

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121321\  
 Data File : VU046314.D  
 Acq On : 13 Dec 2021 14:44  
 Operator : SY/MD  
 Sample : M5062-20  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGL18

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: VU046314.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          | 96           | rVB      | 85062          | 94295         | 16.25%          | 2.058%        |
| 2         | 1.919       | 173           | 180         | 192          | rVB      | 61373          | 76704         | 13.22%          | 1.674%        |
| 3         | 2.571       | 372           | 383         | 398          | rBV      | 126729         | 207528        | 35.76%          | 4.529%        |
| 4         | 4.642       | 1013          | 1027        | 1053         | rBV      | 43673          | 136958        | 23.60%          | 2.989%        |
| 5         | 5.067       | 1144          | 1159        | 1183         | rBV      | 101840         | 234129        | 40.34%          | 5.109%        |
| 6         | 5.378       | 1253          | 1256        | 1259         | rBV2     | 256            | 189           | 0.03%           | 0.004%        |
| 7         | 5.571       | 1313          | 1316        | 1321         | rBV2     | 251            | 256           | 0.04%           | 0.006%        |
| 8         | 5.729       | 1345          | 1365        | 1403         | rVB2     | 215242         | 580365        | 100.00%         | 12.665%       |
| 9         | 5.973       | 1434          | 1441        | 1445         | rBV      | 390            | 521           | 0.09%           | 0.011%        |
| 10        | 6.057       | 1465          | 1467        | 1472         | rVB2     | 320            | 246           | 0.04%           | 0.005%        |
| 11        | 6.089       | 1472          | 1477        | 1480         | rBV2     | 422            | 447           | 0.08%           | 0.010%        |
| 12        | 6.124       | 1484          | 1488        | 1492         | rVV      | 307            | 265           | 0.05%           | 0.006%        |
| 13        | 6.253       | 1510          | 1528        | 1550         | rBV      | 179023         | 342441        | 59.00%          | 7.473%        |
| 14        | 6.530       | 1606          | 1614        | 1624         | rVB5     | 1562           | 2884          | 0.50%           | 0.063%        |
| 15        | 6.587       | 1628          | 1632        | 1639         | rVB2     | 314            | 346           | 0.06%           | 0.008%        |
| 16        | 6.629       | 1639          | 1645        | 1648         | rBV      | 422            | 448           | 0.08%           | 0.010%        |
| 17        | 6.693       | 1652          | 1665        | 1683         | rBV      | 133181         | 253278        | 43.64%          | 5.527%        |
| 18        | 6.864       | 1715          | 1718        | 1720         | rBV      | 154            | 102           | 0.02%           | 0.002%        |
| 19        | 6.886       | 1720          | 1725        | 1727         | rBV      | 243            | 244           | 0.04%           | 0.005%        |
| 20        | 6.993       | 1752          | 1758        | 1760         | rBV      | 199            | 230           | 0.04%           | 0.005%        |
| 21        | 7.009       | 1760          | 1763        | 1766         | rVB2     | 205            | 132           | 0.02%           | 0.003%        |
| 22        | 7.111       | 1792          | 1795        | 1798         | rBV2     | 144            | 83            | 0.01%           | 0.002%        |
| 23        | 7.163       | 1807          | 1811        | 1814         | rBV      | 241            | 172           | 0.03%           | 0.004%        |
| 24        | 7.372       | 1873          | 1876        | 1880         | rVB      | 256            | 192           | 0.03%           | 0.004%        |
| 25        | 7.394       | 1880          | 1883        | 1886         | rBV      | 303            | 209           | 0.04%           | 0.005%        |
| 26        | 7.568       | 1925          | 1937        | 1955         | rBV      | 70965          | 122311        | 21.07%          | 2.669%        |
| 27        | 7.668       | 1966          | 1968        | 1971         | rVB      | 273            | 160           | 0.03%           | 0.003%        |
| 28        | 7.693       | 1971          | 1976        | 1978         | rBV      | 220            | 161           | 0.03%           | 0.004%        |
| 29        | 7.899       | 2023          | 2040        | 2058         | rBV      | 258578         | 449050        | 77.37%          | 9.799%        |
| 30        | 8.179       | 2117          | 2127        | 2144         | rBV      | 50356          | 83127         | 14.32%          | 1.814%        |
| 31        | 8.320       | 2166          | 2171        | 2173         | rBV2     | 268            | 166           | 0.03%           | 0.004%        |
| 32        | 8.343       | 2173          | 2178        | 2182         | rBV2     | 265            | 254           | 0.04%           | 0.006%        |
| 33        | 8.407       | 2195          | 2198        | 2200         | rBV2     | 158            | 89            | 0.02%           | 0.002%        |
| 34        | 8.423       | 2200          | 2203        | 2207         | rBV2     | 217            | 183           | 0.03%           | 0.004%        |
| 35        | 8.472       | 2212          | 2218        | 2226         | rVB2     | 3049           | 4679          | 0.81%           | 0.102%        |
| 36        | 8.552       | 2238          | 2243        | 2254         | rVB3     | 1528           | 2161          | 0.37%           | 0.047%        |

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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 | 8.636  | 2254 | 2269 | 2297 | rBV  | 158562 | 284951 | 49.10% | 6.218%  |
| 38 | 8.848  | 2333 | 2335 | 2339 | rBV2 | 329    | 290    | 0.05%  | 0.006%  |
| 39 | 8.896  | 2346 | 2350 | 2352 | rBV2 | 153    | 121    | 0.02%  | 0.003%  |
| 40 | 9.057  | 2397 | 2400 | 2405 | rBV  | 207    | 165    | 0.03%  | 0.004%  |
| 41 | 9.121  | 2416 | 2420 | 2424 | rBV  | 223    | 255    | 0.04%  | 0.006%  |
| 42 | 9.189  | 2438 | 2441 | 2444 | rVB  | 343    | 199    | 0.03%  | 0.004%  |
| 43 | 9.208  | 2444 | 2447 | 2450 | rVB2 | 143    | 84     | 0.01%  | 0.002%  |
| 44 | 9.227  | 2450 | 2453 | 2455 | rBV2 | 200    | 165    | 0.03%  | 0.004%  |
| 45 | 9.269  | 2463 | 2466 | 2467 | rBV  | 240    | 150    | 0.03%  | 0.003%  |
| 46 | 9.340  | 2486 | 2488 | 2491 | rVB  | 164    | 79     | 0.01%  | 0.002%  |
| 47 | 9.420  | 2500 | 2513 | 2536 | rBV  | 279033 | 463542 | 79.87% | 10.116% |
| 48 | 9.571  | 2557 | 2560 | 2563 | rBV  | 371    | 266    | 0.05%  | 0.006%  |
| 49 | 9.642  | 2580 | 2582 | 2585 | rBV2 | 118    | 72     | 0.01%  | 0.002%  |
| 50 | 9.957  | 2678 | 2680 | 2683 | rVB  | 154    | 76     | 0.01%  | 0.002%  |
| 51 | 9.976  | 2683 | 2686 | 2692 | rVB2 | 196    | 178    | 0.03%  | 0.004%  |
| 52 | 10.012 | 2692 | 2697 | 2700 | rBV  | 203    | 194    | 0.03%  | 0.004%  |
| 53 | 10.031 | 2700 | 2703 | 2707 | rBV  | 158    | 119    | 0.02%  | 0.003%  |
| 54 | 10.102 | 2719 | 2725 | 2728 | rBV2 | 395    | 329    | 0.06%  | 0.007%  |
| 55 | 10.243 | 2763 | 2769 | 2771 | rBV2 | 274    | 270    | 0.05%  | 0.006%  |
| 56 | 10.500 | 2846 | 2849 | 2852 | rBV2 | 356    | 298    | 0.05%  | 0.007%  |
| 57 | 10.555 | 2861 | 2866 | 2869 | rBV  | 432    | 408    | 0.07%  | 0.009%  |
| 58 | 10.668 | 2895 | 2901 | 2910 | rBV2 | 1416   | 2133   | 0.37%  | 0.047%  |
| 59 | 10.758 | 2917 | 2929 | 2948 | rVB  | 193816 | 308001 | 53.07% | 6.721%  |
| 60 | 10.857 | 2958 | 2960 | 2961 | rBV2 | 123    | 57     | 0.01%  | 0.001%  |
| 61 | 10.893 | 2961 | 2971 | 2982 | rVV3 | 6136   | 10133  | 1.75%  | 0.221%  |
| 62 | 11.002 | 3001 | 3005 | 3007 | rBV2 | 280    | 202    | 0.03%  | 0.004%  |
| 63 | 11.127 | 3040 | 3044 | 3046 | rBV2 | 267    | 224    | 0.04%  | 0.005%  |
| 64 | 11.185 | 3057 | 3062 | 3068 | rBV2 | 235    | 296    | 0.05%  | 0.006%  |
| 65 | 11.240 | 3074 | 3079 | 3083 | rBB2 | 351    | 304    | 0.05%  | 0.007%  |
| 66 | 11.266 | 3083 | 3087 | 3091 | rBV  | 283    | 278    | 0.05%  | 0.006%  |
| 67 | 11.356 | 3113 | 3115 | 3119 | rBV2 | 120    | 75     | 0.01%  | 0.002%  |
| 68 | 11.433 | 3134 | 3139 | 3140 | rBV  | 370    | 333    | 0.06%  | 0.007%  |
| 69 | 11.584 | 3183 | 3186 | 3190 | rVB2 | 464    | 332    | 0.06%  | 0.007%  |
| 70 | 11.693 | 3216 | 3220 | 3227 | rVB3 | 425    | 524    | 0.09%  | 0.011%  |
| 71 | 11.735 | 3231 | 3233 | 3235 | rBV  | 213    | 116    | 0.02%  | 0.003%  |
| 72 | 11.751 | 3235 | 3238 | 3241 | rVB  | 305    | 171    | 0.03%  | 0.004%  |
| 73 | 11.812 | 3245 | 3257 | 3276 | rBV  | 304677 | 469294 | 80.86% | 10.241% |
| 74 | 12.060 | 3325 | 3334 | 3341 | rBV4 | 4039   | 6040   | 1.04%  | 0.132%  |
| 75 | 12.153 | 3360 | 3363 | 3364 | rBV  | 470    | 291    | 0.05%  | 0.006%  |
| 76 | 12.195 | 3364 | 3376 | 3393 | rVB  | 264628 | 424741 | 73.19% | 9.269%  |

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 77 | 12.330 | 3411 | 3418 | 3421 | rBV2 | 557  | 590  | 0.10% | 0.013% |
| 78 | 12.378 | 3429 | 3433 | 3435 | rBV2 | 251  | 222  | 0.04% | 0.005% |
| 79 | 12.468 | 3457 | 3461 | 3464 | rBV2 | 271  | 209  | 0.04% | 0.005% |
| 80 | 12.658 | 3518 | 3520 | 3522 | rBV  | 214  | 101  | 0.02% | 0.002% |
| 81 | 12.674 | 3522 | 3525 | 3529 | rVV  | 275  | 199  | 0.03% | 0.004% |
| 82 | 12.774 | 3546 | 3556 | 3563 | rBV3 | 2196 | 2988 | 0.51% | 0.065% |
| 83 | 12.870 | 3583 | 3586 | 3587 | rBV  | 248  | 130  | 0.02% | 0.003% |
| 84 | 12.886 | 3588 | 3591 | 3598 | rVB4 | 638  | 650  | 0.11% | 0.014% |
| 85 | 13.028 | 3632 | 3635 | 3637 | rBV  | 181  | 126  | 0.02% | 0.003% |
| 86 | 13.211 | 3684 | 3692 | 3702 | rVB5 | 2260 | 3239 | 0.56% | 0.071% |
| 87 | 13.420 | 3752 | 3757 | 3762 | rBV2 | 285  | 425  | 0.07% | 0.009% |
| 88 | 13.938 | 3915 | 3918 | 3920 | rBV  | 248  | 155  | 0.03% | 0.003% |
| 89 | 14.063 | 3953 | 3957 | 3961 | rBV2 | 412  | 435  | 0.07% | 0.009% |
| 90 | 14.147 | 3978 | 3983 | 3986 | rBV2 | 322  | 378  | 0.07% | 0.008% |
| 91 | 14.394 | 4056 | 4060 | 4063 | rBV  | 252  | 250  | 0.04% | 0.005% |
| 92 | 14.722 | 4156 | 4162 | 4165 | rBV2 | 440  | 545  | 0.09% | 0.012% |
| 93 | 15.346 | 4353 | 4356 | 4359 | rVB  | 411  | 266  | 0.05% | 0.006% |
| 94 | 15.712 | 4468 | 4470 | 4473 | rVB2 | 290  | 156  | 0.03% | 0.003% |
| 95 | 15.757 | 4481 | 4484 | 4488 | rBV3 | 348  | 334  | 0.06% | 0.007% |
| 96 | 15.831 | 4504 | 4507 | 4511 | rBV  | 312  | 296  | 0.05% | 0.006% |

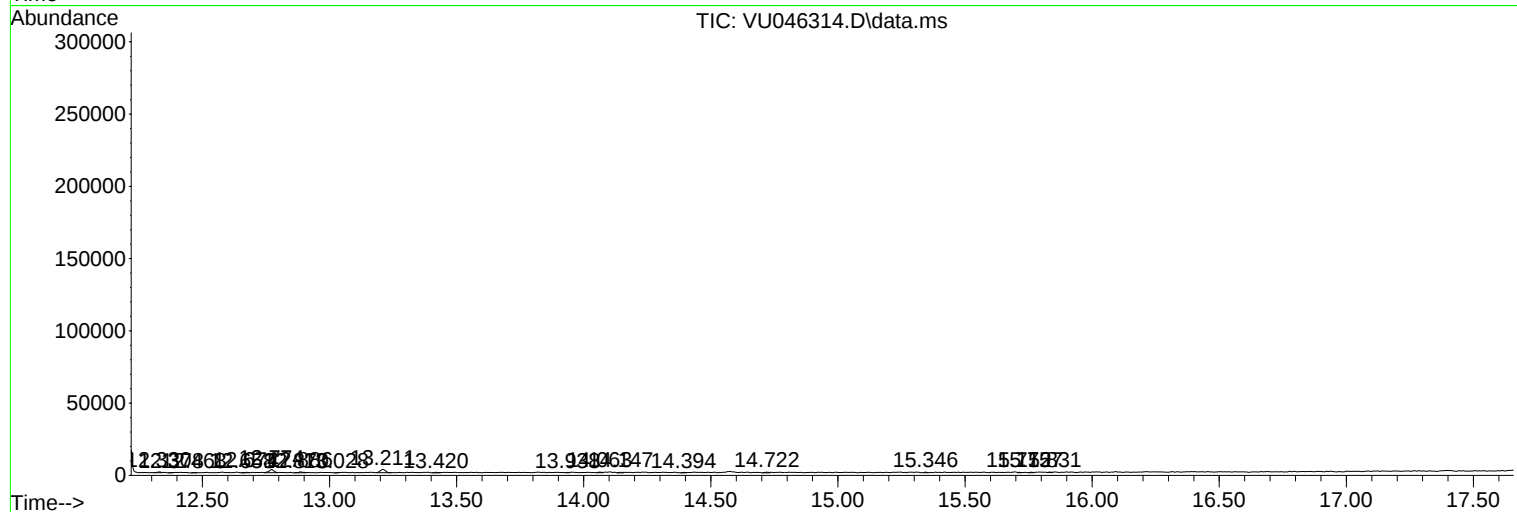
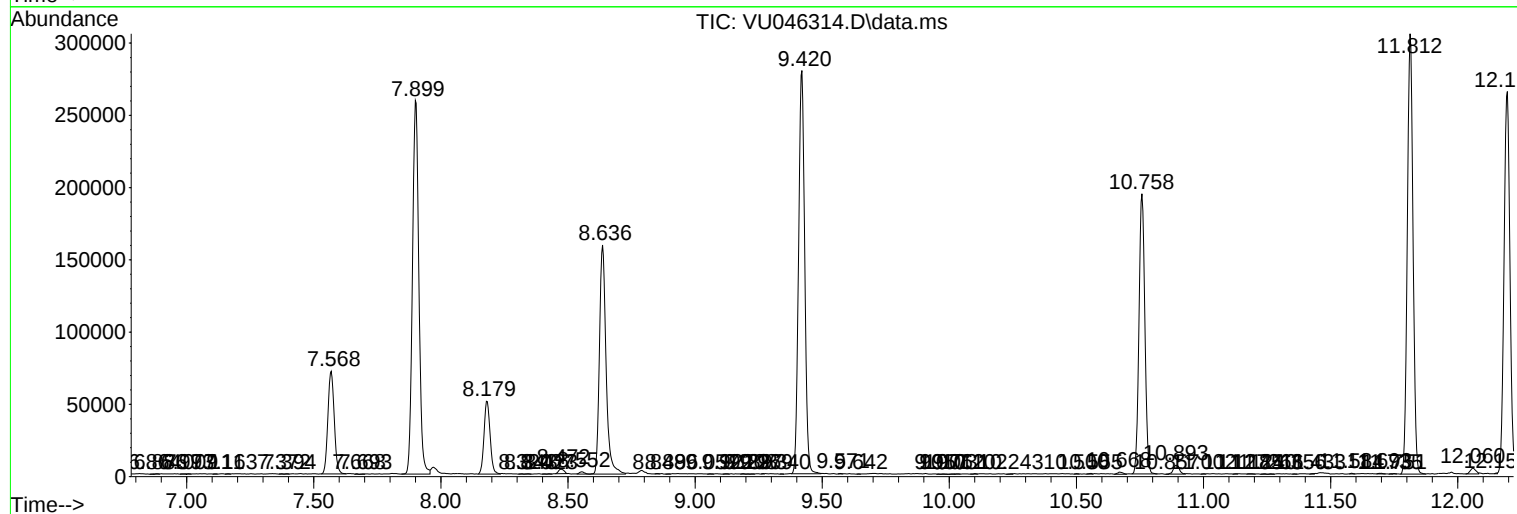
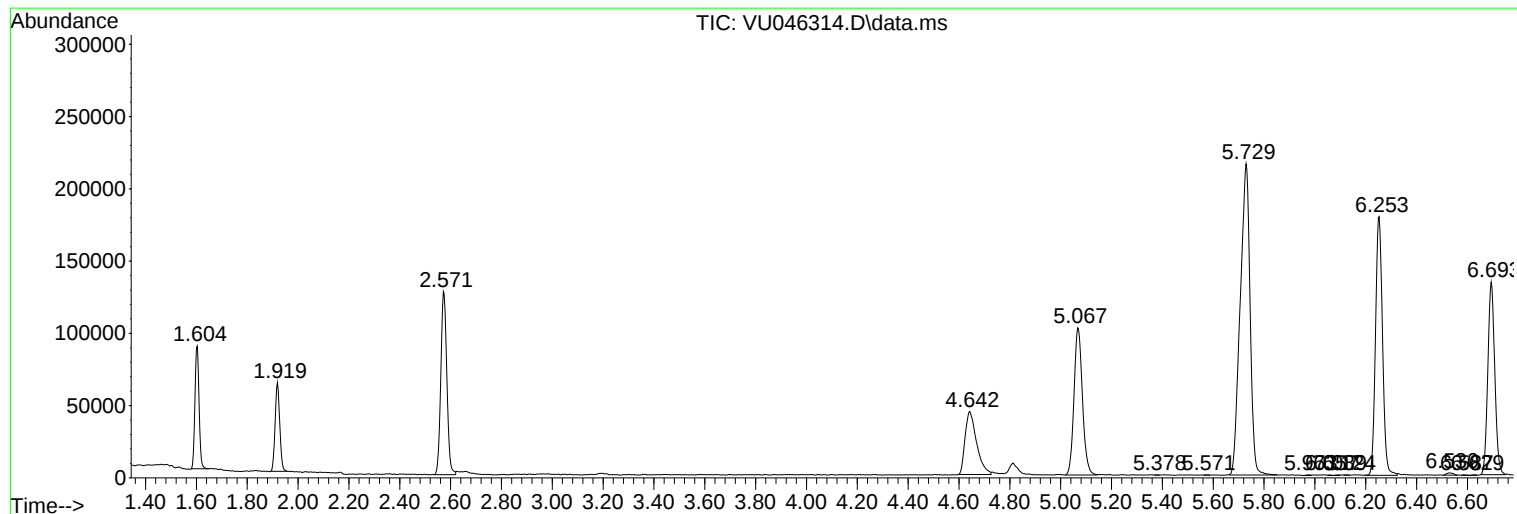
Sum of corrected areas: 4582455

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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121321\  
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No Library Search Compounds Detected

\*\*\*\*\*

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