

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU042923\  
 Data File : VU053966.D  
 Acq On : 28 Apr 2023 12:53  
 Operator : JC/MD  
 Sample : VU0429MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK079

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\_U\Method\SFAMULM033123WMA.M  
 Title : VOC Analysis

Signal : TIC: VU053966.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         | 1.601       | 73            | 81          | 97           | rBV      | 97330          | 119034        | 16.10%          | 1.997%        |
| 2         | 1.912       | 171           | 178         | 196          | rVB      | 105716         | 141379        | 19.12%          | 2.372%        |
| 3         | 2.565       | 368           | 381         | 399          | rBV      | 162295         | 263347        | 35.62%          | 4.419%        |
| 4         | 2.668       | 411           | 413         | 416          | rVB      | 416            | 238           | 0.03%           | 0.004%        |
| 5         | 2.732       | 430           | 433         | 437          | rBV2     | 302            | 215           | 0.03%           | 0.004%        |
| 6         | 2.787       | 447           | 450         | 461          | rVB      | 796            | 972           | 0.13%           | 0.016%        |
| 7         | 3.044       | 521           | 530         | 539          | rVB5     | 2010           | 3681          | 0.50%           | 0.062%        |
| 8         | 3.121       | 549           | 554         | 556          | rBV      | 347            | 326           | 0.04%           | 0.005%        |
| 9         | 3.186       | 569           | 574         | 577          | rBV2     | 288            | 267           | 0.04%           | 0.004%        |
| 10        | 3.456       | 653           | 658         | 661          | rBV      | 215            | 228           | 0.03%           | 0.004%        |
| 11        | 3.629       | 709           | 712         | 717          | rBV      | 190            | 249           | 0.03%           | 0.004%        |
| 12        | 3.719       | 736           | 740         | 741          | rBV      | 219            | 169           | 0.02%           | 0.003%        |
| 13        | 3.764       | 751           | 754         | 759          | rBV2     | 191            | 178           | 0.02%           | 0.003%        |
| 14        | 4.086       | 851           | 854         | 859          | rBB      | 160            | 179           | 0.02%           | 0.003%        |
| 15        | 4.118       | 860           | 864         | 868          | rBV      | 277            | 313           | 0.04%           | 0.005%        |
| 16        | 4.205       | 887           | 891         | 898          | rBV2     | 294            | 406           | 0.05%           | 0.007%        |
| 17        | 4.385       | 945           | 947         | 951          | rBB      | 387            | 190           | 0.03%           | 0.003%        |
| 18        | 4.472       | 969           | 974         | 977          | rBV      | 205            | 240           | 0.03%           | 0.004%        |
| 19        | 4.549       | 995           | 998         | 1001         | rBV      | 286            | 238           | 0.03%           | 0.004%        |
| 20        | 4.626       | 1011          | 1022        | 1045         | rBV      | 43830          | 110094        | 14.89%          | 1.847%        |
| 21        | 4.825       | 1082          | 1084        | 1089         | rBV2     | 316            | 260           | 0.04%           | 0.004%        |
| 22        | 5.057       | 1140          | 1156        | 1182         | rBV      | 141719         | 313276        | 42.38%          | 5.257%        |
| 23        | 5.160       | 1186          | 1188        | 1190         | rBV2     | 393            | 189           | 0.03%           | 0.003%        |
| 24        | 5.224       | 1206          | 1208        | 1211         | rVB2     | 277            | 172           | 0.02%           | 0.003%        |
| 25        | 5.301       | 1229          | 1232        | 1235         | rBB      | 227            | 173           | 0.02%           | 0.003%        |
| 26        | 5.510       | 1292          | 1297        | 1298         | rBV      | 196            | 182           | 0.02%           | 0.003%        |
| 27        | 5.578       | 1314          | 1318        | 1324         | rBB      | 180            | 251           | 0.03%           | 0.004%        |
| 28        | 5.604       | 1324          | 1326        | 1329         | rBB      | 309            | 176           | 0.02%           | 0.003%        |
| 29        | 5.719       | 1342          | 1362        | 1387         | rBV2     | 275978         | 739263        | 100.00%         | 12.405%       |
| 30        | 5.938       | 1428          | 1430        | 1436         | rVB2     | 340            | 301           | 0.04%           | 0.005%        |
| 31        | 5.970       | 1437          | 1440        | 1442         | rBV2     | 314            | 243           | 0.03%           | 0.004%        |
| 32        | 6.044       | 1460          | 1463        | 1465         | rBV      | 298            | 200           | 0.03%           | 0.003%        |
| 33        | 6.124       | 1484          | 1488        | 1493         | rVB      | 264            | 300           | 0.04%           | 0.005%        |
| 34        | 6.163       | 1497          | 1500        | 1505         | rBB      | 196            | 202           | 0.03%           | 0.003%        |
| 35        | 6.243       | 1506          | 1525        | 1549         | rBV      | 295211         | 559441        | 75.68%          | 9.387%        |
| 36        | 6.497       | 1599          | 1604        | 1606         | rBV      | 376            | 329           | 0.04%           | 0.006%        |

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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\_U\Method\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.523  | 1606 | 1612 | 1613 | rBV2 | 2229   | 1818   | 0.25%  | 0.031%  |
| 38 | 6.571  | 1625 | 1627 | 1630 | rBB  | 302    | 183    | 0.02%  | 0.003%  |
| 39 | 6.684  | 1649 | 1662 | 1680 | rBV  | 167381 | 326395 | 44.15% | 5.477%  |
| 40 | 6.800  | 1695 | 1698 | 1701 | rBV  | 390    | 231    | 0.03%  | 0.004%  |
| 41 | 6.944  | 1739 | 1743 | 1746 | rBV  | 303    | 259    | 0.04%  | 0.004%  |
| 42 | 7.092  | 1786 | 1789 | 1793 | rBV  | 166    | 184    | 0.02%  | 0.003%  |
| 43 | 7.295  | 1850 | 1852 | 1857 | rVV  | 291    | 238    | 0.03%  | 0.004%  |
| 44 | 7.372  | 1870 | 1876 | 1879 | rBV  | 380    | 357    | 0.05%  | 0.006%  |
| 45 | 7.391  | 1879 | 1882 | 1885 | rVB  | 261    | 195    | 0.03%  | 0.003%  |
| 46 | 7.475  | 1903 | 1908 | 1911 | rBV2 | 223    | 251    | 0.03%  | 0.004%  |
| 47 | 7.507  | 1915 | 1918 | 1922 | rVV2 | 256    | 196    | 0.03%  | 0.003%  |
| 48 | 7.562  | 1922 | 1935 | 1958 | rVV  | 94033  | 166738 | 22.55% | 2.798%  |
| 49 | 7.645  | 1958 | 1961 | 1962 | rBV  | 354    | 196    | 0.03%  | 0.003%  |
| 50 | 7.713  | 1979 | 1982 | 1986 | rBV  | 266    | 213    | 0.03%  | 0.004%  |
| 51 | 7.793  | 2002 | 2007 | 2008 | rBV  | 270    | 186    | 0.03%  | 0.003%  |
| 52 | 7.848  | 2020 | 2024 | 2025 | rBV  | 239    | 197    | 0.03%  | 0.003%  |
| 53 | 7.893  | 2025 | 2038 | 2058 | rBV  | 346781 | 605561 | 81.91% | 10.161% |
| 54 | 8.063  | 2089 | 2091 | 2095 | rBV2 | 415    | 313    | 0.04%  | 0.005%  |
| 55 | 8.083  | 2095 | 2097 | 2099 | rVB  | 410    | 182    | 0.02%  | 0.003%  |
| 56 | 8.176  | 2113 | 2126 | 2146 | rBV  | 62833  | 109161 | 14.77% | 1.832%  |
| 57 | 8.468  | 2209 | 2217 | 2221 | rVV  | 685    | 818    | 0.11%  | 0.014%  |
| 58 | 8.549  | 2233 | 2242 | 2254 | rVB2 | 10391  | 16638  | 2.25%  | 0.279%  |
| 59 | 8.629  | 2256 | 2267 | 2300 | rBV  | 142555 | 265778 | 35.95% | 4.460%  |
| 60 | 8.854  | 2334 | 2337 | 2342 | rVV2 | 280    | 229    | 0.03%  | 0.004%  |
| 61 | 8.893  | 2345 | 2349 | 2355 | rVB2 | 329    | 406    | 0.05%  | 0.007%  |
| 62 | 9.060  | 2398 | 2401 | 2404 | rVB  | 370    | 241    | 0.03%  | 0.004%  |
| 63 | 9.166  | 2432 | 2434 | 2440 | rVB  | 309    | 190    | 0.03%  | 0.003%  |
| 64 | 9.202  | 2442 | 2445 | 2449 | rVV  | 275    | 194    | 0.03%  | 0.003%  |
| 65 | 9.269  | 2464 | 2466 | 2470 | rBB  | 280    | 196    | 0.03%  | 0.003%  |
| 66 | 9.304  | 2474 | 2477 | 2480 | rBV  | 205    | 204    | 0.03%  | 0.003%  |
| 67 | 9.414  | 2497 | 2511 | 2530 | rBV  | 387491 | 644252 | 87.15% | 10.810% |
| 68 | 9.684  | 2591 | 2595 | 2597 | rBV  | 401    | 261    | 0.04%  | 0.004%  |
| 69 | 9.870  | 2650 | 2653 | 2656 | rBV  | 271    | 223    | 0.03%  | 0.004%  |
| 70 | 9.964  | 2680 | 2682 | 2686 | rVB2 | 534    | 350    | 0.05%  | 0.006%  |
| 71 | 9.992  | 2686 | 2691 | 2694 | rBV  | 269    | 301    | 0.04%  | 0.005%  |
| 72 | 10.012 | 2694 | 2697 | 2703 | rVB  | 296    | 303    | 0.04%  | 0.005%  |
| 73 | 10.063 | 2704 | 2713 | 2716 | rBV  | 311    | 507    | 0.07%  | 0.009%  |
| 74 | 10.108 | 2724 | 2727 | 2729 | rBV3 | 463    | 284    | 0.04%  | 0.005%  |
| 75 | 10.478 | 2837 | 2842 | 2845 | rBV3 | 519    | 481    | 0.07%  | 0.008%  |
| 76 | 10.636 | 2883 | 2891 | 2900 | rVB4 | 3020   | 4730   | 0.64%  | 0.079%  |

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Instrument :  
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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\_U\Method\SFAMULM033123WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 10.751 | 2914 | 2927 | 2944 | rBV  | 234243 | 376959 | 50.99% | 6.325%  |
| 78  | 10.896 | 2967 | 2972 | 2974 | rBV2 | 313    | 298    | 0.04%  | 0.005%  |
| 79  | 10.912 | 2974 | 2977 | 2980 | rVV2 | 405    | 256    | 0.03%  | 0.004%  |
| 80  | 10.992 | 2999 | 3002 | 3005 | rBV2 | 278    | 182    | 0.02%  | 0.003%  |
| 81  | 11.414 | 3127 | 3133 | 3135 | rBV2 | 325    | 371    | 0.05%  | 0.006%  |
| 82  | 11.722 | 3226 | 3229 | 3231 | rBV2 | 441    | 302    | 0.04%  | 0.005%  |
| 83  | 11.745 | 3231 | 3236 | 3243 | rVB3 | 1593   | 1971   | 0.27%  | 0.033%  |
| 84  | 11.806 | 3243 | 3255 | 3280 | rBV  | 372741 | 603746 | 81.67% | 10.131% |
| 85  | 11.957 | 3299 | 3302 | 3306 | rVB2 | 350    | 276    | 0.04%  | 0.005%  |
| 86  | 12.189 | 3361 | 3374 | 3396 | rBV  | 330307 | 537077 | 72.65% | 9.012%  |
| 87  | 12.365 | 3427 | 3429 | 3432 | rBV  | 331    | 200    | 0.03%  | 0.003%  |
| 88  | 12.851 | 3577 | 3580 | 3582 | rBV  | 372    | 219    | 0.03%  | 0.004%  |
| 89  | 13.005 | 3626 | 3628 | 3631 | rVB  | 358    | 171    | 0.02%  | 0.003%  |
| 90  | 13.028 | 3632 | 3635 | 3639 | rBV2 | 277    | 261    | 0.04%  | 0.004%  |
| 91  | 13.221 | 3689 | 3695 | 3699 | rBV3 | 1484   | 1744   | 0.24%  | 0.029%  |
| 92  | 13.555 | 3796 | 3799 | 3801 | rBV  | 353    | 199    | 0.03%  | 0.003%  |
| 93  | 13.645 | 3823 | 3827 | 3830 | rBV  | 333    | 264    | 0.04%  | 0.004%  |
| 94  | 13.844 | 3880 | 3889 | 3898 | rVB4 | 4586   | 6970   | 0.94%  | 0.117%  |
| 95  | 14.086 | 3956 | 3964 | 3984 | rBV3 | 7130   | 12350  | 1.67%  | 0.207%  |
| 96  | 14.330 | 4031 | 4040 | 4052 | rBV5 | 5297   | 8380   | 1.13%  | 0.141%  |
| 97  | 14.394 | 4057 | 4060 | 4064 | rBV  | 255    | 179    | 0.02%  | 0.003%  |
| 98  | 14.799 | 4182 | 4186 | 4188 | rBV  | 367    | 288    | 0.04%  | 0.005%  |
| 99  | 14.918 | 4219 | 4223 | 4225 | rBV2 | 310    | 223    | 0.03%  | 0.004%  |
| 100 | 15.034 | 4256 | 4259 | 4260 | rBV  | 386    | 189    | 0.03%  | 0.003%  |

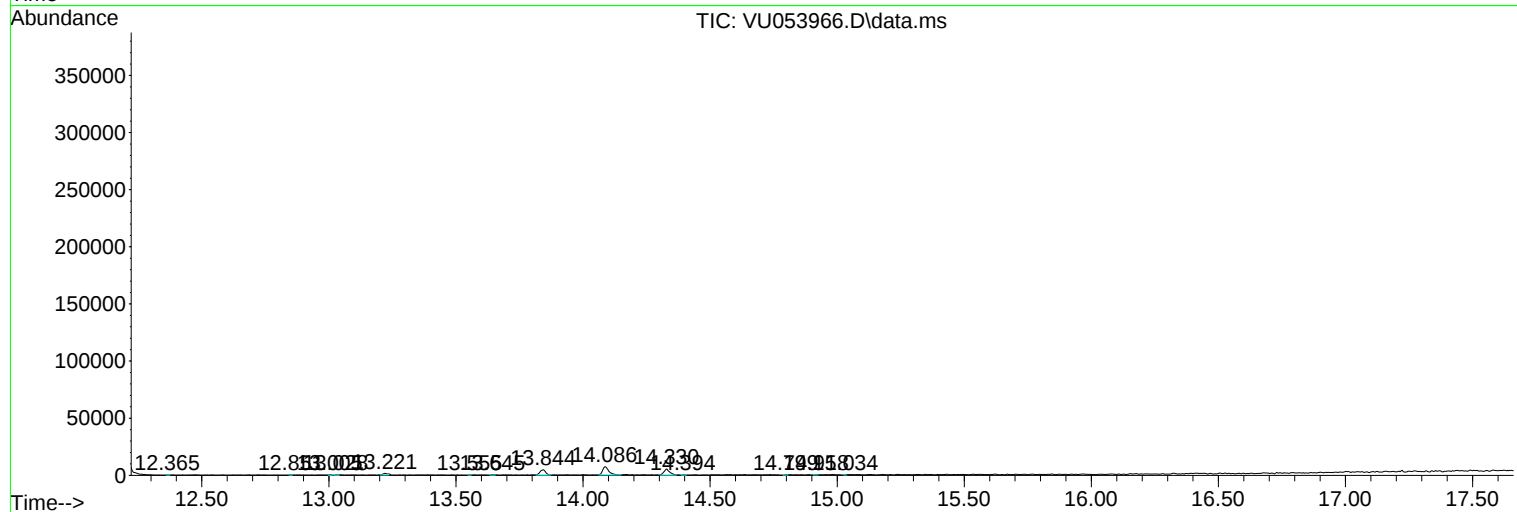
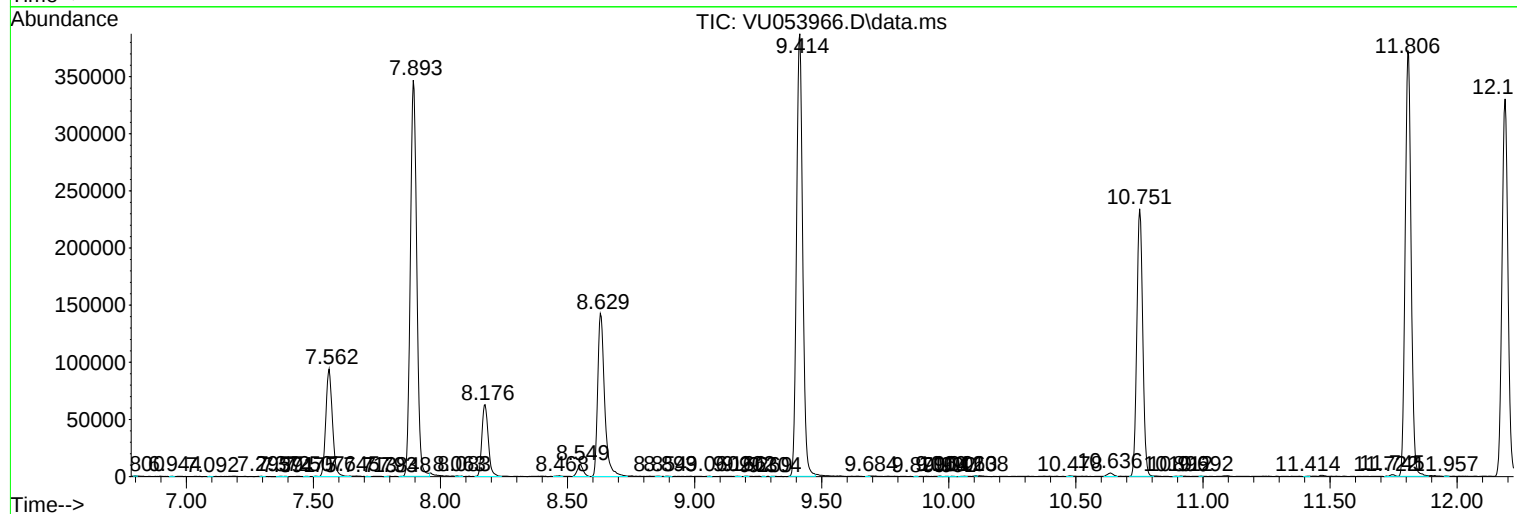
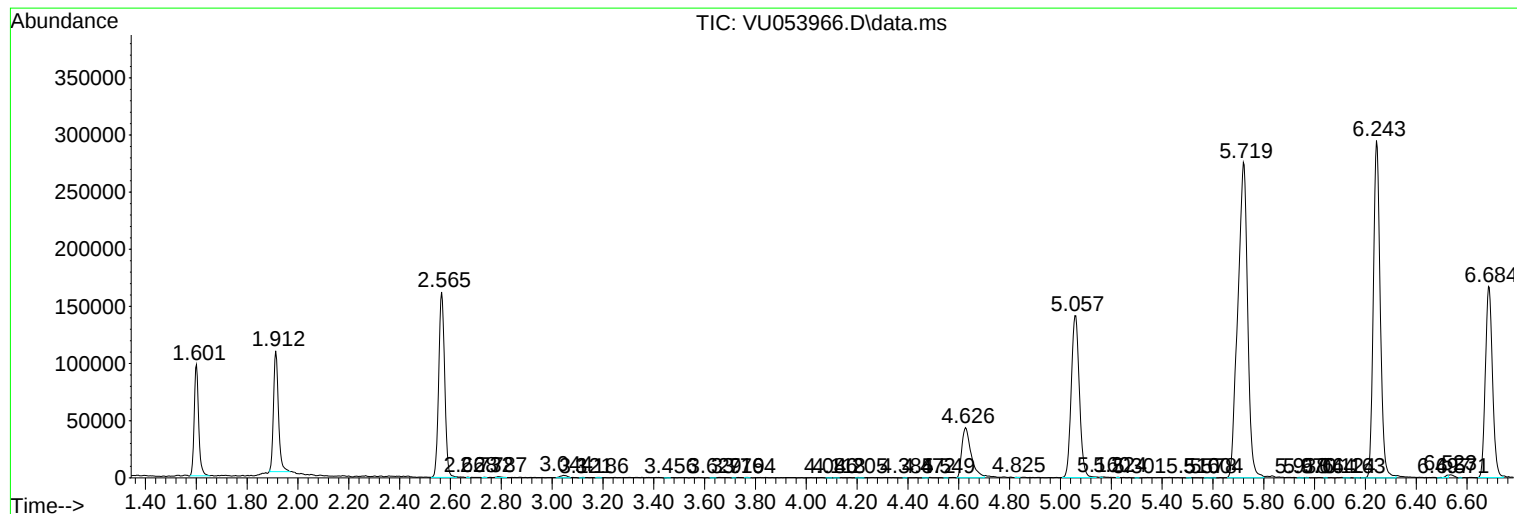
Sum of corrected areas: 5959616

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Instrument :  
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ClientSampleId :  
VBLK079

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU042923\  
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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 |