

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121222\  
 Data File : VU052361.D  
 Acq On : 12 Dec 2022 18:31  
 Operator : JC/MD  
 Sample : N5961-04  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F5N35

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\SFAMUTR111822WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU052361.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         | 1.475       | 32            | 42          | 72           | rBV      | 876915         | 2172372       | 100.00%         | 19.618%       |
| 2         | 1.601       | 76            | 81          | 92           | rVB      | 137090         | 181510        | 8.36%           | 1.639%        |
| 3         | 1.916       | 173           | 179         | 197          | rVB      | 107445         | 156496        | 7.20%           | 1.413%        |
| 4         | 2.568       | 370           | 382         | 399          | rVB      | 198526         | 321533        | 14.80%          | 2.904%        |
| 5         | 3.282       | 583           | 604         | 607          | rBV3     | 9149           | 28674         | 1.32%           | 0.259%        |
| 6         | 4.649       | 1014          | 1029        | 1085         | rBV      | 91553          | 416745        | 19.18%          | 3.764%        |
| 7         | 5.060       | 1141          | 1157        | 1178         | rBV      | 170280         | 377518        | 17.38%          | 3.409%        |
| 8         | 5.723       | 1342          | 1363        | 1378         | rBV2     | 347564         | 906790        | 41.74%          | 8.189%        |
| 9         | 5.790       | 1381          | 1384        | 1403         | rVB3     | 22765          | 40382         | 1.86%           | 0.365%        |
| 10        | 6.247       | 1511          | 1526        | 1550         | rBV      | 269860         | 526708        | 24.25%          | 4.757%        |
| 11        | 6.687       | 1649          | 1663        | 1691         | rBV      | 221336         | 436534        | 20.09%          | 3.942%        |
| 12        | 7.163       | 1788          | 1811        | 1843         | rBV      | 233207         | 505404        | 23.27%          | 4.564%        |
| 13        | 7.562       | 1919          | 1935        | 1956         | rBV      | 98687          | 177572        | 8.17%           | 1.604%        |
| 14        | 7.896       | 2026          | 2039        | 2055         | rVV      | 408988         | 708486        | 32.61%          | 6.398%        |
| 15        | 8.176       | 2114          | 2126        | 2144         | rBV      | 60872          | 106735        | 4.91%           | 0.964%        |
| 16        | 8.481       | 2207          | 2221        | 2234         | rBV4     | 13267          | 30000         | 1.38%           | 0.271%        |
| 17        | 8.636       | 2253          | 2269        | 2287         | rBV      | 551044         | 1087603       | 50.07%          | 9.822%        |
| 18        | 9.414       | 2498          | 2511        | 2537         | rBV      | 401441         | 680371        | 31.32%          | 6.144%        |
| 19        | 10.751      | 2911          | 2927        | 2939         | rBV      | 202274         | 337492        | 15.54%          | 3.048%        |
| 20        | 11.809      | 3243          | 3256        | 3273         | rBV      | 376948         | 611271        | 28.14%          | 5.520%        |
| 21        | 12.057      | 3323          | 3333        | 3352         | rBV3     | 13448          | 29162         | 1.34%           | 0.263%        |
| 22        | 12.189      | 3361          | 3374        | 3394         | rBV      | 412531         | 670574        | 30.87%          | 6.056%        |
| 23        | 12.886      | 3579          | 3591        | 3599         | rBV5     | 12581          | 21919         | 1.01%           | 0.198%        |
| 24        | 14.189      | 3985          | 3996        | 4008         | rVB4     | 19887          | 30609         | 1.41%           | 0.276%        |
| 25        | 14.999      | 4237          | 4248        | 4260         | rBV      | 26563          | 43834         | 2.02%           | 0.396%        |
| 26        | 15.690      | 4452          | 4463        | 4476         | rBV4     | 47681          | 84519         | 3.89%           | 0.763%        |
| 27        | 16.764      | 4786          | 4797        | 4818         | rBV      | 142656         | 252735        | 11.63%          | 2.282%        |
| 28        | 16.883      | 4825          | 4834        | 4849         | rVB      | 82975          | 129690        | 5.97%           | 1.171%        |

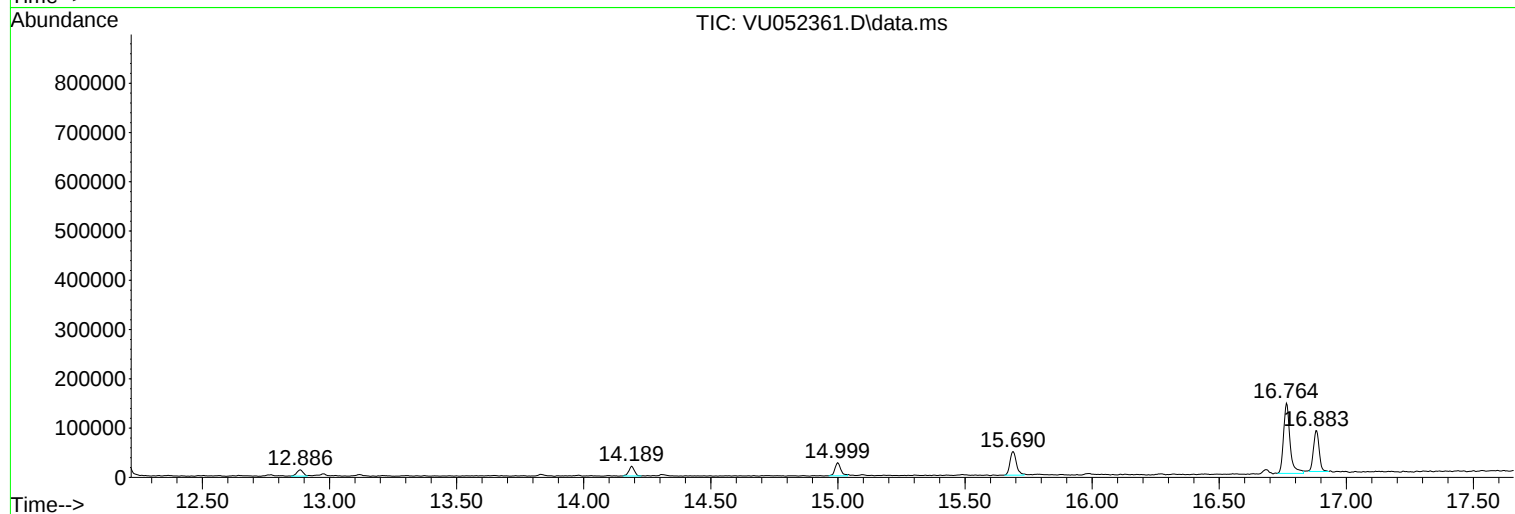
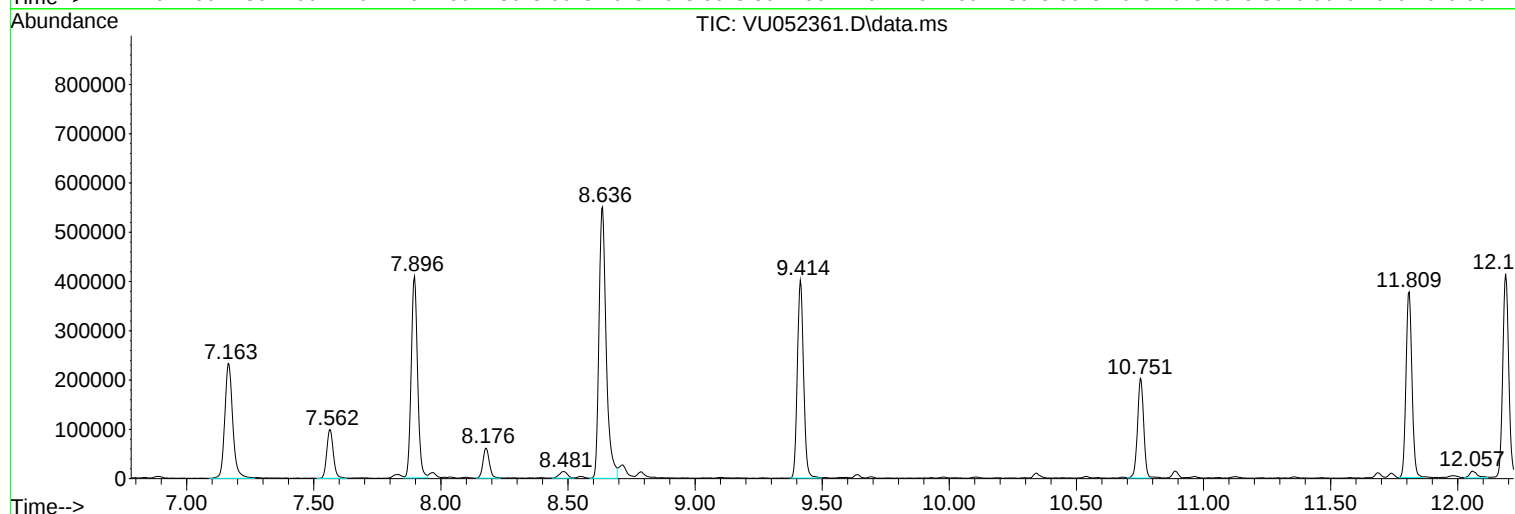
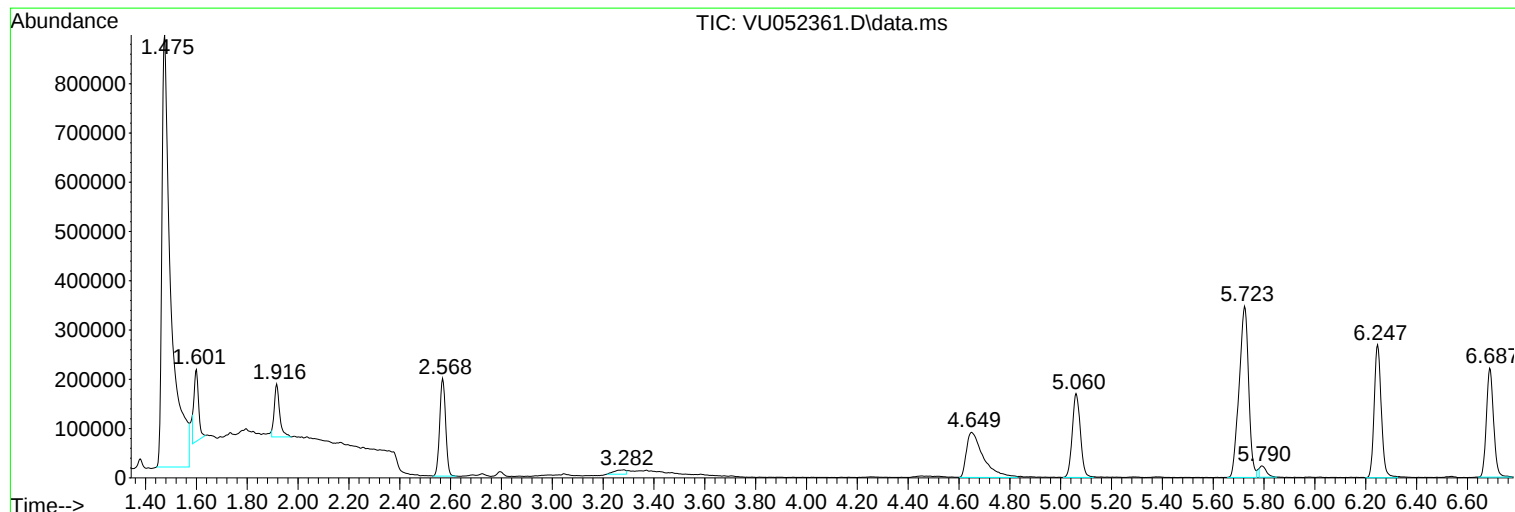
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Sample : N5961-04  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N35

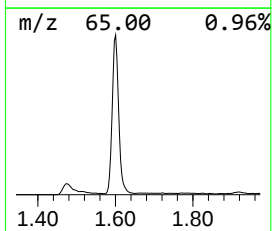
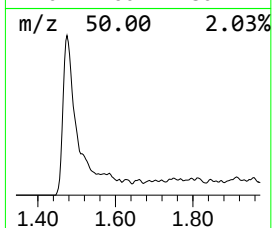
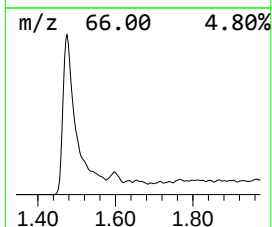
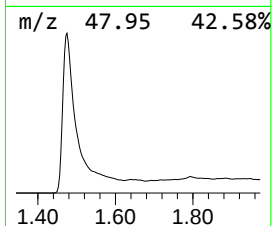
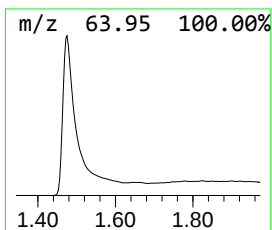
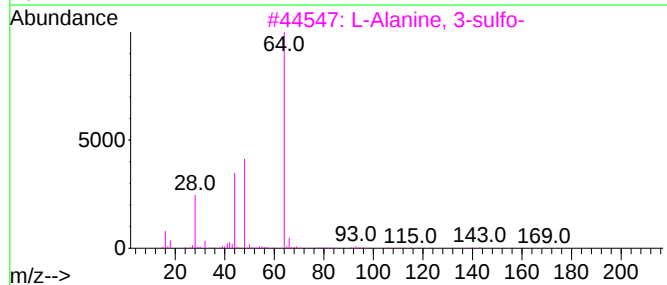
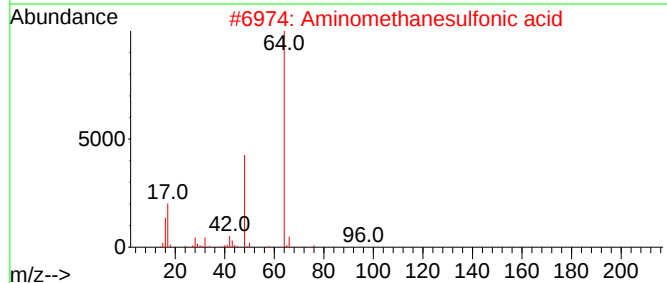
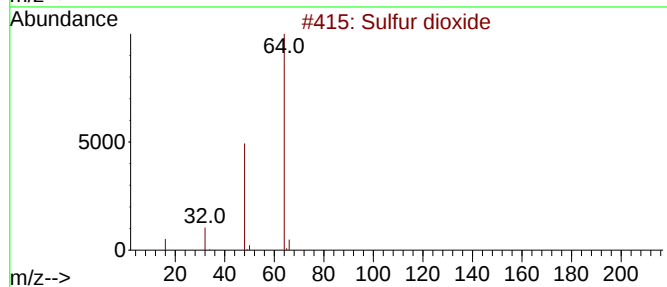
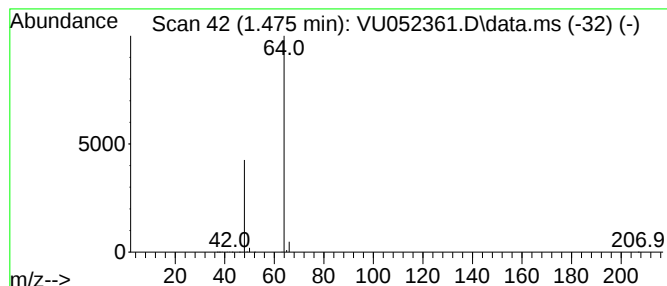
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 1.475 | 20.62 ug/L | 2172370 | 1,4-Difluorobenzene | 6.247 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 83   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |
| 5    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 3    |



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ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N35

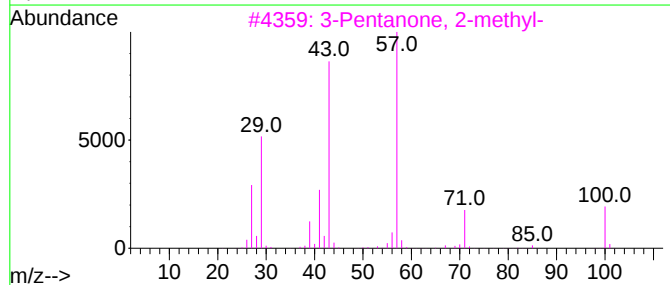
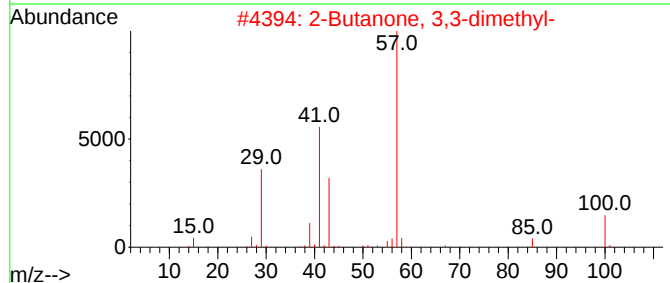
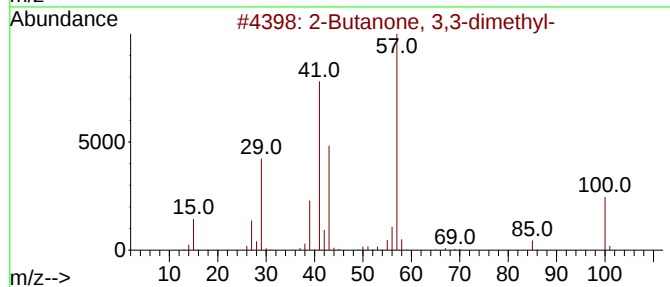
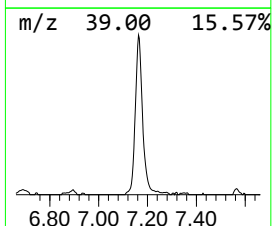
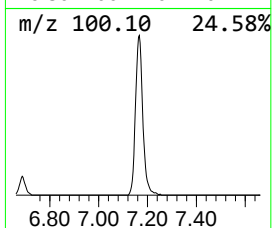
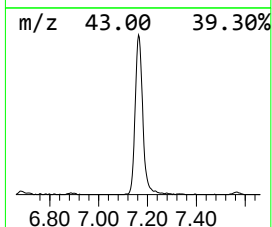
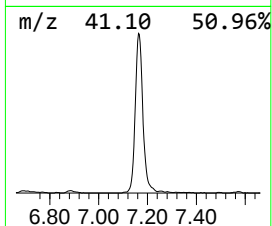
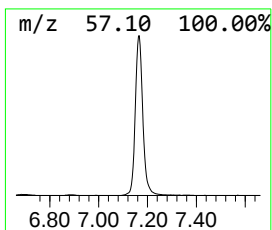
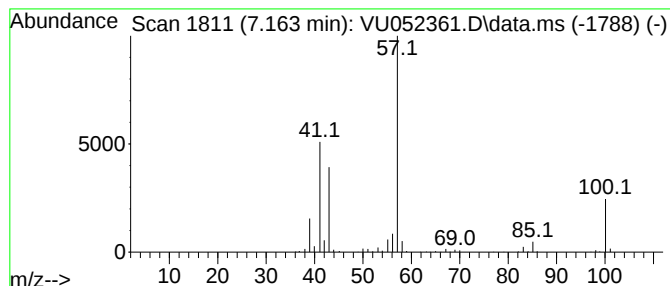
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 7.163 | 4.80 ug/L | 505404 | 1,4-Difluorobenzene | 6.247 |

| Hit# | of                        | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|---------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O       | 000075-97-8 | 90      |      |      |
| 2    | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O       | 000075-97-8 | 80      |      |      |
| 3    | 3-Pentanone, 2-methyl-    | 100 | C6H12O       | 000565-69-5 | 59      |      |      |
| 4    | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O       | 000075-97-8 | 50      |      |      |
| 5    | 3-Pentanone, 2-methyl-    | 100 | C6H12O       | 000565-69-5 | 50      |      |      |



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Sample : N5961-04  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N35

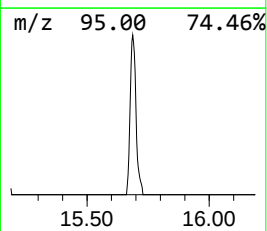
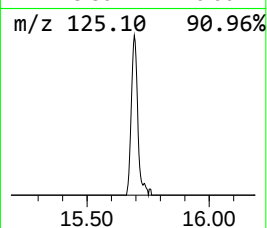
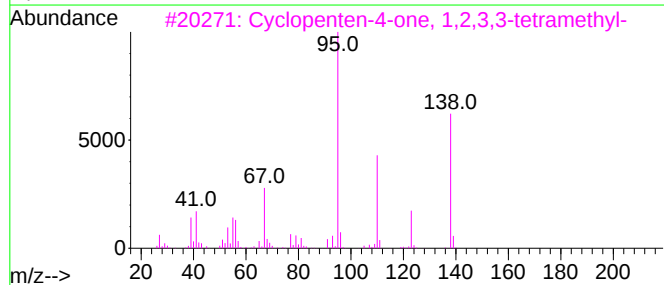
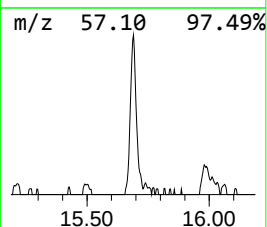
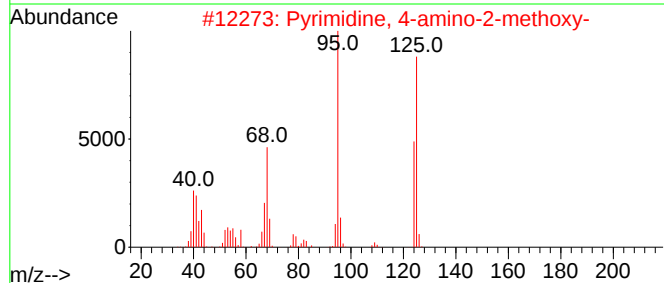
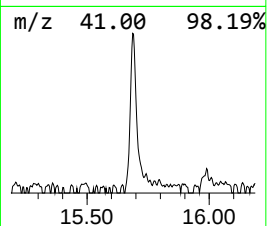
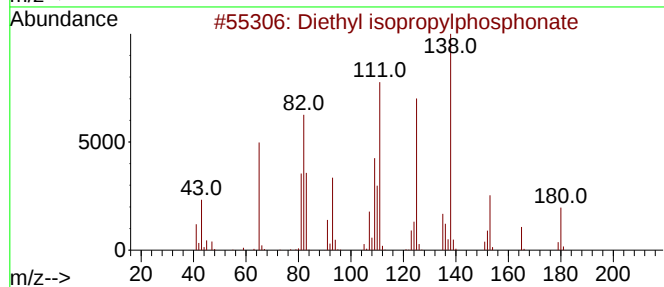
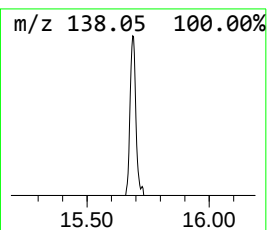
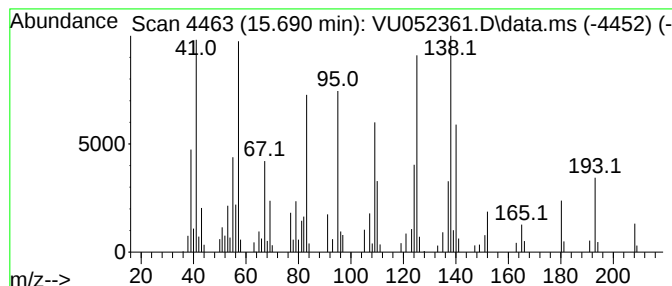
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Diethyl isopropylphosphonate Concentration Rank 6

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 15.690 | 0.69 ug/L | 84519 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Diethyl isopropylphosphonate        | 180 | C7H17O3P | 001538-69-8  | 50   |
| 2    |    |   | Pyrimidine, 4-amino-2-methoxy-      | 125 | C5H7N3O  | 003289-47-2  | 38   |
| 3    |    |   | Cyclopenten-4-one, 1,2,3,3-tetra... | 138 | C9H14O   | 1000163-38-6 | 30   |
| 4    |    |   | Cyclopentanecarboxaldehyde, 2-me... | 124 | C8H12O   | 1000154-24-0 | 25   |
| 5    |    |   | 2,3-Dimethylhydroquinone            | 138 | C8H10O2  | 000608-43-5  | 20   |



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ALS Vial : 22 Sample Multiplier: 1

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MSVOA\_U  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

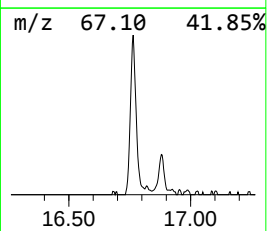
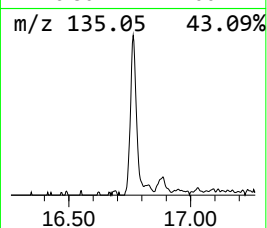
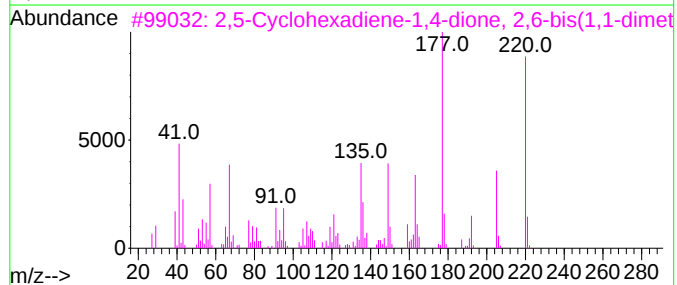
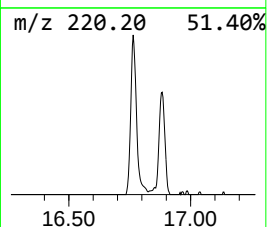
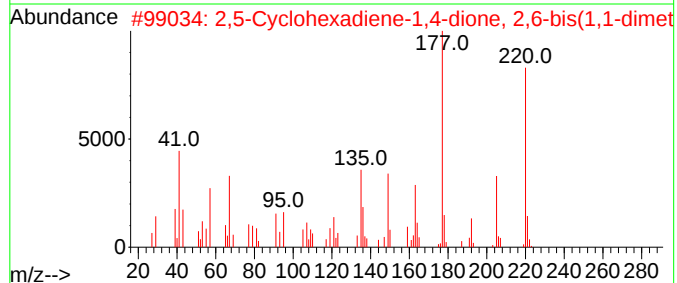
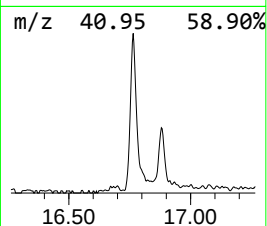
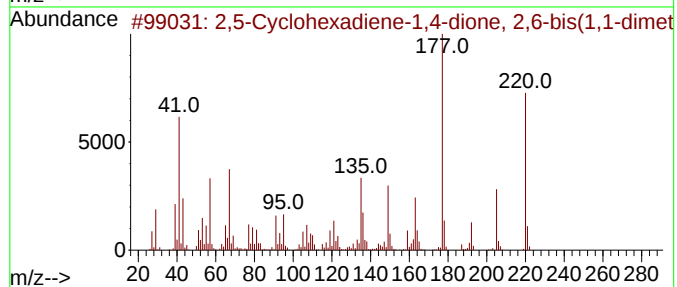
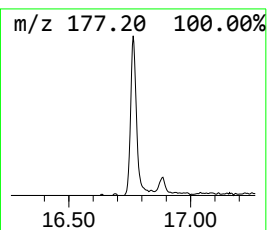
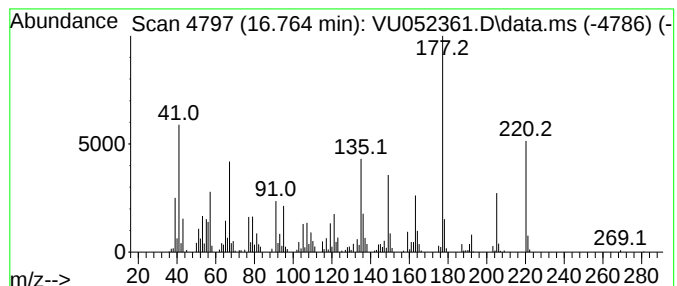
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.764 | 2.07 ug/L | 252735 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 96   |
| 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 | 93   |
| 4    |    |   | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 93   |
| 5    |    |   | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 50   |



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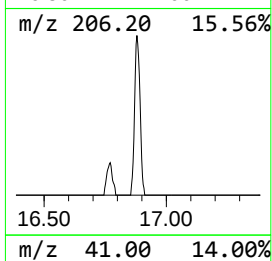
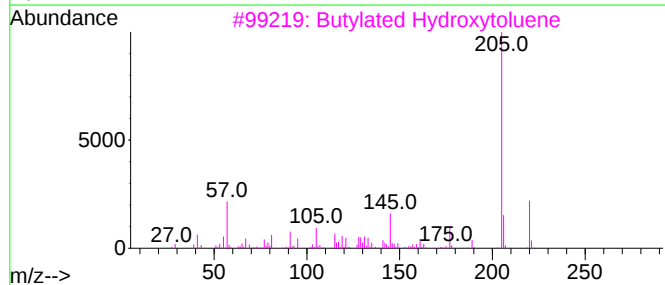
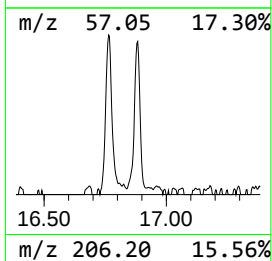
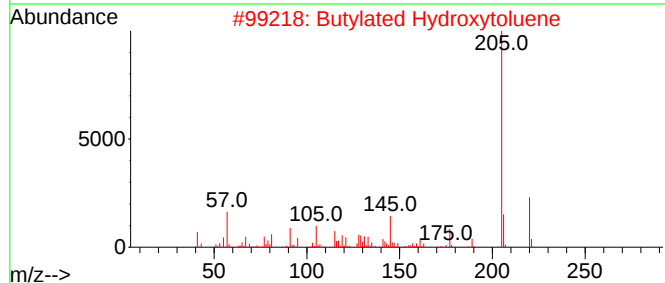
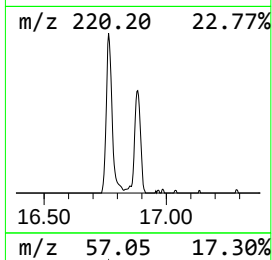
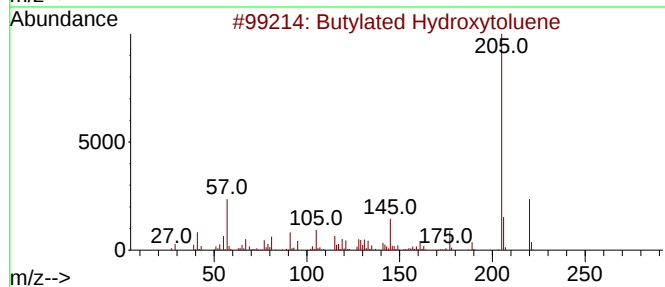
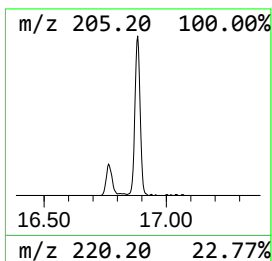
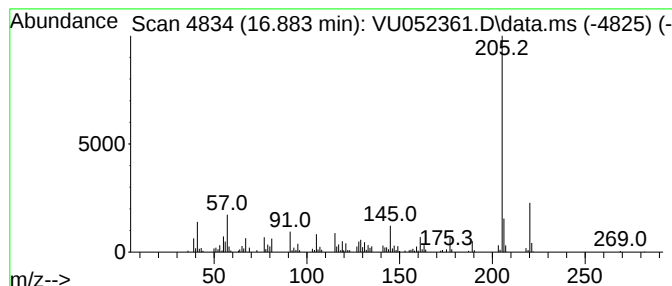
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 6 Butylated Hydroxytoluene Concentration Rank 5

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.883 | 1.06 ug/L | 129690 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm  | CAS#         | Qual |
|------|----|---|--------------------------------|-----|----------|--------------|------|
| 1    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 98   |
| 2    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 97   |
| 3    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 96   |
| 4    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 96   |
| 5    |    |   | Ethyl 4-oxo-2-phenylpentanoate | 220 | C13H16O3 | 1000427-11-2 | 95   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121222\  
Data File : VU052361.D  
Acq On : 12 Dec 2022 18:31  
Operator : JC/MD  
Sample : N5961-04  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Sulfur dioxide     | 1.475  | 20.6    | ug/L  | 2172370  | 1                     | 6.247  | 526708 | 5.0  |
| 2-Butanone, 3,3... | 7.163  | 4.8     | ug/L  | 505404   | 1                     | 6.247  | 526708 | 5.0  |
| Diethyl isoprop... | 15.690 | 0.7     | ug/L  | 84519    | 3                     | 11.809 | 611271 | 5.0  |
| 2,5-Cyclohexadi... | 16.764 | 2.1     | ug/L  | 252735   | 3                     | 11.809 | 611271 | 5.0  |
| Butylated Hydro... | 16.883 | 1.1     | ug/L  | 129690   | 3                     | 11.809 | 611271 | 5.0  |