

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU122021\  
 Data File : VU046513.D  
 Acq On : 20 Dec 2021 16:30  
 Operator : SY/MD  
 Sample : M5150-25  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GBBY1

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\SFAMULM112921WMA.M  
 Title : VOC Analysis

Signal : TIC: VU046513.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 1.475    | 38         | 42       | 47        | rBV   | 1977        | 1926       | 0.01%        | 0.008%     |
| 2      | 1.604    | 74         | 82       | 102       | rBV   | 67185       | 82475      | 0.42%        | 0.327%     |
| 3      | 1.864    | 159        | 163      | 170       | rVB2  | 854         | 1031       | 0.01%        | 0.004%     |
| 4      | 1.919    | 171        | 180      | 200       | rBV   | 44433       | 66571      | 0.34%        | 0.264%     |
| 5      | 2.144    | 244        | 250      | 259       | rVB3  | 1593        | 2064       | 0.01%        | 0.008%     |
| 6      | 2.578    | 372        | 385      | 400       | rBV2  | 147419      | 285825     | 1.46%        | 1.133%     |
| 7      | 2.800    | 446        | 454      | 463       | rVB2  | 2319        | 3512       | 0.02%        | 0.014%     |
| 8      | 2.957    | 500        | 503      | 506       | rBV2  | 409         | 388        | 0.00%        | 0.002%     |
| 9      | 2.970    | 506        | 507      | 512       | rVV   | 473         | 340        | 0.00%        | 0.001%     |
| 10     | 2.989    | 512        | 513      | 517       | rVB   | 274         | 150        | 0.00%        | 0.001%     |
| 11     | 3.051    | 526        | 532      | 542       | rBB4  | 1178        | 2003       | 0.01%        | 0.008%     |
| 12     | 3.192    | 568        | 576      | 579       | rBV2  | 751         | 1119       | 0.01%        | 0.004%     |
| 13     | 3.260    | 594        | 597      | 601       | rBB   | 137         | 139        | 0.00%        | 0.001%     |
| 14     | 3.359    | 616        | 628      | 642       | rVB2  | 10289       | 19646      | 0.10%        | 0.078%     |
| 15     | 3.700    | 729        | 734      | 737       | rBB   | 173         | 190        | 0.00%        | 0.001%     |
| 16     | 3.854    | 780        | 782      | 783       | rBV   | 324         | 159        | 0.00%        | 0.001%     |
| 17     | 3.874    | 783        | 788      | 799       | rVB2  | 705         | 1254       | 0.01%        | 0.005%     |
| 18     | 4.671    | 1012       | 1036     | 1085      | rBV   | 669366      | 1582629    | 8.11%        | 6.275%     |
| 19     | 4.973    | 1126       | 1130     | 1136      | rBV3  | 469         | 695        | 0.00%        | 0.003%     |
| 20     | 5.067    | 1144       | 1159     | 1188      | rBB   | 92270       | 204045     | 1.05%        | 0.809%     |
| 21     | 5.314    | 1231       | 1236     | 1237      | rBV   | 970         | 759        | 0.00%        | 0.003%     |
| 22     | 5.391    | 1250       | 1260     | 1272      | rBB5  | 4725        | 9584       | 0.05%        | 0.038%     |
| 23     | 5.530    | 1296       | 1303     | 1311      | rBB2  | 714         | 1353       | 0.01%        | 0.005%     |
| 24     | 5.729    | 1344       | 1365     | 1395      | rBV2  | 185447      | 508708     | 2.61%        | 2.017%     |
| 25     | 5.870    | 1407       | 1409     | 1412      | rVB   | 171         | 116        | 0.00%        | 0.000%     |
| 26     | 6.253    | 1514       | 1528     | 1552      | rBV   | 157626      | 298123     | 1.53%        | 1.182%     |
| 27     | 6.549    | 1602       | 1620     | 1654      | rBV   | 10286977    | 19517286   | 100.00%      | 77.384%    |
| 28     | 6.694    | 1655       | 1665     | 1681      | rVB   | 116971      | 232136     | 1.19%        | 0.920%     |
| 29     | 6.938    | 1738       | 1741     | 1743      | rBV   | 250         | 178        | 0.00%        | 0.001%     |
| 30     | 7.089    | 1785       | 1788     | 1789      | rBV   | 399         | 207        | 0.00%        | 0.001%     |
| 31     | 7.520    | 1920       | 1922     | 1925      | rBV   | 130         | 119        | 0.00%        | 0.000%     |
| 32     | 7.568    | 1925       | 1937     | 1957      | rVB   | 65332       | 113992     | 0.58%        | 0.452%     |
| 33     | 7.796    | 2001       | 2008     | 2017      | rBB3  | 2110        | 3347       | 0.02%        | 0.013%     |
| 34     | 7.899    | 2027       | 2040     | 2054      | rBV   | 235004      | 396970     | 2.03%        | 1.574%     |
| 35     | 7.970    | 2056       | 2062     | 2076      | rVB   | 5906        | 9779       | 0.05%        | 0.039%     |
| 36     | 8.179    | 2116       | 2127     | 2146      | rBB   | 44875       | 77701      | 0.40%        | 0.308%     |

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 MSVOA\_U  
 ClientSampleId :  
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Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |       |        |
|----|--------|------|------|------|------|--------|--------|-------|--------|
| 37 | 8.266  | 2151 | 2154 | 2157 | rBB2 | 208    | 131    | 0.00% | 0.001% |
| 38 | 8.401  | 2189 | 2196 | 2204 | rBB3 | 3712   | 5241   | 0.03% | 0.021% |
| 39 | 8.468  | 2210 | 2217 | 2218 | rBV2 | 1125   | 1004   | 0.01% | 0.004% |
| 40 | 8.555  | 2234 | 2244 | 2254 | rVB2 | 16621  | 26940  | 0.14% | 0.107% |
| 41 | 8.636  | 2257 | 2269 | 2295 | rBV  | 151618 | 257762 | 1.32% | 1.022% |
| 42 | 8.809  | 2318 | 2323 | 2329 | rVV2 | 749    | 989    | 0.01% | 0.004% |
| 43 | 8.925  | 2353 | 2359 | 2368 | rBB3 | 879    | 1384   | 0.01% | 0.005% |
| 44 | 9.227  | 2450 | 2453 | 2456 | rVB  | 161    | 135    | 0.00% | 0.001% |
| 45 | 9.417  | 2500 | 2512 | 2531 | rBV  | 235349 | 386473 | 1.98% | 1.532% |
| 46 | 9.571  | 2552 | 2560 | 2570 | rBB  | 3228   | 4681   | 0.02% | 0.019% |
| 47 | 9.693  | 2590 | 2598 | 2608 | rVB3 | 3328   | 4811   | 0.02% | 0.019% |
| 48 | 9.796  | 2626 | 2630 | 2633 | rBB  | 139    | 136    | 0.00% | 0.001% |
| 49 | 10.005 | 2693 | 2695 | 2698 | rBV  | 147    | 120    | 0.00% | 0.000% |
| 50 | 10.108 | 2717 | 2727 | 2738 | rBB6 | 4204   | 7891   | 0.04% | 0.031% |
| 51 | 10.169 | 2744 | 2746 | 2751 | rBB  | 190    | 178    | 0.00% | 0.001% |
| 52 | 10.218 | 2758 | 2761 | 2764 | rBV  | 134    | 136    | 0.00% | 0.001% |
| 53 | 10.279 | 2776 | 2780 | 2781 | rBV  | 300    | 195    | 0.00% | 0.001% |
| 54 | 10.295 | 2781 | 2785 | 2790 | rVB  | 843    | 813    | 0.00% | 0.003% |
| 55 | 10.488 | 2836 | 2845 | 2855 | rVB2 | 2859   | 4291   | 0.02% | 0.017% |
| 56 | 10.568 | 2866 | 2870 | 2871 | rBV  | 258    | 134    | 0.00% | 0.001% |
| 57 | 10.578 | 2871 | 2873 | 2876 | rVV  | 255    | 191    | 0.00% | 0.001% |
| 58 | 10.671 | 2895 | 2902 | 2908 | rVB3 | 1083   | 1098   | 0.01% | 0.004% |
| 59 | 10.758 | 2917 | 2929 | 2945 | rBV  | 162887 | 261104 | 1.34% | 1.035% |
| 60 | 10.822 | 2945 | 2949 | 2960 | rVB4 | 1761   | 2333   | 0.01% | 0.009% |
| 61 | 10.890 | 2961 | 2970 | 2977 | rBV2 | 1711   | 2431   | 0.01% | 0.010% |
| 62 | 10.986 | 2997 | 3000 | 3003 | rBB  | 174    | 138    | 0.00% | 0.001% |
| 63 | 11.008 | 3004 | 3007 | 3009 | rBV  | 156    | 129    | 0.00% | 0.001% |
| 64 | 11.025 | 3009 | 3012 | 3019 | rVB  | 216    | 267    | 0.00% | 0.001% |
| 65 | 11.092 | 3024 | 3033 | 3040 | rVV4 | 2316   | 3407   | 0.02% | 0.014% |
| 66 | 11.237 | 3075 | 3078 | 3082 | rVB  | 180    | 172    | 0.00% | 0.001% |
| 67 | 11.291 | 3092 | 3095 | 3099 | rBV  | 160    | 184    | 0.00% | 0.001% |
| 68 | 11.471 | 3141 | 3151 | 3159 | rBV3 | 3441   | 5328   | 0.03% | 0.021% |
| 69 | 11.536 | 3169 | 3171 | 3174 | rVB  | 181    | 121    | 0.00% | 0.000% |
| 70 | 11.555 | 3174 | 3177 | 3180 | rBV  | 160    | 161    | 0.00% | 0.001% |
| 71 | 11.693 | 3216 | 3220 | 3221 | rBV  | 200    | 132    | 0.00% | 0.001% |
| 72 | 11.745 | 3229 | 3236 | 3244 | rBV3 | 3583   | 4994   | 0.03% | 0.020% |
| 73 | 11.812 | 3245 | 3257 | 3275 | rBV  | 253224 | 399835 | 2.05% | 1.585% |
| 74 | 11.973 | 3303 | 3307 | 3314 | rVB2 | 563    | 588    | 0.00% | 0.002% |
| 75 | 12.070 | 3334 | 3337 | 3342 | rVB2 | 345    | 303    | 0.00% | 0.001% |
| 76 | 12.192 | 3363 | 3375 | 3391 | rBV  | 225235 | 373117 | 1.91% | 1.479% |

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Integration Parameters: LSCINT.P

Integrator: RTE  
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 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 12.282 | 3396 | 3403 | 3408 | rBV  | 188  | 371  | 0.00% | 0.001% |
| 78  | 12.590 | 3496 | 3499 | 3500 | rBV  | 202  | 138  | 0.00% | 0.001% |
| 79  | 12.742 | 3542 | 3546 | 3550 | rBV  | 211  | 256  | 0.00% | 0.001% |
| 80  | 12.767 | 3550 | 3554 | 3562 | rVV3 | 511  | 793  | 0.00% | 0.003% |
| 81  | 12.999 | 3620 | 3626 | 3632 | rBV4 | 758  | 1062 | 0.01% | 0.004% |
| 82  | 13.111 | 3658 | 3661 | 3669 | rVB  | 301  | 385  | 0.00% | 0.002% |
| 83  | 13.147 | 3669 | 3672 | 3674 | rBV  | 217  | 173  | 0.00% | 0.001% |
| 84  | 13.221 | 3687 | 3695 | 3704 | rVB3 | 4402 | 6142 | 0.03% | 0.024% |
| 85  | 13.841 | 3881 | 3888 | 3898 | rBB2 | 4539 | 6579 | 0.03% | 0.026% |
| 86  | 14.089 | 3955 | 3965 | 3978 | rVV2 | 5963 | 9009 | 0.05% | 0.036% |
| 87  | 14.330 | 4032 | 4040 | 4050 | rBV3 | 5429 | 7514 | 0.04% | 0.030% |
| 88  | 15.381 | 4364 | 4367 | 4372 | rVB2 | 183  | 151  | 0.00% | 0.001% |
| 89  | 15.452 | 4385 | 4389 | 4392 | rVV2 | 203  | 180  | 0.00% | 0.001% |
| 90  | 15.558 | 4418 | 4422 | 4423 | rBV  | 203  | 132  | 0.00% | 0.001% |
| 91  | 15.571 | 4423 | 4426 | 4430 | rVB2 | 202  | 181  | 0.00% | 0.001% |
| 92  | 15.626 | 4438 | 4443 | 4445 | rBV2 | 158  | 134  | 0.00% | 0.001% |
| 93  | 15.661 | 4450 | 4454 | 4456 | rBV  | 180  | 163  | 0.00% | 0.001% |
| 94  | 15.712 | 4465 | 4470 | 4472 | rBV  | 156  | 179  | 0.00% | 0.001% |
| 95  | 15.848 | 4509 | 4512 | 4516 | rBV  | 298  | 285  | 0.00% | 0.001% |
| 96  | 16.056 | 4575 | 4577 | 4578 | rBV  | 297  | 166  | 0.00% | 0.001% |
| 97  | 16.256 | 4636 | 4639 | 4641 | rBV  | 174  | 116  | 0.00% | 0.000% |
| 98  | 16.346 | 4664 | 4667 | 4670 | rBV2 | 205  | 127  | 0.00% | 0.001% |
| 99  | 16.793 | 4802 | 4806 | 4809 | rBV  | 319  | 285  | 0.00% | 0.001% |
| 100 | 17.523 | 5030 | 5033 | 5038 | rBV4 | 598  | 704  | 0.00% | 0.003% |

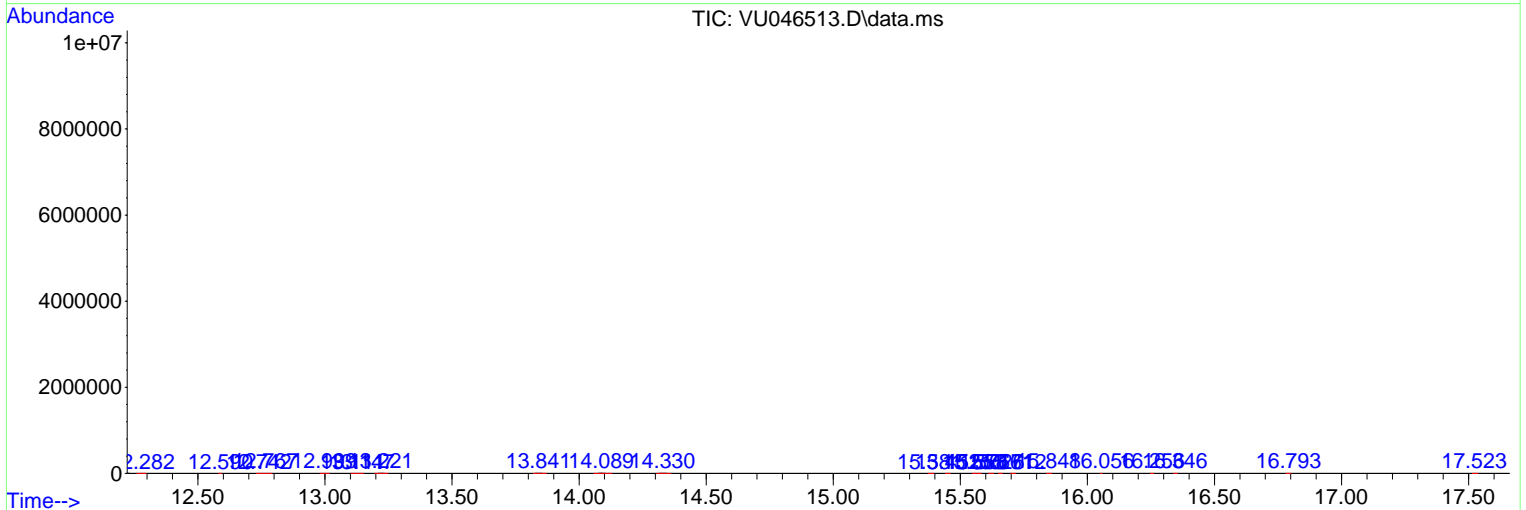
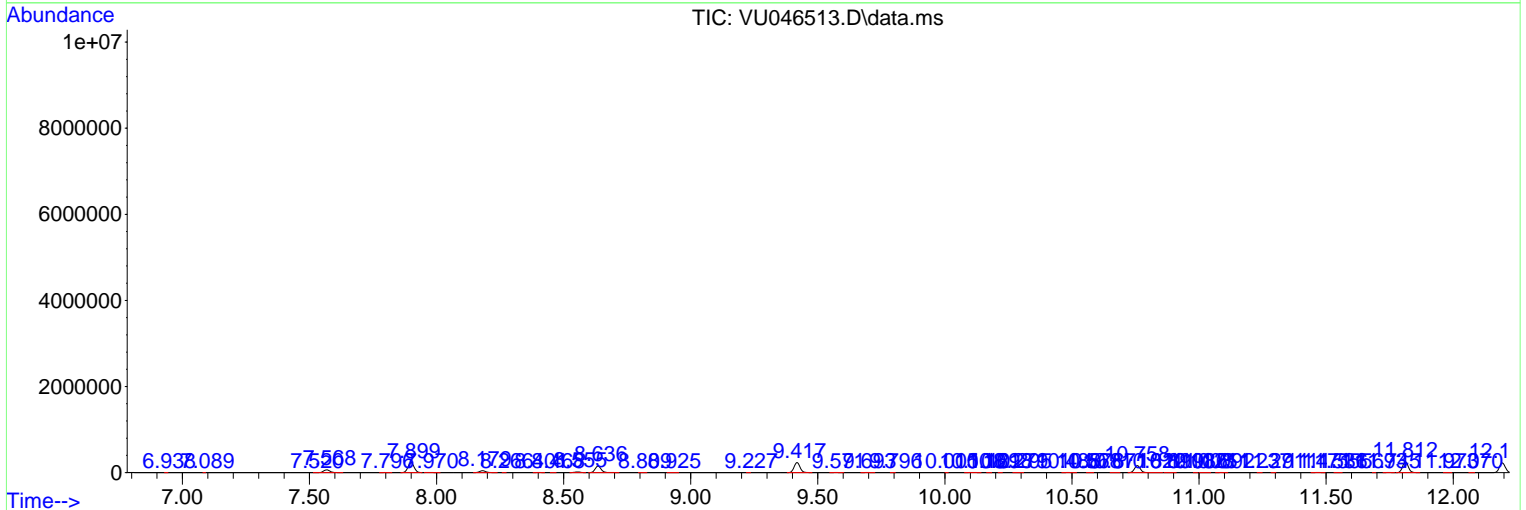
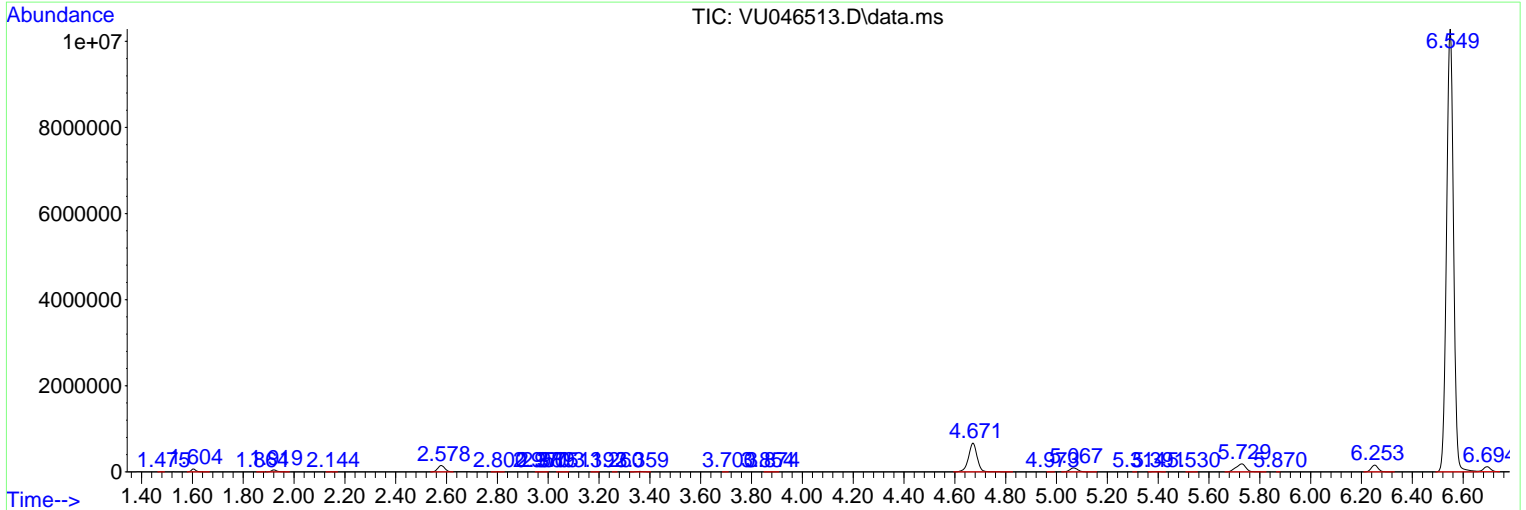
Sum of corrected areas: 25221222

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
 Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU122021\  
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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

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