

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VW123121\  
 Data File : VW024253.D  
 Acq On : 31 Dec 2021 00:33  
 Operator : SY/MD  
 Sample : M5213-14ME  
 Misc : 6.40G/5.0mL/100uL//5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BGLE6ME

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\SFAMVLM123121WMA.M  
 Title : VOC Analysis

Signal : TIC: VW024253.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         | 1.307       | 76            | 83          | 97           | rVB      | 133808         | 161777        | 14.82%          | 2.062%        |
| 2         | 1.568       | 157           | 164         | 180          | rBV      | 92607          | 146020        | 13.37%          | 1.861%        |
| 3         | 2.085       | 316           | 325         | 337          | rVB      | 305399         | 432802        | 39.64%          | 5.515%        |
| 4         | 2.728       | 522           | 525         | 530          | rBV      | 851            | 884           | 0.08%           | 0.011%        |
| 5         | 2.796       | 543           | 546         | 550          | rVB      | 1008           | 788           | 0.07%           | 0.010%        |
| 6         | 3.532       | 771           | 775         | 778          | rBV      | 1078           | 933           | 0.09%           | 0.012%        |
| 7         | 3.902       | 879           | 890         | 919          | rBV2     | 42764          | 167612        | 15.35%          | 2.136%        |
| 8         | 4.346       | 1013          | 1028        | 1054         | rBV      | 175822         | 448964        | 41.12%          | 5.721%        |
| 9         | 4.773       | 1158          | 1161        | 1162         | rBV      | 680            | 380           | 0.03%           | 0.005%        |
| 10        | 4.912       | 1202          | 1204        | 1207         | rBV2     | 542            | 284           | 0.03%           | 0.004%        |
| 11        | 5.040       | 1228          | 1244        | 1278         | rBV2     | 440855         | 1091753       | 100.00%         | 13.913%       |
| 12        | 5.291       | 1317          | 1322        | 1323         | rBV      | 468            | 411           | 0.04%           | 0.005%        |
| 13        | 5.613       | 1411          | 1422        | 1450         | rBV      | 291972         | 613977        | 56.24%          | 7.824%        |
| 14        | 5.905       | 1503          | 1513        | 1528         | rBV5     | 10771          | 22984         | 2.11%           | 0.293%        |
| 15        | 5.989       | 1534          | 1539        | 1540         | rBV2     | 2040           | 1617          | 0.15%           | 0.021%        |
| 16        | 6.069       | 1550          | 1564        | 1595         | rVB      | 216654         | 475355        | 43.54%          | 6.058%        |
| 17        | 6.249       | 1616          | 1620        | 1625         | rBV2     | 743            | 760           | 0.07%           | 0.010%        |
| 18        | 6.458       | 1682          | 1685        | 1688         | rBV2     | 656            | 436           | 0.04%           | 0.006%        |
| 19        | 6.587       | 1722          | 1725        | 1727         | rBV      | 584            | 361           | 0.03%           | 0.005%        |
| 20        | 6.674       | 1749          | 1752        | 1754         | rBV3     | 718            | 532           | 0.05%           | 0.007%        |
| 21        | 6.895       | 1818          | 1821        | 1824         | rBV2     | 626            | 425           | 0.04%           | 0.005%        |
| 22        | 6.947       | 1835          | 1837        | 1838         | rBV      | 432            | 179           | 0.02%           | 0.002%        |
| 23        | 6.985       | 1839          | 1849        | 1877         | rVV      | 125494         | 255558        | 23.41%          | 3.257%        |
| 24        | 7.169       | 1903          | 1906        | 1909         | rBV2     | 628            | 462           | 0.04%           | 0.006%        |
| 25        | 7.313       | 1937          | 1951        | 1969         | rBV      | 495091         | 917917        | 84.08%          | 11.697%       |
| 26        | 7.622       | 2036          | 2047        | 2079         | rBV      | 80476          | 178210        | 16.32%          | 2.271%        |
| 27        | 7.879       | 2122          | 2127        | 2133         | rBV2     | 685            | 817           | 0.07%           | 0.010%        |
| 28        | 7.973       | 2153          | 2156        | 2158         | rBV2     | 504            | 273           | 0.03%           | 0.003%        |
| 29        | 8.095       | 2185          | 2194        | 2198         | rBV3     | 68798          | 106141        | 9.72%           | 1.353%        |
| 30        | 8.538       | 2330          | 2332        | 2338         | rVB      | 634            | 478           | 0.04%           | 0.006%        |
| 31        | 8.567       | 2338          | 2341        | 2346         | rBV      | 787            | 605           | 0.06%           | 0.008%        |
| 32        | 8.629       | 2356          | 2360        | 2362         | rBV      | 512            | 354           | 0.03%           | 0.005%        |
| 33        | 8.712       | 2383          | 2386        | 2387         | rBV      | 484            | 267           | 0.02%           | 0.003%        |
| 34        | 8.776       | 2403          | 2406        | 2408         | rBV      | 449            | 261           | 0.02%           | 0.003%        |
| 35        | 8.854       | 2418          | 2430        | 2458         | rBV      | 346832         | 736837        | 67.49%          | 9.390%        |
| 36        | 9.259       | 2552          | 2556        | 2562         | rVB2     | 469            | 418           | 0.04%           | 0.005%        |

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Instrument :  
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 ClientSampleId :  
 BGLE6ME

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\SFAMVLM123121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 9.288  | 2562 | 2565 | 2567 | rBV2 | 414    | 322    | 0.03%  | 0.004%  |
| 38 | 9.317  | 2572 | 2574 | 2577 | rVB  | 408    | 193    | 0.02%  | 0.002%  |
| 39 | 9.426  | 2605 | 2608 | 2611 | rVB  | 556    | 281    | 0.03%  | 0.004%  |
| 40 | 9.442  | 2611 | 2613 | 2617 | rBV2 | 436    | 298    | 0.03%  | 0.004%  |
| 41 | 9.661  | 2679 | 2681 | 2684 | rBV2 | 540    | 379    | 0.03%  | 0.005%  |
| 42 | 9.719  | 2697 | 2699 | 2702 | rVB  | 335    | 184    | 0.02%  | 0.002%  |
| 43 | 9.744  | 2703 | 2707 | 2712 | rBV2 | 535    | 662    | 0.06%  | 0.008%  |
| 44 | 9.815  | 2726 | 2729 | 2737 | rBV2 | 609    | 793    | 0.07%  | 0.010%  |
| 45 | 9.863  | 2741 | 2744 | 2749 | rBV  | 614    | 614    | 0.06%  | 0.008%  |
| 46 | 9.992  | 2779 | 2784 | 2786 | rBV2 | 477    | 443    | 0.04%  | 0.006%  |
| 47 | 10.008 | 2786 | 2789 | 2791 | rBV  | 504    | 354    | 0.03%  | 0.005%  |
| 48 | 10.127 | 2819 | 2826 | 2835 | rVB4 | 3001   | 4034   | 0.37%  | 0.051%  |
| 49 | 10.227 | 2843 | 2857 | 2875 | rBV  | 257365 | 481885 | 44.14% | 6.141%  |
| 50 | 10.368 | 2898 | 2901 | 2903 | rBV2 | 538    | 414    | 0.04%  | 0.005%  |
| 51 | 10.500 | 2939 | 2942 | 2945 | rBV2 | 548    | 432    | 0.04%  | 0.006%  |
| 52 | 10.538 | 2951 | 2954 | 2956 | rBV  | 869    | 480    | 0.04%  | 0.006%  |
| 53 | 10.574 | 2962 | 2965 | 2971 | rVB4 | 1901   | 1646   | 0.15%  | 0.021%  |
| 54 | 10.786 | 3028 | 3031 | 3035 | rVB  | 852    | 627    | 0.06%  | 0.008%  |
| 55 | 10.818 | 3035 | 3041 | 3044 | rBV  | 499    | 542    | 0.05%  | 0.007%  |
| 56 | 11.088 | 3122 | 3125 | 3130 | rBV  | 581    | 384    | 0.04%  | 0.005%  |
| 57 | 11.178 | 3150 | 3153 | 3155 | rBV2 | 488    | 333    | 0.03%  | 0.004%  |
| 58 | 11.255 | 3166 | 3177 | 3196 | rBV  | 452968 | 717428 | 65.71% | 9.143%  |
| 59 | 11.471 | 3241 | 3244 | 3245 | rBV  | 352    | 216    | 0.02%  | 0.003%  |
| 60 | 11.628 | 3281 | 3293 | 3311 | rBV  | 539495 | 852275 | 78.06% | 10.861% |
| 61 | 11.808 | 3346 | 3349 | 3355 | rVB  | 701    | 529    | 0.05%  | 0.007%  |
| 62 | 11.834 | 3355 | 3357 | 3360 | rBV  | 534    | 405    | 0.04%  | 0.005%  |
| 63 | 12.297 | 3498 | 3501 | 3504 | rBV  | 595    | 474    | 0.04%  | 0.006%  |
| 64 | 12.329 | 3509 | 3511 | 3513 | rVV  | 467    | 185    | 0.02%  | 0.002%  |
| 65 | 12.342 | 3513 | 3515 | 3517 | rVV  | 248    | 127    | 0.01%  | 0.002%  |
| 66 | 12.358 | 3517 | 3520 | 3523 | rVB  | 611    | 385    | 0.04%  | 0.005%  |
| 67 | 12.406 | 3532 | 3535 | 3538 | rBV  | 462    | 407    | 0.04%  | 0.005%  |
| 68 | 12.779 | 3648 | 3651 | 3655 | rBV  | 588    | 461    | 0.04%  | 0.006%  |
| 69 | 13.005 | 3717 | 3721 | 3726 | rBV  | 675    | 581    | 0.05%  | 0.007%  |
| 70 | 13.046 | 3730 | 3734 | 3736 | rBV  | 982    | 667    | 0.06%  | 0.008%  |
| 71 | 13.230 | 3788 | 3791 | 3793 | rBV  | 386    | 217    | 0.02%  | 0.003%  |
| 72 | 13.246 | 3793 | 3796 | 3799 | rVB  | 564    | 372    | 0.03%  | 0.005%  |
| 73 | 13.265 | 3799 | 3802 | 3803 | rBV  | 718    | 379    | 0.03%  | 0.005%  |
| 74 | 13.349 | 3825 | 3828 | 3830 | rBV  | 496    | 260    | 0.02%  | 0.003%  |
| 75 | 13.587 | 3899 | 3902 | 3904 | rBV2 | 507    | 338    | 0.03%  | 0.004%  |
| 76 | 13.670 | 3925 | 3928 | 3931 | rBV2 | 557    | 423    | 0.04%  | 0.005%  |

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 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BGLE6ME

Integration Parameters: LSCINT.P

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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\SFAMVLM123121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 77 | 13.750 | 3949 | 3953 | 3957 | rBV2 | 1000 | 768  | 0.07% | 0.010% |
| 78 | 14.037 | 4035 | 4042 | 4043 | rBV  | 829  | 886  | 0.08% | 0.011% |
| 79 | 14.088 | 4055 | 4058 | 4060 | rBV  | 857  | 553  | 0.05% | 0.007% |
| 80 | 14.345 | 4135 | 4138 | 4142 | rBV2 | 1157 | 1008 | 0.09% | 0.013% |
| 81 | 14.419 | 4157 | 4161 | 4164 | rBV3 | 535  | 517  | 0.05% | 0.007% |
| 82 | 14.513 | 4185 | 4190 | 4193 | rBV2 | 1043 | 961  | 0.09% | 0.012% |
| 83 | 14.718 | 4251 | 4254 | 4261 | rVB2 | 759  | 925  | 0.08% | 0.012% |
| 84 | 14.805 | 4278 | 4281 | 4282 | rBV  | 576  | 328  | 0.03% | 0.004% |
| 85 | 14.963 | 4322 | 4330 | 4334 | rBV2 | 1086 | 1513 | 0.14% | 0.019% |
| 86 | 15.021 | 4345 | 4348 | 4352 | rBV2 | 681  | 437  | 0.04% | 0.006% |

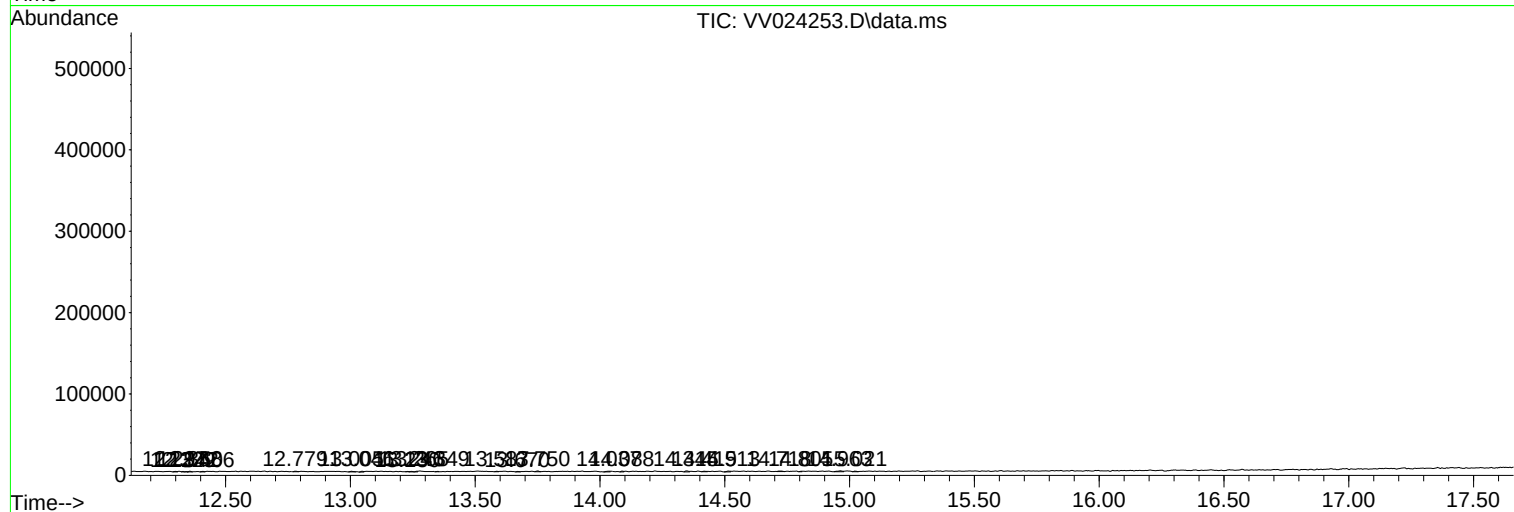
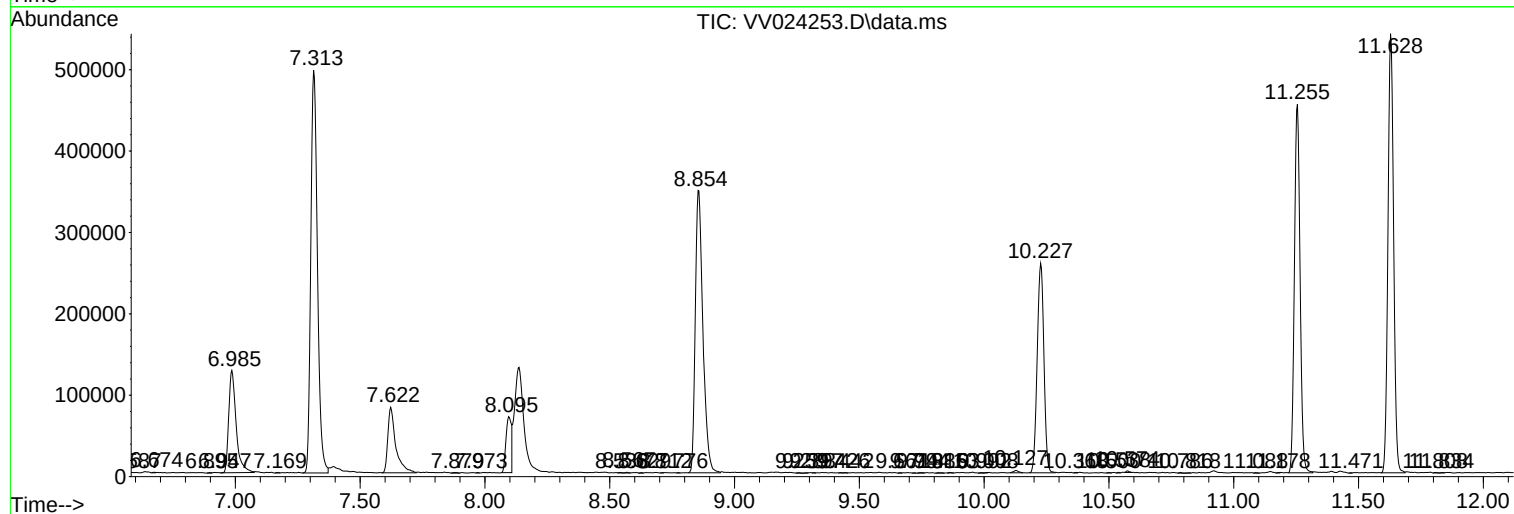
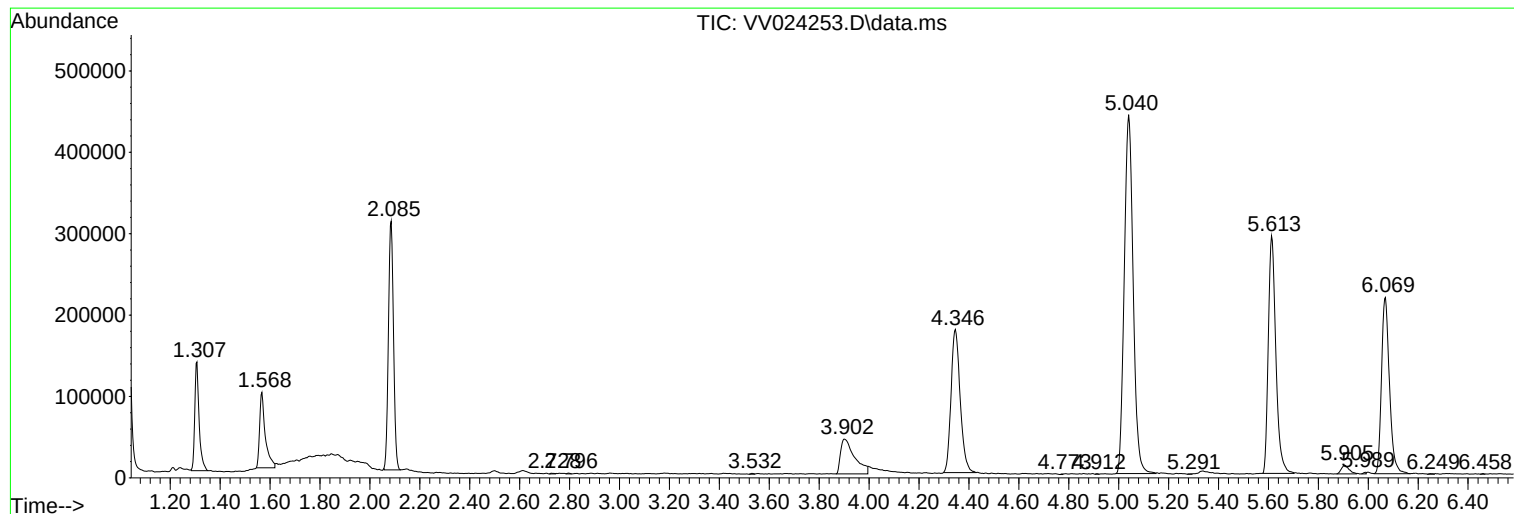
Sum of corrected areas: 7847157

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV123121\  
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ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BGLE6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM123121WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV123121\  
Data File : VV024253.D  
Acq On : 31 Dec 2021 00:33  
Operator : SY/MD  
Sample : M5213-14ME  
Misc : 6.40G/5.0mL/100uL//5.0mL/MSVOA\_V/MEOH  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BGLE6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM123121WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV123121\  
Data File : VV024253.D  
Acq On : 31 Dec 2021 00:33  
Operator : SY/MD  
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Misc : 6.40G/5.0mL/100uL//5.0ml/MSVOA\_V/MEOH  
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Instrument :  
MSVOA\_V  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM123121WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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