

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV020222\  
 Data File : VV024533.D  
 Acq On : 02 Feb 2022 18:33  
 Operator : SY/MD  
 Sample : N1353-11ME  
 Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0VF4ME

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\_V\Method\SFAMVLM020222WMA.M  
 Title : VOC Analysis

Signal : TIC: VV024533.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         | 1.304       | 76            | 82          | 95           | rBV      | 164940         | 187679        | 13.84%          | 1.654%        |
| 2         | 1.568       | 157           | 164         | 181          | rBV      | 120940         | 172444        | 12.72%          | 1.520%        |
| 3         | 2.095       | 320           | 328         | 342          | rVB      | 248340         | 332220        | 24.50%          | 2.928%        |
| 4         | 3.011       | 610           | 613         | 615          | rBV3     | 697            | 420           | 0.03%           | 0.004%        |
| 5         | 3.079       | 630           | 634         | 639          | rBV2     | 799            | 825           | 0.06%           | 0.007%        |
| 6         | 3.179       | 663           | 665         | 667          | rBV2     | 669            | 306           | 0.02%           | 0.003%        |
| 7         | 3.220       | 676           | 678         | 680          | rVB2     | 517            | 166           | 0.01%           | 0.001%        |
| 8         | 3.243       | 683           | 685         | 687          | rBV2     | 304            | 220           | 0.02%           | 0.002%        |
| 9         | 3.272       | 689           | 694         | 696          | rBV4     | 725            | 686           | 0.05%           | 0.006%        |
| 10        | 3.362       | 718           | 722         | 725          | rBV5     | 820            | 674           | 0.05%           | 0.006%        |
| 11        | 3.548       | 777           | 780         | 784          | rBV3     | 463            | 332           | 0.02%           | 0.003%        |
| 12        | 3.580       | 789           | 790         | 791          | rBV      | 453            | 160           | 0.01%           | 0.001%        |
| 13        | 3.616       | 800           | 801         | 803          | rBV2     | 205            | 61            | 0.00%           | 0.001%        |
| 14        | 3.658       | 812           | 814         | 819          | rVB4     | 552            | 383           | 0.03%           | 0.003%        |
| 15        | 3.680       | 819           | 821         | 823          | rBV2     | 549            | 269           | 0.02%           | 0.002%        |
| 16        | 3.735       | 834           | 838         | 839          | rBV2     | 283            | 180           | 0.01%           | 0.002%        |
| 17        | 3.793       | 852           | 856         | 860          | rBV4     | 323            | 352           | 0.03%           | 0.003%        |
| 18        | 3.924       | 885           | 897         | 898          | rBV2     | 36053          | 54637         | 4.03%           | 0.481%        |
| 19        | 4.346       | 1015          | 1028        | 1054         | rVB      | 201704         | 515632        | 38.02%          | 4.544%        |
| 20        | 4.744       | 1150          | 1152        | 1153         | rBV      | 380            | 200           | 0.01%           | 0.002%        |
| 21        | 4.815       | 1173          | 1174        | 1179         | rVB3     | 623            | 481           | 0.04%           | 0.004%        |
| 22        | 4.838       | 1179          | 1181        | 1182         | rVB3     | 299            | 69            | 0.01%           | 0.001%        |
| 23        | 4.854       | 1184          | 1186        | 1191         | rVB3     | 625            | 310           | 0.02%           | 0.003%        |
| 24        | 4.879       | 1191          | 1194        | 1197         | rBV2     | 724            | 457           | 0.03%           | 0.004%        |
| 25        | 4.912       | 1197          | 1204        | 1208         | rBV7     | 711            | 933           | 0.07%           | 0.008%        |
| 26        | 4.982       | 1224          | 1226        | 1228         | rVB3     | 468            | 198           | 0.01%           | 0.002%        |
| 27        | 5.040       | 1228          | 1244        | 1278         | rBV2     | 539745         | 1356096       | 100.00%         | 11.950%       |
| 28        | 5.612       | 1411          | 1422        | 1449         | rBV      | 423788         | 895452        | 66.03%          | 7.891%        |
| 29        | 5.905       | 1502          | 1513        | 1529         | rBV      | 27003          | 59652         | 4.40%           | 0.526%        |
| 30        | 6.069       | 1551          | 1564        | 1593         | rVB      | 288053         | 618456        | 45.61%          | 5.450%        |
| 31        | 6.313       | 1638          | 1640        | 1642         | rBV      | 297            | 141           | 0.01%           | 0.001%        |
| 32        | 6.378       | 1657          | 1660        | 1663         | rBV4     | 858            | 614           | 0.05%           | 0.005%        |
| 33        | 6.429       | 1674          | 1676        | 1678         | rBV3     | 531            | 283           | 0.02%           | 0.002%        |
| 34        | 6.461       | 1685          | 1686        | 1687         | rBV      | 362            | 100           | 0.01%           | 0.001%        |
| 35        | 6.490       | 1692          | 1695        | 1696         | rBV2     | 203            | 114           | 0.01%           | 0.001%        |
| 36        | 6.612       | 1731          | 1733        | 1735         | rVB4     | 338            | 100           | 0.01%           | 0.001%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VW020222\  
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 Sample : N1353-11ME  
 Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0VF4ME

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\_V\Method\SFAMVLM020222WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 6.629  | 1735 | 1738 | 1739 | rBV2 | 1143   | 700     | 0.05%  | 0.006% |
| 38 | 6.818  | 1795 | 1797 | 1798 | rBV2 | 513    | 243     | 0.02%  | 0.002% |
| 39 | 6.915  | 1819 | 1827 | 1830 | rBV6 | 1113   | 1640    | 0.12%  | 0.014% |
| 40 | 6.985  | 1838 | 1849 | 1874 | rBV  | 169011 | 344905  | 25.43% | 3.039% |
| 41 | 7.243  | 1921 | 1929 | 1939 | rBV4 | 13560  | 35043   | 2.58%  | 0.309% |
| 42 | 7.313  | 1941 | 1951 | 1966 | rVV  | 602882 | 1081920 | 79.78% | 9.534% |
| 43 | 7.622  | 2037 | 2047 | 2083 | rBV  | 105797 | 234841  | 17.32% | 2.070% |
| 44 | 7.873  | 2123 | 2125 | 2128 | rBV2 | 422    | 206     | 0.02%  | 0.002% |
| 45 | 7.934  | 2142 | 2144 | 2148 | rBV3 | 667    | 473     | 0.03%  | 0.004% |
| 46 | 7.950  | 2148 | 2149 | 2150 | rBV  | 365    | 124     | 0.01%  | 0.001% |
| 47 | 8.030  | 2170 | 2174 | 2178 | rBV4 | 499    | 250     | 0.02%  | 0.002% |
| 48 | 8.127  | 2185 | 2204 | 2245 | rBV2 | 166564 | 683163  | 50.38% | 6.020% |
| 49 | 8.545  | 2331 | 2334 | 2336 | rBV3 | 585    | 322     | 0.02%  | 0.003% |
| 50 | 8.587  | 2336 | 2347 | 2358 | rVV9 | 3332   | 8743    | 0.64%  | 0.077% |
| 51 | 8.709  | 2383 | 2385 | 2386 | rBV2 | 556    | 220     | 0.02%  | 0.002% |
| 52 | 8.789  | 2403 | 2410 | 2418 | rBV6 | 2404   | 3642    | 0.27%  | 0.032% |
| 53 | 8.854  | 2418 | 2430 | 2460 | rVV  | 572185 | 1098472 | 81.00% | 9.680% |
| 54 | 9.014  | 2471 | 2480 | 2500 | rVB  | 86124  | 156328  | 11.53% | 1.378% |
| 55 | 9.140  | 2508 | 2519 | 2534 | rBV  | 347071 | 622394  | 45.90% | 5.485% |
| 56 | 9.307  | 2569 | 2571 | 2578 | rVB6 | 739    | 603     | 0.04%  | 0.005% |
| 57 | 9.345  | 2582 | 2583 | 2589 | rVV3 | 469    | 278     | 0.02%  | 0.002% |
| 58 | 9.474  | 2611 | 2623 | 2631 | rBV7 | 2015   | 4453    | 0.33%  | 0.039% |
| 59 | 9.548  | 2635 | 2646 | 2664 | rVV  | 121881 | 216234  | 15.95% | 1.906% |
| 60 | 9.889  | 2750 | 2752 | 2754 | rBV3 | 753    | 397     | 0.03%  | 0.003% |
| 61 | 10.014 | 2788 | 2791 | 2793 | rBV4 | 823    | 583     | 0.04%  | 0.005% |
| 62 | 10.223 | 2843 | 2856 | 2876 | rBV  | 324050 | 577598  | 42.59% | 5.090% |
| 63 | 10.455 | 2918 | 2928 | 2940 | rBV2 | 8420   | 18493   | 1.36%  | 0.163% |
| 64 | 10.661 | 2986 | 2992 | 2996 | rBV4 | 1277   | 1508    | 0.11%  | 0.013% |
| 65 | 10.918 | 3065 | 3072 | 3093 | rVB3 | 17198  | 29418   | 2.17%  | 0.259% |
| 66 | 11.037 | 3101 | 3109 | 3117 | rBV7 | 1787   | 3347    | 0.25%  | 0.029% |
| 67 | 11.069 | 3117 | 3119 | 3120 | rBV2 | 567    | 271     | 0.02%  | 0.002% |
| 68 | 11.252 | 3164 | 3176 | 3195 | rBV  | 665190 | 1042564 | 76.88% | 9.187% |
| 69 | 11.538 | 3258 | 3265 | 3267 | rBV4 | 1559   | 1770    | 0.13%  | 0.016% |
| 70 | 11.625 | 3281 | 3292 | 3312 | rBV  | 605223 | 965782  | 71.22% | 8.511% |
| 71 | 11.902 | 3373 | 3378 | 3379 | rBV4 | 584    | 482     | 0.04%  | 0.004% |
| 72 | 12.146 | 3452 | 3454 | 3458 | rBV4 | 410    | 296     | 0.02%  | 0.003% |
| 73 | 12.654 | 3610 | 3612 | 3614 | rBV  | 334    | 170     | 0.01%  | 0.001% |
| 74 | 12.667 | 3614 | 3616 | 3618 | rBV2 | 451    | 214     | 0.02%  | 0.002% |
| 75 | 12.792 | 3649 | 3655 | 3659 | rBV4 | 624    | 772     | 0.06%  | 0.007% |
| 76 | 12.837 | 3666 | 3669 | 3672 | rVB2 | 566    | 361     | 0.03%  | 0.003% |

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 Operator : SY/MD  
 Sample : N1353-11ME  
 Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0VF4ME

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\_V\Method\SFAMVLM020222WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 77 | 12.857 | 3672 | 3675 | 3676 | rBV  | 290  | 153  | 0.01% | 0.001% |
| 78 | 12.963 | 3703 | 3708 | 3711 | rBV4 | 552  | 540  | 0.04% | 0.005% |
| 79 | 13.172 | 3770 | 3773 | 3775 | rBV  | 501  | 342  | 0.03% | 0.003% |
| 80 | 13.258 | 3796 | 3800 | 3805 | rVB5 | 534  | 556  | 0.04% | 0.005% |
|    |        |      |      |      |      |      |      |       |        |
| 81 | 13.291 | 3808 | 3810 | 3812 | rBV  | 297  | 147  | 0.01% | 0.001% |
| 82 | 13.368 | 3830 | 3834 | 3836 | rBV4 | 428  | 372  | 0.03% | 0.003% |
| 83 | 13.410 | 3845 | 3847 | 3850 | rVB2 | 557  | 271  | 0.02% | 0.002% |
| 84 | 13.496 | 3871 | 3874 | 3875 | rBV2 | 418  | 272  | 0.02% | 0.002% |
| 85 | 13.561 | 3892 | 3894 | 3897 | rBV3 | 307  | 164  | 0.01% | 0.001% |
|    |        |      |      |      |      |      |      |       |        |
| 86 | 13.686 | 3930 | 3933 | 3935 | rBV3 | 526  | 309  | 0.02% | 0.003% |
| 87 | 13.702 | 3935 | 3938 | 3941 | rVV2 | 260  | 179  | 0.01% | 0.002% |
| 88 | 13.718 | 3941 | 3943 | 3945 | rBV2 | 358  | 234  | 0.02% | 0.002% |
| 89 | 13.789 | 3963 | 3965 | 3970 | rVB3 | 421  | 289  | 0.02% | 0.003% |
| 90 | 14.040 | 4035 | 4043 | 4049 | rBV5 | 1574 | 2618 | 0.19% | 0.023% |
|    |        |      |      |      |      |      |      |       |        |
| 91 | 14.098 | 4058 | 4061 | 4063 | rBV3 | 474  | 252  | 0.02% | 0.002% |
| 92 | 14.223 | 4098 | 4100 | 4103 | rVB2 | 497  | 254  | 0.02% | 0.002% |
| 93 | 14.455 | 4170 | 4172 | 4175 | rBV2 | 349  | 216  | 0.02% | 0.002% |

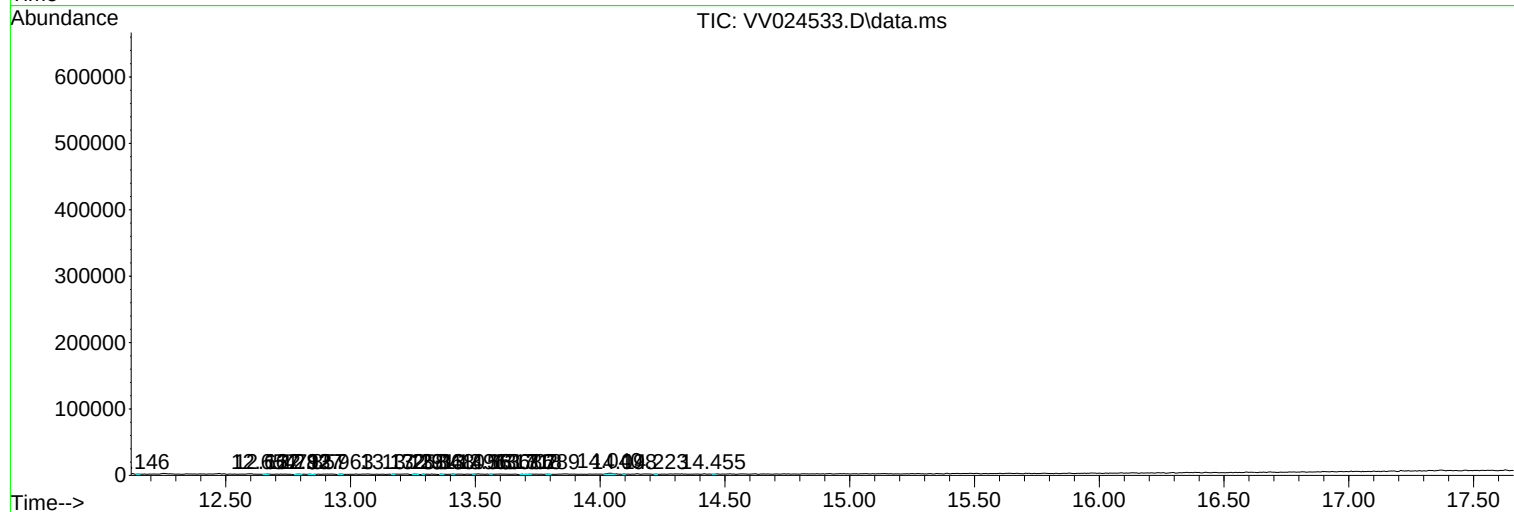
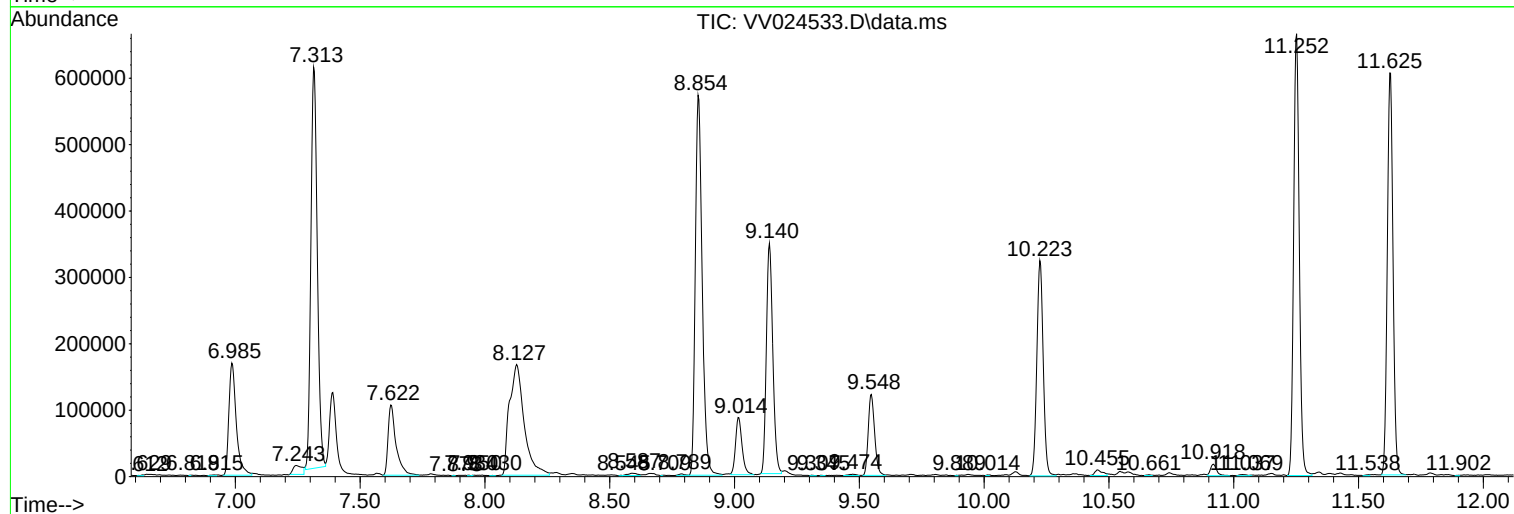
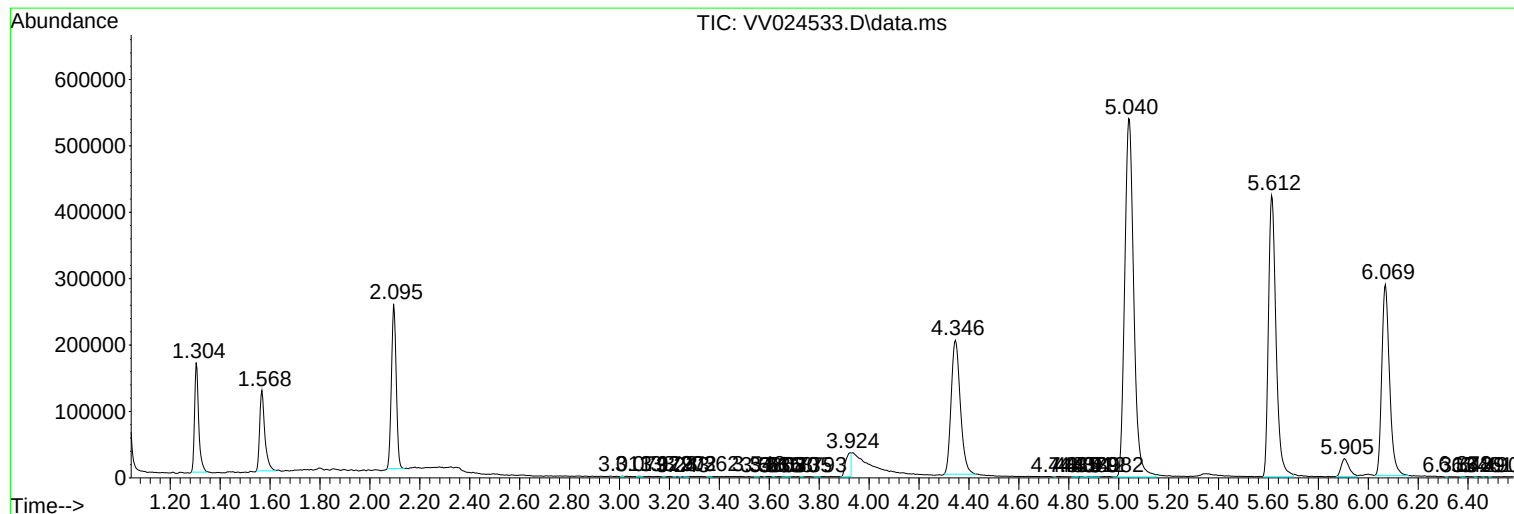
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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV020222\  
Data File : VV024533.D  
Acq On : 02 Feb 2022 18:33  
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Sample : N1353-11ME  
Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
C0VF4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM020222WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV020222\  
Data File : VV024533.D  
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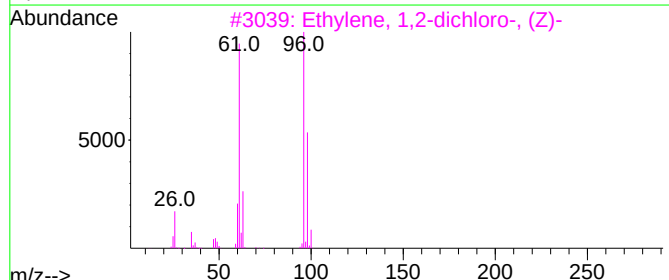
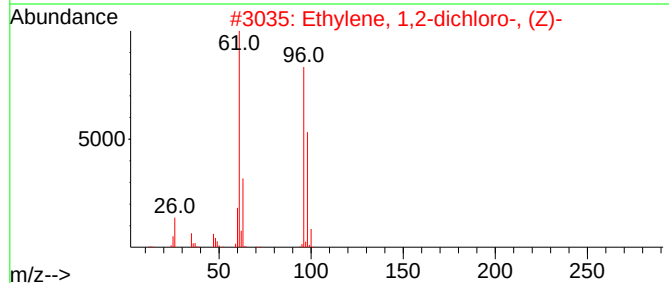
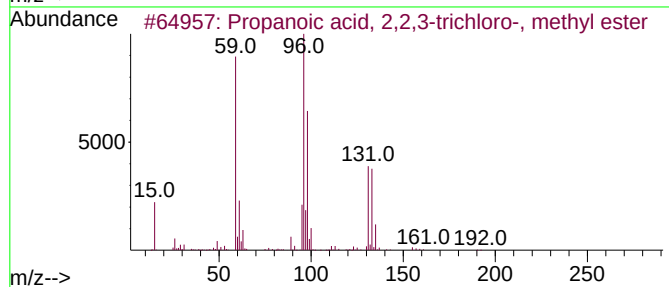
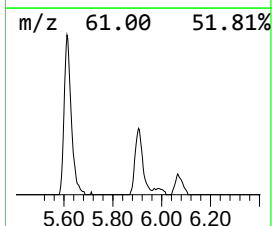
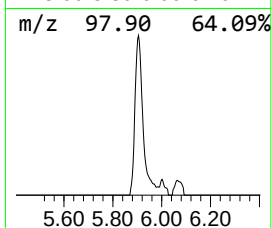
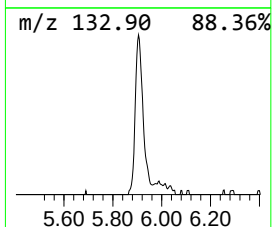
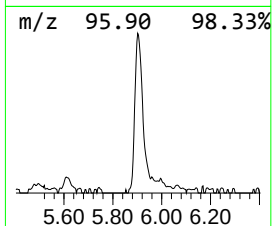
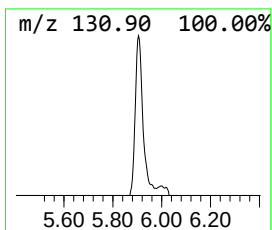
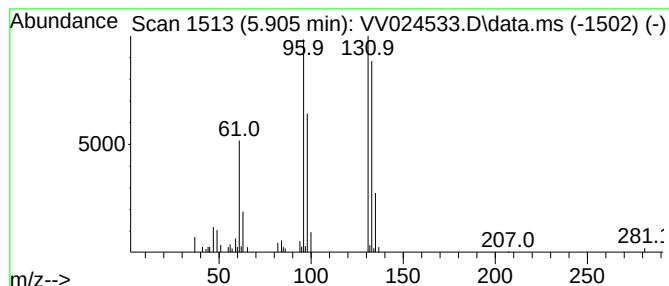
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM020222WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Propanoic acid, 2,2,3-trichloro... Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 5.905 | 3.33 ug/L | 59652 | 1,4-Difluorobenzene | 5.612 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Propanoic acid, 2,2,3-trichloro-... | 190 | C4H5Cl3O2 | 004749-35-3 | 50   |
| 2    |    |   | Ethylene, 1,2-dichloro-, (Z)-       | 96  | C2H2Cl2   | 000156-59-2 | 43   |
| 3    |    |   | Ethylene, 1,2-dichloro-, (Z)-       | 96  | C2H2Cl2   | 000156-59-2 | 38   |
| 4    |    |   | Dihydro-4,5-dichloro-2(3H)furanone  | 154 | C4H4Cl2O2 | 114434-99-0 | 38   |
| 5    |    |   | Ethene, 1,1-dichloro-               | 96  | C2H2Cl2   | 000075-35-4 | 38   |



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Quant Title : VOC Analysis

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

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Propanoic acid,... | 5.905 | 3.3     | ug/L  | 59652    | 1                     | 5.612 | 895452 | 50.0 |