

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX111921\  
 Data File : VX025241.D  
 Acq On : 19 Nov 2021 18:16  
 Operator : JC/MD  
 Sample : M4779-09  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 31 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 F4L21

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\_X\Method\SFAMXML111121WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025241.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         | 1.239       | 22            | 25          | 33           | rBV      | 79532          | 111282        | 19.99%          | 2.414%        |
| 2         | 1.367       | 42            | 46          | 52           | rVB      | 90716          | 86100         | 15.47%          | 1.867%        |
| 3         | 1.666       | 91            | 95          | 109          | rVB      | 68183          | 87293         | 15.68%          | 1.893%        |
| 4         | 2.306       | 194           | 200         | 209          | rBV      | 121268         | 197290        | 35.44%          | 4.279%        |
| 5         | 2.379       | 209           | 212         | 218          | rVB      | 2402           | 4103          | 0.74%           | 0.089%        |
| 6         | 2.538       | 233           | 238         | 245          | rVB2     | 2777           | 4828          | 0.87%           | 0.105%        |
| 7         | 2.635       | 252           | 254         | 260          | rVB4     | 424            | 581           | 0.10%           | 0.013%        |
| 8         | 2.788       | 274           | 279         | 285          | rBV3     | 1286           | 2452          | 0.44%           | 0.053%        |
| 9         | 2.946       | 297           | 305         | 317          | rVB      | 4261           | 10394         | 1.87%           | 0.225%        |
| 10        | 3.215       | 347           | 349         | 353          | rBV2     | 121            | 177           | 0.03%           | 0.004%        |
| 11        | 3.336       | 365           | 369         | 370          | rBV2     | 178            | 197           | 0.04%           | 0.004%        |
| 12        | 3.647       | 417           | 420         | 422          | rVB      | 156            | 160           | 0.03%           | 0.003%        |
| 13        | 3.769       | 436           | 440         | 444          | rBV2     | 167            | 347           | 0.06%           | 0.008%        |
| 14        | 4.245       | 513           | 518         | 523          | rVB2     | 265            | 601           | 0.11%           | 0.013%        |
| 15        | 4.458       | 543           | 553         | 567          | rBV      | 45032          | 125937        | 22.62%          | 2.731%        |
| 16        | 4.720       | 589           | 596         | 601          | rBV3     | 1058           | 2564          | 0.46%           | 0.056%        |
| 17        | 4.970       | 635           | 637         | 640          | rBV2     | 140            | 186           | 0.03%           | 0.004%        |
| 18        | 5.068       | 640           | 653         | 670          | rVV      | 71827          | 220710        | 39.65%          | 4.787%        |
| 19        | 5.391       | 704           | 706         | 708          | rBV2     | 120            | 161           | 0.03%           | 0.003%        |
| 20        | 5.556       | 729           | 733         | 737          | rBV2     | 300            | 473           | 0.08%           | 0.010%        |
| 21        | 5.970       | 788           | 801         | 819          | rBV2     | 187538         | 556706        | 100.00%         | 12.074%       |
| 22        | 6.763       | 920           | 931         | 945          | rBV      | 146620         | 346616        | 62.26%          | 7.518%        |
| 23        | 7.110       | 983           | 988         | 994          | rBV3     | 1796           | 3756          | 0.67%           | 0.081%        |
| 24        | 7.311       | 1012          | 1021        | 1034         | rVV      | 114861         | 248843        | 44.70%          | 5.397%        |
| 25        | 7.464       | 1044          | 1046        | 1053         | rBV4     | 390            | 836           | 0.15%           | 0.018%        |
| 26        | 7.586       | 1060          | 1066        | 1074         | rVV4     | 2707           | 5464          | 0.98%           | 0.119%        |
| 27        | 7.811       | 1098          | 1103        | 1106         | rBV2     | 290            | 582           | 0.10%           | 0.013%        |
| 28        | 7.897       | 1113          | 1117        | 1118         | rBV2     | 400            | 375           | 0.07%           | 0.008%        |
| 29        | 7.927       | 1118          | 1122        | 1126         | rVV3     | 835            | 1527          | 0.27%           | 0.033%        |
| 30        | 8.061       | 1143          | 1144        | 1149         | rBV2     | 106            | 143           | 0.03%           | 0.003%        |
| 31        | 8.329       | 1181          | 1188        | 1200         | rVV      | 78768          | 133822        | 24.04%          | 2.902%        |
| 32        | 8.482       | 1207          | 1213        | 1217         | rBV3     | 542            | 1234          | 0.22%           | 0.027%        |
| 33        | 8.579       | 1226          | 1229        | 1234         | rVB3     | 487            | 671           | 0.12%           | 0.015%        |
| 34        | 8.653       | 1234          | 1241        | 1248         | rBV      | 297379         | 464580        | 83.45%          | 10.076%       |
| 35        | 8.720       | 1248          | 1252        | 1259         | rVB      | 5067           | 8048          | 1.45%           | 0.175%        |
| 36        | 8.811       | 1265          | 1267        | 1268         | rVB      | 237            | 146           | 0.03%           | 0.003%        |

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 ClientSampleId :  
 F4L21

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\_X\Method\SFAMXLM111121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 8.829  | 1268 | 1270 | 1273 | rBV2 | 169    | 216    | 0.04%  | 0.005% |
| 38 | 8.951  | 1284 | 1290 | 1300 | rBV  | 60490  | 86968  | 15.62% | 1.886% |
| 39 | 9.244  | 1336 | 1338 | 1341 | rBV3 | 424    | 518    | 0.09%  | 0.011% |
| 40 | 9.274  | 1341 | 1343 | 1348 | rVB  | 1212   | 1434   | 0.26%  | 0.031% |
| 41 | 9.384  | 1355 | 1361 | 1378 | rBV  | 203308 | 284866 | 51.17% | 6.178% |
| 42 | 9.524  | 1378 | 1384 | 1390 | rBV  | 14374  | 19960  | 3.59%  | 0.433% |
| 43 | 9.890  | 1440 | 1444 | 1446 | rBV2 | 127    | 146    | 0.03%  | 0.003% |
| 44 | 9.994  | 1458 | 1461 | 1465 | rBV  | 231    | 174    | 0.03%  | 0.004% |
| 45 | 10.055 | 1465 | 1471 | 1487 | rVB  | 303145 | 410358 | 73.71% | 8.900% |
| 46 | 10.195 | 1491 | 1494 | 1499 | rVB  | 779    | 1053   | 0.19%  | 0.023% |
| 47 | 10.305 | 1507 | 1512 | 1516 | rVB2 | 1504   | 2075   | 0.37%  | 0.045% |
| 48 | 10.591 | 1556 | 1559 | 1563 | rVB  | 418    | 535    | 0.10%  | 0.012% |
| 49 | 10.652 | 1563 | 1569 | 1576 | rBV4 | 597    | 1143   | 0.21%  | 0.025% |
| 50 | 10.762 | 1583 | 1587 | 1588 | rBV  | 612    | 537    | 0.10%  | 0.012% |
| 51 | 10.817 | 1593 | 1596 | 1600 | rBV2 | 187    | 268    | 0.05%  | 0.006% |
| 52 | 10.853 | 1600 | 1602 | 1607 | rVB2 | 474    | 641    | 0.12%  | 0.014% |
| 53 | 11.024 | 1629 | 1630 | 1632 | rVB  | 262    | 165    | 0.03%  | 0.004% |
| 54 | 11.122 | 1642 | 1646 | 1649 | rVB  | 1625   | 1893   | 0.34%  | 0.041% |
| 55 | 11.195 | 1652 | 1658 | 1667 | rBV  | 216631 | 271924 | 48.85% | 5.898% |
| 56 | 11.274 | 1669 | 1671 | 1672 | rVV  | 308    | 243    | 0.04%  | 0.005% |
| 57 | 11.317 | 1675 | 1678 | 1682 | rVB2 | 962    | 1560   | 0.28%  | 0.034% |
| 58 | 11.378 | 1685 | 1688 | 1689 | rBV2 | 257    | 283    | 0.05%  | 0.006% |
| 59 | 11.451 | 1696 | 1700 | 1702 | rBV2 | 314    | 484    | 0.09%  | 0.010% |
| 60 | 11.555 | 1713 | 1717 | 1720 | rBV  | 185    | 244    | 0.04%  | 0.005% |
| 61 | 11.622 | 1724 | 1728 | 1731 | rBV  | 273    | 393    | 0.07%  | 0.009% |
| 62 | 11.664 | 1731 | 1735 | 1736 | rBV2 | 291    | 304    | 0.05%  | 0.007% |
| 63 | 11.750 | 1742 | 1749 | 1757 | rVB3 | 2676   | 4644   | 0.83%  | 0.101% |
| 64 | 11.841 | 1762 | 1764 | 1770 | rVB2 | 496    | 498    | 0.09%  | 0.011% |
| 65 | 11.933 | 1775 | 1779 | 1782 | rBV3 | 1457   | 1804   | 0.32%  | 0.039% |
| 66 | 11.963 | 1782 | 1784 | 1789 | rVB  | 292    | 191    | 0.03%  | 0.004% |
| 67 | 12.024 | 1789 | 1794 | 1801 | rBV  | 318035 | 393730 | 70.72% | 8.540% |
| 68 | 12.128 | 1808 | 1811 | 1813 | rBV4 | 681    | 1021   | 0.18%  | 0.022% |
| 69 | 12.225 | 1821 | 1827 | 1834 | rBV2 | 6785   | 12170  | 2.19%  | 0.264% |
| 70 | 12.323 | 1837 | 1843 | 1850 | rVB  | 323285 | 405591 | 72.86% | 8.797% |
| 71 | 12.420 | 1855 | 1859 | 1865 | rVB2 | 2246   | 3504   | 0.63%  | 0.076% |
| 72 | 12.463 | 1865 | 1866 | 1867 | rBV  | 266    | 163    | 0.03%  | 0.004% |
| 73 | 12.597 | 1883 | 1888 | 1889 | rBV3 | 325    | 383    | 0.07%  | 0.008% |
| 74 | 12.670 | 1895 | 1900 | 1903 | rVB3 | 389    | 688    | 0.12%  | 0.015% |
| 75 | 12.768 | 1912 | 1916 | 1918 | rBV3 | 269    | 415    | 0.07%  | 0.009% |
| 76 | 12.816 | 1918 | 1924 | 1925 | rBV4 | 430    | 627    | 0.11%  | 0.014% |

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Instrument :  
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 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\_X\Method\SFAMXLM111121WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 12.859 | 1925 | 1931 | 1932 | rBV3 | 3695  | 5167  | 0.93% | 0.112% |
| 78  | 13.054 | 1959 | 1963 | 1964 | rBV2 | 361   | 431   | 0.08% | 0.009% |
| 79  | 13.286 | 2000 | 2001 | 2002 | rBV  | 285   | 164   | 0.03% | 0.004% |
| 80  | 13.347 | 2009 | 2011 | 2013 | rBV2 | 226   | 177   | 0.03% | 0.004% |
| 81  | 13.390 | 2016 | 2018 | 2022 | rBV2 | 170   | 173   | 0.03% | 0.004% |
| 82  | 13.426 | 2022 | 2024 | 2028 | rBV3 | 289   | 284   | 0.05% | 0.006% |
| 83  | 13.572 | 2045 | 2048 | 2049 | rBV  | 128   | 145   | 0.03% | 0.003% |
| 84  | 13.591 | 2049 | 2051 | 2055 | rVV3 | 658   | 701   | 0.13% | 0.015% |
| 85  | 13.780 | 2076 | 2082 | 2094 | rVB  | 32942 | 43953 | 7.90% | 0.953% |
| 86  | 13.871 | 2094 | 2097 | 2107 | rVB  | 877   | 1274  | 0.23% | 0.028% |
| 87  | 14.133 | 2137 | 2140 | 2141 | rBV2 | 311   | 266   | 0.05% | 0.006% |
| 88  | 14.310 | 2167 | 2169 | 2174 | rBV3 | 171   | 197   | 0.04% | 0.004% |
| 89  | 14.444 | 2188 | 2191 | 2195 | rVB2 | 222   | 185   | 0.03% | 0.004% |
| 90  | 14.481 | 2195 | 2197 | 2199 | rBV2 | 180   | 176   | 0.03% | 0.004% |
| 91  | 14.505 | 2199 | 2201 | 2203 | rVB2 | 200   | 145   | 0.03% | 0.003% |
| 92  | 14.639 | 2218 | 2223 | 2227 | rBV2 | 1487  | 2028  | 0.36% | 0.044% |
| 93  | 14.780 | 2242 | 2246 | 2250 | rVV  | 1435  | 1981  | 0.36% | 0.043% |
| 94  | 15.206 | 2314 | 2316 | 2322 | rVB4 | 686   | 959   | 0.17% | 0.021% |
| 95  | 15.389 | 2344 | 2346 | 2348 | rBV3 | 212   | 201   | 0.04% | 0.004% |
| 96  | 15.499 | 2363 | 2364 | 2367 | rVB2 | 259   | 200   | 0.04% | 0.004% |
| 97  | 15.621 | 2383 | 2384 | 2388 | rVB3 | 332   | 206   | 0.04% | 0.004% |
| 98  | 15.810 | 2413 | 2415 | 2417 | rBV  | 383   | 184   | 0.03% | 0.004% |
| 99  | 16.328 | 2495 | 2500 | 2507 | rVB3 | 3069  | 5396  | 0.97% | 0.117% |
| 100 | 16.694 | 2556 | 2560 | 2566 | rVB2 | 1681  | 3016  | 0.54% | 0.065% |

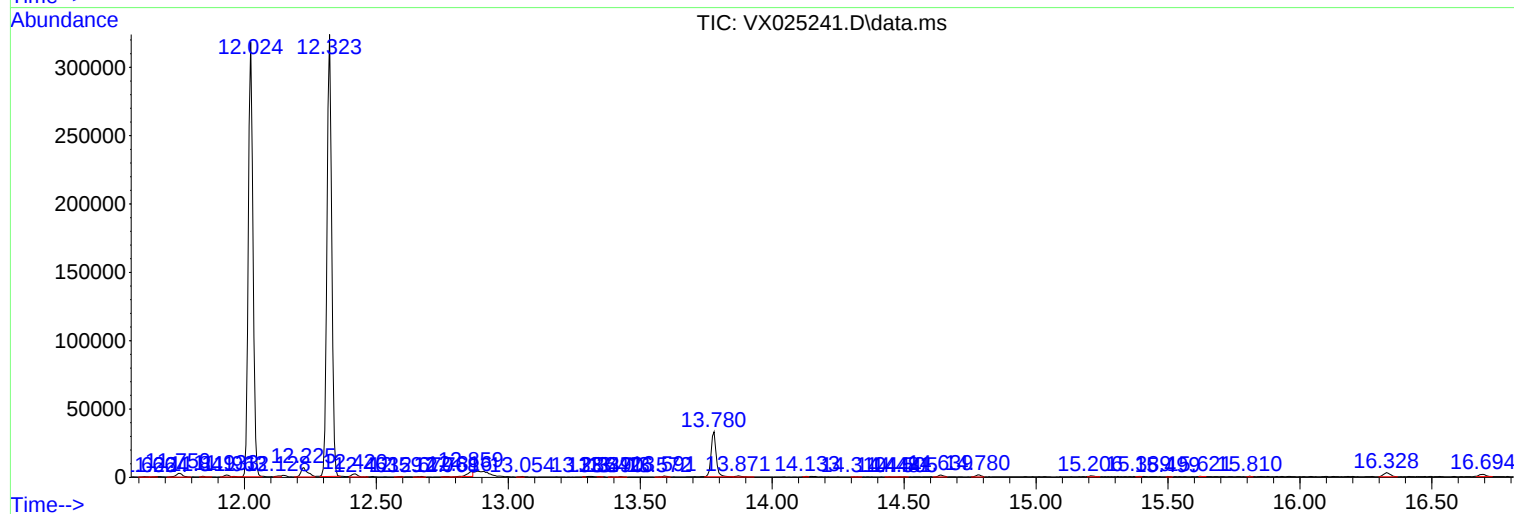
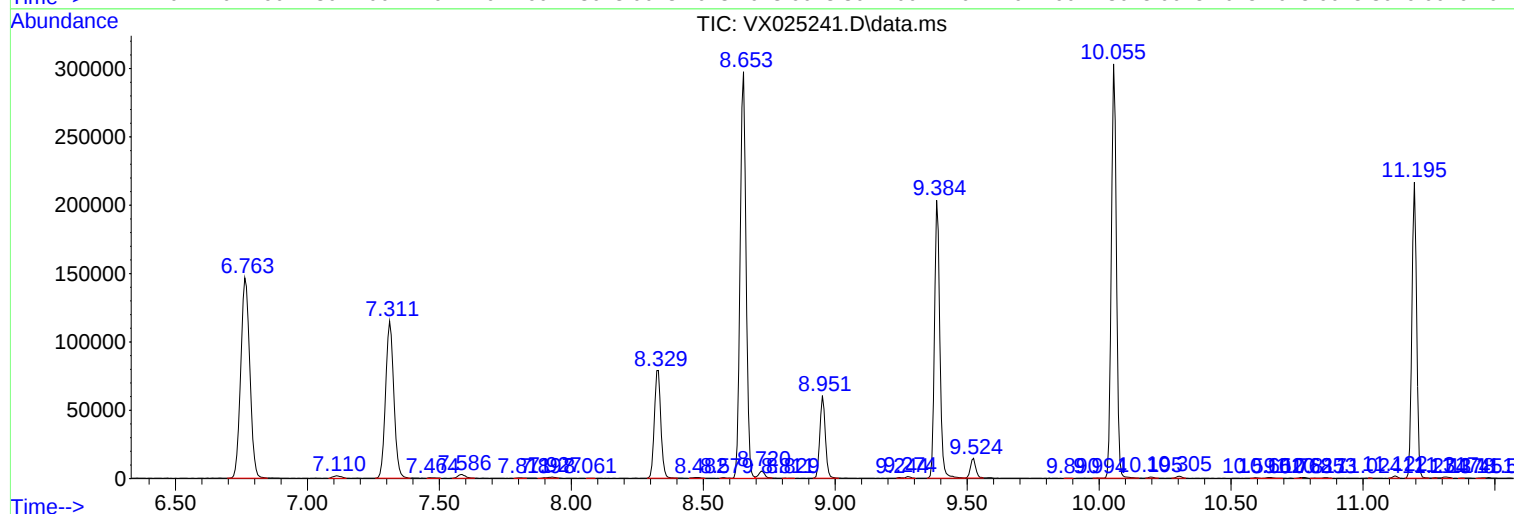
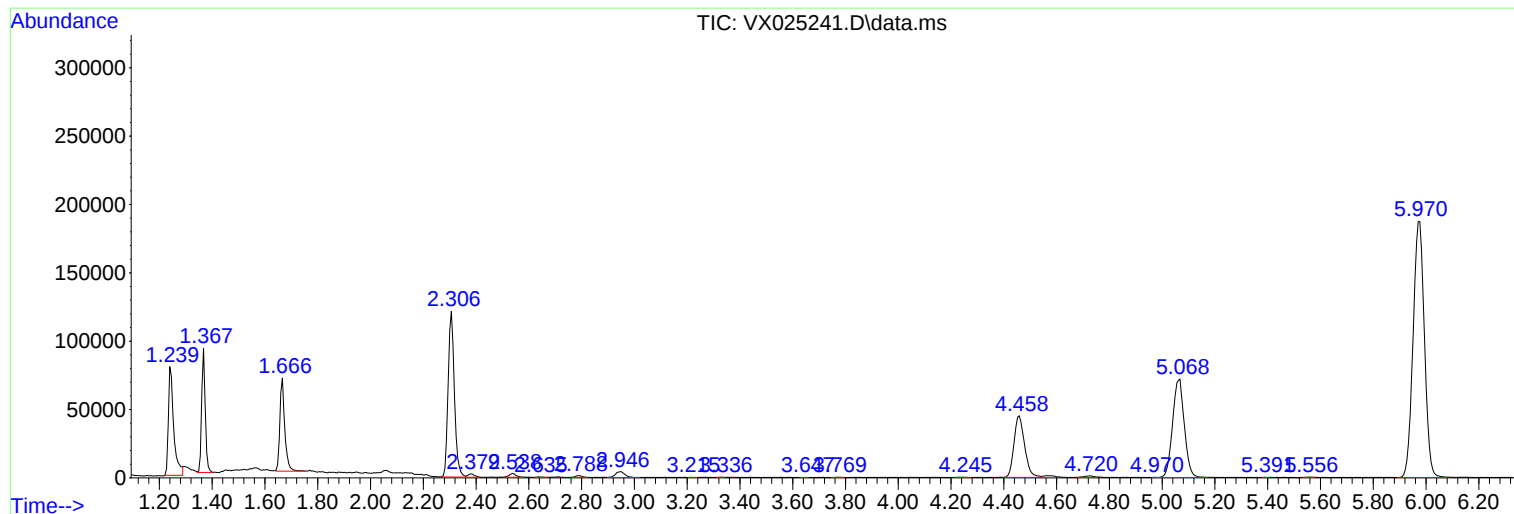
Sum of corrected areas: 4610608

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM111121WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX111921\  
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Instrument :  
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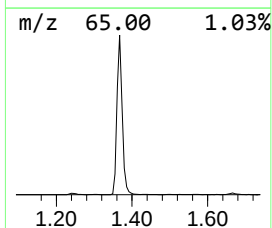
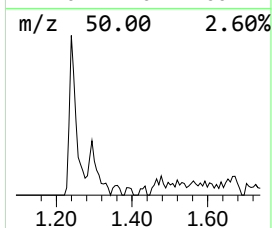
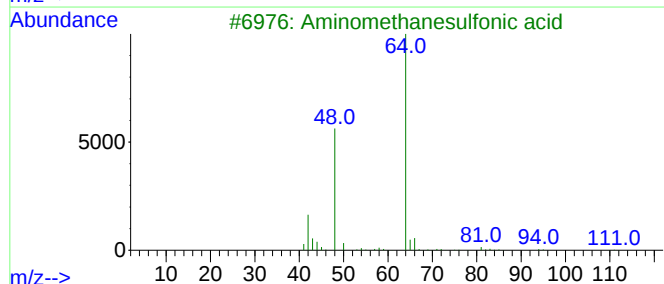
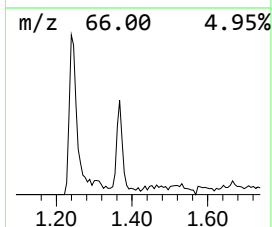
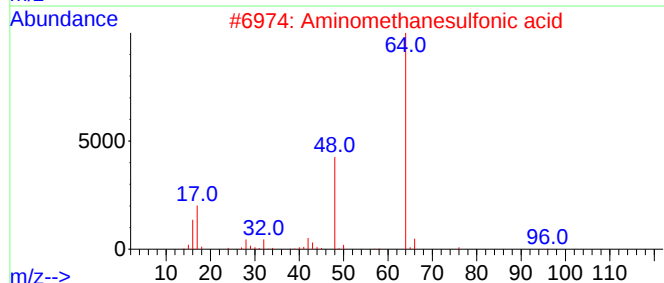
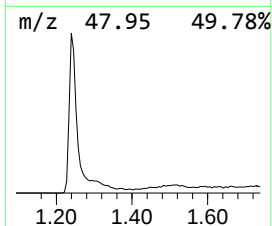
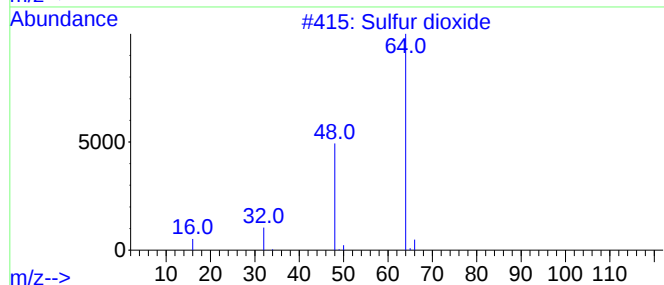
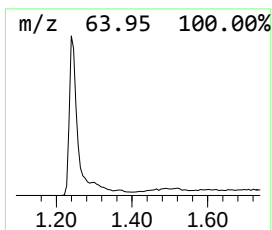
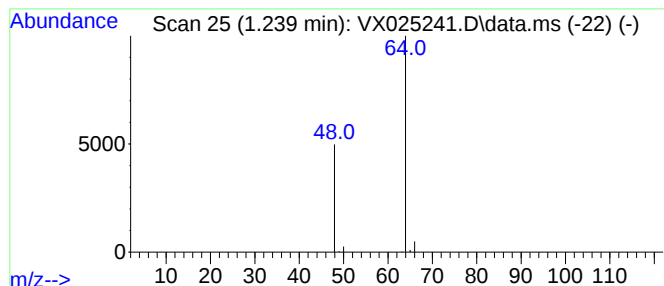
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM111121WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 1.239 | 16.05 ug/L | 111282 | 1,4-Difluorobenzene | 6.763 |

| 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    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 4    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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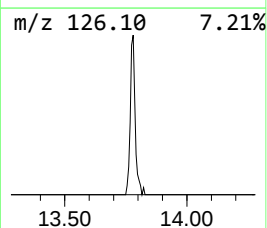
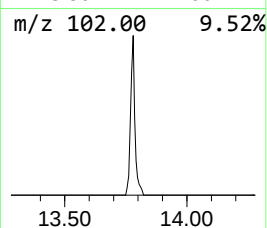
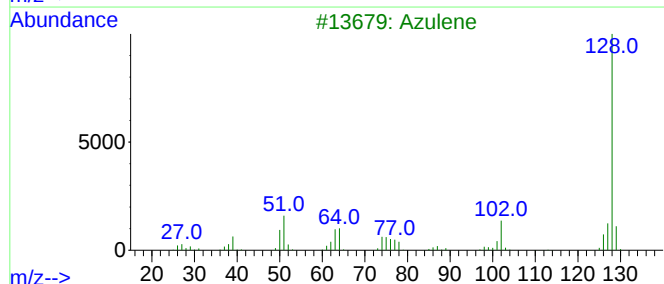
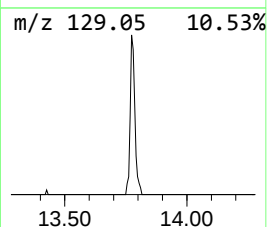
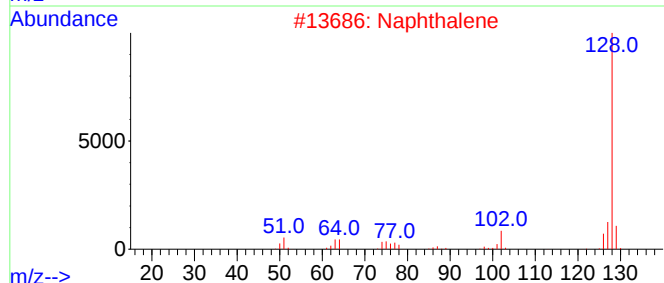
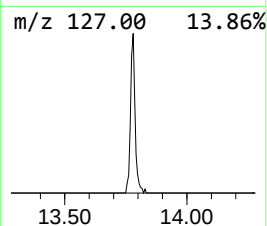
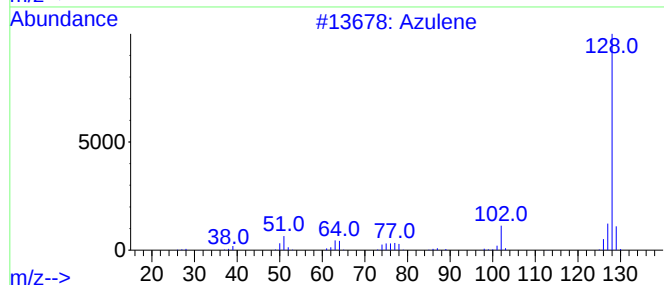
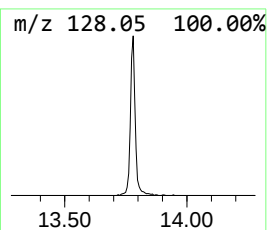
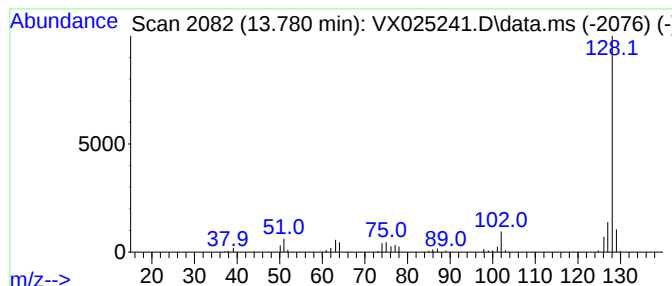
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM111121WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 3 Azulene Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.780 | 5.58 ug/L | 43953 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 95   |
| 2    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 95   |
| 3    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |
| 4    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |
| 5    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 91   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX111921\  
Data File : VX025241.D  
Acq On : 19 Nov 2021 18:16  
Operator : JC/MD  
Sample : M4779-09  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 31 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
F4L21

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML111121WMA.M  
Quant Title : VOC Analysis

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   | 1.239  | 16.1    | ug/L  | 111282   | 1                     | 6.763  | 346616 | 50.0 |
| Azulene          | 13.780 | 5.6     | ug/L  | 43953    | 3                     | 12.024 | 393730 | 50.0 |