

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121823\  
 Data File : VX039337.D  
 Acq On : 19 Dec 2023 01:25  
 Operator : JC/MD  
 Sample : 05835-19 100X  
 Misc : 4.00g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AR9

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: VX039337.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         | 1.240       | 23            | 25          | 27           | rBV2     | 2112           | 1902          | 0.11%           | 0.020%        |
| 2         | 1.368       | 42            | 46          | 57           | rBV      | 85237          | 92931         | 5.54%           | 0.991%        |
| 3         | 1.666       | 91            | 95          | 108          | rVB      | 59019          | 86911         | 5.18%           | 0.926%        |
| 4         | 2.307       | 194           | 200         | 219          | rVB      | 161807         | 257307        | 15.34%          | 2.743%        |
| 5         | 2.617       | 249           | 251         | 255          | rVB      | 363            | 342           | 0.02%           | 0.004%        |
| 6         | 2.752       | 271           | 273         | 274          | rBV      | 201            | 177           | 0.01%           | 0.002%        |
| 7         | 2.788       | 275           | 279         | 286          | rVB3     | 1593           | 3073          | 0.18%           | 0.033%        |
| 8         | 2.843       | 286           | 288         | 291          | rBV2     | 209            | 222           | 0.01%           | 0.002%        |
| 9         | 2.941       | 297           | 304         | 314          | rBV2     | 4227           | 10393         | 0.62%           | 0.111%        |
| 10        | 3.038       | 319           | 320         | 322          | rVB      | 319            | 184           | 0.01%           | 0.002%        |
| 11        | 3.526       | 398           | 400         | 402          | rVB      | 240            | 170           | 0.01%           | 0.002%        |
| 12        | 3.770       | 438           | 440         | 443          | rBV2     | 235            | 288           | 0.02%           | 0.003%        |
| 13        | 4.276       | 521           | 523         | 526          | rVV2     | 192            | 194           | 0.01%           | 0.002%        |
| 14        | 4.312       | 526           | 529         | 533          | rVB2     | 274            | 310           | 0.02%           | 0.003%        |
| 15        | 4.452       | 541           | 552         | 564          | rBV      | 86975          | 244010        | 14.55%          | 2.601%        |
| 16        | 4.837       | 613           | 615         | 618          | rVB2     | 268            | 302           | 0.02%           | 0.003%        |
| 17        | 5.062       | 639           | 652         | 670          | rBV      | 106866         | 332160        | 19.81%          | 3.540%        |
| 18        | 5.397       | 702           | 707         | 709          | rVB      | 179            | 257           | 0.02%           | 0.003%        |
| 19        | 5.562       | 731           | 734         | 735          | rBV2     | 288            | 297           | 0.02%           | 0.003%        |
| 20        | 5.617       | 741           | 743         | 745          | rBV      | 356            | 252           | 0.02%           | 0.003%        |
| 21        | 5.849       | 778           | 781         | 783          | rBV2     | 188            | 206           | 0.01%           | 0.002%        |
| 22        | 5.970       | 788           | 801         | 823          | rBV2     | 274761         | 890754        | 53.12%          | 9.494%        |
| 23        | 6.257       | 846           | 848         | 850          | rBV      | 229            | 180           | 0.01%           | 0.002%        |
| 24        | 6.556       | 894           | 897         | 901          | rBV2     | 425            | 613           | 0.04%           | 0.007%        |
| 25        | 6.757       | 921           | 930         | 947          | rBV      | 217265         | 528759        | 31.53%          | 5.636%        |
| 26        | 6.940       | 959           | 960         | 962          | rBV2     | 332            | 199           | 0.01%           | 0.002%        |
| 27        | 7.111       | 984           | 988         | 996          | rVB7     | 1366           | 3236          | 0.19%           | 0.034%        |
| 28        | 7.251       | 1009          | 1011        | 1012         | rBV2     | 251            | 193           | 0.01%           | 0.002%        |
| 29        | 7.306       | 1012          | 1020        | 1031         | rBV      | 173941         | 380836        | 22.71%          | 4.059%        |
| 30        | 7.489       | 1046          | 1050        | 1052         | rVB2     | 409            | 502           | 0.03%           | 0.005%        |
| 31        | 7.671       | 1077          | 1080        | 1082         | rBV      | 192            | 269           | 0.02%           | 0.003%        |
| 32        | 7.738       | 1087          | 1091        | 1092         | rVV2     | 279            | 332           | 0.02%           | 0.004%        |
| 33        | 7.952       | 1123          | 1126        | 1127         | rBV2     | 350            | 225           | 0.01%           | 0.002%        |
| 34        | 8.190       | 1162          | 1165        | 1166         | rBV2     | 185            | 195           | 0.01%           | 0.002%        |
| 35        | 8.324       | 1181          | 1187        | 1201         | rBV      | 111173         | 187816        | 11.20%          | 2.002%        |
| 36        | 8.574       | 1225          | 1228        | 1233         | rVB2     | 492            | 660           | 0.04%           | 0.007%        |

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 MSVOA\_X  
 ClientSampleId :  
 C0AR9

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 | 8.647  | 1233 | 1240 | 1260 | rBV  | 405694  | 643137  | 38.35%  | 6.855%  |
| 38 | 8.952  | 1284 | 1290 | 1305 | rBV  | 82582   | 125451  | 7.48%   | 1.337%  |
| 39 | 9.141  | 1319 | 1321 | 1325 | rVB  | 293     | 309     | 0.02%   | 0.003%  |
| 40 | 9.196  | 1328 | 1330 | 1331 | rBV2 | 232     | 184     | 0.01%   | 0.002%  |
| 41 | 9.269  | 1340 | 1342 | 1345 | rBV2 | 398     | 486     | 0.03%   | 0.005%  |
| 42 | 9.385  | 1355 | 1361 | 1380 | rBV  | 387017  | 563520  | 33.60%  | 6.006%  |
| 43 | 9.695  | 1409 | 1412 | 1416 | rBV4 | 510     | 790     | 0.05%   | 0.008%  |
| 44 | 9.823  | 1430 | 1433 | 1434 | rBV2 | 219     | 176     | 0.01%   | 0.002%  |
| 45 | 9.903  | 1444 | 1446 | 1450 | rBV  | 168     | 175     | 0.01%   | 0.002%  |
| 46 | 9.945  | 1450 | 1453 | 1458 | rBV2 | 129     | 203     | 0.01%   | 0.002%  |
| 47 | 10.055 | 1465 | 1471 | 1472 | rBV  | 521586  | 686381  | 40.93%  | 7.316%  |
| 48 | 10.080 | 1472 | 1475 | 1491 | rVB  | 1040964 | 1396301 | 83.26%  | 14.883% |
| 49 | 10.293 | 1507 | 1510 | 1511 | rBV  | 280     | 208     | 0.01%   | 0.002%  |
| 50 | 10.311 | 1511 | 1513 | 1516 | rVV2 | 433     | 512     | 0.03%   | 0.005%  |
| 51 | 10.427 | 1530 | 1532 | 1536 | rVB2 | 228     | 168     | 0.01%   | 0.002%  |
| 52 | 10.775 | 1585 | 1589 | 1591 | rBV2 | 221     | 285     | 0.02%   | 0.003%  |
| 53 | 10.872 | 1603 | 1605 | 1607 | rBV2 | 220     | 232     | 0.01%   | 0.002%  |
| 54 | 10.957 | 1617 | 1619 | 1624 | rVB3 | 439     | 573     | 0.03%   | 0.006%  |
| 55 | 11.104 | 1639 | 1643 | 1646 | rBV3 | 284     | 435     | 0.03%   | 0.005%  |
| 56 | 11.189 | 1652 | 1657 | 1673 | rVB  | 339800  | 429077  | 25.59%  | 4.573%  |
| 57 | 11.366 | 1682 | 1686 | 1689 | rBV4 | 1264    | 1545    | 0.09%   | 0.016%  |
| 58 | 11.463 | 1699 | 1702 | 1706 | rVB3 | 570     | 684     | 0.04%   | 0.007%  |
| 59 | 11.555 | 1714 | 1717 | 1719 | rBV2 | 248     | 336     | 0.02%   | 0.004%  |
| 60 | 11.634 | 1729 | 1730 | 1733 | rBV2 | 272     | 196     | 0.01%   | 0.002%  |
| 61 | 11.756 | 1748 | 1750 | 1752 | rVB3 | 380     | 333     | 0.02%   | 0.004%  |
| 62 | 11.823 | 1758 | 1761 | 1762 | rBV  | 300     | 235     | 0.01%   | 0.003%  |
| 63 | 11.841 | 1762 | 1764 | 1766 | rBV2 | 205     | 176     | 0.01%   | 0.002%  |
| 64 | 11.969 | 1779 | 1785 | 1789 | rBV  | 40310   | 51528   | 3.07%   | 0.549%  |
| 65 | 12.036 | 1789 | 1796 | 1805 | rVB2 | 845959  | 1676976 | 100.00% | 17.874% |
| 66 | 12.274 | 1833 | 1835 | 1837 | rBV  | 341     | 222     | 0.01%   | 0.002%  |
| 67 | 12.317 | 1837 | 1842 | 1856 | rVV2 | 469167  | 683012  | 40.73%  | 7.280%  |
| 68 | 12.488 | 1869 | 1870 | 1873 | rVB2 | 249     | 211     | 0.01%   | 0.002%  |
| 69 | 12.671 | 1899 | 1900 | 1903 | rVV2 | 347     | 253     | 0.02%   | 0.003%  |
| 70 | 12.725 | 1906 | 1909 | 1911 | rVB2 | 250     | 220     | 0.01%   | 0.002%  |
| 71 | 12.762 | 1911 | 1915 | 1918 | rBV2 | 576     | 875     | 0.05%   | 0.009%  |
| 72 | 13.061 | 1959 | 1964 | 1970 | rVV3 | 6807    | 12615   | 0.75%   | 0.134%  |
| 73 | 13.109 | 1970 | 1972 | 1976 | rVB2 | 1273    | 1607    | 0.10%   | 0.017%  |
| 74 | 13.298 | 2000 | 2003 | 2004 | rBV  | 374     | 218     | 0.01%   | 0.002%  |
| 75 | 13.317 | 2004 | 2006 | 2009 | rVV  | 295     | 291     | 0.02%   | 0.003%  |
| 76 | 13.384 | 2015 | 2017 | 2020 | rVB2 | 544     | 440     | 0.03%   | 0.005%  |

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 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMXML120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 13.469 | 2029 | 2031 | 2034 | rVB2 | 323   | 320   | 0.02% | 0.003% |
| 78  | 13.591 | 2046 | 2051 | 2057 | rBV2 | 28730 | 38367 | 2.29% | 0.409% |
| 79  | 13.780 | 2078 | 2082 | 2088 | rVB3 | 424   | 753   | 0.04% | 0.008% |
| 80  | 13.963 | 2107 | 2112 | 2118 | rVB  | 18189 | 24766 | 1.48% | 0.264% |
| 81  | 14.128 | 2135 | 2139 | 2146 | rVB2 | 1054  | 1659  | 0.10% | 0.018% |
| 82  | 14.195 | 2146 | 2150 | 2151 | rBV  | 157   | 194   | 0.01% | 0.002% |
| 83  | 14.237 | 2155 | 2157 | 2160 | rBV  | 245   | 309   | 0.02% | 0.003% |
| 84  | 14.408 | 2183 | 2185 | 2187 | rBV  | 286   | 208   | 0.01% | 0.002% |
| 85  | 14.481 | 2196 | 2197 | 2198 | rBV  | 335   | 179   | 0.01% | 0.002% |
| 86  | 14.719 | 2234 | 2236 | 2237 | rBV  | 204   | 195   | 0.01% | 0.002% |
| 87  | 14.768 | 2243 | 2244 | 2246 | rBV2 | 614   | 423   | 0.03% | 0.005% |
| 88  | 14.829 | 2253 | 2254 | 2259 | rVB2 | 375   | 423   | 0.03% | 0.005% |
| 89  | 15.024 | 2284 | 2286 | 2289 | rVB2 | 276   | 231   | 0.01% | 0.002% |
| 90  | 15.054 | 2289 | 2291 | 2293 | rBV2 | 357   | 384   | 0.02% | 0.004% |
| 91  | 15.121 | 2301 | 2302 | 2304 | rVB2 | 366   | 179   | 0.01% | 0.002% |
| 92  | 15.146 | 2304 | 2306 | 2308 | rBV  | 197   | 166   | 0.01% | 0.002% |
| 93  | 15.249 | 2319 | 2323 | 2328 | rBV5 | 3258  | 4367  | 0.26% | 0.047% |
| 94  | 15.359 | 2339 | 2341 | 2343 | rBV2 | 312   | 244   | 0.01% | 0.003% |
| 95  | 15.597 | 2378 | 2380 | 2384 | rVB3 | 322   | 307   | 0.02% | 0.003% |
| 96  | 15.950 | 2437 | 2438 | 2440 | rBV  | 313   | 218   | 0.01% | 0.002% |
| 97  | 16.005 | 2445 | 2447 | 2449 | rBV  | 241   | 193   | 0.01% | 0.002% |
| 98  | 16.188 | 2476 | 2477 | 2480 | rBV2 | 360   | 337   | 0.02% | 0.004% |
| 99  | 16.249 | 2485 | 2487 | 2489 | rBV  | 275   | 217   | 0.01% | 0.002% |
| 100 | 16.725 | 2563 | 2565 | 2567 | rVB2 | 301   | 194   | 0.01% | 0.002% |

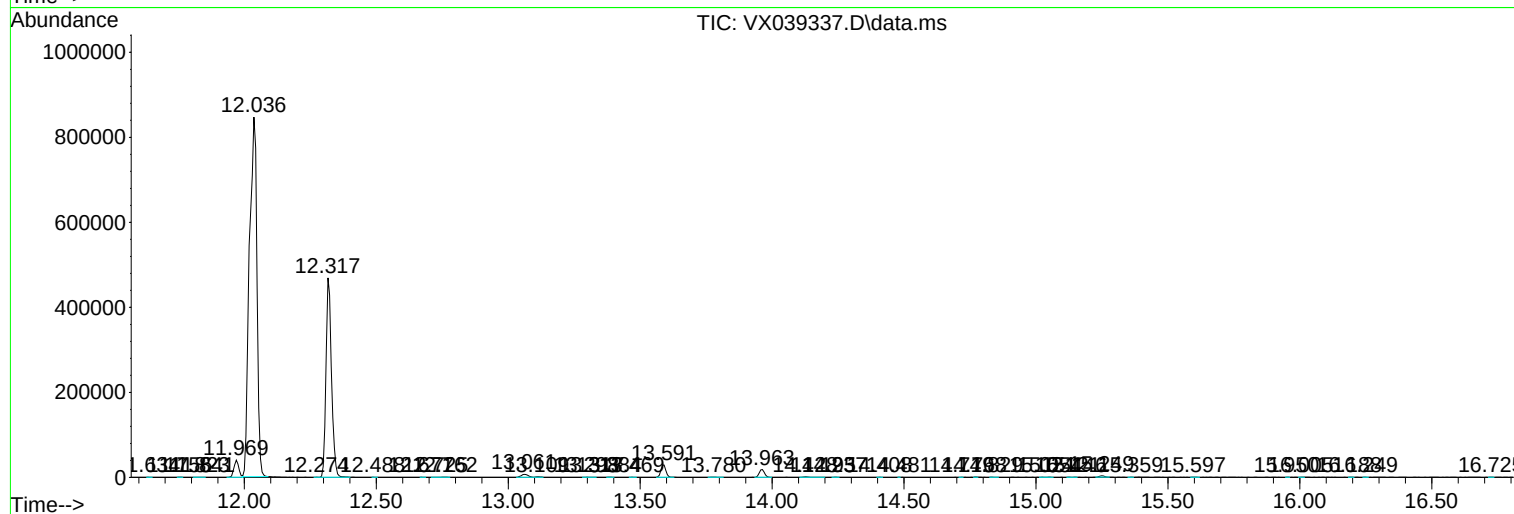
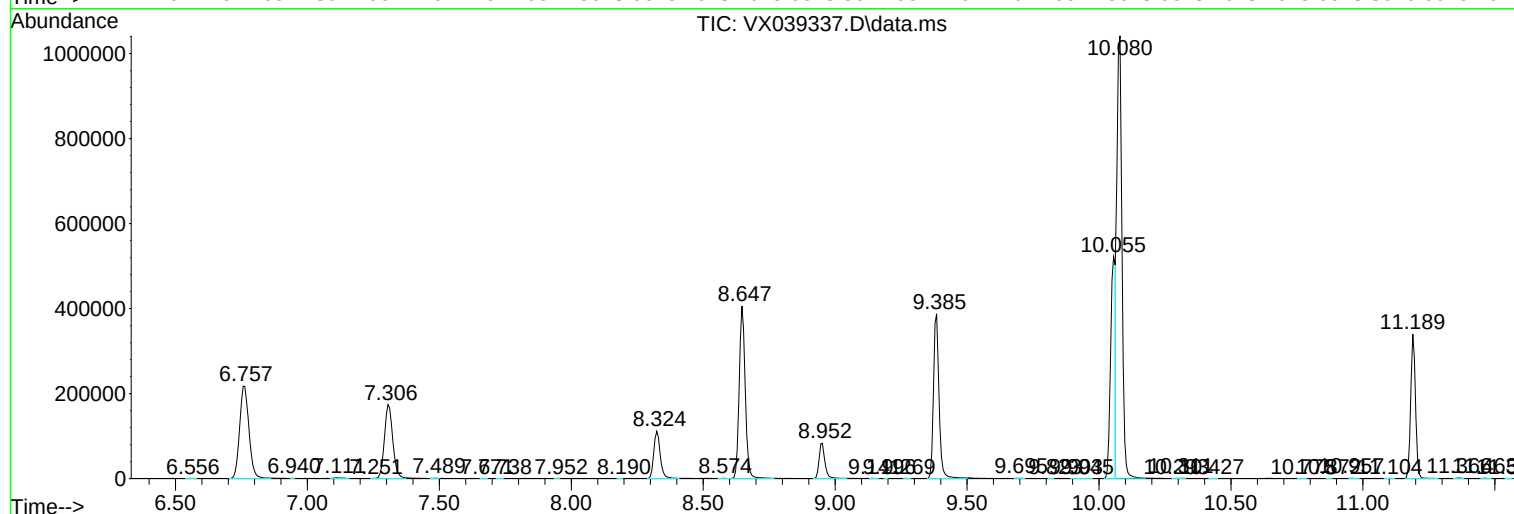
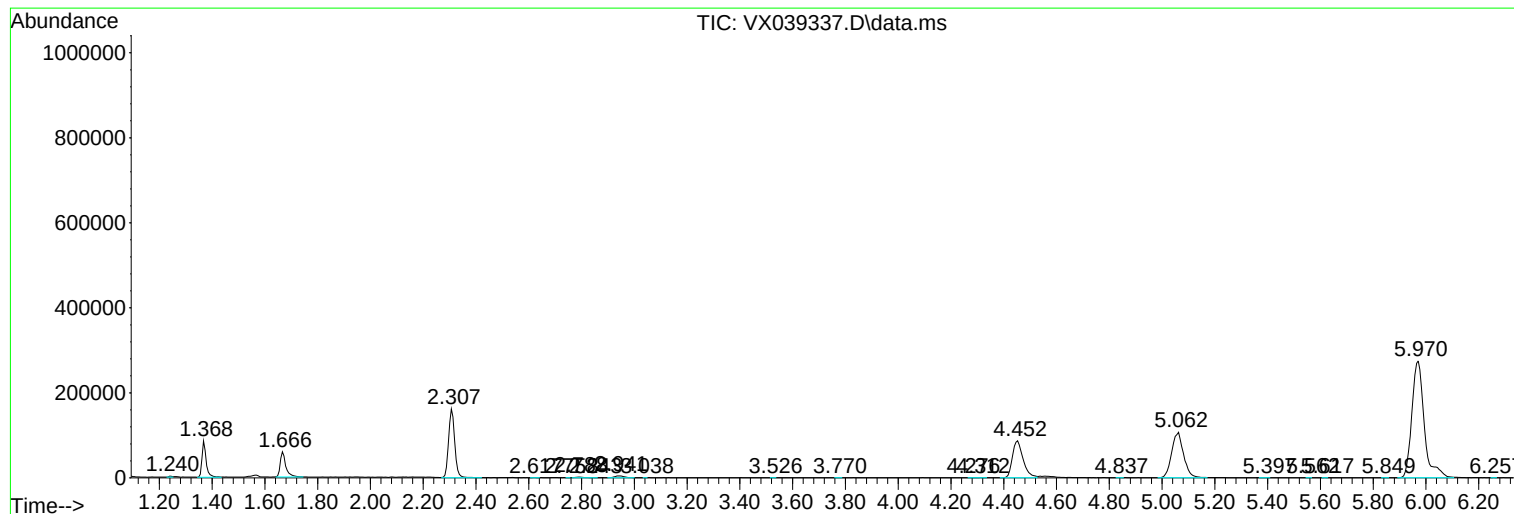
Sum of corrected areas: 9382066

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ALS Vial : 42 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
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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\VX121823\  
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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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| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|