

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041223\  
 Data File : VU053663.D  
 Acq On : 12 Apr 2023 15:43  
 Operator : JC/MD  
 Sample : 02252-07  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 COME3

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\SFAMULM033123WMA.M  
 Title : VOC Analysis

Signal : TIC: VU053663.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         | 1.597       | 73            | 80          | 96           | rVB      | 90538          | 108177        | 13.33%          | 1.710%        |
| 2         | 1.909       | 169           | 177         | 194          | rVB      | 77272          | 109904        | 13.55%          | 1.738%        |
| 3         | 2.565       | 368           | 381         | 395          | rBV      | 146971         | 239913        | 29.57%          | 3.793%        |
| 4         | 2.771       | 443           | 445         | 446          | rBV      | 328            | 100           | 0.01%           | 0.002%        |
| 5         | 2.842       | 464           | 467         | 468          | rBV      | 369            | 209           | 0.03%           | 0.003%        |
| 6         | 3.131       | 555           | 557         | 559          | rBV      | 243            | 142           | 0.02%           | 0.002%        |
| 7         | 3.176       | 566           | 571         | 575          | rBV3     | 520            | 616           | 0.08%           | 0.010%        |
| 8         | 3.305       | 609           | 611         | 614          | rVB      | 304            | 143           | 0.02%           | 0.002%        |
| 9         | 3.687       | 727           | 730         | 732          | rBV2     | 211            | 128           | 0.02%           | 0.002%        |
| 10        | 3.887       | 789           | 792         | 795          | rBV      | 275            | 225           | 0.03%           | 0.004%        |
| 11        | 3.951       | 811           | 812         | 813          | rBV      | 259            | 100           | 0.01%           | 0.002%        |
| 12        | 4.205       | 888           | 891         | 895          | rBV2     | 286            | 207           | 0.03%           | 0.003%        |
| 13        | 4.292       | 916           | 918         | 919          | rBV      | 124            | 47            | 0.01%           | 0.001%        |
| 14        | 4.314       | 922           | 925         | 928          | rBV      | 310            | 239           | 0.03%           | 0.004%        |
| 15        | 4.613       | 1006          | 1018        | 1046         | rBV      | 79543          | 191758        | 23.63%          | 3.032%        |
| 16        | 5.057       | 1137          | 1156        | 1179         | rBV2     | 155702         | 342874        | 42.26%          | 5.421%        |
| 17        | 5.237       | 1210          | 1212        | 1214         | rBV      | 205            | 80            | 0.01%           | 0.001%        |
| 18        | 5.253       | 1214          | 1217        | 1220         | rBV      | 528            | 323           | 0.04%           | 0.005%        |
| 19        | 5.298       | 1230          | 1231        | 1233         | rVB      | 280            | 97            | 0.01%           | 0.002%        |
| 20        | 5.369       | 1251          | 1253        | 1255         | rBV      | 380            | 264           | 0.03%           | 0.004%        |
| 21        | 5.472       | 1283          | 1285        | 1289         | rVB      | 303            | 152           | 0.02%           | 0.002%        |
| 22        | 5.562       | 1310          | 1313        | 1315         | rBV2     | 191            | 143           | 0.02%           | 0.002%        |
| 23        | 5.578       | 1315          | 1318        | 1320         | rVV2     | 195            | 126           | 0.02%           | 0.002%        |
| 24        | 5.604       | 1323          | 1326        | 1331         | rVV      | 355            | 276           | 0.03%           | 0.004%        |
| 25        | 5.719       | 1341          | 1362        | 1374         | rBV2     | 291833         | 811338        | 100.00%         | 12.827%       |
| 26        | 5.935       | 1426          | 1429        | 1433         | rBV3     | 381            | 380           | 0.05%           | 0.006%        |
| 27        | 5.993       | 1444          | 1447        | 1450         | rBV      | 160            | 100           | 0.01%           | 0.002%        |
| 28        | 6.108       | 1479          | 1483        | 1488         | rBV      | 244            | 220           | 0.03%           | 0.003%        |
| 29        | 6.137       | 1488          | 1492        | 1495         | rVV      | 215            | 185           | 0.02%           | 0.003%        |
| 30        | 6.243       | 1512          | 1525        | 1547         | rBV      | 219681         | 416194        | 51.30%          | 6.580%        |
| 31        | 6.459       | 1589          | 1592        | 1594         | rBV      | 359            | 240           | 0.03%           | 0.004%        |
| 32        | 6.523       | 1604          | 1612        | 1614         | rBV4     | 2355           | 2604          | 0.32%           | 0.041%        |
| 33        | 6.684       | 1648          | 1662        | 1688         | rBV      | 188550         | 370980        | 45.72%          | 5.865%        |
| 34        | 6.842       | 1708          | 1711        | 1714         | rVB      | 302            | 197           | 0.02%           | 0.003%        |
| 35        | 6.861       | 1714          | 1717        | 1720         | rBV      | 233            | 153           | 0.02%           | 0.002%        |
| 36        | 6.887       | 1724          | 1725        | 1726         | rBV      | 180            | 40            | 0.00%           | 0.001%        |

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 ClientSampleId :  
 COME3

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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.096  | 1787 | 1790 | 1796 | rVB  | 281    | 190    | 0.02%  | 0.003%  |
| 38 | 7.308  | 1853 | 1856 | 1857 | rBV  | 196    | 112    | 0.01%  | 0.002%  |
| 39 | 7.333  | 1862 | 1864 | 1868 | rVB  | 382    | 288    | 0.04%  | 0.005%  |
| 40 | 7.423  | 1889 | 1892 | 1894 | rBV  | 122    | 63     | 0.01%  | 0.001%  |
| 41 | 7.562  | 1923 | 1935 | 1960 | rBV2 | 101852 | 182601 | 22.51% | 2.887%  |
| 42 | 7.739  | 1986 | 1990 | 1993 | rBV2 | 244    | 201    | 0.02%  | 0.003%  |
| 43 | 7.774  | 1998 | 2001 | 2003 | rBV  | 385    | 224    | 0.03%  | 0.004%  |
| 44 | 7.796  | 2003 | 2008 | 2015 | rVB3 | 978    | 1262   | 0.16%  | 0.020%  |
| 45 | 7.832  | 2015 | 2019 | 2024 | rBV2 | 224    | 222    | 0.03%  | 0.004%  |
| 46 | 7.893  | 2025 | 2038 | 2073 | rBV  | 360712 | 640596 | 78.96% | 10.128% |
| 47 | 8.176  | 2115 | 2126 | 2148 | rBV2 | 73406  | 122710 | 15.12% | 1.940%  |
| 48 | 8.452  | 2210 | 2212 | 2214 | rBV2 | 213    | 122    | 0.02%  | 0.002%  |
| 49 | 8.468  | 2214 | 2217 | 2222 | rVV  | 370    | 319    | 0.04%  | 0.005%  |
| 50 | 8.626  | 2255 | 2266 | 2301 | rBV  | 233144 | 425018 | 52.38% | 6.720%  |
| 51 | 8.874  | 2341 | 2343 | 2346 | rVB  | 282    | 169    | 0.02%  | 0.003%  |
| 52 | 9.034  | 2390 | 2393 | 2396 | rBV  | 199    | 159    | 0.02%  | 0.003%  |
| 53 | 9.128  | 2419 | 2422 | 2425 | rBV  | 273    | 190    | 0.02%  | 0.003%  |
| 54 | 9.333  | 2484 | 2486 | 2490 | rVB2 | 210    | 132    | 0.02%  | 0.002%  |
| 55 | 9.366  | 2494 | 2496 | 2499 | rBV  | 184    | 115    | 0.01%  | 0.002%  |
| 56 | 9.414  | 2499 | 2511 | 2517 | rBV  | 314739 | 549448 | 67.72% | 8.687%  |
| 57 | 9.626  | 2575 | 2577 | 2580 | rVB  | 246    | 104    | 0.01%  | 0.002%  |
| 58 | 9.748  | 2612 | 2615 | 2621 | rBV2 | 347    | 307    | 0.04%  | 0.005%  |
| 59 | 9.841  | 2643 | 2644 | 2645 | rVB  | 205    | 40     | 0.00%  | 0.001%  |
| 60 | 9.906  | 2659 | 2664 | 2667 | rBV  | 268    | 284    | 0.04%  | 0.004%  |
| 61 | 10.070 | 2714 | 2715 | 2716 | rBV  | 159    | 50     | 0.01%  | 0.001%  |
| 62 | 10.414 | 2820 | 2822 | 2823 | rBV  | 106    | 26     | 0.00%  | 0.000%  |
| 63 | 10.751 | 2915 | 2927 | 2945 | rBV  | 302193 | 483648 | 59.61% | 7.646%  |
| 64 | 10.951 | 2987 | 2989 | 2993 | rBV  | 274    | 203    | 0.03%  | 0.003%  |
| 65 | 11.038 | 3013 | 3016 | 3019 | rBV  | 332    | 250    | 0.03%  | 0.004%  |
| 66 | 11.449 | 3142 | 3144 | 3145 | rBV  | 446    | 212    | 0.03%  | 0.003%  |
| 67 | 11.529 | 3161 | 3169 | 3179 | rBV4 | 5494   | 7670   | 0.95%  | 0.121%  |
| 68 | 11.742 | 3229 | 3235 | 3236 | rBV3 | 1532   | 1344   | 0.17%  | 0.021%  |
| 69 | 11.809 | 3243 | 3256 | 3282 | rBV2 | 337932 | 609435 | 75.11% | 9.635%  |
| 70 | 11.941 | 3295 | 3297 | 3300 | rBV2 | 239    | 114    | 0.01%  | 0.002%  |
| 71 | 12.189 | 3363 | 3374 | 3398 | rVB  | 404200 | 696210 | 85.81% | 11.007% |
| 72 | 12.439 | 3450 | 3452 | 3457 | rBV3 | 428    | 336    | 0.04%  | 0.005%  |
| 73 | 12.581 | 3494 | 3496 | 3500 | rBV  | 346    | 217    | 0.03%  | 0.003%  |
| 74 | 12.951 | 3608 | 3611 | 3613 | rBV  | 301    | 166    | 0.02%  | 0.003%  |
| 75 | 13.153 | 3672 | 3674 | 3677 | rBV2 | 300    | 155    | 0.02%  | 0.002%  |
| 76 | 13.282 | 3713 | 3714 | 3715 | rVB  | 386    | 74     | 0.01%  | 0.001%  |

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Instrument :  
MSVOA\_U  
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COME3

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\SFAMULM033123WMA.M  
Title : VOC Analysis

|    |        |      |      |      |      |      |     |       |        |
|----|--------|------|------|------|------|------|-----|-------|--------|
| 77 | 13.346 | 3728 | 3734 | 3735 | rBV2 | 364  | 358 | 0.04% | 0.006% |
| 78 | 13.558 | 3798 | 3800 | 3802 | rBV  | 306  | 173 | 0.02% | 0.003% |
| 79 | 13.844 | 3885 | 3889 | 3890 | rBV2 | 1014 | 712 | 0.09% | 0.011% |

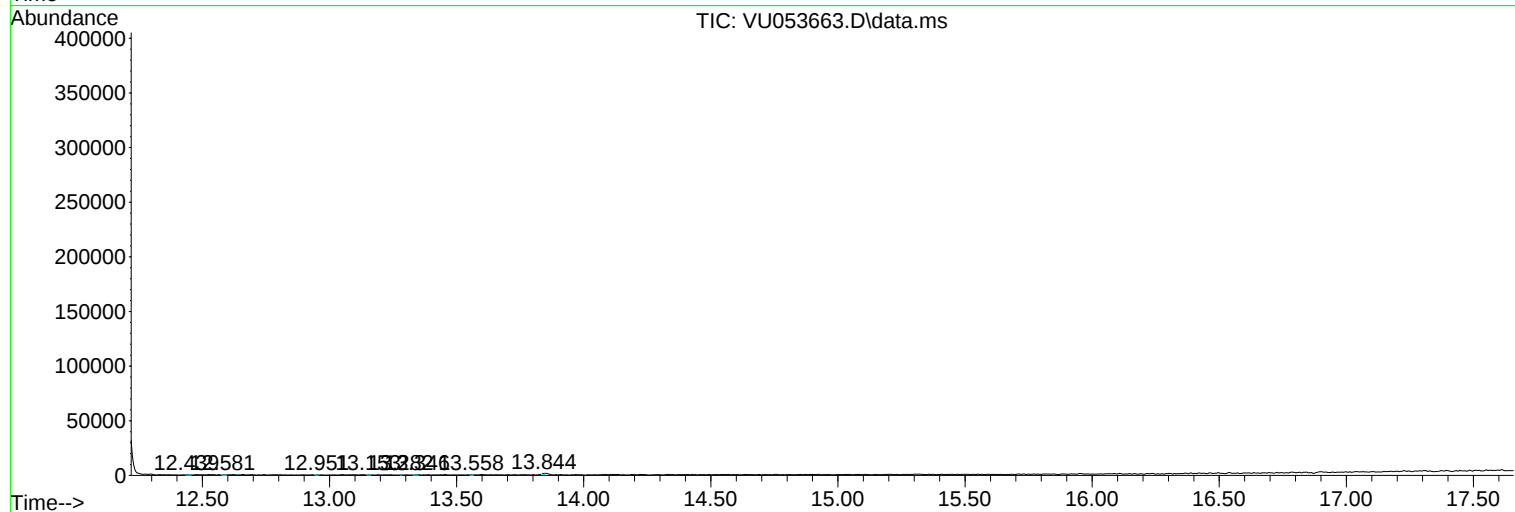
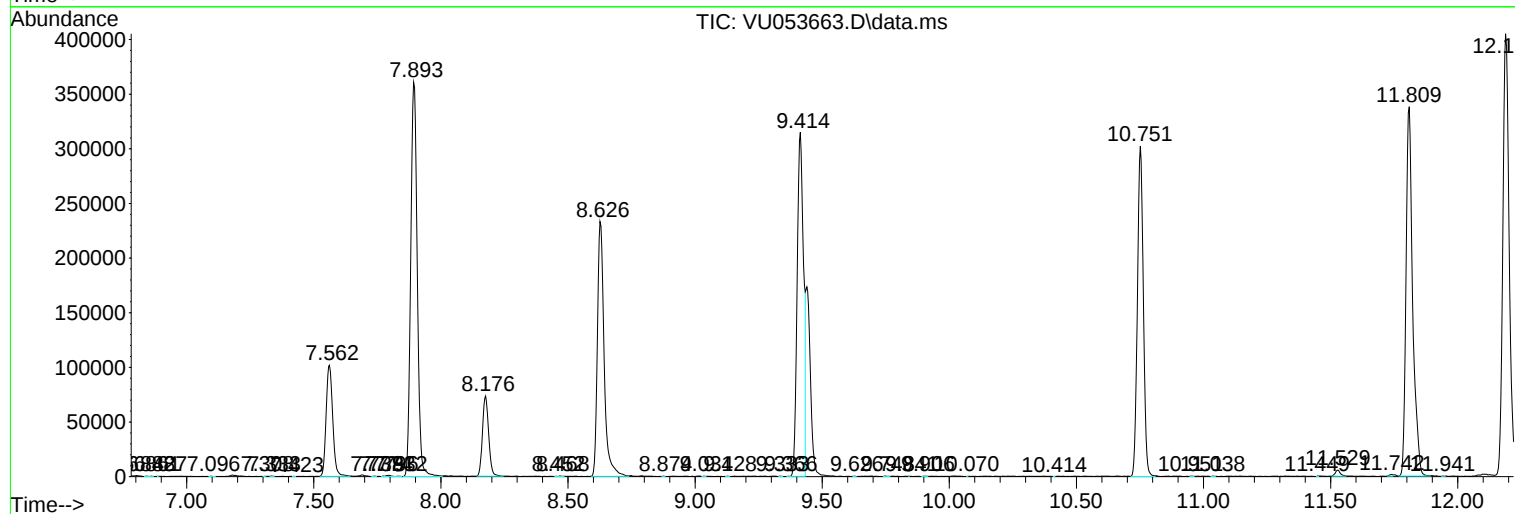
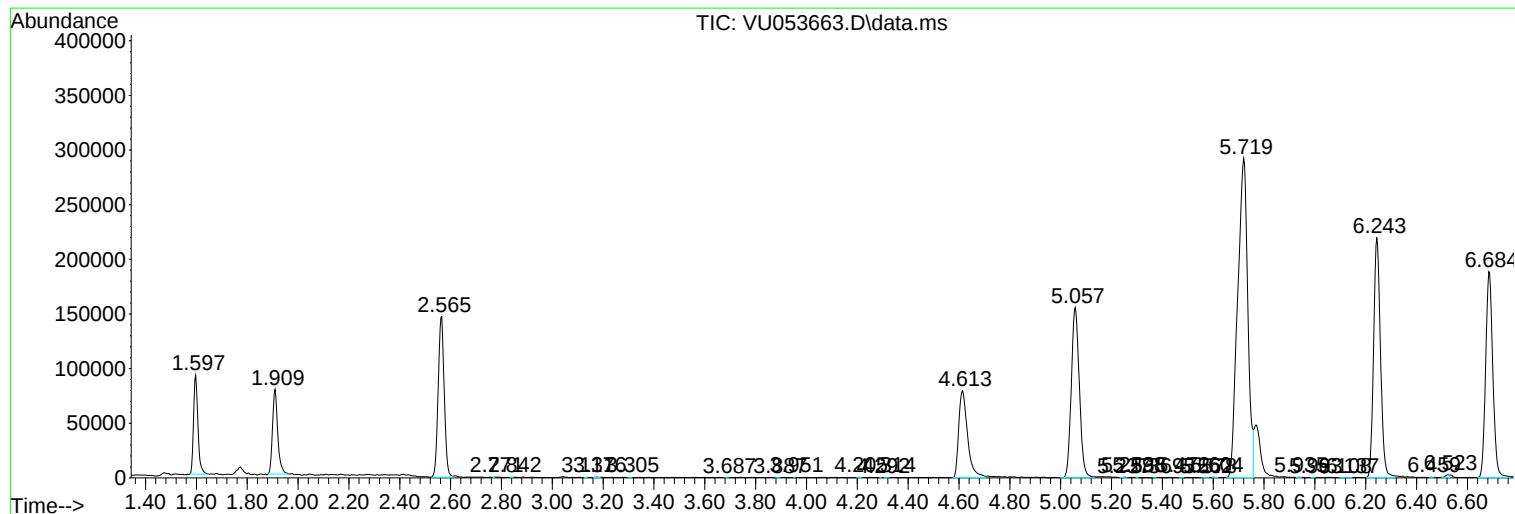
Sum of corrected areas: 6325103

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COME3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041223\  
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Sample : 02252-07  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0ME3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0ME3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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