

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX081722\  
 Data File : VX030654.D  
 Acq On : 17 Aug 2022 12:21  
 Operator : JC/MD  
 Sample : VX0817MBL01  
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK688

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\_X\Method\SFAMXML080422WMA.M

Title : VOC Analysis

Signal : TIC: VX030654.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         | 1.367       | 43            | 46          | 61           | rVB      | 164666         | 171888        | 13.11%          | 1.756%        |
| 2         | 1.666       | 91            | 95          | 105          | rVB      | 115281         | 147950        | 11.28%          | 1.511%        |
| 3         | 2.239       | 187           | 189         | 191          | rBV2     | 613            | 538           | 0.04%           | 0.005%        |
| 4         | 2.306       | 194           | 200         | 211          | rBV      | 292161         | 452140        | 34.47%          | 4.619%        |
| 5         | 2.514       | 231           | 234         | 237          | rVB      | 1945           | 2159          | 0.16%           | 0.022%        |
| 6         | 2.672       | 257           | 260         | 261          | rBV2     | 561            | 544           | 0.04%           | 0.006%        |
| 7         | 2.697       | 262           | 264         | 265          | rBV      | 654            | 330           | 0.03%           | 0.003%        |
| 8         | 2.788       | 273           | 279         | 285          | rBV2     | 4888           | 9310          | 0.71%           | 0.095%        |
| 9         | 2.855       | 288           | 290         | 293          | rVB2     | 532            | 468           | 0.04%           | 0.005%        |
| 10        | 2.892       | 293           | 296         | 298          | rBV2     | 312            | 454           | 0.03%           | 0.005%        |
| 11        | 3.050       | 317           | 322         | 323          | rBV2     | 429            | 574           | 0.04%           | 0.006%        |
| 12        | 3.093       | 323           | 329         | 335          | rBV6     | 1028           | 2537          | 0.19%           | 0.026%        |
| 13        | 3.251       | 353           | 355         | 358          | rVB2     | 448            | 417           | 0.03%           | 0.004%        |
| 14        | 3.294       | 361           | 362         | 364          | rBV      | 711            | 454           | 0.03%           | 0.005%        |
| 15        | 3.483       | 391           | 393         | 395          | rVB2     | 601            | 484           | 0.04%           | 0.005%        |
| 16        | 3.507       | 395           | 397         | 401          | rBV2     | 319            | 443           | 0.03%           | 0.005%        |
| 17        | 3.580       | 407           | 409         | 412          | rVB      | 323            | 385           | 0.03%           | 0.004%        |
| 18        | 3.623       | 414           | 416         | 421          | rVV2     | 377            | 456           | 0.03%           | 0.005%        |
| 19        | 4.007       | 477           | 479         | 483          | rVB2     | 494            | 451           | 0.03%           | 0.005%        |
| 20        | 4.251       | 515           | 519         | 521          | rBV2     | 366            | 452           | 0.03%           | 0.005%        |
| 21        | 4.464       | 545           | 554         | 571          | rVV      | 110967         | 319142        | 24.33%          | 3.260%        |
| 22        | 5.056       | 638           | 651         | 671          | rBV      | 168563         | 529833        | 40.40%          | 5.413%        |
| 23        | 5.391       | 699           | 706         | 710          | rBV4     | 1799           | 4999          | 0.38%           | 0.051%        |
| 24        | 5.489       | 720           | 722         | 725          | rVB      | 411            | 418           | 0.03%           | 0.004%        |
| 25        | 5.550       | 726           | 732         | 738          | rBV4     | 2585           | 5679          | 0.43%           | 0.058%        |
| 26        | 5.665       | 747           | 751         | 752          | rBV      | 427            | 518           | 0.04%           | 0.005%        |
| 27        | 5.793       | 770           | 772         | 775          | rVB2     | 515            | 428           | 0.03%           | 0.004%        |
| 28        | 5.854       | 780           | 782         | 787          | rVB2     | 653            | 608           | 0.05%           | 0.006%        |
| 29        | 5.970       | 787           | 801         | 822          | rBV3     | 442296         | 1311556       | 100.00%         | 13.398%       |
| 30        | 6.306       | 853           | 856         | 858          | rVB3     | 486            | 478           | 0.04%           | 0.005%        |
| 31        | 6.336       | 858           | 861         | 862          | rBV2     | 470            | 591           | 0.05%           | 0.006%        |
| 32        | 6.763       | 921           | 931         | 944          | rBV      | 296311         | 719266        | 54.84%          | 7.348%        |
| 33        | 6.934       | 957           | 959         | 962          | rBV3     | 535            | 570           | 0.04%           | 0.006%        |
| 34        | 7.062       | 977           | 980         | 981          | rBV      | 491            | 477           | 0.04%           | 0.005%        |
| 35        | 7.110       | 981           | 988         | 997          | rVB3     | 10915          | 25806         | 1.97%           | 0.264%        |
| 36        | 7.202       | 1000          | 1003        | 1004         | rBV2     | 339            | 346           | 0.03%           | 0.004%        |

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 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK688

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\_X\Method\SFAMXML080422WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 37 | 7.220  | 1004 | 1006 | 1007 | rBV  | 438    | 336     | 0.03%  | 0.003%  |
| 38 | 7.312  | 1011 | 1021 | 1032 | rBV  | 277564 | 598029  | 45.60% | 6.109%  |
| 39 | 7.537  | 1056 | 1058 | 1061 | rVB2 | 550    | 520     | 0.04%  | 0.005%  |
| 40 | 7.561  | 1061 | 1062 | 1067 | rVB2 | 525    | 626     | 0.05%  | 0.006%  |
| 41 | 7.811  | 1101 | 1103 | 1105 | rBV2 | 371    | 351     | 0.03%  | 0.004%  |
| 42 | 7.854  | 1108 | 1110 | 1112 | rBV  | 576    | 330     | 0.03%  | 0.003%  |
| 43 | 7.878  | 1112 | 1114 | 1117 | rVB2 | 381    | 394     | 0.03%  | 0.004%  |
| 44 | 7.933  | 1120 | 1123 | 1125 | rBV2 | 1451   | 1869    | 0.14%  | 0.019%  |
| 45 | 8.000  | 1131 | 1134 | 1136 | rBV2 | 357    | 401     | 0.03%  | 0.004%  |
| 46 | 8.055  | 1142 | 1143 | 1148 | rBV2 | 728    | 899     | 0.07%  | 0.009%  |
| 47 | 8.171  | 1158 | 1162 | 1163 | rVV2 | 544    | 455     | 0.03%  | 0.005%  |
| 48 | 8.208  | 1166 | 1168 | 1171 | rVB  | 383    | 367     | 0.03%  | 0.004%  |
| 49 | 8.324  | 1181 | 1187 | 1200 | rVB  | 184883 | 303242  | 23.12% | 3.098%  |
| 50 | 8.409  | 1200 | 1201 | 1205 | rBV2 | 781    | 547     | 0.04%  | 0.006%  |
| 51 | 8.470  | 1210 | 1211 | 1212 | rBV  | 740    | 431     | 0.03%  | 0.004%  |
| 52 | 8.580  | 1223 | 1229 | 1234 | rBV3 | 861    | 1681    | 0.13%  | 0.017%  |
| 53 | 8.653  | 1234 | 1241 | 1252 | rBV  | 653142 | 1047778 | 79.89% | 10.704% |
| 54 | 8.878  | 1277 | 1278 | 1283 | rVB  | 586    | 476     | 0.04%  | 0.005%  |
| 55 | 8.951  | 1284 | 1290 | 1301 | rVV  | 138318 | 199865  | 15.24% | 2.042%  |
| 56 | 9.153  | 1321 | 1323 | 1326 | rVB2 | 670    | 683     | 0.05%  | 0.007%  |
| 57 | 9.195  | 1326 | 1330 | 1335 | rBV2 | 461    | 768     | 0.06%  | 0.008%  |
| 58 | 9.275  | 1340 | 1343 | 1347 | rVB3 | 1172   | 1523    | 0.12%  | 0.016%  |
| 59 | 9.384  | 1356 | 1361 | 1376 | rVV  | 509739 | 708290  | 54.00% | 7.236%  |
| 60 | 9.683  | 1409 | 1410 | 1412 | rVV  | 532    | 365     | 0.03%  | 0.004%  |
| 61 | 9.811  | 1429 | 1431 | 1432 | rBV  | 485    | 370     | 0.03%  | 0.004%  |
| 62 | 9.976  | 1456 | 1458 | 1461 | rVB2 | 594    | 456     | 0.03%  | 0.005%  |
| 63 | 10.055 | 1465 | 1471 | 1480 | rBV  | 632509 | 827438  | 63.09% | 8.453%  |
| 64 | 10.305 | 1508 | 1512 | 1515 | rBV3 | 1116   | 1623    | 0.12%  | 0.017%  |
| 65 | 10.573 | 1555 | 1556 | 1558 | rBV  | 490    | 338     | 0.03%  | 0.003%  |
| 66 | 10.646 | 1564 | 1568 | 1569 | rBV3 | 1912   | 2014    | 0.15%  | 0.021%  |
| 67 | 10.884 | 1605 | 1607 | 1611 | rVB  | 550    | 498     | 0.04%  | 0.005%  |
| 68 | 10.933 | 1614 | 1615 | 1617 | rBV2 | 433    | 408     | 0.03%  | 0.004%  |
| 69 | 10.969 | 1617 | 1621 | 1627 | rVB4 | 1705   | 2525    | 0.19%  | 0.026%  |
| 70 | 11.195 | 1652 | 1658 | 1669 | rBV  | 492124 | 622748  | 47.48% | 6.362%  |
| 71 | 11.311 | 1675 | 1677 | 1681 | rBV3 | 549    | 655     | 0.05%  | 0.007%  |
| 72 | 11.451 | 1696 | 1700 | 1703 | rBV2 | 1895   | 2101    | 0.16%  | 0.021%  |
| 73 | 11.695 | 1738 | 1740 | 1743 | rVV2 | 429    | 600     | 0.05%  | 0.006%  |
| 74 | 11.762 | 1747 | 1751 | 1756 | rVB3 | 2309   | 3401    | 0.26%  | 0.035%  |
| 75 | 11.975 | 1782 | 1786 | 1788 | rBV3 | 1632   | 2071    | 0.16%  | 0.021%  |
| 76 | 12.024 | 1789 | 1794 | 1801 | rVV  | 670637 | 800938  | 61.07% | 8.182%  |

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 Sample : VX0817MBL01  
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 VBLK688

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\_X\Method\SFAMXML080422WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.164 | 1815 | 1817 | 1819 | rBV2 | 532    | 356    | 0.03%  | 0.004% |
| 78  | 12.213 | 1823 | 1825 | 1826 | rBV  | 618    | 352    | 0.03%  | 0.004% |
| 79  | 12.323 | 1837 | 1843 | 1859 | rVV  | 736619 | 908707 | 69.28% | 9.283% |
| 80  | 12.457 | 1863 | 1865 | 1868 | rBV2 | 402    | 554    | 0.04%  | 0.006% |
|     |        |      |      |      |      |        |        |        |        |
| 81  | 12.768 | 1913 | 1916 | 1919 | rVB2 | 995    | 1061   | 0.08%  | 0.011% |
| 82  | 13.115 | 1969 | 1973 | 1977 | rVB3 | 3142   | 3516   | 0.27%  | 0.036% |
| 83  | 13.195 | 1984 | 1986 | 1989 | rBV  | 648    | 522    | 0.04%  | 0.005% |
| 84  | 13.304 | 2002 | 2004 | 2007 | rVB2 | 395    | 411    | 0.03%  | 0.004% |
| 85  | 13.384 | 2015 | 2017 | 2021 | rVB  | 539    | 537    | 0.04%  | 0.005% |
|     |        |      |      |      |      |        |        |        |        |
| 86  | 13.432 | 2023 | 2025 | 2028 | rVV2 | 407    | 368    | 0.03%  | 0.004% |
| 87  | 13.591 | 2048 | 2051 | 2056 | rVB3 | 2801   | 3278   | 0.25%  | 0.033% |
| 88  | 13.780 | 2077 | 2082 | 2085 | rBV2 | 3861   | 4857   | 0.37%  | 0.050% |
| 89  | 13.877 | 2096 | 2098 | 2099 | rVB2 | 744    | 450    | 0.03%  | 0.005% |
| 90  | 13.908 | 2101 | 2103 | 2105 | rVV  | 505    | 369    | 0.03%  | 0.004% |
|     |        |      |      |      |      |        |        |        |        |
| 91  | 13.963 | 2108 | 2112 | 2116 | rVV3 | 3917   | 4358   | 0.33%  | 0.045% |
| 92  | 14.073 | 2129 | 2130 | 2132 | rBV  | 405    | 381    | 0.03%  | 0.004% |
| 93  | 14.127 | 2136 | 2139 | 2145 | rVV2 | 1671   | 2772   | 0.21%  | 0.028% |
| 94  | 14.359 | 2175 | 2177 | 2179 | rBV  | 498    | 356    | 0.03%  | 0.004% |
| 95  | 14.713 | 2233 | 2235 | 2238 | rBV2 | 625    | 652    | 0.05%  | 0.007% |
|     |        |      |      |      |      |        |        |        |        |
| 96  | 14.883 | 2262 | 2263 | 2264 | rBV  | 737    | 467    | 0.04%  | 0.005% |
| 97  | 14.963 | 2274 | 2276 | 2277 | rBV  | 946    | 647    | 0.05%  | 0.007% |
| 98  | 15.036 | 2286 | 2288 | 2291 | rBV2 | 855    | 970    | 0.07%  | 0.010% |
| 99  | 15.158 | 2307 | 2308 | 2312 | rBV3 | 589    | 827    | 0.06%  | 0.008% |
| 100 | 16.084 | 2458 | 2460 | 2462 | rVB2 | 811    | 600    | 0.05%  | 0.006% |

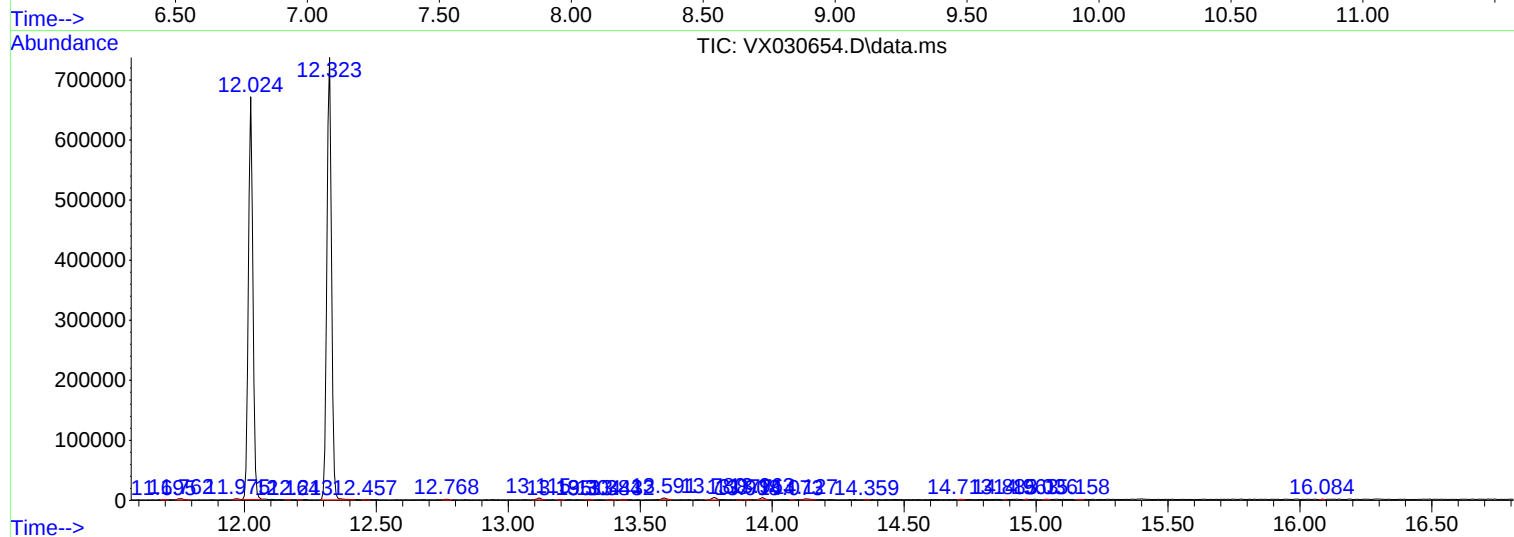
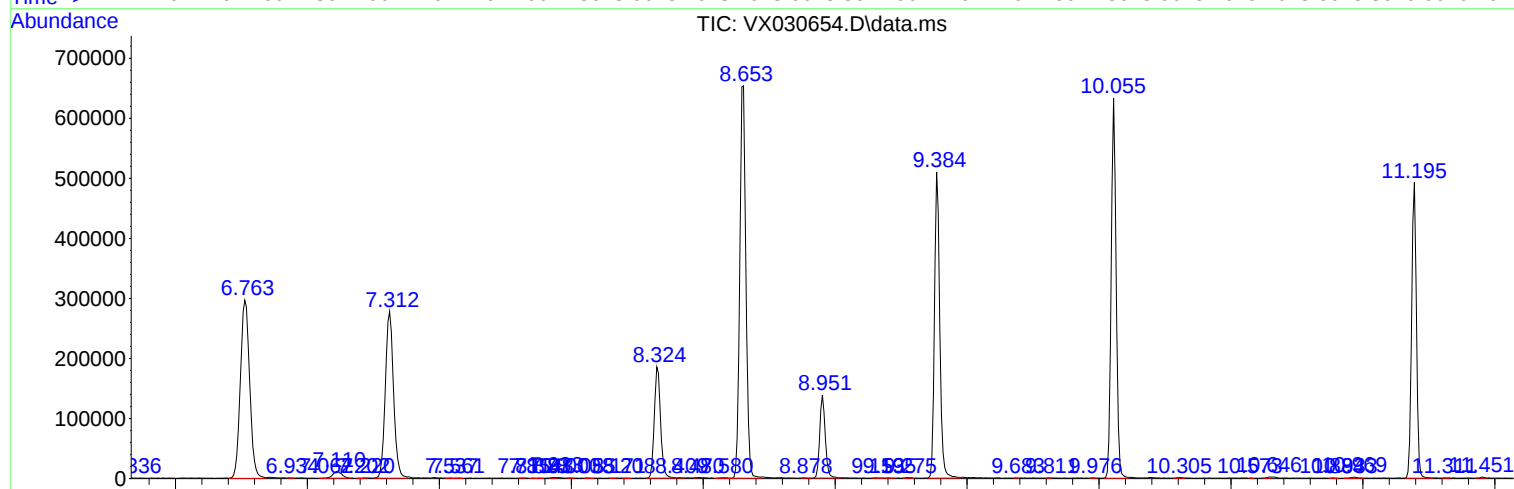
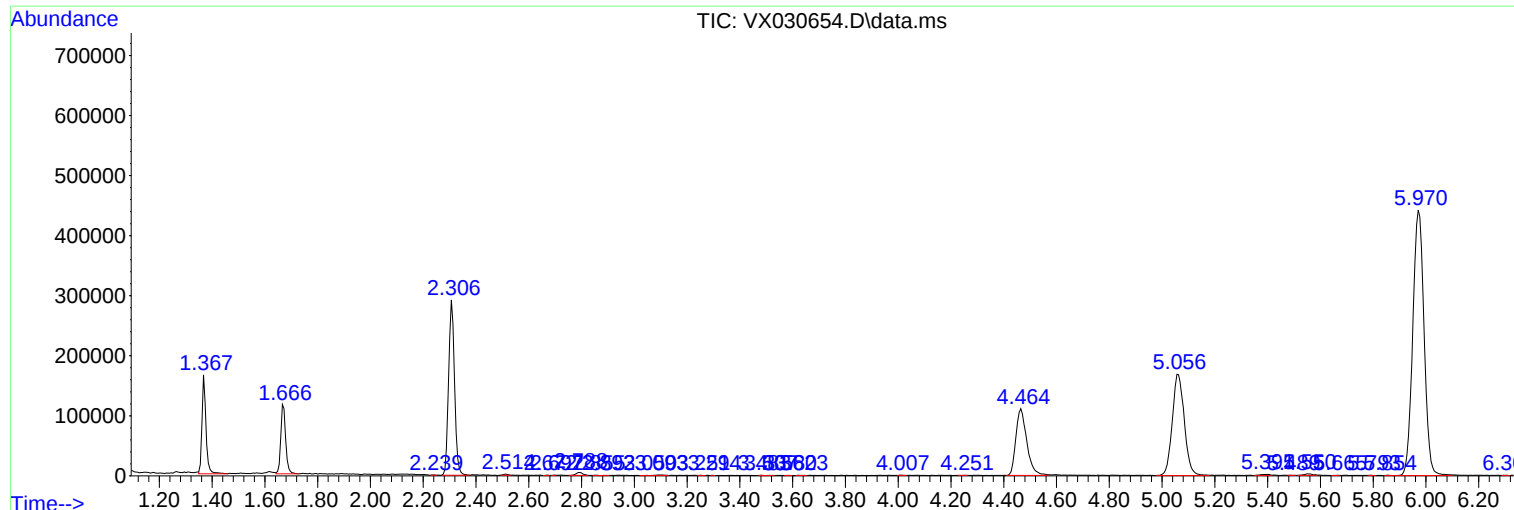
Sum of corrected areas: 9788927

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Instrument :  
MSVOA\_X  
ClientSampleId :  
VBLK688

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.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 |