

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU111722\  
 Data File : VU051885.D  
 Acq On : 17 Nov 2022 10:42  
 Operator : JC/MD  
 Sample : VU1117MBL06  
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK018

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\SFAMULM111522WMA.M  
 Title : VOC Analysis

Signal : TIC: VU051885.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         | 1.597       | 73            | 80          | 95           | rBV      | 157999         | 180546        | 12.17%          | 1.440%        |
| 2         | 1.903       | 166           | 175         | 195          | rVB      | 143300         | 206137        | 13.89%          | 1.644%        |
| 3         | 2.302       | 296           | 299         | 303          | rBV3     | 1496           | 1104          | 0.07%           | 0.009%        |
| 4         | 2.562       | 368           | 380         | 399          | rBV      | 231141         | 380328        | 25.63%          | 3.033%        |
| 5         | 2.704       | 419           | 424         | 431          | rBV3     | 518            | 692           | 0.05%           | 0.006%        |
| 6         | 2.784       | 444           | 449         | 450          | rBV      | 1077           | 900           | 0.06%           | 0.007%        |
| 7         | 2.954       | 497           | 502         | 504          | rBV3     | 384            | 317           | 0.02%           | 0.003%        |
| 8         | 3.044       | 520           | 530         | 539          | rBV4     | 3311           | 5807          | 0.39%           | 0.046%        |
| 9         | 3.179       | 562           | 572         | 590          | rVB2     | 1911           | 4673          | 0.31%           | 0.037%        |
| 10        | 3.704       | 731           | 735         | 737          | rBV2     | 356            | 292           | 0.02%           | 0.002%        |
| 11        | 3.874       | 782           | 788         | 793          | rVB      | 338            | 335           | 0.02%           | 0.003%        |
| 12        | 4.138       | 866           | 870         | 873          | rVB      | 481            | 291           | 0.02%           | 0.002%        |
| 13        | 4.163       | 873           | 878         | 881          | rBV      | 466            | 534           | 0.04%           | 0.004%        |
| 14        | 4.199       | 886           | 889         | 893          | rVB2     | 393            | 299           | 0.02%           | 0.002%        |
| 15        | 4.228       | 893           | 898         | 903          | rVB2     | 245            | 314           | 0.02%           | 0.003%        |
| 16        | 4.295       | 915           | 919         | 929          | rVB2     | 274            | 325           | 0.02%           | 0.003%        |
| 17        | 4.552       | 994           | 999         | 1004         | rVB2     | 420            | 326           | 0.02%           | 0.003%        |
| 18        | 4.617       | 1004          | 1019        | 1057         | rBV      | 191297         | 475326        | 32.04%          | 3.790%        |
| 19        | 5.060       | 1140          | 1157        | 1183         | rBV      | 302021         | 661698        | 44.60%          | 5.276%        |
| 20        | 5.285       | 1221          | 1227        | 1229         | rBV3     | 1225           | 1276          | 0.09%           | 0.010%        |
| 21        | 5.366       | 1248          | 1252        | 1253         | rBV2     | 595            | 353           | 0.02%           | 0.003%        |
| 22        | 5.465       | 1279          | 1283        | 1285         | rBV2     | 555            | 445           | 0.03%           | 0.004%        |
| 23        | 5.507       | 1292          | 1296        | 1303         | rBV2     | 365            | 385           | 0.03%           | 0.003%        |
| 24        | 5.723       | 1342          | 1363        | 1397         | rBV2     | 527115         | 1483672       | 100.00%         | 11.830%       |
| 25        | 5.925       | 1424          | 1426        | 1431         | rVB3     | 553            | 401           | 0.03%           | 0.003%        |
| 26        | 6.012       | 1450          | 1453        | 1456         | rBV2     | 470            | 394           | 0.03%           | 0.003%        |
| 27        | 6.247       | 1511          | 1526        | 1557         | rBV      | 587088         | 1135988       | 76.57%          | 9.058%        |
| 28        | 6.401       | 1572          | 1574        | 1578         | rVB4     | 886            | 547           | 0.04%           | 0.004%        |
| 29        | 6.523       | 1606          | 1612        | 1622         | rVB5     | 2829           | 4903          | 0.33%           | 0.039%        |
| 30        | 6.687       | 1646          | 1663        | 1686         | rBV      | 375755         | 741533        | 49.98%          | 5.913%        |
| 31        | 6.803       | 1695          | 1699        | 1702         | rBV4     | 842            | 852           | 0.06%           | 0.007%        |
| 32        | 6.922       | 1732          | 1736        | 1739         | rBV2     | 393            | 415           | 0.03%           | 0.003%        |
| 33        | 6.961       | 1745          | 1748        | 1757         | rBV2     | 551            | 724           | 0.05%           | 0.006%        |
| 34        | 7.144       | 1800          | 1805        | 1809         | rBV2     | 377            | 334           | 0.02%           | 0.003%        |
| 35        | 7.182       | 1809          | 1817        | 1832         | rBV3     | 6772           | 12885         | 0.87%           | 0.103%        |
| 36        | 7.453       | 1891          | 1901        | 1907         | rBV      | 463            | 771           | 0.05%           | 0.006%        |

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Instrument :  
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 ClientSampleId :  
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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\SFAMULM111522WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 7.562  | 1922 | 1935 | 1958 | rBV  | 168999 | 301157  | 20.30% | 2.401%  |
| 38 | 7.687  | 1964 | 1974 | 1987 | rBV5 | 3956   | 8136    | 0.55%  | 0.065%  |
| 39 | 7.790  | 2002 | 2006 | 2009 | rBV3 | 486    | 444     | 0.03%  | 0.004%  |
| 40 | 7.896  | 2025 | 2039 | 2069 | rVV  | 551913 | 956240  | 64.45% | 7.625%  |
| 41 | 8.176  | 2115 | 2126 | 2146 | rBV  | 119871 | 205328  | 13.84% | 1.637%  |
| 42 | 8.253  | 2148 | 2150 | 2154 | rVB3 | 613    | 315     | 0.02%  | 0.003%  |
| 43 | 8.449  | 2207 | 2211 | 2213 | rBV2 | 500    | 341     | 0.02%  | 0.003%  |
| 44 | 8.514  | 2228 | 2231 | 2235 | rVB3 | 458    | 349     | 0.02%  | 0.003%  |
| 45 | 8.555  | 2236 | 2244 | 2252 | rBV6 | 2043   | 2963    | 0.20%  | 0.024%  |
| 46 | 8.629  | 2256 | 2267 | 2299 | rBV2 | 549225 | 1025753 | 69.14% | 8.179%  |
| 47 | 8.919  | 2355 | 2357 | 2360 | rVV3 | 468    | 291     | 0.02%  | 0.002%  |
| 48 | 8.951  | 2364 | 2367 | 2371 | rVB3 | 532    | 381     | 0.03%  | 0.003%  |
| 49 | 8.986  | 2371 | 2378 | 2381 | rBV2 | 670    | 614     | 0.04%  | 0.005%  |
| 50 | 9.112  | 2411 | 2417 | 2424 | rBV4 | 627    | 891     | 0.06%  | 0.007%  |
| 51 | 9.166  | 2429 | 2434 | 2437 | rBV3 | 290    | 318     | 0.02%  | 0.003%  |
| 52 | 9.279  | 2465 | 2469 | 2475 | rBV2 | 377    | 414     | 0.03%  | 0.003%  |
| 53 | 9.414  | 2498 | 2511 | 2547 | rBV  | 854381 | 1405813 | 94.75% | 11.210% |
| 54 | 9.642  | 2579 | 2582 | 2585 | rBV2 | 708    | 462     | 0.03%  | 0.004%  |
| 55 | 9.658  | 2585 | 2587 | 2592 | rVB2 | 606    | 388     | 0.03%  | 0.003%  |
| 56 | 9.697  | 2597 | 2599 | 2602 | rVB2 | 551    | 315     | 0.02%  | 0.003%  |
| 57 | 9.745  | 2610 | 2614 | 2621 | rVB2 | 484    | 470     | 0.03%  | 0.004%  |
| 58 | 10.009 | 2690 | 2696 | 2702 | rVB2 | 383    | 495     | 0.03%  | 0.004%  |
| 59 | 10.051 | 2702 | 2709 | 2712 | rBV  | 391    | 344     | 0.02%  | 0.003%  |
| 60 | 10.086 | 2717 | 2720 | 2722 | rBV  | 493    | 343     | 0.02%  | 0.003%  |
| 61 | 10.163 | 2739 | 2744 | 2747 | rBV  | 578    | 447     | 0.03%  | 0.004%  |
| 62 | 10.214 | 2754 | 2760 | 2763 | rBV2 | 340    | 355     | 0.02%  | 0.003%  |
| 63 | 10.237 | 2764 | 2767 | 2772 | rVB2 | 414    | 416     | 0.03%  | 0.003%  |
| 64 | 10.340 | 2796 | 2799 | 2805 | rVB2 | 423    | 319     | 0.02%  | 0.003%  |
| 65 | 10.587 | 2872 | 2876 | 2882 | rBV  | 308    | 370     | 0.02%  | 0.003%  |
| 66 | 10.649 | 2891 | 2895 | 2900 | rVB3 | 415    | 303     | 0.02%  | 0.002%  |
| 67 | 10.755 | 2914 | 2928 | 2951 | rBV  | 684165 | 1108408 | 74.71% | 8.838%  |
| 68 | 10.941 | 2979 | 2986 | 2990 | rVB3 | 608    | 641     | 0.04%  | 0.005%  |
| 69 | 10.967 | 2990 | 2994 | 2997 | rBV2 | 408    | 320     | 0.02%  | 0.003%  |
| 70 | 11.089 | 3028 | 3032 | 3034 | rBV2 | 515    | 418     | 0.03%  | 0.003%  |
| 71 | 11.282 | 3088 | 3092 | 3098 | rVB2 | 374    | 333     | 0.02%  | 0.003%  |
| 72 | 11.404 | 3127 | 3130 | 3132 | rBV2 | 719    | 399     | 0.03%  | 0.003%  |
| 73 | 11.578 | 3181 | 3184 | 3190 | rVB2 | 457    | 437     | 0.03%  | 0.003%  |
| 74 | 11.620 | 3194 | 3197 | 3201 | rBV2 | 442    | 335     | 0.02%  | 0.003%  |
| 75 | 11.742 | 3230 | 3235 | 3243 | rBV3 | 1631   | 1758    | 0.12%  | 0.014%  |
| 76 | 11.809 | 3244 | 3256 | 3278 | rBV  | 676064 | 1084679 | 73.11% | 8.649%  |

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 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMULM111522WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 12.089 | 3340 | 3343 | 3347 | rVB2 | 441    | 309     | 0.02%  | 0.002% |
| 78  | 12.192 | 3359 | 3375 | 3395 | rBV  | 670936 | 1086143 | 73.21% | 8.661% |
| 79  | 12.430 | 3446 | 3449 | 3451 | rBV3 | 442    | 294     | 0.02%  | 0.002% |
| 80  | 12.896 | 3591 | 3594 | 3598 | rVB2 | 386    | 286     | 0.02%  | 0.002% |
| 81  | 12.996 | 3623 | 3625 | 3632 | rVB5 | 561    | 505     | 0.03%  | 0.004% |
| 82  | 13.099 | 3653 | 3657 | 3659 | rBV2 | 487    | 384     | 0.03%  | 0.003% |
| 83  | 13.182 | 3680 | 3683 | 3686 | rVB2 | 549    | 355     | 0.02%  | 0.003% |
| 84  | 13.230 | 3686 | 3698 | 3704 | rBV9 | 2335   | 3829    | 0.26%  | 0.031% |
| 85  | 13.311 | 3720 | 3723 | 3726 | rBV  | 429    | 305     | 0.02%  | 0.002% |
| 86  | 13.394 | 3746 | 3749 | 3753 | rBV2 | 365    | 305     | 0.02%  | 0.002% |
| 87  | 13.452 | 3764 | 3767 | 3773 | rVB3 | 433    | 398     | 0.03%  | 0.003% |
| 88  | 13.661 | 3829 | 3832 | 3836 | rVB2 | 377    | 315     | 0.02%  | 0.003% |
| 89  | 13.848 | 3881 | 3890 | 3900 | rVB5 | 4292   | 6491    | 0.44%  | 0.052% |
| 90  | 13.964 | 3923 | 3926 | 3930 | rBV2 | 431    | 401     | 0.03%  | 0.003% |
| 91  | 14.092 | 3957 | 3966 | 3977 | rBV2 | 6550   | 11267   | 0.76%  | 0.090% |
| 92  | 14.166 | 3986 | 3989 | 3993 | rVB2 | 542    | 368     | 0.02%  | 0.003% |
| 93  | 14.333 | 4034 | 4041 | 4049 | rBV5 | 4392   | 6063    | 0.41%  | 0.048% |
| 94  | 14.562 | 4108 | 4112 | 4115 | rBV3 | 552    | 498     | 0.03%  | 0.004% |
| 95  | 14.584 | 4115 | 4119 | 4125 | rVB2 | 555    | 634     | 0.04%  | 0.005% |
| 96  | 14.816 | 4188 | 4191 | 4198 | rBV2 | 482    | 633     | 0.04%  | 0.005% |
| 97  | 15.661 | 4451 | 4454 | 4458 | rBV4 | 689    | 616     | 0.04%  | 0.005% |
| 98  | 15.761 | 4482 | 4485 | 4490 | rBV2 | 798    | 914     | 0.06%  | 0.007% |
| 99  | 15.783 | 4490 | 4492 | 4495 | rVV2 | 667    | 432     | 0.03%  | 0.003% |
| 100 | 16.031 | 4567 | 4569 | 4573 | rBV4 | 941    | 749     | 0.05%  | 0.006% |

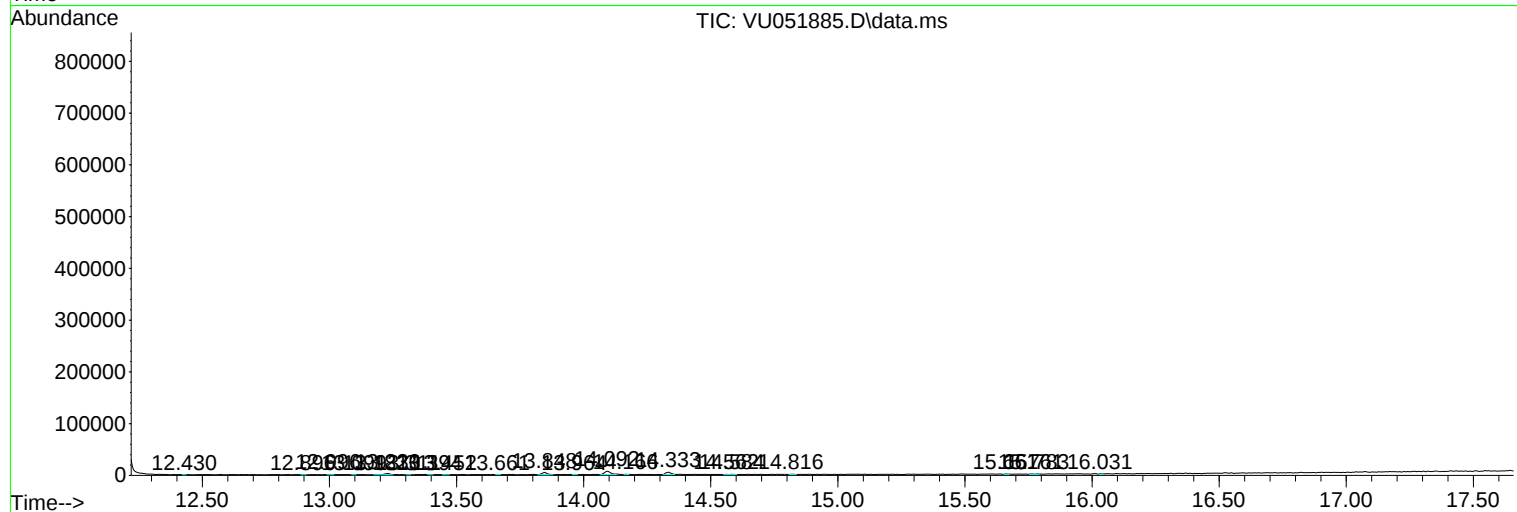
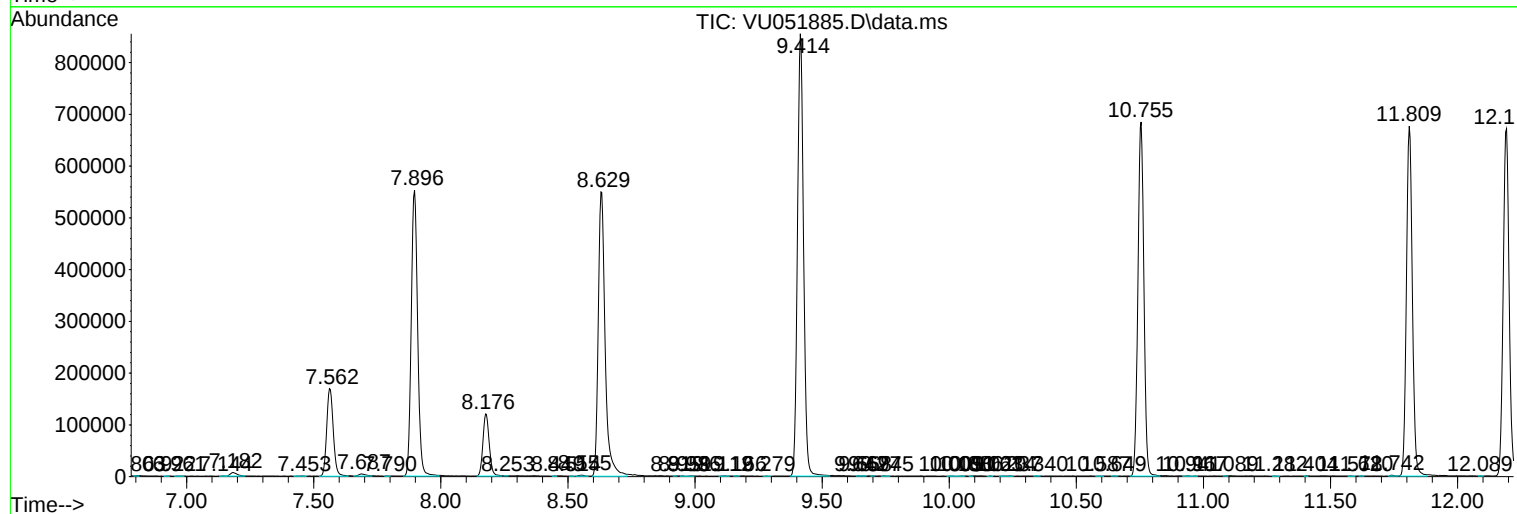
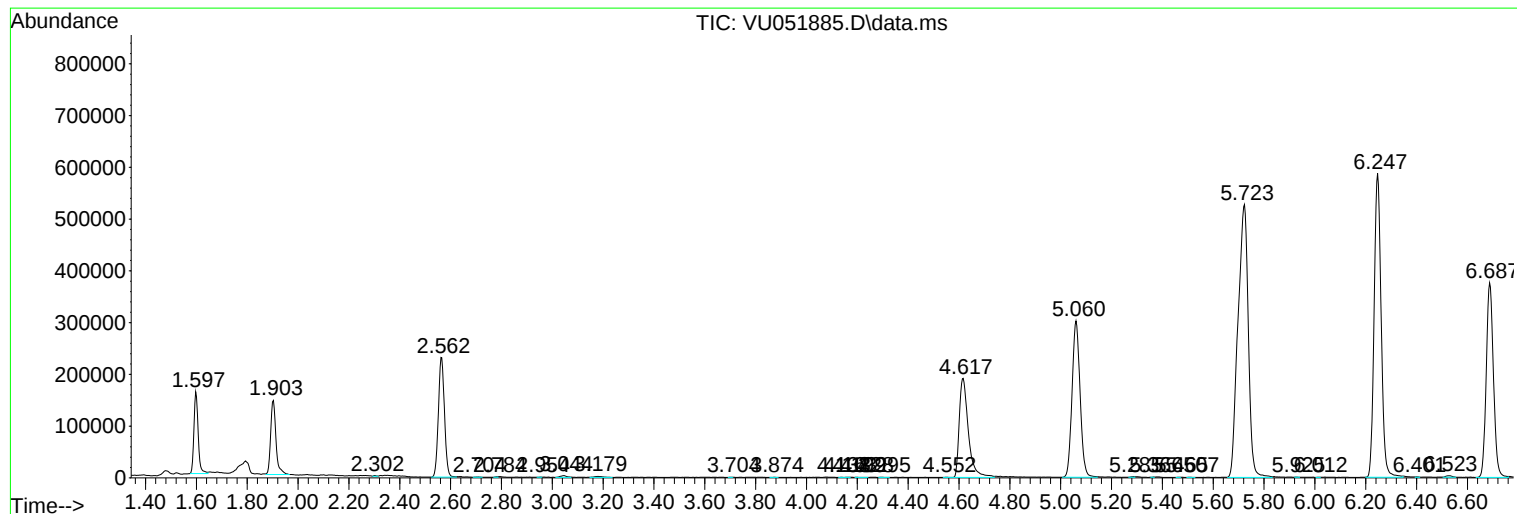
Sum of corrected areas: 12541119

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Instrument :  
MSVOA\_U  
ClientSampleId :  
VBLK018

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM111522WMA.M  
Quant Title : VOC Analysis

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



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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 |