

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
 Data File : VU055905.D  
 Acq On : 26 Oct 2023 15:12  
 Operator : MD/SY  
 Sample : 04961-12MERE  
 Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E0LJ6MERE

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

Signal : TIC: VU055905.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         | 1.483       | 50            | 60          | 66           | rBV3     | 21861          | 44125         | 2.59%           | 0.302%        |
| 2         | 1.599       | 89            | 96          | 128          | rVB2     | 221535         | 343544        | 20.17%          | 2.353%        |
| 3         | 2.493       | 372           | 374         | 377          | rBV2     | 1017           | 558           | 0.03%           | 0.004%        |
| 4         | 2.541       | 377           | 389         | 410          | rBV      | 169646         | 302474        | 17.75%          | 2.071%        |
| 5         | 2.740       | 446           | 451         | 452          | rBV3     | 854            | 786           | 0.05%           | 0.005%        |
| 6         | 2.766       | 455           | 459         | 468          | rVB3     | 2340           | 3880          | 0.23%           | 0.027%        |
| 7         | 2.908       | 500           | 503         | 506          | rBV3     | 564            | 423           | 0.02%           | 0.003%        |
| 8         | 3.030       | 532           | 541         | 555          | rVV7     | 9132           | 25292         | 1.48%           | 0.173%        |
| 9         | 3.110       | 558           | 566         | 574          | rVV2     | 10405          | 20938         | 1.23%           | 0.143%        |
| 10        | 3.175       | 576           | 586         | 607          | rVB2     | 28501          | 67106         | 3.94%           | 0.460%        |
| 11        | 3.332       | 630           | 635         | 655          | rVB8     | 4161           | 9414          | 0.55%           | 0.064%        |
| 12        | 3.676       | 732           | 742         | 747          | rBV4     | 1987           | 3910          | 0.23%           | 0.027%        |
| 13        | 3.779       | 772           | 774         | 779          | rVB3     | 656            | 413           | 0.02%           | 0.003%        |
| 14        | 3.811       | 779           | 784         | 788          | rVB3     | 507            | 516           | 0.03%           | 0.004%        |
| 15        | 3.962       | 827           | 831         | 837          | rBV3     | 613            | 659           | 0.04%           | 0.005%        |
| 16        | 4.056       | 855           | 860         | 866          | rVB3     | 489            | 571           | 0.03%           | 0.004%        |
| 17        | 4.101       | 866           | 874         | 878          | rBV2     | 377            | 484           | 0.03%           | 0.003%        |
| 18        | 4.268       | 920           | 926         | 928          | rBV      | 462            | 479           | 0.03%           | 0.003%        |
| 19        | 4.512       | 987           | 1002        | 1003         | rBV6     | 2575           | 3553          | 0.21%           | 0.024%        |
| 20        | 4.628       | 1026          | 1038        | 1083         | rBV      | 136691         | 487950        | 28.64%          | 3.342%        |
| 21        | 5.056       | 1155          | 1171        | 1196         | rBV2     | 267345         | 642244        | 37.70%          | 4.398%        |
| 22        | 5.284       | 1238          | 1242        | 1243         | rBV2     | 885            | 515           | 0.03%           | 0.004%        |
| 23        | 5.329       | 1247          | 1256        | 1257         | rBV6     | 5430           | 5952          | 0.35%           | 0.041%        |
| 24        | 5.451       | 1284          | 1294        | 1304         | rVB7     | 3575           | 7262          | 0.43%           | 0.050%        |
| 25        | 5.583       | 1328          | 1335        | 1338         | rBV6     | 1387           | 1682          | 0.10%           | 0.012%        |
| 26        | 5.715       | 1356          | 1376        | 1410         | rBV2     | 526401         | 1440422       | 84.55%          | 9.864%        |
| 27        | 5.975       | 1446          | 1457        | 1467         | rBV6     | 5213           | 11580         | 0.68%           | 0.079%        |
| 28        | 6.049       | 1478          | 1480        | 1485         | rVB2     | 685            | 464           | 0.03%           | 0.003%        |
| 29        | 6.126       | 1501          | 1504        | 1508         | rVB3     | 689            | 390           | 0.02%           | 0.003%        |
| 30        | 6.242       | 1527          | 1540        | 1574         | rBV      | 620987         | 1258402       | 73.87%          | 8.618%        |
| 31        | 6.525       | 1614          | 1628        | 1641         | rBV10    | 6909           | 15627         | 0.92%           | 0.107%        |
| 32        | 6.599       | 1641          | 1651        | 1660         | rVV5     | 6461           | 13841         | 0.81%           | 0.095%        |
| 33        | 6.686       | 1664          | 1678        | 1710         | rVB      | 345398         | 723806        | 42.49%          | 4.957%        |
| 34        | 6.859       | 1728          | 1732        | 1735         | rVB4     | 733            | 591           | 0.03%           | 0.004%        |
| 35        | 6.985       | 1765          | 1771        | 1773         | rBV2     | 666            | 534           | 0.03%           | 0.004%        |
| 36        | 7.017       | 1777          | 1781        | 1785         | rVB3     | 691            | 495           | 0.03%           | 0.003%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
 Data File : VU055905.D  
 Acq On : 26 Oct 2023 15:12  
 Operator : MD/SY  
 Sample : 04961-12MERE  
 Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E0LJ6MERE

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 7.072  | 1790 | 1798 | 1800 | rBV5 | 747    | 908     | 0.05%  | 0.006%  |
| 38 | 7.194  | 1827 | 1836 | 1840 | rBV5 | 6141   | 10383   | 0.61%  | 0.071%  |
| 39 | 7.290  | 1864 | 1866 | 1869 | rVB3 | 751    | 414     | 0.02%  | 0.003%  |
| 40 | 7.309  | 1869 | 1872 | 1875 | rBV3 | 788    | 636     | 0.04%  | 0.004%  |
| 41 | 7.335  | 1877 | 1880 | 1884 | rVB4 | 811    | 650     | 0.04%  | 0.004%  |
| 42 | 7.383  | 1893 | 1895 | 1903 | rVB4 | 1126   | 1223    | 0.07%  | 0.008%  |
| 43 | 7.483  | 1921 | 1926 | 1928 | rBV  | 503    | 468     | 0.03%  | 0.003%  |
| 44 | 7.499  | 1928 | 1931 | 1936 | rVB4 | 814    | 779     | 0.05%  | 0.005%  |
| 45 | 7.563  | 1939 | 1951 | 1976 | rBV  | 174275 | 353063  | 20.72% | 2.418%  |
| 46 | 7.660  | 1979 | 1981 | 1985 | rVB3 | 740    | 396     | 0.02%  | 0.003%  |
| 47 | 7.789  | 2010 | 2021 | 2030 | rBV5 | 8213   | 14770   | 0.87%  | 0.101%  |
| 48 | 7.843  | 2035 | 2038 | 2040 | rBV4 | 883    | 508     | 0.03%  | 0.003%  |
| 49 | 7.895  | 2040 | 2054 | 2074 | rBV  | 523456 | 965961  | 56.70% | 6.615%  |
| 50 | 8.123  | 2123 | 2125 | 2130 | rVB4 | 653    | 505     | 0.03%  | 0.003%  |
| 51 | 8.181  | 2131 | 2143 | 2167 | rBV2 | 115210 | 250382  | 14.70% | 1.715%  |
| 52 | 8.325  | 2186 | 2188 | 2191 | rBV3 | 544    | 395     | 0.02%  | 0.003%  |
| 53 | 8.354  | 2191 | 2197 | 2199 | rBV5 | 1400   | 1506    | 0.09%  | 0.010%  |
| 54 | 8.406  | 2210 | 2213 | 2217 | rVB3 | 721    | 539     | 0.03%  | 0.004%  |
| 55 | 8.473  | 2228 | 2234 | 2239 | rBV3 | 1362   | 1684    | 0.10%  | 0.012%  |
| 56 | 8.554  | 2245 | 2259 | 2268 | rBV9 | 9360   | 18110   | 1.06%  | 0.124%  |
| 57 | 8.650  | 2275 | 2289 | 2330 | rBV  | 601921 | 1250563 | 73.41% | 8.564%  |
| 58 | 8.927  | 2371 | 2375 | 2376 | rBV3 | 1459   | 859     | 0.05%  | 0.006%  |
| 59 | 8.997  | 2395 | 2397 | 2401 | rVB3 | 963    | 454     | 0.03%  | 0.003%  |
| 60 | 9.168  | 2446 | 2450 | 2453 | rBV3 | 590    | 556     | 0.03%  | 0.004%  |
| 61 | 9.203  | 2454 | 2461 | 2470 | rVB9 | 2185   | 3784    | 0.22%  | 0.026%  |
| 62 | 9.332  | 2495 | 2501 | 2502 | rBV2 | 1107   | 853     | 0.05%  | 0.006%  |
| 63 | 9.419  | 2514 | 2528 | 2553 | rBV  | 861246 | 1661458 | 97.53% | 11.378% |
| 64 | 9.567  | 2571 | 2574 | 2576 | rBV3 | 1701   | 1199    | 0.07%  | 0.008%  |
| 65 | 9.608  | 2584 | 2587 | 2593 | rVB5 | 927    | 808     | 0.05%  | 0.006%  |
| 66 | 9.702  | 2608 | 2616 | 2622 | rVV6 | 4027   | 6644    | 0.39%  | 0.045%  |
| 67 | 9.743  | 2624 | 2629 | 2644 | rVB7 | 3920   | 5635    | 0.33%  | 0.039%  |
| 68 | 9.891  | 2672 | 2675 | 2677 | rBV2 | 662    | 388     | 0.02%  | 0.003%  |
| 69 | 10.059 | 2724 | 2727 | 2732 | rBV3 | 503    | 460     | 0.03%  | 0.003%  |
| 70 | 10.113 | 2736 | 2744 | 2745 | rBV3 | 1435   | 1385    | 0.08%  | 0.009%  |
| 71 | 10.194 | 2766 | 2769 | 2776 | rBV  | 714    | 797     | 0.05%  | 0.005%  |
| 72 | 10.329 | 2806 | 2811 | 2812 | rBV  | 840    | 632     | 0.04%  | 0.004%  |
| 73 | 10.390 | 2823 | 2830 | 2831 | rBV3 | 1836   | 1737    | 0.10%  | 0.012%  |
| 74 | 10.493 | 2858 | 2862 | 2870 | rVB5 | 1361   | 1778    | 0.10%  | 0.012%  |
| 75 | 10.621 | 2898 | 2902 | 2904 | rBV3 | 1232   | 1104    | 0.06%  | 0.008%  |
| 76 | 10.759 | 2932 | 2945 | 2974 | rVV  | 745855 | 1224933 | 71.90% | 8.388%  |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
 Data File : VU055905.D  
 Acq On : 26 Oct 2023 15:12  
 Operator : MD/SY  
 Sample : 04961-12MERE  
 Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E0LJ6MERE

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\SFAMULM101023WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |       |         |         |         |         |
|-----|--------|------|------|------|-------|---------|---------|---------|---------|
| 77  | 11.052 | 3031 | 3036 | 3044 | rVB9  | 1277    | 1831    | 0.11%   | 0.013%  |
| 78  | 11.113 | 3044 | 3055 | 3068 | rVB7  | 9207    | 17039   | 1.00%   | 0.117%  |
| 79  | 11.168 | 3068 | 3072 | 3074 | rBV3  | 456     | 386     | 0.02%   | 0.003%  |
| 80  | 11.200 | 3077 | 3082 | 3083 | rBV4  | 954     | 944     | 0.06%   | 0.006%  |
| 81  | 11.239 | 3090 | 3094 | 3096 | rBV3  | 753     | 527     | 0.03%   | 0.004%  |
| 82  | 11.313 | 3109 | 3117 | 3127 | rBV8  | 2302    | 3926    | 0.23%   | 0.027%  |
| 83  | 11.374 | 3130 | 3136 | 3141 | rVV5  | 2280    | 3111    | 0.18%   | 0.021%  |
| 84  | 11.415 | 3141 | 3149 | 3156 | rVB6  | 7102    | 11052   | 0.65%   | 0.076%  |
| 85  | 11.624 | 3212 | 3214 | 3216 | rBV3  | 1140    | 690     | 0.04%   | 0.005%  |
| 86  | 11.705 | 3236 | 3239 | 3241 | rBV3  | 941     | 728     | 0.04%   | 0.005%  |
| 87  | 11.811 | 3260 | 3272 | 3300 | rBV   | 1046533 | 1703606 | 100.00% | 11.666% |
| 88  | 12.046 | 3343 | 3345 | 3348 | rVB2  | 873     | 466     | 0.03%   | 0.003%  |
| 89  | 12.094 | 3354 | 3360 | 3368 | rBV8  | 4203    | 5863    | 0.34%   | 0.040%  |
| 90  | 12.193 | 3378 | 3391 | 3408 | rBV   | 827777  | 1359560 | 79.80%  | 9.310%  |
| 91  | 12.329 | 3422 | 3433 | 3443 | rBV4  | 20699   | 33962   | 1.99%   | 0.233%  |
| 92  | 12.464 | 3473 | 3475 | 3477 | rBV3  | 971     | 593     | 0.03%   | 0.004%  |
| 93  | 12.663 | 3530 | 3537 | 3551 | rVB10 | 6269    | 10745   | 0.63%   | 0.074%  |
| 94  | 12.949 | 3606 | 3626 | 3632 | rBV10 | 7125    | 21818   | 1.28%   | 0.149%  |
| 95  | 13.049 | 3652 | 3657 | 3665 | rVB6  | 4884    | 6068    | 0.36%   | 0.042%  |
| 96  | 13.129 | 3676 | 3682 | 3690 | rBV9  | 4167    | 6969    | 0.41%   | 0.048%  |
| 97  | 13.428 | 3767 | 3775 | 3798 | rVB2  | 40953   | 70894   | 4.16%   | 0.485%  |
| 98  | 13.583 | 3813 | 3823 | 3832 | rBV3  | 23169   | 37980   | 2.23%   | 0.260%  |
| 99  | 14.447 | 4084 | 4092 | 4100 | rBV2  | 44438   | 62762   | 3.68%   | 0.430%  |
| 100 | 15.206 | 4323 | 4328 | 4336 | rVB4  | 9123    | 10991   | 0.65%   | 0.075%  |

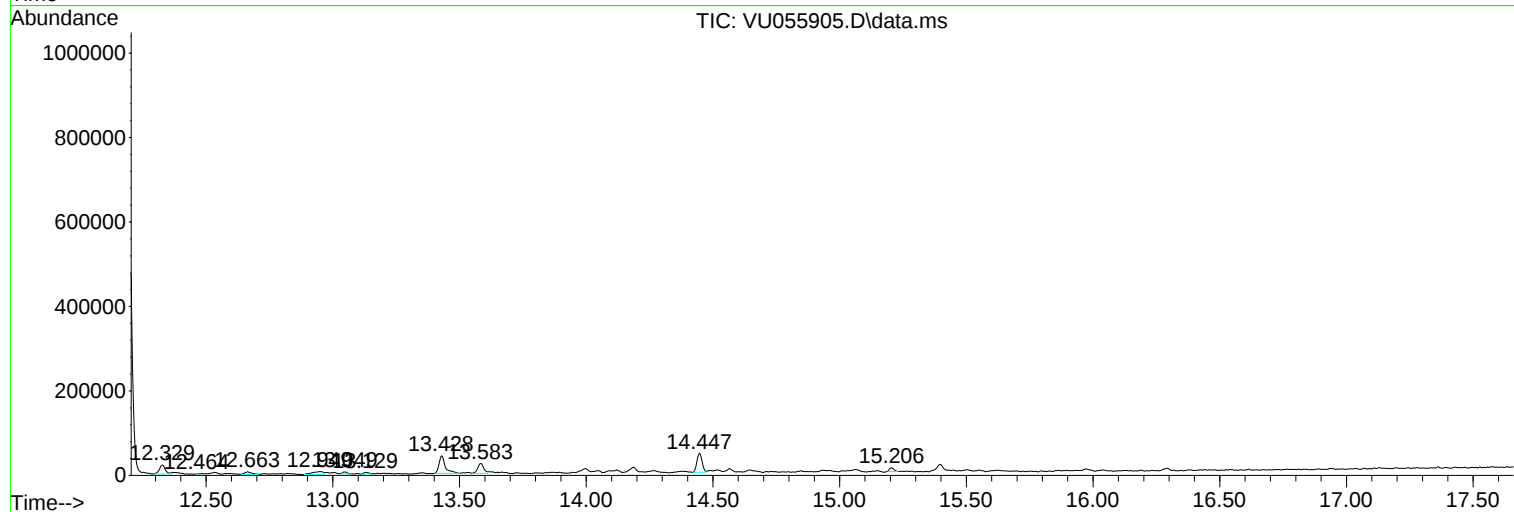
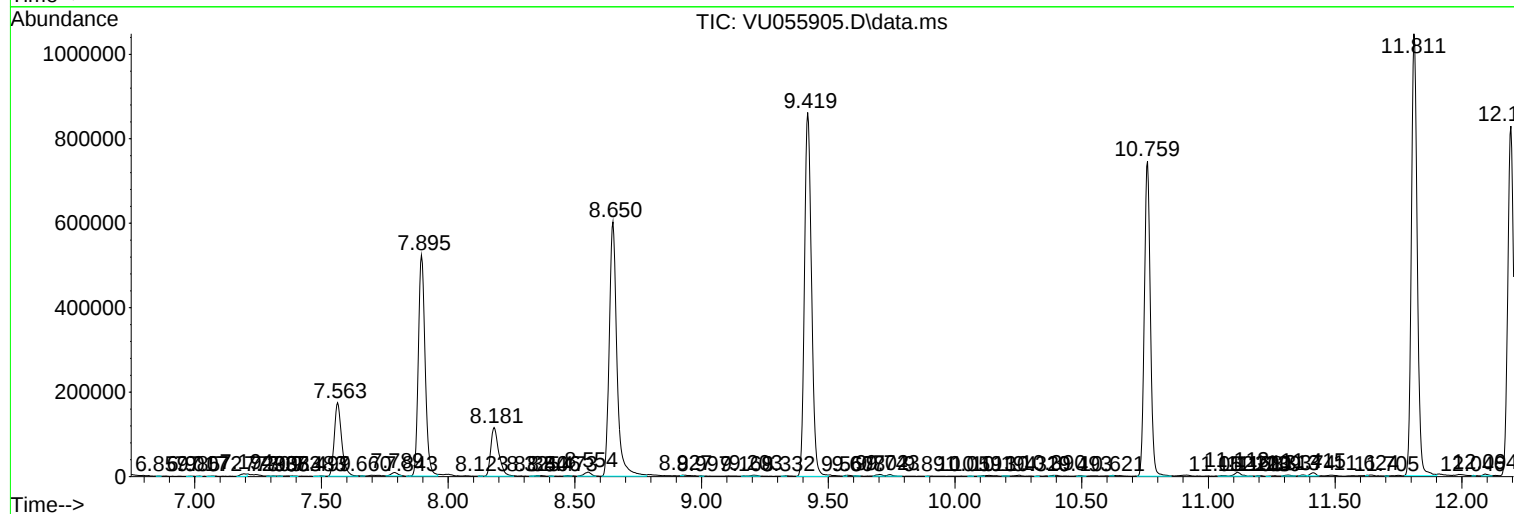
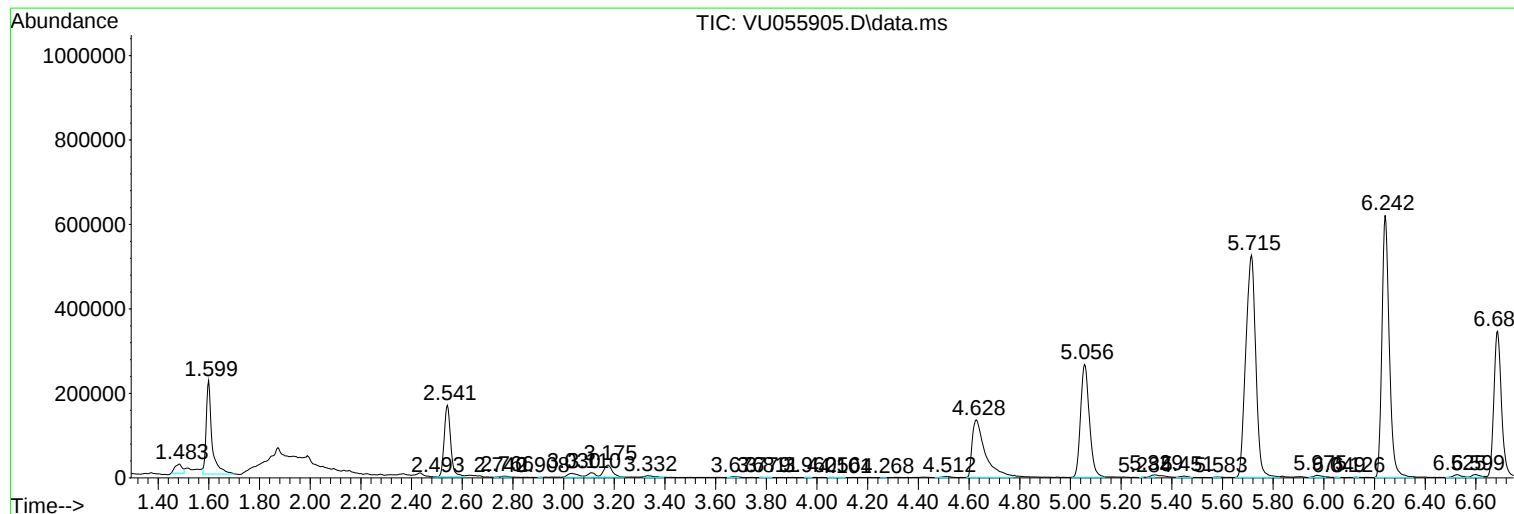
Sum of corrected areas: 14602700

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
Data File : VU055905.D  
Acq On : 26 Oct 2023 15:12  
Operator : MD/SY  
Sample : 04961-12MERE  
Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EOLJ6MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
Data File : VU055905.D  
Acq On : 26 Oct 2023 15:12  
Operator : MD/SY  
Sample : 04961-12MERE  
Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
E0LJ6MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU102623\  
Data File : VU055905.D  
Acq On : 26 Oct 2023 15:12  
Operator : MD/SY  
Sample : 04961-12MERE  
Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
E0LJ6MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM101023WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|