

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV101022\  
 Data File : VV028501.D  
 Acq On : 10 Oct 2022 17:44  
 Operator : SY/MD  
 Sample : N4991-11ME  
 Misc : 4.66g/5.0ml/100ul/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0BL4ME

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\_V\Method\SFAMVLM100722WMA.M  
 Title : VOC Analysis

Signal : TIC: VV028501.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         | 1.304       | 76            | 82          | 105          | rVB      | 87175          | 120351        | 9.04%           | 1.205%        |
| 2         | 1.564       | 158           | 163         | 184          | rVB      | 61371          | 95336         | 7.16%           | 0.954%        |
| 3         | 2.092       | 320           | 327         | 340          | rVB      | 276595         | 388152        | 29.16%          | 3.885%        |
| 4         | 2.934       | 586           | 589         | 593          | rBV4     | 784            | 687           | 0.05%           | 0.007%        |
| 5         | 2.986       | 602           | 605         | 607          | rBV2     | 488            | 378           | 0.03%           | 0.004%        |
| 6         | 3.159       | 656           | 659         | 661          | rBV2     | 312            | 171           | 0.01%           | 0.002%        |
| 7         | 3.195       | 666           | 670         | 673          | rBV4     | 421            | 354           | 0.03%           | 0.004%        |
| 8         | 3.240       | 681           | 684         | 688          | rBV3     | 447            | 297           | 0.02%           | 0.003%        |
| 9         | 3.272       | 690           | 694         | 697          | rVB3     | 447            | 237           | 0.02%           | 0.002%        |
| 10        | 3.301       | 698           | 703         | 707          | rBV4     | 441            | 454           | 0.03%           | 0.005%        |
| 11        | 3.352       | 715           | 719         | 721          | rBV3     | 379            | 328           | 0.02%           | 0.003%        |
| 12        | 3.487       | 757           | 761         | 763          | rBV3     | 452            | 314           | 0.02%           | 0.003%        |
| 13        | 3.532       | 772           | 775         | 778          | rBV2     | 298            | 216           | 0.02%           | 0.002%        |
| 14        | 3.625       | 798           | 804         | 805          | rBV2     | 242            | 220           | 0.02%           | 0.002%        |
| 15        | 3.674       | 817           | 819         | 821          | rVV3     | 306            | 183           | 0.01%           | 0.002%        |
| 16        | 3.709       | 829           | 830         | 834          | rVB      | 494            | 181           | 0.01%           | 0.002%        |
| 17        | 3.732       | 834           | 837         | 841          | rBV3     | 202            | 208           | 0.02%           | 0.002%        |
| 18        | 3.789       | 851           | 855         | 858          | rVB2     | 330            | 266           | 0.02%           | 0.003%        |
| 19        | 3.818       | 862           | 864         | 868          | rVB2     | 345            | 182           | 0.01%           | 0.002%        |
| 20        | 3.851       | 870           | 874         | 876          | rBV      | 191            | 173           | 0.01%           | 0.002%        |
| 21        | 3.870       | 878           | 880         | 881          | rVB      | 492            | 166           | 0.01%           | 0.002%        |
| 22        | 3.918       | 884           | 895         | 897          | rBV2     | 30631          | 50063         | 3.76%           | 0.501%        |
| 23        | 4.770       | 1158          | 1160        | 1163         | rBV2     | 646            | 337           | 0.03%           | 0.003%        |
| 24        | 4.834       | 1176          | 1180        | 1183         | rBV3     | 406            | 361           | 0.03%           | 0.004%        |
| 25        | 4.873       | 1188          | 1192        | 1193         | rBV2     | 754            | 443           | 0.03%           | 0.004%        |
| 26        | 4.969       | 1219          | 1222        | 1226         | rBV      | 380            | 397           | 0.03%           | 0.004%        |
| 27        | 5.037       | 1227          | 1243        | 1271         | rBV2     | 490151         | 1239929       | 93.15%          | 12.410%       |
| 28        | 5.609       | 1409          | 1421        | 1457         | rBV      | 490871         | 1031539       | 77.49%          | 10.324%       |
| 29        | 5.912       | 1505          | 1515        | 1530         | rBV      | 4257           | 10405         | 0.78%           | 0.104%        |
| 30        | 6.063       | 1550          | 1562        | 1589         | rBV      | 269341         | 562970        | 42.29%          | 5.635%        |
| 31        | 6.400       | 1664          | 1667        | 1670         | rVB2     | 746            | 360           | 0.03%           | 0.004%        |
| 32        | 6.449       | 1678          | 1682        | 1683         | rBV2     | 578            | 376           | 0.03%           | 0.004%        |
| 33        | 6.474       | 1688          | 1690        | 1693         | rBV      | 337            | 167           | 0.01%           | 0.002%        |
| 34        | 6.519       | 1701          | 1704        | 1706         | rBV      | 336            | 170           | 0.01%           | 0.002%        |
| 35        | 6.577       | 1718          | 1722        | 1724         | rBV4     | 715            | 446           | 0.03%           | 0.004%        |
| 36        | 6.638       | 1732          | 1741        | 1744         | rBV4     | 3134           | 4139          | 0.31%           | 0.041%        |

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 Misc : 4.66g/5.0ml/100ul/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 COBL4ME

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\_V\Method\SFAMVLM100722WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 6.892  | 1816 | 1820 | 1821 | rBV3 | 383    | 234     | 0.02%  | 0.002%  |
| 38 | 6.918  | 1821 | 1828 | 1831 | rBV5 | 1803   | 1989    | 0.15%  | 0.020%  |
| 39 | 6.982  | 1837 | 1848 | 1870 | rBV  | 164341 | 324658  | 24.39% | 3.249%  |
| 40 | 7.307  | 1938 | 1949 | 1973 | rBV  | 576072 | 1046673 | 78.63% | 10.476% |
| 41 | 7.619  | 2036 | 2046 | 2082 | rBV2 | 107883 | 222781  | 16.74% | 2.230%  |
| 42 | 7.780  | 2093 | 2096 | 2097 | rBV2 | 982    | 485     | 0.04%  | 0.005%  |
| 43 | 7.928  | 2137 | 2142 | 2144 | rBV  | 690    | 658     | 0.05%  | 0.007%  |
| 44 | 7.973  | 2148 | 2156 | 2175 | rVB9 | 7032   | 12526   | 0.94%  | 0.125%  |
| 45 | 8.053  | 2175 | 2181 | 2184 | rBV2 | 483    | 515     | 0.04%  | 0.005%  |
| 46 | 8.114  | 2184 | 2200 | 2235 | rBV  | 187872 | 620304  | 46.60% | 6.208%  |
| 47 | 8.519  | 2324 | 2326 | 2330 | rBV2 | 402    | 289     | 0.02%  | 0.003%  |
| 48 | 8.548  | 2333 | 2335 | 2337 | rBV2 | 464    | 225     | 0.02%  | 0.002%  |
| 49 | 8.580  | 2343 | 2345 | 2347 | rVB3 | 586    | 182     | 0.01%  | 0.002%  |
| 50 | 8.654  | 2366 | 2368 | 2370 | rBV2 | 803    | 414     | 0.03%  | 0.004%  |
| 51 | 8.773  | 2400 | 2405 | 2407 | rBV3 | 951    | 913     | 0.07%  | 0.009%  |
| 52 | 8.847  | 2416 | 2428 | 2454 | rBV  | 699830 | 1269851 | 95.39% | 12.710% |
| 53 | 9.156  | 2514 | 2524 | 2531 | rBV6 | 2798   | 4497    | 0.34%  | 0.045%  |
| 54 | 9.243  | 2549 | 2551 | 2554 | rVB2 | 686    | 333     | 0.03%  | 0.003%  |
| 55 | 9.268  | 2554 | 2559 | 2560 | rBV2 | 562    | 328     | 0.02%  | 0.003%  |
| 56 | 9.297  | 2565 | 2568 | 2571 | rBV2 | 569    | 311     | 0.02%  | 0.003%  |
| 57 | 9.358  | 2585 | 2587 | 2591 | rVB3 | 649    | 337     | 0.03%  | 0.003%  |
| 58 | 9.378  | 2591 | 2593 | 2598 | rVB2 | 357    | 241     | 0.02%  | 0.002%  |
| 59 | 9.407  | 2598 | 2602 | 2603 | rBV2 | 505    | 309     | 0.02%  | 0.003%  |
| 60 | 9.429  | 2604 | 2609 | 2613 | rVB5 | 673    | 605     | 0.05%  | 0.006%  |
| 61 | 9.545  | 2643 | 2645 | 2647 | rBV3 | 783    | 418     | 0.03%  | 0.004%  |
| 62 | 9.632  | 2669 | 2672 | 2678 | rVB2 | 520    | 414     | 0.03%  | 0.004%  |
| 63 | 9.661  | 2678 | 2681 | 2686 | rBV4 | 490    | 515     | 0.04%  | 0.005%  |
| 64 | 9.702  | 2686 | 2694 | 2698 | rBV6 | 951    | 1339    | 0.10%  | 0.013%  |
| 65 | 9.760  | 2705 | 2712 | 2717 | rBV5 | 930    | 1363    | 0.10%  | 0.014%  |
| 66 | 9.841  | 2735 | 2737 | 2744 | rVB3 | 983    | 666     | 0.05%  | 0.007%  |
| 67 | 9.924  | 2760 | 2763 | 2765 | rBV3 | 783    | 564     | 0.04%  | 0.006%  |
| 68 | 9.995  | 2782 | 2785 | 2786 | rBV2 | 664    | 385     | 0.03%  | 0.004%  |
| 69 | 10.217 | 2840 | 2854 | 2877 | rVV  | 352004 | 613941  | 46.12% | 6.145%  |
| 70 | 10.352 | 2891 | 2896 | 2897 | rBV2 | 545    | 511     | 0.04%  | 0.005%  |
| 71 | 10.445 | 2921 | 2925 | 2927 | rBV3 | 578    | 429     | 0.03%  | 0.004%  |
| 72 | 10.477 | 2928 | 2935 | 2938 | rBV5 | 1681   | 2203    | 0.17%  | 0.022%  |
| 73 | 10.661 | 2989 | 2992 | 2995 | rBV3 | 305    | 223     | 0.02%  | 0.002%  |
| 74 | 10.709 | 3004 | 3007 | 3010 | rBV3 | 523    | 395     | 0.03%  | 0.004%  |
| 75 | 10.799 | 3032 | 3035 | 3038 | rBV3 | 588    | 408     | 0.03%  | 0.004%  |
| 76 | 10.985 | 3090 | 3093 | 3094 | rBV2 | 430    | 230     | 0.02%  | 0.002%  |

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 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0BL4ME

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\_V\Method\SFAMVLM100722WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |         |         |
|-----|--------|------|------|------|------|--------|---------|---------|---------|
| 77  | 11.091 | 3122 | 3126 | 3127 | rBV2 | 609    | 431     | 0.03%   | 0.004%  |
| 78  | 11.143 | 3140 | 3142 | 3146 | rVB3 | 1061   | 670     | 0.05%   | 0.007%  |
| 79  | 11.243 | 3161 | 3173 | 3195 | rBV  | 832212 | 1331162 | 100.00% | 13.323% |
| 80  | 11.487 | 3246 | 3249 | 3251 | rBV3 | 479    | 358     | 0.03%   | 0.004%  |
| 81  | 11.513 | 3254 | 3257 | 3259 | rBV3 | 572    | 280     | 0.02%   | 0.003%  |
| 82  | 11.542 | 3262 | 3266 | 3267 | rBV2 | 574    | 357     | 0.03%   | 0.004%  |
| 83  | 11.570 | 3272 | 3275 | 3278 | rBV4 | 765    | 532     | 0.04%   | 0.005%  |
| 84  | 11.619 | 3278 | 3290 | 3314 | rBV  | 620775 | 997216  | 74.91%  | 9.981%  |
| 85  | 11.783 | 3331 | 3341 | 3350 | rVB7 | 3215   | 5136    | 0.39%   | 0.051%  |
| 86  | 11.866 | 3363 | 3367 | 3370 | rVB4 | 633    | 471     | 0.04%   | 0.005%  |
| 87  | 11.937 | 3387 | 3389 | 3392 | rVB2 | 661    | 353     | 0.03%   | 0.004%  |
| 88  | 12.204 | 3470 | 3472 | 3474 | rBV  | 366    | 187     | 0.01%   | 0.002%  |
| 89  | 12.281 | 3492 | 3496 | 3499 | rBV4 | 446    | 302     | 0.02%   | 0.003%  |
| 90  | 12.493 | 3560 | 3562 | 3568 | rVB5 | 598    | 430     | 0.03%   | 0.004%  |
| 91  | 12.558 | 3579 | 3582 | 3584 | rBV3 | 516    | 302     | 0.02%   | 0.003%  |
| 92  | 12.577 | 3585 | 3588 | 3590 | rBV2 | 701    | 457     | 0.03%   | 0.005%  |
| 93  | 12.693 | 3620 | 3624 | 3626 | rBV2 | 501    | 316     | 0.02%   | 0.003%  |
| 94  | 13.156 | 3766 | 3768 | 3773 | rVB2 | 501    | 268     | 0.02%   | 0.003%  |
| 95  | 13.297 | 3810 | 3812 | 3814 | rBV2 | 478    | 248     | 0.02%   | 0.002%  |
| 96  | 13.355 | 3827 | 3830 | 3831 | rBV  | 560    | 301     | 0.02%   | 0.003%  |
| 97  | 13.503 | 3867 | 3876 | 3888 | rBV4 | 3311   | 5708    | 0.43%   | 0.057%  |
| 98  | 13.612 | 3908 | 3910 | 3912 | rBV  | 416    | 226     | 0.02%   | 0.002%  |
| 99  | 13.689 | 3931 | 3934 | 3938 | rVB2 | 824    | 536     | 0.04%   | 0.005%  |
| 100 | 13.815 | 3971 | 3973 | 3976 | rBV  | 455    | 375     | 0.03%   | 0.004%  |

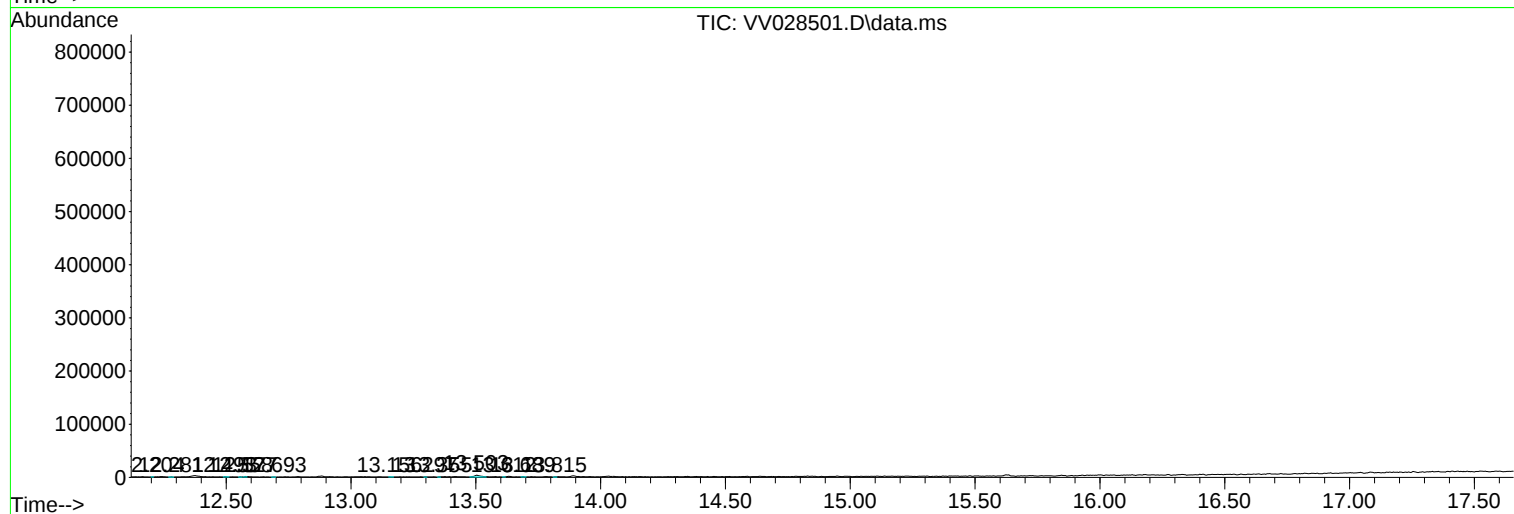
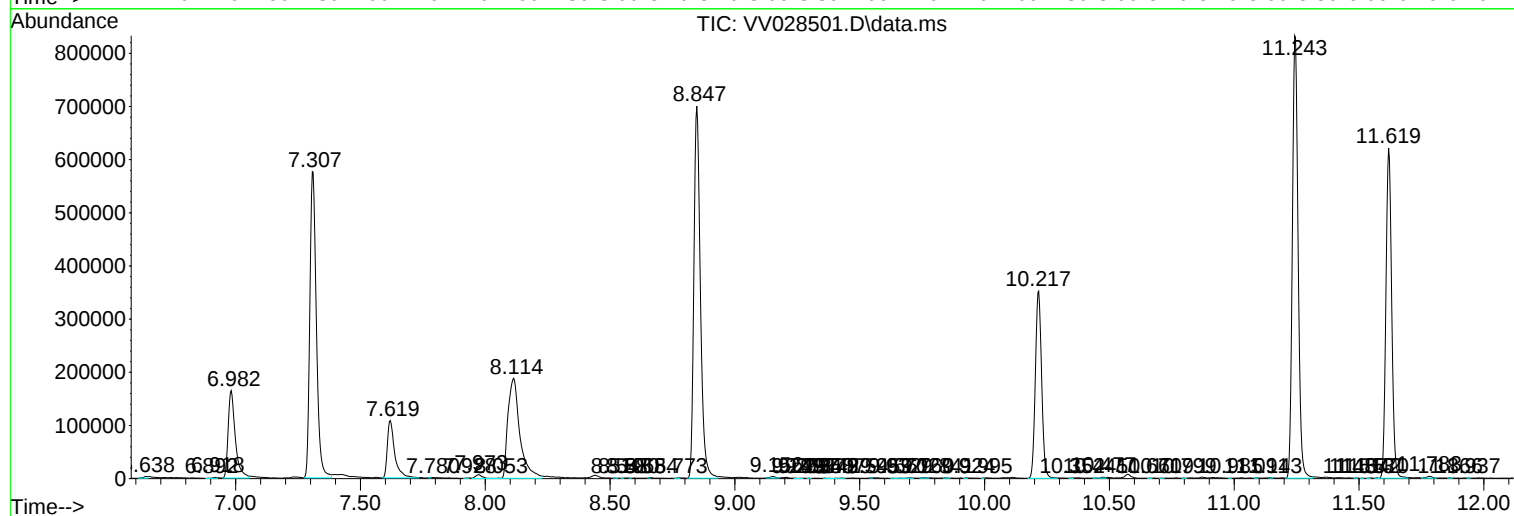
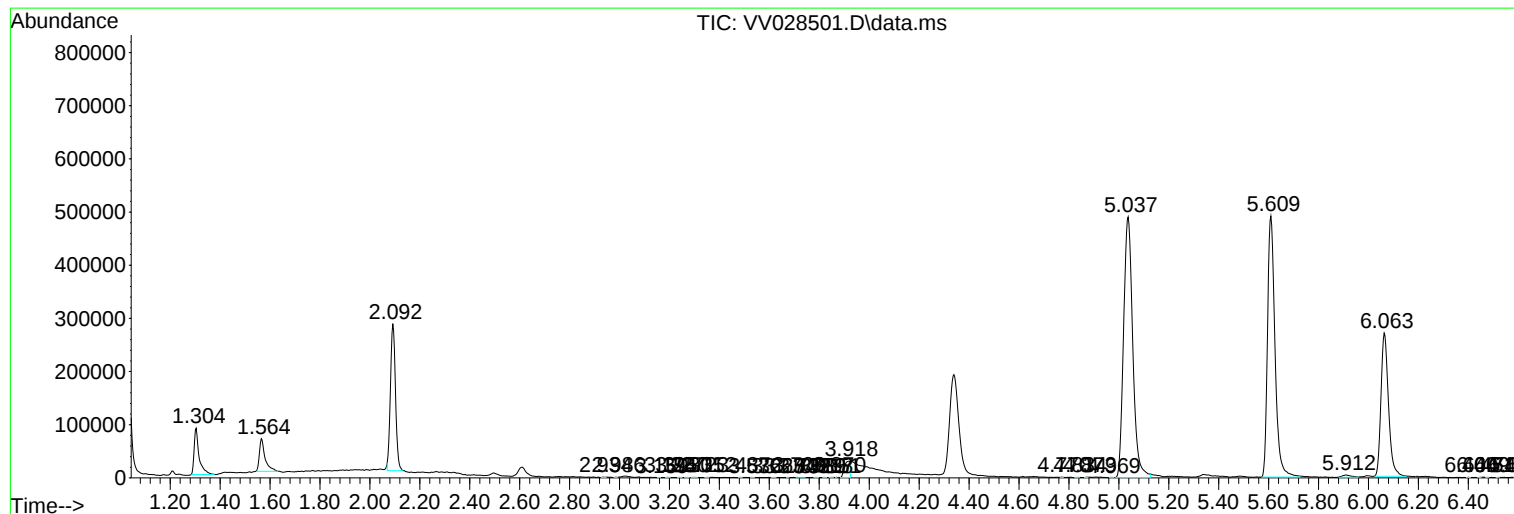
Sum of corrected areas: 9991240

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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
C0BL4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM100722WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV101022\  
Data File : VV028501.D  
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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 |