

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121623\  
 Data File : VX039232.D  
 Acq On : 15 Dec 2023 16:45  
 Operator : JC/MD  
 Sample : VX1216WBL01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK645

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

Signal : TIC: VX039232.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         | 1.368       | 42            | 46          | 57           | rBV      | 122941         | 130164        | 13.39%          | 1.757%        |
| 2         | 1.666       | 91            | 95          | 110          | rBV      | 71641          | 111368        | 11.45%          | 1.503%        |
| 3         | 2.306       | 194           | 200         | 214          | rVB      | 219185         | 339990        | 34.97%          | 4.589%        |
| 4         | 2.508       | 228           | 233         | 242          | rVB2     | 968            | 1813          | 0.19%           | 0.024%        |
| 5         | 2.623       | 249           | 252         | 255          | rBV2     | 281            | 351           | 0.04%           | 0.005%        |
| 6         | 2.782       | 274           | 278         | 286          | rBV4     | 1422           | 2707          | 0.28%           | 0.037%        |
| 7         | 2.867       | 291           | 292         | 295          | rBV2     | 275            | 179           | 0.02%           | 0.002%        |
| 8         | 2.953       | 303           | 306         | 309          | rBV2     | 247            | 356           | 0.04%           | 0.005%        |
| 9         | 3.099       | 327           | 330         | 334          | rVB3     | 329            | 449           | 0.05%           | 0.006%        |
| 10        | 3.245       | 353           | 354         | 357          | rBV2     | 283            | 215           | 0.02%           | 0.003%        |
| 11        | 3.513       | 396           | 398         | 401          | rVV      | 198            | 187           | 0.02%           | 0.003%        |
| 12        | 3.812       | 445           | 447         | 449          | rVB      | 233            | 186           | 0.02%           | 0.003%        |
| 13        | 3.977       | 471           | 474         | 476          | rVB      | 229            | 221           | 0.02%           | 0.003%        |
| 14        | 4.446       | 542           | 551         | 564          | rBV      | 86135          | 244595        | 25.16%          | 3.301%        |
| 15        | 4.910       | 625           | 627         | 630          | rBV      | 302            | 286           | 0.03%           | 0.004%        |
| 16        | 4.934       | 630           | 631         | 636          | rVV      | 280            | 217           | 0.02%           | 0.003%        |
| 17        | 5.050       | 639           | 650         | 673          | rVV      | 117997         | 382680        | 39.36%          | 5.165%        |
| 18        | 5.355       | 698           | 700         | 701          | rBV      | 263            | 179           | 0.02%           | 0.002%        |
| 19        | 5.519       | 724           | 727         | 728          | rBV      | 295            | 304           | 0.03%           | 0.004%        |
| 20        | 5.538       | 728           | 730         | 731          | rBV      | 399            | 292           | 0.03%           | 0.004%        |
| 21        | 5.848       | 779           | 781         | 784          | rBV      | 267            | 250           | 0.03%           | 0.003%        |
| 22        | 5.964       | 788           | 800         | 819          | rBV2     | 322506         | 972255        | 100.00%         | 13.122%       |
| 23        | 6.287       | 851           | 853         | 856          | rVB      | 365            | 273           | 0.03%           | 0.004%        |
| 24        | 6.342       | 860           | 862         | 864          | rBV2     | 204            | 201           | 0.02%           | 0.003%        |
| 25        | 6.757       | 920           | 930         | 946          | rBV      | 223181         | 534204        | 54.94%          | 7.210%        |
| 26        | 7.056       | 975           | 979         | 981          | rVB3     | 239            | 348           | 0.04%           | 0.005%        |
| 27        | 7.117       | 981           | 989         | 998          | rBV5     | 1644           | 3949          | 0.41%           | 0.053%        |
| 28        | 7.196       | 999           | 1002        | 1005         | rVB2     | 219            | 222           | 0.02%           | 0.003%        |
| 29        | 7.305       | 1011          | 1020        | 1037         | rBV      | 197929         | 437170        | 44.96%          | 5.900%        |
| 30        | 7.690       | 1081          | 1083        | 1085         | rVB      | 306            | 202           | 0.02%           | 0.003%        |
| 31        | 8.257       | 1173          | 1176        | 1178         | rBV      | 190            | 207           | 0.02%           | 0.003%        |
| 32        | 8.324       | 1181          | 1187        | 1201         | rBV      | 143462         | 237621        | 24.44%          | 3.207%        |
| 33        | 8.525       | 1219          | 1220        | 1222         | rBV      | 325            | 246           | 0.03%           | 0.003%        |
| 34        | 8.580       | 1225          | 1229        | 1231         | rVB3     | 359            | 460           | 0.05%           | 0.006%        |
| 35        | 8.647       | 1234          | 1240        | 1257         | rVV      | 495447         | 780193        | 80.25%          | 10.530%       |
| 36        | 8.945       | 1284          | 1289        | 1303         | rVV      | 101881         | 157988        | 16.25%          | 2.132%        |

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 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK645

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 9.134  | 1317 | 1320 | 1322 | rVB2 | 240    | 273    | 0.03%  | 0.004% |
| 38 | 9.220  | 1333 | 1334 | 1337 | rBV  | 294    | 213    | 0.02%  | 0.003% |
| 39 | 9.275  | 1339 | 1343 | 1345 | rBV2 | 365    | 531    | 0.05%  | 0.007% |
| 40 | 9.378  | 1355 | 1360 | 1378 | rBV  | 394774 | 582673 | 59.93% | 7.864% |
| 41 | 9.665  | 1406 | 1407 | 1409 | rBV2 | 234    | 201    | 0.02%  | 0.003% |
| 42 | 9.842  | 1435 | 1436 | 1443 | rVB4 | 347    | 526    | 0.05%  | 0.007% |
| 43 | 9.994  | 1460 | 1461 | 1465 | rBV  | 189    | 219    | 0.02%  | 0.003% |
| 44 | 10.049 | 1465 | 1470 | 1483 | rVV  | 458176 | 653414 | 67.21% | 8.819% |
| 45 | 10.183 | 1491 | 1492 | 1496 | rBV3 | 270    | 301    | 0.03%  | 0.004% |
| 46 | 10.305 | 1507 | 1512 | 1518 | rVB3 | 573    | 1000   | 0.10%  | 0.013% |
| 47 | 10.415 | 1528 | 1530 | 1534 | rVB2 | 158    | 185    | 0.02%  | 0.002% |
| 48 | 10.451 | 1534 | 1536 | 1538 | rBV2 | 167    | 195    | 0.02%  | 0.003% |
| 49 | 10.598 | 1559 | 1560 | 1563 | rVB  | 302    | 181    | 0.02%  | 0.002% |
| 50 | 10.634 | 1563 | 1566 | 1567 | rBV  | 462    | 318    | 0.03%  | 0.004% |
| 51 | 10.787 | 1589 | 1591 | 1594 | rVB  | 222    | 206    | 0.02%  | 0.003% |
| 52 | 10.939 | 1615 | 1616 | 1619 | rBV  | 249    | 235    | 0.02%  | 0.003% |
| 53 | 11.043 | 1631 | 1633 | 1636 | rVB2 | 186    | 192    | 0.02%  | 0.003% |
| 54 | 11.085 | 1636 | 1640 | 1646 | rBV2 | 1574   | 2398   | 0.25%  | 0.032% |
| 55 | 11.189 | 1652 | 1657 | 1668 | rBV  | 366586 | 467589 | 48.09% | 6.311% |
| 56 | 11.305 | 1674 | 1676 | 1680 | rVB2 | 381    | 355    | 0.04%  | 0.005% |
| 57 | 11.347 | 1680 | 1683 | 1684 | rVB  | 185    | 184    | 0.02%  | 0.002% |
| 58 | 11.366 | 1684 | 1686 | 1687 | rBV2 | 376    | 265    | 0.03%  | 0.004% |
| 59 | 11.457 | 1697 | 1701 | 1704 | rBV2 | 773    | 828    | 0.09%  | 0.011% |
| 60 | 11.555 | 1713 | 1717 | 1719 | rBV2 | 150    | 190    | 0.02%  | 0.003% |
| 61 | 11.677 | 1735 | 1737 | 1739 | rBV  | 350    | 300    | 0.03%  | 0.004% |
| 62 | 11.756 | 1745 | 1750 | 1753 | rBV4 | 394    | 627    | 0.06%  | 0.008% |
| 63 | 11.963 | 1782 | 1784 | 1788 | rBV  | 532    | 845    | 0.09%  | 0.011% |
| 64 | 12.018 | 1788 | 1793 | 1807 | rBV  | 510604 | 669913 | 68.90% | 9.041% |
| 65 | 12.170 | 1816 | 1818 | 1822 | rVB2 | 213    | 243    | 0.02%  | 0.003% |
| 66 | 12.207 | 1822 | 1824 | 1827 | rVB  | 212    | 213    | 0.02%  | 0.003% |
| 67 | 12.317 | 1837 | 1842 | 1856 | rVV  | 518439 | 668495 | 68.76% | 9.022% |
| 68 | 12.506 | 1871 | 1873 | 1876 | rVB2 | 354    | 251    | 0.03%  | 0.003% |
| 69 | 12.585 | 1883 | 1886 | 1887 | rBV  | 197    | 220    | 0.02%  | 0.003% |
| 70 | 12.756 | 1909 | 1914 | 1916 | rBV2 | 286    | 482    | 0.05%  | 0.007% |
| 71 | 13.128 | 1969 | 1975 | 1976 | rBV2 | 337    | 449    | 0.05%  | 0.006% |
| 72 | 13.286 | 1999 | 2001 | 2006 | rVB2 | 272    | 227    | 0.02%  | 0.003% |
| 73 | 13.512 | 2035 | 2038 | 2039 | rBV  | 263    | 224    | 0.02%  | 0.003% |
| 74 | 13.585 | 2047 | 2050 | 2057 | rBV4 | 1055   | 1582   | 0.16%  | 0.021% |
| 75 | 13.701 | 2067 | 2069 | 2072 | rVV2 | 229    | 253    | 0.03%  | 0.003% |
| 76 | 13.749 | 2073 | 2077 | 2078 | rVV2 | 264    | 300    | 0.03%  | 0.004% |

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 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK645

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 13.780 | 2078 | 2082 | 2087 | rVV  | 1352 | 1961 | 0.20% | 0.026% |
| 78  | 13.877 | 2094 | 2098 | 2102 | rVB2 | 174  | 264  | 0.03% | 0.004% |
| 79  | 13.963 | 2109 | 2112 | 2116 | rVB2 | 944  | 1223 | 0.13% | 0.017% |
| 80  | 13.999 | 2116 | 2118 | 2120 | rBV2 | 160  | 198  | 0.02% | 0.003% |
| 81  | 14.030 | 2120 | 2123 | 2124 | rVB2 | 267  | 251  | 0.03% | 0.003% |
| 82  | 14.054 | 2124 | 2127 | 2131 | rVB2 | 235  | 340  | 0.03% | 0.005% |
| 83  | 14.085 | 2131 | 2132 | 2134 | rBV  | 279  | 237  | 0.02% | 0.003% |
| 84  | 14.134 | 2136 | 2140 | 2143 | rVV  | 608  | 828  | 0.09% | 0.011% |
| 85  | 14.225 | 2153 | 2155 | 2156 | rBV2 | 371  | 211  | 0.02% | 0.003% |
| 86  | 14.280 | 2159 | 2164 | 2165 | rBV  | 210  | 266  | 0.03% | 0.004% |
| 87  | 14.383 | 2179 | 2181 | 2184 | rBV2 | 306  | 327  | 0.03% | 0.004% |
| 88  | 14.420 | 2184 | 2187 | 2193 | rBV  | 209  | 302  | 0.03% | 0.004% |
| 89  | 14.755 | 2240 | 2242 | 2245 | rVB  | 284  | 272  | 0.03% | 0.004% |
| 90  | 14.932 | 2267 | 2271 | 2275 | rBV3 | 257  | 462  | 0.05% | 0.006% |
| 91  | 15.036 | 2286 | 2288 | 2289 | rBV2 | 212  | 188  | 0.02% | 0.003% |
| 92  | 15.456 | 2355 | 2357 | 2358 | rBV2 | 271  | 268  | 0.03% | 0.004% |
| 93  | 15.755 | 2405 | 2406 | 2409 | rBV2 | 277  | 336  | 0.03% | 0.005% |
| 94  | 15.877 | 2424 | 2426 | 2428 | rBV2 | 206  | 190  | 0.02% | 0.003% |
| 95  | 16.097 | 2459 | 2462 | 2465 | rVV2 | 341  | 400  | 0.04% | 0.005% |
| 96  | 16.231 | 2482 | 2484 | 2485 | rVB  | 417  | 234  | 0.02% | 0.003% |
| 97  | 16.401 | 2510 | 2512 | 2513 | rBV  | 249  | 195  | 0.02% | 0.003% |
| 98  | 16.639 | 2550 | 2551 | 2554 | rBV2 | 456  | 383  | 0.04% | 0.005% |
| 99  | 16.670 | 2554 | 2556 | 2558 | rVV2 | 364  | 227  | 0.02% | 0.003% |
| 100 | 16.706 | 2560 | 2562 | 2563 | rBV  | 264  | 188  | 0.02% | 0.003% |

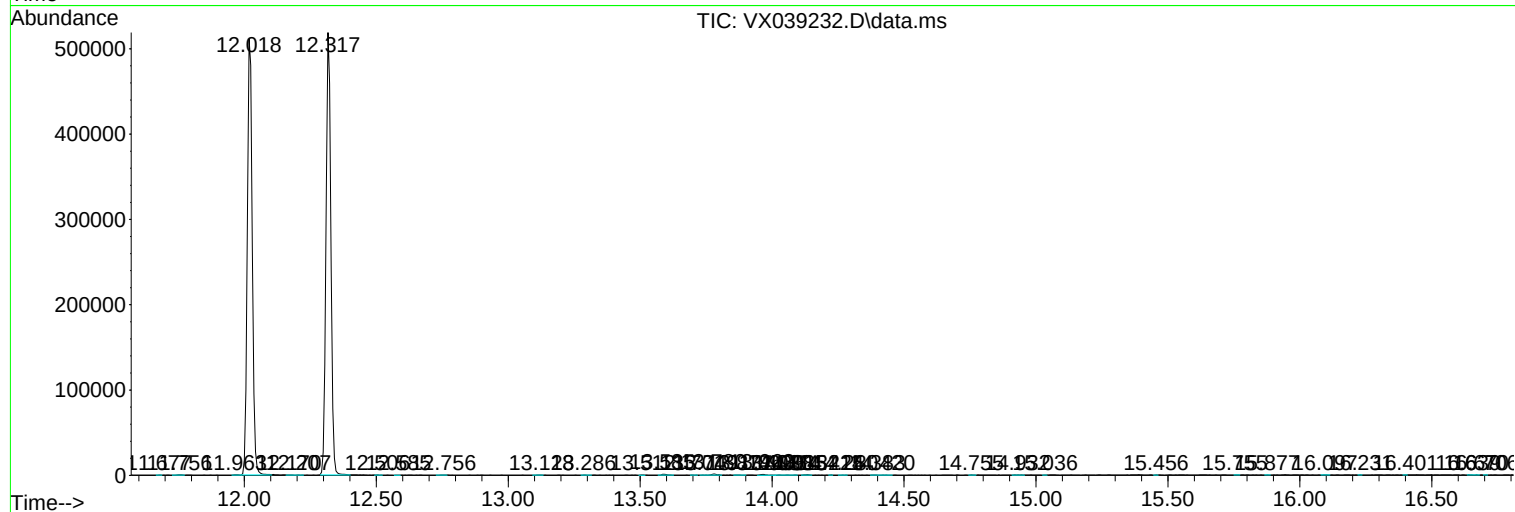
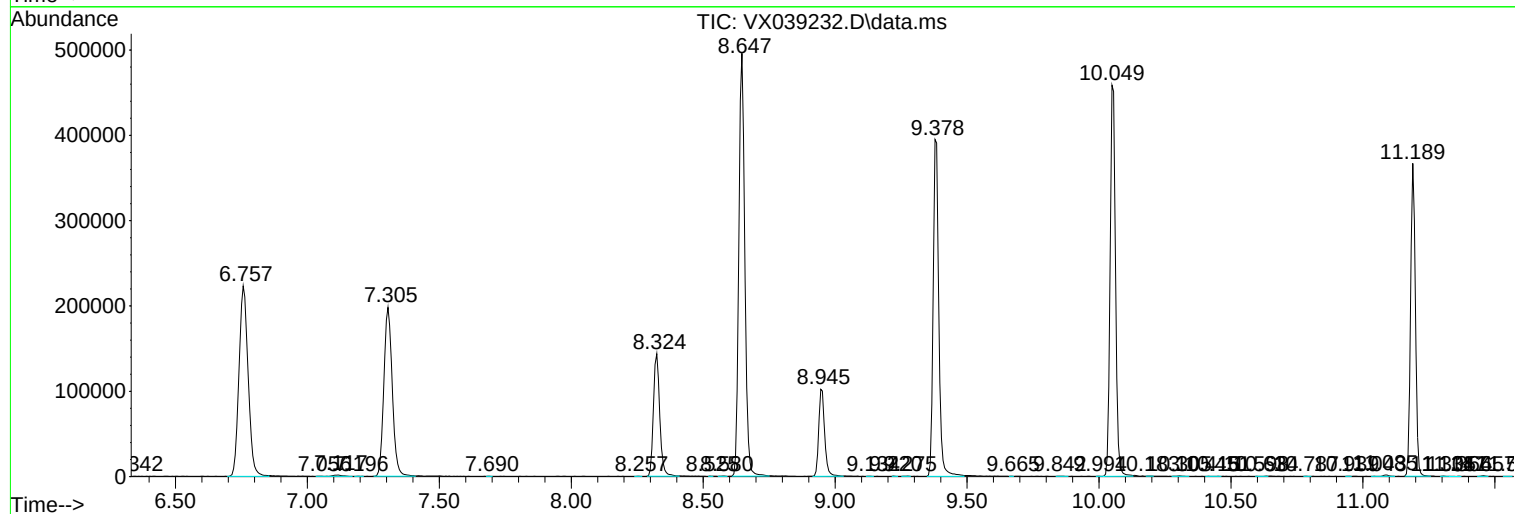
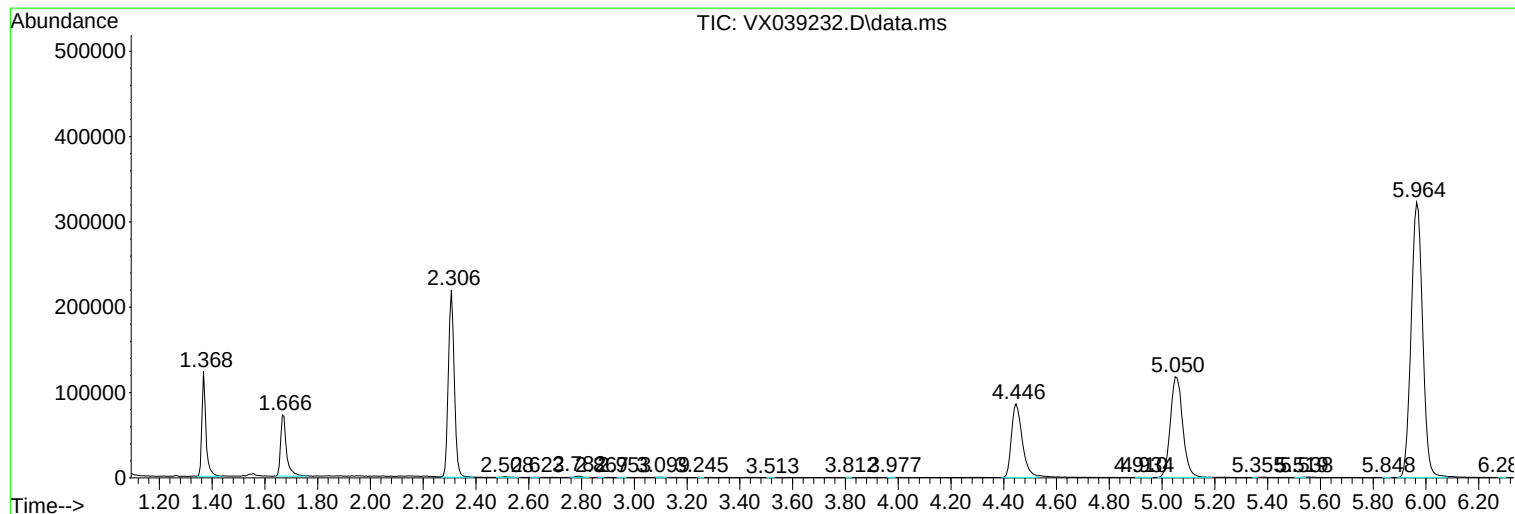
Sum of corrected areas: 7409575

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Instrument :  
MSVOA\_X  
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VBLK645

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121623\  
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
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TIC Library : C:\Database\NIST20.L  
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No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|