

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122721\  
 Data File : VX026071.D  
 Acq On : 27 Dec 2021 18:50  
 Operator : JC/MD  
 Sample : M5174-02ME  
 Misc : 6.41g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 GBC13ME

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\SFAMXLM122321WMA.M  
 Title : VOC Analysis

Signal : TIC: VX026071.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         | 1.373       | 43            | 47          | 53           | rBV      | 108342         | 122709        | 13.72%          | 1.890%        |
| 2         | 1.642       | 87            | 91          | 93           | rBV      | 102722         | 123438        | 13.80%          | 1.902%        |
| 3         | 1.666       | 93            | 95          | 103          | rVB      | 66018          | 90164         | 10.08%          | 1.389%        |
| 4         | 2.294       | 191           | 198         | 206          | rBV      | 192783         | 307031        | 34.33%          | 4.730%        |
| 5         | 2.581       | 243           | 245         | 246          | rBV      | 359            | 318           | 0.04%           | 0.005%        |
| 6         | 2.721       | 260           | 268         | 273          | rBV      | 4850           | 10093         | 1.13%           | 0.155%        |
| 7         | 2.788       | 275           | 279         | 286          | rVB3     | 2698           | 5310          | 0.59%           | 0.082%        |
| 8         | 2.934       | 301           | 303         | 304          | rBV      | 811            | 624           | 0.07%           | 0.010%        |
| 9         | 3.056       | 321           | 323         | 326          | rBV2     | 326            | 319           | 0.04%           | 0.005%        |
| 10        | 3.215       | 347           | 349         | 353          | rBV3     | 332            | 486           | 0.05%           | 0.007%        |
| 11        | 3.306       | 362           | 364         | 367          | rVV      | 358            | 287           | 0.03%           | 0.004%        |
| 12        | 3.513       | 396           | 398         | 401          | rVB      | 267            | 250           | 0.03%           | 0.004%        |
| 13        | 3.836       | 449           | 451         | 452          | rBV      | 298            | 218           | 0.02%           | 0.003%        |
| 14        | 4.489       | 547           | 558         | 590          | rBV      | 37331          | 192766        | 21.55%          | 2.970%        |
| 15        | 5.068       | 639           | 653         | 670          | rBV      | 107326         | 337548        | 37.74%          | 5.200%        |
| 16        | 5.379       | 701           | 704         | 705          | rBV2     | 257            | 237           | 0.03%           | 0.004%        |
| 17        | 5.415       | 708           | 710         | 712          | rBV2     | 274            | 227           | 0.03%           | 0.003%        |
| 18        | 5.495       | 722           | 723         | 725          | rBV      | 294            | 234           | 0.03%           | 0.004%        |
| 19        | 5.970       | 788           | 801         | 818          | rBV2     | 317455         | 894472        | 100.00%         | 13.780%       |
| 20        | 6.178       | 832           | 835         | 837          | rBV2     | 164            | 230           | 0.03%           | 0.004%        |
| 21        | 6.269       | 849           | 850         | 853          | rBV      | 302            | 258           | 0.03%           | 0.004%        |
| 22        | 6.623       | 907           | 908         | 912          | rBV2     | 326            | 327           | 0.04%           | 0.005%        |
| 23        | 6.690       | 915           | 919         | 921          | rBV2     | 233            | 292           | 0.03%           | 0.004%        |
| 24        | 6.763       | 922           | 931         | 944          | rVV      | 188714         | 455882        | 50.97%          | 7.023%        |
| 25        | 6.958       | 959           | 963         | 966          | rVB      | 570            | 697           | 0.08%           | 0.011%        |
| 26        | 6.988       | 966           | 968         | 969          | rBV2     | 318            | 281           | 0.03%           | 0.004%        |
| 27        | 7.110       | 982           | 988         | 995          | rBV6     | 3352           | 8179          | 0.91%           | 0.126%        |
| 28        | 7.311       | 1012          | 1021        | 1035         | rBV      | 180779         | 395366        | 44.20%          | 6.091%        |
| 29        | 7.427       | 1038          | 1040        | 1042         | rBV      | 279            | 346           | 0.04%           | 0.005%        |
| 30        | 7.470       | 1045          | 1047        | 1048         | rBV      | 449            | 307           | 0.03%           | 0.005%        |
| 31        | 7.549       | 1059          | 1060        | 1063         | rBV2     | 244            | 259           | 0.03%           | 0.004%        |
| 32        | 7.817       | 1099          | 1104        | 1105         | rBV2     | 374            | 550           | 0.06%           | 0.008%        |
| 33        | 7.885       | 1112          | 1115        | 1118         | rBV2     | 192            | 251           | 0.03%           | 0.004%        |
| 34        | 8.061       | 1142          | 1144        | 1146         | rBV2     | 281            | 276           | 0.03%           | 0.004%        |
| 35        | 8.159       | 1157          | 1160        | 1161         | rBV2     | 238            | 243           | 0.03%           | 0.004%        |
| 36        | 8.330       | 1181          | 1188        | 1204         | rVB      | 94501          | 161436        | 18.05%          | 2.487%        |

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 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 GBC13ME

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\SFAMXML122321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 8.476  | 1210 | 1212 | 1213 | rBV  | 248    | 220    | 0.02%  | 0.003%  |
| 38 | 8.586  | 1228 | 1230 | 1232 | rVB2 | 297    | 236    | 0.03%  | 0.004%  |
| 39 | 8.653  | 1234 | 1241 | 1248 | rBV  | 437653 | 714219 | 79.85% | 11.003% |
| 40 | 8.951  | 1284 | 1290 | 1301 | rBV  | 58712  | 98899  | 11.06% | 1.524%  |
| 41 | 9.140  | 1319 | 1321 | 1324 | rBV2 | 267    | 263    | 0.03%  | 0.004%  |
| 42 | 9.171  | 1324 | 1326 | 1327 | rBV  | 395    | 221    | 0.02%  | 0.003%  |
| 43 | 9.281  | 1339 | 1344 | 1349 | rBV2 | 3149   | 5386   | 0.60%  | 0.083%  |
| 44 | 9.348  | 1349 | 1355 | 1357 | rVV4 | 1818   | 3020   | 0.34%  | 0.047%  |
| 45 | 9.415  | 1357 | 1366 | 1380 | rVB  | 174433 | 405801 | 45.37% | 6.252%  |
| 46 | 9.726  | 1413 | 1417 | 1419 | rVV3 | 740    | 1021   | 0.11%  | 0.016%  |
| 47 | 9.860  | 1437 | 1439 | 1443 | rVB  | 312    | 371    | 0.04%  | 0.006%  |
| 48 | 10.006 | 1461 | 1463 | 1465 | rBV2 | 234    | 229    | 0.03%  | 0.004%  |
| 49 | 10.055 | 1465 | 1471 | 1482 | rBV  | 366889 | 550068 | 61.50% | 8.474%  |
| 50 | 10.183 | 1490 | 1492 | 1493 | rBV2 | 464    | 381    | 0.04%  | 0.006%  |
| 51 | 10.244 | 1500 | 1502 | 1504 | rVB2 | 259    | 224    | 0.03%  | 0.003%  |
| 52 | 10.311 | 1507 | 1513 | 1516 | rBV2 | 1652   | 2364   | 0.26%  | 0.036%  |
| 53 | 10.445 | 1533 | 1535 | 1539 | rVB2 | 292    | 314    | 0.04%  | 0.005%  |
| 54 | 10.518 | 1544 | 1547 | 1548 | rBV2 | 310    | 288    | 0.03%  | 0.004%  |
| 55 | 10.616 | 1561 | 1563 | 1566 | rBV2 | 160    | 244    | 0.03%  | 0.004%  |
| 56 | 10.652 | 1566 | 1569 | 1570 | rBV3 | 477    | 433    | 0.05%  | 0.007%  |
| 57 | 10.756 | 1584 | 1586 | 1588 | rVV2 | 270    | 278    | 0.03%  | 0.004%  |
| 58 | 10.872 | 1603 | 1605 | 1606 | rBV  | 283    | 243    | 0.03%  | 0.004%  |
| 59 | 10.908 | 1610 | 1611 | 1615 | rVB2 | 209    | 226    | 0.03%  | 0.003%  |
| 60 | 10.963 | 1615 | 1620 | 1622 | rBV2 | 446    | 605    | 0.07%  | 0.009%  |
| 61 | 11.122 | 1641 | 1646 | 1650 | rBV2 | 3661   | 5081   | 0.57%  | 0.078%  |
| 62 | 11.201 | 1653 | 1659 | 1665 | rBV  | 292040 | 387506 | 43.32% | 5.970%  |
| 63 | 11.323 | 1676 | 1679 | 1686 | rVB4 | 3814   | 6163   | 0.69%  | 0.095%  |
| 64 | 11.451 | 1697 | 1700 | 1702 | rBV3 | 629    | 812    | 0.09%  | 0.013%  |
| 65 | 11.481 | 1702 | 1705 | 1713 | rVB3 | 2225   | 3973   | 0.44%  | 0.061%  |
| 66 | 11.548 | 1713 | 1716 | 1719 | rBB3 | 417    | 558    | 0.06%  | 0.009%  |
| 67 | 11.616 | 1725 | 1727 | 1729 | rBV3 | 262    | 283    | 0.03%  | 0.004%  |
| 68 | 11.756 | 1745 | 1750 | 1754 | rVB3 | 3346   | 4787   | 0.54%  | 0.074%  |
| 69 | 11.847 | 1760 | 1765 | 1770 | rVB3 | 886    | 1368   | 0.15%  | 0.021%  |
| 70 | 11.933 | 1774 | 1779 | 1783 | rBV4 | 2266   | 3315   | 0.37%  | 0.051%  |
| 71 | 11.969 | 1783 | 1785 | 1789 | rBV3 | 629    | 903    | 0.10%  | 0.014%  |
| 72 | 12.024 | 1789 | 1794 | 1800 | rBV  | 424092 | 550762 | 61.57% | 8.485%  |
| 73 | 12.146 | 1812 | 1814 | 1826 | rVB2 | 3607   | 6683   | 0.75%  | 0.103%  |
| 74 | 12.262 | 1830 | 1833 | 1836 | rBV3 | 687    | 877    | 0.10%  | 0.014%  |
| 75 | 12.323 | 1836 | 1843 | 1850 | rBV  | 486902 | 602838 | 67.40% | 9.287%  |
| 76 | 12.426 | 1857 | 1860 | 1864 | rVB3 | 1646   | 2235   | 0.25%  | 0.034%  |

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 Misc : 6.41g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 GBC13ME

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\SFAMXML122321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 12.579 | 1882 | 1885 | 1887 | rBV3 | 727  | 661  | 0.07% | 0.010% |
| 78  | 12.768 | 1912 | 1916 | 1920 | rVB  | 1960 | 2115 | 0.24% | 0.033% |
| 79  | 12.914 | 1938 | 1940 | 1942 | rBV2 | 233  | 250  | 0.03% | 0.004% |
| 80  | 13.048 | 1960 | 1962 | 1966 | rVB4 | 794  | 1061 | 0.12% | 0.016% |
| 81  | 13.402 | 2019 | 2020 | 2025 | rVB2 | 409  | 492  | 0.06% | 0.008% |
| 82  | 13.579 | 2047 | 2049 | 2050 | rBV  | 325  | 271  | 0.03% | 0.004% |
| 83  | 13.621 | 2054 | 2056 | 2059 | rVB2 | 392  | 352  | 0.04% | 0.005% |
| 84  | 14.133 | 2136 | 2140 | 2147 | rVB2 | 2223 | 3086 | 0.35% | 0.048% |
| 85  | 14.225 | 2151 | 2155 | 2159 | rBV3 | 500  | 972  | 0.11% | 0.015% |
| 86  | 14.286 | 2163 | 2165 | 2169 | rBV2 | 335  | 572  | 0.06% | 0.009% |
| 87  | 14.316 | 2169 | 2170 | 2174 | rVB  | 356  | 298  | 0.03% | 0.005% |
| 88  | 14.469 | 2194 | 2195 | 2198 | rBV2 | 562  | 437  | 0.05% | 0.007% |
| 89  | 14.621 | 2218 | 2220 | 2221 | rBV  | 569  | 465  | 0.05% | 0.007% |
| 90  | 14.670 | 2226 | 2228 | 2230 | rVV2 | 399  | 271  | 0.03% | 0.004% |
| 91  | 15.139 | 2303 | 2305 | 2307 | rBV3 | 550  | 424  | 0.05% | 0.007% |
| 92  | 15.164 | 2307 | 2309 | 2311 | rBV3 | 866  | 524  | 0.06% | 0.008% |
| 93  | 15.340 | 2336 | 2338 | 2340 | rVB3 | 672  | 430  | 0.05% | 0.007% |
| 94  | 15.469 | 2357 | 2359 | 2360 | rBV  | 375  | 232  | 0.03% | 0.004% |
| 95  | 15.523 | 2366 | 2368 | 2372 | rVB4 | 541  | 447  | 0.05% | 0.007% |
| 96  | 16.334 | 2499 | 2501 | 2504 | rVB  | 543  | 341  | 0.04% | 0.005% |
| 97  | 16.438 | 2517 | 2518 | 2521 | rBV  | 534  | 553  | 0.06% | 0.009% |
| 98  | 16.688 | 2557 | 2559 | 2561 | rBV2 | 323  | 257  | 0.03% | 0.004% |
| 99  | 16.737 | 2565 | 2567 | 2568 | rBV2 | 500  | 279  | 0.03% | 0.004% |
| 100 | 16.755 | 2568 | 2570 | 2572 | rBV4 | 460  | 470  | 0.05% | 0.007% |

Sum of corrected areas: 6490869

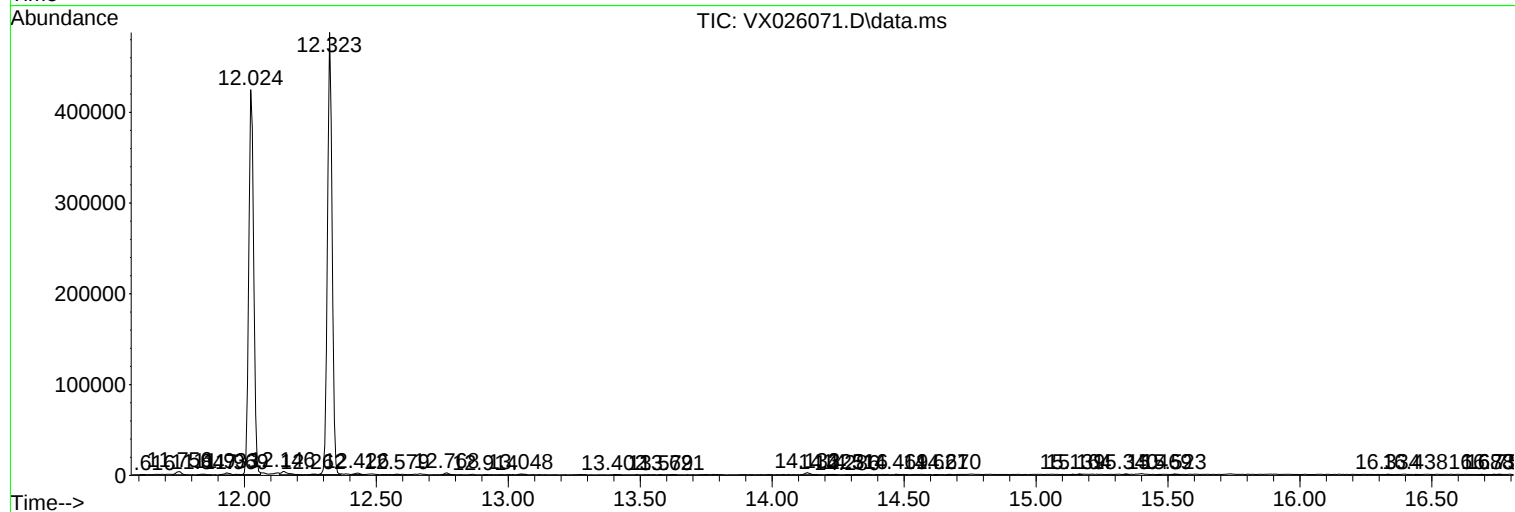
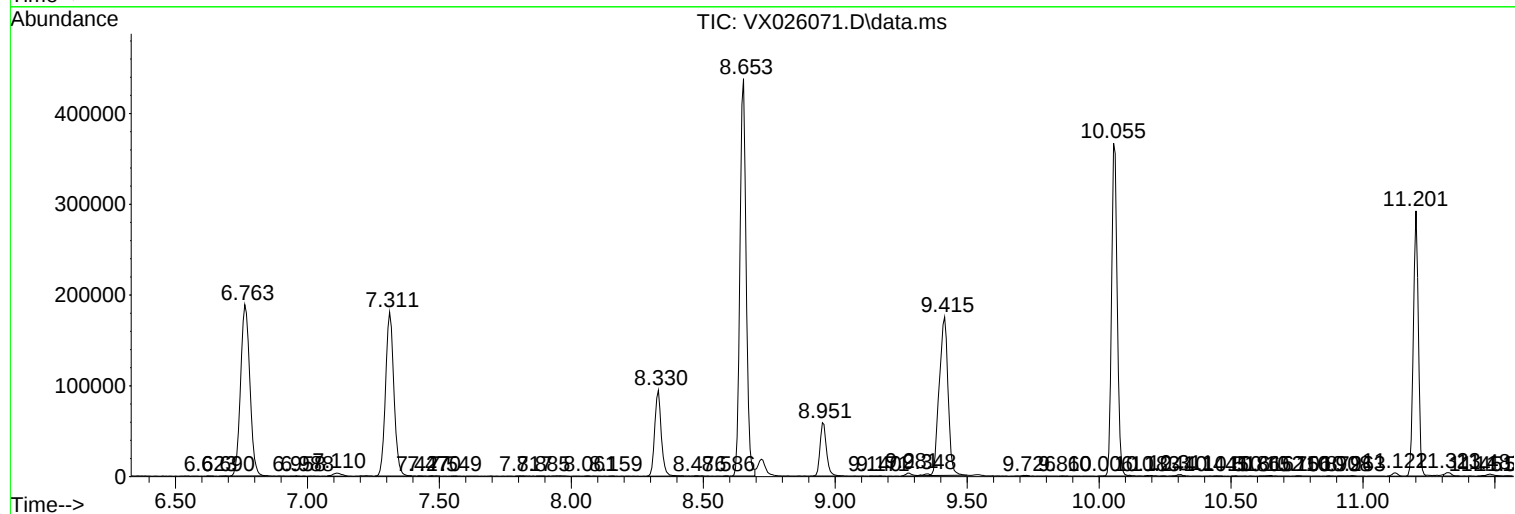
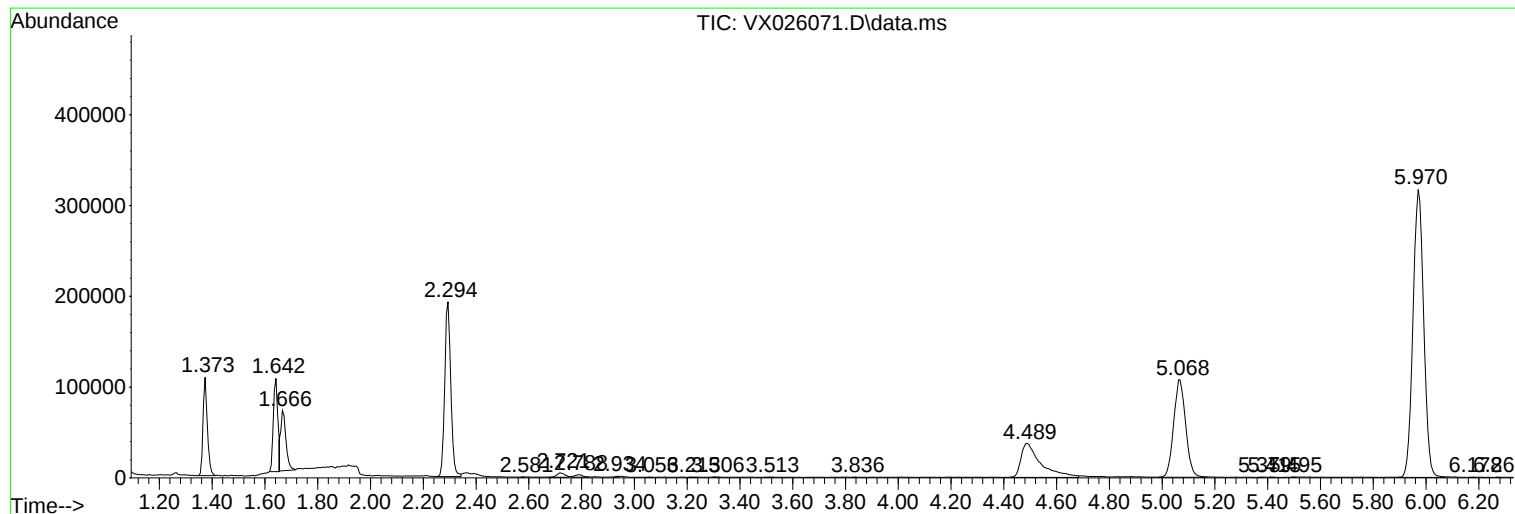
Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122721\  
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ALS Vial : 25 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
GBC13ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122321WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122721\  
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Instrument :  
MSVOA\_X  
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GBC13ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122321WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122321WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |

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