

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VW121423\  
 Data File : VW033336.D  
 Acq On : 14 Dec 2023 15:36  
 Operator : SY/MD  
 Sample : 05794-02  
 Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BGRF8

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\_V\Method\SFAMVLM120123WMA.M  
 Title : VOC Analysis

Signal : TIC: VW033336.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         | 1.278       | 68            | 74          | 83           | rBV      | 93534          | 94981         | 11.92%          | 1.498%        |
| 2         | 1.532       | 146           | 153         | 164          | rVB      | 76073          | 85731         | 10.76%          | 1.352%        |
| 3         | 2.060       | 308           | 317         | 340          | rVB      | 163017         | 237219        | 29.76%          | 3.741%        |
| 4         | 2.278       | 383           | 385         | 387          | rBV      | 388            | 170           | 0.02%           | 0.003%        |
| 5         | 2.333       | 399           | 402         | 406          | rBV      | 429            | 323           | 0.04%           | 0.005%        |
| 6         | 2.449       | 431           | 438         | 445          | rBB3     | 1243           | 1766          | 0.22%           | 0.028%        |
| 7         | 2.481       | 446           | 448         | 451          | rBV      | 271            | 205           | 0.03%           | 0.003%        |
| 8         | 2.552       | 461           | 470         | 473          | rBV4     | 1140           | 1422          | 0.18%           | 0.022%        |
| 9         | 2.632       | 492           | 495         | 497          | rBB2     | 265            | 174           | 0.02%           | 0.003%        |
| 10        | 2.780       | 539           | 541         | 546          | rBV      | 180            | 197           | 0.02%           | 0.003%        |
| 11        | 3.188       | 666           | 668         | 671          | rVB      | 260            | 120           | 0.02%           | 0.002%        |
| 12        | 3.208       | 671           | 674         | 678          | rBV      | 154            | 170           | 0.02%           | 0.003%        |
| 13        | 3.407       | 733           | 736         | 740          | rBB      | 149            | 124           | 0.02%           | 0.002%        |
| 14        | 3.558       | 780           | 783         | 786          | rBB      | 148            | 121           | 0.02%           | 0.002%        |
| 15        | 3.783       | 844           | 853         | 874          | rBV2     | 38056          | 99122         | 12.44%          | 1.563%        |
| 16        | 4.130       | 959           | 961         | 964          | rBV      | 272            | 127           | 0.02%           | 0.002%        |
| 17        | 4.185       | 974           | 978         | 981          | rBV3     | 354            | 259           | 0.03%           | 0.004%        |
| 18        | 4.246       | 982           | 997         | 1034         | rVV2     | 132770         | 346180        | 43.43%          | 5.459%        |
| 19        | 4.767       | 1154          | 1159        | 1161         | rBV2     | 335            | 283           | 0.04%           | 0.004%        |
| 20        | 4.957       | 1201          | 1218        | 1254         | rBV2     | 292318         | 797057        | 100.00%         | 12.570%       |
| 21        | 5.532       | 1383          | 1397        | 1424         | rBV      | 258696         | 531364        | 66.67%          | 8.380%        |
| 22        | 5.892       | 1506          | 1509        | 1513         | rBV2     | 387            | 392           | 0.05%           | 0.006%        |
| 23        | 5.989       | 1526          | 1539        | 1557         | rBV      | 162572         | 334171        | 41.93%          | 5.270%        |
| 24        | 6.246       | 1617          | 1619        | 1622         | rBB      | 298            | 180           | 0.02%           | 0.003%        |
| 25        | 6.342       | 1645          | 1649        | 1652         | rBB2     | 386            | 265           | 0.03%           | 0.004%        |
| 26        | 6.368       | 1653          | 1657        | 1660         | rBB      | 216            | 149           | 0.02%           | 0.002%        |
| 27        | 6.551       | 1712          | 1714        | 1717         | rBB      | 179            | 121           | 0.02%           | 0.002%        |
| 28        | 6.661       | 1745          | 1748        | 1751         | rBV      | 214            | 181           | 0.02%           | 0.003%        |
| 29        | 6.770       | 1779          | 1782        | 1784         | rBV      | 265            | 188           | 0.02%           | 0.003%        |
| 30        | 6.828       | 1795          | 1800        | 1803         | rBB      | 175            | 181           | 0.02%           | 0.003%        |
| 31        | 6.912       | 1814          | 1826        | 1850         | rBV      | 94461          | 177366        | 22.25%          | 2.797%        |
| 32        | 7.243       | 1917          | 1929        | 1957         | rBV      | 382047         | 674220        | 84.59%          | 10.633%       |
| 33        | 7.551       | 2016          | 2025        | 2048         | rBV      | 68397          | 124420        | 15.61%          | 1.962%        |
| 34        | 7.805       | 2102          | 2104        | 2108         | rVB2     | 406            | 251           | 0.03%           | 0.004%        |
| 35        | 7.876       | 2116          | 2126        | 2133         | rBV4     | 1451           | 2254          | 0.28%           | 0.036%        |
| 36        | 7.957       | 2148          | 2151        | 2153         | rBV      | 298            | 218           | 0.03%           | 0.003%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VW121423\  
 Data File : VW033336.D  
 Acq On : 14 Dec 2023 15:36  
 Operator : SY/MD  
 Sample : 05794-02  
 Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BGRF8

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\_V\Method\SFAMVLM120123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.989  | 2157 | 2161 | 2163 | rBV  | 155    | 147    | 0.02%  | 0.002%  |
| 38 | 8.024  | 2163 | 2172 | 2201 | rBV  | 138607 | 259619 | 32.57% | 4.094%  |
| 39 | 8.368  | 2268 | 2279 | 2287 | rBV6 | 1799   | 3541   | 0.44%  | 0.056%  |
| 40 | 8.513  | 2320 | 2324 | 2327 | rBV  | 197    | 211    | 0.03%  | 0.003%  |
| 41 | 8.567  | 2339 | 2341 | 2344 | rBV  | 323    | 215    | 0.03%  | 0.003%  |
| 42 | 8.702  | 2379 | 2383 | 2385 | rBV  | 159    | 129    | 0.02%  | 0.002%  |
| 43 | 8.786  | 2394 | 2409 | 2431 | rBV  | 403404 | 676553 | 84.88% | 10.670% |
| 44 | 9.088  | 2501 | 2503 | 2506 | rBV  | 241    | 163    | 0.02%  | 0.003%  |
| 45 | 9.227  | 2544 | 2546 | 2550 | rBB2 | 312    | 214    | 0.03%  | 0.003%  |
| 46 | 9.297  | 2562 | 2568 | 2571 | rBB  | 161    | 172    | 0.02%  | 0.003%  |
| 47 | 9.323  | 2571 | 2576 | 2579 | rBV  | 175    | 213    | 0.03%  | 0.003%  |
| 48 | 9.362  | 2585 | 2588 | 2593 | rBV  | 238    | 227    | 0.03%  | 0.004%  |
| 49 | 9.439  | 2610 | 2612 | 2616 | rBV  | 158    | 155    | 0.02%  | 0.002%  |
| 50 | 9.632  | 2666 | 2672 | 2674 | rBB2 | 444    | 347    | 0.04%  | 0.005%  |
| 51 | 9.879  | 2744 | 2749 | 2752 | rBV  | 390    | 318    | 0.04%  | 0.005%  |
| 52 | 9.995  | 2782 | 2785 | 2787 | rBV  | 358    | 195    | 0.02%  | 0.003%  |
| 53 | 10.063 | 2799 | 2806 | 2812 | rBB3 | 365    | 472    | 0.06%  | 0.007%  |
| 54 | 10.153 | 2822 | 2834 | 2854 | rBV  | 258106 | 399036 | 50.06% | 6.293%  |
| 55 | 10.265 | 2865 | 2869 | 2872 | rVB2 | 336    | 248    | 0.03%  | 0.004%  |
| 56 | 10.304 | 2879 | 2881 | 2882 | rBV  | 632    | 328    | 0.04%  | 0.005%  |
| 57 | 10.374 | 2900 | 2903 | 2906 | rBV2 | 211    | 169    | 0.02%  | 0.003%  |
| 58 | 10.474 | 2932 | 2934 | 2935 | rBV  | 259    | 146    | 0.02%  | 0.002%  |
| 59 | 10.590 | 2966 | 2970 | 2972 | rBB  | 247    | 183    | 0.02%  | 0.003%  |
| 60 | 10.718 | 3007 | 3010 | 3012 | rBV  | 239    | 174    | 0.02%  | 0.003%  |
| 61 | 10.773 | 3024 | 3027 | 3030 | rBV  | 273    | 207    | 0.03%  | 0.003%  |
| 62 | 10.812 | 3036 | 3039 | 3043 | rBB  | 367    | 248    | 0.03%  | 0.004%  |
| 63 | 10.892 | 3061 | 3064 | 3068 | rBB2 | 382    | 274    | 0.03%  | 0.004%  |
| 64 | 10.950 | 3079 | 3082 | 3083 | rBV2 | 301    | 191    | 0.02%  | 0.003%  |
| 65 | 10.979 | 3087 | 3091 | 3092 | rBV  | 232    | 177    | 0.02%  | 0.003%  |
| 66 | 11.024 | 3101 | 3105 | 3109 | rBB  | 347    | 325    | 0.04%  | 0.005%  |
| 67 | 11.046 | 3109 | 3112 | 3116 | rBB2 | 240    | 186    | 0.02%  | 0.003%  |
| 68 | 11.111 | 3130 | 3132 | 3136 | rBB2 | 382    | 255    | 0.03%  | 0.004%  |
| 69 | 11.133 | 3136 | 3139 | 3141 | rBV2 | 389    | 233    | 0.03%  | 0.004%  |
| 70 | 11.185 | 3141 | 3155 | 3185 | rBV  | 472956 | 732760 | 91.93% | 11.556% |
| 71 | 11.484 | 3245 | 3248 | 3251 | rBB2 | 302    | 220    | 0.03%  | 0.003%  |
| 72 | 11.561 | 3260 | 3272 | 3294 | rBV  | 471684 | 743752 | 93.31% | 11.729% |
| 73 | 11.754 | 3331 | 3332 | 3336 | rBV  | 326    | 221    | 0.03%  | 0.003%  |
| 74 | 11.873 | 3366 | 3369 | 3374 | rBB2 | 274    | 196    | 0.02%  | 0.003%  |
| 75 | 11.918 | 3380 | 3383 | 3385 | rBB  | 295    | 179    | 0.02%  | 0.003%  |
| 76 | 11.992 | 3404 | 3406 | 3410 | rBB  | 251    | 138    | 0.02%  | 0.002%  |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV121423\  
 Data File : VV033336.D  
 Acq On : 14 Dec 2023 15:36  
 Operator : SY/MD  
 Sample : 05794-02  
 Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BGRF8

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\_V\Method\SFAMVLM120123WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |     |     |       |        |
|-----|--------|------|------|------|------|-----|-----|-------|--------|
| 77  | 12.014 | 3411 | 3413 | 3415 | rBV  | 246 | 118 | 0.01% | 0.002% |
| 78  | 12.091 | 3433 | 3437 | 3440 | rBB2 | 280 | 253 | 0.03% | 0.004% |
| 79  | 12.233 | 3479 | 3481 | 3483 | rBV  | 270 | 176 | 0.02% | 0.003% |
| 80  | 12.300 | 3499 | 3502 | 3507 | rBB2 | 374 | 255 | 0.03% | 0.004% |
|     |        |      |      |      |      |     |     |       |        |
| 81  | 12.374 | 3522 | 3525 | 3529 | rBB  | 203 | 122 | 0.02% | 0.002% |
| 82  | 12.429 | 3539 | 3542 | 3545 | rBV  | 412 | 240 | 0.03% | 0.004% |
| 83  | 12.493 | 3560 | 3562 | 3564 | rBV  | 304 | 182 | 0.02% | 0.003% |
| 84  | 12.593 | 3590 | 3593 | 3597 | rBB  | 132 | 134 | 0.02% | 0.002% |
| 85  | 12.628 | 3598 | 3604 | 3608 | rBB2 | 256 | 278 | 0.03% | 0.004% |
|     |        |      |      |      |      |     |     |       |        |
| 86  | 12.799 | 3652 | 3657 | 3660 | rBB2 | 446 | 366 | 0.05% | 0.006% |
| 87  | 12.831 | 3663 | 3667 | 3671 | rBV  | 287 | 265 | 0.03% | 0.004% |
| 88  | 13.021 | 3722 | 3726 | 3728 | rBV  | 402 | 293 | 0.04% | 0.005% |
| 89  | 13.072 | 3739 | 3742 | 3747 | rBV2 | 257 | 245 | 0.03% | 0.004% |
| 90  | 13.130 | 3755 | 3760 | 3762 | rBV2 | 453 | 393 | 0.05% | 0.006% |
|     |        |      |      |      |      |     |     |       |        |
| 91  | 13.223 | 3786 | 3789 | 3792 | rBV  | 137 | 137 | 0.02% | 0.002% |
| 92  | 13.252 | 3794 | 3798 | 3800 | rBV  | 393 | 246 | 0.03% | 0.004% |
| 93  | 13.291 | 3806 | 3810 | 3815 | rBB2 | 354 | 323 | 0.04% | 0.005% |
| 94  | 13.316 | 3815 | 3818 | 3820 | rBV  | 284 | 218 | 0.03% | 0.003% |
| 95  | 13.387 | 3838 | 3840 | 3845 | rVB3 | 479 | 285 | 0.04% | 0.004% |
|     |        |      |      |      |      |     |     |       |        |
| 96  | 13.451 | 3857 | 3860 | 3865 | rBV2 | 477 | 490 | 0.06% | 0.008% |
| 97  | 13.660 | 3920 | 3925 | 3929 | rBV2 | 639 | 595 | 0.07% | 0.009% |
| 98  | 13.747 | 3949 | 3952 | 3957 | rBV  | 294 | 209 | 0.03% | 0.003% |
| 99  | 13.831 | 3975 | 3978 | 3981 | rBV2 | 508 | 301 | 0.04% | 0.005% |
| 100 | 14.024 | 4035 | 4038 | 4041 | rBV2 | 680 | 361 | 0.05% | 0.006% |

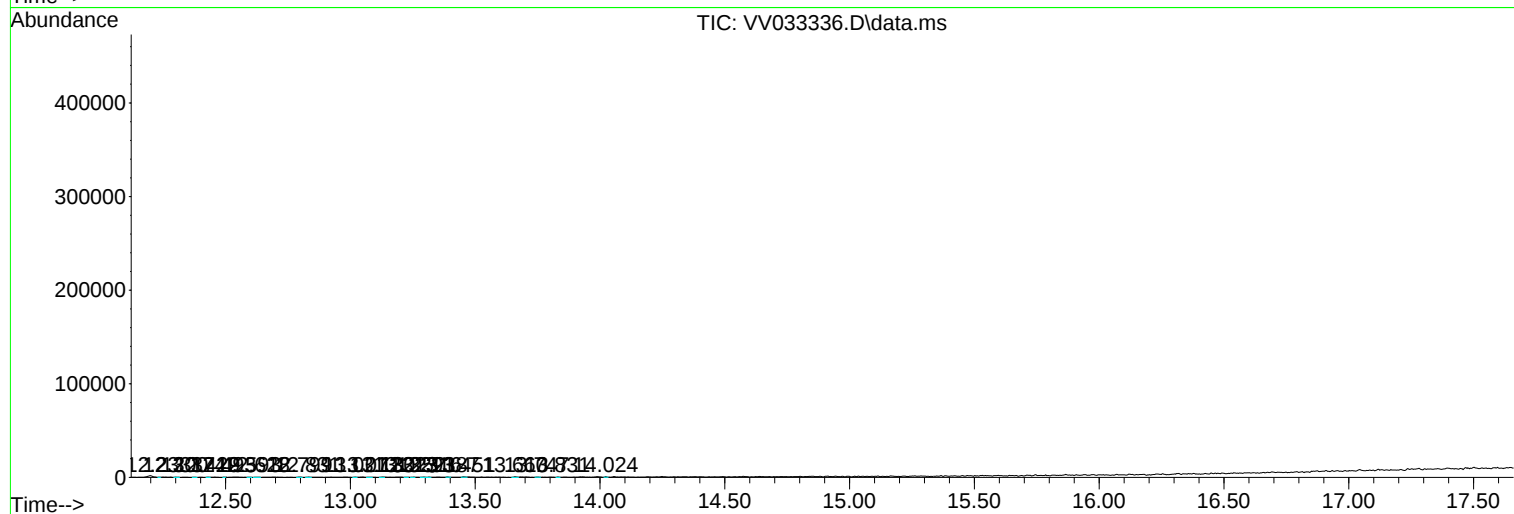
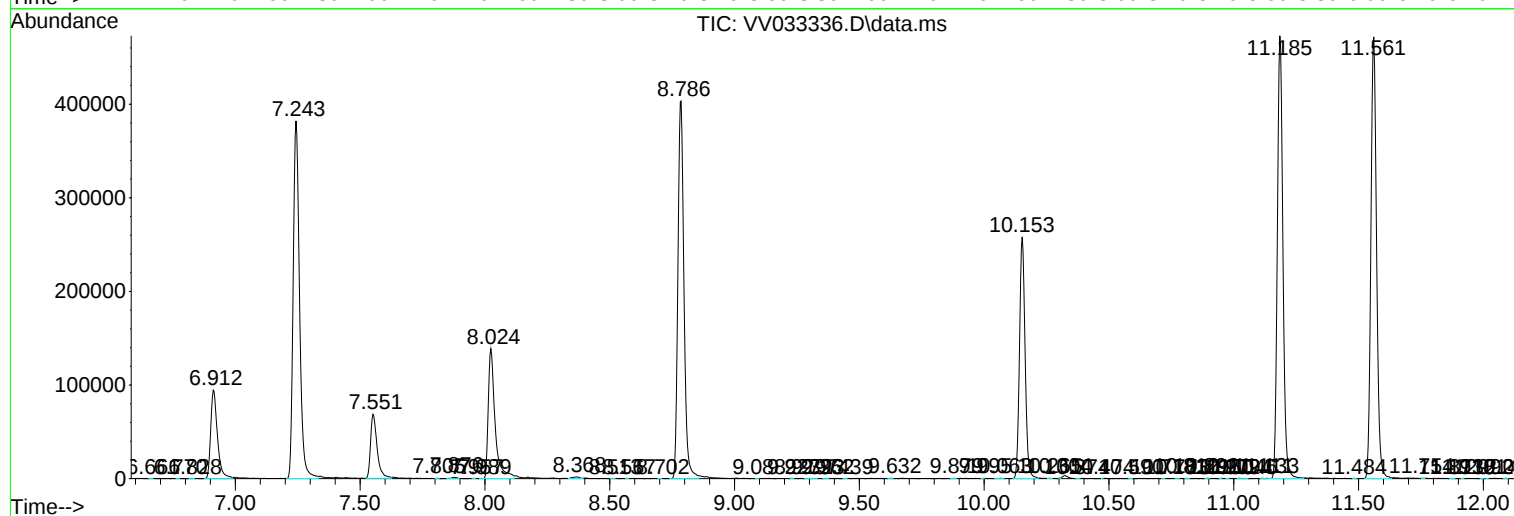
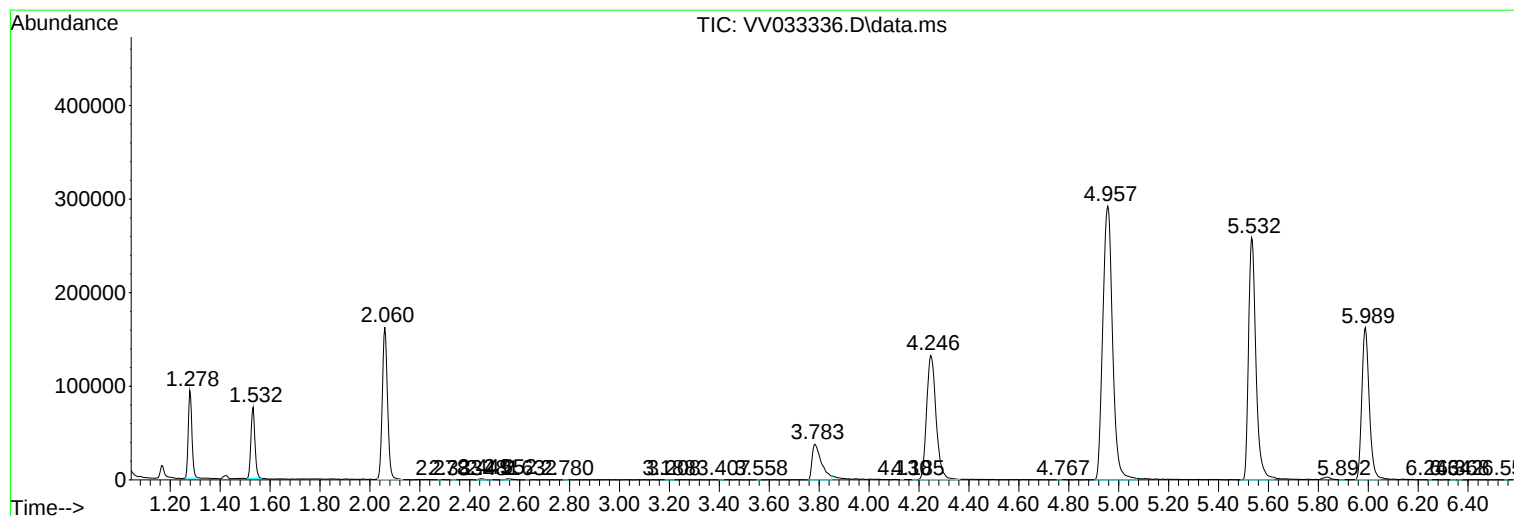
Sum of corrected areas: 6340894

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV121423\  
Data File : VV033336.D  
Acq On : 14 Dec 2023 15:36  
Operator : SY/MD  
Sample : 05794-02  
Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BGRF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM120123WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV121423\  
Data File : VV033336.D  
Acq On : 14 Dec 2023 15:36  
Operator : SY/MD  
Sample : 05794-02  
Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BGRF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM120123WMA.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\_V\Data\VV121423\  
Data File : VV033336.D  
Acq On : 14 Dec 2023 15:36  
Operator : SY/MD  
Sample : 05794-02  
Misc : 4.75g/5.0mL/100uL/5.00mL/MSVOA\_V/MEOH  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BGRF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM120123WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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