

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042921\  
 Data File : VV021226.D  
 Acq On : 29 Apr 2021 17:28  
 Operator : SY/MD  
 Sample : M2177-13ME  
 Misc : 3.93g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BG577ME

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\SFAMVLM042121WMA.M  
 Title : VOC Analysis

Signal : TIC: VV021226.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       | 77            | 83          | 102          | rBV      | 288190         | 395436        | 11.78%          | 1.540%        |
| 2         | 1.568       | 159           | 164         | 174          | rBV      | 172787         | 222350        | 6.62%           | 0.866%        |
| 3         | 2.092       | 319           | 327         | 339          | rVB      | 745431         | 1033213       | 30.78%          | 4.023%        |
| 4         | 2.343       | 403           | 405         | 407          | rBV3     | 9266           | 4224          | 0.13%           | 0.016%        |
| 5         | 2.381       | 415           | 417         | 419          | rVB3     | 9173           | 3365          | 0.10%           | 0.013%        |
| 6         | 2.812       | 548           | 551         | 555          | rBV5     | 6107           | 5088          | 0.15%           | 0.020%        |
| 7         | 2.915       | 581           | 583         | 585          | rBV3     | 6737           | 3044          | 0.09%           | 0.012%        |
| 8         | 3.011       | 611           | 613         | 616          | rVB4     | 9157           | 4019          | 0.12%           | 0.016%        |
| 9         | 3.027       | 616           | 618         | 622          | rBV5     | 8292           | 6436          | 0.19%           | 0.025%        |
| 10        | 3.069       | 630           | 631         | 632          | rBV      | 8697           | 2985          | 0.09%           | 0.012%        |
| 11        | 3.134       | 649           | 651         | 653          | rBV3     | 6794           | 3594          | 0.11%           | 0.014%        |
| 12        | 3.166       | 658           | 661         | 662          | rBV2     | 5624           | 3301          | 0.10%           | 0.013%        |
| 13        | 3.355       | 718           | 720         | 721          | rBV2     | 3779           | 1328          | 0.04%           | 0.005%        |
| 14        | 3.478       | 756           | 758         | 762          | rVB5     | 8021           | 4304          | 0.13%           | 0.017%        |
| 15        | 3.600       | 790           | 796         | 801          | rBV9     | 8938           | 10179         | 0.30%           | 0.040%        |
| 16        | 3.732       | 833           | 837         | 840          | rBV5     | 8966           | 7676          | 0.23%           | 0.030%        |
| 17        | 3.854       | 874           | 875         | 876          | rBV      | 7026           | 2207          | 0.07%           | 0.009%        |
| 18        | 3.902       | 881           | 890         | 913          | rBV      | 135842         | 459343        | 13.69%          | 1.789%        |
| 19        | 4.291       | 1008          | 1011        | 1013         | rBV4     | 9320           | 5431          | 0.16%           | 0.021%        |
| 20        | 4.349       | 1016          | 1029        | 1049         | rVB      | 570189         | 1387260       | 41.33%          | 5.402%        |
| 21        | 4.523       | 1080          | 1083        | 1086         | rBV5     | 7561           | 4546          | 0.14%           | 0.018%        |
| 22        | 4.587       | 1100          | 1103        | 1108         | rVB6     | 10295          | 8952          | 0.27%           | 0.035%        |
| 23        | 4.613       | 1109          | 1111        | 1112         | rBV2     | 6526           | 1886          | 0.06%           | 0.007%        |
| 24        | 4.767       | 1157          | 1159        | 1162         | rBV4     | 7217           | 3045          | 0.09%           | 0.012%        |
| 25        | 4.870       | 1188          | 1191        | 1194         | rBV5     | 4317           | 3273          | 0.10%           | 0.013%        |
| 26        | 4.931       | 1208          | 1210        | 1211         | rBV2     | 4570           | 1594          | 0.05%           | 0.006%        |
| 27        | 4.957       | 1216          | 1218        | 1220         | rBV3     | 6554           | 2857          | 0.09%           | 0.011%        |
| 28        | 4.979       | 1222          | 1225        | 1230         | rVB6     | 8562           | 6078          | 0.18%           | 0.024%        |
| 29        | 5.043       | 1230          | 1245        | 1269         | rBV2     | 1362037        | 3356450       | 100.00%         | 13.069%       |
| 30        | 5.185       | 1287          | 1289        | 1291         | rBV3     | 6829           | 4102          | 0.12%           | 0.016%        |
| 31        | 5.220       | 1298          | 1300        | 1301         | rBV2     | 8864           | 4101          | 0.12%           | 0.016%        |
| 32        | 5.246       | 1306          | 1308        | 1309         | rBV2     | 7995           | 2744          | 0.08%           | 0.011%        |
| 33        | 5.362       | 1338          | 1344        | 1350         | rBV10    | 8891           | 15045         | 0.45%           | 0.059%        |
| 34        | 5.522       | 1392          | 1394        | 1397         | rBV4     | 6405           | 2413          | 0.07%           | 0.009%        |
| 35        | 5.616       | 1412          | 1423        | 1444         | rBV      | 951634         | 1915722       | 57.08%          | 7.459%        |
| 36        | 5.908       | 1504          | 1514        | 1517         | rBV10    | 37786          | 60448         | 1.80%           | 0.235%        |

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 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BG577ME

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\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |         |         |        |         |
|----|-------|------|------|------|------|---------|---------|--------|---------|
| 37 | 6.072 | 1554 | 1565 | 1584 | rVB  | 726694  | 1458831 | 43.46% | 5.680%  |
| 38 | 6.201 | 1598 | 1605 | 1607 | rBV7 | 11002   | 13384   | 0.40%  | 0.052%  |
| 39 | 6.407 | 1667 | 1669 | 1670 | rBV2 | 7518    | 3186    | 0.09%  | 0.012%  |
| 40 | 6.609 | 1730 | 1732 | 1737 | rBV6 | 9290    | 8782    | 0.26%  | 0.034%  |
| 41 | 6.793 | 1786 | 1789 | 1790 | rBV3 | 7823    | 4287    | 0.13%  | 0.017%  |
| 42 | 6.847 | 1804 | 1806 | 1810 | rBV4 | 7910    | 5200    | 0.15%  | 0.020%  |
| 43 | 6.886 | 1813 | 1818 | 1820 | rBV6 | 7770    | 7620    | 0.23%  | 0.030%  |
| 44 | 6.911 | 1825 | 1826 | 1828 | rVV2 | 5780    | 1736    | 0.05%  | 0.007%  |
| 45 | 6.940 | 1834 | 1835 | 1837 | rBV2 | 5979    | 2421    | 0.07%  | 0.009%  |
| 46 | 6.989 | 1840 | 1850 | 1871 | rVV  | 446140  | 822788  | 24.51% | 3.204%  |
| 47 | 7.108 | 1885 | 1887 | 1890 | rBV4 | 8931    | 6782    | 0.20%  | 0.026%  |
| 48 | 7.214 | 1918 | 1920 | 1923 | rBV4 | 6404    | 2796    | 0.08%  | 0.011%  |
| 49 | 7.317 | 1942 | 1952 | 1971 | rBV  | 1604574 | 2795415 | 83.28% | 10.885% |
| 50 | 7.503 | 2008 | 2010 | 2013 | rBV4 | 7637    | 4442    | 0.13%  | 0.017%  |
| 51 | 7.551 | 2023 | 2025 | 2027 | rVB3 | 11853   | 4263    | 0.13%  | 0.017%  |
| 52 | 7.571 | 2027 | 2031 | 2036 | rBV7 | 9929    | 9674    | 0.29%  | 0.038%  |
| 53 | 7.625 | 2040 | 2048 | 2068 | rVB  | 294343  | 542582  | 16.17% | 2.113%  |
| 54 | 7.863 | 2121 | 2122 | 2123 | rBV  | 5525    | 2090    | 0.06%  | 0.008%  |
| 55 | 7.886 | 2127 | 2129 | 2131 | rBV3 | 6243    | 3086    | 0.09%  | 0.012%  |
| 56 | 7.960 | 2149 | 2152 | 2153 | rBV3 | 8757    | 4985    | 0.15%  | 0.019%  |
| 57 | 8.030 | 2171 | 2174 | 2178 | rBV5 | 8665    | 5808    | 0.17%  | 0.023%  |
| 58 | 8.120 | 2187 | 2202 | 2223 | rBV2 | 409992  | 1325779 | 39.50% | 5.162%  |
| 59 | 8.339 | 2268 | 2270 | 2275 | rVB6 | 8706    | 7655    | 0.23%  | 0.030%  |
| 60 | 8.358 | 2275 | 2276 | 2278 | rBV2 | 7028    | 3736    | 0.11%  | 0.015%  |
| 61 | 8.455 | 2304 | 2306 | 2309 | rBV4 | 7024    | 4132    | 0.12%  | 0.016%  |
| 62 | 8.513 | 2322 | 2324 | 2326 | rBV2 | 4268    | 1291    | 0.04%  | 0.005%  |
| 63 | 8.661 | 2368 | 2370 | 2374 | rVB5 | 8785    | 5058    | 0.15%  | 0.020%  |
| 64 | 8.680 | 2374 | 2376 | 2377 | rBV2 | 5438    | 2666    | 0.08%  | 0.010%  |
| 65 | 8.812 | 2410 | 2417 | 2419 | rBV7 | 15160   | 15901   | 0.47%  | 0.062%  |
| 66 | 8.857 | 2421 | 2431 | 2449 | rVV  | 1347140 | 2403024 | 71.59% | 9.357%  |
| 67 | 8.976 | 2464 | 2468 | 2471 | rBV6 | 9135    | 7318    | 0.22%  | 0.028%  |
| 68 | 8.992 | 2471 | 2473 | 2476 | rBV4 | 7328    | 4103    | 0.12%  | 0.016%  |
| 69 | 9.108 | 2505 | 2509 | 2510 | rBV4 | 6570    | 3930    | 0.12%  | 0.015%  |
| 70 | 9.146 | 2517 | 2521 | 2524 | rBV6 | 9013    | 7667    | 0.23%  | 0.030%  |
| 71 | 9.246 | 2550 | 2552 | 2555 | rVB3 | 7777    | 3380    | 0.10%  | 0.013%  |
| 72 | 9.268 | 2557 | 2559 | 2562 | rBV4 | 4245    | 2330    | 0.07%  | 0.009%  |
| 73 | 9.304 | 2567 | 2570 | 2573 | rBV5 | 15016   | 10555   | 0.31%  | 0.041%  |
| 74 | 9.403 | 2600 | 2601 | 2605 | rBV4 | 6731    | 4055    | 0.12%  | 0.016%  |
| 75 | 9.587 | 2656 | 2658 | 2659 | rBV2 | 8407    | 3122    | 0.09%  | 0.012%  |
| 76 | 9.606 | 2663 | 2664 | 2667 | rBV3 | 8232    | 4521    | 0.13%  | 0.018%  |

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Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BG577ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMVLM042121WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 77 | 9.802  | 2721 | 2725 | 2727 | rBV5 | 9280    | 7768    | 0.23%  | 0.030%  |
| 78 | 9.844  | 2736 | 2738 | 2739 | rBV2 | 8481    | 3535    | 0.11%  | 0.014%  |
| 79 | 10.230 | 2846 | 2858 | 2874 | rBV  | 929212  | 1593432 | 47.47% | 6.205%  |
| 80 | 11.001 | 3096 | 3098 | 3100 | rBV3 | 8178    | 3487    | 0.10%  | 0.014%  |
| 81 | 11.040 | 3104 | 3110 | 3114 | rBV7 | 19838   | 27606   | 0.82%  | 0.107%  |
| 82 | 11.259 | 3168 | 3178 | 3194 | rBV  | 1656427 | 2571721 | 76.62% | 10.014% |
| 83 | 11.525 | 3258 | 3261 | 3264 | rBV5 | 13681   | 8433    | 0.25%  | 0.033%  |
| 84 | 11.635 | 3284 | 3295 | 3308 | rBV  | 1900155 | 2966665 | 88.39% | 11.552% |
| 85 | 13.213 | 3781 | 3786 | 3788 | rBV6 | 11135   | 10790   | 0.32%  | 0.042%  |

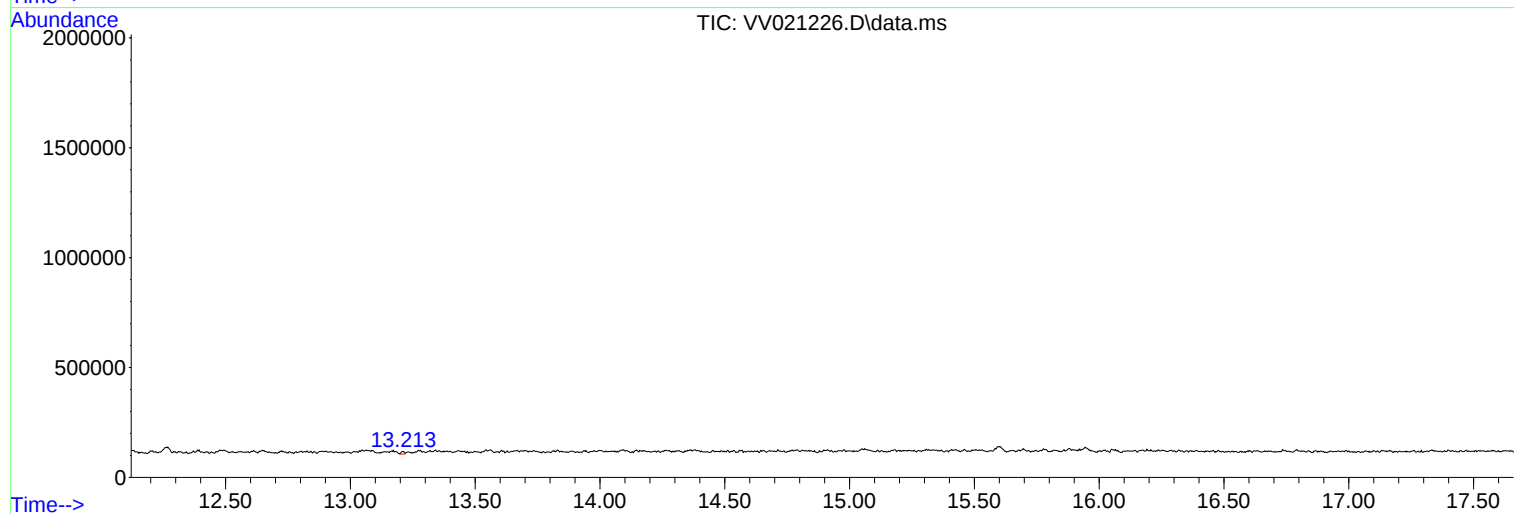
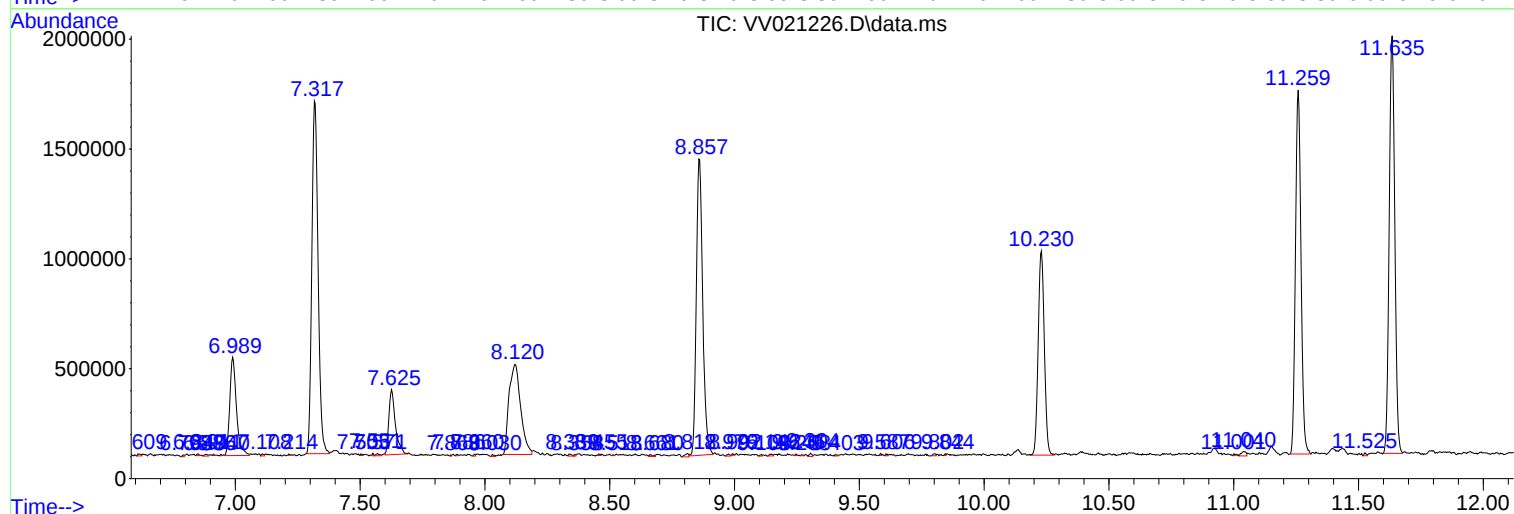
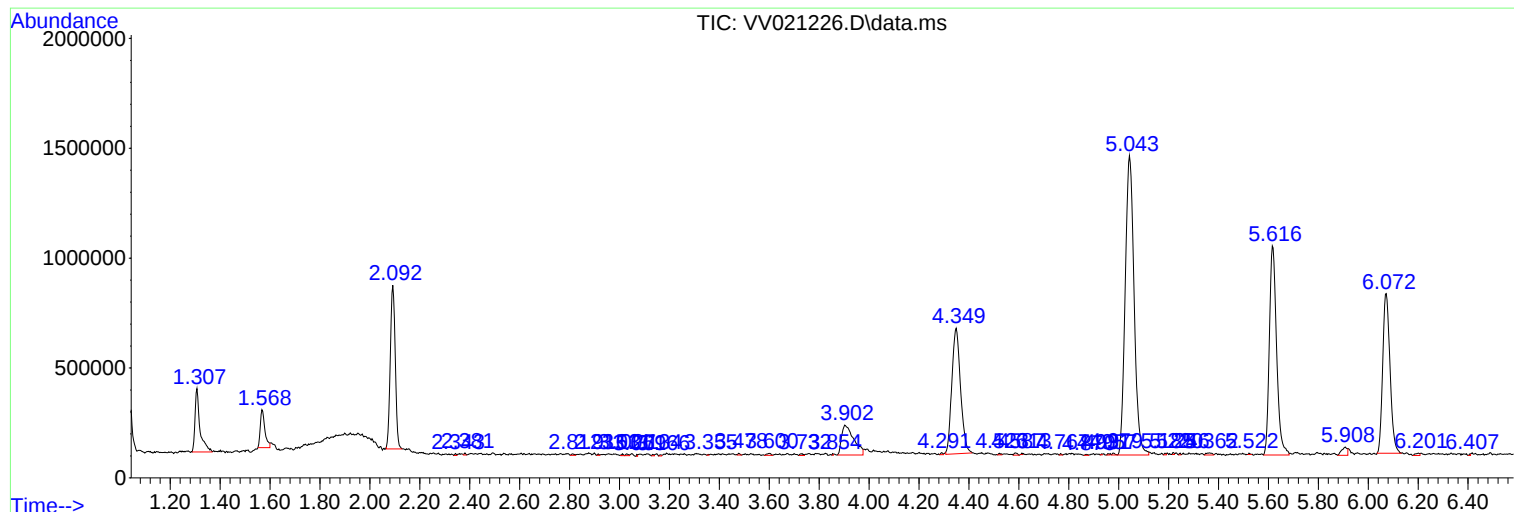
Sum of corrected areas: 25681857

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042921\  
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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BG577ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM042121WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042921\  
Data File : VV021226.D  
Acq On : 29 Apr 2021 17:28  
Operator : SY/MD  
Sample : M2177-13ME  
Misc : 3.93g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
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Instrument :  
MSVOA\_V  
ClientSampleId :  
BG577ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM042121WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042921\  
Data File : VV021226.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM042121WMA.M  
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| TIC Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |

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