

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120722\  
 Data File : VU052232.D  
 Acq On : 08 Dec 2022 06:09  
 Operator : JC/MD  
 Sample : N5916-13  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 44 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F5N31

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: VU052232.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         | 1.600       | 71            | 81          | 92           | rBV      | 106482         | 130630        | 1.08%           | 0.663%        |
| 2         | 1.916       | 170           | 179         | 198          | rBV      | 87971          | 121525        | 1.01%           | 0.617%        |
| 3         | 2.568       | 369           | 382         | 400          | rBV      | 171351         | 280442        | 2.32%           | 1.424%        |
| 4         | 4.655       | 1015          | 1031        | 1077         | rBV2     | 79934          | 378284        | 3.13%           | 1.921%        |
| 5         | 5.063       | 1142          | 1158        | 1192         | rBV      | 150259         | 340504        | 2.82%           | 1.729%        |
| 6         | 5.726       | 1342          | 1364        | 1372         | rBV2     | 293510         | 760673        | 6.29%           | 3.863%        |
| 7         | 5.793       | 1372          | 1385        | 1443         | rVB      | 5917427        | 12087394      | 100.00%         | 61.391%       |
| 8         | 6.247       | 1513          | 1526        | 1546         | rBV      | 267941         | 514365        | 4.26%           | 2.612%        |
| 9         | 6.690       | 1650          | 1664        | 1683         | rBV      | 187760         | 377747        | 3.13%           | 1.919%        |
| 10        | 7.565       | 1924          | 1936        | 1956         | rBV      | 75116          | 135005        | 1.12%           | 0.686%        |
| 11        | 7.896       | 2023          | 2039        | 2054         | rBV      | 316626         | 545655        | 4.51%           | 2.771%        |
| 12        | 8.636       | 2251          | 2269        | 2310         | rBV2     | 457419         | 988278        | 8.18%           | 5.019%        |
| 13        | 9.414       | 2499          | 2511        | 2531         | rBV      | 368210         | 616801        | 5.10%           | 3.133%        |
| 14        | 10.754      | 2911          | 2928        | 2942         | rBV      | 181483         | 301657        | 2.50%           | 1.532%        |
| 15        | 11.809      | 3243          | 3256        | 3274         | rBV      | 332646         | 542728        | 4.49%           | 2.756%        |
| 16        | 12.188      | 3362          | 3374        | 3396         | rBV      | 317243         | 542758        | 4.49%           | 2.757%        |
| 17        | 16.693      | 4764          | 4775        | 4787         | rBV3     | 99220          | 194860        | 1.61%           | 0.990%        |
| 18        | 16.767      | 4789          | 4798        | 4809         | rVV2     | 115833         | 188107        | 1.56%           | 0.955%        |
| 19        | 16.883      | 4824          | 4834        | 4850         | rBV      | 413583         | 641709        | 5.31%           | 3.259%        |

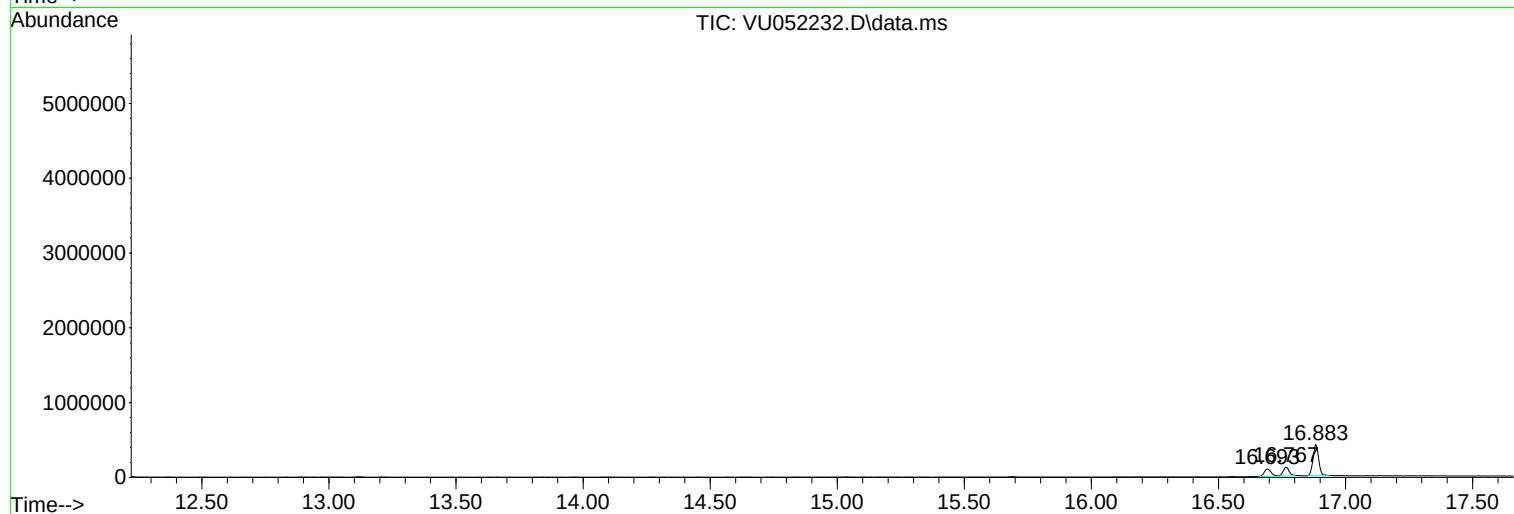
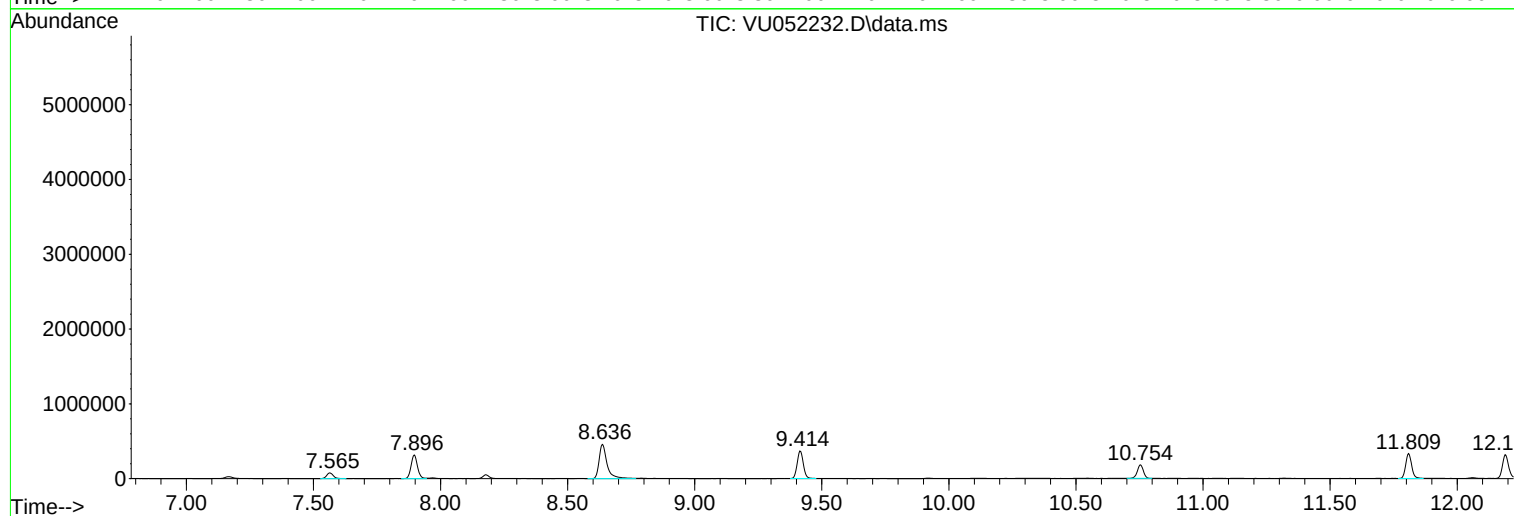
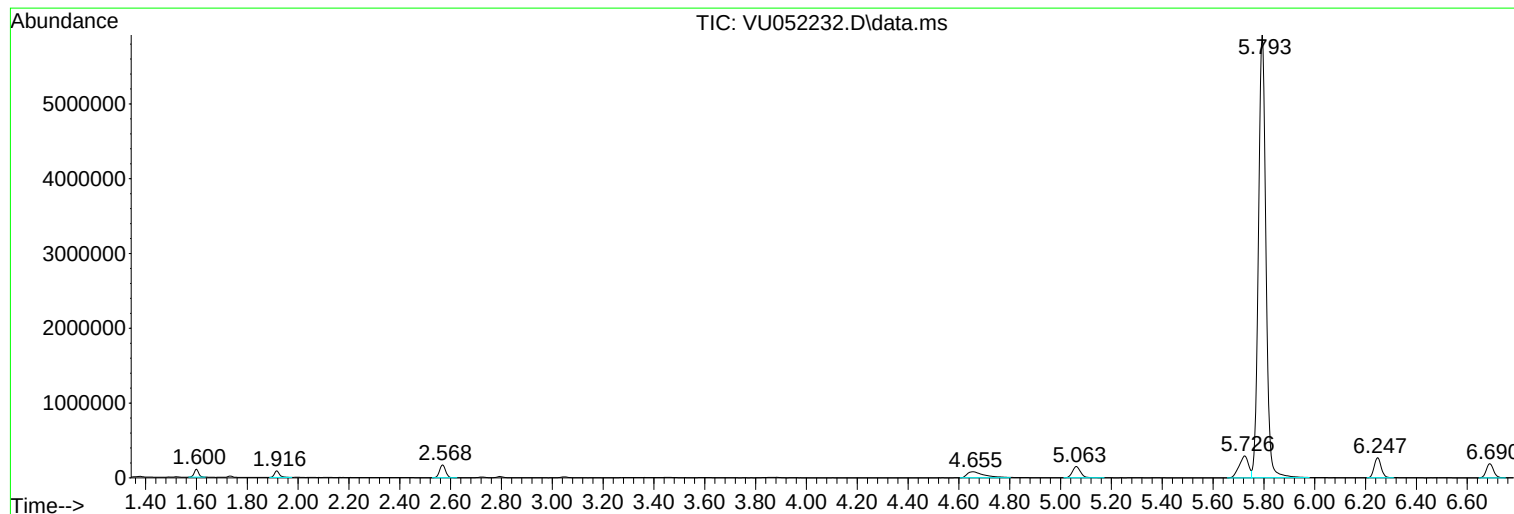
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ALS Vial : 44 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F5N31

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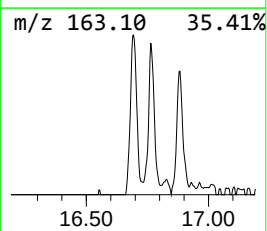
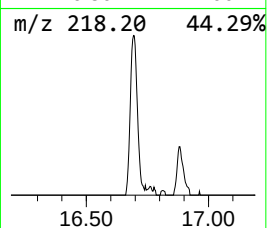
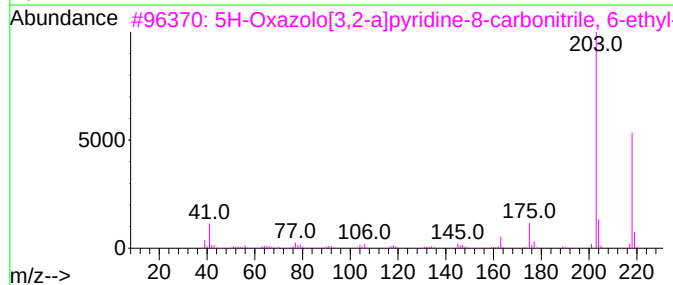
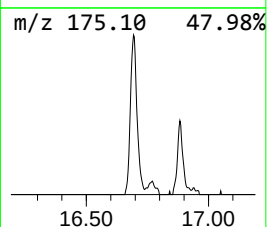
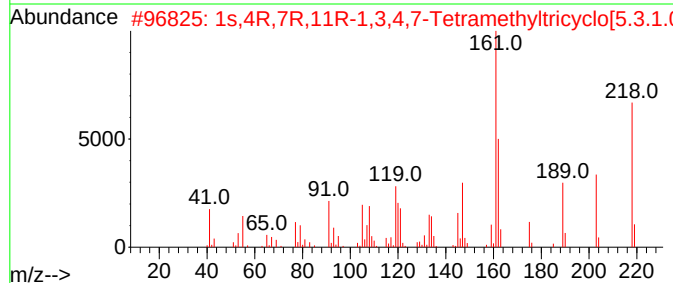
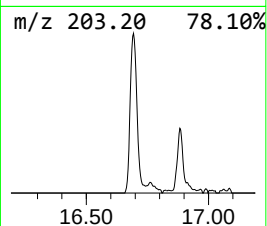
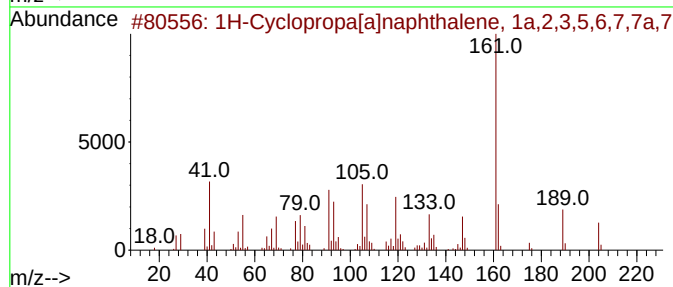
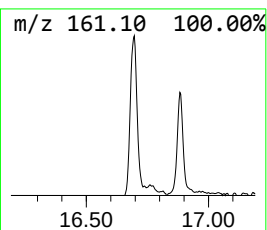
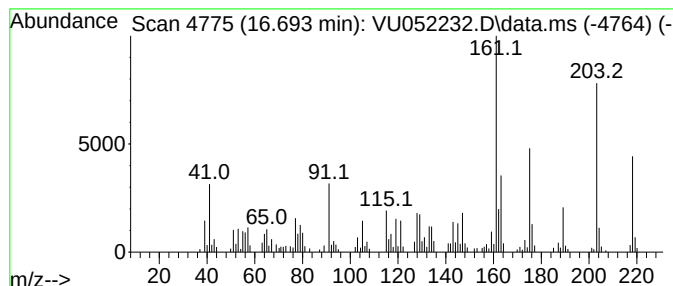
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 unknown-01 Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.693 | 1.80 ug/L | 194860 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 1H-Cyclopropa[a]naphthalene, 1a,... | 204 | C15H24     | 017334-55-3  | 42   |
| 2    |    |   | 1s,4R,7R,11R-1,3,4,7-Tetramethyl... | 218 | C15H22O    | 137235-42-8  | 42   |
| 3    |    |   | 5H-Oxazolo[3,2-a]pyridine-8-carb... | 218 | C12H14N2O2 | 1000337-58-3 | 38   |
| 4    |    |   | 1H-Cyclopropa[a]naphthalene, 1a,... | 204 | C15H24     | 017334-55-3  | 38   |
| 5    |    |   | Acetic acid, trifluoro-, 4-ethyl... | 218 | C10H9F3O2  | 1000376-49-4 | 38   |



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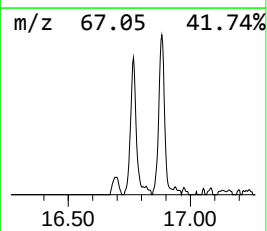
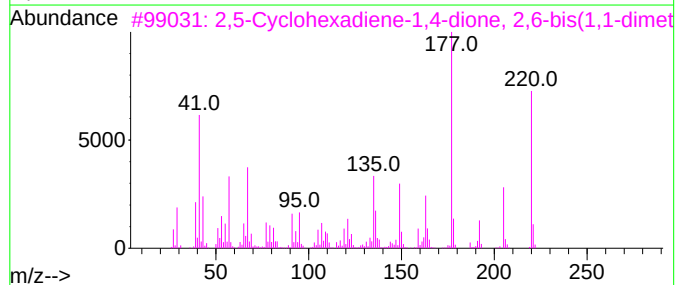
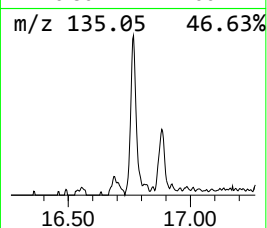
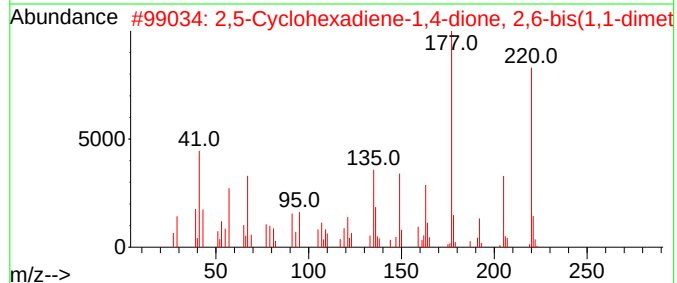
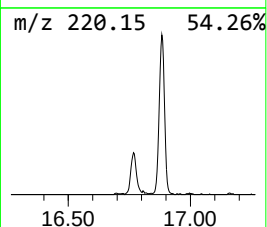
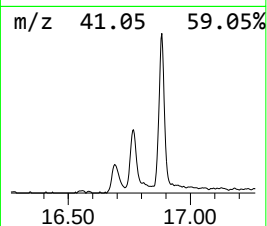
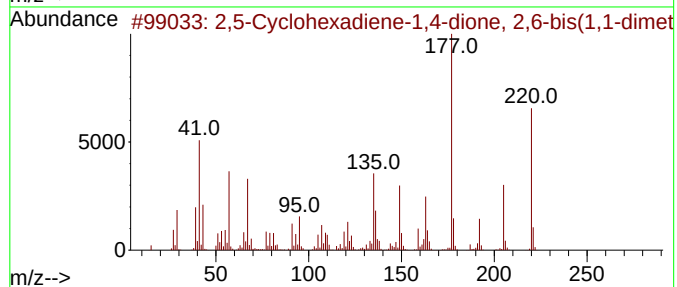
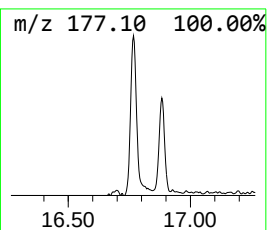
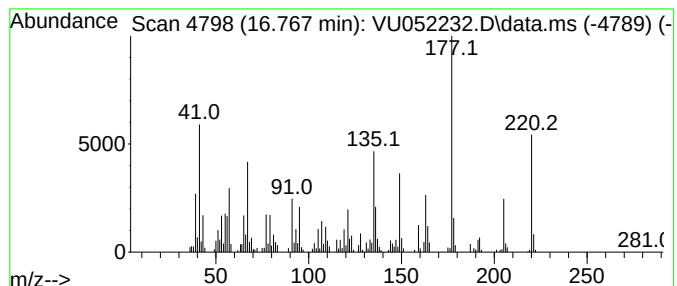
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR111822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.767 | 1.73 ug/L | 188107 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 96      |      |      |
| 2    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 96      |      |      |
| 3    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 95      |      |      |
| 4    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 93      |      |      |
| 5    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 93      |      |      |



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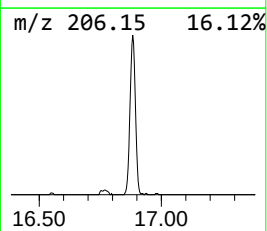
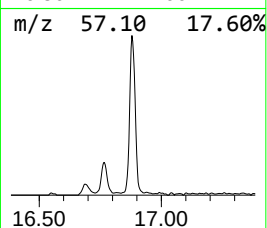
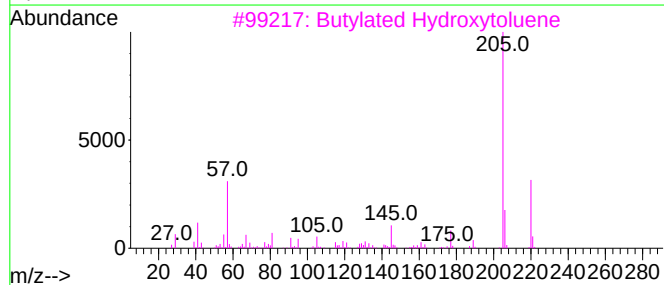
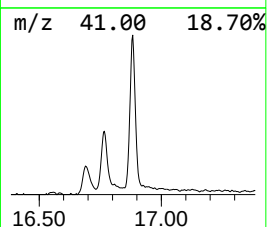
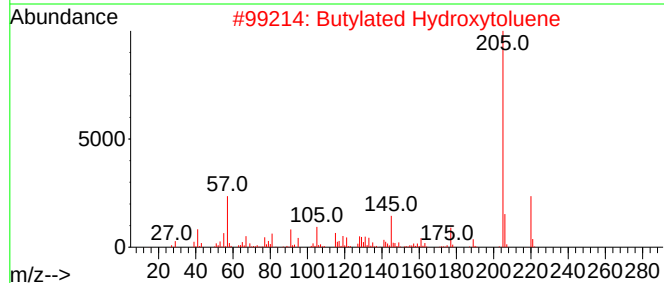
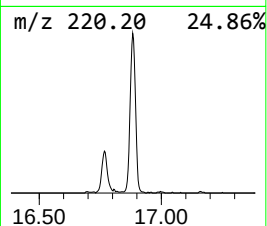
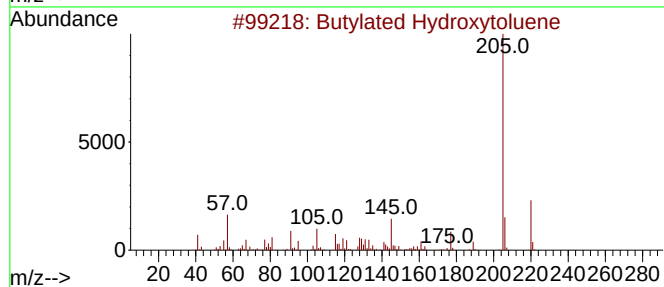
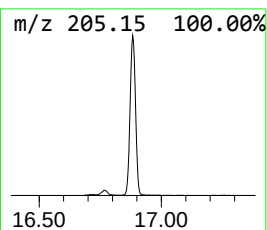
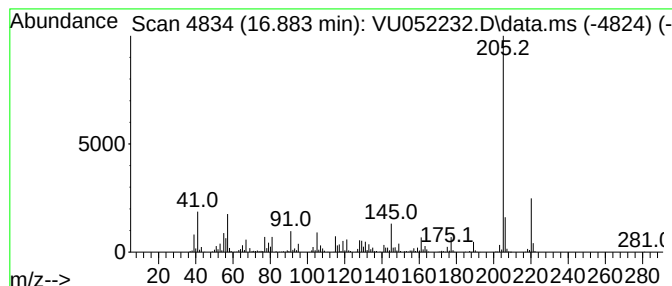
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Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.883 | 5.91 ug/L | 641709 | 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  | 98   |
| 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 | 94   |



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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 |
| unknown-01         | 16.693 | 1.8     | ug/L  | 194860   | 3                     | 11.809 | 542728 | 5.0  |
| 2,5-Cyclohexadi... | 16.767 | 1.7     | ug/L  | 188107   | 3                     | 11.809 | 542728 | 5.0  |
| Butylated Hydro... | 16.883 | 5.9     | ug/L  | 641709   | 3                     | 11.809 | 542728 | 5.0  |