

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU082418\  
 Data File : VU026334.D  
 Acq On : 24 Aug 2018 15:28  
 Operator : MD/SY  
 Sample : J4624-03ME  
 Misc : 6.32g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E4429ME

## 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\SOMULM082218WMA.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         | 0.770       | 51            | 56          | 61           | rBV3     | 258            | 340           | 0.03%           | 0.003%        |
| 2         | 0.825       | 69            | 73          | 77           | rBV3     | 400            | 419           | 0.04%           | 0.004%        |
| 3         | 0.892       | 90            | 94          | 97           | rBV2     | 321            | 316           | 0.03%           | 0.003%        |
| 4         | 1.082       | 136           | 153         | 169          | rBV      | 1127961        | 1195940       | 100.00%         | 11.619%       |
| 5         | 1.394       | 243           | 250         | 265          | rVB      | 109306         | 123096        | 10.29%          | 1.196%        |
| 6         | 1.642       | 322           | 327         | 340          | rBV      | 79553          | 83150         | 6.95%           | 0.808%        |
| 7         | 2.236       | 502           | 512         | 528          | rBV      | 205215         | 313943        | 26.25%          | 3.050%        |
| 8         | 2.442       | 574           | 576         | 581          | rVB2     | 1197           | 834           | 0.07%           | 0.008%        |
| 9         | 2.590       | 618           | 622         | 624          | rBV4     | 436            | 332           | 0.03%           | 0.003%        |
| 10        | 2.690       | 644           | 653         | 662          | rBV5     | 3371           | 5350          | 0.45%           | 0.052%        |
| 11        | 2.831       | 684           | 697         | 711          | rBV2     | 8331           | 19824         | 1.66%           | 0.193%        |
| 12        | 3.015       | 751           | 754         | 760          | rVB2     | 508            | 382           | 0.03%           | 0.004%        |
| 13        | 3.117       | 783           | 786         | 793          | rBV2     | 439            | 504           | 0.04%           | 0.005%        |
| 14        | 3.278       | 830           | 836         | 837          | rBV2     | 631            | 437           | 0.04%           | 0.004%        |
| 15        | 3.436       | 880           | 885         | 889          | rBV2     | 557            | 629           | 0.05%           | 0.006%        |
| 16        | 3.635       | 944           | 947         | 951          | rBV2     | 459            | 339           | 0.03%           | 0.003%        |
| 17        | 3.661       | 951           | 955         | 958          | rBV3     | 494            | 389           | 0.03%           | 0.004%        |
| 18        | 3.741       | 970           | 980         | 981          | rBV2     | 296            | 353           | 0.03%           | 0.003%        |
| 19        | 3.812       | 997           | 1002        | 1007         | rVB3     | 334            | 398           | 0.03%           | 0.004%        |
| 20        | 3.924       | 1033          | 1037        | 1044         | rBV4     | 473            | 623           | 0.05%           | 0.006%        |
| 21        | 4.027       | 1064          | 1069        | 1072         | rBV3     | 284            | 329           | 0.03%           | 0.003%        |
| 22        | 4.201       | 1105          | 1123        | 1168         | rBV2     | 69148          | 278646        | 23.30%          | 2.707%        |
| 23        | 4.484       | 1208          | 1211        | 1217         | rBV3     | 450            | 453           | 0.04%           | 0.004%        |
| 24        | 4.648       | 1243          | 1262        | 1286         | rBV      | 170735         | 424731        | 35.51%          | 4.126%        |
| 25        | 4.809       | 1308          | 1312        | 1315         | rVB4     | 330            | 290           | 0.02%           | 0.003%        |
| 26        | 4.960       | 1347          | 1359        | 1372         | rBV3     | 4327           | 10841         | 0.91%           | 0.105%        |
| 27        | 5.034       | 1377          | 1382        | 1386         | rBV3     | 375            | 326           | 0.03%           | 0.003%        |
| 28        | 5.085       | 1395          | 1398        | 1404         | rVB2     | 416            | 313           | 0.03%           | 0.003%        |
| 29        | 5.140       | 1411          | 1415        | 1417         | rBV3     | 467            | 390           | 0.03%           | 0.004%        |
| 30        | 5.239       | 1443          | 1446        | 1449         | rVV2     | 493            | 331           | 0.03%           | 0.003%        |
| 31        | 5.333       | 1453          | 1475        | 1507         | rVB2     | 362044         | 1038829       | 86.86%          | 10.092%       |
| 32        | 5.564       | 1544          | 1547        | 1552         | rVB3     | 360            | 294           | 0.02%           | 0.003%        |
| 33        | 5.606       | 1552          | 1560        | 1562         | rBV5     | 2294           | 2449          | 0.20%           | 0.024%        |
| 34        | 5.776       | 1609          | 1613        | 1618         | rVB3     | 466            | 401           | 0.03%           | 0.004%        |

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 E4429ME

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 Start Thrs: 0.2  
 Stop Thrs : 0

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\SOMULM082218WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 5.886  | 1628 | 1647 | 1677 | rBV  | 362046 | 754270 | 63.07% | 7.328% |
| 36 | 6.082  | 1702 | 1708 | 1711 | rVB3 | 581    | 458    | 0.04%  | 0.004% |
| 37 | 6.185  | 1727 | 1740 | 1754 | rBV2 | 34291  | 67541  | 5.65%  | 0.656% |
| 38 | 6.252  | 1755 | 1761 | 1769 | rVV4 | 2520   | 4373   | 0.37%  | 0.042% |
| 39 | 6.330  | 1770 | 1785 | 1815 | rVB  | 225718 | 474551 | 39.68% | 4.610% |
| 40 | 6.442  | 1815 | 1820 | 1821 | rBV2 | 416    | 306    | 0.03%  | 0.003% |
| 41 | 6.558  | 1854 | 1856 | 1860 | rVB4 | 490    | 361    | 0.03%  | 0.004% |
| 42 | 6.693  | 1896 | 1898 | 1903 | rVV3 | 381    | 315    | 0.03%  | 0.003% |
| 43 | 6.879  | 1947 | 1956 | 1970 | rVV6 | 2960   | 6811   | 0.57%  | 0.066% |
| 44 | 6.931  | 1970 | 1972 | 1979 | rVB3 | 594    | 545    | 0.05%  | 0.005% |
| 45 | 7.159  | 2039 | 2043 | 2046 | rBV2 | 434    | 330    | 0.03%  | 0.003% |
| 46 | 7.230  | 2052 | 2065 | 2086 | rBV  | 120117 | 237054 | 19.82% | 2.303% |
| 47 | 7.346  | 2097 | 2101 | 2102 | rBV  | 525    | 312    | 0.03%  | 0.003% |
| 48 | 7.400  | 2111 | 2118 | 2123 | rBV5 | 646    | 842    | 0.07%  | 0.008% |
| 49 | 7.567  | 2156 | 2170 | 2190 | rBV  | 454076 | 825635 | 69.04% | 8.021% |
| 50 | 7.854  | 2247 | 2259 | 2277 | rBV2 | 85059  | 167081 | 13.97% | 1.623% |
| 51 | 8.188  | 2343 | 2363 | 2368 | rBV  | 80217  | 169061 | 14.14% | 1.642% |
| 52 | 8.323  | 2396 | 2405 | 2431 | rVB  | 276791 | 529794 | 44.30% | 5.147% |
| 53 | 8.625  | 2493 | 2499 | 2509 | rBV4 | 1649   | 2681   | 0.22%  | 0.026% |
| 54 | 8.789  | 2548 | 2550 | 2556 | rVB3 | 325    | 310    | 0.03%  | 0.003% |
| 55 | 8.886  | 2575 | 2580 | 2584 | rVB3 | 473    | 389    | 0.03%  | 0.004% |
| 56 | 8.911  | 2584 | 2588 | 2594 | rBV4 | 504    | 612    | 0.05%  | 0.006% |
| 57 | 8.963  | 2599 | 2604 | 2606 | rBV3 | 350    | 367    | 0.03%  | 0.004% |
| 58 | 9.050  | 2623 | 2631 | 2632 | rBV4 | 2448   | 2157   | 0.18%  | 0.021% |
| 59 | 9.095  | 2632 | 2645 | 2670 | rVB  | 551130 | 956116 | 79.95% | 9.289% |
| 60 | 9.255  | 2690 | 2695 | 2698 | rBV4 | 1065   | 936    | 0.08%  | 0.009% |
| 61 | 9.352  | 2721 | 2725 | 2729 | rBV4 | 425    | 409    | 0.03%  | 0.004% |
| 62 | 9.374  | 2729 | 2732 | 2733 | rBV2 | 656    | 347    | 0.03%  | 0.003% |
| 63 | 9.574  | 2790 | 2794 | 2797 | rBV2 | 531    | 507    | 0.04%  | 0.005% |
| 64 | 9.712  | 2833 | 2837 | 2840 | rBV  | 422    | 400    | 0.03%  | 0.004% |
| 65 | 9.744  | 2842 | 2847 | 2850 | rBV2 | 424    | 334    | 0.03%  | 0.003% |
| 66 | 9.767  | 2851 | 2854 | 2858 | rBV5 | 413    | 359    | 0.03%  | 0.003% |
| 67 | 9.808  | 2863 | 2867 | 2873 | rVV3 | 677    | 926    | 0.08%  | 0.009% |
| 68 | 9.834  | 2873 | 2875 | 2880 | rVV3 | 505    | 325    | 0.03%  | 0.003% |
| 69 | 9.860  | 2880 | 2883 | 2888 | rVB3 | 511    | 482    | 0.04%  | 0.005% |
| 70 | 9.956  | 2906 | 2913 | 2922 | rVB4 | 2537   | 3833   | 0.32%  | 0.037% |
| 71 | 10.027 | 2930 | 2935 | 2939 | rBV2 | 511    | 566    | 0.05%  | 0.005% |

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Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 E4429ME

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
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Filtering: 5  
 Min Area: 0 % of largest Peak  
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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\SOMULM082218WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 10.268 | 3006 | 3010 | 3014 | rVB2 | 526    | 463    | 0.04%  | 0.004% |
| 73  | 10.300 | 3014 | 3020 | 3022 | rBV2 | 559    | 521    | 0.04%  | 0.005% |
| 74  | 10.439 | 3050 | 3063 | 3077 | rBV  | 366637 | 587213 | 49.10% | 5.705% |
| 75  | 10.525 | 3087 | 3090 | 3092 | rBV  | 443    | 301    | 0.03%  | 0.003% |
| 76  | 10.561 | 3097 | 3101 | 3104 | rBV3 | 318    | 307    | 0.03%  | 0.003% |
| 77  | 10.616 | 3107 | 3118 | 3137 | rVB2 | 27465  | 53894  | 4.51%  | 0.524% |
| 78  | 10.934 | 3213 | 3217 | 3219 | rBV  | 348    | 291    | 0.02%  | 0.003% |
| 79  | 10.956 | 3221 | 3224 | 3229 | rVV3 | 449    | 433    | 0.04%  | 0.004% |
| 80  | 11.265 | 3317 | 3320 | 3323 | rBV  | 353    | 294    | 0.02%  | 0.003% |
| 81  | 11.368 | 3346 | 3352 | 3354 | rBV3 | 406    | 460    | 0.04%  | 0.004% |
| 82  | 11.487 | 3376 | 3389 | 3407 | rBV  | 647281 | 994156 | 83.13% | 9.658% |
| 83  | 11.722 | 3458 | 3462 | 3465 | rBV3 | 371    | 347    | 0.03%  | 0.003% |
| 84  | 11.796 | 3481 | 3485 | 3491 | rVB3 | 505    | 583    | 0.05%  | 0.006% |
| 85  | 11.863 | 3492 | 3506 | 3524 | rBV  | 562921 | 903311 | 75.53% | 8.776% |
| 86  | 12.066 | 3565 | 3569 | 3570 | rBV3 | 525    | 341    | 0.03%  | 0.003% |
| 87  | 12.098 | 3576 | 3579 | 3582 | rBV2 | 753    | 530    | 0.04%  | 0.005% |
| 88  | 12.432 | 3680 | 3683 | 3686 | rBV  | 489    | 350    | 0.03%  | 0.003% |
| 89  | 12.484 | 3689 | 3699 | 3709 | rVB2 | 9174   | 16042  | 1.34%  | 0.156% |
| 90  | 12.570 | 3723 | 3726 | 3731 | rVB3 | 498    | 372    | 0.03%  | 0.004% |
| 91  | 12.892 | 3823 | 3826 | 3830 | rBV2 | 566    | 353    | 0.03%  | 0.003% |
| 92  | 13.149 | 3904 | 3906 | 3910 | rBV  | 404    | 340    | 0.03%  | 0.003% |
| 93  | 13.403 | 3982 | 3985 | 3987 | rBV2 | 500    | 307    | 0.03%  | 0.003% |
| 94  | 13.493 | 4010 | 4013 | 4017 | rBV3 | 451    | 375    | 0.03%  | 0.004% |
| 95  | 13.853 | 4123 | 4125 | 4129 | rVB3 | 507    | 355    | 0.03%  | 0.003% |
| 96  | 13.889 | 4134 | 4136 | 4143 | rVB3 | 534    | 372    | 0.03%  | 0.004% |
| 97  | 14.281 | 4249 | 4258 | 4271 | rVB2 | 6701   | 11483  | 0.96%  | 0.112% |
| 98  | 14.786 | 4412 | 4415 | 4418 | rBV3 | 774    | 509    | 0.04%  | 0.005% |
| 99  | 15.043 | 4492 | 4495 | 4496 | rBV  | 741    | 425    | 0.04%  | 0.004% |
| 100 | 16.020 | 4797 | 4799 | 4802 | rVB2 | 1287   | 596    | 0.05%  | 0.006% |

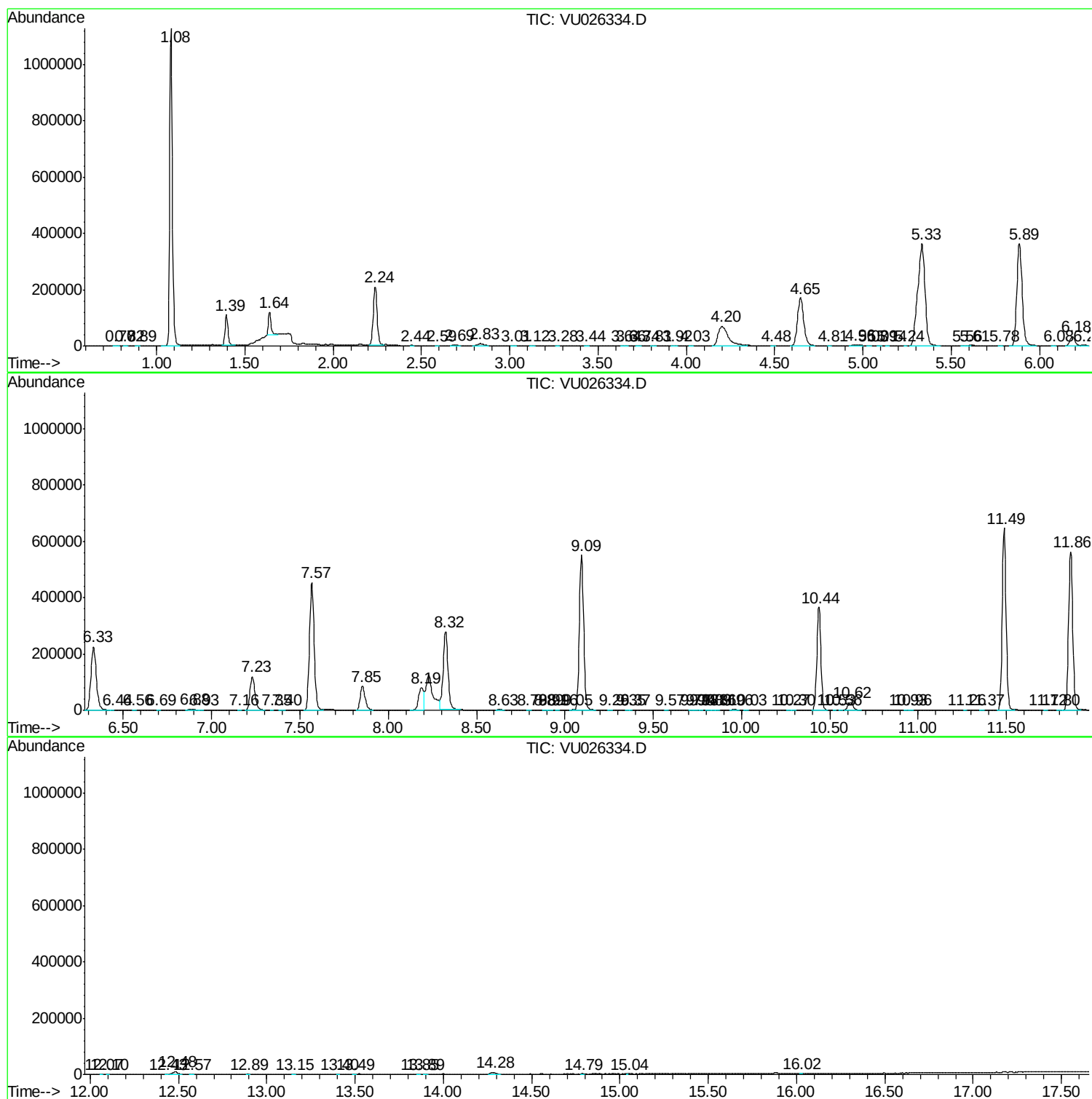
Sum of corrected areas: 10293241

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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
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E4429ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM082218WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU082418\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM082218WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
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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          |