

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100421\  
 Data File : VU045126.D  
 Acq On : 05 Oct 2021 03:37  
 Operator : SY/MD  
 Sample : M4025-03 100X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 44 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AL3

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: VU045126.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         | 1.600       | 74            | 81          | 96           | rVB      | 113677         | 131520        | 11.28%          | 1.417%        |
| 2         | 1.909       | 169           | 177         | 191          | rVB      | 106401         | 135624        | 11.64%          | 1.461%        |
| 3         | 2.568       | 370           | 382         | 411          | rBV      | 204827         | 351132        | 30.13%          | 3.782%        |
| 4         | 2.790       | 448           | 451         | 458          | rVB2     | 408            | 469           | 0.04%           | 0.005%        |
| 5         | 2.887       | 474           | 481         | 484          | rBV2     | 163            | 220           | 0.02%           | 0.002%        |
| 6         | 2.928       | 487           | 494         | 496          | rBV      | 169            | 238           | 0.02%           | 0.003%        |
| 7         | 2.964       | 501           | 505         | 517          | rVB3     | 675            | 1147          | 0.10%           | 0.012%        |
| 8         | 3.015       | 517           | 521         | 524          | rBV2     | 244            | 246           | 0.02%           | 0.003%        |
| 9         | 3.054       | 524           | 533         | 542          | rVB3     | 1512           | 2335          | 0.20%           | 0.025%        |
| 10        | 3.192       | 568           | 576         | 581          | rBV3     | 511            | 776           | 0.07%           | 0.008%        |
| 11        | 3.279       | 598           | 603         | 604          | rBV      | 216            | 180           | 0.02%           | 0.002%        |
| 12        | 3.324       | 611           | 617         | 619          | rBV      | 174            | 220           | 0.02%           | 0.002%        |
| 13        | 3.359       | 625           | 628         | 634          | rVB2     | 265            | 234           | 0.02%           | 0.003%        |
| 14        | 3.395       | 634           | 639         | 642          | rBV      | 220            | 262           | 0.02%           | 0.003%        |
| 15        | 3.501       | 667           | 672         | 675          | rBV2     | 169            | 176           | 0.02%           | 0.002%        |
| 16        | 3.674       | 723           | 726         | 733          | rVB      | 155            | 189           | 0.02%           | 0.002%        |
| 17        | 3.761       | 749           | 753         | 756          | rBV2     | 246            | 226           | 0.02%           | 0.002%        |
| 18        | 4.305       | 919           | 922         | 925          | rVB      | 215            | 164           | 0.01%           | 0.002%        |
| 19        | 4.353       | 931           | 937         | 939          | rBV      | 162            | 174           | 0.01%           | 0.002%        |
| 20        | 4.417       | 954           | 957         | 963          | rBV      | 237            | 262           | 0.02%           | 0.003%        |
| 21        | 4.639       | 1009          | 1026        | 1069         | rBV      | 141795         | 412014        | 35.35%          | 4.438%        |
| 22        | 4.996       | 1135          | 1137        | 1140         | rVB2     | 331            | 167           | 0.01%           | 0.002%        |
| 23        | 5.067       | 1140          | 1159        | 1187         | rBV      | 209891         | 464365        | 39.84%          | 5.001%        |
| 24        | 5.166       | 1188          | 1190        | 1194         | rVB3     | 270            | 198           | 0.02%           | 0.002%        |
| 25        | 5.224       | 1205          | 1208        | 1211         | rVV2     | 299            | 226           | 0.02%           | 0.002%        |
| 26        | 5.288       | 1224          | 1228        | 1230         | rBV2     | 459            | 385           | 0.03%           | 0.004%        |
| 27        | 5.382       | 1250          | 1257        | 1259         | rBV2     | 276            | 301           | 0.03%           | 0.003%        |
| 28        | 5.440       | 1271          | 1275        | 1279         | rBV2     | 160            | 197           | 0.02%           | 0.002%        |
| 29        | 5.517       | 1294          | 1299        | 1301         | rBV      | 206            | 225           | 0.02%           | 0.002%        |
| 30        | 5.539       | 1304          | 1306        | 1311         | rVB2     | 202            | 162           | 0.01%           | 0.002%        |
| 31        | 5.623       | 1326          | 1332        | 1335         | rBV2     | 161            | 182           | 0.02%           | 0.002%        |
| 32        | 5.729       | 1342          | 1365        | 1391         | rBV2     | 429596         | 1165554       | 100.00%         | 12.553%       |
| 33        | 6.041       | 1460          | 1462        | 1465         | rVV      | 276            | 162           | 0.01%           | 0.002%        |
| 34        | 6.079       | 1471          | 1474        | 1482         | rVV      | 175            | 191           | 0.02%           | 0.002%        |
| 35        | 6.115       | 1482          | 1485        | 1488         | rVB2     | 262            | 218           | 0.02%           | 0.002%        |
| 36        | 6.253       | 1513          | 1528        | 1549         | rBV      | 363335         | 683812        | 58.67%          | 7.365%        |

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 ClientSampleId :  
 C0AL3

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

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.446  | 1585 | 1588 | 1592 | rVB2 | 231    | 214    | 0.02%  | 0.002% |
| 38 | 6.539  | 1606 | 1617 | 1627 | rVB8 | 4932   | 9580   | 0.82%  | 0.103% |
| 39 | 6.591  | 1627 | 1633 | 1635 | rBV2 | 155    | 164    | 0.01%  | 0.002% |
| 40 | 6.694  | 1651 | 1665 | 1686 | rBV  | 280177 | 546462 | 46.88% | 5.886% |
| 41 | 6.812  | 1699 | 1702 | 1707 | rVB2 | 725    | 633    | 0.05%  | 0.007% |
| 42 | 6.935  | 1734 | 1740 | 1742 | rBV2 | 184    | 192    | 0.02%  | 0.002% |
| 43 | 6.989  | 1748 | 1757 | 1761 | rBV2 | 236    | 461    | 0.04%  | 0.005% |
| 44 | 7.012  | 1761 | 1764 | 1767 | rBV2 | 228    | 205    | 0.02%  | 0.002% |
| 45 | 7.047  | 1771 | 1775 | 1778 | rBV2 | 405    | 339    | 0.03%  | 0.004% |
| 46 | 7.095  | 1787 | 1790 | 1795 | rVB2 | 209    | 214    | 0.02%  | 0.002% |
| 47 | 7.134  | 1799 | 1802 | 1805 | rVV  | 189    | 170    | 0.01%  | 0.002% |
| 48 | 7.189  | 1809 | 1819 | 1833 | rVB4 | 2794   | 4980   | 0.43%  | 0.054% |
| 49 | 7.433  | 1890 | 1895 | 1897 | rBV2 | 213    | 172    | 0.01%  | 0.002% |
| 50 | 7.452  | 1898 | 1901 | 1904 | rBV  | 178    | 184    | 0.02%  | 0.002% |
| 51 | 7.504  | 1911 | 1917 | 1922 | rBV2 | 183    | 260    | 0.02%  | 0.003% |
| 52 | 7.568  | 1925 | 1937 | 1954 | rBV  | 143701 | 254820 | 21.86% | 2.745% |
| 53 | 7.693  | 1968 | 1976 | 1984 | rVB3 | 1541   | 2702   | 0.23%  | 0.029% |
| 54 | 7.902  | 2027 | 2041 | 2055 | rBV  | 507598 | 869897 | 74.63% | 9.369% |
| 55 | 7.973  | 2058 | 2063 | 2073 | rVB2 | 7594   | 11030  | 0.95%  | 0.119% |
| 56 | 8.182  | 2115 | 2128 | 2147 | rBV  | 103447 | 174400 | 14.96% | 1.878% |
| 57 | 8.558  | 2239 | 2245 | 2250 | rVB6 | 651    | 713    | 0.06%  | 0.008% |
| 58 | 8.584  | 2250 | 2253 | 2256 | rBV  | 272    | 203    | 0.02%  | 0.002% |
| 59 | 8.642  | 2258 | 2271 | 2306 | rBV  | 507560 | 892008 | 76.53% | 9.607% |
| 60 | 8.906  | 2350 | 2353 | 2356 | rBV  | 243    | 221    | 0.02%  | 0.002% |
| 61 | 9.108  | 2413 | 2416 | 2420 | rVB  | 281    | 224    | 0.02%  | 0.002% |
| 62 | 9.263  | 2461 | 2464 | 2469 | rVB  | 285    | 227    | 0.02%  | 0.002% |
| 63 | 9.420  | 2499 | 2513 | 2546 | rBV  | 503699 | 842400 | 72.27% | 9.073% |
| 64 | 9.574  | 2554 | 2561 | 2568 | rVB3 | 492    | 770    | 0.07%  | 0.008% |
| 65 | 9.729  | 2605 | 2609 | 2612 | rVB2 | 219    | 185    | 0.02%  | 0.002% |
| 66 | 9.754  | 2612 | 2617 | 2620 | rBV  | 184    | 204    | 0.02%  | 0.002% |
| 67 | 10.250 | 2767 | 2771 | 2774 | rBV2 | 172    | 173    | 0.01%  | 0.002% |
| 68 | 10.494 | 2844 | 2847 | 2850 | rVB  | 235    | 179    | 0.02%  | 0.002% |
| 69 | 10.677 | 2898 | 2904 | 2910 | rVB3 | 1076   | 1238   | 0.11%  | 0.013% |
| 70 | 10.761 | 2917 | 2930 | 2948 | rVB  | 444808 | 706349 | 60.60% | 7.608% |
| 71 | 10.899 | 2970 | 2973 | 2977 | rVB2 | 246    | 182    | 0.02%  | 0.002% |
| 72 | 10.996 | 3000 | 3003 | 3006 | rBV3 | 248    | 186    | 0.02%  | 0.002% |
| 73 | 11.446 | 3138 | 3143 | 3144 | rBV  | 353    | 268    | 0.02%  | 0.003% |
| 74 | 11.471 | 3145 | 3151 | 3158 | rVV6 | 1218   | 1799   | 0.15%  | 0.019% |
| 75 | 11.536 | 3166 | 3171 | 3176 | rBV2 | 252    | 329    | 0.03%  | 0.004% |
| 76 | 11.639 | 3197 | 3203 | 3206 | rVB2 | 232    | 223    | 0.02%  | 0.002% |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.700 | 3215 | 3222 | 3226 | rBV3 | 541    | 725    | 0.06%  | 0.008% |
| 78  | 11.815 | 3245 | 3258 | 3276 | rBV  | 493221 | 782327 | 67.12% | 8.426% |
| 79  | 11.934 | 3292 | 3295 | 3298 | rBV  | 307    | 212    | 0.02%  | 0.002% |
| 80  | 12.028 | 3321 | 3324 | 3327 | rBV2 | 208    | 197    | 0.02%  | 0.002% |
| 81  | 12.195 | 3364 | 3376 | 3393 | rBV  | 506863 | 816257 | 70.03% | 8.791% |
| 82  | 12.729 | 3538 | 3542 | 3545 | rBV  | 171    | 191    | 0.02%  | 0.002% |
| 83  | 12.770 | 3551 | 3555 | 3560 | rBV2 | 379    | 511    | 0.04%  | 0.006% |
| 84  | 13.352 | 3733 | 3736 | 3738 | rBV  | 204    | 172    | 0.01%  | 0.002% |
| 85  | 13.401 | 3748 | 3751 | 3756 | rVB2 | 213    | 239    | 0.02%  | 0.003% |
| 86  | 13.449 | 3761 | 3766 | 3768 | rBV  | 184    | 176    | 0.02%  | 0.002% |
| 87  | 13.571 | 3797 | 3804 | 3807 | rBV2 | 237    | 370    | 0.03%  | 0.004% |
| 88  | 13.732 | 3848 | 3854 | 3858 | rBV  | 217    | 322    | 0.03%  | 0.003% |
| 89  | 13.803 | 3873 | 3876 | 3878 | rBV  | 258    | 209    | 0.02%  | 0.002% |
| 90  | 13.857 | 3890 | 3893 | 3897 | rVB  | 219    | 178    | 0.02%  | 0.002% |
| 91  | 13.889 | 3901 | 3903 | 3910 | rVB2 | 303    | 285    | 0.02%  | 0.003% |
| 92  | 13.947 | 3916 | 3921 | 3923 | rBV  | 194    | 212    | 0.02%  | 0.002% |
| 93  | 14.012 | 3938 | 3941 | 3944 | rBV  | 245    | 194    | 0.02%  | 0.002% |
| 94  | 14.095 | 3960 | 3967 | 3975 | rBV2 | 680    | 1094   | 0.09%  | 0.012% |
| 95  | 14.272 | 4019 | 4022 | 4027 | rBV  | 327    | 331    | 0.03%  | 0.004% |
| 96  | 14.413 | 4062 | 4066 | 4069 | rBV2 | 394    | 339    | 0.03%  | 0.004% |
| 97  | 14.507 | 4092 | 4095 | 4096 | rBV  | 258    | 167    | 0.01%  | 0.002% |
| 98  | 14.568 | 4110 | 4114 | 4115 | rBV2 | 282    | 183    | 0.02%  | 0.002% |
| 99  | 15.896 | 4524 | 4527 | 4530 | rVB3 | 537    | 369    | 0.03%  | 0.004% |
| 100 | 15.947 | 4541 | 4543 | 4545 | rBV  | 300    | 177    | 0.02%  | 0.002% |

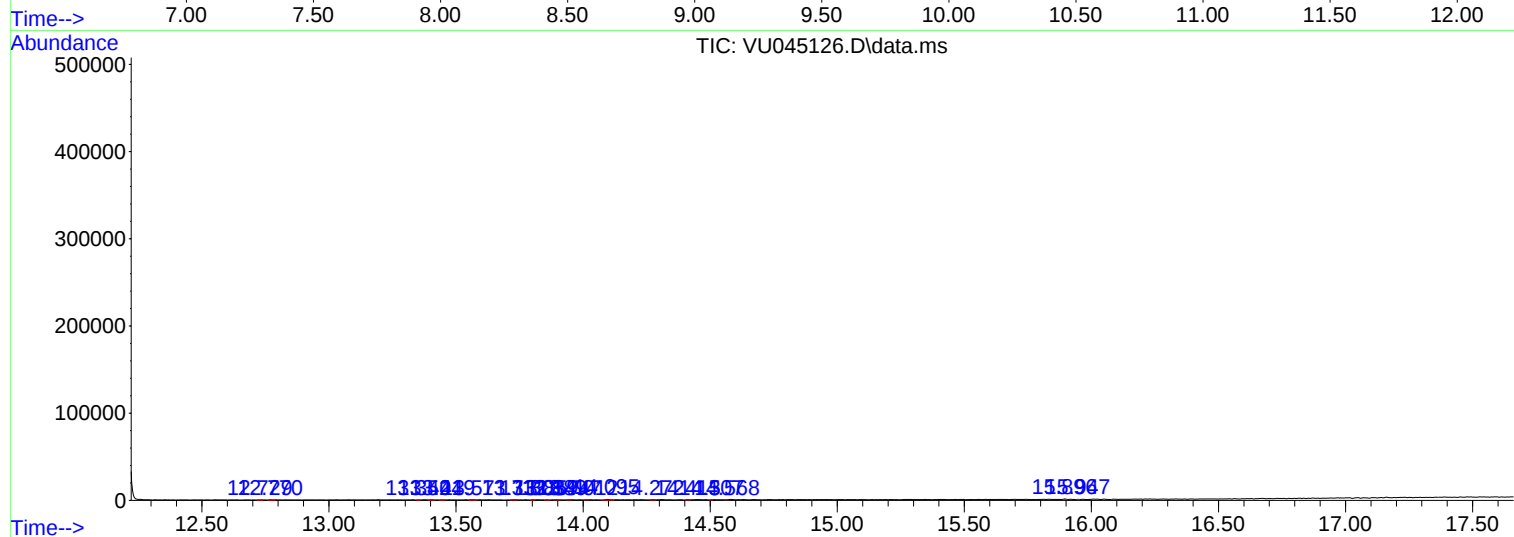
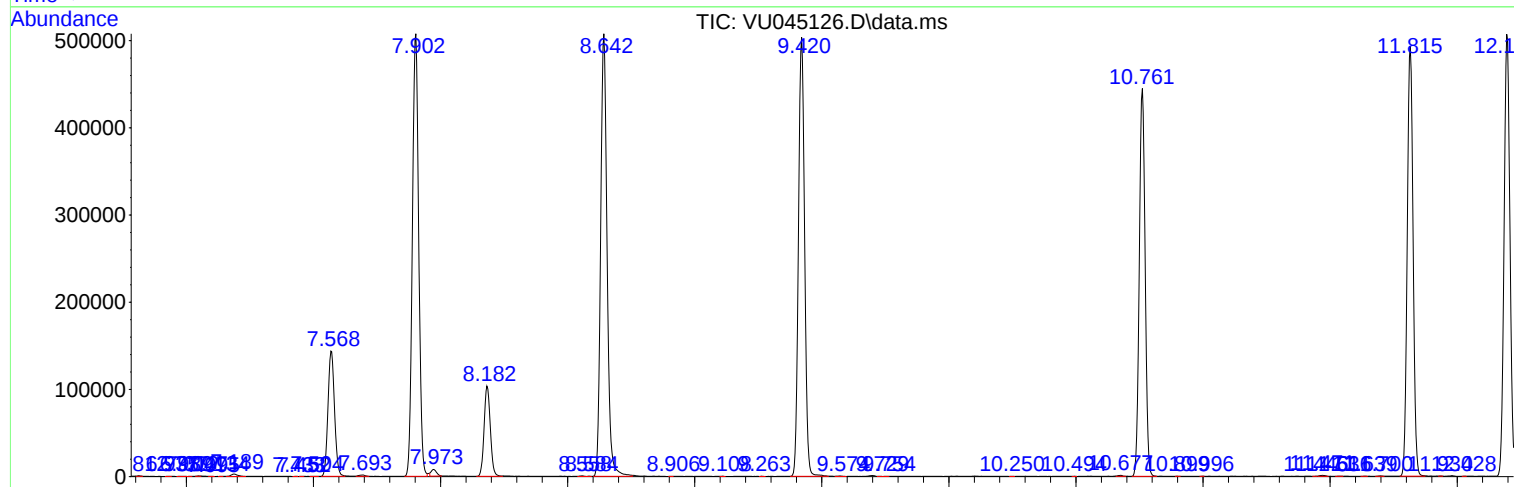
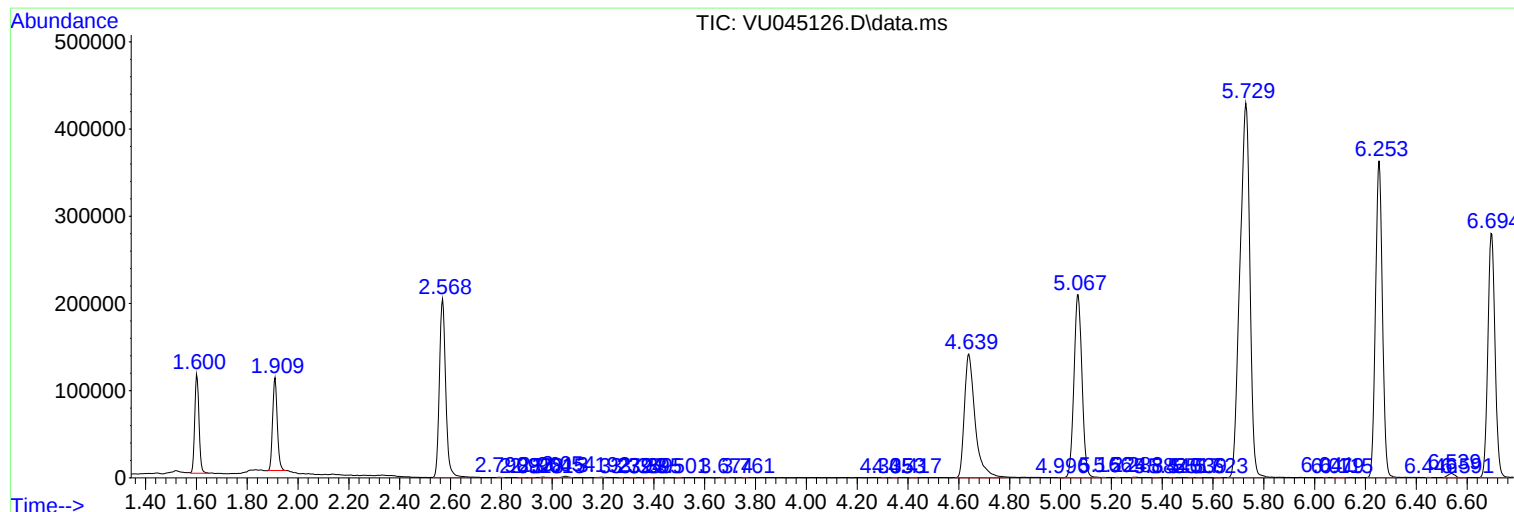
Sum of corrected areas: 9284750

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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100421\  
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No Library Search Compounds Detected

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