

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041123\  
 Data File : VU053634.D  
 Acq On : 11 Apr 2023 14:47  
 Operator : JC/MD  
 Sample : 02251-18  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 COMD6

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\SFAMULM033123WMA.M  
 Title : VOC Analysis

Signal : TIC: VU053634.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         | 1.469       | 33            | 40          | 54           | rBV      | 21228          | 38731         | 5.10%           | 0.620%        |
| 2         | 1.597       | 74            | 80          | 92           | rBV      | 95115          | 110656        | 14.56%          | 1.771%        |
| 3         | 1.909       | 171           | 177         | 190          | rVB      | 80691          | 108123        | 14.23%          | 1.730%        |
| 4         | 2.562       | 369           | 380         | 394          | rBV      | 149020         | 239545        | 31.52%          | 3.833%        |
| 5         | 2.822       | 458           | 461         | 464          | rBV      | 387            | 245           | 0.03%           | 0.004%        |
| 6         | 3.079       | 538           | 541         | 544          | rBV2     | 269            | 149           | 0.02%           | 0.002%        |
| 7         | 3.176       | 565           | 571         | 573          | rBV3     | 716            | 811           | 0.11%           | 0.013%        |
| 8         | 3.494       | 667           | 670         | 673          | rBV      | 236            | 171           | 0.02%           | 0.003%        |
| 9         | 3.604       | 701           | 704         | 706          | rBV      | 334            | 229           | 0.03%           | 0.004%        |
| 10        | 3.645       | 713           | 717         | 719          | rBV      | 230            | 147           | 0.02%           | 0.002%        |
| 11        | 3.658       | 719           | 721         | 722          | rBV      | 213            | 73            | 0.01%           | 0.001%        |
| 12        | 3.790       | 759           | 762         | 766          | rBV      | 245            | 230           | 0.03%           | 0.004%        |
| 13        | 4.166       | 876           | 879         | 884          | rBV2     | 241            | 213           | 0.03%           | 0.003%        |
| 14        | 4.218       | 892           | 895         | 899          | rBV      | 323            | 235           | 0.03%           | 0.004%        |
| 15        | 4.311       | 922           | 924         | 925          | rBV      | 367            | 122           | 0.02%           | 0.002%        |
| 16        | 4.452       | 965           | 968         | 971          | rBV2     | 211            | 123           | 0.02%           | 0.002%        |
| 17        | 4.613       | 1007          | 1018        | 1041         | rBV2     | 63127          | 152423        | 20.05%          | 2.439%        |
| 18        | 5.057       | 1140          | 1156        | 1174         | rBV      | 143923         | 306064        | 40.27%          | 4.897%        |
| 19        | 5.240       | 1210          | 1213        | 1216         | rBV3     | 442            | 348           | 0.05%           | 0.006%        |
| 20        | 5.292       | 1226          | 1229        | 1231         | rBV      | 230            | 167           | 0.02%           | 0.003%        |
| 21        | 5.330       | 1236          | 1241        | 1244         | rBV3     | 337            | 373           | 0.05%           | 0.006%        |
| 22        | 5.401       | 1260          | 1263        | 1266         | rBV      | 413            | 249           | 0.03%           | 0.004%        |
| 23        | 5.449       | 1275          | 1278        | 1280         | rBV      | 146            | 92            | 0.01%           | 0.001%        |
| 24        | 5.504       | 1293          | 1295        | 1296         | rBV      | 134            | 52            | 0.01%           | 0.001%        |
| 25        | 5.603       | 1323          | 1326        | 1329         | rBV      | 275            | 234           | 0.03%           | 0.004%        |
| 26        | 5.719       | 1340          | 1362        | 1393         | rBV2     | 268652         | 760085        | 100.00%         | 12.162%       |
| 27        | 5.996       | 1445          | 1448        | 1449         | rBV2     | 236            | 109           | 0.01%           | 0.002%        |
| 28        | 6.137       | 1487          | 1492        | 1493         | rBV2     | 338            | 295           | 0.04%           | 0.005%        |
| 29        | 6.243       | 1512          | 1525        | 1547         | rBV      | 276605         | 532101        | 70.01%          | 8.514%        |
| 30        | 6.526       | 1608          | 1613        | 1620         | rVB3     | 849            | 887           | 0.12%           | 0.014%        |
| 31        | 6.581       | 1627          | 1630        | 1632         | rBV      | 151            | 77            | 0.01%           | 0.001%        |
| 32        | 6.639       | 1645          | 1648        | 1649         | rBV      | 185            | 98            | 0.01%           | 0.002%        |
| 33        | 6.684       | 1649          | 1662        | 1681         | rVV      | 170731         | 333020        | 43.81%          | 5.329%        |
| 34        | 6.899       | 1728          | 1729        | 1733         | rVB      | 132            | 56            | 0.01%           | 0.001%        |
| 35        | 6.925       | 1734          | 1737        | 1740         | rBV      | 297            | 187           | 0.02%           | 0.003%        |
| 36        | 7.147       | 1803          | 1806        | 1809         | rBV      | 191            | 181           | 0.02%           | 0.003%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMULM033123WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.173  | 1809 | 1814 | 1815 | rBV2 | 473    | 419    | 0.06%  | 0.007%  |
| 38 | 7.285  | 1847 | 1849 | 1852 | rVB  | 221    | 102    | 0.01%  | 0.002%  |
| 39 | 7.385  | 1877 | 1880 | 1882 | rBV  | 186    | 89     | 0.01%  | 0.001%  |
| 40 | 7.420  | 1889 | 1891 | 1892 | rBV  | 141    | 33     | 0.00%  | 0.001%  |
| 41 | 7.562  | 1921 | 1935 | 1953 | rBV  | 93026  | 167073 | 21.98% | 2.673%  |
| 42 | 7.761  | 1994 | 1997 | 2000 | rBV  | 239    | 119    | 0.02%  | 0.002%  |
| 43 | 7.809  | 2010 | 2012 | 2017 | rBB  | 220    | 153    | 0.02%  | 0.002%  |
| 44 | 7.893  | 2024 | 2038 | 2058 | rBV  | 345692 | 601139 | 79.09% | 9.619%  |
| 45 | 8.102  | 2100 | 2103 | 2107 | rVB  | 307    | 159    | 0.02%  | 0.003%  |
| 46 | 8.124  | 2108 | 2110 | 2113 | rVV2 | 247    | 150    | 0.02%  | 0.002%  |
| 47 | 8.176  | 2115 | 2126 | 2144 | rVV2 | 66046  | 110242 | 14.50% | 1.764%  |
| 48 | 8.272  | 2154 | 2156 | 2160 | rVB3 | 254    | 176    | 0.02%  | 0.003%  |
| 49 | 8.304  | 2163 | 2166 | 2168 | rBV2 | 178    | 86     | 0.01%  | 0.001%  |
| 50 | 8.410  | 2197 | 2199 | 2201 | rBV2 | 177    | 99     | 0.01%  | 0.002%  |
| 51 | 8.439  | 2205 | 2208 | 2211 | rBV2 | 244    | 194    | 0.03%  | 0.003%  |
| 52 | 8.626  | 2255 | 2266 | 2300 | rBV  | 189678 | 349107 | 45.93% | 5.586%  |
| 53 | 9.012  | 2383 | 2386 | 2387 | rBV  | 183    | 111    | 0.01%  | 0.002%  |
| 54 | 9.121  | 2417 | 2420 | 2423 | rBV2 | 260    | 161    | 0.02%  | 0.003%  |
| 55 | 9.172  | 2434 | 2436 | 2440 | rBV  | 183    | 77     | 0.01%  | 0.001%  |
| 56 | 9.320  | 2477 | 2482 | 2484 | rBV2 | 269    | 216    | 0.03%  | 0.003%  |
| 57 | 9.353  | 2488 | 2492 | 2496 | rBV2 | 208    | 209    | 0.03%  | 0.003%  |
| 58 | 9.414  | 2498 | 2511 | 2535 | rBV  | 392619 | 703608 | 92.57% | 11.259% |
| 59 | 9.645  | 2580 | 2583 | 2585 | rBV  | 169    | 120    | 0.02%  | 0.002%  |
| 60 | 9.697  | 2593 | 2599 | 2602 | rVB2 | 460    | 428    | 0.06%  | 0.007%  |
| 61 | 9.880  | 2654 | 2656 | 2658 | rVB  | 223    | 94     | 0.01%  | 0.002%  |
| 62 | 10.008 | 2693 | 2696 | 2698 | rBV2 | 247    | 161    | 0.02%  | 0.003%  |
| 63 | 10.118 | 2727 | 2730 | 2733 | rBV2 | 305    | 231    | 0.03%  | 0.004%  |
| 64 | 10.333 | 2794 | 2797 | 2800 | rBV  | 199    | 168    | 0.02%  | 0.003%  |
| 65 | 10.484 | 2841 | 2844 | 2846 | rBV2 | 262    | 181    | 0.02%  | 0.003%  |
| 66 | 10.571 | 2868 | 2871 | 2873 | rBV  | 203    | 138    | 0.02%  | 0.002%  |
| 67 | 10.680 | 2902 | 2905 | 2908 | rBV  | 220    | 134    | 0.02%  | 0.002%  |
| 68 | 10.751 | 2915 | 2927 | 2950 | rBV  | 263109 | 412198 | 54.23% | 6.596%  |
| 69 | 11.237 | 3075 | 3078 | 3080 | rVB  | 216    | 113    | 0.01%  | 0.002%  |
| 70 | 11.256 | 3080 | 3084 | 3086 | rBV  | 309    | 191    | 0.03%  | 0.003%  |
| 71 | 11.478 | 3149 | 3153 | 3157 | rBV  | 405    | 354    | 0.05%  | 0.006%  |
| 72 | 11.748 | 3226 | 3237 | 3244 | rBV4 | 1701   | 2738   | 0.36%  | 0.044%  |
| 73 | 11.809 | 3244 | 3256 | 3275 | rBV  | 413325 | 687297 | 90.42% | 10.998% |
| 74 | 12.089 | 3337 | 3343 | 3344 | rBV2 | 552    | 500    | 0.07%  | 0.008%  |
| 75 | 12.188 | 3362 | 3374 | 3395 | rBV  | 373799 | 617083 | 81.19% | 9.874%  |
| 76 | 12.381 | 3432 | 3434 | 3439 | rVB2 | 391    | 250    | 0.03%  | 0.004%  |

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Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0MD6

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\SFAMULM033123WMA.M

Title : VOC Analysis

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 77 | 12.851 | 3577 | 3580 | 3583 | rBV2 | 341  | 250  | 0.03% | 0.004% |
| 78 | 13.076 | 3647 | 3650 | 3652 | rBV2 | 221  | 117  | 0.02% | 0.002% |
| 79 | 13.095 | 3652 | 3656 | 3659 | rBV  | 288  | 219  | 0.03% | 0.004% |
| 80 | 13.349 | 3733 | 3735 | 3741 | rBV2 | 366  | 262  | 0.03% | 0.004% |
| 81 | 13.462 | 3766 | 3770 | 3775 | rVB  | 370  | 325  | 0.04% | 0.005% |
| 82 | 13.577 | 3803 | 3806 | 3809 | rBV  | 468  | 264  | 0.03% | 0.004% |
| 83 | 13.844 | 3882 | 3889 | 3898 | rVB6 | 3426 | 4862 | 0.64% | 0.078% |
| 84 | 14.024 | 3942 | 3945 | 3946 | rBV  | 330  | 171  | 0.02% | 0.003% |

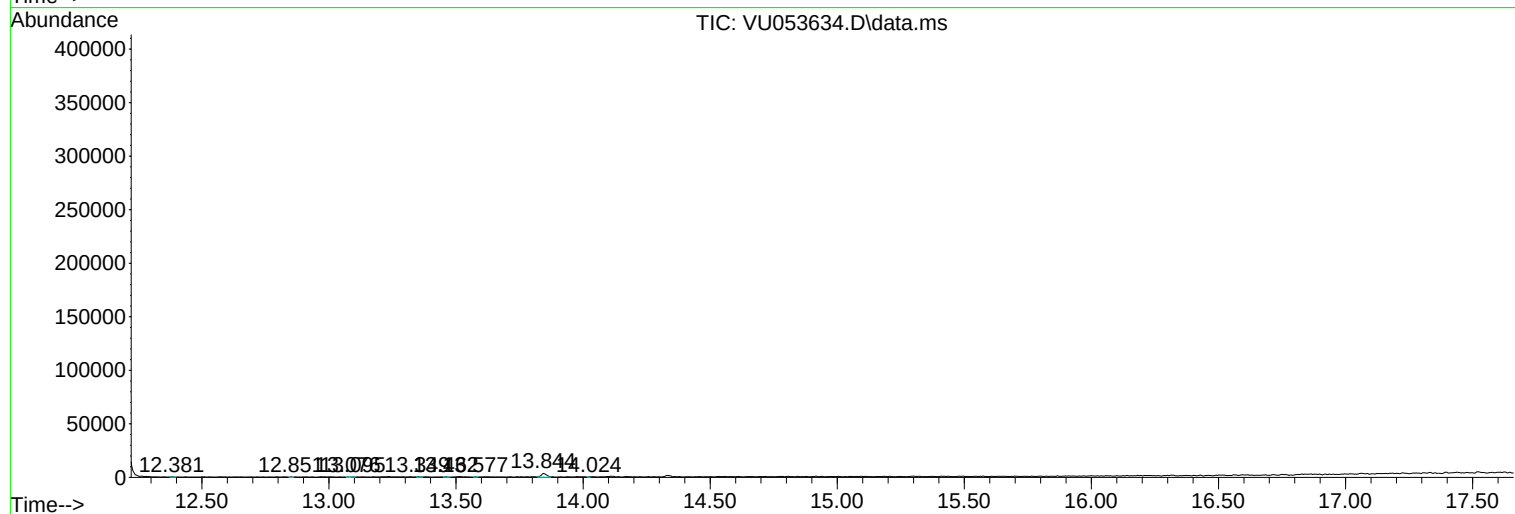
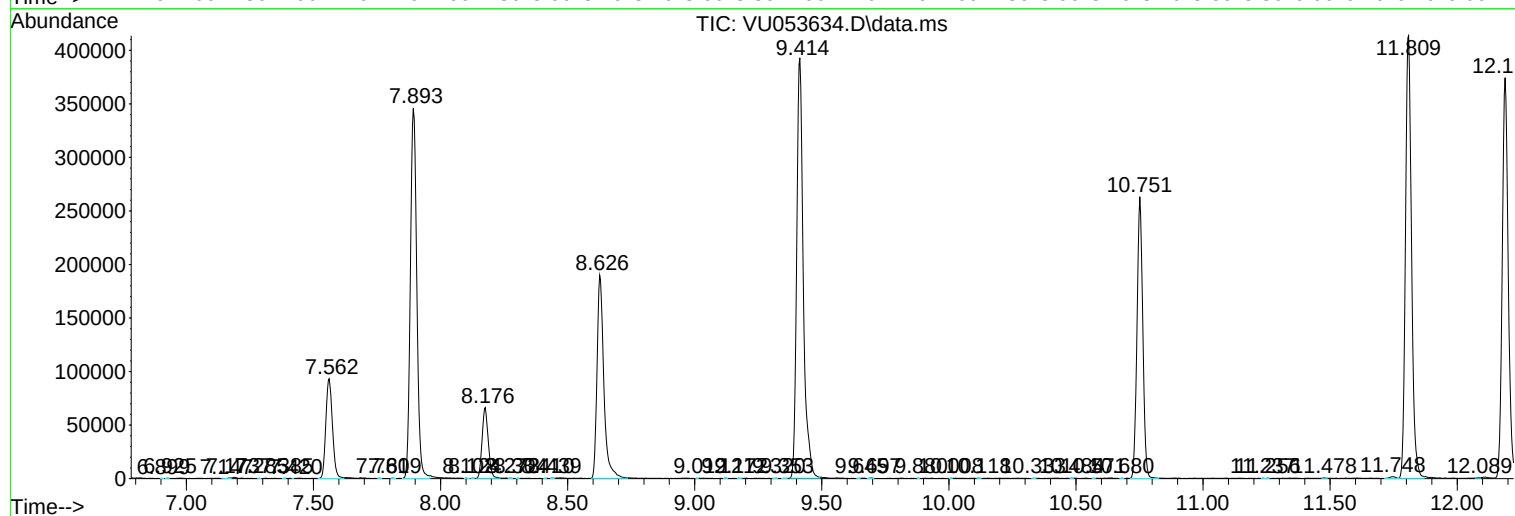
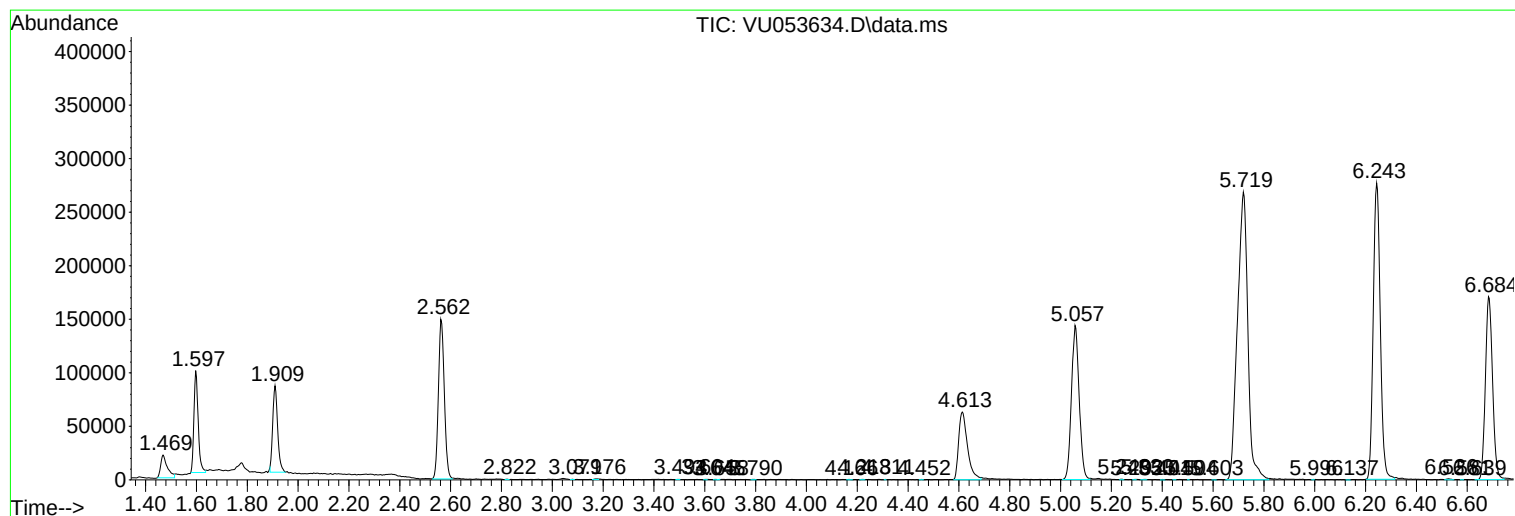
Sum of corrected areas: 6249472

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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



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Instrument :  
MSVOA\_U  
ClientSampleId :  
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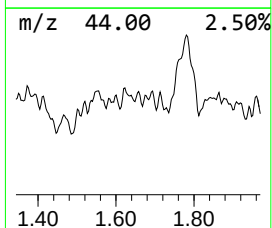
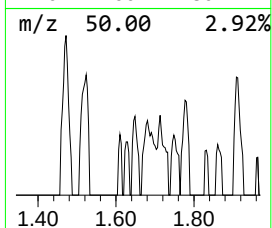
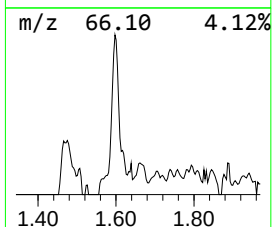
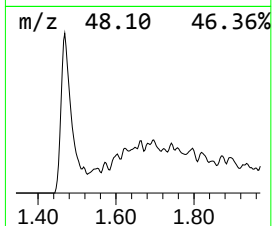
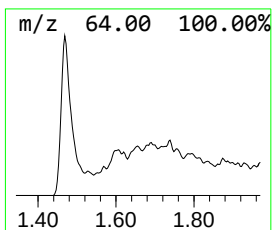
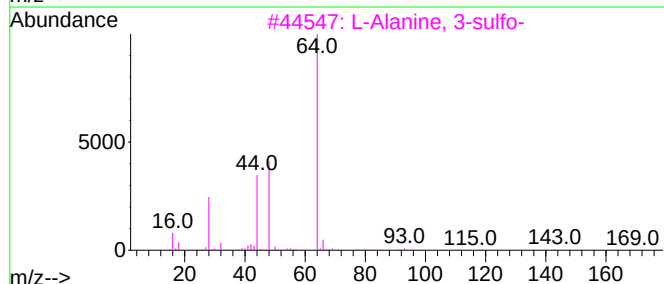
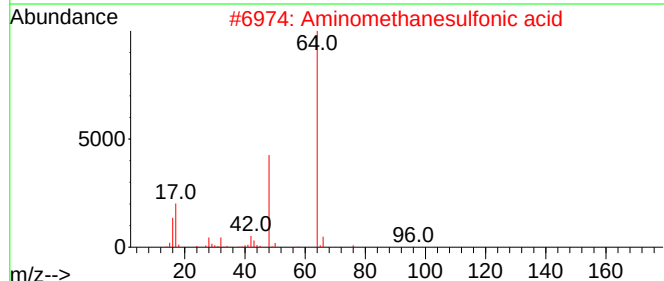
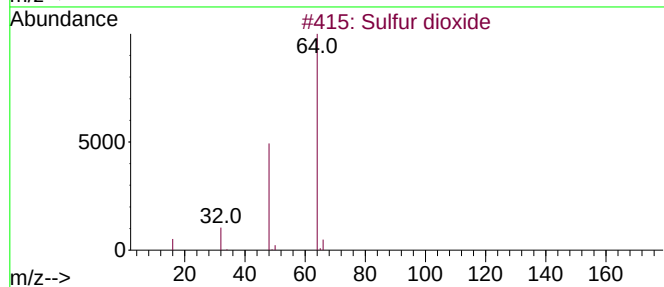
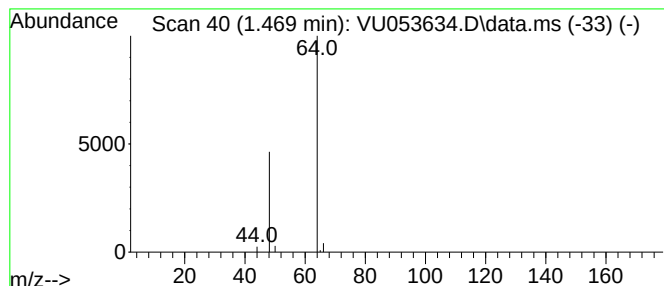
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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

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Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.469 | 3.64 ug/L | 38731 | 1,4-Difluorobenzene | 6.243 |

| 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    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 4    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.469 | 3.6     | ug/L  | 38731    | 1                     | 6.243 | 532101 | 50.0 |