

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120821\  
 Data File : VX025642.D  
 Acq On : 09 Dec 2021 00:09  
 Operator : JC/MD  
 Sample : M4975-07  
 Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGKT1

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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025642.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         | 1.240       | 22            | 25          | 31           | rBV      | 4506           | 7429          | 0.02%           | 0.015%        |
| 2         | 1.368       | 43            | 46          | 57           | rVB      | 53523          | 63031         | 0.19%           | 0.128%        |
| 3         | 1.550       | 69            | 76          | 77           | rBV4     | 6825           | 12245         | 0.04%           | 0.025%        |
| 4         | 1.648       | 89            | 92          | 98           | rVB      | 34802          | 39513         | 0.12%           | 0.080%        |
| 5         | 2.288       | 190           | 197         | 208          | rBV5     | 164075         | 350378        | 1.03%           | 0.712%        |
| 6         | 2.947       | 299           | 305         | 317          | rBV      | 7144           | 19459         | 0.06%           | 0.040%        |
| 7         | 3.526       | 397           | 400         | 403          | rVB2     | 350            | 439           | 0.00%           | 0.001%        |
| 8         | 3.605       | 405           | 413         | 426          | rBV      | 25783          | 62419         | 0.18%           | 0.127%        |
| 9         | 4.190       | 506           | 509         | 510          | rBV2     | 374            | 394           | 0.00%           | 0.001%        |
| 10        | 4.495       | 546           | 559         | 583          | rBV2     | 20828          | 104137        | 0.31%           | 0.212%        |
| 11        | 4.721       | 592           | 596         | 597          | rBV3     | 699            | 894           | 0.00%           | 0.002%        |
| 12        | 5.068       | 641           | 653         | 670          | rBV      | 57743          | 196522        | 0.58%           | 0.399%        |
| 13        | 5.385       | 689           | 705         | 725          | rBV      | 2249074        | 7152925       | 21.09%          | 14.531%       |
| 14        | 5.806       | 772           | 774         | 779          | rBV      | 454            | 485           | 0.00%           | 0.001%        |
| 15        | 5.970       | 790           | 801         | 817          | rBV2     | 165619         | 487825        | 1.44%           | 0.991%        |
| 16        | 6.239       | 844           | 845         | 850          | rBV3     | 429            | 526           | 0.00%           | 0.001%        |
| 17        | 6.373       | 860           | 867         | 872          | rBV6     | 1823           | 5489          | 0.02%           | 0.011%        |
| 18        | 6.513       | 888           | 890         | 892          | rBV2     | 377            | 345           | 0.00%           | 0.001%        |
| 19        | 6.769       | 922           | 932         | 948          | rBV      | 120427         | 330386        | 0.97%           | 0.671%        |
| 20        | 6.940       | 958           | 960         | 962          | rBV      | 397            | 277           | 0.00%           | 0.001%        |
| 21        | 7.129       | 981           | 991         | 1012         | rBV      | 1505303        | 3370773       | 9.94%           | 6.848%        |
| 22        | 7.312       | 1013          | 1021        | 1035         | rVB      | 91395          | 220386        | 0.65%           | 0.448%        |
| 23        | 7.452       | 1043          | 1044        | 1046         | rVB      | 491            | 272           | 0.00%           | 0.001%        |
| 24        | 7.476       | 1046          | 1048        | 1049         | rBV      | 597            | 503           | 0.00%           | 0.001%        |
| 25        | 7.610       | 1069          | 1070        | 1073         | rBV      | 286            | 336           | 0.00%           | 0.001%        |
| 26        | 7.653       | 1076          | 1077        | 1079         | rBV      | 461            | 331           | 0.00%           | 0.001%        |
| 27        | 7.726       | 1085          | 1089        | 1090         | rBV      | 312            | 273           | 0.00%           | 0.001%        |
| 28        | 7.818       | 1102          | 1104        | 1108         | rBV2     | 299            | 424           | 0.00%           | 0.001%        |
| 29        | 7.915       | 1118          | 1120        | 1121         | rBV      | 375            | 295           | 0.00%           | 0.001%        |
| 30        | 8.068       | 1143          | 1145        | 1148         | rBV2     | 290            | 405           | 0.00%           | 0.001%        |
| 31        | 8.330       | 1181          | 1188        | 1201         | rBV      | 58173          | 110848        | 0.33%           | 0.225%        |
| 32        | 8.494       | 1213          | 1215        | 1219         | rVV      | 481            | 666           | 0.00%           | 0.001%        |
| 33        | 8.555       | 1222          | 1225        | 1227         | rBV      | 357            | 328           | 0.00%           | 0.001%        |
| 34        | 8.653       | 1232          | 1241        | 1247         | rBV      | 227418         | 406030        | 1.20%           | 0.825%        |
| 35        | 8.720       | 1247          | 1252        | 1265         | rVB      | 173230         | 305083        | 0.90%           | 0.620%        |
| 36        | 8.958       | 1286          | 1291        | 1299         | rBV2     | 38860          | 68709         | 0.20%           | 0.140%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |          |          |         |         |
|----|--------|------|------|------|------|----------|----------|---------|---------|
| 37 | 9.104  | 1313 | 1315 | 1318 | rBV  | 502      | 432      | 0.00%   | 0.001%  |
| 38 | 9.141  | 1318 | 1321 | 1322 | rBV3 | 506      | 466      | 0.00%   | 0.001%  |
| 39 | 9.287  | 1336 | 1345 | 1351 | rBV  | 19547984 | 33919847 | 100.00% | 68.907% |
| 40 | 9.403  | 1358 | 1364 | 1376 | rVB  | 133866   | 232059   | 0.68%   | 0.471%  |
| 41 | 9.756  | 1420 | 1422 | 1427 | rBV6 | 824      | 1180     | 0.00%   | 0.002%  |
| 42 | 9.878  | 1440 | 1442 | 1444 | rBV2 | 724      | 695      | 0.00%   | 0.001%  |
| 43 | 9.951  | 1450 | 1454 | 1456 | rBV2 | 510      | 712      | 0.00%   | 0.001%  |
| 44 | 10.012 | 1460 | 1464 | 1466 | rBV2 | 1821     | 2621     | 0.01%   | 0.005%  |
| 45 | 10.061 | 1466 | 1472 | 1483 | rVB  | 260547   | 389419   | 1.15%   | 0.791%  |
| 46 | 10.201 | 1490 | 1495 | 1499 | rVB  | 8920     | 12284    | 0.04%   | 0.025%  |
| 47 | 10.305 | 1506 | 1512 | 1519 | rBV  | 81966    | 120466   | 0.36%   | 0.245%  |
| 48 | 10.360 | 1519 | 1521 | 1525 | rVB2 | 1116     | 1121     | 0.00%   | 0.002%  |
| 49 | 10.403 | 1525 | 1528 | 1532 | rBV3 | 979      | 1372     | 0.00%   | 0.003%  |
| 50 | 10.646 | 1563 | 1568 | 1573 | rVV  | 25870    | 34567    | 0.10%   | 0.070%  |
| 51 | 10.854 | 1598 | 1602 | 1607 | rBV4 | 2650     | 3780     | 0.01%   | 0.008%  |
| 52 | 10.896 | 1607 | 1609 | 1614 | rBV2 | 473      | 554      | 0.00%   | 0.001%  |
| 53 | 10.963 | 1619 | 1620 | 1624 | rVB3 | 458      | 435      | 0.00%   | 0.001%  |
| 54 | 11.037 | 1626 | 1632 | 1633 | rBV3 | 470      | 866      | 0.00%   | 0.002%  |
| 55 | 11.067 | 1634 | 1637 | 1639 | rBV3 | 987      | 1262     | 0.00%   | 0.003%  |
| 56 | 11.201 | 1653 | 1659 | 1666 | rBV  | 169411   | 230225   | 0.68%   | 0.468%  |
| 57 | 11.384 | 1685 | 1689 | 1695 | rBV3 | 3680     | 6767     | 0.02%   | 0.014%  |
| 58 | 11.476 | 1702 | 1704 | 1714 | rVB3 | 5456     | 7255     | 0.02%   | 0.015%  |
| 59 | 11.622 | 1724 | 1728 | 1734 | rVB4 | 1613     | 2631     | 0.01%   | 0.005%  |
| 60 | 11.713 | 1740 | 1743 | 1746 | rBV3 | 1776     | 1989     | 0.01%   | 0.004%  |
| 61 | 11.756 | 1746 | 1750 | 1758 | rVB2 | 11032    | 14239    | 0.04%   | 0.029%  |
| 62 | 11.847 | 1761 | 1765 | 1768 | rBV3 | 825      | 1380     | 0.00%   | 0.003%  |
| 63 | 11.939 | 1776 | 1780 | 1784 | rBV3 | 1435     | 2127     | 0.01%   | 0.004%  |
| 64 | 11.975 | 1784 | 1786 | 1789 | rVB2 | 794      | 585      | 0.00%   | 0.001%  |
| 65 | 12.024 | 1789 | 1794 | 1801 | rBV  | 332342   | 413982   | 1.22%   | 0.841%  |
| 66 | 12.091 | 1802 | 1805 | 1809 | rVB  | 2377     | 3266     | 0.01%   | 0.007%  |
| 67 | 12.213 | 1823 | 1825 | 1826 | rBV  | 557      | 449      | 0.00%   | 0.001%  |
| 68 | 12.250 | 1826 | 1831 | 1837 | rVV  | 48748    | 62698    | 0.18%   | 0.127%  |
| 69 | 12.323 | 1838 | 1843 | 1850 | rVB  | 312586   | 390664   | 1.15%   | 0.794%  |
| 70 | 12.427 | 1855 | 1860 | 1864 | rBV  | 7412     | 8808     | 0.03%   | 0.018%  |
| 71 | 12.463 | 1864 | 1866 | 1872 | rVB4 | 1068     | 1715     | 0.01%   | 0.003%  |
| 72 | 12.609 | 1889 | 1890 | 1897 | rBV3 | 640      | 928      | 0.00%   | 0.002%  |
| 73 | 12.762 | 1913 | 1915 | 1917 | rBV  | 346      | 355      | 0.00%   | 0.001%  |
| 74 | 12.896 | 1932 | 1937 | 1939 | rBV2 | 1007     | 1384     | 0.00%   | 0.003%  |
| 75 | 13.048 | 1958 | 1962 | 1966 | rBV4 | 522      | 984      | 0.00%   | 0.002%  |
| 76 | 13.164 | 1976 | 1981 | 1983 | rBV3 | 439      | 646      | 0.00%   | 0.001%  |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGKT1

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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 13.268 | 1994 | 1998 | 2001 | rBV2 | 2360 | 3715 | 0.01% | 0.008% |
| 78  | 13.384 | 2015 | 2017 | 2021 | rVB3 | 641  | 553  | 0.00% | 0.001% |
| 79  | 13.481 | 2032 | 2033 | 2036 | rBV  | 388  | 375  | 0.00% | 0.001% |
| 80  | 13.615 | 2051 | 2055 | 2058 | rVB  | 287  | 383  | 0.00% | 0.001% |
| 81  | 13.780 | 2078 | 2082 | 2089 | rVB  | 3359 | 4033 | 0.01% | 0.008% |
| 82  | 13.841 | 2089 | 2092 | 2096 | rVB4 | 720  | 1103 | 0.00% | 0.002% |
| 83  | 14.042 | 2120 | 2125 | 2129 | rVB3 | 1999 | 2691 | 0.01% | 0.005% |
| 84  | 14.298 | 2165 | 2167 | 2168 | rBV  | 360  | 273  | 0.00% | 0.001% |
| 85  | 14.402 | 2181 | 2184 | 2187 | rBV2 | 392  | 509  | 0.00% | 0.001% |
| 86  | 14.426 | 2187 | 2188 | 2191 | rVV  | 345  | 280  | 0.00% | 0.001% |
| 87  | 14.615 | 2212 | 2219 | 2221 | rBV3 | 494  | 1126 | 0.00% | 0.002% |
| 88  | 14.640 | 2221 | 2223 | 2228 | rVB3 | 1225 | 1340 | 0.00% | 0.003% |
| 89  | 14.755 | 2239 | 2242 | 2246 | rBV4 | 1431 | 1770 | 0.01% | 0.004% |
| 90  | 14.981 | 2278 | 2279 | 2281 | rBV  | 370  | 272  | 0.00% | 0.001% |
| 91  | 15.213 | 2315 | 2317 | 2322 | rVB3 | 523  | 678  | 0.00% | 0.001% |
| 92  | 15.249 | 2322 | 2323 | 2326 | rBV  | 425  | 319  | 0.00% | 0.001% |
| 93  | 15.426 | 2349 | 2352 | 2354 | rVB3 | 1254 | 1207 | 0.00% | 0.002% |
| 94  | 15.450 | 2354 | 2356 | 2357 | rBV  | 405  | 309  | 0.00% | 0.001% |
| 95  | 15.493 | 2357 | 2363 | 2367 | rBV5 | 1487 | 2653 | 0.01% | 0.005% |
| 96  | 15.627 | 2381 | 2385 | 2387 | rBV3 | 615  | 824  | 0.00% | 0.002% |
| 97  | 15.652 | 2387 | 2389 | 2392 | rVB3 | 536  | 466  | 0.00% | 0.001% |
| 98  | 15.841 | 2418 | 2420 | 2424 | rBV3 | 302  | 295  | 0.00% | 0.001% |
| 99  | 16.383 | 2503 | 2509 | 2514 | rVB4 | 1222 | 2086 | 0.01% | 0.004% |
| 100 | 16.664 | 2553 | 2555 | 2556 | rBV  | 425  | 345  | 0.00% | 0.001% |

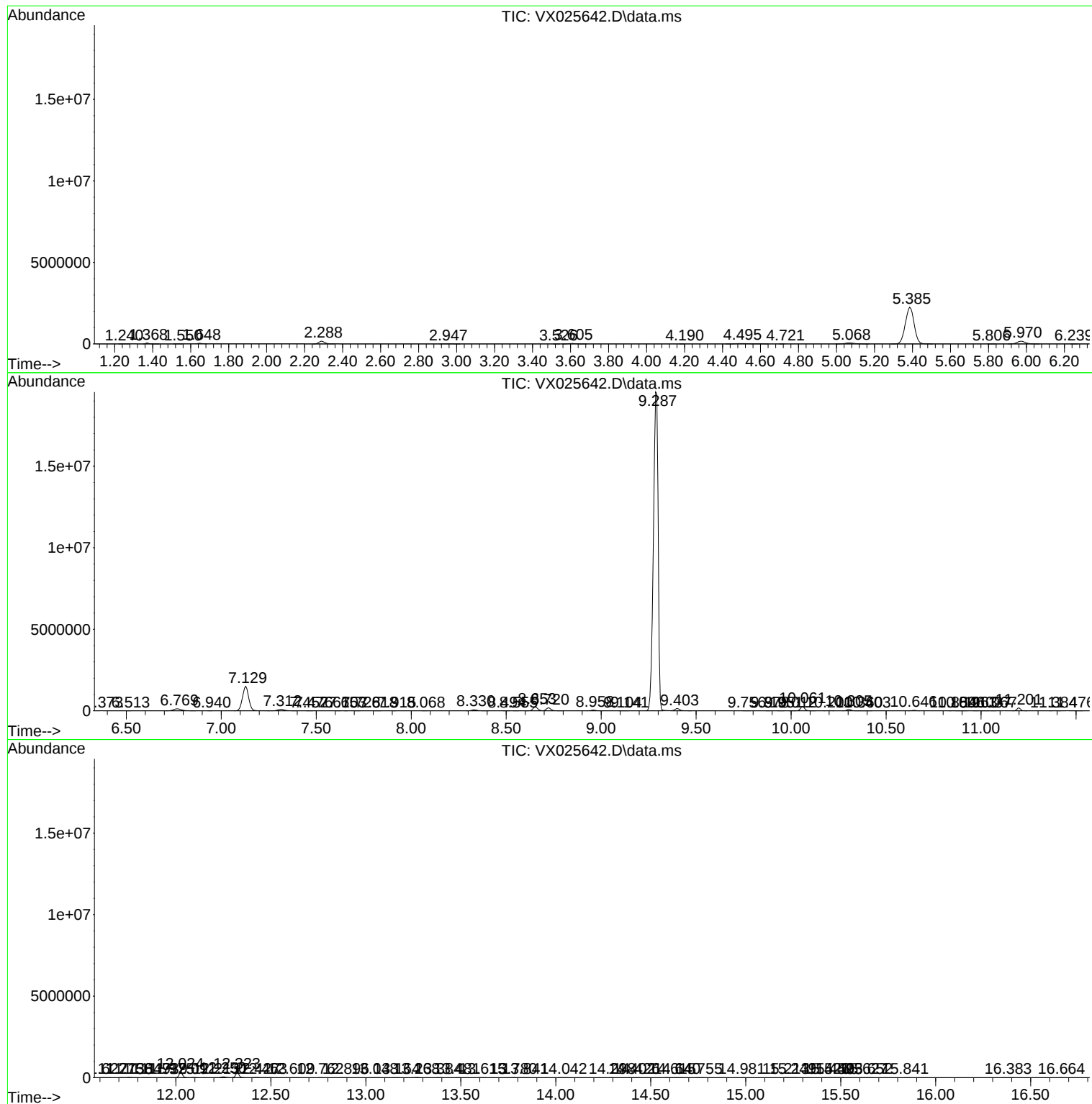
Sum of corrected areas: 49225600

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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120821\  
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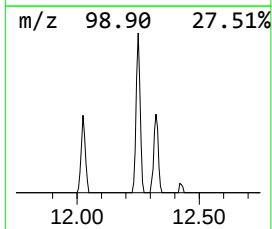
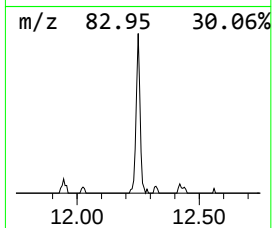
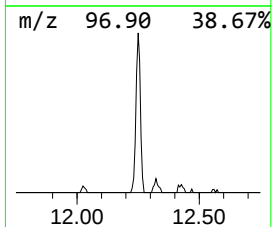
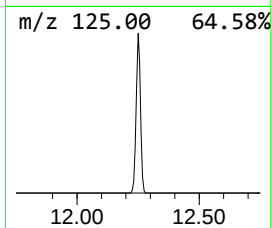
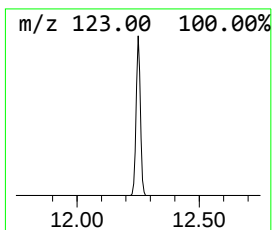
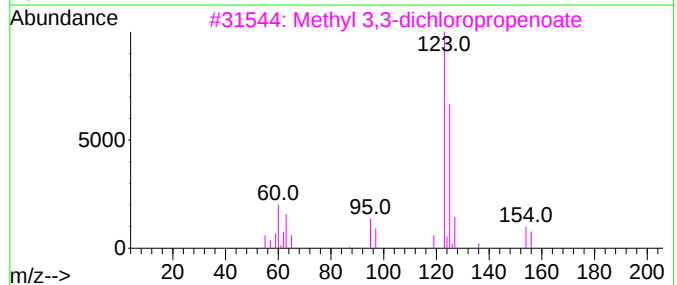
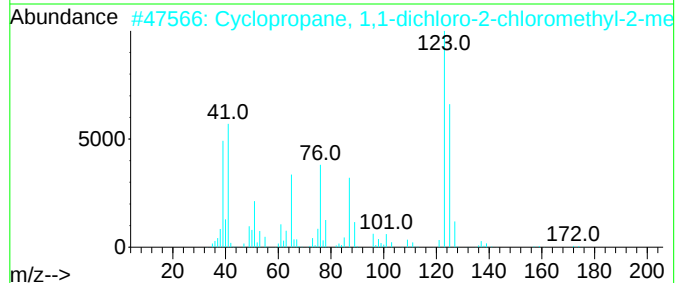
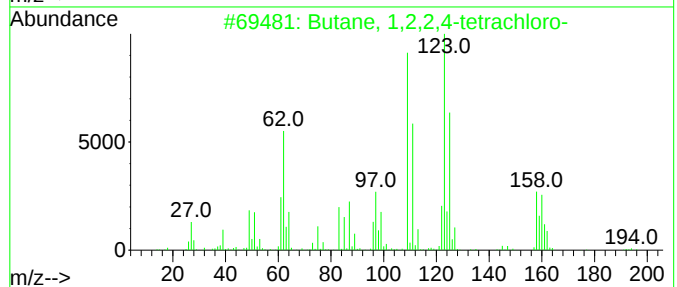
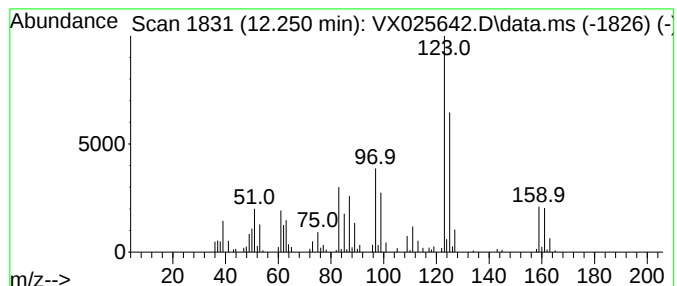
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 3 unknown-01 Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.250 | 7.57 ug/L | 62698 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Butane, 1,2,2,4-tetrachloro-        | 194 | C4H6Cl4   | 042525-60-0 | 40   |
| 2    |    |   | Cyclopropane, 1,1-dichloro-2-chl... | 172 | C5H7Cl3   | 015997-19-0 | 32   |
| 3    |    |   | Methyl 3,3-dichloropropenoate       | 154 | C4H4Cl2O2 | 002257-46-7 | 25   |
| 4    |    |   | 1-Propene, 3,3,3-trichloro-2-met... | 158 | C4H5Cl3   | 004749-27-3 | 16   |
| 5    |    |   | 1-Propene, 1,1,3-trichloro-2-met... | 158 | C4H5Cl3   | 031702-33-7 | 16   |



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

| TIC Top Hit name | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                  |        |         |       |          | #                     | RT     | Resp   | Conc |
| unknown-01       | 12.250 | 7.6     | ug/L  | 62698    | 3                     | 12.024 | 413982 | 50.0 |