

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\  
 Data File : VU023748.D  
 Acq On : 08 May 2018 20:29  
 Operator : MD/SY  
 Sample : J2746-02  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

## 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 : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
 Title : VOC Analysis

Signal : TIC

| 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         | 0.638       | 9             | 15          | 17           | rBV2     | 198            | 181           | 0.001%          | 0.001%        |
| 2         | 0.844       | 75            | 79          | 84           | rBV2     | 116            | 108           | 0.00%           | 0.001%        |
| 3         | 0.973       | 113           | 119         | 122          | rBV2     | 154            | 175           | 0.00%           | 0.001%        |
| 4         | 1.088       | 148           | 155         | 175          | rBV      | 354442         | 410860        | 11.41%          | 2.777%        |
| 5         | 1.182       | 179           | 184         | 195          | rVV2     | 13166          | 14524         | 0.40%           | 0.098%        |
| 6         | 1.281       | 207           | 215         | 231          | rBV      | 105329         | 262345        | 7.28%           | 1.773%        |
| 7         | 1.397       | 246           | 251         | 284          | rVB      | 203805         | 307874        | 8.55%           | 2.081%        |
| 8         | 1.680       | 332           | 339         | 353          | rVB      | 132678         | 169863        | 4.72%           | 1.148%        |
| 9         | 1.886       | 397           | 403         | 418          | rVB      | 30281          | 42932         | 1.19%           | 0.290%        |
| 10        | 2.272       | 512           | 523         | 536          | rBV      | 300018         | 450553        | 12.51%          | 3.046%        |
| 11        | 2.445       | 569           | 577         | 578          | rBV3     | 494            | 566           | 0.02%           | 0.004%        |
| 12        | 2.474       | 579           | 586         | 591          | rBV      | 928            | 1293          | 0.04%           | 0.009%        |
| 13        | 2.619       | 625           | 631         | 639          | rBV2     | 557            | 825           | 0.02%           | 0.006%        |
| 14        | 2.703       | 651           | 657         | 664          | rVB4     | 936            | 1043          | 0.03%           | 0.007%        |
| 15        | 2.834       | 690           | 698         | 706          | rVB3     | 701            | 1214          | 0.03%           | 0.008%        |
| 16        | 2.886       | 711           | 714         | 716          | rBV      | 443            | 304           | 0.01%           | 0.002%        |
| 17        | 2.953       | 732           | 735         | 738          | rVV2     | 143            | 102           | 0.00%           | 0.001%        |
| 18        | 2.985       | 738           | 745         | 753          | rVB3     | 1074           | 1517          | 0.04%           | 0.010%        |
| 19        | 3.072       | 767           | 772         | 779          | rBV2     | 131            | 214           | 0.01%           | 0.001%        |
| 20        | 3.355       | 855           | 860         | 863          | rBV2     | 155            | 153           | 0.00%           | 0.001%        |
| 21        | 3.384       | 864           | 869         | 874          | rBV2     | 320            | 392           | 0.01%           | 0.003%        |
| 22        | 3.529       | 911           | 914         | 916          | rBV2     | 166            | 98            | 0.00%           | 0.001%        |
| 23        | 3.590       | 930           | 933         | 938          | rVB2     | 123            | 109           | 0.00%           | 0.001%        |
| 24        | 3.821       | 1003          | 1005        | 1017         | rVB2     | 175            | 233           | 0.01%           | 0.002%        |
| 25        | 3.870       | 1017          | 1020        | 1023         | rBV      | 119            | 91            | 0.00%           | 0.001%        |
| 26        | 4.120       | 1096          | 1098        | 1101         | rBV2     | 153            | 104           | 0.00%           | 0.001%        |
| 27        | 4.178       | 1101          | 1116        | 1124         | rBV      | 123385         | 293933        | 8.16%           | 1.987%        |
| 28        | 4.532       | 1224          | 1226        | 1228         | rBV      | 246            | 165           | 0.00%           | 0.001%        |
| 29        | 4.571       | 1234          | 1238        | 1240         | rBV2     | 149            | 91            | 0.00%           | 0.001%        |
| 30        | 4.590       | 1240          | 1244        | 1246         | rBV      | 215            | 189           | 0.01%           | 0.001%        |
| 31        | 4.651       | 1246          | 1263        | 1289         | rBV      | 209333         | 488594        | 13.56%          | 3.303%        |
| 32        | 4.886       | 1330          | 1336        | 1344         | rBV2     | 737            | 1047          | 0.03%           | 0.007%        |
| 33        | 4.969       | 1359          | 1362        | 1364         | rBV      | 187            | 133           | 0.00%           | 0.001%        |
| 34        | 4.995       | 1368          | 1370        | 1372         | rVV2     | 388            | 222           | 0.01%           | 0.002%        |

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |         |         |         |         |
|----|-------|------|------|------|------|---------|---------|---------|---------|
| 35 | 5.030 | 1376 | 1381 | 1385 | rVB2 | 110     | 114     | 0.00%   | 0.001%  |
| 36 | 5.114 | 1405 | 1407 | 1410 | rBV  | 140     | 95      | 0.00%   | 0.001%  |
| 37 | 5.165 | 1419 | 1423 | 1426 | rBV2 | 181     | 134     | 0.00%   | 0.001%  |
| 38 | 5.188 | 1427 | 1430 | 1432 | rBV  | 142     | 100     | 0.00%   | 0.001%  |
| 39 | 5.227 | 1439 | 1442 | 1447 | rBV2 | 128     | 124     | 0.00%   | 0.001%  |
| 40 | 5.345 | 1453 | 1479 | 1516 | rBV2 | 434686  | 1295980 | 35.98%  | 8.760%  |
| 41 | 5.661 | 1573 | 1577 | 1579 | rBV2 | 230     | 173     | 0.00%   | 0.001%  |
| 42 | 5.699 | 1586 | 1589 | 1592 | rBV  | 125     | 118     | 0.00%   | 0.001%  |
| 43 | 5.718 | 1592 | 1595 | 1598 | rVV3 | 212     | 154     | 0.00%   | 0.001%  |
| 44 | 5.747 | 1601 | 1604 | 1610 | rVV2 | 294     | 378     | 0.01%   | 0.003%  |
| 45 | 5.889 | 1633 | 1648 | 1690 | rBV  | 400876  | 824941  | 22.90%  | 5.576%  |
| 46 | 6.191 | 1725 | 1742 | 1773 | rBV  | 1846434 | 3601874 | 100.00% | 24.347% |
| 47 | 6.336 | 1775 | 1787 | 1808 | rVB  | 290289  | 586687  | 16.29%  | 3.966%  |
| 48 | 6.551 | 1851 | 1854 | 1862 | rVB4 | 338     | 412     | 0.01%   | 0.003%  |
| 49 | 6.654 | 1881 | 1886 | 1889 | rBV2 | 220     | 169     | 0.00%   | 0.001%  |
| 50 | 6.670 | 1889 | 1891 | 1896 | rVB2 | 200     | 151     | 0.00%   | 0.001%  |
| 51 | 6.757 | 1916 | 1918 | 1921 | rVV  | 252     | 156     | 0.00%   | 0.001%  |
| 52 | 6.776 | 1922 | 1924 | 1927 | rVV  | 245     | 132     | 0.00%   | 0.001%  |
| 53 | 6.796 | 1928 | 1930 | 1935 | rVB  | 160     | 122     | 0.00%   | 0.001%  |
| 54 | 6.866 | 1943 | 1952 | 1959 | rBV2 | 519     | 728     | 0.02%   | 0.005%  |
| 55 | 6.902 | 1959 | 1963 | 1966 | rBV  | 171     | 149     | 0.00%   | 0.001%  |
| 56 | 6.953 | 1975 | 1979 | 1985 | rVB2 | 228     | 140     | 0.00%   | 0.001%  |
| 57 | 7.056 | 2008 | 2011 | 2015 | rVV2 | 188     | 118     | 0.00%   | 0.001%  |
| 58 | 7.165 | 2042 | 2045 | 2050 | rBV2 | 153     | 160     | 0.00%   | 0.001%  |
| 59 | 7.233 | 2053 | 2066 | 2088 | rBV  | 157484  | 281622  | 7.82%   | 1.904%  |
| 60 | 7.390 | 2113 | 2115 | 2119 | rVB2 | 266     | 175     | 0.00%   | 0.001%  |
| 61 | 7.432 | 2126 | 2128 | 2131 | rVB2 | 310     | 158     | 0.00%   | 0.001%  |
| 62 | 7.452 | 2131 | 2134 | 2136 | rBV2 | 190     | 135     | 0.00%   | 0.001%  |
| 63 | 7.487 | 2140 | 2145 | 2149 | rVV2 | 172     | 172     | 0.00%   | 0.001%  |
| 64 | 7.570 | 2154 | 2171 | 2217 | rBV  | 589047  | 1063145 | 29.52%  | 7.186%  |
| 65 | 7.853 | 2246 | 2259 | 2282 | rBV  | 105884  | 182577  | 5.07%   | 1.234%  |
| 66 | 8.075 | 2323 | 2328 | 2329 | rBV2 | 958     | 814     | 0.02%   | 0.006%  |
| 67 | 8.181 | 2352 | 2361 | 2366 | rBV3 | 2570    | 3748    | 0.10%   | 0.025%  |
| 68 | 8.233 | 2366 | 2377 | 2391 | rVV  | 80903   | 137507  | 3.82%   | 0.929%  |
| 69 | 8.313 | 2391 | 2402 | 2436 | rVV  | 410638  | 704798  | 19.57%  | 4.764%  |
| 70 | 8.490 | 2455 | 2457 | 2461 | rVB  | 413     | 311     | 0.01%   | 0.002%  |
| 71 | 8.599 | 2488 | 2491 | 2498 | rBV3 | 185     | 261     | 0.01%   | 0.002%  |

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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
 Title : VOC Analysis

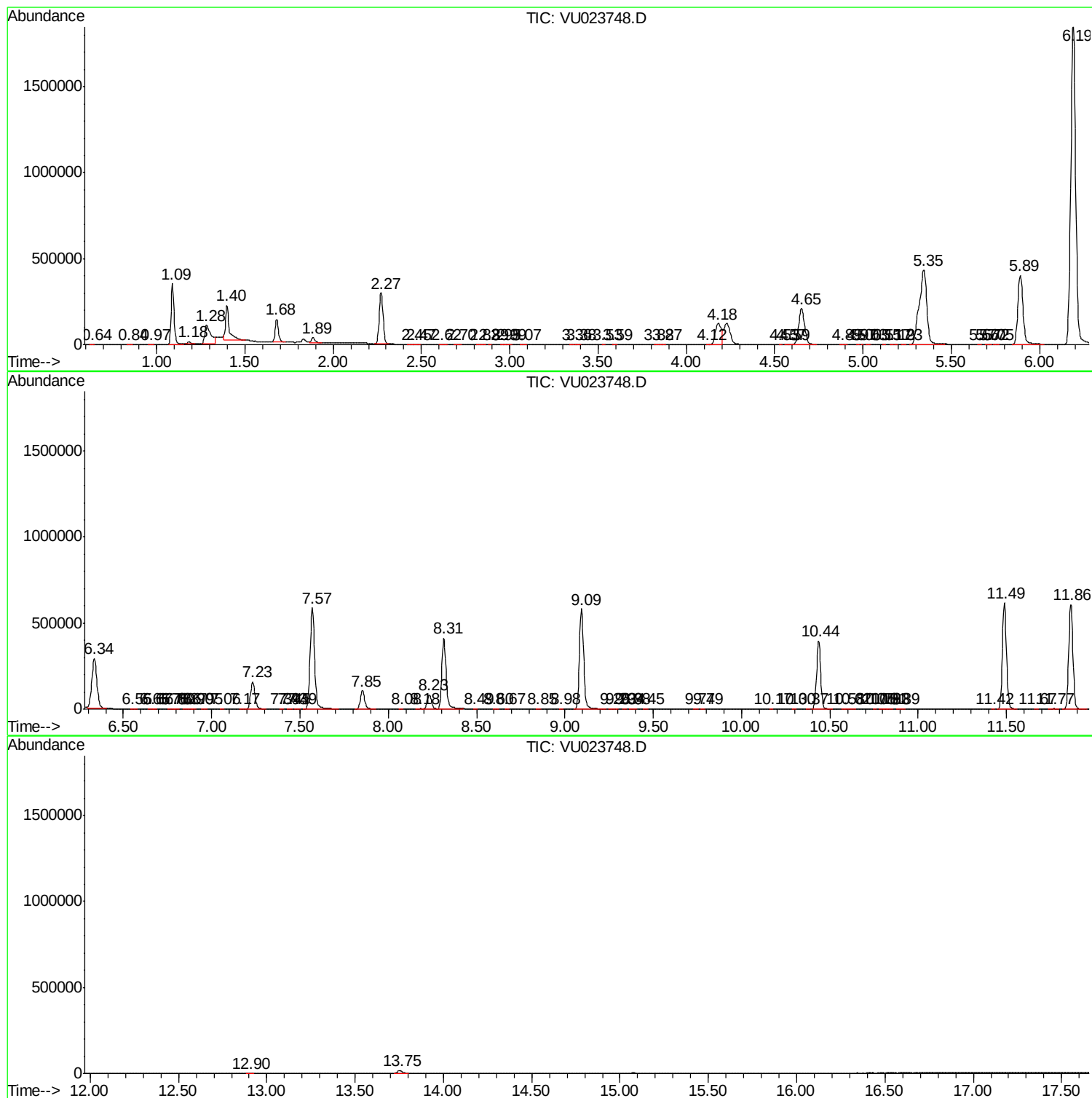
|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 72  | 8.667  | 2510 | 2512 | 2516 | rVB2 | 182    | 100     | 0.00%  | 0.001% |
| 73  | 8.850  | 2565 | 2569 | 2572 | rBV2 | 138    | 143     | 0.00%  | 0.001% |
| 74  | 8.979  | 2606 | 2609 | 2612 | rBV2 | 167    | 150     | 0.00%  | 0.001% |
| 75  | 9.095  | 2632 | 2645 | 2687 | rBV  | 582895 | 1002675 | 27.84% | 6.778% |
| 76  | 9.262  | 2692 | 2697 | 2704 | rVB3 | 794    | 988     | 0.03%  | 0.007% |
| 77  | 9.294  | 2705 | 2707 | 2709 | rBV  | 223    | 118     | 0.00%  | 0.001% |
| 78  | 9.342  | 2717 | 2722 | 2724 | rBV2 | 293    | 243     | 0.01%  | 0.002% |
| 79  | 9.377  | 2728 | 2733 | 2742 | rBV3 | 1215   | 1786    | 0.05%  | 0.012% |
| 80  | 9.455  | 2753 | 2757 | 2761 | rBV  | 212    | 167     | 0.00%  | 0.001% |
| 81  | 9.738  | 2842 | 2845 | 2849 | rVV2 | 172    | 119     | 0.00%  | 0.001% |
| 82  | 9.786  | 2855 | 2860 | 2861 | rBV2 | 483    | 426     | 0.01%  | 0.003% |
| 83  | 10.168 | 2976 | 2979 | 2981 | rBV3 | 345    | 210     | 0.01%  | 0.001% |
| 84  | 10.297 | 3015 | 3019 | 3022 | rBV  | 249    | 235     | 0.01%  | 0.002% |
| 85  | 10.374 | 3040 | 3043 | 3046 | rBV  | 219    | 119     | 0.00%  | 0.001% |
| 86  | 10.435 | 3050 | 3062 | 3086 | rVV  | 397043 | 633984  | 17.60% | 4.285% |
| 87  | 10.577 | 3103 | 3106 | 3108 | rBV2 | 148    | 98      | 0.00%  | 0.001% |
| 88  | 10.615 | 3108 | 3118 | 3127 | rVB3 | 1990   | 3321    | 0.09%  | 0.022% |
| 89  | 10.750 | 3158 | 3160 | 3163 | rBV  | 178    | 104     | 0.00%  | 0.001% |
| 90  | 10.786 | 3168 | 3171 | 3176 | rVB2 | 246    | 231     | 0.01%  | 0.002% |
| 91  | 10.815 | 3176 | 3180 | 3183 | rBV  | 245    | 165     | 0.00%  | 0.001% |
| 92  | 10.834 | 3183 | 3186 | 3192 | rBV  | 134    | 152     | 0.00%  | 0.001% |
| 93  | 10.892 | 3200 | 3204 | 3214 | rBV2 | 649    | 1057    | 0.03%  | 0.007% |
| 94  | 11.422 | 3367 | 3369 | 3372 | rBV3 | 349    | 152     | 0.00%  | 0.001% |
| 95  | 11.487 | 3377 | 3389 | 3411 | rBV  | 618035 | 990766  | 27.51% | 6.697% |
| 96  | 11.667 | 3442 | 3445 | 3448 | rBV  | 251    | 175     | 0.00%  | 0.001% |
| 97  | 11.766 | 3466 | 3476 | 3485 | rBV7 | 2191   | 3822    | 0.11%  | 0.026% |
| 98  | 11.863 | 3492 | 3506 | 3534 | rBV  | 607320 | 981111  | 27.24% | 6.632% |
| 99  | 12.898 | 3823 | 3828 | 3836 | rVB4 | 642    | 814     | 0.02%  | 0.006% |
| 100 | 13.754 | 4084 | 4094 | 4108 | rBV  | 17663  | 29824   | 0.83%  | 0.202% |

Sum of corrected areas: 14794034

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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



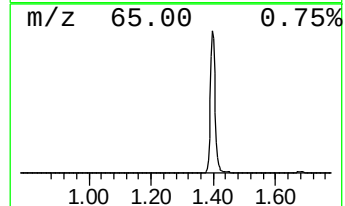
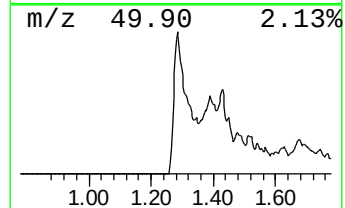
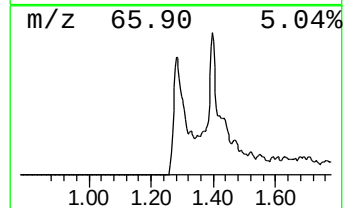
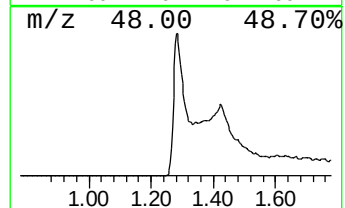
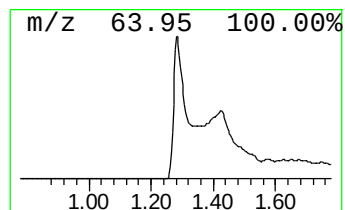
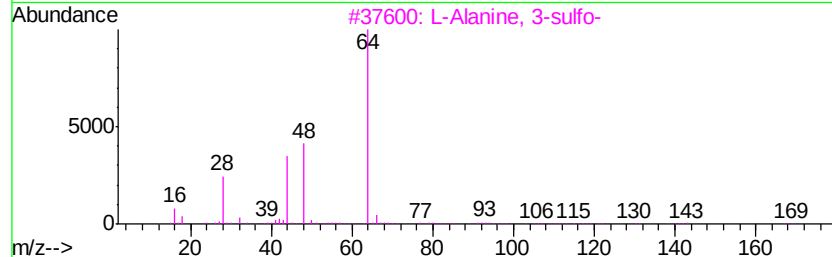
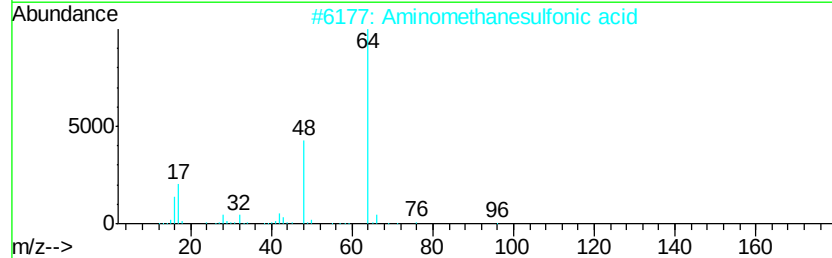
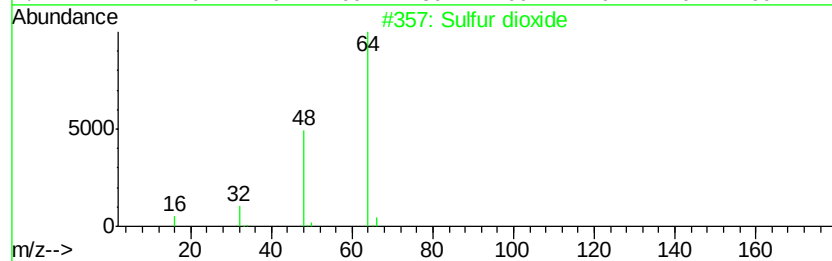
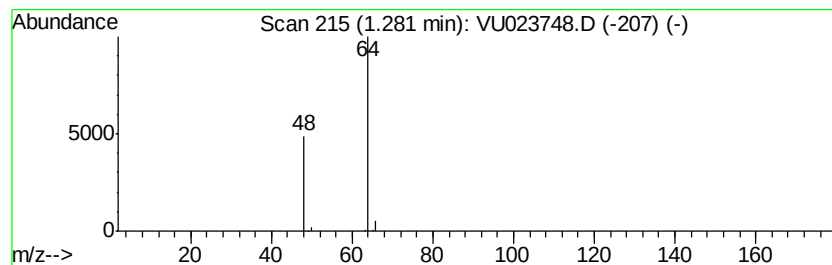
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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Sulfur dioxide Concentration Rank 3

| R.T.    | EstConc                   | Area         | Relative to ISTD    | R.T.      |
|---------|---------------------------|--------------|---------------------|-----------|
| 1.28    | 15.90 ug/L                | 262345       | 1,4-Difluorobenzene | 5.89      |
| Hit# of | 5                         | Tentative ID | MW MolForm          | CAS# Qual |
| 1       | Sulfur dioxide            | 64 O2S       | 007446-09-5         | 83        |
| 2       | Aminomethanesulfonic acid | 111 CH5NO3S  | 013881-91-9         | 74        |
| 3       | L-Alanine, 3-sulfo-       | 169 C3H7NO5S | 000498-40-8         | 9         |
| 4       | Sulfur dioxide            | 64 O2S       | 007446-09-5         | 5         |
| 5       | Ethene, 1,1-difluoro-     | 64 C2H2F2    | 000075-38-7         | 4         |



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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| Sulfur dioxide   | 1.28 | 15.9    | ug/L  | 262345   | 1                     | 5.89 | 824941 | 50.0 |