

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX041923\  
 Data File : VX035177.D  
 Acq On : 19 Apr 2023 18:10  
 Operator : JC/MD  
 Sample : 02333-17  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 COMH2

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\_X\Method\SFAMXML041823WMA.M  
 Title : VOC Analysis

Signal : TIC: VX035177.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         | 1.258       | 24            | 28          | 42           | rBV      | 90711          | 255408        | 18.48%          | 2.337%        |
| 2         | 1.368       | 43            | 46          | 58           | rVB      | 164093         | 189405        | 13.71%          | 1.733%        |
| 3         | 1.672       | 92            | 96          | 108          | rVB      | 122316         | 154988        | 11.22%          | 1.418%        |
| 4         | 2.306       | 194           | 200         | 210          | rBV      | 309095         | 483092        | 34.96%          | 4.421%        |
| 5         | 2.520       | 230           | 235         | 239          | rVB2     | 525            | 880           | 0.06%           | 0.008%        |
| 6         | 2.721       | 264           | 268         | 271          | rBV2     | 320            | 427           | 0.03%           | 0.004%        |
| 7         | 2.794       | 276           | 280         | 283          | rVB4     | 861            | 1431          | 0.10%           | 0.013%        |
| 8         | 2.940       | 297           | 304         | 317          | rVB      | 7559           | 18511         | 1.34%           | 0.169%        |
| 9         | 3.026       | 317           | 318         | 320          | rBV2     | 264            | 235           | 0.02%           | 0.002%        |
| 10        | 3.111       | 330           | 332         | 333          | rVV      | 469            | 249           | 0.02%           | 0.002%        |
| 11        | 3.184       | 340           | 344         | 347          | rVB      | 205            | 312           | 0.02%           | 0.003%        |
| 12        | 3.233       | 350           | 352         | 359          | rVB2     | 285            | 533           | 0.04%           | 0.005%        |
| 13        | 3.361       | 370           | 373         | 375          | rVV2     | 192            | 199           | 0.01%           | 0.002%        |
| 14        | 3.574       | 404           | 408         | 411          | rBV2     | 245            | 346           | 0.03%           | 0.003%        |
| 15        | 3.654       | 420           | 421         | 427          | rVB2     | 199            | 342           | 0.02%           | 0.003%        |
| 16        | 3.715       | 427           | 431         | 434          | rBV2     | 325            | 476           | 0.03%           | 0.004%        |
| 17        | 3.782       | 438           | 442         | 443          | rBV2     | 300            | 337           | 0.02%           | 0.003%        |
| 18        | 3.946       | 467           | 469         | 470          | rVV      | 403            | 217           | 0.02%           | 0.002%        |
| 19        | 4.001       | 474           | 478         | 480          | rBV2     | 244            | 304           | 0.02%           | 0.003%        |
| 20        | 4.160       | 502           | 504         | 506          | rBV      | 360            | 257           | 0.02%           | 0.002%        |
| 21        | 4.404       | 542           | 544         | 546          | rVB2     | 321            | 246           | 0.02%           | 0.002%        |
| 22        | 4.471       | 546           | 555         | 572          | rBV2     | 74029          | 252429        | 18.27%          | 2.310%        |
| 23        | 4.763       | 601           | 603         | 607          | rVB2     | 447            | 394           | 0.03%           | 0.004%        |
| 24        | 4.800       | 607           | 609         | 613          | rBV2     | 279            | 310           | 0.02%           | 0.003%        |
| 25        | 5.056       | 639           | 651         | 666          | rBV      | 172824         | 518837        | 37.55%          | 4.748%        |
| 26        | 5.452       | 713           | 716         | 719          | rVB2     | 234            | 253           | 0.02%           | 0.002%        |
| 27        | 5.550       | 727           | 732         | 736          | rBV3     | 1029           | 2120          | 0.15%           | 0.019%        |
| 28        | 5.702       | 755           | 757         | 758          | rVB2     | 313            | 205           | 0.01%           | 0.002%        |
| 29        | 5.775       | 768           | 769         | 770          | rBV      | 429            | 205           | 0.01%           | 0.002%        |
| 30        | 5.800       | 771           | 773         | 777          | rVB2     | 329            | 279           | 0.02%           | 0.003%        |
| 31        | 5.970       | 789           | 801         | 820          | rBV2     | 463526         | 1381901       | 100.00%         | 12.645%       |
| 32        | 6.275       | 849           | 851         | 852          | rBV2     | 329            | 290           | 0.02%           | 0.003%        |
| 33        | 6.312       | 856           | 857         | 860          | rBV      | 417            | 312           | 0.02%           | 0.003%        |
| 34        | 6.452       | 878           | 880         | 882          | rBV      | 368            | 228           | 0.02%           | 0.002%        |
| 35        | 6.550       | 891           | 896         | 898          | rBV2     | 292            | 447           | 0.03%           | 0.004%        |
| 36        | 6.763       | 921           | 931         | 944          | rBV      | 459794         | 1110368       | 80.35%          | 10.160%       |

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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\_X\Method\SFAMXML041823WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 7.080  | 980  | 983  | 984  | rBV2 | 183    | 239     | 0.02%  | 0.002%  |
| 38 | 7.104  | 984  | 987  | 988  | rBV  | 1339   | 1172    | 0.08%  | 0.011%  |
| 39 | 7.305  | 1012 | 1020 | 1037 | rVV  | 277366 | 613731  | 44.41% | 5.616%  |
| 40 | 7.446  | 1041 | 1043 | 1045 | rVB2 | 408    | 326     | 0.02%  | 0.003%  |
| 41 | 7.482  | 1045 | 1049 | 1050 | rBV2 | 705    | 790     | 0.06%  | 0.007%  |
| 42 | 7.702  | 1082 | 1085 | 1087 | rBV2 | 302    | 262     | 0.02%  | 0.002%  |
| 43 | 7.757  | 1092 | 1094 | 1095 | rVB  | 370    | 212     | 0.02%  | 0.002%  |
| 44 | 7.879  | 1112 | 1114 | 1117 | rBV2 | 285    | 291     | 0.02%  | 0.003%  |
| 45 | 7.940  | 1122 | 1124 | 1125 | rBV2 | 399    | 371     | 0.03%  | 0.003%  |
| 46 | 8.110  | 1149 | 1152 | 1153 | rBV  | 203    | 207     | 0.01%  | 0.002%  |
| 47 | 8.165  | 1159 | 1161 | 1164 | rBV2 | 163    | 214     | 0.02%  | 0.002%  |
| 48 | 8.238  | 1170 | 1173 | 1176 | rBV2 | 159    | 236     | 0.02%  | 0.002%  |
| 49 | 8.324  | 1181 | 1187 | 1202 | rBV  | 132356 | 228442  | 16.53% | 2.090%  |
| 50 | 8.488  | 1212 | 1214 | 1216 | rBV3 | 347    | 264     | 0.02%  | 0.002%  |
| 51 | 8.519  | 1216 | 1219 | 1223 | rVB5 | 665    | 984     | 0.07%  | 0.009%  |
| 52 | 8.555  | 1223 | 1225 | 1229 | rVB2 | 443    | 617     | 0.04%  | 0.006%  |
| 53 | 8.592  | 1229 | 1231 | 1232 | rBV  | 211    | 211     | 0.02%  | 0.002%  |
| 54 | 8.647  | 1234 | 1240 | 1259 | rBV  | 720332 | 1120218 | 81.06% | 10.251% |
| 55 | 8.878  | 1276 | 1278 | 1281 | rVB  | 359    | 325     | 0.02%  | 0.003%  |
| 56 | 8.952  | 1284 | 1290 | 1302 | rBV  | 91234  | 140519  | 10.17% | 1.286%  |
| 57 | 9.104  | 1313 | 1315 | 1317 | rVB  | 560    | 394     | 0.03%  | 0.004%  |
| 58 | 9.183  | 1325 | 1328 | 1332 | rVB2 | 309    | 400     | 0.03%  | 0.004%  |
| 59 | 9.220  | 1332 | 1334 | 1337 | rBV3 | 221    | 268     | 0.02%  | 0.002%  |
| 60 | 9.275  | 1339 | 1343 | 1350 | rVB5 | 1134   | 1632    | 0.12%  | 0.015%  |
| 61 | 9.384  | 1356 | 1361 | 1375 | rBV  | 372504 | 539062  | 39.01% | 4.933%  |
| 62 | 9.677  | 1407 | 1409 | 1411 | rBV2 | 384    | 353     | 0.03%  | 0.003%  |
| 63 | 9.866  | 1438 | 1440 | 1443 | rVB2 | 500    | 537     | 0.04%  | 0.005%  |
| 64 | 9.909  | 1443 | 1447 | 1448 | rBV2 | 234    | 256     | 0.02%  | 0.002%  |
| 65 | 10.055 | 1465 | 1471 | 1483 | rBV  | 899751 | 1260892 | 91.24% | 11.538% |
| 66 | 10.281 | 1506 | 1508 | 1509 | rBV  | 320    | 196     | 0.01%  | 0.002%  |
| 67 | 10.299 | 1509 | 1511 | 1515 | rVB3 | 373    | 474     | 0.03%  | 0.004%  |
| 68 | 10.409 | 1526 | 1529 | 1530 | rBV2 | 287    | 323     | 0.02%  | 0.003%  |
| 69 | 10.427 | 1530 | 1532 | 1534 | rVV  | 354    | 205     | 0.01%  | 0.002%  |
| 70 | 10.537 | 1548 | 1550 | 1552 | rVB2 | 366    | 264     | 0.02%  | 0.002%  |
| 71 | 10.567 | 1552 | 1555 | 1556 | rBV2 | 230    | 220     | 0.02%  | 0.002%  |
| 72 | 10.628 | 1561 | 1565 | 1566 | rBV2 | 174    | 199     | 0.01%  | 0.002%  |
| 73 | 11.043 | 1632 | 1633 | 1637 | rVB  | 453    | 286     | 0.02%  | 0.003%  |
| 74 | 11.189 | 1652 | 1657 | 1668 | rBV  | 433210 | 578445  | 41.86% | 5.293%  |
| 75 | 11.427 | 1693 | 1696 | 1700 | rBV2 | 432    | 737     | 0.05%  | 0.007%  |
| 76 | 11.707 | 1740 | 1742 | 1744 | rBV  | 325    | 214     | 0.02%  | 0.002%  |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_X\Method\SFAMXML041823WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |         |
|-----|--------|------|------|------|------|--------|---------|--------|---------|
| 77  | 11.969 | 1782 | 1785 | 1788 | rBV2 | 1597   | 2155    | 0.16%  | 0.020%  |
| 78  | 12.024 | 1788 | 1794 | 1806 | rVV  | 860222 | 1126702 | 81.53% | 10.310% |
| 79  | 12.219 | 1822 | 1826 | 1829 | rBV4 | 1485   | 1973    | 0.14%  | 0.018%  |
| 80  | 12.317 | 1837 | 1842 | 1854 | rBV  | 683602 | 909626  | 65.82% | 8.323%  |
| 81  | 12.731 | 1908 | 1910 | 1912 | rVB  | 323    | 230     | 0.02%  | 0.002%  |
| 82  | 12.768 | 1912 | 1916 | 1917 | rBV3 | 392    | 519     | 0.04%  | 0.005%  |
| 83  | 12.884 | 1933 | 1935 | 1938 | rBV  | 313    | 371     | 0.03%  | 0.003%  |
| 84  | 13.109 | 1970 | 1972 | 1976 | rVB  | 411    | 361     | 0.03%  | 0.003%  |
| 85  | 13.182 | 1983 | 1984 | 1986 | rBV2 | 244    | 203     | 0.01%  | 0.002%  |
| 86  | 13.274 | 1997 | 1999 | 2004 | rBV2 | 250    | 391     | 0.03%  | 0.004%  |
| 87  | 13.432 | 2020 | 2025 | 2026 | rBV  | 278    | 451     | 0.03%  | 0.004%  |
| 88  | 13.499 | 2034 | 2036 | 2039 | rVB2 | 246    | 226     | 0.02%  | 0.002%  |
| 89  | 13.591 | 2045 | 2051 | 2056 | rBV2 | 5135   | 7544    | 0.55%  | 0.069%  |
| 90  | 13.859 | 2093 | 2095 | 2098 | rVB2 | 383    | 372     | 0.03%  | 0.003%  |
| 91  | 13.896 | 2098 | 2101 | 2105 | rBV2 | 424    | 631     | 0.05%  | 0.006%  |
| 92  | 13.926 | 2105 | 2106 | 2109 | rVV2 | 286    | 251     | 0.02%  | 0.002%  |
| 93  | 13.963 | 2109 | 2112 | 2117 | rVV3 | 1724   | 2104    | 0.15%  | 0.019%  |
| 94  | 14.054 | 2125 | 2127 | 2130 | rBV3 | 183    | 212     | 0.02%  | 0.002%  |
| 95  | 14.152 | 2139 | 2143 | 2145 | rBV  | 357    | 544     | 0.04%  | 0.005%  |
| 96  | 14.390 | 2181 | 2182 | 2185 | rBV  | 370    | 324     | 0.02%  | 0.003%  |
| 97  | 14.505 | 2197 | 2201 | 2202 | rBV2 | 429    | 461     | 0.03%  | 0.004%  |
| 98  | 14.597 | 2215 | 2216 | 2219 | rBV2 | 399    | 295     | 0.02%  | 0.003%  |
| 99  | 15.036 | 2286 | 2288 | 2291 | rBV3 | 413    | 274     | 0.02%  | 0.003%  |
| 100 | 16.517 | 2529 | 2531 | 2534 | rVB3 | 778    | 434     | 0.03%  | 0.004%  |

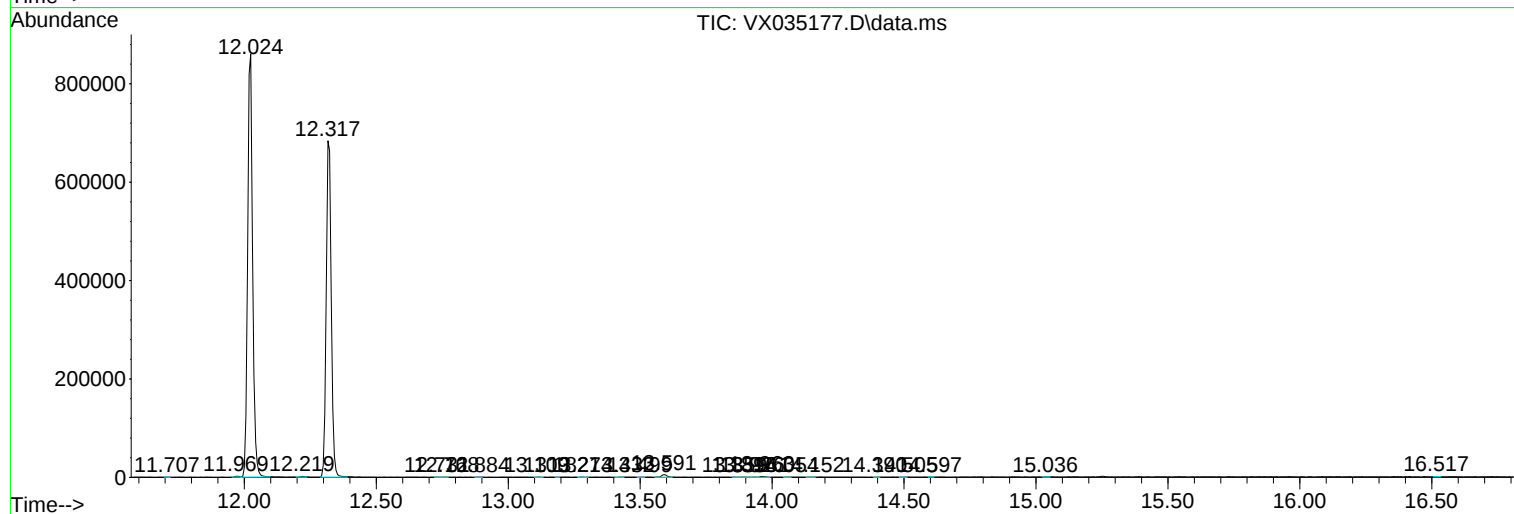
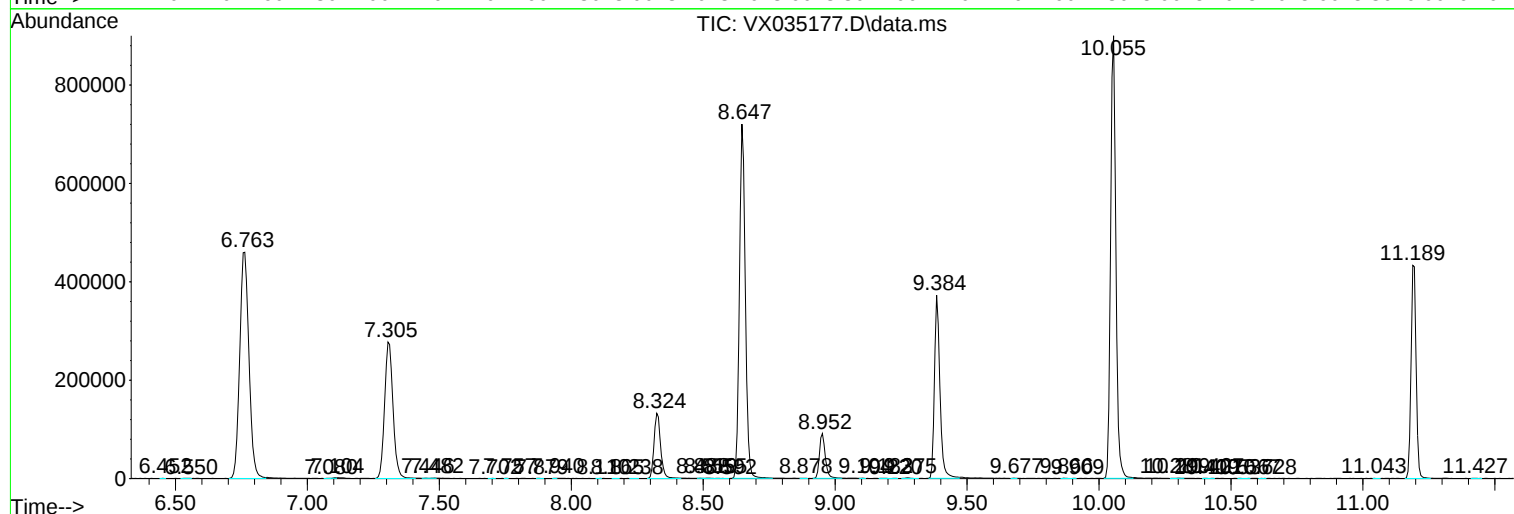
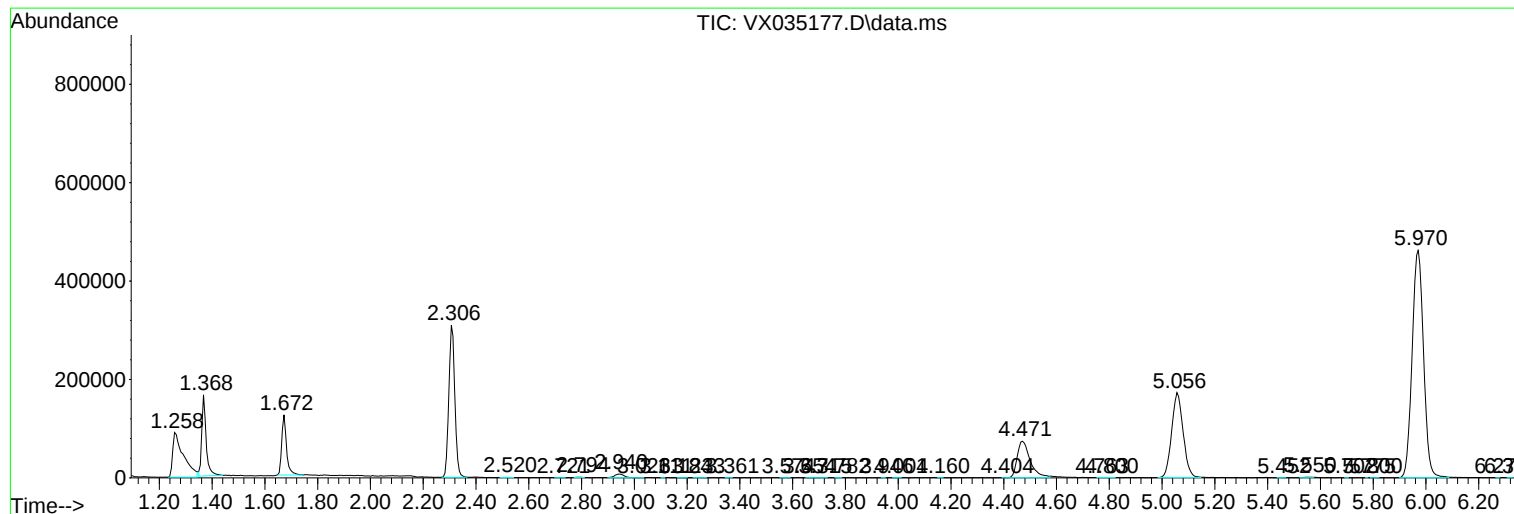
Sum of corrected areas: 10928415

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML041823WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX041923\  
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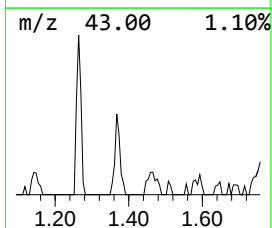
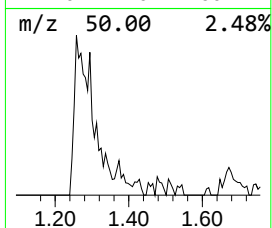
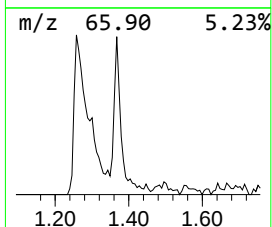
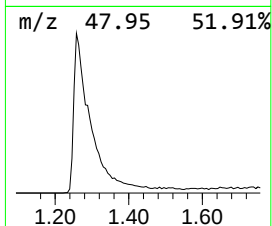
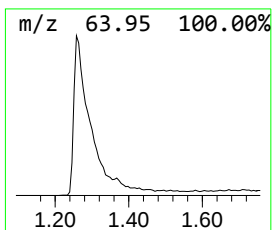
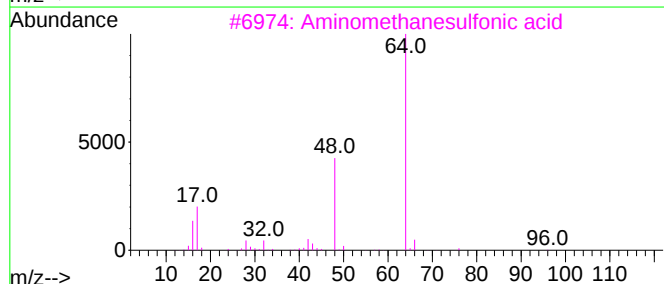
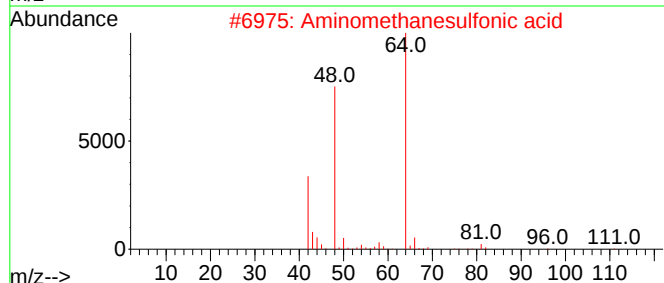
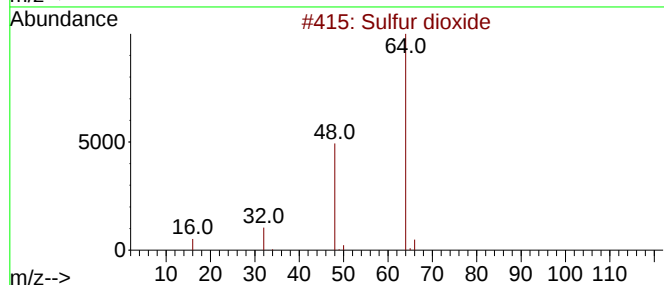
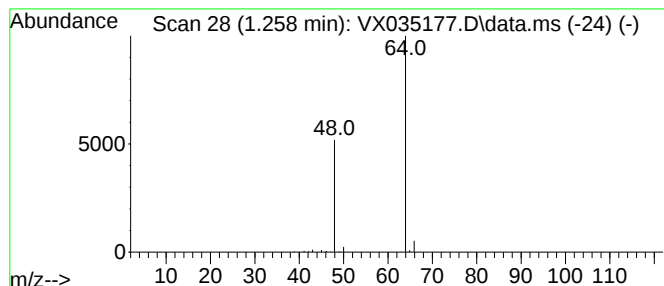
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML041823WMA.M  
Quant Title : VOC Analysis

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

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

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 1.258 | 11.50 ug/L | 255408 | 1,4-Difluorobenzene | 6.763 |

| 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    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                  |       |         |       |          | #                     | RT    | Resp    | Conc |
| Sulfur dioxide   | 1.258 | 11.5    | ug/L  | 255408   | 1                     | 6.763 | 1110370 | 50.0 |