

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100421\  
 Data File : VU045114.D  
 Acq On : 04 Oct 2021 22:58  
 Operator : SY/MD  
 Sample : M4023-11 100X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AK0

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045114.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       | 74            | 82          | 97           | rVB2     | 130919         | 158860        | 2.38%           | 0.668%        |
| 2         | 1.896       | 167           | 173         | 190          | rVB      | 69825          | 93436         | 1.40%           | 0.393%        |
| 3         | 2.240       | 276           | 280         | 288          | rVB2     | 6361           | 7664          | 0.11%           | 0.032%        |
| 4         | 2.575       | 368           | 384         | 401          | rBV4     | 445136         | 877919        | 13.14%          | 3.693%        |
| 5         | 2.800       | 446           | 454         | 459          | rVB      | 498            | 784           | 0.01%           | 0.003%        |
| 6         | 2.848       | 465           | 469         | 473          | rVB2     | 206            | 225           | 0.00%           | 0.001%        |
| 7         | 2.871       | 473           | 476         | 479          | rBV2     | 378            | 280           | 0.00%           | 0.001%        |
| 8         | 2.948       | 496           | 500         | 501          | rBV2     | 425            | 303           | 0.00%           | 0.001%        |
| 9         | 2.957       | 501           | 503         | 509          | rVB2     | 446            | 452           | 0.01%           | 0.002%        |
| 10        | 3.048       | 516           | 531         | 562          | rBV      | 1199660        | 2352009       | 35.21%          | 9.893%        |
| 11        | 3.321       | 612           | 616         | 618          | rBV      | 354            | 241           | 0.00%           | 0.001%        |
| 12        | 3.356       | 618           | 627         | 636          | rVV3     | 2658           | 4902          | 0.07%           | 0.021%        |
| 13        | 3.414       | 641           | 645         | 646          | rBV      | 283            | 213           | 0.00%           | 0.001%        |
| 14        | 3.472       | 659           | 663         | 666          | rBV2     | 191            | 181           | 0.00%           | 0.001%        |
| 15        | 3.736       | 742           | 745         | 752          | rVB2     | 231            | 294           | 0.00%           | 0.001%        |
| 16        | 3.771       | 752           | 756         | 759          | rBV      | 203            | 202           | 0.00%           | 0.001%        |
| 17        | 3.874       | 771           | 788         | 806          | rVV      | 52276          | 123009        | 1.84%           | 0.517%        |
| 18        | 3.977       | 816           | 820         | 822          | rBV      | 220            | 195           | 0.00%           | 0.001%        |
| 19        | 4.137       | 865           | 870         | 875          | rBV2     | 207            | 315           | 0.00%           | 0.001%        |
| 20        | 4.440       | 959           | 964         | 968          | rBV2     | 186            | 246           | 0.00%           | 0.001%        |
| 21        | 4.671       | 1008          | 1036        | 1083         | rBV2     | 1167960        | 2953970       | 44.22%          | 12.425%       |
| 22        | 4.973       | 1127          | 1130        | 1137         | rVV3     | 290            | 264           | 0.00%           | 0.001%        |
| 23        | 5.067       | 1142          | 1159        | 1182         | rVV      | 219444         | 478452        | 7.16%           | 2.012%        |
| 24        | 5.321       | 1219          | 1238        | 1262         | rBV      | 765494         | 1715579       | 25.68%          | 7.216%        |
| 25        | 5.462       | 1276          | 1282        | 1284         | rBV3     | 214            | 245           | 0.00%           | 0.001%        |
| 26        | 5.729       | 1343          | 1365        | 1381         | rBV2     | 437629         | 1188708       | 17.79%          | 5.000%        |
| 27        | 5.980       | 1440          | 1443        | 1446         | rBV2     | 294            | 186           | 0.00%           | 0.001%        |
| 28        | 6.096       | 1474          | 1479        | 1482         | rBV2     | 193            | 177           | 0.00%           | 0.001%        |
| 29        | 6.115       | 1482          | 1485        | 1486         | rVV      | 280            | 202           | 0.00%           | 0.001%        |
| 30        | 6.134       | 1488          | 1491        | 1499         | rVB4     | 616            | 751           | 0.01%           | 0.003%        |
| 31        | 6.253       | 1512          | 1528        | 1548         | rBV      | 387396         | 718080        | 10.75%          | 3.020%        |
| 32        | 6.546       | 1602          | 1619        | 1651         | rBV      | 3612805        | 6680061       | 100.00%         | 28.098%       |
| 33        | 6.694       | 1653          | 1665        | 1683         | rVB      | 288221         | 560261        | 8.39%           | 2.357%        |
| 34        | 6.996       | 1754          | 1759        | 1763         | rBV3     | 368            | 461           | 0.01%           | 0.002%        |
| 35        | 7.054       | 1770          | 1777        | 1784         | rVB2     | 724            | 929           | 0.01%           | 0.004%        |
| 36        | 7.189       | 1809          | 1819        | 1830         | rVB5     | 3391           | 6224          | 0.09%           | 0.026%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 7.369  | 1871 | 1875 | 1878 | rBV2 | 211    | 217    | 0.00%  | 0.001% |
| 38 | 7.504  | 1910 | 1917 | 1922 | rBV2 | 308    | 274    | 0.00%  | 0.001% |
| 39 | 7.568  | 1923 | 1937 | 1955 | rBV  | 157271 | 276293 | 4.14%  | 1.162% |
| 40 | 7.690  | 1968 | 1975 | 1985 | rVB4 | 1582   | 2598   | 0.04%  | 0.011% |
| 41 | 7.771  | 1993 | 2000 | 2003 | rBV2 | 157    | 204    | 0.00%  | 0.001% |
| 42 | 7.800  | 2003 | 2009 | 2019 | rBV4 | 1417   | 2012   | 0.03%  | 0.008% |
| 43 | 7.903  | 2027 | 2041 | 2055 | rBV  | 515264 | 891832 | 13.35% | 3.751% |
| 44 | 7.973  | 2055 | 2063 | 2075 | rVB  | 15843  | 26534  | 0.40%  | 0.112% |
| 45 | 8.137  | 2108 | 2114 | 2116 | rBV2 | 366    | 326    | 0.00%  | 0.001% |
| 46 | 8.182  | 2116 | 2128 | 2144 | rVV  | 111640 | 185522 | 2.78%  | 0.780% |
| 47 | 8.404  | 2187 | 2197 | 2215 | rBV2 | 16566  | 27056  | 0.41%  | 0.114% |
| 48 | 8.475  | 2216 | 2219 | 2225 | rVB2 | 338    | 311    | 0.00%  | 0.001% |
| 49 | 8.555  | 2238 | 2244 | 2251 | rVB4 | 1940   | 2649   | 0.04%  | 0.011% |
| 50 | 8.642  | 2257 | 2271 | 2306 | rBV  | 504438 | 918537 | 13.75% | 3.864% |
| 51 | 8.796  | 2318 | 2319 | 2322 | rVB  | 477    | 214    | 0.00%  | 0.001% |
| 52 | 8.893  | 2346 | 2349 | 2356 | rVB2 | 173    | 192    | 0.00%  | 0.001% |
| 53 | 9.095  | 2406 | 2412 | 2415 | rBV2 | 213    | 277    | 0.00%  | 0.001% |
| 54 | 9.131  | 2420 | 2423 | 2427 | rBV  | 202    | 198    | 0.00%  | 0.001% |
| 55 | 9.420  | 2499 | 2513 | 2533 | rBV  | 537397 | 878860 | 13.16% | 3.697% |
| 56 | 9.536  | 2543 | 2549 | 2553 | rBV3 | 2104   | 2680   | 0.04%  | 0.011% |
| 57 | 9.575  | 2553 | 2561 | 2570 | rVB  | 10090  | 15237  | 0.23%  | 0.064% |
| 58 | 9.642  | 2579 | 2582 | 2587 | rBV2 | 192    | 181    | 0.00%  | 0.001% |
| 59 | 9.697  | 2587 | 2599 | 2613 | rVV  | 36991  | 60232  | 0.90%  | 0.253% |
| 60 | 9.771  | 2619 | 2622 | 2628 | rVB2 | 954    | 780    | 0.01%  | 0.003% |
| 61 | 9.832  | 2638 | 2641 | 2646 | rVB2 | 211    | 186    | 0.00%  | 0.001% |
| 62 | 9.867  | 2646 | 2652 | 2656 | rBV2 | 183    | 220    | 0.00%  | 0.001% |
| 63 | 9.922  | 2666 | 2669 | 2675 | rBV  | 172    | 233    | 0.00%  | 0.001% |
| 64 | 10.105 | 2712 | 2726 | 2738 | rBV  | 17722  | 28508  | 0.43%  | 0.120% |
| 65 | 10.227 | 2760 | 2764 | 2767 | rBV2 | 267    | 183    | 0.00%  | 0.001% |
| 66 | 10.259 | 2770 | 2774 | 2779 | rBV  | 192    | 195    | 0.00%  | 0.001% |
| 67 | 10.491 | 2842 | 2846 | 2849 | rVB2 | 264    | 206    | 0.00%  | 0.001% |
| 68 | 10.575 | 2868 | 2872 | 2881 | rVB3 | 689    | 938    | 0.01%  | 0.004% |
| 69 | 10.674 | 2896 | 2903 | 2909 | rVB3 | 1661   | 2339   | 0.04%  | 0.010% |
| 70 | 10.761 | 2917 | 2930 | 2952 | rVV  | 468795 | 747274 | 11.19% | 3.143% |
| 71 | 11.005 | 2996 | 3006 | 3008 | rBV2 | 650    | 953    | 0.01%  | 0.004% |
| 72 | 11.070 | 3022 | 3026 | 3028 | rBV  | 227    | 186    | 0.00%  | 0.001% |
| 73 | 11.095 | 3028 | 3034 | 3037 | rVV4 | 499    | 645    | 0.01%  | 0.003% |
| 74 | 11.250 | 3078 | 3082 | 3085 | rBV2 | 220    | 246    | 0.00%  | 0.001% |
| 75 | 11.295 | 3092 | 3096 | 3103 | rBB2 | 308    | 337    | 0.01%  | 0.001% |
| 76 | 11.468 | 3142 | 3150 | 3159 | rVB4 | 2190   | 3375   | 0.05%  | 0.014% |

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.558 | 3170 | 3178 | 3182 | rBV2 | 259    | 397    | 0.01%  | 0.002% |
| 78  | 11.581 | 3182 | 3185 | 3192 | rVB  | 351    | 320    | 0.00%  | 0.001% |
| 79  | 11.636 | 3200 | 3202 | 3209 | rVB2 | 170    | 190    | 0.00%  | 0.001% |
| 80  | 11.700 | 3209 | 3222 | 3225 | rBV3 | 984    | 1489   | 0.02%  | 0.006% |
|     |        |      |      |      |      |        |        |        |        |
| 81  | 11.816 | 3246 | 3258 | 3276 | rBV  | 542404 | 866781 | 12.98% | 3.646% |
| 82  | 11.902 | 3282 | 3285 | 3288 | rBV3 | 421    | 242    | 0.00%  | 0.001% |
| 83  | 12.198 | 3363 | 3377 | 3396 | rBV  | 541561 | 887090 | 13.28% | 3.731% |
| 84  | 12.333 | 3416 | 3419 | 3425 | rVB  | 337    | 359    | 0.01%  | 0.002% |
| 85  | 12.372 | 3425 | 3431 | 3438 | rBV2 | 331    | 584    | 0.01%  | 0.002% |
|     |        |      |      |      |      |        |        |        |        |
| 86  | 12.427 | 3444 | 3448 | 3451 | rBV  | 321    | 241    | 0.00%  | 0.001% |
| 87  | 12.539 | 3477 | 3483 | 3486 | rBV2 | 234    | 232    | 0.00%  | 0.001% |
| 88  | 12.581 | 3491 | 3496 | 3499 | rVV3 | 283    | 305    | 0.00%  | 0.001% |
| 89  | 12.748 | 3545 | 3548 | 3551 | rBV  | 308    | 302    | 0.00%  | 0.001% |
| 90  | 12.854 | 3575 | 3581 | 3587 | rVB  | 325    | 410    | 0.01%  | 0.002% |
|     |        |      |      |      |      |        |        |        |        |
| 91  | 12.886 | 3587 | 3591 | 3598 | rBV2 | 257    | 359    | 0.01%  | 0.002% |
| 92  | 13.449 | 3761 | 3766 | 3768 | rBV2 | 442    | 418    | 0.01%  | 0.002% |
| 93  | 14.095 | 3959 | 3967 | 3977 | rVB2 | 1585   | 2444   | 0.04%  | 0.010% |
| 94  | 14.156 | 3983 | 3986 | 3990 | rBV  | 321    | 238    | 0.00%  | 0.001% |
| 95  | 14.304 | 4026 | 4032 | 4034 | rBV2 | 358    | 330    | 0.00%  | 0.001% |
|     |        |      |      |      |      |        |        |        |        |
| 96  | 14.584 | 4111 | 4119 | 4128 | rVB4 | 904    | 1804   | 0.03%  | 0.008% |
| 97  | 14.623 | 4128 | 4131 | 4134 | rBV3 | 377    | 367    | 0.01%  | 0.002% |
| 98  | 14.870 | 4204 | 4208 | 4216 | rBV  | 414    | 695    | 0.01%  | 0.003% |
| 99  | 15.230 | 4312 | 4320 | 4328 | rBV3 | 1585   | 2704   | 0.04%  | 0.011% |
| 100 | 15.742 | 4477 | 4479 | 4481 | rBV2 | 435    | 244    | 0.00%  | 0.001% |

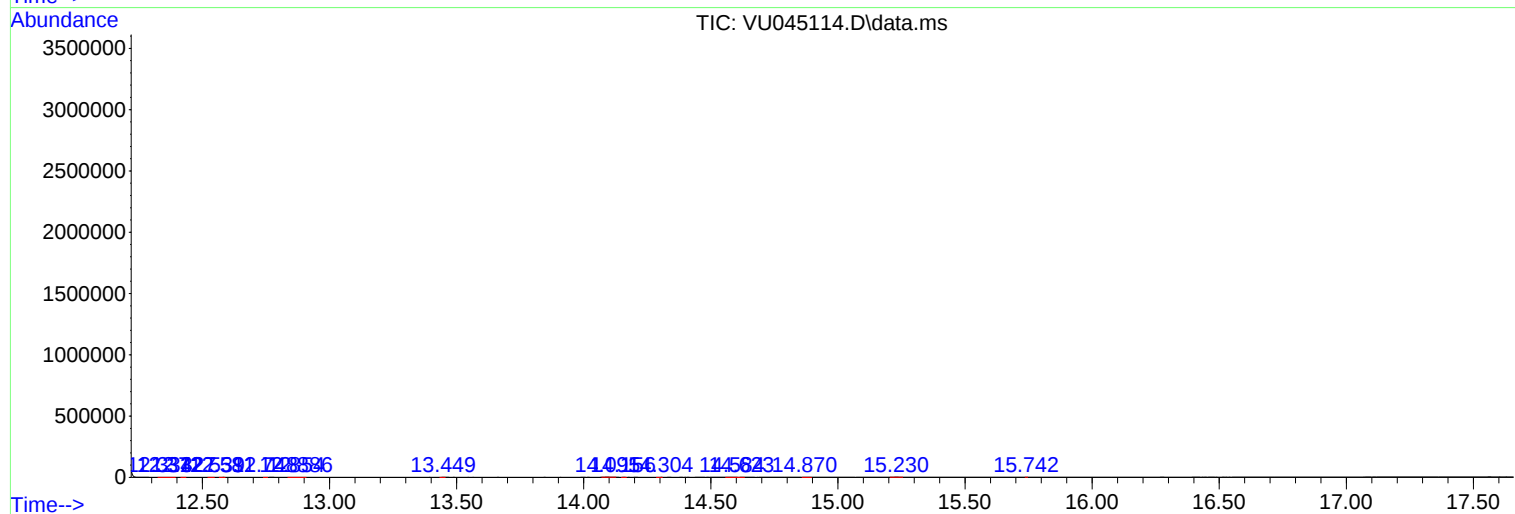
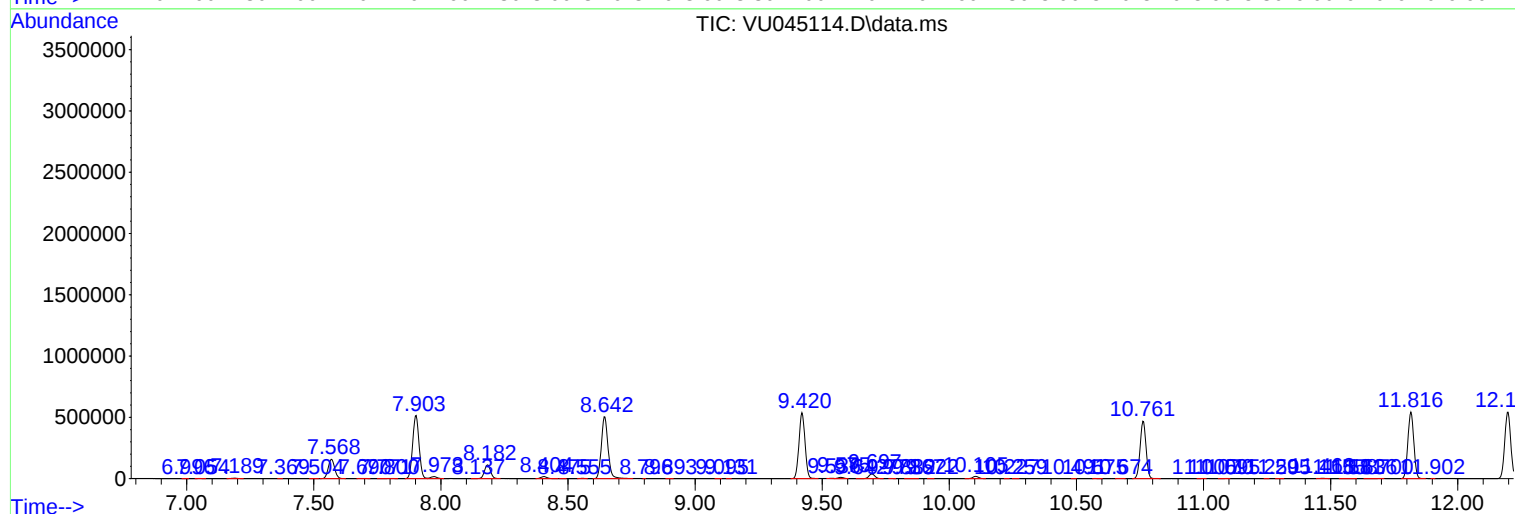
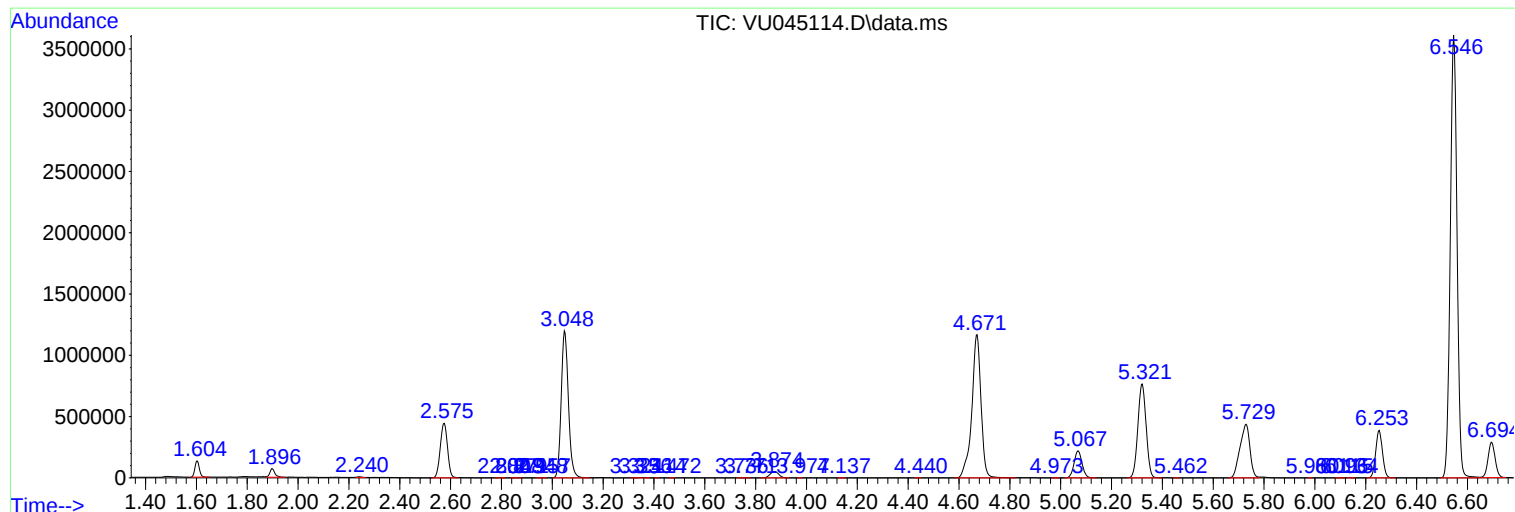
Sum of corrected areas: 23774065

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.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 |

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