

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050618\  
 Data File : VU023695.D  
 Acq On : 06 May 2018 17:42  
 Operator : MD/SY  
 Sample : J2721-11  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 16 Sample Multiplier: 1

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.M  
 Title : VOC Analysis

Signal : TIC

| 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         | 0.969       | 115           | 118         | 121          | rVV2     | 187            | 148           | 0.01%           | 0.001%        |
| 2         | 1.088       | 148           | 155         | 178          | rBV      | 255286         | 291471        | 23.73%          | 2.839%        |
| 3         | 1.182       | 180           | 184         | 194          | rVV2     | 8263           | 9400          | 0.77%           | 0.092%        |
| 4         | 1.400       | 245           | 252         | 267          | rVV      | 159461         | 169773        | 13.82%          | 1.654%        |
| 5         | 1.474       | 269           | 275         | 288          | rVB      | 19993          | 23823         | 1.94%           | 0.232%        |
| 6         | 1.680       | 331           | 339         | 356          | rBV      | 122896         | 154771        | 12.60%          | 1.508%        |
| 7         | 2.271       | 512           | 523         | 534          | rBV      | 274140         | 420385        | 34.23%          | 4.095%        |
| 8         | 2.442       | 566           | 576         | 595          | rBV2     | 12954          | 25981         | 2.12%           | 0.253%        |
| 9         | 2.548       | 605           | 609         | 613          | rBV3     | 423            | 493           | 0.04%           | 0.005%        |
| 10        | 2.599       | 621           | 625         | 626          | rBV2     | 312            | 193           | 0.02%           | 0.002%        |
| 11        | 2.706       | 652           | 658         | 664          | rBV3     | 530            | 646           | 0.05%           | 0.006%        |
| 12        | 2.773       | 673           | 679         | 680          | rBV      | 188            | 194           | 0.02%           | 0.002%        |
| 13        | 2.841       | 687           | 700         | 713          | rVB2     | 3865           | 7833          | 0.64%           | 0.076%        |
| 14        | 2.927       | 723           | 727         | 729          | rBV      | 170            | 146           | 0.01%           | 0.001%        |
| 15        | 2.982       | 737           | 744         | 747          | rBV3     | 279            | 302           | 0.02%           | 0.003%        |
| 16        | 3.046       | 758           | 764         | 768          | rVB2     | 202            | 208           | 0.02%           | 0.002%        |
| 17        | 3.188       | 804           | 808         | 811          | rVB3     | 172            | 149           | 0.01%           | 0.001%        |
| 18        | 3.300       | 840           | 843         | 845          | rBV2     | 328            | 179           | 0.01%           | 0.002%        |
| 19        | 3.384       | 866           | 869         | 872          | rBV      | 235            | 158           | 0.01%           | 0.002%        |
| 20        | 4.001       | 1052          | 1061        | 1066         | rBV4     | 972            | 1605          | 0.13%           | 0.016%        |
| 21        | 4.178       | 1101          | 1116        | 1149         | rBV      | 122233         | 327756        | 26.69%          | 3.193%        |
| 22        | 4.394       | 1176          | 1183        | 1186         | rBV3     | 497            | 696           | 0.06%           | 0.007%        |
| 23        | 4.423       | 1190          | 1192        | 1196         | rVB3     | 495            | 312           | 0.03%           | 0.003%        |
| 24        | 4.564       | 1232          | 1236        | 1239         | rBV2     | 351            | 294           | 0.02%           | 0.003%        |
| 25        | 4.651       | 1243          | 1263        | 1285         | rBV      | 196076         | 465598        | 37.91%          | 4.535%        |
| 26        | 4.886       | 1329          | 1336        | 1337         | rBV      | 444            | 419           | 0.03%           | 0.004%        |
| 27        | 4.992       | 1361          | 1369        | 1379         | rVB6     | 1501           | 2497          | 0.20%           | 0.024%        |
| 28        | 5.223       | 1432          | 1441        | 1442         | rBV3     | 1308           | 1436          | 0.12%           | 0.014%        |
| 29        | 5.345       | 1454          | 1479        | 1504         | rBV2     | 412560         | 1228068       | 100.00%         | 11.963%       |
| 30        | 5.558       | 1542          | 1545        | 1551         | rVB2     | 421            | 348           | 0.03%           | 0.003%        |
| 31        | 5.680       | 1580          | 1583        | 1587         | rBV2     | 199            | 150           | 0.01%           | 0.001%        |
| 32        | 5.754       | 1603          | 1606        | 1609         | rBV      | 232            | 207           | 0.02%           | 0.002%        |
| 33        | 5.792       | 1609          | 1618        | 1629         | rVB5     | 3224           | 5456          | 0.44%           | 0.053%        |
| 34        | 5.892       | 1633          | 1649        | 1684         | rBV      | 398030         | 805401        | 65.58%          | 7.845%        |

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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 6.336  | 1771 | 1787 | 1811 | rBV  | 276393 | 562670 | 45.82% | 5.481% |
| 36 | 6.644  | 1880 | 1883 | 1889 | rVB2 | 339    | 248    | 0.02%  | 0.002% |
| 37 | 6.680  | 1889 | 1894 | 1897 | rBV2 | 156    | 165    | 0.01%  | 0.002% |
| 38 | 6.863  | 1943 | 1951 | 1954 | rBV3 | 607    | 698    | 0.06%  | 0.007% |
| 39 | 7.127  | 2029 | 2033 | 2037 | rBV2 | 179    | 182    | 0.01%  | 0.002% |
| 40 | 7.233  | 2053 | 2066 | 2092 | rVV  | 143773 | 264130 | 21.51% | 2.573% |
| 41 | 7.387  | 2110 | 2114 | 2117 | rBV3 | 600    | 541    | 0.04%  | 0.005% |
| 42 | 7.467  | 2129 | 2139 | 2148 | rBV2 | 882    | 1338   | 0.11%  | 0.013% |
| 43 | 7.570  | 2154 | 2171 | 2187 | rBV  | 556306 | 983340 | 80.07% | 9.579% |
| 44 | 7.853  | 2244 | 2259 | 2291 | rBV  | 100480 | 175510 | 14.29% | 1.710% |
| 45 | 8.178  | 2354 | 2360 | 2370 | rVB3 | 664    | 1256   | 0.10%  | 0.012% |
| 46 | 8.239  | 2375 | 2379 | 2382 | rVB2 | 346    | 231    | 0.02%  | 0.002% |
| 47 | 8.313  | 2390 | 2402 | 2448 | rBV  | 399340 | 692325 | 56.38% | 6.744% |
| 48 | 8.593  | 2487 | 2489 | 2493 | rVB2 | 354    | 297    | 0.02%  | 0.003% |
| 49 | 8.615  | 2493 | 2496 | 2499 | rBV2 | 283    | 237    | 0.02%  | 0.002% |
| 50 | 8.676  | 2512 | 2515 | 2520 | rVB2 | 320    | 225    | 0.02%  | 0.002% |
| 51 | 8.847  | 2565 | 2568 | 2572 | rBV2 | 220    | 161    | 0.01%  | 0.002% |
| 52 | 8.995  | 2610 | 2614 | 2617 | rBV  | 181    | 150    | 0.01%  | 0.001% |
| 53 | 9.043  | 2624 | 2629 | 2632 | rBV2 | 196    | 237    | 0.02%  | 0.002% |
| 54 | 9.094  | 2632 | 2645 | 2686 | rVV  | 573297 | 966552 | 78.71% | 9.415% |
| 55 | 9.255  | 2687 | 2695 | 2707 | rVB  | 8671   | 13609  | 1.11%  | 0.133% |
| 56 | 9.377  | 2722 | 2733 | 2745 | rBV  | 22715  | 37582  | 3.06%  | 0.366% |
| 57 | 9.442  | 2750 | 2753 | 2757 | rBV3 | 402    | 398    | 0.03%  | 0.004% |
| 58 | 9.786  | 2850 | 2860 | 2873 | rBV2 | 9739   | 15499  | 1.26%  | 0.151% |
| 59 | 9.844  | 2875 | 2878 | 2882 | rBV2 | 217    | 144    | 0.01%  | 0.001% |
| 60 | 9.975  | 2916 | 2919 | 2922 | rVB  | 211    | 157    | 0.01%  | 0.002% |
| 61 | 10.001 | 2922 | 2927 | 2929 | rBV  | 187    | 155    | 0.01%  | 0.002% |
| 62 | 10.175 | 2974 | 2981 | 2985 | rBV3 | 488    | 570    | 0.05%  | 0.006% |
| 63 | 10.332 | 3027 | 3030 | 3034 | rVB3 | 405    | 301    | 0.02%  | 0.003% |
| 64 | 10.435 | 3050 | 3062 | 3084 | rVB  | 378256 | 609843 | 49.66% | 5.941% |
| 65 | 10.599 | 3104 | 3113 | 3115 | rBV3 | 1374   | 1999   | 0.16%  | 0.019% |
| 66 | 10.686 | 3134 | 3140 | 3141 | rBV2 | 1151   | 1003   | 0.08%  | 0.010% |
| 67 | 10.818 | 3175 | 3181 | 3193 | rVB2 | 4066   | 5055   | 0.41%  | 0.049% |
| 68 | 10.889 | 3200 | 3203 | 3205 | rBV  | 249    | 177    | 0.01%  | 0.002% |
| 69 | 11.075 | 3258 | 3261 | 3267 | rBV3 | 457    | 435    | 0.04%  | 0.004% |
| 70 | 11.120 | 3268 | 3275 | 3280 | rVV4 | 1981   | 2603   | 0.21%  | 0.025% |
| 71 | 11.155 | 3280 | 3286 | 3297 | rVB  | 3451   | 4839   | 0.39%  | 0.047% |

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Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.M  
 Title : VOC Analysis

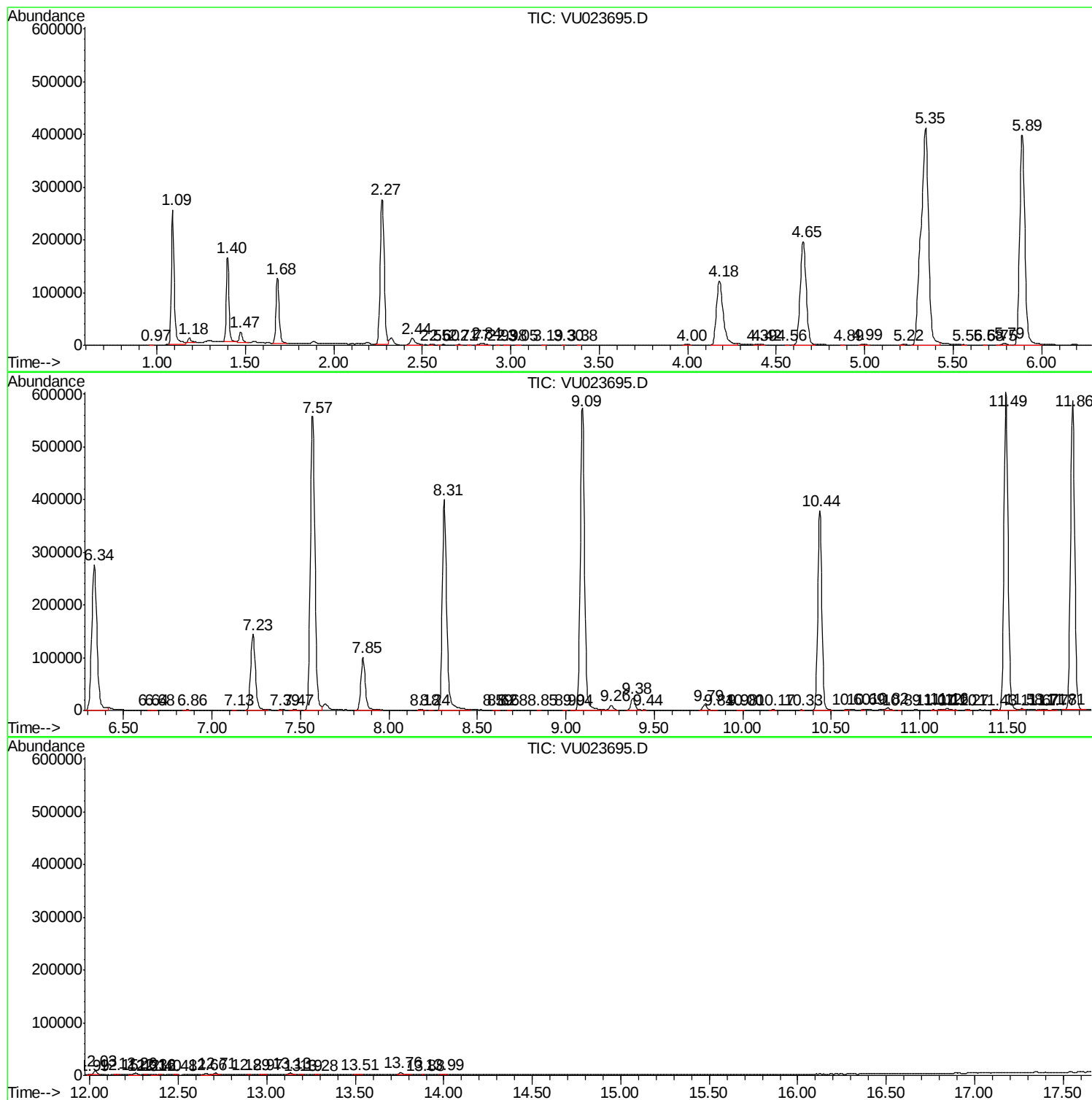
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 11.204 | 3297 | 3301 | 3303 | rBV2 | 417    | 230    | 0.02%  | 0.002% |
| 73  | 11.271 | 3319 | 3322 | 3328 | rVB3 | 668    | 586    | 0.05%  | 0.006% |
| 74  | 11.429 | 3366 | 3371 | 3376 | rVB3 | 718    | 873    | 0.07%  | 0.009% |
| 75  | 11.487 | 3376 | 3389 | 3410 | rBV  | 602812 | 967572 | 78.79% | 9.425% |
| 76  | 11.577 | 3413 | 3417 | 3423 | rVB5 | 1514   | 1610   | 0.13%  | 0.016% |
| 77  | 11.670 | 3443 | 3446 | 3450 | rBV2 | 365    | 285    | 0.02%  | 0.003% |
| 78  | 11.708 | 3450 | 3458 | 3467 | rVB6 | 1465   | 2221   | 0.18%  | 0.022% |
| 79  | 11.766 | 3468 | 3476 | 3479 | rBV2 | 531    | 703    | 0.06%  | 0.007% |
| 80  | 11.815 | 3488 | 3491 | 3494 | rBV2 | 1034   | 698    | 0.06%  | 0.007% |
| 81  | 11.863 | 3494 | 3506 | 3530 | rVB  | 587129 | 951306 | 77.46% | 9.267% |
| 82  | 11.991 | 3543 | 3546 | 3548 | rBV2 | 288    | 184    | 0.01%  | 0.002% |
| 83  | 12.030 | 3548 | 3558 | 3565 | rBV3 | 8284   | 11487  | 0.94%  | 0.112% |
| 84  | 12.152 | 3590 | 3596 | 3600 | rBV4 | 1039   | 1456   | 0.12%  | 0.014% |
| 85  | 12.258 | 3616 | 3629 | 3637 | rVB5 | 3596   | 6158   | 0.50%  | 0.060% |
| 86  | 12.310 | 3643 | 3645 | 3649 | rBV2 | 405    | 221    | 0.02%  | 0.002% |
| 87  | 12.364 | 3657 | 3662 | 3667 | rVB3 | 1063   | 1122   | 0.09%  | 0.011% |
| 88  | 12.396 | 3669 | 3672 | 3675 | rBV  | 509    | 368    | 0.03%  | 0.004% |
| 89  | 12.483 | 3696 | 3699 | 3703 | rBV  | 380    | 284    | 0.02%  | 0.003% |
| 90  | 12.657 | 3744 | 3753 | 3761 | rBV4 | 2579   | 4249   | 0.35%  | 0.041% |
| 91  | 12.708 | 3762 | 3769 | 3777 | rVB2 | 3787   | 4715   | 0.38%  | 0.046% |
| 92  | 12.895 | 3825 | 3827 | 3831 | rVB2 | 781    | 438    | 0.04%  | 0.004% |
| 93  | 12.972 | 3846 | 3851 | 3860 | rVB5 | 1200   | 1373   | 0.11%  | 0.013% |
| 94  | 13.130 | 3894 | 3900 | 3911 | rBV4 | 3776   | 5233   | 0.43%  | 0.051% |
| 95  | 13.191 | 3917 | 3919 | 3923 | rVB  | 375    | 250    | 0.02%  | 0.002% |
| 96  | 13.281 | 3944 | 3947 | 3951 | rBV3 | 419    | 332    | 0.03%  | 0.003% |
| 97  | 13.512 | 4013 | 4019 | 4027 | rBV5 | 1465   | 2049   | 0.17%  | 0.020% |
| 98  | 13.757 | 4088 | 4095 | 4113 | rVB2 | 4210   | 6938   | 0.56%  | 0.068% |
| 99  | 13.882 | 4132 | 4134 | 4135 | rBV2 | 378    | 144    | 0.01%  | 0.001% |
| 100 | 13.994 | 4164 | 4169 | 4176 | rVB5 | 1157   | 1408   | 0.11%  | 0.014% |

Sum of corrected areas: 10265851

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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050118WMA.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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