

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100521\  
 Data File : VU045168.D  
 Acq On : 06 Oct 2021 00:43  
 Operator : SY/MD  
 Sample : M3996-15  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 37 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F4A30

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045168.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         | 1.481       | 36            | 44          | 67           | rBV      | 31837          | 99708         | 7.82%           | 0.922%        |
| 2         | 1.604       | 75            | 82          | 95           | rBV      | 147393         | 169337        | 13.28%          | 1.566%        |
| 3         | 1.912       | 171           | 178         | 197          | rVB      | 134069         | 183466        | 14.39%          | 1.697%        |
| 4         | 2.497       | 357           | 360         | 363          | rBV      | 460            | 379           | 0.03%           | 0.004%        |
| 5         | 2.571       | 371           | 383         | 404          | rBV      | 253949         | 428187        | 33.59%          | 3.961%        |
| 6         | 2.742       | 434           | 436         | 442          | rVB2     | 240            | 223           | 0.02%           | 0.002%        |
| 7         | 2.764       | 442           | 443         | 448          | rBV2     | 273            | 227           | 0.02%           | 0.002%        |
| 8         | 2.803       | 448           | 455         | 456          | rBV3     | 550            | 623           | 0.05%           | 0.006%        |
| 9         | 2.954       | 499           | 502         | 503          | rBV2     | 324            | 233           | 0.02%           | 0.002%        |
| 10        | 3.192       | 559           | 576         | 595          | rBV2     | 14127          | 34371         | 2.70%           | 0.318%        |
| 11        | 3.372       | 622           | 632         | 644          | rVB3     | 1285           | 2819          | 0.22%           | 0.026%        |
| 12        | 3.632       | 710           | 713         | 718          | rVB      | 249            | 214           | 0.02%           | 0.002%        |
| 13        | 3.671       | 721           | 725         | 730          | rBV2     | 177            | 215           | 0.02%           | 0.002%        |
| 14        | 3.870       | 783           | 787         | 790          | rVB2     | 218            | 192           | 0.02%           | 0.002%        |
| 15        | 3.909       | 796           | 799         | 803          | rBV      | 255            | 241           | 0.02%           | 0.002%        |
| 16        | 4.105       | 855           | 860         | 864          | rBV2     | 150            | 228           | 0.02%           | 0.002%        |
| 17        | 4.282       | 912           | 915         | 920          | rVB2     | 238            | 239           | 0.02%           | 0.002%        |
| 18        | 4.349       | 928           | 936         | 939          | rBV      | 217            | 309           | 0.02%           | 0.003%        |
| 19        | 4.520       | 986           | 989         | 993          | rBV2     | 219            | 194           | 0.02%           | 0.002%        |
| 20        | 4.636       | 1009          | 1025        | 1062         | rBV      | 145009         | 415013        | 32.55%          | 3.839%        |
| 21        | 4.870       | 1094          | 1098        | 1101         | rBV2     | 421            | 276           | 0.02%           | 0.003%        |
| 22        | 4.970       | 1126          | 1129        | 1134         | rVB3     | 271            | 242           | 0.02%           | 0.002%        |
| 23        | 4.999       | 1134          | 1138        | 1142         | rBV3     | 250            | 251           | 0.02%           | 0.002%        |
| 24        | 5.070       | 1143          | 1160        | 1184         | rBV      | 226150         | 492585        | 38.64%          | 4.557%        |
| 25        | 5.176       | 1191          | 1193        | 1197         | rVB2     | 363            | 251           | 0.02%           | 0.002%        |
| 26        | 5.205       | 1198          | 1202        | 1209         | rBV4     | 405            | 512           | 0.04%           | 0.005%        |
| 27        | 5.292       | 1225          | 1229        | 1235         | rVB4     | 454            | 538           | 0.04%           | 0.005%        |
| 28        | 5.481       | 1282          | 1288        | 1292         | rBV2     | 188            | 269           | 0.02%           | 0.002%        |
| 29        | 5.732       | 1343          | 1366        | 1394         | rBV2     | 469914         | 1274896       | 100.00%         | 11.793%       |
| 30        | 6.070       | 1465          | 1471        | 1475         | rBV2     | 269            | 368           | 0.03%           | 0.003%        |
| 31        | 6.111       | 1478          | 1484        | 1485         | rBV3     | 402            | 393           | 0.03%           | 0.004%        |
| 32        | 6.253       | 1512          | 1528        | 1549         | rBV      | 371451         | 693129        | 54.37%          | 6.412%        |
| 33        | 6.417       | 1573          | 1579        | 1582         | rVB3     | 263            | 319           | 0.03%           | 0.003%        |
| 34        | 6.439       | 1582          | 1586        | 1588         | rBV      | 269            | 228           | 0.02%           | 0.002%        |
| 35        | 6.542       | 1604          | 1618        | 1626         | rBV9     | 3072           | 6151          | 0.48%           | 0.057%        |
| 36        | 6.697       | 1651          | 1666        | 1691         | rBV      | 296957         | 586463        | 46.00%          | 5.425%        |

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 7.041  | 1769 | 1773 | 1774 | rBV  | 302    | 231    | 0.02%  | 0.002% |
| 38 | 7.185  | 1811 | 1818 | 1828 | rBV3 | 1674   | 2609   | 0.20%  | 0.024% |
| 39 | 7.365  | 1871 | 1874 | 1881 | rVB2 | 171    | 210    | 0.02%  | 0.002% |
| 40 | 7.427  | 1889 | 1893 | 1896 | rBV2 | 204    | 199    | 0.02%  | 0.002% |
| 41 | 7.449  | 1896 | 1900 | 1905 | rVB2 | 228    | 267    | 0.02%  | 0.002% |
| 42 | 7.571  | 1922 | 1938 | 1958 | rBV  | 158720 | 281998 | 22.12% | 2.609% |
| 43 | 7.690  | 1970 | 1975 | 1983 | rVB2 | 1190   | 1791   | 0.14%  | 0.017% |
| 44 | 7.902  | 2027 | 2041 | 2056 | rBV  | 578399 | 984104 | 77.19% | 9.103% |
| 45 | 7.970  | 2058 | 2062 | 2075 | rVB  | 8331   | 13432  | 1.05%  | 0.124% |
| 46 | 8.182  | 2116 | 2128 | 2147 | rBV  | 111365 | 190188 | 14.92% | 1.759% |
| 47 | 8.488  | 2215 | 2223 | 2229 | rVB3 | 371    | 618    | 0.05%  | 0.006% |
| 48 | 8.555  | 2231 | 2244 | 2258 | rBV  | 563371 | 952849 | 74.74% | 8.814% |
| 49 | 8.639  | 2259 | 2270 | 2307 | rVB  | 453913 | 801636 | 62.88% | 7.415% |
| 50 | 8.896  | 2344 | 2350 | 2354 | rBV2 | 192    | 295    | 0.02%  | 0.003% |
| 51 | 9.005  | 2379 | 2384 | 2387 | rVV2 | 179    | 195    | 0.02%  | 0.002% |
| 52 | 9.266  | 2461 | 2465 | 2468 | rBV2 | 211    | 236    | 0.02%  | 0.002% |
| 53 | 9.353  | 2488 | 2492 | 2498 | rVB  | 299    | 255    | 0.02%  | 0.002% |
| 54 | 9.420  | 2498 | 2513 | 2535 | rBV  | 514406 | 851834 | 66.82% | 7.880% |
| 55 | 9.645  | 2576 | 2583 | 2590 | rBV2 | 346    | 480    | 0.04%  | 0.004% |
| 56 | 9.697  | 2590 | 2599 | 2605 | rBV3 | 652    | 1052   | 0.08%  | 0.010% |
| 57 | 10.098 | 2717 | 2724 | 2726 | rBV2 | 349    | 272    | 0.02%  | 0.003% |
| 58 | 10.455 | 2829 | 2835 | 2838 | rBV2 | 211    | 220    | 0.02%  | 0.002% |
| 59 | 10.475 | 2838 | 2841 | 2846 | rVB2 | 189    | 207    | 0.02%  | 0.002% |
| 60 | 10.520 | 2846 | 2855 | 2860 | rBV2 | 269    | 380    | 0.03%  | 0.004% |
| 61 | 10.568 | 2867 | 2870 | 2875 | rBV  | 253    | 312    | 0.02%  | 0.003% |
| 62 | 10.635 | 2888 | 2891 | 2894 | rVV  | 249    | 205    | 0.02%  | 0.002% |
| 63 | 10.671 | 2894 | 2902 | 2911 | rVV2 | 2876   | 3999   | 0.31%  | 0.037% |
| 64 | 10.761 | 2917 | 2930 | 2953 | rVB  | 415767 | 673222 | 52.81% | 6.228% |
| 65 | 10.870 | 2957 | 2964 | 2969 | rBV4 | 601    | 667    | 0.05%  | 0.006% |
| 66 | 10.944 | 2985 | 2987 | 2993 | rVB2 | 203    | 194    | 0.02%  | 0.002% |
| 67 | 11.021 | 3008 | 3011 | 3015 | rVB2 | 228    | 197    | 0.02%  | 0.002% |
| 68 | 11.060 | 3017 | 3023 | 3027 | rBV  | 215    | 307    | 0.02%  | 0.003% |
| 69 | 11.150 | 3048 | 3051 | 3055 | rBV2 | 389    | 295    | 0.02%  | 0.003% |
| 70 | 11.208 | 3064 | 3069 | 3072 | rBV  | 214    | 223    | 0.02%  | 0.002% |
| 71 | 11.243 | 3076 | 3080 | 3086 | rBV2 | 199    | 214    | 0.02%  | 0.002% |
| 72 | 11.295 | 3089 | 3096 | 3100 | rVB3 | 309    | 377    | 0.03%  | 0.003% |
| 73 | 11.407 | 3123 | 3131 | 3136 | rBV2 | 236    | 413    | 0.03%  | 0.004% |
| 74 | 11.465 | 3139 | 3149 | 3158 | rVB6 | 1825   | 3256   | 0.26%  | 0.030% |
| 75 | 11.578 | 3181 | 3184 | 3190 | rVB3 | 301    | 356    | 0.03%  | 0.003% |
| 76 | 11.700 | 3215 | 3222 | 3231 | rVV6 | 1090   | 1621   | 0.13%  | 0.015% |

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.815 | 3244 | 3258 | 3275 | rBV  | 486642 | 762863 | 59.84% | 7.057% |
| 78  | 11.941 | 3294 | 3297 | 3302 | rVV2 | 401    | 355    | 0.03%  | 0.003% |
| 79  | 11.976 | 3302 | 3308 | 3315 | rVB2 | 1667   | 2228   | 0.17%  | 0.021% |
| 80  | 12.195 | 3360 | 3376 | 3395 | rBV  | 539419 | 868389 | 68.11% | 8.033% |
| 81  | 12.295 | 3404 | 3407 | 3410 | rBB2 | 407    | 309    | 0.02%  | 0.003% |
| 82  | 12.336 | 3416 | 3420 | 3423 | rBV3 | 422    | 271    | 0.02%  | 0.003% |
| 83  | 12.442 | 3449 | 3453 | 3456 | rBV2 | 264    | 193    | 0.02%  | 0.002% |
| 84  | 12.574 | 3491 | 3494 | 3498 | rBV2 | 230    | 206    | 0.02%  | 0.002% |
| 85  | 12.642 | 3512 | 3515 | 3521 | rBV2 | 248    | 277    | 0.02%  | 0.003% |
| 86  | 12.719 | 3536 | 3539 | 3542 | rVV2 | 233    | 203    | 0.02%  | 0.002% |
| 87  | 12.822 | 3567 | 3571 | 3576 | rBV  | 292    | 273    | 0.02%  | 0.003% |
| 88  | 12.938 | 3603 | 3607 | 3613 | rBV2 | 231    | 276    | 0.02%  | 0.003% |
| 89  | 13.140 | 3663 | 3670 | 3673 | rBV2 | 206    | 302    | 0.02%  | 0.003% |
| 90  | 13.288 | 3710 | 3716 | 3724 | rVB  | 404    | 494    | 0.04%  | 0.005% |
| 91  | 13.368 | 3738 | 3741 | 3744 | rVB  | 300    | 195    | 0.02%  | 0.002% |
| 92  | 13.507 | 3782 | 3784 | 3789 | rVB  | 263    | 194    | 0.02%  | 0.002% |
| 93  | 13.558 | 3798 | 3800 | 3805 | rVB2 | 319    | 258    | 0.02%  | 0.002% |
| 94  | 13.883 | 3897 | 3901 | 3904 | rBV2 | 241    | 210    | 0.02%  | 0.002% |
| 95  | 13.938 | 3915 | 3918 | 3921 | rBV  | 287    | 250    | 0.02%  | 0.002% |
| 96  | 14.005 | 3934 | 3939 | 3942 | rVB2 | 281    | 241    | 0.02%  | 0.002% |
| 97  | 14.092 | 3956 | 3966 | 3977 | rBV  | 2830   | 4279   | 0.34%  | 0.040% |
| 98  | 14.725 | 4160 | 4163 | 4164 | rBV  | 316    | 213    | 0.02%  | 0.002% |
| 99  | 15.175 | 4299 | 4303 | 4306 | rBV  | 309    | 258    | 0.02%  | 0.002% |
| 100 | 15.413 | 4370 | 4377 | 4388 | rVB5 | 1823   | 2976   | 0.23%  | 0.028% |

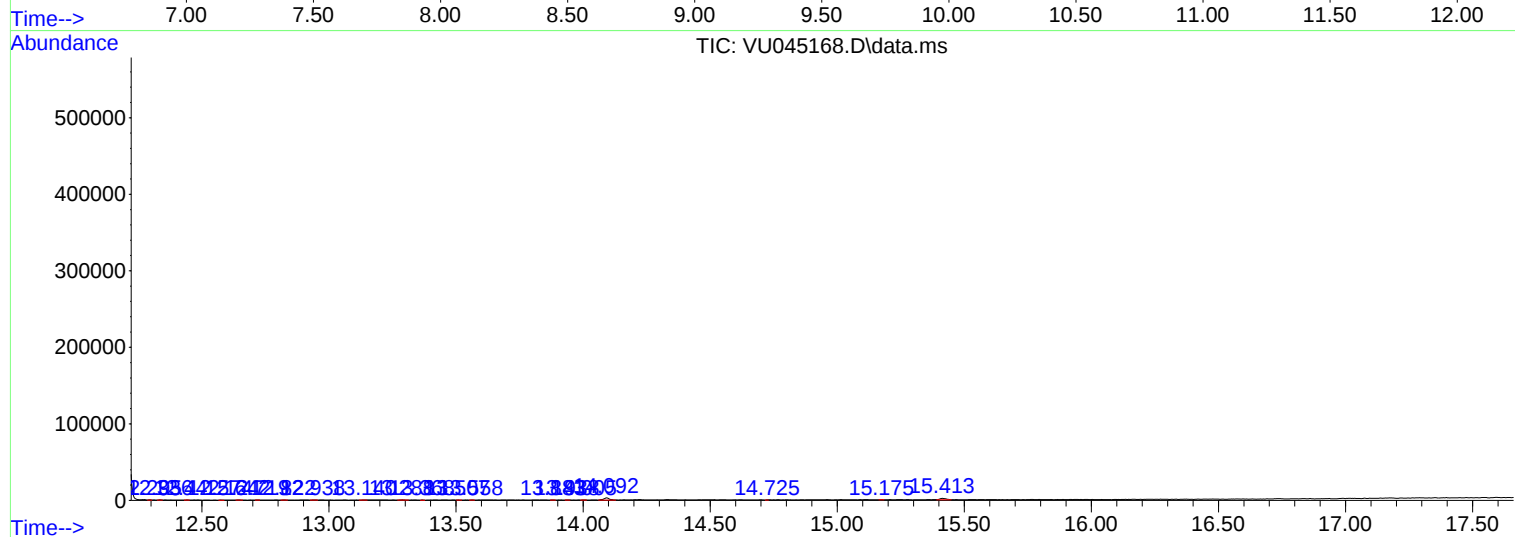
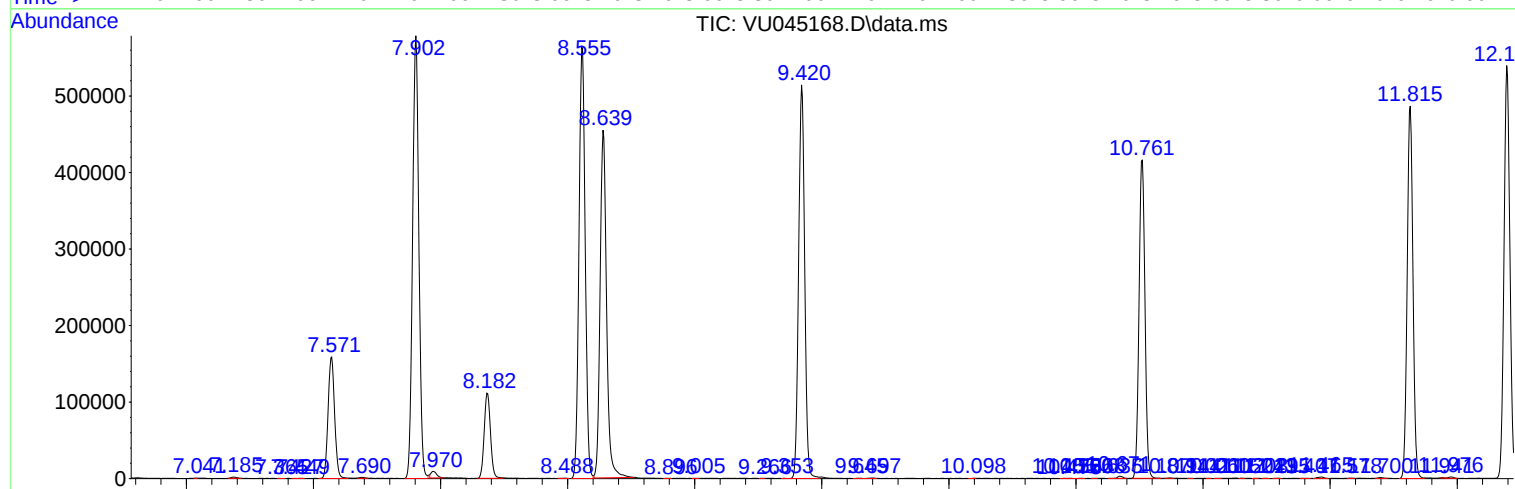
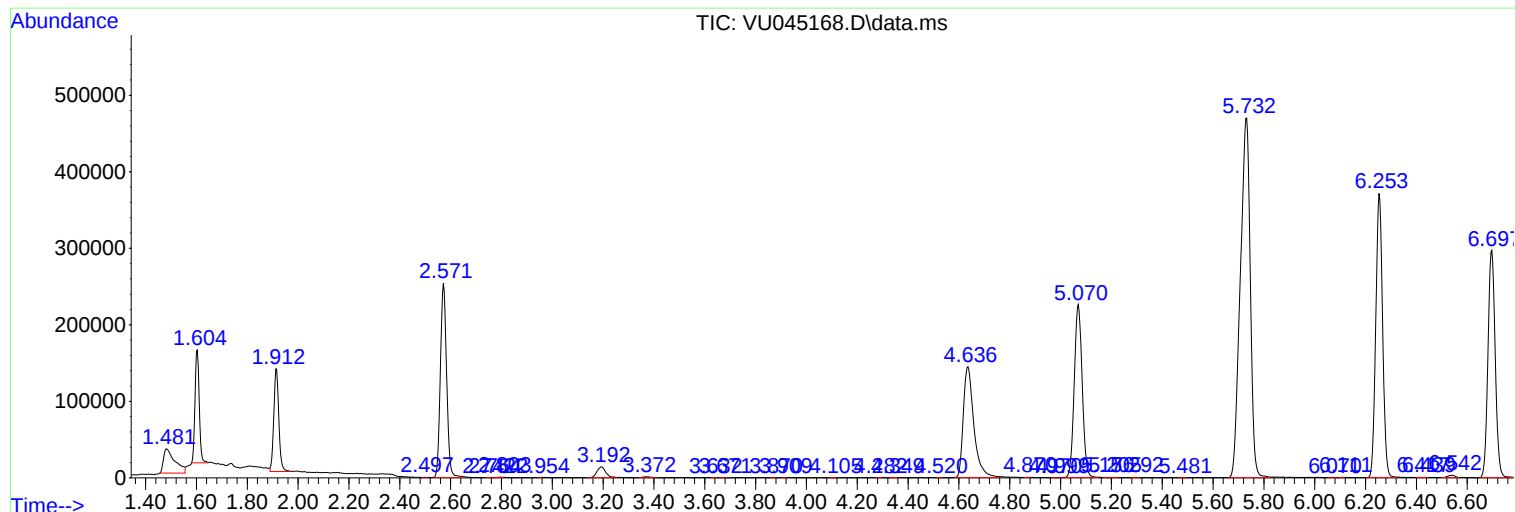
Sum of corrected areas: 10810418

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
Quant Title : VOC Analysis

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



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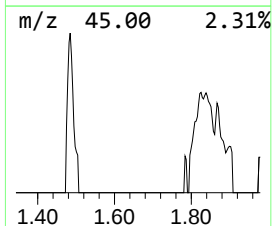
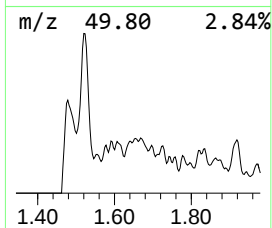
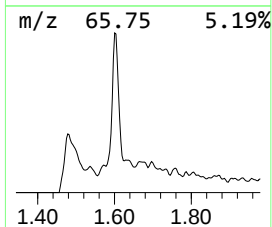
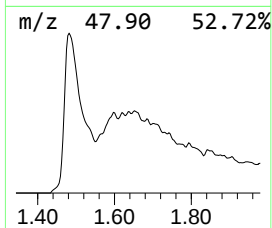
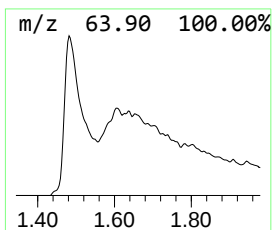
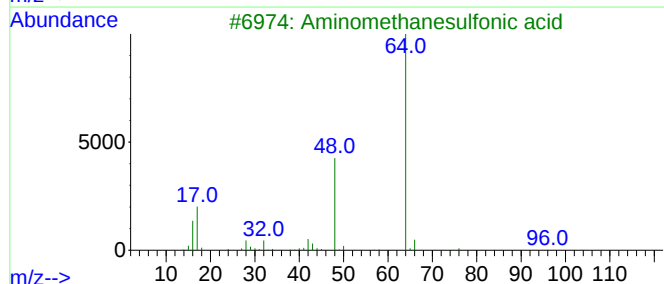
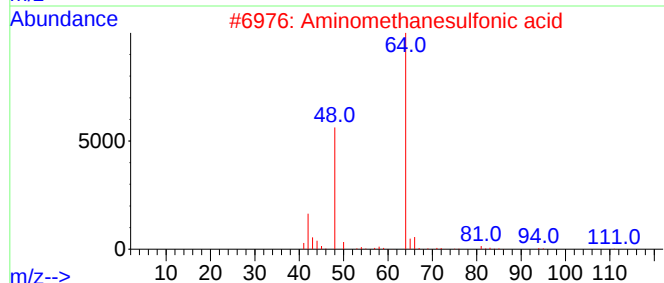
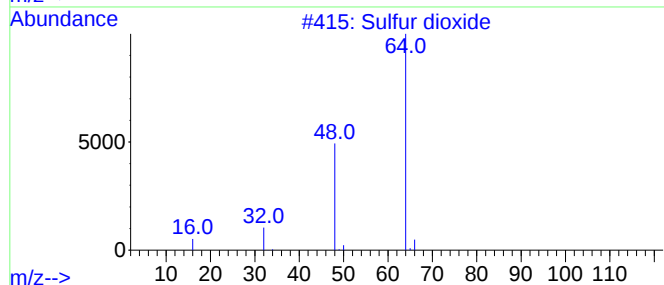
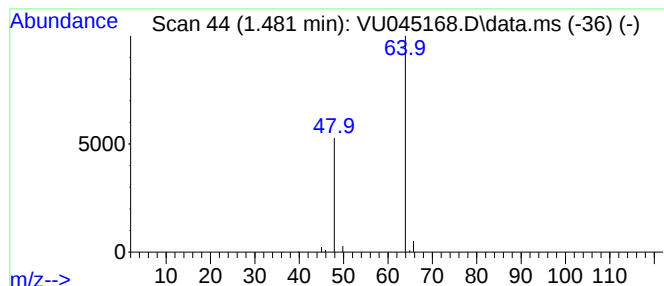
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.481 | 7.19 ug/L | 99708 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 64   |
| 3    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 64   |
| 4    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 7    |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.481 | 7.2     | ug/L  | 99708    | 1                     | 6.253 | 693129 | 50.0 |