

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU071723\  
 Data File : VU054794.D  
 Acq On : 17 Jul 2023 15:40  
 Operator : MD/SY  
 Sample : VU0717MBL01  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK097

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\SFAMULM071723WMA.M  
 Title : VOC Analysis

Signal : TIC: VU054794.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         | 1.595       | 90            | 95          | 111          | rBV      | 101338         | 123239        | 16.03%          | 1.893%        |
| 2         | 2.554       | 383           | 393         | 412          | rVB      | 153449         | 248017        | 32.27%          | 3.809%        |
| 3         | 3.309       | 625           | 628         | 630          | rBV3     | 884            | 554           | 0.07%           | 0.009%        |
| 4         | 3.534       | 695           | 698         | 699          | rBV2     | 615            | 257           | 0.03%           | 0.004%        |
| 5         | 3.801       | 779           | 781         | 783          | rBV4     | 757            | 396           | 0.05%           | 0.006%        |
| 6         | 3.856       | 796           | 798         | 801          | rBV2     | 639            | 336           | 0.04%           | 0.005%        |
| 7         | 3.888       | 806           | 808         | 811          | rBV3     | 427            | 296           | 0.04%           | 0.005%        |
| 8         | 3.920       | 816           | 818         | 821          | rBV      | 518            | 201           | 0.03%           | 0.003%        |
| 9         | 4.068       | 862           | 864         | 872          | rVB6     | 795            | 841           | 0.11%           | 0.013%        |
| 10        | 4.103       | 872           | 875         | 877          | rBV4     | 732            | 455           | 0.06%           | 0.007%        |
| 11        | 4.119       | 877           | 880         | 883          | rBV4     | 708            | 580           | 0.08%           | 0.009%        |
| 12        | 4.229       | 911           | 914         | 917          | rBV2     | 479            | 289           | 0.04%           | 0.004%        |
| 13        | 4.283       | 929           | 931         | 933          | rBV2     | 569            | 253           | 0.03%           | 0.004%        |
| 14        | 4.441       | 977           | 980         | 981          | rBV2     | 451            | 290           | 0.04%           | 0.004%        |
| 15        | 4.476       | 987           | 991         | 993          | rBV2     | 637            | 550           | 0.07%           | 0.008%        |
| 16        | 4.505       | 998           | 1000        | 1002         | rBV2     | 629            | 338           | 0.04%           | 0.005%        |
| 17        | 4.618       | 1025          | 1035        | 1071         | rBV      | 80856          | 199271        | 25.92%          | 3.061%        |
| 18        | 5.055       | 1156          | 1171        | 1198         | rBV      | 141433         | 314779        | 40.95%          | 4.835%        |
| 19        | 5.341       | 1258          | 1260        | 1265         | rBV4     | 530            | 430           | 0.06%           | 0.007%        |
| 20        | 5.489       | 1304          | 1306        | 1308         | rBV3     | 633            | 410           | 0.05%           | 0.006%        |
| 21        | 5.576       | 1331          | 1333        | 1334         | rBV      | 427            | 197           | 0.03%           | 0.003%        |
| 22        | 5.717       | 1353          | 1377        | 1399         | rBV3     | 282130         | 768685        | 100.00%         | 11.807%       |
| 23        | 6.197       | 1521          | 1526        | 1527         | rBV3     | 848            | 740           | 0.10%           | 0.011%        |
| 24        | 6.245       | 1528          | 1541        | 1561         | rVV      | 280437         | 534443        | 69.53%          | 8.209%        |
| 25        | 6.476       | 1611          | 1613        | 1617         | rVB2     | 630            | 368           | 0.05%           | 0.006%        |
| 26        | 6.512       | 1621          | 1624        | 1625         | rBV3     | 978            | 487           | 0.06%           | 0.007%        |
| 27        | 6.685       | 1665          | 1678        | 1694         | rBV      | 177228         | 351445        | 45.72%          | 5.398%        |
| 28        | 6.852       | 1728          | 1730        | 1733         | rVB2     | 878            | 404           | 0.05%           | 0.006%        |
| 29        | 6.936       | 1751          | 1756        | 1760         | rBV4     | 653            | 724           | 0.09%           | 0.011%        |
| 30        | 6.959       | 1760          | 1763        | 1766         | rVB4     | 831            | 545           | 0.07%           | 0.008%        |
| 31        | 6.978       | 1766          | 1769        | 1770         | rBV2     | 344            | 202           | 0.03%           | 0.003%        |
| 32        | 7.090       | 1801          | 1804        | 1806         | rBV2     | 881            | 547           | 0.07%           | 0.008%        |
| 33        | 7.145       | 1817          | 1821        | 1822         | rBV2     | 671            | 443           | 0.06%           | 0.007%        |
| 34        | 7.322       | 1874          | 1876        | 1879         | rBV4     | 504            | 304           | 0.04%           | 0.005%        |
| 35        | 7.341       | 1879          | 1882        | 1889         | rVV4     | 719            | 912           | 0.12%           | 0.014%        |
| 36        | 7.386       | 1893          | 1896        | 1899         | rVB2     | 828            | 606           | 0.08%           | 0.009%        |

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 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK097

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\SFAMULM071723WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.470  | 1919 | 1922 | 1924 | rBV3 | 747    | 465    | 0.06%  | 0.007%  |
| 38 | 7.563  | 1938 | 1951 | 1971 | rBV2 | 108081 | 192678 | 25.07% | 2.959%  |
| 39 | 7.894  | 2042 | 2054 | 2071 | rBV  | 365317 | 629583 | 81.90% | 9.670%  |
| 40 | 8.135  | 2126 | 2129 | 2131 | rBV2 | 978    | 524    | 0.07%  | 0.008%  |
| 41 | 8.177  | 2131 | 2142 | 2157 | rBV  | 75483  | 128382 | 16.70% | 1.972%  |
| 42 | 8.383  | 2204 | 2206 | 2209 | rBV3 | 669    | 511    | 0.07%  | 0.008%  |
| 43 | 8.630  | 2272 | 2283 | 2318 | rBV  | 241589 | 450295 | 58.58% | 6.916%  |
| 44 | 8.913  | 2365 | 2371 | 2374 | rBV6 | 832    | 936    | 0.12%  | 0.014%  |
| 45 | 9.023  | 2400 | 2405 | 2409 | rBV4 | 1032   | 987    | 0.13%  | 0.015%  |
| 46 | 9.126  | 2433 | 2437 | 2438 | rBV2 | 468    | 353    | 0.05%  | 0.005%  |
| 47 | 9.193  | 2455 | 2458 | 2461 | rVB  | 925    | 590    | 0.08%  | 0.009%  |
| 48 | 9.212  | 2461 | 2464 | 2468 | rBV3 | 992    | 764    | 0.10%  | 0.012%  |
| 49 | 9.283  | 2482 | 2486 | 2489 | rBV4 | 851    | 702    | 0.09%  | 0.011%  |
| 50 | 9.322  | 2495 | 2498 | 2499 | rBV  | 560    | 301    | 0.04%  | 0.005%  |
| 51 | 9.415  | 2513 | 2527 | 2547 | rVV  | 407114 | 682548 | 88.79% | 10.484% |
| 52 | 9.692  | 2606 | 2613 | 2625 | rBV7 | 2562   | 4790   | 0.62%  | 0.074%  |
| 53 | 9.884  | 2670 | 2673 | 2676 | rVB3 | 1098   | 765    | 0.10%  | 0.012%  |
| 54 | 9.901  | 2676 | 2678 | 2679 | rBV2 | 527    | 231    | 0.03%  | 0.004%  |
| 55 | 9.952  | 2692 | 2694 | 2696 | rBV3 | 591    | 332    | 0.04%  | 0.005%  |
| 56 | 10.219 | 2775 | 2777 | 2779 | rBV3 | 466    | 316    | 0.04%  | 0.005%  |
| 57 | 10.261 | 2787 | 2790 | 2793 | rVB3 | 461    | 283    | 0.04%  | 0.004%  |
| 58 | 10.280 | 2793 | 2796 | 2799 | rBV3 | 622    | 557    | 0.07%  | 0.009%  |
| 59 | 10.418 | 2836 | 2839 | 2840 | rBV2 | 477    | 248    | 0.03%  | 0.004%  |
| 60 | 10.550 | 2876 | 2880 | 2886 | rBV3 | 491    | 558    | 0.07%  | 0.009%  |
| 61 | 10.605 | 2894 | 2897 | 2900 | rBV3 | 670    | 508    | 0.07%  | 0.008%  |
| 62 | 10.753 | 2931 | 2943 | 2959 | rBV  | 304082 | 492229 | 64.04% | 7.561%  |
| 63 | 10.962 | 3005 | 3008 | 3010 | rBV3 | 527    | 293    | 0.04%  | 0.005%  |
| 64 | 10.984 | 3011 | 3015 | 3020 | rBV6 | 640    | 797    | 0.10%  | 0.012%  |
| 65 | 11.023 | 3025 | 3027 | 3030 | rVB2 | 517    | 320    | 0.04%  | 0.005%  |
| 66 | 11.045 | 3030 | 3034 | 3036 | rBV2 | 518    | 430    | 0.06%  | 0.007%  |
| 67 | 11.138 | 3061 | 3063 | 3067 | rVB4 | 981    | 752    | 0.10%  | 0.012%  |
| 68 | 11.167 | 3069 | 3072 | 3074 | rBV3 | 426    | 318    | 0.04%  | 0.005%  |
| 69 | 11.328 | 3121 | 3122 | 3126 | rVB2 | 628    | 351    | 0.05%  | 0.005%  |
| 70 | 11.357 | 3128 | 3131 | 3137 | rBV4 | 959    | 1059   | 0.14%  | 0.016%  |
| 71 | 11.396 | 3140 | 3143 | 3145 | rVB3 | 485    | 193    | 0.03%  | 0.003%  |
| 72 | 11.405 | 3145 | 3146 | 3148 | rBV3 | 434    | 235    | 0.03%  | 0.004%  |
| 73 | 11.466 | 3161 | 3163 | 3166 | rBV  | 2249   | 1219   | 0.16%  | 0.019%  |
| 74 | 11.621 | 3211 | 3213 | 3215 | rVB2 | 619    | 260    | 0.03%  | 0.004%  |
| 75 | 11.646 | 3219 | 3221 | 3226 | rVB3 | 882    | 529    | 0.07%  | 0.008%  |
| 76 | 11.669 | 3226 | 3228 | 3230 | rBV2 | 547    | 300    | 0.04%  | 0.005%  |

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 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK097

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\SFAMULM071723WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.746 | 3247 | 3252 | 3257 | rBV6 | 2479   | 2593   | 0.34%  | 0.040%  |
| 78  | 11.810 | 3260 | 3272 | 3292 | rVV  | 443785 | 713609 | 92.84% | 10.961% |
| 79  | 12.010 | 3333 | 3334 | 3340 | rBV4 | 780    | 539    | 0.07%  | 0.008%  |
| 80  | 12.074 | 3351 | 3354 | 3358 | rVB5 | 753    | 652    | 0.08%  | 0.010%  |
|     |        |      |      |      |      |        |        |        |         |
| 81  | 12.106 | 3358 | 3364 | 3367 | rBV5 | 868    | 883    | 0.11%  | 0.014%  |
| 82  | 12.135 | 3371 | 3373 | 3377 | rVB4 | 923    | 563    | 0.07%  | 0.009%  |
| 83  | 12.190 | 3377 | 3390 | 3408 | rBV  | 381243 | 616650 | 80.22% | 9.472%  |
| 84  | 12.601 | 3515 | 3518 | 3523 | rVB4 | 1088   | 810    | 0.11%  | 0.012%  |
| 85  | 12.662 | 3533 | 3537 | 3538 | rBV3 | 716    | 471    | 0.06%  | 0.007%  |
|     |        |      |      |      |      |        |        |        |         |
| 86  | 12.962 | 3627 | 3630 | 3632 | rBV4 | 383    | 269    | 0.03%  | 0.004%  |
| 87  | 12.971 | 3632 | 3633 | 3635 | rBV2 | 523    | 233    | 0.03%  | 0.004%  |
| 88  | 13.023 | 3647 | 3649 | 3653 | rBV4 | 697    | 426    | 0.06%  | 0.007%  |
| 89  | 13.164 | 3690 | 3693 | 3694 | rBV2 | 689    | 275    | 0.04%  | 0.004%  |
| 90  | 13.421 | 3770 | 3773 | 3776 | rBV  | 586    | 427    | 0.06%  | 0.007%  |
|     |        |      |      |      |      |        |        |        |         |
| 91  | 13.563 | 3814 | 3817 | 3819 | rBV2 | 872    | 646    | 0.08%  | 0.010%  |
| 92  | 13.714 | 3862 | 3864 | 3865 | rBV2 | 545    | 247    | 0.03%  | 0.004%  |
| 93  | 13.846 | 3898 | 3905 | 3915 | rVB8 | 4771   | 7884   | 1.03%  | 0.121%  |
| 94  | 14.026 | 3959 | 3961 | 3964 | rBV2 | 689    | 477    | 0.06%  | 0.007%  |
| 95  | 14.158 | 3998 | 4002 | 4011 | rBV5 | 1333   | 1838   | 0.24%  | 0.028%  |
|     |        |      |      |      |      |        |        |        |         |
| 96  | 14.209 | 4016 | 4018 | 4020 | rBV  | 462    | 224    | 0.03%  | 0.003%  |
| 97  | 14.328 | 4046 | 4055 | 4068 | rBV8 | 5166   | 8955   | 1.16%  | 0.138%  |
| 98  | 14.492 | 4103 | 4106 | 4109 | rBV3 | 760    | 528    | 0.07%  | 0.008%  |
| 99  | 14.675 | 4160 | 4163 | 4165 | rBV2 | 817    | 443    | 0.06%  | 0.007%  |
| 100 | 14.691 | 4165 | 4168 | 4171 | rBV3 | 711    | 551    | 0.07%  | 0.008%  |

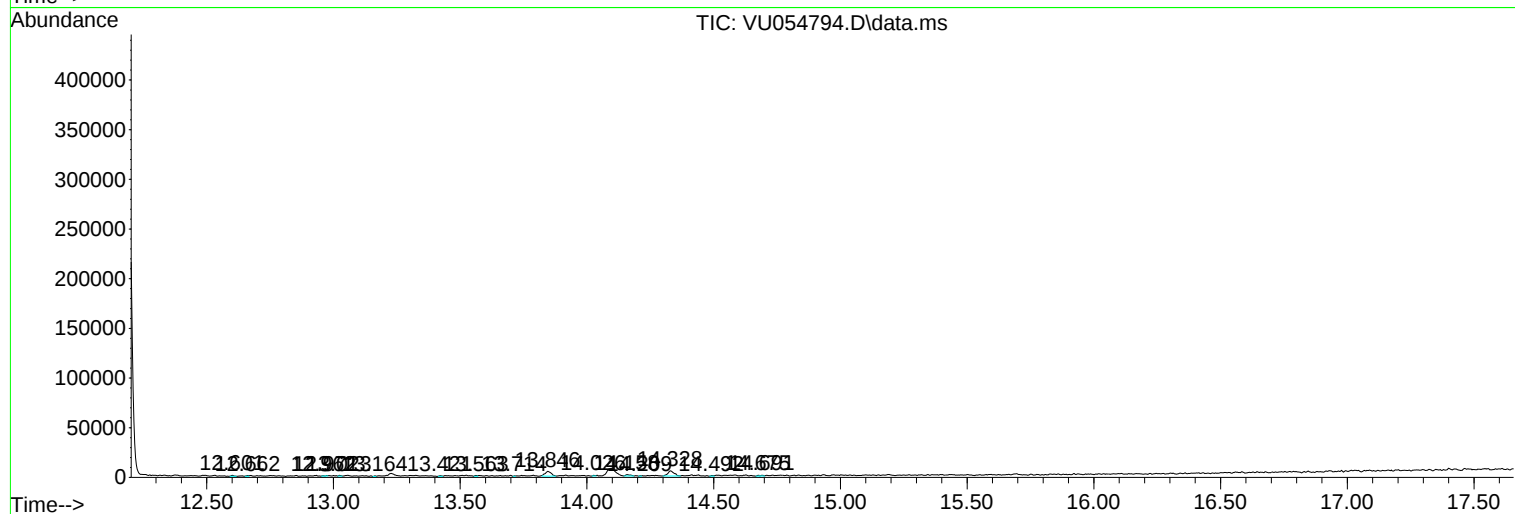
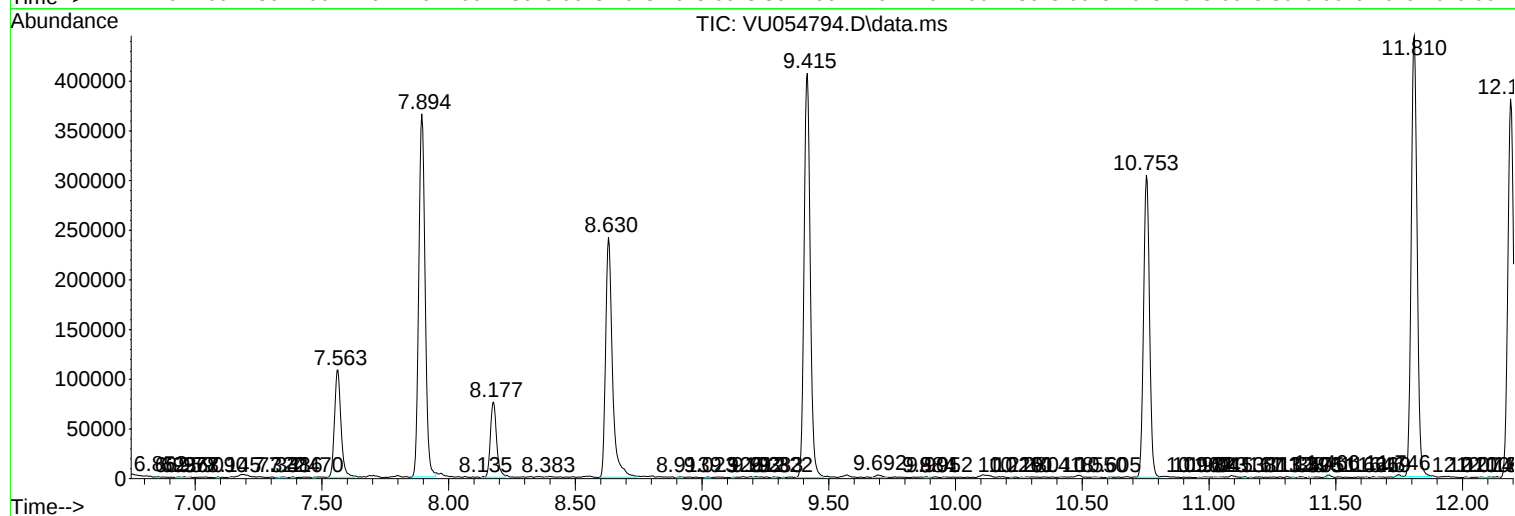
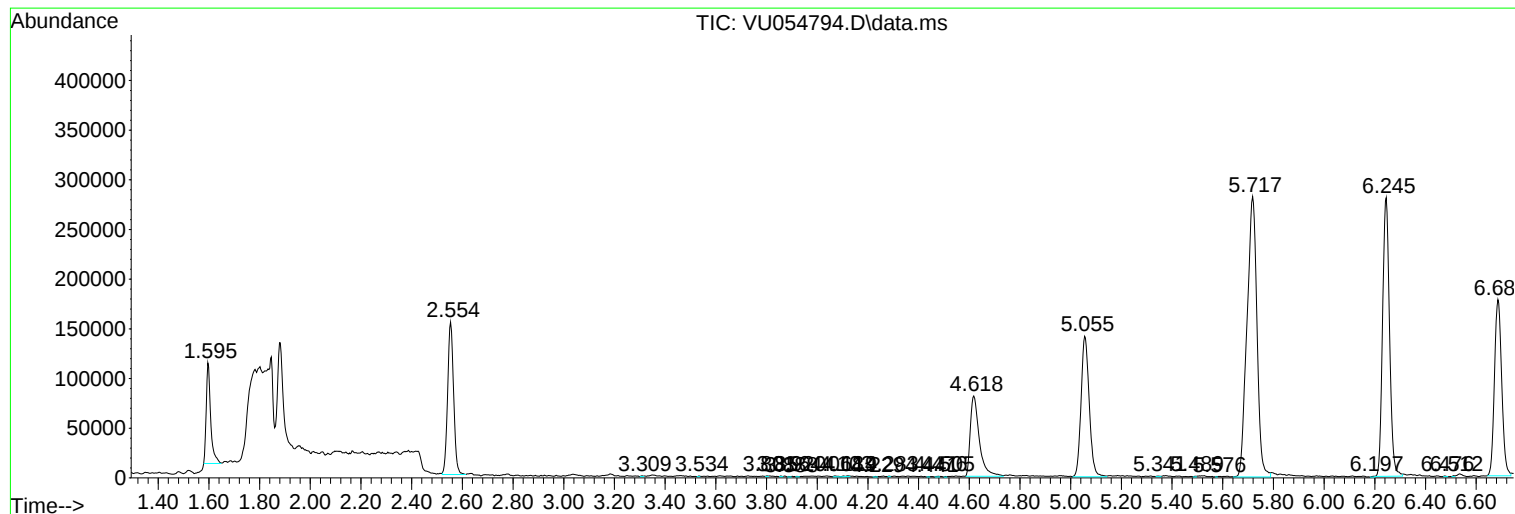
Sum of corrected areas: 6510519

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU071723\  
Data File : VU054794.D  
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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK097

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM071723WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU071723\  
Data File : VU054794.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM071723WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM071723WMA.M  
Quant Title : VOC Analysis

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

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