

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050923\  
 Data File : VU054115.D  
 Acq On : 09 May 2023 10:29  
 Operator : JC/MD  
 Sample : VU0509MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK094

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\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

Signal : TIC: VU054115.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         | 1.597       | 73            | 80          | 99           | rVB      | 103012         | 128659        | 14.77%          | 2.011%        |
| 2         | 1.903       | 168           | 175         | 198          | rVB      | 75591          | 109692        | 12.59%          | 1.715%        |
| 3         | 2.562       | 368           | 380         | 398          | rBV      | 185594         | 304320        | 34.94%          | 4.758%        |
| 4         | 2.784       | 443           | 449         | 452          | rBV2     | 902            | 1085          | 0.12%           | 0.017%        |
| 5         | 2.948       | 497           | 500         | 503          | rBV3     | 362            | 271           | 0.03%           | 0.004%        |
| 6         | 3.041       | 517           | 529         | 543          | rBV      | 8792           | 16787         | 1.93%           | 0.262%        |
| 7         | 3.102       | 546           | 548         | 549          | rBV      | 278            | 79            | 0.01%           | 0.001%        |
| 8         | 3.182       | 561           | 573         | 584          | rBV3     | 2814           | 6592          | 0.76%           | 0.103%        |
| 9         | 3.356       | 619           | 627         | 637          | rVV4     | 1687           | 2601          | 0.30%           | 0.041%        |
| 10        | 3.407       | 641           | 643         | 649          | rVB      | 279            | 154           | 0.02%           | 0.002%        |
| 11        | 3.610       | 704           | 706         | 709          | rVB      | 214            | 92            | 0.01%           | 0.001%        |
| 12        | 3.661       | 719           | 722         | 724          | rVB      | 265            | 146           | 0.02%           | 0.002%        |
| 13        | 3.780       | 758           | 759         | 761          | rVB      | 248            | 89            | 0.01%           | 0.001%        |
| 14        | 3.793       | 761           | 763         | 769          | rBV2     | 165            | 123           | 0.01%           | 0.002%        |
| 15        | 3.861       | 778           | 784         | 787          | rBV2     | 440            | 555           | 0.06%           | 0.009%        |
| 16        | 3.951       | 809           | 812         | 819          | rBV2     | 260            | 251           | 0.03%           | 0.004%        |
| 17        | 3.983       | 819           | 822         | 827          | rVV      | 159            | 107           | 0.01%           | 0.002%        |
| 18        | 4.018       | 830           | 833         | 835          | rBV2     | 263            | 179           | 0.02%           | 0.003%        |
| 19        | 4.147       | 870           | 873         | 875          | rBV      | 198            | 137           | 0.02%           | 0.002%        |
| 20        | 4.189       | 884           | 886         | 890          | rVB      | 154            | 57            | 0.01%           | 0.001%        |
| 21        | 4.237       | 899           | 901         | 903          | rBV      | 149            | 88            | 0.01%           | 0.001%        |
| 22        | 4.276       | 910           | 913         | 914          | rBV      | 165            | 87            | 0.01%           | 0.001%        |
| 23        | 4.340       | 930           | 933         | 935          | rBV      | 162            | 135           | 0.02%           | 0.002%        |
| 24        | 4.423       | 956           | 959         | 961          | rBV      | 238            | 130           | 0.01%           | 0.002%        |
| 25        | 4.459       | 967           | 970         | 974          | rVB      | 292            | 182           | 0.02%           | 0.003%        |
| 26        | 4.478       | 974           | 976         | 980          | rVB      | 160            | 71            | 0.01%           | 0.001%        |
| 27        | 4.523       | 989           | 990         | 991          | rBV      | 224            | 71            | 0.01%           | 0.001%        |
| 28        | 4.620       | 1009          | 1020        | 1051         | rBV      | 64632          | 169737        | 19.49%          | 2.654%        |
| 29        | 4.935       | 1114          | 1118        | 1119         | rBV      | 192            | 123           | 0.01%           | 0.002%        |
| 30        | 4.967       | 1121          | 1128        | 1130         | rBV4     | 468            | 551           | 0.06%           | 0.009%        |
| 31        | 5.057       | 1140          | 1156        | 1176         | rBV      | 156733         | 350320        | 40.22%          | 5.477%        |
| 32        | 5.263       | 1219          | 1220        | 1223         | rBV      | 234            | 154           | 0.02%           | 0.002%        |
| 33        | 5.288       | 1226          | 1228        | 1231         | rBV2     | 219            | 154           | 0.02%           | 0.002%        |
| 34        | 5.301       | 1231          | 1232        | 1233         | rBV2     | 403            | 125           | 0.01%           | 0.002%        |
| 35        | 5.375       | 1250          | 1255        | 1257         | rBV      | 545            | 443           | 0.05%           | 0.007%        |
| 36        | 5.465       | 1277          | 1283        | 1284         | rBV2     | 296            | 261           | 0.03%           | 0.004%        |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
 VBLK094

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\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |         |         |
|----|-------|------|------|------|------|--------|--------|---------|---------|
| 37 | 5.507 | 1293 | 1296 | 1297 | rBV  | 415    | 224    | 0.03%   | 0.004%  |
| 38 | 5.719 | 1339 | 1362 | 1390 | rBV2 | 314996 | 870987 | 100.00% | 13.617% |
| 39 | 6.009 | 1444 | 1452 | 1456 | rBV  | 359    | 616    | 0.07%   | 0.010%  |
| 40 | 6.054 | 1463 | 1466 | 1470 | rVB  | 383    | 314    | 0.04%   | 0.005%  |
| 41 | 6.076 | 1470 | 1473 | 1475 | rBV  | 260    | 212    | 0.02%   | 0.003%  |
| 42 | 6.108 | 1479 | 1483 | 1486 | rVB2 | 286    | 242    | 0.03%   | 0.004%  |
| 43 | 6.189 | 1506 | 1508 | 1510 | rBV2 | 151    | 69     | 0.01%   | 0.001%  |
| 44 | 6.243 | 1511 | 1525 | 1555 | rBV  | 265788 | 512213 | 58.81%  | 8.008%  |
| 45 | 6.481 | 1597 | 1599 | 1604 | rBV2 | 189    | 104    | 0.01%   | 0.002%  |
| 46 | 6.529 | 1604 | 1614 | 1626 | rVB7 | 4172   | 8644   | 0.99%   | 0.135%  |
| 47 | 6.578 | 1627 | 1629 | 1631 | rBV2 | 156    | 86     | 0.01%   | 0.001%  |
| 48 | 6.684 | 1649 | 1662 | 1680 | rBV  | 199968 | 389709 | 44.74%  | 6.093%  |
| 49 | 6.828 | 1706 | 1707 | 1708 | rBV  | 245    | 69     | 0.01%   | 0.001%  |
| 50 | 6.877 | 1720 | 1722 | 1723 | rBV  | 290    | 139    | 0.02%   | 0.002%  |
| 51 | 6.960 | 1744 | 1748 | 1752 | rBV  | 347    | 462    | 0.05%   | 0.007%  |
| 52 | 7.012 | 1761 | 1764 | 1766 | rBV  | 202    | 110    | 0.01%   | 0.002%  |
| 53 | 7.025 | 1766 | 1768 | 1770 | rVV  | 169    | 72     | 0.01%   | 0.001%  |
| 54 | 7.092 | 1787 | 1789 | 1791 | rBV2 | 433    | 268    | 0.03%   | 0.004%  |
| 55 | 7.185 | 1815 | 1818 | 1819 | rBV  | 445    | 273    | 0.03%   | 0.004%  |
| 56 | 7.288 | 1848 | 1850 | 1851 | rBV  | 142    | 64     | 0.01%   | 0.001%  |
| 57 | 7.317 | 1857 | 1859 | 1862 | rBV  | 133    | 95     | 0.01%   | 0.001%  |
| 58 | 7.462 | 1902 | 1904 | 1906 | rBV2 | 220    | 128    | 0.01%   | 0.002%  |
| 59 | 7.558 | 1922 | 1934 | 1960 | rBV  | 102025 | 185174 | 21.26%  | 2.895%  |
| 60 | 7.793 | 2000 | 2007 | 2013 | rBV5 | 1775   | 2562   | 0.29%   | 0.040%  |
| 61 | 7.893 | 2024 | 2038 | 2058 | rBV  | 389385 | 673781 | 77.36%  | 10.534% |
| 62 | 8.127 | 2108 | 2111 | 2113 | rBV  | 166    | 96     | 0.01%   | 0.002%  |
| 63 | 8.172 | 2113 | 2125 | 2147 | rBV  | 74915  | 128763 | 14.78%  | 2.013%  |
| 64 | 8.475 | 2217 | 2219 | 2221 | rBV2 | 170    | 115    | 0.01%   | 0.002%  |
| 65 | 8.549 | 2236 | 2242 | 2253 | rVB4 | 1867   | 2220   | 0.25%   | 0.035%  |
| 66 | 8.629 | 2256 | 2267 | 2297 | rBV2 | 187970 | 361549 | 41.51%  | 5.652%  |
| 67 | 8.841 | 2330 | 2333 | 2335 | rBV2 | 321    | 174    | 0.02%   | 0.003%  |
| 68 | 8.915 | 2351 | 2356 | 2364 | rBV2 | 555    | 1022   | 0.12%   | 0.016%  |
| 69 | 9.021 | 2385 | 2389 | 2393 | rBV2 | 254    | 245    | 0.03%   | 0.004%  |
| 70 | 9.041 | 2393 | 2395 | 2398 | rBV  | 209    | 105    | 0.01%   | 0.002%  |
| 71 | 9.060 | 2398 | 2401 | 2406 | rBV  | 162    | 161    | 0.02%   | 0.003%  |
| 72 | 9.150 | 2426 | 2429 | 2432 | rBV  | 256    | 189    | 0.02%   | 0.003%  |
| 73 | 9.240 | 2453 | 2457 | 2459 | rBV  | 272    | 246    | 0.03%   | 0.004%  |
| 74 | 9.410 | 2498 | 2510 | 2534 | rBV  | 351020 | 593613 | 68.15%  | 9.281%  |
| 75 | 9.652 | 2583 | 2585 | 2587 | rBV  | 163    | 73     | 0.01%   | 0.001%  |
| 76 | 9.838 | 2641 | 2643 | 2646 | rBV  | 149    | 64     | 0.01%   | 0.001%  |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK094

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_U\Method\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 77 | 9.963  | 2677 | 2682 | 2687 | rBV  | 311    | 363    | 0.04%  | 0.006% |
| 78 | 10.105 | 2716 | 2726 | 2740 | rVB6 | 2384   | 5436   | 0.62%  | 0.085% |
| 79 | 10.160 | 2740 | 2743 | 2745 | rBV  | 199    | 113    | 0.01%  | 0.002% |
| 80 | 10.214 | 2757 | 2760 | 2761 | rBV  | 173    | 72     | 0.01%  | 0.001% |
| 81 | 10.639 | 2890 | 2892 | 2899 | rVB3 | 421    | 318    | 0.04%  | 0.005% |
| 82 | 10.751 | 2914 | 2927 | 2942 | rBV  | 257961 | 417203 | 47.90% | 6.523% |
| 83 | 11.082 | 3023 | 3030 | 3040 | rBV4 | 1544   | 2390   | 0.27%  | 0.037% |
| 84 | 11.468 | 3141 | 3150 | 3158 | rBV2 | 2150   | 3262   | 0.37%  | 0.051% |
| 85 | 11.745 | 3228 | 3236 | 3243 | rBV4 | 2940   | 4176   | 0.48%  | 0.065% |
| 86 | 11.806 | 3244 | 3255 | 3272 | rBV  | 333960 | 530182 | 60.87% | 8.289% |
| 87 | 12.012 | 3317 | 3319 | 3323 | rBV2 | 213    | 159    | 0.02%  | 0.002% |
| 88 | 12.188 | 3361 | 3374 | 3395 | rBV  | 342463 | 562394 | 64.57% | 8.793% |
| 89 | 13.221 | 3688 | 3695 | 3709 | rBV6 | 2964   | 5088   | 0.58%  | 0.080% |
| 90 | 13.442 | 3762 | 3764 | 3765 | rBV6 | 263    | 94     | 0.01%  | 0.001% |
| 91 | 13.735 | 3853 | 3855 | 3856 | rBV6 | 243    | 100    | 0.01%  | 0.002% |
| 92 | 13.767 | 3861 | 3865 | 3868 | rBV3 | 499    | 408    | 0.05%  | 0.006% |
| 93 | 13.841 | 3880 | 3888 | 3899 | rVB3 | 5774   | 9235   | 1.06%  | 0.144% |
| 94 | 14.089 | 3957 | 3965 | 3982 | rVB  | 9254   | 15285  | 1.75%  | 0.239% |
| 95 | 14.330 | 4032 | 4040 | 4051 | rBV4 | 6559   | 10134  | 1.16%  | 0.158% |

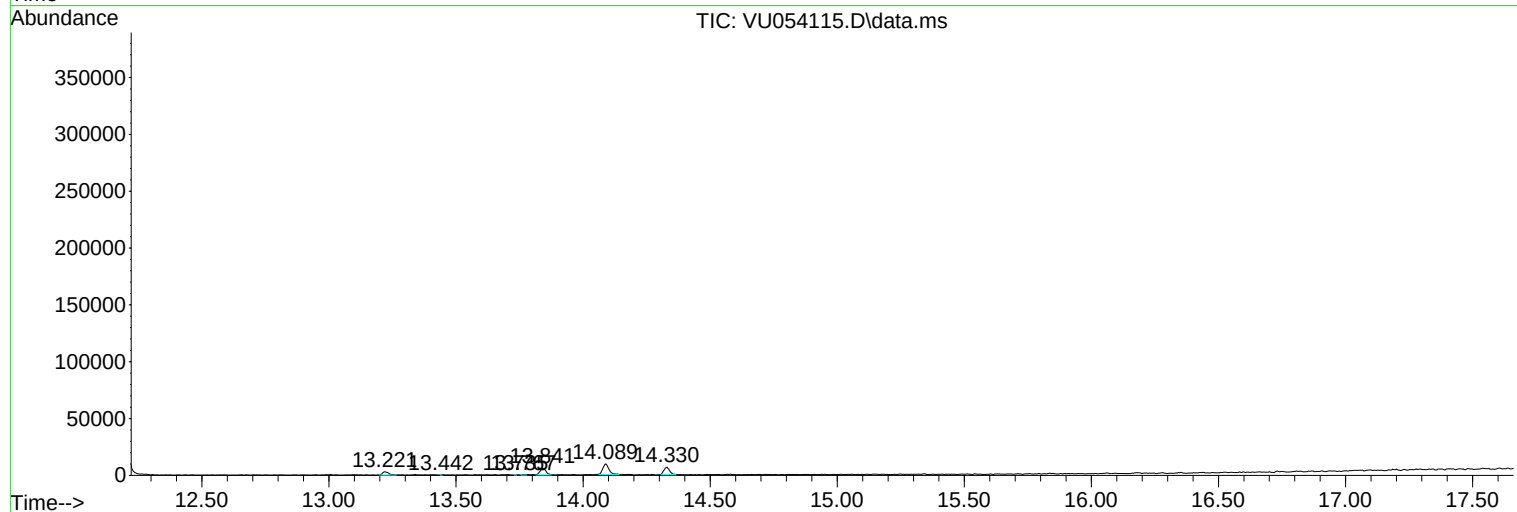
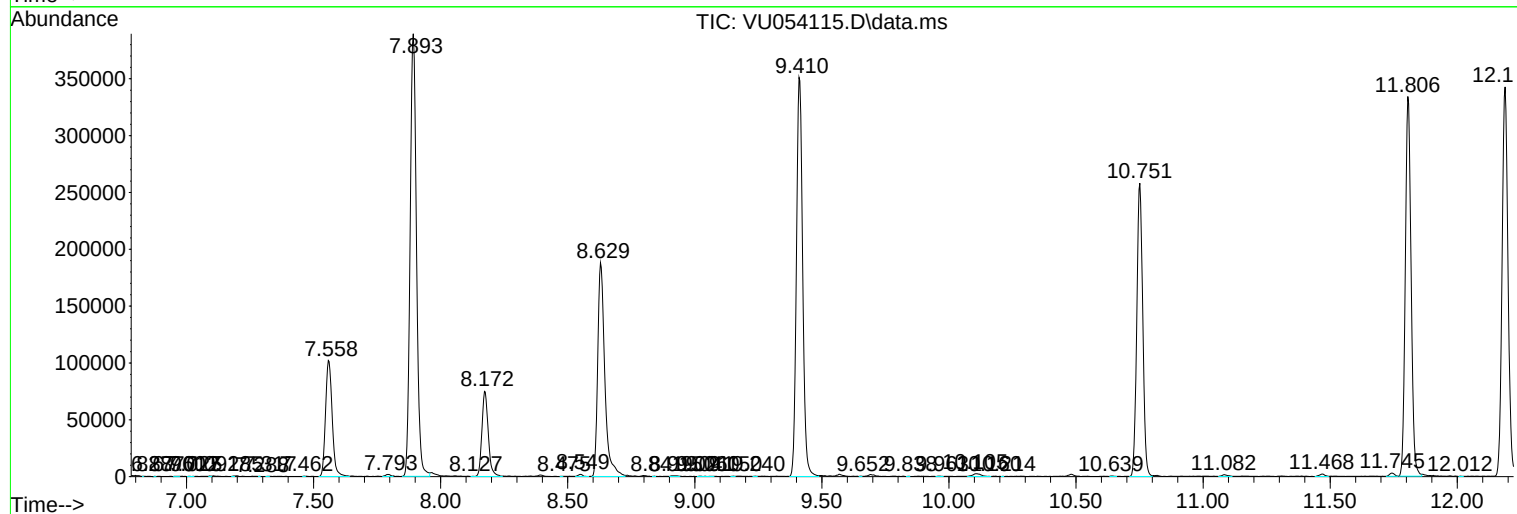
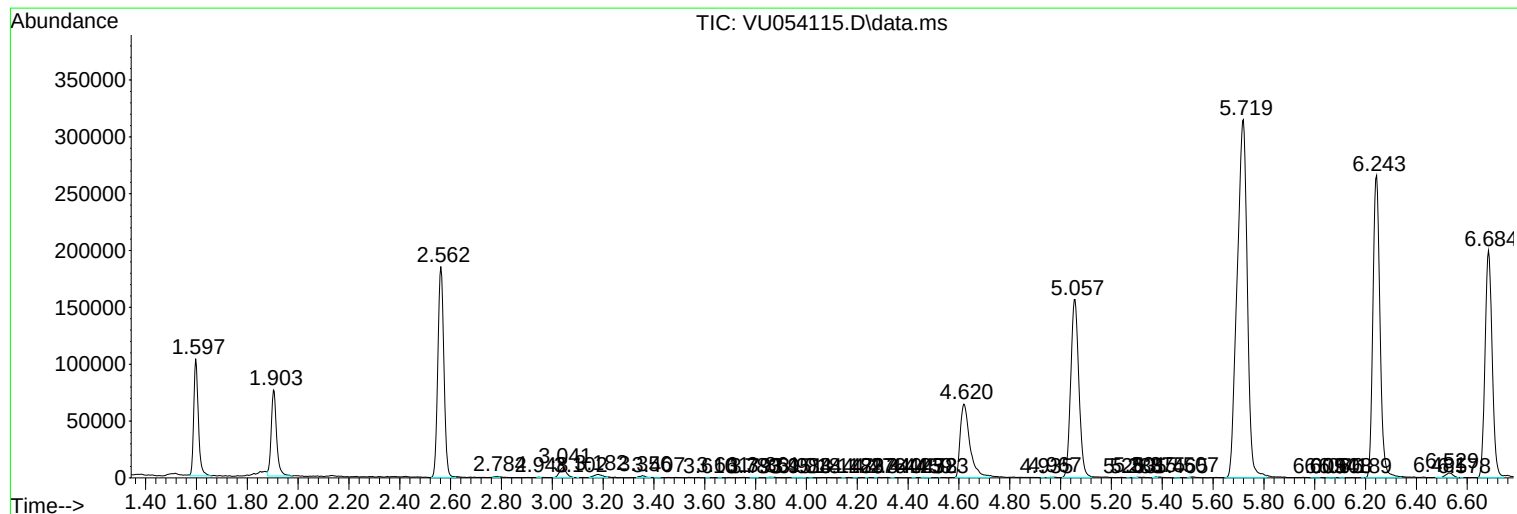
Sum of corrected areas: 6396272

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ALS Vial : 4 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK094

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU050923\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

\*\*\*\*\*

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