

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
 Data File : VX025669.D  
 Acq On : 09 Dec 2021 19:07  
 Operator : JC/MD  
 Sample : M4975-12ME  
 Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGKT6ME

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: VX025669.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         | 1.368       | 43            | 46          | 54           | rBV      | 74792          | 87159         | 13.32%          | 1.770%        |
| 2         | 1.648       | 88            | 92          | 100          | rBV      | 49491          | 58974         | 9.01%           | 1.198%        |
| 3         | 2.282       | 189           | 196         | 207          | rBV      | 140892         | 240104        | 36.69%          | 4.876%        |
| 4         | 2.587       | 244           | 246         | 250          | rBV      | 287            | 417           | 0.06%           | 0.008%        |
| 5         | 2.630       | 252           | 253         | 254          | rBV      | 461            | 300           | 0.05%           | 0.006%        |
| 6         | 2.697       | 262           | 264         | 265          | rBV      | 403            | 319           | 0.05%           | 0.006%        |
| 7         | 2.947       | 297           | 305         | 311          | rBV2     | 4071           | 10662         | 1.63%           | 0.217%        |
| 8         | 3.715       | 427           | 431         | 433          | rBV      | 280            | 315           | 0.05%           | 0.006%        |
| 9         | 3.788       | 441           | 443         | 445          | rVB      | 314            | 210           | 0.03%           | 0.004%        |
| 10        | 4.142       | 499           | 501         | 505          | rVB2     | 347            | 310           | 0.05%           | 0.006%        |
| 11        | 4.263       | 517           | 521         | 522          | rBV      | 311            | 326           | 0.05%           | 0.007%        |
| 12        | 4.300       | 525           | 527         | 529          | rVB      | 346            | 271           | 0.04%           | 0.006%        |
| 13        | 4.495       | 549           | 559         | 588          | rBV      | 27055          | 122112        | 18.66%          | 2.480%        |
| 14        | 4.763       | 601           | 603         | 604          | rBV      | 313            | 233           | 0.04%           | 0.005%        |
| 15        | 4.806       | 609           | 610         | 612          | rBV      | 310            | 210           | 0.03%           | 0.004%        |
| 16        | 4.946       | 631           | 633         | 634          | rVB      | 330            | 209           | 0.03%           | 0.004%        |
| 17        | 4.977       | 634           | 638         | 639          | rBV      | 292            | 461           | 0.07%           | 0.009%        |
| 18        | 5.068       | 641           | 653         | 671          | rVB      | 76605          | 260000        | 39.73%          | 5.280%        |
| 19        | 5.239       | 680           | 681         | 683          | rBV      | 293            | 197           | 0.03%           | 0.004%        |
| 20        | 5.306       | 689           | 692         | 693          | rBV      | 199            | 210           | 0.03%           | 0.004%        |
| 21        | 5.391       | 705           | 706         | 710          | rBV2     | 269            | 351           | 0.05%           | 0.007%        |
| 22        | 5.513       | 720           | 726         | 727          | rBV      | 442            | 752           | 0.11%           | 0.015%        |
| 23        | 5.629       | 743           | 745         | 748          | rVB      | 254            | 205           | 0.03%           | 0.004%        |
| 24        | 5.702       | 754           | 757         | 761          | rBV2     | 233            | 341           | 0.05%           | 0.007%        |
| 25        | 5.800       | 771           | 773         | 777          | rBV2     | 232            | 337           | 0.05%           | 0.007%        |
| 26        | 5.970       | 789           | 801         | 817          | rBV2     | 225953         | 654358        | 100.00%         | 13.288%       |
| 27        | 6.306       | 853           | 856         | 857          | rBV      | 262            | 214           | 0.03%           | 0.004%        |
| 28        | 6.367       | 860           | 866         | 873          | rBV4     | 1610           | 5205          | 0.80%           | 0.106%        |
| 29        | 6.519       | 889           | 891         | 893          | rBV      | 257            | 213           | 0.03%           | 0.004%        |
| 30        | 6.556       | 895           | 897         | 901          | rVB2     | 453            | 457           | 0.07%           | 0.009%        |
| 31        | 6.592       | 901           | 903         | 904          | rBV      | 357            | 273           | 0.04%           | 0.006%        |
| 32        | 6.659       | 911           | 914         | 917          | rVB      | 351            | 506           | 0.08%           | 0.010%        |
| 33        | 6.690       | 917           | 919         | 920          | rBV2     | 259            | 242           | 0.04%           | 0.005%        |
| 34        | 6.763       | 922           | 931         | 950          | rVV      | 148225         | 386265        | 59.03%          | 7.844%        |
| 35        | 6.915       | 954           | 956         | 958          | rBV      | 359            | 288           | 0.04%           | 0.006%        |
| 36        | 7.104       | 981           | 987         | 1000         | rVB7     | 2361           | 7055          | 1.08%           | 0.143%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
 Data File : VX025669.D  
 Acq On : 09 Dec 2021 19:07  
 Operator : JC/MD  
 Sample : M4975-12ME  
 Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGKT6ME

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.226  | 1000 | 1007 | 1008 | rBV6 | 953    | 1866   | 0.29%  | 0.038%  |
| 38 | 7.312  | 1012 | 1021 | 1036 | rVV  | 123968 | 287629 | 43.96% | 5.841%  |
| 39 | 7.495  | 1049 | 1051 | 1054 | rVB  | 429    | 330    | 0.05%  | 0.007%  |
| 40 | 7.696  | 1083 | 1084 | 1086 | rBV  | 333    | 253    | 0.04%  | 0.005%  |
| 41 | 7.781  | 1097 | 1098 | 1101 | rBV2 | 361    | 369    | 0.06%  | 0.007%  |
| 42 | 7.970  | 1127 | 1129 | 1130 | rBV  | 307    | 203    | 0.03%  | 0.004%  |
| 43 | 8.019  | 1135 | 1137 | 1139 | rBV  | 299    | 280    | 0.04%  | 0.006%  |
| 44 | 8.269  | 1176 | 1178 | 1179 | rVV  | 230    | 194    | 0.03%  | 0.004%  |
| 45 | 8.330  | 1182 | 1188 | 1198 | rVV  | 83814  | 151405 | 23.14% | 3.075%  |
| 46 | 8.653  | 1232 | 1241 | 1249 | rBV  | 327906 | 555170 | 84.84% | 11.274% |
| 47 | 8.958  | 1285 | 1291 | 1300 | rVV  | 54021  | 93382  | 14.27% | 1.896%  |
| 48 | 9.080  | 1309 | 1311 | 1312 | rBV2 | 310    | 246    | 0.04%  | 0.005%  |
| 49 | 9.147  | 1320 | 1322 | 1327 | rVB2 | 254    | 355    | 0.05%  | 0.007%  |
| 50 | 9.275  | 1340 | 1343 | 1348 | rVB3 | 3100   | 4595   | 0.70%  | 0.093%  |
| 51 | 9.403  | 1356 | 1364 | 1379 | rBV  | 158305 | 270476 | 41.33% | 5.493%  |
| 52 | 9.641  | 1401 | 1403 | 1406 | rVB2 | 322    | 322    | 0.05%  | 0.007%  |
| 53 | 9.677  | 1406 | 1409 | 1411 | rBV  | 336    | 478    | 0.07%  | 0.010%  |
| 54 | 9.915  | 1446 | 1448 | 1450 | rBV  | 256    | 240    | 0.04%  | 0.005%  |
| 55 | 9.988  | 1458 | 1460 | 1462 | rVB  | 240    | 198    | 0.03%  | 0.004%  |
| 56 | 10.061 | 1466 | 1472 | 1485 | rVB  | 303611 | 455439 | 69.60% | 9.249%  |
| 57 | 10.244 | 1500 | 1502 | 1503 | rBV  | 379    | 250    | 0.04%  | 0.005%  |
| 58 | 10.305 | 1510 | 1512 | 1516 | rVB2 | 579    | 721    | 0.11%  | 0.015%  |
| 59 | 10.390 | 1524 | 1526 | 1528 | rBV2 | 286    | 237    | 0.04%  | 0.005%  |
| 60 | 10.415 | 1528 | 1530 | 1532 | rBV  | 336    | 305    | 0.05%  | 0.006%  |
| 61 | 10.500 | 1542 | 1544 | 1545 | rBV  | 266    | 211    | 0.03%  | 0.004%  |
| 62 | 10.671 | 1571 | 1572 | 1576 | rVB2 | 312    | 260    | 0.04%  | 0.005%  |
| 63 | 10.750 | 1582 | 1585 | 1587 | rVB2 | 306    | 312    | 0.05%  | 0.006%  |
| 64 | 10.775 | 1587 | 1589 | 1592 | rBV2 | 224    | 312    | 0.05%  | 0.006%  |
| 65 | 10.976 | 1621 | 1622 | 1625 | rBV2 | 308    | 222    | 0.03%  | 0.005%  |
| 66 | 11.012 | 1625 | 1628 | 1630 | rVV2 | 297    | 330    | 0.05%  | 0.007%  |
| 67 | 11.122 | 1642 | 1646 | 1651 | rVB2 | 3053   | 3909   | 0.60%  | 0.079%  |
| 68 | 11.195 | 1653 | 1658 | 1669 | rVB  | 231769 | 299717 | 45.80% | 6.087%  |
| 69 | 11.281 | 1669 | 1672 | 1673 | rBV2 | 478    | 451    | 0.07%  | 0.009%  |
| 70 | 11.451 | 1699 | 1700 | 1701 | rBV  | 418    | 236    | 0.04%  | 0.005%  |
| 71 | 11.622 | 1726 | 1728 | 1730 | rBV2 | 329    | 270    | 0.04%  | 0.005%  |
| 72 | 11.750 | 1746 | 1749 | 1755 | rVB3 | 2400   | 2893   | 0.44%  | 0.059%  |
| 73 | 11.933 | 1776 | 1779 | 1783 | rVB2 | 1269   | 1471   | 0.22%  | 0.030%  |
| 74 | 12.024 | 1789 | 1794 | 1801 | rBV  | 374067 | 454670 | 69.48% | 9.233%  |
| 75 | 12.122 | 1807 | 1810 | 1812 | rBV3 | 945    | 1188   | 0.18%  | 0.024%  |
| 76 | 12.152 | 1812 | 1815 | 1818 | rVB2 | 2163   | 2696   | 0.41%  | 0.055%  |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
 Data File : VX025669.D  
 Acq On : 09 Dec 2021 19:07  
 Operator : JC/MD  
 Sample : M4975-12ME  
 Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGKT6ME

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\SFAMXML112221WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.323 | 1836 | 1843 | 1849 | rBV  | 383519 | 478570 | 73.14% | 9.719% |
| 78  | 12.433 | 1858 | 1861 | 1865 | rVB4 | 924    | 1109   | 0.17%  | 0.023% |
| 79  | 12.561 | 1878 | 1882 | 1884 | rBV2 | 177    | 254    | 0.04%  | 0.005% |
| 80  | 12.634 | 1892 | 1894 | 1896 | rVV2 | 401    | 350    | 0.05%  | 0.007% |
| 81  | 12.664 | 1896 | 1899 | 1903 | rVB2 | 599    | 899    | 0.14%  | 0.018% |
| 82  | 12.756 | 1912 | 1914 | 1920 | rVB3 | 495    | 703    | 0.11%  | 0.014% |
| 83  | 12.957 | 1945 | 1947 | 1951 | rBV2 | 252    | 304    | 0.05%  | 0.006% |
| 84  | 13.048 | 1960 | 1962 | 1968 | rVB3 | 533    | 775    | 0.12%  | 0.016% |
| 85  | 13.329 | 2004 | 2008 | 2009 | rVB  | 374    | 393    | 0.06%  | 0.008% |
| 86  | 13.445 | 2026 | 2027 | 2030 | rBV2 | 211    | 227    | 0.03%  | 0.005% |
| 87  | 13.548 | 2042 | 2044 | 2047 | rBV2 | 426    | 390    | 0.06%  | 0.008% |
| 88  | 13.603 | 2051 | 2053 | 2055 | rBV  | 265    | 289    | 0.04%  | 0.006% |
| 89  | 13.743 | 2074 | 2076 | 2078 | rBV  | 396    | 319    | 0.05%  | 0.006% |
| 90  | 13.780 | 2078 | 2082 | 2084 | rBV  | 665    | 816    | 0.12%  | 0.017% |
| 91  | 13.847 | 2091 | 2093 | 2095 | rBV2 | 300    | 389    | 0.06%  | 0.008% |
| 92  | 13.908 | 2100 | 2103 | 2104 | rBV  | 372    | 430    | 0.07%  | 0.009% |
| 93  | 14.128 | 2135 | 2139 | 2144 | rBV2 | 1236   | 2079   | 0.32%  | 0.042% |
| 94  | 14.615 | 2217 | 2219 | 2220 | rBV2 | 262    | 198    | 0.03%  | 0.004% |
| 95  | 14.743 | 2238 | 2240 | 2241 | rBV  | 317    | 224    | 0.03%  | 0.005% |
| 96  | 15.603 | 2379 | 2381 | 2383 | rVB2 | 411    | 323    | 0.05%  | 0.007% |
| 97  | 15.713 | 2397 | 2399 | 2400 | rBV  | 489    | 356    | 0.05%  | 0.007% |
| 98  | 16.072 | 2456 | 2458 | 2459 | rBV2 | 291    | 202    | 0.03%  | 0.004% |
| 99  | 16.603 | 2543 | 2545 | 2546 | rBV2 | 280    | 219    | 0.03%  | 0.004% |
| 100 | 16.767 | 2570 | 2572 | 2573 | rBV  | 332    | 303    | 0.05%  | 0.006% |

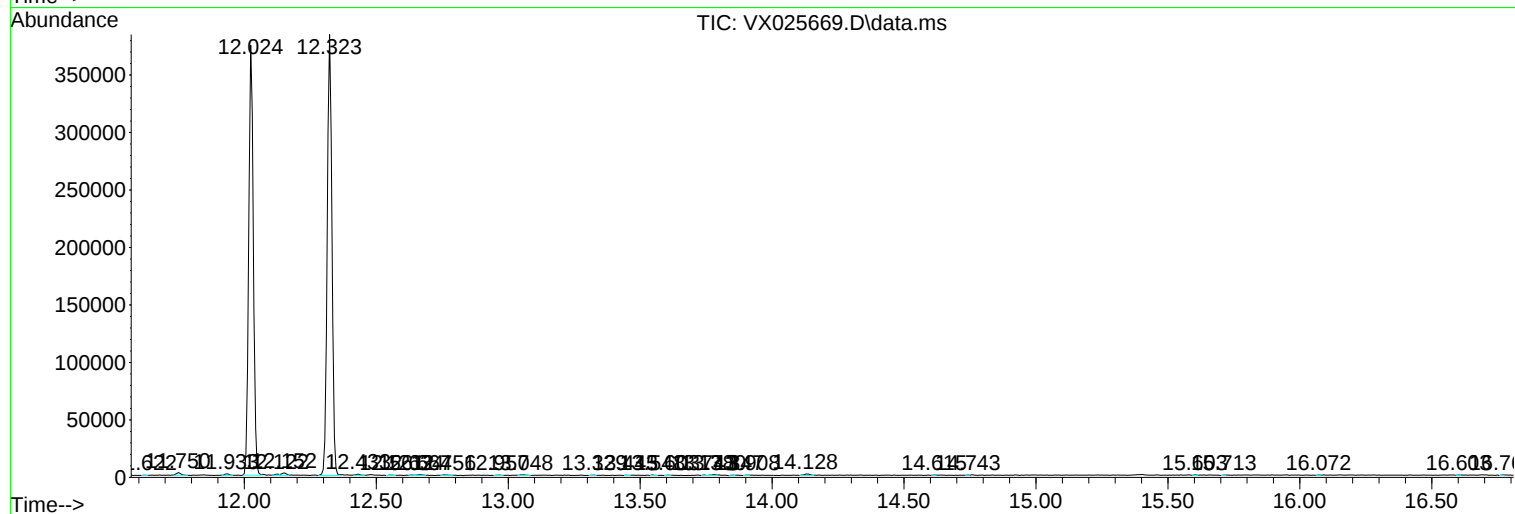
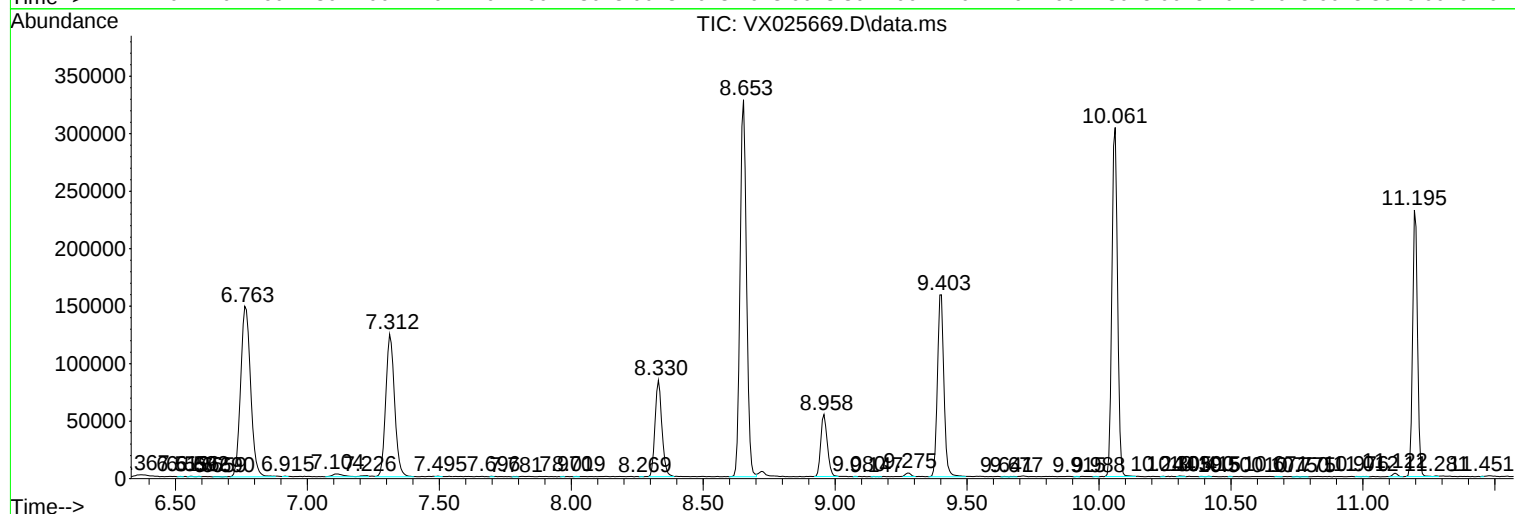
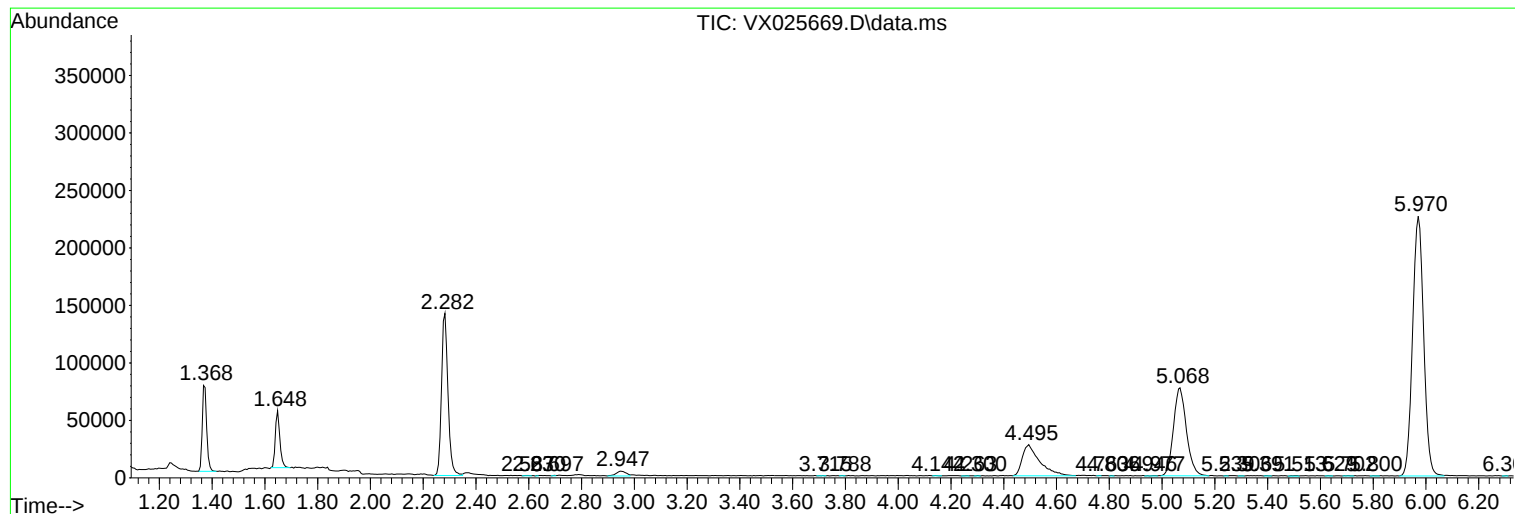
Sum of corrected areas: 4924273

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
Data File : VX025669.D  
Acq On : 09 Dec 2021 19:07  
Operator : JC/MD  
Sample : M4975-12ME  
Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
BGKT6ME

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

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
Data File : VX025669.D  
Acq On : 09 Dec 2021 19:07  
Operator : JC/MD  
Sample : M4975-12ME  
Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
BGKT6ME

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

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120921\  
Data File : VX025669.D  
Acq On : 09 Dec 2021 19:07  
Operator : JC/MD  
Sample : M4975-12ME  
Misc : 5.53g/5mL/100uL/5.0mL/MSVOA\_X/MEOH  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
BGKT6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.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 |