

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU042622\  
 Data File : VU048295.D  
 Acq On : 26 Apr 2022 12:44  
 Operator : SY/MD  
 Sample : VU0426WBL01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK113

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\SFAMULM042522WMA.M  
 Title : VOC Analysis

Signal : TIC: VU048295.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         | 1.485       | 40            | 45          | 51           | rBV2     | 4042           | 5027          | 0.29%           | 0.040%        |
| 2         | 1.520       | 52            | 56          | 68           | rVB      | 3791           | 5850          | 0.34%           | 0.046%        |
| 3         | 1.601       | 73            | 81          | 102          | rVV      | 194017         | 259295        | 15.13%          | 2.050%        |
| 4         | 1.903       | 168           | 175         | 204          | rVB      | 160522         | 254083        | 14.82%          | 2.009%        |
| 5         | 2.510       | 361           | 364         | 366          | rBV4     | 441            | 279           | 0.02%           | 0.002%        |
| 6         | 2.565       | 368           | 381         | 400          | rBV      | 356812         | 585728        | 34.18%          | 4.631%        |
| 7         | 2.690       | 418           | 420         | 424          | rVB2     | 367            | 254           | 0.01%           | 0.002%        |
| 8         | 2.736       | 431           | 434         | 437          | rBV2     | 364            | 308           | 0.02%           | 0.002%        |
| 9         | 2.793       | 448           | 452         | 455          | rVV2     | 526            | 548           | 0.03%           | 0.004%        |
| 10        | 2.945       | 496           | 499         | 500          | rBV      | 375            | 193           | 0.01%           | 0.002%        |
| 11        | 3.044       | 522           | 530         | 547          | rVB4     | 2168           | 3873          | 0.23%           | 0.031%        |
| 12        | 3.186       | 564           | 574         | 586          | rBV3     | 3161           | 6322          | 0.37%           | 0.050%        |
| 13        | 3.362       | 627           | 629         | 634          | rVV2     | 280            | 219           | 0.01%           | 0.002%        |
| 14        | 3.388       | 634           | 637         | 643          | rVB2     | 380            | 289           | 0.02%           | 0.002%        |
| 15        | 3.485       | 662           | 667         | 673          | rBV2     | 171            | 207           | 0.01%           | 0.002%        |
| 16        | 3.639       | 711           | 715         | 719          | rBV      | 266            | 276           | 0.02%           | 0.002%        |
| 17        | 3.719       | 738           | 740         | 745          | rVB2     | 366            | 242           | 0.01%           | 0.002%        |
| 18        | 3.758       | 745           | 752         | 753          | rBV2     | 279            | 243           | 0.01%           | 0.002%        |
| 19        | 3.797       | 760           | 764         | 768          | rBV2     | 195            | 211           | 0.01%           | 0.002%        |
| 20        | 4.002       | 822           | 828         | 833          | rVB2     | 221            | 280           | 0.02%           | 0.002%        |
| 21        | 4.031       | 833           | 837         | 841          | rBV2     | 189            | 202           | 0.01%           | 0.002%        |
| 22        | 4.131       | 865           | 868         | 871          | rVB      | 297            | 218           | 0.01%           | 0.002%        |
| 23        | 4.311       | 921           | 924         | 930          | rBV2     | 198            | 224           | 0.01%           | 0.002%        |
| 24        | 4.629       | 1008          | 1023        | 1069         | rBV      | 173517         | 471137        | 27.49%          | 3.725%        |
| 25        | 5.063       | 1142          | 1158        | 1184         | rBV      | 302401         | 668221        | 38.99%          | 5.284%        |
| 26        | 5.240       | 1209          | 1213        | 1217         | rVB2     | 314            | 218           | 0.01%           | 0.002%        |
| 27        | 5.279       | 1220          | 1225        | 1226         | rBV2     | 435            | 313           | 0.02%           | 0.002%        |
| 28        | 5.382       | 1254          | 1257        | 1262         | rBV3     | 417            | 430           | 0.03%           | 0.003%        |
| 29        | 5.459       | 1278          | 1281        | 1284         | rVB      | 324            | 240           | 0.01%           | 0.002%        |
| 30        | 5.523       | 1297          | 1301        | 1304         | rBV2     | 421            | 283           | 0.02%           | 0.002%        |
| 31        | 5.726       | 1342          | 1364        | 1394         | rBV2     | 643565         | 1713895       | 100.00%         | 13.552%       |
| 32        | 6.034       | 1456          | 1460        | 1468         | rVB4     | 553            | 729           | 0.04%           | 0.006%        |
| 33        | 6.118       | 1481          | 1486        | 1489         | rBV3     | 445            | 450           | 0.03%           | 0.004%        |
| 34        | 6.250       | 1511          | 1527        | 1547         | rBV      | 417952         | 792300        | 46.23%          | 6.265%        |
| 35        | 6.530       | 1606          | 1614        | 1627         | rVB6     | 1742           | 3282          | 0.19%           | 0.026%        |
| 36        | 6.600       | 1631          | 1636        | 1638         | rBV2     | 223            | 239           | 0.01%           | 0.002%        |

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042522WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.690  | 1648 | 1664 | 1693 | rBV  | 395908 | 775435  | 45.24% | 6.131%  |
| 38 | 6.806  | 1696 | 1700 | 1708 | rVV5 | 1270   | 1806    | 0.11%  | 0.014%  |
| 39 | 7.012  | 1761 | 1764 | 1769 | rVV2 | 225    | 209     | 0.01%  | 0.002%  |
| 40 | 7.044  | 1769 | 1774 | 1780 | rVB2 | 307    | 419     | 0.02%  | 0.003%  |
| 41 | 7.076  | 1780 | 1784 | 1787 | rBV3 | 225    | 206     | 0.01%  | 0.002%  |
| 42 | 7.189  | 1807 | 1819 | 1835 | rBV3 | 2844   | 6402    | 0.37%  | 0.051%  |
| 43 | 7.488  | 1908 | 1912 | 1915 | rBV  | 332    | 265     | 0.02%  | 0.002%  |
| 44 | 7.565  | 1923 | 1936 | 1964 | rVV2 | 208603 | 373539  | 21.79% | 2.954%  |
| 45 | 7.755  | 1990 | 1995 | 1997 | rBV  | 431    | 410     | 0.02%  | 0.003%  |
| 46 | 7.800  | 2002 | 2009 | 2018 | rVB5 | 1359   | 2346    | 0.14%  | 0.019%  |
| 47 | 7.899  | 2025 | 2040 | 2056 | rBV  | 780570 | 1349444 | 78.74% | 10.670% |
| 48 | 8.179  | 2115 | 2127 | 2142 | rBV  | 147571 | 252649  | 14.74% | 1.998%  |
| 49 | 8.411  | 2196 | 2199 | 2202 | rBV2 | 472    | 394     | 0.02%  | 0.003%  |
| 50 | 8.456  | 2209 | 2213 | 2215 | rBV3 | 230    | 211     | 0.01%  | 0.002%  |
| 51 | 8.555  | 2238 | 2244 | 2248 | rBV3 | 713    | 717     | 0.04%  | 0.006%  |
| 52 | 8.594  | 2252 | 2256 | 2257 | rBV3 | 368    | 211     | 0.01%  | 0.002%  |
| 53 | 8.639  | 2257 | 2270 | 2303 | rBV  | 558945 | 1035974 | 60.45% | 8.192%  |
| 54 | 8.793  | 2315 | 2318 | 2324 | rVB3 | 844    | 632     | 0.04%  | 0.005%  |
| 55 | 8.915  | 2352 | 2356 | 2357 | rBV2 | 330    | 227     | 0.01%  | 0.002%  |
| 56 | 8.954  | 2365 | 2368 | 2378 | rVB4 | 587    | 743     | 0.04%  | 0.006%  |
| 57 | 8.996  | 2378 | 2381 | 2384 | rBV2 | 485    | 282     | 0.02%  | 0.002%  |
| 58 | 9.015  | 2384 | 2387 | 2390 | rVB3 | 433    | 315     | 0.02%  | 0.002%  |
| 59 | 9.041  | 2390 | 2395 | 2398 | rBV  | 529    | 449     | 0.03%  | 0.004%  |
| 60 | 9.160  | 2429 | 2432 | 2436 | rVV3 | 296    | 263     | 0.02%  | 0.002%  |
| 61 | 9.311  | 2474 | 2479 | 2483 | rVB2 | 354    | 351     | 0.02%  | 0.003%  |
| 62 | 9.417  | 2496 | 2512 | 2539 | rBV  | 601868 | 1007131 | 58.76% | 7.964%  |
| 63 | 9.571  | 2554 | 2560 | 2572 | rVB3 | 822    | 1339    | 0.08%  | 0.011%  |
| 64 | 9.636  | 2577 | 2580 | 2582 | rBV2 | 284    | 226     | 0.01%  | 0.002%  |
| 65 | 9.655  | 2584 | 2586 | 2589 | rVB  | 445    | 193     | 0.01%  | 0.002%  |
| 66 | 9.693  | 2589 | 2598 | 2606 | rBV4 | 1222   | 1843    | 0.11%  | 0.015%  |
| 67 | 10.095 | 2719 | 2723 | 2725 | rBV2 | 486    | 408     | 0.02%  | 0.003%  |
| 68 | 10.108 | 2725 | 2727 | 2732 | rVB4 | 607    | 489     | 0.03%  | 0.004%  |
| 69 | 10.481 | 2840 | 2843 | 2847 | rBV3 | 587    | 498     | 0.03%  | 0.004%  |
| 70 | 10.671 | 2895 | 2902 | 2911 | rBV3 | 2629   | 3567    | 0.21%  | 0.028%  |
| 71 | 10.758 | 2916 | 2929 | 2947 | rBV  | 611331 | 982214  | 57.31% | 7.766%  |
| 72 | 10.864 | 2959 | 2962 | 2966 | rBV3 | 588    | 409     | 0.02%  | 0.003%  |
| 73 | 10.896 | 2966 | 2972 | 2974 | rBV3 | 596    | 535     | 0.03%  | 0.004%  |
| 74 | 10.960 | 2986 | 2992 | 2994 | rBV2 | 322    | 288     | 0.02%  | 0.002%  |
| 75 | 11.115 | 3038 | 3040 | 3042 | rBV  | 419    | 247     | 0.01%  | 0.002%  |
| 76 | 11.150 | 3047 | 3051 | 3056 | rVB2 | 326    | 309     | 0.02%  | 0.002%  |

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042522WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 11.414 | 3129 | 3133 | 3136 | rBV  | 468    | 395     | 0.02%  | 0.003% |
| 78  | 11.471 | 3140 | 3151 | 3156 | rBV5 | 2019   | 3641    | 0.21%  | 0.029% |
| 79  | 11.574 | 3179 | 3183 | 3186 | rBV3 | 397    | 279     | 0.02%  | 0.002% |
| 80  | 11.697 | 3216 | 3221 | 3226 | rBV  | 1203   | 1079    | 0.06%  | 0.009% |
| 81  | 11.745 | 3231 | 3236 | 3244 | rBV4 | 1362   | 2057    | 0.12%  | 0.016% |
| 82  | 11.812 | 3244 | 3257 | 3277 | rBV  | 561299 | 884101  | 51.58% | 6.991% |
| 83  | 11.973 | 3303 | 3307 | 3313 | rVB3 | 1457   | 1524    | 0.09%  | 0.012% |
| 84  | 12.025 | 3318 | 3323 | 3326 | rBV  | 367    | 355     | 0.02%  | 0.003% |
| 85  | 12.070 | 3335 | 3337 | 3341 | rVB2 | 414    | 275     | 0.02%  | 0.002% |
| 86  | 12.092 | 3341 | 3344 | 3346 | rBV2 | 415    | 267     | 0.02%  | 0.002% |
| 87  | 12.195 | 3362 | 3376 | 3396 | rVV  | 700656 | 1130840 | 65.98% | 8.942% |
| 88  | 12.330 | 3415 | 3418 | 3426 | rBV3 | 763    | 598     | 0.03%  | 0.005% |
| 89  | 12.362 | 3426 | 3428 | 3432 | rBV3 | 372    | 200     | 0.01%  | 0.002% |
| 90  | 12.423 | 3443 | 3447 | 3452 | rBV3 | 338    | 385     | 0.02%  | 0.003% |
| 91  | 12.539 | 3480 | 3483 | 3487 | rVB3 | 424    | 326     | 0.02%  | 0.003% |
| 92  | 12.742 | 3543 | 3546 | 3549 | rBV2 | 260    | 252     | 0.01%  | 0.002% |
| 93  | 12.774 | 3550 | 3556 | 3563 | rVB4 | 925    | 1499    | 0.09%  | 0.012% |
| 94  | 13.224 | 3689 | 3696 | 3703 | rBV7 | 1743   | 2382    | 0.14%  | 0.019% |
| 95  | 13.552 | 3796 | 3798 | 3801 | rVB2 | 408    | 196     | 0.01%  | 0.002% |
| 96  | 13.844 | 3880 | 3889 | 3899 | rVB4 | 5106   | 7513    | 0.44%  | 0.059% |
| 97  | 14.089 | 3956 | 3965 | 3978 | rBV2 | 11328  | 19094   | 1.11%  | 0.151% |
| 98  | 14.333 | 4032 | 4041 | 4053 | rVB3 | 5592   | 9025    | 0.53%  | 0.071% |
| 99  | 14.864 | 4204 | 4206 | 4211 | rVB3 | 564    | 312     | 0.02%  | 0.002% |
| 100 | 15.018 | 4250 | 4254 | 4258 | rBV3 | 554    | 527     | 0.03%  | 0.004% |

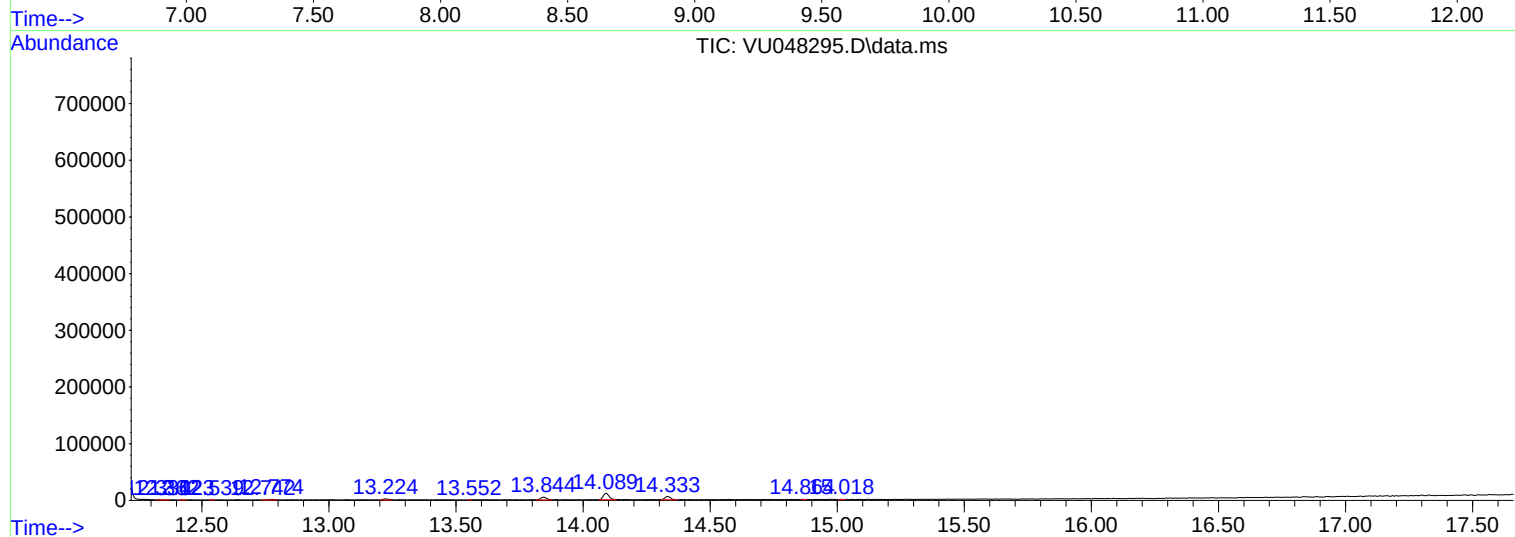
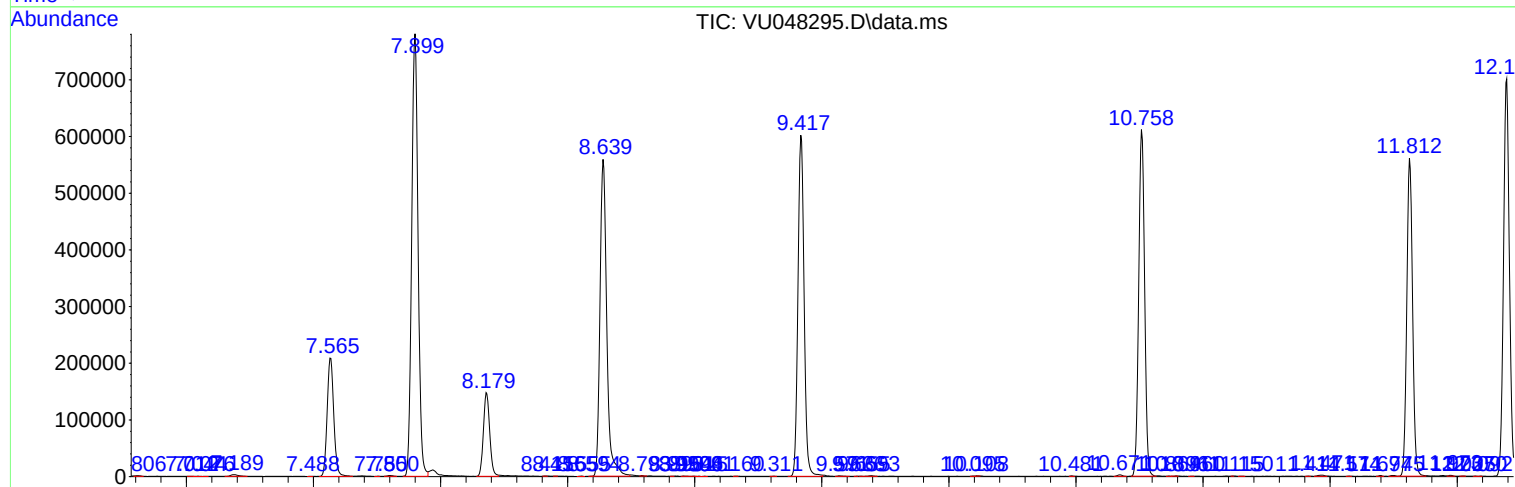
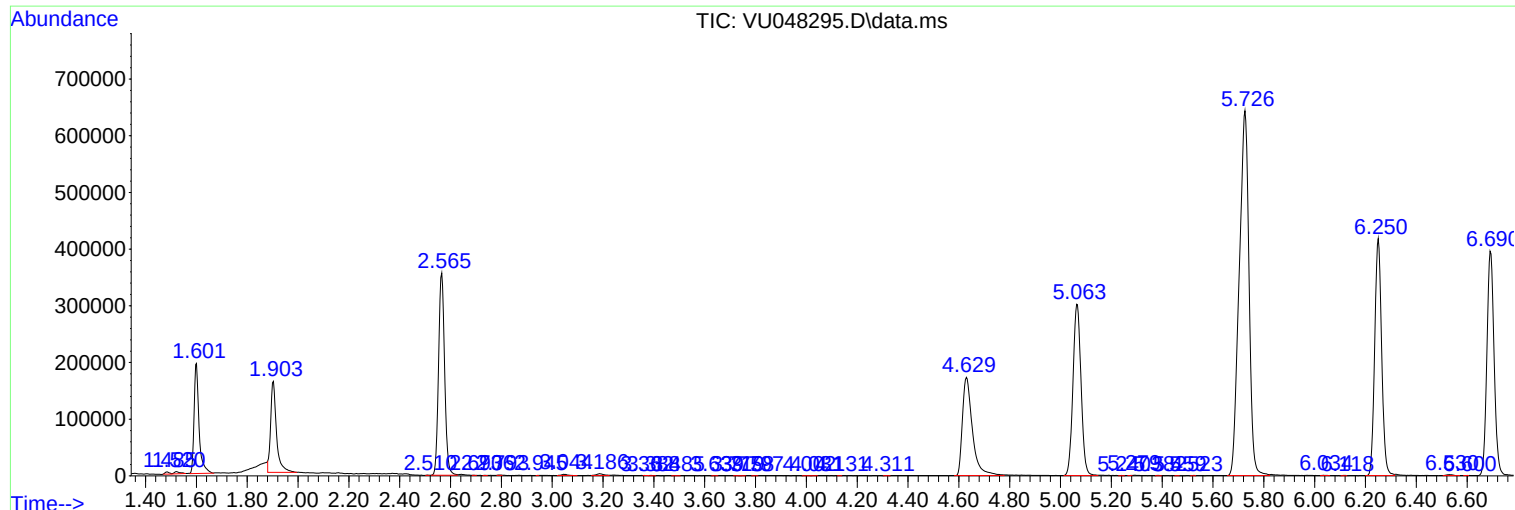
Sum of corrected areas: 12646825

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042522WMA.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 | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|