

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100421\  
 Data File : VU045091.D  
 Acq On : 04 Oct 2021 13:15  
 Operator : SY/MD  
 Sample : M3996-20DL 4X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F4A41DL

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045091.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         | 1.475       | 35            | 42          | 52           | rBV      | 127698         | 126939        | 10.92%          | 1.396%        |
| 2         | 1.601       | 74            | 81          | 94           | rBV      | 138266         | 153204        | 13.18%          | 1.685%        |
| 3         | 1.906       | 168           | 176         | 195          | rVB      | 111928         | 157582        | 13.56%          | 1.733%        |
| 4         | 2.568       | 369           | 382         | 400          | rBV      | 226718         | 373586        | 32.15%          | 4.109%        |
| 5         | 2.707       | 423           | 425         | 429          | rVB2     | 253            | 200           | 0.02%           | 0.002%        |
| 6         | 2.742       | 434           | 436         | 438          | rBV      | 199            | 133           | 0.01%           | 0.001%        |
| 7         | 2.790       | 446           | 451         | 455          | rBV3     | 511            | 564           | 0.05%           | 0.006%        |
| 8         | 2.835       | 461           | 465         | 469          | rBV      | 156            | 170           | 0.01%           | 0.002%        |
| 9         | 2.948       | 495           | 500         | 503          | rBV3     | 391            | 380           | 0.03%           | 0.004%        |
| 10        | 3.051       | 523           | 532         | 541          | rBV2     | 2915           | 5401          | 0.46%           | 0.059%        |
| 11        | 3.112       | 549           | 551         | 554          | rBV      | 172            | 132           | 0.01%           | 0.001%        |
| 12        | 3.186       | 561           | 574         | 576          | rBV      | 5719           | 7691          | 0.66%           | 0.085%        |
| 13        | 3.285       | 600           | 605         | 608          | rVB2     | 224            | 204           | 0.02%           | 0.002%        |
| 14        | 3.366       | 622           | 630         | 633          | rBV3     | 698            | 949           | 0.08%           | 0.010%        |
| 15        | 3.414       | 644           | 645         | 650          | rVB3     | 203            | 167           | 0.01%           | 0.002%        |
| 16        | 3.601       | 699           | 703         | 707          | rBV2     | 150            | 141           | 0.01%           | 0.002%        |
| 17        | 3.626       | 707           | 711         | 715          | rVB2     | 186            | 200           | 0.02%           | 0.002%        |
| 18        | 3.668       | 719           | 724         | 728          | rBV2     | 236            | 316           | 0.03%           | 0.003%        |
| 19        | 3.858       | 780           | 783         | 787          | rVB2     | 219            | 188           | 0.02%           | 0.002%        |
| 20        | 3.880       | 787           | 790         | 793          | rBV2     | 202            | 152           | 0.01%           | 0.002%        |
| 21        | 3.977       | 817           | 820         | 823          | rVB2     | 220            | 173           | 0.01%           | 0.002%        |
| 22        | 4.067       | 844           | 848         | 854          | rBV      | 182            | 277           | 0.02%           | 0.003%        |
| 23        | 4.240       | 898           | 902         | 907          | rBV      | 180            | 202           | 0.02%           | 0.002%        |
| 24        | 4.334       | 927           | 931         | 934          | rBV2     | 153            | 148           | 0.01%           | 0.002%        |
| 25        | 4.379       | 939           | 945         | 948          | rBV2     | 143            | 192           | 0.02%           | 0.002%        |
| 26        | 4.478       | 973           | 976         | 981          | rVB2     | 247            | 191           | 0.02%           | 0.002%        |
| 27        | 4.623       | 1007          | 1021        | 1048         | rBV      | 143613         | 340368        | 29.29%          | 3.743%        |
| 28        | 4.922       | 1110          | 1114        | 1117         | rVB2     | 298            | 256           | 0.02%           | 0.003%        |
| 29        | 4.951       | 1119          | 1123        | 1129         | rVB2     | 321            | 287           | 0.02%           | 0.003%        |
| 30        | 4.999       | 1134          | 1138        | 1140         | rBV      | 201            | 157           | 0.01%           | 0.002%        |
| 31        | 5.067       | 1140          | 1159        | 1186         | rBV      | 211747         | 463046        | 39.85%          | 5.093%        |
| 32        | 5.224       | 1206          | 1208        | 1211         | rVB      | 247            | 152           | 0.01%           | 0.002%        |
| 33        | 5.282       | 1223          | 1226        | 1228         | rBV2     | 497            | 419           | 0.04%           | 0.005%        |
| 34        | 5.340       | 1239          | 1244        | 1250         | rBV2     | 206            | 311           | 0.03%           | 0.003%        |
| 35        | 5.379       | 1250          | 1256        | 1259         | rVV4     | 487            | 553           | 0.05%           | 0.006%        |
| 36        | 5.411       | 1263          | 1266        | 1269         | rVV      | 168            | 167           | 0.01%           | 0.002%        |

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |         |         |
|----|--------|------|------|------|------|--------|---------|---------|---------|
| 37 | 5.443  | 1272 | 1276 | 1279 | rVB  | 243    | 196     | 0.02%   | 0.002%  |
| 38 | 5.462  | 1279 | 1282 | 1287 | rBV2 | 174    | 220     | 0.02%   | 0.002%  |
| 39 | 5.530  | 1299 | 1303 | 1305 | rVV2 | 194    | 173     | 0.01%   | 0.002%  |
| 40 | 5.729  | 1343 | 1365 | 1399 | rVV2 | 425423 | 1162011 | 100.00% | 12.780% |
| 41 | 6.044  | 1460 | 1463 | 1466 | rBV  | 398    | 317     | 0.03%   | 0.003%  |
| 42 | 6.253  | 1508 | 1528 | 1545 | rBV  | 350182 | 648270  | 55.79%  | 7.130%  |
| 43 | 6.539  | 1606 | 1617 | 1631 | rVB9 | 5343   | 11022   | 0.95%   | 0.121%  |
| 44 | 6.636  | 1641 | 1647 | 1651 | rVB2 | 213    | 247     | 0.02%   | 0.003%  |
| 45 | 6.694  | 1651 | 1665 | 1686 | rBV  | 281709 | 545730  | 46.96%  | 6.002%  |
| 46 | 6.806  | 1695 | 1700 | 1701 | rBV  | 590    | 436     | 0.04%   | 0.005%  |
| 47 | 6.854  | 1712 | 1715 | 1722 | rVB2 | 323    | 320     | 0.03%   | 0.004%  |
| 48 | 6.896  | 1722 | 1728 | 1731 | rBV2 | 186    | 240     | 0.02%   | 0.003%  |
| 49 | 6.983  | 1750 | 1755 | 1757 | rBV  | 178    | 164     | 0.01%   | 0.002%  |
| 50 | 7.041  | 1767 | 1773 | 1774 | rBV2 | 488    | 422     | 0.04%   | 0.005%  |
| 51 | 7.051  | 1774 | 1776 | 1781 | rVB2 | 528    | 335     | 0.03%   | 0.004%  |
| 52 | 7.182  | 1809 | 1817 | 1825 | rBV4 | 2124   | 3377    | 0.29%   | 0.037%  |
| 53 | 7.237  | 1831 | 1834 | 1838 | rBV2 | 150    | 149     | 0.01%   | 0.002%  |
| 54 | 7.282  | 1845 | 1848 | 1853 | rBV  | 184    | 146     | 0.01%   | 0.002%  |
| 55 | 7.321  | 1857 | 1860 | 1867 | rBV2 | 211    | 267     | 0.02%   | 0.003%  |
| 56 | 7.375  | 1874 | 1877 | 1879 | rBV2 | 177    | 142     | 0.01%   | 0.002%  |
| 57 | 7.472  | 1901 | 1907 | 1910 | rBV2 | 223    | 300     | 0.03%   | 0.003%  |
| 58 | 7.504  | 1914 | 1917 | 1920 | rVB2 | 200    | 151     | 0.01%   | 0.002%  |
| 59 | 7.568  | 1925 | 1937 | 1955 | rBV  | 150976 | 262502  | 22.59%  | 2.887%  |
| 60 | 7.661  | 1962 | 1966 | 1968 | rBV2 | 279    | 245     | 0.02%   | 0.003%  |
| 61 | 7.687  | 1968 | 1974 | 1984 | rVV5 | 1561   | 2704    | 0.23%   | 0.030%  |
| 62 | 7.903  | 2026 | 2041 | 2055 | rBV  | 501325 | 854043  | 73.50%  | 9.393%  |
| 63 | 7.973  | 2057 | 2063 | 2076 | rVB  | 6962   | 11742   | 1.01%   | 0.129%  |
| 64 | 8.182  | 2116 | 2128 | 2149 | rBV  | 106677 | 177051  | 15.24%  | 1.947%  |
| 65 | 8.555  | 2233 | 2244 | 2256 | rBV  | 60349  | 100686  | 8.66%   | 1.107%  |
| 66 | 8.636  | 2256 | 2269 | 2312 | rBV  | 422590 | 736803  | 63.41%  | 8.104%  |
| 67 | 8.925  | 2355 | 2359 | 2361 | rBV  | 164    | 143     | 0.01%   | 0.002%  |
| 68 | 9.005  | 2380 | 2384 | 2386 | rBV2 | 214    | 213     | 0.02%   | 0.002%  |
| 69 | 9.420  | 2499 | 2513 | 2548 | rBV  | 487778 | 799488  | 68.80%  | 8.793%  |
| 70 | 9.616  | 2572 | 2574 | 2577 | rVB2 | 313    | 159     | 0.01%   | 0.002%  |
| 71 | 9.642  | 2577 | 2582 | 2588 | rBV2 | 200    | 280     | 0.02%   | 0.003%  |
| 72 | 9.697  | 2593 | 2599 | 2609 | rVB  | 734    | 1054    | 0.09%   | 0.012%  |
| 73 | 9.890  | 2653 | 2659 | 2664 | rBV2 | 210    | 286     | 0.02%   | 0.003%  |
| 74 | 10.012 | 2693 | 2697 | 2701 | rBV2 | 183    | 220     | 0.02%   | 0.002%  |
| 75 | 10.105 | 2722 | 2726 | 2730 | rBV  | 493    | 417     | 0.04%   | 0.005%  |
| 76 | 10.250 | 2769 | 2771 | 2776 | rBV2 | 220    | 255     | 0.02%   | 0.003%  |

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 MSVOA\_U  
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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

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 10.340 | 2796 | 2799 | 2802 | rVB2 | 230    | 179    | 0.02%  | 0.002% |
| 78  | 10.359 | 2802 | 2805 | 2807 | rBV2 | 226    | 183    | 0.02%  | 0.002% |
| 79  | 10.484 | 2841 | 2844 | 2848 | rBV  | 317    | 246    | 0.02%  | 0.003% |
| 80  | 10.578 | 2867 | 2873 | 2877 | rBV2 | 272    | 428    | 0.04%  | 0.005% |
| 81  | 10.639 | 2888 | 2892 | 2894 | rBV3 | 230    | 157    | 0.01%  | 0.002% |
| 82  | 10.671 | 2896 | 2902 | 2911 | rVV2 | 1531   | 1973   | 0.17%  | 0.022% |
| 83  | 10.761 | 2914 | 2930 | 2948 | rBV  | 395322 | 640487 | 55.12% | 7.044% |
| 84  | 10.867 | 2960 | 2963 | 2965 | rBV2 | 372    | 274    | 0.02%  | 0.003% |
| 85  | 11.005 | 3002 | 3006 | 3008 | rBV2 | 262    | 205    | 0.02%  | 0.002% |
| 86  | 11.224 | 3068 | 3074 | 3077 | rBV2 | 236    | 278    | 0.02%  | 0.003% |
| 87  | 11.247 | 3077 | 3081 | 3084 | rBV2 | 190    | 160    | 0.01%  | 0.002% |
| 88  | 11.301 | 3094 | 3098 | 3100 | rBV2 | 197    | 168    | 0.01%  | 0.002% |
| 89  | 11.465 | 3142 | 3149 | 3159 | rVB5 | 1511   | 2633   | 0.23%  | 0.029% |
| 90  | 11.700 | 3213 | 3222 | 3230 | rBV4 | 757    | 1188   | 0.10%  | 0.013% |
| 91  | 11.816 | 3245 | 3258 | 3273 | rBV  | 447276 | 715824 | 61.60% | 7.873% |
| 92  | 11.944 | 3295 | 3298 | 3302 | rBV2 | 453    | 316    | 0.03%  | 0.003% |
| 93  | 11.970 | 3303 | 3306 | 3308 | rBV2 | 777    | 571    | 0.05%  | 0.006% |
| 94  | 12.086 | 3338 | 3342 | 3346 | rBV2 | 193    | 224    | 0.02%  | 0.002% |
| 95  | 12.195 | 3363 | 3376 | 3397 | rBV  | 467099 | 766344 | 65.95% | 8.429% |
| 96  | 12.337 | 3415 | 3420 | 3425 | rBV2 | 247    | 327    | 0.03%  | 0.004% |
| 97  | 12.404 | 3438 | 3441 | 3444 | rBV  | 253    | 214    | 0.02%  | 0.002% |
| 98  | 12.494 | 3465 | 3469 | 3471 | rBV2 | 231    | 187    | 0.02%  | 0.002% |
| 99  | 14.095 | 3960 | 3967 | 3974 | rBV2 | 659    | 1175   | 0.10%  | 0.013% |
| 100 | 14.925 | 4221 | 4225 | 4229 | rBV2 | 375    | 411    | 0.04%  | 0.005% |

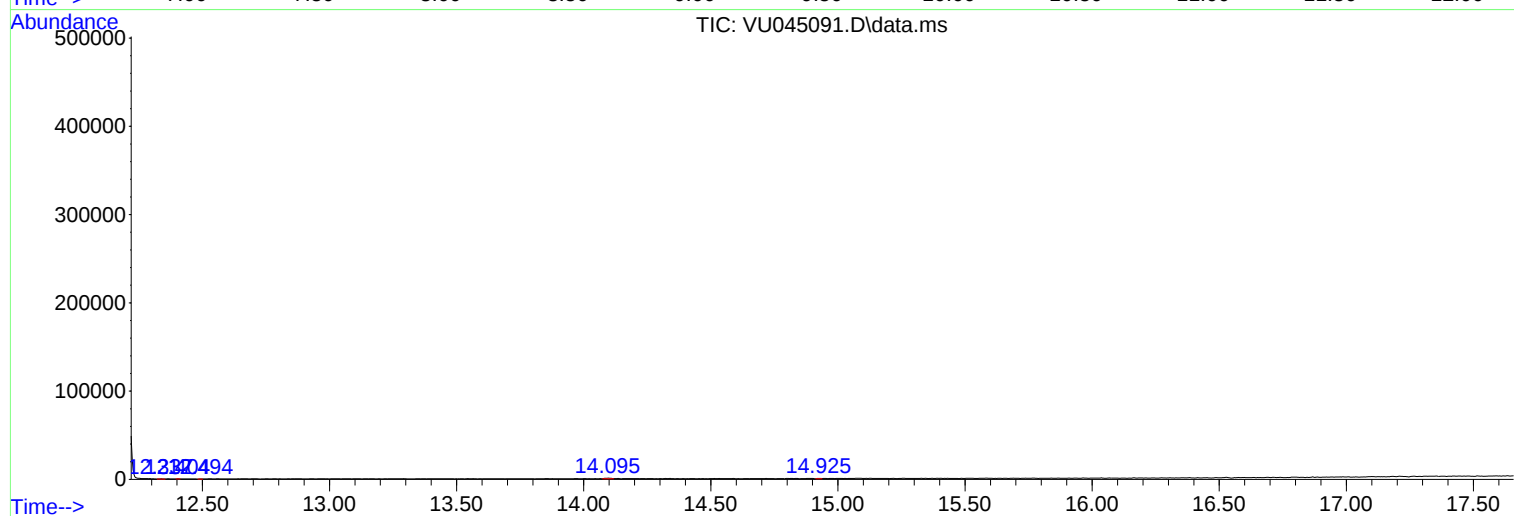
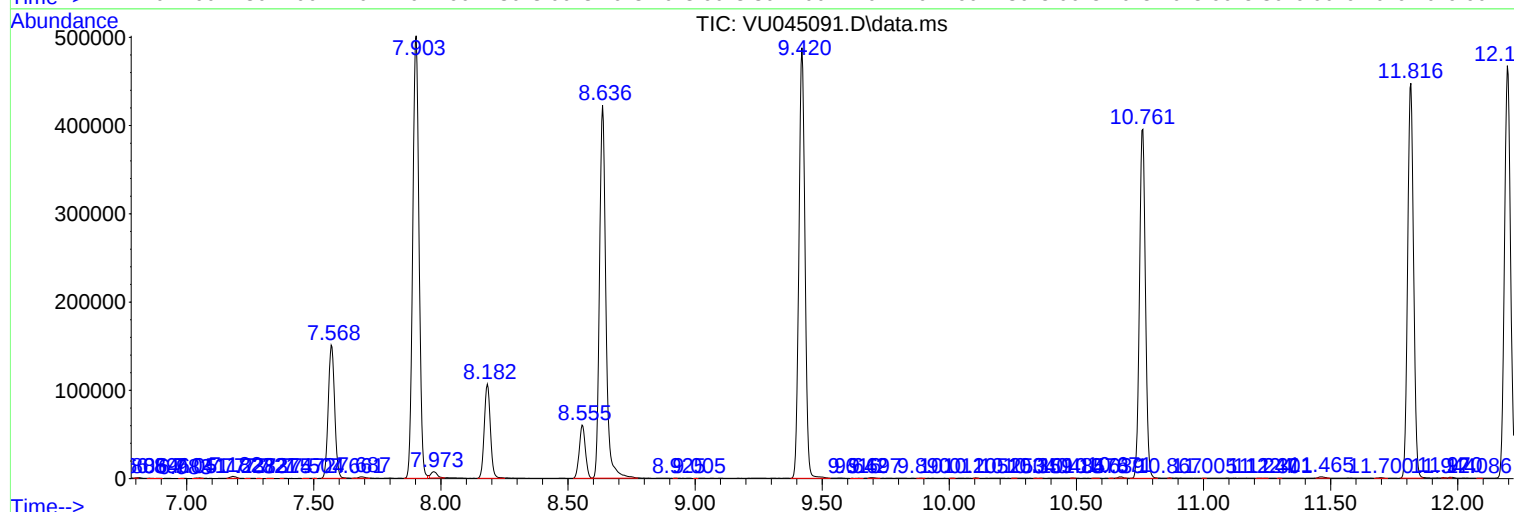
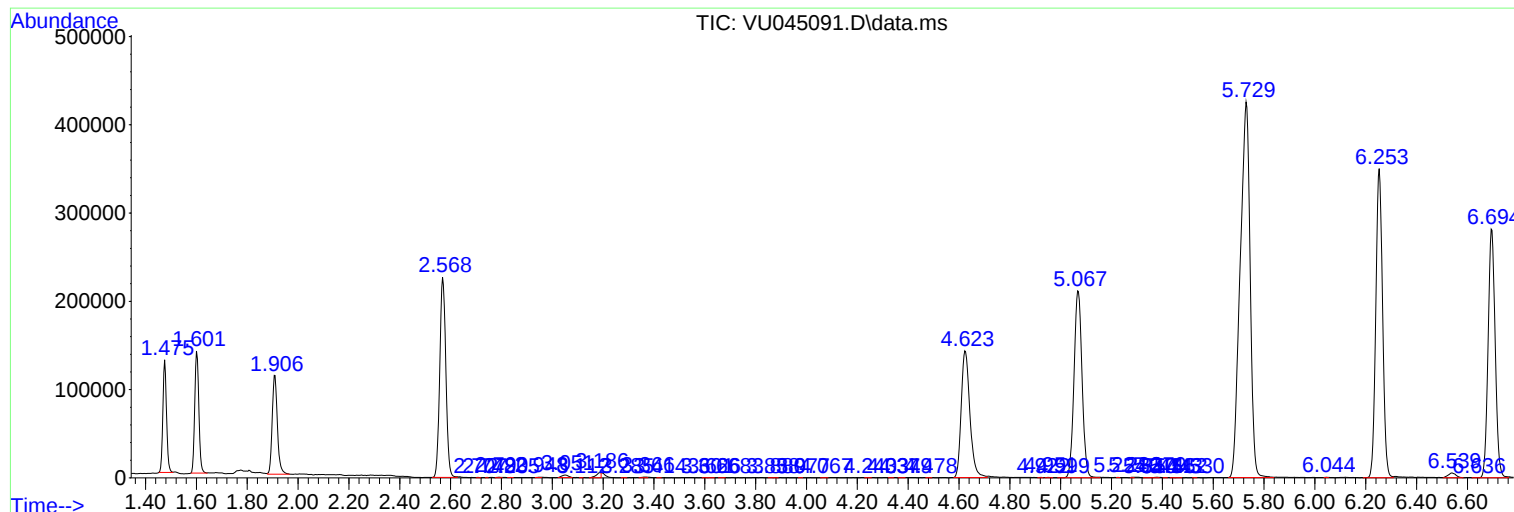
Sum of corrected areas: 9092276

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
Quant Title : VOC Analysis

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



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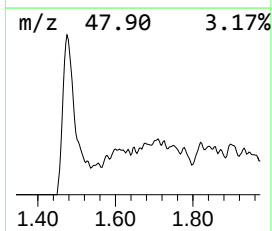
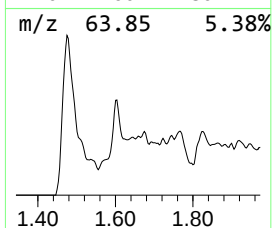
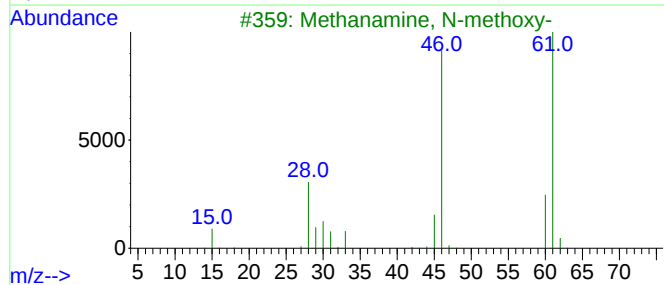
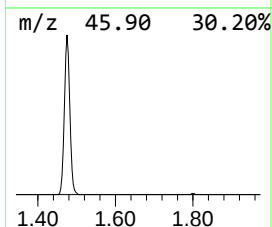
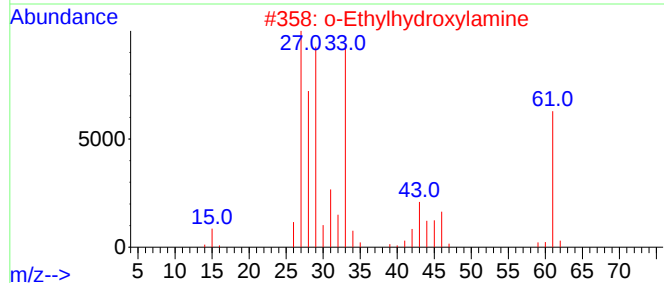
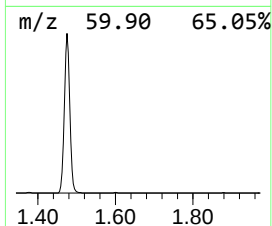
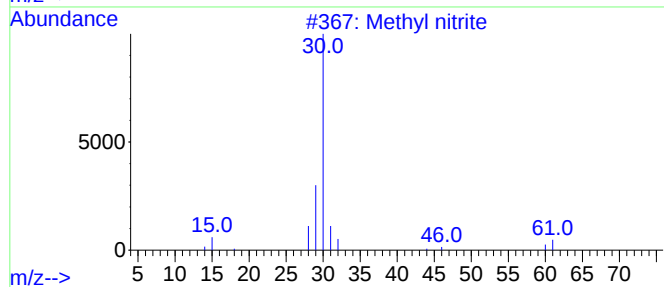
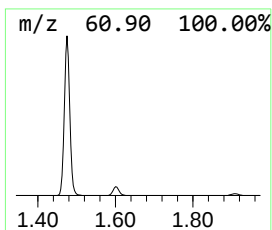
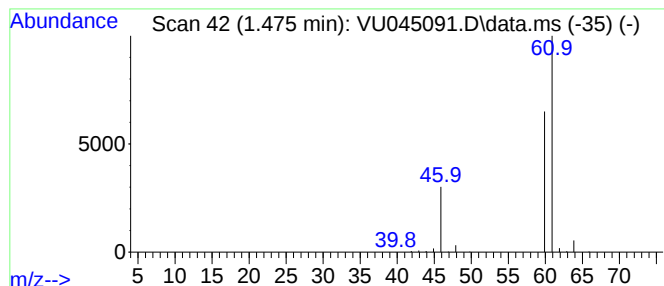
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
Quant Title : VOC Analysis

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.  |
|-------|-----------|--------|---------------------|-------|
| 1.475 | 9.79 ug/L | 126939 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID            | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------|-----|---------|-------------|------|
| 1    |    |   | Methyl nitrite          | 61  | CH3NO2  | 000624-91-9 | 5    |
| 2    |    |   | o-Ethylhydroxylamine    | 61  | C2H7NO  | 000624-86-2 | 4    |
| 3    |    |   | Methanamine, N-methoxy- | 61  | C2H7NO  | 001117-97-1 | 4    |
| 4    |    |   | Trifluoroguanidine      | 113 | CH2F3N3 | 037950-72-4 | 4    |
| 5    |    |   | Cyanogen chloride       | 61  | CClN    | 000506-77-4 | 4    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown-01       | 1.475 | 9.8     | ug/L  | 126939   | 1                     | 6.253 | 648270 | 50.0 |