

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU041023\  
 Data File : VU053623.D  
 Acq On : 10 Apr 2023 19:12  
 Operator : JC/MD  
 Sample : 02251-20  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 COMD8

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: VU053623.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          | 63           | rBV      | 34057          | 71457         | 8.76%           | 1.078%        |
| 2         | 1.597       | 74            | 80          | 93           | rVB      | 103961         | 120764        | 14.80%          | 1.822%        |
| 3         | 1.909       | 170           | 177         | 193          | rVB      | 90019          | 120430        | 14.76%          | 1.817%        |
| 4         | 2.565       | 369           | 381         | 395          | rBV      | 163730         | 262477        | 32.17%          | 3.960%        |
| 5         | 3.131       | 555           | 557         | 559          | rBV      | 242            | 103           | 0.01%           | 0.002%        |
| 6         | 3.337       | 619           | 621         | 623          | rBV      | 297            | 124           | 0.02%           | 0.002%        |
| 7         | 3.459       | 656           | 659         | 660          | rBV      | 325            | 190           | 0.02%           | 0.003%        |
| 8         | 3.613       | 704           | 707         | 712          | rVB2     | 332            | 199           | 0.02%           | 0.003%        |
| 9         | 3.700       | 732           | 734         | 737          | rVB      | 182            | 79            | 0.01%           | 0.001%        |
| 10        | 3.800       | 762           | 765         | 768          | rBV2     | 331            | 218           | 0.03%           | 0.003%        |
| 11        | 3.887       | 789           | 792         | 794          | rBV      | 272            | 144           | 0.02%           | 0.002%        |
| 12        | 3.935       | 805           | 807         | 808          | rBV      | 247            | 80            | 0.01%           | 0.001%        |
| 13        | 4.189       | 878           | 886         | 890          | rBV2     | 212            | 362           | 0.04%           | 0.005%        |
| 14        | 4.250       | 903           | 905         | 908          | rBV2     | 173            | 112           | 0.01%           | 0.002%        |
| 15        | 4.343       | 931           | 934         | 938          | rBV2     | 168            | 128           | 0.02%           | 0.002%        |
| 16        | 4.462       | 968           | 971         | 974          | rBV      | 233            | 137           | 0.02%           | 0.002%        |
| 17        | 4.617       | 1007          | 1019        | 1047         | rBV      | 66123          | 161627        | 19.81%          | 2.439%        |
| 18        | 4.967       | 1124          | 1128        | 1129         | rBV2     | 217            | 138           | 0.02%           | 0.002%        |
| 19        | 4.980       | 1129          | 1132        | 1138         | rVB2     | 267            | 197           | 0.02%           | 0.003%        |
| 20        | 5.054       | 1140          | 1155        | 1174         | rBV      | 147882         | 329463        | 40.38%          | 4.971%        |
| 21        | 5.330       | 1238          | 1241        | 1244         | rBV2     | 277            | 264           | 0.03%           | 0.004%        |
| 22        | 5.408       | 1263          | 1265        | 1267         | rBV      | 179            | 71            | 0.01%           | 0.001%        |
| 23        | 5.443       | 1275          | 1276        | 1279         | rVB      | 257            | 96            | 0.01%           | 0.001%        |
| 24        | 5.465       | 1279          | 1283        | 1285         | rBV      | 194            | 195           | 0.02%           | 0.003%        |
| 25        | 5.719       | 1341          | 1362        | 1394         | rBV2     | 293202         | 815974        | 100.00%         | 12.311%       |
| 26        | 5.973       | 1438          | 1441        | 1443         | rBV2     | 176            | 115           | 0.01%           | 0.002%        |
| 27        | 5.986       | 1443          | 1445        | 1448         | rVB      | 225            | 90            | 0.01%           | 0.001%        |
| 28        | 6.006       | 1448          | 1451        | 1452         | rBV      | 227            | 125           | 0.02%           | 0.002%        |
| 29        | 6.051       | 1462          | 1465        | 1469         | rVB      | 275            | 148           | 0.02%           | 0.002%        |
| 30        | 6.076       | 1469          | 1473        | 1474         | rBV      | 126            | 84            | 0.01%           | 0.001%        |
| 31        | 6.244       | 1510          | 1525        | 1546         | rBV      | 283944         | 539018        | 66.06%          | 8.133%        |
| 32        | 6.523       | 1608          | 1612        | 1614         | rBV2     | 975            | 933           | 0.11%           | 0.014%        |
| 33        | 6.565       | 1622          | 1625        | 1627         | rBV      | 175            | 101           | 0.01%           | 0.002%        |
| 34        | 6.684       | 1648          | 1662        | 1683         | rBV      | 183984         | 359704        | 44.08%          | 5.427%        |
| 35        | 6.944       | 1741          | 1743        | 1746         | rBV      | 173            | 85            | 0.01%           | 0.001%        |
| 36        | 7.012       | 1762          | 1764        | 1766         | rBV      | 196            | 122           | 0.01%           | 0.002%        |

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 COMD8

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.035  | 1770 | 1771 | 1772 | rBV  | 93     | 22     | 0.00%  | 0.000%  |
| 38 | 7.125  | 1796 | 1799 | 1801 | rBV  | 209    | 119    | 0.01%  | 0.002%  |
| 39 | 7.153  | 1805 | 1808 | 1810 | rBV  | 255    | 184    | 0.02%  | 0.003%  |
| 40 | 7.221  | 1827 | 1829 | 1833 | rBV2 | 242    | 163    | 0.02%  | 0.002%  |
| 41 | 7.240  | 1833 | 1835 | 1838 | rBV  | 171    | 115    | 0.01%  | 0.002%  |
| 42 | 7.414  | 1886 | 1889 | 1895 | rBV2 | 220    | 180    | 0.02%  | 0.003%  |
| 43 | 7.436  | 1895 | 1896 | 1897 | rVB  | 167    | 32     | 0.00%  | 0.000%  |
| 44 | 7.452  | 1898 | 1901 | 1903 | rVV  | 174    | 104    | 0.01%  | 0.002%  |
| 45 | 7.562  | 1920 | 1935 | 1953 | rBV  | 104326 | 181612 | 22.26% | 2.740%  |
| 46 | 7.893  | 2025 | 2038 | 2061 | rBV  | 379545 | 653363 | 80.07% | 9.858%  |
| 47 | 8.083  | 2094 | 2097 | 2099 | rBV  | 247    | 146    | 0.02%  | 0.002%  |
| 48 | 8.173  | 2114 | 2125 | 2143 | rBV  | 72161  | 121227 | 14.86% | 1.829%  |
| 49 | 8.536  | 2235 | 2238 | 2240 | rBV2 | 233    | 150    | 0.02%  | 0.002%  |
| 50 | 8.549  | 2240 | 2242 | 2250 | rVB2 | 187    | 185    | 0.02%  | 0.003%  |
| 51 | 8.629  | 2254 | 2267 | 2294 | rBV  | 200433 | 368612 | 45.17% | 5.562%  |
| 52 | 9.067  | 2400 | 2403 | 2405 | rBV  | 174    | 120    | 0.01%  | 0.002%  |
| 53 | 9.137  | 2422 | 2425 | 2426 | rBV  | 181    | 90     | 0.01%  | 0.001%  |
| 54 | 9.414  | 2498 | 2511 | 2539 | rBV  | 384524 | 695933 | 85.29% | 10.500% |
| 55 | 10.025 | 2698 | 2701 | 2704 | rVB  | 250    | 142    | 0.02%  | 0.002%  |
| 56 | 10.362 | 2803 | 2806 | 2809 | rBV  | 248    | 167    | 0.02%  | 0.003%  |
| 57 | 10.385 | 2810 | 2813 | 2815 | rBV  | 344    | 166    | 0.02%  | 0.003%  |
| 58 | 10.555 | 2863 | 2866 | 2869 | rBV  | 205    | 187    | 0.02%  | 0.003%  |
| 59 | 10.568 | 2869 | 2870 | 2872 | rVB  | 259    | 85     | 0.01%  | 0.001%  |
| 60 | 10.616 | 2882 | 2885 | 2888 | rBV2 | 206    | 137    | 0.02%  | 0.002%  |
| 61 | 10.751 | 2915 | 2927 | 2950 | rVB  | 275022 | 438487 | 53.74% | 6.616%  |
| 62 | 10.973 | 2994 | 2996 | 3003 | rVB  | 249    | 178    | 0.02%  | 0.003%  |
| 63 | 11.005 | 3003 | 3006 | 3008 | rBV  | 204    | 103    | 0.01%  | 0.002%  |
| 64 | 11.240 | 3077 | 3079 | 3081 | rVB2 | 339    | 155    | 0.02%  | 0.002%  |
| 65 | 11.275 | 3088 | 3090 | 3093 | rBV  | 161    | 70     | 0.01%  | 0.001%  |
| 66 | 11.472 | 3147 | 3151 | 3154 | rBV2 | 312    | 226    | 0.03%  | 0.003%  |
| 67 | 11.565 | 3178 | 3180 | 3183 | rVB2 | 185    | 102    | 0.01%  | 0.002%  |
| 68 | 11.626 | 3195 | 3199 | 3202 | rBV  | 286    | 172    | 0.02%  | 0.003%  |
| 69 | 11.706 | 3222 | 3224 | 3228 | rBV  | 238    | 133    | 0.02%  | 0.002%  |
| 70 | 11.742 | 3228 | 3235 | 3243 | rBV3 | 2766   | 3825   | 0.47%  | 0.058%  |
| 71 | 11.806 | 3243 | 3255 | 3277 | rBV  | 418970 | 707530 | 86.71% | 10.675% |
| 72 | 12.076 | 3335 | 3339 | 3341 | rBV  | 594    | 427    | 0.05%  | 0.006%  |
| 73 | 12.189 | 3362 | 3374 | 3393 | rBV  | 389722 | 659130 | 80.78% | 9.945%  |
| 74 | 12.523 | 3476 | 3478 | 3480 | rBV  | 293    | 190    | 0.02%  | 0.003%  |
| 75 | 12.584 | 3494 | 3497 | 3500 | rBV  | 268    | 169    | 0.02%  | 0.003%  |
| 76 | 12.742 | 3545 | 3546 | 3554 | rBV2 | 316    | 292    | 0.04%  | 0.004%  |

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ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0MD8

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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 | 12.870 | 3583 | 3586 | 3587 | rBV  | 286  | 117  | 0.01% | 0.002% |
| 78 | 13.121 | 3662 | 3664 | 3665 | rBV  | 274  | 110  | 0.01% | 0.002% |
| 79 | 13.253 | 3703 | 3705 | 3706 | rBV  | 314  | 102  | 0.01% | 0.002% |
| 80 | 13.385 | 3744 | 3746 | 3747 | rBV  | 322  | 133  | 0.02% | 0.002% |
| 81 | 13.783 | 3866 | 3870 | 3875 | rBV2 | 556  | 558  | 0.07% | 0.008% |
| 82 | 13.845 | 3881 | 3889 | 3898 | rBV5 | 4576 | 6829 | 0.84% | 0.103% |

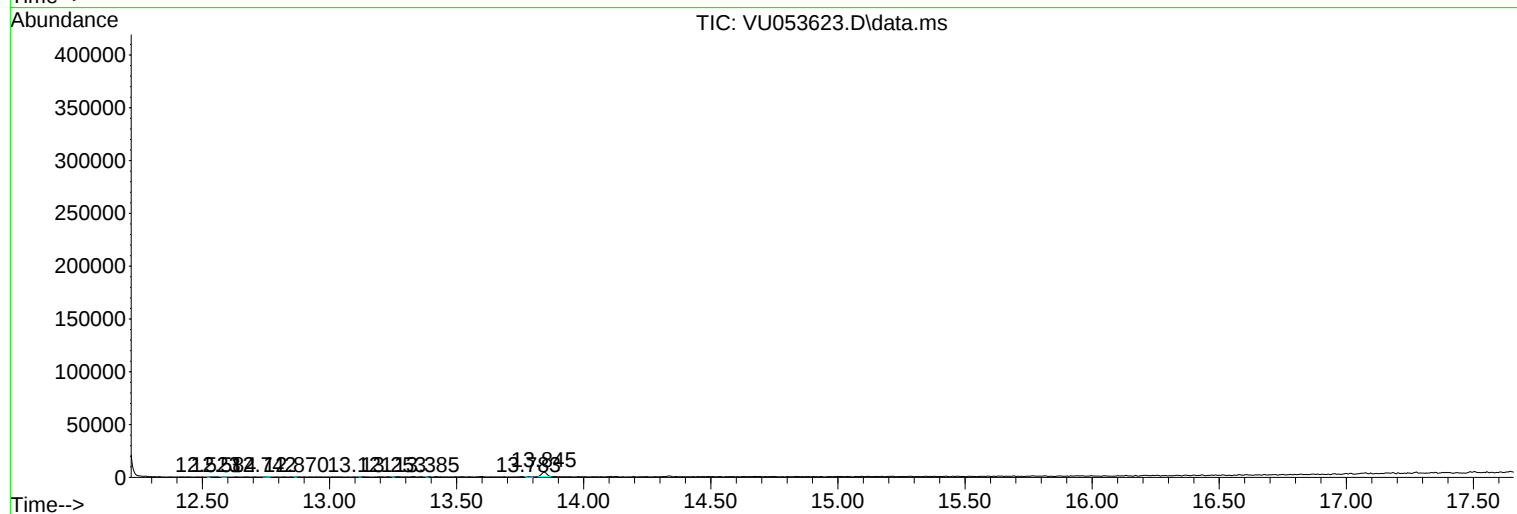
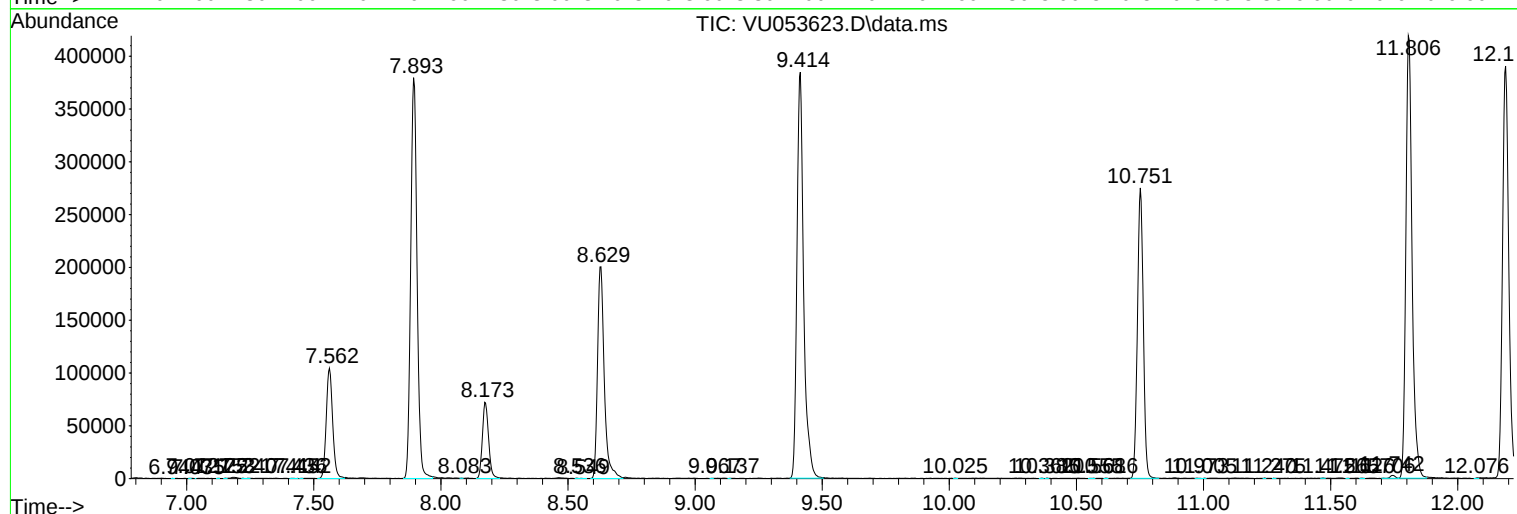
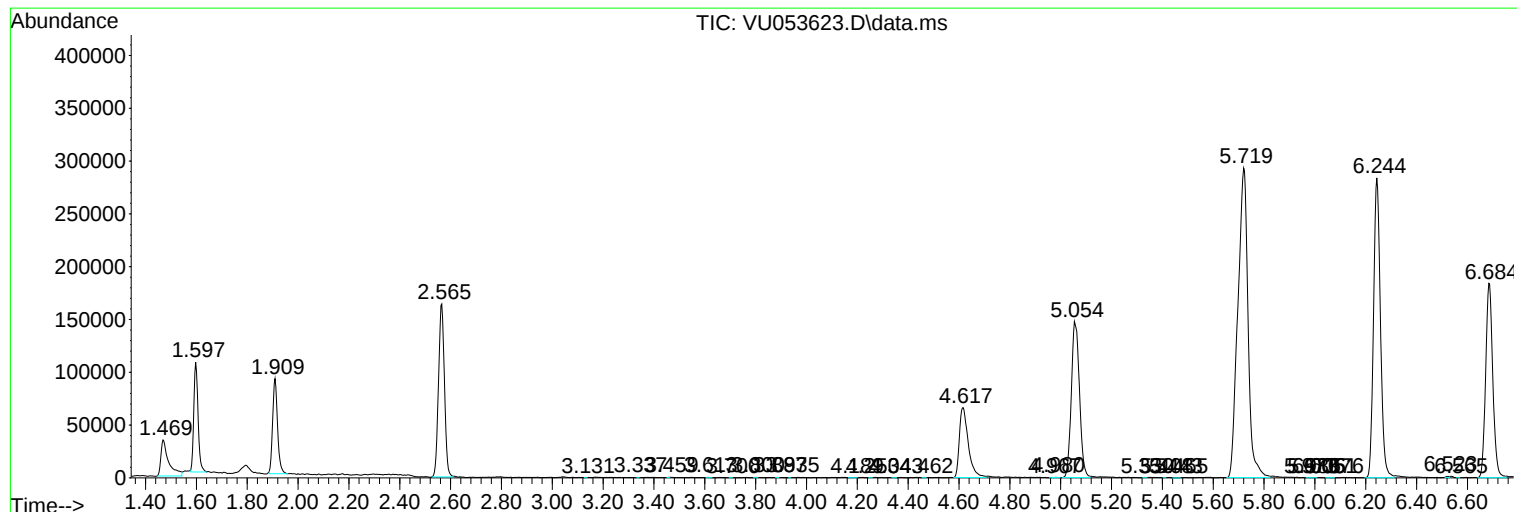
Sum of corrected areas: 6627833

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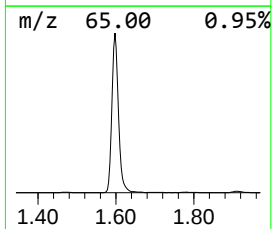
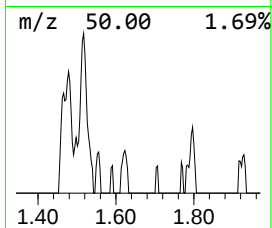
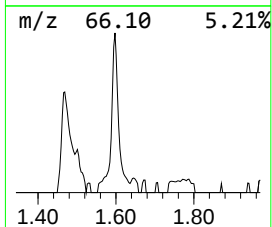
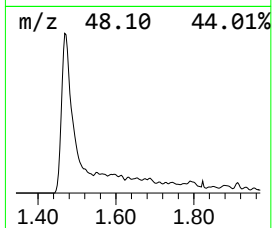
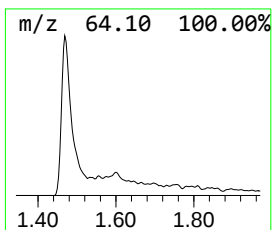
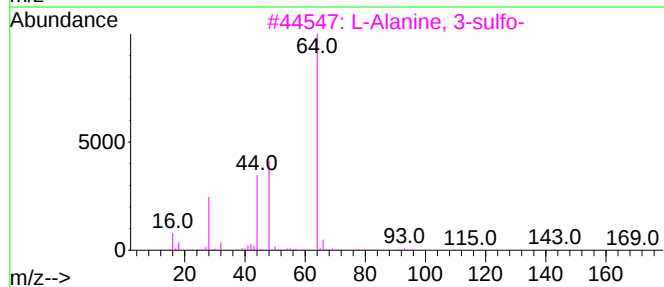
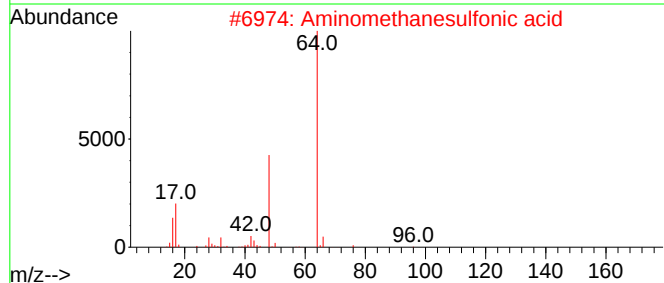
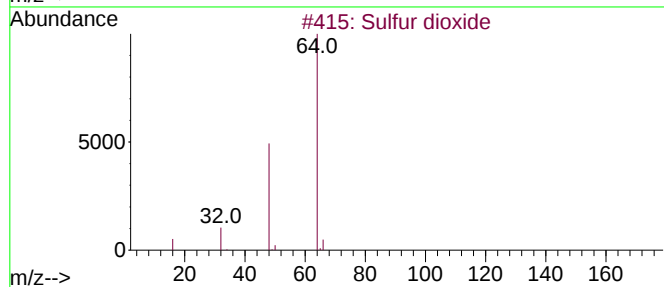
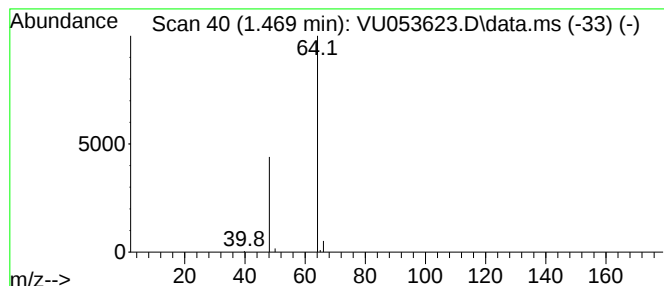
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM033123WMA.M  
Quant Title : VOC Analysis

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

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

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.469 | 6.63 ug/L | 71457 | 1,4-Difluorobenzene | 6.244 |

| 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    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.469 | 6.6     | ug/L  | 71457    | 1                     | 6.244 | 539018 | 50.0 |