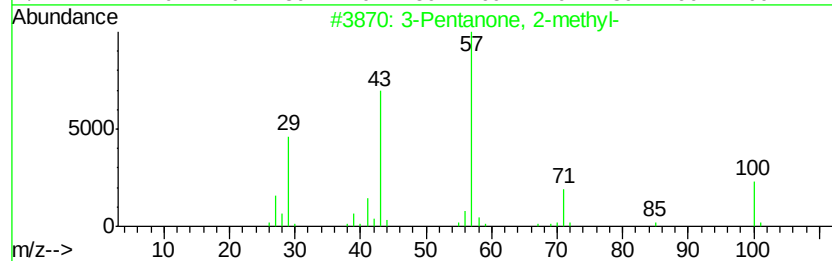
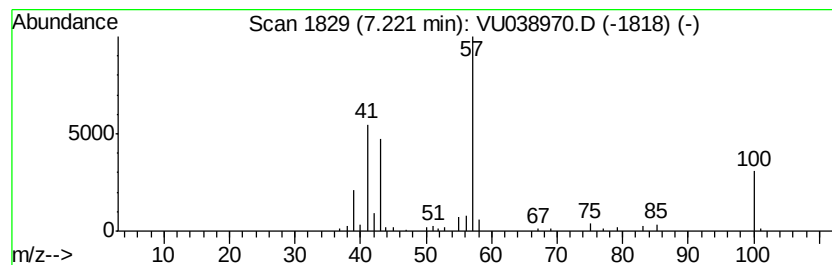
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 3-Pentanone, 2-methyl- Concentration Rank 5

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 7.22 | 0.64 ug/L | 79701 | 1,4-Difluorobenzene | 6.30 |

| Hit# | of | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------------|-----|---------|-------------|------|
| 1    | 5  | 3-Pentanone, 2-methyl-    | 100 | C6H12O  | 000565-69-5 | 72   |
| 2    |    | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O  | 000075-97-8 | 64   |
| 3    |    | 3-Pentanone, 2-methyl-    | 100 | C6H12O  | 000565-69-5 | 64   |
| 4    |    | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O  | 000075-97-8 | 59   |
| 5    |    | 3-Hexanone                | 100 | C6H12O  | 000589-38-8 | 50   |



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Misc : 25.0mL/MSVOA U/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
Quant Title : TRACE VOA SOM01.0

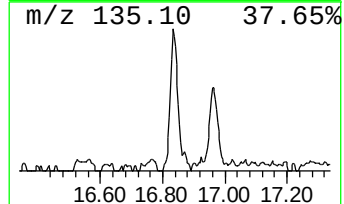
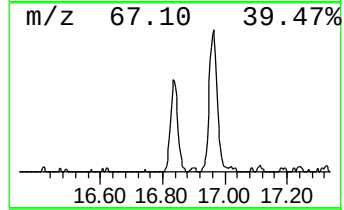
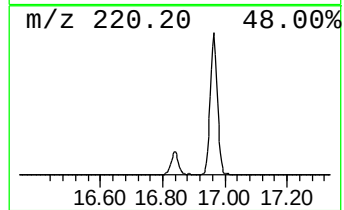
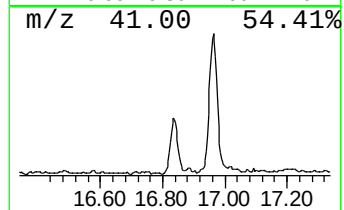
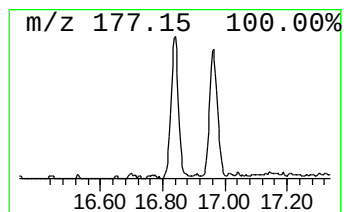
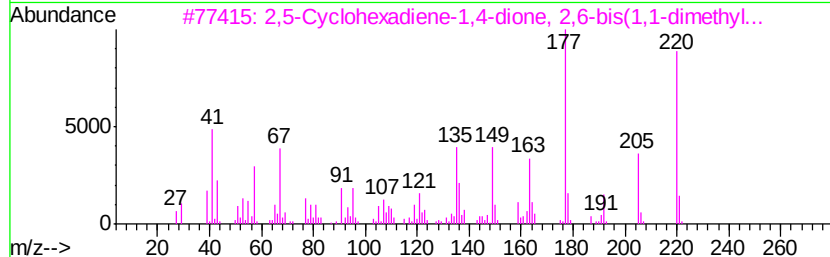
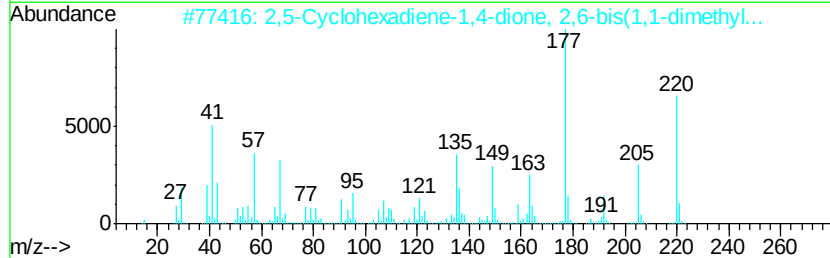
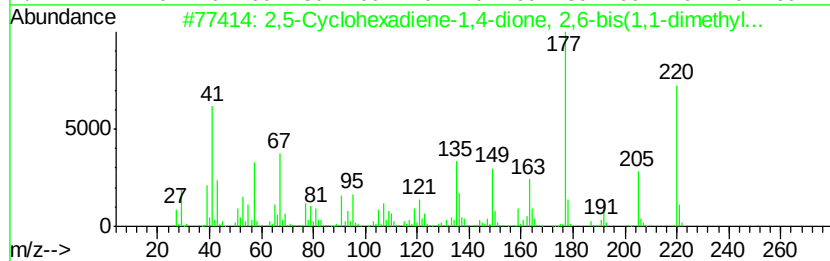
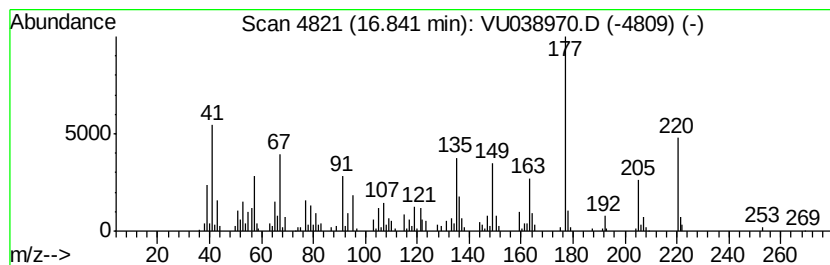
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 16.84 | 0.80 ug/L | 125587 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 98   |
| 2    |    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 95   |
| 3    |    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 60   |
| 4    |    | 2-Butanone, 3-(4-tert-butylpheno... | 220 | C14H20O2 | 160875-28-5 | 50   |
| 5    |    | 3-Buten-2-one, 4-(2,6,6-trimethy... | 192 | C13H20O  | 014901-07-6 | 38   |



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ALS Vial : 1 Sample Multiplier: 1

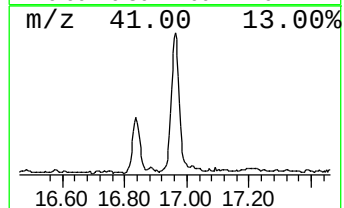
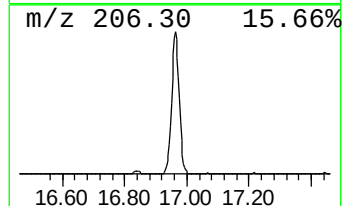
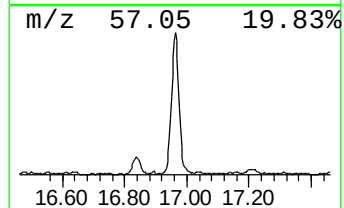
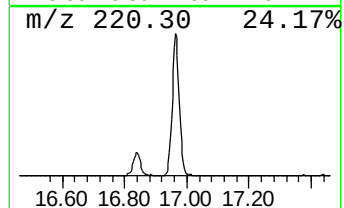
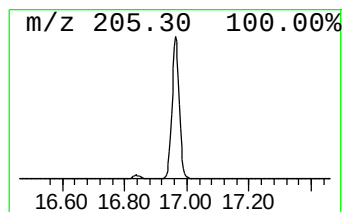
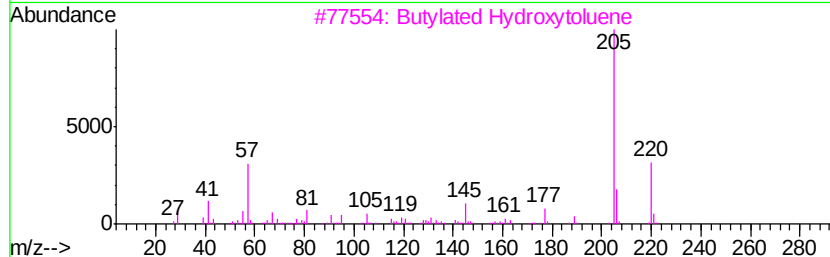
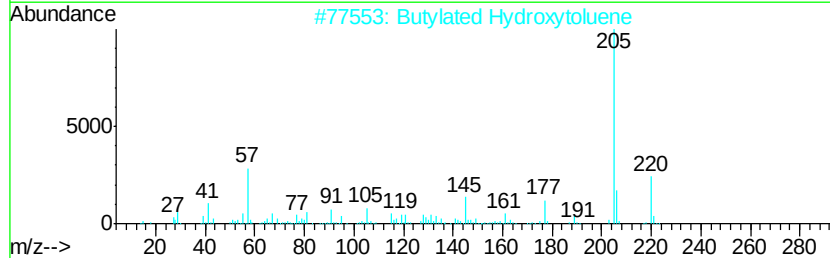
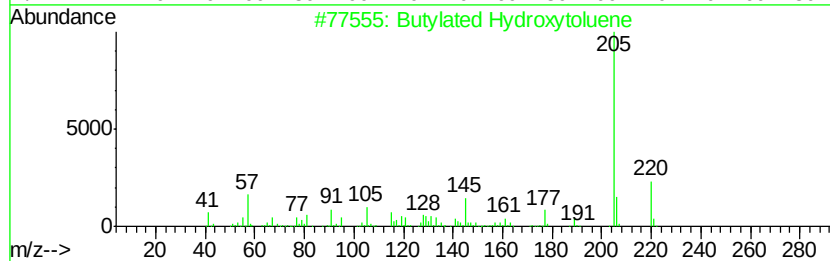
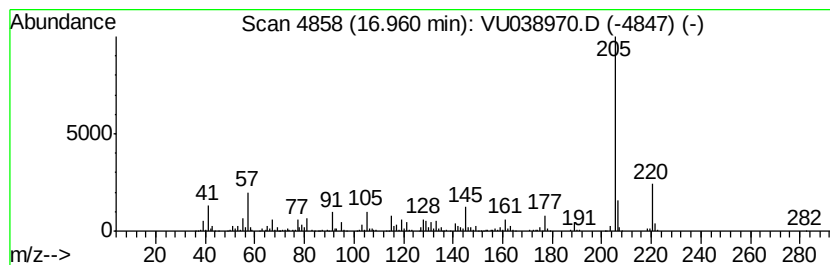
Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
Quant Title : TRACE VOA SOM01.0

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

\*\*\*\*\*  
Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

| R.T.    | EstConc                            | Area           | Relative to ISTD       | R.T.    |             |      |
|---------|------------------------------------|----------------|------------------------|---------|-------------|------|
| 16.96   | 3.81 ug/L                          | 597577         | 1,4-Dichlorobenzene-d4 | 11.83   |             |      |
| Hit# of | 5                                  | Tentative ID   | MW                     | MolForm | CAS#        | Qual |
| 1       | Butylated                          | Hydroxytoluene | 220                    | C15H24O | 000128-37-0 | 99   |
| 2       | Butylated                          | Hydroxytoluene | 220                    | C15H24O | 000128-37-0 | 97   |
| 3       | Butylated                          | Hydroxytoluene | 220                    | C15H24O | 000128-37-0 | 97   |
| 4       | Butylated                          | Hydroxytoluene | 220                    | C15H24O | 000128-37-0 | 94   |
| 5       | Phenol, 2,4,6-tris(1-methylethyl)- |                | 220                    | C15H24O | 002934-07-8 | 83   |





Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU061820\  
Data File : VU038970.D  
Acq On : 18 Jun 2020 15:18  
Operator : SY/MD  
Sample : L3058-04  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F9L31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR061720WMA.M  
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 |
| L-Alanine, 3-sulfo-  | 2.18  | 0.8     | ug/L  | 104992   | 1                     | 6.30  | 621983 | 5.0  |
| unknown-01           | 3.54  | 0.5     | ug/L  | 66466    | 1                     | 6.30  | 621983 | 5.0  |
| 3-Pentanone, 2-me... | 7.22  | 0.6     | ug/L  | 79701    | 1                     | 6.30  | 621983 | 5.0  |
| 2,5-Cyclohexadien... | 16.84 | 0.8     | ug/L  | 125587   | 3                     | 11.83 | 783848 | 5.0  |
| Butylated Hydroxy... | 16.96 | 3.8     | ug/L  | 597577   | 3                     | 11.83 | 783848 | 5.0  |