

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV111323\  
 Data File : VV032928.D  
 Acq On : 13 Nov 2023 13:32  
 Operator : SY/MD  
 Sample : VV1113MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK218

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\_V\Method\SFAMVLM111323WMA.M

Title : VOC Analysis

Signal : TIC: VV032928.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         | 1.281       | 69            | 75          | 85           | rVB      | 198441         | 203162        | 16.90%          | 2.033%        |
| 2         | 1.532       | 147           | 153         | 172          | rVB      | 163813         | 203392        | 16.92%          | 2.035%        |
| 3         | 2.059       | 309           | 317         | 336          | rVB      | 328917         | 480867        | 40.00%          | 4.812%        |
| 4         | 2.442       | 433           | 436         | 437          | rBV3     | 2580           | 1669          | 0.14%           | 0.017%        |
| 5         | 2.503       | 451           | 455         | 456          | rBV4     | 2015           | 1418          | 0.12%           | 0.014%        |
| 6         | 2.613       | 487           | 489         | 490          | rBV2     | 1254           | 648           | 0.05%           | 0.006%        |
| 7         | 2.629       | 492           | 494         | 498          | rVB5     | 2058           | 1376          | 0.11%           | 0.014%        |
| 8         | 2.799       | 541           | 547         | 548          | rBV5     | 1572           | 1071          | 0.09%           | 0.011%        |
| 9         | 2.941       | 590           | 591         | 596          | rVB4     | 1686           | 1285          | 0.11%           | 0.013%        |
| 10        | 2.966       | 596           | 599         | 601          | rBV4     | 1111           | 768           | 0.06%           | 0.008%        |
| 11        | 2.989       | 604           | 606         | 608          | rBV3     | 945            | 448           | 0.04%           | 0.004%        |
| 12        | 3.088       | 635           | 637         | 642          | rVB5     | 1824           | 980           | 0.08%           | 0.010%        |
| 13        | 3.130       | 647           | 650         | 653          | rBV5     | 1673           | 1231          | 0.10%           | 0.012%        |
| 14        | 3.175       | 661           | 664         | 665          | rBV3     | 1111           | 729           | 0.06%           | 0.007%        |
| 15        | 3.207       | 672           | 674         | 678          | rBV4     | 1187           | 1007          | 0.08%           | 0.010%        |
| 16        | 3.278       | 693           | 696         | 697          | rBV3     | 1117           | 386           | 0.03%           | 0.004%        |
| 17        | 3.288       | 697           | 699         | 700          | rVV2     | 570            | 184           | 0.02%           | 0.002%        |
| 18        | 3.323       | 708           | 710         | 712          | rBV3     | 2247           | 991           | 0.08%           | 0.010%        |
| 19        | 3.368       | 720           | 724         | 726          | rBV5     | 1633           | 1575          | 0.13%           | 0.016%        |
| 20        | 3.513       | 764           | 769         | 772          | rBV7     | 1394           | 1149          | 0.10%           | 0.011%        |
| 21        | 3.571       | 784           | 787         | 789          | rBV4     | 1499           | 844           | 0.07%           | 0.008%        |
| 22        | 3.613       | 798           | 800         | 803          | rBV4     | 1034           | 599           | 0.05%           | 0.006%        |
| 23        | 3.641       | 807           | 809         | 819          | rVB10    | 1837           | 2274          | 0.19%           | 0.023%        |
| 24        | 3.680       | 819           | 821         | 823          | rBV3     | 1403           | 708           | 0.06%           | 0.007%        |
| 25        | 3.709       | 827           | 830         | 832          | rBV3     | 1873           | 965           | 0.08%           | 0.010%        |
| 26        | 3.719       | 832           | 833         | 838          | rVB5     | 1767           | 1176          | 0.10%           | 0.012%        |
| 27        | 3.744       | 838           | 841         | 842          | rBV3     | 1374           | 594           | 0.05%           | 0.006%        |
| 28        | 3.786       | 842           | 854         | 877          | rBV      | 63792          | 178523        | 14.85%          | 1.787%        |
| 29        | 4.124       | 956           | 959         | 962          | rBV5     | 1013           | 788           | 0.07%           | 0.008%        |
| 30        | 4.249       | 985           | 998         | 1021         | rBV      | 194019         | 485472        | 40.38%          | 4.858%        |
| 31        | 4.625       | 1112          | 1115        | 1119         | rVB6     | 2862           | 1620          | 0.13%           | 0.016%        |
| 32        | 4.751       | 1152          | 1154        | 1157         | rVV4     | 2008           | 1214          | 0.10%           | 0.012%        |
| 33        | 4.773       | 1157          | 1161        | 1165         | rVB5     | 2076           | 1977          | 0.16%           | 0.020%        |
| 34        | 4.825       | 1173          | 1177        | 1181         | rVB5     | 1340           | 927           | 0.08%           | 0.009%        |
| 35        | 4.847       | 1181          | 1184        | 1185         | rBV3     | 1344           | 665           | 0.06%           | 0.007%        |
| 36        | 4.957       | 1203          | 1218        | 1242         | rBV2     | 456044         | 1202294       | 100.00%         | 12.032%       |

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Instrument :  
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 ClientSampleId :  
 VBLK218

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\_V\Method\SFAMVLM111323WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 5.535  | 1383 | 1398 | 1430 | rBV  | 450364 | 938055  | 78.02% | 9.387%  |
| 38 | 5.989  | 1526 | 1539 | 1563 | rBV  | 261652 | 546782  | 45.48% | 5.472%  |
| 39 | 6.339  | 1645 | 1648 | 1651 | rBV5 | 1603   | 1236    | 0.10%  | 0.012%  |
| 40 | 6.407  | 1667 | 1669 | 1670 | rBV2 | 1417   | 580     | 0.05%  | 0.006%  |
| 41 | 6.535  | 1707 | 1709 | 1711 | rBV3 | 1916   | 819     | 0.07%  | 0.008%  |
| 42 | 6.780  | 1782 | 1785 | 1791 | rVB7 | 2266   | 2170    | 0.18%  | 0.022%  |
| 43 | 6.809  | 1791 | 1794 | 1795 | rBV3 | 1595   | 837     | 0.07%  | 0.008%  |
| 44 | 6.915  | 1816 | 1827 | 1842 | rBV  | 146122 | 265617  | 22.09% | 2.658%  |
| 45 | 7.243  | 1916 | 1929 | 1955 | rBV  | 549018 | 987991  | 82.18% | 9.887%  |
| 46 | 7.516  | 2012 | 2014 | 2016 | rVB3 | 2284   | 963     | 0.08%  | 0.010%  |
| 47 | 7.554  | 2017 | 2026 | 2045 | rBV  | 104287 | 188815  | 15.70% | 1.889%  |
| 48 | 7.870  | 2122 | 2124 | 2127 | rBV3 | 1739   | 964     | 0.08%  | 0.010%  |
| 49 | 8.024  | 2164 | 2172 | 2200 | rBV  | 228928 | 409940  | 34.10% | 4.102%  |
| 50 | 8.519  | 2322 | 2326 | 2330 | rBV7 | 1521   | 1512    | 0.13%  | 0.015%  |
| 51 | 8.535  | 2330 | 2331 | 2334 | rBV3 | 1297   | 762     | 0.06%  | 0.008%  |
| 52 | 8.786  | 2399 | 2409 | 2436 | rBV  | 719579 | 1174478 | 97.69% | 11.753% |
| 53 | 9.143  | 2518 | 2520 | 2523 | rBV3 | 1325   | 1019    | 0.08%  | 0.010%  |
| 54 | 9.233  | 2547 | 2548 | 2550 | rBV2 | 1035   | 428     | 0.04%  | 0.004%  |
| 55 | 9.429  | 2606 | 2609 | 2610 | rBV3 | 1561   | 990     | 0.08%  | 0.010%  |
| 56 | 9.702  | 2692 | 2694 | 2696 | rBV3 | 1326   | 484     | 0.04%  | 0.005%  |
| 57 | 9.741  | 2704 | 2706 | 2709 | rBV4 | 1607   | 1182    | 0.10%  | 0.012%  |
| 58 | 10.021 | 2791 | 2793 | 2794 | rBV  | 851    | 436     | 0.04%  | 0.004%  |
| 59 | 10.091 | 2809 | 2815 | 2818 | rBV6 | 1567   | 1745    | 0.15%  | 0.017%  |
| 60 | 10.152 | 2824 | 2834 | 2854 | rBV  | 352919 | 561441  | 46.70% | 5.618%  |
| 61 | 10.323 | 2882 | 2887 | 2889 | rBV6 | 1296   | 1166    | 0.10%  | 0.012%  |
| 62 | 10.406 | 2911 | 2913 | 2916 | rBV4 | 1070   | 458     | 0.04%  | 0.005%  |
| 63 | 10.477 | 2932 | 2935 | 2944 | rBV4 | 3051   | 3746    | 0.31%  | 0.037%  |
| 64 | 10.619 | 2977 | 2979 | 2982 | rBV3 | 1330   | 858     | 0.07%  | 0.009%  |
| 65 | 10.657 | 2989 | 2991 | 2992 | rBV2 | 994    | 335     | 0.03%  | 0.003%  |
| 66 | 10.722 | 3009 | 3011 | 3012 | rBV2 | 1241   | 599     | 0.05%  | 0.006%  |
| 67 | 10.837 | 3044 | 3047 | 3049 | rBV3 | 1377   | 855     | 0.07%  | 0.009%  |
| 68 | 10.969 | 3085 | 3088 | 3089 | rBV3 | 1199   | 724     | 0.06%  | 0.007%  |
| 69 | 11.040 | 3108 | 3110 | 3111 | rBV2 | 740    | 304     | 0.03%  | 0.003%  |
| 70 | 11.053 | 3112 | 3114 | 3115 | rVB2 | 1202   | 331     | 0.03%  | 0.003%  |
| 71 | 11.085 | 3120 | 3124 | 3126 | rBV5 | 1557   | 1365    | 0.11%  | 0.014%  |
| 72 | 11.185 | 3145 | 3155 | 3175 | rBV  | 743152 | 1163791 | 96.80% | 11.646% |
| 73 | 11.561 | 3261 | 3272 | 3294 | rBV  | 584862 | 933868  | 77.67% | 9.345%  |
| 74 | 12.088 | 3435 | 3436 | 3437 | rBV  | 1060   | 279     | 0.02%  | 0.003%  |
| 75 | 12.101 | 3438 | 3440 | 3442 | rVV3 | 1441   | 561     | 0.05%  | 0.006%  |
| 76 | 12.172 | 3458 | 3462 | 3463 | rBV3 | 1655   | 1114    | 0.09%  | 0.011%  |

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ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
VBLK218

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM111323WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 77 | 12.432 | 3541 | 3543 | 3545 | rBV3 | 1529 | 730  | 0.06% | 0.007% |
| 78 | 12.635 | 3603 | 3606 | 3609 | rBV5 | 2295 | 1379 | 0.11% | 0.014% |
| 79 | 12.702 | 3624 | 3627 | 3628 | rBV3 | 1049 | 603  | 0.05% | 0.006% |
| 80 | 12.908 | 3688 | 3691 | 3693 | rBV4 | 1751 | 1145 | 0.10% | 0.011% |
| 81 | 12.950 | 3701 | 3704 | 3705 | rBV3 | 1678 | 1054 | 0.09% | 0.011% |
| 82 | 13.037 | 3729 | 3731 | 3733 | rBV3 | 1110 | 733  | 0.06% | 0.007% |
| 83 | 13.863 | 3986 | 3988 | 3989 | rBV2 | 1444 | 475  | 0.04% | 0.005% |
| 84 | 14.339 | 4134 | 4136 | 4137 | rBV2 | 1602 | 591  | 0.05% | 0.006% |
| 85 | 14.680 | 4239 | 4242 | 4245 | rBV5 | 1931 | 1584 | 0.13% | 0.016% |

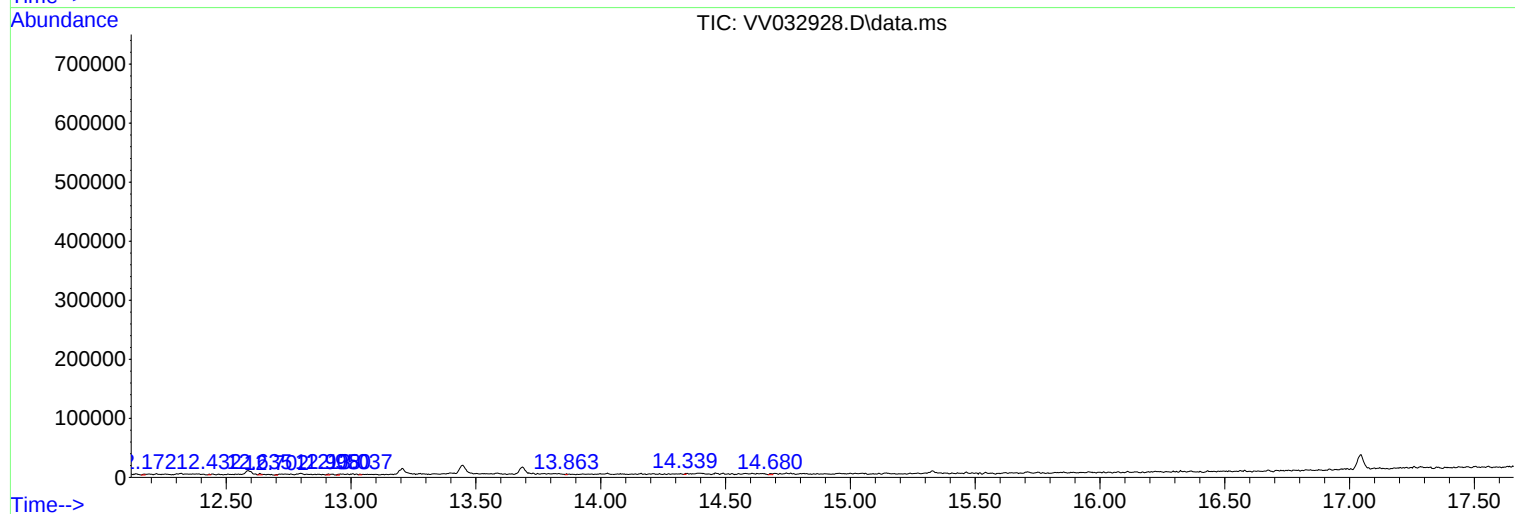
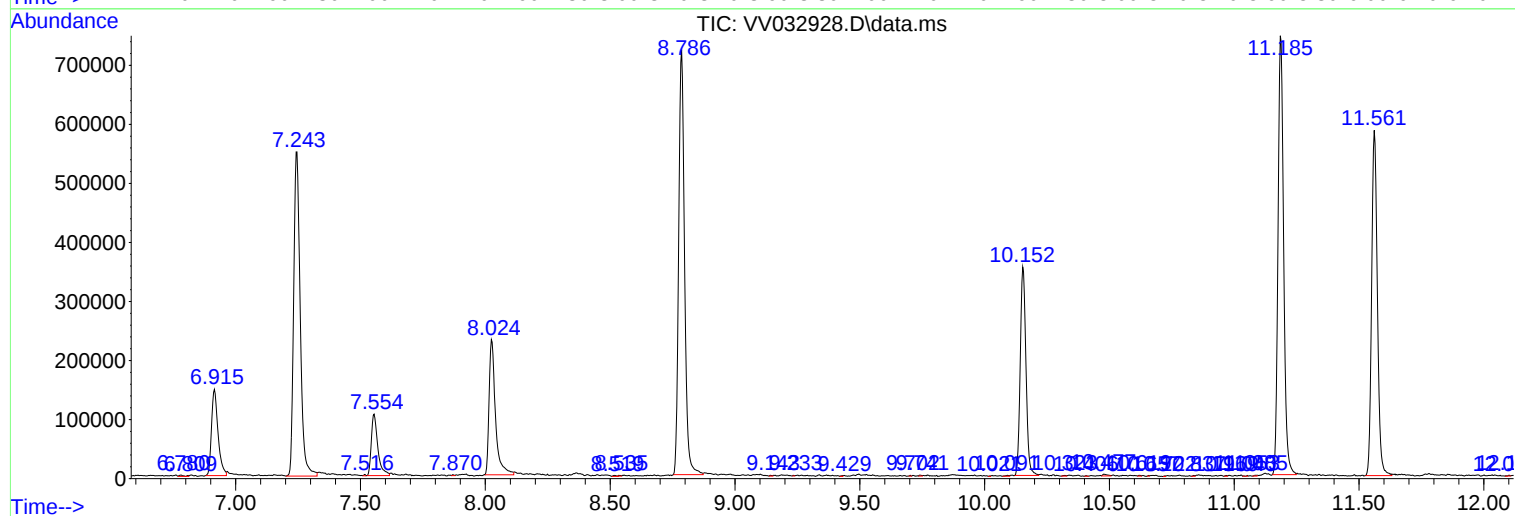
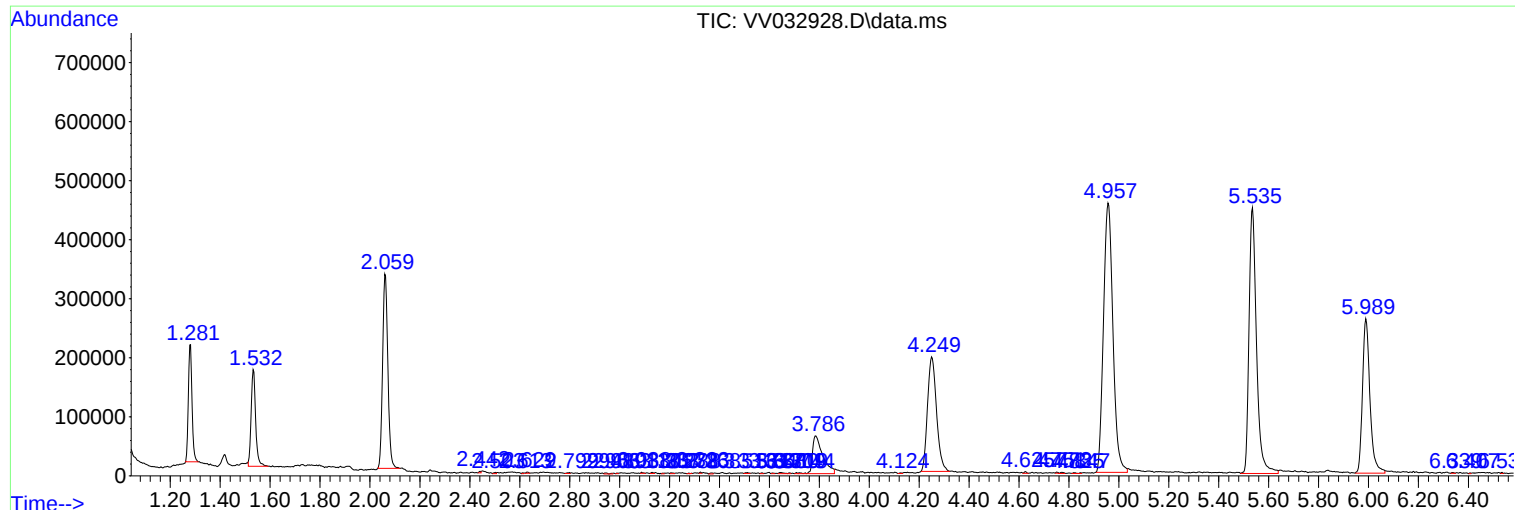
Sum of corrected areas: 9992870

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ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
VBLK218

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM111323WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV111323\  
Data File : VV032928.D  
Acq On : 13 Nov 2023 13:32  
Operator : SY/MD  
Sample : VV1113MBL01  
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
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Instrument :  
MSVOA\_V  
ClientSampleId :  
VBLK218

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM111323WMA.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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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV111323\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM111323WMA.M  
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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 |