

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061422\  
 Data File : VX029478.D  
 Acq On : 14 Jun 2022 20:23  
 Operator : JC/MD  
 Sample : N3313-07  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 YB7L5

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\SFAMXML061322WMA.M  
 Title : VOC Analysis

Signal : TIC: VX029478.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         | 1.270       | 27            | 30          | 32           | rBV3     | 4900           | 7566          | 0.01%           | 0.006%        |
| 2         | 1.368       | 42            | 46          | 54           | rVB      | 195156         | 194225        | 0.20%           | 0.164%        |
| 3         | 1.453       | 57            | 60          | 64           | rVV      | 13115          | 13673         | 0.01%           | 0.012%        |
| 4         | 1.666       | 91            | 95          | 103          | rBV      | 135204         | 160974        | 0.16%           | 0.136%        |
| 5         | 1.996       | 146           | 149         | 156          | rVB      | 7830           | 10223         | 0.01%           | 0.009%        |
| 6         | 2.319       | 193           | 202         | 212          | rBV2     | 1533070        | 2623209       | 2.65%           | 2.211%        |
| 7         | 2.508       | 230           | 233         | 236          | rBV3     | 563            | 811           | 0.00%           | 0.001%        |
| 8         | 2.666       | 257           | 259         | 261          | rBV2     | 258            | 301           | 0.00%           | 0.000%        |
| 9         | 2.794       | 272           | 280         | 287          | rVB3     | 4360           | 8112          | 0.01%           | 0.007%        |
| 10        | 2.849       | 287           | 289         | 290          | rBV      | 341            | 268           | 0.00%           | 0.000%        |
| 11        | 2.947       | 297           | 305         | 315          | rBV2     | 12667          | 35550         | 0.04%           | 0.030%        |
| 12        | 3.099       | 322           | 330         | 338          | rVB2     | 7973           | 16954         | 0.02%           | 0.014%        |
| 13        | 3.221       | 348           | 350         | 353          | rBV2     | 307            | 369           | 0.00%           | 0.000%        |
| 14        | 3.361       | 371           | 373         | 375          | rBV2     | 300            | 329           | 0.00%           | 0.000%        |
| 15        | 3.611       | 406           | 414         | 426          | rVB      | 25103          | 59056         | 0.06%           | 0.050%        |
| 16        | 4.001       | 475           | 478         | 479          | rBV2     | 343            | 285           | 0.00%           | 0.000%        |
| 17        | 4.489       | 545           | 558         | 581          | rBV2     | 1345371        | 3892229       | 3.94%           | 3.281%        |
| 18        | 4.812       | 608           | 611         | 613          | rBV2     | 392            | 450           | 0.00%           | 0.000%        |
| 19        | 4.867       | 619           | 620         | 623          | rBV2     | 306            | 331           | 0.00%           | 0.000%        |
| 20        | 4.922       | 627           | 629         | 633          | rBV2     | 302            | 327           | 0.00%           | 0.000%        |
| 21        | 5.062       | 638           | 652         | 671          | rBV      | 180429         | 600897        | 0.61%           | 0.506%        |
| 22        | 5.269       | 683           | 686         | 688          | rBV2     | 228            | 288           | 0.00%           | 0.000%        |
| 23        | 5.306       | 691           | 692         | 694          | rBV      | 322            | 267           | 0.00%           | 0.000%        |
| 24        | 5.385       | 703           | 705         | 708          | rBV3     | 787            | 867           | 0.00%           | 0.001%        |
| 25        | 5.477       | 718           | 720         | 721          | rBV2     | 383            | 374           | 0.00%           | 0.000%        |
| 26        | 5.550       | 726           | 732         | 733          | rBV2     | 1091           | 1643          | 0.00%           | 0.001%        |
| 27        | 5.562       | 733           | 734         | 736          | rVV2     | 801            | 400           | 0.00%           | 0.000%        |
| 28        | 5.684       | 746           | 754         | 761          | rBV6     | 2610           | 6788          | 0.01%           | 0.006%        |
| 29        | 5.842       | 778           | 780         | 783          | rBV2     | 296            | 378           | 0.00%           | 0.000%        |
| 30        | 5.976       | 789           | 802         | 814          | rBV2     | 467498         | 1414726       | 1.43%           | 1.192%        |
| 31        | 6.239       | 843           | 845         | 846          | rBV      | 327            | 263           | 0.00%           | 0.000%        |
| 32        | 6.269       | 848           | 850         | 854          | rVB3     | 687            | 688           | 0.00%           | 0.001%        |
| 33        | 6.318       | 856           | 858         | 860          | rBV2     | 302            | 324           | 0.00%           | 0.000%        |
| 34        | 6.342       | 860           | 862         | 863          | rBV      | 452            | 370           | 0.00%           | 0.000%        |
| 35        | 6.361       | 863           | 865         | 867          | rVV2     | 664            | 687           | 0.00%           | 0.001%        |
| 36        | 6.385       | 867           | 869         | 875          | rVV4     | 1000           | 1493          | 0.00%           | 0.001%        |

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 Title : VOC Analysis

|    |        |      |      |      |      |          |          |         |         |
|----|--------|------|------|------|------|----------|----------|---------|---------|
| 37 | 6.550  | 893  | 896  | 901  | rBV2 | 449      | 801      | 0.00%   | 0.001%  |
| 38 | 6.769  | 922  | 932  | 946  | rVV  | 320165   | 776879   | 0.79%   | 0.655%  |
| 39 | 7.153  | 980  | 995  | 1014 | rBV  | 33765535 | 98806923 | 100.00% | 83.284% |
| 40 | 7.312  | 1015 | 1021 | 1034 | rVB  | 276528   | 616129   | 0.62%   | 0.519%  |
| 41 | 7.671  | 1074 | 1080 | 1092 | rVB  | 52365    | 113643   | 0.12%   | 0.096%  |
| 42 | 7.940  | 1120 | 1124 | 1125 | rBV4 | 953      | 1050     | 0.00%   | 0.001%  |
| 43 | 8.330  | 1181 | 1188 | 1202 | rVB  | 184793   | 303971   | 0.31%   | 0.256%  |
| 44 | 8.482  | 1211 | 1213 | 1218 | rBV4 | 1204     | 2077     | 0.00%   | 0.002%  |
| 45 | 8.653  | 1234 | 1241 | 1248 | rBV  | 762183   | 1173447  | 1.19%   | 0.989%  |
| 46 | 8.720  | 1249 | 1252 | 1260 | rVB  | 14043    | 21814    | 0.02%   | 0.018%  |
| 47 | 8.952  | 1285 | 1290 | 1299 | rBV  | 127623   | 188759   | 0.19%   | 0.159%  |
| 48 | 9.061  | 1307 | 1308 | 1310 | rBV2 | 523      | 350      | 0.00%   | 0.000%  |
| 49 | 9.153  | 1317 | 1323 | 1331 | rBV  | 82669    | 123473   | 0.12%   | 0.104%  |
| 50 | 9.275  | 1333 | 1343 | 1356 | rBV  | 2070474  | 3000065  | 3.04%   | 2.529%  |
| 51 | 9.384  | 1356 | 1361 | 1371 | rBV  | 495250   | 715393   | 0.72%   | 0.603%  |
| 52 | 9.525  | 1381 | 1384 | 1394 | rVB2 | 5589     | 9016     | 0.01%   | 0.008%  |
| 53 | 9.714  | 1413 | 1415 | 1416 | rBV2 | 389      | 252      | 0.00%   | 0.000%  |
| 54 | 9.738  | 1416 | 1419 | 1421 | rVV3 | 926      | 997      | 0.00%   | 0.001%  |
| 55 | 9.775  | 1423 | 1425 | 1427 | rVV2 | 369      | 279      | 0.00%   | 0.000%  |
| 56 | 9.805  | 1427 | 1430 | 1434 | rVB3 | 477      | 609      | 0.00%   | 0.001%  |
| 57 | 9.909  | 1445 | 1447 | 1449 | rVV  | 417      | 253      | 0.00%   | 0.000%  |
| 58 | 9.951  | 1450 | 1454 | 1456 | rVB4 | 403      | 553      | 0.00%   | 0.000%  |
| 59 | 10.055 | 1465 | 1471 | 1481 | rBV  | 690780   | 922068   | 0.93%   | 0.777%  |
| 60 | 10.165 | 1486 | 1489 | 1492 | rBV3 | 3786     | 4528     | 0.00%   | 0.004%  |
| 61 | 10.305 | 1507 | 1512 | 1519 | rVB2 | 3634     | 5555     | 0.01%   | 0.005%  |
| 62 | 10.378 | 1520 | 1524 | 1529 | rVB2 | 5523     | 7777     | 0.01%   | 0.007%  |
| 63 | 10.646 | 1562 | 1568 | 1574 | rBV  | 76424    | 102166   | 0.10%   | 0.086%  |
| 64 | 10.750 | 1581 | 1585 | 1591 | rBV5 | 304      | 566      | 0.00%   | 0.000%  |
| 65 | 10.854 | 1600 | 1602 | 1605 | rBV2 | 479      | 509      | 0.00%   | 0.000%  |
| 66 | 10.969 | 1617 | 1621 | 1625 | rVB2 | 1178     | 1628     | 0.00%   | 0.001%  |
| 67 | 11.018 | 1625 | 1629 | 1634 | rVB3 | 1242     | 2389     | 0.00%   | 0.002%  |
| 68 | 11.122 | 1642 | 1646 | 1652 | rVB  | 6720     | 8543     | 0.01%   | 0.007%  |
| 69 | 11.195 | 1652 | 1658 | 1666 | rBV  | 524699   | 675965   | 0.68%   | 0.570%  |
| 70 | 11.311 | 1674 | 1677 | 1678 | rBV3 | 2665     | 2983     | 0.00%   | 0.003%  |
| 71 | 11.427 | 1694 | 1696 | 1697 | rBV2 | 475      | 412      | 0.00%   | 0.000%  |
| 72 | 11.549 | 1714 | 1716 | 1719 | rVB2 | 942      | 701      | 0.00%   | 0.001%  |
| 73 | 11.610 | 1724 | 1726 | 1733 | rVV3 | 2003     | 3000     | 0.00%   | 0.003%  |
| 74 | 11.695 | 1736 | 1740 | 1745 | rVV5 | 3214     | 5511     | 0.01%   | 0.005%  |
| 75 | 11.750 | 1745 | 1749 | 1754 | rVB2 | 7784     | 10170    | 0.01%   | 0.009%  |
| 76 | 11.841 | 1760 | 1764 | 1768 | rVB3 | 1775     | 2278     | 0.00%   | 0.002%  |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 YB7L5

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\SFAMXML061322WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |       |        |
|-----|--------|------|------|------|------|--------|--------|-------|--------|
| 77  | 11.933 | 1776 | 1779 | 1783 | rBV2 | 4335   | 5466   | 0.01% | 0.005% |
| 78  | 11.975 | 1783 | 1786 | 1789 | rVB3 | 1443   | 1574   | 0.00% | 0.001% |
| 79  | 12.024 | 1789 | 1794 | 1800 | rBV  | 787474 | 939513 | 0.95% | 0.792% |
| 80  | 12.225 | 1823 | 1827 | 1830 | rBV3 | 2342   | 3049   | 0.00% | 0.003% |
| 81  | 12.323 | 1836 | 1843 | 1850 | rBV  | 787183 | 994014 | 1.01% | 0.838% |
| 82  | 12.427 | 1856 | 1860 | 1864 | rVB5 | 2352   | 3297   | 0.00% | 0.003% |
| 83  | 12.524 | 1874 | 1876 | 1878 | rBV2 | 505    | 388    | 0.00% | 0.000% |
| 84  | 12.609 | 1888 | 1890 | 1892 | rBV3 | 656    | 633    | 0.00% | 0.001% |
| 85  | 12.768 | 1914 | 1916 | 1919 | rVB2 | 1290   | 1291   | 0.00% | 0.001% |
| 86  | 12.859 | 1927 | 1931 | 1937 | rBV4 | 5527   | 8292   | 0.01% | 0.007% |
| 87  | 12.908 | 1937 | 1939 | 1940 | rBV2 | 587    | 503    | 0.00% | 0.000% |
| 88  | 13.054 | 1958 | 1963 | 1969 | rVB5 | 1822   | 3009   | 0.00% | 0.003% |
| 89  | 13.122 | 1969 | 1974 | 1976 | rVV2 | 745    | 875    | 0.00% | 0.001% |
| 90  | 13.152 | 1977 | 1979 | 1982 | rVB2 | 398    | 257    | 0.00% | 0.000% |
| 91  | 13.530 | 2038 | 2041 | 2044 | rBV2 | 242    | 348    | 0.00% | 0.000% |
| 92  | 13.695 | 2065 | 2068 | 2070 | rBV  | 640    | 748    | 0.00% | 0.001% |
| 93  | 13.780 | 2078 | 2082 | 2085 | rBV2 | 1061   | 1329   | 0.00% | 0.001% |
| 94  | 13.975 | 2109 | 2114 | 2115 | rVV  | 692    | 710    | 0.00% | 0.001% |
| 95  | 14.134 | 2137 | 2140 | 2144 | rVB2 | 1441   | 1908   | 0.00% | 0.002% |
| 96  | 14.188 | 2146 | 2149 | 2150 | rBV2 | 482    | 484    | 0.00% | 0.000% |
| 97  | 14.243 | 2156 | 2158 | 2161 | rBV2 | 499    | 638    | 0.00% | 0.001% |
| 98  | 14.914 | 2266 | 2268 | 2270 | rVB  | 547    | 380    | 0.00% | 0.000% |
| 99  | 14.957 | 2272 | 2275 | 2276 | rBV2 | 571    | 671    | 0.00% | 0.001% |
| 100 | 16.603 | 2544 | 2545 | 2547 | rBV2 | 470    | 339    | 0.00% | 0.000% |

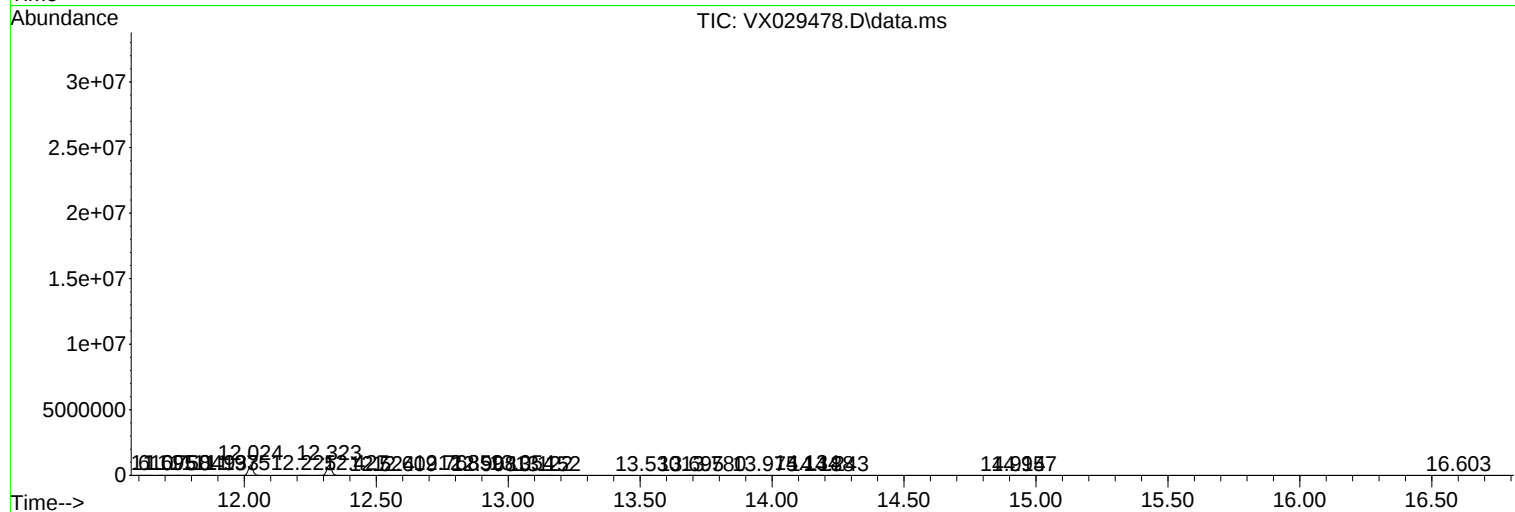
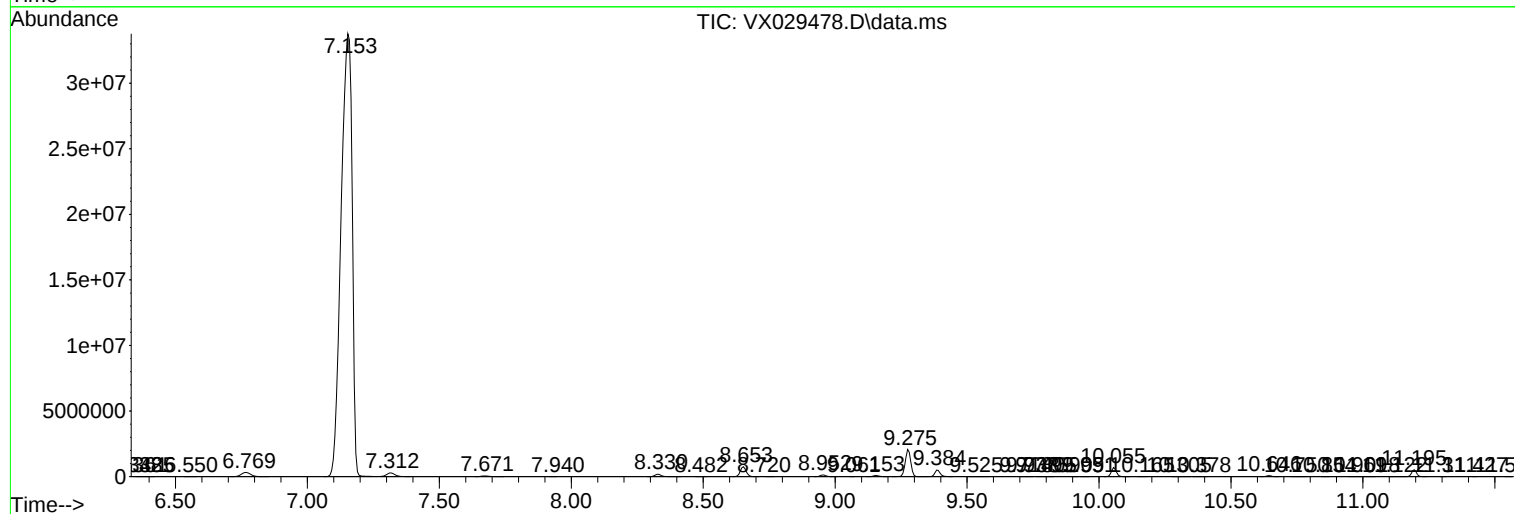
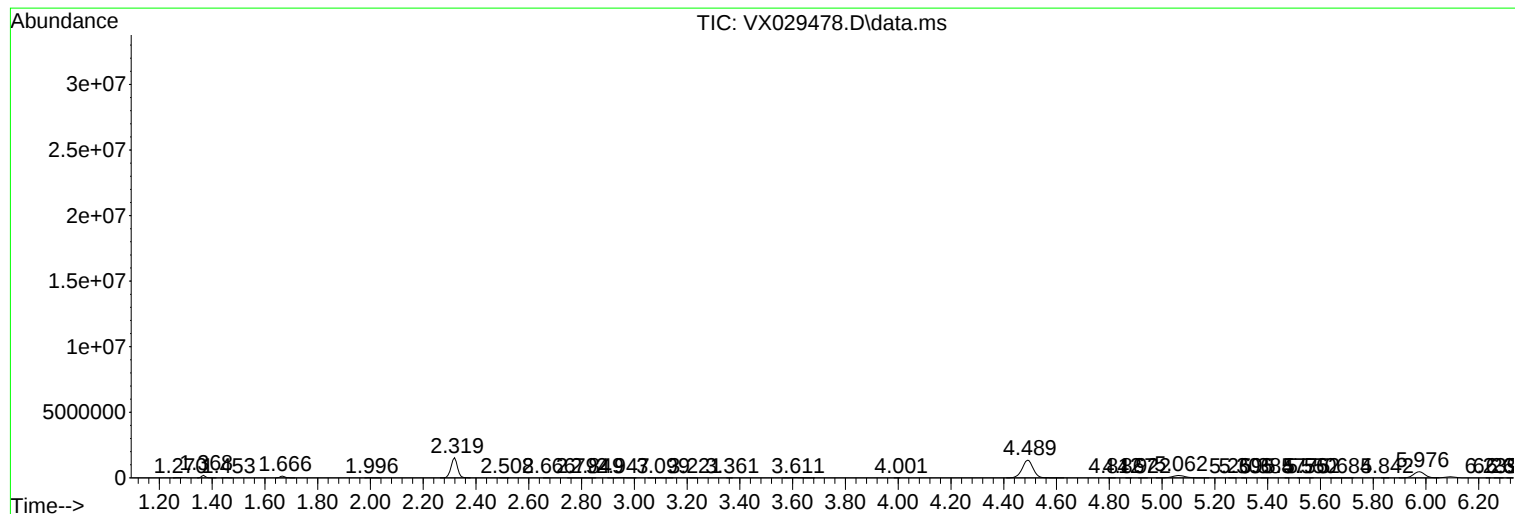
Sum of corrected areas: 118638893

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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML061322WMA.M  
Quant Title : VOC Analysis

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



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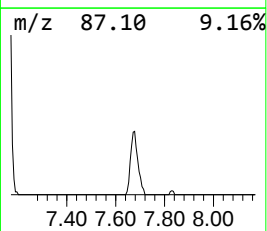
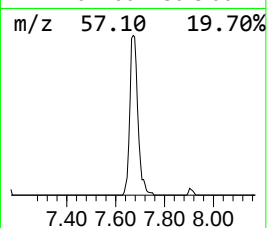
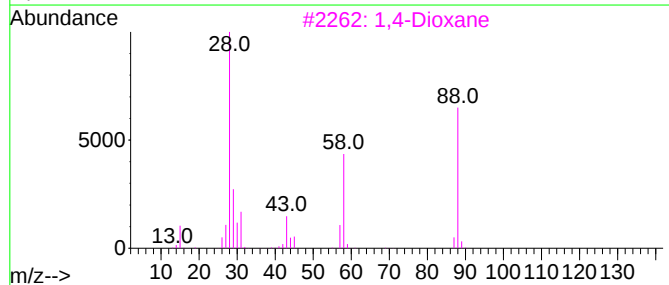
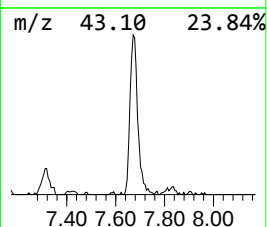
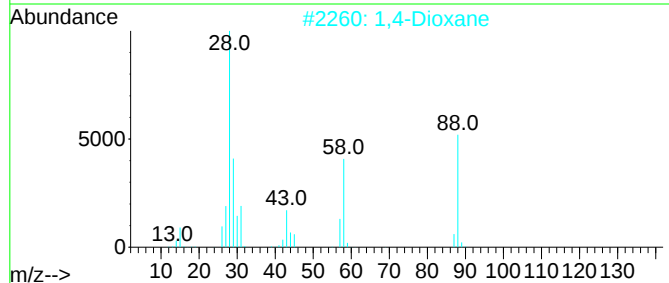
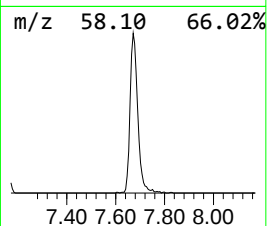
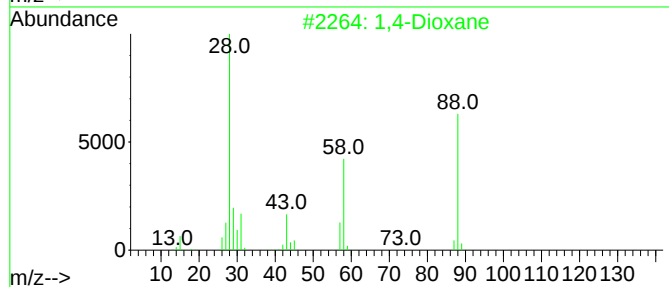
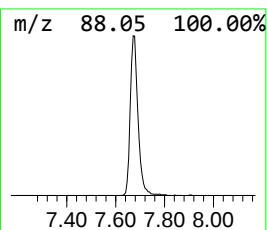
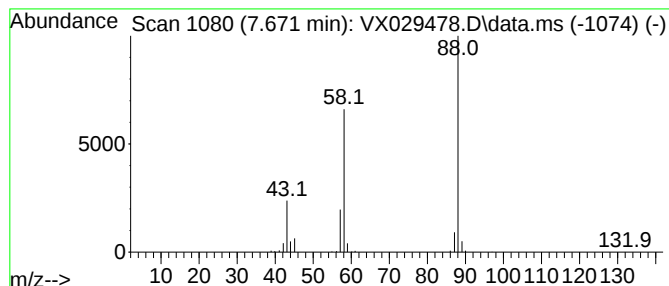
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML061322WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 1,3,6-Trioxocane Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 7.671 | 7.31 ug/L | 113643 | 1,4-Difluorobenzene | 6.769 |

| Hit# | of | 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------|-----|---------|-------------|------|
| 1    |    |   | 1,4-Dioxane      | 88  | C4H8O2  | 000123-91-1 | 91   |
| 2    |    |   | 1,4-Dioxane      | 88  | C4H8O2  | 000123-91-1 | 90   |
| 3    |    |   | 1,4-Dioxane      | 88  | C4H8O2  | 000123-91-1 | 83   |
| 4    |    |   | 1,4-Dioxane      | 88  | C4H8O2  | 000123-91-1 | 78   |
| 5    |    |   | 1,3,6-Trioxocane | 118 | C5H10O3 | 001779-19-7 | 64   |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| 1,3,6-Trioxocane | 7.671 | 7.3     | ug/L  | 113643   | 1                     | 6.769 | 776879 | 50.0 |