

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
 Data File : VU042174.D  
 Acq On : 22 Jan 2021 16:58  
 Operator : SY/MD  
 Sample : M1222-09  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F1E16

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\SOMUTR012021WMA.M  
 Title : TRACE VOA SOM01.0

Signal : TIC: VU042174.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         | 1.601       | 71            | 81          | 93           | rVB2     | 44151          | 58928         | 11.99%          | 1.514%        |
| 2         | 1.916       | 172           | 179         | 192          | rVB      | 33882          | 43064         | 8.76%           | 1.107%        |
| 3         | 2.572       | 370           | 383         | 396          | rBV      | 73691          | 119463        | 24.30%          | 3.070%        |
| 4         | 3.253       | 575           | 595         | 601          | rBV7     | 4613           | 14419         | 2.93%           | 0.371%        |
| 5         | 4.652       | 1010          | 1030        | 1032         | rBV      | 45172          | 86956         | 17.69%          | 2.235%        |
| 6         | 5.073       | 1146          | 1161        | 1182         | rBV      | 69554          | 149420        | 30.40%          | 3.840%        |
| 7         | 5.735       | 1345          | 1367        | 1387         | rBV2     | 133414         | 349463        | 71.09%          | 8.980%        |
| 8         | 6.256       | 1516          | 1529        | 1549         | rBV      | 131982         | 243599        | 49.55%          | 6.260%        |
| 9         | 6.549       | 1611          | 1620        | 1631         | rVB6     | 4894           | 9256          | 1.88%           | 0.238%        |
| 10        | 6.700       | 1654          | 1667        | 1684         | rVB      | 86939          | 164624        | 33.49%          | 4.230%        |
| 11        | 7.179       | 1801          | 1816        | 1825         | rBV4     | 4507           | 9042          | 1.84%           | 0.232%        |
| 12        | 7.575       | 1927          | 1939        | 1955         | rBV      | 48765          | 86114         | 17.52%          | 2.213%        |
| 13        | 7.906       | 2028          | 2042        | 2056         | rBV      | 169137         | 286849        | 58.35%          | 7.371%        |
| 14        | 8.185       | 2119          | 2129        | 2143         | rBV      | 31130          | 53146         | 10.81%          | 1.366%        |
| 15        | 8.558       | 2237          | 2245        | 2255         | rVB3     | 6510           | 10074         | 2.05%           | 0.259%        |
| 16        | 8.642       | 2255          | 2271        | 2316         | rBV      | 217264         | 467271        | 95.06%          | 12.008%       |
| 17        | 9.423       | 2502          | 2514        | 2534         | rBV      | 185908         | 307236        | 62.50%          | 7.895%        |
| 18        | 9.989       | 2680          | 2690        | 2702         | rBV2     | 14958          | 25504         | 5.19%           | 0.655%        |
| 19        | 10.552      | 2855          | 2865        | 2875         | rBV      | 8342           | 14140         | 2.88%           | 0.363%        |
| 20        | 10.693      | 2902          | 2909        | 2919         | rVB3     | 3753           | 5929          | 1.21%           | 0.152%        |
| 21        | 10.764      | 2919          | 2931        | 2947         | rBV      | 68130          | 112279        | 22.84%          | 2.885%        |
| 22        | 11.819      | 3247          | 3259        | 3273         | rBV      | 209968         | 326874        | 66.50%          | 8.400%        |
| 23        | 12.070      | 3328          | 3337        | 3357         | rBV3     | 6376           | 13337         | 2.71%           | 0.343%        |
| 24        | 12.201      | 3366          | 3378        | 3394         | rVB      | 177223         | 284888        | 57.95%          | 7.321%        |
| 25        | 12.333      | 3402          | 3419        | 3429         | rBV      | 6846           | 12638         | 2.57%           | 0.325%        |
| 26        | 12.896      | 3585          | 3594        | 3604         | rVV3     | 12165          | 18022         | 3.67%           | 0.463%        |
| 27        | 14.201      | 3990          | 4000        | 4010         | rBV2     | 26928          | 40206         | 8.18%           | 1.033%        |
| 28        | 14.323      | 4031          | 4038        | 4049         | rBV6     | 4839           | 8210          | 1.67%           | 0.211%        |
| 29        | 15.703      | 4455          | 4467        | 4479         | rBV7     | 6816           | 11145         | 2.27%           | 0.286%        |
| 30        | 16.143      | 4597          | 4604        | 4614         | rVB5     | 6512           | 9257          | 1.88%           | 0.238%        |
| 31        | 16.783      | 4791          | 4803        | 4816         | rBV2     | 33957          | 58452         | 11.89%          | 1.502%        |
| 32        | 16.899      | 4827          | 4839        | 4856         | rBV      | 332260         | 491575        | 100.00%         | 12.632%       |

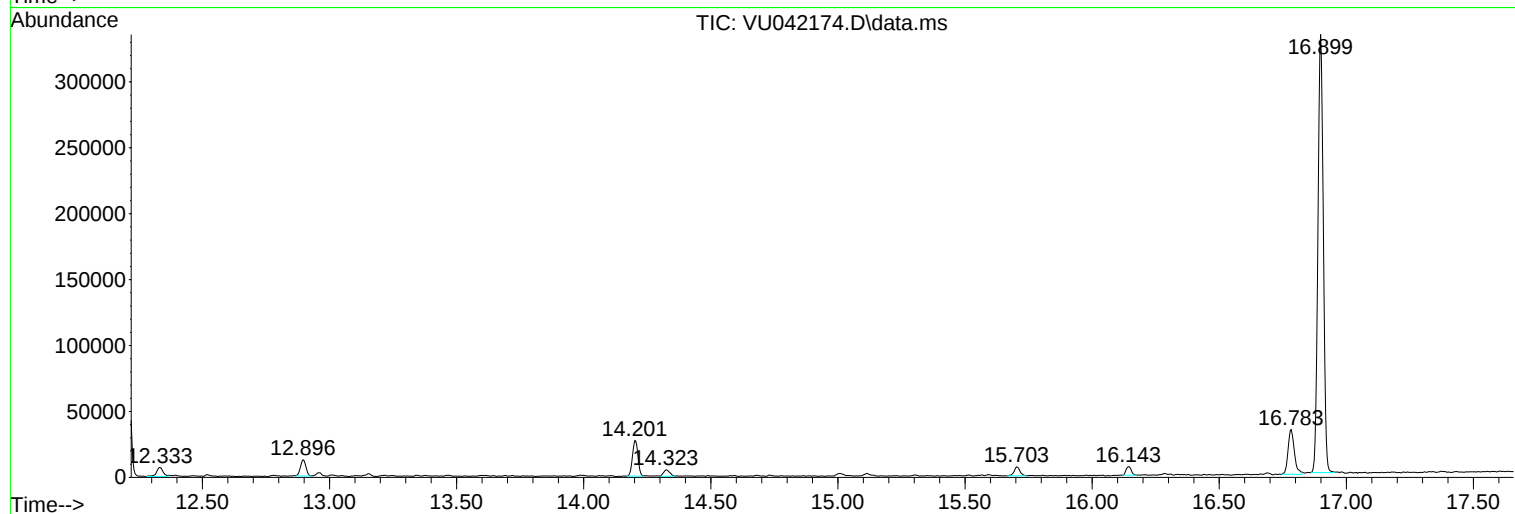
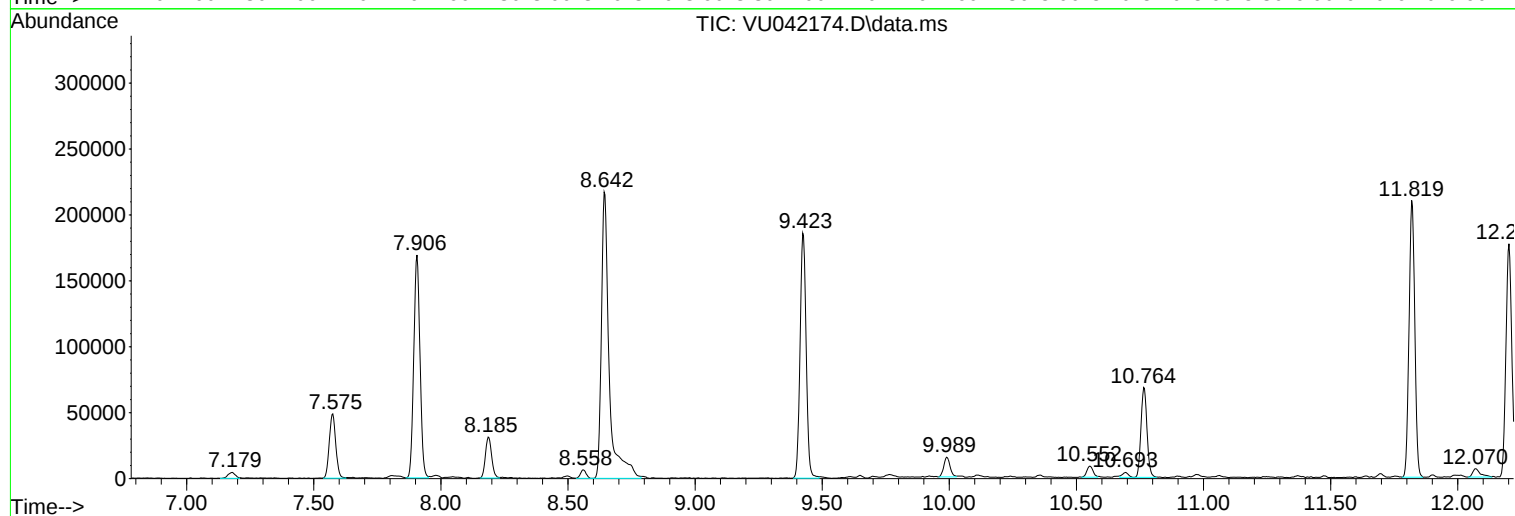
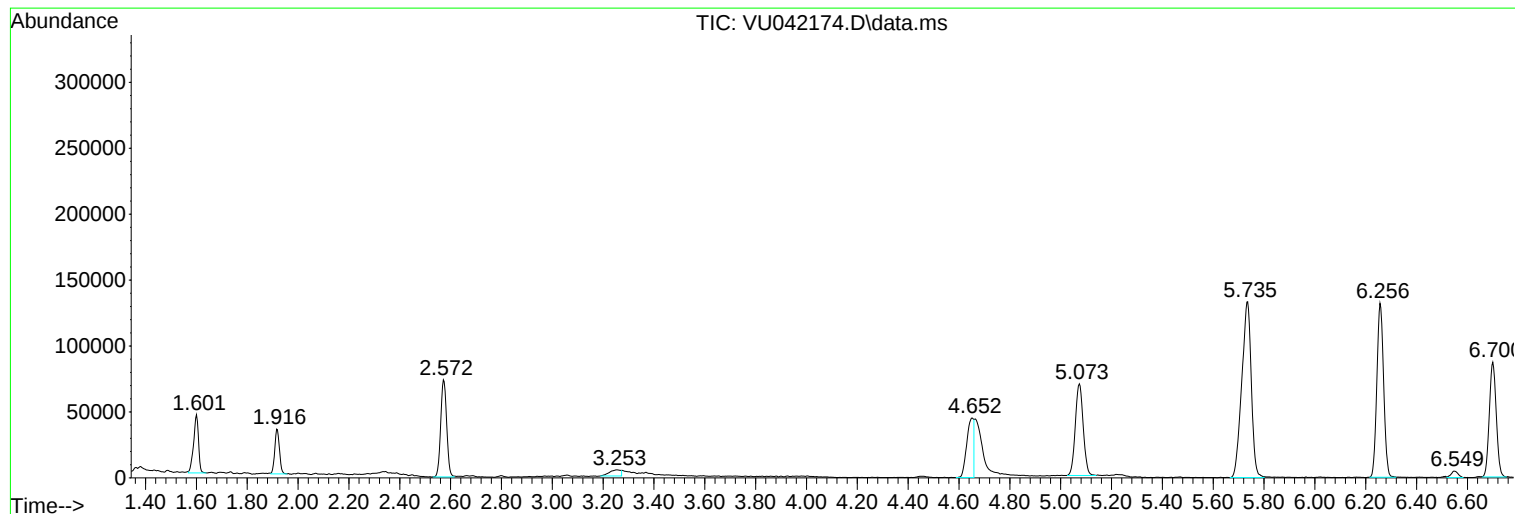
Sum of corrected areas: 3891380

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
Data File : VU042174.D  
Acq On : 22 Jan 2021 16:58  
Operator : SY/MD  
Sample : M1222-09  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
Data File : VU042174.D  
Acq On : 22 Jan 2021 16:58  
Operator : SY/MD  
Sample : M1222-09  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E16

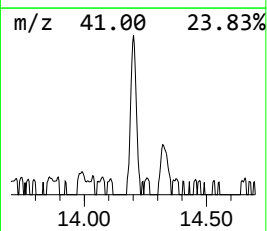
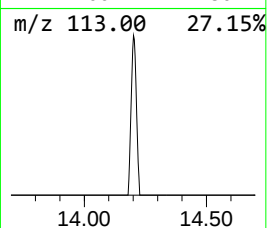
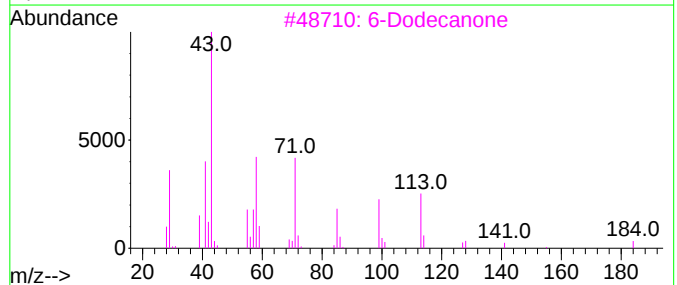
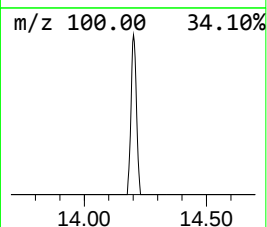
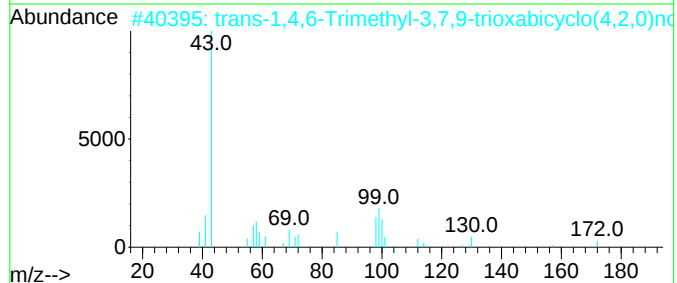
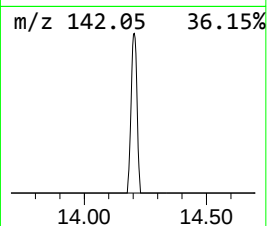
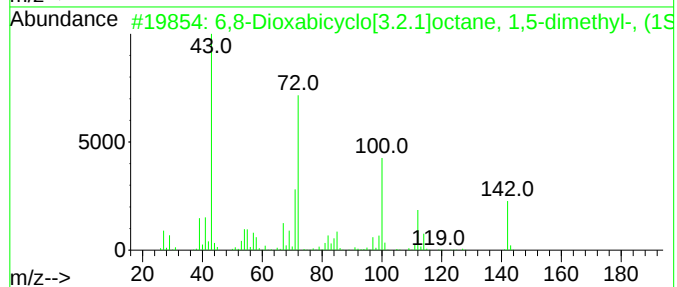
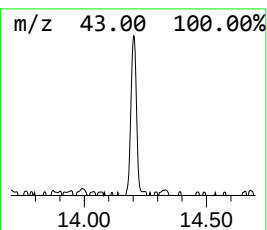
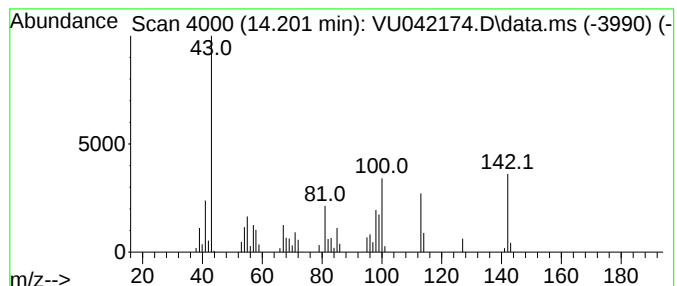
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

\*\*\*\*\*  
Peak Number 2 unknown-01 Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 14.201 | 0.62 ug/L | 40206 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 6,8-Dioxabicyclo[3.2.1]octane, 1... | 142 | C8H14O2      | 028401-39-0  | 27      |      |      |
| 2    | trans-1,4,6-Trimethyl-3,7,9-trio... | 172 | C9H16O3      | 062759-59-5  | 16      |      |      |
| 3    | 6-Dodecanone                        | 184 | C12H24O      | 006064-27-3  | 16      |      |      |
| 4    | 3-t-Butylhexan-2-one                | 156 | C10H20O      | 1000202-22-9 | 10      |      |      |
| 5    | 1,4,6-Trimethyl-3,7,9-trioxabicy... | 172 | C9H16O3      | 062759-58-4  | 10      |      |      |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
Data File : VU042174.D  
Acq On : 22 Jan 2021 16:58  
Operator : SY/MD  
Sample : M1222-09  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E16

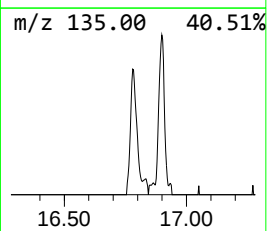
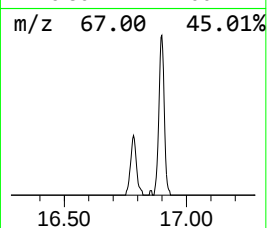
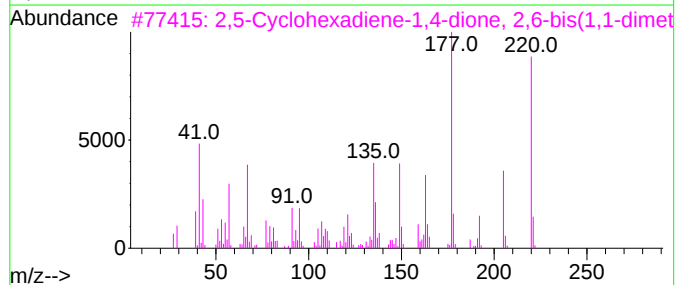
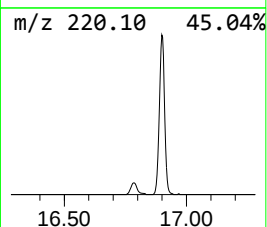
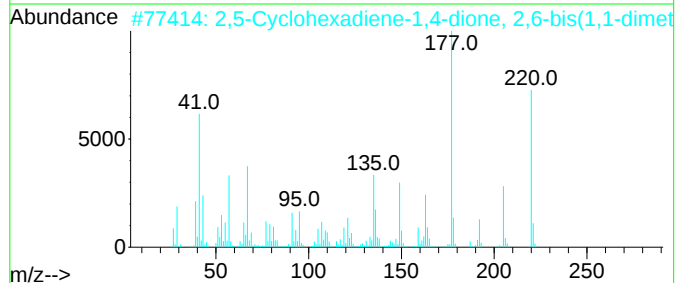
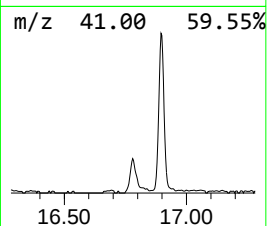
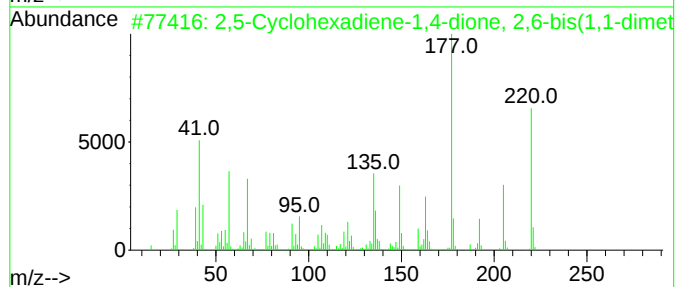
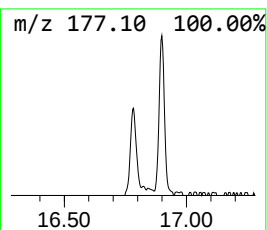
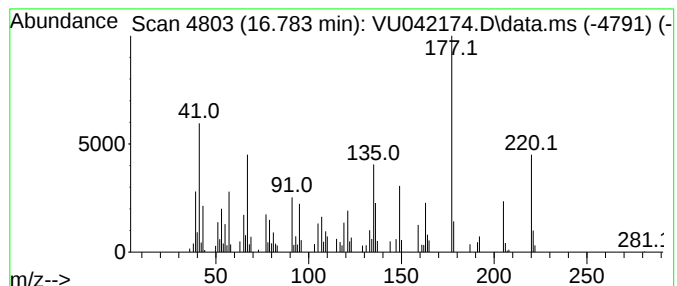
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

\*\*\*\*\*

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

| R.T.      | EstConc                             | Area  | Relative to ISTD       |          | R.T.         |      |
|-----------|-------------------------------------|-------|------------------------|----------|--------------|------|
| 16.783    | 0.89 ug/L                           | 58452 | 1,4-Dichlorobenzene-d4 |          | 11.819       |      |
| Hit# of 5 | Tentative ID                        |       | MW                     | MolForm  | CAS#         | Qual |
| 1         | 2,5-Cyclohexadiene-1,4-dione, 2,... |       | 220                    | C14H20O2 | 000719-22-2  | 94   |
| 2         | 2,5-Cyclohexadiene-1,4-dione, 2,... |       | 220                    | C14H20O2 | 000719-22-2  | 87   |
| 3         | 2,5-Cyclohexadiene-1,4-dione, 2,... |       | 220                    | C14H20O2 | 000719-22-2  | 83   |
| 4         | trans-.beta.-Ionone                 |       | 192                    | C13H20O  | 000079-77-6  | 38   |
| 5         | Thiocoumarin, 4,4,6,8-tetramethyl-  |       | 220                    | C13H16OS | 1000128-90-3 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
Data File : VU042174.D  
Acq On : 22 Jan 2021 16:58  
Operator : SY/MD  
Sample : M1222-09  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E16

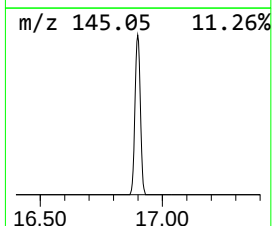
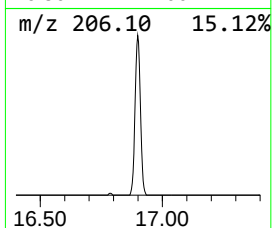
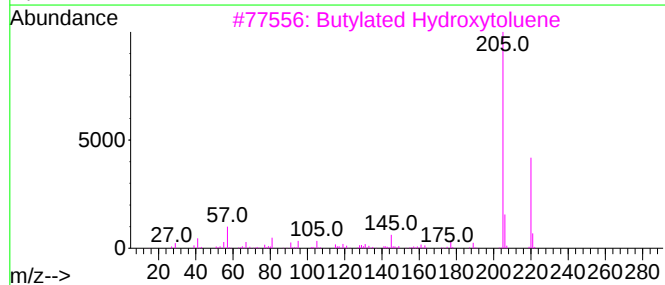
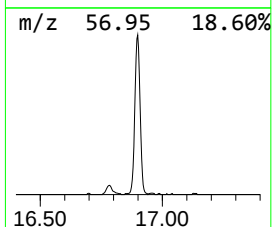
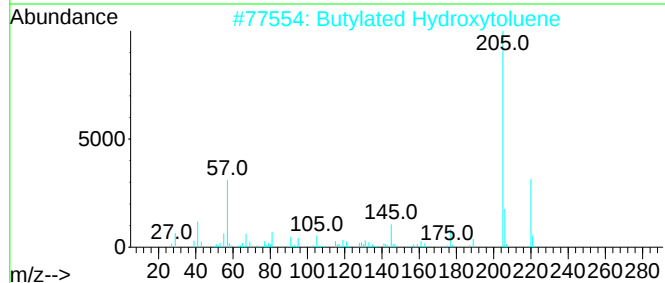
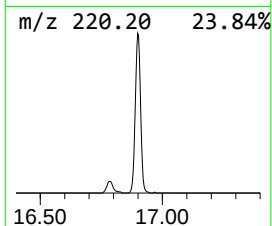
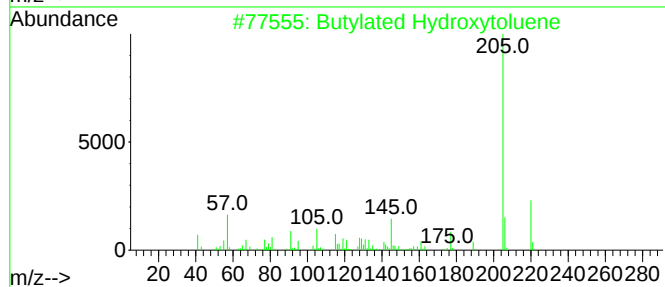
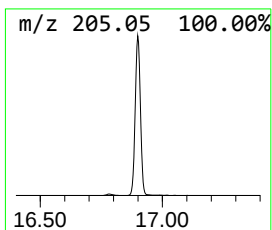
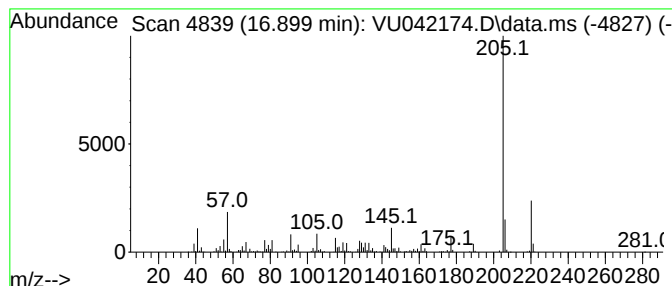
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

\*\*\*\*\*  
Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.899 | 7.52 ug/L | 491575 | 1,4-Dichlorobenzene-d4 | 11.819 |

| 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 | 96   |
| 3    |    |   | Butylated Hydroxytoluene            | 220 | C15H24O | 000128-37-0 | 94   |
| 4    |    |   | Butylated Hydroxytoluene            | 220 | C15H24O | 000128-37-0 | 94   |
| 5    |    |   | Phenol, 4,6-di(1,1-dimethylethyl... | 220 | C15H24O | 000616-55-7 | 81   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
Data File : VU042174.D  
Acq On : 22 Jan 2021 16:58  
Operator : SY/MD  
Sample : M1222-09  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.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 |
| unknown-01         | 14.201 | 0.6     | ug/L  | 40206    | 3                     | 11.819 | 326874 | 5.0  |
| 2,5-Cyclohexadi... | 16.783 | 0.9     | ug/L  | 58452    | 3                     | 11.819 | 326874 | 5.0  |
| Butylated Hydro... | 16.899 | 7.5     | ug/L  | 491575   | 3                     | 11.819 | 326874 | 5.0  |