

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU060324\  
 Data File : VU059128.D  
 Acq On : 03 Jun 2024 17:32  
 Operator : MD/SY  
 Sample : P2659-18ME  
 Misc : 4.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BHC39ME

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: VU059128.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         | 1.483       | 56            | 60          | 66           | rVB2     | 2828           | 2834          | 0.25%           | 0.032%        |
| 2         | 1.592       | 86            | 94          | 119          | rVB      | 86821          | 130818        | 11.65%          | 1.475%        |
| 3         | 1.821       | 136           | 165         | 166          | rBV3     | 58038          | 188768        | 16.82%          | 2.128%        |
| 4         | 1.872       | 177           | 181         | 198          | rVB      | 77125          | 101473        | 9.04%           | 1.144%        |
| 5         | 2.538       | 376           | 388         | 409          | rVB      | 190563         | 309032        | 27.53%          | 3.484%        |
| 6         | 2.769       | 456           | 460         | 467          | rVB2     | 937            | 1093          | 0.10%           | 0.012%        |
| 7         | 2.801       | 467           | 470         | 473          | rBV      | 239            | 240           | 0.02%           | 0.003%        |
| 8         | 2.885       | 491           | 496         | 500          | rBV3     | 229            | 269           | 0.02%           | 0.003%        |
| 9         | 2.962       | 518           | 520         | 524          | rVB2     | 389            | 279           | 0.02%           | 0.003%        |
| 10        | 3.026       | 526           | 540         | 556          | rBV5     | 3687           | 8575          | 0.76%           | 0.097%        |
| 11        | 3.171       | 572           | 585         | 599          | rBV      | 9230           | 21112         | 1.88%           | 0.238%        |
| 12        | 3.303       | 624           | 626         | 630          | rVB2     | 480            | 269           | 0.02%           | 0.003%        |
| 13        | 3.660       | 733           | 737         | 739          | rBV      | 380            | 293           | 0.03%           | 0.003%        |
| 14        | 3.676       | 739           | 742         | 745          | rVB2     | 388            | 268           | 0.02%           | 0.003%        |
| 15        | 3.833       | 787           | 791         | 796          | rBV2     | 266            | 237           | 0.02%           | 0.003%        |
| 16        | 4.332       | 940           | 946         | 950          | rBV2     | 270            | 239           | 0.02%           | 0.003%        |
| 17        | 4.425       | 971           | 975         | 980          | rVB2     | 285            | 246           | 0.02%           | 0.003%        |
| 18        | 4.502       | 995           | 999         | 1003         | rBV2     | 193            | 198           | 0.02%           | 0.002%        |
| 19        | 4.618       | 1024          | 1035        | 1080         | rBV      | 130007         | 387154        | 34.49%          | 4.365%        |
| 20        | 4.930       | 1129          | 1132        | 1135         | rBV2     | 265            | 194           | 0.02%           | 0.002%        |
| 21        | 5.049       | 1153          | 1169        | 1194         | rBV      | 204189         | 458735        | 40.87%          | 5.172%        |
| 22        | 5.284       | 1238          | 1242        | 1245         | rBV4     | 464            | 423           | 0.04%           | 0.005%        |
| 23        | 5.358       | 1261          | 1265        | 1267         | rVV2     | 318            | 230           | 0.02%           | 0.003%        |
| 24        | 5.383       | 1271          | 1273        | 1276         | rVV2     | 255            | 201           | 0.02%           | 0.002%        |
| 25        | 5.415       | 1280          | 1283        | 1289         | rVV2     | 280            | 306           | 0.03%           | 0.003%        |
| 26        | 5.557       | 1323          | 1327        | 1332         | rBV      | 185            | 212           | 0.02%           | 0.002%        |
| 27        | 5.711       | 1356          | 1375        | 1409         | rBV2     | 417268         | 1122499       | 100.00%         | 12.655%       |
| 28        | 5.933       | 1437          | 1444        | 1447         | rBV2     | 329            | 393           | 0.04%           | 0.004%        |
| 29        | 5.949       | 1447          | 1449        | 1450         | rBV2     | 489            | 216           | 0.02%           | 0.002%        |
| 30        | 5.972       | 1450          | 1456        | 1461         | rVV7     | 1146           | 1517          | 0.14%           | 0.017%        |
| 31        | 6.120       | 1498          | 1502        | 1505         | rVV2     | 202            | 199           | 0.02%           | 0.002%        |
| 32        | 6.239       | 1527          | 1539        | 1564         | rBV      | 277172         | 542009        | 48.29%          | 6.110%        |
| 33        | 6.354       | 1572          | 1575        | 1581         | rVB3     | 494            | 449           | 0.04%           | 0.005%        |
| 34        | 6.425       | 1594          | 1597        | 1600         | rVB2     | 337            | 261           | 0.02%           | 0.003%        |
| 35        | 6.473       | 1609          | 1612        | 1616         | rBV3     | 297            | 225           | 0.02%           | 0.003%        |
| 36        | 6.521       | 1618          | 1627        | 1643         | rBV4     | 8143           | 16479         | 1.47%           | 0.186%        |

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 BHC39ME

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Integrator: RTE

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Filtering: 5

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Start Thrs: 0.2

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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

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.599  | 1643 | 1651 | 1663 | rBV5 | 2353   | 5146   | 0.46%  | 0.058% |
| 38 | 6.682  | 1663 | 1677 | 1700 | rBV  | 267419 | 537176 | 47.86% | 6.056% |
| 39 | 6.939  | 1753 | 1757 | 1763 | rBV2 | 258    | 217    | 0.02%  | 0.002% |
| 40 | 7.193  | 1828 | 1836 | 1841 | rBV5 | 1284   | 1907   | 0.17%  | 0.021% |
| 41 | 7.271  | 1856 | 1860 | 1865 | rVB2 | 368    | 249    | 0.02%  | 0.003% |
| 42 | 7.322  | 1872 | 1876 | 1882 | rBV2 | 251    | 236    | 0.02%  | 0.003% |
| 43 | 7.377  | 1890 | 1893 | 1898 | rVB  | 266    | 253    | 0.02%  | 0.003% |
| 44 | 7.415  | 1898 | 1905 | 1908 | rBV  | 321    | 357    | 0.03%  | 0.004% |
| 45 | 7.499  | 1926 | 1931 | 1934 | rVB3 | 529    | 393    | 0.04%  | 0.004% |
| 46 | 7.560  | 1937 | 1950 | 1972 | rBV2 | 132530 | 245921 | 21.91% | 2.772% |
| 47 | 7.701  | 1987 | 1994 | 1999 | rBV4 | 838    | 1229   | 0.11%  | 0.014% |
| 48 | 7.792  | 2018 | 2022 | 2029 | rVB2 | 327    | 361    | 0.03%  | 0.004% |
| 49 | 7.891  | 2038 | 2053 | 2076 | rBV  | 462737 | 812797 | 72.41% | 9.163% |
| 50 | 8.078  | 2108 | 2111 | 2114 | rBV2 | 392    | 219    | 0.02%  | 0.002% |
| 51 | 8.174  | 2130 | 2141 | 2167 | rVV2 | 91402  | 167612 | 14.93% | 1.890% |
| 52 | 8.300  | 2175 | 2180 | 2184 | rBV2 | 274    | 275    | 0.02%  | 0.003% |
| 53 | 8.345  | 2190 | 2194 | 2196 | rBV  | 316    | 280    | 0.02%  | 0.003% |
| 54 | 8.637  | 2272 | 2285 | 2321 | rBV  | 364640 | 815151 | 72.62% | 9.190% |
| 55 | 8.836  | 2345 | 2347 | 2356 | rVB4 | 636    | 688    | 0.06%  | 0.008% |
| 56 | 8.933  | 2375 | 2377 | 2383 | rBV2 | 463    | 437    | 0.04%  | 0.005% |
| 57 | 8.988  | 2390 | 2394 | 2396 | rBV  | 273    | 203    | 0.02%  | 0.002% |
| 58 | 9.090  | 2423 | 2426 | 2430 | rBV  | 231    | 213    | 0.02%  | 0.002% |
| 59 | 9.139  | 2436 | 2441 | 2442 | rBV  | 329    | 209    | 0.02%  | 0.002% |
| 60 | 9.412  | 2514 | 2526 | 2551 | rBV  | 403571 | 706338 | 62.93% | 7.963% |
| 61 | 9.502  | 2552 | 2554 | 2561 | rVB3 | 1215   | 1078   | 0.10%  | 0.012% |
| 62 | 9.560  | 2570 | 2572 | 2574 | rBV2 | 378    | 234    | 0.02%  | 0.003% |
| 63 | 9.666  | 2598 | 2605 | 2607 | rBV2 | 171    | 206    | 0.02%  | 0.002% |
| 64 | 9.698  | 2607 | 2615 | 2617 | rBV2 | 1358   | 1521   | 0.14%  | 0.017% |
| 65 | 9.798  | 2641 | 2646 | 2649 | rBV2 | 295    | 261    | 0.02%  | 0.003% |
| 66 | 10.078 | 2728 | 2733 | 2735 | rBV2 | 274    | 298    | 0.03%  | 0.003% |
| 67 | 10.110 | 2739 | 2743 | 2748 | rVV2 | 254    | 294    | 0.03%  | 0.003% |
| 68 | 10.213 | 2772 | 2775 | 2779 | rVB  | 272    | 246    | 0.02%  | 0.003% |
| 69 | 10.406 | 2830 | 2835 | 2841 | rBV2 | 288    | 352    | 0.03%  | 0.004% |
| 70 | 10.753 | 2929 | 2943 | 2966 | rBV  | 461041 | 761603 | 67.85% | 8.586% |
| 71 | 10.923 | 2994 | 2996 | 3000 | rVV2 | 368    | 248    | 0.02%  | 0.003% |
| 72 | 10.984 | 3004 | 3015 | 3018 | rBV2 | 381    | 524    | 0.05%  | 0.006% |
| 73 | 11.299 | 3108 | 3113 | 3115 | rBV2 | 308    | 268    | 0.02%  | 0.003% |
| 74 | 11.479 | 3165 | 3169 | 3173 | rBV  | 276    | 291    | 0.03%  | 0.003% |
| 75 | 11.711 | 3237 | 3241 | 3244 | rBV2 | 360    | 234    | 0.02%  | 0.003% |
| 76 | 11.753 | 3251 | 3254 | 3258 | rBV  | 419    | 258    | 0.02%  | 0.003% |

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Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BHC39ME

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  | 11.811 | 3259 | 3272 | 3291 | rBV  | 408248 | 661453 | 58.93% | 7.457% |
| 78  | 11.959 | 3314 | 3318 | 3322 | rVB3 | 271    | 271    | 0.02%  | 0.003% |
| 79  | 12.007 | 3330 | 3333 | 3337 | rVB2 | 373    | 243    | 0.02%  | 0.003% |
| 80  | 12.045 | 3342 | 3345 | 3350 | rVB3 | 371    | 372    | 0.03%  | 0.004% |
| 81  | 12.190 | 3377 | 3390 | 3411 | rBV  | 506450 | 836535 | 74.52% | 9.431% |
| 82  | 12.322 | 3428 | 3431 | 3434 | rBV2 | 395    | 238    | 0.02%  | 0.003% |
| 83  | 12.592 | 3512 | 3515 | 3520 | rBV2 | 346    | 312    | 0.03%  | 0.004% |
| 84  | 13.698 | 3856 | 3859 | 3864 | rVB  | 386    | 285    | 0.03%  | 0.003% |
| 85  | 14.055 | 3968 | 3970 | 3977 | rVB2 | 272    | 224    | 0.02%  | 0.003% |
| 86  | 14.119 | 3987 | 3990 | 3994 | rBV2 | 372    | 299    | 0.03%  | 0.003% |
| 87  | 14.151 | 3994 | 4000 | 4005 | rBV  | 660    | 577    | 0.05%  | 0.007% |
| 88  | 14.212 | 4015 | 4019 | 4021 | rBV  | 279    | 210    | 0.02%  | 0.002% |
| 89  | 14.229 | 4021 | 4024 | 4026 | rVV  | 343    | 242    | 0.02%  | 0.003% |
| 90  | 14.328 | 4048 | 4055 | 4061 | rBV  | 393    | 564    | 0.05%  | 0.006% |
| 91  | 14.441 | 4088 | 4090 | 4092 | rBV  | 313    | 200    | 0.02%  | 0.002% |
| 92  | 14.573 | 4125 | 4131 | 4135 | rBV3 | 880    | 968    | 0.09%  | 0.011% |
| 93  | 14.640 | 4148 | 4152 | 4158 | rBV3 | 300    | 355    | 0.03%  | 0.004% |
| 94  | 14.933 | 4240 | 4243 | 4245 | rBV2 | 338    | 256    | 0.02%  | 0.003% |
| 95  | 15.055 | 4277 | 4281 | 4284 | rBV  | 333    | 320    | 0.03%  | 0.004% |
| 96  | 15.740 | 4491 | 4494 | 4497 | rBV2 | 357    | 258    | 0.02%  | 0.003% |
| 97  | 15.971 | 4563 | 4566 | 4568 | rBV2 | 852    | 414    | 0.04%  | 0.005% |
| 98  | 15.987 | 4568 | 4571 | 4574 | rVV2 | 642    | 419    | 0.04%  | 0.005% |
| 99  | 16.016 | 4576 | 4580 | 4586 | rBV3 | 584    | 763    | 0.07%  | 0.009% |
| 100 | 16.415 | 4701 | 4704 | 4707 | rBV2 | 829    | 638    | 0.06%  | 0.007% |

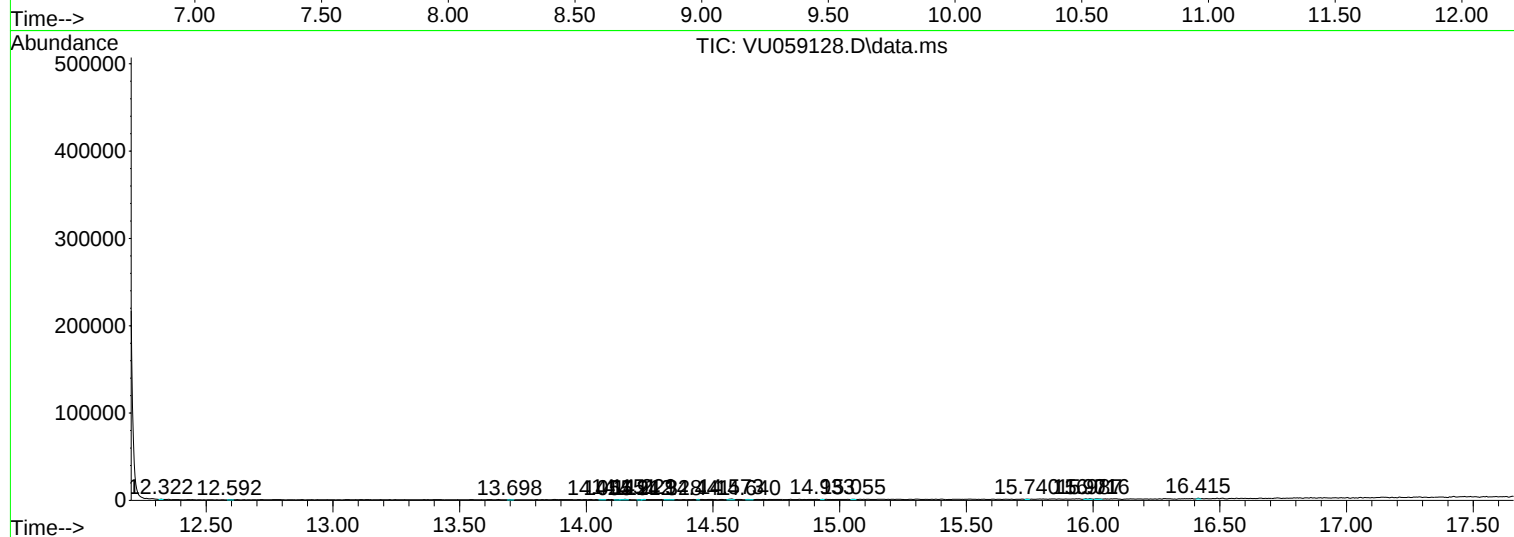
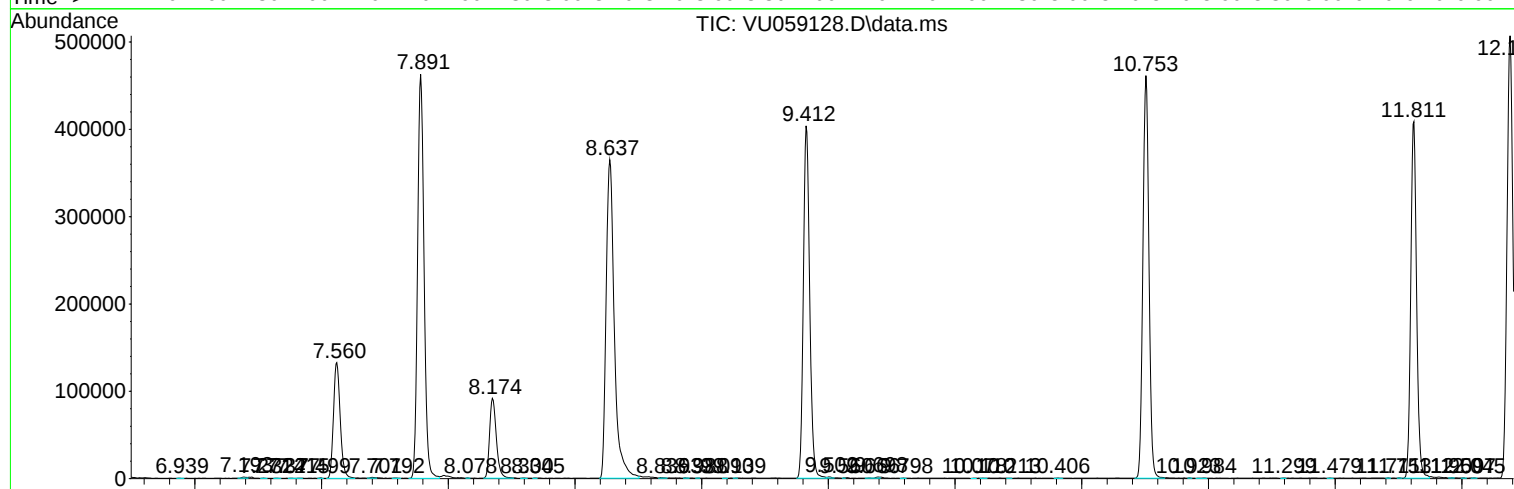
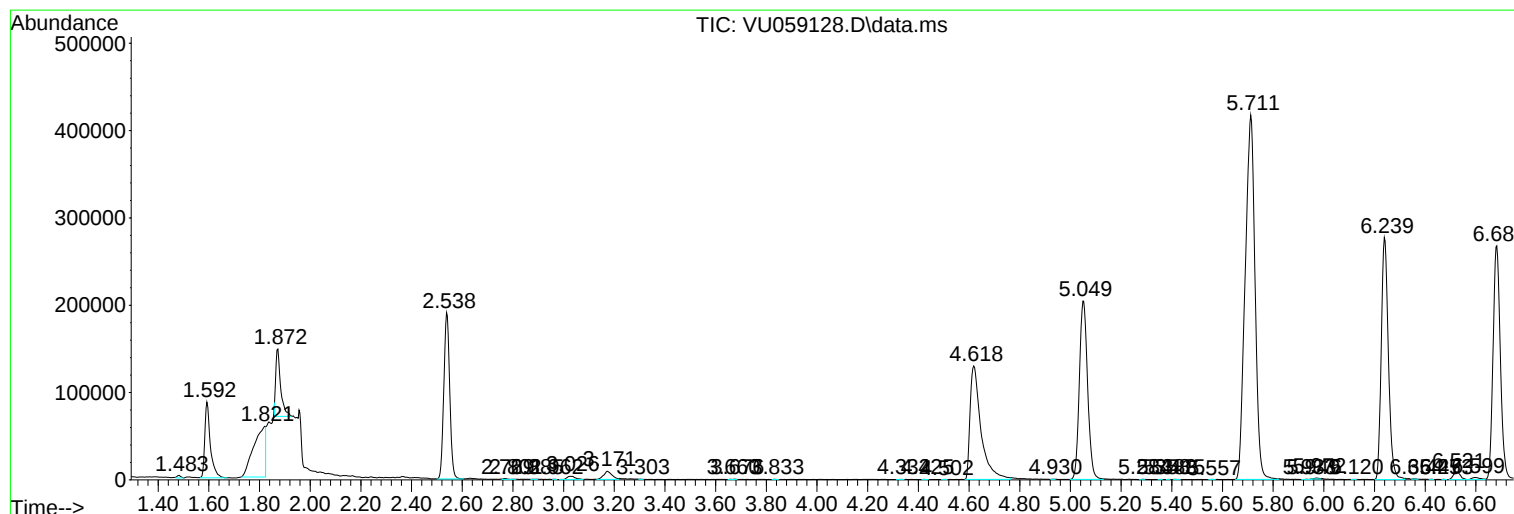
Sum of corrected areas: 8870144

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Instrument :  
MSVOA\_U  
ClientSampleId :  
BHC39ME

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\VU060324\  
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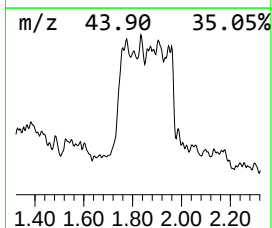
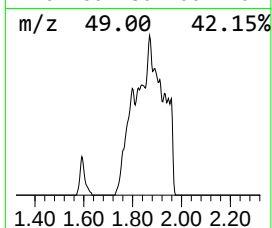
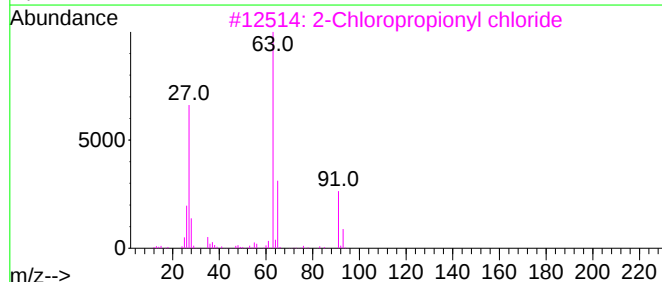
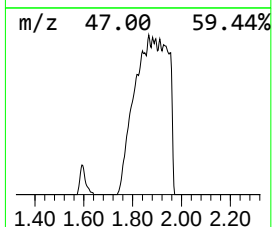
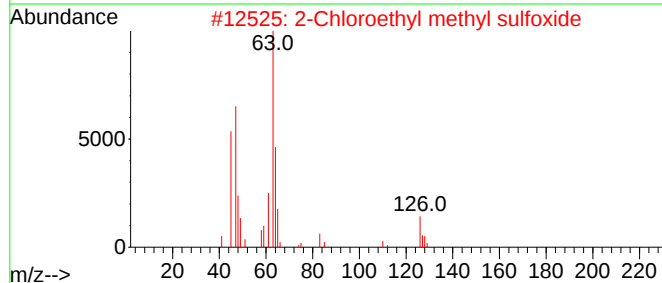
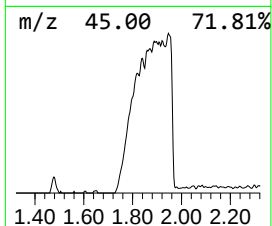
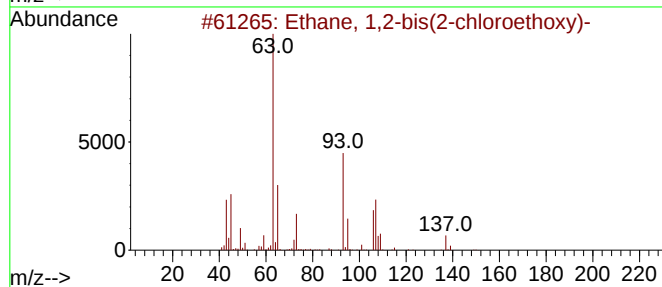
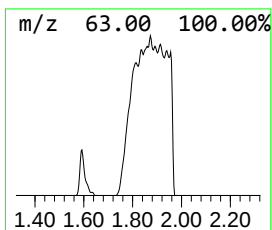
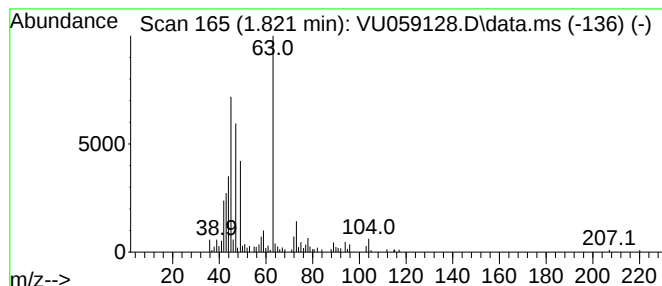
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052924WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 unknown-01 Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 1.821 | 17.41 ug/L | 188768 | 1,4-Difluorobenzene | 6.239 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Ethane, 1,2-bis(2-chloroethoxy)-    | 186 | C6H12Cl2O2  | 000112-26-5  | 36   |
| 2    |    |   | 2-Chloroethyl methyl sulfoxide      | 126 | C3H7ClOS    | 005331-57-7  | 33   |
| 3    |    |   | 2-Chloropropionyl chloride          | 126 | C3H4Cl2O    | 007623-09-8  | 32   |
| 4    |    |   | 3,6,9,12-tetraoxatetradecane, 1,... | 274 | C10H20Cl2O4 | 1000401-80-9 | 25   |
| 5    |    |   | Bis(2-chloroethyl) sulfone          | 190 | C4H8Cl2O2S  | 000471-03-4  | 23   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown-01       | 1.821 | 17.4    | ug/L  | 188768   | 1                     | 6.239 | 542009 | 50.0 |