

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062022\  
 Data File : VU049298.D  
 Acq On : 20 Jun 2022 12:17  
 Operator : SY/MD  
 Sample : N3395-03  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0152

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\SFAMULM061022WMA.M  
 Title : VOC Analysis

Signal : TIC: VU049298.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         | 1.485       | 35            | 45          | 56           | rBV2     | 16240          | 40516         | 4.11%           | 0.485%        |
| 2         | 1.601       | 74            | 81          | 99           | rVB      | 126061         | 141533        | 14.35%          | 1.693%        |
| 3         | 1.913       | 170           | 178         | 192          | rVB      | 95965          | 123039        | 12.47%          | 1.472%        |
| 4         | 2.569       | 369           | 382         | 395          | rBV      | 188196         | 303432        | 30.76%          | 3.629%        |
| 5         | 2.755       | 434           | 440         | 446          | rBV5     | 1505           | 2052          | 0.21%           | 0.025%        |
| 6         | 2.874       | 469           | 477         | 482          | rBV3     | 322            | 560           | 0.06%           | 0.007%        |
| 7         | 2.964       | 502           | 505         | 509          | rBV2     | 359            | 235           | 0.02%           | 0.003%        |
| 8         | 3.025       | 521           | 524         | 527          | rBV3     | 295            | 222           | 0.02%           | 0.003%        |
| 9         | 3.151       | 560           | 563         | 566          | rBV2     | 392            | 268           | 0.03%           | 0.003%        |
| 10        | 3.170       | 566           | 569         | 570          | rBV2     | 555            | 355           | 0.04%           | 0.004%        |
| 11        | 3.334       | 616           | 620         | 624          | rBV3     | 268            | 297           | 0.03%           | 0.004%        |
| 12        | 3.552       | 682           | 688         | 691          | rBV2     | 297            | 318           | 0.03%           | 0.004%        |
| 13        | 3.614       | 704           | 707         | 711          | rVB2     | 299            | 245           | 0.02%           | 0.003%        |
| 14        | 3.655       | 714           | 720         | 725          | rBV2     | 251            | 295           | 0.03%           | 0.004%        |
| 15        | 3.761       | 746           | 753         | 756          | rBV3     | 295            | 354           | 0.04%           | 0.004%        |
| 16        | 3.806       | 761           | 767         | 771          | rVV2     | 272            | 345           | 0.03%           | 0.004%        |
| 17        | 3.848       | 776           | 780         | 787          | rVB2     | 309            | 272           | 0.03%           | 0.003%        |
| 18        | 3.880       | 787           | 790         | 795          | rBV2     | 260            | 258           | 0.03%           | 0.003%        |
| 19        | 3.938       | 805           | 808         | 814          | rVB2     | 292            | 314           | 0.03%           | 0.004%        |
| 20        | 3.964       | 814           | 816         | 819          | rBV2     | 358            | 251           | 0.03%           | 0.003%        |
| 21        | 4.176       | 881           | 882         | 887          | rVB2     | 501            | 332           | 0.03%           | 0.004%        |
| 22        | 4.205       | 887           | 891         | 895          | rBV2     | 437            | 432           | 0.04%           | 0.005%        |
| 23        | 4.244       | 895           | 903         | 904          | rVV2     | 222            | 248           | 0.03%           | 0.003%        |
| 24        | 4.263       | 906           | 909         | 913          | rVB3     | 399            | 300           | 0.03%           | 0.004%        |
| 25        | 4.385       | 942           | 947         | 949          | rBV2     | 375            | 286           | 0.03%           | 0.003%        |
| 26        | 4.408       | 949           | 954         | 958          | rVV2     | 253            | 316           | 0.03%           | 0.004%        |
| 27        | 4.446       | 960           | 966         | 969          | rVB2     | 246            | 283           | 0.03%           | 0.003%        |
| 28        | 4.533       | 988           | 993         | 998          | rBV3     | 368            | 328           | 0.03%           | 0.004%        |
| 29        | 4.620       | 1007          | 1020        | 1047         | rBV      | 117357         | 291314        | 29.53%          | 3.484%        |
| 30        | 4.858       | 1091          | 1094        | 1097         | rVB2     | 464            | 331           | 0.03%           | 0.004%        |
| 31        | 5.064       | 1142          | 1158        | 1179         | rBV      | 179730         | 394118        | 39.96%          | 4.714%        |
| 32        | 5.298       | 1229          | 1231        | 1234         | rVB2     | 504            | 248           | 0.03%           | 0.003%        |
| 33        | 5.372       | 1238          | 1254        | 1276         | rBV      | 212617         | 431420        | 43.74%          | 5.160%        |
| 34        | 5.472       | 1283          | 1285        | 1293         | rVB3     | 398            | 340           | 0.03%           | 0.004%        |
| 35        | 5.565       | 1312          | 1314        | 1319         | rVB2     | 501            | 320           | 0.03%           | 0.004%        |
| 36        | 5.726       | 1341          | 1364        | 1392         | rBV2     | 361238         | 986386        | 100.00%         | 11.798%       |

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM061022WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 5.848  | 1399 | 1402 | 1405 | rBV4 | 363    | 262    | 0.03%  | 0.003% |
| 38 | 5.967  | 1436 | 1439 | 1443 | rBV4 | 413    | 368    | 0.04%  | 0.004% |
| 39 | 6.048  | 1461 | 1464 | 1469 | rBV2 | 338    | 270    | 0.03%  | 0.003% |
| 40 | 6.131  | 1487 | 1490 | 1493 | rVB2 | 434    | 261    | 0.03%  | 0.003% |
| 41 | 6.173  | 1499 | 1503 | 1506 | rVB  | 379    | 276    | 0.03%  | 0.003% |
| 42 | 6.250  | 1513 | 1527 | 1555 | rVV  | 336409 | 643240 | 65.21% | 7.693% |
| 43 | 6.411  | 1572 | 1577 | 1580 | rBV3 | 354    | 294    | 0.03%  | 0.004% |
| 44 | 6.533  | 1606 | 1615 | 1621 | rVB6 | 1808   | 2865   | 0.29%  | 0.034% |
| 45 | 6.691  | 1647 | 1664 | 1685 | rBV  | 237724 | 470033 | 47.65% | 5.622% |
| 46 | 6.800  | 1694 | 1698 | 1700 | rBV4 | 437    | 314    | 0.03%  | 0.004% |
| 47 | 6.851  | 1712 | 1714 | 1718 | rVB2 | 315    | 232    | 0.02%  | 0.003% |
| 48 | 6.880  | 1718 | 1723 | 1726 | rBV  | 383    | 391    | 0.04%  | 0.005% |
| 49 | 6.948  | 1741 | 1744 | 1746 | rBV2 | 353    | 243    | 0.02%  | 0.003% |
| 50 | 7.189  | 1811 | 1819 | 1825 | rBV4 | 1112   | 1855   | 0.19%  | 0.022% |
| 51 | 7.398  | 1882 | 1884 | 1892 | rVB2 | 241    | 275    | 0.03%  | 0.003% |
| 52 | 7.475  | 1902 | 1908 | 1914 | rBV3 | 357    | 494    | 0.05%  | 0.006% |
| 53 | 7.565  | 1924 | 1936 | 1959 | rBV  | 104641 | 188276 | 19.09% | 2.252% |
| 54 | 7.691  | 1968 | 1975 | 1980 | rBV4 | 1166   | 1578   | 0.16%  | 0.019% |
| 55 | 7.742  | 1985 | 1991 | 1996 | rVB3 | 323    | 414    | 0.04%  | 0.005% |
| 56 | 7.784  | 1996 | 2004 | 2007 | rBV3 | 429    | 592    | 0.06%  | 0.007% |
| 57 | 7.810  | 2010 | 2012 | 2015 | rVB3 | 595    | 323    | 0.03%  | 0.004% |
| 58 | 7.896  | 2025 | 2039 | 2060 | rBV  | 442439 | 771748 | 78.24% | 9.230% |
| 59 | 8.179  | 2114 | 2127 | 2149 | rBV2 | 71915  | 124685 | 12.64% | 1.491% |
| 60 | 8.308  | 2164 | 2167 | 2177 | rVB3 | 654    | 626    | 0.06%  | 0.007% |
| 61 | 8.414  | 2197 | 2200 | 2206 | rVB3 | 332    | 318    | 0.03%  | 0.004% |
| 62 | 8.472  | 2212 | 2218 | 2220 | rBV2 | 499    | 548    | 0.06%  | 0.007% |
| 63 | 8.533  | 2231 | 2237 | 2239 | rBV2 | 282    | 276    | 0.03%  | 0.003% |
| 64 | 8.633  | 2255 | 2268 | 2302 | rBV2 | 322602 | 645923 | 65.48% | 7.726% |
| 65 | 9.218  | 2448 | 2450 | 2455 | rVB3 | 310    | 234    | 0.02%  | 0.003% |
| 66 | 9.417  | 2499 | 2512 | 2543 | rBV  | 465317 | 780956 | 79.17% | 9.341% |
| 67 | 9.610  | 2569 | 2572 | 2576 | rVB2 | 340    | 262    | 0.03%  | 0.003% |
| 68 | 9.655  | 2581 | 2586 | 2589 | rBV2 | 318    | 288    | 0.03%  | 0.003% |
| 69 | 9.761  | 2615 | 2619 | 2622 | rBV3 | 352    | 296    | 0.03%  | 0.004% |
| 70 | 10.102 | 2722 | 2725 | 2728 | rBV2 | 369    | 240    | 0.02%  | 0.003% |
| 71 | 10.292 | 2781 | 2784 | 2788 | rVB2 | 331    | 251    | 0.03%  | 0.003% |
| 72 | 10.321 | 2788 | 2793 | 2795 | rBV2 | 310    | 257    | 0.03%  | 0.003% |
| 73 | 10.485 | 2840 | 2844 | 2846 | rBV  | 407    | 368    | 0.04%  | 0.004% |
| 74 | 10.755 | 2916 | 2928 | 2944 | rBV  | 339785 | 549848 | 55.74% | 6.576% |
| 75 | 10.890 | 2966 | 2970 | 2981 | rVB5 | 1573   | 2072   | 0.21%  | 0.025% |
| 76 | 10.977 | 2991 | 2997 | 3000 | rBV2 | 311    | 373    | 0.04%  | 0.004% |

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM061022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.276 | 3087 | 3090 | 3096 | rVB2 | 388    | 403    | 0.04%  | 0.005% |
| 78  | 11.546 | 3171 | 3174 | 3177 | rBV  | 331    | 226    | 0.02%  | 0.003% |
| 79  | 11.694 | 3215 | 3220 | 3223 | rBV2 | 354    | 333    | 0.03%  | 0.004% |
| 80  | 11.729 | 3227 | 3231 | 3234 | rBV3 | 323    | 308    | 0.03%  | 0.004% |
| 81  | 11.813 | 3244 | 3257 | 3276 | rBV  | 443414 | 716886 | 72.68% | 8.574% |
| 82  | 12.063 | 3331 | 3335 | 3339 | rVB  | 499    | 317    | 0.03%  | 0.004% |
| 83  | 12.089 | 3339 | 3343 | 3344 | rBV  | 338    | 256    | 0.03%  | 0.003% |
| 84  | 12.192 | 3362 | 3375 | 3398 | rBV  | 437692 | 712516 | 72.24% | 8.522% |
| 85  | 12.430 | 3446 | 3449 | 3451 | rBV3 | 312    | 225    | 0.02%  | 0.003% |
| 86  | 12.636 | 3510 | 3513 | 3517 | rVV  | 382    | 303    | 0.03%  | 0.004% |
| 87  | 12.848 | 3576 | 3579 | 3584 | rBV2 | 378    | 404    | 0.04%  | 0.005% |
| 88  | 13.067 | 3643 | 3647 | 3651 | rBV2 | 349    | 391    | 0.04%  | 0.005% |
| 89  | 13.224 | 3691 | 3696 | 3701 | rBV4 | 833    | 973    | 0.10%  | 0.012% |
| 90  | 13.346 | 3731 | 3734 | 3738 | rVB2 | 343    | 308    | 0.03%  | 0.004% |
| 91  | 13.423 | 3754 | 3758 | 3760 | rBV2 | 306    | 312    | 0.03%  | 0.004% |
| 92  | 13.507 | 3780 | 3784 | 3787 | rBV  | 499    | 526    | 0.05%  | 0.006% |
| 93  | 13.848 | 3884 | 3890 | 3899 | rBV6 | 1456   | 2068   | 0.21%  | 0.025% |
| 94  | 14.009 | 3936 | 3940 | 3941 | rBV2 | 518    | 406    | 0.04%  | 0.005% |
| 95  | 14.092 | 3961 | 3966 | 3975 | rBV4 | 3073   | 4274   | 0.43%  | 0.051% |
| 96  | 14.333 | 4035 | 4041 | 4053 | rVB5 | 1668   | 2816   | 0.29%  | 0.034% |
| 97  | 14.385 | 4053 | 4057 | 4063 | rBV2 | 351    | 425    | 0.04%  | 0.005% |
| 98  | 15.632 | 4442 | 4445 | 4447 | rBV3 | 630    | 440    | 0.04%  | 0.005% |
| 99  | 16.230 | 4629 | 4631 | 4634 | rBV3 | 890    | 542    | 0.05%  | 0.006% |
| 100 | 16.295 | 4648 | 4651 | 4655 | rBV4 | 857    | 666    | 0.07%  | 0.008% |

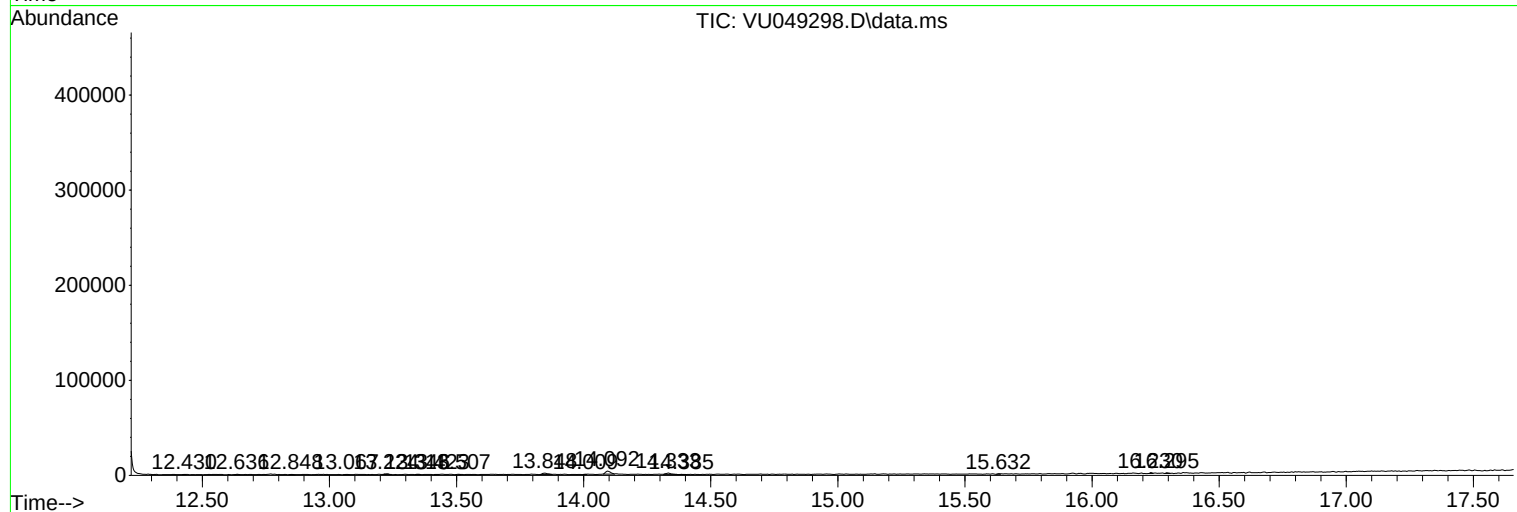
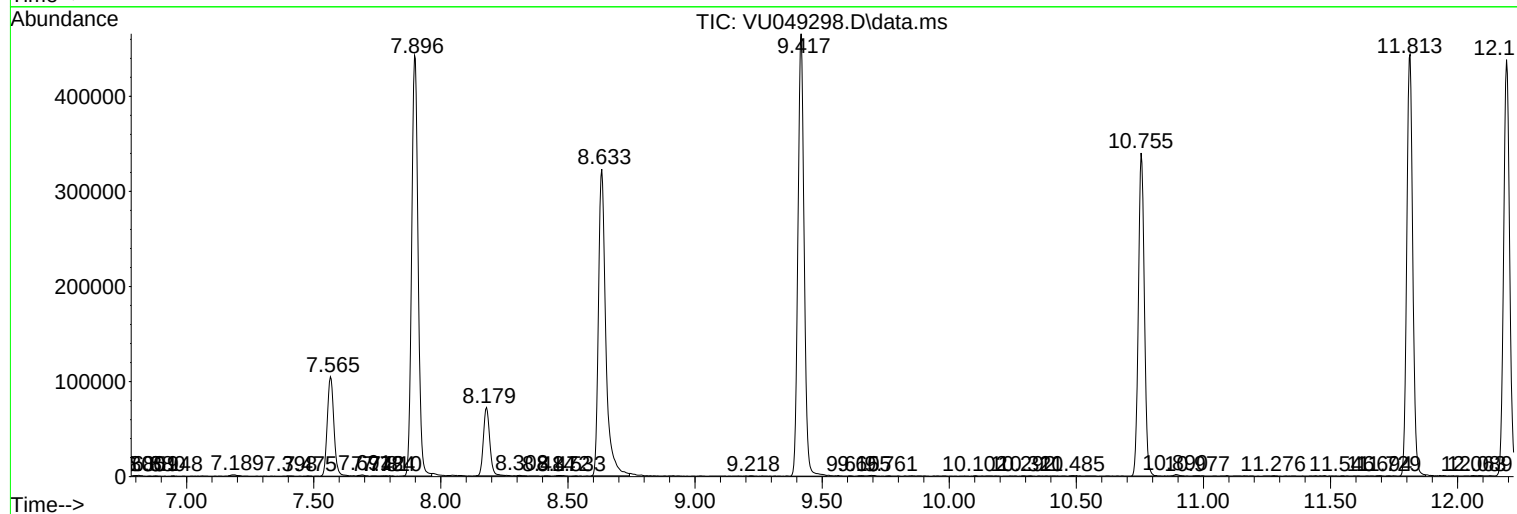
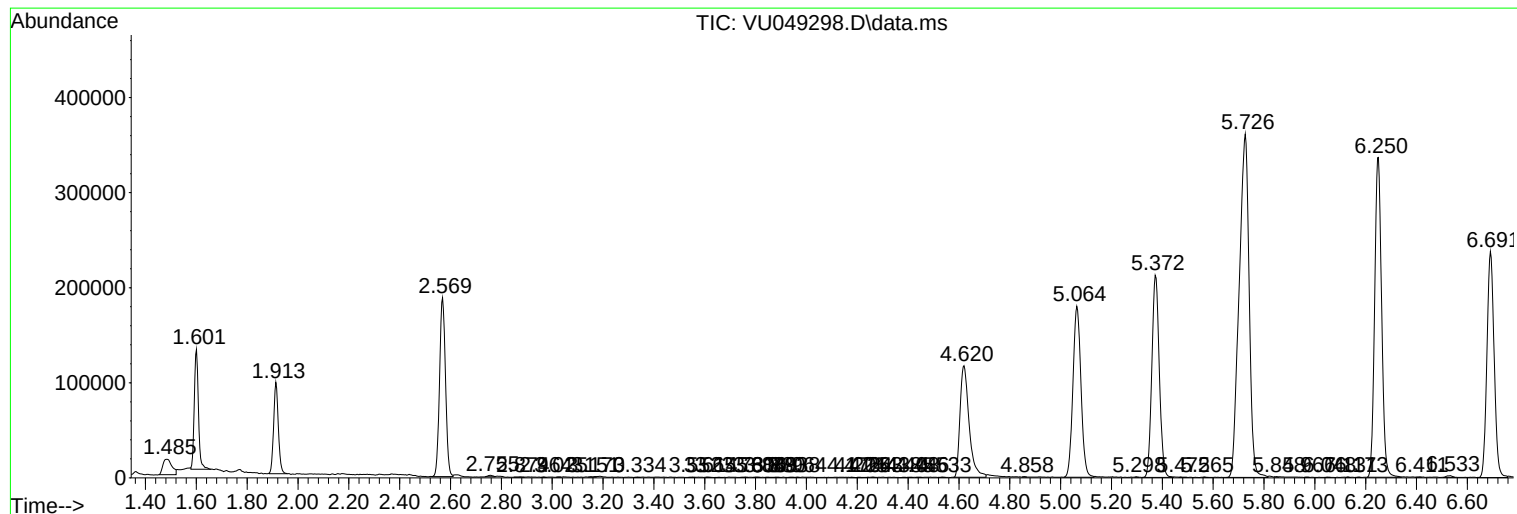
Sum of corrected areas: 8360912

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM061022WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062022\  
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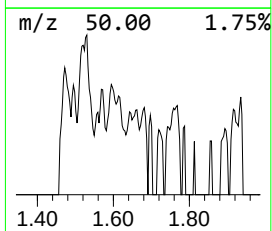
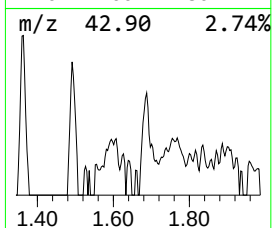
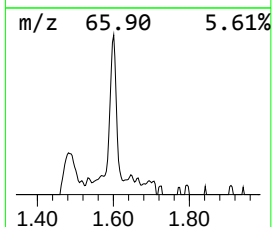
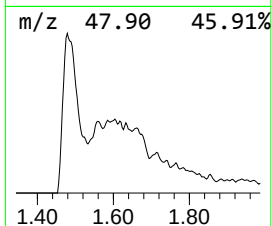
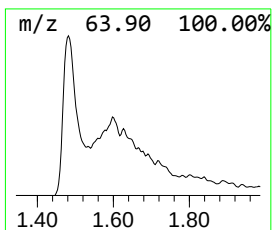
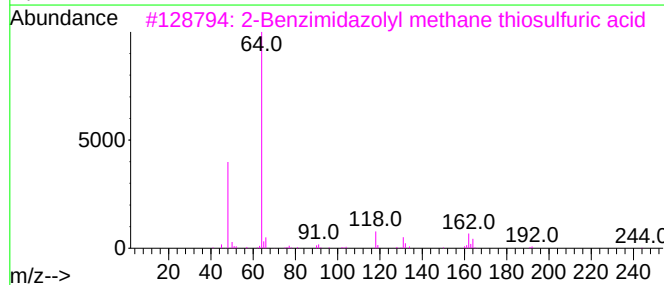
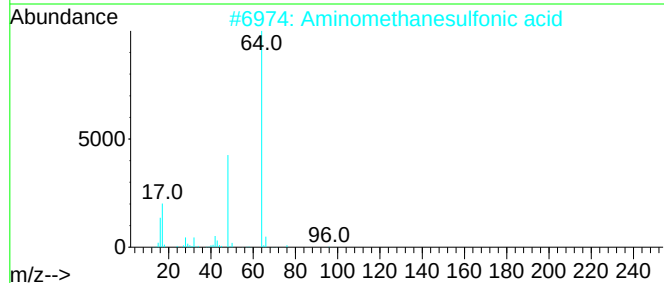
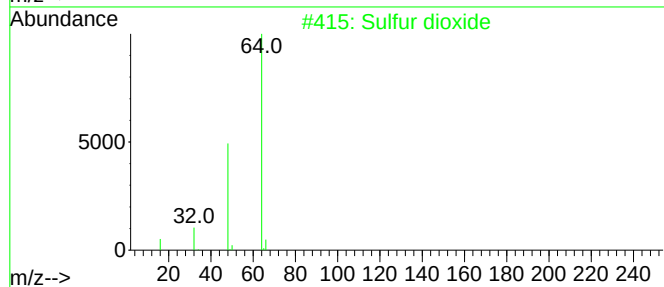
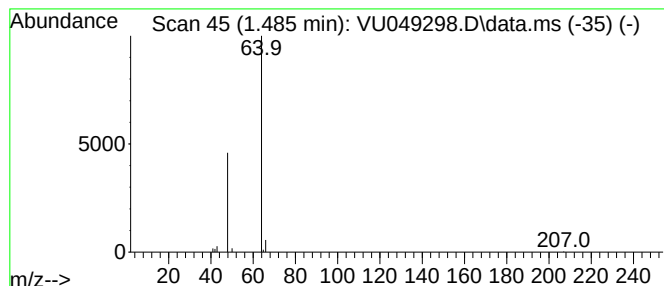
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM061022WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.485 | 3.15 ug/L | 40516 | 1,4-Difluorobenzene | 6.250 |

| 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  | 74   |
| 3    |    |   | 2-Benzimidazolyl methane thiosul... | 244 | C8H8N2O3S2   | 1010256-39-2 | 9    |
| 4    |    |   | (N-(-2-Acetamido))-2-aminoethane... | 182 | C4H10N2O4S   | 007365-82-4  | 9    |
| 5    |    |   | S-2-[4-Glutarimidobutylamino]eth... | 324 | C11H20N2O5S2 | 031701-78-7  | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.485 | 3.1     | ug/L  | 40516    | 1                     | 6.250 | 643240 | 50.0 |