

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051822\  
 Data File : VU048610.D  
 Acq On : 18 May 2022 13:48  
 Operator : SY/MD  
 Sample : N2843-22ME  
 Misc : 5.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 EW4K2ME

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\SFAMULM051622WMA.M  
 Title : VOC Analysis

Signal : TIC: VU048610.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         | 1.597       | 73            | 80          | 103          | rVB      | 26245          | 47385         | 6.95%           | 0.821%        |
| 2         | 1.809       | 124           | 146         | 148          | rBV10    | 14332          | 34191         | 5.01%           | 0.592%        |
| 3         | 2.453       | 340           | 346         | 350          | rVB2     | 766            | 892           | 0.13%           | 0.015%        |
| 4         | 2.536       | 360           | 372         | 384          | rBV      | 84995          | 138615        | 20.33%          | 2.401%        |
| 5         | 2.700       | 418           | 423         | 426          | rBV2     | 435            | 343           | 0.05%           | 0.006%        |
| 6         | 2.723       | 426           | 430         | 431          | rBV2     | 428            | 340           | 0.05%           | 0.006%        |
| 7         | 2.748       | 435           | 438         | 440          | rBV      | 556            | 347           | 0.05%           | 0.006%        |
| 8         | 2.819       | 456           | 460         | 464          | rBV      | 127            | 173           | 0.03%           | 0.003%        |
| 9         | 2.935       | 493           | 496         | 499          | rBV      | 330            | 295           | 0.04%           | 0.005%        |
| 10        | 2.951       | 499           | 501         | 505          | rVV3     | 487            | 311           | 0.05%           | 0.005%        |
| 11        | 3.031       | 518           | 526         | 539          | rBV4     | 2666           | 4426          | 0.65%           | 0.077%        |
| 12        | 3.105       | 544           | 549         | 552          | rBB      | 173            | 189           | 0.03%           | 0.003%        |
| 13        | 3.179       | 558           | 572         | 589          | rBV2     | 12531          | 30358         | 4.45%           | 0.526%        |
| 14        | 3.317       | 613           | 615         | 620          | rVB2     | 252            | 181           | 0.03%           | 0.003%        |
| 15        | 3.478       | 662           | 665         | 668          | rBB      | 206            | 161           | 0.02%           | 0.003%        |
| 16        | 3.665       | 720           | 723         | 724          | rBV2     | 286            | 160           | 0.02%           | 0.003%        |
| 17        | 3.678       | 724           | 727         | 729          | rVB      | 301            | 185           | 0.03%           | 0.003%        |
| 18        | 4.372       | 940           | 943         | 947          | rBB      | 246            | 214           | 0.03%           | 0.004%        |
| 19        | 4.633       | 1011          | 1024        | 1043         | rBV2     | 65057          | 197025        | 28.89%          | 3.413%        |
| 20        | 4.870       | 1096          | 1098        | 1099         | rBV2     | 394            | 155           | 0.02%           | 0.003%        |
| 21        | 5.060       | 1139          | 1157        | 1182         | rBV      | 116941         | 274474        | 40.25%          | 4.754%        |
| 22        | 5.186       | 1194          | 1196        | 1198         | rBV      | 296            | 163           | 0.02%           | 0.003%        |
| 23        | 5.279       | 1223          | 1225        | 1229         | rBV      | 278            | 245           | 0.04%           | 0.004%        |
| 24        | 5.324       | 1233          | 1239        | 1241         | rBV2     | 390            | 330           | 0.05%           | 0.006%        |
| 25        | 5.346       | 1241          | 1246        | 1249         | rVV2     | 454            | 403           | 0.06%           | 0.007%        |
| 26        | 5.378       | 1254          | 1256        | 1259         | rVV2     | 549            | 360           | 0.05%           | 0.006%        |
| 27        | 5.391       | 1259          | 1260        | 1263         | rVV      | 370            | 180           | 0.03%           | 0.003%        |
| 28        | 5.552       | 1306          | 1310        | 1311         | rBV      | 208            | 162           | 0.02%           | 0.003%        |
| 29        | 5.716       | 1342          | 1361        | 1380         | rBV2     | 213641         | 568385        | 83.35%          | 9.846%        |
| 30        | 5.829       | 1394          | 1396        | 1400         | rVB      | 347            | 159           | 0.02%           | 0.003%        |
| 31        | 5.973       | 1430          | 1441        | 1462         | rBV4     | 6710           | 16042         | 2.35%           | 0.278%        |
| 32        | 6.050       | 1462          | 1465        | 1467         | rVB2     | 392            | 215           | 0.03%           | 0.004%        |
| 33        | 6.160       | 1494          | 1499        | 1500         | rBV      | 318            | 236           | 0.03%           | 0.004%        |
| 34        | 6.247       | 1509          | 1526        | 1551         | rBV      | 212683         | 430920        | 63.19%          | 7.464%        |
| 35        | 6.417       | 1575          | 1579        | 1581         | rBB      | 173            | 142           | 0.02%           | 0.002%        |
| 36        | 6.523       | 1604          | 1612        | 1623         | rBB7     | 4861           | 8631          | 1.27%           | 0.150%        |

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 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 EW4K2ME

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\SFAMULM051622WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |        |        |
|----|-------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.591 | 1625 | 1633 | 1650 | rBV6 | 2759   | 6876   | 1.01%  | 0.119% |
| 38 | 6.690 | 1650 | 1664 | 1683 | rVB  | 132095 | 273434 | 40.10% | 4.736% |
| 39 | 6.800 | 1693 | 1698 | 1703 | rBV2 | 519    | 453    | 0.07%  | 0.008% |
| 40 | 6.922 | 1733 | 1736 | 1738 | rBV  | 272    | 185    | 0.03%  | 0.003% |
| 41 | 7.028 | 1764 | 1769 | 1770 | rBV  | 194    | 199    | 0.03%  | 0.003% |
| 42 | 7.041 | 1771 | 1773 | 1776 | rVV3 | 298    | 158    | 0.02%  | 0.003% |
| 43 | 7.189 | 1811 | 1819 | 1821 | rBV3 | 4472   | 5365   | 0.79%  | 0.093% |
| 44 | 7.298 | 1851 | 1853 | 1854 | rBV  | 258    | 145    | 0.02%  | 0.003% |
| 45 | 7.346 | 1864 | 1868 | 1870 | rBV  | 324    | 236    | 0.03%  | 0.004% |
| 46 | 7.501 | 1913 | 1916 | 1918 | rBV  | 273    | 211    | 0.03%  | 0.004% |
| 47 | 7.565 | 1924 | 1936 | 1960 | rVB  | 72664  | 143618 | 21.06% | 2.488% |
| 48 | 7.661 | 1961 | 1966 | 1968 | rBV2 | 280    | 214    | 0.03%  | 0.004% |
| 49 | 7.684 | 1971 | 1973 | 1976 | rBV2 | 309    | 172    | 0.03%  | 0.003% |
| 50 | 7.700 | 1976 | 1978 | 1981 | rVV2 | 285    | 157    | 0.02%  | 0.003% |
| 51 | 7.790 | 1998 | 2006 | 2009 | rBV2 | 1217   | 1555   | 0.23%  | 0.027% |
| 52 | 7.829 | 2016 | 2018 | 2021 | rBV2 | 349    | 218    | 0.03%  | 0.004% |
| 53 | 7.899 | 2025 | 2040 | 2055 | rBV  | 222209 | 401167 | 58.83% | 6.949% |
| 54 | 8.047 | 2084 | 2086 | 2091 | rVB3 | 516    | 327    | 0.05%  | 0.006% |
| 55 | 8.083 | 2094 | 2097 | 2100 | rBB  | 270    | 154    | 0.02%  | 0.003% |
| 56 | 8.182 | 2116 | 2128 | 2145 | rBV2 | 50721  | 104655 | 15.35% | 1.813% |
| 57 | 8.292 | 2161 | 2162 | 2167 | rVB2 | 262    | 195    | 0.03%  | 0.003% |
| 58 | 8.343 | 2171 | 2178 | 2181 | rBV3 | 422    | 570    | 0.08%  | 0.010% |
| 59 | 8.404 | 2195 | 2197 | 2199 | rVB  | 394    | 171    | 0.03%  | 0.003% |
| 60 | 8.510 | 2228 | 2230 | 2233 | rVB2 | 298    | 160    | 0.02%  | 0.003% |
| 61 | 8.529 | 2233 | 2236 | 2241 | rBV2 | 317    | 335    | 0.05%  | 0.006% |
| 62 | 8.655 | 2258 | 2275 | 2302 | rBV  | 213412 | 501270 | 73.50% | 8.683% |
| 63 | 8.777 | 2310 | 2313 | 2315 | rBV3 | 648    | 400    | 0.06%  | 0.007% |
| 64 | 8.883 | 2343 | 2346 | 2348 | rBV  | 198    | 164    | 0.02%  | 0.003% |
| 65 | 8.928 | 2352 | 2360 | 2365 | rBV4 | 1004   | 1603   | 0.24%  | 0.028% |
| 66 | 8.999 | 2381 | 2382 | 2387 | rBV  | 287    | 227    | 0.03%  | 0.004% |
| 67 | 9.153 | 2428 | 2430 | 2434 | rVB  | 243    | 146    | 0.02%  | 0.003% |
| 68 | 9.214 | 2448 | 2449 | 2451 | rVB  | 586    | 218    | 0.03%  | 0.004% |
| 69 | 9.272 | 2463 | 2467 | 2470 | rBV  | 262    | 261    | 0.04%  | 0.005% |
| 70 | 9.333 | 2483 | 2486 | 2491 | rBV2 | 714    | 517    | 0.08%  | 0.009% |
| 71 | 9.420 | 2498 | 2513 | 2534 | rBV  | 287742 | 557184 | 81.70% | 9.652% |
| 72 | 9.568 | 2556 | 2559 | 2561 | rVV  | 430    | 296    | 0.04%  | 0.005% |
| 73 | 9.639 | 2577 | 2581 | 2583 | rBV  | 202    | 180    | 0.03%  | 0.003% |
| 74 | 9.742 | 2607 | 2613 | 2615 | rBV3 | 1337   | 1263   | 0.19%  | 0.022% |
| 75 | 9.825 | 2637 | 2639 | 2640 | rBV3 | 341    | 158    | 0.02%  | 0.003% |
| 76 | 9.867 | 2649 | 2652 | 2656 | rVB2 | 590    | 353    | 0.05%  | 0.006% |

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 Sample : N2843-22ME  
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 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 EW4K2ME

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\SFAMULM051622WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |         |         |
|-----|--------|------|------|------|------|--------|--------|---------|---------|
| 77  | 9.893  | 2656 | 2660 | 2664 | rBV  | 369    | 334    | 0.05%   | 0.006%  |
| 78  | 9.954  | 2676 | 2679 | 2684 | rVB  | 398    | 273    | 0.04%   | 0.005%  |
| 79  | 10.021 | 2695 | 2700 | 2703 | rBV2 | 540    | 504    | 0.07%   | 0.009%  |
| 80  | 10.108 | 2723 | 2727 | 2729 | rBV3 | 499    | 446    | 0.07%   | 0.008%  |
| 81  | 10.246 | 2764 | 2770 | 2778 | rVB5 | 2019   | 2947   | 0.43%   | 0.051%  |
| 82  | 10.349 | 2798 | 2802 | 2806 | rBV3 | 547    | 492    | 0.07%   | 0.009%  |
| 83  | 10.394 | 2809 | 2816 | 2825 | rVB5 | 2180   | 3428   | 0.50%   | 0.059%  |
| 84  | 10.452 | 2828 | 2834 | 2837 | rBV2 | 555    | 512    | 0.08%   | 0.009%  |
| 85  | 10.555 | 2861 | 2866 | 2873 | rBV3 | 747    | 909    | 0.13%   | 0.016%  |
| 86  | 10.607 | 2879 | 2882 | 2884 | rBV  | 498    | 375    | 0.05%   | 0.006%  |
| 87  | 10.626 | 2884 | 2888 | 2892 | rVV3 | 1411   | 1189   | 0.17%   | 0.021%  |
| 88  | 10.764 | 2917 | 2931 | 2953 | rBV  | 290536 | 486968 | 71.41%  | 8.435%  |
| 89  | 11.057 | 3017 | 3022 | 3023 | rBV2 | 1080   | 746    | 0.11%   | 0.013%  |
| 90  | 11.118 | 3033 | 3041 | 3058 | rVB5 | 9660   | 17132  | 2.51%   | 0.297%  |
| 91  | 11.311 | 3095 | 3101 | 3102 | rBV2 | 1168   | 902    | 0.13%   | 0.016%  |
| 92  | 11.417 | 3126 | 3134 | 3142 | rBV5 | 5731   | 8248   | 1.21%   | 0.143%  |
| 93  | 11.542 | 3170 | 3173 | 3174 | rBV2 | 286    | 170    | 0.02%   | 0.003%  |
| 94  | 11.558 | 3176 | 3178 | 3180 | rVV2 | 538    | 235    | 0.03%   | 0.004%  |
| 95  | 11.816 | 3247 | 3258 | 3272 | rBV  | 437681 | 681962 | 100.00% | 11.813% |
| 96  | 12.089 | 3339 | 3343 | 3348 | rBV4 | 1011   | 1231   | 0.18%   | 0.021%  |
| 97  | 12.195 | 3365 | 3376 | 3389 | rBV  | 367807 | 602946 | 88.41%  | 10.444% |
| 98  | 12.330 | 3412 | 3418 | 3429 | rVB3 | 18387  | 25818  | 3.79%   | 0.447%  |
| 99  | 13.430 | 3754 | 3760 | 3783 | rVB3 | 50483  | 86043  | 12.62%  | 1.490%  |
| 100 | 14.449 | 4072 | 4077 | 4087 | rVB  | 66396  | 86968  | 12.75%  | 1.506%  |

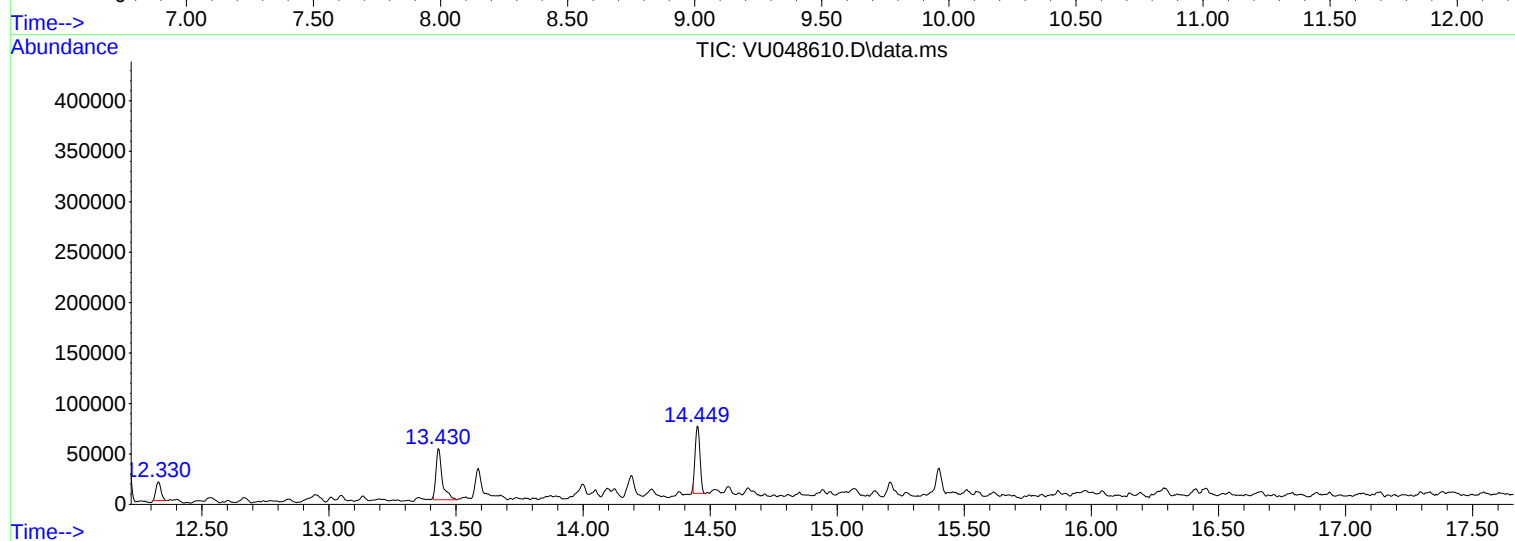
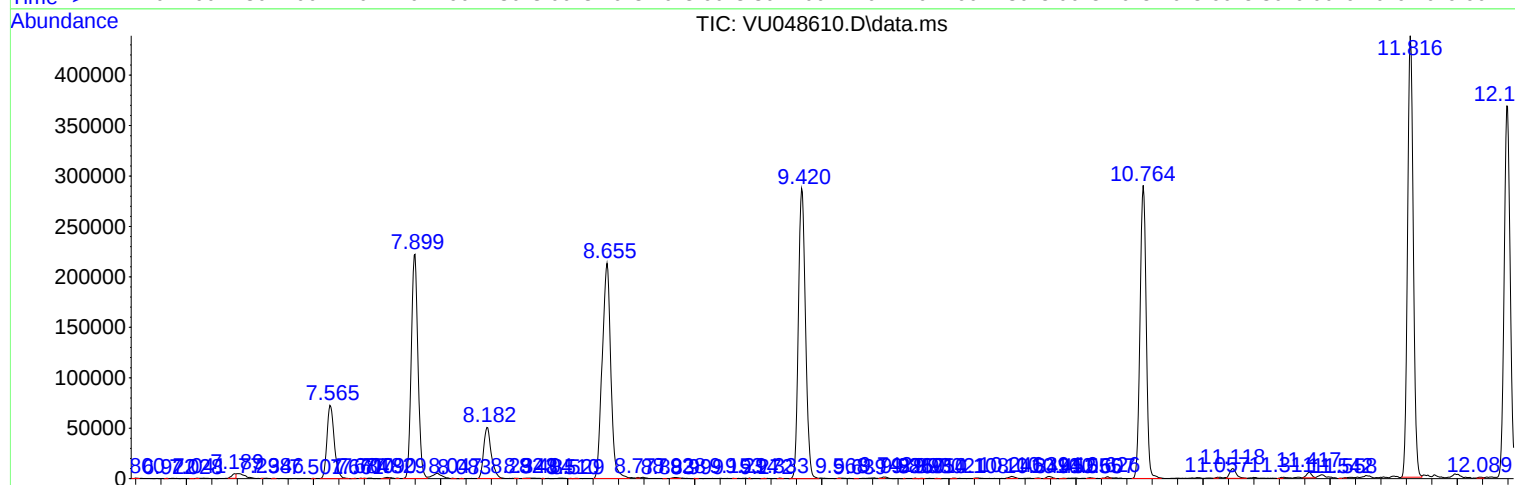
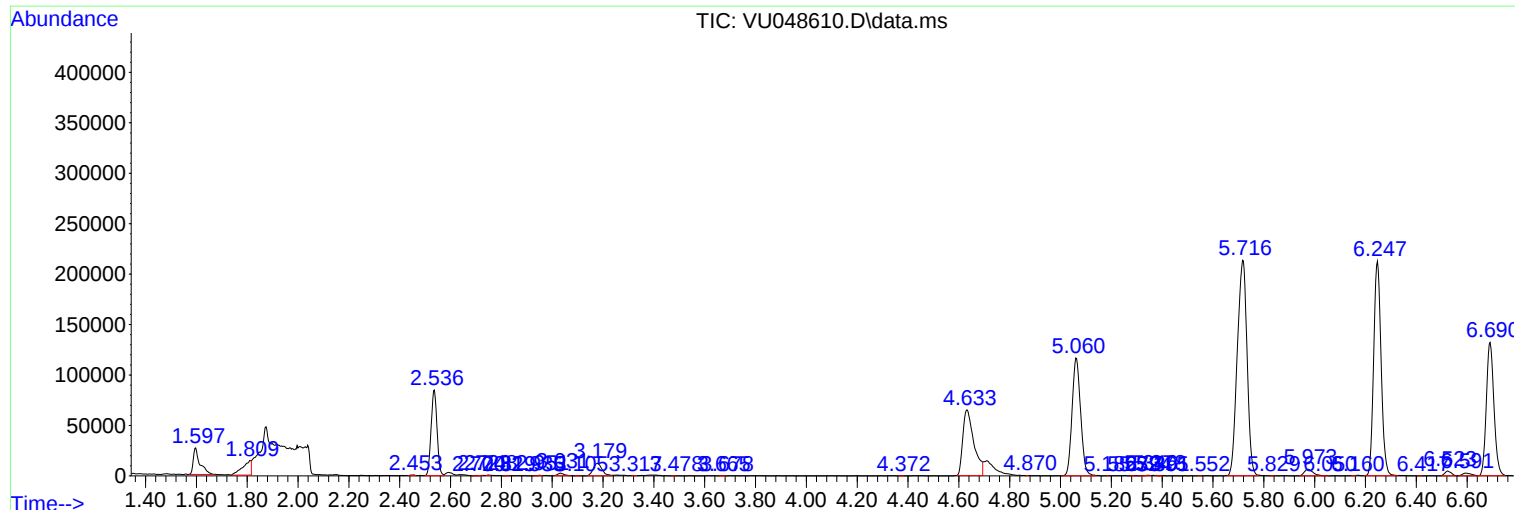
Sum of corrected areas: 5772941

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Data File : VU048610.D  
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Sample : N2843-22ME  
Misc : 5.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EW4K2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM051622WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051822\  
Data File : VU048610.D  
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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EW4K2ME

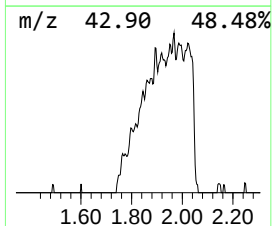
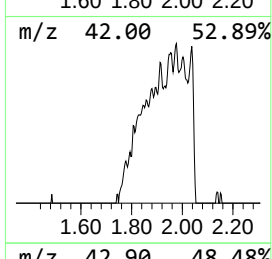
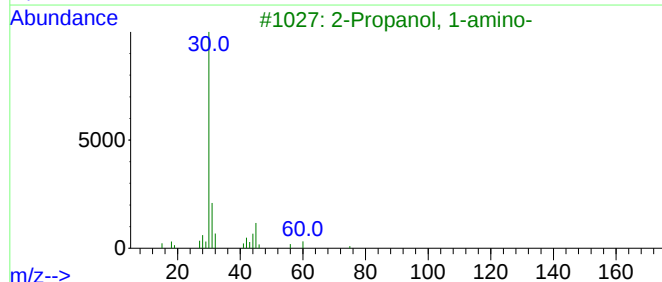
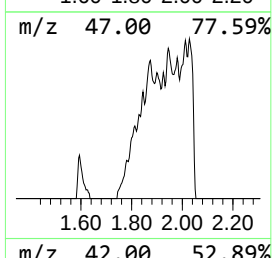
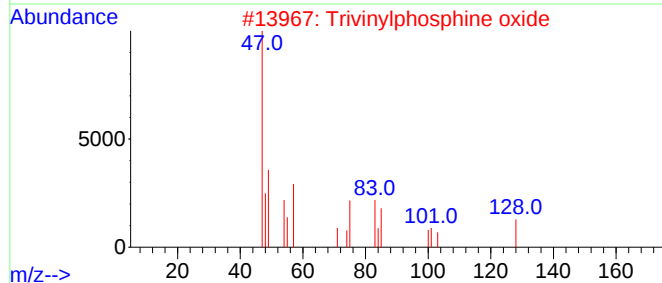
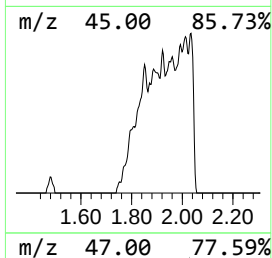
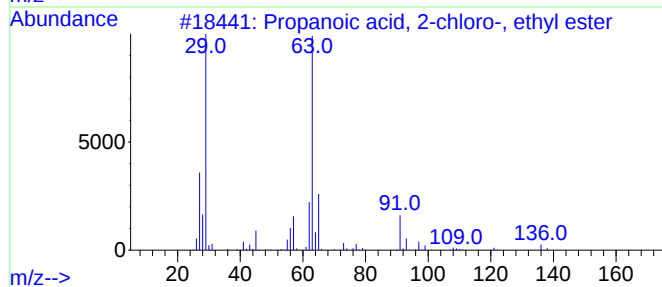
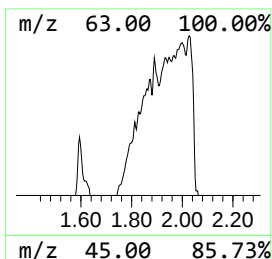
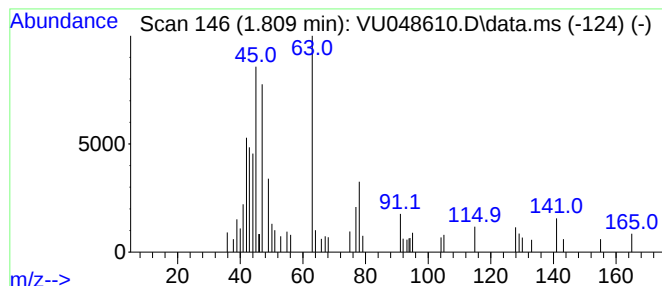
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM051622WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 unknown-01 Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.809 | 3.97 ug/L | 34191 | 1,4-Difluorobenzene | 6.247 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Propanoic acid, 2-chloro-, ethyl... | 136 | C5H9ClO2   | 000535-13-7 | 17   |
| 2    |    |   | Trivinylphosphine oxide             | 128 | C6H9OP     | 013699-67-7 | 14   |
| 3    |    |   | 2-Propanol, 1-amino-                | 75  | C3H9NO     | 000078-96-6 | 9    |
| 4    |    |   | Azetidine, 1-chloro-                | 91  | C3H6ClN    | 032115-53-0 | 9    |
| 5    |    |   | dl-Cystathionine                    | 222 | C7H14N2O4S | 000535-34-2 | 9    |



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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EW4K2ME

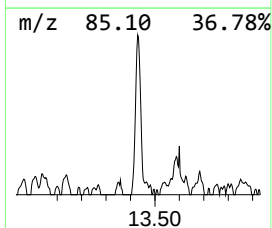
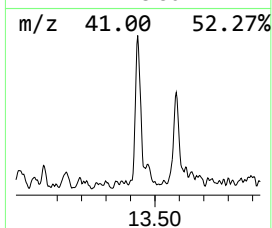
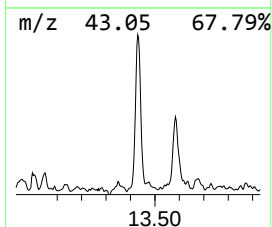
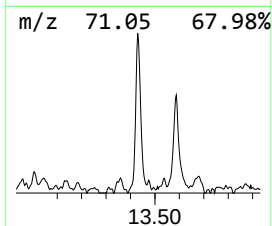
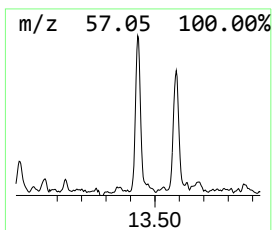
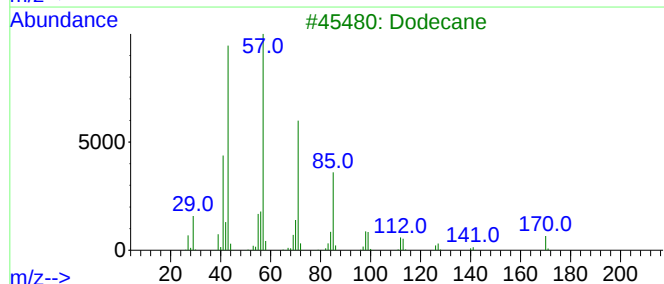
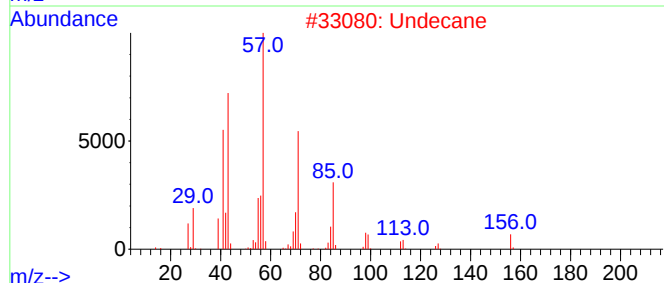
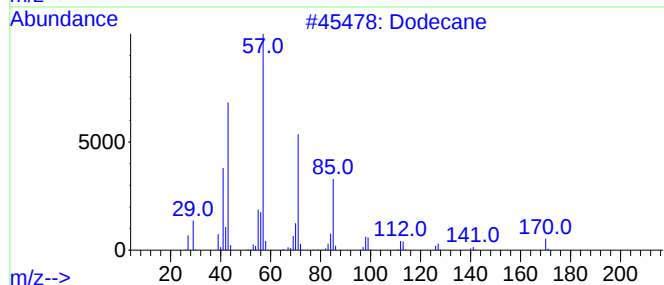
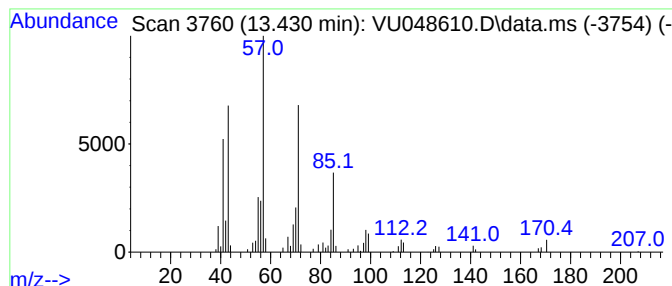
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM051622WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.430 | 6.31 ug/L | 86043 | 1,4-Dichlorobenzene-d4 | 11.816 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Dodecane     | 170 | C12H26  | 000112-40-3 | 94   |
| 2    |    |   | Undecane     | 156 | C11H24  | 001120-21-4 | 90   |
| 3    |    |   | Dodecane     | 170 | C12H26  | 000112-40-3 | 87   |
| 4    |    |   | Tridecane    | 184 | C13H28  | 000629-50-5 | 86   |
| 5    |    |   | Tetradecane  | 198 | C14H30  | 000629-59-4 | 80   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051822\  
Data File : VU048610.D  
Acq On : 18 May 2022 13:48  
Operator : SY/MD  
Sample : N2843-22ME  
Misc : 5.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EW4K2ME

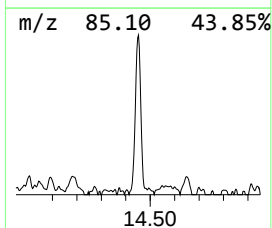
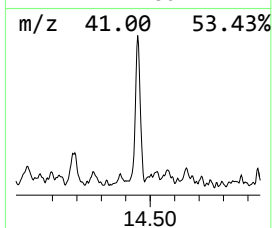
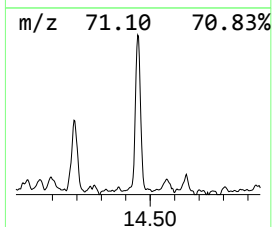
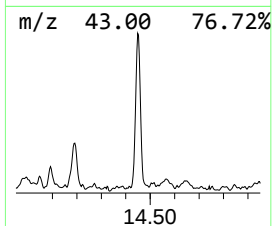
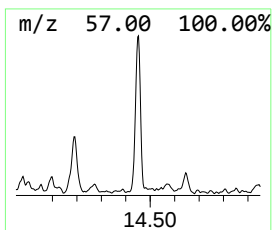
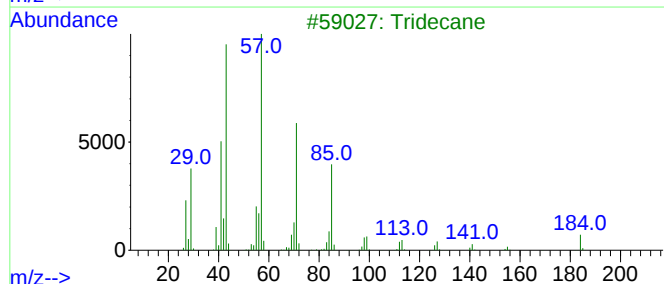
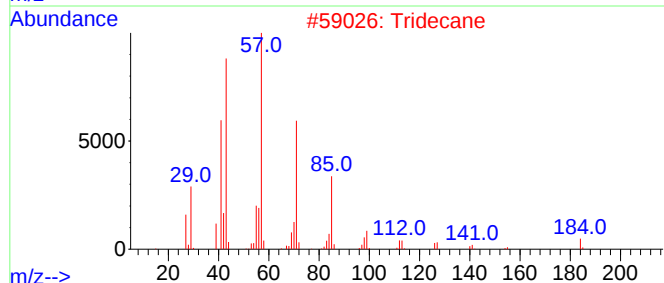
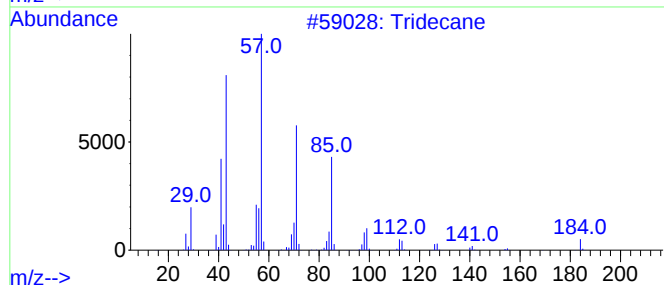
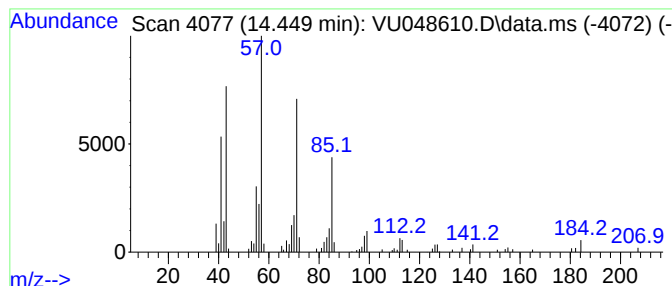
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Quant Title : VOC Analysis

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

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Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 14.449 | 6.38 ug/L | 86968 | 1,4-Dichlorobenzene-d4 | 11.816 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Tridecane    | 184 | C13H28  | 000629-50-5 | 98   |
| 2    |    |   | Tridecane    | 184 | C13H28  | 000629-50-5 | 95   |
| 3    |    |   | Tridecane    | 184 | C13H28  | 000629-50-5 | 93   |
| 4    |    |   | Hexadecane   | 226 | C16H34  | 000544-76-3 | 90   |
| 5    |    |   | Dodecane     | 170 | C12H26  | 000112-40-3 | 90   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU051822\  
Data File : VU048610.D  
Acq On : 18 May 2022 13:48  
Operator : SY/MD  
Sample : N2843-22ME  
Misc : 5.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
EW4K2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM051622WMA.M  
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 |
| unknown-01         | 1.809  | 4.0     | ug/L  | 34191    | 1                     | 6.247  | 430920 | 50.0 |
| (DEL) Alkane: S... | 13.430 | 6.3     | ug/L  | 86043    | 3                     | 11.816 | 681962 | 50.0 |
| (DEL) Alkane: S... | 14.449 | 6.4     | ug/L  | 86968    | 3                     | 11.816 | 681962 | 50.0 |