

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU052424\  
 Data File : VU058983.D  
 Acq On : 24 May 2024 20:13  
 Operator : MD/SY  
 Sample : P2566-13 1000X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BHHS0

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\SFAMULM052324WMA.M

Title : VOC Analysis

Signal : TIC: VU058983.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         | 1.592       | 86            | 94          | 110          | rBV      | 104521         | 124741        | 14.55%          | 1.983%        |
| 2         | 1.827       | 139           | 167         | 175          | rBV4     | 52522          | 185247        | 21.60%          | 2.945%        |
| 3         | 1.885       | 177           | 185         | 205          | rVB      | 84332          | 121948        | 14.22%          | 1.939%        |
| 4         | 2.502       | 373           | 377         | 381          | rBV2     | 369            | 337           | 0.04%           | 0.005%        |
| 5         | 2.554       | 381           | 393         | 409          | rBV      | 157928         | 256500        | 29.91%          | 4.077%        |
| 6         | 2.676       | 429           | 431         | 435          | rBV2     | 447            | 348           | 0.04%           | 0.006%        |
| 7         | 2.750       | 451           | 454         | 455          | rVV      | 455            | 306           | 0.04%           | 0.005%        |
| 8         | 2.779       | 455           | 463         | 474          | rVB4     | 1499           | 2925          | 0.34%           | 0.046%        |
| 9         | 3.033       | 533           | 542         | 553          | rVB3     | 4731           | 7995          | 0.93%           | 0.127%        |
| 10        | 3.174       | 572           | 586         | 605          | rVB      | 14963          | 34919         | 4.07%           | 0.555%        |
| 11        | 3.348       | 637           | 640         | 645          | rVB2     | 257            | 225           | 0.03%           | 0.004%        |
| 12        | 3.435       | 663           | 667         | 673          | rVB2     | 229            | 193           | 0.02%           | 0.003%        |
| 13        | 3.512       | 685           | 691         | 695          | rBV2     | 262            | 340           | 0.04%           | 0.005%        |
| 14        | 3.644       | 726           | 732         | 736          | rBV2     | 248            | 211           | 0.02%           | 0.003%        |
| 15        | 3.962       | 829           | 831         | 838          | rVB2     | 266            | 255           | 0.03%           | 0.004%        |
| 16        | 4.004       | 838           | 844         | 847          | rBV      | 295            | 306           | 0.04%           | 0.005%        |
| 17        | 4.062       | 858           | 862         | 865          | rBV2     | 229            | 204           | 0.02%           | 0.003%        |
| 18        | 4.116       | 875           | 879         | 886          | rVB2     | 251            | 305           | 0.04%           | 0.005%        |
| 19        | 4.203       | 900           | 906         | 910          | rVB      | 255            | 255           | 0.03%           | 0.004%        |
| 20        | 4.367       | 953           | 957         | 961          | rVB2     | 237            | 233           | 0.03%           | 0.004%        |
| 21        | 4.409       | 961           | 970         | 972          | rBV      | 239            | 257           | 0.03%           | 0.004%        |
| 22        | 4.608       | 1019          | 1032        | 1063         | rBV      | 98413          | 243994        | 28.46%          | 3.879%        |
| 23        | 5.052       | 1153          | 1170        | 1198         | rVB      | 156139         | 341566        | 39.84%          | 5.430%        |
| 24        | 5.235       | 1222          | 1227        | 1230         | rBV2     | 406            | 330           | 0.04%           | 0.005%        |
| 25        | 5.287       | 1238          | 1243        | 1245         | rBV3     | 286            | 218           | 0.03%           | 0.003%        |
| 26        | 5.348       | 1259          | 1262        | 1264         | rVB3     | 318            | 194           | 0.02%           | 0.003%        |
| 27        | 5.473       | 1297          | 1301        | 1305         | rBV2     | 250            | 303           | 0.04%           | 0.005%        |
| 28        | 5.541       | 1319          | 1322        | 1325         | rVB      | 285            | 203           | 0.02%           | 0.003%        |
| 29        | 5.714       | 1353          | 1376        | 1401         | rBV2     | 311216         | 857439        | 100.00%         | 13.630%       |
| 30        | 5.853       | 1417          | 1419        | 1425         | rVB3     | 265            | 197           | 0.02%           | 0.003%        |
| 31        | 5.923       | 1438          | 1441        | 1444         | rBV2     | 350            | 301           | 0.04%           | 0.005%        |
| 32        | 5.981       | 1455          | 1459        | 1462         | rVB      | 442            | 346           | 0.04%           | 0.006%        |
| 33        | 6.242       | 1528          | 1540        | 1559         | rBV      | 210286         | 408073        | 47.59%          | 6.487%        |
| 34        | 6.354       | 1572          | 1575        | 1579         | rVB3     | 373            | 241           | 0.03%           | 0.004%        |
| 35        | 6.460       | 1602          | 1608        | 1617         | rVB3     | 328            | 437           | 0.05%           | 0.007%        |
| 36        | 6.531       | 1620          | 1630        | 1645         | rVB7     | 5911           | 12541         | 1.46%           | 0.199%        |

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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\SFAMULM052324WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.682  | 1662 | 1677 | 1697 | rBV  | 205281 | 399049 | 46.54% | 6.343% |
| 38 | 6.811  | 1714 | 1717 | 1718 | rBV2 | 340    | 212    | 0.02%  | 0.003% |
| 39 | 7.094  | 1800 | 1805 | 1808 | rVB2 | 205    | 199    | 0.02%  | 0.003% |
| 40 | 7.197  | 1831 | 1837 | 1840 | rBV3 | 236    | 299    | 0.03%  | 0.005% |
| 41 | 7.258  | 1853 | 1856 | 1860 | rBV2 | 228    | 220    | 0.03%  | 0.003% |
| 42 | 7.389  | 1893 | 1897 | 1908 | rVB2 | 302    | 592    | 0.07%  | 0.009% |
| 43 | 7.447  | 1908 | 1915 | 1917 | rBV2 | 205    | 220    | 0.03%  | 0.003% |
| 44 | 7.515  | 1930 | 1936 | 1939 | rBV2 | 248    | 223    | 0.03%  | 0.004% |
| 45 | 7.560  | 1939 | 1950 | 1968 | rBV  | 96840  | 173766 | 20.27% | 2.762% |
| 46 | 7.656  | 1978 | 1980 | 1990 | rBV3 | 459    | 470    | 0.05%  | 0.007% |
| 47 | 7.779  | 2013 | 2018 | 2024 | rVB4 | 704    | 789    | 0.09%  | 0.013% |
| 48 | 7.891  | 2040 | 2053 | 2077 | rBV  | 341448 | 599003 | 69.86% | 9.522% |
| 49 | 8.094  | 2113 | 2116 | 2118 | rBV2 | 286    | 224    | 0.03%  | 0.004% |
| 50 | 8.107  | 2118 | 2120 | 2124 | rVV4 | 340    | 203    | 0.02%  | 0.003% |
| 51 | 8.174  | 2129 | 2141 | 2163 | rBV  | 67012  | 115806 | 13.51% | 1.841% |
| 52 | 8.422  | 2215 | 2218 | 2225 | rVB  | 232    | 241    | 0.03%  | 0.004% |
| 53 | 8.473  | 2225 | 2234 | 2240 | rBV3 | 694    | 1192   | 0.14%  | 0.019% |
| 54 | 8.512  | 2240 | 2246 | 2250 | rBV  | 249    | 249    | 0.03%  | 0.004% |
| 55 | 8.627  | 2269 | 2282 | 2307 | rBV  | 265294 | 489423 | 57.08% | 7.780% |
| 56 | 8.939  | 2377 | 2379 | 2385 | rVV2 | 398    | 289    | 0.03%  | 0.005% |
| 57 | 9.213  | 2461 | 2464 | 2468 | rVB2 | 291    | 235    | 0.03%  | 0.004% |
| 58 | 9.287  | 2484 | 2487 | 2493 | rVB  | 285    | 267    | 0.03%  | 0.004% |
| 59 | 9.412  | 2513 | 2526 | 2549 | rBV  | 300908 | 506871 | 59.11% | 8.057% |
| 60 | 9.560  | 2568 | 2572 | 2574 | rBV  | 435    | 338    | 0.04%  | 0.005% |
| 61 | 9.576  | 2574 | 2577 | 2583 | rVB2 | 760    | 572    | 0.07%  | 0.009% |
| 62 | 9.685  | 2606 | 2611 | 2612 | rBV2 | 581    | 439    | 0.05%  | 0.007% |
| 63 | 9.740  | 2625 | 2628 | 2632 | rBV  | 272    | 242    | 0.03%  | 0.004% |
| 64 | 9.955  | 2687 | 2695 | 2698 | rBV2 | 334    | 442    | 0.05%  | 0.007% |
| 65 | 10.103 | 2736 | 2741 | 2745 | rBV3 | 306    | 338    | 0.04%  | 0.005% |
| 66 | 10.171 | 2754 | 2762 | 2765 | rBV2 | 242    | 302    | 0.04%  | 0.005% |
| 67 | 10.216 | 2773 | 2776 | 2782 | rVB2 | 195    | 211    | 0.02%  | 0.003% |
| 68 | 10.248 | 2782 | 2786 | 2794 | rBV  | 215    | 258    | 0.03%  | 0.004% |
| 69 | 10.434 | 2841 | 2844 | 2850 | rVB2 | 348    | 249    | 0.03%  | 0.004% |
| 70 | 10.692 | 2920 | 2924 | 2928 | rVB2 | 269    | 238    | 0.03%  | 0.004% |
| 71 | 10.749 | 2928 | 2942 | 2966 | rBV  | 286801 | 471059 | 54.94% | 7.488% |
| 72 | 10.878 | 2977 | 2982 | 2985 | rBV3 | 446    | 457    | 0.05%  | 0.007% |
| 73 | 10.894 | 2985 | 2987 | 2990 | rVV  | 432    | 226    | 0.03%  | 0.004% |
| 74 | 11.219 | 3085 | 3088 | 3091 | rBV  | 257    | 205    | 0.02%  | 0.003% |
| 75 | 11.383 | 3136 | 3139 | 3145 | rVB  | 380    | 389    | 0.05%  | 0.006% |
| 76 | 11.627 | 3212 | 3215 | 3216 | rBV  | 360    | 213    | 0.02%  | 0.003% |

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Integration Parameters: LSCINT.P

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.807 | 3260 | 3271 | 3293 | rBV  | 261176 | 418860 | 48.85% | 6.658% |
| 78  | 11.962 | 3317 | 3319 | 3325 | rVB2 | 447    | 387    | 0.05%  | 0.006% |
| 79  | 12.032 | 3339 | 3341 | 3348 | rVB2 | 322    | 272    | 0.03%  | 0.004% |
| 80  | 12.187 | 3377 | 3389 | 3407 | rBV  | 292586 | 492580 | 57.45% | 7.830% |
| 81  | 12.367 | 3442 | 3445 | 3449 | rVB2 | 408    | 283    | 0.03%  | 0.004% |
| 82  | 12.393 | 3449 | 3453 | 3458 | rBV2 | 643    | 526    | 0.06%  | 0.008% |
| 83  | 12.672 | 3538 | 3540 | 3545 | rVB  | 417    | 293    | 0.03%  | 0.005% |
| 84  | 12.701 | 3545 | 3549 | 3552 | rBV  | 252    | 206    | 0.02%  | 0.003% |
| 85  | 12.765 | 3560 | 3569 | 3575 | rVB3 | 886    | 1314   | 0.15%  | 0.021% |
| 86  | 12.798 | 3575 | 3579 | 3584 | rBV  | 489    | 504    | 0.06%  | 0.008% |
| 87  | 12.974 | 3630 | 3634 | 3637 | rBV  | 332    | 250    | 0.03%  | 0.004% |
| 88  | 13.100 | 3670 | 3673 | 3679 | rVB  | 330    | 224    | 0.03%  | 0.004% |
| 89  | 13.212 | 3703 | 3708 | 3709 | rBV  | 410    | 327    | 0.04%  | 0.005% |
| 90  | 13.640 | 3838 | 3841 | 3844 | rBV2 | 359    | 216    | 0.03%  | 0.003% |
| 91  | 13.801 | 3888 | 3891 | 3898 | rVB  | 412    | 411    | 0.05%  | 0.007% |
| 92  | 14.019 | 3956 | 3959 | 3961 | rBV  | 404    | 273    | 0.03%  | 0.004% |
| 93  | 14.161 | 4000 | 4003 | 4008 | rBV3 | 434    | 352    | 0.04%  | 0.006% |
| 94  | 14.325 | 4050 | 4054 | 4057 | rBV3 | 369    | 367    | 0.04%  | 0.006% |
| 95  | 14.392 | 4072 | 4075 | 4078 | rBV2 | 352    | 280    | 0.03%  | 0.004% |
| 96  | 14.486 | 4101 | 4104 | 4113 | rVB2 | 657    | 885    | 0.10%  | 0.014% |
| 97  | 14.740 | 4179 | 4183 | 4184 | rBV2 | 319    | 254    | 0.03%  | 0.004% |
| 98  | 15.039 | 4273 | 4276 | 4279 | rBV2 | 441    | 342    | 0.04%  | 0.005% |
| 99  | 15.945 | 4555 | 4558 | 4559 | rBV  | 583    | 377    | 0.04%  | 0.006% |
| 100 | 16.145 | 4618 | 4620 | 4623 | rBV2 | 533    | 284    | 0.03%  | 0.005% |

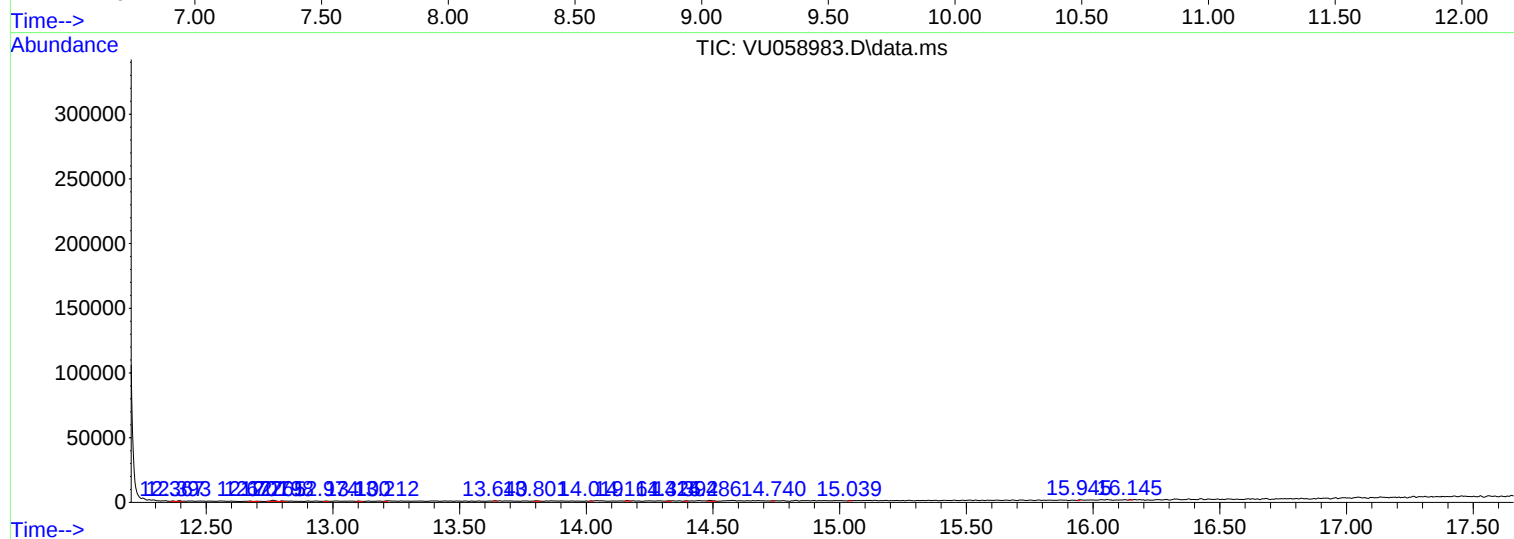
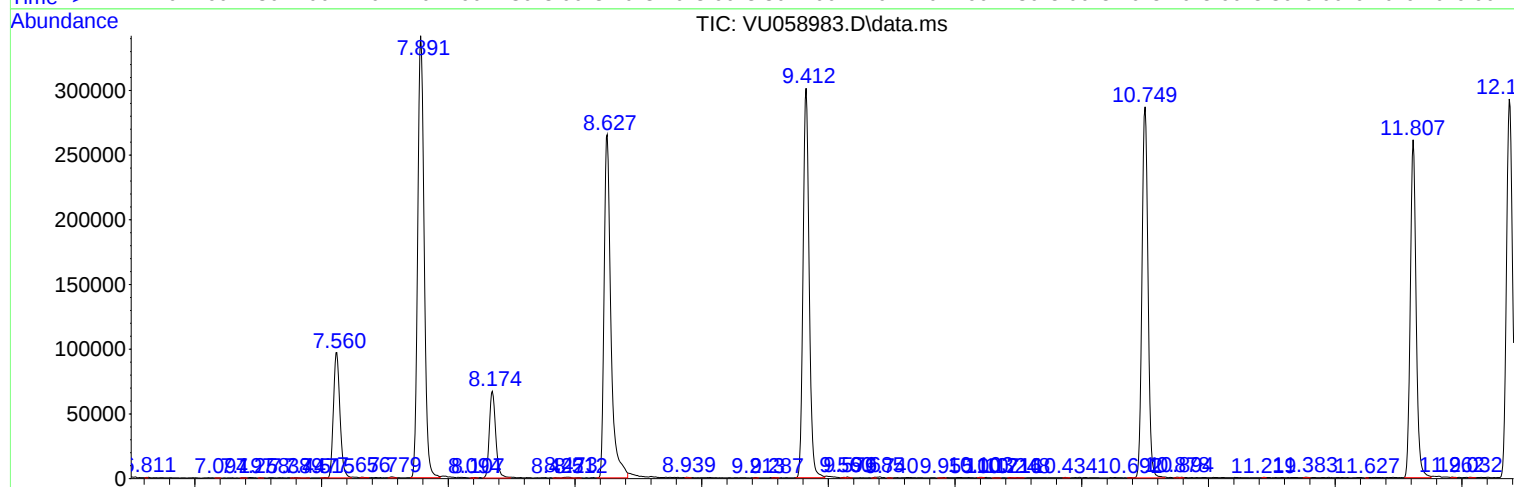
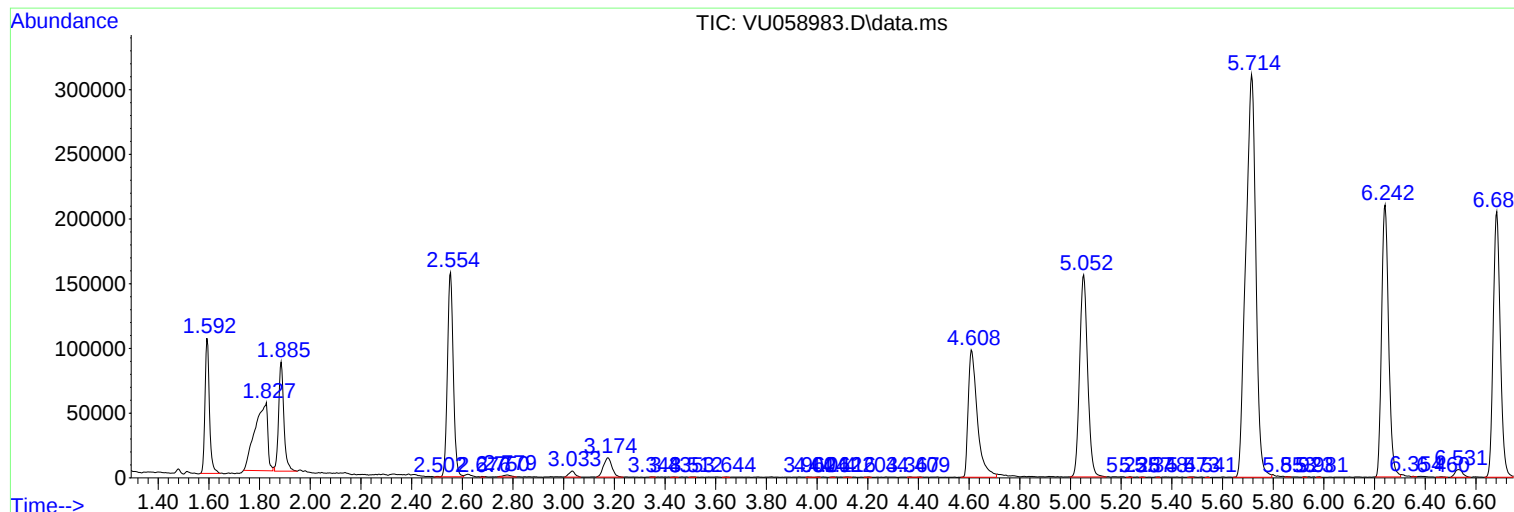
Sum of corrected areas: 6290720

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052324WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU052424\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM052324WMA.M  
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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 | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|