

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU112122\  
 Data File : VU052028.D  
 Acq On : 22 Nov 2022 06:11  
 Operator : JC/MD  
 Sample : N5658-10ME  
 Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 ESQT0ME

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\_U\Method\SFAMULM112122WMA.M  
 Title : VOC Analysis

Signal : TIC: VU052028.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         | 1.478       | 35            | 43          | 50           | rBV3     | 7279           | 12359         | 0.34%           | 0.048%        |
| 2         | 1.601       | 73            | 81          | 112          | rVB      | 327550         | 511892        | 14.20%          | 1.991%        |
| 3         | 1.797       | 121           | 142         | 143          | rBV4     | 26468          | 67099         | 1.86%           | 0.261%        |
| 4         | 1.871       | 160           | 165         | 188          | rVB      | 134685         | 207929        | 5.77%           | 0.809%        |
| 5         | 2.543       | 361           | 374         | 396          | rBV      | 711585         | 1147333       | 31.82%          | 4.463%        |
| 6         | 2.768       | 438           | 444         | 448          | rBV3     | 994            | 1239          | 0.03%           | 0.005%        |
| 7         | 2.916       | 487           | 490         | 493          | rBV3     | 409            | 322           | 0.01%           | 0.001%        |
| 8         | 3.035       | 512           | 527         | 540          | rBV4     | 6655           | 13510         | 0.37%           | 0.053%        |
| 9         | 3.176       | 557           | 571         | 588          | rBV2     | 22202          | 51481         | 1.43%           | 0.200%        |
| 10        | 3.436       | 646           | 652         | 656          | rBV3     | 264            | 314           | 0.01%           | 0.001%        |
| 11        | 3.539       | 678           | 684         | 688          | rBV2     | 595            | 497           | 0.01%           | 0.002%        |
| 12        | 3.681       | 722           | 728         | 735          | rBV5     | 1160           | 1803          | 0.05%           | 0.007%        |
| 13        | 3.797       | 761           | 764         | 771          | rVB2     | 352            | 386           | 0.01%           | 0.002%        |
| 14        | 3.867       | 778           | 786         | 787          | rBV      | 484            | 455           | 0.01%           | 0.002%        |
| 15        | 4.253       | 902           | 906         | 912          | rVB2     | 406            | 331           | 0.01%           | 0.001%        |
| 16        | 4.623       | 1008          | 1021        | 1085         | rBV      | 246469         | 868392        | 24.08%          | 3.378%        |
| 17        | 5.057       | 1139          | 1156        | 1183         | rBV      | 614167         | 1393052       | 38.63%          | 5.419%        |
| 18        | 5.581       | 1314          | 1319        | 1325         | rVB3     | 299            | 381           | 0.01%           | 0.001%        |
| 19        | 5.716       | 1339          | 1361        | 1393         | rBV2     | 1406692        | 3605867       | 100.00%         | 14.027%       |
| 20        | 5.880       | 1409          | 1412        | 1414         | rVB3     | 512            | 283           | 0.01%           | 0.001%        |
| 21        | 6.099       | 1475          | 1480        | 1482         | rBV4     | 470            | 379           | 0.01%           | 0.001%        |
| 22        | 6.112       | 1482          | 1484        | 1491         | rVB2     | 529            | 571           | 0.02%           | 0.002%        |
| 23        | 6.243       | 1509          | 1525        | 1552         | rBV      | 643052         | 1274435       | 35.34%          | 4.958%        |
| 24        | 6.526       | 1599          | 1613        | 1623         | rBV9     | 7630           | 15394         | 0.43%           | 0.060%        |
| 25        | 6.597       | 1624          | 1635        | 1647         | rBV3     | 5044           | 11106         | 0.31%           | 0.043%        |
| 26        | 6.687       | 1647          | 1663        | 1690         | rVV      | 815244         | 1637366       | 45.41%          | 6.369%        |
| 27        | 6.845       | 1708          | 1712        | 1719         | rVB5     | 920            | 986           | 0.03%           | 0.004%        |
| 28        | 7.044       | 1771          | 1774        | 1776         | rBV      | 436            | 306           | 0.01%           | 0.001%        |
| 29        | 7.089       | 1781          | 1788        | 1789         | rBV2     | 290            | 304           | 0.01%           | 0.001%        |
| 30        | 7.192       | 1812          | 1820        | 1822         | rBV4     | 5215           | 6085          | 0.17%           | 0.024%        |
| 31        | 7.562       | 1919          | 1935        | 1958         | rBV      | 392372         | 748300        | 20.75%          | 2.911%        |
| 32        | 7.658       | 1963          | 1965        | 1970         | rVV4     | 689            | 523           | 0.01%           | 0.002%        |
| 33        | 7.703       | 1970          | 1979        | 1986         | rVV5     | 1465           | 2744          | 0.08%           | 0.011%        |
| 34        | 7.732       | 1986          | 1988        | 1991         | rVB4     | 808            | 448           | 0.01%           | 0.002%        |
| 35        | 7.784       | 1996          | 2004        | 2013         | rBV5     | 2601           | 4391          | 0.12%           | 0.017%        |
| 36        | 7.896       | 2022          | 2039        | 2060         | rBV      | 1655085        | 2985490       | 82.80%          | 11.614%       |

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 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 ESQTOME

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\_U\Method\SFAMULM112122WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 37 | 8.179  | 2110 | 2127 | 2154 | rBV  | 256068  | 526589  | 14.60% | 2.048%  |
| 38 | 8.276  | 2154 | 2157 | 2159 | rBV3 | 498     | 337     | 0.01%  | 0.001%  |
| 39 | 8.330  | 2170 | 2174 | 2175 | rBV2 | 392     | 288     | 0.01%  | 0.001%  |
| 40 | 8.423  | 2201 | 2203 | 2210 | rBV4 | 365     | 391     | 0.01%  | 0.002%  |
| 41 | 8.555  | 2236 | 2244 | 2248 | rBV4 | 1757    | 2287    | 0.06%  | 0.009%  |
| 42 | 8.581  | 2248 | 2252 | 2257 | rVB3 | 625     | 684     | 0.02%  | 0.003%  |
| 43 | 8.645  | 2257 | 2272 | 2303 | rBV  | 1113605 | 2191262 | 60.77% | 8.524%  |
| 44 | 8.989  | 2374 | 2379 | 2384 | rBV4 | 310     | 311     | 0.01%  | 0.001%  |
| 45 | 9.073  | 2402 | 2405 | 2407 | rBV  | 535     | 361     | 0.01%  | 0.001%  |
| 46 | 9.420  | 2497 | 2513 | 2533 | rBV  | 922274  | 1663032 | 46.12% | 6.469%  |
| 47 | 9.652  | 2578 | 2585 | 2586 | rBV4 | 1810    | 1580    | 0.04%  | 0.006%  |
| 48 | 9.944  | 2672 | 2676 | 2679 | rBV  | 366     | 293     | 0.01%  | 0.001%  |
| 49 | 9.964  | 2679 | 2682 | 2692 | rVB3 | 428     | 491     | 0.01%  | 0.002%  |
| 50 | 10.108 | 2720 | 2727 | 2731 | rBV3 | 609     | 724     | 0.02%  | 0.003%  |
| 51 | 10.230 | 2757 | 2765 | 2767 | rBV3 | 264     | 312     | 0.01%  | 0.001%  |
| 52 | 10.317 | 2780 | 2792 | 2804 | rVB2 | 14200   | 23905   | 0.66%  | 0.093%  |
| 53 | 10.462 | 2828 | 2837 | 2852 | rVB5 | 6336    | 10771   | 0.30%  | 0.042%  |
| 54 | 10.533 | 2855 | 2859 | 2865 | rBV3 | 344     | 375     | 0.01%  | 0.001%  |
| 55 | 10.619 | 2882 | 2886 | 2890 | rVV4 | 865     | 945     | 0.03%  | 0.004%  |
| 56 | 10.645 | 2890 | 2894 | 2901 | rVB4 | 557     | 753     | 0.02%  | 0.003%  |
| 57 | 10.758 | 2914 | 2929 | 2947 | rBV  | 1467333 | 2387821 | 66.22% | 9.289%  |
| 58 | 11.066 | 3021 | 3025 | 3028 | rBV3 | 315     | 285     | 0.01%  | 0.001%  |
| 59 | 11.118 | 3028 | 3041 | 3052 | rVB8 | 2198    | 4502    | 0.12%  | 0.018%  |
| 60 | 11.169 | 3052 | 3057 | 3059 | rBV  | 444     | 438     | 0.01%  | 0.002%  |
| 61 | 11.250 | 3077 | 3082 | 3084 | rBV3 | 374     | 297     | 0.01%  | 0.001%  |
| 62 | 11.272 | 3084 | 3089 | 3093 | rBV2 | 387     | 297     | 0.01%  | 0.001%  |
| 63 | 11.314 | 3093 | 3102 | 3103 | rBV4 | 606     | 814     | 0.02%  | 0.003%  |
| 64 | 11.362 | 3113 | 3117 | 3119 | rBV2 | 536     | 353     | 0.01%  | 0.001%  |
| 65 | 11.417 | 3127 | 3134 | 3137 | rVB5 | 2019    | 2090    | 0.06%  | 0.008%  |
| 66 | 11.472 | 3149 | 3151 | 3157 | rVB2 | 766     | 639     | 0.02%  | 0.002%  |
| 67 | 11.552 | 3174 | 3176 | 3180 | rVB  | 463     | 318     | 0.01%  | 0.001%  |
| 68 | 11.578 | 3180 | 3184 | 3188 | rVB2 | 402     | 329     | 0.01%  | 0.001%  |
| 69 | 11.632 | 3193 | 3201 | 3203 | rBV3 | 337     | 376     | 0.01%  | 0.001%  |
| 70 | 11.648 | 3203 | 3206 | 3208 | rBV2 | 626     | 353     | 0.01%  | 0.001%  |
| 71 | 11.706 | 3219 | 3224 | 3229 | rBV3 | 306     | 338     | 0.01%  | 0.001%  |
| 72 | 11.742 | 3229 | 3235 | 3241 | rBV6 | 1379    | 1875    | 0.05%  | 0.007%  |
| 73 | 11.812 | 3244 | 3257 | 3291 | rBV  | 924596  | 1480135 | 41.05% | 5.758%  |
| 74 | 11.992 | 3310 | 3313 | 3314 | rBV2 | 834     | 536     | 0.01%  | 0.002%  |
| 75 | 12.002 | 3314 | 3316 | 3324 | rVB3 | 1284    | 1395    | 0.04%  | 0.005%  |
| 76 | 12.192 | 3361 | 3375 | 3400 | rBV  | 1733782 | 2769443 | 76.80% | 10.773% |

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 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 ESQT0ME

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\_U\Method\SFAMULM112122WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 12.404 | 3438 | 3441 | 3445 | rBV3 | 437   | 349   | 0.01% | 0.001% |
| 78  | 12.697 | 3527 | 3532 | 3538 | rVB4 | 681   | 858   | 0.02% | 0.003% |
| 79  | 12.928 | 3600 | 3604 | 3609 | rBV2 | 462   | 576   | 0.02% | 0.002% |
| 80  | 13.057 | 3636 | 3644 | 3647 | rVB3 | 546   | 623   | 0.02% | 0.002% |
| 81  | 13.076 | 3647 | 3650 | 3652 | rBV2 | 516   | 367   | 0.01% | 0.001% |
| 82  | 13.143 | 3668 | 3671 | 3673 | rBV  | 439   | 306   | 0.01% | 0.001% |
| 83  | 13.224 | 3691 | 3696 | 3705 | rBV5 | 1873  | 2440  | 0.07% | 0.009% |
| 84  | 13.298 | 3716 | 3719 | 3728 | rVB3 | 758   | 908   | 0.03% | 0.004% |
| 85  | 13.340 | 3728 | 3732 | 3737 | rBV3 | 424   | 428   | 0.01% | 0.002% |
| 86  | 13.697 | 3838 | 3843 | 3844 | rBV2 | 536   | 397   | 0.01% | 0.002% |
| 87  | 13.735 | 3851 | 3855 | 3866 | rVB6 | 776   | 1324  | 0.04% | 0.005% |
| 88  | 13.812 | 3876 | 3879 | 3882 | rBV3 | 566   | 341   | 0.01% | 0.001% |
| 89  | 13.844 | 3883 | 3889 | 3892 | rBV5 | 1375  | 1619  | 0.04% | 0.006% |
| 90  | 13.902 | 3903 | 3907 | 3911 | rBV3 | 442   | 542   | 0.02% | 0.002% |
| 91  | 14.037 | 3945 | 3949 | 3951 | rBV2 | 528   | 395   | 0.01% | 0.002% |
| 92  | 14.089 | 3963 | 3965 | 3967 | rBV2 | 564   | 321   | 0.01% | 0.001% |
| 93  | 14.208 | 3999 | 4002 | 4006 | rVB3 | 414   | 316   | 0.01% | 0.001% |
| 94  | 14.336 | 4035 | 4042 | 4052 | rBV5 | 1597  | 2580  | 0.07% | 0.010% |
| 95  | 14.500 | 4090 | 4093 | 4097 | rVB2 | 463   | 316   | 0.01% | 0.001% |
| 96  | 14.568 | 4110 | 4114 | 4119 | rBV3 | 737   | 887   | 0.02% | 0.003% |
| 97  | 14.909 | 4212 | 4220 | 4234 | rVB4 | 18058 | 27611 | 0.77% | 0.107% |
| 98  | 15.452 | 4380 | 4389 | 4398 | rBV4 | 3934  | 6543  | 0.18% | 0.025% |
| 99  | 15.507 | 4403 | 4406 | 4408 | rBV3 | 743   | 561   | 0.02% | 0.002% |
| 100 | 15.651 | 4444 | 4451 | 4458 | rBV7 | 2837  | 4344  | 0.12% | 0.017% |

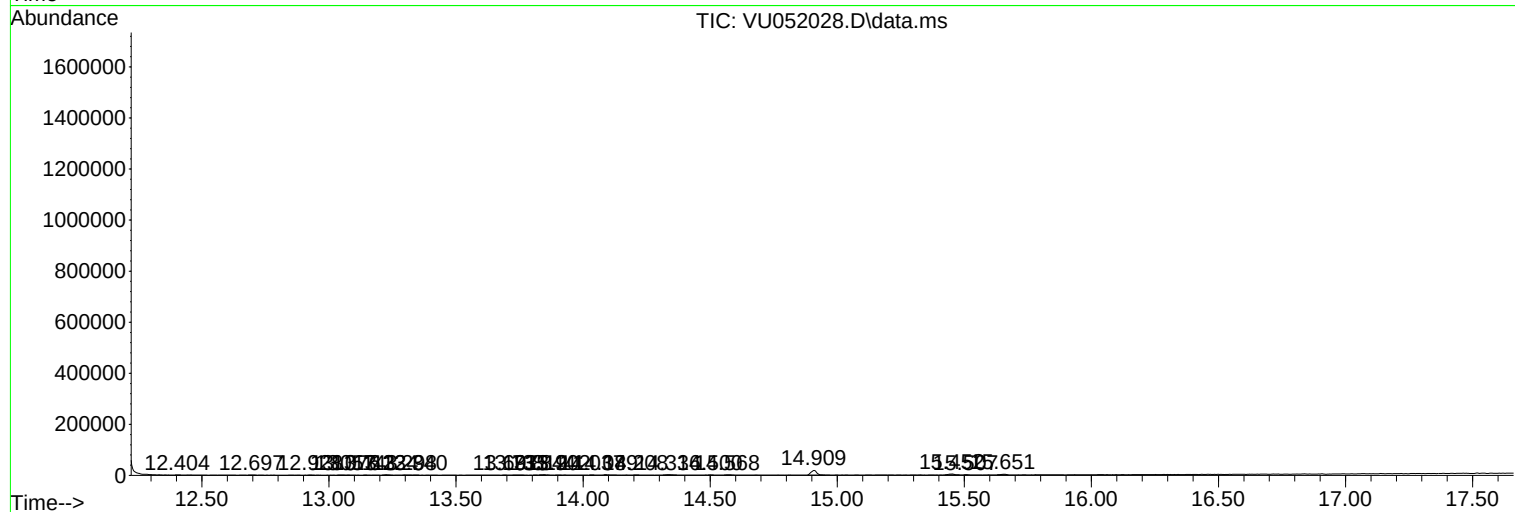
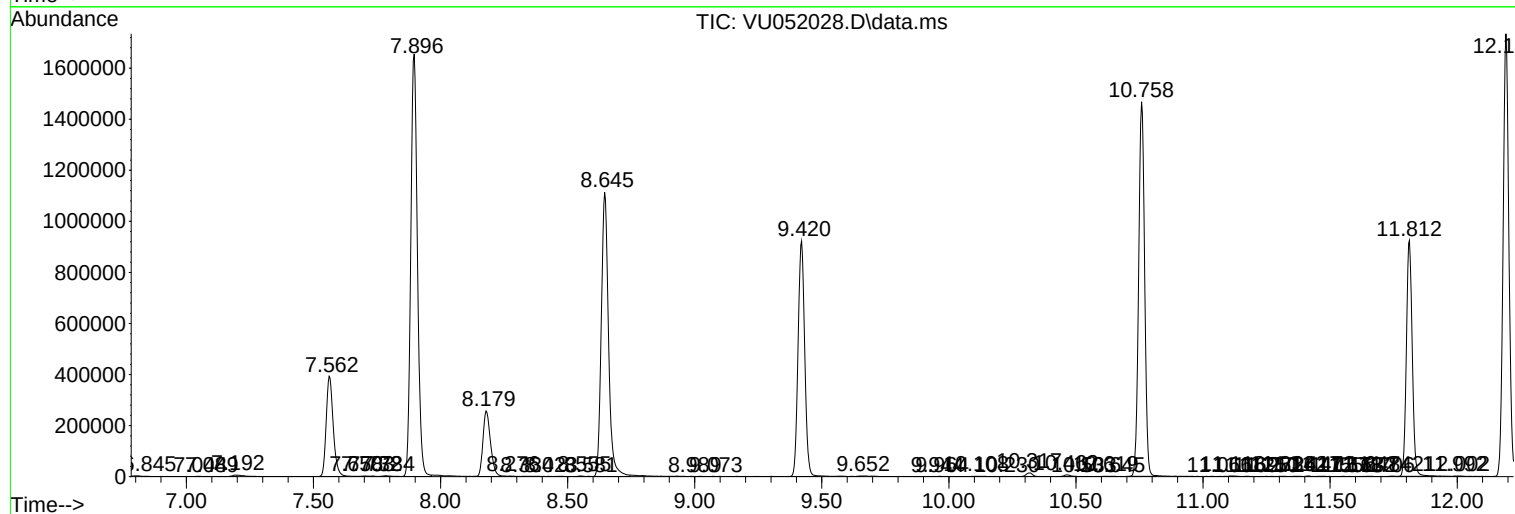
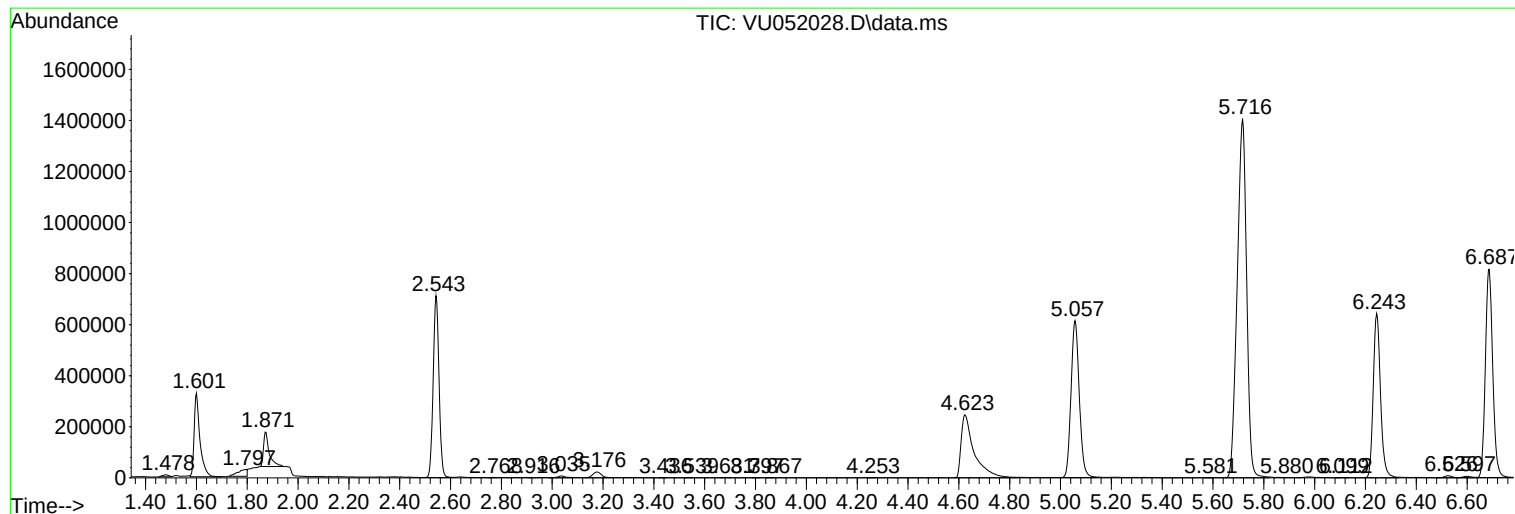
Sum of corrected areas: 25707030

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ClientSampleId :  
ESQT0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112122WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU112122\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112122WMA.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 | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |