

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX060823\  
 Data File : VX036080.D  
 Acq On : 08 Jun 2023 19:02  
 Operator : JC/MD  
 Sample : 03097-05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EZEN2

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\_X\Method\SFAMXML060623WMA.M  
 Title : VOC Analysis

Signal : TIC: VX036080.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         | 1.142       | 6             | 9           | 16           | rVB      | 9661           | 10031         | 0.77%           | 0.104%        |
| 2         | 1.270       | 26            | 30          | 33           | rBV4     | 1051           | 1584          | 0.12%           | 0.016%        |
| 3         | 1.368       | 42            | 46          | 59           | rBV      | 135324         | 163082        | 12.49%          | 1.688%        |
| 4         | 1.672       | 91            | 96          | 111          | rBV      | 105165         | 155986        | 11.94%          | 1.615%        |
| 5         | 2.307       | 194           | 200         | 211          | rBV      | 279449         | 434988        | 33.31%          | 4.503%        |
| 6         | 2.508       | 231           | 233         | 235          | rBV3     | 342            | 344           | 0.03%           | 0.004%        |
| 7         | 2.624       | 250           | 252         | 256          | rVB      | 318            | 388           | 0.03%           | 0.004%        |
| 8         | 2.654       | 256           | 257         | 259          | rBV      | 209            | 148           | 0.01%           | 0.002%        |
| 9         | 2.709       | 264           | 266         | 269          | rVB      | 312            | 285           | 0.02%           | 0.003%        |
| 10        | 2.739       | 269           | 271         | 273          | rVB3     | 323            | 296           | 0.02%           | 0.003%        |
| 11        | 2.794       | 275           | 280         | 283          | rVV2     | 569            | 860           | 0.07%           | 0.009%        |
| 12        | 2.843       | 286           | 288         | 289          | rBV      | 214            | 158           | 0.01%           | 0.002%        |
| 13        | 2.892       | 293           | 296         | 299          | rBV2     | 253            | 367           | 0.03%           | 0.004%        |
| 14        | 2.965       | 306           | 308         | 310          | rVB2     | 243            | 184           | 0.01%           | 0.002%        |
| 15        | 3.123       | 332           | 334         | 335          | rBV      | 276            | 148           | 0.01%           | 0.002%        |
| 16        | 3.166       | 338           | 341         | 343          | rBV2     | 234            | 254           | 0.02%           | 0.003%        |
| 17        | 3.251       | 352           | 355         | 358          | rBV2     | 154            | 190           | 0.01%           | 0.002%        |
| 18        | 3.556       | 403           | 405         | 408          | rBV      | 196            | 257           | 0.02%           | 0.003%        |
| 19        | 3.587       | 408           | 410         | 412          | rVV2     | 161            | 190           | 0.01%           | 0.002%        |
| 20        | 3.703       | 424           | 429         | 430          | rBV2     | 221            | 286           | 0.02%           | 0.003%        |
| 21        | 3.757       | 437           | 438         | 440          | rBV      | 178            | 155           | 0.01%           | 0.002%        |
| 22        | 3.776       | 440           | 441         | 443          | rVB      | 318            | 162           | 0.01%           | 0.002%        |
| 23        | 3.806       | 443           | 446         | 448          | rBV      | 200            | 255           | 0.02%           | 0.003%        |
| 24        | 3.885       | 457           | 459         | 462          | rVB      | 205            | 202           | 0.02%           | 0.002%        |
| 25        | 4.032       | 481           | 483         | 485          | rVB2     | 233            | 172           | 0.01%           | 0.002%        |
| 26        | 4.123       | 494           | 498         | 499          | rBV2     | 248            | 268           | 0.02%           | 0.003%        |
| 27        | 4.471       | 545           | 555         | 575          | rBV      | 77244          | 262461        | 20.10%          | 2.717%        |
| 28        | 4.910       | 624           | 627         | 630          | rBV2     | 215            | 279           | 0.02%           | 0.003%        |
| 29        | 5.056       | 638           | 651         | 668          | rBV2     | 161141         | 519655        | 39.79%          | 5.379%        |
| 30        | 5.538       | 726           | 730         | 731          | rBV3     | 821            | 1050          | 0.08%           | 0.011%        |
| 31        | 5.653       | 747           | 749         | 752          | rVB2     | 295            | 218           | 0.02%           | 0.002%        |
| 32        | 5.836       | 776           | 779         | 781          | rBV2     | 165            | 193           | 0.01%           | 0.002%        |
| 33        | 5.970       | 788           | 801         | 820          | rBV2     | 434323         | 1306021       | 100.00%         | 13.519%       |
| 34        | 6.166       | 831           | 833         | 837          | rBV2     | 356            | 431           | 0.03%           | 0.004%        |
| 35        | 6.355       | 861           | 864         | 866          | rBV      | 247            | 250           | 0.02%           | 0.003%        |
| 36        | 6.763       | 920           | 931         | 949          | rBV      | 313941         | 752234        | 57.60%          | 7.787%        |

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML060623WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.976  | 964  | 966  | 967  | rBV  | 330    | 165     | 0.01%  | 0.002%  |
| 38 | 7.104  | 983  | 987  | 993  | rVV2 | 1316   | 2752    | 0.21%  | 0.028%  |
| 39 | 7.306  | 1010 | 1020 | 1034 | rBV  | 272539 | 601492  | 46.06% | 6.226%  |
| 40 | 7.482  | 1044 | 1049 | 1052 | rBV4 | 923    | 1523    | 0.12%  | 0.016%  |
| 41 | 7.860  | 1110 | 1111 | 1114 | rBV  | 224    | 168     | 0.01%  | 0.002%  |
| 42 | 7.927  | 1119 | 1122 | 1124 | rBV3 | 768    | 899     | 0.07%  | 0.009%  |
| 43 | 8.116  | 1150 | 1153 | 1155 | rBV2 | 195    | 227     | 0.02%  | 0.002%  |
| 44 | 8.220  | 1168 | 1170 | 1172 | rBV  | 272    | 157     | 0.01%  | 0.002%  |
| 45 | 8.324  | 1179 | 1187 | 1200 | rBV  | 166494 | 274470  | 21.02% | 2.841%  |
| 46 | 8.470  | 1207 | 1211 | 1212 | rBV4 | 591    | 707     | 0.05%  | 0.007%  |
| 47 | 8.525  | 1217 | 1220 | 1222 | rBV2 | 347    | 423     | 0.03%  | 0.004%  |
| 48 | 8.568  | 1226 | 1227 | 1229 | rBV  | 385    | 279     | 0.02%  | 0.003%  |
| 49 | 8.647  | 1233 | 1240 | 1255 | rBV  | 675505 | 1034338 | 79.20% | 10.707% |
| 50 | 8.811  | 1265 | 1267 | 1272 | rVB4 | 476    | 601     | 0.05%  | 0.006%  |
| 51 | 8.854  | 1272 | 1274 | 1278 | rBV3 | 332    | 468     | 0.04%  | 0.005%  |
| 52 | 8.952  | 1284 | 1290 | 1300 | rBV  | 120301 | 179588  | 13.75% | 1.859%  |
| 53 | 9.122  | 1316 | 1318 | 1319 | rBV2 | 226    | 164     | 0.01%  | 0.002%  |
| 54 | 9.208  | 1330 | 1332 | 1337 | rVB3 | 333    | 241     | 0.02%  | 0.002%  |
| 55 | 9.269  | 1337 | 1342 | 1343 | rBV2 | 805    | 804     | 0.06%  | 0.008%  |
| 56 | 9.336  | 1351 | 1353 | 1355 | rBV2 | 361    | 321     | 0.02%  | 0.003%  |
| 57 | 9.385  | 1355 | 1361 | 1375 | rBV  | 418907 | 594625  | 45.53% | 6.155%  |
| 58 | 9.647  | 1402 | 1404 | 1406 | rBV2 | 214    | 174     | 0.01%  | 0.002%  |
| 59 | 9.799  | 1427 | 1429 | 1432 | rBV2 | 222    | 257     | 0.02%  | 0.003%  |
| 60 | 9.891  | 1442 | 1444 | 1445 | rBV  | 278    | 173     | 0.01%  | 0.002%  |
| 61 | 10.055 | 1465 | 1471 | 1487 | rBV  | 660491 | 896955  | 68.68% | 9.285%  |
| 62 | 10.238 | 1498 | 1501 | 1505 | rBV2 | 369    | 460     | 0.04%  | 0.005%  |
| 63 | 10.299 | 1509 | 1511 | 1515 | rVB3 | 428    | 532     | 0.04%  | 0.006%  |
| 64 | 10.336 | 1515 | 1517 | 1518 | rBV  | 318    | 147     | 0.01%  | 0.002%  |
| 65 | 10.421 | 1529 | 1531 | 1533 | rVB  | 247    | 153     | 0.01%  | 0.002%  |
| 66 | 10.543 | 1548 | 1551 | 1555 | rBV2 | 270    | 481     | 0.04%  | 0.005%  |
| 67 | 10.689 | 1571 | 1575 | 1578 | rVB2 | 749    | 937     | 0.07%  | 0.010%  |
| 68 | 11.079 | 1637 | 1639 | 1642 | rBV2 | 421    | 351     | 0.03%  | 0.004%  |
| 69 | 11.152 | 1649 | 1651 | 1652 | rBV  | 246    | 166     | 0.01%  | 0.002%  |
| 70 | 11.189 | 1652 | 1657 | 1665 | rVV  | 464908 | 594968  | 45.56% | 6.159%  |
| 71 | 11.305 | 1674 | 1676 | 1682 | rVB2 | 553    | 807     | 0.06%  | 0.008%  |
| 72 | 11.427 | 1692 | 1696 | 1699 | rBV3 | 955    | 1338    | 0.10%  | 0.014%  |
| 73 | 11.683 | 1736 | 1738 | 1747 | rVB2 | 264    | 459     | 0.04%  | 0.005%  |
| 74 | 11.963 | 1782 | 1784 | 1786 | rBV2 | 180    | 149     | 0.01%  | 0.002%  |
| 75 | 12.018 | 1788 | 1793 | 1800 | rBV  | 663373 | 841684  | 64.45% | 8.713%  |
| 76 | 12.219 | 1821 | 1826 | 1837 | rBV  | 67372  | 113750  | 8.71%  | 1.177%  |

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Peak Location: TOP

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

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Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML060623WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.317 | 1837 | 1842 | 1853 | rVB  | 711524 | 890255 | 68.17% | 9.215% |
| 78  | 12.750 | 1911 | 1913 | 1915 | rBV3 | 610    | 451    | 0.03%  | 0.005% |
| 79  | 12.969 | 1947 | 1949 | 1950 | rBV  | 245    | 181    | 0.01%  | 0.002% |
| 80  | 13.042 | 1960 | 1961 | 1965 | rBV2 | 294    | 305    | 0.02%  | 0.003% |
| 81  | 13.158 | 1978 | 1980 | 1981 | rBV  | 455    | 323    | 0.02%  | 0.003% |
| 82  | 13.195 | 1985 | 1986 | 1989 | rBV2 | 373    | 404    | 0.03%  | 0.004% |
| 83  | 13.244 | 1992 | 1994 | 1996 | rVV  | 462    | 293    | 0.02%  | 0.003% |
| 84  | 13.262 | 1996 | 1997 | 2000 | rVB3 | 548    | 506    | 0.04%  | 0.005% |
| 85  | 13.445 | 2025 | 2027 | 2031 | rVB2 | 387    | 291    | 0.02%  | 0.003% |
| 86  | 13.500 | 2033 | 2036 | 2037 | rBV2 | 313    | 318    | 0.02%  | 0.003% |
| 87  | 13.561 | 2042 | 2046 | 2047 | rBV3 | 393    | 391    | 0.03%  | 0.004% |
| 88  | 13.689 | 2062 | 2067 | 2071 | rBV3 | 444    | 701    | 0.05%  | 0.007% |
| 89  | 13.853 | 2091 | 2094 | 2095 | rBV  | 245    | 229    | 0.02%  | 0.002% |
| 90  | 14.158 | 2143 | 2144 | 2146 | rBV  | 316    | 207    | 0.02%  | 0.002% |
| 91  | 14.329 | 2171 | 2172 | 2177 | rBV2 | 394    | 528    | 0.04%  | 0.005% |
| 92  | 14.457 | 2192 | 2193 | 2196 | rVB2 | 413    | 237    | 0.02%  | 0.002% |
| 93  | 14.634 | 2220 | 2222 | 2225 | rVB  | 489    | 293    | 0.02%  | 0.003% |
| 94  | 14.816 | 2251 | 2252 | 2253 | rBV  | 360    | 176    | 0.01%  | 0.002% |
| 95  | 14.908 | 2264 | 2267 | 2269 | rBV2 | 333    | 412    | 0.03%  | 0.004% |
| 96  | 15.012 | 2282 | 2284 | 2285 | rBV  | 433    | 252    | 0.02%  | 0.003% |
| 97  | 15.597 | 2379 | 2380 | 2382 | rBV  | 571    | 380    | 0.03%  | 0.004% |
| 98  | 15.725 | 2399 | 2401 | 2402 | rBV2 | 765    | 506    | 0.04%  | 0.005% |
| 99  | 16.359 | 2503 | 2505 | 2506 | rBV  | 438    | 281    | 0.02%  | 0.003% |
| 100 | 16.578 | 2540 | 2541 | 2543 | rBV  | 424    | 312    | 0.02%  | 0.003% |

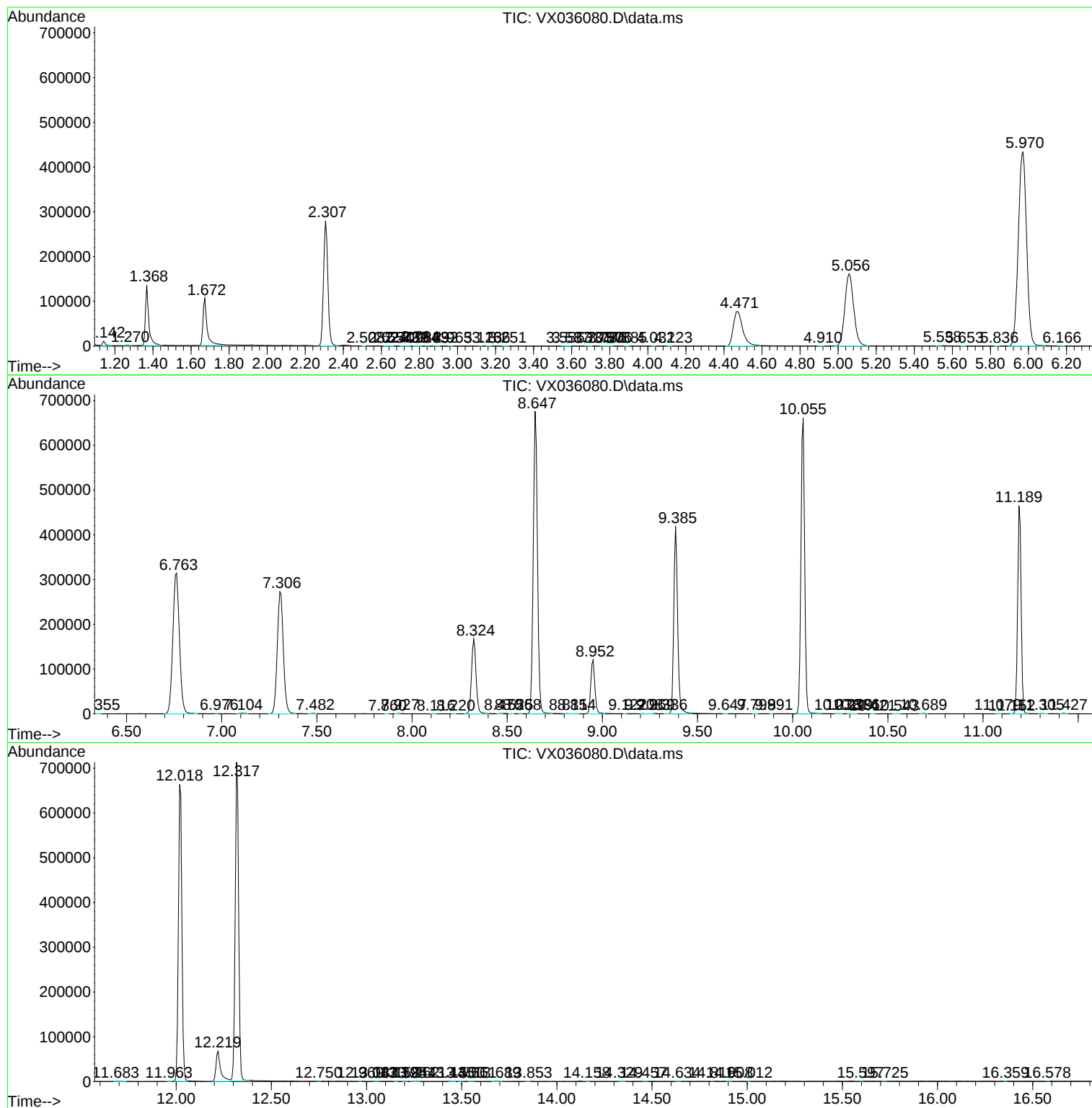
Sum of corrected areas: 9660617

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML060623WMA.M  
Quant Title : VOC Analysis

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



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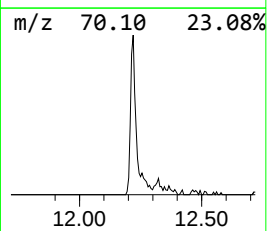
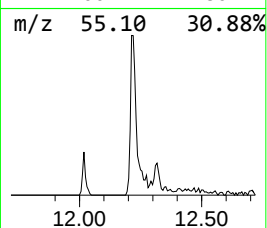
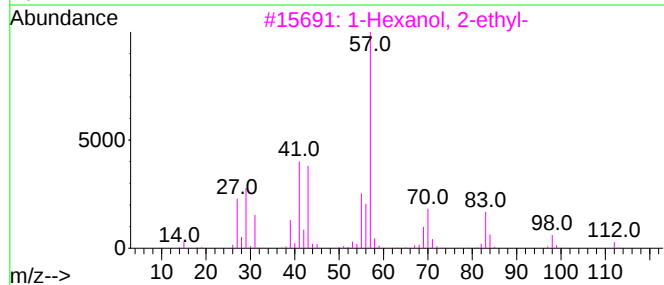
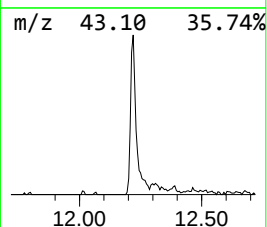
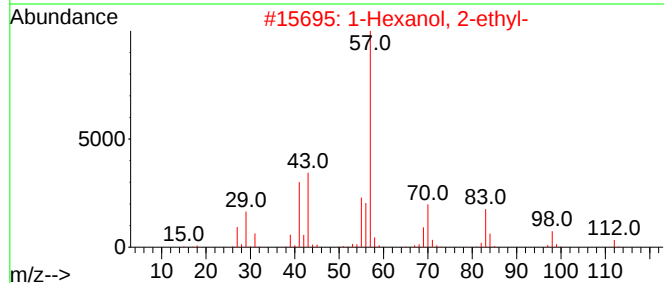
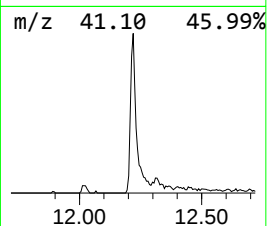
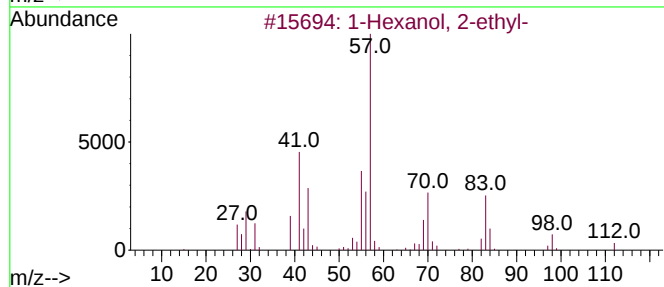
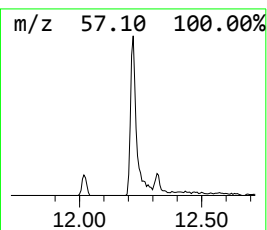
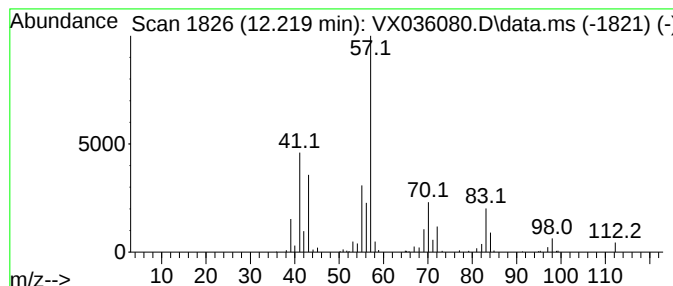
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML060623WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.219 | 6.76 ug/L | 113750 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 78   |
| 3    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 72   |
| 4    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 64   |
| 5    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 64   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 1-Hexanol, 2-et... | 12.219 | 6.8     | ug/L  | 113750   | 3                     | 12.024 | 841684 | 50.0 |