LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122718\
Data File : VU028955.D
Acq On : 27 Dec 2018 09:30
Operator : MD/SY
Sample : VU1227MBL01
Misc : 5.00g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** VBLK46

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\SOMULM122018WMA.M
Title : VOC Analysis

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.398 | 63 | 70 | 83 | rBV | 139328 | 139699 | 14.74% | 1.928% |
| 2 | 1.675 | 149 | 156 | 173 | rVB | 106449 | 134577 | 14.20% | 1.857% |
| 3 | 2.270 | 331 | 341 | 356 | rVB | 242087 | 362413 | 38.25% | 5.001% |
| 4 | 2.437 | 390 | 393 | 396 | rBV2 | 328 | 260 | 0.03% | 0.004% |
| 5 | 2.704 | 466 | 476 | 484 | rVB | 2593 | 4386 | 0.46% | 0.061% |
| 6 | 2.832 | 507 | 516 | 517 | rBV | 941 | 1148 | 0.12% | 0.016% |
| 7 | 2.993 | 563 | 566 | 568 | rBV2 | 195 | 120 | 0.01% | 0.002% |
| 8 | 3.019 | 572 | 574 | 576 | rBV2 | 155 | 93 | 0.01% | 0.001% |
| 9 | 3.353 | 674 | 678 | 686 | rBV2 | 412 | 583 | 0.06% | 0.008% |
| 10 | 3.517 | 722 | 729 | 735 | rVB2 | 273 | 361 | 0.04% | 0.005% |
| 11 | 3.549 | 735 | 739 | 742 | rBV | 129 | 117 | 0.01% | 0.002% |
| 12 | 3.678 | 776 | 779 | 783 | rVB2 | 170 | 126 | 0.01% | 0.002% |
| 13 | 3.781 | 806 | 811 | 814 | rVB3 | 235 | 178 | 0.02% | 0.002% |
| 14 | 3.826 | 820 | 825 | 829 | rVB2 | 163 | 158 | 0.02% | 0.002% |
| 15 | 4.119 | 914 | 916 | 920 | rBV | 186 | 136 | 0.01% | 0.002% |
| 16 | 4.173 | 920 | 933 | 971 | rBV | 87265 | 229120 | 24.18% | 3.162% |
| 17 | 4.546 | 1044 | 1049 | 1051 | rBV2 | 210 | 184 | 0.02% | 0.003% |
| 18 | 4.578 | 1056 | 1059 | 1063 | rBV2 | 199 | 153 | 0.02% | 0.002% |
| 19 | 4.646 | 1063 | 1080 | 1104 | rBV | 153448 | 364986 | 38.52% | 5.036% |
| 20 | 4.877 | 1148 | 1152 | 1155 | rBV2 | 457 | 486 | 0.05% | 0.007% |
| 21 | 4.977 | 1179 | 1183 | 1185 | rBV2 | 341 | 271 | 0.03% | 0.004% |
| 22 | 5.086 | 1214 | 1217 | 1221 | rBV2 | 180 | 123 | 0.01% | 0.002% |
| 23 | 5.337 | 1271 | 1295 | 1324 | rBV2 | 328655 | 947562 | 100.00% | 13.075% |
| 24 | 5.662 | 1393 | 1396 | 1397 | rBV | 265 | 131 | 0.01% | 0.002% |
| 25 | 5.739 | 1416 | 1420 | 1421 | rBV2 | 218 | 153 | 0.02% | 0.002% |
| 26 | 5.752 | 1421 | 1424 | 1428 | rVV2 | 208 | 186 | 0.02% | 0.003% |
| 27 | 5.823 | 1444 | 1446 | 1450 | rVB | 165 | 102 | 0.01% | 0.001% |
| 28 | 5.884 | 1450 | 1465 | 1487 | rBV | 274862 | 537364 | 56.71% | 7.415% |
| 29 | 6.173 | 1547 | 1555 | 1564 | rVB4 | 1076 | 1538 | 0.16% | 0.021% |
| 30 | 6.327 | 1589 | 1603 | 1626 | rBV | 215194 | 428026 | 45.17% | 5.906% |
| 31 | 6.601 | 1685 | 1688 | 1689 | rBV | 208 | 100 | 0.01% | 0.001% |
| 32 | 6.614 | 1690 | 1692 | 1696 | rVB2 | 175 | 124 | 0.01% | 0.002% |
| 33 | 6.662 | 1705 | 1707 | 1712 | rVB | 141 | 101 | 0.01% | 0.001% |
| 34 | 6.716 | 1719 | 1724 | 1728 | rVB | 212 | 228 | 0.02% | 0.003% |

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Acq On : 27 Dec 2018 09:30
Operator : MD/SY
Sample : VU1227MBL01
Misc : 5.00g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** VBLK46

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\SOMULM122018WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 6.774 | 1735 | 1742 | 1747 | rBV2 | 244 | 321 | 0.03% | 0.004% |
| 36 | 6.813 | 1752 | 1754 | 1757 | rBV | 161 | 107 | 0.01% | 0.001% |
| 37 | 6.864 | 1763 | 1770 | 1772 | rBV2 | 436 | 591 | 0.06% | 0.008% |
| 38 | 6.951 | 1796 | 1797 | 1800 | rBV | 203 | 94 | 0.01% | 0.001% |
| 39 | 7.022 | 1813 | 1819 | 1821 | rVB2 | 293 | 234 | 0.02% | 0.003% |
| 40 | 7.035 | 1821 | 1823 | 1827 | rVB | 166 | 134 | 0.01% | 0.002% |
| 41 | 7.057 | 1827 | 1830 | 1835 | rBV | 121 | 116 | 0.01% | 0.002% |
| 42 | 7.083 | 1835 | 1838 | 1839 | rBV | 131 | 93 | 0.01% | 0.001% |
| 43 | 7.224 | 1870 | 1882 | 1910 | rVB | 130559 | 231832 | 24.47% | 3.199% |
| 44 | 7.398 | 1932 | 1936 | 1940 | rVB3 | 551 | 498 | 0.05% | 0.007% |
| 45 | 7.459 | 1951 | 1955 | 1956 | rBV | 409 | 324 | 0.03% | 0.004% |
| 46 | 7.514 | 1969 | 1972 | 1974 | rBV | 139 | 108 | 0.01% | 0.001% |
| 47 | 7.562 | 1974 | 1987 | 2008 | rBV | 439897 | 781500 | 82.47% | 10.784% |
| 48 | 7.848 | 2065 | 2076 | 2098 | rBV | 88310 | 150438 | 15.88% | 2.076% |
| 49 | 8.054 | 2137 | 2140 | 2141 | rBV | 246 | 124 | 0.01% | 0.002% |
| 50 | 8.157 | 2168 | 2172 | 2173 | rBV | 266 | 148 | 0.02% | 0.002% |
| 51 | 8.221 | 2190 | 2192 | 2193 | rBV | 313 | 108 | 0.01% | 0.001% |
| 52 | 8.269 | 2204 | 2207 | 2208 | rBV | 223 | 110 | 0.01% | 0.002% |
| 53 | 8.308 | 2208 | 2219 | 2256 | rVV | 297792 | 513050 | 54.14% | 7.080% |
| 54 | 8.620 | 2310 | 2316 | 2322 | rVB2 | 691 | 819 | 0.09% | 0.011% |
| 55 | 8.700 | 2338 | 2341 | 2346 | rVB2 | 216 | 202 | 0.02% | 0.003% |
| 56 | 8.736 | 2350 | 2352 | 2357 | rBV2 | 162 | 149 | 0.02% | 0.002% |
| 57 | 8.790 | 2367 | 2369 | 2373 | rVB | 168 | 91 | 0.01% | 0.001% |
| 58 | 8.816 | 2374 | 2377 | 2380 | rBV | 197 | 111 | 0.01% | 0.002% |
| 59 | 8.835 | 2380 | 2383 | 2386 | rBV | 170 | 154 | 0.02% | 0.002% |
| 60 | 8.900 | 2399 | 2403 | 2408 | rBV2 | 203 | 228 | 0.02% | 0.003% |
| 61 | 8.938 | 2411 | 2415 | 2419 | rVB | 223 | 199 | 0.02% | 0.003% |
| 62 | 9.086 | 2449 | 2461 | 2490 | rBV | 379279 | 637734 | 67.30% | 8.800% |
| 63 | 9.327 | 2533 | 2536 | 2537 | rBV | 168 | 101 | 0.01% | 0.001% |
| 64 | 9.376 | 2544 | 2551 | 2552 | rBV | 780 | 659 | 0.07% | 0.009% |
| 65 | 9.433 | 2562 | 2569 | 2572 | rBV2 | 144 | 140 | 0.01% | 0.002% |
| 66 | 9.469 | 2577 | 2580 | 2586 | rBV | 84 | 95 | 0.01% | 0.001% |
| 67 | 9.533 | 2598 | 2600 | 2604 | rVB2 | 182 | 132 | 0.01% | 0.002% |
| 68 | 9.742 | 2662 | 2665 | 2667 | rVB2 | 164 | 93 | 0.01% | 0.001% |
| 69 | 9.777 | 2670 | 2676 | 2678 | rBV3 | 859 | 775 | 0.08% | 0.011% |
| 70 | 9.842 | 2693 | 2696 | 2698 | rVB2 | 230 | 132 | 0.01% | 0.002% |
| 71 | 9.871 | 2698 | 2705 | 2712 | rBV | 173 | 218 | 0.02% | 0.003% |

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Operator : MD/SY
Sample : VU1227MBL01
Misc : 5.00g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** VBLK46

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\SOMULM122018WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 9.948 | 2727 | 2729 | 2735 | rVB2 | 191 | 158 | 0.02% | 0.002% |
| 73 | 9.977 | 2735 | 2738 | 2741 | rBV | 187 | 151 | 0.02% | 0.002% |
| 74 | 10.157 | 2791 | 2794 | 2795 | rBV | 476 | 261 | 0.03% | 0.004% |
| 75 | 10.234 | 2812 | 2818 | 2824 | rVB2 | 242 | 399 | 0.04% | 0.006% |
| 76 | 10.295 | 2834 | 2837 | 2840 | rVB2 | 231 | 153 | 0.02% | 0.002% |
| 77 | 10.314 | 2840 | 2843 | 2846 | rBV2 | 211 | 163 | 0.02% | 0.002% |
| 78 | 10.430 | 2866 | 2879 | 2901 | rBV | 311729 | 497783 | 52.53% | 6.869% |
| 79 | 10.610 | 2925 | 2935 | 2942 | rBV4 | 2433 | 3669 | 0.39% | 0.051% |
| 80 | 10.707 | 2963 | 2965 | 2968 | rVB | 209 | 111 | 0.01% | 0.002% |
| 81 | 10.758 | 2977 | 2981 | 2983 | rBV | 202 | 111 | 0.01% | 0.002% |
| 82 | 10.774 | 2983 | 2986 | 2988 | rVV | 173 | 103 | 0.01% | 0.001% |
| 83 | 10.797 | 2991 | 2993 | 2995 | rBV | 175 | 94 | 0.01% | 0.001% |
| 84 | 10.855 | 3009 | 3011 | 3013 | rBV | 286 | 126 | 0.01% | 0.002% |
| 85 | 11.086 | 3081 | 3083 | 3087 | rVB | 191 | 92 | 0.01% | 0.001% |
| 86 | 11.160 | 3104 | 3106 | 3113 | rVB2 | 323 | 241 | 0.03% | 0.003% |
| 87 | 11.240 | 3129 | 3131 | 3135 | rBV | 164 | 93 | 0.01% | 0.001% |
| 88 | 11.305 | 3149 | 3151 | 3155 | rVB2 | 236 | 153 | 0.02% | 0.002% |
| 89 | 11.327 | 3155 | 3158 | 3160 | rBV | 276 | 195 | 0.02% | 0.003% |
| 90 | 11.379 | 3171 | 3174 | 3178 | rBV | 173 | 151 | 0.02% | 0.002% |
| 91 | 11.420 | 3182 | 3187 | 3194 | rVB5 | 1209 | 1594 | 0.17% | 0.022% |
| 92 | 11.482 | 3194 | 3206 | 3227 | rBV | 365120 | 587833 | 62.04% | 8.112% |
| 93 | 11.636 | 3250 | 3254 | 3259 | rBV4 | 403 | 356 | 0.04% | 0.005% |
| 94 | 11.697 | 3270 | 3273 | 3278 | rBV3 | 296 | 241 | 0.03% | 0.003% |
| 95 | 11.755 | 3289 | 3291 | 3295 | rVB2 | 316 | 250 | 0.03% | 0.003% |
| 96 | 11.858 | 3310 | 3323 | 3346 | rBV | 413009 | 669116 | 70.61% | 9.233% |
| 97 | 12.070 | 3387 | 3389 | 3391 | rBV | 280 | 136 | 0.01% | 0.002% |
| 98 | 12.478 | 3507 | 3516 | 3527 | rVB2 | 3289 | 5439 | 0.57% | 0.075% |
| 99 | 12.520 | 3527 | 3529 | 3532 | rBV2 | 159 | 98 | 0.01% | 0.001% |
| 100 | 12.555 | 3534 | 3540 | 3543 | rBV2 | 291 | 342 | 0.04% | 0.005% |

Sum of corrected areas: 7246867

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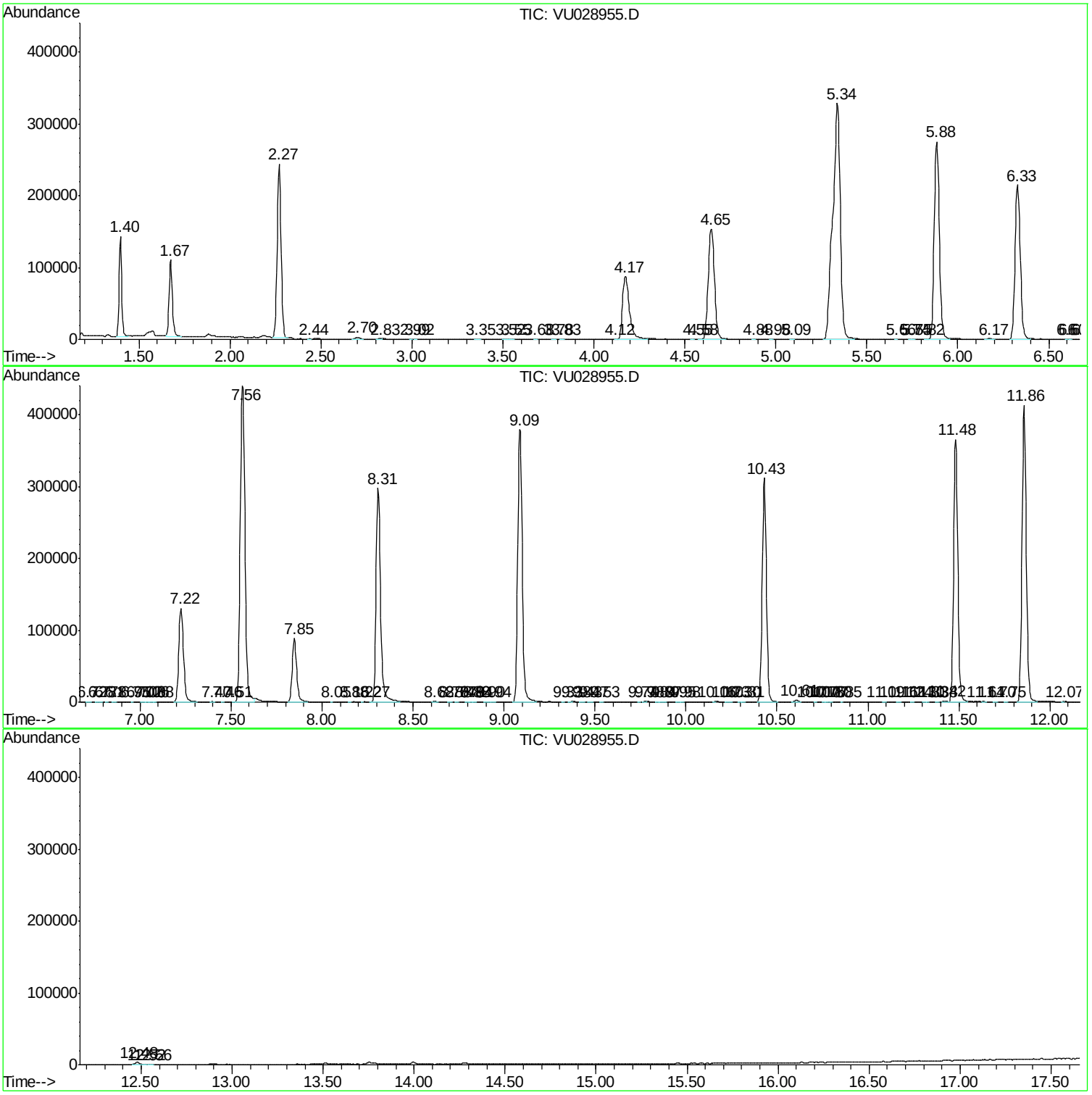
Misc : 5.00g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** VBLK46

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122718\
Data File : VU028955.D
Acq On : 27 Dec 2018 09:30
Operator : MD/SY
Sample : VU1227MBL01
Misc : 5.00g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
VBLK46

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

**********

Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122718\
Data File : VU028955.D
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ALS Vial : 3 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** VBLK46

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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