

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX070624\  
 Data File : VX042215.D  
 Acq On : 05 Jul 2024 16:52  
 Operator : JC/MD  
 Sample : P3087-13ME  
 Misc : 4.61g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 A4BP1ME

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: VX042215.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         | 1.258       | 23            | 28          | 33           | rBV2     | 14778          | 17813         | 2.84%           | 0.352%        |
| 2         | 1.368       | 43            | 46          | 48           | rBV      | 20578          | 25210         | 4.02%           | 0.498%        |
| 3         | 2.276       | 190           | 195         | 214          | rBV      | 97511          | 181511        | 28.97%          | 3.585%        |
| 4         | 2.721       | 262           | 268         | 273          | rBV      | 7698           | 15218         | 2.43%           | 0.301%        |
| 5         | 2.947       | 299           | 305         | 314          | rVB      | 3983           | 9624          | 1.54%           | 0.190%        |
| 6         | 3.050       | 318           | 322         | 324          | rBV2     | 161            | 262           | 0.04%           | 0.005%        |
| 7         | 3.075       | 324           | 326         | 331          | rVB2     | 282            | 370           | 0.06%           | 0.007%        |
| 8         | 3.276       | 356           | 359         | 362          | rBV      | 200            | 172           | 0.03%           | 0.003%        |
| 9         | 3.373       | 373           | 375         | 377          | rBV2     | 109            | 112           | 0.02%           | 0.002%        |
| 10        | 3.422       | 377           | 383         | 386          | rBV4     | 493            | 879           | 0.14%           | 0.017%        |
| 11        | 3.623       | 413           | 416         | 418          | rBV2     | 94             | 124           | 0.02%           | 0.002%        |
| 12        | 3.782       | 439           | 442         | 445          | rBV2     | 93             | 106           | 0.02%           | 0.002%        |
| 13        | 3.940       | 465           | 468         | 469          | rBV2     | 139            | 153           | 0.02%           | 0.003%        |
| 14        | 4.026       | 479           | 482         | 484          | rBV2     | 97             | 137           | 0.02%           | 0.003%        |
| 15        | 4.123       | 495           | 498         | 499          | rBV2     | 112            | 119           | 0.02%           | 0.002%        |
| 16        | 4.190       | 507           | 509         | 512          | rBV2     | 122            | 167           | 0.03%           | 0.003%        |
| 17        | 4.227       | 512           | 515         | 516          | rVB      | 189            | 170           | 0.03%           | 0.003%        |
| 18        | 4.391       | 538           | 542         | 547          | rBV2     | 129            | 308           | 0.05%           | 0.006%        |
| 19        | 4.489       | 549           | 558         | 576          | rBV      | 37903          | 129902        | 20.73%          | 2.566%        |
| 20        | 5.056       | 638           | 651         | 667          | rBV      | 74297          | 236566        | 37.75%          | 4.673%        |
| 21        | 5.391       | 700           | 706         | 707          | rBV2     | 961            | 1436          | 0.23%           | 0.028%        |
| 22        | 5.550       | 725           | 732         | 737          | rBV3     | 1752           | 4281          | 0.68%           | 0.085%        |
| 23        | 5.684       | 752           | 754         | 756          | rBV2     | 131            | 126           | 0.02%           | 0.002%        |
| 24        | 5.836       | 776           | 779         | 784          | rBV2     | 177            | 264           | 0.04%           | 0.005%        |
| 25        | 5.964       | 789           | 800         | 814          | rBV2     | 217570         | 626598        | 100.00%         | 12.377%       |
| 26        | 6.379       | 862           | 868         | 876          | rBV4     | 771            | 1922          | 0.31%           | 0.038%        |
| 27        | 6.489       | 884           | 886         | 887          | rBV      | 194            | 142           | 0.02%           | 0.003%        |
| 28        | 6.531       | 891           | 893         | 895          | rVB2     | 151            | 154           | 0.02%           | 0.003%        |
| 29        | 6.556       | 895           | 897         | 900          | rBV2     | 189            | 214           | 0.03%           | 0.004%        |
| 30        | 6.757       | 921           | 930         | 953          | rBV      | 217868         | 538430        | 85.93%          | 10.635%       |
| 31        | 7.117       | 984           | 989         | 999          | rVB7     | 1323           | 3776          | 0.60%           | 0.075%        |
| 32        | 7.220       | 999           | 1006        | 1012         | rBV3     | 1326           | 3184          | 0.51%           | 0.063%        |
| 33        | 7.312       | 1012          | 1021        | 1042         | rVB      | 121496         | 281507        | 44.93%          | 5.560%        |
| 34        | 7.653       | 1076          | 1077        | 1080         | rVB      | 157            | 114           | 0.02%           | 0.002%        |
| 35        | 7.726       | 1087          | 1089        | 1092         | rVV2     | 133            | 131           | 0.02%           | 0.003%        |
| 36        | 7.933       | 1119          | 1123        | 1124         | rBV2     | 111            | 132           | 0.02%           | 0.003%        |

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Integration Parameters: LSCINT.P

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Smoothing : OFF

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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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 7.970  | 1124 | 1129 | 1131 | rBV2 | 562    | 1063   | 0.17%  | 0.021%  |
| 38 | 8.238  | 1171 | 1173 | 1174 | rBV  | 190    | 193    | 0.03%  | 0.004%  |
| 39 | 8.263  | 1174 | 1177 | 1181 | rVV2 | 1306   | 1584   | 0.25%  | 0.031%  |
| 40 | 8.324  | 1181 | 1187 | 1205 | rVV  | 65853  | 119240 | 19.03% | 2.355%  |
| 41 | 8.507  | 1213 | 1217 | 1218 | rBV2 | 260    | 228    | 0.04%  | 0.005%  |
| 42 | 8.525  | 1218 | 1220 | 1226 | rVB4 | 363    | 471    | 0.08%  | 0.009%  |
| 43 | 8.647  | 1234 | 1240 | 1250 | rBV  | 319022 | 511015 | 81.55% | 10.094% |
| 44 | 8.952  | 1285 | 1290 | 1306 | rBV  | 48729  | 78766  | 12.57% | 1.556%  |
| 45 | 9.110  | 1314 | 1316 | 1319 | rBV2 | 348    | 279    | 0.04%  | 0.006%  |
| 46 | 9.275  | 1338 | 1343 | 1348 | rBV2 | 2077   | 3036   | 0.48%  | 0.060%  |
| 47 | 9.390  | 1357 | 1362 | 1381 | rBV  | 150275 | 303272 | 48.40% | 5.990%  |
| 48 | 9.683  | 1409 | 1410 | 1411 | rBV  | 335    | 176    | 0.03%  | 0.003%  |
| 49 | 9.714  | 1411 | 1415 | 1419 | rVB3 | 1226   | 2026   | 0.32%  | 0.040%  |
| 50 | 9.836  | 1433 | 1435 | 1438 | rVB  | 134    | 115    | 0.02%  | 0.002%  |
| 51 | 9.872  | 1438 | 1441 | 1442 | rBV2 | 149    | 147    | 0.02%  | 0.003%  |
| 52 | 9.909  | 1445 | 1447 | 1448 | rBV2 | 143    | 109    | 0.02%  | 0.002%  |
| 53 | 9.994  | 1457 | 1461 | 1462 | rBV2 | 205    | 183    | 0.03%  | 0.004%  |
| 54 | 10.055 | 1465 | 1471 | 1492 | rBV  | 435358 | 606044 | 96.72% | 11.971% |
| 55 | 10.201 | 1492 | 1495 | 1499 | rVV3 | 665    | 941    | 0.15%  | 0.019%  |
| 56 | 10.244 | 1499 | 1502 | 1508 | rVB2 | 1546   | 2243   | 0.36%  | 0.044%  |
| 57 | 10.311 | 1509 | 1513 | 1516 | rBV2 | 1956   | 2442   | 0.39%  | 0.048%  |
| 58 | 10.390 | 1524 | 1526 | 1530 | rVB2 | 129    | 159    | 0.03%  | 0.003%  |
| 59 | 10.537 | 1547 | 1550 | 1552 | rVB2 | 142    | 180    | 0.03%  | 0.004%  |
| 60 | 10.579 | 1554 | 1557 | 1560 | rBV  | 173    | 191    | 0.03%  | 0.004%  |
| 61 | 10.652 | 1565 | 1569 | 1573 | rBV4 | 567    | 1025   | 0.16%  | 0.020%  |
| 62 | 10.939 | 1611 | 1616 | 1617 | rBV2 | 228    | 256    | 0.04%  | 0.005%  |
| 63 | 11.012 | 1626 | 1628 | 1631 | rVB2 | 121    | 126    | 0.02%  | 0.002%  |
| 64 | 11.091 | 1637 | 1641 | 1647 | rVB3 | 1599   | 2545   | 0.41%  | 0.050%  |
| 65 | 11.195 | 1652 | 1658 | 1669 | rBV  | 250918 | 327035 | 52.19% | 6.460%  |
| 66 | 11.311 | 1674 | 1677 | 1682 | rVV3 | 1083   | 1343   | 0.21%  | 0.027%  |
| 67 | 11.372 | 1685 | 1687 | 1690 | rBV2 | 109    | 159    | 0.03%  | 0.003%  |
| 68 | 11.457 | 1697 | 1701 | 1704 | rBV3 | 318    | 614    | 0.10%  | 0.012%  |
| 69 | 11.622 | 1726 | 1728 | 1730 | rVV2 | 134    | 135    | 0.02%  | 0.003%  |
| 70 | 11.689 | 1737 | 1739 | 1743 | rVV  | 166    | 155    | 0.02%  | 0.003%  |
| 71 | 11.762 | 1747 | 1751 | 1754 | rVB2 | 478    | 567    | 0.09%  | 0.011%  |
| 72 | 11.829 | 1760 | 1762 | 1765 | rVB  | 127    | 110    | 0.02%  | 0.002%  |
| 73 | 11.951 | 1779 | 1782 | 1783 | rBV2 | 89     | 113    | 0.02%  | 0.002%  |
| 74 | 11.969 | 1783 | 1785 | 1789 | rBV  | 572    | 789    | 0.13%  | 0.016%  |
| 75 | 12.024 | 1789 | 1794 | 1805 | rVV  | 443371 | 555071 | 88.58% | 10.964% |
| 76 | 12.238 | 1827 | 1829 | 1831 | rVB2 | 350    | 288    | 0.05%  | 0.006%  |

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Instrument :  
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Integration Parameters: LSCINT.P

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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\SFAMXMLM070324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.323 | 1837 | 1843 | 1854 | rBV  | 347948 | 449131 | 71.68% | 8.871% |
| 78  | 12.530 | 1875 | 1877 | 1879 | rBV  | 202    | 219    | 0.03%  | 0.004% |
| 79  | 12.628 | 1891 | 1893 | 1896 | rVV2 | 130    | 142    | 0.02%  | 0.003% |
| 80  | 12.762 | 1913 | 1915 | 1921 | rVB3 | 446    | 516    | 0.08%  | 0.010% |
| 81  | 12.841 | 1926 | 1928 | 1932 | rVB2 | 92     | 130    | 0.02%  | 0.003% |
| 82  | 12.884 | 1932 | 1935 | 1940 | rVB2 | 241    | 292    | 0.05%  | 0.006% |
| 83  | 12.939 | 1942 | 1944 | 1946 | rVB  | 192    | 139    | 0.02%  | 0.003% |
| 84  | 13.030 | 1958 | 1959 | 1961 | rBV2 | 218    | 174    | 0.03%  | 0.003% |
| 85  | 13.048 | 1961 | 1962 | 1966 | rVV  | 251    | 214    | 0.03%  | 0.004% |
| 86  | 13.115 | 1971 | 1973 | 1980 | rVV3 | 314    | 496    | 0.08%  | 0.010% |
| 87  | 13.439 | 2024 | 2026 | 2029 | rBV2 | 115    | 157    | 0.03%  | 0.003% |
| 88  | 13.597 | 2049 | 2052 | 2056 | rVB3 | 506    | 666    | 0.11%  | 0.013% |
| 89  | 13.743 | 2074 | 2076 | 2077 | rBV2 | 127    | 105    | 0.02%  | 0.002% |
| 90  | 13.786 | 2077 | 2083 | 2087 | rVV2 | 815    | 1514   | 0.24%  | 0.030% |
| 91  | 13.841 | 2090 | 2092 | 2098 | rBV2 | 174    | 267    | 0.04%  | 0.005% |
| 92  | 13.963 | 2110 | 2112 | 2115 | rVB  | 591    | 681    | 0.11%  | 0.013% |
| 93  | 14.079 | 2129 | 2131 | 2134 | rBV2 | 166    | 240    | 0.04%  | 0.005% |
| 94  | 14.127 | 2136 | 2139 | 2141 | rBV  | 360    | 566    | 0.09%  | 0.011% |
| 95  | 14.182 | 2146 | 2148 | 2151 | rBV2 | 222    | 234    | 0.04%  | 0.005% |
| 96  | 14.274 | 2161 | 2163 | 2166 | rBV2 | 190    | 224    | 0.04%  | 0.004% |
| 97  | 14.341 | 2172 | 2174 | 2175 | rBV2 | 186    | 119    | 0.02%  | 0.002% |
| 98  | 14.414 | 2184 | 2186 | 2188 | rBV2 | 296    | 301    | 0.05%  | 0.006% |
| 99  | 14.530 | 2203 | 2205 | 2209 | rVB3 | 303    | 341    | 0.05%  | 0.007% |
| 100 | 14.841 | 2254 | 2256 | 2257 | rBV  | 262    | 141    | 0.02%  | 0.003% |

Sum of corrected areas: 5062777

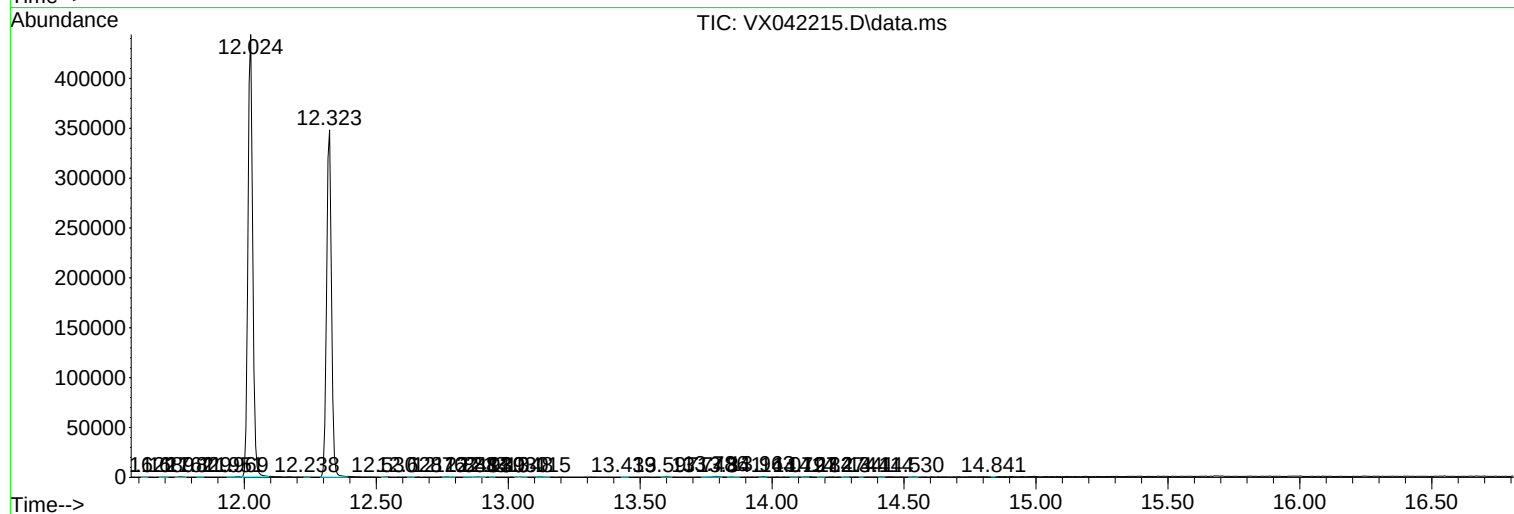
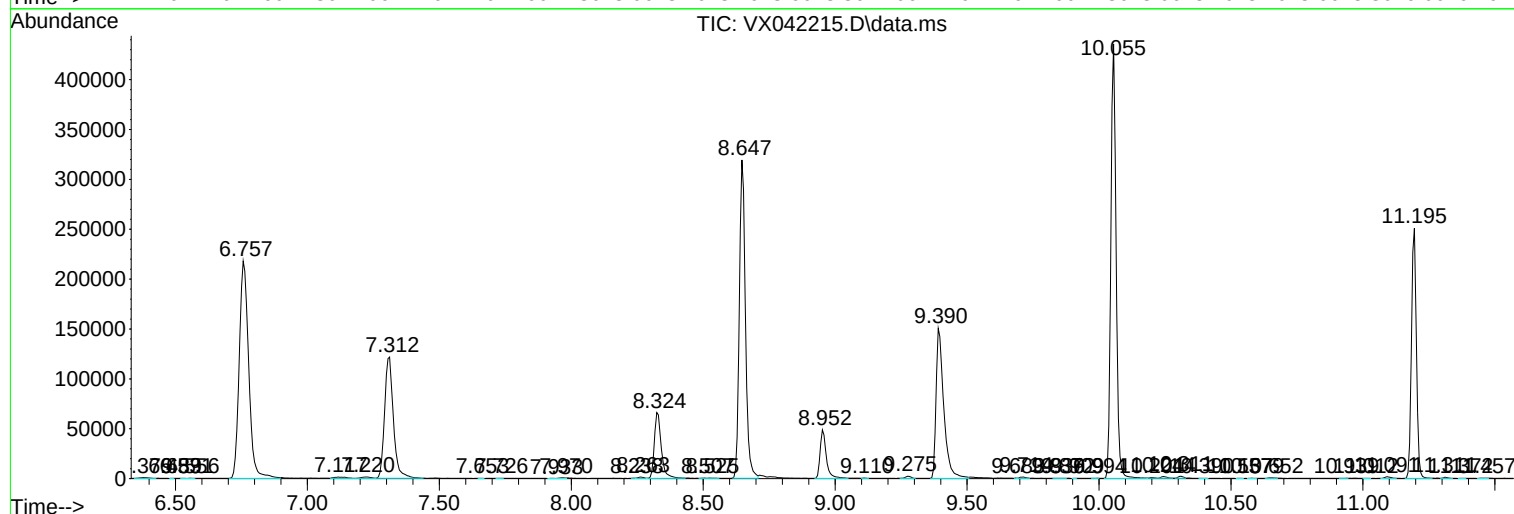
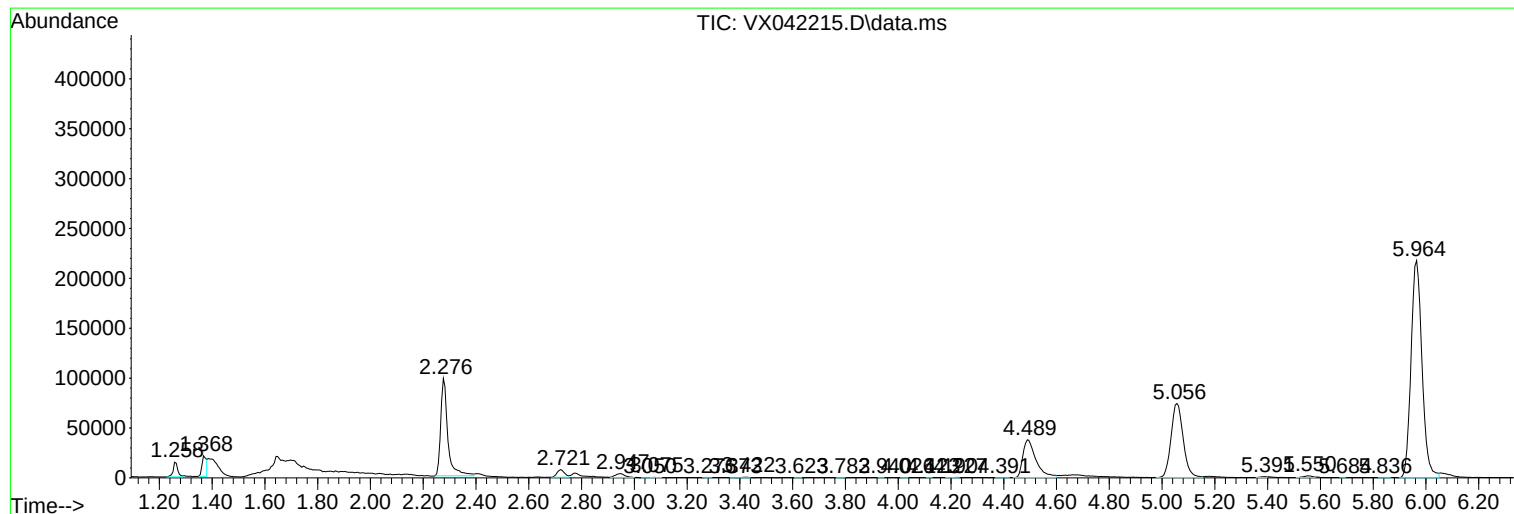
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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 |

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