

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092322\  
 Data File : VU050929.D  
 Acq On : 23 Sep 2022 19:05  
 Operator : JC/MD  
 Sample : N4747-13  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E45B1

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\SFAMULM092022WMA.M  
 Title : VOC Analysis

Signal : TIC: VU050929.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         | 1.597       | 73            | 80          | 96           | rVB      | 215669         | 255513        | 14.75%          | 1.945%        |
| 2         | 1.912       | 170           | 178         | 214          | rVB      | 201970         | 288068        | 16.63%          | 2.192%        |
| 3         | 2.565       | 368           | 381         | 395          | rBV      | 344808         | 572353        | 33.05%          | 4.356%        |
| 4         | 2.642       | 396           | 405         | 424          | rVB2     | 31953          | 70935         | 4.10%           | 0.540%        |
| 5         | 2.793       | 442           | 452         | 463          | rBV      | 7646           | 13371         | 0.77%           | 0.102%        |
| 6         | 2.903       | 483           | 486         | 492          | rVB4     | 572            | 559           | 0.03%           | 0.004%        |
| 7         | 3.038       | 522           | 528         | 529          | rBV2     | 1649           | 1304          | 0.08%           | 0.010%        |
| 8         | 3.186       | 559           | 574         | 589          | rBV2     | 5459           | 12717         | 0.73%           | 0.097%        |
| 9         | 3.279       | 598           | 603         | 606          | rBV3     | 438            | 363           | 0.02%           | 0.003%        |
| 10        | 3.327       | 616           | 618         | 623          | rVB2     | 409            | 299           | 0.02%           | 0.002%        |
| 11        | 3.790       | 758           | 762         | 766          | rBV3     | 294            | 299           | 0.02%           | 0.002%        |
| 12        | 3.871       | 784           | 787         | 791          | rVB2     | 490            | 369           | 0.02%           | 0.003%        |
| 13        | 3.900       | 791           | 796         | 801          | rBV2     | 303            | 385           | 0.02%           | 0.003%        |
| 14        | 4.131       | 864           | 868         | 870          | rBV      | 453            | 359           | 0.02%           | 0.003%        |
| 15        | 4.301       | 917           | 921         | 924          | rBV      | 330            | 288           | 0.02%           | 0.002%        |
| 16        | 4.629       | 1009          | 1023        | 1075         | rBV      | 199711         | 555787        | 32.09%          | 4.230%        |
| 17        | 5.060       | 1141          | 1157        | 1186         | rBV      | 313493         | 695439        | 40.15%          | 5.292%        |
| 18        | 5.276       | 1221          | 1224        | 1228         | rBV2     | 859            | 953           | 0.06%           | 0.007%        |
| 19        | 5.372       | 1252          | 1254        | 1257         | rBV2     | 570            | 369           | 0.02%           | 0.003%        |
| 20        | 5.407       | 1262          | 1265        | 1268         | rVV3     | 435            | 284           | 0.02%           | 0.002%        |
| 21        | 5.723       | 1341          | 1363        | 1385         | rBV2     | 638693         | 1731965       | 100.00%         | 13.181%       |
| 22        | 6.028       | 1454          | 1458        | 1460         | rBV3     | 571            | 423           | 0.02%           | 0.003%        |
| 23        | 6.112       | 1480          | 1484        | 1488         | rBV3     | 339            | 332           | 0.02%           | 0.003%        |
| 24        | 6.153       | 1493          | 1497        | 1498         | rBV2     | 787            | 590           | 0.03%           | 0.004%        |
| 25        | 6.247       | 1512          | 1526        | 1547         | rBV      | 502625         | 960353        | 55.45%          | 7.309%        |
| 26        | 6.526       | 1604          | 1613        | 1626         | rVB5     | 11324          | 21393         | 1.24%           | 0.163%        |
| 27        | 6.610       | 1635          | 1639        | 1644         | rVB2     | 365            | 404           | 0.02%           | 0.003%        |
| 28        | 6.690       | 1649          | 1664        | 1683         | rBV      | 423618         | 815418        | 47.08%          | 6.206%        |
| 29        | 6.780       | 1684          | 1692        | 1705         | rVB2     | 6589           | 13697         | 0.79%           | 0.104%        |
| 30        | 6.874       | 1719          | 1721        | 1724         | rVB2     | 605            | 374           | 0.02%           | 0.003%        |
| 31        | 6.896       | 1724          | 1728        | 1731         | rBV3     | 515            | 412           | 0.02%           | 0.003%        |
| 32        | 7.009       | 1759          | 1763        | 1768         | rVB2     | 453            | 339           | 0.02%           | 0.003%        |
| 33        | 7.044       | 1768          | 1774        | 1776         | rBV4     | 729            | 616           | 0.04%           | 0.005%        |
| 34        | 7.096       | 1786          | 1790        | 1796         | rVV2     | 502            | 388           | 0.02%           | 0.003%        |
| 35        | 7.157       | 1805          | 1809        | 1811         | rBV2     | 387            | 289           | 0.02%           | 0.002%        |
| 36        | 7.186       | 1811          | 1818        | 1828         | rVV8     | 2206           | 4673          | 0.27%           | 0.036%        |

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Integrator: RTE

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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\SFAMULM092022WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 7.295  | 1850 | 1852 | 1857 | rVB2 | 405    | 291     | 0.02%  | 0.002% |
| 38 | 7.333  | 1857 | 1864 | 1867 | rBV2 | 228    | 304     | 0.02%  | 0.002% |
| 39 | 7.414  | 1883 | 1889 | 1894 | rBV2 | 375    | 390     | 0.02%  | 0.003% |
| 40 | 7.565  | 1917 | 1936 | 1961 | rBV  | 200523 | 359592  | 20.76% | 2.737% |
| 41 | 7.697  | 1972 | 1977 | 1978 | rBV3 | 982    | 776     | 0.04%  | 0.006% |
| 42 | 7.793  | 1996 | 2007 | 2022 | rVB3 | 7400   | 13700   | 0.79%  | 0.104% |
| 43 | 7.896  | 2025 | 2039 | 2055 | rBV  | 724793 | 1243359 | 71.79% | 9.462% |
| 44 | 8.179  | 2114 | 2127 | 2147 | rBV  | 140231 | 245836  | 14.19% | 1.871% |
| 45 | 8.340  | 2176 | 2177 | 2182 | rVB2 | 487    | 304     | 0.02%  | 0.002% |
| 46 | 8.366  | 2182 | 2185 | 2190 | rVB3 | 334    | 310     | 0.02%  | 0.002% |
| 47 | 8.411  | 2195 | 2199 | 2204 | rVB3 | 509    | 484     | 0.03%  | 0.004% |
| 48 | 8.449  | 2207 | 2211 | 2212 | rBV  | 487    | 333     | 0.02%  | 0.003% |
| 49 | 8.472  | 2212 | 2218 | 2226 | rVB6 | 2320   | 3216    | 0.19%  | 0.024% |
| 50 | 8.555  | 2240 | 2244 | 2250 | rVB4 | 1332   | 1000    | 0.06%  | 0.008% |
| 51 | 8.636  | 2255 | 2269 | 2302 | rBV2 | 540810 | 1129732 | 65.23% | 8.598% |
| 52 | 8.877  | 2337 | 2344 | 2348 | rVB4 | 883    | 1131    | 0.07%  | 0.009% |
| 53 | 8.899  | 2348 | 2351 | 2355 | rBV2 | 308    | 264     | 0.02%  | 0.002% |
| 54 | 9.028  | 2386 | 2391 | 2394 | rBV3 | 537    | 375     | 0.02%  | 0.003% |
| 55 | 9.166  | 2429 | 2434 | 2437 | rBV2 | 335    | 376     | 0.02%  | 0.003% |
| 56 | 9.414  | 2498 | 2511 | 2534 | rBV  | 698311 | 1167558 | 67.41% | 8.885% |
| 57 | 9.568  | 2554 | 2559 | 2562 | rBV4 | 610    | 584     | 0.03%  | 0.004% |
| 58 | 9.687  | 2591 | 2596 | 2597 | rBV  | 751    | 633     | 0.04%  | 0.005% |
| 59 | 9.787  | 2625 | 2627 | 2632 | rVB4 | 453    | 357     | 0.02%  | 0.003% |
| 60 | 9.848  | 2644 | 2646 | 2651 | rVB2 | 439    | 290     | 0.02%  | 0.002% |
| 61 | 9.938  | 2668 | 2674 | 2677 | rBV2 | 366    | 409     | 0.02%  | 0.003% |
| 62 | 10.025 | 2698 | 2701 | 2704 | rBV2 | 433    | 345     | 0.02%  | 0.003% |
| 63 | 10.134 | 2731 | 2735 | 2743 | rVB3 | 978    | 1212    | 0.07%  | 0.009% |
| 64 | 10.240 | 2762 | 2768 | 2782 | rBV2 | 2097   | 3220    | 0.19%  | 0.025% |
| 65 | 10.478 | 2836 | 2842 | 2846 | rVB3 | 458    | 544     | 0.03%  | 0.004% |
| 66 | 10.542 | 2857 | 2862 | 2865 | rBV2 | 274    | 289     | 0.02%  | 0.002% |
| 67 | 10.568 | 2866 | 2870 | 2872 | rBV3 | 542    | 436     | 0.03%  | 0.003% |
| 68 | 10.665 | 2897 | 2900 | 2902 | rBV2 | 912    | 655     | 0.04%  | 0.005% |
| 69 | 10.755 | 2915 | 2928 | 2947 | rBV  | 601977 | 971971  | 56.12% | 7.397% |
| 70 | 10.890 | 2962 | 2970 | 2981 | rVB5 | 8908   | 15069   | 0.87%  | 0.115% |
| 71 | 11.044 | 3015 | 3018 | 3021 | rBV2 | 512    | 315     | 0.02%  | 0.002% |
| 72 | 11.118 | 3030 | 3041 | 3049 | rBV8 | 2102   | 3708    | 0.21%  | 0.028% |
| 73 | 11.259 | 3083 | 3085 | 3092 | rVB2 | 405    | 410     | 0.02%  | 0.003% |
| 74 | 11.308 | 3095 | 3100 | 3102 | rBV3 | 776    | 645     | 0.04%  | 0.005% |
| 75 | 11.375 | 3115 | 3121 | 3122 | rBV3 | 620    | 596     | 0.03%  | 0.005% |
| 76 | 11.388 | 3122 | 3125 | 3126 | rBV2 | 448    | 263     | 0.02%  | 0.002% |

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.455 | 3142 | 3146 | 3148 | rBV2 | 1172   | 841    | 0.05%  | 0.006% |
| 78  | 11.558 | 3170 | 3178 | 3179 | rBV4 | 2174   | 2177   | 0.13%  | 0.017% |
| 79  | 11.693 | 3214 | 3220 | 3226 | rBV4 | 939    | 1347   | 0.08%  | 0.010% |
| 80  | 11.754 | 3235 | 3239 | 3243 | rBV3 | 319    | 301    | 0.02%  | 0.002% |
| 81  | 11.809 | 3243 | 3256 | 3280 | rBV  | 547125 | 872810 | 50.39% | 6.642% |
| 82  | 11.970 | 3302 | 3306 | 3313 | rVB7 | 1812   | 2042   | 0.12%  | 0.016% |
| 83  | 12.060 | 3324 | 3334 | 3346 | rBV3 | 10317  | 19684  | 1.14%  | 0.150% |
| 84  | 12.192 | 3359 | 3375 | 3393 | rBV  | 611891 | 997264 | 57.58% | 7.589% |
| 85  | 12.452 | 3452 | 3456 | 3463 | rVB5 | 709    | 741    | 0.04%  | 0.006% |
| 86  | 12.864 | 3581 | 3584 | 3585 | rBV  | 475    | 270    | 0.02%  | 0.002% |
| 87  | 12.889 | 3588 | 3592 | 3594 | rBV3 | 1240   | 937    | 0.05%  | 0.007% |
| 88  | 12.947 | 3602 | 3610 | 3617 | rBV4 | 4099   | 5689   | 0.33%  | 0.043% |
| 89  | 12.996 | 3623 | 3625 | 3628 | rBV  | 493    | 285    | 0.02%  | 0.002% |
| 90  | 13.082 | 3649 | 3652 | 3653 | rBV2 | 427    | 261    | 0.02%  | 0.002% |
| 91  | 13.288 | 3709 | 3716 | 3727 | rVB7 | 3614   | 6038   | 0.35%  | 0.046% |
| 92  | 13.484 | 3774 | 3777 | 3783 | rBV3 | 477    | 453    | 0.03%  | 0.003% |
| 93  | 13.684 | 3836 | 3839 | 3842 | rBV3 | 506    | 432    | 0.02%  | 0.003% |
| 94  | 13.735 | 3845 | 3855 | 3866 | rVB5 | 19426  | 33382  | 1.93%  | 0.254% |
| 95  | 13.799 | 3873 | 3875 | 3876 | rBV2 | 603    | 264    | 0.02%  | 0.002% |
| 96  | 14.651 | 4137 | 4140 | 4142 | rBV  | 588    | 344    | 0.02%  | 0.003% |
| 97  | 14.700 | 4152 | 4155 | 4158 | rBV2 | 451    | 287    | 0.02%  | 0.002% |
| 98  | 15.041 | 4258 | 4261 | 4263 | rBV2 | 550    | 311    | 0.02%  | 0.002% |
| 99  | 15.336 | 4351 | 4353 | 4356 | rBV3 | 593    | 401    | 0.02%  | 0.003% |
| 100 | 15.880 | 4520 | 4522 | 4525 | rBV3 | 987    | 595    | 0.03%  | 0.005% |

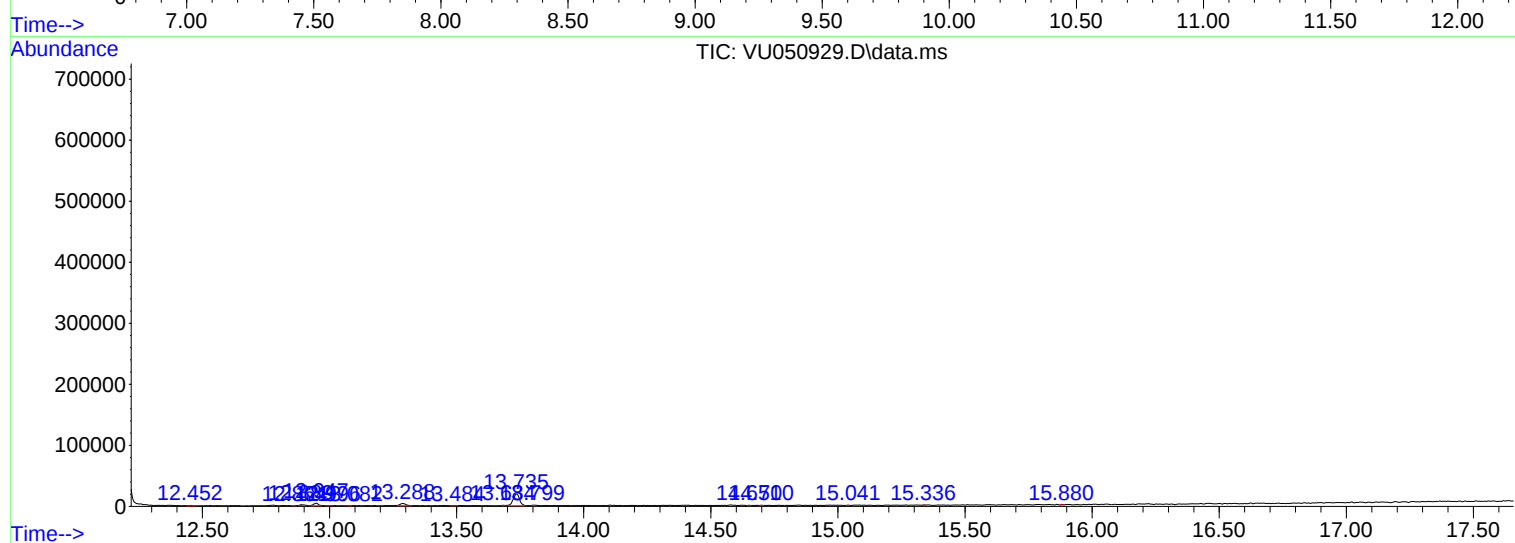
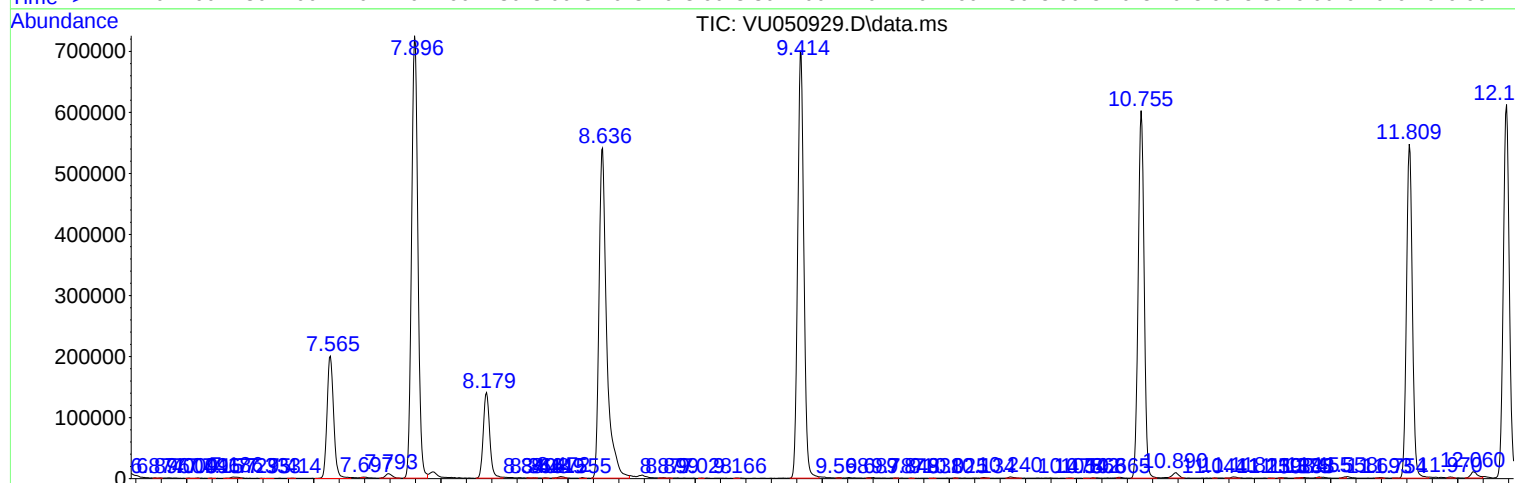
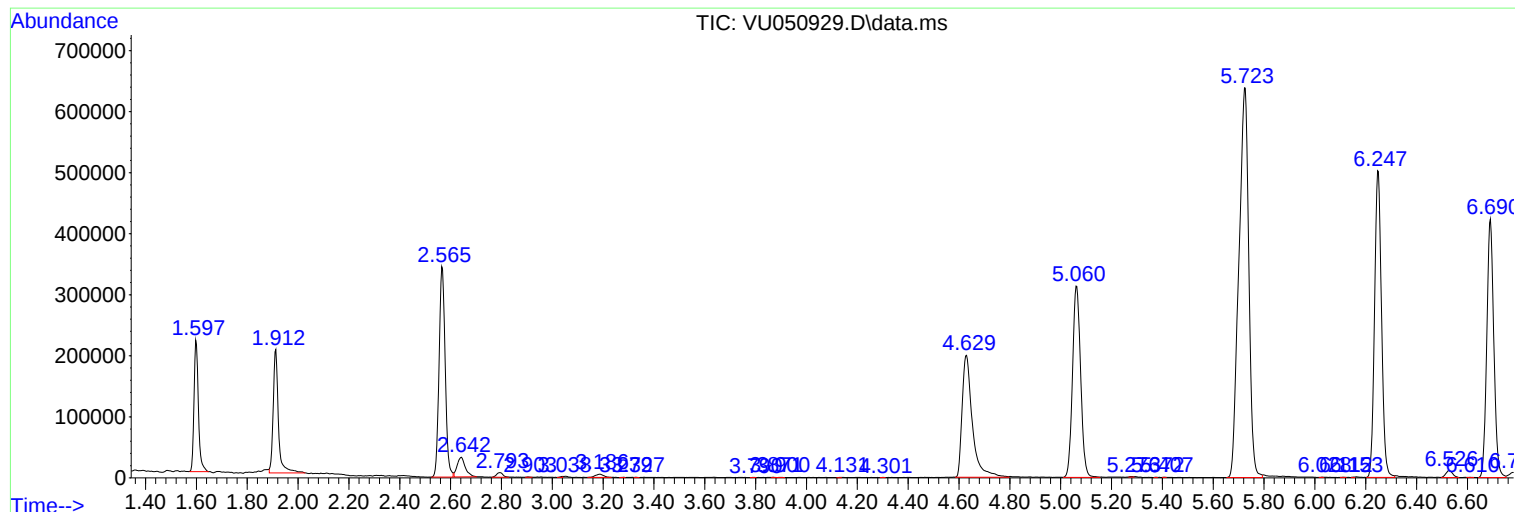
Sum of corrected areas: 13140118

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.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 |