

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU102918\  
 Data File : VU027855.D  
 Acq On : 29 Oct 2018 14:54  
 Operator : MD/SY  
 Sample : J5635-26ME  
 Misc : 5.64g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A40G2ME

## 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 : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
 Title : VOC Analysis

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 1.395    | 62         | 69       | 91        | rVB   | 76486       | 111574     | 13.19%       | 1.408%     |
| 2      | 1.575    | 110        | 125      | 126       | rBV5  | 6507        | 10178      | 1.20%        | 0.128%     |
| 3      | 1.640    | 140        | 145      | 163       | rBV   | 64287       | 97862      | 11.57%       | 1.235%     |
| 4      | 2.141    | 296        | 301      | 309       | rBV5  | 1941        | 2767       | 0.33%        | 0.035%     |
| 5      | 2.228    | 318        | 328      | 345       | rBV   | 156185      | 250602     | 29.62%       | 3.162%     |
| 6      | 2.411    | 382        | 385      | 392       | rVB2  | 379         | 370        | 0.04%        | 0.005%     |
| 7      | 2.530    | 419        | 422      | 424       | rBV   | 181         | 127        | 0.02%        | 0.002%     |
| 8      | 2.630    | 444        | 453      | 465       | rVB2  | 475         | 1164       | 0.14%        | 0.015%     |
| 9      | 2.682    | 465        | 469      | 470       | rBV   | 464         | 319        | 0.04%        | 0.004%     |
| 10     | 2.836    | 505        | 517      | 528       | rBV   | 2680        | 5733       | 0.68%        | 0.072%     |
| 11     | 2.878    | 528        | 530      | 534       | rVB2  | 295         | 205        | 0.02%        | 0.003%     |
| 12     | 3.305    | 657        | 663      | 669       | rBV   | 96          | 138        | 0.02%        | 0.002%     |
| 13     | 3.363    | 676        | 681      | 685       | rBV2  | 178         | 192        | 0.02%        | 0.002%     |
| 14     | 3.907    | 845        | 850      | 856       | rBV   | 99          | 126        | 0.01%        | 0.002%     |
| 15     | 4.051    | 891        | 895      | 898       | rBV   | 202         | 219        | 0.03%        | 0.003%     |
| 16     | 4.199    | 927        | 941      | 987       | rBV   | 55476       | 213494     | 25.23%       | 2.694%     |
| 17     | 4.646    | 1062       | 1080     | 1112      | rVB   | 125702      | 320880     | 37.92%       | 4.049%     |
| 18     | 4.800    | 1121       | 1128     | 1129      | rBV2  | 275         | 302        | 0.04%        | 0.004%     |
| 19     | 4.855    | 1142       | 1145     | 1150      | rVB2  | 300         | 293        | 0.03%        | 0.004%     |
| 20     | 4.897    | 1154       | 1158     | 1161      | rBV2  | 256         | 256        | 0.03%        | 0.003%     |
| 21     | 4.952    | 1170       | 1175     | 1177      | rBV   | 629         | 575        | 0.07%        | 0.007%     |
| 22     | 5.231    | 1259       | 1262     | 1266      | rBV   | 171         | 176        | 0.02%        | 0.002%     |
| 23     | 5.331    | 1270       | 1293     | 1326      | rVV2  | 293762      | 841111     | 99.41%       | 10.613%    |
| 24     | 5.492    | 1339       | 1343     | 1346      | rVB2  | 146         | 132        | 0.02%        | 0.002%     |
| 25     | 5.617    | 1378       | 1382     | 1386      | rBV2  | 684         | 762        | 0.09%        | 0.010%     |
| 26     | 5.649    | 1389       | 1392     | 1397      | rVV   | 279         | 255        | 0.03%        | 0.003%     |
| 27     | 5.762    | 1423       | 1427     | 1435      | rVV   | 109         | 152        | 0.02%        | 0.002%     |
| 28     | 5.884    | 1450       | 1465     | 1495      | rBV   | 256507      | 539523     | 63.76%       | 6.808%     |
| 29     | 6.170    | 1547       | 1554     | 1562      | rVB4  | 884         | 1410       | 0.17%        | 0.018%     |
| 30     | 6.257    | 1574       | 1581     | 1587      | rBV3  | 705         | 1262       | 0.15%        | 0.016%     |
| 31     | 6.331    | 1589       | 1604     | 1630      | rVV   | 181941      | 394160     | 46.58%       | 4.973%     |
| 32     | 6.424    | 1630       | 1633     | 1638      | rVB2  | 278         | 250        | 0.03%        | 0.003%     |
| 33     | 6.453    | 1638       | 1642     | 1644      | rBV   | 394         | 227        | 0.03%        | 0.003%     |
| 34     | 6.466    | 1644       | 1646     | 1649      | rVB2  | 274         | 156        | 0.02%        | 0.002%     |

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 ClientSampleId :  
 A40G2ME

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Filtering: 5  
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 Max Peaks: 100  
 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |         |         |
|----|--------|------|------|------|------|--------|--------|---------|---------|
| 35 | 6.550  | 1668 | 1672 | 1674 | rBV  | 155    | 155    | 0.02%   | 0.002%  |
| 36 | 6.829  | 1757 | 1759 | 1761 | rBV  | 240    | 163    | 0.02%   | 0.002%  |
| 37 | 6.865  | 1762 | 1770 | 1774 | rBV4 | 1233   | 1690   | 0.20%   | 0.021%  |
| 38 | 7.228  | 1870 | 1883 | 1908 | rBV  | 105400 | 209310 | 24.74%  | 2.641%  |
| 39 | 7.386  | 1924 | 1932 | 1938 | rBV4 | 818    | 1280   | 0.15%   | 0.016%  |
| 40 | 7.492  | 1962 | 1965 | 1967 | rBV2 | 275    | 159    | 0.02%   | 0.002%  |
| 41 | 7.566  | 1974 | 1988 | 2007 | rBV  | 376130 | 680835 | 80.47%  | 8.591%  |
| 42 | 7.681  | 2015 | 2024 | 2036 | rVB3 | 1062   | 2394   | 0.28%   | 0.030%  |
| 43 | 7.852  | 2066 | 2077 | 2105 | rBV2 | 73633  | 144440 | 17.07%  | 1.822%  |
| 44 | 8.061  | 2138 | 2142 | 2149 | rBV  | 122    | 141    | 0.02%   | 0.002%  |
| 45 | 8.183  | 2166 | 2180 | 2190 | rBV  | 18757  | 43844  | 5.18%   | 0.553%  |
| 46 | 8.328  | 2213 | 2225 | 2252 | rVB  | 295041 | 567194 | 67.03%  | 7.157%  |
| 47 | 8.562  | 2295 | 2298 | 2302 | rVB  | 243    | 191    | 0.02%   | 0.002%  |
| 48 | 8.633  | 2311 | 2320 | 2328 | rBV2 | 1487   | 2358   | 0.28%   | 0.030%  |
| 49 | 9.093  | 2445 | 2463 | 2482 | rBV  | 399499 | 697949 | 82.49%  | 8.806%  |
| 50 | 9.202  | 2493 | 2497 | 2502 | rVB3 | 487    | 460    | 0.05%   | 0.006%  |
| 51 | 9.289  | 2521 | 2524 | 2525 | rBV2 | 295    | 189    | 0.02%   | 0.002%  |
| 52 | 9.434  | 2567 | 2569 | 2574 | rVB3 | 287    | 212    | 0.03%   | 0.003%  |
| 53 | 9.543  | 2600 | 2603 | 2609 | rBV4 | 272    | 350    | 0.04%   | 0.004%  |
| 54 | 9.668  | 2638 | 2642 | 2644 | rBV2 | 318    | 295    | 0.03%   | 0.004%  |
| 55 | 9.733  | 2660 | 2662 | 2665 | rBV2 | 254    | 152    | 0.02%   | 0.002%  |
| 56 | 9.955  | 2726 | 2731 | 2739 | rVB4 | 828    | 1113   | 0.13%   | 0.014%  |
| 57 | 10.173 | 2792 | 2799 | 2805 | rVB2 | 726    | 1112   | 0.13%   | 0.014%  |
| 58 | 10.244 | 2817 | 2821 | 2830 | rVB2 | 324    | 524    | 0.06%   | 0.007%  |
| 59 | 10.353 | 2851 | 2855 | 2860 | rBV  | 138    | 153    | 0.02%   | 0.002%  |
| 60 | 10.437 | 2869 | 2881 | 2901 | rBV  | 296316 | 467639 | 55.27%  | 5.901%  |
| 61 | 10.614 | 2924 | 2936 | 2951 | rVV3 | 8411   | 17589  | 2.08%   | 0.222%  |
| 62 | 10.774 | 2981 | 2986 | 2992 | rBV2 | 412    | 480    | 0.06%   | 0.006%  |
| 63 | 10.813 | 2995 | 2998 | 3000 | rBV  | 275    | 137    | 0.02%   | 0.002%  |
| 64 | 10.874 | 3009 | 3017 | 3024 | rVB3 | 622    | 807    | 0.10%   | 0.010%  |
| 65 | 11.385 | 3172 | 3176 | 3180 | rBV3 | 650    | 616    | 0.07%   | 0.008%  |
| 66 | 11.424 | 3180 | 3188 | 3195 | rVV2 | 6464   | 9112   | 1.08%   | 0.115%  |
| 67 | 11.485 | 3195 | 3207 | 3230 | rVB  | 498807 | 846124 | 100.00% | 10.676% |
| 68 | 11.630 | 3248 | 3252 | 3255 | rBV2 | 594    | 464    | 0.05%   | 0.006%  |
| 69 | 11.762 | 3289 | 3293 | 3294 | rBV  | 237    | 144    | 0.02%   | 0.002%  |
| 70 | 11.864 | 3312 | 3325 | 3344 | rBV  | 450774 | 718691 | 84.94%  | 9.068%  |
| 71 | 12.025 | 3373 | 3375 | 3378 | rVB  | 255    | 145    | 0.02%   | 0.002%  |

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Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 A40G2ME

## Integration Parameters: LSCINT.P

Integrator: RTE  
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Filtering: 5  
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 Max Peaks: 100  
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 12.160 | 3413 | 3417 | 3419 | rBV  | 326    | 300    | 0.04%  | 0.004% |
| 73  | 12.234 | 3419 | 3440 | 3441 | rBV4 | 4251   | 9300   | 1.10%  | 0.117% |
| 74  | 12.572 | 3543 | 3545 | 3552 | rVB2 | 194    | 175    | 0.02%  | 0.002% |
| 75  | 12.639 | 3563 | 3566 | 3569 | rBV  | 184    | 148    | 0.02%  | 0.002% |
| 76  | 12.839 | 3622 | 3628 | 3630 | rBV2 | 485    | 447    | 0.05%  | 0.006% |
| 77  | 13.167 | 3728 | 3730 | 3734 | rBV  | 146    | 124    | 0.01%  | 0.002% |
| 78  | 13.189 | 3734 | 3737 | 3738 | rBV2 | 265    | 168    | 0.02%  | 0.002% |
| 79  | 13.202 | 3738 | 3741 | 3744 | rVB3 | 264    | 157    | 0.02%  | 0.002% |
| 80  | 13.295 | 3768 | 3770 | 3774 | rVB  | 281    | 130    | 0.02%  | 0.002% |
| 81  | 14.015 | 3991 | 3994 | 3996 | rBV  | 198    | 117    | 0.01%  | 0.001% |
| 82  | 14.054 | 4003 | 4006 | 4009 | rBV2 | 231    | 176    | 0.02%  | 0.002% |
| 83  | 14.115 | 4023 | 4025 | 4031 | rVB  | 275    | 185    | 0.02%  | 0.002% |
| 84  | 14.141 | 4031 | 4033 | 4036 | rBV  | 327    | 144    | 0.02%  | 0.002% |
| 85  | 14.196 | 4044 | 4050 | 4051 | rBV  | 507    | 454    | 0.05%  | 0.006% |
| 86  | 14.276 | 4069 | 4075 | 4089 | rVB2 | 5888   | 10073  | 1.19%  | 0.127% |
| 87  | 14.360 | 4097 | 4101 | 4103 | rVB2 | 312    | 223    | 0.03%  | 0.003% |
| 88  | 14.382 | 4106 | 4108 | 4110 | rBV  | 237    | 132    | 0.02%  | 0.002% |
| 89  | 14.524 | 4147 | 4152 | 4153 | rBV2 | 869    | 739    | 0.09%  | 0.009% |
| 90  | 14.591 | 4155 | 4173 | 4176 | rBV4 | 13303  | 30515  | 3.61%  | 0.385% |
| 91  | 14.787 | 4227 | 4234 | 4241 | rBV3 | 5368   | 6977   | 0.82%  | 0.088% |
| 92  | 14.832 | 4241 | 4248 | 4260 | rVV  | 9034   | 13546  | 1.60%  | 0.171% |
| 93  | 14.890 | 4262 | 4266 | 4275 | rVB5 | 2147   | 2628   | 0.31%  | 0.033% |
| 94  | 15.015 | 4296 | 4305 | 4316 | rBV3 | 6569   | 11568  | 1.37%  | 0.146% |
| 95  | 15.089 | 4321 | 4328 | 4338 | rVB3 | 10344  | 14042  | 1.66%  | 0.177% |
| 96  | 15.179 | 4349 | 4356 | 4368 | rBV3 | 3906   | 5477   | 0.65%  | 0.069% |
| 97  | 15.614 | 4483 | 4491 | 4500 | rBV2 | 6664   | 10799  | 1.28%  | 0.136% |
| 98  | 15.880 | 4566 | 4574 | 4587 | rVB2 | 4800   | 7212   | 0.85%  | 0.091% |
| 99  | 16.552 | 4773 | 4783 | 4797 | rVB  | 337140 | 491291 | 58.06% | 6.199% |
| 100 | 16.703 | 4820 | 4830 | 4846 | rVB  | 59382  | 92597  | 10.94% | 1.168% |

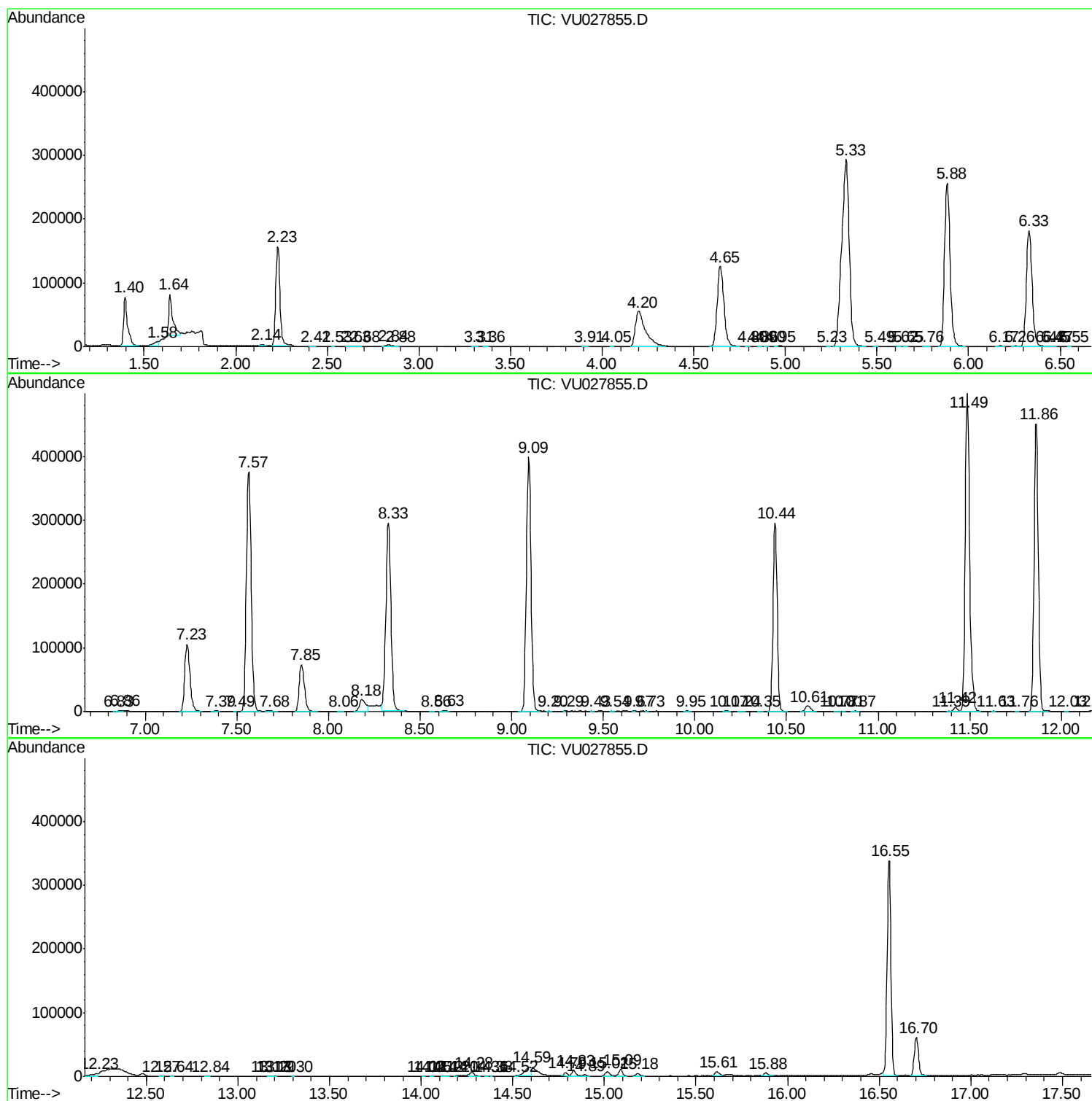
Sum of corrected areas: 7925407

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Instrument :  
MSVOA\_U  
ClientSampled :  
A40G2ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU102918\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
 Quant Title : VOC Analysis

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

\*\*\*\*\*  
 Peak Number 1 Butylated Hydroxytoluene Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD       | R.T.  |
|-------|------------|--------|------------------------|-------|
| 16.55 | 29.03 ug/L | 491291 | 1,4-Dichlorobenzene-d4 | 11.49 |

| Hit# of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|---------|---|------------------------------------|-----|---------|-------------|------|
| 1       |   | Butylated Hydroxytoluene           | 220 | C15H24O | 000128-37-0 | 98   |
| 2       |   | Butylated Hydroxytoluene           | 220 | C15H24O | 000128-37-0 | 96   |
| 3       |   | Butylated Hydroxytoluene           | 220 | C15H24O | 000128-37-0 | 95   |
| 4       |   | Butylated Hydroxytoluene           | 220 | C15H24O | 000128-37-0 | 94   |
| 5       |   | Phenol, 2,4,6-tris(1-methylethyl)- | 220 | C15H24O | 002934-07-8 | 87   |

\*\*\*\*\*  
 Peak Number 2 1,1'-Biphenyl, 2-chloro- Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 16.70 | 5.47 ug/L | 92597 | 1,4-Dichlorobenzene-d4 | 11.49 |

| Hit# of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|---------|---|--------------------------|-----|---------|-------------|------|
| 1       |   | 1,1'-Biphenyl, 2-chloro- | 188 | C12H9Cl | 002051-60-7 | 98   |
| 2       |   | 1,1'-Biphenyl, 4-chloro- | 188 | C12H9Cl | 002051-62-9 | 97   |
| 3       |   | 1,1'-Biphenyl, 4-chloro- | 188 | C12H9Cl | 002051-62-9 | 96   |
| 4       |   | 1,1'-Biphenyl, 4-chloro- | 188 | C12H9Cl | 002051-62-9 | 94   |
| 5       |   | 3-Chlorobiphenyl         | 188 | C12H9Cl | 002051-61-8 | 94   |

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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 |
| Butylated Hydroxy... | 16.55 | 29.0    | ug/L  | 491291   | 3                     | 11.49 | 846124 | 50.0 |
| 1,1'-Biphenyl, 2-... | 16.70 | 5.5     | ug/L  | 92597    | 3                     | 11.49 | 846124 | 50.0 |