

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012221\  
 Data File : VU042176.D  
 Acq On : 22 Jan 2021 17:46  
 Operator : SY/MD  
 Sample : M1222-11  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F1E18

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: VU042176.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          | 91           | rVB      | 41641          | 48119         | 7.94%           | 1.165%        |
| 2         | 1.916       | 171           | 179         | 192          | rVB      | 33773          | 42485         | 7.01%           | 1.028%        |
| 3         | 2.298       | 291           | 298         | 305          | rBV      | 8614           | 13024         | 2.15%           | 0.315%        |
| 4         | 2.572       | 372           | 383         | 396          | rBV      | 72865          | 117261        | 19.36%          | 2.838%        |
| 5         | 4.655       | 1014          | 1031        | 1084         | rBV      | 48341          | 202196        | 33.38%          | 4.894%        |
| 6         | 5.073       | 1146          | 1161        | 1178         | rBV      | 69074          | 152785        | 25.22%          | 3.698%        |
| 7         | 5.732       | 1345          | 1366        | 1393         | rBV2     | 136183         | 354121        | 58.45%          | 8.572%        |
| 8         | 6.256       | 1515          | 1529        | 1547         | rBV      | 131605         | 247142        | 40.79%          | 5.982%        |
| 9         | 6.700       | 1654          | 1667        | 1682         | rVB      | 86046          | 166733        | 27.52%          | 4.036%        |
| 10        | 7.176       | 1800          | 1815        | 1832         | rVB      | 18632          | 37819         | 6.24%           | 0.915%        |
| 11        | 7.575       | 1927          | 1939        | 1951         | rBV      | 50758          | 88936         | 14.68%          | 2.153%        |
| 12        | 7.838       | 1998          | 2021        | 2030         | rBV5     | 8508           | 24447         | 4.04%           | 0.592%        |
| 13        | 7.906       | 2030          | 2042        | 2057         | rVB      | 167591         | 287074        | 47.39%          | 6.949%        |
| 14        | 8.041       | 2075          | 2084        | 2094         | rVB3     | 3598           | 6718          | 1.11%           | 0.163%        |
| 15        | 8.186       | 2117          | 2129        | 2141         | rBV      | 32866          | 54172         | 8.94%           | 1.311%        |
| 16        | 8.497       | 2216          | 2226        | 2235         | rBV4     | 4077           | 6581          | 1.09%           | 0.159%        |
| 17        | 8.559       | 2235          | 2245        | 2255         | rVB2     | 11704          | 19192         | 3.17%           | 0.465%        |
| 18        | 8.645       | 2255          | 2272        | 2292         | rBV      | 241480         | 451420        | 74.51%          | 10.927%       |
| 19        | 9.423       | 2502          | 2514        | 2534         | rBV      | 183975         | 308464        | 50.92%          | 7.466%        |
| 20        | 9.649       | 2578          | 2584        | 2593         | rVB2     | 4974           | 7049          | 1.16%           | 0.171%        |
| 21        | 9.768       | 2612          | 2621        | 2634         | rBV3     | 4159           | 8109          | 1.34%           | 0.196%        |
| 22        | 10.694      | 2901          | 2909        | 2919         | rVB3     | 5716           | 9268          | 1.53%           | 0.224%        |
| 23        | 10.764      | 2919          | 2931        | 2946         | rBV      | 70381          | 112988        | 18.65%          | 2.735%        |
| 24        | 10.976      | 2982          | 2997        | 3010         | rBV3     | 5674           | 11676         | 1.93%           | 0.283%        |
| 25        | 11.819      | 3247          | 3259        | 3274         | rVB      | 211067         | 328961        | 54.30%          | 7.963%        |
| 26        | 12.073      | 3328          | 3338        | 3346         | rBV2     | 8789           | 16265         | 2.68%           | 0.394%        |
| 27        | 12.202      | 3362          | 3378        | 3393         | rVB      | 178387         | 286963        | 47.37%          | 6.946%        |
| 28        | 12.330      | 3409          | 3418        | 3431         | rBV2     | 7133           | 10363         | 1.71%           | 0.251%        |
| 29        | 14.201      | 3988          | 4000        | 4014         | rBV      | 38764          | 59163         | 9.77%           | 1.432%        |
| 30        | 15.706      | 4459          | 4468        | 4478         | rBV8     | 7134           | 12610         | 2.08%           | 0.305%        |
| 31        | 16.143      | 4595          | 4604        | 4614         | rBV3     | 14053          | 22429         | 3.70%           | 0.543%        |
| 32        | 16.780      | 4795          | 4802        | 4813         | rBV5     | 7615           | 10969         | 1.81%           | 0.266%        |
| 33        | 16.899      | 4827          | 4839        | 4854         | rBV      | 412290         | 605827        | 100.00%         | 14.664%       |

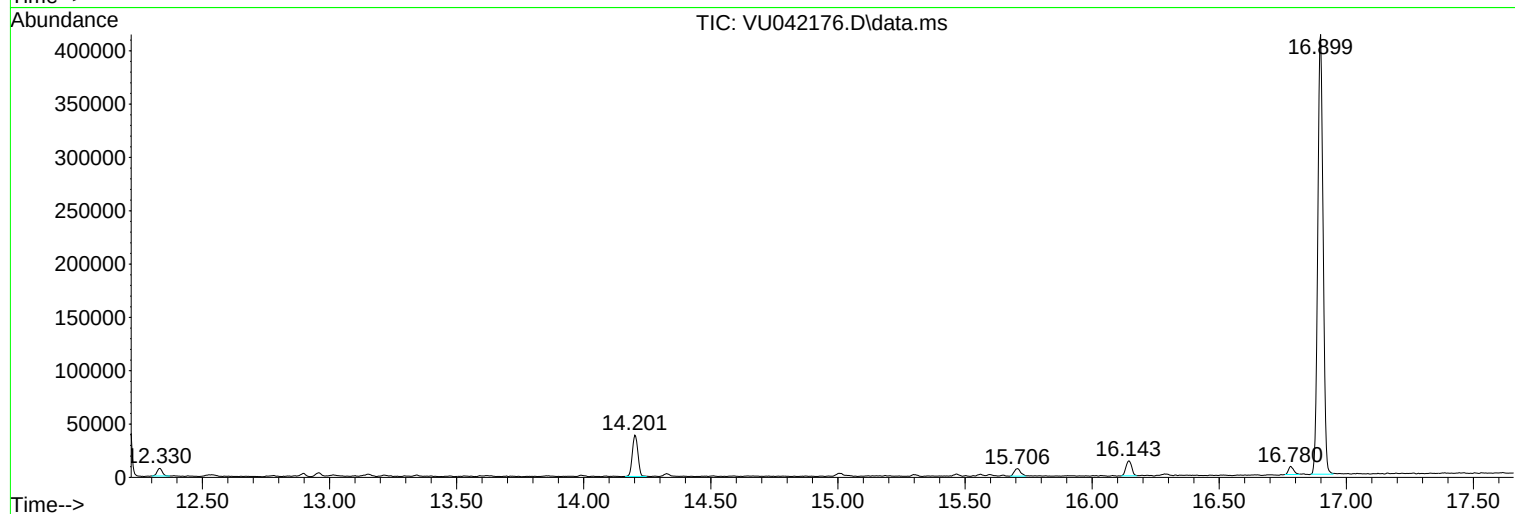
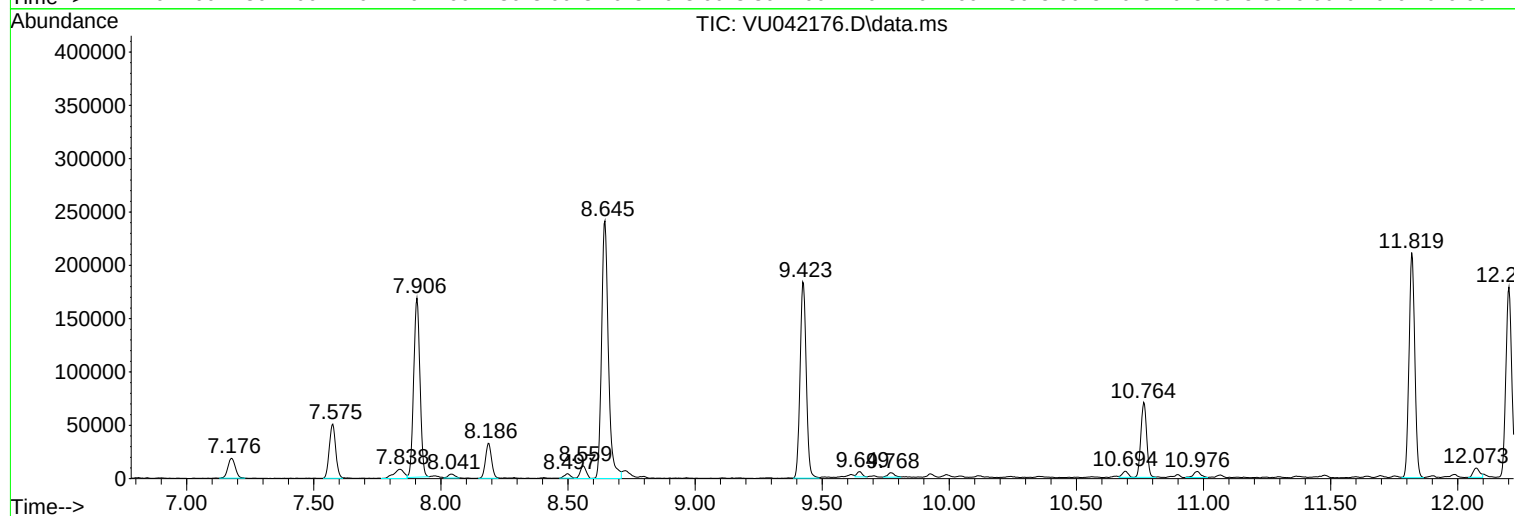
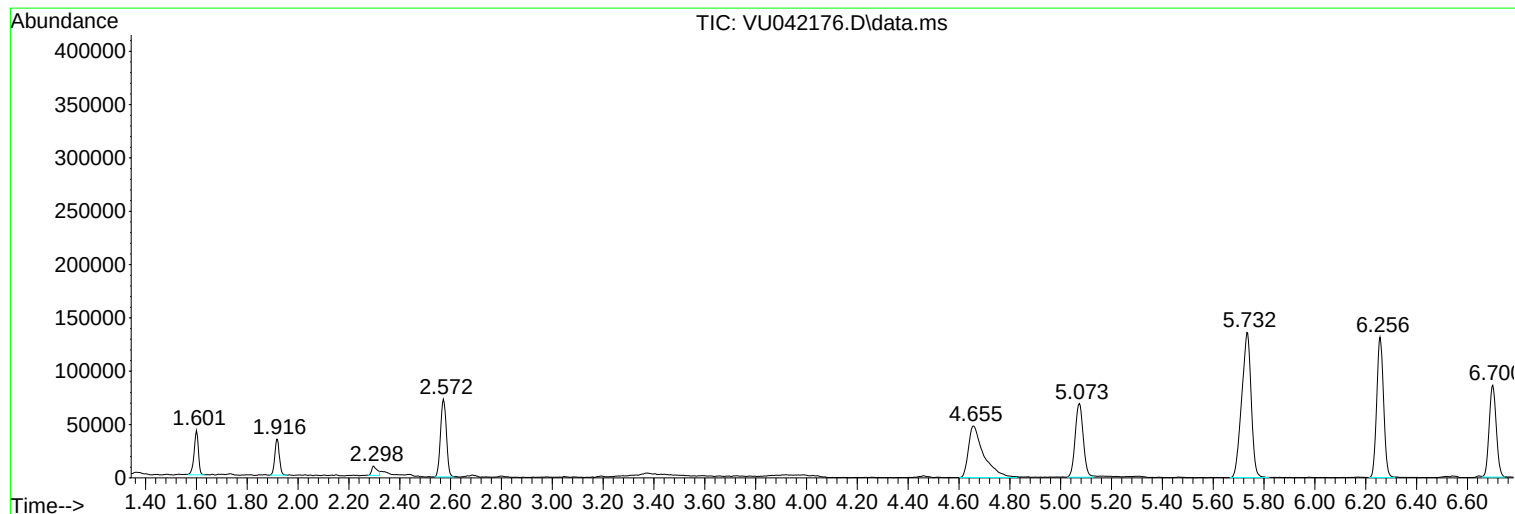
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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F1E18

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



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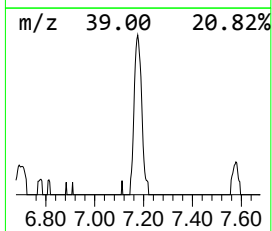
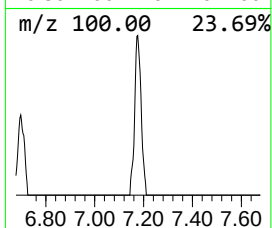
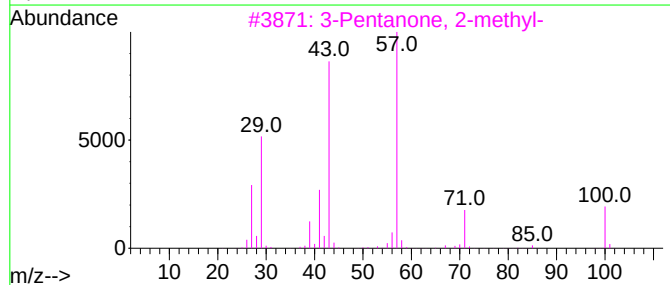
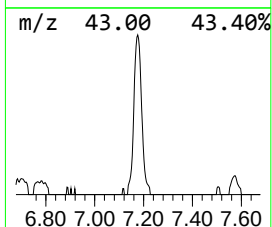
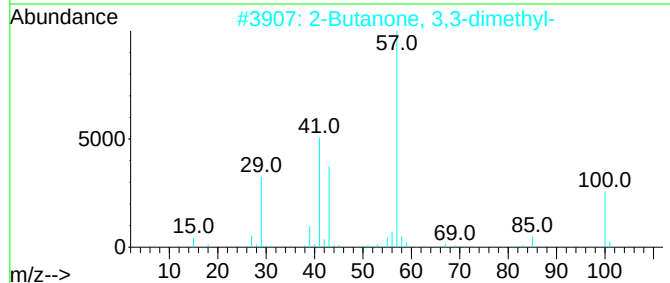
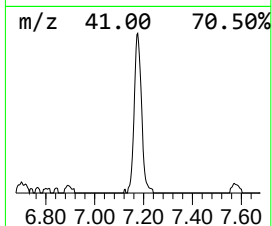
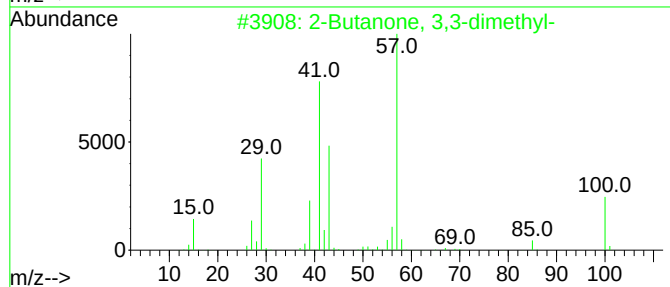
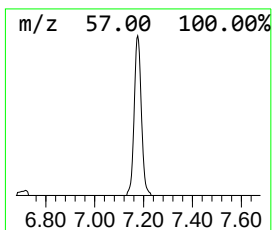
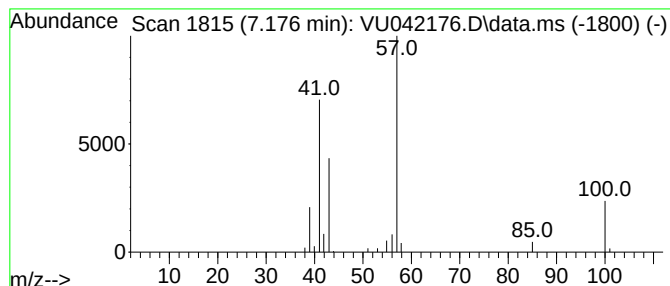
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 7.176 | 0.77 ug/L | 37819 | 1,4-Difluorobenzene | 6.256 |

| Hit# | of 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------------|-----|---------|-------------|------|
| 1    |      | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O  | 000075-97-8 | 91   |
| 2    |      | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O  | 000075-97-8 | 90   |
| 3    |      | 3-Pentanone, 2-methyl-    | 100 | C6H12O  | 000565-69-5 | 64   |
| 4    |      | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O  | 000075-97-8 | 64   |
| 5    |      | 3-Pentanone, 2-methyl-    | 100 | C6H12O  | 000565-69-5 | 64   |



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MSVOA\_U  
ClientSampleId :  
F1E18

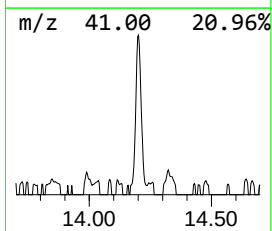
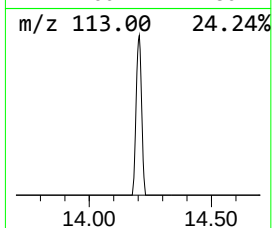
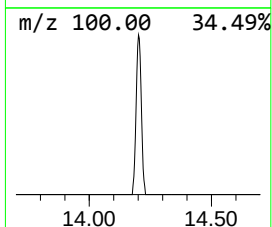
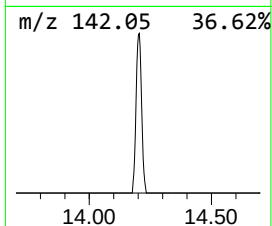
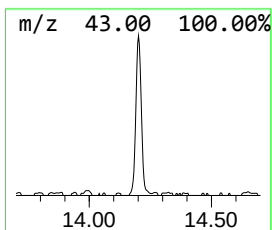
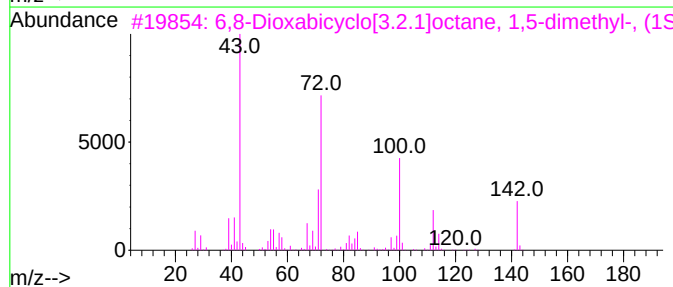
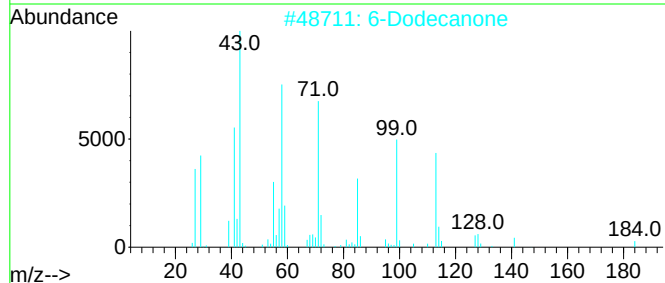
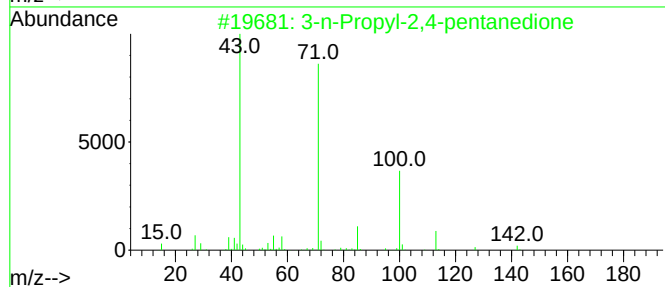
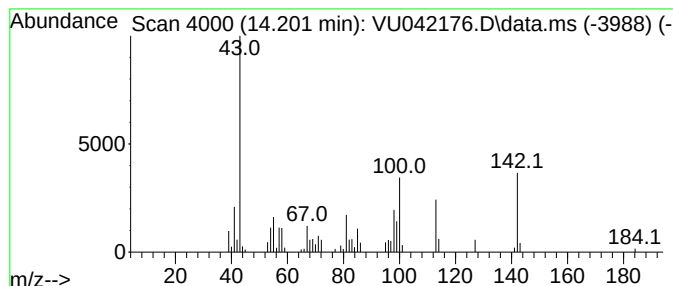
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 3 unknown-01 Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 14.201 | 0.90 ug/L | 59163 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-n-Propyl-2,4-pentanedione         | 142 | C8H14O2 | 001540-35-8 | 25   |
| 2    |    |   | 6-Dodecanone                        | 184 | C12H24O | 006064-27-3 | 22   |
| 3    |    |   | 6,8-Dioxabicyclo[3.2.1]octane, 1... | 142 | C8H14O2 | 028401-39-0 | 22   |
| 4    |    |   | Heptane, 4-ethyl-                   | 128 | C9H20   | 002216-32-2 | 12   |
| 5    |    |   | Cyclohexanemethylamine              | 113 | C7H15N  | 003218-02-8 | 11   |



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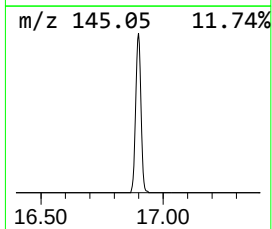
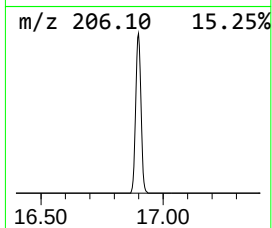
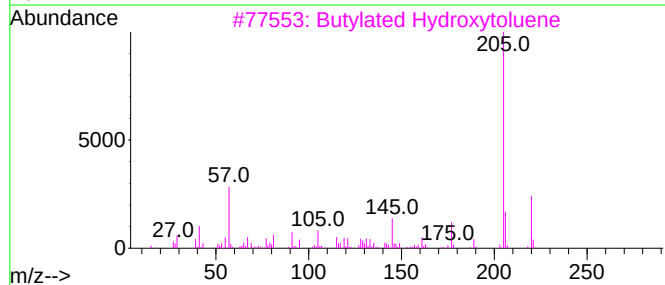
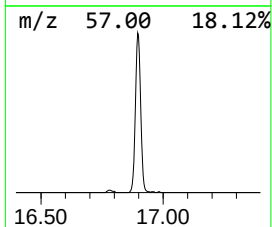
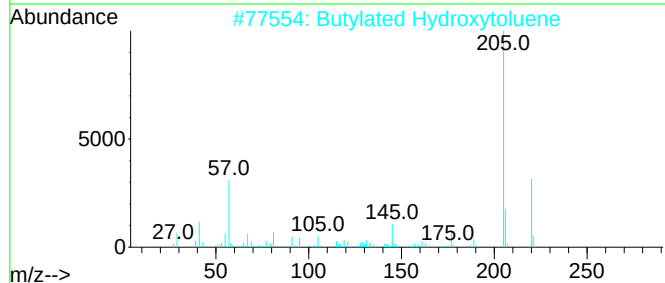
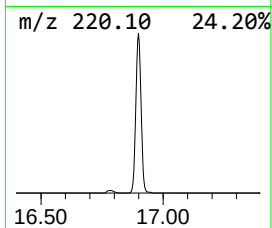
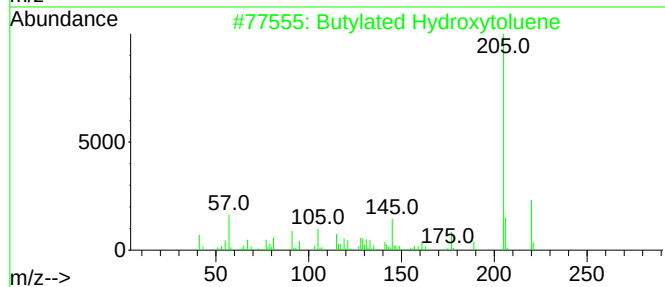
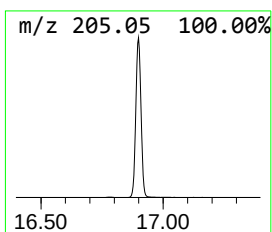
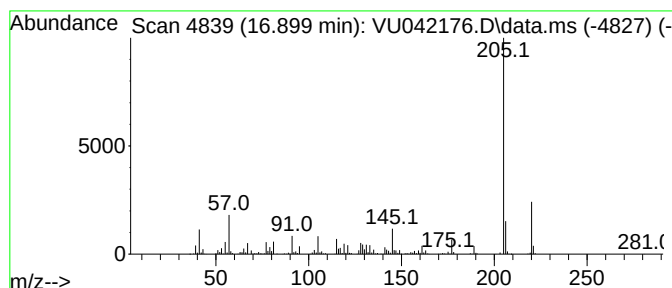
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 16.899 | 9.21 ug/L | 605827 | 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 | 97   |
| 3    |    |   | Butylated Hydroxytoluene            | 220 | C15H24O | 000128-37-0 | 96   |
| 4    |    |   | Butylated Hydroxytoluene            | 220 | C15H24O | 000128-37-0 | 94   |
| 5    |    |   | Phenol, 4,6-di(1,1-dimethylethyl... | 220 | C15H24O | 000616-55-7 | 93   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Butanone, 3,3... | 7.176  | 0.8     | ug/L  | 37819    | 1                     | 6.256  | 247142 | 5.0  |
| unknown-01         | 14.201 | 0.9     | ug/L  | 59163    | 3                     | 11.819 | 328961 | 5.0  |
| Butylated Hydro... | 16.899 | 9.2     | ug/L  | 605827   | 3                     | 11.819 | 328961 | 5.0  |