

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\  
 Data File : VU023740.D  
 Acq On : 08 May 2018 16:32  
 Operator : MD/SY  
 Sample : J2691-12  
 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\SOMULM050818WMA.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         | 0.635       | 12            | 14          | 19           | rVB      | 136            | 92            | 0.01%           | 0.001%        |
| 2         | 0.735       | 40            | 45          | 51           | rBV2     | 187            | 224           | 0.02%           | 0.002%        |
| 3         | 0.822       | 66            | 72          | 77           | rBV2     | 105            | 116           | 0.01%           | 0.001%        |
| 4         | 0.995       | 117           | 126         | 130          | rBV2     | 178            | 232           | 0.02%           | 0.002%        |
| 5         | 1.088       | 134           | 155         | 180          | rBV      | 1206299        | 1390201       | 100.00%         | 12.011%       |
| 6         | 1.185       | 181           | 185         | 190          | rVB      | 6864           | 6318          | 0.45%           | 0.055%        |
| 7         | 1.400       | 245           | 252         | 271          | rBV      | 195472         | 200062        | 14.39%          | 1.729%        |
| 8         | 1.680       | 332           | 339         | 355          | rVB      | 134416         | 173240        | 12.46%          | 1.497%        |
| 9         | 2.275       | 512           | 524         | 538          | rBV      | 291712         | 449449        | 32.33%          | 3.883%        |
| 10        | 2.529       | 600           | 603         | 608          | rBV2     | 246            | 249           | 0.02%           | 0.002%        |
| 11        | 2.629       | 627           | 634         | 639          | rVB      | 572            | 704           | 0.05%           | 0.006%        |
| 12        | 2.654       | 639           | 642         | 644          | rBV      | 197            | 126           | 0.01%           | 0.001%        |
| 13        | 2.699       | 651           | 656         | 658          | rBV2     | 562            | 557           | 0.04%           | 0.005%        |
| 14        | 2.796       | 683           | 686         | 689          | rVB      | 172            | 102           | 0.01%           | 0.001%        |
| 15        | 2.841       | 689           | 700         | 711          | rBV2     | 1477           | 3220          | 0.23%           | 0.028%        |
| 16        | 2.908       | 718           | 721         | 725          | rBV2     | 148            | 91            | 0.01%           | 0.001%        |
| 17        | 2.947       | 731           | 733         | 737          | rVB2     | 211            | 145           | 0.01%           | 0.001%        |
| 18        | 2.992       | 744           | 747         | 749          | rVB2     | 259            | 146           | 0.01%           | 0.001%        |
| 19        | 3.027       | 755           | 758         | 761          | rBV2     | 133            | 108           | 0.01%           | 0.001%        |
| 20        | 3.075       | 770           | 773         | 777          | rVB2     | 194            | 133           | 0.01%           | 0.001%        |
| 21        | 3.133       | 783           | 791         | 793          | rBV      | 129            | 176           | 0.01%           | 0.002%        |
| 22        | 3.182       | 800           | 806         | 809          | rBV      | 121            | 154           | 0.01%           | 0.001%        |
| 23        | 3.291       | 836           | 840         | 844          | rBV2     | 149            | 132           | 0.01%           | 0.001%        |
| 24        | 3.394       | 868           | 872         | 876          | rVB3     | 240            | 259           | 0.02%           | 0.002%        |
| 25        | 3.455       | 888           | 891         | 895          | rVB2     | 158            | 141           | 0.01%           | 0.001%        |
| 26        | 3.481       | 895           | 899         | 902          | rBV2     | 125            | 96            | 0.01%           | 0.001%        |
| 27        | 3.574       | 924           | 928         | 932          | rVV2     | 141            | 123           | 0.01%           | 0.001%        |
| 28        | 3.850       | 1008          | 1014        | 1015         | rBV      | 194            | 160           | 0.01%           | 0.001%        |
| 29        | 4.034       | 1067          | 1071        | 1073         | rBV      | 126            | 108           | 0.01%           | 0.001%        |
| 30        | 4.088       | 1084          | 1088        | 1093         | rVB      | 137            | 112           | 0.01%           | 0.001%        |
| 31        | 4.182       | 1101          | 1117        | 1149         | rBV      | 127706         | 336950        | 24.24%          | 2.911%        |
| 32        | 4.436       | 1194          | 1196        | 1200         | rVB2     | 408            | 291           | 0.02%           | 0.003%        |
| 33        | 4.577       | 1236          | 1240        | 1244         | rBV2     | 256            | 270           | 0.02%           | 0.002%        |
| 34        | 4.654       | 1247          | 1264        | 1292         | rBV      | 209785         | 497496        | 35.79%          | 4.298%        |

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\  
 Data File : VU023740.D  
 Acq On : 08 May 2018 16:32  
 Operator : MD/SY  
 Sample : J2691-12  
 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\SOMULM050818WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 4.828 | 1316 | 1318 | 1322 | rVB2 | 227    | 119     | 0.01%  | 0.001%  |
| 36 | 4.889 | 1331 | 1337 | 1338 | rBV  | 446    | 426     | 0.03%  | 0.004%  |
| 37 | 4.992 | 1363 | 1369 | 1372 | rBV3 | 481    | 516     | 0.04%  | 0.004%  |
| 38 | 5.008 | 1372 | 1374 | 1378 | rVB  | 378    | 191     | 0.01%  | 0.002%  |
| 39 | 5.069 | 1390 | 1393 | 1402 | rBV2 | 108    | 156     | 0.01%  | 0.001%  |
| 40 | 5.124 | 1402 | 1410 | 1413 | rBV2 | 142    | 159     | 0.01%  | 0.001%  |
| 41 | 5.220 | 1435 | 1440 | 1443 | rBV2 | 122    | 112     | 0.01%  | 0.001%  |
| 42 | 5.346 | 1453 | 1479 | 1534 | rBV2 | 445493 | 1333825 | 95.94% | 11.524% |
| 43 | 5.667 | 1576 | 1579 | 1582 | rVB2 | 209    | 135     | 0.01%  | 0.001%  |
| 44 | 5.738 | 1596 | 1601 | 1603 | rBV2 | 127    | 105     | 0.01%  | 0.001%  |
| 45 | 5.892 | 1627 | 1649 | 1683 | rBV  | 385286 | 782891  | 56.31% | 6.764%  |
| 46 | 6.140 | 1723 | 1726 | 1731 | rVV2 | 217    | 138     | 0.01%  | 0.001%  |
| 47 | 6.188 | 1731 | 1741 | 1750 | rVV8 | 1646   | 3208    | 0.23%  | 0.028%  |
| 48 | 6.223 | 1750 | 1752 | 1755 | rVB  | 234    | 99      | 0.01%  | 0.001%  |
| 49 | 6.336 | 1773 | 1787 | 1811 | rBV  | 292329 | 595493  | 42.84% | 5.145%  |
| 50 | 6.561 | 1854 | 1857 | 1862 | rVB  | 169    | 147     | 0.01%  | 0.001%  |
| 51 | 6.609 | 1866 | 1872 | 1875 | rBV2 | 167    | 158     | 0.01%  | 0.001%  |
| 52 | 6.638 | 1879 | 1881 | 1884 | rVB  | 189    | 93      | 0.01%  | 0.001%  |
| 53 | 6.799 | 1925 | 1931 | 1934 | rBV  | 177    | 163     | 0.01%  | 0.001%  |
| 54 | 6.828 | 1937 | 1940 | 1943 | rVB  | 167    | 95      | 0.01%  | 0.001%  |
| 55 | 6.863 | 1948 | 1951 | 1952 | rBV2 | 203    | 118     | 0.01%  | 0.001%  |
| 56 | 6.921 | 1966 | 1969 | 1972 | rVB2 | 207    | 139     | 0.01%  | 0.001%  |
| 57 | 6.944 | 1972 | 1976 | 1980 | rBV2 | 152    | 129     | 0.01%  | 0.001%  |
| 58 | 7.075 | 2011 | 2017 | 2022 | rVB  | 202    | 196     | 0.01%  | 0.002%  |
| 59 | 7.104 | 2022 | 2026 | 2033 | rVB  | 187    | 215     | 0.02%  | 0.002%  |
| 60 | 7.140 | 2033 | 2037 | 2042 | rBV2 | 197    | 246     | 0.02%  | 0.002%  |
| 61 | 7.233 | 2052 | 2066 | 2098 | rBV  | 154974 | 285694  | 20.55% | 2.468%  |
| 62 | 7.387 | 2111 | 2114 | 2115 | rBV  | 219    | 112     | 0.01%  | 0.001%  |
| 63 | 7.571 | 2156 | 2171 | 2209 | rBV  | 596237 | 1063212 | 76.48% | 9.186%  |
| 64 | 7.853 | 2245 | 2259 | 2280 | rBV  | 107953 | 186071  | 13.38% | 1.608%  |
| 65 | 8.040 | 2315 | 2317 | 2325 | rVB  | 241    | 207     | 0.01%  | 0.002%  |
| 66 | 8.159 | 2350 | 2354 | 2357 | rBV  | 156    | 139     | 0.01%  | 0.001%  |
| 67 | 8.178 | 2357 | 2360 | 2362 | rBV2 | 215    | 181     | 0.01%  | 0.002%  |
| 68 | 8.236 | 2369 | 2378 | 2380 | rBV2 | 372    | 367     | 0.03%  | 0.003%  |
| 69 | 8.255 | 2381 | 2384 | 2387 | rBV2 | 145    | 109     | 0.01%  | 0.001%  |
| 70 | 8.313 | 2390 | 2402 | 2442 | rBV  | 420266 | 732598  | 52.70% | 6.330%  |
| 71 | 8.603 | 2488 | 2492 | 2494 | rBV2 | 161    | 109     | 0.01%  | 0.001%  |

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\  
 Data File : VU023740.D  
 Acq On : 08 May 2018 16:32  
 Operator : MD/SY  
 Sample : J2691-12  
 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\SOMULM050818WMA.M  
 Title : VOC Analysis

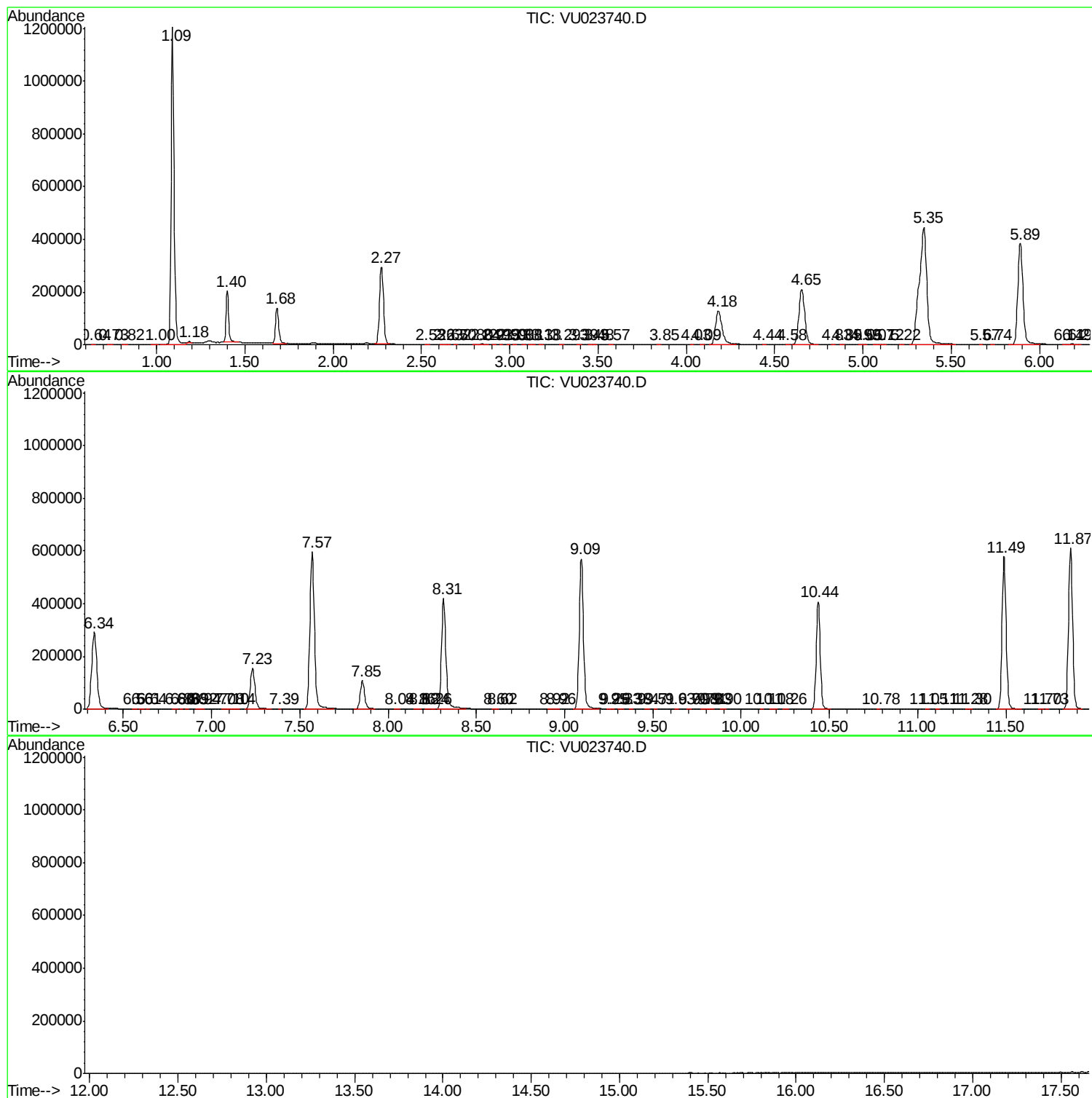
|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 8.622  | 2494 | 2498 | 2499 | rBV  | 541    | 379    | 0.03%  | 0.003% |
| 73  | 8.918  | 2586 | 2590 | 2598 | rBV2 | 231    | 349    | 0.03%  | 0.003% |
| 74  | 8.956  | 2599 | 2602 | 2605 | rVV  | 177    | 122    | 0.01%  | 0.001% |
| 75  | 9.095  | 2631 | 2645 | 2676 | rBV  | 569613 | 958438 | 68.94% | 8.281% |
| 76  | 9.252  | 2690 | 2694 | 2695 | rBV  | 437    | 319    | 0.02%  | 0.003% |
| 77  | 9.262  | 2695 | 2697 | 2702 | rVB2 | 505    | 403    | 0.03%  | 0.003% |
| 78  | 9.326  | 2709 | 2717 | 2719 | rBV2 | 166    | 183    | 0.01%  | 0.002% |
| 79  | 9.381  | 2728 | 2734 | 2735 | rBV  | 663    | 604    | 0.04%  | 0.005% |
| 80  | 9.471  | 2756 | 2762 | 2765 | rBV2 | 203    | 222    | 0.02%  | 0.002% |
| 81  | 9.513  | 2773 | 2775 | 2778 | rVB  | 174    | 96     | 0.01%  | 0.001% |
| 82  | 9.632  | 2809 | 2812 | 2815 | rBV  | 224    | 143    | 0.01%  | 0.001% |
| 83  | 9.702  | 2830 | 2834 | 2838 | rBV2 | 202    | 173    | 0.01%  | 0.001% |
| 84  | 9.786  | 2855 | 2860 | 2866 | rBV2 | 416    | 535    | 0.04%  | 0.005% |
| 85  | 9.812  | 2866 | 2868 | 2870 | rVB2 | 344    | 166    | 0.01%  | 0.001% |
| 86  | 9.834  | 2870 | 2875 | 2878 | rVB  | 136    | 139    | 0.01%  | 0.001% |
| 87  | 9.895  | 2889 | 2894 | 2899 | rBV2 | 538    | 671    | 0.05%  | 0.006% |
| 88  | 10.114 | 2960 | 2962 | 2965 | rBV  | 158    | 107    | 0.01%  | 0.001% |
| 89  | 10.178 | 2977 | 2982 | 2990 | rVB3 | 333    | 451    | 0.03%  | 0.004% |
| 90  | 10.255 | 2999 | 3006 | 3010 | rBV2 | 222    | 301    | 0.02%  | 0.003% |
| 91  | 10.435 | 3050 | 3062 | 3084 | rBV  | 407461 | 649700 | 46.73% | 5.613% |
| 92  | 10.779 | 3166 | 3169 | 3171 | rBV2 | 207    | 154    | 0.01%  | 0.001% |
| 93  | 11.049 | 3251 | 3253 | 3258 | rVB  | 188    | 103    | 0.01%  | 0.001% |
| 94  | 11.107 | 3268 | 3271 | 3275 | rBV2 | 222    | 164    | 0.01%  | 0.001% |
| 95  | 11.278 | 3321 | 3324 | 3327 | rVB2 | 308    | 185    | 0.01%  | 0.002% |
| 96  | 11.297 | 3328 | 3330 | 3333 | rBV2 | 174    | 109    | 0.01%  | 0.001% |
| 97  | 11.487 | 3376 | 3389 | 3419 | rBV  | 577964 | 926188 | 66.62% | 8.002% |
| 98  | 11.696 | 3449 | 3454 | 3459 | rBV2 | 292    | 283    | 0.02%  | 0.002% |
| 99  | 11.734 | 3463 | 3466 | 3467 | rBV2 | 211    | 116    | 0.01%  | 0.001% |
| 100 | 11.866 | 3493 | 3507 | 3527 | rBV  | 610138 | 983331 | 70.73% | 8.496% |

Sum of corrected areas: 11574188

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\  
Data File : VU023740.D  
Acq On : 08 May 2018 16:32  
Operator : MD/SY  
Sample : J2691-12  
Misc : 5.0mL/MSVOA U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
Quant Title : VOC Analysis

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



Data Path : W:\HPCHEM1\MSVOA\_U\DATA\VU050818\  
Data File : VU023740.D  
Acq On : 08 May 2018 16:32  
Operator : MD/SY  
Sample : J2691-12  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : W:\HPCHEM1\MSVOA\_U\DATA\VU050818\  
Data File : VU023740.D  
Acq On : 08 May 2018 16:32  
Operator : MD/SY  
Sample : J2691-12  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 16 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA\_U\METHOD\SOMULM050818WMA.M  
Quant Title : VOC Analysis

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

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

-----