

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122023\  
 Data File : VX039412.D  
 Acq On : 20 Dec 2023 19:16  
 Operator : JC/MD  
 Sample : 05834-05ME  
 Misc : 3.13g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BGQZ8ME

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

Signal : TIC: VX039412.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         | 1.368       | 43            | 46          | 63           | rVB      | 89086          | 145459        | 12.63%          | 1.704%        |
| 2         | 1.648       | 89            | 92          | 109          | rBV      | 27919          | 67219         | 5.84%           | 0.787%        |
| 3         | 2.282       | 189           | 196         | 221          | rBV      | 217180         | 375582        | 32.61%          | 4.400%        |
| 4         | 2.666       | 257           | 259         | 261          | rBV2     | 301            | 296           | 0.03%           | 0.003%        |
| 5         | 2.709       | 261           | 266         | 268          | rBV3     | 378            | 517           | 0.04%           | 0.006%        |
| 6         | 2.782       | 272           | 278         | 284          | rBV3     | 2798           | 6210          | 0.54%           | 0.073%        |
| 7         | 2.947       | 297           | 305         | 313          | rVB2     | 2692           | 6123          | 0.53%           | 0.072%        |
| 8         | 3.056       | 320           | 323         | 329          | rVB2     | 198            | 338           | 0.03%           | 0.004%        |
| 9         | 3.221       | 347           | 350         | 353          | rBV2     | 281            | 324           | 0.03%           | 0.004%        |
| 10        | 3.251       | 353           | 355         | 357          | rVV2     | 186            | 200           | 0.02%           | 0.002%        |
| 11        | 3.312       | 362           | 365         | 370          | rVV2     | 308            | 415           | 0.04%           | 0.005%        |
| 12        | 3.398       | 375           | 379         | 380          | rVV2     | 186            | 232           | 0.02%           | 0.003%        |
| 13        | 3.428       | 380           | 384         | 388          | rVB4     | 986            | 1788          | 0.16%           | 0.021%        |
| 14        | 3.605       | 411           | 413         | 417          | rVB2     | 182            | 226           | 0.02%           | 0.003%        |
| 15        | 3.733       | 431           | 434         | 437          | rVB2     | 270            | 299           | 0.03%           | 0.004%        |
| 16        | 3.770       | 437           | 440         | 441          | rBV2     | 211            | 200           | 0.02%           | 0.002%        |
| 17        | 3.849       | 450           | 453         | 457          | rBV2     | 171            | 271           | 0.02%           | 0.003%        |
| 18        | 4.020       | 479           | 481         | 485          | rVB2     | 237            | 286           | 0.02%           | 0.003%        |
| 19        | 4.050       | 485           | 486         | 491          | rBV2     | 321            | 435           | 0.04%           | 0.005%        |
| 20        | 4.349       | 531           | 535         | 537          | rBV2     | 143            | 194           | 0.02%           | 0.002%        |
| 21        | 4.483       | 547           | 557         | 591          | rBV2     | 63617          | 300916        | 26.13%          | 3.525%        |
| 22        | 4.910       | 624           | 627         | 629          | rBV2     | 288            | 318           | 0.03%           | 0.004%        |
| 23        | 5.056       | 639           | 651         | 671          | rBV      | 135674         | 447984        | 38.90%          | 5.248%        |
| 24        | 5.544       | 730           | 731         | 732          | rBV      | 363            | 236           | 0.02%           | 0.003%        |
| 25        | 5.727       | 759           | 761         | 764          | rVB2     | 289            | 228           | 0.02%           | 0.003%        |
| 26        | 5.751       | 764           | 765         | 767          | rBV      | 323            | 226           | 0.02%           | 0.003%        |
| 27        | 5.830       | 777           | 778         | 780          | rBV      | 256            | 194           | 0.02%           | 0.002%        |
| 28        | 5.873       | 783           | 785         | 786          | rBV      | 295            | 206           | 0.02%           | 0.002%        |
| 29        | 5.964       | 789           | 800         | 823          | rBV2     | 393423         | 1151717       | 100.00%         | 13.492%       |
| 30        | 6.257       | 846           | 848         | 850          | rBV      | 267            | 198           | 0.02%           | 0.002%        |
| 31        | 6.348       | 860           | 863         | 864          | rBV2     | 397            | 407           | 0.04%           | 0.005%        |
| 32        | 6.373       | 864           | 867         | 868          | rBV3     | 641            | 696           | 0.06%           | 0.008%        |
| 33        | 6.623       | 906           | 908         | 909          | rBV2     | 271            | 211           | 0.02%           | 0.002%        |
| 34        | 6.757       | 921           | 930         | 950          | rBV      | 252941         | 631635        | 54.84%          | 7.400%        |
| 35        | 7.111       | 982           | 988         | 989          | rBV5     | 2150           | 3180          | 0.28%           | 0.037%        |
| 36        | 7.306       | 1012          | 1020        | 1041         | rVB      | 224654         | 519445        | 45.10%          | 6.085%        |

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 BGQZ8ME

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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.708  | 1084 | 1086 | 1090 | rBV2 | 237    | 326    | 0.03%  | 0.004%  |
| 38 | 7.854  | 1109 | 1110 | 1113 | rBV  | 286    | 217    | 0.02%  | 0.003%  |
| 39 | 7.970  | 1123 | 1129 | 1132 | rBV4 | 907    | 1469   | 0.13%  | 0.017%  |
| 40 | 8.263  | 1173 | 1177 | 1180 | rBV  | 391    | 425    | 0.04%  | 0.005%  |
| 41 | 8.324  | 1180 | 1187 | 1202 | rBV  | 144534 | 253137 | 21.98% | 2.966%  |
| 42 | 8.513  | 1215 | 1218 | 1220 | rBV2 | 480    | 597    | 0.05%  | 0.007%  |
| 43 | 8.647  | 1233 | 1240 | 1256 | rBV  | 536804 | 872602 | 75.77% | 10.223% |
| 44 | 8.891  | 1279 | 1280 | 1284 | rBV  | 284    | 397    | 0.03%  | 0.005%  |
| 45 | 8.952  | 1284 | 1290 | 1300 | rBV  | 102258 | 164785 | 14.31% | 1.930%  |
| 46 | 9.122  | 1315 | 1318 | 1321 | rBV3 | 701    | 734    | 0.06%  | 0.009%  |
| 47 | 9.275  | 1338 | 1343 | 1348 | rVB2 | 5431   | 8611   | 0.75%  | 0.101%  |
| 48 | 9.330  | 1351 | 1352 | 1356 | rVB2 | 361    | 288    | 0.03%  | 0.003%  |
| 49 | 9.403  | 1356 | 1364 | 1383 | rBV  | 337577 | 679055 | 58.96% | 7.955%  |
| 50 | 9.616  | 1397 | 1399 | 1405 | rVV3 | 439    | 536    | 0.05%  | 0.006%  |
| 51 | 9.665  | 1405 | 1407 | 1412 | rVV3 | 451    | 624    | 0.05%  | 0.007%  |
| 52 | 9.714  | 1412 | 1415 | 1421 | rVB3 | 959    | 1428   | 0.12%  | 0.017%  |
| 53 | 10.055 | 1465 | 1471 | 1488 | rBV  | 522006 | 749487 | 65.08% | 8.780%  |
| 54 | 10.275 | 1505 | 1507 | 1509 | rVB2 | 263    | 200    | 0.02%  | 0.002%  |
| 55 | 10.311 | 1510 | 1513 | 1519 | rVB3 | 633    | 877    | 0.08%  | 0.010%  |
| 56 | 10.647 | 1565 | 1568 | 1569 | rBV  | 306    | 371    | 0.03%  | 0.004%  |
| 57 | 10.854 | 1601 | 1602 | 1606 | rVB  | 333    | 217    | 0.02%  | 0.003%  |
| 58 | 10.884 | 1606 | 1607 | 1611 | rVB2 | 239    | 214    | 0.02%  | 0.003%  |
| 59 | 10.976 | 1616 | 1622 | 1625 | rBV3 | 371    | 643    | 0.06%  | 0.008%  |
| 60 | 11.092 | 1638 | 1641 | 1644 | rBV2 | 248    | 259    | 0.02%  | 0.003%  |
| 61 | 11.195 | 1652 | 1658 | 1672 | rVV  | 408499 | 539450 | 46.84% | 6.320%  |
| 62 | 11.311 | 1673 | 1677 | 1681 | rVV2 | 1490   | 1993   | 0.17%  | 0.023%  |
| 63 | 11.457 | 1697 | 1701 | 1703 | rBV3 | 439    | 487    | 0.04%  | 0.006%  |
| 64 | 11.476 | 1703 | 1704 | 1707 | rVB  | 325    | 214    | 0.02%  | 0.003%  |
| 65 | 11.622 | 1727 | 1728 | 1729 | rBV  | 300    | 209    | 0.02%  | 0.002%  |
| 66 | 11.683 | 1734 | 1738 | 1740 | rBV2 | 534    | 578    | 0.05%  | 0.007%  |
| 67 | 11.756 | 1747 | 1750 | 1754 | rVB3 | 541    | 730    | 0.06%  | 0.009%  |
| 68 | 11.787 | 1754 | 1755 | 1759 | rBV2 | 256    | 273    | 0.02%  | 0.003%  |
| 69 | 11.915 | 1774 | 1776 | 1778 | rBV2 | 203    | 195    | 0.02%  | 0.002%  |
| 70 | 11.976 | 1783 | 1786 | 1789 | rBV3 | 752    | 1035   | 0.09%  | 0.012%  |
| 71 | 12.024 | 1789 | 1794 | 1805 | rBV  | 618877 | 768079 | 66.69% | 8.998%  |
| 72 | 12.171 | 1815 | 1818 | 1821 | rBV2 | 325    | 409    | 0.04%  | 0.005%  |
| 73 | 12.232 | 1826 | 1828 | 1831 | rBV  | 323    | 399    | 0.03%  | 0.005%  |
| 74 | 12.323 | 1837 | 1843 | 1857 | rVV  | 585191 | 775175 | 67.31% | 9.081%  |
| 75 | 12.762 | 1910 | 1915 | 1921 | rBV2 | 6015   | 8039   | 0.70%  | 0.094%  |
| 76 | 13.030 | 1957 | 1959 | 1961 | rBV  | 367    | 346    | 0.03%  | 0.004%  |

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 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
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 BGQZ8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 13.116 | 1971 | 1973 | 1978 | rVB3 | 438   | 502   | 0.04% | 0.006% |
| 78  | 13.323 | 2006 | 2007 | 2009 | rVV  | 376   | 227   | 0.02% | 0.003% |
| 79  | 13.463 | 2027 | 2030 | 2032 | rBV  | 204   | 226   | 0.02% | 0.003% |
| 80  | 13.548 | 2040 | 2044 | 2045 | rVB2 | 230   | 253   | 0.02% | 0.003% |
| 81  | 13.591 | 2047 | 2051 | 2056 | rVV2 | 3925  | 4884  | 0.42% | 0.057% |
| 82  | 13.756 | 2076 | 2078 | 2080 | rBV  | 223   | 273   | 0.02% | 0.003% |
| 83  | 13.786 | 2080 | 2083 | 2085 | rVV2 | 542   | 611   | 0.05% | 0.007% |
| 84  | 13.865 | 2094 | 2096 | 2099 | rVB  | 297   | 282   | 0.02% | 0.003% |
| 85  | 13.969 | 2108 | 2113 | 2118 | rVB4 | 1241  | 1921  | 0.17% | 0.023% |
| 86  | 14.128 | 2134 | 2139 | 2144 | rBV  | 10009 | 14067 | 1.22% | 0.165% |
| 87  | 14.292 | 2162 | 2166 | 2168 | rBV2 | 264   | 350   | 0.03% | 0.004% |
| 88  | 14.499 | 2198 | 2200 | 2204 | rBV2 | 216   | 277   | 0.02% | 0.003% |
| 89  | 14.536 | 2204 | 2206 | 2208 | rVB2 | 276   | 204   | 0.02% | 0.002% |
| 90  | 14.688 | 2228 | 2231 | 2232 | rVB2 | 272   | 212   | 0.02% | 0.002% |
| 91  | 14.713 | 2234 | 2235 | 2237 | rVB  | 377   | 277   | 0.02% | 0.003% |
| 92  | 14.890 | 2263 | 2264 | 2266 | rBV2 | 267   | 212   | 0.02% | 0.002% |
| 93  | 15.249 | 2318 | 2323 | 2329 | rBV2 | 5098  | 7137  | 0.62% | 0.084% |
| 94  | 15.341 | 2336 | 2338 | 2340 | rBV2 | 245   | 248   | 0.02% | 0.003% |
| 95  | 15.390 | 2342 | 2346 | 2352 | rVB3 | 1655  | 2738  | 0.24% | 0.032% |
| 96  | 15.737 | 2401 | 2403 | 2405 | rBV2 | 349   | 256   | 0.02% | 0.003% |
| 97  | 15.841 | 2419 | 2420 | 2423 | rBV2 | 374   | 406   | 0.04% | 0.005% |
| 98  | 15.975 | 2441 | 2442 | 2445 | rBV2 | 352   | 349   | 0.03% | 0.004% |
| 99  | 16.139 | 2467 | 2469 | 2470 | rBV  | 450   | 317   | 0.03% | 0.004% |
| 100 | 16.633 | 2548 | 2550 | 2551 | rBV  | 381   | 249   | 0.02% | 0.003% |

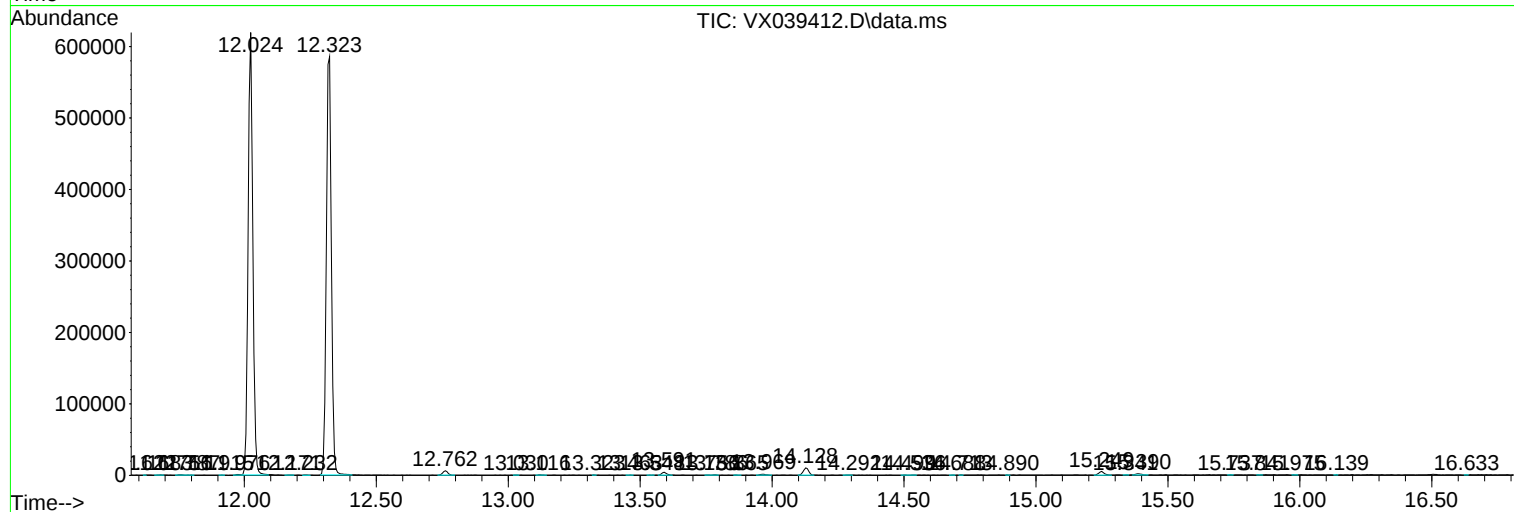
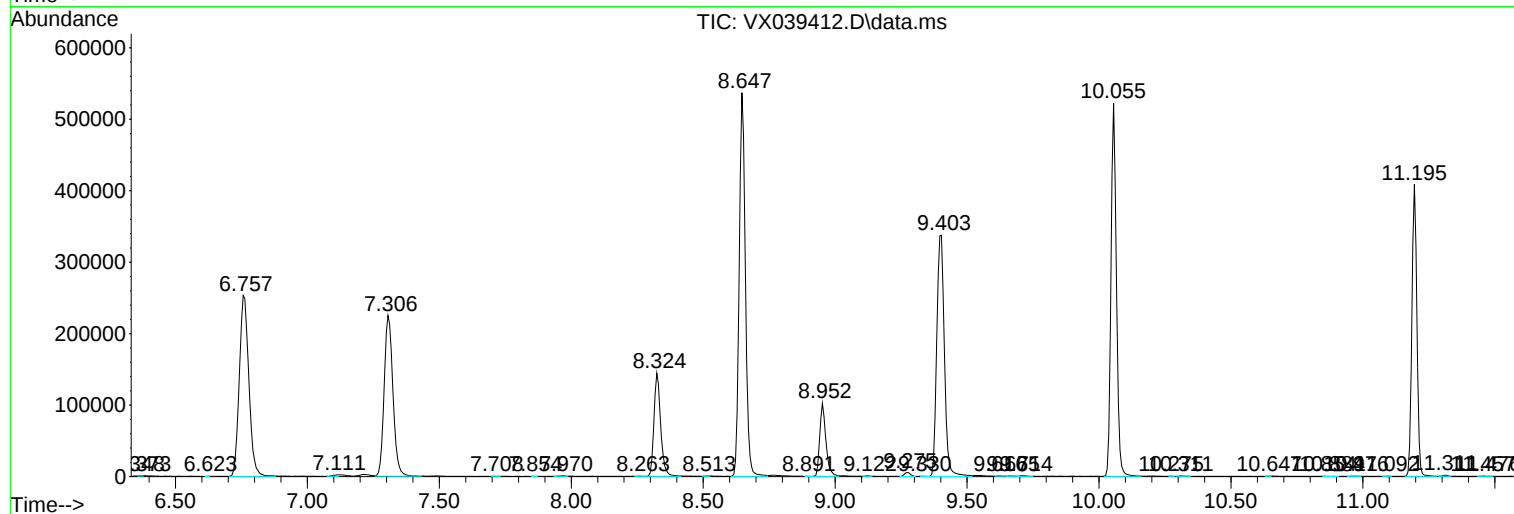
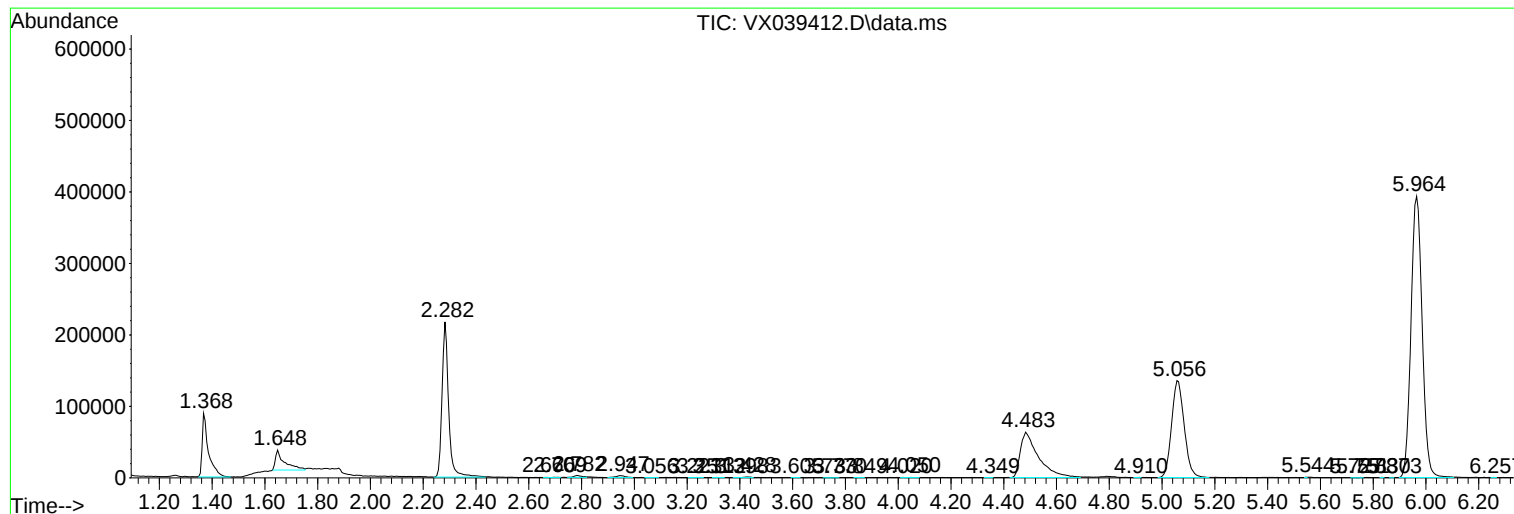
Sum of corrected areas: 8535999

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM120523WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122023\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
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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          |