

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011022\  
 Data File : VU046714.D  
 Acq On : 10 Jan 2022 14:22  
 Operator : SY/MD  
 Sample : N1053-25ME  
 Misc : 6.55g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGLL2ME

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\SFAMULM010522WMA.M  
 Title : VOC Analysis

Signal : TIC: VU046714.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         | 1.604       | 74            | 82          | 108          | rVB      | 48603          | 99621         | 12.92%          | 1.708%        |
| 2         | 1.919       | 171           | 180         | 220          | rVB      | 29424          | 92433         | 11.99%          | 1.585%        |
| 3         | 2.559       | 368           | 379         | 393          | rBV      | 124616         | 209148        | 27.13%          | 3.586%        |
| 4         | 2.777       | 444           | 447         | 449          | rBV      | 298            | 219           | 0.03%           | 0.004%        |
| 5         | 2.793       | 450           | 452         | 454          | rVB      | 459            | 210           | 0.03%           | 0.004%        |
| 6         | 2.832       | 461           | 464         | 466          | rBV      | 175            | 150           | 0.02%           | 0.003%        |
| 7         | 2.900       | 482           | 485         | 488          | rVB2     | 211            | 138           | 0.02%           | 0.002%        |
| 8         | 2.967       | 501           | 506         | 509          | rBV2     | 326            | 255           | 0.03%           | 0.004%        |
| 9         | 3.041       | 525           | 529         | 537          | rVB2     | 686            | 899           | 0.12%           | 0.015%        |
| 10        | 3.186       | 559           | 574         | 589          | rBV      | 4980           | 11482         | 1.49%           | 0.197%        |
| 11        | 3.533       | 679           | 682         | 686          | rBB      | 135            | 145           | 0.02%           | 0.002%        |
| 12        | 3.655       | 716           | 720         | 724          | rBB      | 144            | 169           | 0.02%           | 0.003%        |
| 13        | 3.681       | 725           | 728         | 731          | rBB      | 175            | 137           | 0.02%           | 0.002%        |
| 14        | 3.816       | 768           | 770         | 773          | rBV      | 138            | 121           | 0.02%           | 0.002%        |
| 15        | 4.234       | 898           | 900         | 904          | rBV      | 114            | 126           | 0.02%           | 0.002%        |
| 16        | 4.665       | 1017          | 1034        | 1104         | rBV2     | 36257          | 231263        | 30.00%          | 3.965%        |
| 17        | 5.070       | 1144          | 1160        | 1187         | rVB      | 133455         | 315005        | 40.86%          | 5.401%        |
| 18        | 5.726       | 1344          | 1364        | 1393         | rBV2     | 302234         | 770999        | 100.00%         | 13.218%       |
| 19        | 5.983       | 1434          | 1444        | 1445         | rBV4     | 2854           | 3279          | 0.43%           | 0.056%        |
| 20        | 6.186       | 1505          | 1507        | 1509         | rVV      | 233            | 132           | 0.02%           | 0.002%        |
| 21        | 6.198       | 1509          | 1511        | 1513         | rVB      | 254            | 135           | 0.02%           | 0.002%        |
| 22        | 6.253       | 1514          | 1528        | 1552         | rBV      | 172207         | 343649        | 44.57%          | 5.892%        |
| 23        | 6.543       | 1608          | 1618        | 1630         | rBB5     | 8397           | 15356         | 1.99%           | 0.263%        |
| 24        | 6.604       | 1630          | 1637        | 1639         | rBV      | 1267           | 1437          | 0.19%           | 0.025%        |
| 25        | 6.694       | 1651          | 1665        | 1691         | rVB      | 168036         | 347727        | 45.10%          | 5.962%        |
| 26        | 6.973       | 1749          | 1752        | 1755         | rBB      | 160            | 134           | 0.02%           | 0.002%        |
| 27        | 7.018       | 1763          | 1766        | 1770         | rVB      | 171            | 162           | 0.02%           | 0.003%        |
| 28        | 7.192       | 1812          | 1820        | 1827         | rVV2     | 587            | 775           | 0.10%           | 0.013%        |
| 29        | 7.221       | 1827          | 1829        | 1831         | rBV      | 354            | 192           | 0.02%           | 0.003%        |
| 30        | 7.256       | 1839          | 1840        | 1843         | rVB      | 312            | 146           | 0.02%           | 0.003%        |
| 31        | 7.272       | 1843          | 1845        | 1849         | rVB2     | 245            | 121           | 0.02%           | 0.002%        |
| 32        | 7.571       | 1925          | 1938        | 1969         | rBB      | 86926          | 178240        | 23.12%          | 3.056%        |
| 33        | 7.694       | 1972          | 1976        | 1977         | rBV2     | 163            | 121           | 0.02%           | 0.002%        |
| 34        | 7.706       | 1977          | 1980        | 1982         | rBV      | 209            | 123           | 0.02%           | 0.002%        |
| 35        | 7.800       | 2000          | 2009        | 2017         | rBB3     | 1238           | 2314          | 0.30%           | 0.040%        |
| 36        | 7.903       | 2027          | 2041        | 2058         | rBV      | 339133         | 618860        | 80.27%          | 10.610%       |

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGLL2ME

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\SFAMULM010522WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 8.073  | 2093 | 2094 | 2096 | rBV  | 345    | 146    | 0.02%  | 0.003% |
| 38 | 8.186  | 2116 | 2129 | 2159 | rBV  | 47682  | 123425 | 16.01% | 2.116% |
| 39 | 8.330  | 2170 | 2174 | 2176 | rBV  | 161    | 153    | 0.02%  | 0.003% |
| 40 | 8.440  | 2205 | 2208 | 2211 | rBV  | 131    | 131    | 0.02%  | 0.002% |
| 41 | 8.478  | 2211 | 2220 | 2227 | rVB4 | 912    | 1426   | 0.18%  | 0.024% |
| 42 | 8.523  | 2231 | 2234 | 2236 | rBV  | 150    | 128    | 0.02%  | 0.002% |
| 43 | 8.555  | 2236 | 2244 | 2254 | rVB2 | 12236  | 18861  | 2.45%  | 0.323% |
| 44 | 8.687  | 2262 | 2285 | 2317 | rBV  | 163525 | 474969 | 61.60% | 8.143% |
| 45 | 8.915  | 2353 | 2356 | 2359 | rBV  | 155    | 153    | 0.02%  | 0.003% |
| 46 | 8.954  | 2365 | 2368 | 2372 | rBB3 | 343    | 292    | 0.04%  | 0.005% |
| 47 | 8.976  | 2372 | 2375 | 2378 | rBV  | 145    | 145    | 0.02%  | 0.002% |
| 48 | 9.095  | 2408 | 2412 | 2414 | rBV  | 135    | 137    | 0.02%  | 0.002% |
| 49 | 9.276  | 2465 | 2468 | 2472 | rBV  | 153    | 179    | 0.02%  | 0.003% |
| 50 | 9.369  | 2493 | 2497 | 2501 | rBB  | 178    | 158    | 0.02%  | 0.003% |
| 51 | 9.427  | 2502 | 2515 | 2538 | rBV  | 184946 | 441890 | 57.31% | 7.576% |
| 52 | 9.552  | 2550 | 2554 | 2556 | rBB  | 180    | 144    | 0.02%  | 0.002% |
| 53 | 9.581  | 2560 | 2563 | 2566 | rBB2 | 297    | 238    | 0.03%  | 0.004% |
| 54 | 9.639  | 2578 | 2581 | 2585 | rVB  | 170    | 159    | 0.02%  | 0.003% |
| 55 | 9.690  | 2594 | 2597 | 2599 | rVV  | 249    | 168    | 0.02%  | 0.003% |
| 56 | 9.790  | 2625 | 2628 | 2631 | rBV  | 156    | 150    | 0.02%  | 0.003% |
| 57 | 9.825  | 2635 | 2639 | 2642 | rBB  | 165    | 158    | 0.02%  | 0.003% |
| 58 | 9.864  | 2648 | 2651 | 2655 | rBB  | 155    | 151    | 0.02%  | 0.003% |
| 59 | 9.915  | 2665 | 2667 | 2671 | rBB  | 136    | 119    | 0.02%  | 0.002% |
| 60 | 10.018 | 2696 | 2699 | 2705 | rBV  | 175    | 252    | 0.03%  | 0.004% |
| 61 | 10.259 | 2771 | 2774 | 2776 | rBV  | 138    | 120    | 0.02%  | 0.002% |
| 62 | 10.452 | 2832 | 2834 | 2839 | rVB  | 184    | 173    | 0.02%  | 0.003% |
| 63 | 10.478 | 2839 | 2842 | 2845 | rBB  | 180    | 136    | 0.02%  | 0.002% |
| 64 | 10.674 | 2895 | 2903 | 2909 | rBB3 | 1303   | 1640   | 0.21%  | 0.028% |
| 65 | 10.703 | 2910 | 2912 | 2914 | rBV  | 189    | 132    | 0.02%  | 0.002% |
| 66 | 10.774 | 2920 | 2934 | 2949 | rBV  | 276441 | 465399 | 60.36% | 7.979% |
| 67 | 10.870 | 2961 | 2964 | 2966 | rBV  | 141    | 121    | 0.02%  | 0.002% |
| 68 | 10.896 | 2967 | 2972 | 2980 | rVB3 | 697    | 897    | 0.12%  | 0.015% |
| 69 | 10.960 | 2987 | 2992 | 2993 | rBV  | 179    | 178    | 0.02%  | 0.003% |
| 70 | 11.076 | 3025 | 3028 | 3031 | rVB  | 208    | 159    | 0.02%  | 0.003% |
| 71 | 11.111 | 3034 | 3039 | 3040 | rBV2 | 760    | 495    | 0.06%  | 0.008% |
| 72 | 11.465 | 3139 | 3149 | 3152 | rBV3 | 691    | 1161   | 0.15%  | 0.020% |
| 73 | 11.584 | 3184 | 3186 | 3188 | rBV  | 181    | 128    | 0.02%  | 0.002% |
| 74 | 11.697 | 3217 | 3221 | 3226 | rVB2 | 334    | 382    | 0.05%  | 0.007% |
| 75 | 11.758 | 3237 | 3240 | 3241 | rBV  | 170    | 121    | 0.02%  | 0.002% |
| 76 | 11.822 | 3247 | 3260 | 3276 | rBV  | 267906 | 426371 | 55.30% | 7.310% |

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 Misc : 6.55g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGLL2ME

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\SFAMULM010522WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.944 | 3293 | 3298 | 3303 | rBV3 | 389    | 585    | 0.08%  | 0.010%  |
| 78  | 11.976 | 3306 | 3308 | 3315 | rVB3 | 881    | 683    | 0.09%  | 0.012%  |
| 79  | 12.156 | 3361 | 3364 | 3366 | rBV  | 192    | 137    | 0.02%  | 0.002%  |
| 80  | 12.201 | 3366 | 3378 | 3394 | rVV  | 385168 | 618323 | 80.20% | 10.601% |
| 81  | 12.327 | 3412 | 3417 | 3421 | rBV  | 142    | 127    | 0.02%  | 0.002%  |
| 82  | 12.443 | 3449 | 3453 | 3455 | rBV  | 147    | 123    | 0.02%  | 0.002%  |
| 83  | 12.774 | 3550 | 3556 | 3559 | rBV2 | 379    | 407    | 0.05%  | 0.007%  |
| 84  | 12.867 | 3579 | 3585 | 3587 | rBV  | 245    | 292    | 0.04%  | 0.005%  |
| 85  | 13.224 | 3693 | 3696 | 3702 | rVB2 | 383    | 369    | 0.05%  | 0.006%  |
| 86  | 13.661 | 3826 | 3832 | 3835 | rBV  | 140    | 131    | 0.02%  | 0.002%  |
| 87  | 13.851 | 3885 | 3891 | 3896 | rBB3 | 524    | 748    | 0.10%  | 0.013%  |
| 88  | 14.095 | 3960 | 3967 | 3975 | rVV  | 698    | 1000   | 0.13%  | 0.017%  |
| 89  | 14.333 | 4037 | 4041 | 4047 | rVB3 | 569    | 568    | 0.07%  | 0.010%  |
| 90  | 14.578 | 4111 | 4117 | 4127 | rBV  | 450    | 673    | 0.09%  | 0.012%  |
| 91  | 14.713 | 4156 | 4159 | 4168 | rBV  | 147    | 159    | 0.02%  | 0.003%  |
| 92  | 15.381 | 4364 | 4367 | 4369 | rBV2 | 213    | 136    | 0.02%  | 0.002%  |
| 93  | 15.500 | 4401 | 4404 | 4408 | rVB2 | 228    | 179    | 0.02%  | 0.003%  |
| 94  | 15.532 | 4411 | 4414 | 4420 | rBV  | 312    | 338    | 0.04%  | 0.006%  |
| 95  | 15.584 | 4427 | 4430 | 4433 | rBV  | 211    | 170    | 0.02%  | 0.003%  |
| 96  | 15.642 | 4444 | 4448 | 4452 | rBV  | 211    | 196    | 0.03%  | 0.003%  |
| 97  | 15.819 | 4500 | 4503 | 4505 | rBV  | 194    | 129    | 0.02%  | 0.002%  |
| 98  | 15.941 | 4538 | 4541 | 4545 | rBV2 | 217    | 141    | 0.02%  | 0.002%  |
| 99  | 15.963 | 4545 | 4548 | 4550 | rBV  | 218    | 150    | 0.02%  | 0.003%  |
| 100 | 16.922 | 4844 | 4846 | 4849 | rBV  | 341    | 228    | 0.03%  | 0.004%  |

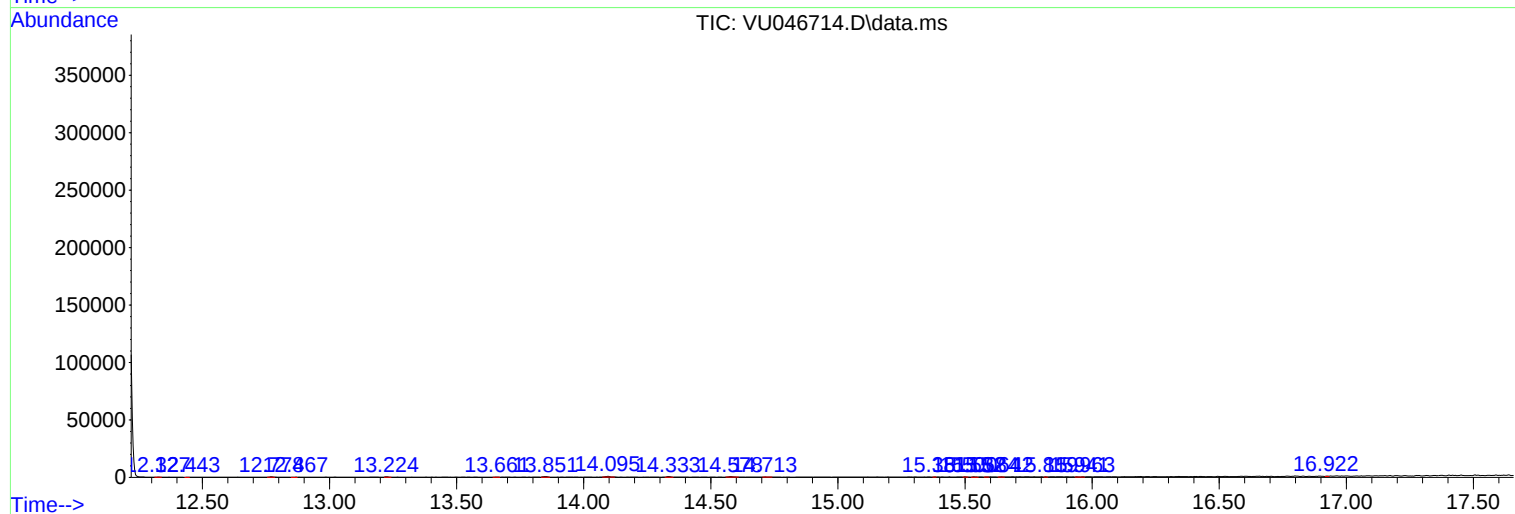
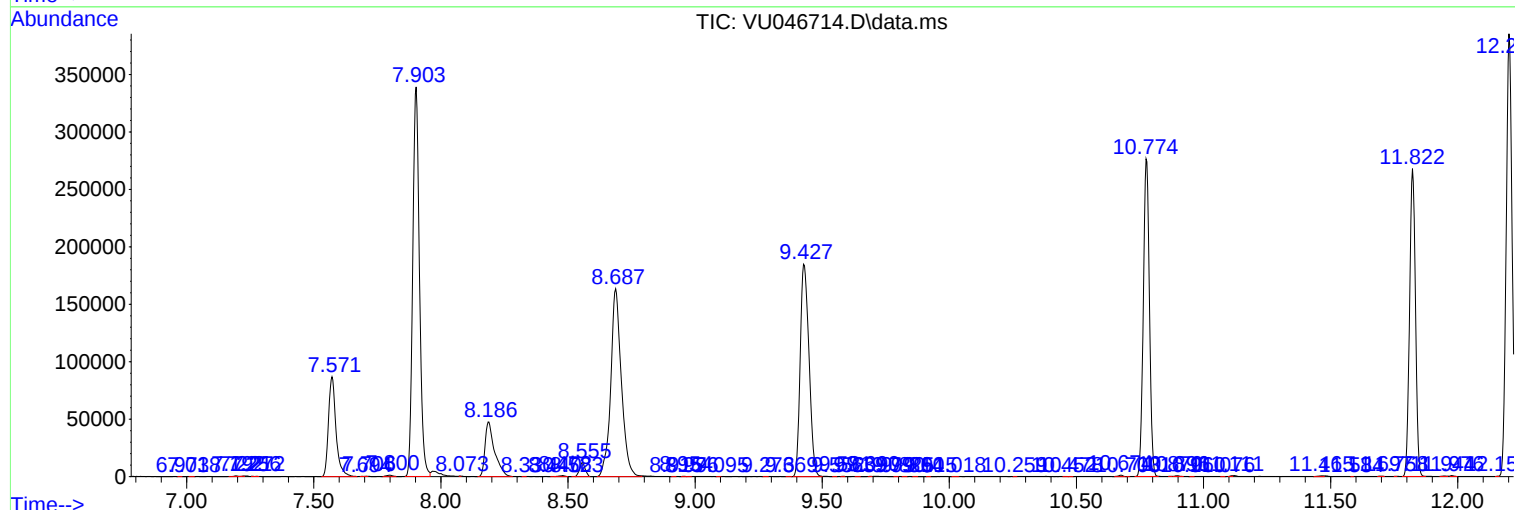
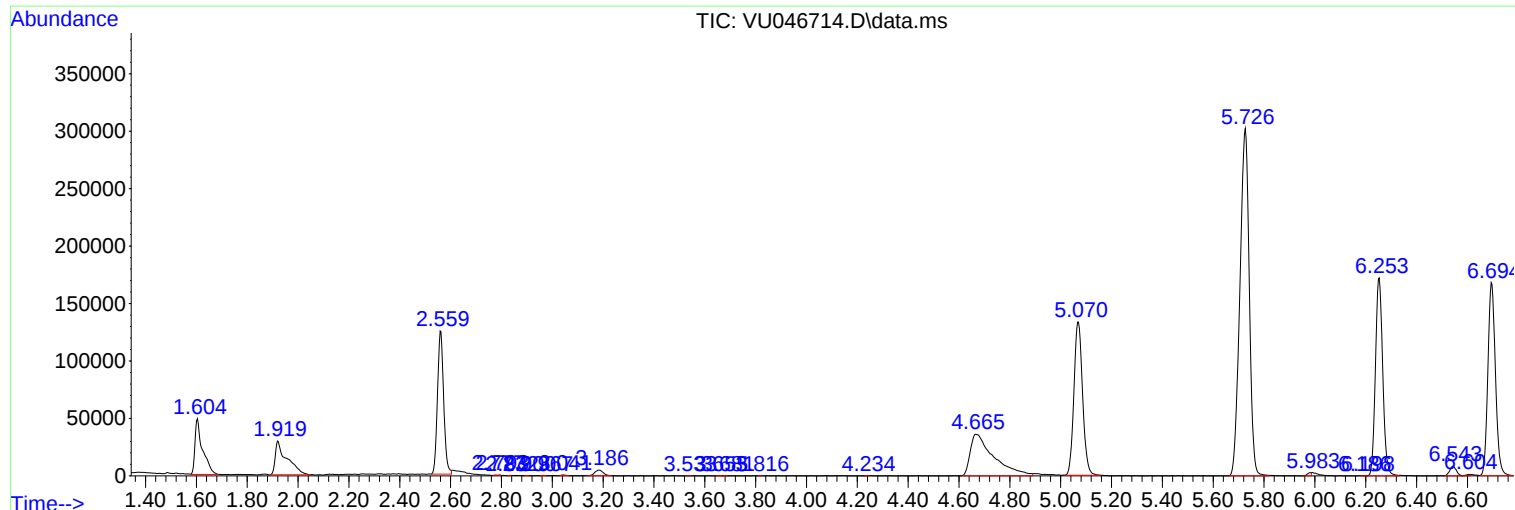
Sum of corrected areas: 5832760

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011022\  
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Sample : N1053-25ME  
Misc : 6.55g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BGLL2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM010522WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU011022\  
Data File : VU046714.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM010522WMA.M  
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No Library Search Compounds Detected

\*\*\*\*\*

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