

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU022224\  
 Data File : VU057930.D  
 Acq On : 22 Feb 2024 17:22  
 Operator : MD/SY  
 Sample : P1567-07  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 JWAB5

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\SFAMULM021924WMA.M

Title : VOC Analysis

Signal : TIC: VU057930.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       | 87            | 94          | 115          | rVB      | 109359         | 127687        | 14.29%          | 1.790%        |
| 2         | 1.907       | 183           | 192         | 207          | rVB      | 89047          | 116276        | 13.01%          | 1.630%        |
| 3         | 2.399       | 342           | 345         | 351          | rBV2     | 910            | 843           | 0.09%           | 0.012%        |
| 4         | 2.560       | 383           | 395         | 407          | rBV      | 177249         | 289645        | 32.41%          | 4.061%        |
| 5         | 2.615       | 407           | 412         | 428          | rVB      | 8113           | 14249         | 1.59%           | 0.200%        |
| 6         | 2.740       | 440           | 451         | 461          | rBV2     | 5117           | 10053         | 1.12%           | 0.141%        |
| 7         | 2.943       | 511           | 514         | 519          | rBV3     | 517            | 508           | 0.06%           | 0.007%        |
| 8         | 3.039       | 536           | 544         | 552          | rVB2     | 1331           | 1991          | 0.22%           | 0.028%        |
| 9         | 3.171       | 571           | 585         | 590          | rBV6     | 2172           | 4641          | 0.52%           | 0.065%        |
| 10        | 3.264       | 611           | 614         | 618          | rBV2     | 227            | 256           | 0.03%           | 0.004%        |
| 11        | 3.316       | 627           | 630         | 637          | rVB2     | 229            | 272           | 0.03%           | 0.004%        |
| 12        | 3.354       | 637           | 642         | 645          | rBV2     | 436            | 379           | 0.04%           | 0.005%        |
| 13        | 3.441       | 667           | 669         | 673          | rVB2     | 208            | 158           | 0.02%           | 0.002%        |
| 14        | 3.467       | 673           | 677         | 680          | rBV      | 232            | 226           | 0.03%           | 0.003%        |
| 15        | 3.708       | 748           | 752         | 755          | rBV2     | 230            | 215           | 0.02%           | 0.003%        |
| 16        | 3.743       | 760           | 763         | 768          | rBV      | 192            | 201           | 0.02%           | 0.003%        |
| 17        | 3.840       | 788           | 793         | 795          | rBV      | 172            | 174           | 0.02%           | 0.002%        |
| 18        | 4.094       | 867           | 872         | 878          | rVB2     | 302            | 378           | 0.04%           | 0.005%        |
| 19        | 4.136       | 878           | 885         | 887          | rBV2     | 156            | 170           | 0.02%           | 0.002%        |
| 20        | 4.284       | 927           | 931         | 935          | rVB2     | 207            | 172           | 0.02%           | 0.002%        |
| 21        | 4.374       | 956           | 959         | 965          | rVV2     | 170            | 213           | 0.02%           | 0.003%        |
| 22        | 4.457       | 983           | 985         | 992          | rVB2     | 198            | 188           | 0.02%           | 0.003%        |
| 23        | 4.566       | 1016          | 1019        | 1022         | rVB      | 243            | 161           | 0.02%           | 0.002%        |
| 24        | 4.611       | 1022          | 1033        | 1064         | rBV2     | 58178          | 158082        | 17.69%          | 2.216%        |
| 25        | 5.052       | 1154          | 1170        | 1191         | rBV      | 159943         | 353324        | 39.54%          | 4.954%        |
| 26        | 5.271       | 1235          | 1238        | 1241         | rVB3     | 293            | 160           | 0.02%           | 0.002%        |
| 27        | 5.364       | 1265          | 1267        | 1270         | rBV2     | 266            | 186           | 0.02%           | 0.003%        |
| 28        | 5.492       | 1303          | 1307        | 1310         | rBV      | 173            | 153           | 0.02%           | 0.002%        |
| 29        | 5.534       | 1315          | 1320        | 1324         | rBV2     | 163            | 145           | 0.02%           | 0.002%        |
| 30        | 5.624       | 1343          | 1348        | 1351         | rBV      | 155            | 143           | 0.02%           | 0.002%        |
| 31        | 5.714       | 1356          | 1376        | 1413         | rBV2     | 320461         | 893672        | 100.00%         | 12.530%       |
| 32        | 6.045       | 1476          | 1479        | 1483         | rVB      | 464            | 347           | 0.04%           | 0.005%        |
| 33        | 6.074       | 1483          | 1488        | 1492         | rVB3     | 245            | 204           | 0.02%           | 0.003%        |
| 34        | 6.116       | 1492          | 1501        | 1502         | rBV2     | 356            | 402           | 0.04%           | 0.006%        |
| 35        | 6.242       | 1527          | 1540        | 1569         | rBV      | 348765         | 678974        | 75.98%          | 9.520%        |
| 36        | 6.537       | 1623          | 1632        | 1647         | rVB5     | 6736           | 12839         | 1.44%           | 0.180%        |

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Integration Parameters: LSCINT.P

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Smoothing : OFF

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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\_U\Method\SFAMULM021924WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.682  | 1662 | 1677 | 1706 | rBV  | 202874 | 405265 | 45.35% | 5.682%  |
| 38 | 7.058  | 1788 | 1794 | 1799 | rBV2 | 228    | 380    | 0.04%  | 0.005%  |
| 39 | 7.119  | 1810 | 1813 | 1816 | rVB2 | 275    | 190    | 0.02%  | 0.003%  |
| 40 | 7.148  | 1816 | 1822 | 1829 | rBV2 | 331    | 466    | 0.05%  | 0.007%  |
| 41 | 7.312  | 1866 | 1873 | 1878 | rBV2 | 149    | 231    | 0.03%  | 0.003%  |
| 42 | 7.454  | 1914 | 1917 | 1923 | rVB  | 269    | 283    | 0.03%  | 0.004%  |
| 43 | 7.560  | 1938 | 1950 | 1980 | rBV2 | 110437 | 201390 | 22.54% | 2.824%  |
| 44 | 7.705  | 1993 | 1995 | 2005 | rVB5 | 908    | 1010   | 0.11%  | 0.014%  |
| 45 | 7.785  | 2017 | 2020 | 2023 | rBV  | 280    | 217    | 0.02%  | 0.003%  |
| 46 | 7.891  | 2041 | 2053 | 2071 | rBV  | 389680 | 690754 | 77.29% | 9.685%  |
| 47 | 8.174  | 2130 | 2141 | 2165 | rBV  | 73481  | 132000 | 14.77% | 1.851%  |
| 48 | 8.367  | 2199 | 2201 | 2206 | rVB  | 405    | 328    | 0.04%  | 0.005%  |
| 49 | 8.402  | 2210 | 2212 | 2217 | rBV  | 232    | 214    | 0.02%  | 0.003%  |
| 50 | 8.454  | 2225 | 2228 | 2230 | rBV  | 345    | 231    | 0.03%  | 0.003%  |
| 51 | 8.553  | 2256 | 2259 | 2261 | rBV2 | 502    | 333    | 0.04%  | 0.005%  |
| 52 | 8.627  | 2271 | 2282 | 2326 | rBV3 | 179616 | 401679 | 44.95% | 5.632%  |
| 53 | 8.872  | 2354 | 2358 | 2361 | rVB2 | 303    | 261    | 0.03%  | 0.004%  |
| 54 | 8.933  | 2374 | 2377 | 2380 | rVB2 | 321    | 210    | 0.02%  | 0.003%  |
| 55 | 9.161  | 2443 | 2448 | 2452 | rBV  | 300    | 322    | 0.04%  | 0.005%  |
| 56 | 9.229  | 2465 | 2469 | 2474 | rBV  | 271    | 258    | 0.03%  | 0.004%  |
| 57 | 9.254  | 2474 | 2477 | 2481 | rBV2 | 281    | 190    | 0.02%  | 0.003%  |
| 58 | 9.412  | 2513 | 2526 | 2566 | rBV  | 480345 | 837411 | 93.70% | 11.741% |
| 59 | 9.688  | 2610 | 2612 | 2615 | rBV2 | 351    | 260    | 0.03%  | 0.004%  |
| 60 | 9.942  | 2688 | 2691 | 2696 | rBV2 | 130    | 143    | 0.02%  | 0.002%  |
| 61 | 10.074 | 2729 | 2732 | 2735 | rBV2 | 182    | 146    | 0.02%  | 0.002%  |
| 62 | 10.129 | 2744 | 2749 | 2752 | rVV2 | 311    | 260    | 0.03%  | 0.004%  |
| 63 | 10.254 | 2784 | 2788 | 2791 | rBV  | 376    | 329    | 0.04%  | 0.005%  |
| 64 | 10.528 | 2871 | 2873 | 2881 | rVB2 | 165    | 147    | 0.02%  | 0.002%  |
| 65 | 10.563 | 2881 | 2884 | 2888 | rVB2 | 179    | 168    | 0.02%  | 0.002%  |
| 66 | 10.589 | 2888 | 2892 | 2895 | rBV2 | 191    | 151    | 0.02%  | 0.002%  |
| 67 | 10.666 | 2913 | 2916 | 2919 | rVV  | 181    | 162    | 0.02%  | 0.002%  |
| 68 | 10.749 | 2930 | 2942 | 2961 | rBV  | 248044 | 407694 | 45.62% | 5.716%  |
| 69 | 10.885 | 2978 | 2984 | 2990 | rVB3 | 459    | 493    | 0.06%  | 0.007%  |
| 70 | 11.087 | 3044 | 3047 | 3054 | rVB2 | 232    | 237    | 0.03%  | 0.003%  |
| 71 | 11.290 | 3106 | 3110 | 3112 | rBV2 | 268    | 264    | 0.03%  | 0.004%  |
| 72 | 11.344 | 3123 | 3127 | 3128 | rBV2 | 273    | 179    | 0.02%  | 0.003%  |
| 73 | 11.463 | 3162 | 3164 | 3168 | rBV2 | 222    | 189    | 0.02%  | 0.003%  |
| 74 | 11.550 | 3187 | 3191 | 3196 | rBV  | 217    | 275    | 0.03%  | 0.004%  |
| 75 | 11.749 | 3247 | 3253 | 3257 | rVB3 | 741    | 763    | 0.09%  | 0.011%  |
| 76 | 11.807 | 3258 | 3271 | 3296 | rBV  | 480554 | 781720 | 87.47% | 10.960% |

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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\SFAMULM021924WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 12.020 | 3332 | 3337 | 3338 | rBV2 | 246    | 216    | 0.02%  | 0.003% |
| 78  | 12.071 | 3345 | 3353 | 3354 | rBV4 | 2640   | 2764   | 0.31%  | 0.039% |
| 79  | 12.187 | 3377 | 3389 | 3411 | rBV  | 349181 | 588707 | 65.88% | 8.254% |
| 80  | 12.762 | 3563 | 3568 | 3569 | rBV2 | 349    | 294    | 0.03%  | 0.004% |
| 81  | 12.827 | 3585 | 3588 | 3593 | rBV2 | 180    | 165    | 0.02%  | 0.002% |
| 82  | 12.862 | 3593 | 3599 | 3604 | rBV  | 311    | 408    | 0.05%  | 0.006% |
| 83  | 12.913 | 3613 | 3615 | 3625 | rVV2 | 263    | 278    | 0.03%  | 0.004% |
| 84  | 13.222 | 3708 | 3711 | 3713 | rBV  | 258    | 179    | 0.02%  | 0.003% |
| 85  | 13.306 | 3733 | 3737 | 3740 | rBV2 | 374    | 306    | 0.03%  | 0.004% |
| 86  | 13.328 | 3741 | 3744 | 3747 | rVV  | 401    | 269    | 0.03%  | 0.004% |
| 87  | 13.351 | 3748 | 3751 | 3755 | rVB2 | 370    | 302    | 0.03%  | 0.004% |
| 88  | 13.862 | 3905 | 3910 | 3914 | rVB3 | 399    | 353    | 0.04%  | 0.005% |
| 89  | 13.981 | 3945 | 3947 | 3951 | rBV2 | 190    | 149    | 0.02%  | 0.002% |
| 90  | 14.177 | 4005 | 4008 | 4011 | rVB2 | 407    | 250    | 0.03%  | 0.004% |
| 91  | 14.196 | 4011 | 4014 | 4015 | rBV  | 272    | 151    | 0.02%  | 0.002% |
| 92  | 14.280 | 4038 | 4040 | 4046 | rVB2 | 261    | 167    | 0.02%  | 0.002% |
| 93  | 14.351 | 4058 | 4062 | 4064 | rVB2 | 462    | 297    | 0.03%  | 0.004% |
| 94  | 14.450 | 4090 | 4093 | 4099 | rVB2 | 327    | 260    | 0.03%  | 0.004% |
| 95  | 14.537 | 4116 | 4120 | 4124 | rBV2 | 401    | 387    | 0.04%  | 0.005% |
| 96  | 15.093 | 4288 | 4293 | 4296 | rBV  | 452    | 441    | 0.05%  | 0.006% |
| 97  | 15.560 | 4436 | 4438 | 4442 | rBV2 | 383    | 221    | 0.02%  | 0.003% |
| 98  | 15.598 | 4447 | 4450 | 4451 | rBV  | 360    | 206    | 0.02%  | 0.003% |
| 99  | 15.669 | 4469 | 4472 | 4474 | rBV2 | 391    | 244    | 0.03%  | 0.003% |
| 100 | 16.254 | 4651 | 4654 | 4656 | rVB  | 554    | 313    | 0.04%  | 0.004% |

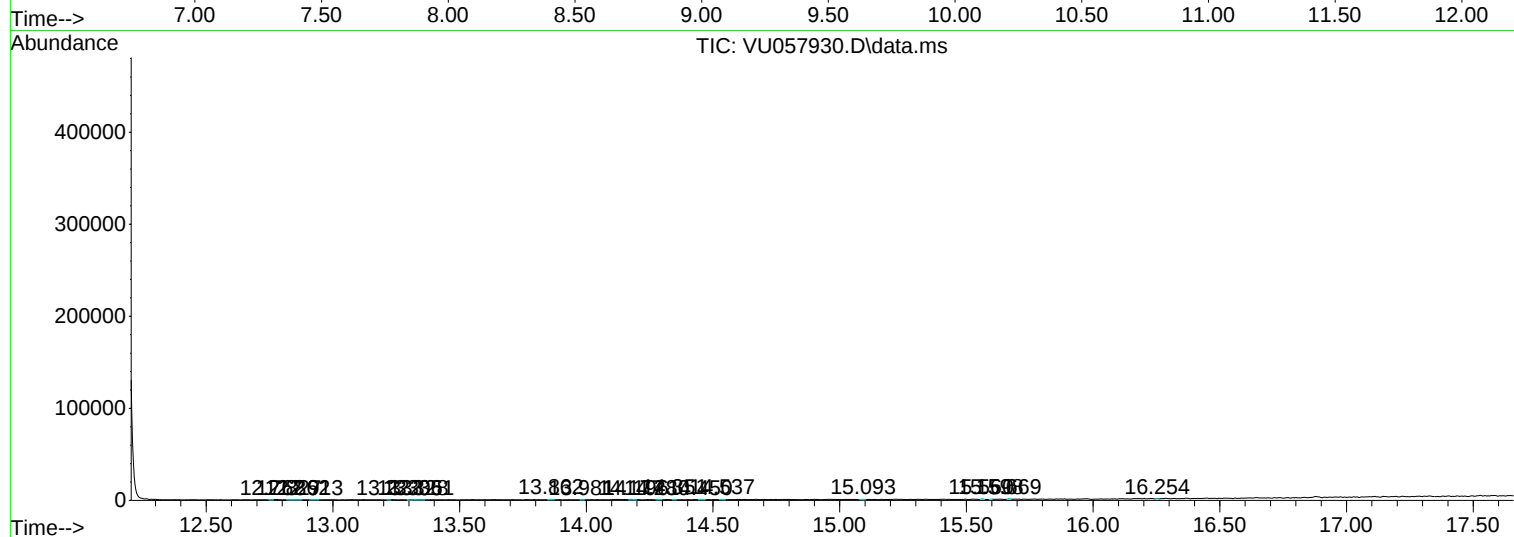
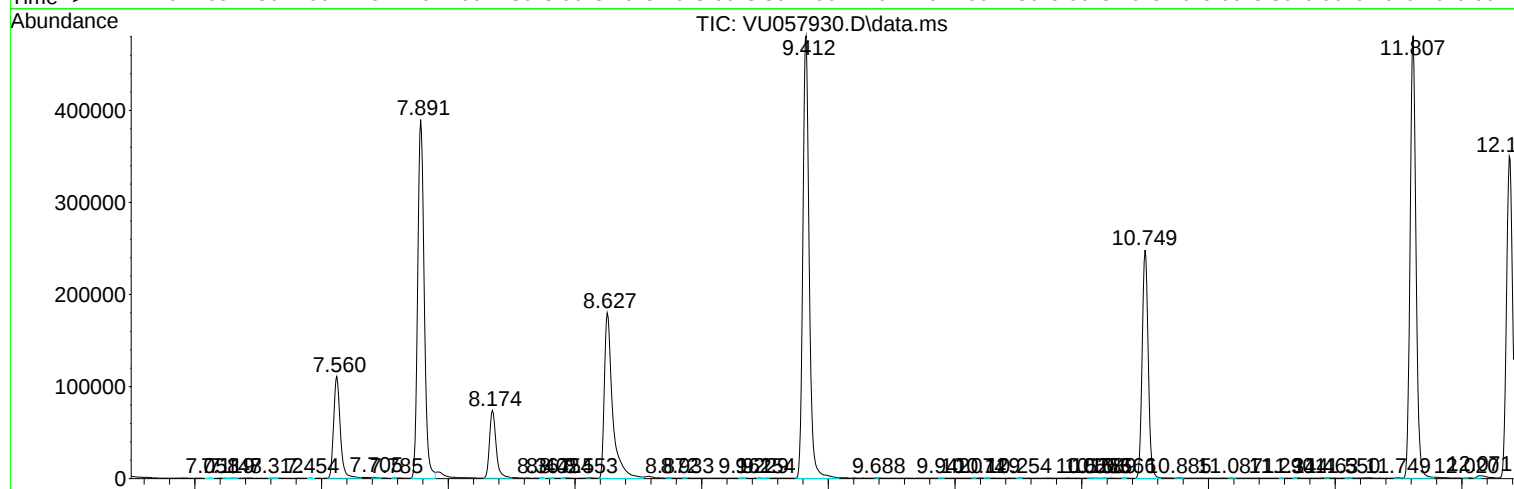
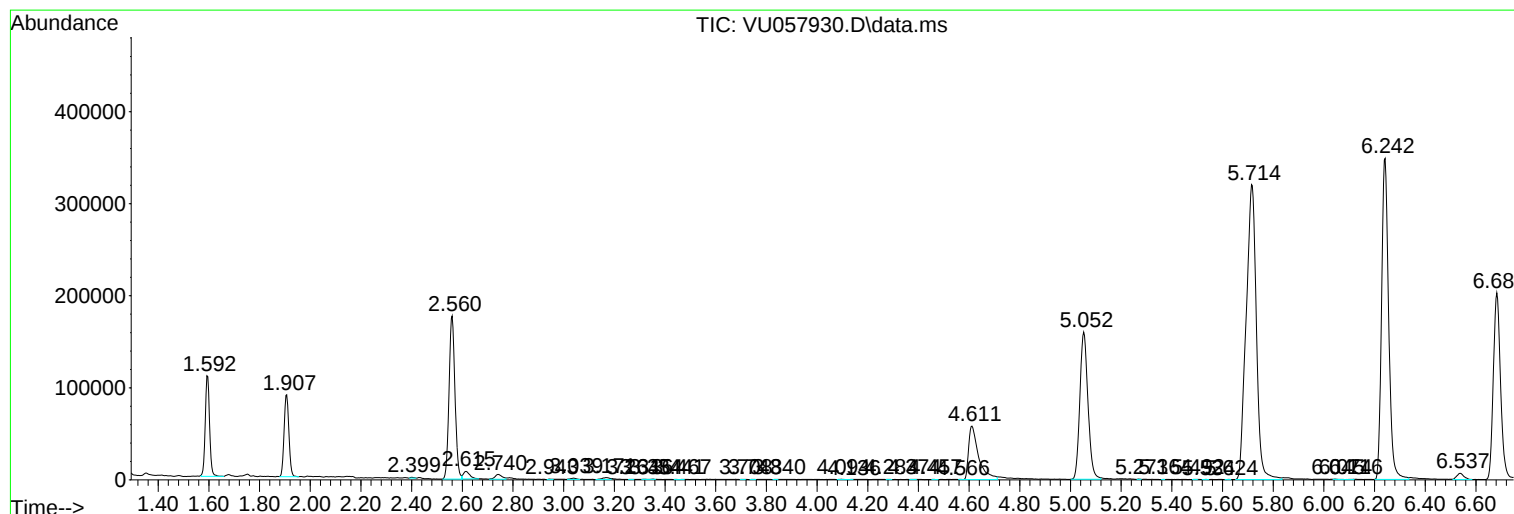
Sum of corrected areas: 7132217

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM021924WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU022224\  
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No Library Search Compounds Detected

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