

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121923\  
 Data File : VX039345.D  
 Acq On : 19 Dec 2023 11:00  
 Operator : JC/MD  
 Sample : 05835-02ME  
 Misc : 2.26g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B32ME

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: VX039345.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         | 1.374       | 43            | 47          | 64           | rVB      | 71653          | 129334        | 14.57%          | 2.012%        |
| 2         | 1.648       | 89            | 92          | 97           | rBV      | 21021          | 32546         | 3.67%           | 0.506%        |
| 3         | 2.282       | 190           | 196         | 214          | rBV      | 171160         | 303650        | 34.22%          | 4.724%        |
| 4         | 2.605       | 248           | 249         | 252          | rBV2     | 509            | 506           | 0.06%           | 0.008%        |
| 5         | 2.636       | 252           | 254         | 255          | rBV      | 284            | 186           | 0.02%           | 0.003%        |
| 6         | 2.940       | 298           | 304         | 310          | rBV3     | 1383           | 3444          | 0.39%           | 0.054%        |
| 7         | 3.087       | 326           | 328         | 333          | rBV2     | 300            | 343           | 0.04%           | 0.005%        |
| 8         | 3.135       | 333           | 336         | 341          | rVB4     | 310            | 462           | 0.05%           | 0.007%        |
| 9         | 3.392       | 376           | 378         | 380          | rBV      | 245            | 186           | 0.02%           | 0.003%        |
| 10        | 3.471       | 389           | 391         | 393          | rVB      | 267            | 240           | 0.03%           | 0.004%        |
| 11        | 3.587       | 408           | 410         | 412          | rVV      | 181            | 200           | 0.02%           | 0.003%        |
| 12        | 3.928       | 462           | 466         | 470          | rBV      | 276            | 329           | 0.04%           | 0.005%        |
| 13        | 4.123       | 496           | 498         | 501          | rBV2     | 302            | 360           | 0.04%           | 0.006%        |
| 14        | 4.166       | 504           | 505         | 508          | rBV2     | 206            | 206           | 0.02%           | 0.003%        |
| 15        | 4.483       | 548           | 557         | 594          | rBV      | 37359          | 197638        | 22.27%          | 3.075%        |
| 16        | 4.903       | 624           | 626         | 627          | rBV      | 265            | 201           | 0.02%           | 0.003%        |
| 17        | 5.056       | 639           | 651         | 668          | rBV      | 99076          | 335682        | 37.83%          | 5.222%        |
| 18        | 5.263       | 681           | 685         | 687          | rBV2     | 221            | 295           | 0.03%           | 0.005%        |
| 19        | 5.294       | 688           | 690         | 693          | rVV      | 545            | 343           | 0.04%           | 0.005%        |
| 20        | 5.336       | 696           | 697         | 701          | rBV      | 237            | 246           | 0.03%           | 0.004%        |
| 21        | 5.367       | 701           | 702         | 704          | rBV      | 244            | 177           | 0.02%           | 0.003%        |
| 22        | 5.385       | 704           | 705         | 709          | rBV3     | 229            | 177           | 0.02%           | 0.003%        |
| 23        | 5.544       | 729           | 731         | 733          | rBV2     | 282            | 322           | 0.04%           | 0.005%        |
| 24        | 5.666       | 747           | 751         | 753          | rBV      | 236            | 248           | 0.03%           | 0.004%        |
| 25        | 5.958       | 787           | 799         | 822          | rBV3     | 306349         | 887422        | 100.00%         | 13.806%       |
| 26        | 6.257       | 844           | 848         | 849          | rBV      | 344            | 408           | 0.05%           | 0.006%        |
| 27        | 6.470       | 880           | 883         | 885          | rBV2     | 168            | 222           | 0.03%           | 0.003%        |
| 28        | 6.757       | 920           | 930         | 943          | rBV      | 198991         | 489345        | 55.14%          | 7.613%        |
| 29        | 6.927       | 956           | 958         | 960          | rBV2     | 201            | 196           | 0.02%           | 0.003%        |
| 30        | 6.988       | 966           | 968         | 970          | rBV      | 233            | 188           | 0.02%           | 0.003%        |
| 31        | 7.104       | 983           | 987         | 997          | rVB4     | 1399           | 3643          | 0.41%           | 0.057%        |
| 32        | 7.177       | 997           | 999         | 1001         | rVB2     | 243            | 173           | 0.02%           | 0.003%        |
| 33        | 7.202       | 1001          | 1003        | 1004         | rBV      | 395            | 275           | 0.03%           | 0.004%        |
| 34        | 7.305       | 1011          | 1020        | 1035         | rBV      | 170570         | 391686        | 44.14%          | 6.093%        |
| 35        | 7.458       | 1044          | 1045        | 1046         | rBV      | 305            | 211           | 0.02%           | 0.003%        |
| 36        | 7.952       | 1124          | 1126        | 1128         | rBV      | 249            | 172           | 0.02%           | 0.003%        |

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 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B32ME

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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.982  | 1128 | 1131 | 1133 | rBV2 | 286    | 266    | 0.03%  | 0.004%  |
| 38 | 8.324  | 1181 | 1187 | 1200 | rBV  | 106229 | 190065 | 21.42% | 2.957%  |
| 39 | 8.452  | 1205 | 1208 | 1209 | rBV3 | 342    | 349    | 0.04%  | 0.005%  |
| 40 | 8.586  | 1227 | 1230 | 1233 | rBV2 | 155    | 199    | 0.02%  | 0.003%  |
| 41 | 8.647  | 1233 | 1240 | 1257 | rBV  | 419285 | 692832 | 78.07% | 10.778% |
| 42 | 8.952  | 1284 | 1290 | 1302 | rBV  | 74323  | 126257 | 14.23% | 1.964%  |
| 43 | 9.220  | 1331 | 1334 | 1337 | rVB2 | 253    | 321    | 0.04%  | 0.005%  |
| 44 | 9.250  | 1337 | 1339 | 1340 | rBV2 | 319    | 200    | 0.02%  | 0.003%  |
| 45 | 9.269  | 1340 | 1342 | 1343 | rBV2 | 522    | 300    | 0.03%  | 0.005%  |
| 46 | 9.397  | 1356 | 1363 | 1380 | rBV  | 216570 | 456238 | 51.41% | 7.098%  |
| 47 | 9.805  | 1429 | 1430 | 1432 | rVB2 | 279    | 187    | 0.02%  | 0.003%  |
| 48 | 10.055 | 1465 | 1471 | 1482 | rBV  | 391058 | 583149 | 65.71% | 9.072%  |
| 49 | 10.305 | 1510 | 1512 | 1514 | rVV  | 550    | 349    | 0.04%  | 0.005%  |
| 50 | 10.494 | 1540 | 1543 | 1544 | rVB2 | 219    | 194    | 0.02%  | 0.003%  |
| 51 | 10.646 | 1566 | 1568 | 1570 | rBV2 | 383    | 445    | 0.05%  | 0.007%  |
| 52 | 10.811 | 1592 | 1595 | 1598 | rBV2 | 163    | 257    | 0.03%  | 0.004%  |
| 53 | 10.963 | 1617 | 1620 | 1625 | rVB2 | 427    | 758    | 0.09%  | 0.012%  |
| 54 | 11.091 | 1638 | 1641 | 1645 | rBV  | 271    | 311    | 0.04%  | 0.005%  |
| 55 | 11.195 | 1652 | 1658 | 1667 | rBV  | 291952 | 381244 | 42.96% | 5.931%  |
| 56 | 11.311 | 1674 | 1677 | 1683 | rVB2 | 688    | 973    | 0.11%  | 0.015%  |
| 57 | 11.463 | 1697 | 1702 | 1704 | rVB3 | 421    | 683    | 0.08%  | 0.011%  |
| 58 | 11.579 | 1719 | 1721 | 1722 | rBV2 | 350    | 316    | 0.04%  | 0.005%  |
| 59 | 11.756 | 1748 | 1750 | 1752 | rVB2 | 451    | 341    | 0.04%  | 0.005%  |
| 60 | 11.939 | 1777 | 1780 | 1783 | rBV2 | 461    | 682    | 0.08%  | 0.011%  |
| 61 | 11.975 | 1783 | 1786 | 1789 | rBV3 | 632    | 486    | 0.05%  | 0.008%  |
| 62 | 12.024 | 1789 | 1794 | 1809 | rVV  | 470895 | 597040 | 67.28% | 9.288%  |
| 63 | 12.231 | 1825 | 1828 | 1829 | rBV2 | 324    | 258    | 0.03%  | 0.004%  |
| 64 | 12.250 | 1829 | 1831 | 1833 | rVB2 | 295    | 186    | 0.02%  | 0.003%  |
| 65 | 12.323 | 1837 | 1843 | 1858 | rVV  | 447875 | 582628 | 65.65% | 9.064%  |
| 66 | 12.567 | 1882 | 1883 | 1887 | rBV2 | 253    | 271    | 0.03%  | 0.004%  |
| 67 | 12.701 | 1901 | 1905 | 1908 | rVV2 | 189    | 320    | 0.04%  | 0.005%  |
| 68 | 12.762 | 1911 | 1915 | 1920 | rVB2 | 1377   | 2081   | 0.23%  | 0.032%  |
| 69 | 13.054 | 1962 | 1963 | 1966 | rVV  | 218    | 192    | 0.02%  | 0.003%  |
| 70 | 13.097 | 1968 | 1970 | 1977 | rVV3 | 1565   | 2832   | 0.32%  | 0.044%  |
| 71 | 13.268 | 1995 | 1998 | 2000 | rBV2 | 314    | 332    | 0.04%  | 0.005%  |
| 72 | 13.359 | 2012 | 2013 | 2016 | rBV  | 211    | 192    | 0.02%  | 0.003%  |
| 73 | 13.591 | 2048 | 2051 | 2056 | rBV2 | 1778   | 2186   | 0.25%  | 0.034%  |
| 74 | 13.749 | 2074 | 2077 | 2080 | rVV2 | 1151   | 1393   | 0.16%  | 0.022%  |
| 75 | 13.798 | 2082 | 2085 | 2091 | rVB3 | 1902   | 2613   | 0.29%  | 0.041%  |
| 76 | 13.963 | 2109 | 2112 | 2120 | rVV3 | 1794   | 2413   | 0.27%  | 0.038%  |

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 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0B32ME

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  | 14.024 | 2120 | 2122 | 2124 | rVB  | 269  | 197  | 0.02% | 0.003% |
| 78  | 14.127 | 2133 | 2139 | 2145 | rVB  | 3553 | 4530 | 0.51% | 0.070% |
| 79  | 14.225 | 2153 | 2155 | 2157 | rBV2 | 174  | 196  | 0.02% | 0.003% |
| 80  | 14.335 | 2170 | 2173 | 2174 | rBV2 | 248  | 241  | 0.03% | 0.004% |
| 81  | 14.396 | 2180 | 2183 | 2184 | rBV2 | 339  | 252  | 0.03% | 0.004% |
| 82  | 14.579 | 2211 | 2213 | 2216 | rVB2 | 184  | 191  | 0.02% | 0.003% |
| 83  | 14.682 | 2228 | 2230 | 2231 | rBV  | 236  | 183  | 0.02% | 0.003% |
| 84  | 14.719 | 2235 | 2236 | 2238 | rBV  | 289  | 209  | 0.02% | 0.003% |
| 85  | 14.755 | 2240 | 2242 | 2244 | rVB  | 278  | 235  | 0.03% | 0.004% |
| 86  | 14.786 | 2244 | 2247 | 2252 | rBV4 | 970  | 1539 | 0.17% | 0.024% |
| 87  | 14.847 | 2255 | 2257 | 2261 | rVV3 | 194  | 205  | 0.02% | 0.003% |
| 88  | 14.999 | 2280 | 2282 | 2285 | rBV2 | 277  | 295  | 0.03% | 0.005% |
| 89  | 15.042 | 2285 | 2289 | 2290 | rBV2 | 186  | 207  | 0.02% | 0.003% |
| 90  | 15.127 | 2302 | 2303 | 2306 | rBV2 | 218  | 196  | 0.02% | 0.003% |
| 91  | 15.249 | 2319 | 2323 | 2327 | rBV3 | 1011 | 1261 | 0.14% | 0.020% |
| 92  | 15.389 | 2340 | 2346 | 2352 | rBV2 | 1227 | 2210 | 0.25% | 0.034% |
| 93  | 15.609 | 2380 | 2382 | 2384 | rBV  | 250  | 279  | 0.03% | 0.004% |
| 94  | 15.706 | 2396 | 2398 | 2402 | rBV2 | 252  | 361  | 0.04% | 0.006% |
| 95  | 15.932 | 2433 | 2435 | 2436 | rBV  | 311  | 186  | 0.02% | 0.003% |
| 96  | 15.969 | 2439 | 2441 | 2443 | rBV2 | 408  | 286  | 0.03% | 0.004% |
| 97  | 16.206 | 2478 | 2480 | 2484 | rBV2 | 311  | 288  | 0.03% | 0.004% |
| 98  | 16.517 | 2529 | 2531 | 2532 | rVB2 | 365  | 194  | 0.02% | 0.003% |
| 99  | 16.536 | 2532 | 2534 | 2536 | rBV2 | 290  | 282  | 0.03% | 0.004% |
| 100 | 16.621 | 2546 | 2548 | 2551 | rBV3 | 310  | 334  | 0.04% | 0.005% |

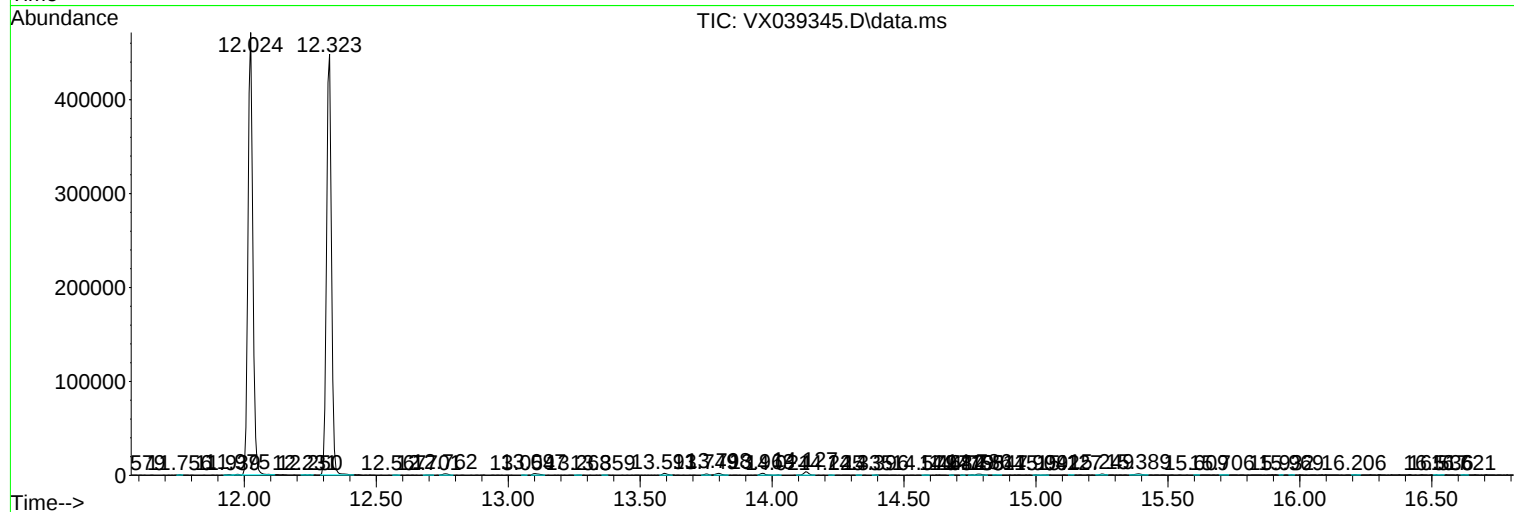
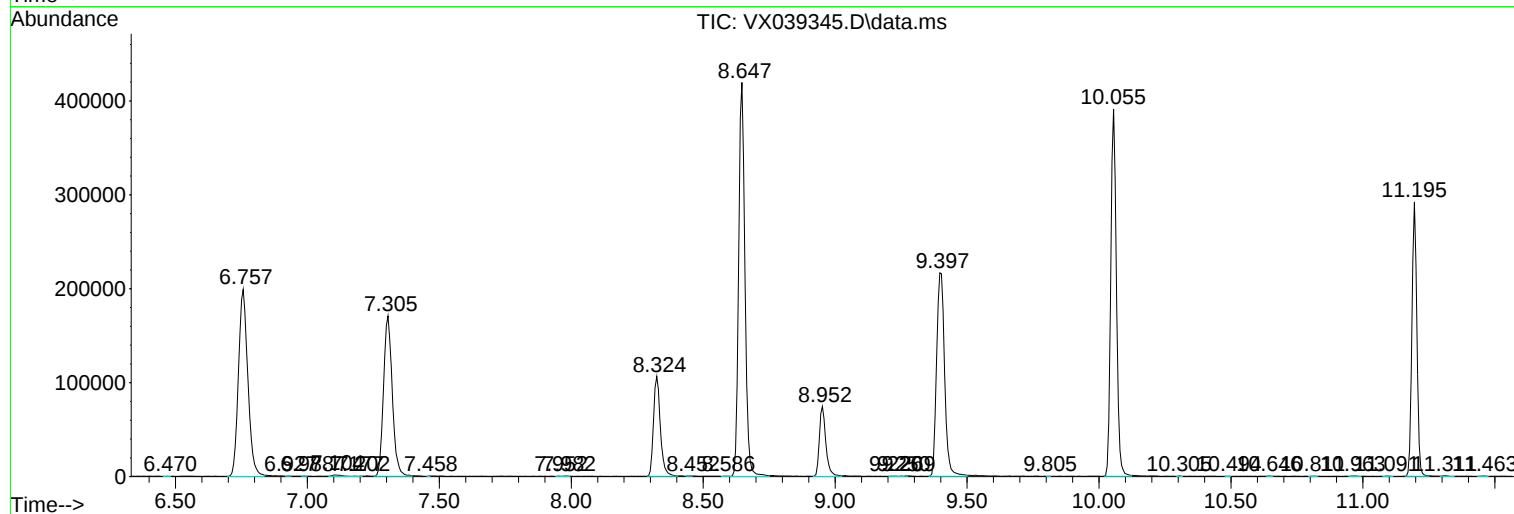
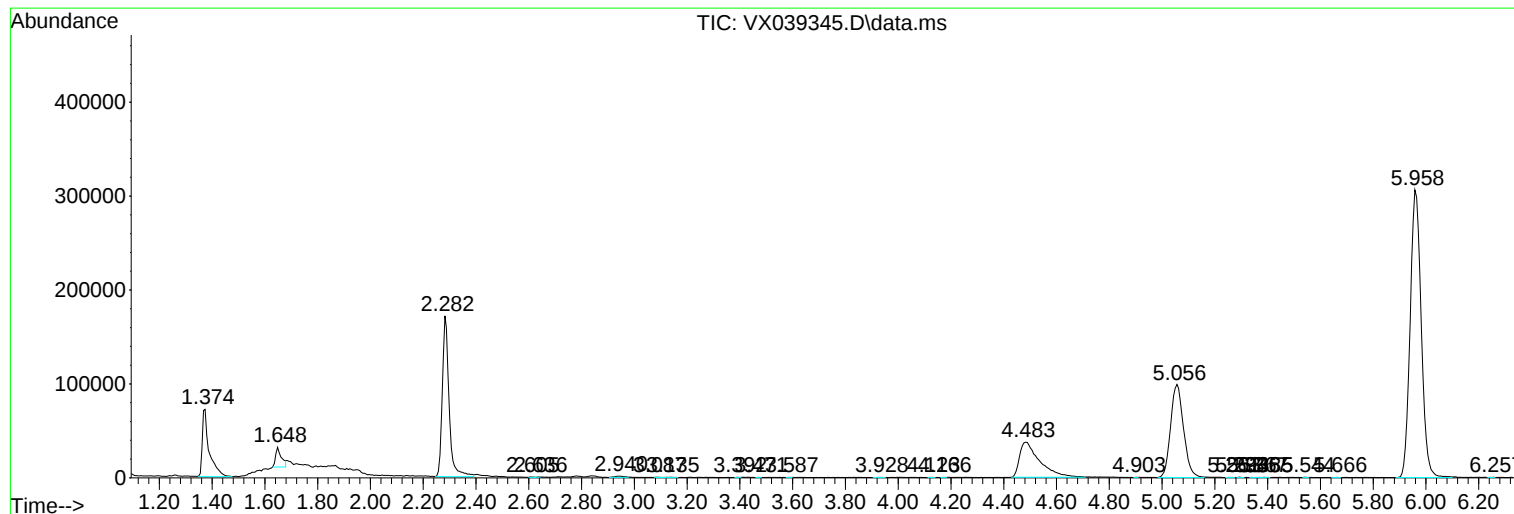
Sum of corrected areas: 6427958

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Misc : 2.26g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
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Instrument :  
MSVOA\_X  
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C0B32ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM120523WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121923\  
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Instrument :  
MSVOA\_X  
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C0B32ME

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

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 | --Internal Standard-- |
|------------------|----|---------|-------|----------|-----------------------|
|                  |    |         |       | #        | RT Resp Conc          |