

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU111522\  
 Data File : VU051862.D  
 Acq On : 15 Nov 2022 16:22  
 Operator : JC/MD  
 Sample : VU1115MBL02  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK010

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\SFAMULM111522WMA.M  
 Title : VOC Analysis

Signal : TIC: VU051862.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         | 1.481       | 35            | 44          | 53           | rBV3     | 19620          | 38494         | 2.46%           | 0.298%        |
| 2         | 1.600       | 74            | 81          | 92           | rVB      | 170695         | 189579        | 12.14%          | 1.468%        |
| 3         | 1.909       | 169           | 177         | 194          | rVB      | 150002         | 213040        | 13.64%          | 1.649%        |
| 4         | 2.565       | 368           | 381         | 394          | rBV      | 243246         | 401502        | 25.71%          | 3.108%        |
| 5         | 2.748       | 435           | 438         | 440          | rBV3     | 894            | 646           | 0.04%           | 0.005%        |
| 6         | 2.880       | 476           | 479         | 482          | rVV2     | 337            | 262           | 0.02%           | 0.002%        |
| 7         | 2.967       | 504           | 506         | 510          | rVB4     | 427            | 236           | 0.02%           | 0.002%        |
| 8         | 3.041       | 524           | 529         | 532          | rBV4     | 1789           | 1789          | 0.11%           | 0.014%        |
| 9         | 3.179       | 562           | 572         | 589          | rVB2     | 4562           | 9890          | 0.63%           | 0.077%        |
| 10        | 3.276       | 599           | 602         | 605          | rVB2     | 337            | 253           | 0.02%           | 0.002%        |
| 11        | 3.330       | 615           | 619         | 621          | rBV2     | 364            | 306           | 0.02%           | 0.002%        |
| 12        | 3.697       | 730           | 733         | 736          | rBV2     | 436            | 336           | 0.02%           | 0.003%        |
| 13        | 3.989       | 821           | 824         | 828          | rVB2     | 333            | 266           | 0.02%           | 0.002%        |
| 14        | 4.054       | 838           | 844         | 847          | rVB2     | 380            | 470           | 0.03%           | 0.004%        |
| 15        | 4.102       | 855           | 859         | 862          | rBV2     | 337            | 345           | 0.02%           | 0.003%        |
| 16        | 4.462       | 968           | 971         | 975          | rVV      | 335            | 254           | 0.02%           | 0.002%        |
| 17        | 4.539       | 990           | 995         | 998          | rVB2     | 351            | 277           | 0.02%           | 0.002%        |
| 18        | 4.559       | 998           | 1001        | 1005         | rBV      | 510            | 396           | 0.03%           | 0.003%        |
| 19        | 4.616       | 1007          | 1019        | 1046         | rBV      | 195150         | 471074        | 30.16%          | 3.647%        |
| 20        | 4.967       | 1123          | 1128        | 1132         | rBV3     | 326            | 493           | 0.03%           | 0.004%        |
| 21        | 5.060       | 1141          | 1157        | 1180         | rBV      | 310841         | 678672        | 43.46%          | 5.254%        |
| 22        | 5.276       | 1220          | 1224        | 1226         | rBV2     | 971            | 811           | 0.05%           | 0.006%        |
| 23        | 5.292       | 1226          | 1229        | 1238         | rVB4     | 1436           | 2011          | 0.13%           | 0.016%        |
| 24        | 5.356       | 1245          | 1249        | 1251         | rBV      | 441            | 398           | 0.03%           | 0.003%        |
| 25        | 5.722       | 1342          | 1363        | 1388         | rBV2     | 553781         | 1561683       | 100.00%         | 12.089%       |
| 26        | 5.973       | 1438          | 1441        | 1445         | rBV2     | 473            | 357           | 0.02%           | 0.003%        |
| 27        | 6.002       | 1448          | 1450        | 1454         | rVB      | 565            | 378           | 0.02%           | 0.003%        |
| 28        | 6.025       | 1454          | 1457        | 1459         | rBV2     | 624            | 387           | 0.02%           | 0.003%        |
| 29        | 6.050       | 1459          | 1465        | 1467         | rBV3     | 556            | 585           | 0.04%           | 0.005%        |
| 30        | 6.108       | 1479          | 1483        | 1490         | rVB4     | 387            | 508           | 0.03%           | 0.004%        |
| 31        | 6.182       | 1501          | 1506        | 1511         | rBV2     | 348            | 272           | 0.02%           | 0.002%        |
| 32        | 6.247       | 1511          | 1526        | 1561         | rBV      | 616441         | 1191614       | 76.30%          | 9.224%        |
| 33        | 6.536       | 1609          | 1616        | 1623         | rVB6     | 2408           | 3802          | 0.24%           | 0.029%        |
| 34        | 6.687       | 1649          | 1663        | 1685         | rBV      | 394052         | 776532        | 49.72%          | 6.011%        |
| 35        | 6.800       | 1695          | 1698        | 1701         | rBV4     | 555            | 318           | 0.02%           | 0.002%        |
| 36        | 6.822       | 1701          | 1705        | 1710         | rVB3     | 817            | 658           | 0.04%           | 0.005%        |

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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\_U\Method\SFAMULM111522WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.906  | 1727 | 1731 | 1732 | rBV2 | 639    | 400     | 0.03%  | 0.003%  |
| 38 | 7.025  | 1765 | 1768 | 1770 | rBV  | 349    | 251     | 0.02%  | 0.002%  |
| 39 | 7.060  | 1776 | 1779 | 1787 | rVB3 | 447    | 568     | 0.04%  | 0.004%  |
| 40 | 7.189  | 1808 | 1819 | 1836 | rVB4 | 5836   | 11706   | 0.75%  | 0.091%  |
| 41 | 7.282  | 1845 | 1848 | 1852 | rVB  | 389    | 272     | 0.02%  | 0.002%  |
| 42 | 7.308  | 1852 | 1856 | 1859 | rBV2 | 419    | 365     | 0.02%  | 0.003%  |
| 43 | 7.488  | 1910 | 1912 | 1916 | rVB  | 422    | 286     | 0.02%  | 0.002%  |
| 44 | 7.513  | 1916 | 1920 | 1923 | rBV2 | 376    | 421     | 0.03%  | 0.003%  |
| 45 | 7.565  | 1923 | 1936 | 1961 | rBV  | 173034 | 312077  | 19.98% | 2.416%  |
| 46 | 7.690  | 1968 | 1975 | 1986 | rBV3 | 4036   | 6856    | 0.44%  | 0.053%  |
| 47 | 7.790  | 2004 | 2006 | 2009 | rVV4 | 537    | 341     | 0.02%  | 0.003%  |
| 48 | 7.896  | 2021 | 2039 | 2059 | rBV  | 580778 | 1004967 | 64.35% | 7.779%  |
| 49 | 8.176  | 2115 | 2126 | 2149 | rBV  | 125392 | 213899  | 13.70% | 1.656%  |
| 50 | 8.468  | 2211 | 2217 | 2229 | rVB3 | 2907   | 4536    | 0.29%  | 0.035%  |
| 51 | 8.555  | 2236 | 2244 | 2252 | rBV7 | 3179   | 4514    | 0.29%  | 0.035%  |
| 52 | 8.629  | 2255 | 2267 | 2301 | rBV2 | 549359 | 1030841 | 66.01% | 7.980%  |
| 53 | 8.880  | 2341 | 2345 | 2350 | rVB4 | 576    | 517     | 0.03%  | 0.004%  |
| 54 | 8.967  | 2370 | 2372 | 2374 | rBV2 | 433    | 276     | 0.02%  | 0.002%  |
| 55 | 9.002  | 2381 | 2383 | 2387 | rVB2 | 392    | 245     | 0.02%  | 0.002%  |
| 56 | 9.025  | 2387 | 2390 | 2393 | rBV  | 464    | 262     | 0.02%  | 0.002%  |
| 57 | 9.160  | 2427 | 2432 | 2439 | rVB3 | 359    | 406     | 0.03%  | 0.003%  |
| 58 | 9.414  | 2498 | 2511 | 2549 | rBV  | 873046 | 1462628 | 93.66% | 11.322% |
| 59 | 9.568  | 2557 | 2559 | 2565 | rVB4 | 987    | 858     | 0.05%  | 0.007%  |
| 60 | 9.635  | 2579 | 2580 | 2584 | rBV2 | 396    | 281     | 0.02%  | 0.002%  |
| 61 | 9.693  | 2595 | 2598 | 2607 | rVB4 | 1271   | 1673    | 0.11%  | 0.013%  |
| 62 | 9.812  | 2630 | 2635 | 2639 | rBV  | 281    | 301     | 0.02%  | 0.002%  |
| 63 | 10.002 | 2691 | 2694 | 2699 | rVB2 | 301    | 271     | 0.02%  | 0.002%  |
| 64 | 10.102 | 2721 | 2725 | 2727 | rBV4 | 472    | 382     | 0.02%  | 0.003%  |
| 65 | 10.279 | 2775 | 2780 | 2787 | rVB2 | 306    | 426     | 0.03%  | 0.003%  |
| 66 | 10.327 | 2791 | 2795 | 2800 | rBV2 | 319    | 418     | 0.03%  | 0.003%  |
| 67 | 10.404 | 2816 | 2819 | 2823 | rBV2 | 316    | 298     | 0.02%  | 0.002%  |
| 68 | 10.423 | 2823 | 2825 | 2832 | rVB  | 481    | 313     | 0.02%  | 0.002%  |
| 69 | 10.481 | 2839 | 2843 | 2844 | rBV2 | 522    | 394     | 0.03%  | 0.003%  |
| 70 | 10.597 | 2874 | 2879 | 2882 | rVV2 | 327    | 346     | 0.02%  | 0.003%  |
| 71 | 10.754 | 2915 | 2928 | 2951 | rBV  | 676426 | 1088733 | 69.72% | 8.428%  |
| 72 | 10.889 | 2961 | 2970 | 2978 | rVB2 | 3177   | 4882    | 0.31%  | 0.038%  |
| 73 | 11.018 | 3006 | 3010 | 3013 | rVB  | 327    | 258     | 0.02%  | 0.002%  |
| 74 | 11.041 | 3013 | 3017 | 3022 | rBV2 | 257    | 274     | 0.02%  | 0.002%  |
| 75 | 11.414 | 3128 | 3133 | 3135 | rBV  | 388    | 314     | 0.02%  | 0.002%  |
| 76 | 11.610 | 3192 | 3194 | 3198 | rBV2 | 350    | 253     | 0.02%  | 0.002%  |

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Instrument :  
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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SFAMULM111522WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 11.745 | 3230 | 3236 | 3244 | rBV3 | 1363   | 1963    | 0.13%  | 0.015% |
| 78  | 11.809 | 3244 | 3256 | 3290 | rBV  | 687697 | 1100131 | 70.45% | 8.516% |
| 79  | 12.073 | 3329 | 3338 | 3343 | rBV8 | 2211   | 3337    | 0.21%  | 0.026% |
| 80  | 12.192 | 3361 | 3375 | 3404 | rBV  | 653963 | 1082990 | 69.35% | 8.383% |
| 81  | 12.758 | 3548 | 3551 | 3553 | rBV2 | 422    | 284     | 0.02%  | 0.002% |
| 82  | 12.841 | 3572 | 3577 | 3581 | rBV3 | 591    | 704     | 0.05%  | 0.005% |
| 83  | 13.044 | 3637 | 3640 | 3641 | rBV3 | 411    | 265     | 0.02%  | 0.002% |
| 84  | 13.221 | 3686 | 3695 | 3708 | rBV6 | 2181   | 4338    | 0.28%  | 0.034% |
| 85  | 13.336 | 3729 | 3731 | 3734 | rVB  | 446    | 270     | 0.02%  | 0.002% |
| 86  | 13.552 | 3795 | 3798 | 3802 | rVB3 | 499    | 400     | 0.03%  | 0.003% |
| 87  | 13.584 | 3802 | 3808 | 3810 | rBV3 | 389    | 405     | 0.03%  | 0.003% |
| 88  | 13.613 | 3815 | 3817 | 3822 | rVB2 | 439    | 318     | 0.02%  | 0.002% |
| 89  | 13.648 | 3826 | 3828 | 3831 | rBV  | 395    | 283     | 0.02%  | 0.002% |
| 90  | 13.706 | 3843 | 3846 | 3852 | rBV3 | 588    | 710     | 0.05%  | 0.005% |
| 91  | 13.732 | 3852 | 3854 | 3859 | rVB2 | 439    | 309     | 0.02%  | 0.002% |
| 92  | 13.848 | 3883 | 3890 | 3899 | rVB6 | 2429   | 3255    | 0.21%  | 0.025% |
| 93  | 14.095 | 3957 | 3967 | 3972 | rBV4 | 3394   | 5427    | 0.35%  | 0.042% |
| 94  | 14.272 | 4020 | 4022 | 4026 | rVB  | 586    | 377     | 0.02%  | 0.003% |
| 95  | 14.294 | 4026 | 4029 | 4031 | rBV2 | 386    | 258     | 0.02%  | 0.002% |
| 96  | 14.336 | 4032 | 4042 | 4052 | rVV6 | 2282   | 3845    | 0.25%  | 0.030% |
| 97  | 14.616 | 4126 | 4129 | 4131 | rBV2 | 430    | 240     | 0.02%  | 0.002% |
| 98  | 15.417 | 4375 | 4378 | 4381 | rVB2 | 867    | 490     | 0.03%  | 0.004% |
| 99  | 15.825 | 4501 | 4505 | 4508 | rBV4 | 873    | 969     | 0.06%  | 0.008% |
| 100 | 16.532 | 4723 | 4725 | 4728 | rBV2 | 1247   | 696     | 0.04%  | 0.005% |

Sum of corrected areas: 12918467

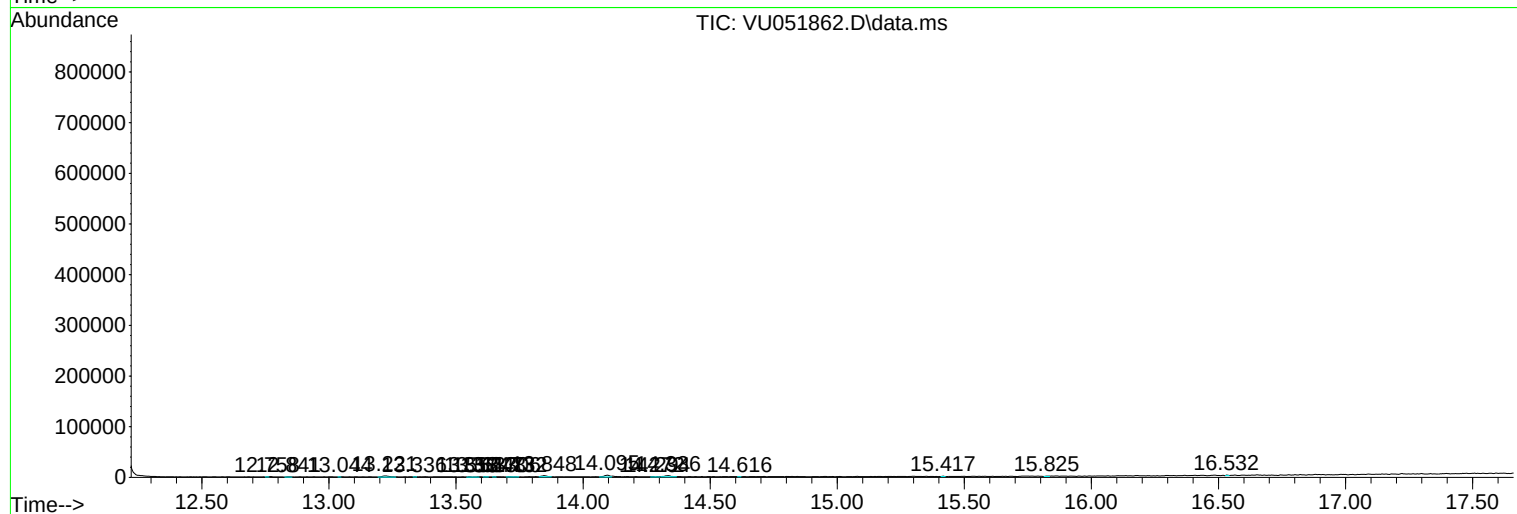
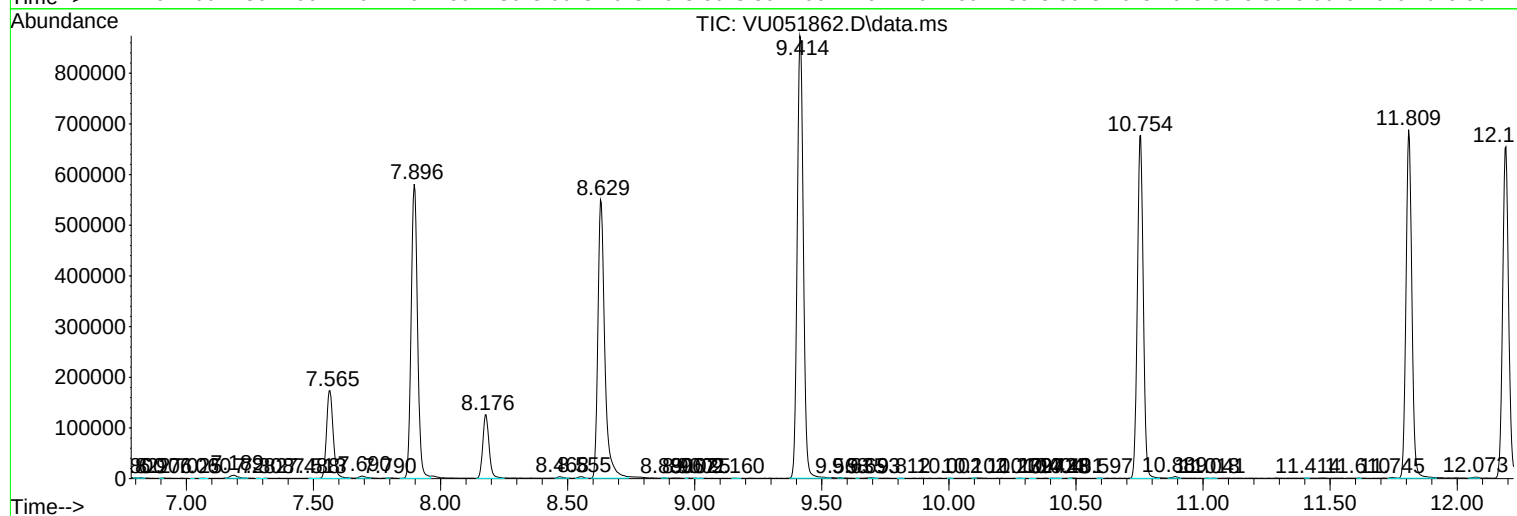
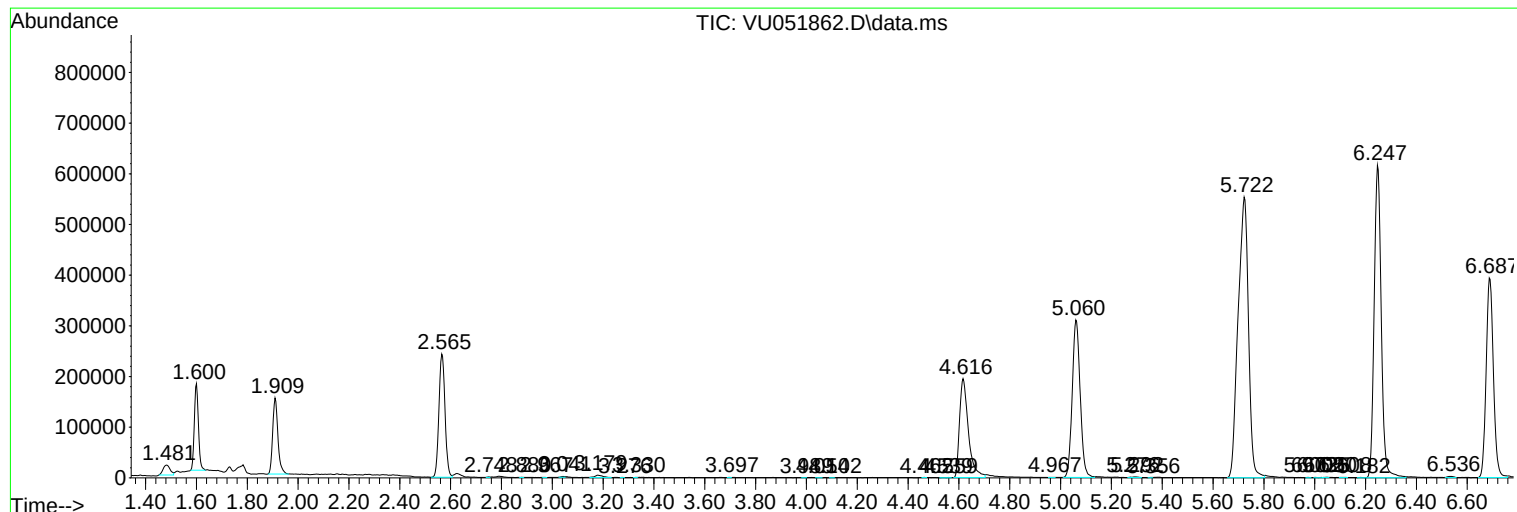
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM111522WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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No Library Search Compounds Detected

\*\*\*\*\*

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