

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120821\  
 Data File : VU046199.D  
 Acq On : 09 Dec 2021 00:27  
 Operator : SY/MD  
 Sample : M4982-03  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0CQ6

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: VU046199.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         | 1.604       | 75            | 82          | 97           | rVB      | 80793          | 89744         | 12.46%          | 1.474%        |
| 2         | 1.919       | 172           | 180         | 193          | rBV      | 63590          | 80182         | 11.14%          | 1.317%        |
| 3         | 2.141       | 246           | 249         | 251          | rBV      | 491            | 319           | 0.04%           | 0.005%        |
| 4         | 2.212       | 268           | 271         | 274          | rBV3     | 325            | 176           | 0.02%           | 0.003%        |
| 5         | 2.260       | 284           | 286         | 290          | rBV      | 275            | 265           | 0.04%           | 0.004%        |
| 6         | 2.331       | 306           | 308         | 312          | rBV2     | 386            | 249           | 0.03%           | 0.004%        |
| 7         | 2.427       | 334           | 338         | 340          | rBV2     | 434            | 284           | 0.04%           | 0.005%        |
| 8         | 2.575       | 372           | 384         | 403          | rBV      | 141664         | 236914        | 32.90%          | 3.890%        |
| 9         | 3.086       | 538           | 543         | 548          | rBV2     | 505            | 663           | 0.09%           | 0.011%        |
| 10        | 3.347       | 621           | 624         | 626          | rBV      | 402            | 266           | 0.04%           | 0.004%        |
| 11        | 3.691       | 727           | 731         | 737          | rBV2     | 401            | 381           | 0.05%           | 0.006%        |
| 12        | 3.787       | 758           | 761         | 765          | rBV2     | 344            | 273           | 0.04%           | 0.004%        |
| 13        | 3.848       | 775           | 780         | 782          | rBV2     | 558            | 539           | 0.07%           | 0.009%        |
| 14        | 3.941       | 806           | 809         | 813          | rBV      | 416            | 293           | 0.04%           | 0.005%        |
| 15        | 3.964       | 813           | 816         | 819          | rVV      | 390            | 254           | 0.04%           | 0.004%        |
| 16        | 4.138       | 868           | 870         | 875          | rVB      | 270            | 231           | 0.03%           | 0.004%        |
| 17        | 4.215       | 891           | 894         | 898          | rBV      | 403            | 408           | 0.06%           | 0.007%        |
| 18        | 4.269       | 908           | 911         | 915          | rBV2     | 426            | 312           | 0.04%           | 0.005%        |
| 19        | 4.639       | 1007          | 1026        | 1055         | rBV      | 75060          | 229318        | 31.85%          | 3.765%        |
| 20        | 4.948       | 1118          | 1122        | 1126         | rBV2     | 450            | 374           | 0.05%           | 0.006%        |
| 21        | 4.990       | 1132          | 1135        | 1136         | rBV      | 204            | 130           | 0.02%           | 0.002%        |
| 22        | 5.067       | 1141          | 1159        | 1179         | rBV      | 130340         | 292686        | 40.65%          | 4.806%        |
| 23        | 5.292       | 1226          | 1229        | 1232         | rBV4     | 532            | 436           | 0.06%           | 0.007%        |
| 24        | 5.379       | 1251          | 1256        | 1257         | rBV      | 332            | 249           | 0.03%           | 0.004%        |
| 25        | 5.456       | 1278          | 1280        | 1282         | rBV      | 178            | 108           | 0.01%           | 0.002%        |
| 26        | 5.472       | 1282          | 1285        | 1288         | rVV      | 329            | 233           | 0.03%           | 0.004%        |
| 27        | 5.552       | 1307          | 1310        | 1311         | rBV      | 210            | 127           | 0.02%           | 0.002%        |
| 28        | 5.565       | 1311          | 1314        | 1315         | rBV      | 239            | 129           | 0.02%           | 0.002%        |
| 29        | 5.729       | 1342          | 1365        | 1387         | rBV2     | 263799         | 720041        | 100.00%         | 11.822%       |
| 30        | 6.019       | 1449          | 1455        | 1458         | rBV2     | 643            | 571           | 0.08%           | 0.009%        |
| 31        | 6.253       | 1513          | 1528        | 1544         | rBV      | 258965         | 488124        | 67.79%          | 8.015%        |
| 32        | 6.536       | 1606          | 1616        | 1629         | rBV7     | 4847           | 10137         | 1.41%           | 0.166%        |
| 33        | 6.694       | 1651          | 1665        | 1682         | rBV      | 166001         | 320801        | 44.55%          | 5.267%        |
| 34        | 6.945       | 1738          | 1743        | 1748         | rBV2     | 443            | 478           | 0.07%           | 0.008%        |
| 35        | 6.977       | 1748          | 1753        | 1755         | rBV2     | 576            | 565           | 0.08%           | 0.009%        |
| 36        | 7.009       | 1760          | 1763        | 1766         | rVB      | 418            | 246           | 0.03%           | 0.004%        |

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 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0CQ6

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.028  | 1766 | 1769 | 1773 | rBV  | 404    | 349    | 0.05%  | 0.006%  |
| 38 | 7.086  | 1781 | 1787 | 1791 | rBV2 | 480    | 653    | 0.09%  | 0.011%  |
| 39 | 7.282  | 1845 | 1848 | 1853 | rBV  | 295    | 311    | 0.04%  | 0.005%  |
| 40 | 7.334  | 1862 | 1864 | 1866 | rBV  | 159    | 90     | 0.01%  | 0.001%  |
| 41 | 7.350  | 1866 | 1869 | 1875 | rVB  | 414    | 323    | 0.04%  | 0.005%  |
| 42 | 7.382  | 1875 | 1879 | 1880 | rBV  | 276    | 194    | 0.03%  | 0.003%  |
| 43 | 7.498  | 1913 | 1915 | 1919 | rVB2 | 311    | 212    | 0.03%  | 0.003%  |
| 44 | 7.520  | 1919 | 1922 | 1924 | rBV  | 415    | 274    | 0.04%  | 0.004%  |
| 45 | 7.568  | 1924 | 1937 | 1959 | rVV  | 95178  | 168416 | 23.39% | 2.765%  |
| 46 | 7.899  | 2025 | 2040 | 2056 | rBV  | 332311 | 585050 | 81.25% | 9.606%  |
| 47 | 8.179  | 2116 | 2127 | 2144 | rBV  | 66545  | 109791 | 15.25% | 1.803%  |
| 48 | 8.340  | 2174 | 2177 | 2183 | rVB2 | 522    | 520    | 0.07%  | 0.009%  |
| 49 | 8.443  | 2206 | 2209 | 2211 | rBV  | 587    | 432    | 0.06%  | 0.007%  |
| 50 | 8.539  | 2236 | 2239 | 2243 | rBV  | 350    | 316    | 0.04%  | 0.005%  |
| 51 | 8.633  | 2256 | 2268 | 2295 | rBV  | 235691 | 425089 | 59.04% | 6.980%  |
| 52 | 8.906  | 2350 | 2353 | 2356 | rBV  | 336    | 240    | 0.03%  | 0.004%  |
| 53 | 9.018  | 2386 | 2388 | 2391 | rBV2 | 305    | 258    | 0.04%  | 0.004%  |
| 54 | 9.089  | 2404 | 2410 | 2412 | rBV  | 504    | 432    | 0.06%  | 0.007%  |
| 55 | 9.163  | 2430 | 2433 | 2435 | rBV  | 284    | 172    | 0.02%  | 0.003%  |
| 56 | 9.221  | 2447 | 2451 | 2453 | rBV  | 546    | 495    | 0.07%  | 0.008%  |
| 57 | 9.343  | 2485 | 2489 | 2494 | rBV2 | 585    | 554    | 0.08%  | 0.009%  |
| 58 | 9.417  | 2499 | 2512 | 2536 | rBV  | 365546 | 613033 | 85.14% | 10.065% |
| 59 | 9.568  | 2553 | 2559 | 2561 | rBV2 | 670    | 699    | 0.10%  | 0.011%  |
| 60 | 9.697  | 2591 | 2599 | 2606 | rVB3 | 2010   | 3196   | 0.44%  | 0.052%  |
| 61 | 9.915  | 2660 | 2667 | 2668 | rBV  | 293    | 303    | 0.04%  | 0.005%  |
| 62 | 10.102 | 2719 | 2725 | 2731 | rBV4 | 876    | 1288   | 0.18%  | 0.021%  |
| 63 | 10.362 | 2800 | 2806 | 2810 | rBV  | 550    | 749    | 0.10%  | 0.012%  |
| 64 | 10.424 | 2822 | 2825 | 2828 | rVB2 | 393    | 225    | 0.03%  | 0.004%  |
| 65 | 10.443 | 2828 | 2831 | 2833 | rBV2 | 359    | 273    | 0.04%  | 0.004%  |
| 66 | 10.549 | 2861 | 2864 | 2866 | rBV  | 310    | 201    | 0.03%  | 0.003%  |
| 67 | 10.636 | 2888 | 2891 | 2892 | rBV  | 193    | 120    | 0.02%  | 0.002%  |
| 68 | 10.758 | 2917 | 2929 | 2948 | rVB  | 265928 | 419819 | 58.30% | 6.893%  |
| 69 | 10.825 | 2948 | 2950 | 2952 | rBV  | 364    | 220    | 0.03%  | 0.004%  |
| 70 | 10.893 | 2964 | 2971 | 2984 | rVB4 | 4658   | 7784   | 1.08%  | 0.128%  |
| 71 | 11.468 | 3142 | 3150 | 3161 | rVB2 | 4659   | 6568   | 0.91%  | 0.108%  |
| 72 | 11.813 | 3245 | 3257 | 3274 | rBV  | 424270 | 663993 | 92.22% | 10.902% |
| 73 | 12.092 | 3342 | 3344 | 3346 | rBV  | 446    | 234    | 0.03%  | 0.004%  |
| 74 | 12.192 | 3363 | 3375 | 3391 | rBV  | 372970 | 600046 | 83.33% | 9.852%  |
| 75 | 12.684 | 3524 | 3528 | 3532 | rBV2 | 490    | 480    | 0.07%  | 0.008%  |
| 76 | 12.861 | 3580 | 3583 | 3588 | rBV  | 440    | 387    | 0.05%  | 0.006%  |

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Sample : M4982-03  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0CQ6

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

|    |        |      |      |      |     |     |     |       |        |
|----|--------|------|------|------|-----|-----|-----|-------|--------|
| 77 | 12.912 | 3596 | 3599 | 3601 | rBV | 318 | 192 | 0.03% | 0.003% |
|----|--------|------|------|------|-----|-----|-----|-------|--------|

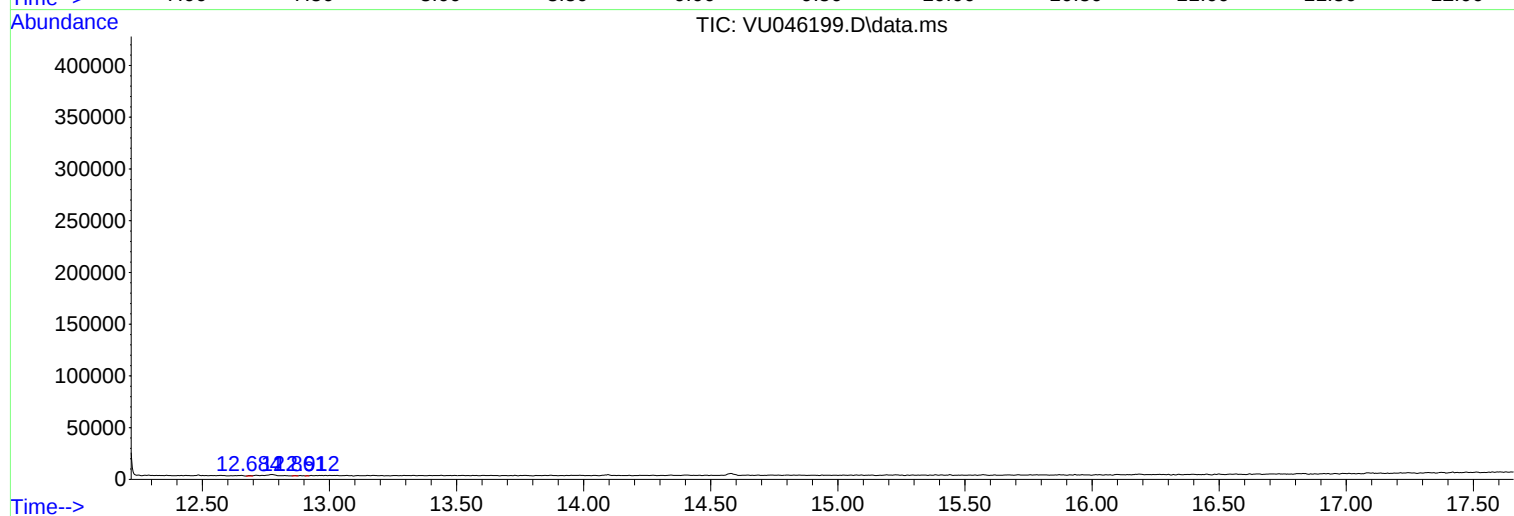
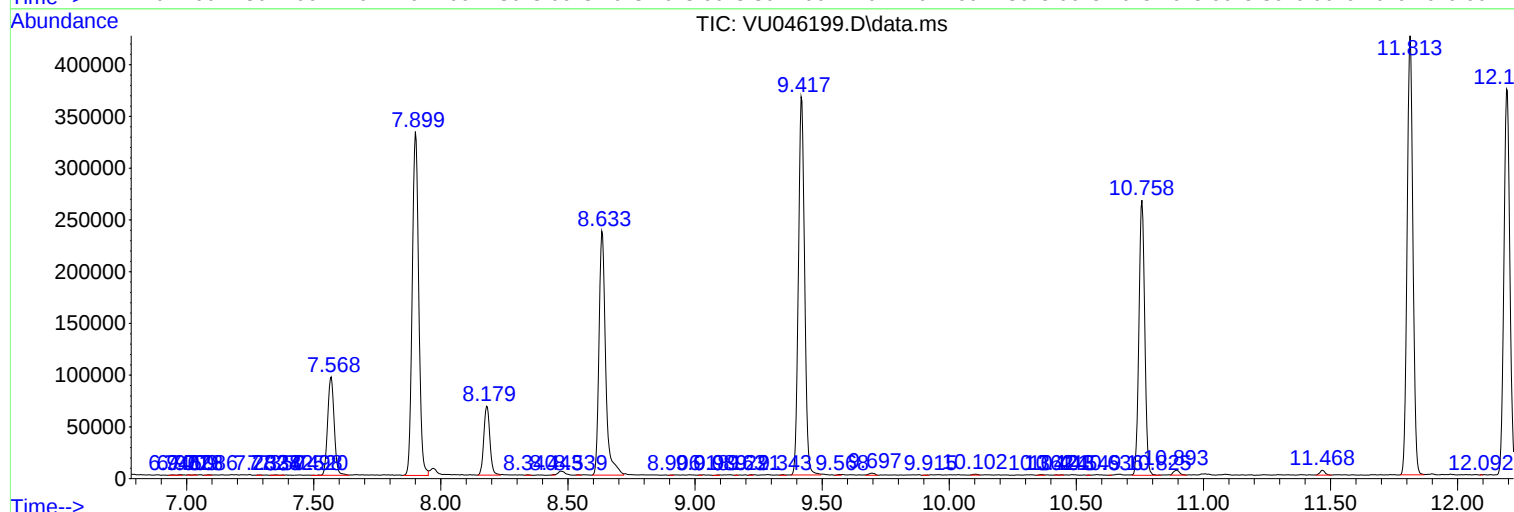
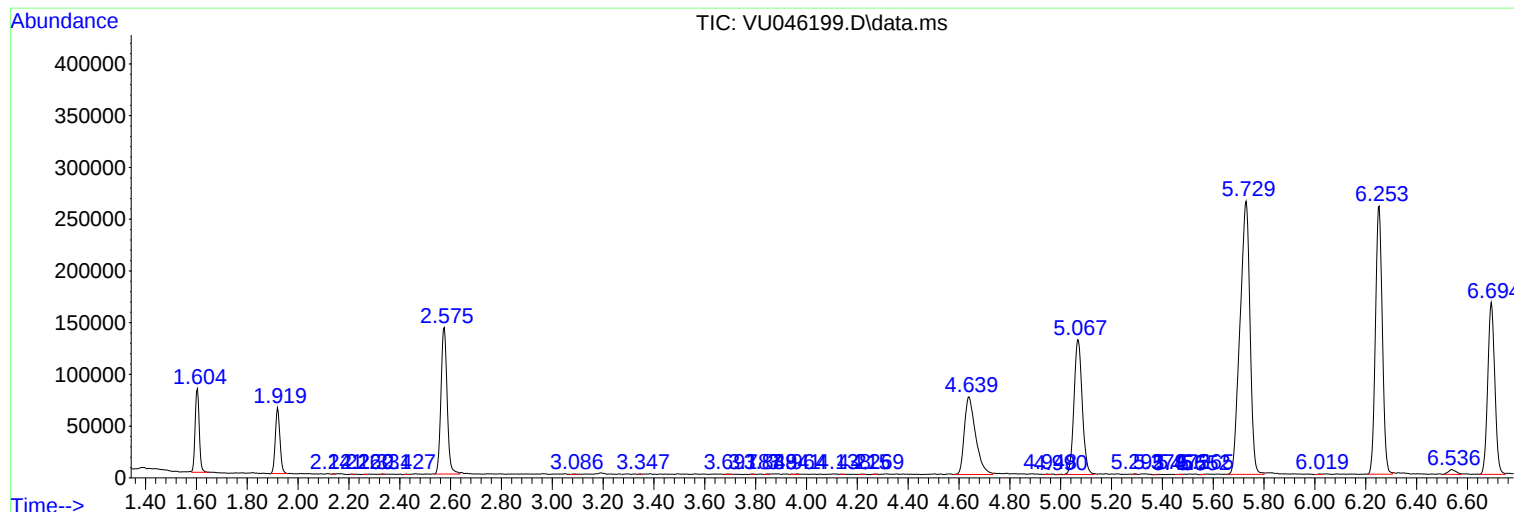
Sum of corrected areas: 6090487

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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0CQ6

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120821\  
Data File : VU046199.D  
Acq On : 09 Dec 2021 00:27  
Operator : SY/MD  
Sample : M4982-03  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
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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

No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
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TIC Integration Parameters: LSCINT.P

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