

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV032921\  
 Data File : VV020792.D  
 Acq On : 29 Mar 2021 10:08  
 Operator : SY/MD  
 Sample : VV0329MBL01  
 Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK82

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\SOMVLM032321WMA.M

Title : VOC Analysis

Signal : TIC: VV020792.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          | 94           | rVB      | 320114         | 313405        | 12.79%          | 1.647%        |
| 2         | 1.568       | 157           | 164         | 179          | rVB      | 245830         | 281714        | 11.50%          | 1.481%        |
| 3         | 2.108       | 322           | 332         | 358          | rVB      | 567519         | 862433        | 35.21%          | 4.533%        |
| 4         | 2.298       | 384           | 391         | 400          | rVB      | 2872           | 5013          | 0.20%           | 0.026%        |
| 5         | 2.510       | 449           | 457         | 465          | rBV6     | 3581           | 6011          | 0.25%           | 0.032%        |
| 6         | 2.609       | 487           | 488         | 492          | rBV2     | 454            | 342           | 0.01%           | 0.002%        |
| 7         | 2.661       | 500           | 504         | 507          | rBV3     | 492            | 368           | 0.02%           | 0.002%        |
| 8         | 2.677       | 507           | 509         | 511          | rBV3     | 495            | 227           | 0.01%           | 0.001%        |
| 9         | 2.725       | 520           | 524         | 527          | rBV3     | 327            | 265           | 0.01%           | 0.001%        |
| 10        | 2.767       | 527           | 537         | 542          | rBV7     | 2367           | 3824          | 0.16%           | 0.020%        |
| 11        | 2.818       | 551           | 553         | 559          | rBV2     | 652            | 434           | 0.02%           | 0.002%        |
| 12        | 2.851       | 561           | 563         | 565          | rVV2     | 734            | 334           | 0.01%           | 0.002%        |
| 13        | 2.912       | 579           | 582         | 585          | rBV2     | 466            | 331           | 0.01%           | 0.002%        |
| 14        | 2.973       | 598           | 601         | 604          | rVB      | 680            | 392           | 0.02%           | 0.002%        |
| 15        | 2.992       | 604           | 607         | 608          | rBV2     | 544            | 281           | 0.01%           | 0.001%        |
| 16        | 3.146       | 653           | 655         | 658          | rVB      | 496            | 252           | 0.01%           | 0.001%        |
| 17        | 3.172       | 658           | 663         | 664          | rBV2     | 509            | 310           | 0.01%           | 0.002%        |
| 18        | 3.320       | 704           | 709         | 710          | rBV2     | 468            | 349           | 0.01%           | 0.002%        |
| 19        | 3.445       | 745           | 748         | 755          | rBV3     | 627            | 726           | 0.03%           | 0.004%        |
| 20        | 3.539       | 774           | 777         | 780          | rVB2     | 613            | 427           | 0.02%           | 0.002%        |
| 21        | 3.555       | 780           | 782         | 784          | rBV3     | 344            | 217           | 0.01%           | 0.001%        |
| 22        | 3.580       | 786           | 790         | 792          | rVV2     | 562            | 434           | 0.02%           | 0.002%        |
| 23        | 3.597       | 792           | 795         | 797          | rVV      | 621            | 382           | 0.02%           | 0.002%        |
| 24        | 3.609       | 797           | 799         | 803          | rVB2     | 782            | 441           | 0.02%           | 0.002%        |
| 25        | 3.632       | 803           | 806         | 810          | rBV      | 466            | 415           | 0.02%           | 0.002%        |
| 26        | 3.716       | 830           | 832         | 835          | rVB2     | 546            | 303           | 0.01%           | 0.002%        |
| 27        | 3.889       | 875           | 886         | 927          | rBV      | 157193         | 476409        | 19.45%          | 2.504%        |
| 28        | 4.349       | 1013          | 1029        | 1055         | rBV      | 414800         | 1030842       | 42.08%          | 5.418%        |
| 29        | 4.722       | 1141          | 1145        | 1149         | rBV4     | 1059           | 931           | 0.04%           | 0.005%        |
| 30        | 4.741       | 1149          | 1151        | 1153         | rVV3     | 545            | 220           | 0.01%           | 0.001%        |
| 31        | 4.783       | 1162          | 1164        | 1168         | rBV2     | 407            | 317           | 0.01%           | 0.002%        |
| 32        | 4.822       | 1171          | 1176        | 1178         | rBV3     | 1178           | 937           | 0.04%           | 0.005%        |
| 33        | 4.902       | 1197          | 1201        | 1202         | rBV2     | 620            | 337           | 0.01%           | 0.002%        |
| 34        | 5.047       | 1229          | 1246        | 1280         | rBV2     | 942476         | 2449531       | 100.00%         | 12.874%       |
| 35        | 5.342       | 1336          | 1338        | 1339         | rBV      | 842            | 310           | 0.01%           | 0.002%        |
| 36        | 5.413       | 1355          | 1360        | 1365         | rBV6     | 1046           | 1406          | 0.06%           | 0.007%        |

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 ClientSampleId :  
 VBLK82

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SOMVLM032321WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |         |         |        |         |
|----|-------|------|------|------|------|---------|---------|--------|---------|
| 37 | 5.545 | 1397 | 1401 | 1404 | rBV3 | 729     | 547     | 0.02%  | 0.003%  |
| 38 | 5.564 | 1404 | 1407 | 1409 | rBV3 | 796     | 432     | 0.02%  | 0.002%  |
| 39 | 5.619 | 1411 | 1424 | 1446 | rBV  | 751597  | 1503994 | 61.40% | 7.905%  |
| 40 | 5.908 | 1507 | 1514 | 1531 | rVB4 | 18286   | 37461   | 1.53%  | 0.197%  |
| 41 | 5.989 | 1537 | 1539 | 1541 | rBV2 | 516     | 209     | 0.01%  | 0.001%  |
| 42 | 6.072 | 1551 | 1565 | 1594 | rBV  | 534753  | 1082964 | 44.21% | 5.692%  |
| 43 | 6.439 | 1677 | 1679 | 1682 | rVB2 | 861     | 449     | 0.02%  | 0.002%  |
| 44 | 6.529 | 1703 | 1707 | 1710 | rBV3 | 988     | 759     | 0.03%  | 0.004%  |
| 45 | 6.574 | 1719 | 1721 | 1722 | rBV  | 480     | 218     | 0.01%  | 0.001%  |
| 46 | 6.600 | 1727 | 1729 | 1732 | rVB2 | 520     | 267     | 0.01%  | 0.001%  |
| 47 | 6.619 | 1732 | 1735 | 1737 | rBV2 | 445     | 305     | 0.01%  | 0.002%  |
| 48 | 6.751 | 1773 | 1776 | 1778 | rBV2 | 362     | 225     | 0.01%  | 0.001%  |
| 49 | 6.764 | 1778 | 1780 | 1784 | rBV2 | 600     | 423     | 0.02%  | 0.002%  |
| 50 | 6.860 | 1807 | 1810 | 1814 | rBV3 | 592     | 354     | 0.01%  | 0.002%  |
| 51 | 6.944 | 1834 | 1836 | 1839 | rVB3 | 829     | 349     | 0.01%  | 0.002%  |
| 52 | 6.989 | 1839 | 1850 | 1873 | rBV  | 302290  | 549468  | 22.43% | 2.888%  |
| 53 | 7.317 | 1939 | 1952 | 1976 | rBV  | 1117122 | 1960617 | 80.04% | 10.305% |
| 54 | 7.539 | 2019 | 2021 | 2024 | rBV3 | 705     | 341     | 0.01%  | 0.002%  |
| 55 | 7.625 | 2037 | 2048 | 2080 | rBV  | 222063  | 392840  | 16.04% | 2.065%  |
| 56 | 7.857 | 2115 | 2120 | 2123 | rBV6 | 1687    | 1820    | 0.07%  | 0.010%  |
| 57 | 7.937 | 2142 | 2145 | 2147 | rBV2 | 1195    | 713     | 0.03%  | 0.004%  |
| 58 | 8.092 | 2182 | 2193 | 2222 | rBV  | 597437  | 1096859 | 44.78% | 5.765%  |
| 59 | 8.420 | 2293 | 2295 | 2301 | rBV4 | 883     | 780     | 0.03%  | 0.004%  |
| 60 | 8.600 | 2348 | 2351 | 2352 | rBV2 | 687     | 396     | 0.02%  | 0.002%  |
| 61 | 8.632 | 2356 | 2361 | 2366 | rVV3 | 980     | 885     | 0.04%  | 0.005%  |
| 62 | 8.696 | 2379 | 2381 | 2386 | rVB  | 997     | 858     | 0.04%  | 0.005%  |
| 63 | 8.722 | 2386 | 2389 | 2390 | rBV  | 910     | 459     | 0.02%  | 0.002%  |
| 64 | 8.760 | 2399 | 2401 | 2406 | rBV2 | 433     | 288     | 0.01%  | 0.002%  |
| 65 | 8.789 | 2406 | 2410 | 2413 | rBV2 | 499     | 428     | 0.02%  | 0.002%  |
| 66 | 8.857 | 2418 | 2431 | 2455 | rBV  | 1145226 | 1882291 | 76.84% | 9.893%  |
| 67 | 9.153 | 2515 | 2523 | 2525 | rBV5 | 1537    | 2127    | 0.09%  | 0.011%  |
| 68 | 9.194 | 2533 | 2536 | 2539 | rBV3 | 621     | 466     | 0.02%  | 0.002%  |
| 69 | 9.239 | 2548 | 2550 | 2552 | rBV2 | 388     | 209     | 0.01%  | 0.001%  |
| 70 | 9.281 | 2561 | 2563 | 2565 | rVB2 | 672     | 271     | 0.01%  | 0.001%  |
| 71 | 9.320 | 2572 | 2575 | 2582 | rBV4 | 989     | 886     | 0.04%  | 0.005%  |
| 72 | 9.432 | 2605 | 2610 | 2611 | rBV  | 824     | 646     | 0.03%  | 0.003%  |
| 73 | 9.484 | 2623 | 2626 | 2627 | rBV  | 833     | 364     | 0.01%  | 0.002%  |
| 74 | 9.535 | 2640 | 2642 | 2643 | rBV  | 617     | 259     | 0.01%  | 0.001%  |
| 75 | 9.670 | 2682 | 2684 | 2687 | rVB2 | 768     | 338     | 0.01%  | 0.002%  |
| 76 | 9.770 | 2711 | 2715 | 2721 | rBV4 | 645     | 735     | 0.03%  | 0.004%  |

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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SOMVLM032321WMA.M

Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |         |
|-----|--------|------|------|------|------|---------|---------|--------|---------|
| 77  | 10.130 | 2825 | 2827 | 2829 | rBV4 | 690     | 335     | 0.01%  | 0.002%  |
| 78  | 10.220 | 2843 | 2855 | 2875 | rBV  | 775854  | 1205706 | 49.22% | 6.337%  |
| 79  | 10.355 | 2895 | 2897 | 2899 | rBV2 | 678     | 342     | 0.01%  | 0.002%  |
| 80  | 10.384 | 2903 | 2906 | 2907 | rBV  | 537     | 255     | 0.01%  | 0.001%  |
| 81  | 10.513 | 2944 | 2946 | 2948 | rBV3 | 462     | 220     | 0.01%  | 0.001%  |
| 82  | 10.554 | 2952 | 2959 | 2964 | rBV5 | 1963    | 2663    | 0.11%  | 0.014%  |
| 83  | 10.606 | 2973 | 2975 | 2977 | rBV  | 517     | 228     | 0.01%  | 0.001%  |
| 84  | 10.725 | 3010 | 3012 | 3015 | rVB2 | 430     | 215     | 0.01%  | 0.001%  |
| 85  | 10.741 | 3015 | 3017 | 3021 | rBV3 | 700     | 533     | 0.02%  | 0.003%  |
| 86  | 10.802 | 3033 | 3036 | 3038 | rBV  | 528     | 263     | 0.01%  | 0.001%  |
| 87  | 10.863 | 3051 | 3055 | 3056 | rBV3 | 608     | 396     | 0.02%  | 0.002%  |
| 88  | 10.931 | 3068 | 3076 | 3084 | rVB5 | 2394    | 3645    | 0.15%  | 0.019%  |
| 89  | 11.030 | 3105 | 3107 | 3108 | rBV  | 432     | 233     | 0.01%  | 0.001%  |
| 90  | 11.069 | 3115 | 3119 | 3121 | rBV  | 651     | 438     | 0.02%  | 0.002%  |
| 91  | 11.255 | 3165 | 3177 | 3196 | rBV  | 1245527 | 1878670 | 76.70% | 9.874%  |
| 92  | 11.484 | 3247 | 3248 | 3250 | rBV  | 728     | 265     | 0.01%  | 0.001%  |
| 93  | 11.632 | 3281 | 3294 | 3314 | rBV  | 1239905 | 1927040 | 78.67% | 10.128% |
| 94  | 12.657 | 3607 | 3613 | 3623 | rVB9 | 6336    | 9533    | 0.39%  | 0.050%  |
| 95  | 12.995 | 3715 | 3718 | 3722 | rBV3 | 1149    | 933     | 0.04%  | 0.005%  |
| 96  | 13.271 | 3799 | 3804 | 3814 | rVB7 | 6145    | 9846    | 0.40%  | 0.052%  |
| 97  | 13.374 | 3834 | 3836 | 3838 | rBV  | 532     | 318     | 0.01%  | 0.002%  |
| 98  | 13.468 | 3862 | 3865 | 3866 | rBV  | 732     | 367     | 0.01%  | 0.002%  |
| 99  | 13.519 | 3875 | 3881 | 3891 | rVB4 | 5524    | 8842    | 0.36%  | 0.046%  |
| 100 | 13.757 | 3949 | 3955 | 3963 | rVB6 | 7590    | 9950    | 0.41%  | 0.052%  |

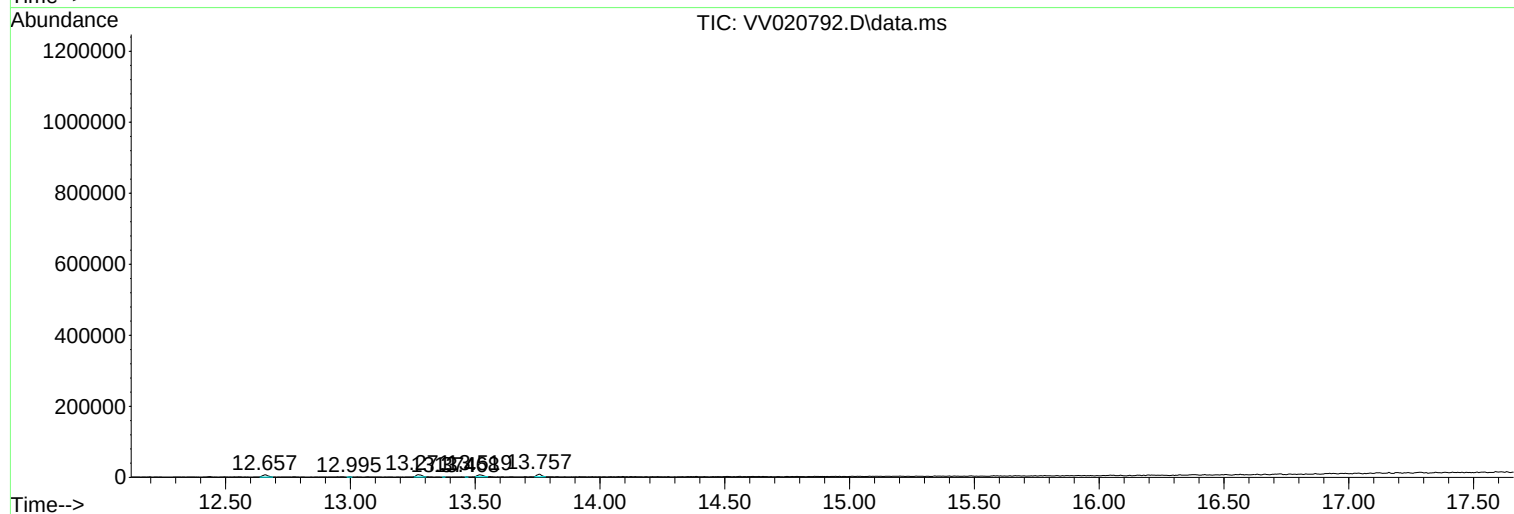
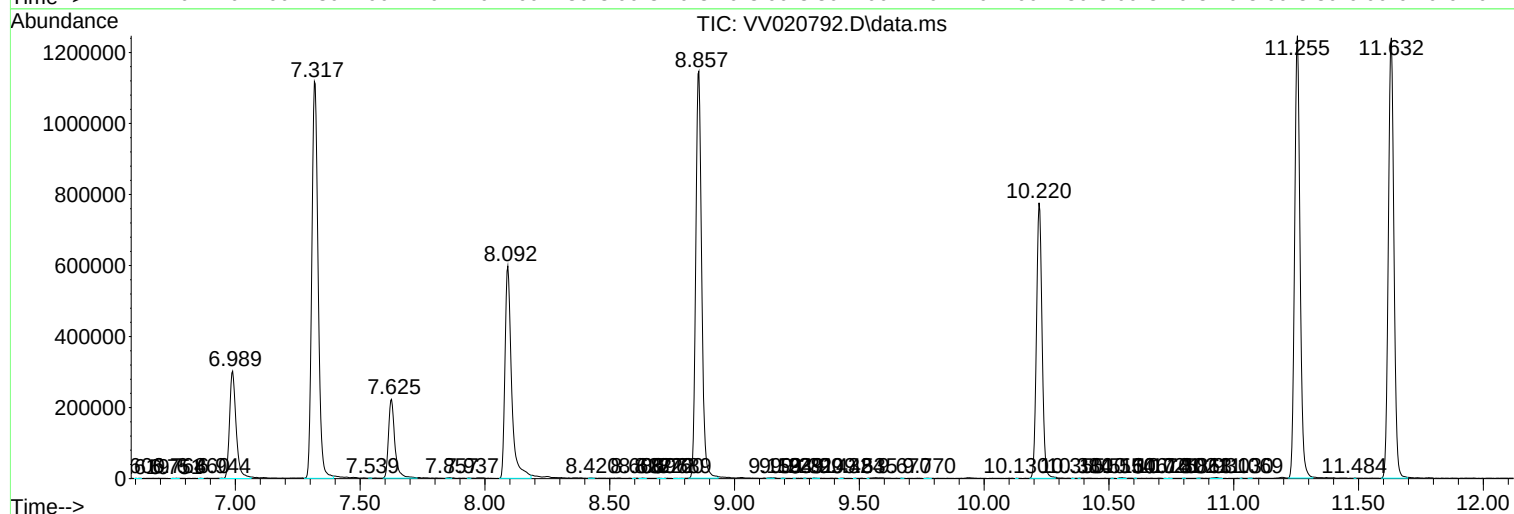
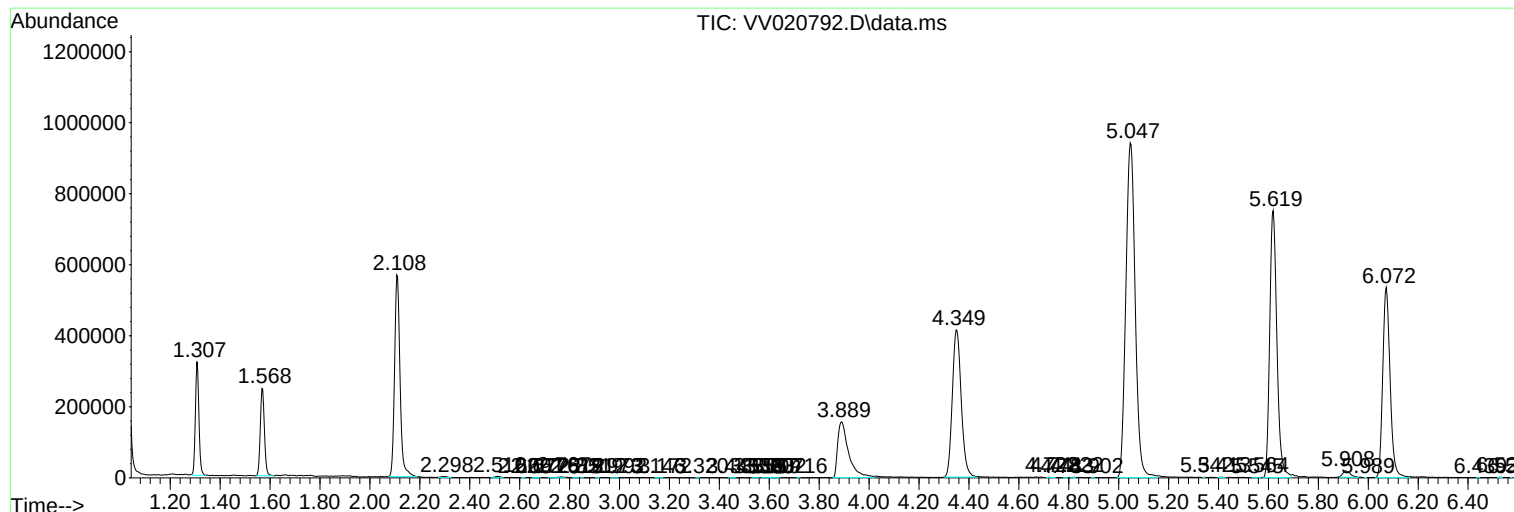
Sum of corrected areas: 19026406

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SOMVLM032321WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV032921\  
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No Library Search Compounds Detected

\*\*\*\*\*

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