

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062424\  
 Data File : VU059448.D  
 Acq On : 24 Jun 2024 14:31  
 Operator : MD/SY  
 Sample : P2963-15ME  
 Misc : 4.59g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A4CR9ME

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059448.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         | 1.480       | 55            | 59          | 65           | rVB3     | 2077           | 2108          | 0.32%           | 0.042%        |
| 2         | 1.592       | 86            | 94          | 114          | rVB      | 32200          | 52386         | 7.99%           | 1.047%        |
| 3         | 1.814       | 136           | 163         | 164          | rBV5     | 37379          | 114185        | 17.42%          | 2.282%        |
| 4         | 2.538       | 377           | 388         | 405          | rVB      | 81152          | 132288        | 20.18%          | 2.644%        |
| 5         | 2.631       | 408           | 417         | 420          | rBV3     | 1949           | 2852          | 0.44%           | 0.057%        |
| 6         | 2.753       | 452           | 455         | 456          | rBV2     | 279            | 165           | 0.03%           | 0.003%        |
| 7         | 2.850       | 483           | 485         | 487          | rVV2     | 285            | 178           | 0.03%           | 0.004%        |
| 8         | 2.875       | 490           | 493         | 497          | rVV      | 634            | 511           | 0.08%           | 0.010%        |
| 9         | 2.898       | 497           | 500         | 505          | rVB2     | 390            | 278           | 0.04%           | 0.006%        |
| 10        | 2.943       | 505           | 514         | 532          | rBV      | 20195          | 39960         | 6.10%           | 0.799%        |
| 11        | 3.026       | 532           | 540         | 557          | rVB6     | 3603           | 8077          | 1.23%           | 0.161%        |
| 12        | 3.107       | 562           | 565         | 569          | rBV3     | 423            | 373           | 0.06%           | 0.007%        |
| 13        | 3.171       | 572           | 585         | 605          | rBV2     | 8588           | 23091         | 3.52%           | 0.462%        |
| 14        | 3.428       | 663           | 665         | 668          | rVB      | 327            | 175           | 0.03%           | 0.003%        |
| 15        | 3.448       | 668           | 671         | 673          | rBV      | 259            | 176           | 0.03%           | 0.004%        |
| 16        | 3.859       | 795           | 799         | 801          | rBV2     | 188            | 160           | 0.02%           | 0.003%        |
| 17        | 3.927       | 816           | 820         | 826          | rBV2     | 231            | 241           | 0.04%           | 0.005%        |
| 18        | 4.055       | 858           | 860         | 865          | rBV2     | 168            | 187           | 0.03%           | 0.004%        |
| 19        | 4.084       | 865           | 869         | 873          | rVV2     | 192            | 218           | 0.03%           | 0.004%        |
| 20        | 4.126       | 880           | 882         | 889          | rVB      | 206            | 168           | 0.03%           | 0.003%        |
| 21        | 4.538       | 1004          | 1010        | 1013         | rBV2     | 275            | 260           | 0.04%           | 0.005%        |
| 22        | 4.621       | 1022          | 1036        | 1077         | rBV      | 53973          | 164244        | 25.05%          | 3.283%        |
| 23        | 5.052       | 1154          | 1170        | 1195         | rVV2     | 96212          | 217554        | 33.18%          | 4.349%        |
| 24        | 5.145       | 1196          | 1199        | 1205         | rVB3     | 407            | 384           | 0.06%           | 0.008%        |
| 25        | 5.290       | 1239          | 1244        | 1249         | rVB3     | 298            | 232           | 0.04%           | 0.005%        |
| 26        | 5.711       | 1357          | 1375        | 1401         | rBV3     | 189261         | 513911        | 78.39%          | 10.273%       |
| 27        | 5.917       | 1436          | 1439        | 1443         | rBV3     | 297            | 209           | 0.03%           | 0.004%        |
| 28        | 5.978       | 1451          | 1458        | 1463         | rVV5     | 738            | 1136          | 0.17%           | 0.023%        |
| 29        | 6.238       | 1527          | 1539        | 1568         | rBV      | 258545         | 500743        | 76.38%          | 10.009%       |
| 30        | 6.528       | 1620          | 1629        | 1640         | rVB6     | 3109           | 5484          | 0.84%           | 0.110%        |
| 31        | 6.602       | 1640          | 1652        | 1660         | rBV5     | 1315           | 2394          | 0.37%           | 0.048%        |
| 32        | 6.682       | 1664          | 1677        | 1696         | rBV      | 121344         | 241865        | 36.89%          | 4.835%        |
| 33        | 6.775       | 1704          | 1706        | 1711         | rVB2     | 370            | 205           | 0.03%           | 0.004%        |
| 34        | 6.808       | 1712          | 1716        | 1717         | rBV      | 312            | 193           | 0.03%           | 0.004%        |
| 35        | 6.875       | 1734          | 1737        | 1740         | rVV2     | 315            | 255           | 0.04%           | 0.005%        |
| 36        | 7.036       | 1784          | 1787        | 1791         | rBV      | 428            | 367           | 0.06%           | 0.007%        |

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Integrator: RTE

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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\SFAMULM052924WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |         |         |
|----|--------|------|------|------|------|--------|--------|---------|---------|
| 37 | 7.197  | 1830 | 1837 | 1842 | rBV6 | 2198   | 3270   | 0.50%   | 0.065%  |
| 38 | 7.415  | 1900 | 1905 | 1909 | rBV2 | 230    | 232    | 0.04%   | 0.005%  |
| 39 | 7.560  | 1938 | 1950 | 1968 | rBV2 | 56514  | 103964 | 15.86%  | 2.078%  |
| 40 | 7.698  | 1987 | 1993 | 2000 | rBV4 | 980    | 1711   | 0.26%   | 0.034%  |
| 41 | 7.788  | 2017 | 2021 | 2024 | rVB3 | 305    | 242    | 0.04%   | 0.005%  |
| 42 | 7.891  | 2041 | 2053 | 2071 | rBV  | 200255 | 356097 | 54.32%  | 7.118%  |
| 43 | 8.045  | 2099 | 2101 | 2105 | rVB  | 301    | 203    | 0.03%   | 0.004%  |
| 44 | 8.177  | 2130 | 2142 | 2160 | rBV  | 39390  | 70139  | 10.70%  | 1.402%  |
| 45 | 8.299  | 2177 | 2180 | 2183 | rBV  | 185    | 144    | 0.02%   | 0.003%  |
| 46 | 8.351  | 2191 | 2196 | 2200 | rVB  | 216    | 167    | 0.03%   | 0.003%  |
| 47 | 8.451  | 2223 | 2227 | 2229 | rBV  | 261    | 196    | 0.03%   | 0.004%  |
| 48 | 8.541  | 2252 | 2255 | 2256 | rBV  | 243    | 157    | 0.02%   | 0.003%  |
| 49 | 8.637  | 2274 | 2285 | 2312 | rBV2 | 157072 | 344617 | 52.57%  | 6.889%  |
| 50 | 8.988  | 2391 | 2394 | 2396 | rBV2 | 255    | 179    | 0.03%   | 0.004%  |
| 51 | 9.094  | 2423 | 2427 | 2431 | rVB  | 265    | 206    | 0.03%   | 0.004%  |
| 52 | 9.119  | 2431 | 2435 | 2438 | rBV2 | 193    | 155    | 0.02%   | 0.003%  |
| 53 | 9.142  | 2439 | 2442 | 2445 | rVV  | 201    | 163    | 0.02%   | 0.003%  |
| 54 | 9.219  | 2462 | 2466 | 2472 | rVV  | 261    | 284    | 0.04%   | 0.006%  |
| 55 | 9.348  | 2503 | 2506 | 2510 | rVB  | 384    | 301    | 0.05%   | 0.006%  |
| 56 | 9.412  | 2514 | 2526 | 2558 | rBV  | 379385 | 655592 | 100.00% | 13.105% |
| 57 | 9.602  | 2583 | 2585 | 2592 | rVB5 | 700    | 628    | 0.10%   | 0.013%  |
| 58 | 9.631  | 2592 | 2594 | 2598 | rVB2 | 259    | 141    | 0.02%   | 0.003%  |
| 59 | 9.695  | 2608 | 2614 | 2626 | rVB3 | 1091   | 1857   | 0.28%   | 0.037%  |
| 60 | 9.817  | 2649 | 2652 | 2658 | rBV  | 206    | 171    | 0.03%   | 0.003%  |
| 61 | 9.894  | 2672 | 2676 | 2680 | rBV2 | 191    | 193    | 0.03%   | 0.004%  |
| 62 | 10.033 | 2715 | 2719 | 2726 | rBV2 | 191    | 210    | 0.03%   | 0.004%  |
| 63 | 10.068 | 2726 | 2730 | 2733 | rBV2 | 225    | 180    | 0.03%   | 0.004%  |
| 64 | 10.103 | 2738 | 2741 | 2744 | rBV3 | 344    | 315    | 0.05%   | 0.006%  |
| 65 | 10.174 | 2759 | 2763 | 2766 | rBV2 | 203    | 174    | 0.03%   | 0.003%  |
| 66 | 10.348 | 2809 | 2817 | 2821 | rVB2 | 300    | 392    | 0.06%   | 0.008%  |
| 67 | 10.370 | 2821 | 2824 | 2829 | rBV2 | 250    | 260    | 0.04%   | 0.005%  |
| 68 | 10.454 | 2847 | 2850 | 2851 | rBV  | 329    | 179    | 0.03%   | 0.004%  |
| 69 | 10.467 | 2852 | 2854 | 2855 | rBV  | 414    | 184    | 0.03%   | 0.004%  |
| 70 | 10.753 | 2930 | 2943 | 2963 | rBV  | 235986 | 384455 | 58.64%  | 7.685%  |
| 71 | 10.859 | 2973 | 2976 | 2980 | rBV  | 289    | 182    | 0.03%   | 0.004%  |
| 72 | 10.881 | 2980 | 2983 | 2984 | rVV  | 426    | 201    | 0.03%   | 0.004%  |
| 73 | 10.891 | 2984 | 2986 | 2994 | rVB2 | 628    | 604    | 0.09%   | 0.012%  |
| 74 | 11.000 | 3017 | 3020 | 3027 | rBV2 | 203    | 170    | 0.03%   | 0.003%  |
| 75 | 11.119 | 3050 | 3057 | 3059 | rBV  | 226    | 246    | 0.04%   | 0.005%  |
| 76 | 11.209 | 3082 | 3085 | 3090 | rVB2 | 194    | 170    | 0.03%   | 0.003%  |

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 A4CR9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\_U\Method\SFAMULM052924WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.415 | 3143 | 3149 | 3152 | rBV2 | 229    | 277    | 0.04%  | 0.006%  |
| 78  | 11.659 | 3222 | 3225 | 3228 | rVB2 | 343    | 210    | 0.03%  | 0.004%  |
| 79  | 11.692 | 3233 | 3235 | 3241 | rVB  | 332    | 159    | 0.02%  | 0.003%  |
| 80  | 11.811 | 3259 | 3272 | 3294 | rVV  | 389259 | 631327 | 96.30% | 12.620% |
| 81  | 12.032 | 3338 | 3341 | 3344 | rBV2 | 309    | 210    | 0.03%  | 0.004%  |
| 82  | 12.190 | 3378 | 3390 | 3410 | rBV  | 247037 | 407130 | 62.10% | 8.138%  |
| 83  | 12.412 | 3457 | 3459 | 3467 | rVB  | 385    | 311    | 0.05%  | 0.006%  |
| 84  | 12.457 | 3467 | 3473 | 3475 | rBV2 | 234    | 253    | 0.04%  | 0.005%  |
| 85  | 12.521 | 3491 | 3493 | 3498 | rBV  | 281    | 251    | 0.04%  | 0.005%  |
| 86  | 12.766 | 3566 | 3569 | 3570 | rBV  | 296    | 173    | 0.03%  | 0.003%  |
| 87  | 12.862 | 3597 | 3599 | 3606 | rVB2 | 386    | 257    | 0.04%  | 0.005%  |
| 88  | 12.933 | 3611 | 3621 | 3627 | rBV4 | 1386   | 2290   | 0.35%  | 0.046%  |
| 89  | 13.039 | 3651 | 3654 | 3657 | rBV  | 359    | 272    | 0.04%  | 0.005%  |
| 90  | 13.524 | 3802 | 3805 | 3807 | rBV2 | 278    | 169    | 0.03%  | 0.003%  |
| 91  | 13.720 | 3863 | 3866 | 3869 | rBV  | 401    | 267    | 0.04%  | 0.005%  |
| 92  | 13.798 | 3886 | 3890 | 3891 | rBV  | 308    | 230    | 0.04%  | 0.005%  |
| 93  | 13.823 | 3896 | 3898 | 3902 | rVB  | 372    | 218    | 0.03%  | 0.004%  |
| 94  | 14.010 | 3954 | 3956 | 3958 | rVB  | 405    | 200    | 0.03%  | 0.004%  |
| 95  | 14.032 | 3958 | 3963 | 3965 | rBV2 | 397    | 328    | 0.05%  | 0.007%  |
| 96  | 14.110 | 3982 | 3987 | 3988 | rBV2 | 586    | 417    | 0.06%  | 0.008%  |
| 97  | 14.782 | 4193 | 4196 | 4198 | rBV2 | 329    | 216    | 0.03%  | 0.004%  |
| 98  | 15.132 | 4303 | 4305 | 4308 | rBV2 | 319    | 248    | 0.04%  | 0.005%  |
| 99  | 15.518 | 4422 | 4425 | 4433 | rBV2 | 718    | 746    | 0.11%  | 0.015%  |
| 100 | 16.183 | 4629 | 4632 | 4633 | rBV3 | 724    | 392    | 0.06%  | 0.008%  |

Sum of corrected areas: 5002695

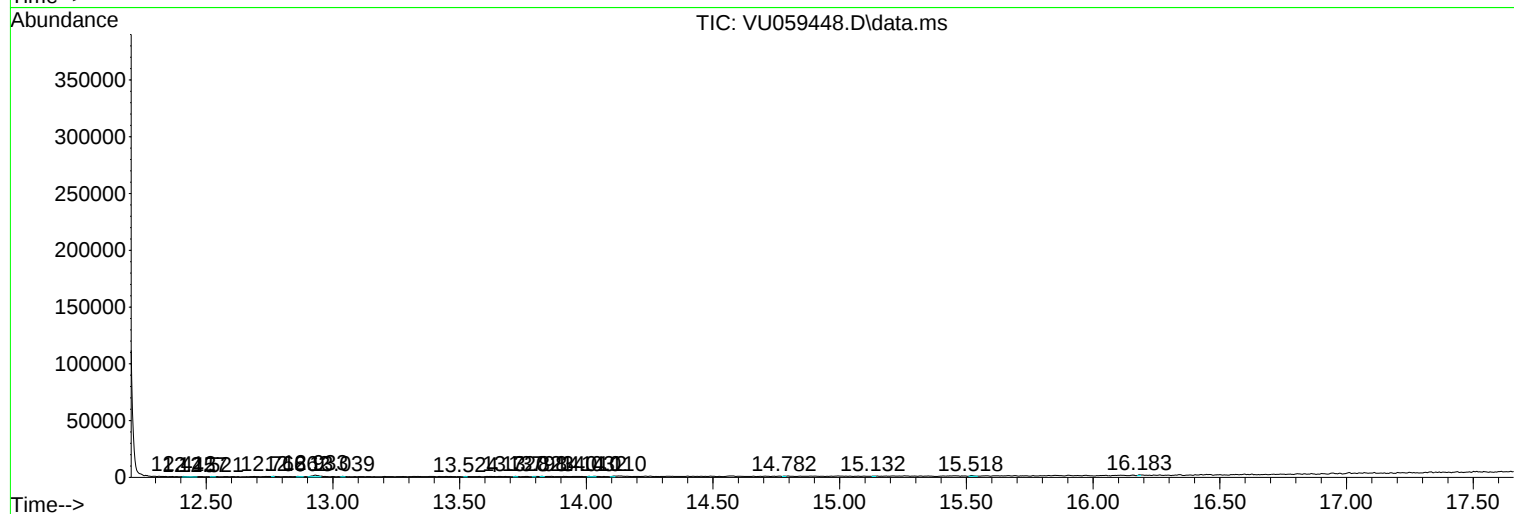
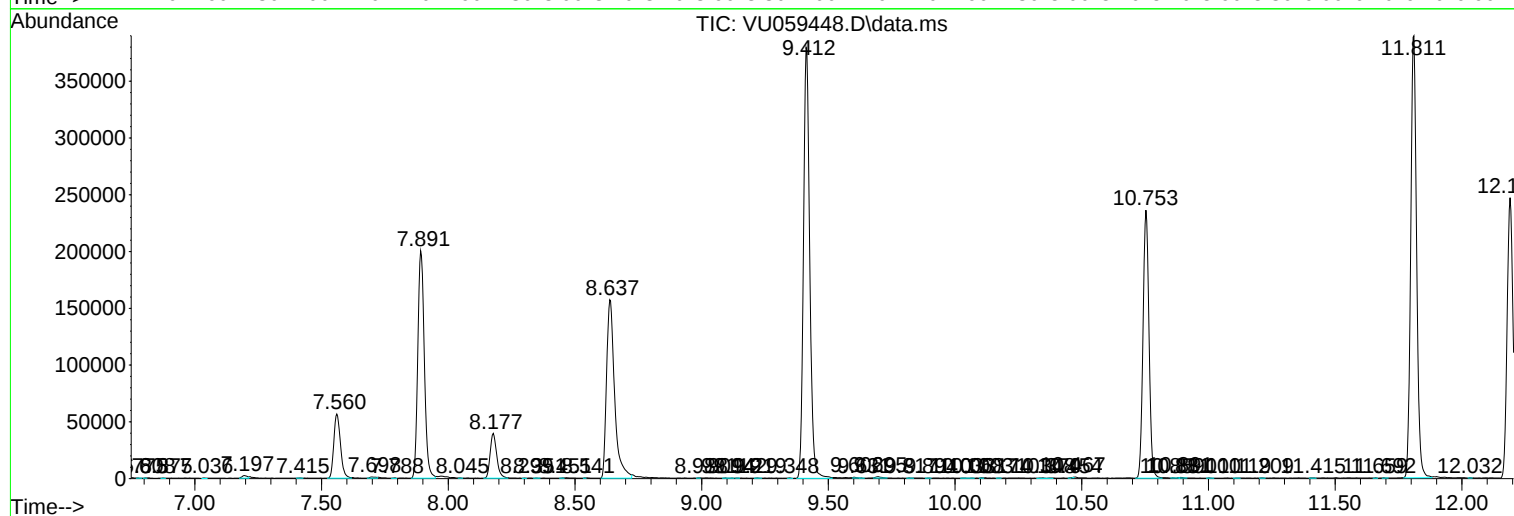
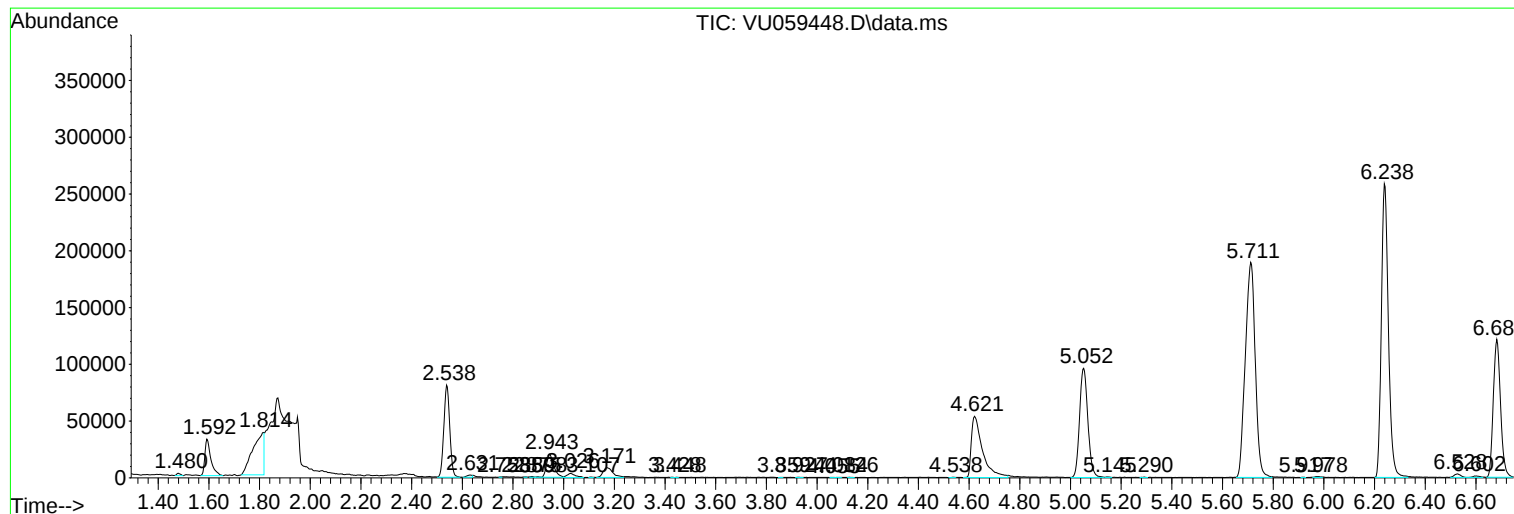
Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062424\  
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Instrument :  
MSVOA\_U  
ClientSampleId :  
A4CR9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052924WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062424\  
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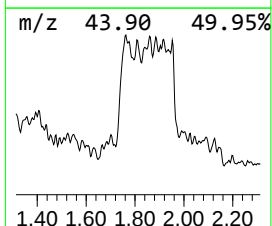
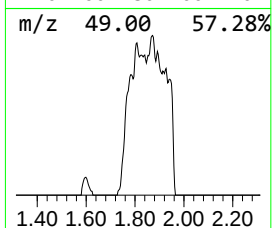
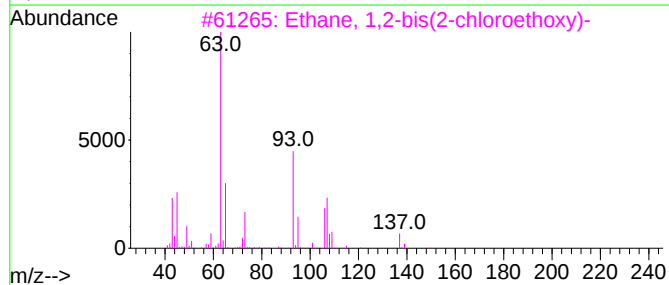
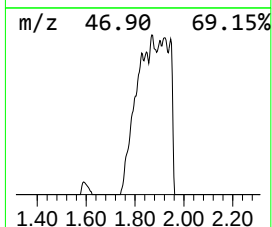
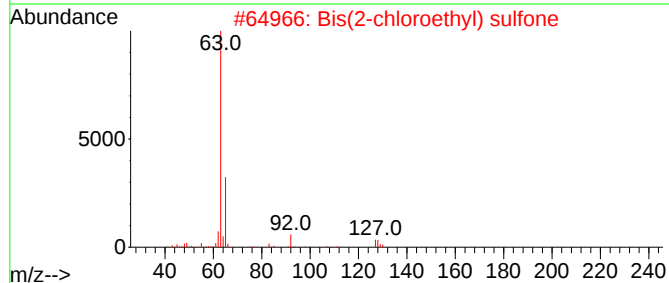
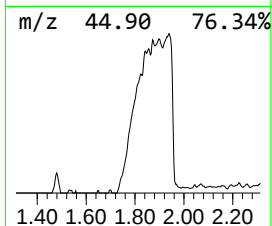
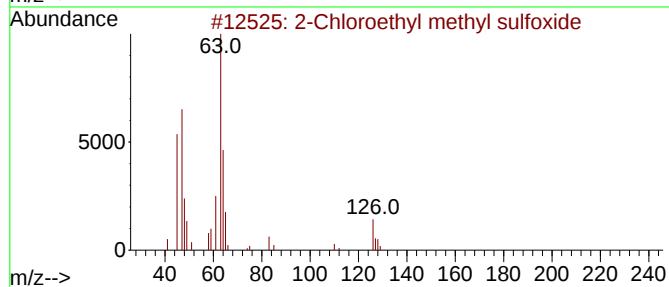
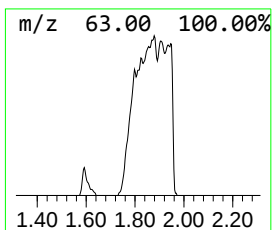
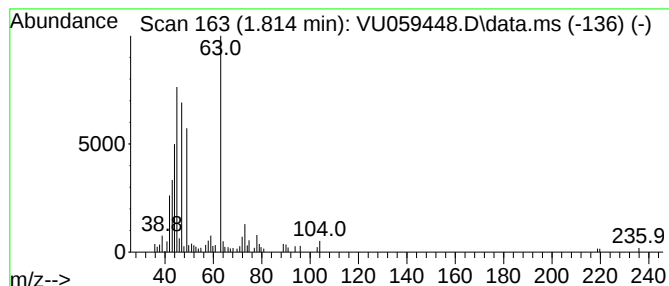
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052924WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 unknown-01 Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 1.814 | 11.40 ug/L | 114185 | 1,4-Difluorobenzene | 6.238 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | 2-Chloroethyl methyl sulfoxide      | 126 | C3H7ClOS    | 005331-57-7  | 33   |
| 2    |    |   | Bis(2-chloroethyl) sulfone          | 190 | C4H8Cl2O2S  | 000471-03-4  | 23   |
| 3    |    |   | Ethane, 1,2-bis(2-chloroethoxy)-    | 186 | C6H12Cl2O2  | 000112-26-5  | 23   |
| 4    |    |   | 3,6,9,12-tetraoxatetradecane, 1,... | 274 | C10H20Cl2O4 | 1000401-80-9 | 23   |
| 5    |    |   | Ethylamine                          | 45  | C2H7N       | 000075-04-7  | 9    |



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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown-01       | 1.814 | 11.4    | ug/L  | 114185   | 1                     | 6.238 | 500743 | 50.0 |