

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
 Data File : VX025701.D  
 Acq On : 10 Dec 2021 15:04  
 Operator : JC/MD  
 Sample : M4888-05ME  
 Misc : 4.76g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX8B2ME

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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025701.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          | 53           | rVB      | 44990          | 52099         | 13.29%          | 1.514%        |
| 2         | 1.648       | 89            | 92          | 99           | rVB      | 31508          | 36378         | 9.28%           | 1.057%        |
| 3         | 2.276       | 189           | 195         | 205          | rBV      | 82945          | 139148        | 35.50%          | 4.044%        |
| 4         | 2.367       | 208           | 210         | 212          | rBV2     | 1350           | 1454          | 0.37%           | 0.042%        |
| 5         | 2.532       | 235           | 237         | 239          | rBV      | 390            | 412           | 0.11%           | 0.012%        |
| 6         | 2.593       | 244           | 247         | 250          | rBV      | 365            | 566           | 0.14%           | 0.016%        |
| 7         | 2.660       | 255           | 258         | 260          | rBV2     | 360            | 480           | 0.12%           | 0.014%        |
| 8         | 2.782       | 275           | 278         | 279          | rBV2     | 1222           | 1462          | 0.37%           | 0.042%        |
| 9         | 2.947       | 298           | 305         | 321          | rBV      | 6095           | 18946         | 4.83%           | 0.551%        |
| 10        | 4.166       | 502           | 505         | 510          | rBV      | 285            | 490           | 0.12%           | 0.014%        |
| 11        | 4.288       | 520           | 525         | 527          | rBV5     | 502            | 881           | 0.22%           | 0.026%        |
| 12        | 4.495       | 547           | 559         | 581          | rBV      | 16800          | 76638         | 19.55%          | 2.228%        |
| 13        | 5.062       | 641           | 652         | 669          | rBV      | 48703          | 157815        | 40.26%          | 4.587%        |
| 14        | 5.343       | 695           | 698         | 700          | rBV2     | 315            | 447           | 0.11%           | 0.013%        |
| 15        | 5.458       | 711           | 717         | 718          | rBV3     | 836            | 1252          | 0.32%           | 0.036%        |
| 16        | 5.970       | 790           | 801         | 816          | rVB2     | 138075         | 392008        | 100.00%         | 11.394%       |
| 17        | 6.074       | 816           | 818         | 821          | rBV2     | 396            | 450           | 0.11%           | 0.013%        |
| 18        | 6.153       | 827           | 831         | 833          | rBV2     | 425            | 436           | 0.11%           | 0.013%        |
| 19        | 6.251       | 846           | 847         | 850          | rVB3     | 489            | 369           | 0.09%           | 0.011%        |
| 20        | 6.367       | 860           | 866         | 877          | rVB6     | 2048           | 5777          | 1.47%           | 0.168%        |
| 21        | 6.483       | 883           | 885         | 889          | rVB2     | 266            | 366           | 0.09%           | 0.011%        |
| 22        | 6.763       | 921           | 931         | 944          | rBV      | 99953          | 254077        | 64.81%          | 7.385%        |
| 23        | 7.001       | 967           | 970         | 972          | rBV2     | 286            | 343           | 0.09%           | 0.010%        |
| 24        | 7.129       | 983           | 991         | 1001         | rBV3     | 10446          | 24251         | 6.19%           | 0.705%        |
| 25        | 7.214       | 1001          | 1005        | 1013         | rBV4     | 853            | 1992          | 0.51%           | 0.058%        |
| 26        | 7.312       | 1013          | 1021        | 1030         | rBV      | 75145          | 176523        | 45.03%          | 5.131%        |
| 27        | 7.775       | 1092          | 1097        | 1102         | rBV2     | 497            | 1311          | 0.33%           | 0.038%        |
| 28        | 7.952       | 1123          | 1126        | 1128         | rBV3     | 508            | 574           | 0.15%           | 0.017%        |
| 29        | 8.129       | 1152          | 1155        | 1157         | rBV      | 332            | 428           | 0.11%           | 0.012%        |
| 30        | 8.177       | 1160          | 1163        | 1167         | rVB      | 308            | 434           | 0.11%           | 0.013%        |
| 31        | 8.330       | 1182          | 1188        | 1197         | rBV      | 50086          | 88071         | 22.47%          | 2.560%        |
| 32        | 8.537       | 1219          | 1222        | 1225         | rBV2     | 281            | 326           | 0.08%           | 0.009%        |
| 33        | 8.604       | 1225          | 1233        | 1234         | rBV2     | 966            | 1719          | 0.44%           | 0.050%        |
| 34        | 8.653       | 1234          | 1241        | 1249         | rVV      | 206951         | 328551        | 83.81%          | 9.549%        |
| 35        | 8.720       | 1249          | 1252        | 1258         | rVV      | 3817           | 6518          | 1.66%           | 0.189%        |
| 36        | 8.775       | 1258          | 1261        | 1266         | rVV4     | 1046           | 1394          | 0.36%           | 0.041%        |

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 ALS Vial : 11 Sample Multiplier: 1

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 MSVOA\_X  
 ClientSampleId :  
 EX8B2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 8.842  | 1270 | 1272 | 1276 | rBV2 | 567    | 576    | 0.15%  | 0.017% |
| 38 | 8.915  | 1281 | 1284 | 1285 | rVV  | 412    | 507    | 0.13%  | 0.015% |
| 39 | 8.958  | 1285 | 1291 | 1304 | rVB  | 32055  | 56052  | 14.30% | 1.629% |
| 40 | 9.220  | 1332 | 1334 | 1337 | rBV  | 273    | 318    | 0.08%  | 0.009% |
| 41 | 9.275  | 1337 | 1343 | 1352 | rVV  | 183929 | 263227 | 67.15% | 7.651% |
| 42 | 9.403  | 1357 | 1364 | 1376 | rBV  | 101257 | 166357 | 42.44% | 4.835% |
| 43 | 9.561  | 1387 | 1390 | 1394 | rVB3 | 1409   | 2011   | 0.51%  | 0.058% |
| 44 | 9.616  | 1394 | 1399 | 1403 | rBV2 | 1893   | 2708   | 0.69%  | 0.079% |
| 45 | 9.708  | 1412 | 1414 | 1417 | rVV2 | 487    | 568    | 0.14%  | 0.017% |
| 46 | 9.817  | 1428 | 1432 | 1438 | rBV5 | 940    | 1890   | 0.48%  | 0.055% |
| 47 | 9.909  | 1444 | 1447 | 1450 | rVB2 | 313    | 438    | 0.11%  | 0.013% |
| 48 | 10.061 | 1466 | 1472 | 1480 | rBV  | 207255 | 303100 | 77.32% | 8.810% |
| 49 | 10.201 | 1491 | 1495 | 1500 | rBV2 | 667    | 1029   | 0.26%  | 0.030% |
| 50 | 10.305 | 1506 | 1512 | 1517 | rBV2 | 2853   | 4250   | 1.08%  | 0.124% |
| 51 | 10.360 | 1519 | 1521 | 1526 | rVB4 | 1105   | 1266   | 0.32%  | 0.037% |
| 52 | 10.451 | 1534 | 1536 | 1538 | rVB  | 390    | 341    | 0.09%  | 0.010% |
| 53 | 10.494 | 1541 | 1543 | 1545 | rBV  | 362    | 324    | 0.08%  | 0.009% |
| 54 | 10.646 | 1565 | 1568 | 1573 | rVB2 | 2531   | 3358   | 0.86%  | 0.098% |
| 55 | 10.756 | 1583 | 1586 | 1587 | rVV2 | 614    | 721    | 0.18%  | 0.021% |
| 56 | 10.781 | 1587 | 1590 | 1592 | rVV3 | 1144   | 1477   | 0.38%  | 0.043% |
| 57 | 10.805 | 1592 | 1594 | 1596 | rVV  | 362    | 336    | 0.09%  | 0.010% |
| 58 | 10.854 | 1599 | 1602 | 1605 | rVV3 | 668    | 872    | 0.22%  | 0.025% |
| 59 | 10.896 | 1606 | 1609 | 1612 | rVV  | 949    | 1044   | 0.27%  | 0.030% |
| 60 | 10.951 | 1614 | 1618 | 1626 | rVB4 | 1357   | 2743   | 0.70%  | 0.080% |
| 61 | 11.085 | 1637 | 1640 | 1641 | rBV2 | 405    | 346    | 0.09%  | 0.010% |
| 62 | 11.122 | 1642 | 1646 | 1650 | rVB  | 2623   | 3448   | 0.88%  | 0.100% |
| 63 | 11.201 | 1653 | 1659 | 1666 | rBV  | 135333 | 185407 | 47.30% | 5.389% |
| 64 | 11.274 | 1669 | 1671 | 1672 | rBV2 | 506    | 408    | 0.10%  | 0.012% |
| 65 | 11.390 | 1687 | 1690 | 1695 | rVB3 | 1008   | 1373   | 0.35%  | 0.040% |
| 66 | 11.439 | 1695 | 1698 | 1702 | rVV4 | 1331   | 2300   | 0.59%  | 0.067% |
| 67 | 11.482 | 1702 | 1705 | 1711 | rVB4 | 2101   | 3459   | 0.88%  | 0.101% |
| 68 | 11.616 | 1725 | 1727 | 1733 | rVB2 | 866    | 1229   | 0.31%  | 0.036% |
| 69 | 11.689 | 1737 | 1739 | 1740 | rVV2 | 385    | 320    | 0.08%  | 0.009% |
| 70 | 11.713 | 1741 | 1743 | 1746 | rVV2 | 1431   | 1901   | 0.48%  | 0.055% |
| 71 | 11.750 | 1746 | 1749 | 1756 | rVB3 | 3382   | 5108   | 1.30%  | 0.148% |
| 72 | 11.841 | 1761 | 1764 | 1766 | rBV2 | 565    | 695    | 0.18%  | 0.020% |
| 73 | 11.933 | 1776 | 1779 | 1785 | rBV4 | 1255   | 1774   | 0.45%  | 0.052% |
| 74 | 12.024 | 1789 | 1794 | 1800 | rBV  | 245783 | 308123 | 78.60% | 8.956% |
| 75 | 12.323 | 1836 | 1843 | 1850 | rVV  | 231924 | 294248 | 75.06% | 8.552% |
| 76 | 12.427 | 1856 | 1860 | 1865 | rBV2 | 3448   | 4465   | 1.14%  | 0.130% |

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Instrument :  
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 EX8B2ME

Integration Parameters: LSCINT.P

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Min Area: 0 % of largest Peak

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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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 12.658 | 1896 | 1898 | 1902 | rBV2 | 531  | 897  | 0.23% | 0.026% |
| 78  | 12.719 | 1906 | 1908 | 1912 | rBV3 | 413  | 562  | 0.14% | 0.016% |
| 79  | 12.768 | 1912 | 1916 | 1920 | rVB3 | 614  | 742  | 0.19% | 0.022% |
| 80  | 12.890 | 1933 | 1936 | 1940 | rBV3 | 343  | 581  | 0.15% | 0.017% |
| 81  | 12.975 | 1945 | 1950 | 1955 | rVB4 | 1106 | 1959 | 0.50% | 0.057% |
| 82  | 13.048 | 1960 | 1962 | 1965 | rBV3 | 547  | 527  | 0.13% | 0.015% |
| 83  | 13.268 | 1994 | 1998 | 2007 | rVB2 | 3019 | 3976 | 1.01% | 0.116% |
| 84  | 13.384 | 2014 | 2017 | 2022 | rVB3 | 1427 | 1983 | 0.51% | 0.058% |
| 85  | 13.780 | 2078 | 2082 | 2087 | rVB  | 3150 | 4623 | 1.18% | 0.134% |
| 86  | 13.847 | 2087 | 2093 | 2097 | rBV3 | 2172 | 3061 | 0.78% | 0.089% |
| 87  | 14.042 | 2122 | 2125 | 2128 | rVB  | 2395 | 2518 | 0.64% | 0.073% |
| 88  | 14.103 | 2133 | 2135 | 2136 | rBV  | 490  | 373  | 0.10% | 0.011% |
| 89  | 14.420 | 2186 | 2187 | 2191 | rVB2 | 527  | 404  | 0.10% | 0.012% |
| 90  | 14.615 | 2216 | 2219 | 2221 | rBV3 | 693  | 796  | 0.20% | 0.023% |
| 91  | 14.640 | 2221 | 2223 | 2227 | rVB2 | 1987 | 1845 | 0.47% | 0.054% |
| 92  | 14.762 | 2237 | 2243 | 2244 | rBV5 | 1254 | 2023 | 0.52% | 0.059% |
| 93  | 14.780 | 2244 | 2246 | 2251 | rVB2 | 2222 | 2973 | 0.76% | 0.086% |
| 94  | 14.853 | 2254 | 2258 | 2260 | rBV2 | 611  | 604  | 0.15% | 0.018% |
| 95  | 14.999 | 2278 | 2282 | 2284 | rBV3 | 282  | 425  | 0.11% | 0.012% |
| 96  | 15.213 | 2313 | 2317 | 2321 | rBV3 | 868  | 1341 | 0.34% | 0.039% |
| 97  | 15.493 | 2358 | 2363 | 2367 | rVB5 | 914  | 1678 | 0.43% | 0.049% |
| 98  | 15.621 | 2380 | 2384 | 2386 | rBV3 | 991  | 1139 | 0.29% | 0.033% |
| 99  | 15.810 | 2412 | 2415 | 2416 | rBV2 | 655  | 600  | 0.15% | 0.017% |
| 100 | 16.066 | 2456 | 2457 | 2460 | rBV  | 410  | 387  | 0.10% | 0.011% |

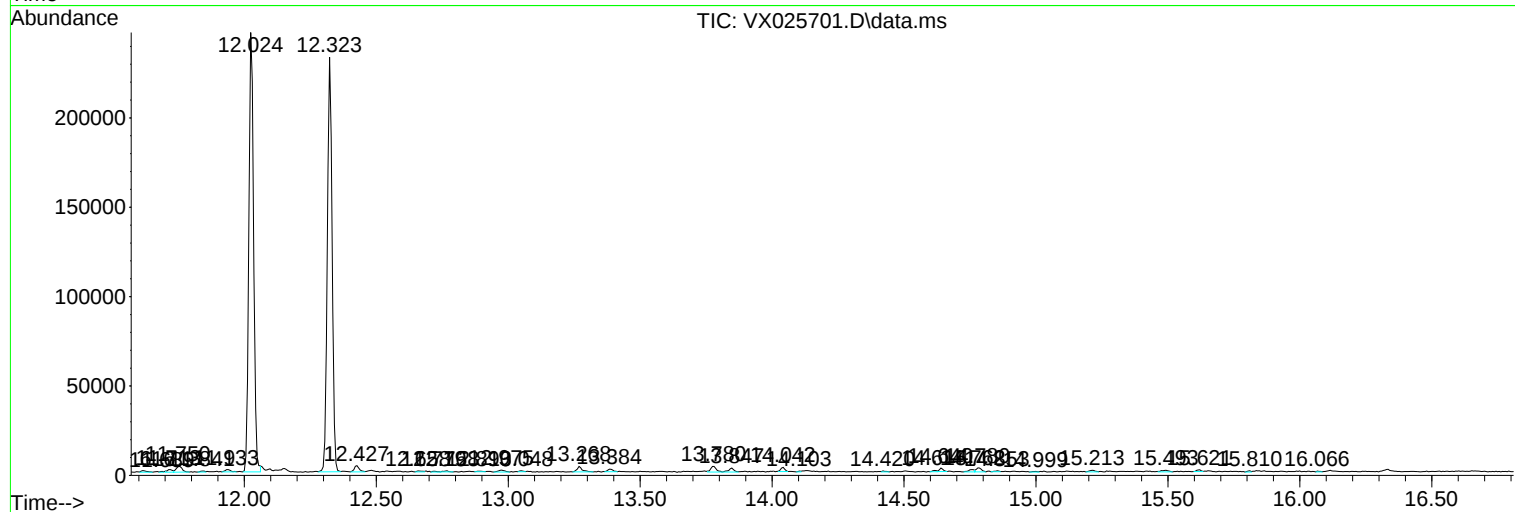
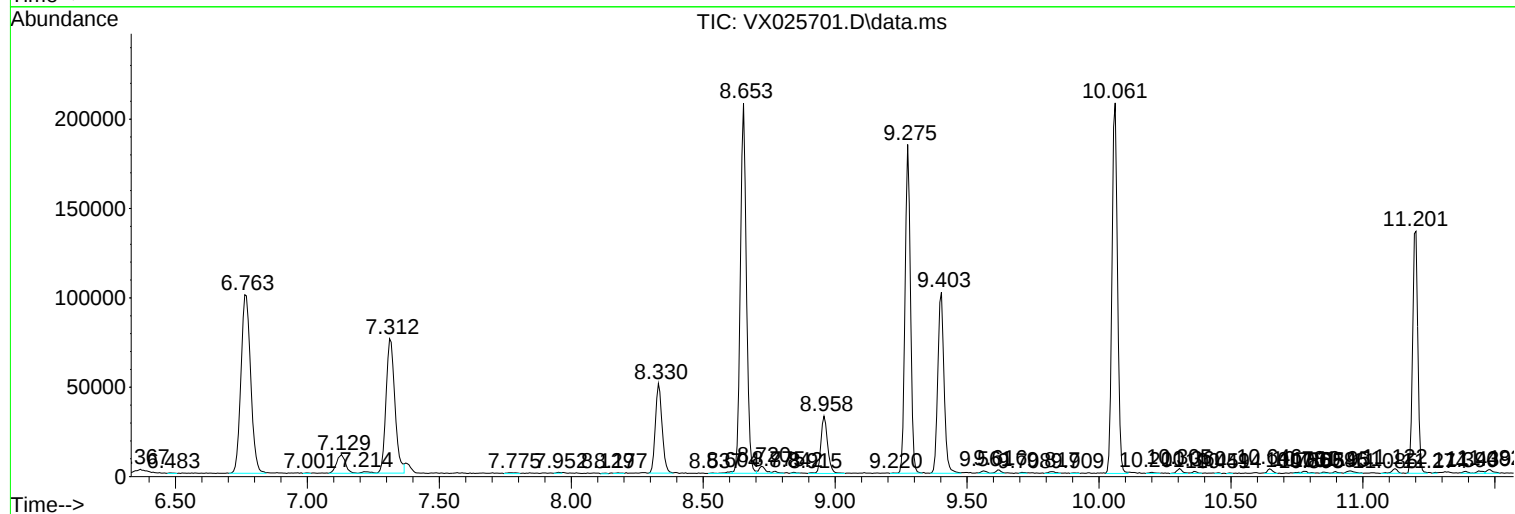
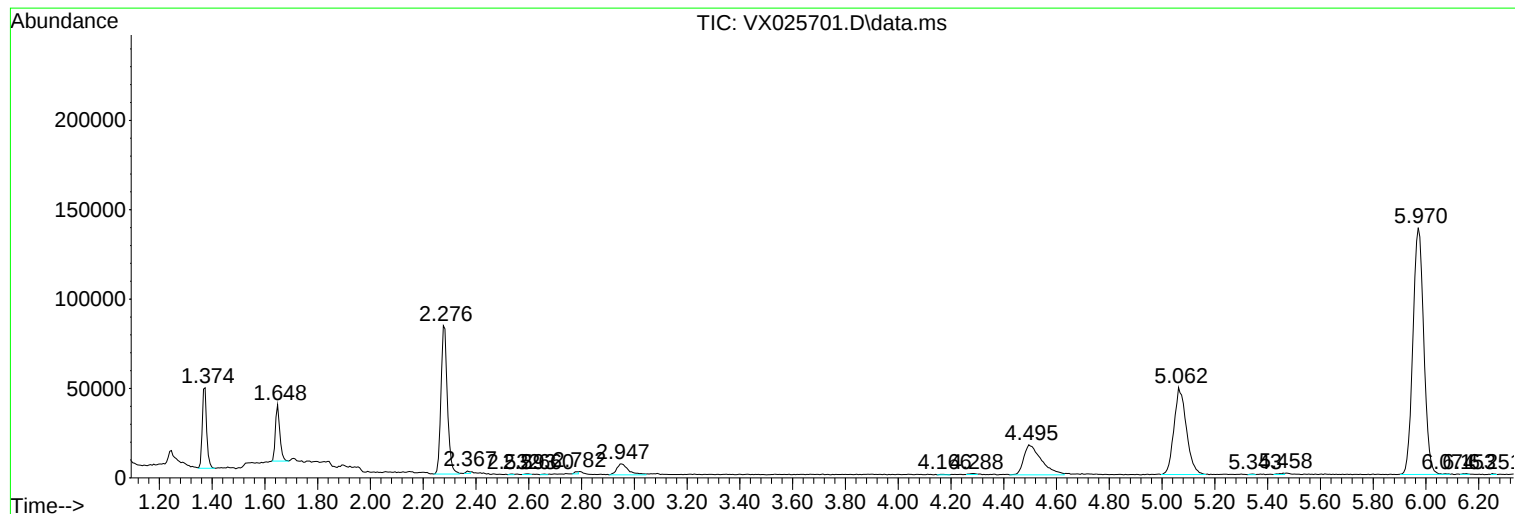
Sum of corrected areas: 3440520

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Instrument :  
MSVOA\_X  
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EX8B2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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TIC Library : C:\Database\NIST20.L  
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| TIC Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |

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