

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX070424\  
 Data File : VX042189.D  
 Acq On : 04 Jul 2024 02:04  
 Operator : JC/MD  
 Sample : P3087-17ME  
 Misc : 4.63g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 39 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 A4BR2ME

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\SFAMXML070324WMA.M  
 Title : VOC Analysis

Signal : TIC: VX042189.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         | 1.264       | 22            | 29          | 40           | rBV2     | 19306          | 26473         | 3.84%           | 0.482%        |
| 2         | 1.374       | 42            | 47          | 48           | rBV      | 29003          | 34833         | 5.06%           | 0.635%        |
| 3         | 1.599       | 71            | 84          | 85           | rBV6     | 6480           | 17472         | 2.54%           | 0.318%        |
| 4         | 1.648       | 86            | 92          | 94           | rBV2     | 16155          | 27193         | 3.95%           | 0.495%        |
| 5         | 2.282       | 190           | 196         | 212          | rBV      | 111143         | 204010        | 29.62%          | 3.717%        |
| 6         | 2.617       | 248           | 251         | 253          | rBV3     | 289            | 271           | 0.04%           | 0.005%        |
| 7         | 2.660       | 256           | 258         | 260          | rVB3     | 357            | 273           | 0.04%           | 0.005%        |
| 8         | 2.715       | 260           | 267         | 273          | rBV2     | 6026           | 12416         | 1.80%           | 0.226%        |
| 9         | 2.782       | 273           | 278         | 286          | rVB2     | 3664           | 7549          | 1.10%           | 0.138%        |
| 10        | 2.941       | 297           | 304         | 315          | rVB      | 3469           | 8607          | 1.25%           | 0.157%        |
| 11        | 3.410       | 379           | 381         | 383          | rBV2     | 402            | 438           | 0.06%           | 0.008%        |
| 12        | 3.629       | 415           | 417         | 420          | rBV      | 242            | 228           | 0.03%           | 0.004%        |
| 13        | 3.666       | 421           | 423         | 426          | rVB2     | 183            | 186           | 0.03%           | 0.003%        |
| 14        | 3.703       | 426           | 429         | 431          | rBV2     | 142            | 181           | 0.03%           | 0.003%        |
| 15        | 4.081       | 490           | 491         | 494          | rBV2     | 136            | 159           | 0.02%           | 0.003%        |
| 16        | 4.184       | 503           | 508         | 510          | rBV2     | 122            | 202           | 0.03%           | 0.004%        |
| 17        | 4.245       | 517           | 518         | 522          | rBV2     | 208            | 206           | 0.03%           | 0.004%        |
| 18        | 4.343       | 530           | 534         | 536          | rBV      | 196            | 200           | 0.03%           | 0.004%        |
| 19        | 4.489       | 550           | 558         | 577          | rBV      | 37298          | 133655        | 19.40%          | 2.435%        |
| 20        | 5.056       | 638           | 651         | 669          | rBV2     | 81931          | 259483        | 37.67%          | 4.727%        |
| 21        | 5.385       | 703           | 705         | 706          | rBV2     | 251            | 150           | 0.02%           | 0.003%        |
| 22        | 5.964       | 787           | 800         | 815          | rBV2     | 237980         | 688842        | 100.00%         | 12.550%       |
| 23        | 6.245       | 844           | 846         | 849          | rVB3     | 253            | 197           | 0.03%           | 0.004%        |
| 24        | 6.385       | 861           | 869         | 877          | rBV3     | 1075           | 2816          | 0.41%           | 0.051%        |
| 25        | 6.556       | 893           | 897         | 899          | rBV2     | 168            | 221           | 0.03%           | 0.004%        |
| 26        | 6.757       | 921           | 930         | 943          | rBV      | 221438         | 535722        | 77.77%          | 9.760%        |
| 27        | 7.104       | 982           | 987         | 988          | rBV3     | 1332           | 1541          | 0.22%           | 0.028%        |
| 28        | 7.214       | 999           | 1005        | 1012         | rBV3     | 1612           | 3739          | 0.54%           | 0.068%        |
| 29        | 7.306       | 1012          | 1020        | 1043         | rVB      | 137756         | 304863        | 44.26%          | 5.554%        |
| 30        | 7.489       | 1048          | 1050        | 1054         | rVB3     | 287            | 352           | 0.05%           | 0.006%        |
| 31        | 7.958       | 1124          | 1127        | 1130         | rBV4     | 672            | 856           | 0.12%           | 0.016%        |
| 32        | 8.324       | 1181          | 1187        | 1202         | rBV      | 70226          | 124320        | 18.05%          | 2.265%        |
| 33        | 8.531       | 1218          | 1221        | 1223         | rBV3     | 249            | 398           | 0.06%           | 0.007%        |
| 34        | 8.647       | 1233          | 1240        | 1249         | rBV      | 349210         | 553712        | 80.38%          | 10.088%       |
| 35        | 8.720       | 1249          | 1252        | 1257         | rVB      | 5633           | 9240          | 1.34%           | 0.168%        |
| 36        | 8.952       | 1284          | 1290        | 1307         | rBV      | 52308          | 81548         | 11.84%          | 1.486%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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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\SFAMXML070324WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 9.061  | 1307 | 1308 | 1311 | rVB2 | 236    | 187    | 0.03%  | 0.003%  |
| 38 | 9.275  | 1336 | 1343 | 1350 | rVB3 | 1780   | 2849   | 0.41%  | 0.052%  |
| 39 | 9.391  | 1357 | 1362 | 1382 | rBV  | 153514 | 312634 | 45.39% | 5.696%  |
| 40 | 9.634  | 1400 | 1402 | 1403 | rVB2 | 242    | 169    | 0.02%  | 0.003%  |
| 41 | 9.708  | 1410 | 1414 | 1423 | rVB3 | 2005   | 3384   | 0.49%  | 0.062%  |
| 42 | 9.805  | 1427 | 1430 | 1431 | rBV2 | 258    | 154    | 0.02%  | 0.003%  |
| 43 | 10.055 | 1465 | 1471 | 1483 | rBV  | 440924 | 612956 | 88.98% | 11.167% |
| 44 | 10.201 | 1491 | 1495 | 1498 | rVB3 | 601    | 784    | 0.11%  | 0.014%  |
| 45 | 10.244 | 1498 | 1502 | 1508 | rVB3 | 920    | 1764   | 0.26%  | 0.032%  |
| 46 | 10.305 | 1508 | 1512 | 1521 | rVB2 | 1890   | 3172   | 0.46%  | 0.058%  |
| 47 | 10.372 | 1521 | 1523 | 1525 | rVB  | 159    | 162    | 0.02%  | 0.003%  |
| 48 | 10.567 | 1552 | 1555 | 1556 | rBV  | 225    | 159    | 0.02%  | 0.003%  |
| 49 | 10.586 | 1556 | 1558 | 1561 | rVB2 | 134    | 151    | 0.02%  | 0.003%  |
| 50 | 10.653 | 1565 | 1569 | 1571 | rBV2 | 583    | 832    | 0.12%  | 0.015%  |
| 51 | 10.671 | 1571 | 1572 | 1574 | rVB2 | 277    | 202    | 0.03%  | 0.004%  |
| 52 | 10.860 | 1602 | 1603 | 1606 | rBV2 | 135    | 178    | 0.03%  | 0.003%  |
| 53 | 10.957 | 1618 | 1619 | 1623 | rBV2 | 194    | 273    | 0.04%  | 0.005%  |
| 54 | 11.024 | 1628 | 1630 | 1633 | rVB2 | 153    | 200    | 0.03%  | 0.004%  |
| 55 | 11.055 | 1633 | 1635 | 1637 | rBV  | 266    | 215    | 0.03%  | 0.004%  |
| 56 | 11.104 | 1640 | 1643 | 1648 | rVB3 | 334    | 562    | 0.08%  | 0.010%  |
| 57 | 11.195 | 1652 | 1658 | 1671 | rBV  | 256326 | 352143 | 51.12% | 6.416%  |
| 58 | 11.311 | 1674 | 1677 | 1682 | rVB2 | 1180   | 1509   | 0.22%  | 0.027%  |
| 59 | 11.360 | 1684 | 1685 | 1689 | rBV2 | 233    | 288    | 0.04%  | 0.005%  |
| 60 | 11.439 | 1694 | 1698 | 1699 | rBV2 | 191    | 193    | 0.03%  | 0.004%  |
| 61 | 11.482 | 1699 | 1705 | 1709 | rBV4 | 696    | 916    | 0.13%  | 0.017%  |
| 62 | 11.524 | 1709 | 1712 | 1715 | rVB2 | 420    | 480    | 0.07%  | 0.009%  |
| 63 | 11.628 | 1727 | 1729 | 1732 | rBV3 | 231    | 290    | 0.04%  | 0.005%  |
| 64 | 11.683 | 1735 | 1738 | 1744 | rBV3 | 691    | 1046   | 0.15%  | 0.019%  |
| 65 | 11.738 | 1744 | 1747 | 1754 | rBV4 | 498    | 960    | 0.14%  | 0.017%  |
| 66 | 11.872 | 1765 | 1769 | 1773 | rBV4 | 517    | 872    | 0.13%  | 0.016%  |
| 67 | 11.933 | 1775 | 1779 | 1782 | rVB3 | 743    | 759    | 0.11%  | 0.014%  |
| 68 | 11.976 | 1782 | 1786 | 1788 | rBV4 | 683    | 837    | 0.12%  | 0.015%  |
| 69 | 12.024 | 1788 | 1794 | 1806 | rBV  | 442498 | 581763 | 84.46% | 10.599% |
| 70 | 12.122 | 1808 | 1810 | 1812 | rVV2 | 564    | 644    | 0.09%  | 0.012%  |
| 71 | 12.152 | 1812 | 1815 | 1820 | rVB4 | 2519   | 3791   | 0.55%  | 0.069%  |
| 72 | 12.195 | 1820 | 1822 | 1825 | rVB2 | 365    | 254    | 0.04%  | 0.005%  |
| 73 | 12.225 | 1825 | 1827 | 1828 | rBV2 | 202    | 197    | 0.03%  | 0.004%  |
| 74 | 12.262 | 1828 | 1833 | 1834 | rBV2 | 522    | 550    | 0.08%  | 0.010%  |
| 75 | 12.317 | 1837 | 1842 | 1856 | rVB  | 376562 | 497947 | 72.29% | 9.072%  |
| 76 | 12.433 | 1856 | 1861 | 1863 | rBV4 | 876    | 1215   | 0.18%  | 0.022%  |

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Instrument :  
 MSVOA\_X  
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 A4BR2ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

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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\SFAMXML070324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 12.463 | 1863 | 1866 | 1873 | rVB7 | 2486 | 4431 | 0.64% | 0.081% |
| 78  | 12.512 | 1873 | 1874 | 1877 | rVB2 | 482  | 262  | 0.04% | 0.005% |
| 79  | 12.573 | 1877 | 1884 | 1886 | rBV5 | 666  | 1286 | 0.19% | 0.023% |
| 80  | 12.628 | 1890 | 1893 | 1895 | rVB3 | 327  | 378  | 0.05% | 0.007% |
| 81  | 12.664 | 1896 | 1899 | 1901 | rBV3 | 811  | 1030 | 0.15% | 0.019% |
| 82  | 12.731 | 1909 | 1910 | 1913 | rBV3 | 373  | 436  | 0.06% | 0.008% |
| 83  | 12.762 | 1913 | 1915 | 1918 | rVB2 | 632  | 678  | 0.10% | 0.012% |
| 84  | 12.805 | 1918 | 1922 | 1923 | rBV4 | 987  | 1143 | 0.17% | 0.021% |
| 85  | 12.884 | 1932 | 1935 | 1936 | rBV2 | 434  | 424  | 0.06% | 0.008% |
| 86  | 13.000 | 1949 | 1954 | 1957 | rBV5 | 982  | 1826 | 0.27% | 0.033% |
| 87  | 13.055 | 1959 | 1963 | 1970 | rVB6 | 2080 | 3748 | 0.54% | 0.068% |
| 88  | 13.207 | 1983 | 1988 | 1992 | rBV7 | 1054 | 2167 | 0.31% | 0.039% |
| 89  | 13.292 | 2000 | 2002 | 2006 | rVB3 | 1573 | 1736 | 0.25% | 0.032% |
| 90  | 13.366 | 2011 | 2014 | 2016 | rBV4 | 754  | 746  | 0.11% | 0.014% |
| 91  | 13.414 | 2019 | 2022 | 2024 | rBV3 | 1860 | 2301 | 0.33% | 0.042% |
| 92  | 13.555 | 2042 | 2045 | 2048 | rBV4 | 710  | 671  | 0.10% | 0.012% |
| 93  | 13.701 | 2066 | 2069 | 2077 | rVB7 | 4012 | 6392 | 0.93% | 0.116% |
| 94  | 13.762 | 2077 | 2079 | 2080 | rBV2 | 1195 | 958  | 0.14% | 0.017% |
| 95  | 13.841 | 2089 | 2092 | 2095 | rBV5 | 3465 | 4428 | 0.64% | 0.081% |
| 96  | 13.987 | 2114 | 2116 | 2119 | rBV4 | 1773 | 1605 | 0.23% | 0.029% |
| 97  | 14.615 | 2216 | 2219 | 2225 | rBV6 | 4130 | 6034 | 0.88% | 0.110% |
| 98  | 14.756 | 2239 | 2242 | 2244 | rBV4 | 3132 | 3336 | 0.48% | 0.061% |
| 99  | 15.213 | 2314 | 2317 | 2322 | rVB6 | 4834 | 5640 | 0.82% | 0.103% |
| 100 | 15.743 | 2400 | 2404 | 2411 | rVB8 | 3947 | 7068 | 1.03% | 0.129% |

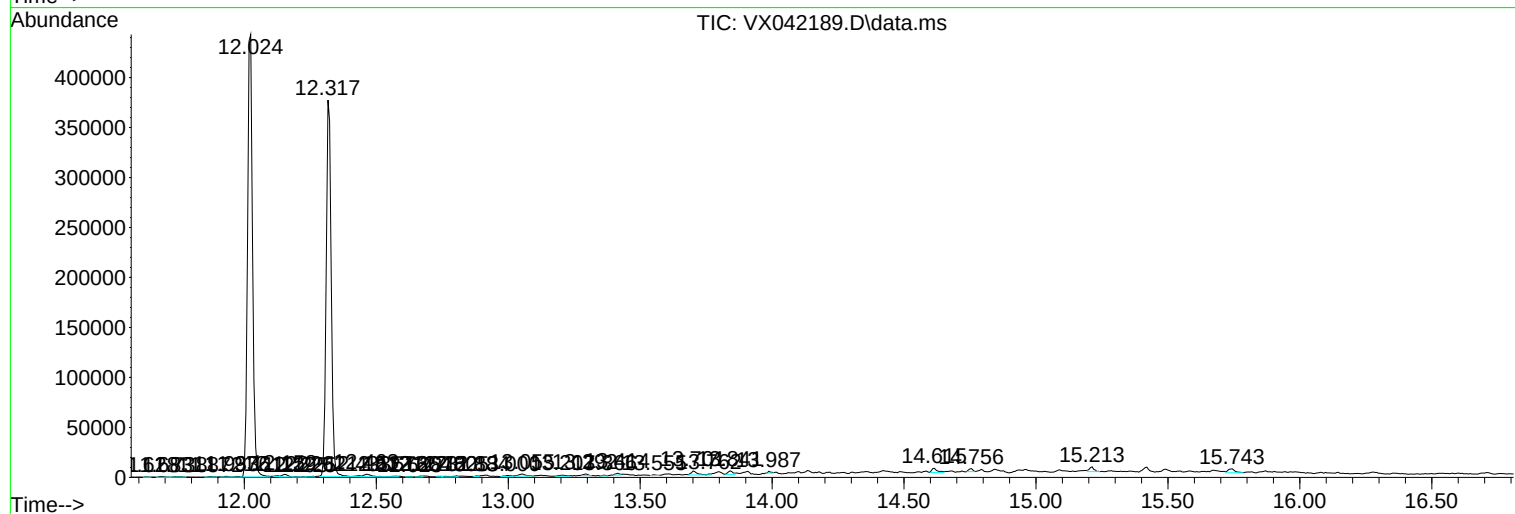
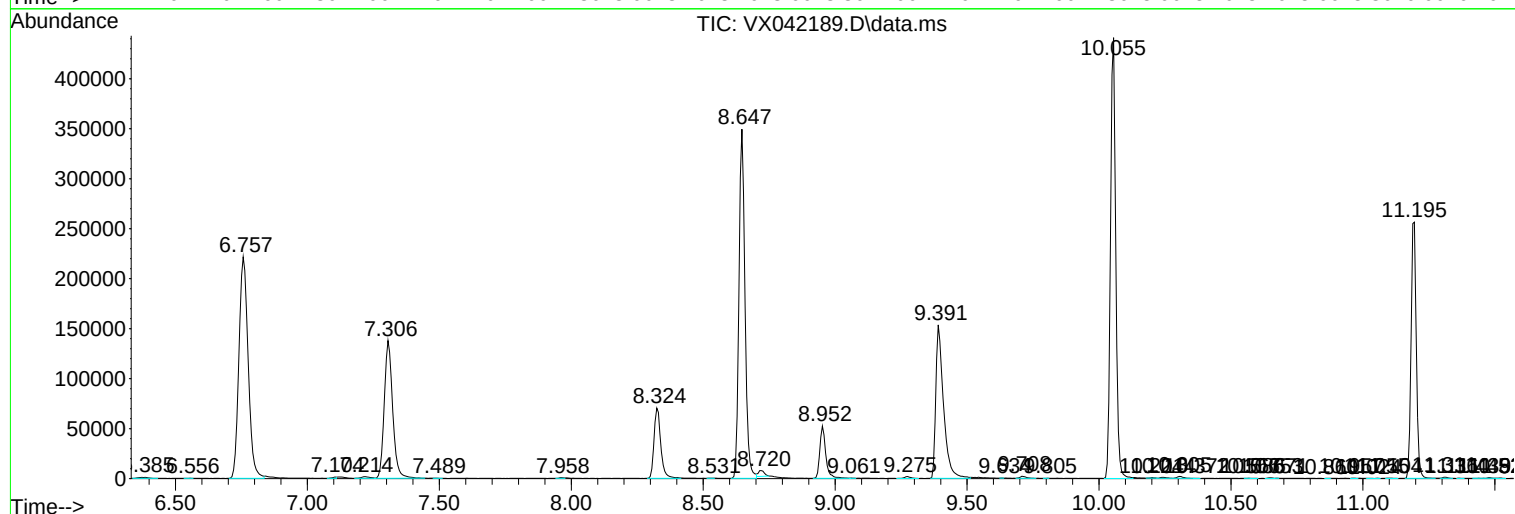
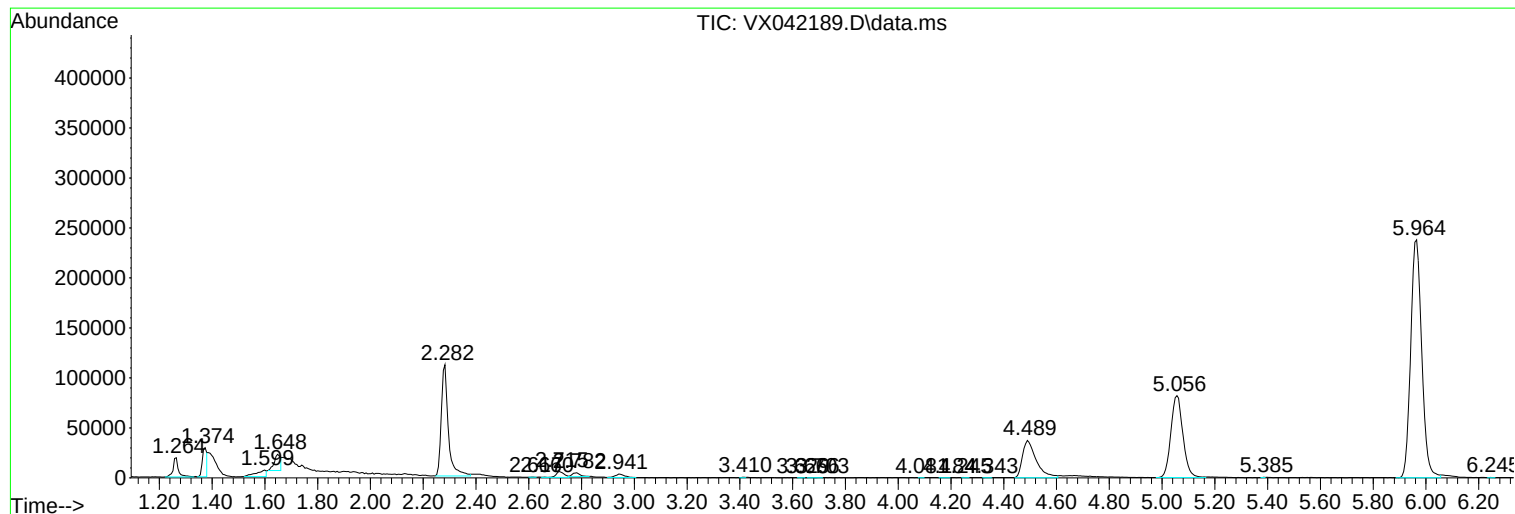
Sum of corrected areas: 5488917

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.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 |