

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV081920\  
 Data File : VV018060.D  
 Acq On : 19 Aug 2020 12:51  
 Operator : SY/MD  
 Sample : L3709-13ME 10X  
 Misc : 7.10g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BFWQ6ME

## 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\_V\METHOD\SOMVLM081120WMA.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         | 1.315       | 63            | 70          | 89           | rVB      | 126566         | 131091        | 14.37%          | 1.754%        |
| 2         | 1.573       | 143           | 150         | 171          | rVB      | 113392         | 129815        | 14.23%          | 1.737%        |
| 3         | 2.122       | 310           | 321         | 350          | rVB      | 222969         | 344849        | 37.79%          | 4.615%        |
| 4         | 2.299       | 373           | 376         | 377          | rBV2     | 308            | 198           | 0.02%           | 0.003%        |
| 5         | 2.309       | 377           | 379         | 387          | rVB2     | 719            | 840           | 0.09%           | 0.011%        |
| 6         | 2.454       | 419           | 424         | 431          | rBV2     | 194            | 283           | 0.03%           | 0.004%        |
| 7         | 2.524       | 437           | 446         | 457          | rVB      | 5858           | 9077          | 0.99%           | 0.121%        |
| 8         | 2.637       | 471           | 481         | 492          | rBV4     | 1368           | 3053          | 0.33%           | 0.041%        |
| 9         | 2.794       | 524           | 530         | 534          | rBV2     | 223            | 285           | 0.03%           | 0.004%        |
| 10        | 2.836       | 539           | 543         | 546          | rBV2     | 114            | 110           | 0.01%           | 0.001%        |
| 11        | 2.955       | 576           | 580         | 583          | rBV      | 168            | 124           | 0.01%           | 0.002%        |
| 12        | 2.978       | 583           | 587         | 590          | rBV      | 109            | 98            | 0.01%           | 0.001%        |
| 13        | 3.183       | 643           | 651         | 655          | rBV2     | 113            | 171           | 0.02%           | 0.002%        |
| 14        | 3.312       | 688           | 691         | 699          | rBV2     | 110            | 141           | 0.02%           | 0.002%        |
| 15        | 3.351       | 699           | 703         | 709          | rVV2     | 127            | 136           | 0.01%           | 0.002%        |
| 16        | 3.402       | 714           | 719         | 723          | rBV      | 176            | 174           | 0.02%           | 0.002%        |
| 17        | 3.534       | 757           | 760         | 766          | rVB      | 163            | 142           | 0.02%           | 0.002%        |
| 18        | 3.666       | 796           | 801         | 805          | rBV2     | 74             | 104           | 0.01%           | 0.001%        |
| 19        | 3.762       | 827           | 831         | 836          | rBV      | 120            | 120           | 0.01%           | 0.002%        |
| 20        | 3.823       | 846           | 850         | 853          | rBV      | 142            | 107           | 0.01%           | 0.001%        |
| 21        | 3.862       | 857           | 862         | 864          | rBV2     | 95             | 95            | 0.01%           | 0.001%        |
| 22        | 3.900       | 864           | 874         | 923          | rBV      | 69609          | 202362        | 22.18%          | 2.708%        |
| 23        | 4.129       | 942           | 945         | 946          | rBV2     | 259            | 109           | 0.01%           | 0.001%        |
| 24        | 4.376       | 1005          | 1022        | 1054         | rBV      | 147686         | 370425        | 40.59%          | 4.957%        |
| 25        | 4.505       | 1061          | 1062        | 1066         | rVB      | 305            | 151           | 0.02%           | 0.002%        |
| 26        | 4.524       | 1066          | 1068        | 1070         | rVB      | 222            | 107           | 0.01%           | 0.001%        |
| 27        | 4.540       | 1070          | 1073        | 1076         | rBV2     | 177            | 105           | 0.01%           | 0.001%        |
| 28        | 4.556       | 1076          | 1078        | 1081         | rVB      | 273            | 130           | 0.01%           | 0.002%        |
| 29        | 4.849       | 1163          | 1169        | 1175         | rBV2     | 175            | 206           | 0.02%           | 0.003%        |
| 30        | 5.071       | 1221          | 1238        | 1269         | rBV2     | 356061         | 912519        | 100.00%         | 12.211%       |
| 31        | 5.222       | 1283          | 1285        | 1288         | rVB2     | 168            | 108           | 0.01%           | 0.001%        |
| 32        | 5.328       | 1316          | 1318        | 1323         | rVB2     | 222            | 110           | 0.01%           | 0.001%        |
| 33        | 5.376       | 1331          | 1333        | 1338         | rVB3     | 247            | 180           | 0.02%           | 0.002%        |
| 34        | 5.421       | 1345          | 1347        | 1350         | rBV2     | 132            | 90            | 0.01%           | 0.001%        |

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 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVLM081120WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |        |         |
|----|-------|------|------|------|------|--------|--------|--------|---------|
| 35 | 5.502 | 1371 | 1372 | 1376 | rVB2 | 251    | 137    | 0.02%  | 0.002%  |
| 36 | 5.524 | 1376 | 1379 | 1383 | rBV2 | 237    | 161    | 0.02%  | 0.002%  |
| 37 | 5.640 | 1397 | 1415 | 1442 | rBV  | 331535 | 658610 | 72.17% | 8.814%  |
| 38 | 5.929 | 1495 | 1505 | 1530 | rVB2 | 19673  | 39636  | 4.34%  | 0.530%  |
| 39 | 6.093 | 1542 | 1556 | 1580 | rBV  | 211535 | 422735 | 46.33% | 5.657%  |
| 40 | 6.228 | 1596 | 1598 | 1602 | rVB2 | 245    | 171    | 0.02%  | 0.002%  |
| 41 | 6.318 | 1623 | 1626 | 1632 | rVB2 | 171    | 193    | 0.02%  | 0.003%  |
| 42 | 6.354 | 1632 | 1637 | 1640 | rBV  | 232    | 197    | 0.02%  | 0.003%  |
| 43 | 6.373 | 1640 | 1643 | 1647 | rVB  | 126    | 100    | 0.01%  | 0.001%  |
| 44 | 6.412 | 1647 | 1655 | 1658 | rBV2 | 108    | 128    | 0.01%  | 0.002%  |
| 45 | 6.531 | 1686 | 1692 | 1697 | rVB2 | 108    | 154    | 0.02%  | 0.002%  |
| 46 | 6.736 | 1752 | 1756 | 1763 | rVB2 | 163    | 178    | 0.02%  | 0.002%  |
| 47 | 7.006 | 1824 | 1840 | 1863 | rBV  | 108207 | 195347 | 21.41% | 2.614%  |
| 48 | 7.158 | 1885 | 1887 | 1890 | rBV3 | 190    | 145    | 0.02%  | 0.002%  |
| 49 | 7.215 | 1902 | 1905 | 1909 | rVB2 | 221    | 102    | 0.01%  | 0.001%  |
| 50 | 7.254 | 1913 | 1917 | 1918 | rBV2 | 154    | 94     | 0.01%  | 0.001%  |
| 51 | 7.338 | 1931 | 1943 | 1965 | rBV  | 398725 | 681801 | 74.72% | 9.124%  |
| 52 | 7.553 | 2007 | 2010 | 2013 | rBV3 | 266    | 168    | 0.02%  | 0.002%  |
| 53 | 7.643 | 2027 | 2038 | 2061 | rBV  | 78484  | 134526 | 14.74% | 1.800%  |
| 54 | 7.910 | 2119 | 2121 | 2127 | rBV2 | 133    | 117    | 0.01%  | 0.002%  |
| 55 | 7.997 | 2137 | 2148 | 2167 | rVB  | 101967 | 170977 | 18.74% | 2.288%  |
| 56 | 8.109 | 2172 | 2183 | 2219 | rBV2 | 167404 | 340816 | 37.35% | 4.561%  |
| 57 | 8.347 | 2253 | 2257 | 2260 | rVB3 | 181    | 165    | 0.02%  | 0.002%  |
| 58 | 8.437 | 2277 | 2285 | 2298 | rVB4 | 1170   | 2036   | 0.22%  | 0.027%  |
| 59 | 8.550 | 2315 | 2320 | 2324 | rBV  | 186    | 177    | 0.02%  | 0.002%  |
| 60 | 8.691 | 2359 | 2364 | 2366 | rBV2 | 89     | 90     | 0.01%  | 0.001%  |
| 61 | 8.743 | 2377 | 2380 | 2385 | rBV  | 163    | 106    | 0.01%  | 0.001%  |
| 62 | 8.801 | 2392 | 2398 | 2401 | rBV2 | 138    | 135    | 0.01%  | 0.002%  |
| 63 | 8.871 | 2408 | 2420 | 2446 | rBV  | 506047 | 817926 | 89.63% | 10.946% |
| 64 | 9.158 | 2504 | 2509 | 2515 | rVB2 | 266    | 302    | 0.03%  | 0.004%  |
| 65 | 9.238 | 2529 | 2534 | 2537 | rBV2 | 135    | 119    | 0.01%  | 0.002%  |
| 66 | 9.440 | 2592 | 2597 | 2601 | rBV2 | 84     | 99     | 0.01%  | 0.001%  |
| 67 | 9.566 | 2631 | 2636 | 2639 | rBV2 | 135    | 139    | 0.02%  | 0.002%  |
| 68 | 9.649 | 2657 | 2662 | 2665 | rVV2 | 146    | 126    | 0.01%  | 0.002%  |
| 69 | 9.765 | 2696 | 2698 | 2704 | rVB  | 120    | 94     | 0.01%  | 0.001%  |
| 70 | 9.830 | 2714 | 2718 | 2721 | rBV2 | 152    | 121    | 0.01%  | 0.002%  |
| 71 | 9.903 | 2738 | 2741 | 2744 | rBV  | 133    | 106    | 0.01%  | 0.001%  |

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 ClientSampleId :  
 BFWQ6ME

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Filtering: 5  
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 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVLM081120WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 72  | 10.238 | 2833 | 2845 | 2866 | rBV  | 256273 | 406381 | 44.53% | 5.438%  |
| 73  | 10.347 | 2875 | 2879 | 2883 | rBV2 | 116    | 113    | 0.01%  | 0.002%  |
| 74  | 10.373 | 2885 | 2887 | 2892 | rVB2 | 155    | 134    | 0.01%  | 0.002%  |
| 75  | 10.482 | 2917 | 2921 | 2926 | rBV2 | 162    | 154    | 0.02%  | 0.002%  |
| 76  | 10.550 | 2938 | 2942 | 2945 | rBV  | 124    | 130    | 0.01%  | 0.002%  |
| 77  | 10.585 | 2950 | 2953 | 2956 | rBV2 | 117    | 99     | 0.01%  | 0.001%  |
| 78  | 10.936 | 3058 | 3062 | 3065 | rBV2 | 179    | 138    | 0.02%  | 0.002%  |
| 79  | 11.090 | 3105 | 3110 | 3115 | rBV2 | 124    | 163    | 0.02%  | 0.002%  |
| 80  | 11.270 | 3155 | 3166 | 3193 | rBV  | 515001 | 783621 | 85.87% | 10.486% |
| 81  | 11.514 | 3237 | 3242 | 3245 | rBV2 | 133    | 140    | 0.02%  | 0.002%  |
| 82  | 11.646 | 3271 | 3283 | 3308 | rBV  | 453740 | 702142 | 76.95% | 9.396%  |
| 83  | 11.820 | 3333 | 3337 | 3340 | rBV3 | 183    | 137    | 0.02%  | 0.002%  |
| 84  | 12.048 | 3406 | 3408 | 3412 | rBV  | 162    | 98     | 0.01%  | 0.001%  |
| 85  | 12.077 | 3413 | 3417 | 3421 | rVB2 | 149    | 146    | 0.02%  | 0.002%  |
| 86  | 12.170 | 3442 | 3446 | 3448 | rBV3 | 211    | 176    | 0.02%  | 0.002%  |
| 87  | 12.456 | 3531 | 3535 | 3538 | rBV  | 181    | 178    | 0.02%  | 0.002%  |
| 88  | 12.608 | 3580 | 3582 | 3586 | rBV2 | 212    | 97     | 0.01%  | 0.001%  |
| 89  | 12.646 | 3592 | 3594 | 3595 | rBV2 | 214    | 95     | 0.01%  | 0.001%  |
| 90  | 12.733 | 3619 | 3621 | 3627 | rBV  | 291    | 245    | 0.03%  | 0.003%  |
| 91  | 13.061 | 3720 | 3723 | 3726 | rBV2 | 211    | 131    | 0.01%  | 0.002%  |
| 92  | 13.292 | 3792 | 3795 | 3800 | rBV2 | 392    | 360    | 0.04%  | 0.005%  |
| 93  | 13.553 | 3872 | 3876 | 3878 | rBV2 | 230    | 138    | 0.02%  | 0.002%  |
| 94  | 13.669 | 3909 | 3912 | 3914 | rBV  | 239    | 153    | 0.02%  | 0.002%  |
| 95  | 13.842 | 3964 | 3966 | 3970 | rVB2 | 297    | 153    | 0.02%  | 0.002%  |
| 96  | 13.861 | 3970 | 3972 | 3973 | rBV2 | 206    | 90     | 0.01%  | 0.001%  |
| 97  | 14.083 | 4039 | 4041 | 4043 | rBV  | 199    | 141    | 0.02%  | 0.002%  |
| 98  | 14.209 | 4078 | 4080 | 4082 | rBV  | 292    | 170    | 0.02%  | 0.002%  |
| 99  | 14.646 | 4213 | 4216 | 4219 | rBV2 | 283    | 228    | 0.02%  | 0.003%  |
| 100 | 16.045 | 4647 | 4651 | 4660 | rBV5 | 658    | 885    | 0.10%  | 0.012%  |

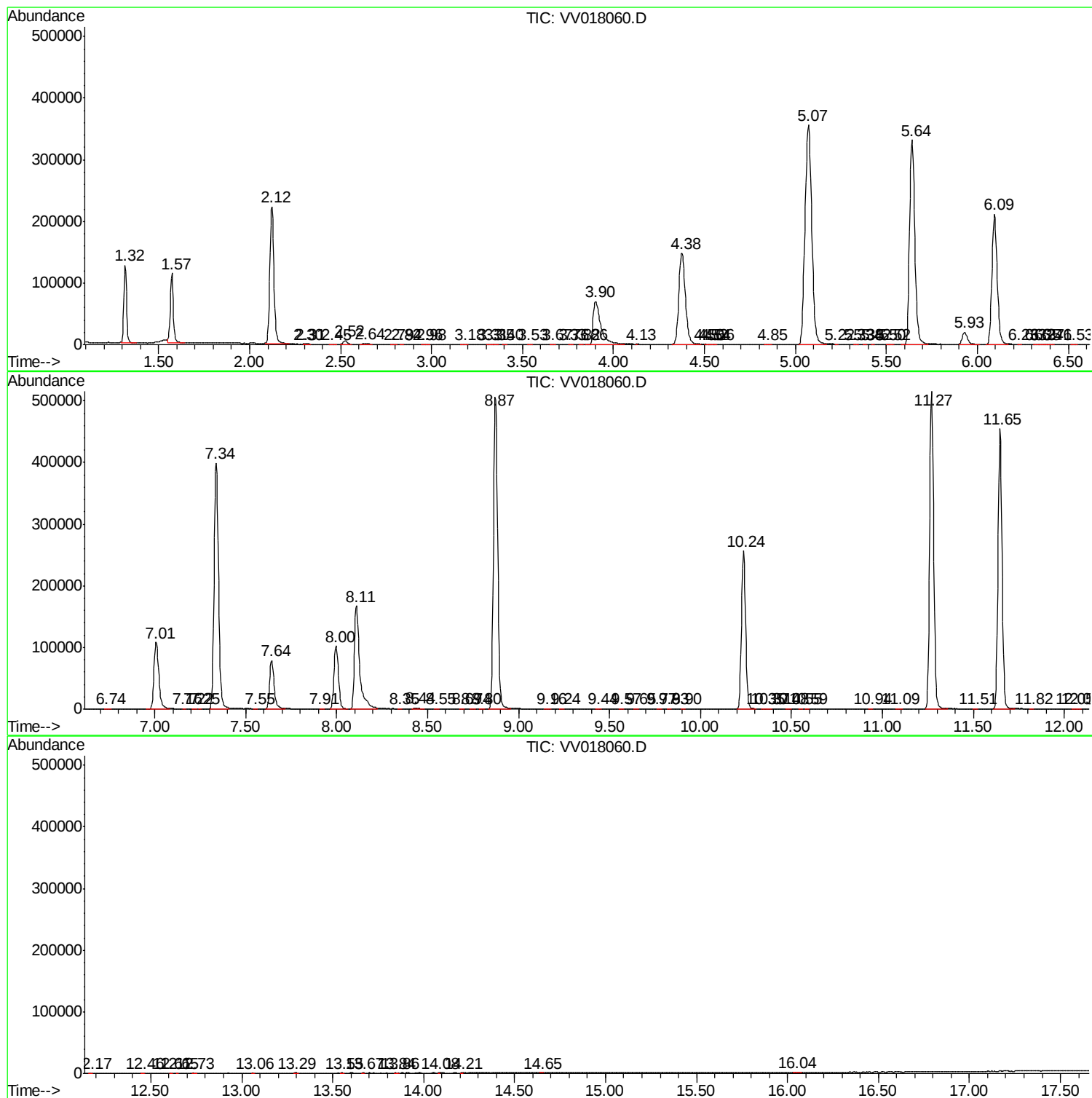
Sum of corrected areas: 7472685

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Instrument :  
MSVOA\_V  
ClientSampled :  
BFWQ6ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVLM081120WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV081920\  
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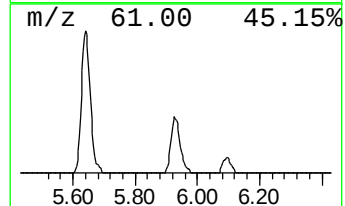
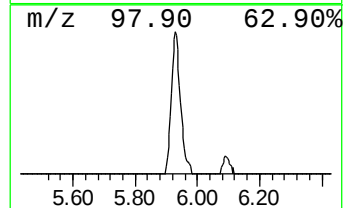
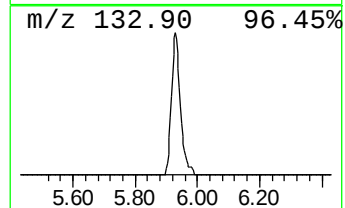
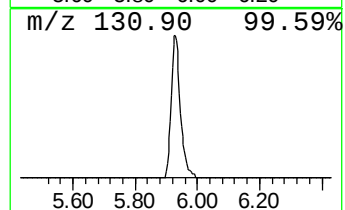
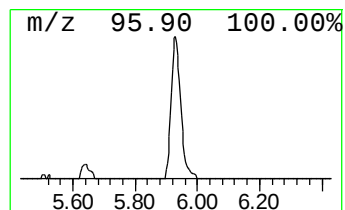
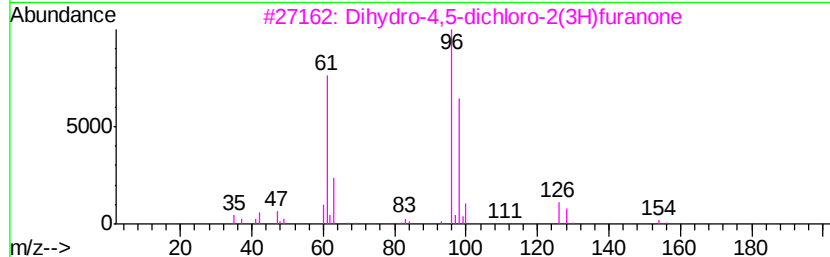
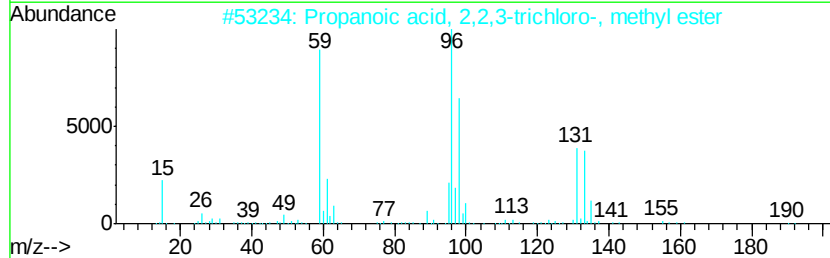
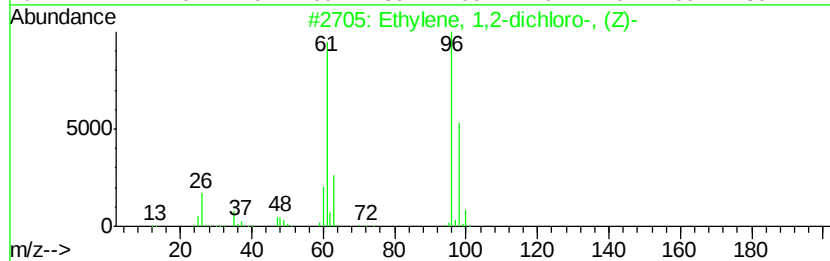
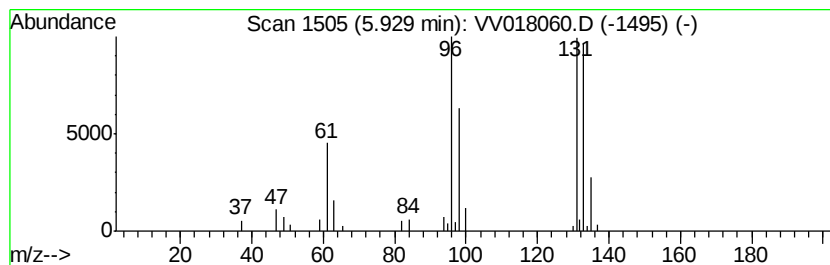
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVLM081120WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 unknown-01 Concentration Rank 2

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 5.93 | 3.01 ug/L | 39636 | 1,4-Difluorobenzene | 5.64 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | Ethylene, 1,2-dichloro-, (Z)-       | 96  | C2H2Cl2   | 000156-59-2 | 38   |
| 2    |    | Propanoic acid, 2,2,3-trichloro-... | 190 | C4H5Cl3O2 | 004749-35-3 | 37   |
| 3    |    | Dihydro-4,5-dichloro-2(3H)furanone  | 154 | C4H4Cl2O2 | 114434-99-0 | 25   |
| 4    |    | Heptanoic acid, heptyl ester        | 228 | C14H28O2  | 000624-09-9 | 12   |
| 5    |    | Pyrimidine, 4-hydroxy-              | 96  | C4H4N2O   | 051953-18-5 | 9    |



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| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown-01       | 5.93 | 3.0     | ug/L  | 39636    | 1                     | 5.64 | 658610 | 50.0 |