

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042623\  
 Data File : VX035304.D  
 Acq On : 26 Apr 2023 11:45  
 Operator : JC/MD  
 Sample : 02479-03ME  
 Misc : 4.26g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EW944ME

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\SFAMXML041823WMA.M  
 Title : VOC Analysis

Signal : TIC: VX035304.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       | 26            | 29          | 33           | rBV3     | 2171           | 2761          | 0.16%           | 0.021%        |
| 2         | 1.368       | 42            | 46          | 69           | rVB      | 75197          | 172926        | 10.13%          | 1.316%        |
| 3         | 1.642       | 87            | 91          | 92           | rBV      | 2995           | 3144          | 0.18%           | 0.024%        |
| 4         | 1.672       | 92            | 96          | 100          | rBV      | 36690          | 58499         | 3.43%           | 0.445%        |
| 5         | 2.288       | 191           | 197         | 211          | rBV      | 316375         | 517196        | 30.29%          | 3.937%        |
| 6         | 2.715       | 261           | 267         | 271          | rVV2     | 1227           | 2207          | 0.13%           | 0.017%        |
| 7         | 2.782       | 273           | 278         | 286          | rVV5     | 3987           | 9431          | 0.55%           | 0.072%        |
| 8         | 3.428       | 378           | 384         | 392          | rVB6     | 1291           | 2804          | 0.16%           | 0.021%        |
| 9         | 4.477       | 547           | 556         | 578          | rBV      | 86889          | 317496        | 18.59%          | 2.417%        |
| 10        | 5.056       | 638           | 651         | 668          | rBV      | 204188         | 656401        | 38.44%          | 4.997%        |
| 11        | 5.550       | 725           | 732         | 737          | rBV2     | 1725           | 4039          | 0.24%           | 0.031%        |
| 12        | 5.964       | 788           | 800         | 824          | rVV2     | 591253         | 1707428       | 100.00%         | 12.999%       |
| 13        | 6.135       | 826           | 828         | 838          | rVB5     | 1008           | 2304          | 0.13%           | 0.018%        |
| 14        | 6.354       | 856           | 864         | 874          | rVV7     | 3648           | 10974         | 0.64%           | 0.084%        |
| 15        | 6.757       | 919           | 930         | 954          | rBV      | 466157         | 1111806       | 65.12%          | 8.464%        |
| 16        | 7.013       | 965           | 972         | 979          | rVV4     | 1123           | 2497          | 0.15%           | 0.019%        |
| 17        | 7.117       | 981           | 989         | 997          | rVV7     | 5357           | 15590         | 0.91%           | 0.119%        |
| 18        | 7.208       | 999           | 1004        | 1011         | rVV3     | 4300           | 10604         | 0.62%           | 0.081%        |
| 19        | 7.306       | 1011          | 1020        | 1040         | rVV      | 356102         | 798462        | 46.76%          | 6.079%        |
| 20        | 7.476       | 1045          | 1048        | 1056         | rVB6     | 1072           | 2493          | 0.15%           | 0.019%        |
| 21        | 7.769       | 1091          | 1096        | 1101         | rVB3     | 1246           | 2291          | 0.13%           | 0.017%        |
| 22        | 7.958       | 1120          | 1127        | 1141         | rBV6     | 4941           | 14506         | 0.85%           | 0.110%        |
| 23        | 8.324       | 1181          | 1187        | 1201         | rBV      | 205139         | 328085        | 19.22%          | 2.498%        |
| 24        | 8.433       | 1202          | 1205        | 1211         | rVB5     | 2329           | 4070          | 0.24%           | 0.031%        |
| 25        | 8.500       | 1211          | 1216        | 1226         | rVB6     | 1333           | 3450          | 0.20%           | 0.026%        |
| 26        | 8.598       | 1226          | 1232        | 1233         | rBV4     | 1769           | 2585          | 0.15%           | 0.020%        |
| 27        | 8.647       | 1233          | 1240        | 1248         | rBV      | 893257         | 1406873       | 82.40%          | 10.711%       |
| 28        | 8.720       | 1249          | 1252        | 1256         | rVB2     | 4831           | 6818          | 0.40%           | 0.052%        |
| 29        | 8.842       | 1270          | 1272        | 1279         | rVB4     | 1456           | 2236          | 0.13%           | 0.017%        |
| 30        | 8.952       | 1284          | 1290        | 1308         | rVB      | 136921         | 223034        | 13.06%          | 1.698%        |
| 31        | 9.110       | 1310          | 1316        | 1318         | rBV6     | 1484           | 2121          | 0.12%           | 0.016%        |
| 32        | 9.275       | 1338          | 1343        | 1349         | rBV4     | 5401           | 8289          | 0.49%           | 0.063%        |
| 33        | 9.391       | 1356          | 1362        | 1363         | rBV      | 141615         | 182100        | 10.67%          | 1.386%        |
| 34        | 9.421       | 1363          | 1367        | 1380         | rVB      | 276002         | 507531        | 29.72%          | 3.864%        |
| 35        | 9.561       | 1387          | 1390        | 1394         | rVB4     | 2701           | 3943          | 0.23%           | 0.030%        |
| 36        | 9.616       | 1394          | 1399        | 1403         | rBV2     | 6140           | 10186         | 0.60%           | 0.078%        |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EW944ME

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\SFAMXML041823WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 37 | 9.762  | 1419 | 1423 | 1426 | rVB5 | 1150    | 1704    | 0.10%  | 0.013% |
| 38 | 9.823  | 1428 | 1433 | 1436 | rBV4 | 1965    | 3609    | 0.21%  | 0.027% |
| 39 | 10.012 | 1457 | 1464 | 1465 | rBV4 | 1079    | 1863    | 0.11%  | 0.014% |
| 40 | 10.055 | 1465 | 1471 | 1482 | rBV  | 855625  | 1229798 | 72.03% | 9.362% |
| 41 | 10.305 | 1502 | 1512 | 1517 | rBV7 | 4767    | 10421   | 0.61%  | 0.079% |
| 42 | 10.360 | 1517 | 1521 | 1528 | rVB3 | 3461    | 5725    | 0.34%  | 0.044% |
| 43 | 10.457 | 1533 | 1537 | 1542 | rBV5 | 1334    | 2077    | 0.12%  | 0.016% |
| 44 | 10.561 | 1551 | 1554 | 1556 | rBV3 | 1121    | 1588    | 0.09%  | 0.012% |
| 45 | 10.585 | 1556 | 1558 | 1564 | rVB3 | 1478    | 1947    | 0.11%  | 0.015% |
| 46 | 10.646 | 1564 | 1568 | 1571 | rBV2 | 2123    | 3399    | 0.20%  | 0.026% |
| 47 | 10.781 | 1582 | 1590 | 1593 | rBV7 | 4820    | 7962    | 0.47%  | 0.061% |
| 48 | 10.860 | 1599 | 1603 | 1605 | rBV3 | 1944    | 2491    | 0.15%  | 0.019% |
| 49 | 10.890 | 1605 | 1608 | 1614 | rVB3 | 4343    | 6361    | 0.37%  | 0.048% |
| 50 | 10.951 | 1614 | 1618 | 1622 | rVB5 | 1637    | 2783    | 0.16%  | 0.021% |
| 51 | 11.000 | 1622 | 1626 | 1629 | rBV3 | 1079    | 1864    | 0.11%  | 0.014% |
| 52 | 11.085 | 1634 | 1640 | 1642 | rBV5 | 2973    | 5317    | 0.31%  | 0.040% |
| 53 | 11.201 | 1651 | 1659 | 1673 | rBV  | 514705  | 780538  | 45.71% | 5.942% |
| 54 | 11.323 | 1675 | 1679 | 1681 | rBV3 | 1229    | 1775    | 0.10%  | 0.014% |
| 55 | 11.390 | 1687 | 1690 | 1694 | rVB4 | 3527    | 4563    | 0.27%  | 0.035% |
| 56 | 11.433 | 1694 | 1697 | 1699 | rBV3 | 1479    | 2155    | 0.13%  | 0.016% |
| 57 | 11.476 | 1701 | 1704 | 1710 | rVB2 | 11210   | 14332   | 0.84%  | 0.109% |
| 58 | 11.628 | 1725 | 1729 | 1734 | rVB6 | 2512    | 4061    | 0.24%  | 0.031% |
| 59 | 11.683 | 1734 | 1738 | 1740 | rBV3 | 2305    | 3178    | 0.19%  | 0.024% |
| 60 | 11.713 | 1740 | 1743 | 1746 | rVV3 | 8024    | 9415    | 0.55%  | 0.072% |
| 61 | 11.750 | 1746 | 1749 | 1757 | rVB7 | 5864    | 13108   | 0.77%  | 0.100% |
| 62 | 11.890 | 1769 | 1772 | 1777 | rVB4 | 3499    | 4456    | 0.26%  | 0.034% |
| 63 | 11.951 | 1777 | 1782 | 1783 | rBV4 | 1474    | 2230    | 0.13%  | 0.017% |
| 64 | 11.969 | 1783 | 1785 | 1788 | rVB4 | 3325    | 3280    | 0.19%  | 0.025% |
| 65 | 12.024 | 1789 | 1794 | 1803 | rBV  | 981156  | 1226872 | 71.85% | 9.340% |
| 66 | 12.158 | 1812 | 1816 | 1822 | rVB6 | 4497    | 7548    | 0.44%  | 0.057% |
| 67 | 12.250 | 1827 | 1831 | 1836 | rBV6 | 2279    | 4597    | 0.27%  | 0.035% |
| 68 | 12.323 | 1837 | 1843 | 1854 | rVV  | 1003361 | 1264373 | 74.05% | 9.626% |
| 69 | 12.420 | 1856 | 1859 | 1863 | rVV  | 12594   | 14800   | 0.87%  | 0.113% |
| 70 | 12.463 | 1863 | 1866 | 1874 | rVB6 | 4369    | 8976    | 0.53%  | 0.068% |
| 71 | 12.530 | 1874 | 1877 | 1880 | rBV5 | 3184    | 5240    | 0.31%  | 0.040% |
| 72 | 12.683 | 1899 | 1902 | 1904 | rVB4 | 2921    | 2554    | 0.15%  | 0.019% |
| 73 | 12.762 | 1913 | 1915 | 1919 | rVB6 | 3106    | 3638    | 0.21%  | 0.028% |
| 74 | 12.884 | 1932 | 1935 | 1937 | rBV3 | 3562    | 4887    | 0.29%  | 0.037% |
| 75 | 12.969 | 1947 | 1949 | 1956 | rVB7 | 5585    | 9516    | 0.56%  | 0.072% |
| 76 | 13.042 | 1958 | 1961 | 1964 | rVB5 | 2181    | 2462    | 0.14%  | 0.019% |

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Instrument :  
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 EW944ME

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\SFAMXML041823WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 13.268 | 1994 | 1998 | 2001 | rBV  | 16336 | 21396 | 1.25% | 0.163% |
| 78  | 13.384 | 2013 | 2017 | 2020 | rBV  | 14206 | 16670 | 0.98% | 0.127% |
| 79  | 13.707 | 2066 | 2070 | 2073 | rBV5 | 5762  | 7228  | 0.42% | 0.055% |
| 80  | 13.780 | 2077 | 2082 | 2088 | rVB  | 17321 | 30279 | 1.77% | 0.231% |
| 81  | 13.841 | 2088 | 2092 | 2096 | rVB5 | 4936  | 6566  | 0.38% | 0.050% |
| 82  | 14.036 | 2121 | 2124 | 2127 | rVB  | 13892 | 15319 | 0.90% | 0.117% |
| 83  | 14.103 | 2133 | 2135 | 2138 | rVV4 | 4615  | 4353  | 0.25% | 0.033% |
| 84  | 14.134 | 2138 | 2140 | 2144 | rVB5 | 4445  | 5847  | 0.34% | 0.045% |
| 85  | 14.615 | 2216 | 2219 | 2220 | rBV3 | 4141  | 5015  | 0.29% | 0.038% |
| 86  | 14.640 | 2220 | 2223 | 2226 | rVB  | 16574 | 19414 | 1.14% | 0.148% |
| 87  | 14.755 | 2239 | 2242 | 2244 | rBV3 | 9228  | 13196 | 0.77% | 0.100% |
| 88  | 14.780 | 2244 | 2246 | 2251 | rVV  | 20998 | 25508 | 1.49% | 0.194% |
| 89  | 14.847 | 2255 | 2257 | 2260 | rVV4 | 4586  | 4428  | 0.26% | 0.034% |
| 90  | 14.883 | 2260 | 2263 | 2267 | rVB4 | 5193  | 6377  | 0.37% | 0.049% |
| 91  | 15.133 | 2300 | 2304 | 2307 | rBV2 | 6343  | 9627  | 0.56% | 0.073% |
| 92  | 15.408 | 2347 | 2349 | 2354 | rVB6 | 4824  | 6312  | 0.37% | 0.048% |
| 93  | 15.481 | 2356 | 2361 | 2367 | rBV3 | 12227 | 21669 | 1.27% | 0.165% |
| 94  | 15.615 | 2378 | 2383 | 2385 | rBV2 | 17147 | 26451 | 1.55% | 0.201% |
| 95  | 15.841 | 2411 | 2420 | 2428 | rVV7 | 6326  | 16991 | 1.00% | 0.129% |
| 96  | 15.981 | 2439 | 2443 | 2448 | rVB8 | 6151  | 10625 | 0.62% | 0.081% |
| 97  | 16.084 | 2458 | 2460 | 2466 | rVB5 | 2791  | 4068  | 0.24% | 0.031% |
| 98  | 16.328 | 2487 | 2500 | 2510 | rVB5 | 13580 | 40360 | 2.36% | 0.307% |
| 99  | 16.597 | 2541 | 2544 | 2550 | rVB7 | 3554  | 6184  | 0.36% | 0.047% |
| 100 | 16.664 | 2550 | 2555 | 2556 | rBV4 | 4657  | 6841  | 0.40% | 0.052% |

Sum of corrected areas: 13135367



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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
EW944ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXMLM041823WMA.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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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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