

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042821\  
 Data File : VV021194.D  
 Acq On : 28 Apr 2021 12:20  
 Operator : SY/MD  
 Sample : M2165-11 500X  
 Misc : 6.72g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GB3F2

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: VV021194.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          | 95           | rBV      | 401528         | 403449        | 0.62%           | 0.461%        |
| 2         | 1.571       | 158           | 165         | 180          | rVB      | 330421         | 374260        | 0.58%           | 0.428%        |
| 3         | 2.111       | 323           | 333         | 351          | rBV      | 709876         | 1026582       | 1.58%           | 1.174%        |
| 4         | 2.365       | 410           | 412         | 415          | rBV3     | 683            | 318           | 0.00%           | 0.000%        |
| 5         | 2.420       | 427           | 429         | 433          | rVB2     | 844            | 477           | 0.00%           | 0.001%        |
| 6         | 2.513       | 451           | 458         | 471          | rVB5     | 10659          | 18987         | 0.03%           | 0.022%        |
| 7         | 2.564       | 471           | 474         | 476          | rBV      | 666            | 431           | 0.00%           | 0.000%        |
| 8         | 2.703       | 514           | 517         | 518          | rBV2     | 417            | 235           | 0.00%           | 0.000%        |
| 9         | 2.728       | 522           | 525         | 527          | rBV4     | 713            | 396           | 0.00%           | 0.000%        |
| 10        | 2.812       | 548           | 551         | 553          | rBV3     | 495            | 291           | 0.00%           | 0.000%        |
| 11        | 2.957       | 592           | 596         | 599          | rVB3     | 722            | 549           | 0.00%           | 0.001%        |
| 12        | 3.040       | 619           | 622         | 625          | rBV4     | 544            | 369           | 0.00%           | 0.000%        |
| 13        | 3.092       | 635           | 638         | 640          | rBV3     | 480            | 308           | 0.00%           | 0.000%        |
| 14        | 3.111       | 640           | 644         | 646          | rBV2     | 523            | 391           | 0.00%           | 0.000%        |
| 15        | 3.191       | 664           | 669         | 671          | rBV2     | 504            | 482           | 0.00%           | 0.001%        |
| 16        | 3.236       | 680           | 683         | 684          | rBV3     | 361            | 219           | 0.00%           | 0.000%        |
| 17        | 3.262       | 687           | 691         | 695          | rVV3     | 799            | 592           | 0.00%           | 0.001%        |
| 18        | 3.320       | 708           | 709         | 712          | rBV2     | 339            | 231           | 0.00%           | 0.000%        |
| 19        | 3.339       | 712           | 715         | 719          | rVB3     | 793            | 687           | 0.00%           | 0.001%        |
| 20        | 3.420       | 737           | 740         | 743          | rVV2     | 447            | 317           | 0.00%           | 0.000%        |
| 21        | 3.449       | 747           | 749         | 751          | rVB      | 319            | 126           | 0.00%           | 0.000%        |
| 22        | 3.468       | 751           | 755         | 757          | rBV      | 347            | 244           | 0.00%           | 0.000%        |
| 23        | 3.587       | 789           | 792         | 794          | rBV      | 369            | 238           | 0.00%           | 0.000%        |
| 24        | 3.629       | 803           | 805         | 808          | rVB2     | 515            | 347           | 0.00%           | 0.000%        |
| 25        | 3.648       | 808           | 811         | 813          | rBV2     | 242            | 148           | 0.00%           | 0.000%        |
| 26        | 3.661       | 813           | 815         | 818          | rVV2     | 682            | 394           | 0.00%           | 0.000%        |
| 27        | 3.693       | 821           | 825         | 828          | rVV3     | 520            | 435           | 0.00%           | 0.000%        |
| 28        | 3.709       | 828           | 830         | 833          | rVB2     | 753            | 321           | 0.00%           | 0.000%        |
| 29        | 3.735       | 836           | 838         | 840          | rBV      | 406            | 249           | 0.00%           | 0.000%        |
| 30        | 3.761       | 843           | 846         | 852          | rVB3     | 991            | 847           | 0.00%           | 0.001%        |
| 31        | 3.867       | 877           | 879         | 880          | rBV3     | 574            | 227           | 0.00%           | 0.000%        |
| 32        | 3.905       | 881           | 891         | 941          | rVV      | 125676         | 503816        | 0.77%           | 0.576%        |
| 33        | 4.352       | 1015          | 1030        | 1056         | rBV2     | 476416         | 1172104       | 1.80%           | 1.341%        |
| 34        | 4.767       | 1156          | 1159        | 1163         | rBV4     | 1019           | 695           | 0.00%           | 0.001%        |
| 35        | 4.908       | 1201          | 1203        | 1206         | rBV3     | 514            | 216           | 0.00%           | 0.000%        |
| 36        | 4.944       | 1212          | 1214        | 1215         | rBV      | 414            | 154           | 0.00%           | 0.000%        |

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 GB3F2

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |          |          |         |         |
|----|-------|------|------|------|------|----------|----------|---------|---------|
| 37 | 4.989 | 1222 | 1228 | 1230 | rBV3 | 592      | 588      | 0.00%   | 0.001%  |
| 38 | 5.050 | 1230 | 1247 | 1278 | rBV2 | 1102907  | 2804891  | 4.31%   | 3.208%  |
| 39 | 5.339 | 1334 | 1337 | 1339 | rBV3 | 787      | 521      | 0.00%   | 0.001%  |
| 40 | 5.368 | 1343 | 1346 | 1350 | rBV4 | 1486     | 1272     | 0.00%   | 0.001%  |
| 41 | 5.571 | 1402 | 1409 | 1412 | rBV5 | 1260     | 1343     | 0.00%   | 0.002%  |
| 42 | 5.622 | 1412 | 1425 | 1446 | rBV  | 900164   | 1813198  | 2.79%   | 2.074%  |
| 43 | 5.912 | 1505 | 1515 | 1538 | rVB4 | 31018    | 70880    | 0.11%   | 0.081%  |
| 44 | 6.072 | 1552 | 1565 | 1594 | rBV  | 611093   | 1248160  | 1.92%   | 1.428%  |
| 45 | 6.375 | 1657 | 1659 | 1661 | rVB3 | 630      | 246      | 0.00%   | 0.000%  |
| 46 | 6.407 | 1668 | 1669 | 1670 | rBV  | 546      | 192      | 0.00%   | 0.000%  |
| 47 | 6.452 | 1681 | 1683 | 1686 | rVB2 | 874      | 334      | 0.00%   | 0.000%  |
| 48 | 6.494 | 1694 | 1696 | 1697 | rBV2 | 217      | 108      | 0.00%   | 0.000%  |
| 49 | 6.503 | 1697 | 1699 | 1702 | rVB2 | 775      | 363      | 0.00%   | 0.000%  |
| 50 | 6.526 | 1702 | 1706 | 1709 | rBV4 | 960      | 926      | 0.00%   | 0.001%  |
| 51 | 6.558 | 1713 | 1716 | 1719 | rBV3 | 900      | 458      | 0.00%   | 0.001%  |
| 52 | 6.574 | 1719 | 1721 | 1723 | rBV3 | 779      | 350      | 0.00%   | 0.000%  |
| 53 | 6.632 | 1736 | 1739 | 1742 | rBV2 | 598      | 380      | 0.00%   | 0.000%  |
| 54 | 6.651 | 1743 | 1745 | 1747 | rVV2 | 658      | 262      | 0.00%   | 0.000%  |
| 55 | 6.690 | 1755 | 1757 | 1762 | rVB3 | 1372     | 851      | 0.00%   | 0.001%  |
| 56 | 6.722 | 1765 | 1767 | 1770 | rVV3 | 870      | 399      | 0.00%   | 0.000%  |
| 57 | 6.799 | 1787 | 1791 | 1792 | rBV2 | 669      | 418      | 0.00%   | 0.000%  |
| 58 | 6.828 | 1797 | 1800 | 1801 | rBV2 | 392      | 209      | 0.00%   | 0.000%  |
| 59 | 6.992 | 1838 | 1851 | 1878 | rBV  | 337783   | 633026   | 0.97%   | 0.724%  |
| 60 | 7.320 | 1940 | 1953 | 1972 | rBV  | 1348072  | 2351519  | 3.62%   | 2.689%  |
| 61 | 7.625 | 2039 | 2048 | 2074 | rBV  | 233691   | 421422   | 0.65%   | 0.482%  |
| 62 | 7.918 | 2136 | 2139 | 2140 | rBV2 | 619      | 349      | 0.00%   | 0.000%  |
| 63 | 7.982 | 2143 | 2159 | 2184 | rBV  | 38663605 | 65024533 | 100.00% | 74.368% |
| 64 | 8.095 | 2186 | 2194 | 2226 | rVB  | 646265   | 1217043  | 1.87%   | 1.392%  |
| 65 | 8.738 | 2391 | 2394 | 2398 | rBV4 | 997      | 735      | 0.00%   | 0.001%  |
| 66 | 8.857 | 2419 | 2431 | 2460 | rBV  | 1392090  | 2282930  | 3.51%   | 2.611%  |
| 67 | 9.268 | 2556 | 2559 | 2561 | rBV2 | 657      | 543      | 0.00%   | 0.001%  |
| 68 | 9.304 | 2567 | 2570 | 2572 | rBV2 | 611      | 374      | 0.00%   | 0.000%  |
| 69 | 9.487 | 2624 | 2627 | 2630 | rVB4 | 922      | 591      | 0.00%   | 0.001%  |
| 70 | 9.500 | 2630 | 2631 | 2634 | rBV  | 551      | 241      | 0.00%   | 0.000%  |
| 71 | 9.545 | 2642 | 2645 | 2647 | rBV4 | 740      | 534      | 0.00%   | 0.001%  |
| 72 | 9.590 | 2655 | 2659 | 2663 | rVB5 | 1024     | 749      | 0.00%   | 0.001%  |
| 73 | 9.628 | 2669 | 2671 | 2674 | rVB3 | 634      | 256      | 0.00%   | 0.000%  |
| 74 | 9.648 | 2674 | 2677 | 2681 | rBV2 | 773      | 610      | 0.00%   | 0.001%  |
| 75 | 9.712 | 2692 | 2697 | 2700 | rBV  | 977      | 890      | 0.00%   | 0.001%  |
| 76 | 9.757 | 2709 | 2711 | 2717 | rVB3 | 969      | 576      | 0.00%   | 0.001%  |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |       |        |
|-----|--------|------|------|------|------|---------|---------|-------|--------|
| 77  | 9.809  | 2724 | 2727 | 2729 | rVB  | 878     | 472     | 0.00% | 0.001% |
| 78  | 10.133 | 2818 | 2828 | 2838 | rBV4 | 7182    | 10522   | 0.02% | 0.012% |
| 79  | 10.220 | 2844 | 2855 | 2877 | rBV  | 916293  | 1446157 | 2.22% | 1.654% |
| 80  | 10.390 | 2905 | 2908 | 2915 | rVB5 | 2240    | 1817    | 0.00% | 0.002% |
| 81  | 10.609 | 2973 | 2976 | 2983 | rVB5 | 2087    | 2080    | 0.00% | 0.002% |
| 82  | 10.638 | 2983 | 2985 | 2987 | rBV2 | 415     | 125     | 0.00% | 0.000% |
| 83  | 10.715 | 3005 | 3009 | 3010 | rBV  | 488     | 327     | 0.00% | 0.000% |
| 84  | 10.841 | 3046 | 3048 | 3050 | rBV3 | 914     | 494     | 0.00% | 0.001% |
| 85  | 10.927 | 3067 | 3075 | 3083 | rBV9 | 5468    | 8663    | 0.01% | 0.010% |
| 86  | 11.034 | 3104 | 3108 | 3111 | rBV3 | 1396    | 1167    | 0.00% | 0.001% |
| 87  | 11.072 | 3118 | 3120 | 3121 | rBV  | 547     | 242     | 0.00% | 0.000% |
| 88  | 11.146 | 3140 | 3143 | 3144 | rBV3 | 2593    | 1465    | 0.00% | 0.002% |
| 89  | 11.255 | 3165 | 3177 | 3201 | rBV  | 1445887 | 2252992 | 3.46% | 2.577% |
| 90  | 11.632 | 3282 | 3294 | 3319 | rBV  | 1459160 | 2308537 | 3.55% | 2.640% |
| 91  | 12.024 | 3414 | 3416 | 3420 | rBV3 | 987     | 678     | 0.00% | 0.001% |
| 92  | 12.249 | 3482 | 3486 | 3489 | rBV5 | 1597    | 1648    | 0.00% | 0.002% |
| 93  | 12.468 | 3552 | 3554 | 3556 | rBV2 | 754     | 296     | 0.00% | 0.000% |
| 94  | 12.484 | 3557 | 3559 | 3562 | rVB2 | 1390    | 746     | 0.00% | 0.001% |
| 95  | 12.648 | 3607 | 3610 | 3612 | rBV4 | 1208    | 881     | 0.00% | 0.001% |
| 96  | 12.773 | 3646 | 3649 | 3654 | rVB4 | 1215    | 923     | 0.00% | 0.001% |
| 97  | 12.873 | 3678 | 3680 | 3682 | rBV  | 840     | 438     | 0.00% | 0.001% |
| 98  | 13.120 | 3754 | 3757 | 3762 | rBV4 | 780     | 772     | 0.00% | 0.001% |
| 99  | 13.191 | 3776 | 3779 | 3783 | rBV2 | 933     | 575     | 0.00% | 0.001% |
| 100 | 14.030 | 4038 | 4040 | 4042 | rBV2 | 1050    | 517     | 0.00% | 0.001% |

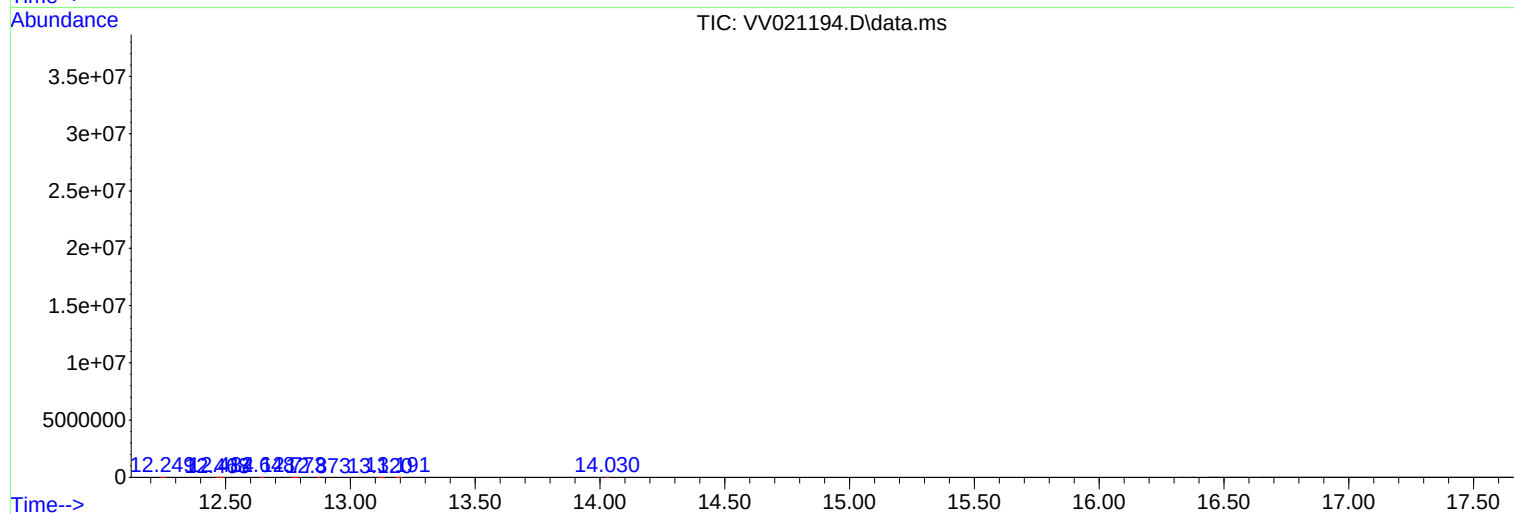
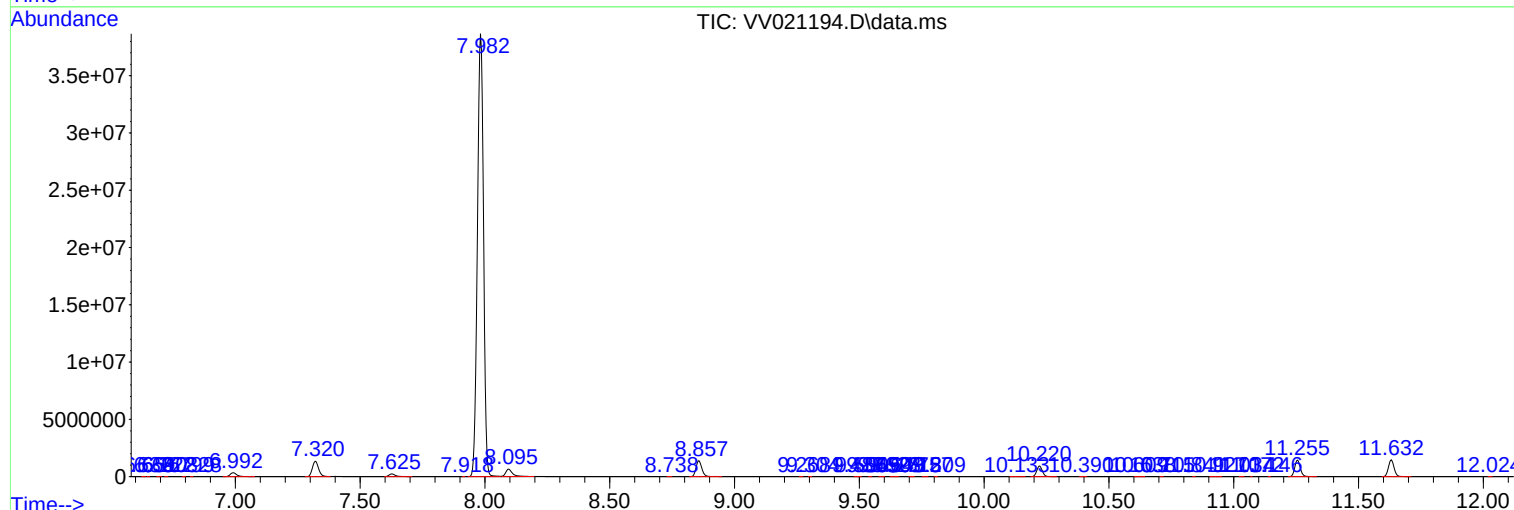
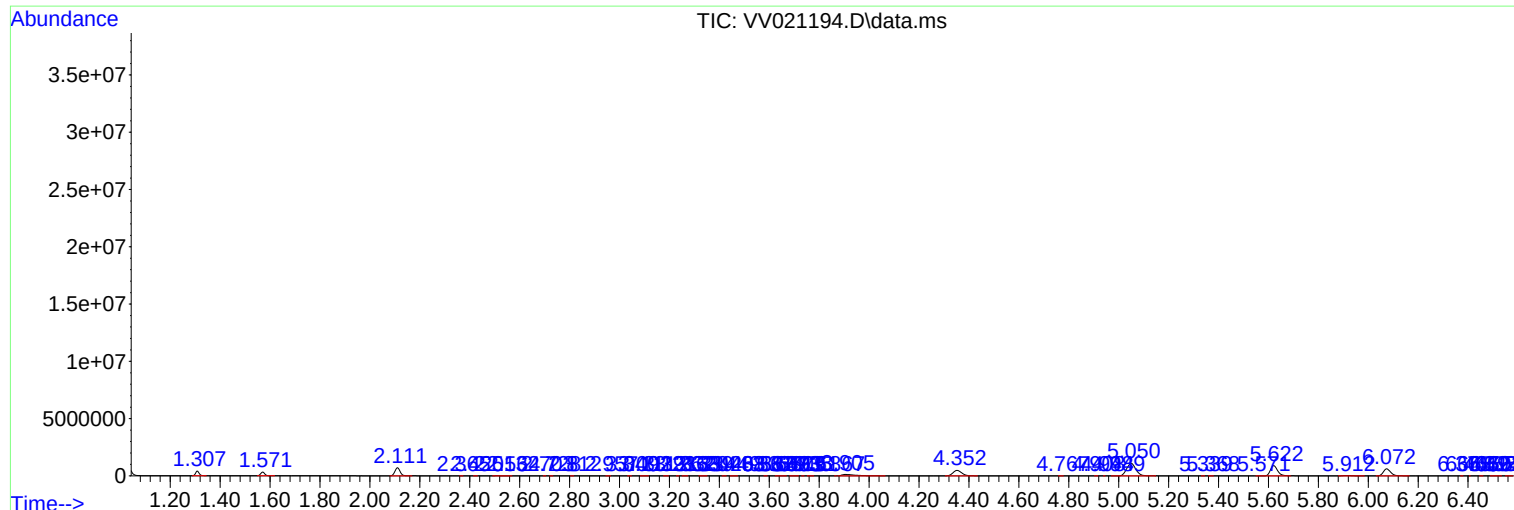
Sum of corrected areas: 87435936

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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



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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 |

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