

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121321\  
 Data File : VU046320.D  
 Acq On : 13 Dec 2021 17:03  
 Operator : SY/MD  
 Sample : VU1213WBL02  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK059

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: VU046320.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         | 1.601       | 74            | 81          | 96           | rBV      | 94790          | 105003        | 16.73%          | 2.173%        |
| 2         | 1.919       | 172           | 180         | 193          | rVB      | 67769          | 85649         | 13.64%          | 1.773%        |
| 3         | 2.231       | 273           | 277         | 281          | rVB      | 301            | 284           | 0.05%           | 0.006%        |
| 4         | 2.257       | 283           | 285         | 290          | rVB      | 438            | 302           | 0.05%           | 0.006%        |
| 5         | 2.286       | 290           | 294         | 298          | rVB      | 369            | 306           | 0.05%           | 0.006%        |
| 6         | 2.408       | 328           | 332         | 337          | rVB      | 422            | 373           | 0.06%           | 0.008%        |
| 7         | 2.433       | 337           | 340         | 344          | rBV2     | 533            | 390           | 0.06%           | 0.008%        |
| 8         | 2.572       | 371           | 383         | 406          | rBV      | 138039         | 231281        | 36.84%          | 4.786%        |
| 9         | 2.761       | 437           | 442         | 447          | rBV2     | 445            | 461           | 0.07%           | 0.010%        |
| 10        | 3.002       | 511           | 517         | 519          | rBV2     | 252            | 311           | 0.05%           | 0.006%        |
| 11        | 3.054       | 527           | 533         | 539          | rVB3     | 783            | 1017          | 0.16%           | 0.021%        |
| 12        | 3.093       | 541           | 545         | 548          | rVV      | 398            | 266           | 0.04%           | 0.006%        |
| 13        | 3.179       | 567           | 572         | 574          | rBV      | 645            | 594           | 0.09%           | 0.012%        |
| 14        | 3.359       | 625           | 628         | 633          | rVB      | 356            | 280           | 0.04%           | 0.006%        |
| 15        | 3.401       | 636           | 641         | 644          | rBV      | 382            | 349           | 0.06%           | 0.007%        |
| 16        | 3.449       | 653           | 656         | 659          | rVB2     | 430            | 297           | 0.05%           | 0.006%        |
| 17        | 3.478       | 659           | 665         | 668          | rBV      | 548            | 590           | 0.09%           | 0.012%        |
| 18        | 3.501       | 668           | 672         | 673          | rBV      | 423            | 293           | 0.05%           | 0.006%        |
| 19        | 3.581       | 692           | 697         | 704          | rVB2     | 539            | 643           | 0.10%           | 0.013%        |
| 20        | 3.671       | 722           | 725         | 730          | rVB2     | 379            | 290           | 0.05%           | 0.006%        |
| 21        | 3.884       | 788           | 791         | 795          | rVB      | 381            | 273           | 0.04%           | 0.006%        |
| 22        | 4.060       | 840           | 846         | 849          | rVB2     | 314            | 323           | 0.05%           | 0.007%        |
| 23        | 4.083       | 849           | 853         | 858          | rBV2     | 282            | 296           | 0.05%           | 0.006%        |
| 24        | 4.131       | 865           | 868         | 876          | rVB      | 442            | 440           | 0.07%           | 0.009%        |
| 25        | 4.179       | 876           | 883         | 887          | rBV2     | 360            | 520           | 0.08%           | 0.011%        |
| 26        | 4.237       | 896           | 901         | 908          | rBV2     | 344            | 467           | 0.07%           | 0.010%        |
| 27        | 4.324       | 924           | 928         | 933          | rVB      | 328            | 284           | 0.05%           | 0.006%        |
| 28        | 4.366       | 938           | 941         | 947          | rBV      | 329            | 418           | 0.07%           | 0.009%        |
| 29        | 4.465       | 966           | 972         | 976          | rVB2     | 528            | 574           | 0.09%           | 0.012%        |
| 30        | 4.639       | 1012          | 1026        | 1060         | rBV2     | 48973          | 148492        | 23.65%          | 3.073%        |
| 31        | 4.864       | 1093          | 1096        | 1100         | rVB2     | 415            | 302           | 0.05%           | 0.006%        |
| 32        | 4.893       | 1100          | 1105        | 1110         | rBV3     | 468            | 397           | 0.06%           | 0.008%        |
| 33        | 4.932       | 1110          | 1117        | 1119         | rBV2     | 265            | 370           | 0.06%           | 0.008%        |
| 34        | 4.990       | 1132          | 1135        | 1137         | rBV      | 475            | 337           | 0.05%           | 0.007%        |
| 35        | 5.067       | 1144          | 1159        | 1183         | rBV2     | 106637         | 254034        | 40.47%          | 5.257%        |
| 36        | 5.182       | 1192          | 1195        | 1200         | rBV2     | 463            | 460           | 0.07%           | 0.010%        |

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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

|    |        |      |      |      |      |        |        |         |         |
|----|--------|------|------|------|------|--------|--------|---------|---------|
| 37 | 5.224  | 1203 | 1208 | 1213 | rVB2 | 312    | 408    | 0.06%   | 0.008%  |
| 38 | 5.285  | 1219 | 1227 | 1228 | rBV2 | 275    | 313    | 0.05%   | 0.006%  |
| 39 | 5.588  | 1318 | 1321 | 1327 | rVB  | 430    | 353    | 0.06%   | 0.007%  |
| 40 | 5.626  | 1327 | 1333 | 1337 | rBV  | 491    | 495    | 0.08%   | 0.010%  |
| 41 | 5.729  | 1343 | 1365 | 1382 | rBV2 | 233992 | 627765 | 100.00% | 12.992% |
| 42 | 5.883  | 1410 | 1413 | 1419 | rVB2 | 364    | 330    | 0.05%   | 0.007%  |
| 43 | 6.060  | 1462 | 1468 | 1472 | rBV  | 445    | 624    | 0.10%   | 0.013%  |
| 44 | 6.118  | 1483 | 1486 | 1490 | rVB2 | 490    | 404    | 0.06%   | 0.008%  |
| 45 | 6.141  | 1490 | 1493 | 1499 | rBV  | 302    | 388    | 0.06%   | 0.008%  |
| 46 | 6.253  | 1512 | 1528 | 1553 | rBV  | 178479 | 340199 | 54.19%  | 7.041%  |
| 47 | 6.424  | 1578 | 1581 | 1587 | rBV  | 302    | 266    | 0.04%   | 0.006%  |
| 48 | 6.530  | 1607 | 1614 | 1622 | rVB5 | 1957   | 3329   | 0.53%   | 0.069%  |
| 49 | 6.565  | 1622 | 1625 | 1629 | rVB  | 447    | 341    | 0.05%   | 0.007%  |
| 50 | 6.694  | 1651 | 1665 | 1685 | rBV  | 145408 | 278055 | 44.29%  | 5.754%  |
| 51 | 6.813  | 1696 | 1702 | 1703 | rBV2 | 311    | 280    | 0.04%   | 0.006%  |
| 52 | 6.871  | 1717 | 1720 | 1723 | rBV2 | 449    | 281    | 0.04%   | 0.006%  |
| 53 | 7.006  | 1757 | 1762 | 1765 | rBV  | 331    | 352    | 0.06%   | 0.007%  |
| 54 | 7.520  | 1916 | 1922 | 1925 | rBV  | 517    | 624    | 0.10%   | 0.013%  |
| 55 | 7.568  | 1925 | 1937 | 1956 | rVV  | 77512  | 134400 | 21.41%  | 2.781%  |
| 56 | 7.697  | 1974 | 1977 | 1982 | rVB  | 450    | 292    | 0.05%   | 0.006%  |
| 57 | 7.784  | 2001 | 2004 | 2007 | rVB2 | 371    | 272    | 0.04%   | 0.006%  |
| 58 | 7.899  | 2027 | 2040 | 2057 | rBV  | 285257 | 488639 | 77.84%  | 10.113% |
| 59 | 8.131  | 2109 | 2112 | 2115 | rBV  | 373    | 276    | 0.04%   | 0.006%  |
| 60 | 8.182  | 2115 | 2128 | 2142 | rVV  | 55065  | 91252  | 14.54%  | 1.889%  |
| 61 | 8.308  | 2163 | 2167 | 2170 | rVB3 | 450    | 312    | 0.05%   | 0.006%  |
| 62 | 8.337  | 2170 | 2176 | 2180 | rBV  | 324    | 328    | 0.05%   | 0.007%  |
| 63 | 8.382  | 2186 | 2190 | 2195 | rVB2 | 337    | 369    | 0.06%   | 0.008%  |
| 64 | 8.636  | 2256 | 2269 | 2300 | rBV  | 173801 | 307096 | 48.92%  | 6.355%  |
| 65 | 8.912  | 2349 | 2355 | 2362 | rBV2 | 891    | 1350   | 0.22%   | 0.028%  |
| 66 | 9.089  | 2405 | 2410 | 2415 | rVV  | 537    | 547    | 0.09%   | 0.011%  |
| 67 | 9.189  | 2437 | 2441 | 2446 | rVB  | 634    | 677    | 0.11%   | 0.014%  |
| 68 | 9.237  | 2452 | 2456 | 2461 | rBV2 | 363    | 522    | 0.08%   | 0.011%  |
| 69 | 9.288  | 2469 | 2472 | 2476 | rBV  | 446    | 328    | 0.05%   | 0.007%  |
| 70 | 9.311  | 2476 | 2479 | 2484 | rVB2 | 427    | 333    | 0.05%   | 0.007%  |
| 71 | 9.420  | 2500 | 2513 | 2535 | rBV  | 274112 | 456591 | 72.73%  | 9.449%  |
| 72 | 9.568  | 2551 | 2559 | 2564 | rBV2 | 846    | 1217   | 0.19%   | 0.025%  |
| 73 | 9.658  | 2581 | 2587 | 2590 | rBV2 | 485    | 546    | 0.09%   | 0.011%  |
| 74 | 9.838  | 2640 | 2643 | 2647 | rVB2 | 396    | 270    | 0.04%   | 0.006%  |
| 75 | 9.864  | 2647 | 2651 | 2654 | rBV  | 496    | 464    | 0.07%   | 0.010%  |
| 76 | 10.022 | 2696 | 2700 | 2704 | rBV2 | 483    | 405    | 0.06%   | 0.008%  |

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 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 10.276 | 2776 | 2779 | 2782 | rBV  | 437    | 323    | 0.05%  | 0.007% |
| 78  | 10.446 | 2829 | 2832 | 2835 | rBV  | 430    | 335    | 0.05%  | 0.007% |
| 79  | 10.674 | 2898 | 2903 | 2910 | rVB3 | 1389   | 1489   | 0.24%  | 0.031% |
| 80  | 10.758 | 2917 | 2929 | 2947 | rVB  | 208888 | 333016 | 53.05% | 6.892% |
| 81  | 10.893 | 2969 | 2971 | 2978 | rVB2 | 555    | 428    | 0.07%  | 0.009% |
| 82  | 11.009 | 3003 | 3007 | 3011 | rVB2 | 598    | 538    | 0.09%  | 0.011% |
| 83  | 11.256 | 3080 | 3084 | 3090 | rVB2 | 360    | 453    | 0.07%  | 0.009% |
| 84  | 11.459 | 3141 | 3147 | 3148 | rBV4 | 798    | 822    | 0.13%  | 0.017% |
| 85  | 11.530 | 3165 | 3169 | 3175 | rBV  | 488    | 710    | 0.11%  | 0.015% |
| 86  | 11.812 | 3242 | 3257 | 3273 | rBV  | 290216 | 454746 | 72.44% | 9.411% |
| 87  | 11.896 | 3279 | 3283 | 3285 | rBV  | 451    | 375    | 0.06%  | 0.008% |
| 88  | 12.195 | 3363 | 3376 | 3391 | rVB  | 287596 | 454230 | 72.36% | 9.401% |
| 89  | 12.771 | 3552 | 3555 | 3561 | rVB3 | 717    | 738    | 0.12%  | 0.015% |
| 90  | 12.816 | 3565 | 3569 | 3573 | rBV2 | 385    | 370    | 0.06%  | 0.008% |
| 91  | 13.423 | 3755 | 3758 | 3761 | rBV  | 462    | 290    | 0.05%  | 0.006% |
| 92  | 13.533 | 3790 | 3792 | 3797 | rBV2 | 403    | 296    | 0.05%  | 0.006% |
| 93  | 13.668 | 3831 | 3834 | 3836 | rBV  | 379    | 272    | 0.04%  | 0.006% |
| 94  | 13.931 | 3913 | 3916 | 3920 | rBV2 | 471    | 356    | 0.06%  | 0.007% |
| 95  | 14.089 | 3960 | 3965 | 3969 | rBV3 | 738    | 855    | 0.14%  | 0.018% |
| 96  | 14.574 | 4110 | 4116 | 4124 | rVB2 | 1145   | 1778   | 0.28%  | 0.037% |
| 97  | 14.713 | 4156 | 4159 | 4162 | rVB2 | 580    | 378    | 0.06%  | 0.008% |
| 98  | 15.217 | 4314 | 4316 | 4319 | rBV2 | 496    | 283    | 0.05%  | 0.006% |
| 99  | 15.729 | 4472 | 4475 | 4478 | rBV2 | 471    | 338    | 0.05%  | 0.007% |
| 100 | 15.783 | 4490 | 4492 | 4495 | rBV2 | 430    | 297    | 0.05%  | 0.006% |

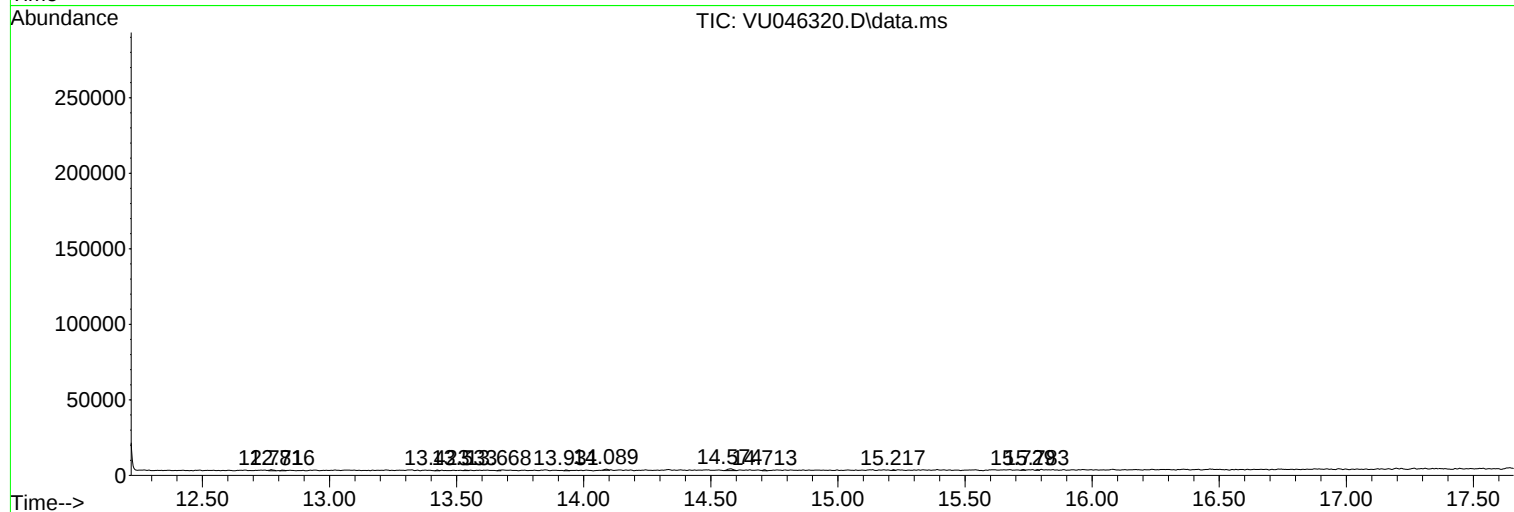
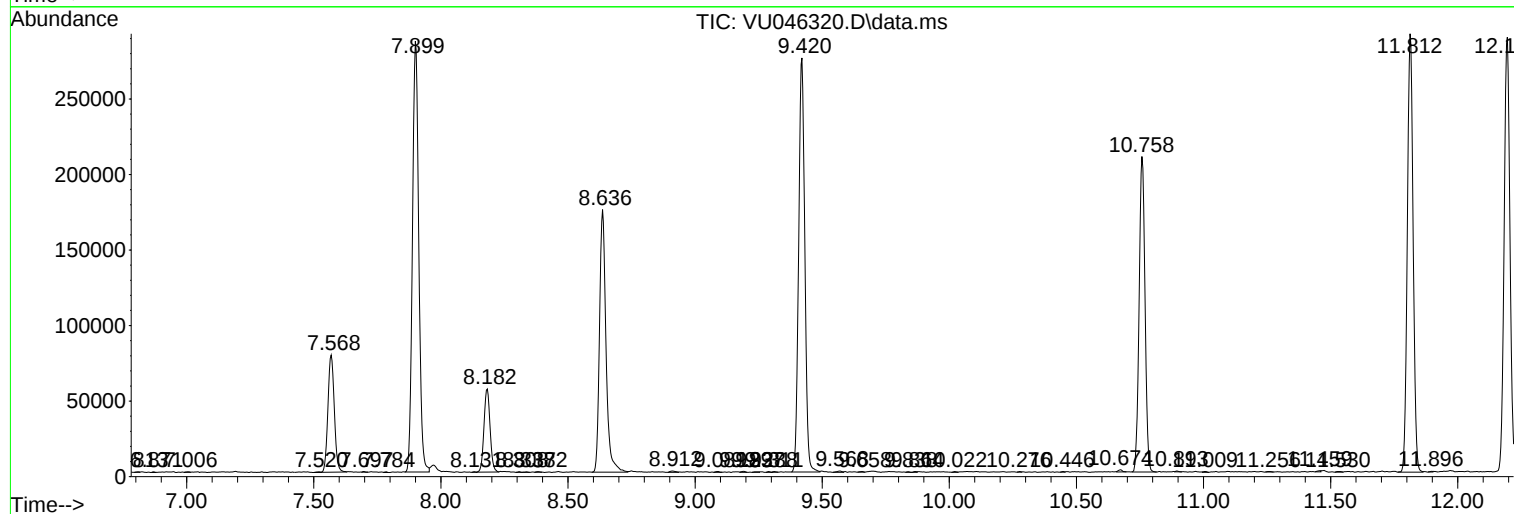
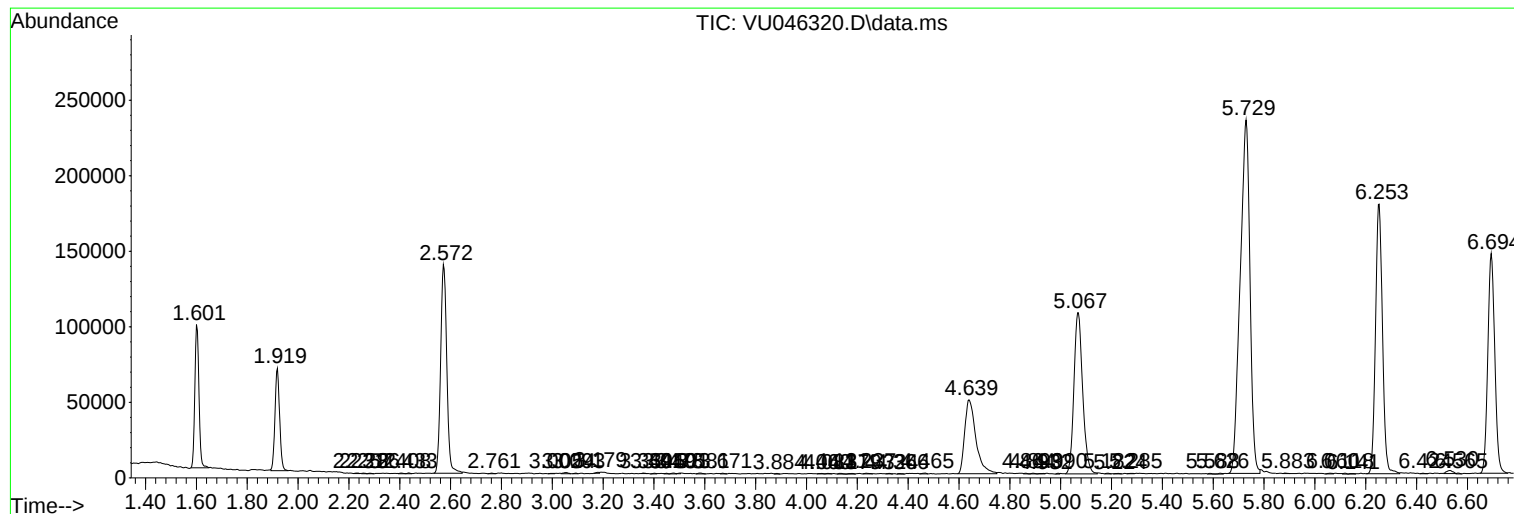
Sum of corrected areas: 4831975

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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 | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |