

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU113021\  
 Data File : VU046029.D  
 Acq On : 30 Nov 2021 12:59  
 Operator : SY/MD  
 Sample : M4833-20ME  
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 ESQN7ME

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\SFAMULM112921WMA.M  
 Title : VOC Analysis

Signal : TIC: VU046029.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         | 1.600       | 73            | 81          | 103          | rVB      | 89966          | 117957        | 15.06%          | 1.936%        |
| 2         | 1.919       | 171           | 180         | 199          | rBV      | 53663          | 92857         | 11.85%          | 1.524%        |
| 3         | 1.996       | 200           | 204         | 212          | rVB3     | 1944           | 2464          | 0.31%           | 0.040%        |
| 4         | 2.028       | 212           | 214         | 219          | rBV      | 368            | 340           | 0.04%           | 0.006%        |
| 5         | 2.552       | 366           | 377         | 391          | rBV      | 138603         | 222244        | 28.37%          | 3.647%        |
| 6         | 3.041       | 523           | 529         | 538          | rBV4     | 1145           | 2157          | 0.28%           | 0.035%        |
| 7         | 3.115       | 550           | 552         | 559          | rVB      | 274            | 144           | 0.02%           | 0.002%        |
| 8         | 3.186       | 559           | 574         | 584          | rBV2     | 4181           | 10657         | 1.36%           | 0.175%        |
| 9         | 3.314       | 612           | 614         | 616          | rBV2     | 250            | 184           | 0.02%           | 0.003%        |
| 10        | 3.446       | 652           | 655         | 660          | rBB      | 192            | 186           | 0.02%           | 0.003%        |
| 11        | 3.594       | 699           | 701         | 706          | rBB      | 160            | 133           | 0.02%           | 0.002%        |
| 12        | 3.623       | 707           | 710         | 713          | rBB      | 175            | 137           | 0.02%           | 0.002%        |
| 13        | 3.748       | 745           | 749         | 754          | rBB      | 143            | 193           | 0.02%           | 0.003%        |
| 14        | 4.176       | 879           | 882         | 884          | rBV      | 149            | 124           | 0.02%           | 0.002%        |
| 15        | 4.497       | 979           | 982         | 984          | rBV      | 151            | 124           | 0.02%           | 0.002%        |
| 16        | 4.665       | 1016          | 1034        | 1088         | rBV      | 33860          | 184948        | 23.61%          | 3.035%        |
| 17        | 5.066       | 1142          | 1159        | 1187         | rVV      | 123773         | 303473        | 38.74%          | 4.980%        |
| 18        | 5.169       | 1187          | 1191        | 1194         | rVB2     | 270            | 232           | 0.03%           | 0.004%        |
| 19        | 5.285       | 1225          | 1227        | 1231         | rBB      | 245            | 192           | 0.02%           | 0.003%        |
| 20        | 5.722       | 1343          | 1363        | 1387         | rBV2     | 311299         | 783391        | 100.00%         | 12.855%       |
| 21        | 5.803       | 1387          | 1388        | 1396         | rVB2     | 327            | 257           | 0.03%           | 0.004%        |
| 22        | 5.883       | 1412          | 1413        | 1419         | rBB      | 220            | 162           | 0.02%           | 0.003%        |
| 23        | 5.983       | 1433          | 1444        | 1467         | rBV6     | 3436           | 10211         | 1.30%           | 0.168%        |
| 24        | 6.250       | 1512          | 1527        | 1551         | rBV      | 236925         | 486596        | 62.11%          | 7.984%        |
| 25        | 6.533       | 1605          | 1615        | 1625         | rBV6     | 3902           | 9115          | 1.16%           | 0.150%        |
| 26        | 6.693       | 1651          | 1665        | 1692         | rVB      | 164923         | 343317        | 43.82%          | 5.633%        |
| 27        | 6.806       | 1697          | 1700        | 1701         | rBV      | 249            | 125           | 0.02%           | 0.002%        |
| 28        | 7.034       | 1768          | 1771        | 1774         | rBV      | 147            | 145           | 0.02%           | 0.002%        |
| 29        | 7.160       | 1807          | 1810        | 1812         | rBV      | 146            | 118           | 0.02%           | 0.002%        |
| 30        | 7.192       | 1812          | 1820        | 1826         | rVV4     | 880            | 1403          | 0.18%           | 0.023%        |
| 31        | 7.218       | 1826          | 1828        | 1831         | rVV2     | 231            | 168           | 0.02%           | 0.003%        |
| 32        | 7.308       | 1853          | 1856        | 1860         | rBB      | 145            | 147           | 0.02%           | 0.002%        |
| 33        | 7.568       | 1924          | 1937        | 1967         | rVB      | 86091          | 173076        | 22.09%          | 2.840%        |
| 34        | 7.693       | 1968          | 1976        | 1982         | rBV3     | 522            | 924           | 0.12%           | 0.015%        |
| 35        | 7.748       | 1990          | 1993        | 1996         | rBV2     | 246            | 211           | 0.03%           | 0.003%        |
| 36        | 7.793       | 2000          | 2007        | 2017         | rVB2     | 660            | 1371          | 0.18%           | 0.022%        |

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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.899  | 2026 | 2040 | 2060 | rBV  | 330865 | 647793 | 82.69% | 10.630% |
| 38 | 8.185  | 2117 | 2129 | 2157 | rVB2 | 50084  | 118233 | 15.09% | 1.940%  |
| 39 | 8.298  | 2158 | 2164 | 2165 | rBV  | 136    | 146    | 0.02%  | 0.002%  |
| 40 | 8.333  | 2171 | 2175 | 2178 | rBV  | 178    | 191    | 0.02%  | 0.003%  |
| 41 | 8.423  | 2201 | 2203 | 2206 | rBV  | 162    | 132    | 0.02%  | 0.002%  |
| 42 | 8.478  | 2213 | 2220 | 2226 | rVB2 | 389    | 710    | 0.09%  | 0.012%  |
| 43 | 8.587  | 2252 | 2254 | 2259 | rBB  | 138    | 141    | 0.02%  | 0.002%  |
| 44 | 8.684  | 2260 | 2284 | 2317 | rBV2 | 115794 | 378680 | 48.34% | 6.214%  |
| 45 | 8.835  | 2327 | 2331 | 2336 | rVB  | 204    | 250    | 0.03%  | 0.004%  |
| 46 | 8.889  | 2346 | 2348 | 2353 | rVB  | 162    | 170    | 0.02%  | 0.003%  |
| 47 | 8.931  | 2356 | 2361 | 2363 | rBB  | 137    | 144    | 0.02%  | 0.002%  |
| 48 | 8.951  | 2364 | 2367 | 2370 | rBV2 | 428    | 288    | 0.04%  | 0.005%  |
| 49 | 9.102  | 2411 | 2414 | 2417 | rBB  | 142    | 120    | 0.02%  | 0.002%  |
| 50 | 9.169  | 2432 | 2435 | 2437 | rBV  | 184    | 152    | 0.02%  | 0.002%  |
| 51 | 9.275  | 2463 | 2468 | 2471 | rBB  | 217    | 214    | 0.03%  | 0.004%  |
| 52 | 9.301  | 2471 | 2476 | 2486 | rBV  | 158    | 385    | 0.05%  | 0.006%  |
| 53 | 9.426  | 2499 | 2515 | 2539 | rBV  | 259078 | 618936 | 79.01% | 10.156% |
| 54 | 9.574  | 2557 | 2561 | 2567 | rBB2 | 312    | 415    | 0.05%  | 0.007%  |
| 55 | 9.606  | 2567 | 2571 | 2575 | rBV  | 157    | 209    | 0.03%  | 0.003%  |
| 56 | 9.697  | 2594 | 2599 | 2610 | rVB3 | 580    | 1118   | 0.14%  | 0.018%  |
| 57 | 9.745  | 2611 | 2614 | 2616 | rBV  | 161    | 131    | 0.02%  | 0.002%  |
| 58 | 9.809  | 2631 | 2634 | 2636 | rBV  | 161    | 130    | 0.02%  | 0.002%  |
| 59 | 9.857  | 2646 | 2649 | 2653 | rBV  | 152    | 174    | 0.02%  | 0.003%  |
| 60 | 9.947  | 2674 | 2677 | 2681 | rVB  | 202    | 191    | 0.02%  | 0.003%  |
| 61 | 10.250 | 2768 | 2771 | 2774 | rBV  | 145    | 148    | 0.02%  | 0.002%  |
| 62 | 10.311 | 2784 | 2790 | 2793 | rBV  | 178    | 263    | 0.03%  | 0.004%  |
| 63 | 10.414 | 2820 | 2822 | 2826 | rVB  | 233    | 173    | 0.02%  | 0.003%  |
| 64 | 10.436 | 2826 | 2829 | 2831 | rBV  | 154    | 130    | 0.02%  | 0.002%  |
| 65 | 10.478 | 2840 | 2842 | 2845 | rVB  | 192    | 126    | 0.02%  | 0.002%  |
| 66 | 10.497 | 2845 | 2848 | 2851 | rBV  | 158    | 156    | 0.02%  | 0.003%  |
| 67 | 10.616 | 2882 | 2885 | 2890 | rVV  | 151    | 150    | 0.02%  | 0.002%  |
| 68 | 10.671 | 2894 | 2902 | 2910 | rVB3 | 3193   | 4513   | 0.58%  | 0.074%  |
| 69 | 10.774 | 2921 | 2934 | 2948 | rBV  | 226112 | 378478 | 48.31% | 6.210%  |
| 70 | 10.867 | 2956 | 2963 | 2966 | rVV3 | 537    | 619    | 0.08%  | 0.010%  |
| 71 | 10.896 | 2966 | 2972 | 2976 | rVV4 | 687    | 902    | 0.12%  | 0.015%  |
| 72 | 10.925 | 2979 | 2981 | 2987 | rVB2 | 340    | 256    | 0.03%  | 0.004%  |
| 73 | 11.118 | 3036 | 3041 | 3043 | rBV2 | 650    | 564    | 0.07%  | 0.009%  |
| 74 | 11.143 | 3046 | 3049 | 3050 | rBV  | 297    | 118    | 0.02%  | 0.002%  |
| 75 | 11.153 | 3050 | 3052 | 3055 | rVB3 | 384    | 248    | 0.03%  | 0.004%  |
| 76 | 11.205 | 3065 | 3068 | 3073 | rBV2 | 223    | 228    | 0.03%  | 0.004%  |

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Instrument :  
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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.459 | 3138 | 3147 | 3160 | rVB3 | 1931   | 3155   | 0.40%  | 0.052% |
| 78  | 11.581 | 3179 | 3185 | 3191 | rVV  | 381    | 467    | 0.06%  | 0.008% |
| 79  | 11.696 | 3214 | 3221 | 3228 | rBV3 | 1458   | 1736   | 0.22%  | 0.028% |
| 80  | 11.819 | 3246 | 3259 | 3279 | rVB  | 386513 | 607301 | 77.52% | 9.965% |
| 81  | 11.918 | 3286 | 3290 | 3291 | rBV2 | 176    | 130    | 0.02%  | 0.002% |
| 82  | 11.944 | 3291 | 3298 | 3301 | rVV4 | 1342   | 1897   | 0.24%  | 0.031% |
| 83  | 11.976 | 3303 | 3308 | 3317 | rVB4 | 2141   | 2958   | 0.38%  | 0.049% |
| 84  | 12.121 | 3349 | 3353 | 3356 | rVB2 | 216    | 150    | 0.02%  | 0.002% |
| 85  | 12.201 | 3359 | 3378 | 3393 | rVB  | 352506 | 565903 | 72.24% | 9.286% |
| 86  | 12.275 | 3398 | 3401 | 3404 | rVB  | 246    | 155    | 0.02%  | 0.003% |
| 87  | 12.330 | 3412 | 3418 | 3423 | rBV4 | 969    | 1035   | 0.13%  | 0.017% |
| 88  | 12.394 | 3434 | 3438 | 3441 | rBV  | 260    | 225    | 0.03%  | 0.004% |
| 89  | 13.140 | 3668 | 3670 | 3672 | rBV  | 173    | 119    | 0.02%  | 0.002% |
| 90  | 14.098 | 3963 | 3968 | 3973 | rVB2 | 649    | 687    | 0.09%  | 0.011% |
| 91  | 15.085 | 4271 | 4275 | 4279 | rBV2 | 184    | 161    | 0.02%  | 0.003% |
| 92  | 15.143 | 4290 | 4293 | 4297 | rBV2 | 222    | 199    | 0.03%  | 0.003% |
| 93  | 15.590 | 4428 | 4432 | 4434 | rBV  | 312    | 265    | 0.03%  | 0.004% |
| 94  | 15.632 | 4440 | 4445 | 4446 | rBV  | 260    | 235    | 0.03%  | 0.004% |
| 95  | 16.291 | 4646 | 4650 | 4653 | rBV  | 309    | 256    | 0.03%  | 0.004% |
| 96  | 16.355 | 4667 | 4670 | 4672 | rBV2 | 426    | 196    | 0.03%  | 0.003% |
| 97  | 16.455 | 4699 | 4701 | 4703 | rBV2 | 344    | 161    | 0.02%  | 0.003% |
| 98  | 16.616 | 4748 | 4751 | 4753 | rBV  | 456    | 366    | 0.05%  | 0.006% |
| 99  | 16.690 | 4771 | 4774 | 4779 | rVB3 | 545    | 375    | 0.05%  | 0.006% |
| 100 | 16.880 | 4830 | 4833 | 4837 | rBV  | 790    | 552    | 0.07%  | 0.009% |

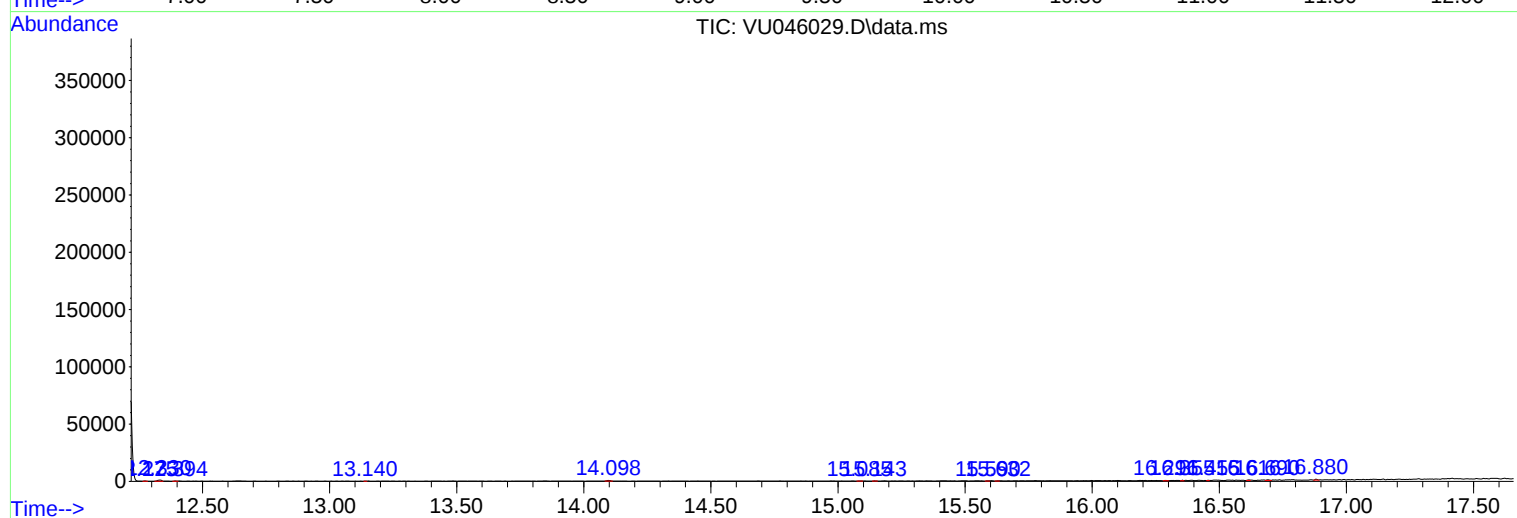
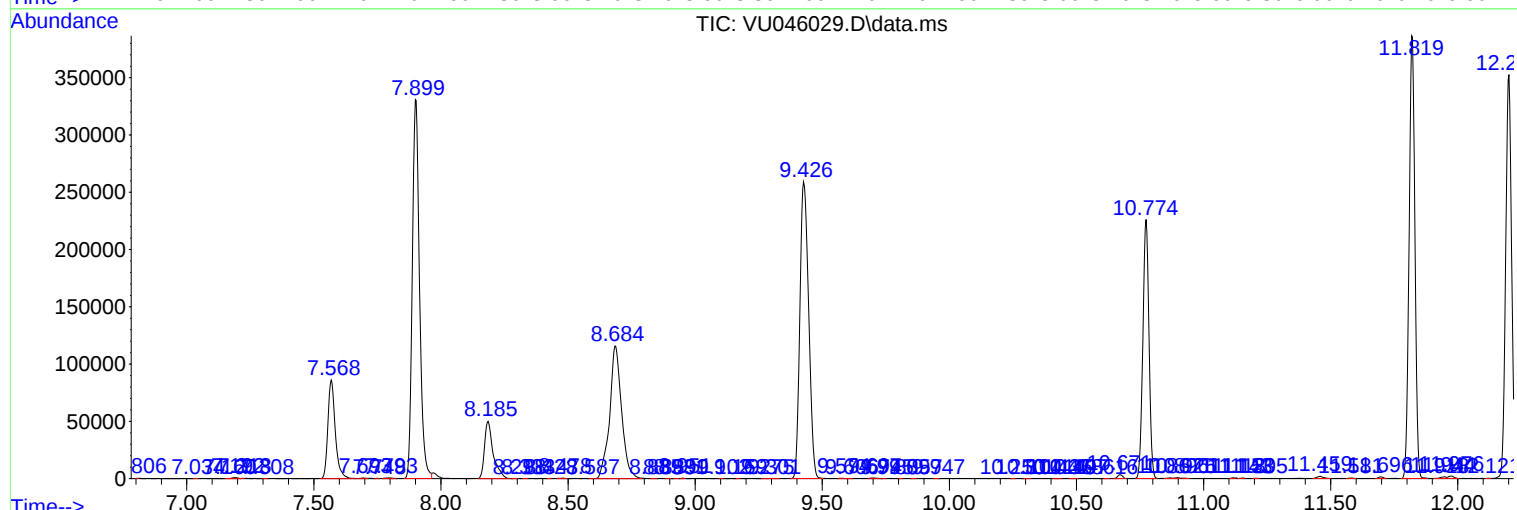
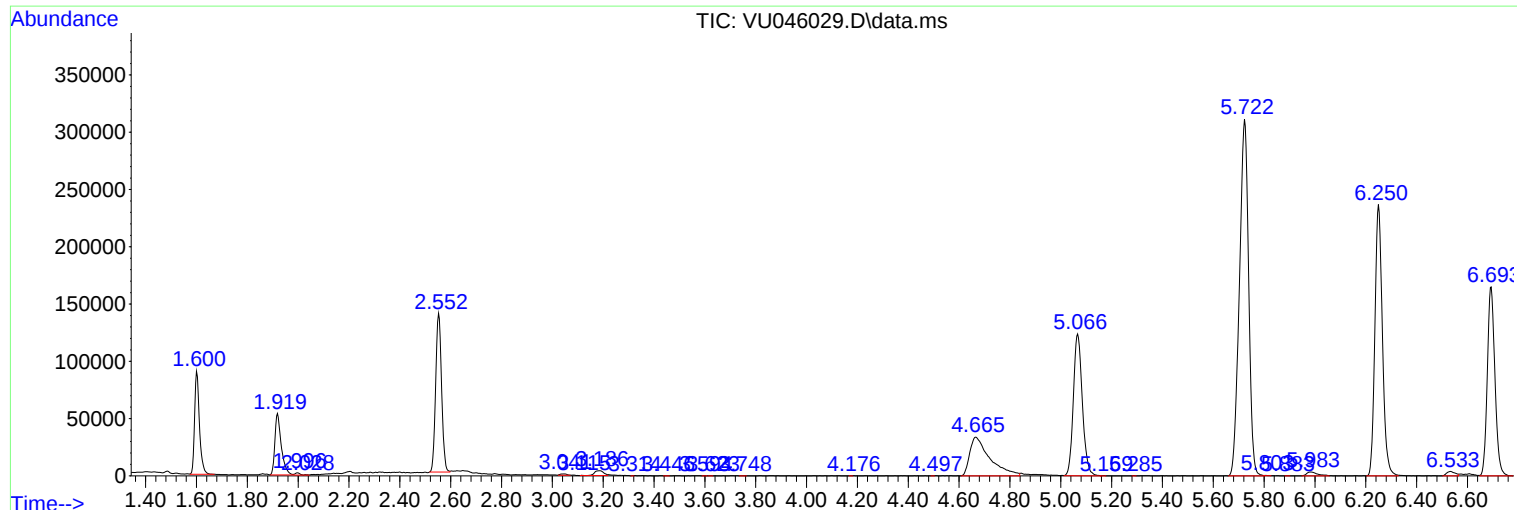
Sum of corrected areas: 6094292

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.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 |