

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU043023\  
 Data File : VU054006.D  
 Acq On : 29 Apr 2023 23:08  
 Operator : JC/MD  
 Sample : 02526-10ME  
 Misc : 5.87g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DCCF4ME

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\SFAMULM042923WMA.M

Title : VOC Analysis

Signal : TIC: VU054006.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       | 72            | 80          | 102          | rBV      | 121437         | 184635        | 13.51%          | 1.934%        |
| 2         | 1.906       | 168           | 176         | 192          | rBV      | 69446          | 134632        | 9.85%           | 1.410%        |
| 3         | 2.420       | 333           | 336         | 340          | rBV3     | 641            | 538           | 0.04%           | 0.006%        |
| 4         | 2.549       | 363           | 376         | 396          | rBV      | 293512         | 466764        | 34.15%          | 4.890%        |
| 5         | 2.642       | 398           | 405         | 419          | rBV      | 4110           | 8019          | 0.59%           | 0.084%        |
| 6         | 2.726       | 428           | 431         | 434          | rBV3     | 650            | 467           | 0.03%           | 0.005%        |
| 7         | 2.880       | 476           | 479         | 483          | rVB2     | 463            | 292           | 0.02%           | 0.003%        |
| 8         | 2.906       | 483           | 487         | 491          | rBV2     | 436            | 554           | 0.04%           | 0.006%        |
| 9         | 2.990       | 510           | 513         | 518          | rVB2     | 342            | 326           | 0.02%           | 0.003%        |
| 10        | 3.044       | 518           | 530         | 537          | rBV6     | 2662           | 5754          | 0.42%           | 0.060%        |
| 11        | 3.150       | 557           | 563         | 566          | rBV2     | 287            | 399           | 0.03%           | 0.004%        |
| 12        | 3.237       | 586           | 590         | 593          | rBV2     | 247            | 222           | 0.02%           | 0.002%        |
| 13        | 3.260       | 594           | 597         | 602          | rBV3     | 209            | 224           | 0.02%           | 0.002%        |
| 14        | 3.318       | 612           | 615         | 619          | rBV2     | 207            | 192           | 0.01%           | 0.002%        |
| 15        | 3.366       | 625           | 630         | 634          | rVB3     | 334            | 357           | 0.03%           | 0.004%        |
| 16        | 3.404       | 639           | 642         | 647          | rVB2     | 334            | 326           | 0.02%           | 0.003%        |
| 17        | 3.475       | 659           | 664         | 668          | rBV      | 469            | 418           | 0.03%           | 0.004%        |
| 18        | 3.520       | 676           | 678         | 682          | rVB      | 440            | 271           | 0.02%           | 0.003%        |
| 19        | 3.546       | 682           | 686         | 691          | rBV      | 256            | 290           | 0.02%           | 0.003%        |
| 20        | 3.649       | 711           | 718         | 723          | rBV2     | 486            | 597           | 0.04%           | 0.006%        |
| 21        | 3.671       | 723           | 725         | 727          | rBV      | 287            | 194           | 0.01%           | 0.002%        |
| 22        | 3.691       | 727           | 731         | 741          | rVV5     | 479            | 624           | 0.05%           | 0.007%        |
| 23        | 4.096       | 851           | 857         | 860          | rBV2     | 214            | 256           | 0.02%           | 0.003%        |
| 24        | 4.433       | 957           | 962         | 966          | rBV2     | 233            | 238           | 0.02%           | 0.002%        |
| 25        | 4.565       | 1000          | 1003        | 1005         | rBV      | 244            | 205           | 0.01%           | 0.002%        |
| 26        | 4.633       | 1011          | 1024        | 1069         | rBV      | 62533          | 246279        | 18.02%          | 2.580%        |
| 27        | 4.954       | 1120          | 1124        | 1125         | rBV3     | 380            | 244           | 0.02%           | 0.003%        |
| 28        | 5.054       | 1139          | 1155        | 1184         | rVV      | 227693         | 534589        | 39.11%          | 5.600%        |
| 29        | 5.208       | 1197          | 1203        | 1204         | rBV4     | 779            | 839           | 0.06%           | 0.009%        |
| 30        | 5.446       | 1272          | 1277        | 1280         | rBV2     | 226            | 232           | 0.02%           | 0.002%        |
| 31        | 5.520       | 1297          | 1300        | 1303         | rBV2     | 328            | 263           | 0.02%           | 0.003%        |
| 32        | 5.568       | 1312          | 1315        | 1320         | rBV2     | 209            | 243           | 0.02%           | 0.003%        |
| 33        | 5.716       | 1339          | 1361        | 1381         | rBV2     | 519379         | 1366823       | 100.00%         | 14.319%       |
| 34        | 5.980       | 1434          | 1443        | 1444         | rBV3     | 1572           | 1982          | 0.15%           | 0.021%        |
| 35        | 6.240       | 1510          | 1524        | 1550         | rBV      | 289106         | 568437        | 41.59%          | 5.955%        |
| 36        | 6.523       | 1603          | 1612        | 1625         | rVB4     | 4296           | 8049          | 0.59%           | 0.084%        |

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Instrument :  
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 ClientSampleId :  
 DCCF4ME

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.597  | 1625 | 1635 | 1636 | rBV2 | 2385   | 2841    | 0.21%  | 0.030%  |
| 38 | 6.684  | 1648 | 1662 | 1688 | rBV  | 313502 | 619242  | 45.31% | 6.487%  |
| 39 | 6.838  | 1708 | 1710 | 1717 | rVB2 | 337    | 308     | 0.02%  | 0.003%  |
| 40 | 7.195  | 1814 | 1821 | 1828 | rBV6 | 1591   | 2952    | 0.22%  | 0.031%  |
| 41 | 7.411  | 1883 | 1888 | 1891 | rVB2 | 250    | 226     | 0.02%  | 0.002%  |
| 42 | 7.559  | 1922 | 1934 | 1962 | rBV  | 154936 | 305986  | 22.39% | 3.206%  |
| 43 | 7.716  | 1978 | 1983 | 1985 | rVB2 | 268    | 219     | 0.02%  | 0.002%  |
| 44 | 7.835  | 2015 | 2020 | 2023 | rBV3 | 351    | 287     | 0.02%  | 0.003%  |
| 45 | 7.893  | 2023 | 2038 | 2066 | rBV  | 620056 | 1142757 | 83.61% | 11.972% |
| 46 | 8.099  | 2096 | 2102 | 2106 | rBV4 | 353    | 315     | 0.02%  | 0.003%  |
| 47 | 8.176  | 2114 | 2126 | 2154 | rVV  | 94924  | 217009  | 15.88% | 2.273%  |
| 48 | 8.462  | 2211 | 2215 | 2218 | rBV2 | 511    | 517     | 0.04%  | 0.005%  |
| 49 | 8.546  | 2232 | 2241 | 2247 | rBV7 | 1580   | 2496    | 0.18%  | 0.026%  |
| 50 | 8.658  | 2258 | 2276 | 2306 | rBV  | 274674 | 582653  | 42.63% | 6.104%  |
| 51 | 8.931  | 2359 | 2361 | 2365 | rVB2 | 544    | 314     | 0.02%  | 0.003%  |
| 52 | 9.073  | 2402 | 2405 | 2408 | rBV  | 321    | 223     | 0.02%  | 0.002%  |
| 53 | 9.202  | 2439 | 2445 | 2449 | rBV3 | 483    | 502     | 0.04%  | 0.005%  |
| 54 | 9.247  | 2455 | 2459 | 2466 | rVB2 | 224    | 244     | 0.02%  | 0.003%  |
| 55 | 9.349  | 2488 | 2491 | 2497 | rVB2 | 275    | 308     | 0.02%  | 0.003%  |
| 56 | 9.417  | 2498 | 2512 | 2534 | rBV  | 351767 | 700314  | 51.24% | 7.337%  |
| 57 | 9.568  | 2552 | 2559 | 2562 | rBV3 | 605    | 592     | 0.04%  | 0.006%  |
| 58 | 9.645  | 2578 | 2583 | 2588 | rBV2 | 280    | 398     | 0.03%  | 0.004%  |
| 59 | 9.690  | 2590 | 2597 | 2599 | rBV3 | 1511   | 1573    | 0.12%  | 0.016%  |
| 60 | 9.890  | 2656 | 2659 | 2667 | rVV2 | 254    | 295     | 0.02%  | 0.003%  |
| 61 | 9.938  | 2671 | 2674 | 2680 | rVB  | 198    | 242     | 0.02%  | 0.003%  |
| 62 | 10.038 | 2701 | 2705 | 2708 | rBV2 | 249    | 240     | 0.02%  | 0.003%  |
| 63 | 10.066 | 2712 | 2714 | 2720 | rVB2 | 229    | 197     | 0.01%  | 0.002%  |
| 64 | 10.099 | 2720 | 2724 | 2726 | rBV2 | 553    | 431     | 0.03%  | 0.005%  |
| 65 | 10.115 | 2727 | 2729 | 2731 | rBV3 | 310    | 187     | 0.01%  | 0.002%  |
| 66 | 10.478 | 2839 | 2842 | 2849 | rBV2 | 324    | 350     | 0.03%  | 0.004%  |
| 67 | 10.648 | 2892 | 2895 | 2898 | rVB2 | 530    | 382     | 0.03%  | 0.004%  |
| 68 | 10.668 | 2898 | 2901 | 2905 | rVB2 | 399    | 272     | 0.02%  | 0.003%  |
| 69 | 10.700 | 2905 | 2911 | 2912 | rBV  | 267    | 233     | 0.02%  | 0.002%  |
| 70 | 10.758 | 2916 | 2929 | 2950 | rBV  | 415205 | 662369  | 48.46% | 6.939%  |
| 71 | 10.922 | 2977 | 2980 | 2986 | rVB2 | 282    | 253     | 0.02%  | 0.003%  |
| 72 | 11.012 | 3002 | 3008 | 3010 | rBV  | 202    | 227     | 0.02%  | 0.002%  |
| 73 | 11.108 | 3035 | 3038 | 3039 | rBV2 | 586    | 335     | 0.02%  | 0.004%  |
| 74 | 11.153 | 3048 | 3052 | 3057 | rBV2 | 304    | 334     | 0.02%  | 0.003%  |
| 75 | 11.192 | 3058 | 3064 | 3068 | rVV  | 345    | 331     | 0.02%  | 0.003%  |
| 76 | 11.304 | 3095 | 3099 | 3102 | rBV2 | 447    | 350     | 0.03%  | 0.004%  |

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 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DCCF4ME

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\SFAMULM042923WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |         |
|-----|--------|------|------|------|------|--------|---------|--------|---------|
| 77  | 11.365 | 3114 | 3118 | 3124 | rVV4 | 719    | 860     | 0.06%  | 0.009%  |
| 78  | 11.394 | 3124 | 3127 | 3135 | rVB3 | 470    | 495     | 0.04%  | 0.005%  |
| 79  | 11.751 | 3233 | 3238 | 3243 | rBV4 | 547    | 562     | 0.04%  | 0.006%  |
| 80  | 11.812 | 3244 | 3257 | 3277 | rBV  | 437897 | 696703  | 50.97% | 7.299%  |
| 81  | 12.121 | 3350 | 3353 | 3357 | rBV2 | 214    | 213     | 0.02%  | 0.002%  |
| 82  | 12.192 | 3362 | 3375 | 3396 | rBV  | 651216 | 1056607 | 77.30% | 11.069% |
| 83  | 12.401 | 3435 | 3440 | 3443 | rBV  | 291    | 306     | 0.02%  | 0.003%  |
| 84  | 12.619 | 3504 | 3508 | 3512 | rBV2 | 226    | 231     | 0.02%  | 0.002%  |
| 85  | 12.722 | 3537 | 3540 | 3545 | rBV2 | 345    | 268     | 0.02%  | 0.003%  |
| 86  | 12.873 | 3585 | 3587 | 3592 | rVB2 | 300    | 200     | 0.01%  | 0.002%  |
| 87  | 12.970 | 3614 | 3617 | 3620 | rBV2 | 306    | 238     | 0.02%  | 0.002%  |
| 88  | 13.095 | 3653 | 3656 | 3659 | rBV2 | 270    | 230     | 0.02%  | 0.002%  |
| 89  | 13.230 | 3693 | 3698 | 3699 | rBV2 | 584    | 513     | 0.04%  | 0.005%  |
| 90  | 13.375 | 3740 | 3743 | 3744 | rBV  | 318    | 187     | 0.01%  | 0.002%  |
| 91  | 13.542 | 3792 | 3795 | 3801 | rBV2 | 310    | 287     | 0.02%  | 0.003%  |
| 92  | 13.571 | 3801 | 3804 | 3809 | rVV3 | 291    | 343     | 0.03%  | 0.004%  |
| 93  | 13.626 | 3818 | 3821 | 3824 | rVB  | 335    | 204     | 0.01%  | 0.002%  |
| 94  | 13.706 | 3843 | 3846 | 3850 | rBV2 | 267    | 218     | 0.02%  | 0.002%  |
| 95  | 13.841 | 3885 | 3888 | 3893 | rBV3 | 873    | 939     | 0.07%  | 0.010%  |
| 96  | 13.992 | 3933 | 3935 | 3938 | rBV2 | 332    | 264     | 0.02%  | 0.003%  |
| 97  | 14.092 | 3962 | 3966 | 3967 | rBV  | 479    | 335     | 0.02%  | 0.004%  |
| 98  | 14.635 | 4129 | 4135 | 4136 | rBV2 | 440    | 437     | 0.03%  | 0.005%  |
| 99  | 14.870 | 4205 | 4208 | 4210 | rBV  | 287    | 209     | 0.02%  | 0.002%  |
| 100 | 15.449 | 4385 | 4388 | 4393 | rBV3 | 587    | 488     | 0.04%  | 0.005%  |

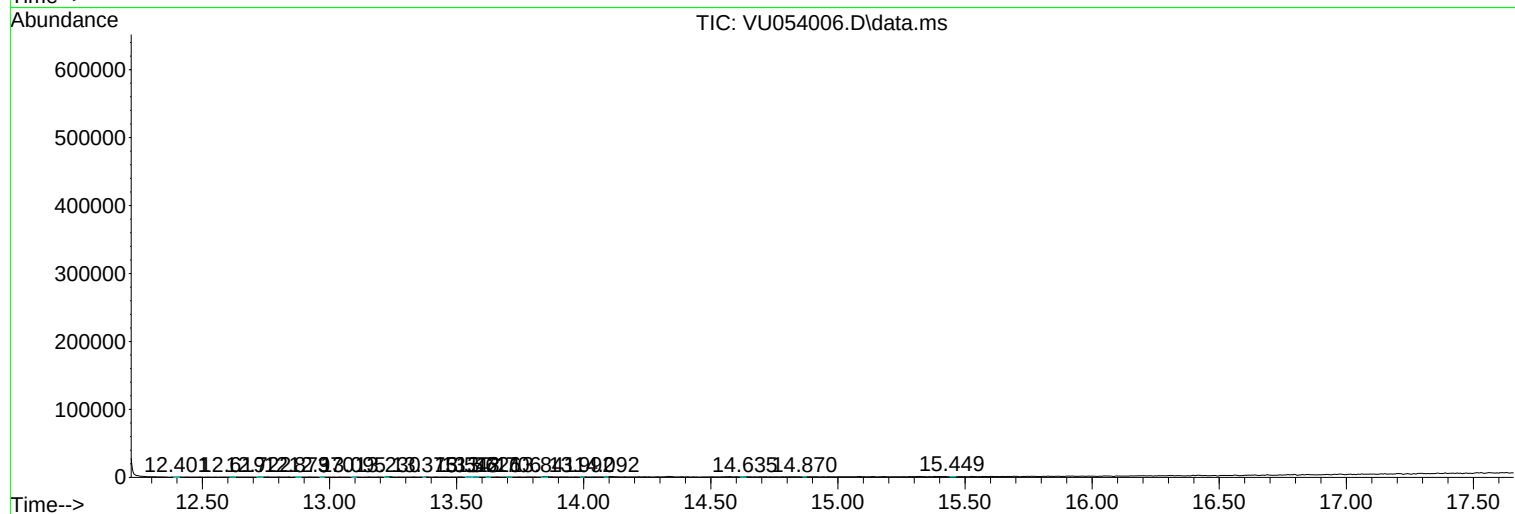
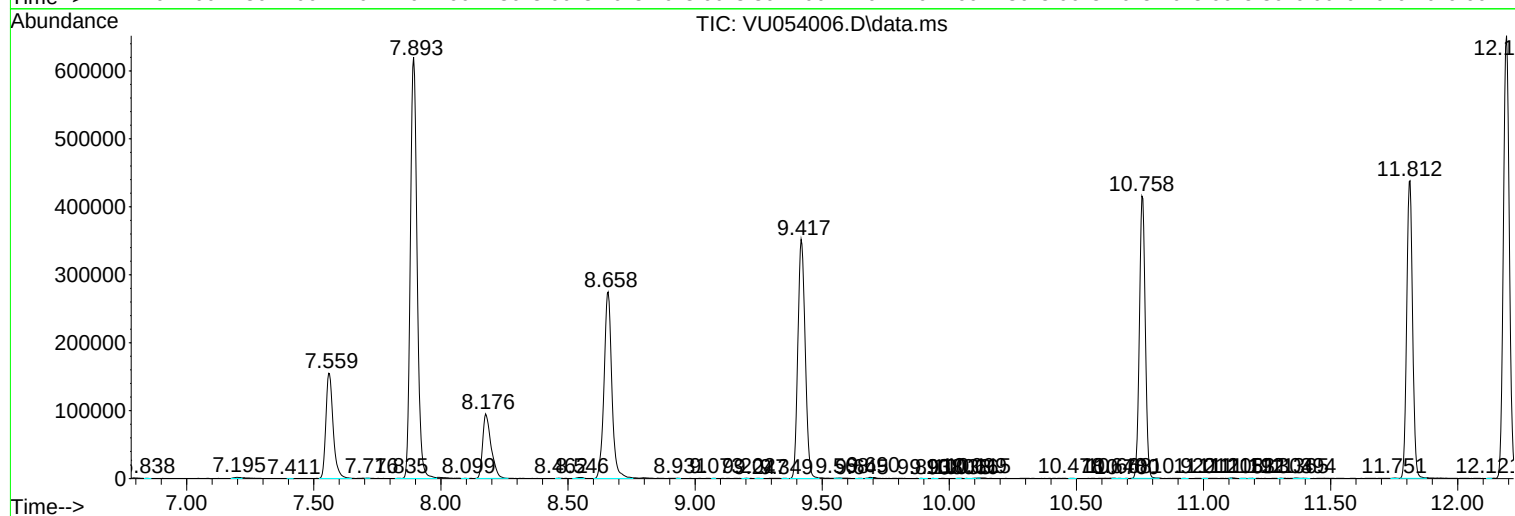
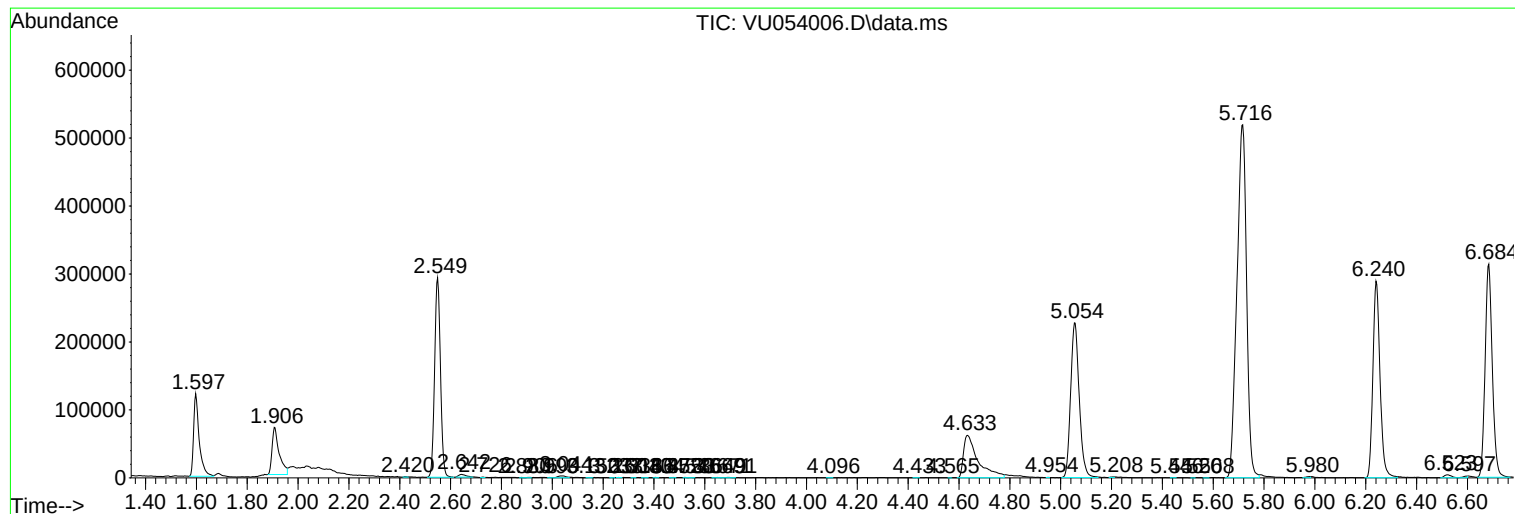
Sum of corrected areas: 9545415

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Instrument :  
MSVOA\_U  
ClientSampleId :  
DCCF4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU043023\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM042923WMA.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 |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|