

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121421\  
 Data File : VU046349.D  
 Acq On : 14 Dec 2021 12:43  
 Operator : SY/MD  
 Sample : M5002-14  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 5 Sample Multiplier: 1

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\_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046349.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         | 1.604       | 75            | 82          | 97           | rVB      | 67911          | 76875         | 15.34%          | 1.890%        |
| 2         | 1.919       | 172           | 180         | 198          | rVB      | 49917          | 66268         | 13.23%          | 1.629%        |
| 3         | 2.244       | 277           | 281         | 285          | rVB3     | 246            | 185           | 0.04%           | 0.005%        |
| 4         | 2.324       | 303           | 306         | 309          | rBV2     | 281            | 209           | 0.04%           | 0.005%        |
| 5         | 2.575       | 372           | 384         | 412          | rBV      | 107418         | 184614        | 36.85%          | 4.539%        |
| 6         | 2.771       | 441           | 445         | 447          | rBV      | 176            | 170           | 0.03%           | 0.004%        |
| 7         | 2.800       | 450           | 454         | 461          | rVB2     | 234            | 292           | 0.06%           | 0.007%        |
| 8         | 2.967       | 501           | 506         | 510          | rBV2     | 315            | 254           | 0.05%           | 0.006%        |
| 9         | 3.025       | 519           | 524         | 530          | rVB      | 117            | 129           | 0.03%           | 0.003%        |
| 10        | 3.054       | 530           | 533         | 540          | rVB3     | 474            | 425           | 0.08%           | 0.010%        |
| 11        | 3.105       | 547           | 549         | 552          | rBB      | 176            | 117           | 0.02%           | 0.003%        |
| 12        | 3.150       | 560           | 563         | 564          | rBV      | 178            | 119           | 0.02%           | 0.003%        |
| 13        | 3.186       | 564           | 574         | 576          | rBV2     | 1400           | 1738          | 0.35%           | 0.043%        |
| 14        | 3.263       | 594           | 598         | 600          | rBV      | 183            | 179           | 0.04%           | 0.004%        |
| 15        | 3.379       | 632           | 634         | 637          | rBV      | 152            | 121           | 0.02%           | 0.003%        |
| 16        | 3.530       | 677           | 681         | 684          | rBB      | 166            | 159           | 0.03%           | 0.004%        |
| 17        | 3.575       | 692           | 695         | 698          | rBV      | 178            | 159           | 0.03%           | 0.004%        |
| 18        | 3.658       | 718           | 721         | 725          | rBB      | 168            | 165           | 0.03%           | 0.004%        |
| 19        | 3.703       | 732           | 735         | 740          | rBV      | 155            | 197           | 0.04%           | 0.005%        |
| 20        | 3.855       | 777           | 782         | 785          | rBB      | 142            | 171           | 0.03%           | 0.004%        |
| 21        | 4.211       | 890           | 893         | 895          | rBV      | 144            | 126           | 0.03%           | 0.003%        |
| 22        | 4.646       | 1012          | 1028        | 1072         | rBV      | 41050          | 136609        | 27.27%          | 3.358%        |
| 23        | 4.848       | 1087          | 1091        | 1098         | rBV2     | 183            | 276           | 0.06%           | 0.007%        |
| 24        | 5.070       | 1143          | 1160        | 1178         | rBV      | 92762          | 203274        | 40.57%          | 4.997%        |
| 25        | 5.195       | 1195          | 1199        | 1201         | rBV      | 136            | 118           | 0.02%           | 0.003%        |
| 26        | 5.215       | 1203          | 1205        | 1208         | rVV2     | 195            | 139           | 0.03%           | 0.003%        |
| 27        | 5.285       | 1224          | 1227        | 1229         | rBV      | 267            | 197           | 0.04%           | 0.005%        |
| 28        | 5.350       | 1245          | 1247        | 1250         | rBV      | 243            | 168           | 0.03%           | 0.004%        |
| 29        | 5.401       | 1260          | 1263        | 1267         | rBV      | 136            | 162           | 0.03%           | 0.004%        |
| 30        | 5.729       | 1343          | 1365        | 1387         | rBV2     | 185730         | 500986        | 100.00%         | 12.316%       |
| 31        | 5.993       | 1444          | 1447        | 1449         | rBV      | 164            | 128           | 0.03%           | 0.003%        |
| 32        | 6.076       | 1471          | 1473        | 1477         | rBV      | 120            | 127           | 0.03%           | 0.003%        |
| 33        | 6.253       | 1514          | 1528        | 1547         | rBV      | 175986         | 329489        | 65.77%          | 8.100%        |
| 34        | 6.356       | 1557          | 1560        | 1564         | rVB2     | 204            | 170           | 0.03%           | 0.004%        |
| 35        | 6.588       | 1627          | 1632        | 1634         | rBV      | 170            | 181           | 0.04%           | 0.004%        |
| 36        | 6.633       | 1641          | 1646        | 1651         | rBV      | 151            | 243           | 0.05%           | 0.006%        |

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 ALS Vial : 5 Sample Multiplier: 1

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\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.694  | 1651 | 1665 | 1685 | rVV  | 117506 | 224955 | 44.90% | 5.530%  |
| 38 | 6.813  | 1699 | 1702 | 1705 | rBV2 | 259    | 241    | 0.05%  | 0.006%  |
| 39 | 7.031  | 1767 | 1770 | 1773 | rBV  | 169    | 178    | 0.04%  | 0.004%  |
| 40 | 7.108  | 1790 | 1794 | 1798 | rBV  | 138    | 184    | 0.04%  | 0.005%  |
| 41 | 7.147  | 1802 | 1806 | 1808 | rBV  | 152    | 147    | 0.03%  | 0.004%  |
| 42 | 7.179  | 1814 | 1816 | 1819 | rVB  | 218    | 130    | 0.03%  | 0.003%  |
| 43 | 7.211  | 1823 | 1826 | 1829 | rBV  | 174    | 161    | 0.03%  | 0.004%  |
| 44 | 7.276  | 1843 | 1846 | 1849 | rBV  | 146    | 148    | 0.03%  | 0.004%  |
| 45 | 7.443  | 1895 | 1898 | 1901 | rBB  | 174    | 138    | 0.03%  | 0.003%  |
| 46 | 7.491  | 1911 | 1913 | 1916 | rBV  | 143    | 123    | 0.02%  | 0.003%  |
| 47 | 7.568  | 1924 | 1937 | 1954 | rBV2 | 58666  | 101489 | 20.26% | 2.495%  |
| 48 | 7.899  | 2025 | 2040 | 2056 | rBV  | 223750 | 377980 | 75.45% | 9.292%  |
| 49 | 8.060  | 2088 | 2090 | 2096 | rBV  | 143    | 193    | 0.04%  | 0.005%  |
| 50 | 8.182  | 2116 | 2128 | 2142 | rBV  | 42922  | 70224  | 14.02% | 1.726%  |
| 51 | 8.234  | 2142 | 2144 | 2148 | rVB  | 327    | 223    | 0.04%  | 0.005%  |
| 52 | 8.298  | 2162 | 2164 | 2168 | rVB2 | 231    | 133    | 0.03%  | 0.003%  |
| 53 | 8.321  | 2169 | 2171 | 2174 | rBV  | 142    | 117    | 0.02%  | 0.003%  |
| 54 | 8.407  | 2194 | 2198 | 2200 | rBV  | 176    | 169    | 0.03%  | 0.004%  |
| 55 | 8.475  | 2208 | 2219 | 2232 | rBV  | 8274   | 14143  | 2.82%  | 0.348%  |
| 56 | 8.555  | 2242 | 2244 | 2249 | rBV2 | 154    | 154    | 0.03%  | 0.004%  |
| 57 | 8.636  | 2258 | 2269 | 2290 | rBV  | 148444 | 257539 | 51.41% | 6.331%  |
| 58 | 8.854  | 2332 | 2337 | 2342 | rBB  | 194    | 284    | 0.06%  | 0.007%  |
| 59 | 8.906  | 2348 | 2353 | 2356 | rBV  | 176    | 204    | 0.04%  | 0.005%  |
| 60 | 8.973  | 2368 | 2374 | 2378 | rBB  | 167    | 238    | 0.05%  | 0.006%  |
| 61 | 9.009  | 2382 | 2385 | 2388 | rBV  | 166    | 156    | 0.03%  | 0.004%  |
| 62 | 9.153  | 2425 | 2430 | 2436 | rBV  | 172    | 307    | 0.06%  | 0.008%  |
| 63 | 9.211  | 2445 | 2448 | 2453 | rBV  | 181    | 220    | 0.04%  | 0.005%  |
| 64 | 9.321  | 2479 | 2482 | 2485 | rBV  | 141    | 136    | 0.03%  | 0.003%  |
| 65 | 9.420  | 2500 | 2513 | 2533 | rBV  | 261665 | 436624 | 87.15% | 10.734% |
| 66 | 9.681  | 2591 | 2594 | 2596 | rBV  | 152    | 133    | 0.03%  | 0.003%  |
| 67 | 9.768  | 2618 | 2621 | 2626 | rVB  | 169    | 182    | 0.04%  | 0.004%  |
| 68 | 9.803  | 2627 | 2632 | 2634 | rBV  | 153    | 195    | 0.04%  | 0.005%  |
| 69 | 9.851  | 2642 | 2647 | 2650 | rBV  | 153    | 194    | 0.04%  | 0.005%  |
| 70 | 9.915  | 2661 | 2667 | 2670 | rBV  | 217    | 281    | 0.06%  | 0.007%  |
| 71 | 9.983  | 2685 | 2688 | 2692 | rBV  | 162    | 189    | 0.04%  | 0.005%  |
| 72 | 10.243 | 2767 | 2769 | 2774 | rBV  | 167    | 208    | 0.04%  | 0.005%  |
| 73 | 10.327 | 2791 | 2795 | 2800 | rBV  | 183    | 268    | 0.05%  | 0.007%  |
| 74 | 10.523 | 2852 | 2856 | 2861 | rBV  | 207    | 275    | 0.05%  | 0.007%  |
| 75 | 10.629 | 2886 | 2889 | 2893 | rVV  | 201    | 194    | 0.04%  | 0.005%  |
| 76 | 10.671 | 2897 | 2902 | 2909 | rVV2 | 658    | 814    | 0.16%  | 0.020%  |

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 ALS Vial : 5 Sample Multiplier: 1

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\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 10.758 | 2917 | 2929 | 2945 | rVB  | 173133 | 273332 | 54.56% | 6.720%  |
| 78  | 10.845 | 2953 | 2956 | 2960 | rBV  | 164    | 188    | 0.04%  | 0.005%  |
| 79  | 10.893 | 2961 | 2971 | 2981 | rVB  | 7231   | 11755  | 2.35%  | 0.289%  |
| 80  | 10.973 | 2987 | 2996 | 3002 | rBB  | 220    | 416    | 0.08%  | 0.010%  |
| 81  | 11.324 | 3100 | 3105 | 3108 | rBV  | 219    | 283    | 0.06%  | 0.007%  |
| 82  | 11.456 | 3140 | 3146 | 3148 | rBV  | 391    | 344    | 0.07%  | 0.008%  |
| 83  | 11.812 | 3245 | 3257 | 3274 | rBV  | 274194 | 422863 | 84.41% | 10.396% |
| 84  | 11.973 | 3302 | 3307 | 3313 | rVB  | 298    | 349    | 0.07%  | 0.009%  |
| 85  | 12.195 | 3363 | 3376 | 3391 | rBV  | 221000 | 354814 | 70.82% | 8.723%  |
| 86  | 12.771 | 3547 | 3555 | 3566 | rVB2 | 2184   | 3178   | 0.63%  | 0.078%  |
| 87  | 13.230 | 3696 | 3698 | 3703 | rVB  | 196    | 117    | 0.02%  | 0.003%  |
| 88  | 13.986 | 3930 | 3933 | 3940 | rBV  | 158    | 200    | 0.04%  | 0.005%  |
| 89  | 14.092 | 3960 | 3966 | 3972 | rVB  | 405    | 547    | 0.11%  | 0.013%  |
| 90  | 14.324 | 4035 | 4038 | 4046 | rVB  | 152    | 166    | 0.03%  | 0.004%  |
| 91  | 14.578 | 4105 | 4117 | 4127 | rBV2 | 1491   | 2623   | 0.52%  | 0.064%  |
| 92  | 15.381 | 4364 | 4367 | 4371 | rBV2 | 214    | 172    | 0.03%  | 0.004%  |
| 93  | 15.552 | 4417 | 4420 | 4422 | rBV  | 224    | 142    | 0.03%  | 0.003%  |
| 94  | 15.623 | 4438 | 4442 | 4446 | rVB2 | 254    | 250    | 0.05%  | 0.006%  |
| 95  | 15.684 | 4457 | 4461 | 4464 | rBV2 | 218    | 182    | 0.04%  | 0.004%  |
| 96  | 16.179 | 4611 | 4615 | 4616 | rBV2 | 369    | 270    | 0.05%  | 0.007%  |
| 97  | 16.372 | 4672 | 4675 | 4676 | rBV  | 258    | 136    | 0.03%  | 0.003%  |
| 98  | 16.500 | 4713 | 4715 | 4718 | rBV2 | 273    | 126    | 0.03%  | 0.003%  |
| 99  | 16.668 | 4764 | 4767 | 4769 | rBV3 | 213    | 152    | 0.03%  | 0.004%  |
| 100 | 17.018 | 4874 | 4876 | 4879 | rBV2 | 361    | 257    | 0.05%  | 0.006%  |

Sum of corrected areas: 4067672



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ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.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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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU121421\  
Data File : VU046349.D  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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

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

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