

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV012221\  
 Data File : VV020140.D  
 Acq On : 22 Jan 2021 17:02  
 Operator : SY/MD  
 Sample : M1181-21  
 Misc : 5.0mL/MSVOA\_V/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 F1E52

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\_V\Method\SOMVLM012121WMA.M

Title : VOC Analysis

Signal : TIC: VV020140.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         | 1.309       | 62            | 68          | 84           | rVB      | 246833         | 253239        | 16.27%          | 1.887%        |
| 2         | 1.569       | 142           | 149         | 165          | rVB      | 174943         | 197319        | 12.68%          | 1.470%        |
| 3         | 2.110       | 307           | 317         | 347          | rVB      | 370053         | 562196        | 36.13%          | 4.189%        |
| 4         | 2.460       | 423           | 426         | 429          | rBV2     | 224            | 141           | 0.01%           | 0.001%        |
| 5         | 2.566       | 456           | 459         | 460          | rBV2     | 220            | 152           | 0.01%           | 0.001%        |
| 6         | 2.698       | 498           | 500         | 503          | rBV2     | 308            | 159           | 0.01%           | 0.001%        |
| 7         | 2.730       | 506           | 510         | 513          | rVB2     | 390            | 337           | 0.02%           | 0.003%        |
| 8         | 2.766       | 513           | 521         | 522          | rBV4     | 2832           | 2683          | 0.17%           | 0.020%        |
| 9         | 2.849       | 545           | 547         | 549          | rBV3     | 247            | 114           | 0.01%           | 0.001%        |
| 10        | 2.904       | 562           | 564         | 571          | rVB4     | 607            | 575           | 0.04%           | 0.004%        |
| 11        | 2.936       | 571           | 574         | 576          | rBV2     | 419            | 270           | 0.02%           | 0.002%        |
| 12        | 3.042       | 605           | 607         | 610          | rBV2     | 508            | 319           | 0.02%           | 0.002%        |
| 13        | 3.103       | 622           | 626         | 630          | rBV3     | 393            | 345           | 0.02%           | 0.003%        |
| 14        | 3.142       | 635           | 638         | 641          | rBV3     | 382            | 285           | 0.02%           | 0.002%        |
| 15        | 3.213       | 657           | 660         | 664          | rBV2     | 624            | 503           | 0.03%           | 0.004%        |
| 16        | 3.241       | 667           | 669         | 670          | rBV2     | 340            | 108           | 0.01%           | 0.001%        |
| 17        | 3.303       | 685           | 688         | 690          | rBV2     | 263            | 161           | 0.01%           | 0.001%        |
| 18        | 3.402       | 717           | 719         | 724          | rVV4     | 540            | 453           | 0.03%           | 0.003%        |
| 19        | 3.434       | 727           | 729         | 732          | rVB3     | 436            | 249           | 0.02%           | 0.002%        |
| 20        | 3.460       | 732           | 737         | 740          | rVB3     | 761            | 575           | 0.04%           | 0.004%        |
| 21        | 3.476       | 740           | 742         | 745          | rBV2     | 247            | 165           | 0.01%           | 0.001%        |
| 22        | 3.531       | 757           | 759         | 764          | rVB2     | 278            | 173           | 0.01%           | 0.001%        |
| 23        | 3.563       | 767           | 769         | 773          | rVB2     | 431            | 280           | 0.02%           | 0.002%        |
| 24        | 3.585       | 773           | 776         | 779          | rBV3     | 297            | 268           | 0.02%           | 0.002%        |
| 25        | 3.627       | 787           | 789         | 793          | rVB      | 260            | 142           | 0.01%           | 0.001%        |
| 26        | 3.647       | 793           | 795         | 797          | rBV      | 190            | 115           | 0.01%           | 0.001%        |
| 27        | 3.676       | 799           | 804         | 807          | rBV3     | 708            | 539           | 0.03%           | 0.004%        |
| 28        | 3.714       | 814           | 816         | 818          | rBV      | 215            | 148           | 0.01%           | 0.001%        |
| 29        | 3.788       | 837           | 839         | 841          | rVB      | 307            | 135           | 0.01%           | 0.001%        |
| 30        | 3.897       | 858           | 873         | 908          | rBV2     | 140817         | 533633        | 34.29%          | 3.976%        |
| 31        | 4.354       | 998           | 1015        | 1046         | rBV      | 282881         | 697176        | 44.80%          | 5.195%        |
| 32        | 4.772       | 1143          | 1145        | 1147         | rBV      | 378            | 197           | 0.01%           | 0.001%        |
| 33        | 4.801       | 1152          | 1154        | 1156         | rBV      | 421            | 187           | 0.01%           | 0.001%        |
| 34        | 4.875       | 1174          | 1177        | 1180         | rBV2     | 253            | 209           | 0.01%           | 0.002%        |
| 35        | 4.917       | 1188          | 1190        | 1193         | rBV2     | 439            | 240           | 0.02%           | 0.002%        |
| 36        | 4.962       | 1200          | 1204        | 1208         | rBV5     | 651            | 630           | 0.04%           | 0.005%        |

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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\_V\Method\SOMVLM012121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |         |         |
|----|--------|------|------|------|------|--------|---------|---------|---------|
| 37 | 5.052  | 1214 | 1232 | 1261 | rBV2 | 598210 | 1556169 | 100.00% | 11.595% |
| 38 | 5.376  | 1331 | 1333 | 1336 | rBV3 | 766    | 503     | 0.03%   | 0.004%  |
| 39 | 5.621  | 1397 | 1409 | 1435 | rBV  | 413624 | 826770  | 53.13%  | 6.160%  |
| 40 | 5.859  | 1481 | 1483 | 1485 | rVB3 | 528    | 162     | 0.01%   | 0.001%  |
| 41 | 5.917  | 1485 | 1501 | 1528 | rBV4 | 75015  | 177970  | 11.44%  | 1.326%  |
| 42 | 6.074  | 1536 | 1550 | 1577 | rBV  | 347049 | 709814  | 45.61%  | 5.289%  |
| 43 | 6.402  | 1649 | 1652 | 1654 | rBV  | 760    | 455     | 0.03%   | 0.003%  |
| 44 | 6.476  | 1673 | 1675 | 1679 | rBV3 | 523    | 466     | 0.03%   | 0.003%  |
| 45 | 6.508  | 1683 | 1685 | 1686 | rBV  | 453    | 142     | 0.01%   | 0.001%  |
| 46 | 6.531  | 1690 | 1692 | 1693 | rBV  | 543    | 203     | 0.01%   | 0.002%  |
| 47 | 6.592  | 1709 | 1711 | 1714 | rBV3 | 764    | 394     | 0.03%   | 0.003%  |
| 48 | 6.634  | 1720 | 1724 | 1727 | rBV6 | 767    | 720     | 0.05%   | 0.005%  |
| 49 | 6.704  | 1744 | 1746 | 1750 | rVB4 | 486    | 321     | 0.02%   | 0.002%  |
| 50 | 6.862  | 1791 | 1795 | 1796 | rBV3 | 890    | 436     | 0.03%   | 0.003%  |
| 51 | 6.900  | 1805 | 1807 | 1810 | rBV3 | 444    | 238     | 0.02%   | 0.002%  |
| 52 | 6.923  | 1812 | 1814 | 1818 | rVV2 | 565    | 274     | 0.02%   | 0.002%  |
| 53 | 6.990  | 1824 | 1835 | 1865 | rBV  | 197161 | 352810  | 22.67%  | 2.629%  |
| 54 | 7.322  | 1926 | 1938 | 1958 | rBV  | 699013 | 1214629 | 78.05%  | 9.050%  |
| 55 | 7.627  | 2022 | 2033 | 2057 | rBV  | 126941 | 228165  | 14.66%  | 1.700%  |
| 56 | 7.862  | 2104 | 2106 | 2109 | rBV2 | 610    | 325     | 0.02%   | 0.002%  |
| 57 | 7.981  | 2129 | 2143 | 2163 | rBV  | 887193 | 1486406 | 95.52%  | 11.075% |
| 58 | 8.093  | 2168 | 2178 | 2213 | rBV2 | 346544 | 686138  | 44.09%  | 5.112%  |
| 59 | 8.460  | 2289 | 2292 | 2294 | rBV2 | 651    | 346     | 0.02%   | 0.003%  |
| 60 | 8.617  | 2339 | 2341 | 2344 | rBV3 | 857    | 430     | 0.03%   | 0.003%  |
| 61 | 8.859  | 2403 | 2416 | 2438 | rBV  | 638558 | 1045688 | 67.20%  | 7.791%  |
| 62 | 9.158  | 2507 | 2509 | 2515 | rVB5 | 623    | 336     | 0.02%   | 0.003%  |
| 63 | 9.334  | 2560 | 2564 | 2565 | rBV2 | 490    | 330     | 0.02%   | 0.002%  |
| 64 | 9.383  | 2577 | 2579 | 2580 | rBV2 | 571    | 193     | 0.01%   | 0.001%  |
| 65 | 9.515  | 2617 | 2620 | 2621 | rBV2 | 461    | 267     | 0.02%   | 0.002%  |
| 66 | 9.707  | 2678 | 2680 | 2681 | rBV  | 339    | 149     | 0.01%   | 0.001%  |
| 67 | 9.730  | 2685 | 2687 | 2690 | rVV3 | 366    | 166     | 0.01%   | 0.001%  |
| 68 | 9.862  | 2726 | 2728 | 2730 | rBV  | 996    | 563     | 0.04%   | 0.004%  |
| 69 | 10.000 | 2768 | 2771 | 2773 | rBV3 | 579    | 380     | 0.02%   | 0.003%  |
| 70 | 10.096 | 2799 | 2801 | 2803 | rBV3 | 513    | 306     | 0.02%   | 0.002%  |
| 71 | 10.148 | 2815 | 2817 | 2820 | rBV2 | 441    | 266     | 0.02%   | 0.002%  |
| 72 | 10.164 | 2820 | 2822 | 2823 | rBV  | 537    | 205     | 0.01%   | 0.002%  |
| 73 | 10.222 | 2828 | 2840 | 2857 | rBV  | 478611 | 709138  | 45.57%  | 5.284%  |
| 74 | 10.466 | 2913 | 2916 | 2920 | rVB3 | 664    | 423     | 0.03%   | 0.003%  |
| 75 | 10.521 | 2931 | 2933 | 2935 | rVB2 | 601    | 254     | 0.02%   | 0.002%  |
| 76 | 10.910 | 3050 | 3054 | 3056 | rBV3 | 739    | 592     | 0.04%   | 0.004%  |

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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\_V\Method\SOMVLM012121WMA.M

Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 11.022 | 3083 | 3089 | 3093 | rBV5 | 755    | 933     | 0.06%  | 0.007% |
| 78  | 11.138 | 3123 | 3125 | 3126 | rVB  | 586    | 122     | 0.01%  | 0.001% |
| 79  | 11.177 | 3135 | 3137 | 3140 | rBV3 | 758    | 526     | 0.03%  | 0.004% |
| 80  | 11.257 | 3149 | 3162 | 3182 | rBV  | 657917 | 1022657 | 65.72% | 7.620% |
| 81  | 11.630 | 3266 | 3278 | 3298 | rBV  | 719754 | 1132282 | 72.76% | 8.436% |
| 82  | 11.823 | 3336 | 3338 | 3341 | rBV2 | 663    | 343     | 0.02%  | 0.003% |
| 83  | 11.891 | 3357 | 3359 | 3362 | rBV2 | 538    | 288     | 0.02%  | 0.002% |
| 84  | 11.971 | 3382 | 3384 | 3386 | rBV2 | 458    | 227     | 0.01%  | 0.002% |
| 85  | 12.058 | 3409 | 3411 | 3414 | rBV3 | 795    | 394     | 0.03%  | 0.003% |
| 86  | 12.154 | 3439 | 3441 | 3442 | rBV  | 628    | 300     | 0.02%  | 0.002% |
| 87  | 12.241 | 3466 | 3468 | 3471 | rVB3 | 647    | 307     | 0.02%  | 0.002% |
| 88  | 12.421 | 3522 | 3524 | 3525 | rBV  | 530    | 234     | 0.02%  | 0.002% |
| 89  | 12.518 | 3551 | 3554 | 3556 | rBV2 | 804    | 388     | 0.02%  | 0.003% |
| 90  | 12.627 | 3585 | 3588 | 3589 | rBV2 | 416    | 193     | 0.01%  | 0.001% |
| 91  | 12.640 | 3590 | 3592 | 3595 | rVV4 | 650    | 332     | 0.02%  | 0.002% |
| 92  | 12.936 | 3681 | 3684 | 3686 | rBV4 | 874    | 565     | 0.04%  | 0.004% |
| 93  | 13.058 | 3720 | 3722 | 3724 | rBV2 | 471    | 222     | 0.01%  | 0.002% |
| 94  | 13.138 | 3745 | 3747 | 3750 | rBV2 | 429    | 244     | 0.02%  | 0.002% |
| 95  | 13.164 | 3753 | 3755 | 3757 | rVB2 | 522    | 227     | 0.01%  | 0.002% |
| 96  | 13.479 | 3850 | 3853 | 3856 | rBV4 | 781    | 577     | 0.04%  | 0.004% |
| 97  | 13.868 | 3969 | 3974 | 3978 | rBV6 | 827    | 936     | 0.06%  | 0.007% |
| 98  | 13.968 | 4003 | 4005 | 4006 | rBV2 | 576    | 275     | 0.02%  | 0.002% |
| 99  | 14.135 | 4052 | 4057 | 4058 | rBV3 | 815    | 690     | 0.04%  | 0.005% |
| 100 | 14.309 | 4109 | 4111 | 4113 | rBV  | 507    | 197     | 0.01%  | 0.001% |

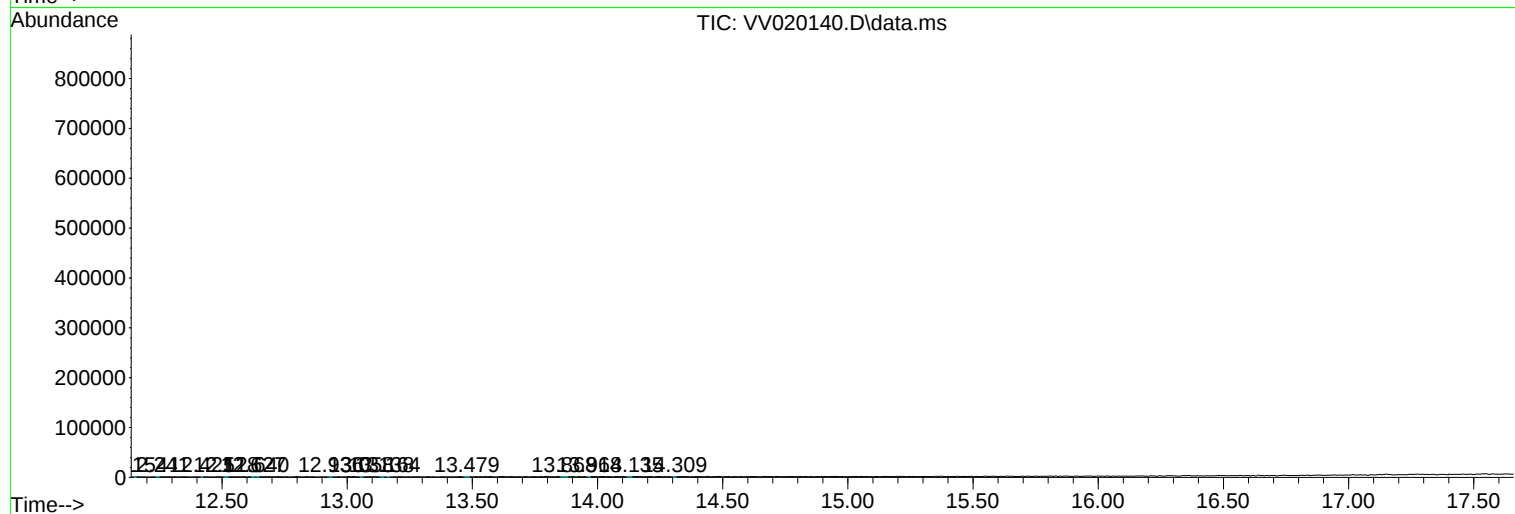
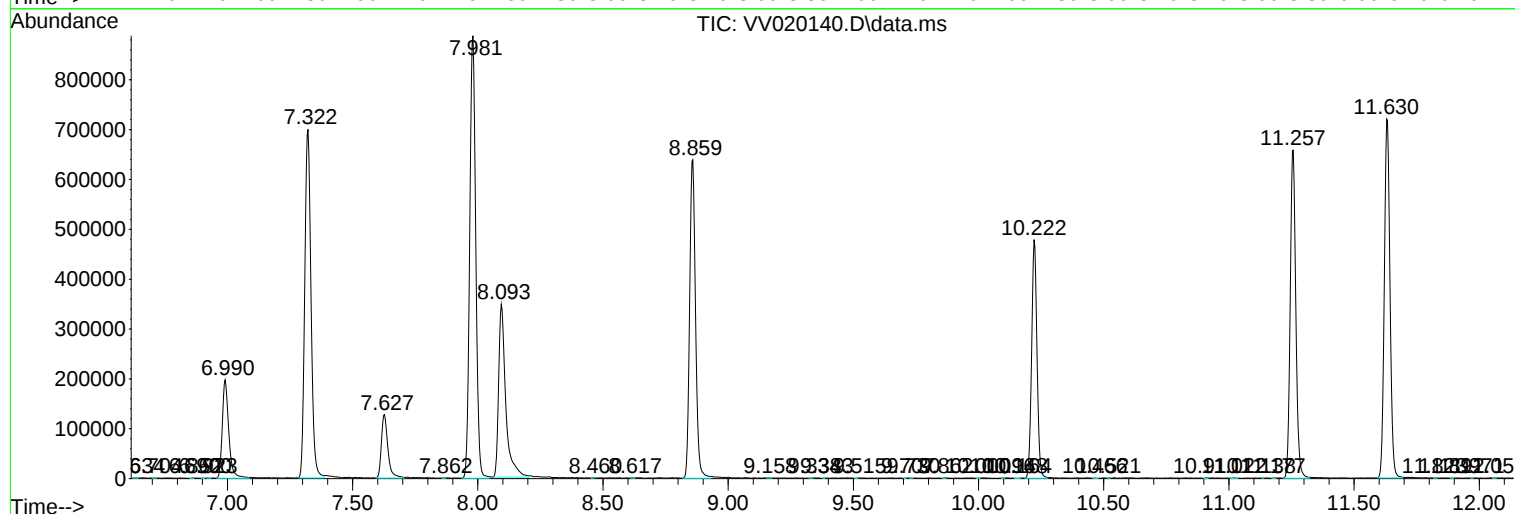
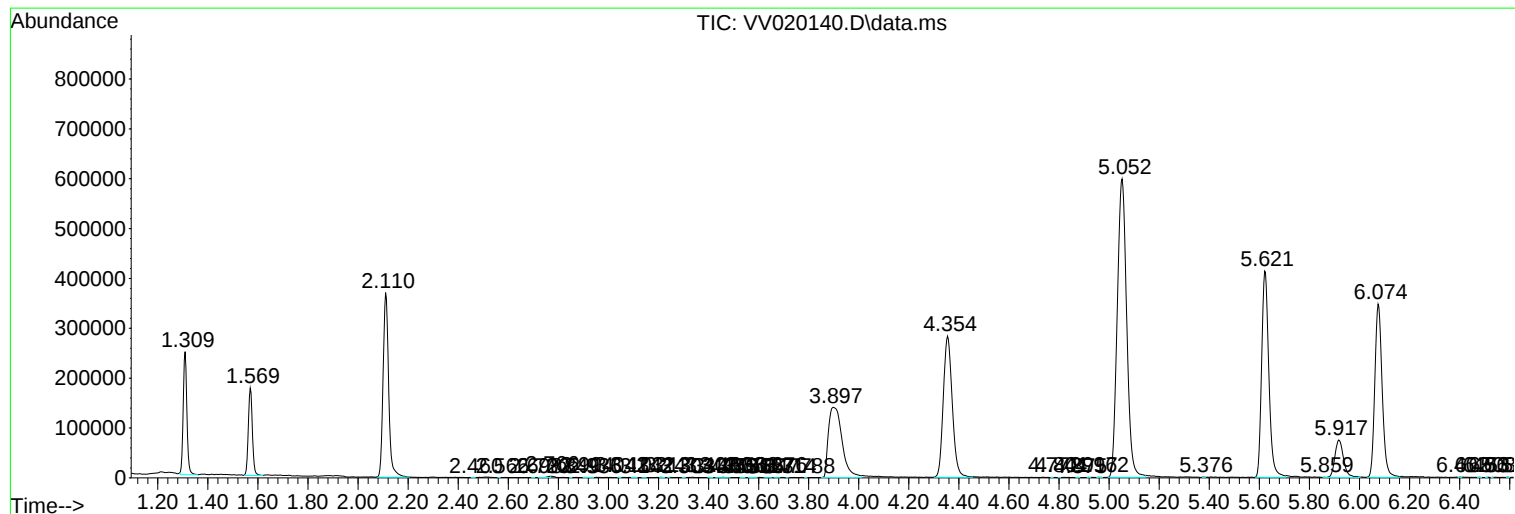
Sum of corrected areas: 13421421

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SOMVLM012121WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV012221\  
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No Library Search Compounds Detected

\*\*\*\*\*

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