

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV061322\  
 Data File : VV026213.D  
 Acq On : 13 Jun 2022 16:46  
 Operator : SY/MD  
 Sample : N3272-14  
 Misc : 25.0mL/MSVOA\_V/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0B58

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\_V\Method\SFAMVTR061222WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV026213.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         | 1.314       | 74            | 85          | 107          | rBV2     | 158523         | 235782        | 4.29%           | 1.947%        |
| 2         | 1.577       | 158           | 167         | 183          | rBV      | 115108         | 133868        | 2.44%           | 1.106%        |
| 3         | 1.715       | 202           | 210         | 216          | rBV      | 98667          | 118154        | 2.15%           | 0.976%        |
| 4         | 1.761       | 216           | 224         | 246          | rVB      | 605554         | 788507        | 14.36%          | 6.512%        |
| 5         | 2.114       | 323           | 334         | 354          | rVB      | 233538         | 336380        | 6.13%           | 2.778%        |
| 6         | 3.915       | 881           | 894         | 927          | rBV      | 54606          | 203139        | 3.70%           | 1.678%        |
| 7         | 4.358       | 1016          | 1032        | 1068         | rVB      | 136593         | 359162        | 6.54%           | 2.966%        |
| 8         | 5.053       | 1232          | 1248        | 1274         | rBV2     | 294083         | 721658        | 13.14%          | 5.960%        |
| 9         | 5.622       | 1412          | 1425        | 1449         | rBV      | 186039         | 379430        | 6.91%           | 3.134%        |
| 10        | 5.915       | 1501          | 1516        | 1549         | rBV      | 2885196        | 5490836       | 100.00%         | 45.348%       |
| 11        | 6.072       | 1553          | 1565        | 1589         | rVB      | 166268         | 350878        | 6.39%           | 2.898%        |
| 12        | 6.992       | 1840          | 1851        | 1875         | rBV2     | 68892          | 132584        | 2.41%           | 1.095%        |
| 13        | 7.317       | 1940          | 1952        | 1973         | rBV      | 327201         | 578024        | 10.53%          | 4.774%        |
| 14        | 7.628       | 2039          | 2049        | 2070         | rBV2     | 38216          | 71773         | 1.31%           | 0.593%        |
| 15        | 7.979       | 2149          | 2158        | 2177         | rVB      | 85182          | 148370        | 2.70%           | 1.225%        |
| 16        | 8.091       | 2182          | 2193        | 2232         | rBV2     | 231358         | 517559        | 9.43%           | 4.274%        |
| 17        | 8.853       | 2419          | 2430        | 2453         | rBV      | 285831         | 466962        | 8.50%           | 3.857%        |
| 18        | 10.217      | 2839          | 2854        | 2869         | rBV      | 106484         | 168244        | 3.06%           | 1.390%        |
| 19        | 11.249      | 3164          | 3175        | 3194         | rBV      | 245803         | 379959        | 6.92%           | 3.138%        |
| 20        | 11.625      | 3281          | 3292        | 3312         | rBV      | 271593         | 432817        | 7.88%           | 3.575%        |
| 21        | 16.178      | 4696          | 4708        | 4723         | rBV2     | 62059          | 94052         | 1.71%           | 0.777%        |

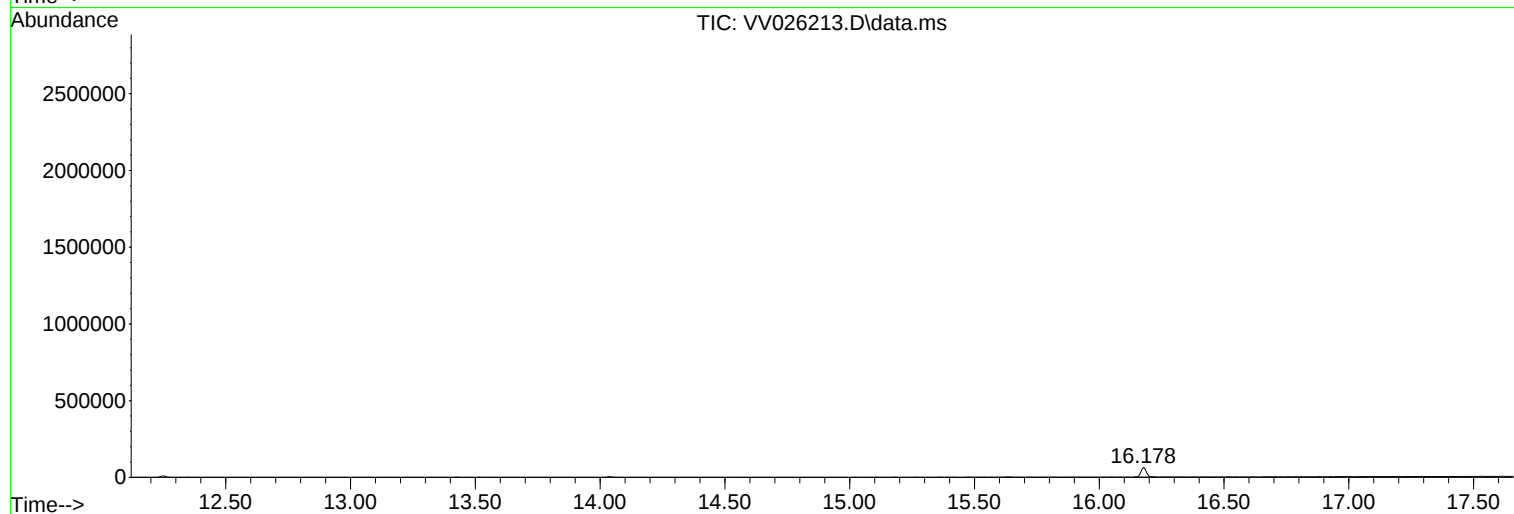
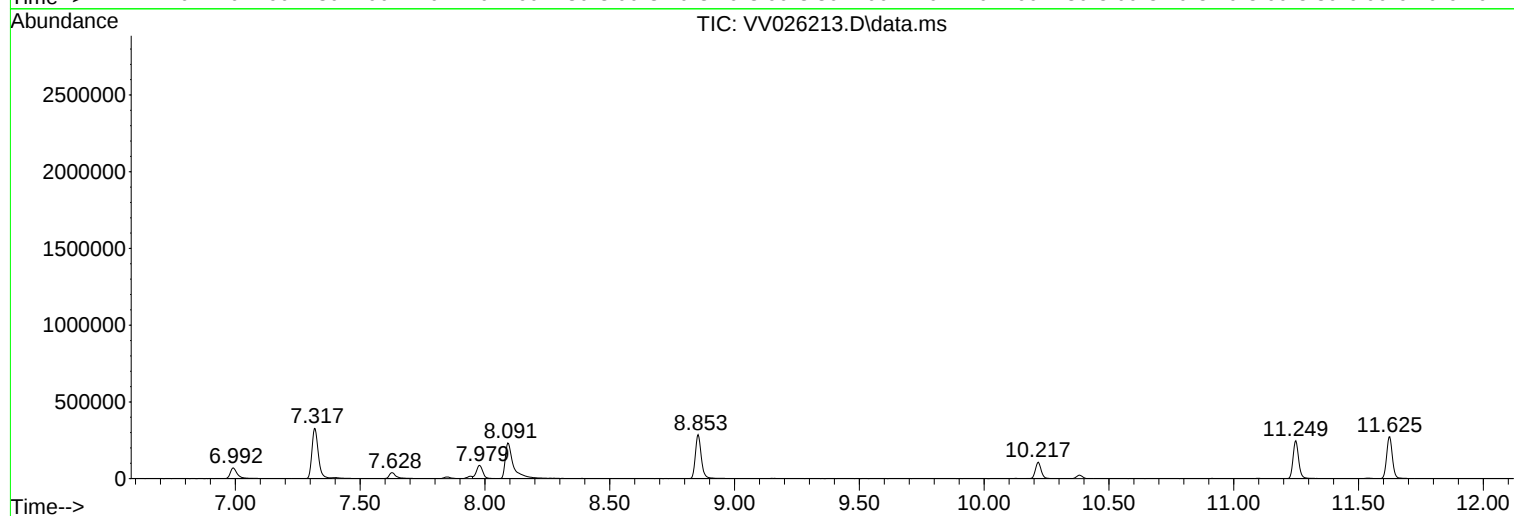
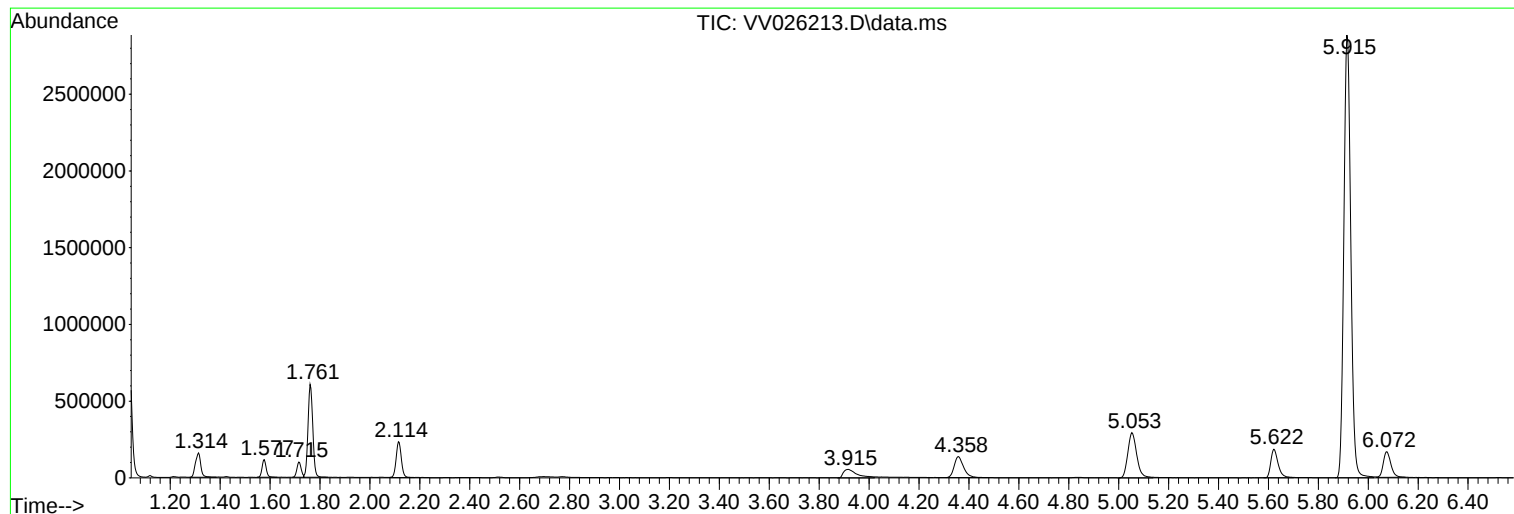
Sum of corrected areas: 12108138

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ClientSampleId :  
C0B58

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR061222WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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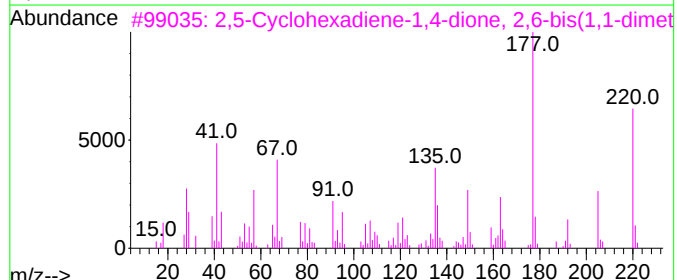
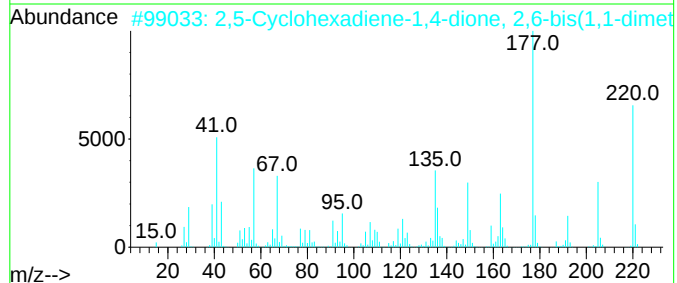
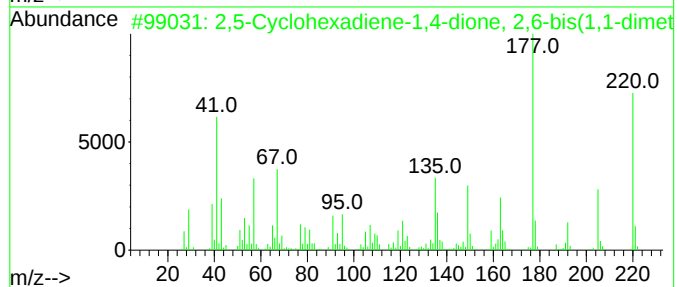
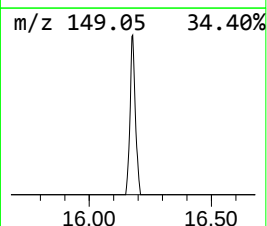
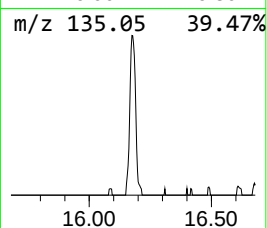
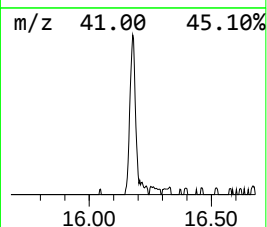
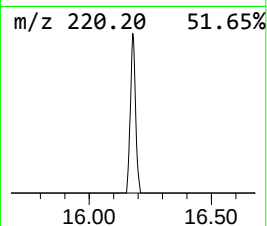
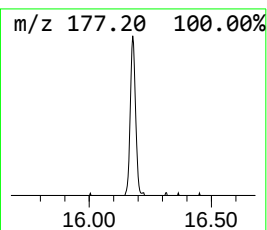
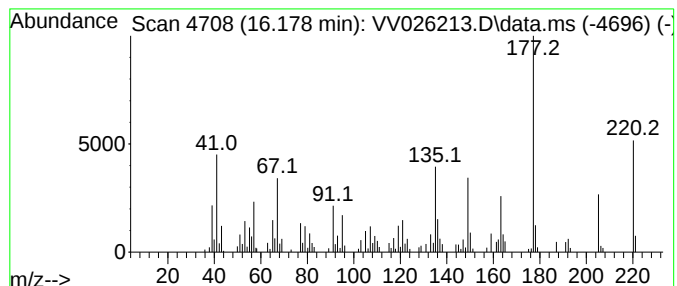
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 16.178 | 1.24 ug/L | 94052 | 1,4-Dichlorobenzene-d4 | 11.249 |

| 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 | 95      |      |      |
| 3    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 94      |      |      |
| 4    | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H2002     | 000719-22-2 | 94      |      |      |
| 5    | trans-.beta.-Ionone                 | 192 | C13H200      | 000079-77-6 | 66      |      |      |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2,5-Cyclohexadi... | 16.178 | 1.2     | ug/L  | 94052    | 3                     | 11.249 | 379959 | 5.0  |