

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120721\  
 Data File : VU046147.D  
 Acq On : 07 Dec 2021 18:27  
 Operator : SY/MD  
 Sample : VU1207WBL02  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 21 Sample Multiplier: 1

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: VU046147.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       | 73            | 81          | 94           | rBV      | 122224         | 135033        | 14.96%          | 1.938%        |
| 2         | 1.919       | 171           | 180         | 193          | rVB      | 85791          | 109651        | 12.14%          | 1.574%        |
| 3         | 2.224       | 273           | 275         | 278          | rVB      | 242            | 129           | 0.01%           | 0.002%        |
| 4         | 2.257       | 281           | 285         | 286          | rBV      | 285            | 208           | 0.02%           | 0.003%        |
| 5         | 2.572       | 371           | 383         | 407          | rBV      | 199429         | 332246        | 36.80%          | 4.768%        |
| 6         | 2.745       | 434           | 437         | 442          | rVB2     | 163            | 135           | 0.01%           | 0.002%        |
| 7         | 2.800       | 447           | 454         | 460          | rVV2     | 590            | 869           | 0.10%           | 0.012%        |
| 8         | 2.951       | 499           | 501         | 507          | rVB2     | 203            | 191           | 0.02%           | 0.003%        |
| 9         | 3.051       | 525           | 532         | 538          | rVV3     | 817            | 1179          | 0.13%           | 0.017%        |
| 10        | 3.192       | 571           | 576         | 581          | rVB2     | 193            | 276           | 0.03%           | 0.004%        |
| 11        | 3.459       | 656           | 659         | 662          | rBV      | 139            | 143           | 0.02%           | 0.002%        |
| 12        | 3.597       | 697           | 702         | 704          | rBV      | 168            | 202           | 0.02%           | 0.003%        |
| 13        | 3.642       | 710           | 716         | 720          | rBV      | 163            | 233           | 0.03%           | 0.003%        |
| 14        | 3.845       | 774           | 779         | 785          | rBV      | 177            | 289           | 0.03%           | 0.004%        |
| 15        | 3.954       | 807           | 813         | 815          | rBB      | 140            | 146           | 0.02%           | 0.002%        |
| 16        | 3.983       | 819           | 822         | 825          | rBV      | 163            | 164           | 0.02%           | 0.002%        |
| 17        | 4.006       | 827           | 829         | 833          | rBV      | 128            | 136           | 0.02%           | 0.002%        |
| 18        | 4.044       | 839           | 841         | 845          | rBV      | 132            | 146           | 0.02%           | 0.002%        |
| 19        | 4.247       | 900           | 904         | 908          | rBB      | 154            | 174           | 0.02%           | 0.002%        |
| 20        | 4.279       | 912           | 914         | 918          | rBV      | 188            | 165           | 0.02%           | 0.002%        |
| 21        | 4.494       | 977           | 981         | 986          | rBV      | 186            | 255           | 0.03%           | 0.004%        |
| 22        | 4.639       | 1009          | 1026        | 1065         | rVV      | 76252          | 228374        | 25.29%          | 3.278%        |
| 23        | 4.800       | 1073          | 1076        | 1079         | rBV2     | 171            | 144           | 0.02%           | 0.002%        |
| 24        | 4.951       | 1120          | 1123        | 1126         | rBV      | 251            | 249           | 0.03%           | 0.004%        |
| 25        | 5.067       | 1142          | 1159        | 1182         | rBV      | 149237         | 348166        | 38.56%          | 4.997%        |
| 26        | 5.289       | 1225          | 1228        | 1234         | rVB3     | 274            | 280           | 0.03%           | 0.004%        |
| 27        | 5.408       | 1259          | 1265        | 1270         | rBV      | 147            | 246           | 0.03%           | 0.004%        |
| 28        | 5.491       | 1288          | 1291        | 1296         | rVB      | 203            | 208           | 0.02%           | 0.003%        |
| 29        | 5.530       | 1299          | 1303        | 1304         | rBV      | 160            | 129           | 0.01%           | 0.002%        |
| 30        | 5.584       | 1316          | 1320        | 1323         | rBV      | 176            | 185           | 0.02%           | 0.003%        |
| 31        | 5.604       | 1323          | 1326        | 1328         | rVB      | 261            | 163           | 0.02%           | 0.002%        |
| 32        | 5.633       | 1332          | 1335        | 1340         | rBV      | 166            | 199           | 0.02%           | 0.003%        |
| 33        | 5.729       | 1342          | 1365        | 1385         | rBV2     | 336521         | 902884        | 100.00%         | 12.958%       |
| 34        | 6.105       | 1480          | 1482        | 1484         | rVB      | 263            | 138           | 0.02%           | 0.002%        |
| 35        | 6.131       | 1485          | 1490        | 1493         | rBB      | 162            | 153           | 0.02%           | 0.002%        |
| 36        | 6.160       | 1497          | 1499        | 1503         | rVB      | 286            | 195           | 0.02%           | 0.003%        |

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 ALS Vial : 21 Sample Multiplier: 1

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.192  | 1505 | 1509 | 1513 | rBB  | 138    | 170    | 0.02%  | 0.002%  |
| 38 | 6.250  | 1513 | 1527 | 1547 | rBV  | 247352 | 470672 | 52.13% | 6.755%  |
| 39 | 6.408  | 1574 | 1576 | 1581 | rVB2 | 243    | 181    | 0.02%  | 0.003%  |
| 40 | 6.443  | 1583 | 1587 | 1592 | rVV2 | 191    | 211    | 0.02%  | 0.003%  |
| 41 | 6.530  | 1600 | 1614 | 1626 | rBV4 | 3598   | 7185   | 0.80%  | 0.103%  |
| 42 | 6.694  | 1650 | 1665 | 1682 | rBV  | 202760 | 393714 | 43.61% | 5.651%  |
| 43 | 6.806  | 1697 | 1700 | 1708 | rVB3 | 930    | 1199   | 0.13%  | 0.017%  |
| 44 | 6.845  | 1709 | 1712 | 1714 | rBV  | 173    | 147    | 0.02%  | 0.002%  |
| 45 | 7.015  | 1759 | 1765 | 1768 | rBV  | 167    | 238    | 0.03%  | 0.003%  |
| 46 | 7.041  | 1768 | 1773 | 1780 | rVV2 | 355    | 510    | 0.06%  | 0.007%  |
| 47 | 7.134  | 1799 | 1802 | 1806 | rBB  | 175    | 166    | 0.02%  | 0.002%  |
| 48 | 7.163  | 1807 | 1811 | 1812 | rBV2 | 284    | 216    | 0.02%  | 0.003%  |
| 49 | 7.179  | 1812 | 1816 | 1818 | rBV  | 382    | 315    | 0.03%  | 0.005%  |
| 50 | 7.311  | 1854 | 1857 | 1858 | rBV  | 275    | 146    | 0.02%  | 0.002%  |
| 51 | 7.568  | 1922 | 1937 | 1957 | rBV  | 119173 | 206105 | 22.83% | 2.958%  |
| 52 | 7.636  | 1957 | 1958 | 1961 | rVV2 | 501    | 260    | 0.03%  | 0.004%  |
| 53 | 7.649  | 1961 | 1962 | 1969 | rVV  | 220    | 298    | 0.03%  | 0.004%  |
| 54 | 7.687  | 1971 | 1974 | 1983 | rVB3 | 336    | 505    | 0.06%  | 0.007%  |
| 55 | 7.803  | 2003 | 2010 | 2014 | rBV2 | 529    | 725    | 0.08%  | 0.010%  |
| 56 | 7.899  | 2026 | 2040 | 2057 | rBV  | 434056 | 758563 | 84.02% | 10.887% |
| 57 | 8.134  | 2109 | 2113 | 2116 | rBV  | 203    | 224    | 0.02%  | 0.003%  |
| 58 | 8.179  | 2116 | 2127 | 2143 | rBV  | 81241  | 134799 | 14.93% | 1.935%  |
| 59 | 8.314  | 2165 | 2169 | 2176 | rVB2 | 255    | 236    | 0.03%  | 0.003%  |
| 60 | 8.465  | 2210 | 2216 | 2217 | rBV  | 271    | 247    | 0.03%  | 0.004%  |
| 61 | 8.633  | 2255 | 2268 | 2297 | rBV  | 265339 | 476577 | 52.78% | 6.840%  |
| 62 | 9.160  | 2425 | 2432 | 2434 | rBV2 | 302    | 300    | 0.03%  | 0.004%  |
| 63 | 9.417  | 2500 | 2512 | 2542 | rBV  | 357461 | 593240 | 65.71% | 8.514%  |
| 64 | 9.568  | 2553 | 2559 | 2566 | rVB2 | 447    | 533    | 0.06%  | 0.008%  |
| 65 | 9.645  | 2578 | 2583 | 2586 | rBV  | 187    | 168    | 0.02%  | 0.002%  |
| 66 | 9.694  | 2591 | 2598 | 2606 | rVV  | 1126   | 1690   | 0.19%  | 0.024%  |
| 67 | 10.102 | 2721 | 2725 | 2727 | rBV3 | 379    | 351    | 0.04%  | 0.005%  |
| 68 | 10.481 | 2839 | 2843 | 2850 | rBV  | 198    | 245    | 0.03%  | 0.004%  |
| 69 | 10.671 | 2894 | 2902 | 2912 | rBB4 | 2641   | 3523   | 0.39%  | 0.051%  |
| 70 | 10.758 | 2916 | 2929 | 2947 | rBV  | 295770 | 471180 | 52.19% | 6.762%  |
| 71 | 10.922 | 2976 | 2980 | 2983 | rBV  | 189    | 156    | 0.02%  | 0.002%  |
| 72 | 10.951 | 2986 | 2989 | 2993 | rVB2 | 156    | 129    | 0.01%  | 0.002%  |
| 73 | 10.999 | 3001 | 3004 | 3009 | rBV2 | 294    | 234    | 0.03%  | 0.003%  |
| 74 | 11.089 | 3027 | 3032 | 3036 | rBV2 | 501    | 520    | 0.06%  | 0.007%  |
| 75 | 11.118 | 3036 | 3041 | 3043 | rBV3 | 349    | 260    | 0.03%  | 0.004%  |
| 76 | 11.456 | 3140 | 3146 | 3158 | rVB4 | 2035   | 3446   | 0.38%  | 0.049%  |

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 ALS Vial : 21 Sample Multiplier: 1

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

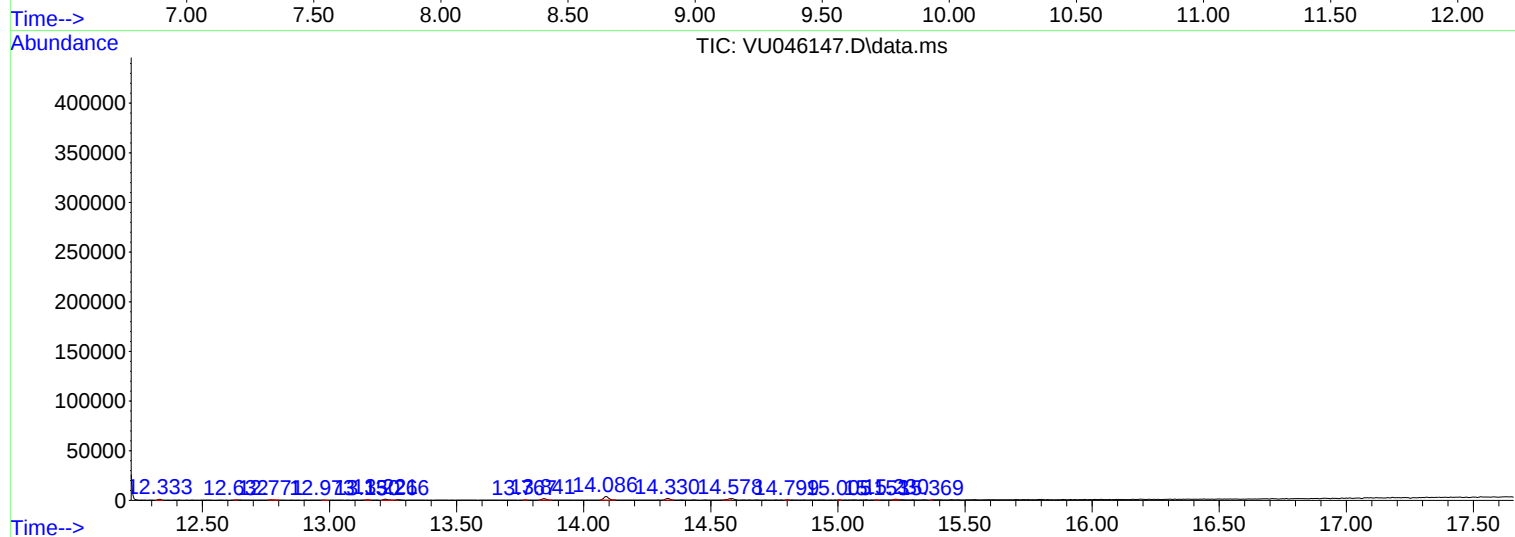
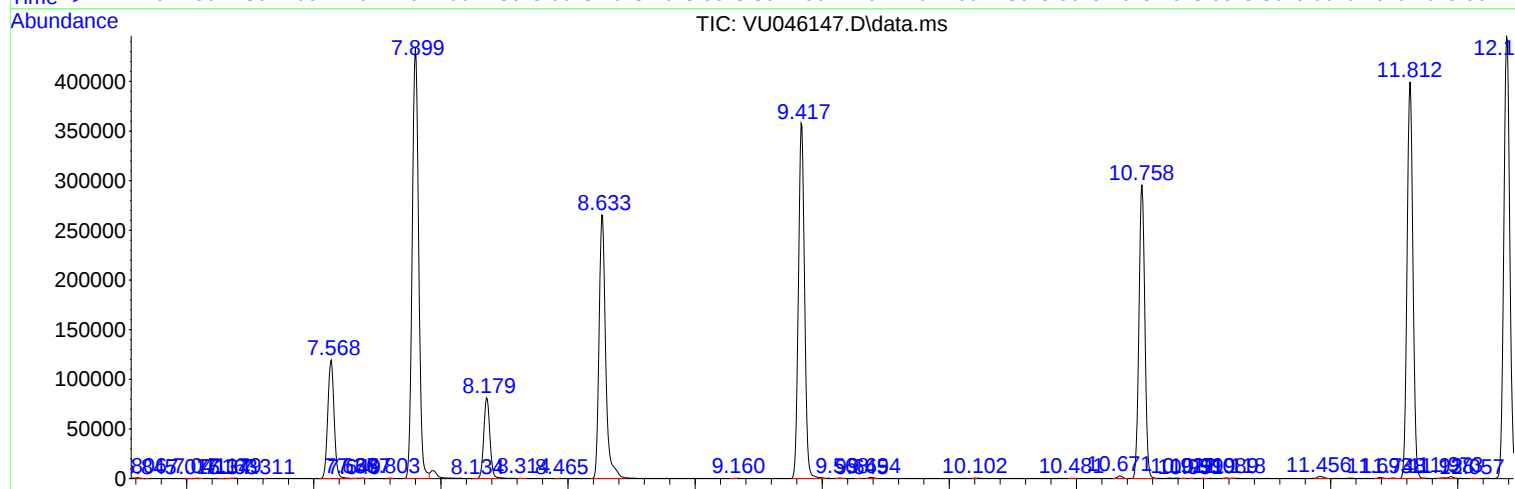
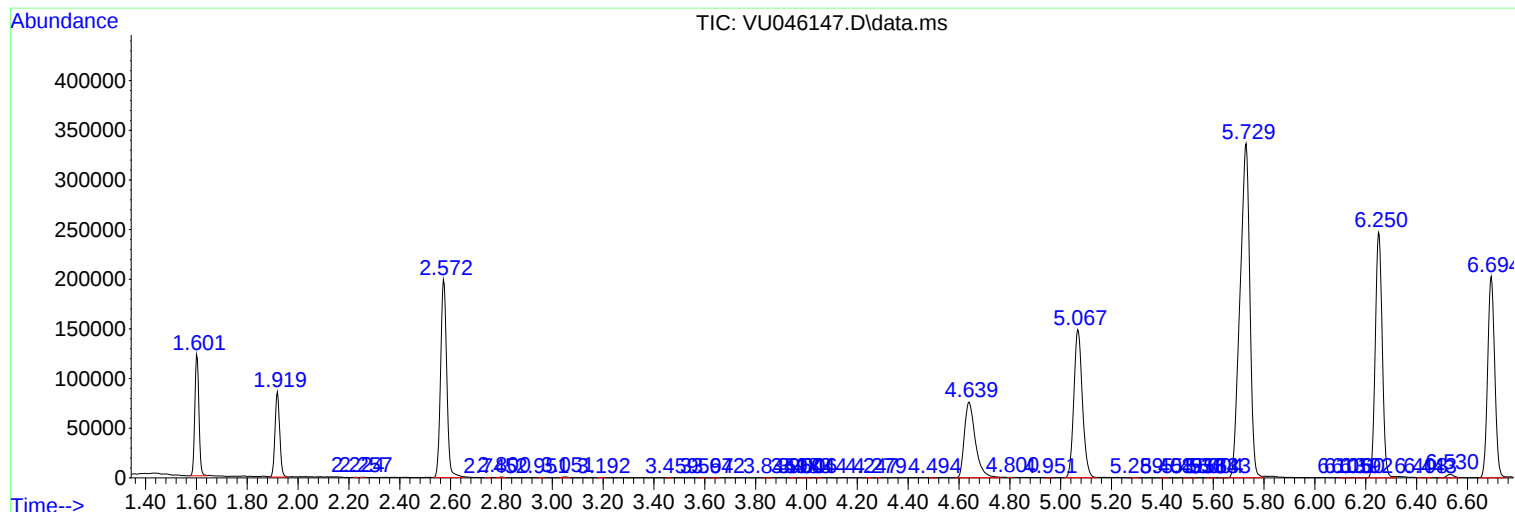
|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.693 | 3213 | 3220 | 3230 | rBV3 | 1058   | 1428   | 0.16%  | 0.020%  |
| 78  | 11.748 | 3231 | 3237 | 3242 | rVB3 | 548    | 596    | 0.07%  | 0.009%  |
| 79  | 11.812 | 3242 | 3257 | 3275 | rBV  | 399475 | 633997 | 70.22% | 9.099%  |
| 80  | 11.938 | 3291 | 3296 | 3298 | rVV2 | 625    | 591    | 0.07%  | 0.008%  |
| 81  | 11.973 | 3301 | 3307 | 3314 | rVB3 | 1891   | 2337   | 0.26%  | 0.034%  |
| 82  | 12.057 | 3330 | 3333 | 3342 | rVB  | 130    | 145    | 0.02%  | 0.002%  |
| 83  | 12.192 | 3360 | 3375 | 3394 | rBV  | 445802 | 719606 | 79.70% | 10.328% |
| 84  | 12.333 | 3413 | 3419 | 3422 | rBV2 | 878    | 780    | 0.09%  | 0.011%  |
| 85  | 12.632 | 3509 | 3512 | 3514 | rBV  | 294    | 194    | 0.02%  | 0.003%  |
| 86  | 12.771 | 3551 | 3555 | 3565 | rVB2 | 376    | 450    | 0.05%  | 0.006%  |
| 87  | 12.973 | 3616 | 3618 | 3625 | rBV  | 200    | 144    | 0.02%  | 0.002%  |
| 88  | 13.150 | 3669 | 3673 | 3677 | rVB3 | 338    | 316    | 0.03%  | 0.005%  |
| 89  | 13.221 | 3689 | 3695 | 3705 | rBV3 | 1015   | 1253   | 0.14%  | 0.018%  |
| 90  | 13.266 | 3706 | 3709 | 3710 | rBV2 | 326    | 185    | 0.02%  | 0.003%  |
| 91  | 13.767 | 3863 | 3865 | 3869 | rBV2 | 208    | 133    | 0.01%  | 0.002%  |
| 92  | 13.841 | 3882 | 3888 | 3899 | rVB3 | 1560   | 1917   | 0.21%  | 0.028%  |
| 93  | 14.086 | 3957 | 3964 | 3977 | rVB2 | 3551   | 5045   | 0.56%  | 0.072%  |
| 94  | 14.330 | 4034 | 4040 | 4047 | rBV4 | 1644   | 1993   | 0.22%  | 0.029%  |
| 95  | 14.578 | 4107 | 4117 | 4118 | rBV  | 1424   | 1536   | 0.17%  | 0.022%  |
| 96  | 14.799 | 4183 | 4186 | 4189 | rBV  | 273    | 264    | 0.03%  | 0.004%  |
| 97  | 15.005 | 4247 | 4250 | 4253 | rBV  | 275    | 197    | 0.02%  | 0.003%  |
| 98  | 15.153 | 4293 | 4296 | 4299 | rBV2 | 170    | 140    | 0.02%  | 0.002%  |
| 99  | 15.230 | 4314 | 4320 | 4324 | rBV2 | 721    | 919    | 0.10%  | 0.013%  |
| 100 | 15.369 | 4360 | 4363 | 4364 | rBV  | 230    | 134    | 0.01%  | 0.002%  |

Sum of corrected areas: 6967567

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ALS Vial : 21 Sample Multiplier: 1

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\VU120721\  
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TIC Library : C:\Database\NIST20.L  
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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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