

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121923\  
 Data File : VX039381.D  
 Acq On : 20 Dec 2023 00:40  
 Operator : JC/MD  
 Sample : 05869-07 100X  
 Misc : 4.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 41 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AT3

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: VX039381.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          | 59           | rVB      | 94312          | 102856        | 13.44%          | 1.746%        |
| 2         | 1.672       | 91            | 96          | 112          | rVB      | 61965          | 94935         | 12.40%          | 1.612%        |
| 3         | 2.306       | 194           | 200         | 210          | rBV      | 163828         | 260773        | 34.07%          | 4.427%        |
| 4         | 2.794       | 275           | 280         | 285          | rVV5     | 1565           | 3107          | 0.41%           | 0.053%        |
| 5         | 2.837       | 285           | 287         | 289          | rVB2     | 333            | 281           | 0.04%           | 0.005%        |
| 6         | 2.892       | 294           | 296         | 297          | rBV      | 256            | 179           | 0.02%           | 0.003%        |
| 7         | 2.940       | 299           | 304         | 313          | rVB2     | 4234           | 9110          | 1.19%           | 0.155%        |
| 8         | 3.215       | 348           | 349         | 350          | rBV      | 384            | 171           | 0.02%           | 0.003%        |
| 9         | 3.306       | 361           | 364         | 367          | rBV      | 167            | 201           | 0.03%           | 0.003%        |
| 10        | 3.361       | 369           | 373         | 375          | rBV      | 212            | 258           | 0.03%           | 0.004%        |
| 11        | 3.440       | 384           | 386         | 389          | rVB2     | 195            | 187           | 0.02%           | 0.003%        |
| 12        | 3.916       | 462           | 464         | 466          | rVV      | 231            | 175           | 0.02%           | 0.003%        |
| 13        | 3.946       | 467           | 469         | 471          | rVB      | 304            | 169           | 0.02%           | 0.003%        |
| 14        | 3.965       | 471           | 472         | 475          | rBV2     | 132            | 166           | 0.02%           | 0.003%        |
| 15        | 4.026       | 479           | 482         | 484          | rBV2     | 204            | 255           | 0.03%           | 0.004%        |
| 16        | 4.190       | 507           | 509         | 511          | rBV2     | 185            | 194           | 0.03%           | 0.003%        |
| 17        | 4.306       | 526           | 528         | 530          | rBV      | 150            | 195           | 0.03%           | 0.003%        |
| 18        | 4.446       | 543           | 551         | 564          | rBV      | 67426          | 194554        | 25.42%          | 3.303%        |
| 19        | 5.056       | 639           | 651         | 666          | rBV      | 94818          | 303710        | 39.68%          | 5.155%        |
| 20        | 5.355       | 699           | 700         | 705          | rBV2     | 148            | 202           | 0.03%           | 0.003%        |
| 21        | 5.403       | 705           | 708         | 709          | rBV      | 182            | 159           | 0.02%           | 0.003%        |
| 22        | 5.562       | 730           | 734         | 735          | rBV3     | 261            | 253           | 0.03%           | 0.004%        |
| 23        | 5.970       | 789           | 801         | 819          | rBV2     | 253605         | 765337        | 100.00%         | 12.992%       |
| 24        | 6.226       | 840           | 843         | 847          | rBV2     | 224            | 383           | 0.05%           | 0.007%        |
| 25        | 6.379       | 866           | 868         | 870          | rVB      | 271            | 158           | 0.02%           | 0.003%        |
| 26        | 6.446       | 877           | 879         | 881          | rBV2     | 251            | 276           | 0.04%           | 0.005%        |
| 27        | 6.592       | 902           | 903         | 906          | rBV      | 312            | 222           | 0.03%           | 0.004%        |
| 28        | 6.757       | 921           | 930         | 946          | rBV      | 180698         | 440906        | 57.61%          | 7.484%        |
| 29        | 7.062       | 977           | 980         | 981          | rBV2     | 185            | 201           | 0.03%           | 0.003%        |
| 30        | 7.116       | 984           | 989         | 994          | rVB3     | 1095           | 2235          | 0.29%           | 0.038%        |
| 31        | 7.305       | 1012          | 1020        | 1036         | rBV      | 158470         | 348219        | 45.50%          | 5.911%        |
| 32        | 7.488       | 1047          | 1050        | 1055         | rVB4     | 459            | 659           | 0.09%           | 0.011%        |
| 33        | 7.629       | 1071          | 1073        | 1075         | rBV2     | 188            | 167           | 0.02%           | 0.003%        |
| 34        | 7.964       | 1125          | 1128        | 1131         | rVB2     | 145            | 198           | 0.03%           | 0.003%        |
| 35        | 8.232       | 1170          | 1172        | 1174         | rBV2     | 150            | 175           | 0.02%           | 0.003%        |
| 36        | 8.324       | 1181          | 1187        | 1201         | rBV      | 102445         | 170390        | 22.26%          | 2.892%        |

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 MSVOA\_X  
 ClientSampleId :  
 C0AT3

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 | 8.574  | 1227 | 1228 | 1233 | rVB3 | 513    | 631    | 0.08%  | 0.011%  |
| 38 | 8.647  | 1233 | 1240 | 1256 | rBV  | 374670 | 595393 | 77.79% | 10.107% |
| 39 | 8.891  | 1277 | 1280 | 1283 | rBV3 | 171    | 257    | 0.03%  | 0.004%  |
| 40 | 8.952  | 1284 | 1290 | 1307 | rVV  | 73121  | 112435 | 14.69% | 1.909%  |
| 41 | 9.275  | 1337 | 1343 | 1349 | rVB3 | 292    | 610    | 0.08%  | 0.010%  |
| 42 | 9.384  | 1355 | 1361 | 1374 | rBV  | 312710 | 463682 | 60.59% | 7.871%  |
| 43 | 9.579  | 1391 | 1393 | 1395 | rBV3 | 339    | 182    | 0.02%  | 0.003%  |
| 44 | 10.055 | 1465 | 1471 | 1483 | rBV  | 377765 | 554606 | 72.47% | 9.414%  |
| 45 | 10.311 | 1510 | 1513 | 1517 | rBV3 | 212    | 295    | 0.04%  | 0.005%  |
| 46 | 10.402 | 1525 | 1528 | 1529 | rBV2 | 154    | 168    | 0.02%  | 0.003%  |
| 47 | 10.463 | 1536 | 1538 | 1540 | rBV  | 195    | 166    | 0.02%  | 0.003%  |
| 48 | 10.512 | 1544 | 1546 | 1548 | rVB2 | 237    | 184    | 0.02%  | 0.003%  |
| 49 | 10.591 | 1558 | 1559 | 1562 | rVV  | 277    | 242    | 0.03%  | 0.004%  |
| 50 | 10.652 | 1566 | 1569 | 1571 | rVV2 | 320    | 412    | 0.05%  | 0.007%  |
| 51 | 10.677 | 1571 | 1573 | 1576 | rVB2 | 310    | 327    | 0.04%  | 0.006%  |
| 52 | 10.726 | 1579 | 1581 | 1584 | rVB  | 186    | 176    | 0.02%  | 0.003%  |
| 53 | 10.835 | 1597 | 1599 | 1604 | rVB2 | 141    | 159    | 0.02%  | 0.003%  |
| 54 | 10.957 | 1617 | 1619 | 1621 | rBV3 | 206    | 237    | 0.03%  | 0.004%  |
| 55 | 11.055 | 1632 | 1635 | 1636 | rBV  | 194    | 211    | 0.03%  | 0.004%  |
| 56 | 11.091 | 1639 | 1641 | 1645 | rVB2 | 310    | 315    | 0.04%  | 0.005%  |
| 57 | 11.140 | 1646 | 1649 | 1652 | rBV  | 164    | 254    | 0.03%  | 0.004%  |
| 58 | 11.189 | 1652 | 1657 | 1668 | rVV  | 288170 | 370923 | 48.47% | 6.296%  |
| 59 | 11.360 | 1683 | 1685 | 1688 | rBV3 | 550    | 615    | 0.08%  | 0.010%  |
| 60 | 11.445 | 1697 | 1699 | 1700 | rBV  | 284    | 192    | 0.03%  | 0.003%  |
| 61 | 11.762 | 1748 | 1751 | 1755 | rVB3 | 396    | 554    | 0.07%  | 0.009%  |
| 62 | 11.805 | 1755 | 1758 | 1759 | rBV2 | 163    | 158    | 0.02%  | 0.003%  |
| 63 | 11.975 | 1782 | 1786 | 1788 | rVB3 | 612    | 523    | 0.07%  | 0.009%  |
| 64 | 12.018 | 1788 | 1793 | 1802 | rBV  | 412966 | 549325 | 71.78% | 9.325%  |
| 65 | 12.317 | 1837 | 1842 | 1855 | rBV  | 396254 | 514487 | 67.22% | 8.733%  |
| 66 | 12.445 | 1862 | 1863 | 1866 | rBV2 | 219    | 158    | 0.02%  | 0.003%  |
| 67 | 12.634 | 1892 | 1894 | 1896 | rBV  | 283    | 215    | 0.03%  | 0.004%  |
| 68 | 12.762 | 1911 | 1915 | 1919 | rVB3 | 1085   | 1612   | 0.21%  | 0.027%  |
| 69 | 12.798 | 1919 | 1921 | 1925 | rVB2 | 171    | 157    | 0.02%  | 0.003%  |
| 70 | 12.926 | 1940 | 1942 | 1946 | rBV2 | 290    | 398    | 0.05%  | 0.007%  |
| 71 | 13.115 | 1971 | 1973 | 1975 | rVB  | 368    | 239    | 0.03%  | 0.004%  |
| 72 | 13.323 | 2006 | 2007 | 2009 | rBV2 | 179    | 166    | 0.02%  | 0.003%  |
| 73 | 13.420 | 2021 | 2023 | 2026 | rVB  | 180    | 177    | 0.02%  | 0.003%  |
| 74 | 13.591 | 2047 | 2051 | 2055 | rVV2 | 4034   | 4833   | 0.63%  | 0.082%  |
| 75 | 13.682 | 2064 | 2066 | 2069 | rBV  | 168    | 195    | 0.03%  | 0.003%  |
| 76 | 13.786 | 2080 | 2083 | 2086 | rVB2 | 458    | 646    | 0.08%  | 0.011%  |

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Instrument :  
 MSVOA\_X  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 13.823 | 2086 | 2089 | 2090 | rBV  | 221  | 289  | 0.04% | 0.005% |
| 78  | 13.969 | 2108 | 2113 | 2117 | rVB3 | 928  | 1386 | 0.18% | 0.024% |
| 79  | 14.054 | 2124 | 2127 | 2128 | rBV  | 208  | 202  | 0.03% | 0.003% |
| 80  | 14.073 | 2128 | 2130 | 2132 | rVV2 | 211  | 157  | 0.02% | 0.003% |
| 81  | 14.127 | 2133 | 2139 | 2144 | rVV  | 2332 | 3263 | 0.43% | 0.055% |
| 82  | 14.188 | 2146 | 2149 | 2152 | rBV2 | 296  | 401  | 0.05% | 0.007% |
| 83  | 14.298 | 2165 | 2167 | 2171 | rBV2 | 206  | 217  | 0.03% | 0.004% |
| 84  | 14.359 | 2174 | 2177 | 2180 | rBV2 | 266  | 423  | 0.06% | 0.007% |
| 85  | 14.463 | 2191 | 2194 | 2195 | rBV  | 346  | 362  | 0.05% | 0.006% |
| 86  | 14.633 | 2221 | 2222 | 2224 | rVB  | 408  | 174  | 0.02% | 0.003% |
| 87  | 14.664 | 2224 | 2227 | 2229 | rBV3 | 443  | 502  | 0.07% | 0.009% |
| 88  | 14.725 | 2236 | 2237 | 2240 | rVV  | 243  | 179  | 0.02% | 0.003% |
| 89  | 14.761 | 2240 | 2243 | 2246 | rVV3 | 220  | 344  | 0.04% | 0.006% |
| 90  | 14.786 | 2246 | 2247 | 2249 | rVV  | 223  | 173  | 0.02% | 0.003% |
| 91  | 14.804 | 2249 | 2250 | 2253 | rVB2 | 303  | 263  | 0.03% | 0.004% |
| 92  | 15.017 | 2283 | 2285 | 2287 | rBV2 | 178  | 187  | 0.02% | 0.003% |
| 93  | 15.249 | 2319 | 2323 | 2327 | rVB3 | 2192 | 2618 | 0.34% | 0.044% |
| 94  | 15.597 | 2378 | 2380 | 2382 | rBV2 | 350  | 239  | 0.03% | 0.004% |
| 95  | 15.853 | 2420 | 2422 | 2424 | rVB  | 360  | 229  | 0.03% | 0.004% |
| 96  | 15.908 | 2428 | 2431 | 2432 | rBV  | 266  | 263  | 0.03% | 0.004% |
| 97  | 16.182 | 2474 | 2476 | 2478 | rBV2 | 296  | 229  | 0.03% | 0.004% |
| 98  | 16.225 | 2482 | 2483 | 2485 | rBV2 | 240  | 200  | 0.03% | 0.003% |
| 99  | 16.481 | 2523 | 2525 | 2527 | rVB2 | 428  | 339  | 0.04% | 0.006% |
| 100 | 16.761 | 2569 | 2571 | 2575 | rBV3 | 221  | 284  | 0.04% | 0.005% |

Sum of corrected areas: 5891054

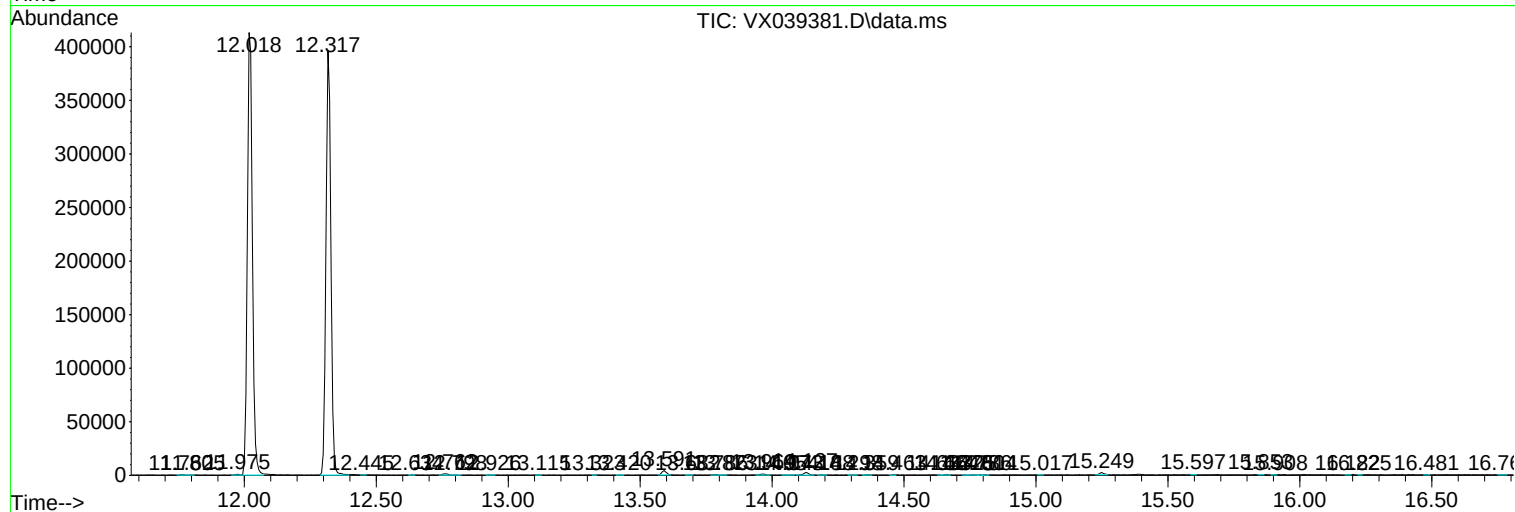
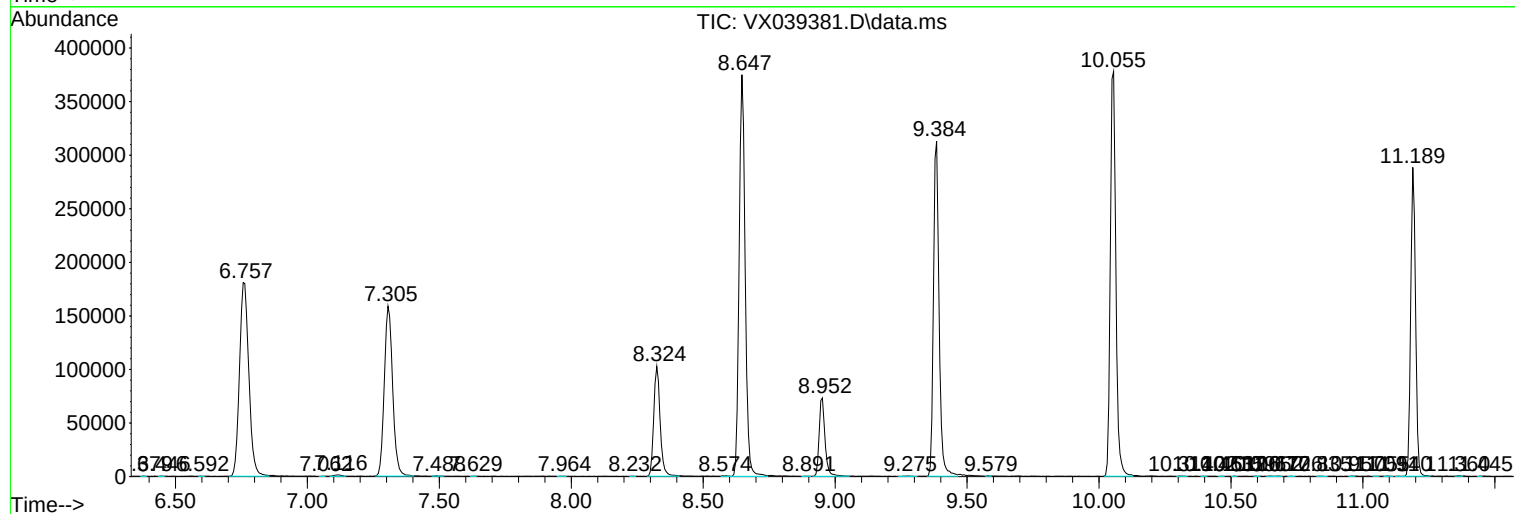
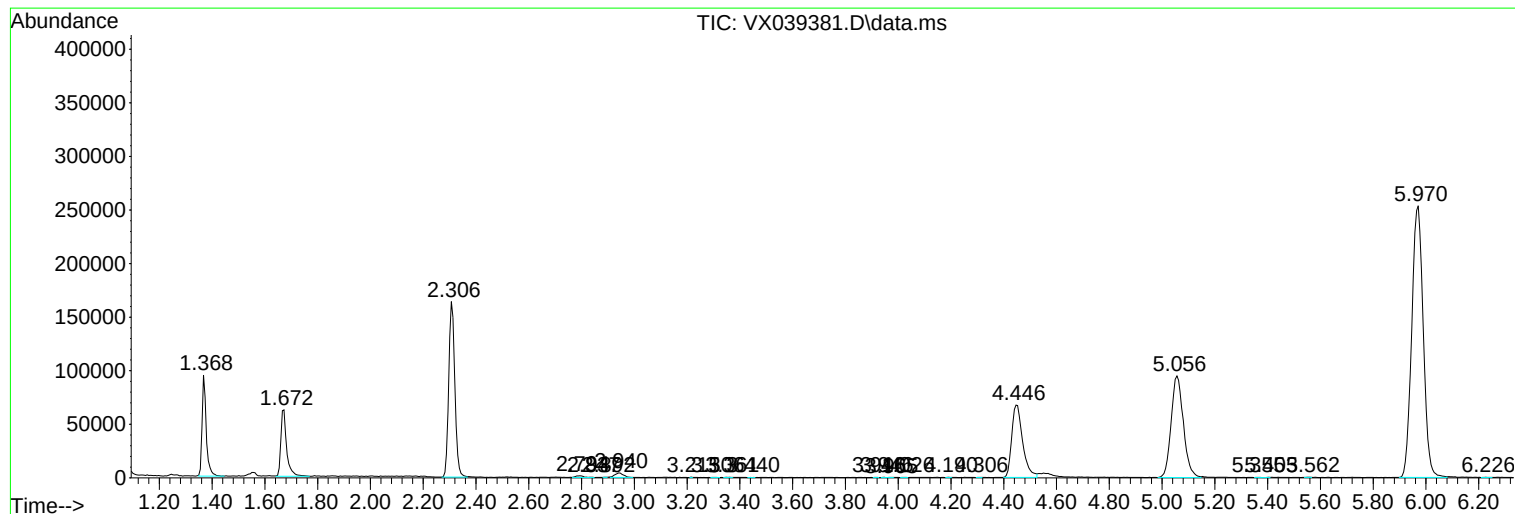
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML120523WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121923\  
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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 | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |