

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
 Data File : VU050566.D  
 Acq On : 31 Aug 2022 22:04  
 Operator : SY/MD  
 Sample : N4345-03ME 100X  
 Misc : 6.13g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBVS3ME

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\SFAMULM083022WMA.M  
 Title : VOC Analysis

Signal : TIC: VU050566.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       | 72            | 80          | 105          | rVB      | 93097          | 118366        | 12.87%          | 1.535%        |
| 2         | 1.903       | 167           | 175         | 191          | rVB      | 66145          | 91171         | 9.91%           | 1.182%        |
| 3         | 2.350       | 312           | 314         | 316          | rBV      | 351            | 93            | 0.01%           | 0.001%        |
| 4         | 2.562       | 365           | 380         | 399          | rBV      | 172222         | 276503        | 30.06%          | 3.585%        |
| 5         | 2.710       | 423           | 426         | 434          | rVB3     | 361            | 323           | 0.04%           | 0.004%        |
| 6         | 2.761       | 440           | 442         | 445          | rBV      | 174            | 121           | 0.01%           | 0.002%        |
| 7         | 2.797       | 449           | 453         | 455          | rVB      | 445            | 302           | 0.03%           | 0.004%        |
| 8         | 2.842       | 464           | 467         | 468          | rBV2     | 232            | 146           | 0.02%           | 0.002%        |
| 9         | 2.893       | 480           | 483         | 486          | rVB      | 278            | 161           | 0.02%           | 0.002%        |
| 10        | 3.041       | 522           | 529         | 545          | rVV4     | 2002           | 3113          | 0.34%           | 0.040%        |
| 11        | 3.118       | 549           | 553         | 555          | rVB2     | 250            | 176           | 0.02%           | 0.002%        |
| 12        | 3.182       | 555           | 573         | 590          | rBV2     | 7304           | 16858         | 1.83%           | 0.219%        |
| 13        | 3.266       | 596           | 599         | 603          | rBV      | 429            | 261           | 0.03%           | 0.003%        |
| 14        | 3.356       | 625           | 627         | 629          | rBV      | 167            | 93            | 0.01%           | 0.001%        |
| 15        | 3.404       | 637           | 642         | 643          | rBV2     | 250            | 178           | 0.02%           | 0.002%        |
| 16        | 3.414       | 643           | 645         | 648          | rVB      | 97             | 53            | 0.01%           | 0.001%        |
| 17        | 3.443       | 648           | 654         | 658          | rBV      | 259            | 383           | 0.04%           | 0.005%        |
| 18        | 3.469       | 659           | 662         | 666          | rVV2     | 255            | 218           | 0.02%           | 0.003%        |
| 19        | 3.504       | 669           | 673         | 677          | rVB2     | 213            | 204           | 0.02%           | 0.003%        |
| 20        | 3.526       | 677           | 680         | 682          | rBV2     | 246            | 138           | 0.02%           | 0.002%        |
| 21        | 3.575       | 691           | 695         | 698          | rBV      | 121            | 119           | 0.01%           | 0.002%        |
| 22        | 3.633       | 708           | 713         | 715          | rBV2     | 221            | 173           | 0.02%           | 0.002%        |
| 23        | 3.645       | 715           | 717         | 720          | rVB      | 119            | 58            | 0.01%           | 0.001%        |
| 24        | 3.665       | 721           | 723         | 727          | rVB2     | 198            | 137           | 0.01%           | 0.002%        |
| 25        | 3.687       | 727           | 730         | 732          | rBV2     | 203            | 144           | 0.02%           | 0.002%        |
| 26        | 3.703       | 732           | 735         | 740          | rVB      | 319            | 213           | 0.02%           | 0.003%        |
| 27        | 3.732       | 742           | 744         | 746          | rBV      | 110            | 62            | 0.01%           | 0.001%        |
| 28        | 3.761       | 751           | 753         | 755          | rBV      | 131            | 50            | 0.01%           | 0.001%        |
| 29        | 3.800       | 762           | 765         | 767          | rBV      | 190            | 102           | 0.01%           | 0.001%        |
| 30        | 3.851       | 779           | 781         | 784          | rBV2     | 141            | 97            | 0.01%           | 0.001%        |
| 31        | 3.890       | 790           | 793         | 796          | rBV      | 120            | 89            | 0.01%           | 0.001%        |
| 32        | 3.909       | 796           | 799         | 800          | rBV      | 137            | 84            | 0.01%           | 0.001%        |
| 33        | 3.964       | 814           | 816         | 819          | rVB2     | 271            | 171           | 0.02%           | 0.002%        |
| 34        | 3.993       | 819           | 825         | 827          | rBV      | 78             | 83            | 0.01%           | 0.001%        |
| 35        | 4.022       | 831           | 834         | 845          | rVB2     | 278            | 453           | 0.05%           | 0.006%        |
| 36        | 4.070       | 845           | 849         | 851          | rBV      | 217            | 141           | 0.02%           | 0.002%        |

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 ClientSampleId :  
 DBVS3ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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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\SFAMULM083022WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |         |         |
|----|-------|------|------|------|------|--------|--------|---------|---------|
| 37 | 4.102 | 855  | 859  | 864  | rVB2 | 198    | 159    | 0.02%   | 0.002%  |
| 38 | 4.198 | 885  | 889  | 890  | rBV  | 200    | 170    | 0.02%   | 0.002%  |
| 39 | 4.227 | 895  | 898  | 903  | rVB  | 179    | 155    | 0.02%   | 0.002%  |
| 40 | 4.263 | 905  | 909  | 912  | rVB2 | 192    | 132    | 0.01%   | 0.002%  |
| 41 | 4.288 | 912  | 917  | 921  | rBV  | 93     | 95     | 0.01%   | 0.001%  |
| 42 | 4.308 | 921  | 923  | 928  | rBV  | 141    | 91     | 0.01%   | 0.001%  |
| 43 | 4.366 | 934  | 941  | 945  | rVB2 | 193    | 196    | 0.02%   | 0.003%  |
| 44 | 4.385 | 945  | 947  | 952  | rVB2 | 171    | 173    | 0.02%   | 0.002%  |
| 45 | 4.423 | 952  | 959  | 962  | rBV2 | 193    | 264    | 0.03%   | 0.003%  |
| 46 | 4.459 | 965  | 970  | 973  | rBV2 | 168    | 134    | 0.01%   | 0.002%  |
| 47 | 4.491 | 976  | 980  | 982  | rVB  | 184    | 114    | 0.01%   | 0.001%  |
| 48 | 4.510 | 982  | 986  | 988  | rBV2 | 153    | 125    | 0.01%   | 0.002%  |
| 49 | 4.526 | 988  | 991  | 992  | rBV  | 132    | 77     | 0.01%   | 0.001%  |
| 50 | 4.542 | 993  | 996  | 999  | rVB  | 144    | 61     | 0.01%   | 0.001%  |
| 51 | 4.559 | 999  | 1001 | 1005 | rBV2 | 151    | 118    | 0.01%   | 0.002%  |
| 52 | 4.629 | 1010 | 1023 | 1061 | rBV  | 88176  | 248602 | 27.03%  | 3.224%  |
| 53 | 5.060 | 1142 | 1157 | 1182 | rBV  | 172177 | 381958 | 41.52%  | 4.953%  |
| 54 | 5.214 | 1200 | 1205 | 1207 | rBV3 | 413    | 326    | 0.04%   | 0.004%  |
| 55 | 5.292 | 1223 | 1229 | 1238 | rBV3 | 809    | 1033   | 0.11%   | 0.013%  |
| 56 | 5.404 | 1261 | 1264 | 1265 | rBV  | 151    | 102    | 0.01%   | 0.001%  |
| 57 | 5.430 | 1269 | 1272 | 1278 | rBV  | 182    | 226    | 0.02%   | 0.003%  |
| 58 | 5.504 | 1292 | 1295 | 1298 | rBV  | 166    | 101    | 0.01%   | 0.001%  |
| 59 | 5.533 | 1301 | 1304 | 1306 | rBV  | 170    | 103    | 0.01%   | 0.001%  |
| 60 | 5.616 | 1320 | 1330 | 1337 | rBV  | 633    | 1077   | 0.12%   | 0.014%  |
| 61 | 5.722 | 1342 | 1363 | 1389 | rVV2 | 340968 | 919874 | 100.00% | 11.928% |
| 62 | 5.964 | 1434 | 1438 | 1440 | rBV  | 183    | 178    | 0.02%   | 0.002%  |
| 63 | 6.034 | 1453 | 1460 | 1461 | rBV2 | 346    | 341    | 0.04%   | 0.004%  |
| 64 | 6.066 | 1467 | 1470 | 1474 | rBV2 | 192    | 180    | 0.02%   | 0.002%  |
| 65 | 6.108 | 1482 | 1483 | 1486 | rBV2 | 182    | 70     | 0.01%   | 0.001%  |
| 66 | 6.247 | 1508 | 1526 | 1551 | rBV  | 323779 | 615499 | 66.91%  | 7.981%  |
| 67 | 6.520 | 1608 | 1611 | 1612 | rBV  | 884    | 515    | 0.06%   | 0.007%  |
| 68 | 6.591 | 1631 | 1633 | 1636 | rVB2 | 271    | 169    | 0.02%   | 0.002%  |
| 69 | 6.607 | 1636 | 1638 | 1639 | rBV  | 153    | 84     | 0.01%   | 0.001%  |
| 70 | 6.690 | 1650 | 1664 | 1688 | rBV  | 227750 | 439876 | 47.82%  | 5.704%  |
| 71 | 7.282 | 1842 | 1848 | 1849 | rBV2 | 203    | 211    | 0.02%   | 0.003%  |
| 72 | 7.410 | 1882 | 1888 | 1891 | rBV  | 282    | 263    | 0.03%   | 0.003%  |
| 73 | 7.523 | 1920 | 1923 | 1924 | rBV2 | 149    | 104    | 0.01%   | 0.001%  |
| 74 | 7.565 | 1924 | 1936 | 1957 | rVV  | 98078  | 172221 | 18.72%  | 2.233%  |
| 75 | 7.899 | 2027 | 2040 | 2062 | rBV  | 404501 | 701226 | 76.23%  | 9.093%  |
| 76 | 8.140 | 2112 | 2115 | 2116 | rBV2 | 284    | 188    | 0.02%   | 0.002%  |

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Integration Parameters: LSCINT.P

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\SFAMULM083022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 8.179  | 2116 | 2127 | 2149 | rVB  | 67088  | 114482 | 12.45% | 1.484%  |
| 78  | 8.407  | 2195 | 2198 | 2202 | rBV2 | 210    | 225    | 0.02%  | 0.003%  |
| 79  | 8.552  | 2230 | 2243 | 2258 | rBV  | 463405 | 783261 | 85.15% | 10.156% |
| 80  | 8.639  | 2259 | 2270 | 2300 | rVV3 | 202059 | 465286 | 50.58% | 6.033%  |
| 81  | 8.918  | 2355 | 2357 | 2360 | rBV2 | 192    | 113    | 0.01%  | 0.001%  |
| 82  | 8.944  | 2360 | 2365 | 2368 | rVV2 | 261    | 261    | 0.03%  | 0.003%  |
| 83  | 8.986  | 2374 | 2378 | 2381 | rBV2 | 333    | 302    | 0.03%  | 0.004%  |
| 84  | 9.169  | 2431 | 2435 | 2438 | rBV  | 161    | 146    | 0.02%  | 0.002%  |
| 85  | 9.214  | 2443 | 2449 | 2456 | rBV2 | 251    | 506    | 0.06%  | 0.007%  |
| 86  | 9.417  | 2499 | 2512 | 2540 | rBV  | 429462 | 715683 | 77.80% | 9.280%  |
| 87  | 9.677  | 2589 | 2593 | 2595 | rBV2 | 221    | 168    | 0.02%  | 0.002%  |
| 88  | 9.774  | 2619 | 2623 | 2625 | rBV2 | 156    | 139    | 0.02%  | 0.002%  |
| 89  | 9.960  | 2678 | 2681 | 2685 | rBV2 | 406    | 357    | 0.04%  | 0.005%  |
| 90  | 10.047 | 2702 | 2708 | 2711 | rBV2 | 329    | 463    | 0.05%  | 0.006%  |
| 91  | 10.346 | 2799 | 2801 | 2802 | rBV  | 142    | 76     | 0.01%  | 0.001%  |
| 92  | 10.758 | 2916 | 2929 | 2948 | rBV  | 322689 | 524484 | 57.02% | 6.801%  |
| 93  | 10.899 | 2970 | 2973 | 2975 | rBV  | 279    | 190    | 0.02%  | 0.002%  |
| 94  | 11.629 | 3198 | 3200 | 3201 | rBV  | 163    | 67     | 0.01%  | 0.001%  |
| 95  | 11.812 | 3245 | 3257 | 3278 | rBV  | 348385 | 553076 | 60.13% | 7.172%  |
| 96  | 12.192 | 3363 | 3375 | 3400 | rBV  | 339473 | 554312 | 60.26% | 7.188%  |
| 97  | 12.648 | 3514 | 3517 | 3520 | rBV2 | 338    | 221    | 0.02%  | 0.003%  |
| 98  | 12.925 | 3601 | 3603 | 3605 | rBV2 | 309    | 193    | 0.02%  | 0.003%  |
| 99  | 13.266 | 3707 | 3709 | 3712 | rBV2 | 322    | 178    | 0.02%  | 0.002%  |
| 100 | 13.372 | 3740 | 3742 | 3745 | rBV2 | 259    | 141    | 0.02%  | 0.002%  |

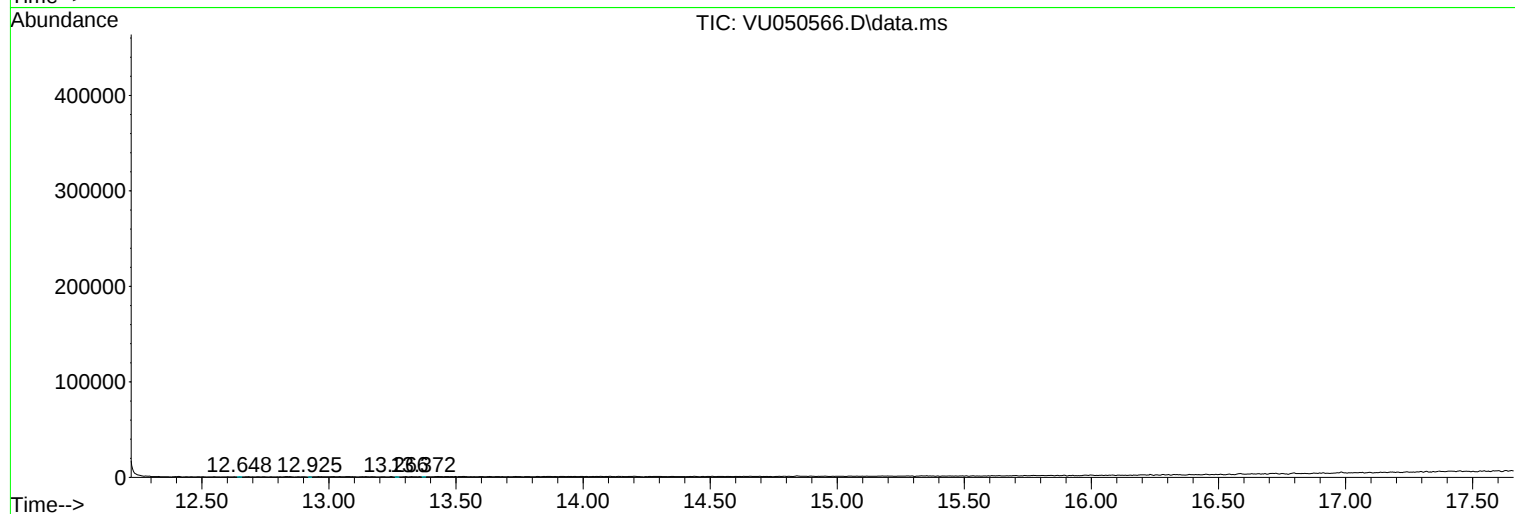
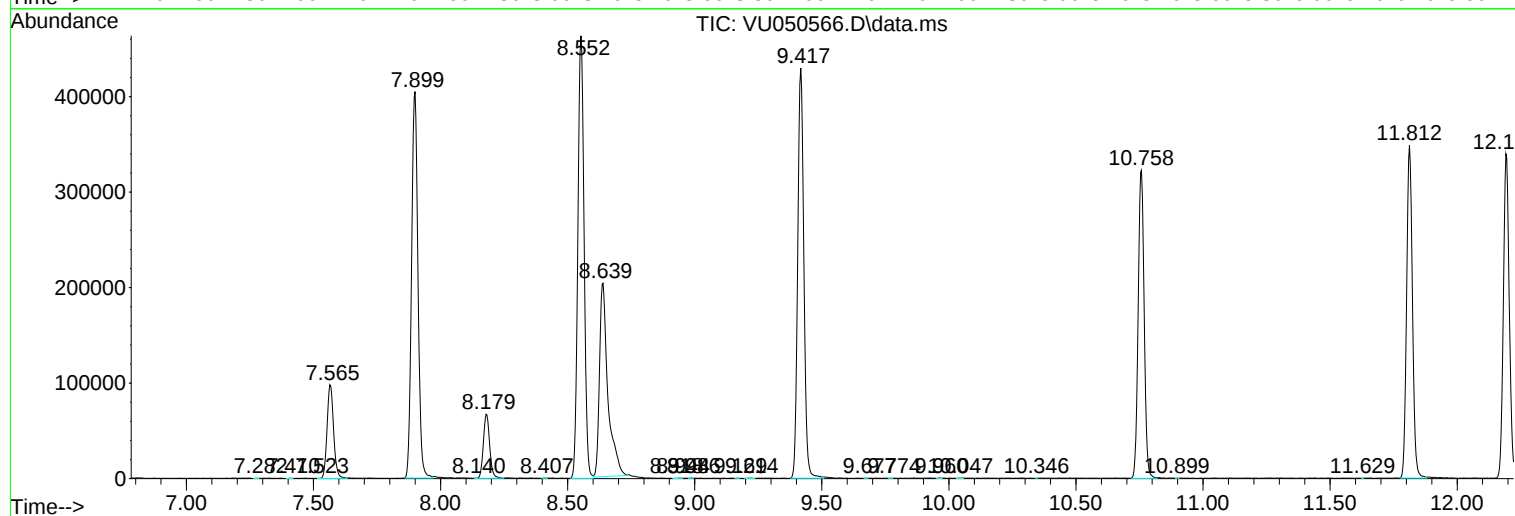
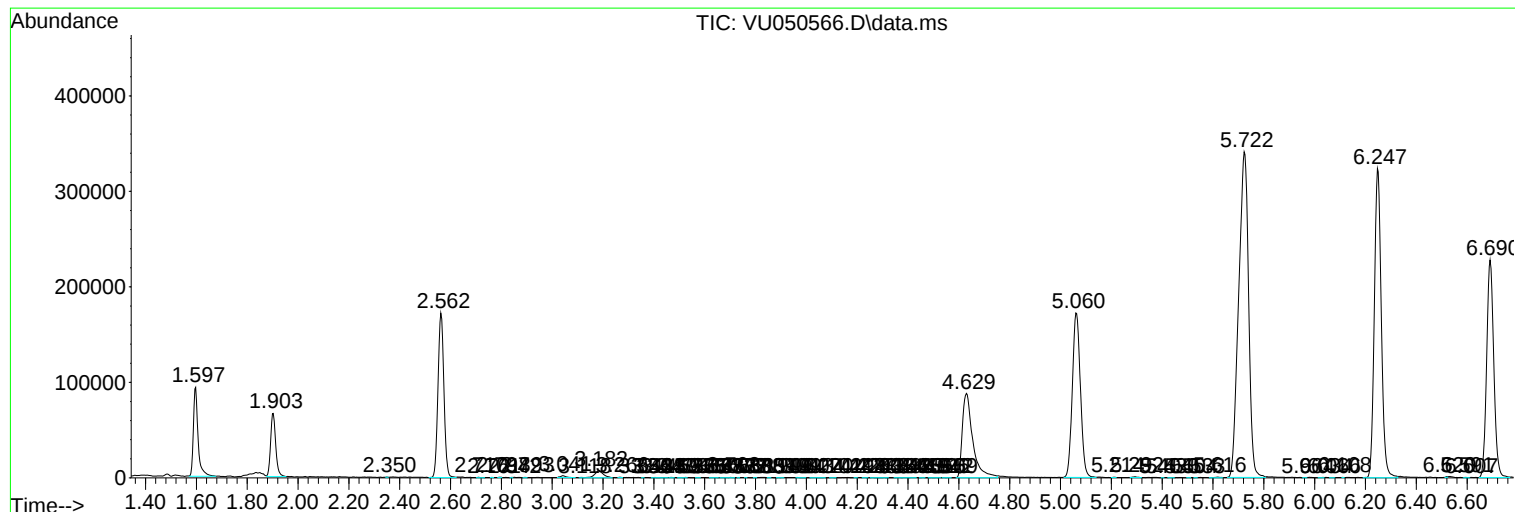
Sum of corrected areas: 7711958

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Instrument :  
MSVOA\_U  
ClientSampleId :  
DBVS3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM083022WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
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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 |