

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121521\  
 Data File : VU046393.D  
 Acq On : 15 Dec 2021 13:37  
 Operator : SY/MD  
 Sample : M4971-14DL 10X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BG3D1DL

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\SFAMULM112921WMA.M  
 Title : VOC Analysis

Signal : TIC: VU046393.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         | 1.363       | 3             | 7           | 23           | rVB      | 7973           | 8698          | 1.76%           | 0.191%        |
| 2         | 1.475       | 35            | 42          | 54           | rBV      | 65797          | 67660         | 13.68%          | 1.485%        |
| 3         | 1.604       | 74            | 82          | 103          | rVB2     | 66077          | 83685         | 16.91%          | 1.837%        |
| 4         | 1.919       | 172           | 180         | 198          | rBV      | 39366          | 56240         | 11.37%          | 1.234%        |
| 5         | 2.089       | 231           | 233         | 236          | rBV2     | 372            | 266           | 0.05%           | 0.006%        |
| 6         | 2.314       | 299           | 303         | 309          | rBV3     | 372            | 440           | 0.09%           | 0.010%        |
| 7         | 2.340       | 309           | 311         | 313          | rBV      | 255            | 144           | 0.03%           | 0.003%        |
| 8         | 2.572       | 372           | 383         | 396          | rBV      | 92062          | 152815        | 30.89%          | 3.354%        |
| 9         | 2.752       | 435           | 439         | 442          | rBV      | 184            | 201           | 0.04%           | 0.004%        |
| 10        | 2.842       | 464           | 467         | 470          | rBB      | 145            | 120           | 0.02%           | 0.003%        |
| 11        | 2.887       | 471           | 481         | 482          | rBV2     | 299            | 475           | 0.10%           | 0.010%        |
| 12        | 2.970       | 505           | 507         | 511          | rVB      | 331            | 237           | 0.05%           | 0.005%        |
| 13        | 2.996       | 511           | 515         | 518          | rBV2     | 146            | 153           | 0.03%           | 0.003%        |
| 14        | 3.051       | 526           | 532         | 542          | rVB3     | 1244           | 2035          | 0.41%           | 0.045%        |
| 15        | 3.189       | 561           | 575         | 584          | rBV2     | 2639           | 5374          | 1.09%           | 0.118%        |
| 16        | 3.359       | 616           | 628         | 643          | rBB2     | 21748          | 41458         | 8.38%           | 0.910%        |
| 17        | 4.141       | 867           | 871         | 873          | rBB      | 151            | 123           | 0.02%           | 0.003%        |
| 18        | 4.671       | 1012          | 1036        | 1065         | rBV3     | 135583         | 414464        | 83.77%          | 9.097%        |
| 19        | 4.838       | 1086          | 1088        | 1092         | rVV2     | 165            | 128           | 0.03%           | 0.003%        |
| 20        | 4.883       | 1099          | 1102        | 1105         | rVB2     | 255            | 183           | 0.04%           | 0.004%        |
| 21        | 5.067       | 1144          | 1159        | 1182         | rBV      | 95277          | 206711        | 41.78%          | 4.537%        |
| 22        | 5.321       | 1236          | 1238        | 1241         | rVB      | 284            | 143           | 0.03%           | 0.003%        |
| 23        | 5.340       | 1241          | 1244        | 1247         | rBB      | 146            | 123           | 0.02%           | 0.003%        |
| 24        | 5.729       | 1344          | 1365        | 1383         | rBV2     | 179527         | 494768        | 100.00%         | 10.859%       |
| 25        | 6.121       | 1483          | 1487        | 1491         | rBV      | 183            | 233           | 0.05%           | 0.005%        |
| 26        | 6.141       | 1491          | 1493        | 1495         | rVB      | 239            | 133           | 0.03%           | 0.003%        |
| 27        | 6.157       | 1496          | 1498        | 1501         | rBB      | 255            | 124           | 0.03%           | 0.003%        |
| 28        | 6.253       | 1513          | 1528        | 1546         | rBV      | 181701         | 341058        | 68.93%          | 7.485%        |
| 29        | 6.407       | 1574          | 1576        | 1579         | rBB      | 219            | 127           | 0.03%           | 0.003%        |
| 30        | 6.694       | 1651          | 1665        | 1682         | rBV      | 118767         | 229976        | 46.48%          | 5.047%        |
| 31        | 6.752       | 1682          | 1683        | 1686         | rVB      | 265            | 121           | 0.02%           | 0.003%        |
| 32        | 6.806       | 1694          | 1700        | 1702         | rBV2     | 270            | 266           | 0.05%           | 0.006%        |
| 33        | 7.170       | 1810          | 1813        | 1815         | rBV      | 132            | 115           | 0.02%           | 0.003%        |
| 34        | 7.186       | 1815          | 1818        | 1819         | rVV      | 201            | 143           | 0.03%           | 0.003%        |
| 35        | 7.195       | 1819          | 1821        | 1825         | rVB      | 283            | 209           | 0.04%           | 0.005%        |
| 36        | 7.568       | 1925          | 1937        | 1958         | rBB      | 63280          | 110342        | 22.30%          | 2.422%        |

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 BG3D1DL

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Integrator: RTE

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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 7.710  | 1979 | 1981 | 1984 | rBB  | 169    | 111    | 0.02%  | 0.002% |
| 38 | 7.899  | 2027 | 2040 | 2056 | rBV  | 213081 | 363937 | 73.56% | 7.988% |
| 39 | 7.973  | 2057 | 2063 | 2072 | rVB2 | 2622   | 4173   | 0.84%  | 0.092% |
| 40 | 8.179  | 2117 | 2127 | 2142 | rBV  | 45339  | 74733  | 15.10% | 1.640% |
| 41 | 8.234  | 2142 | 2144 | 2149 | rVB2 | 240    | 154    | 0.03%  | 0.003% |
| 42 | 8.481  | 2210 | 2221 | 2226 | rBV4 | 2121   | 4096   | 0.83%  | 0.090% |
| 43 | 8.636  | 2258 | 2269 | 2291 | rBV  | 178192 | 295751 | 59.78% | 6.491% |
| 44 | 8.780  | 2311 | 2314 | 2319 | rVB2 | 279    | 267    | 0.05%  | 0.006% |
| 45 | 8.803  | 2319 | 2321 | 2323 | rBV  | 230    | 131    | 0.03%  | 0.003% |
| 46 | 8.867  | 2338 | 2341 | 2344 | rBV  | 177    | 174    | 0.04%  | 0.004% |
| 47 | 8.954  | 2364 | 2368 | 2371 | rBB  | 125    | 134    | 0.03%  | 0.003% |
| 48 | 8.996  | 2377 | 2381 | 2385 | rBB  | 192    | 200    | 0.04%  | 0.004% |
| 49 | 9.034  | 2389 | 2393 | 2396 | rBB  | 200    | 175    | 0.04%  | 0.004% |
| 50 | 9.092  | 2409 | 2411 | 2414 | rBV  | 133    | 116    | 0.02%  | 0.003% |
| 51 | 9.372  | 2494 | 2498 | 2500 | rBV  | 138    | 115    | 0.02%  | 0.003% |
| 52 | 9.417  | 2500 | 2512 | 2531 | rBV  | 274576 | 446539 | 90.25% | 9.801% |
| 53 | 9.517  | 2541 | 2543 | 2547 | rVB2 | 270    | 184    | 0.04%  | 0.004% |
| 54 | 9.571  | 2558 | 2560 | 2563 | rBB  | 261    | 162    | 0.03%  | 0.004% |
| 55 | 9.652  | 2582 | 2585 | 2588 | rBV  | 161    | 159    | 0.03%  | 0.003% |
| 56 | 9.697  | 2594 | 2599 | 2603 | rBB2 | 417    | 397    | 0.08%  | 0.009% |
| 57 | 9.938  | 2671 | 2674 | 2678 | rBB  | 133    | 141    | 0.03%  | 0.003% |
| 58 | 9.964  | 2679 | 2682 | 2687 | rBV  | 152    | 196    | 0.04%  | 0.004% |
| 59 | 9.989  | 2687 | 2690 | 2695 | rVB  | 178    | 208    | 0.04%  | 0.005% |
| 60 | 10.041 | 2702 | 2706 | 2710 | rBB  | 131    | 141    | 0.03%  | 0.003% |
| 61 | 10.067 | 2710 | 2714 | 2716 | rBV  | 149    | 145    | 0.03%  | 0.003% |
| 62 | 10.157 | 2738 | 2742 | 2748 | rBB  | 186    | 257    | 0.05%  | 0.006% |
| 63 | 10.198 | 2751 | 2755 | 2760 | rBV  | 182    | 239    | 0.05%  | 0.005% |
| 64 | 10.243 | 2766 | 2769 | 2771 | rBV  | 133    | 118    | 0.02%  | 0.003% |
| 65 | 10.317 | 2790 | 2792 | 2796 | rBV  | 123    | 135    | 0.03%  | 0.003% |
| 66 | 10.507 | 2848 | 2851 | 2854 | rVB  | 189    | 143    | 0.03%  | 0.003% |
| 67 | 10.575 | 2869 | 2872 | 2877 | rBV  | 153    | 193    | 0.04%  | 0.004% |
| 68 | 10.629 | 2884 | 2889 | 2890 | rBV  | 140    | 121    | 0.02%  | 0.003% |
| 69 | 10.674 | 2895 | 2903 | 2910 | rBV2 | 445    | 712    | 0.14%  | 0.016% |
| 70 | 10.758 | 2917 | 2929 | 2945 | rBV  | 188170 | 300920 | 60.82% | 6.605% |
| 71 | 10.902 | 2963 | 2974 | 2985 | rVB4 | 1818   | 3519   | 0.71%  | 0.077% |
| 72 | 10.947 | 2985 | 2988 | 2994 | rBV  | 177    | 249    | 0.05%  | 0.005% |
| 73 | 11.102 | 3033 | 3036 | 3038 | rBV  | 144    | 120    | 0.02%  | 0.003% |
| 74 | 11.317 | 3100 | 3103 | 3109 | rBV  | 166    | 240    | 0.05%  | 0.005% |
| 75 | 11.465 | 3143 | 3149 | 3150 | rBV  | 268    | 222    | 0.04%  | 0.005% |
| 76 | 11.710 | 3221 | 3225 | 3230 | rBV  | 173    | 246    | 0.05%  | 0.005% |

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Instrument :  
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 ClientSampleId :  
 BG3D1DL

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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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\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.812 | 3245 | 3257 | 3276 | rBV  | 288597 | 449934 | 90.94% | 9.875% |
| 78  | 11.928 | 3291 | 3293 | 3298 | rBB  | 193    | 178    | 0.04%  | 0.004% |
| 79  | 11.957 | 3298 | 3302 | 3304 | rBV2 | 298    | 276    | 0.06%  | 0.006% |
| 80  | 12.041 | 3325 | 3328 | 3333 | rVV  | 109    | 113    | 0.02%  | 0.002% |
| 81  | 12.195 | 3363 | 3376 | 3393 | rVB  | 241255 | 380894 | 76.98% | 8.360% |
| 82  | 12.636 | 3507 | 3513 | 3517 | rBV  | 218    | 322    | 0.07%  | 0.007% |
| 83  | 12.777 | 3549 | 3557 | 3562 | rVB3 | 609    | 830    | 0.17%  | 0.018% |
| 84  | 12.867 | 3579 | 3585 | 3587 | rBV  | 127    | 138    | 0.03%  | 0.003% |
| 85  | 13.005 | 3625 | 3628 | 3630 | rBV  | 175    | 142    | 0.03%  | 0.003% |
| 86  | 13.279 | 3711 | 3713 | 3715 | rBV  | 161    | 113    | 0.02%  | 0.002% |
| 87  | 14.581 | 4111 | 4118 | 4123 | rVB2 | 332    | 430    | 0.09%  | 0.009% |
| 88  | 15.243 | 4320 | 4324 | 4331 | rBV  | 183    | 224    | 0.05%  | 0.005% |
| 89  | 15.455 | 4386 | 4390 | 4392 | rBV  | 208    | 139    | 0.03%  | 0.003% |
| 90  | 15.642 | 4445 | 4448 | 4450 | rBV2 | 196    | 161    | 0.03%  | 0.004% |
| 91  | 15.697 | 4460 | 4465 | 4468 | rBV2 | 156    | 156    | 0.03%  | 0.003% |
| 92  | 15.719 | 4468 | 4472 | 4474 | rBV  | 206    | 201    | 0.04%  | 0.004% |
| 93  | 15.854 | 4510 | 4514 | 4516 | rBV  | 243    | 243    | 0.05%  | 0.005% |
| 94  | 16.012 | 4559 | 4563 | 4565 | rBV  | 182    | 161    | 0.03%  | 0.004% |
| 95  | 16.028 | 4566 | 4568 | 4576 | rVB2 | 372    | 334    | 0.07%  | 0.007% |
| 96  | 16.095 | 4582 | 4589 | 4593 | rBV3 | 746    | 826    | 0.17%  | 0.018% |
| 97  | 16.211 | 4617 | 4625 | 4628 | rBV2 | 242    | 385    | 0.08%  | 0.008% |
| 98  | 16.545 | 4726 | 4729 | 4733 | rBV  | 285    | 268    | 0.05%  | 0.006% |
| 99  | 16.584 | 4738 | 4741 | 4744 | rBV  | 227    | 115    | 0.02%  | 0.003% |
| 100 | 16.616 | 4748 | 4751 | 4756 | rBV2 | 271    | 232    | 0.05%  | 0.005% |

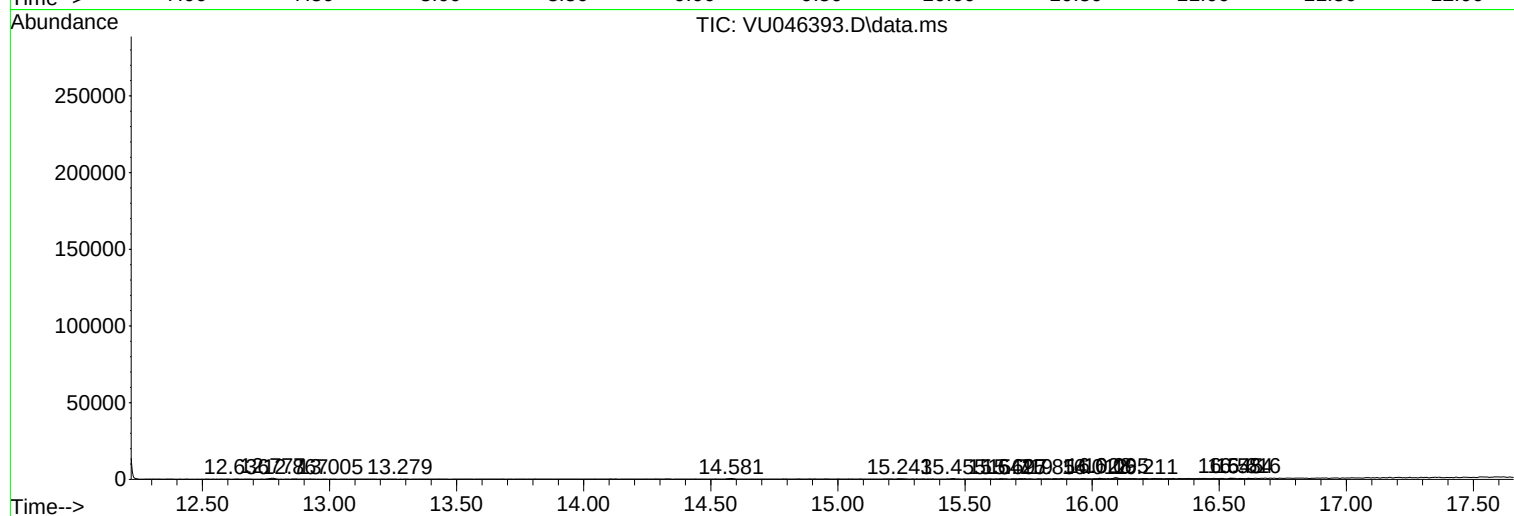
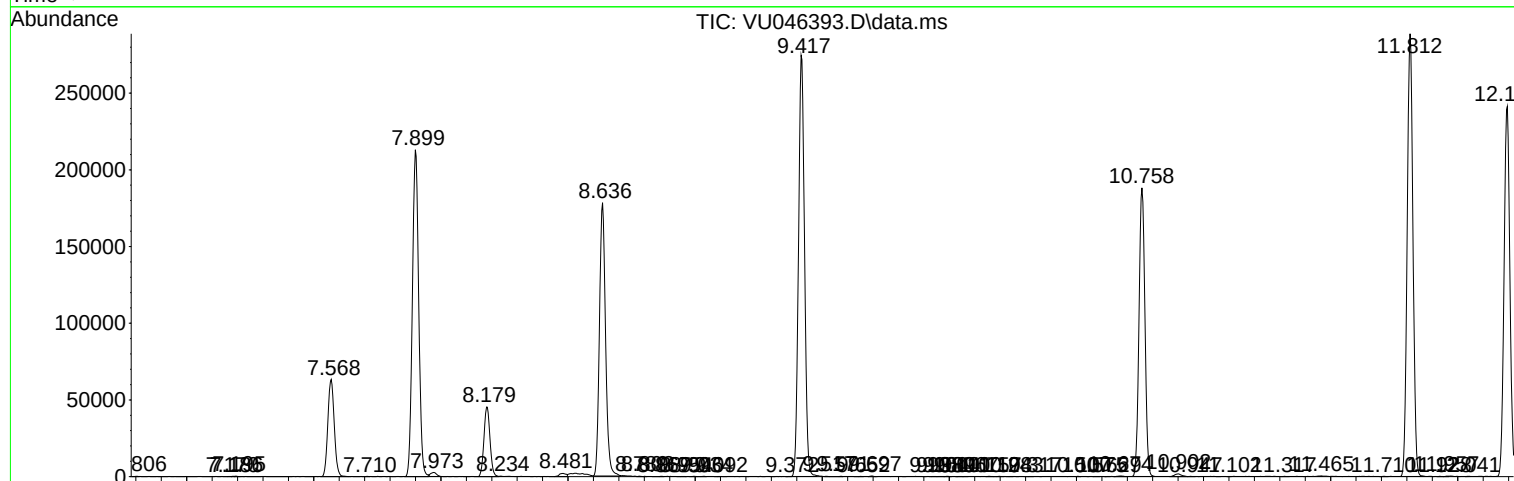
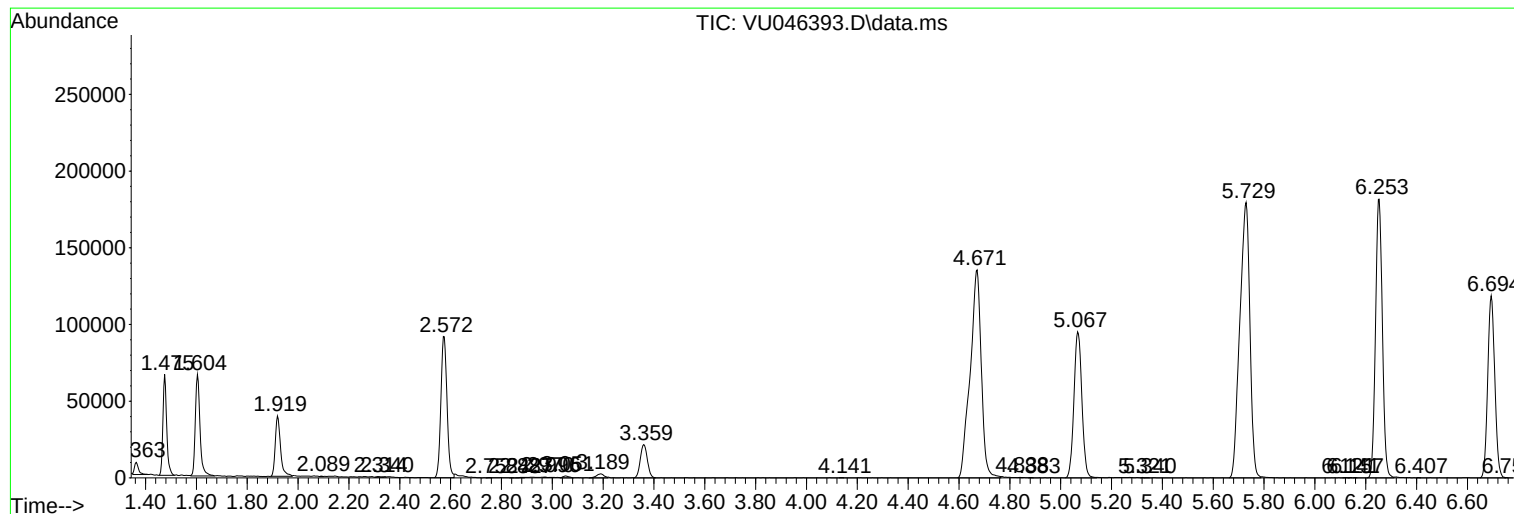
Sum of corrected areas: 4556279

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121521\  
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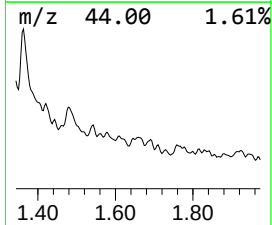
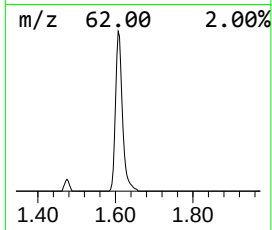
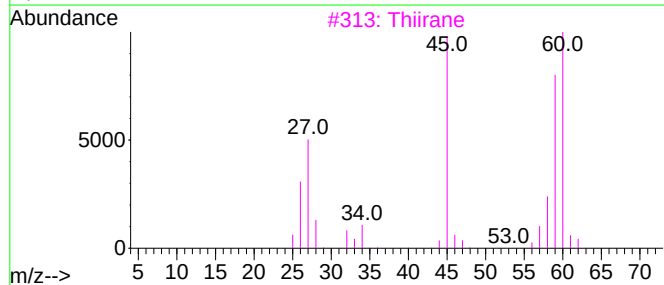
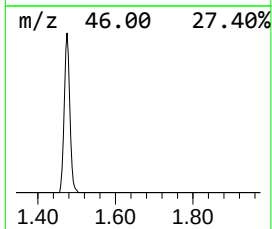
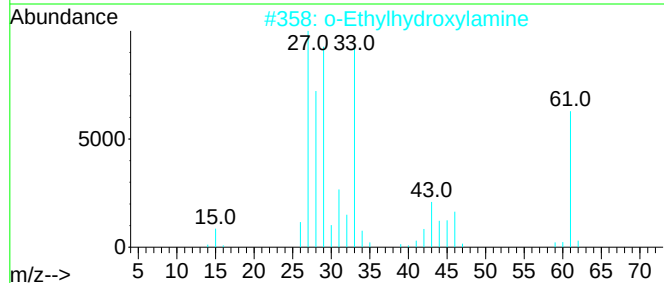
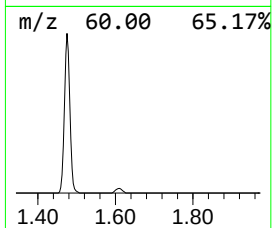
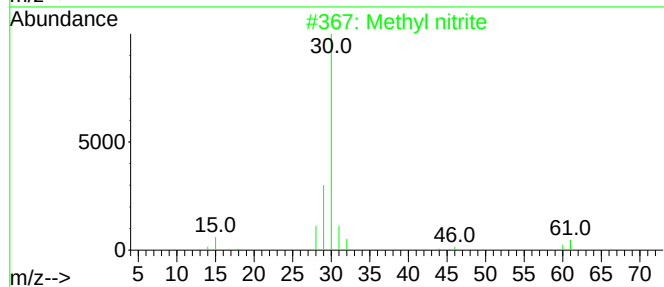
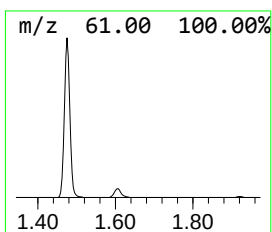
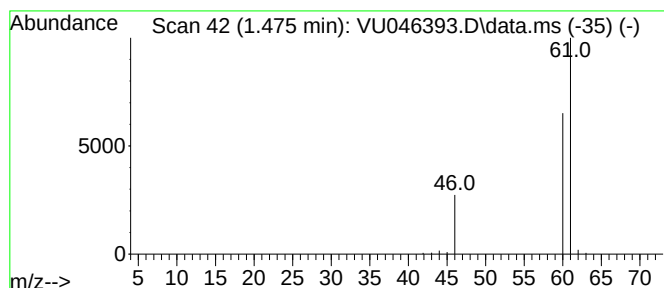
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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 | 9.92 ug/L | 67660 | 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    |    |   | Thiirane                | 60 | C2H4S   | 000420-12-2 | 4    |
| 4    |    |   | Carbonyl sulfide        | 60 | COS     | 000463-58-1 | 4    |
| 5    |    |   | Methanamine, N-methoxy- | 61 | C2H7NO  | 001117-97-1 | 4    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown-01       | 1.475 | 9.9     | ug/L  | 67660    | 1                     | 6.253 | 341058 | 50.0 |