

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012723\  
 Data File : VU052855.D  
 Acq On : 27 Jan 2023 18:29  
 Operator : JC/MD  
 Sample : 01314-15  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44P0

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\SFAMULM012623WMA.M  
 Title : VOC Analysis

Signal : TIC: VU052855.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         | 1.597       | 73            | 80          | 93           | rBV      | 98529          | 117939        | 6.85%           | 1.315%        |
| 2         | 1.909       | 169           | 177         | 200          | rVB      | 102308         | 145221        | 8.44%           | 1.620%        |
| 3         | 2.565       | 368           | 381         | 396          | rBV      | 217164         | 354236        | 20.58%          | 3.951%        |
| 4         | 3.173       | 565           | 570         | 572          | rBV2     | 475            | 466           | 0.03%           | 0.005%        |
| 5         | 3.655       | 711           | 720         | 722          | rBV2     | 382            | 593           | 0.03%           | 0.007%        |
| 6         | 3.890       | 788           | 793         | 795          | rBV2     | 253            | 233           | 0.01%           | 0.003%        |
| 7         | 3.922       | 801           | 803         | 806          | rBV      | 225            | 166           | 0.01%           | 0.002%        |
| 8         | 4.089       | 851           | 855         | 859          | rBV2     | 214            | 262           | 0.02%           | 0.003%        |
| 9         | 4.211       | 890           | 893         | 897          | rBV2     | 243            | 222           | 0.01%           | 0.002%        |
| 10        | 4.388       | 943           | 948         | 951          | rBV2     | 232            | 276           | 0.02%           | 0.003%        |
| 11        | 4.420       | 954           | 958         | 961          | rBV      | 270            | 252           | 0.01%           | 0.003%        |
| 12        | 4.623       | 1009          | 1021        | 1056         | rBV      | 74473          | 224022        | 13.01%          | 2.498%        |
| 13        | 5.057       | 1141          | 1156        | 1175         | rBV      | 194174         | 422855        | 24.56%          | 4.716%        |
| 14        | 5.202       | 1198          | 1201        | 1204         | rVB2     | 297            | 172           | 0.01%           | 0.002%        |
| 15        | 5.234       | 1204          | 1211        | 1214         | rVB      | 248            | 271           | 0.02%           | 0.003%        |
| 16        | 5.276       | 1215          | 1224        | 1225         | rBV2     | 558            | 556           | 0.03%           | 0.006%        |
| 17        | 5.301       | 1225          | 1232        | 1235         | rBV5     | 1861           | 2386          | 0.14%           | 0.027%        |
| 18        | 5.369       | 1249          | 1253        | 1260         | rBV2     | 654            | 774           | 0.04%           | 0.009%        |
| 19        | 5.719       | 1338          | 1362        | 1389         | rBV2     | 373293         | 1023441       | 59.45%          | 11.414%       |
| 20        | 5.989       | 1440          | 1446        | 1449         | rBV      | 412            | 412           | 0.02%           | 0.005%        |
| 21        | 6.243       | 1504          | 1525        | 1544         | rBV      | 328234         | 611072        | 35.49%          | 6.815%        |
| 22        | 6.459       | 1589          | 1592        | 1596         | rBV2     | 233            | 234           | 0.01%           | 0.003%        |
| 23        | 6.536       | 1602          | 1616        | 1648         | rBV      | 913994         | 1721607       | 100.00%         | 19.200%       |
| 24        | 6.687       | 1649          | 1663        | 1684         | rVB      | 234923         | 458176        | 26.61%          | 5.110%        |
| 25        | 6.854       | 1710          | 1715        | 1718         | rBV      | 273            | 238           | 0.01%           | 0.003%        |
| 26        | 6.883       | 1722          | 1724        | 1728         | rBV2     | 310            | 167           | 0.01%           | 0.002%        |
| 27        | 7.134       | 1800          | 1802        | 1807         | rBV2     | 369            | 307           | 0.02%           | 0.003%        |
| 28        | 7.189       | 1809          | 1819        | 1829         | rVB4     | 1536           | 2784          | 0.16%           | 0.031%        |
| 29        | 7.298       | 1847          | 1853        | 1855         | rBV2     | 300            | 319           | 0.02%           | 0.004%        |
| 30        | 7.314       | 1855          | 1858        | 1861         | rVV2     | 268            | 185           | 0.01%           | 0.002%        |
| 31        | 7.333       | 1861          | 1864        | 1868         | rVB2     | 282            | 242           | 0.01%           | 0.003%        |
| 32        | 7.404       | 1884          | 1886        | 1888         | rBV      | 313            | 200           | 0.01%           | 0.002%        |
| 33        | 7.562       | 1923          | 1935        | 1957         | rVB      | 107130         | 185259        | 10.76%          | 2.066%        |
| 34        | 7.694       | 1966          | 1976        | 1977         | rBV4     | 682            | 746           | 0.04%           | 0.008%        |
| 35        | 7.735       | 1987          | 1989        | 1991         | rBV2     | 273            | 198           | 0.01%           | 0.002%        |
| 36        | 7.803       | 2007          | 2010        | 2013         | rVB      | 345            | 244           | 0.01%           | 0.003%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012723\  
 Data File : VU052855.D  
 Acq On : 27 Jan 2023 18:29  
 Operator : JC/MD  
 Sample : 01314-15  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44P0

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\SFAMULM012623WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 7.825  | 2014 | 2017 | 2019 | rBB  | 307    | 165    | 0.01%  | 0.002% |
| 38 | 7.893  | 2024 | 2038 | 2058 | rBV  | 401044 | 688907 | 40.02% | 7.683% |
| 39 | 8.060  | 2088 | 2090 | 2094 | rVB  | 415    | 246    | 0.01%  | 0.003% |
| 40 | 8.086  | 2095 | 2098 | 2101 | rBV  | 434    | 315    | 0.02%  | 0.004% |
| 41 | 8.128  | 2110 | 2111 | 2114 | rBV  | 387    | 274    | 0.02%  | 0.003% |
| 42 | 8.176  | 2114 | 2126 | 2142 | rVV  | 75879  | 128046 | 7.44%  | 1.428% |
| 43 | 8.243  | 2142 | 2147 | 2151 | rVB3 | 547    | 632    | 0.04%  | 0.007% |
| 44 | 8.279  | 2156 | 2158 | 2159 | rBV3 | 350    | 164    | 0.01%  | 0.002% |
| 45 | 8.311  | 2164 | 2168 | 2171 | rBV2 | 464    | 409    | 0.02%  | 0.005% |
| 46 | 8.372  | 2183 | 2187 | 2193 | rBV2 | 421    | 441    | 0.03%  | 0.005% |
| 47 | 8.456  | 2210 | 2213 | 2214 | rBV  | 725    | 395    | 0.02%  | 0.004% |
| 48 | 8.497  | 2224 | 2226 | 2228 | rBV2 | 271    | 173    | 0.01%  | 0.002% |
| 49 | 8.549  | 2238 | 2242 | 2249 | rVB5 | 783    | 728    | 0.04%  | 0.008% |
| 50 | 8.632  | 2255 | 2268 | 2297 | rBV3 | 186238 | 361332 | 20.99% | 4.030% |
| 51 | 8.915  | 2351 | 2356 | 2357 | rBV3 | 279    | 220    | 0.01%  | 0.002% |
| 52 | 9.021  | 2386 | 2389 | 2393 | rBV2 | 231    | 169    | 0.01%  | 0.002% |
| 53 | 9.124  | 2416 | 2421 | 2426 | rVB2 | 318    | 425    | 0.02%  | 0.005% |
| 54 | 9.150  | 2426 | 2429 | 2433 | rBV  | 302    | 303    | 0.02%  | 0.003% |
| 55 | 9.176  | 2433 | 2437 | 2440 | rVV2 | 209    | 182    | 0.01%  | 0.002% |
| 56 | 9.240  | 2454 | 2457 | 2460 | rBV2 | 271    | 222    | 0.01%  | 0.002% |
| 57 | 9.414  | 2498 | 2511 | 2529 | rBV  | 402089 | 659975 | 38.33% | 7.360% |
| 58 | 9.597  | 2564 | 2568 | 2571 | rVV2 | 392    | 352    | 0.02%  | 0.004% |
| 59 | 9.809  | 2632 | 2634 | 2637 | rVB2 | 248    | 164    | 0.01%  | 0.002% |
| 60 | 9.925  | 2666 | 2670 | 2673 | rVB  | 265    | 199    | 0.01%  | 0.002% |
| 61 | 10.018 | 2696 | 2699 | 2705 | rBV2 | 174    | 171    | 0.01%  | 0.002% |
| 62 | 10.153 | 2736 | 2741 | 2742 | rBV  | 345    | 281    | 0.02%  | 0.003% |
| 63 | 10.247 | 2766 | 2770 | 2772 | rBV2 | 294    | 226    | 0.01%  | 0.003% |
| 64 | 10.282 | 2778 | 2781 | 2785 | rVB  | 275    | 248    | 0.01%  | 0.003% |
| 65 | 10.417 | 2820 | 2823 | 2826 | rBB2 | 277    | 193    | 0.01%  | 0.002% |
| 66 | 10.449 | 2827 | 2833 | 2836 | rBV2 | 353    | 496    | 0.03%  | 0.006% |
| 67 | 10.501 | 2845 | 2849 | 2853 | rBV  | 268    | 205    | 0.01%  | 0.002% |
| 68 | 10.751 | 2914 | 2927 | 2941 | rBV  | 282344 | 447035 | 25.97% | 4.985% |
| 69 | 10.854 | 2956 | 2959 | 2962 | rVV2 | 275    | 234    | 0.01%  | 0.003% |
| 70 | 10.890 | 2962 | 2970 | 2977 | rVB3 | 1009   | 1614   | 0.09%  | 0.018% |
| 71 | 10.954 | 2986 | 2990 | 2994 | rVB2 | 339    | 308    | 0.02%  | 0.003% |
| 72 | 10.992 | 2994 | 3002 | 3005 | rBV2 | 390    | 572    | 0.03%  | 0.006% |
| 73 | 11.192 | 3056 | 3064 | 3066 | rBV2 | 310    | 413    | 0.02%  | 0.005% |
| 74 | 11.279 | 3084 | 3091 | 3095 | rBV2 | 261    | 321    | 0.02%  | 0.004% |
| 75 | 11.333 | 3105 | 3108 | 3111 | rBV  | 369    | 354    | 0.02%  | 0.004% |
| 76 | 11.709 | 3222 | 3225 | 3226 | rBV  | 309    | 212    | 0.01%  | 0.002% |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012723\  
 Data File : VU052855.D  
 Acq On : 27 Jan 2023 18:29  
 Operator : JC/MD  
 Sample : 01314-15  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A44P0

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\SFAMULM012623WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.748 | 3227 | 3237 | 3243 | rVB4 | 4775   | 7193   | 0.42%  | 0.080% |
| 78  | 11.806 | 3243 | 3255 | 3273 | rBV  | 386306 | 626607 | 36.40% | 6.988% |
| 79  | 11.976 | 3306 | 3308 | 3311 | rBV  | 299    | 197    | 0.01%  | 0.002% |
| 80  | 12.057 | 3327 | 3333 | 3343 | rVB6 | 1710   | 2704   | 0.16%  | 0.030% |
| 81  | 12.189 | 3361 | 3374 | 3398 | rBV2 | 404590 | 735461 | 42.72% | 8.202% |
| 82  | 12.494 | 3465 | 3469 | 3471 | rBV2 | 265    | 229    | 0.01%  | 0.003% |
| 83  | 12.652 | 3515 | 3518 | 3522 | rBV  | 302    | 246    | 0.01%  | 0.003% |
| 84  | 12.668 | 3522 | 3523 | 3533 | rVV2 | 239    | 320    | 0.02%  | 0.004% |
| 85  | 12.732 | 3538 | 3543 | 3546 | rBV  | 353    | 376    | 0.02%  | 0.004% |
| 86  | 12.854 | 3579 | 3581 | 3583 | rVV2 | 291    | 179    | 0.01%  | 0.002% |
| 87  | 13.018 | 3629 | 3632 | 3634 | rBV2 | 278    | 170    | 0.01%  | 0.002% |
| 88  | 13.208 | 3681 | 3691 | 3702 | rBV2 | 6840   | 12935  | 0.75%  | 0.144% |
| 89  | 13.282 | 3712 | 3714 | 3719 | rBV2 | 176    | 176    | 0.01%  | 0.002% |
| 90  | 13.446 | 3762 | 3765 | 3768 | rBV  | 327    | 245    | 0.01%  | 0.003% |
| 91  | 13.526 | 3786 | 3790 | 3795 | rVB2 | 229    | 261    | 0.02%  | 0.003% |
| 92  | 13.610 | 3813 | 3816 | 3821 | rVB3 | 409    | 396    | 0.02%  | 0.004% |
| 93  | 13.771 | 3862 | 3866 | 3867 | rBV  | 231    | 167    | 0.01%  | 0.002% |
| 94  | 13.841 | 3881 | 3888 | 3901 | rBV5 | 1592   | 2745   | 0.16%  | 0.031% |
| 95  | 14.025 | 3941 | 3945 | 3950 | rVB2 | 333    | 306    | 0.02%  | 0.003% |
| 96  | 14.089 | 3962 | 3965 | 3967 | rBV  | 639    | 461    | 0.03%  | 0.005% |
| 97  | 14.407 | 4061 | 4064 | 4067 | rBV3 | 355    | 246    | 0.01%  | 0.003% |
| 98  | 14.439 | 4071 | 4074 | 4076 | rBV2 | 359    | 218    | 0.01%  | 0.002% |
| 99  | 14.574 | 4113 | 4116 | 4120 | rVB2 | 634    | 440    | 0.03%  | 0.005% |
| 100 | 14.613 | 4123 | 4128 | 4129 | rBV2 | 423    | 410    | 0.02%  | 0.005% |

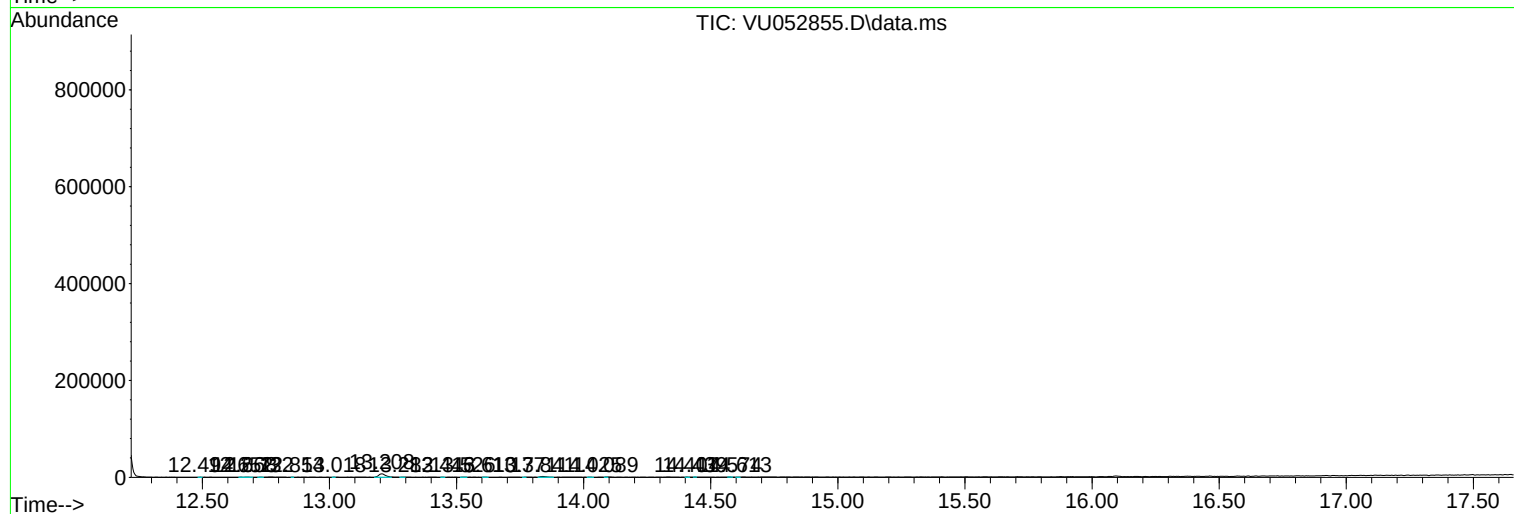
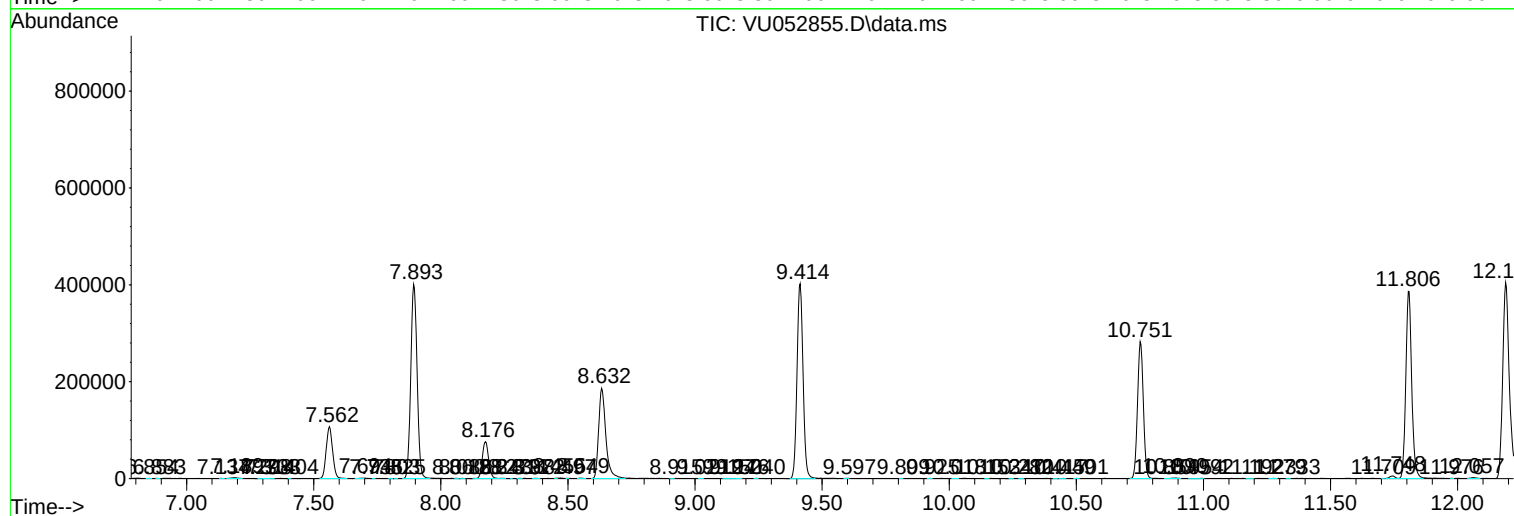
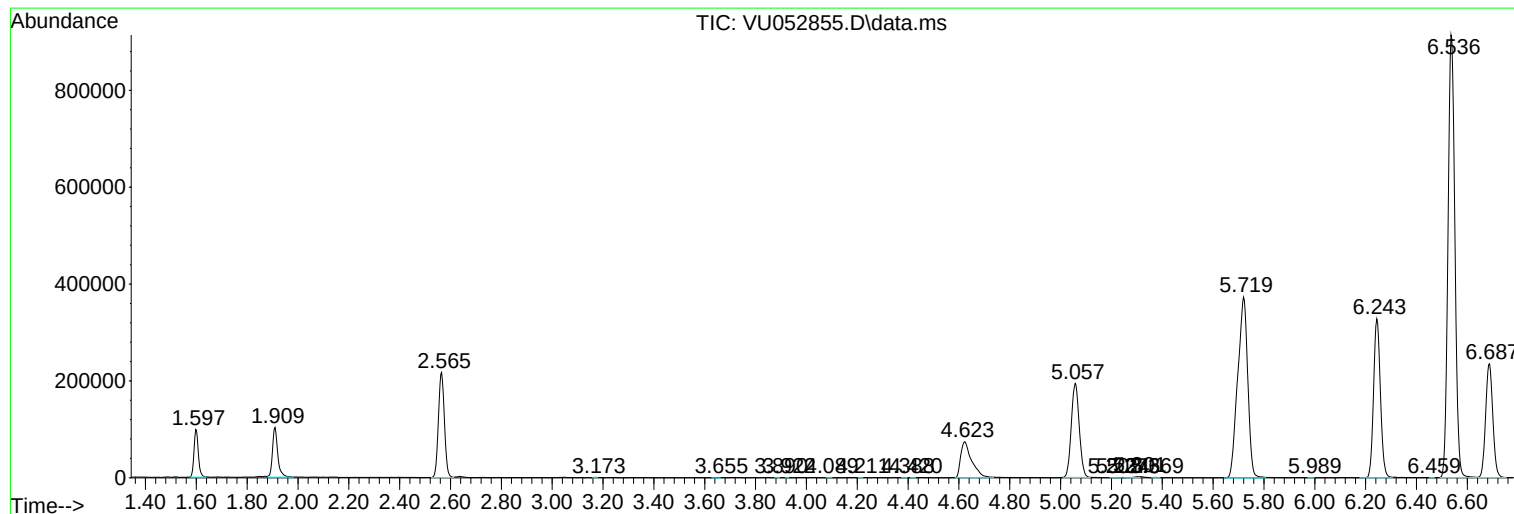
Sum of corrected areas: 8966742

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012723\  
Data File : VU052855.D  
Acq On : 27 Jan 2023 18:29  
Operator : JC/MD  
Sample : 01314-15  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
A44P0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012723\  
Data File : VU052855.D  
Acq On : 27 Jan 2023 18:29  
Operator : JC/MD  
Sample : 01314-15  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
A44P0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.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\VU012723\  
Data File : VU052855.D  
Acq On : 27 Jan 2023 18:29  
Operator : JC/MD  
Sample : 01314-15  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
A44P0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM012623WMA.M  
Quant Title : VOC Analysis

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

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