

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU050719\  
 Data File : VU031805.D  
 Acq On : 07 May 2019 15:27  
 Operator : JC/SP  
 Sample : K2690-06  
 Misc : 4.89g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A5152

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM042719WMA.M  
 Title : VOC Analysis

Signal : TIC

| 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         | 1.392       | 87            | 94          | 109          | rBV      | 198275         | 301772        | 11.62%          | 1.456%        |
| 2         | 1.640       | 165           | 171         | 175          | rBV      | 61755          | 78276         | 3.01%           | 0.378%        |
| 3         | 1.669       | 175           | 180         | 193          | rVV      | 161726         | 260028        | 10.01%          | 1.254%        |
| 4         | 2.241       | 348           | 358         | 372          | rBV      | 460438         | 720511        | 27.75%          | 3.475%        |
| 5         | 2.437       | 414           | 419         | 430          | rVB6     | 3953           | 6983          | 0.27%           | 0.034%        |
| 6         | 2.685       | 490           | 496         | 509          | rVB9     | 6610           | 13663         | 0.53%           | 0.066%        |
| 7         | 3.009       | 593           | 597         | 600          | rVV2     | 1068           | 933           | 0.04%           | 0.005%        |
| 8         | 3.026       | 600           | 602         | 606          | rVB2     | 1464           | 814           | 0.03%           | 0.004%        |
| 9         | 3.125       | 628           | 633         | 635          | rBV2     | 1247           | 1134          | 0.04%           | 0.005%        |
| 10        | 3.167       | 641           | 646         | 649          | rVB5     | 1183           | 1034          | 0.04%           | 0.005%        |
| 11        | 3.264       | 673           | 676         | 680          | rBV      | 2139           | 1903          | 0.07%           | 0.009%        |
| 12        | 3.354       | 700           | 704         | 708          | rBV2     | 995            | 913           | 0.04%           | 0.004%        |
| 13        | 3.550       | 758           | 765         | 768          | rBV4     | 1686           | 1763          | 0.07%           | 0.009%        |
| 14        | 3.688       | 805           | 808         | 810          | rBV      | 1077           | 751           | 0.03%           | 0.004%        |
| 15        | 3.723       | 816           | 819         | 824          | rBV4     | 1326           | 1348          | 0.05%           | 0.007%        |
| 16        | 3.884       | 867           | 869         | 873          | rVB2     | 1292           | 904           | 0.03%           | 0.004%        |
| 17        | 3.916       | 873           | 879         | 882          | rVB3     | 1567           | 1617          | 0.06%           | 0.008%        |
| 18        | 3.948       | 882           | 889         | 895          | rBV4     | 2427           | 3370          | 0.13%           | 0.016%        |
| 19        | 4.054       | 919           | 922         | 925          | rBV2     | 1215           | 989           | 0.04%           | 0.005%        |
| 20        | 4.206       | 956           | 969         | 1015         | rBV2     | 169411         | 822910        | 31.69%          | 3.969%        |
| 21        | 4.643       | 1088          | 1105        | 1131         | rBV2     | 385488         | 1036230       | 39.91%          | 4.998%        |
| 22        | 4.807       | 1153          | 1156        | 1160         | rVB3     | 1627           | 1081          | 0.04%           | 0.005%        |
| 23        | 4.868       | 1173          | 1175        | 1178         | rVV2     | 1357           | 929           | 0.04%           | 0.004%        |
| 24        | 5.032       | 1222          | 1226        | 1229         | rBV5     | 1009           | 1184          | 0.05%           | 0.006%        |
| 25        | 5.189       | 1271          | 1275        | 1278         | rBV2     | 1429           | 1253          | 0.05%           | 0.006%        |
| 26        | 5.328       | 1292          | 1318        | 1343         | rBV2     | 871445         | 2596618       | 100.00%         | 12.524%       |
| 27        | 5.611       | 1403          | 1406        | 1409         | rBV4     | 1197           | 937           | 0.04%           | 0.005%        |
| 28        | 5.694       | 1429          | 1432        | 1437         | rVB5     | 1920           | 1648          | 0.06%           | 0.008%        |
| 29        | 5.717       | 1437          | 1439        | 1441         | rBV2     | 1350           | 813           | 0.03%           | 0.004%        |
| 30        | 5.881       | 1477          | 1490        | 1512         | rBV      | 807063         | 1786856       | 68.81%          | 8.618%        |
| 31        | 6.061       | 1544          | 1546        | 1550         | rBV3     | 1687           | 1200          | 0.05%           | 0.006%        |
| 32        | 6.180       | 1569          | 1583        | 1607         | rBV2     | 312162         | 674674        | 25.98%          | 3.254%        |
| 33        | 6.328       | 1614          | 1629        | 1657         | rBV      | 569233         | 1262214       | 48.61%          | 6.088%        |
| 34        | 6.508       | 1682          | 1685        | 1690         | rBV5     | 1630           | 1524          | 0.06%           | 0.007%        |

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 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM042719WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 35 | 6.562  | 1699 | 1702 | 1704 | rBV3 | 1489    | 915     | 0.04%  | 0.004%  |
| 36 | 6.649  | 1723 | 1729 | 1730 | rBV3 | 1614    | 1407    | 0.05%  | 0.007%  |
| 37 | 6.701  | 1742 | 1745 | 1751 | rVB4 | 1389    | 1324    | 0.05%  | 0.006%  |
| 38 | 6.823  | 1781 | 1783 | 1788 | rVB3 | 1480    | 1254    | 0.05%  | 0.006%  |
| 39 | 6.865  | 1793 | 1796 | 1798 | rBV  | 1270    | 773     | 0.03%  | 0.004%  |
| 40 | 6.900  | 1804 | 1807 | 1808 | rBV2 | 1767    | 898     | 0.03%  | 0.004%  |
| 41 | 7.058  | 1854 | 1856 | 1862 | rVB5 | 1109    | 1143    | 0.04%  | 0.006%  |
| 42 | 7.132  | 1877 | 1879 | 1885 | rVB5 | 962     | 753     | 0.03%  | 0.004%  |
| 43 | 7.170  | 1889 | 1891 | 1894 | rVB  | 1955    | 881     | 0.03%  | 0.004%  |
| 44 | 7.228  | 1895 | 1909 | 1932 | rBV  | 261847  | 574463  | 22.12% | 2.771%  |
| 45 | 7.398  | 1959 | 1962 | 1967 | rBV5 | 1399    | 987     | 0.04%  | 0.005%  |
| 46 | 7.488  | 1988 | 1990 | 1998 | rVB7 | 1851    | 1621    | 0.06%  | 0.008%  |
| 47 | 7.562  | 1998 | 2013 | 2048 | rBV  | 863064  | 1757315 | 67.68% | 8.476%  |
| 48 | 7.852  | 2092 | 2103 | 2129 | rBV2 | 175185  | 385610  | 14.85% | 1.860%  |
| 49 | 8.154  | 2194 | 2197 | 2198 | rBV  | 1733    | 928     | 0.04%  | 0.004%  |
| 50 | 8.231  | 2214 | 2221 | 2223 | rBV6 | 4090    | 4482    | 0.17%  | 0.022%  |
| 51 | 8.286  | 2232 | 2238 | 2239 | rBV4 | 1736    | 1449    | 0.06%  | 0.007%  |
| 52 | 8.334  | 2239 | 2253 | 2297 | rVV  | 719653  | 1756920 | 67.66% | 8.474%  |
| 53 | 8.636  | 2343 | 2347 | 2349 | rBV4 | 1632    | 1327    | 0.05%  | 0.006%  |
| 54 | 8.736  | 2375 | 2378 | 2381 | rBV2 | 1814    | 1165    | 0.04%  | 0.006%  |
| 55 | 8.755  | 2381 | 2384 | 2387 | rBV4 | 1359    | 899     | 0.03%  | 0.004%  |
| 56 | 8.861  | 2414 | 2417 | 2424 | rVB7 | 1715    | 1657    | 0.06%  | 0.008%  |
| 57 | 8.893  | 2424 | 2427 | 2433 | rBV6 | 2001    | 2509    | 0.10%  | 0.012%  |
| 58 | 9.090  | 2475 | 2488 | 2525 | rVV  | 1164365 | 2222466 | 85.59% | 10.719% |
| 59 | 9.324  | 2558 | 2561 | 2564 | rVB3 | 1757    | 1115    | 0.04%  | 0.005%  |
| 60 | 9.350  | 2565 | 2569 | 2572 | rBV2 | 1554    | 1323    | 0.05%  | 0.006%  |
| 61 | 9.459  | 2600 | 2603 | 2605 | rBV2 | 1564    | 981     | 0.04%  | 0.005%  |
| 62 | 9.514  | 2618 | 2620 | 2622 | rBV2 | 1332    | 767     | 0.03%  | 0.004%  |
| 63 | 9.614  | 2648 | 2651 | 2657 | rBV6 | 1354    | 1620    | 0.06%  | 0.008%  |
| 64 | 9.713  | 2680 | 2682 | 2686 | rVB4 | 1287    | 783     | 0.03%  | 0.004%  |
| 65 | 9.922  | 2742 | 2747 | 2750 | rBV3 | 1667    | 1538    | 0.06%  | 0.007%  |
| 66 | 9.945  | 2750 | 2754 | 2757 | rVV3 | 916     | 855     | 0.03%  | 0.004%  |
| 67 | 9.967  | 2757 | 2761 | 2765 | rVB2 | 1688    | 1310    | 0.05%  | 0.006%  |
| 68 | 10.038 | 2780 | 2783 | 2787 | rBV5 | 1070    | 821     | 0.03%  | 0.004%  |
| 69 | 10.112 | 2803 | 2806 | 2811 | rBV3 | 1871    | 1330    | 0.05%  | 0.006%  |
| 70 | 10.196 | 2827 | 2832 | 2838 | rBV5 | 2219    | 2184    | 0.08%  | 0.011%  |
| 71 | 10.241 | 2842 | 2846 | 2849 | rVB2 | 1449    | 1195    | 0.05%  | 0.006%  |

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## Integration Parameters: LSCINT.P

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 Start Thrs: 0.2  
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 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM042719WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 72  | 10.437 | 2894 | 2907 | 2931 | rBV  | 780407  | 1307396 | 50.35% | 6.306% |
| 73  | 10.723 | 2992 | 2996 | 2999 | rBV4 | 1031    | 1157    | 0.04%  | 0.006% |
| 74  | 10.903 | 3049 | 3052 | 3055 | rVB3 | 1460    | 1086    | 0.04%  | 0.005% |
| 75  | 10.983 | 3074 | 3077 | 3080 | rBV2 | 1489    | 1016    | 0.04%  | 0.005% |
| 76  | 11.083 | 3105 | 3108 | 3111 | rBV3 | 1968    | 1578    | 0.06%  | 0.008% |
| 77  | 11.337 | 3183 | 3187 | 3192 | rBV3 | 1386    | 1483    | 0.06%  | 0.007% |
| 78  | 11.485 | 3221 | 3233 | 3264 | rVV  | 1024660 | 1670219 | 64.32% | 8.056% |
| 79  | 11.710 | 3301 | 3303 | 3306 | rBV3 | 1508    | 1059    | 0.04%  | 0.005% |
| 80  | 11.861 | 3338 | 3350 | 3367 | rBV  | 834376  | 1394104 | 53.69% | 6.724% |
| 81  | 12.353 | 3496 | 3503 | 3506 | rVB4 | 1913    | 2032    | 0.08%  | 0.010% |
| 82  | 12.372 | 3507 | 3509 | 3512 | rBV3 | 1205    | 822     | 0.03%  | 0.004% |
| 83  | 12.456 | 3530 | 3535 | 3540 | rBV6 | 1975    | 2616    | 0.10%  | 0.013% |
| 84  | 12.553 | 3562 | 3565 | 3567 | rBV3 | 1427    | 951     | 0.04%  | 0.005% |
| 85  | 12.739 | 3621 | 3623 | 3626 | rBV2 | 1875    | 1100    | 0.04%  | 0.005% |
| 86  | 12.758 | 3626 | 3629 | 3632 | rVV3 | 1131    | 817     | 0.03%  | 0.004% |
| 87  | 12.813 | 3644 | 3646 | 3649 | rBV2 | 1500    | 787     | 0.03%  | 0.004% |
| 88  | 12.932 | 3678 | 3683 | 3685 | rBV3 | 1231    | 1173    | 0.05%  | 0.006% |
| 89  | 13.006 | 3703 | 3706 | 3707 | rBV2 | 1398    | 814     | 0.03%  | 0.004% |
| 90  | 13.295 | 3793 | 3796 | 3799 | rBV3 | 985     | 915     | 0.04%  | 0.004% |
| 91  | 13.334 | 3804 | 3808 | 3811 | rBV2 | 1608    | 1232    | 0.05%  | 0.006% |
| 92  | 13.392 | 3823 | 3826 | 3831 | rBV4 | 1788    | 1445    | 0.06%  | 0.007% |
| 93  | 13.559 | 3874 | 3878 | 3880 | rBV3 | 1328    | 1295    | 0.05%  | 0.006% |
| 94  | 13.713 | 3921 | 3926 | 3929 | rBV3 | 1480    | 1582    | 0.06%  | 0.008% |
| 95  | 13.761 | 3937 | 3941 | 3946 | rVB2 | 1921    | 1745    | 0.07%  | 0.008% |
| 96  | 13.977 | 4004 | 4008 | 4010 | rBV3 | 1937    | 1313    | 0.05%  | 0.006% |
| 97  | 14.176 | 4067 | 4070 | 4072 | rBV2 | 1225    | 795     | 0.03%  | 0.004% |
| 98  | 14.218 | 4080 | 4083 | 4090 | rVB3 | 2068    | 2112    | 0.08%  | 0.010% |
| 99  | 14.964 | 4312 | 4315 | 4319 | rBV3 | 1772    | 1318    | 0.05%  | 0.006% |
| 100 | 15.147 | 4370 | 4372 | 4375 | rBV4 | 1797    | 1501    | 0.06%  | 0.007% |

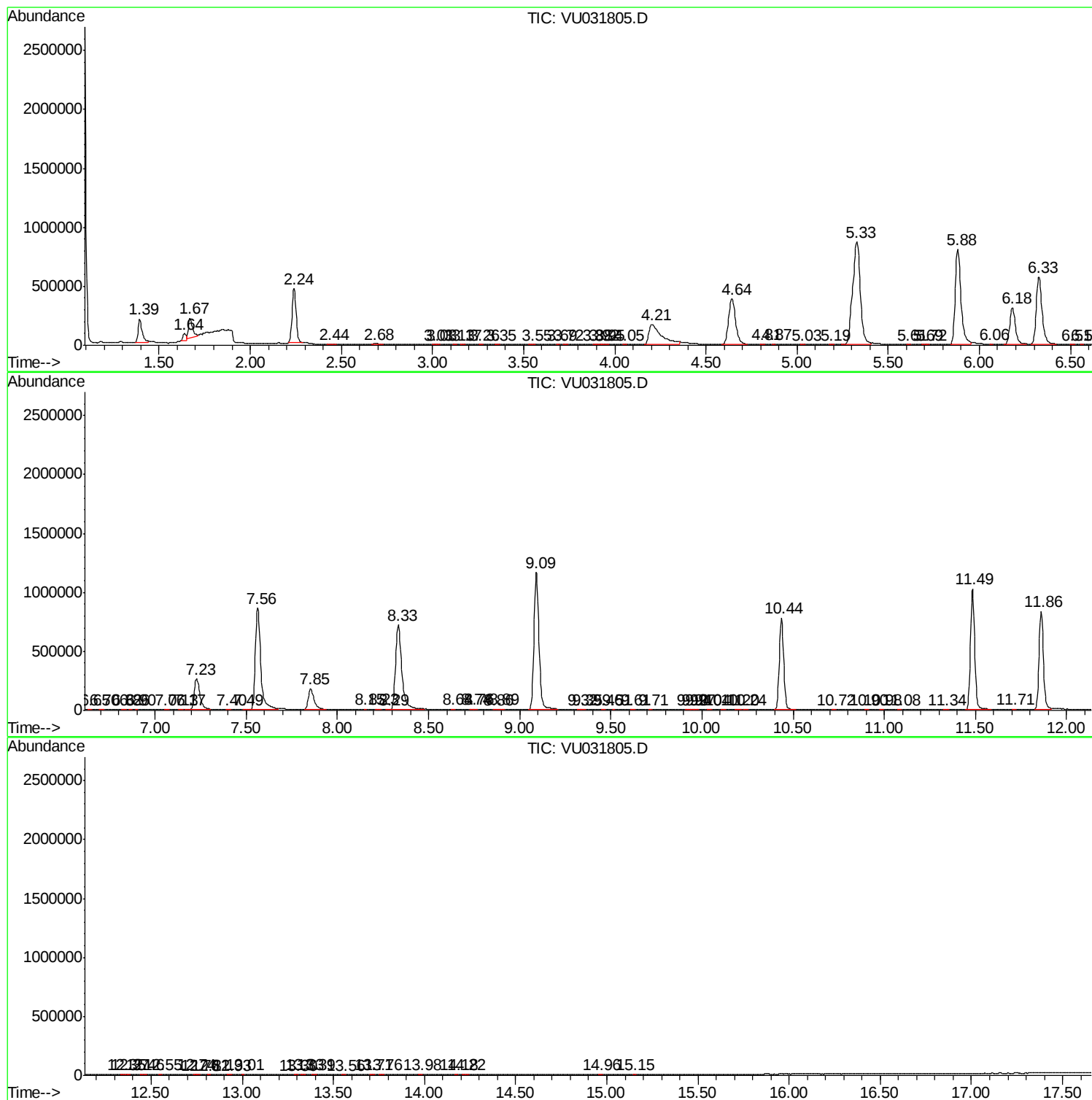
Sum of corrected areas: 20733208

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM042719WMA.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        |