

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100721\  
 Data File : VU045202.D  
 Acq On : 07 Oct 2021 11:19  
 Operator : SY/MD  
 Sample : M4023-12 25X  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AK1

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045202.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         | 1.469       | 34            | 40          | 53           | rBV2     | 11378          | 20797         | 1.07%           | 0.148%        |
| 2         | 1.601       | 73            | 81          | 97           | rBV      | 189853         | 205680        | 10.57%          | 1.463%        |
| 3         | 1.896       | 164           | 173         | 184          | rBV      | 131824         | 177599        | 9.13%           | 1.263%        |
| 4         | 2.491       | 352           | 358         | 360          | rBV2     | 214            | 271           | 0.01%           | 0.002%        |
| 5         | 2.565       | 368           | 381         | 403          | rBV3     | 317508         | 603259        | 31.00%          | 4.290%        |
| 6         | 2.768       | 433           | 444         | 445          | rBV3     | 411            | 637           | 0.03%           | 0.005%        |
| 7         | 2.787       | 445           | 450         | 458          | rVB4     | 644            | 1081          | 0.06%           | 0.008%        |
| 8         | 2.954       | 496           | 502         | 511          | rVB2     | 449            | 770           | 0.04%           | 0.005%        |
| 9         | 3.048       | 519           | 531         | 551          | rVB      | 54034          | 103874        | 5.34%           | 0.739%        |
| 10        | 3.141       | 557           | 560         | 563          | rBV2     | 257            | 213           | 0.01%           | 0.002%        |
| 11        | 3.183       | 563           | 573         | 575          | rBV2     | 1633           | 1967          | 0.10%           | 0.014%        |
| 12        | 3.356       | 614           | 627         | 642          | rBV2     | 15727          | 31074         | 1.60%           | 0.221%        |
| 13        | 3.536       | 680           | 683         | 686          | rBV2     | 167            | 171           | 0.01%           | 0.001%        |
| 14        | 3.736       | 740           | 745         | 749          | rBV      | 149            | 181           | 0.01%           | 0.001%        |
| 15        | 3.784       | 757           | 760         | 765          | rVB2     | 183            | 195           | 0.01%           | 0.001%        |
| 16        | 3.874       | 773           | 788         | 804          | rBV      | 18037          | 40379         | 2.07%           | 0.287%        |
| 17        | 4.163       | 873           | 878         | 879          | rBV      | 227            | 162           | 0.01%           | 0.001%        |
| 18        | 4.472       | 970           | 974         | 976          | rBV2     | 212            | 188           | 0.01%           | 0.001%        |
| 19        | 4.668       | 1005          | 1035        | 1060         | rBV2     | 705994         | 1879457       | 96.58%          | 13.367%       |
| 20        | 4.864       | 1092          | 1096        | 1100         | rVB2     | 441            | 320           | 0.02%           | 0.002%        |
| 21        | 4.900       | 1105          | 1107        | 1110         | rBV3     | 211            | 172           | 0.01%           | 0.001%        |
| 22        | 5.067       | 1143          | 1159        | 1182         | rBV      | 223685         | 489482        | 25.15%          | 3.481%        |
| 23        | 5.173       | 1189          | 1192        | 1197         | rBV2     | 279            | 273           | 0.01%           | 0.002%        |
| 24        | 5.221       | 1203          | 1207        | 1208         | rVV      | 462            | 267           | 0.01%           | 0.002%        |
| 25        | 5.253       | 1212          | 1217        | 1220         | rBV2     | 201            | 157           | 0.01%           | 0.001%        |
| 26        | 5.321       | 1220          | 1238        | 1262         | rBV      | 228739         | 518098        | 26.62%          | 3.685%        |
| 27        | 5.507       | 1293          | 1296        | 1300         | rVB2     | 259            | 202           | 0.01%           | 0.001%        |
| 28        | 5.729       | 1343          | 1365        | 1382         | rBV2     | 469981         | 1265313       | 65.02%          | 8.999%        |
| 29        | 6.012       | 1449          | 1453        | 1454         | rBV      | 211            | 160           | 0.01%           | 0.001%        |
| 30        | 6.041       | 1459          | 1462        | 1464         | rBV2     | 209            | 171           | 0.01%           | 0.001%        |
| 31        | 6.109       | 1479          | 1483        | 1486         | rBV3     | 286            | 193           | 0.01%           | 0.001%        |
| 32        | 6.121       | 1486          | 1487        | 1491         | rVB      | 299            | 155           | 0.01%           | 0.001%        |
| 33        | 6.150       | 1491          | 1496        | 1500         | rBV2     | 275            | 257           | 0.01%           | 0.002%        |
| 34        | 6.253       | 1513          | 1528        | 1547         | rBV      | 389051         | 726159        | 37.31%          | 5.164%        |
| 35        | 6.546       | 1603          | 1619        | 1645         | rBV      | 1044051        | 1946096       | 100.00%         | 13.840%       |
| 36        | 6.694       | 1651          | 1665        | 1685         | rVB      | 297326         | 573592        | 29.47%          | 4.079%        |

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Integrator: RTE

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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\SFAMULM092321WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 6.854  | 1711 | 1715 | 1718 | rVB3 | 317    | 256     | 0.01%  | 0.002% |
| 38 | 6.996  | 1756 | 1759 | 1762 | rBV2 | 222    | 182     | 0.01%  | 0.001% |
| 39 | 7.047  | 1769 | 1775 | 1782 | rBV  | 466    | 654     | 0.03%  | 0.005% |
| 40 | 7.179  | 1805 | 1816 | 1823 | rBV3 | 994    | 1748    | 0.09%  | 0.012% |
| 41 | 7.250  | 1834 | 1838 | 1840 | rBV2 | 168    | 175     | 0.01%  | 0.001% |
| 42 | 7.263  | 1840 | 1842 | 1847 | rVB2 | 221    | 162     | 0.01%  | 0.001% |
| 43 | 7.568  | 1923 | 1937 | 1957 | rVV  | 158537 | 274567  | 14.11% | 1.953% |
| 44 | 7.639  | 1957 | 1959 | 1963 | rVV2 | 392    | 264     | 0.01%  | 0.002% |
| 45 | 7.690  | 1969 | 1975 | 1981 | rVV2 | 616    | 940     | 0.05%  | 0.007% |
| 46 | 7.719  | 1981 | 1984 | 1988 | rVB2 | 278    | 230     | 0.01%  | 0.002% |
| 47 | 7.793  | 2003 | 2007 | 2011 | rBV3 | 246    | 247     | 0.01%  | 0.002% |
| 48 | 7.903  | 2027 | 2041 | 2056 | rBV  | 582215 | 1001093 | 51.44% | 7.120% |
| 49 | 7.973  | 2057 | 2063 | 2075 | rVB  | 9765   | 14603   | 0.75%  | 0.104% |
| 50 | 8.182  | 2115 | 2128 | 2145 | rBV2 | 112000 | 184430  | 9.48%  | 1.312% |
| 51 | 8.404  | 2189 | 2197 | 2207 | rVB2 | 5136   | 8254    | 0.42%  | 0.059% |
| 52 | 8.636  | 2257 | 2269 | 2300 | rBV  | 414551 | 715711  | 36.78% | 5.090% |
| 53 | 8.848  | 2331 | 2335 | 2340 | rVB2 | 246    | 213     | 0.01%  | 0.002% |
| 54 | 8.899  | 2347 | 2351 | 2353 | rBV2 | 247    | 166     | 0.01%  | 0.001% |
| 55 | 8.993  | 2378 | 2380 | 2383 | rBV  | 288    | 217     | 0.01%  | 0.002% |
| 56 | 9.038  | 2391 | 2394 | 2399 | rVB2 | 269    | 290     | 0.01%  | 0.002% |
| 57 | 9.070  | 2399 | 2404 | 2408 | rVB2 | 268    | 264     | 0.01%  | 0.002% |
| 58 | 9.153  | 2427 | 2430 | 2435 | rVB2 | 255    | 245     | 0.01%  | 0.002% |
| 59 | 9.192  | 2438 | 2442 | 2448 | rVV2 | 219    | 287     | 0.01%  | 0.002% |
| 60 | 9.260  | 2457 | 2463 | 2465 | rBV2 | 193    | 210     | 0.01%  | 0.001% |
| 61 | 9.288  | 2465 | 2472 | 2478 | rVB3 | 957    | 1151    | 0.06%  | 0.008% |
| 62 | 9.420  | 2500 | 2513 | 2528 | rBV  | 559659 | 902964  | 46.40% | 6.422% |
| 63 | 9.578  | 2558 | 2562 | 2568 | rVB2 | 806    | 992     | 0.05%  | 0.007% |
| 64 | 9.613  | 2568 | 2573 | 2576 | rBV  | 247    | 207     | 0.01%  | 0.001% |
| 65 | 9.694  | 2592 | 2598 | 2607 | rVB3 | 2994   | 4128    | 0.21%  | 0.029% |
| 66 | 9.829  | 2631 | 2640 | 2648 | rVB2 | 212    | 403     | 0.02%  | 0.003% |
| 67 | 9.877  | 2648 | 2655 | 2657 | rBV2 | 189    | 247     | 0.01%  | 0.002% |
| 68 | 10.009 | 2692 | 2696 | 2699 | rBV  | 225    | 186     | 0.01%  | 0.001% |
| 69 | 10.102 | 2715 | 2725 | 2733 | rBV3 | 3465   | 5229    | 0.27%  | 0.037% |
| 70 | 10.240 | 2760 | 2768 | 2771 | rBV  | 295    | 389     | 0.02%  | 0.003% |
| 71 | 10.385 | 2808 | 2813 | 2816 | rBV  | 192    | 203     | 0.01%  | 0.001% |
| 72 | 10.481 | 2841 | 2843 | 2849 | rVB2 | 303    | 219     | 0.01%  | 0.002% |
| 73 | 10.674 | 2893 | 2903 | 2910 | rBV5 | 1932   | 2806    | 0.14%  | 0.020% |
| 74 | 10.761 | 2917 | 2930 | 2948 | rBV  | 415584 | 669864  | 34.42% | 4.764% |
| 75 | 10.864 | 2959 | 2962 | 2966 | rBV2 | 274    | 292     | 0.02%  | 0.002% |
| 76 | 10.922 | 2976 | 2980 | 2983 | rBV  | 204    | 196     | 0.01%  | 0.001% |

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Integration Parameters: LSCINT.P

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.038 | 3013 | 3016 | 3019 | rBV2 | 173    | 170    | 0.01%  | 0.001% |
| 78  | 11.131 | 3041 | 3045 | 3047 | rBV2 | 227    | 194    | 0.01%  | 0.001% |
| 79  | 11.224 | 3069 | 3074 | 3077 | rBV2 | 240    | 200    | 0.01%  | 0.001% |
| 80  | 11.301 | 3095 | 3098 | 3103 | rBV2 | 313    | 302    | 0.02%  | 0.002% |
| 81  | 11.378 | 3118 | 3122 | 3124 | rBV  | 218    | 192    | 0.01%  | 0.001% |
| 82  | 11.465 | 3140 | 3149 | 3156 | rBV4 | 1457   | 2255   | 0.12%  | 0.016% |
| 83  | 11.620 | 3193 | 3197 | 3203 | rVB  | 307    | 356    | 0.02%  | 0.003% |
| 84  | 11.655 | 3203 | 3208 | 3211 | rBV  | 271    | 214    | 0.01%  | 0.002% |
| 85  | 11.697 | 3211 | 3221 | 3227 | rBV3 | 817    | 1142   | 0.06%  | 0.008% |
| 86  | 11.816 | 3243 | 3258 | 3280 | rBV  | 515458 | 812847 | 41.77% | 5.781% |
| 87  | 11.906 | 3284 | 3286 | 3289 | rVB2 | 293    | 160    | 0.01%  | 0.001% |
| 88  | 11.931 | 3289 | 3294 | 3297 | rBV3 | 388    | 401    | 0.02%  | 0.003% |
| 89  | 11.976 | 3303 | 3308 | 3316 | rVB4 | 1008   | 1307   | 0.07%  | 0.009% |
| 90  | 12.099 | 3343 | 3346 | 3352 | rVB2 | 203    | 230    | 0.01%  | 0.002% |
| 91  | 12.195 | 3361 | 3376 | 3395 | rBV  | 533523 | 852469 | 43.80% | 6.063% |
| 92  | 12.362 | 3425 | 3428 | 3432 | rVB2 | 242    | 209    | 0.01%  | 0.001% |
| 93  | 12.629 | 3506 | 3511 | 3513 | rBV  | 552    | 564    | 0.03%  | 0.004% |
| 94  | 13.224 | 3694 | 3696 | 3699 | rVB  | 249    | 170    | 0.01%  | 0.001% |
| 95  | 13.652 | 3826 | 3829 | 3835 | rBV2 | 244    | 209    | 0.01%  | 0.001% |
| 96  | 13.780 | 3866 | 3869 | 3871 | rBV2 | 182    | 155    | 0.01%  | 0.001% |
| 97  | 13.845 | 3884 | 3889 | 3890 | rBV  | 622    | 508    | 0.03%  | 0.004% |
| 98  | 14.089 | 3959 | 3965 | 3975 | rBV2 | 1433   | 2358   | 0.12%  | 0.017% |
| 99  | 14.324 | 4036 | 4038 | 4040 | rBV2 | 340    | 200    | 0.01%  | 0.001% |
| 100 | 14.783 | 4178 | 4181 | 4184 | rBV2 | 266    | 189    | 0.01%  | 0.001% |

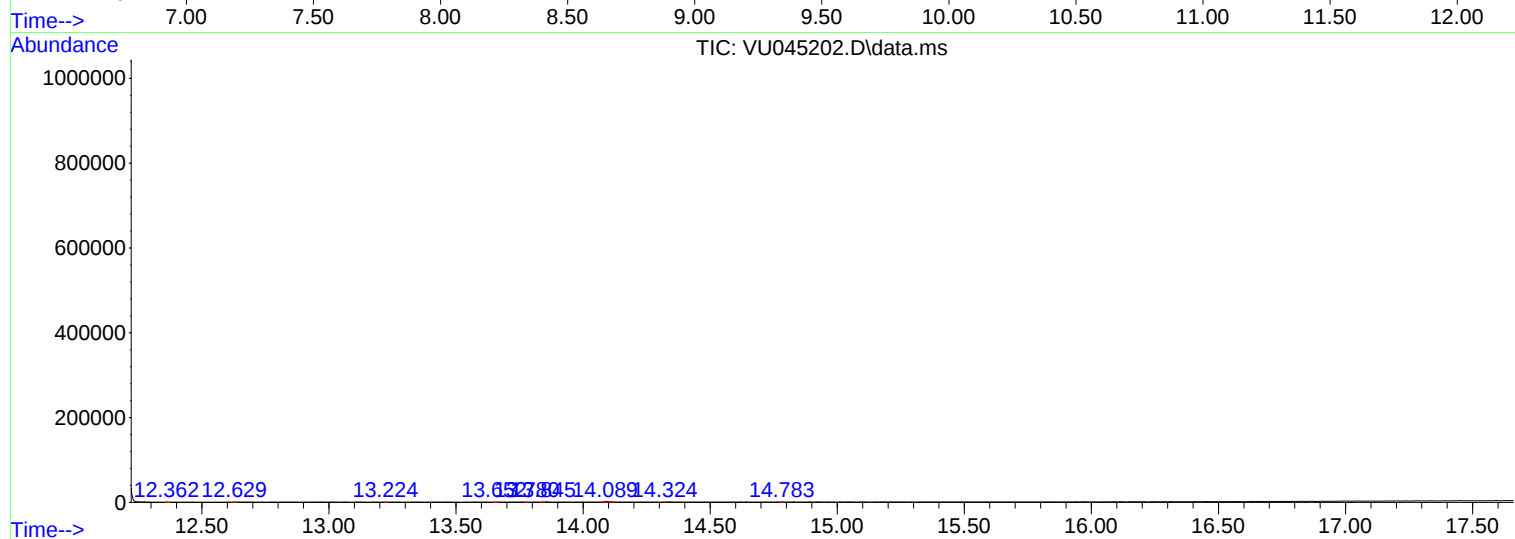
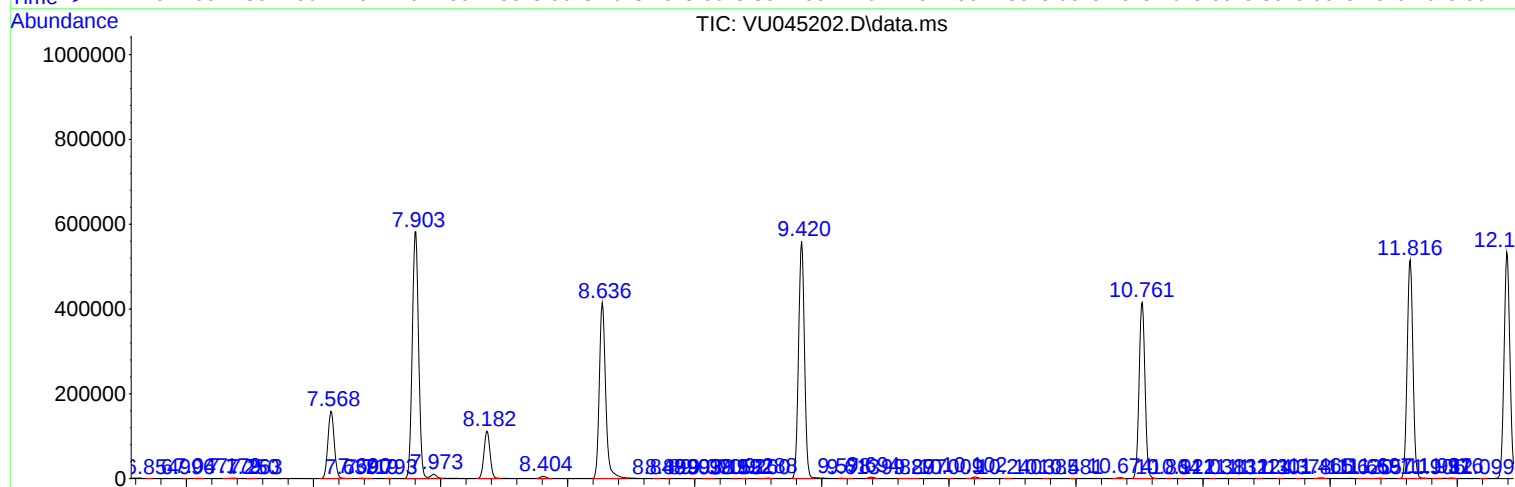
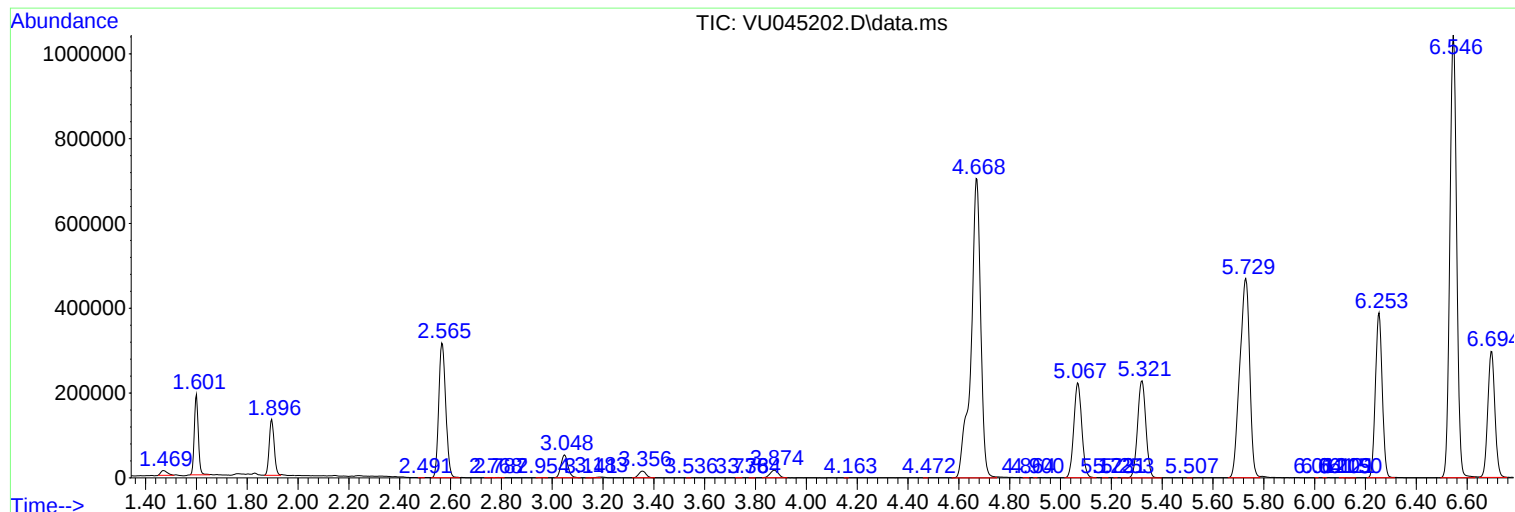
Sum of corrected areas: 14060907

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100721\  
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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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