

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042821\  
 Data File : VV021211.D  
 Acq On : 28 Apr 2021 19:23  
 Operator : SY/MD  
 Sample : M2166-01ME  
 Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GB3G4ME

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\_V\Method\SFAMVLM042121WMA.M

Title : VOC Analysis

Signal : TIC: VV021211.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         | 1.307       | 77            | 83          | 104          | rVB      | 236020         | 337048        | 7.26%           | 1.290%        |
| 2         | 1.568       | 158           | 164         | 192          | rVB      | 147296         | 263689        | 5.68%           | 1.009%        |
| 3         | 2.089       | 318           | 326         | 339          | rVB      | 590227         | 832715        | 17.95%          | 3.186%        |
| 4         | 2.757       | 532           | 534         | 537          | rBV4     | 1199           | 680           | 0.01%           | 0.003%        |
| 5         | 2.790       | 541           | 544         | 547          | rBV3     | 1049           | 840           | 0.02%           | 0.003%        |
| 6         | 2.822       | 552           | 554         | 560          | rVB3     | 1489           | 1093          | 0.02%           | 0.004%        |
| 7         | 3.092       | 635           | 638         | 640          | rBV      | 824            | 415           | 0.01%           | 0.002%        |
| 8         | 3.150       | 654           | 656         | 661          | rVB3     | 800            | 529           | 0.01%           | 0.002%        |
| 9         | 3.191       | 666           | 669         | 673          | rBV2     | 446            | 375           | 0.01%           | 0.001%        |
| 10        | 3.214       | 673           | 676         | 677          | rBV      | 742            | 393           | 0.01%           | 0.002%        |
| 11        | 3.298       | 699           | 702         | 705          | rBV2     | 497            | 399           | 0.01%           | 0.002%        |
| 12        | 3.375       | 723           | 726         | 729          | rVB3     | 467            | 311           | 0.01%           | 0.001%        |
| 13        | 3.404       | 731           | 735         | 738          | rBV4     | 1054           | 885           | 0.02%           | 0.003%        |
| 14        | 3.439       | 744           | 746         | 748          | rBV2     | 752            | 383           | 0.01%           | 0.001%        |
| 15        | 3.468       | 753           | 755         | 757          | rBV      | 557            | 331           | 0.01%           | 0.001%        |
| 16        | 3.519       | 768           | 771         | 773          | rBV2     | 638            | 388           | 0.01%           | 0.001%        |
| 17        | 3.587       | 790           | 792         | 794          | rBV2     | 545            | 325           | 0.01%           | 0.001%        |
| 18        | 3.622       | 801           | 803         | 807          | rVB3     | 928            | 355           | 0.01%           | 0.001%        |
| 19        | 3.667       | 813           | 817         | 819          | rBV2     | 1061           | 678           | 0.01%           | 0.003%        |
| 20        | 3.783       | 849           | 853         | 856          | rBV3     | 706            | 498           | 0.01%           | 0.002%        |
| 21        | 3.870       | 875           | 880         | 881          | rBV      | 520            | 376           | 0.01%           | 0.001%        |
| 22        | 3.915       | 881           | 894         | 918          | rBV      | 94074          | 368063        | 7.93%           | 1.408%        |
| 23        | 4.349       | 1015          | 1029        | 1060         | rVB2     | 424814         | 1088735       | 23.47%          | 4.166%        |
| 24        | 4.777       | 1156          | 1162        | 1167         | rBV5     | 1209           | 1472          | 0.03%           | 0.006%        |
| 25        | 4.802       | 1167          | 1170        | 1171         | rBV      | 659            | 336           | 0.01%           | 0.001%        |
| 26        | 4.844       | 1175          | 1183        | 1187         | rBV7     | 1158           | 1554          | 0.03%           | 0.006%        |
| 27        | 4.928       | 1204          | 1209        | 1210         | rBV2     | 830            | 515           | 0.01%           | 0.002%        |
| 28        | 5.043       | 1229          | 1245        | 1286         | rBV2     | 1072357        | 2707979       | 58.37%          | 10.361%       |
| 29        | 5.339       | 1334          | 1337        | 1340         | rBV4     | 1059           | 597           | 0.01%           | 0.002%        |
| 30        | 5.378       | 1347          | 1349        | 1352         | rBV3     | 946            | 682           | 0.01%           | 0.003%        |
| 31        | 5.468       | 1373          | 1377        | 1382         | rBV4     | 1147           | 1170          | 0.03%           | 0.004%        |
| 32        | 5.503       | 1385          | 1388        | 1390         | rBV2     | 915            | 541           | 0.01%           | 0.002%        |
| 33        | 5.619       | 1411          | 1424        | 1456         | rBV      | 856359         | 1822283       | 39.28%          | 6.972%        |
| 34        | 5.908       | 1505          | 1514        | 1531         | rVB3     | 37718          | 84741         | 1.83%           | 0.324%        |
| 35        | 6.072       | 1551          | 1565        | 1592         | rBV      | 547466         | 1188856       | 25.62%          | 4.549%        |
| 36        | 6.326       | 1642          | 1644        | 1646         | rBV2     | 789            | 388           | 0.01%           | 0.001%        |

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 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GB3G4ME

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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 6.365  | 1654 | 1656 | 1662 | rVB5 | 1193    | 938     | 0.02%   | 0.004%  |
| 38 | 6.404  | 1662 | 1668 | 1670 | rVB4 | 719     | 648     | 0.01%   | 0.002%  |
| 39 | 6.423  | 1670 | 1674 | 1676 | rBV2 | 708     | 614     | 0.01%   | 0.002%  |
| 40 | 6.455  | 1681 | 1684 | 1685 | rBV2 | 507     | 327     | 0.01%   | 0.001%  |
| 41 | 6.494  | 1692 | 1696 | 1699 | rBV3 | 769     | 609     | 0.01%   | 0.002%  |
| 42 | 6.568  | 1716 | 1719 | 1721 | rBV3 | 1173    | 702     | 0.02%   | 0.003%  |
| 43 | 6.632  | 1737 | 1739 | 1741 | rBV2 | 975     | 528     | 0.01%   | 0.002%  |
| 44 | 6.918  | 1824 | 1828 | 1830 | rBV  | 676     | 487     | 0.01%   | 0.002%  |
| 45 | 6.992  | 1837 | 1851 | 1885 | rBV  | 285182  | 598134  | 12.89%  | 2.289%  |
| 46 | 7.204  | 1915 | 1917 | 1920 | rBV4 | 769     | 490     | 0.01%   | 0.002%  |
| 47 | 7.320  | 1939 | 1953 | 1972 | rBV  | 1237950 | 2250091 | 48.50%  | 8.609%  |
| 48 | 7.629  | 2039 | 2049 | 2074 | rBV  | 184172  | 405882  | 8.75%   | 1.553%  |
| 49 | 7.979  | 2143 | 2158 | 2183 | rBV  | 2710394 | 4639474 | 100.00% | 17.751% |
| 50 | 8.127  | 2188 | 2204 | 2237 | rVV  | 322029  | 1165159 | 25.11%  | 4.458%  |
| 51 | 8.719  | 2385 | 2388 | 2390 | rVV3 | 845     | 468     | 0.01%   | 0.002%  |
| 52 | 8.809  | 2413 | 2416 | 2417 | rBV2 | 1069    | 617     | 0.01%   | 0.002%  |
| 53 | 8.860  | 2419 | 2432 | 2460 | rVV  | 1238161 | 2324225 | 50.10%  | 8.893%  |
| 54 | 9.137  | 2515 | 2518 | 2520 | rBV4 | 1448    | 1151    | 0.02%   | 0.004%  |
| 55 | 9.153  | 2520 | 2523 | 2528 | rVV5 | 1919    | 2317    | 0.05%   | 0.009%  |
| 56 | 9.310  | 2569 | 2572 | 2575 | rVB3 | 1336    | 668     | 0.01%   | 0.003%  |
| 57 | 9.329  | 2575 | 2578 | 2581 | rBV3 | 603     | 474     | 0.01%   | 0.002%  |
| 58 | 9.349  | 2581 | 2584 | 2587 | rVV4 | 1094    | 647     | 0.01%   | 0.002%  |
| 59 | 9.490  | 2625 | 2628 | 2632 | rBV2 | 1119    | 873     | 0.02%   | 0.003%  |
| 60 | 9.674  | 2681 | 2685 | 2691 | rBV5 | 750     | 857     | 0.02%   | 0.003%  |
| 61 | 9.754  | 2703 | 2710 | 2715 | rBV2 | 954     | 1010    | 0.02%   | 0.004%  |
| 62 | 9.802  | 2723 | 2725 | 2729 | rVB  | 569     | 377     | 0.01%   | 0.001%  |
| 63 | 9.831  | 2731 | 2734 | 2735 | rBV2 | 584     | 339     | 0.01%   | 0.001%  |
| 64 | 9.873  | 2743 | 2747 | 2750 | rBV3 | 580     | 508     | 0.01%   | 0.002%  |
| 65 | 9.892  | 2750 | 2753 | 2755 | rBV2 | 566     | 356     | 0.01%   | 0.001%  |
| 66 | 9.934  | 2764 | 2766 | 2768 | rBV2 | 991     | 535     | 0.01%   | 0.002%  |
| 67 | 10.018 | 2782 | 2792 | 2793 | rBV2 | 893     | 1037    | 0.02%   | 0.004%  |
| 68 | 10.053 | 2797 | 2803 | 2807 | rVB5 | 675     | 747     | 0.02%   | 0.003%  |
| 69 | 10.104 | 2814 | 2819 | 2820 | rBV2 | 1008    | 881     | 0.02%   | 0.003%  |
| 70 | 10.130 | 2822 | 2827 | 2835 | rVB4 | 6327    | 8609    | 0.19%   | 0.033%  |
| 71 | 10.230 | 2845 | 2858 | 2880 | rBV  | 798505  | 1407865 | 30.35%  | 5.387%  |
| 72 | 10.445 | 2919 | 2925 | 2928 | rBV4 | 988     | 1386    | 0.03%   | 0.005%  |
| 73 | 10.461 | 2928 | 2930 | 2933 | rVV2 | 1348    | 823     | 0.02%   | 0.003%  |
| 74 | 10.481 | 2933 | 2936 | 2944 | rVB5 | 1113    | 1279    | 0.03%   | 0.005%  |
| 75 | 10.538 | 2952 | 2954 | 2956 | rBV3 | 1007    | 525     | 0.01%   | 0.002%  |
| 76 | 10.699 | 3001 | 3004 | 3006 | rBV  | 835     | 489     | 0.01%   | 0.002%  |

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 Sample : M2166-01ME  
 Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GB3G4ME

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\_V\Method\SFAMVLM042121WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 77  | 10.844 | 3047 | 3049 | 3051 | rBV3 | 668     | 333     | 0.01%  | 0.001% |
| 78  | 10.992 | 3093 | 3095 | 3099 | rBV2 | 620     | 423     | 0.01%  | 0.002% |
| 79  | 11.046 | 3106 | 3112 | 3115 | rBV4 | 1520    | 1789    | 0.04%  | 0.007% |
| 80  | 11.156 | 3140 | 3146 | 3152 | rVB5 | 3951    | 4513    | 0.10%  | 0.017% |
| 81  | 11.259 | 3166 | 3178 | 3198 | rBV  | 1478967 | 2330066 | 50.22% | 8.915% |
| 82  | 11.635 | 3283 | 3295 | 3312 | rBV  | 1423814 | 2235667 | 48.19% | 8.554% |
| 83  | 12.050 | 3420 | 3424 | 3426 | rBV5 | 1104    | 766     | 0.02%  | 0.003% |
| 84  | 12.091 | 3434 | 3437 | 3441 | rBV6 | 1374    | 1286    | 0.03%  | 0.005% |
| 85  | 12.255 | 3480 | 3488 | 3496 | rBV8 | 2468    | 4702    | 0.10%  | 0.018% |
| 86  | 12.381 | 3524 | 3527 | 3533 | rBV4 | 754     | 816     | 0.02%  | 0.003% |
| 87  | 12.458 | 3548 | 3551 | 3553 | rBV2 | 718     | 520     | 0.01%  | 0.002% |
| 88  | 12.532 | 3571 | 3574 | 3578 | rBV3 | 956     | 976     | 0.02%  | 0.004% |
| 89  | 12.657 | 3607 | 3613 | 3616 | rBV5 | 2154    | 2628    | 0.06%  | 0.010% |
| 90  | 12.715 | 3629 | 3631 | 3637 | rVB3 | 1212    | 855     | 0.02%  | 0.003% |
| 91  | 12.779 | 3648 | 3651 | 3656 | rVB2 | 1303    | 843     | 0.02%  | 0.003% |
| 92  | 12.870 | 3676 | 3679 | 3683 | rVB3 | 959     | 615     | 0.01%  | 0.002% |
| 93  | 12.898 | 3683 | 3688 | 3690 | rBV3 | 1583    | 1523    | 0.03%  | 0.006% |
| 94  | 13.156 | 3765 | 3768 | 3773 | rBV4 | 950     | 855     | 0.02%  | 0.003% |
| 95  | 13.223 | 3786 | 3789 | 3793 | rBV4 | 934     | 731     | 0.02%  | 0.003% |
| 96  | 13.281 | 3799 | 3807 | 3818 | rVB4 | 4466    | 6989    | 0.15%  | 0.027% |
| 97  | 13.432 | 3850 | 3854 | 3857 | rBV2 | 1490    | 1074    | 0.02%  | 0.004% |
| 98  | 13.689 | 3932 | 3934 | 3938 | rBV2 | 978     | 531     | 0.01%  | 0.002% |
| 99  | 13.754 | 3950 | 3954 | 3968 | rBV8 | 2711    | 3889    | 0.08%  | 0.015% |
| 100 | 14.101 | 4060 | 4062 | 4063 | rBV  | 854     | 345     | 0.01%  | 0.001% |

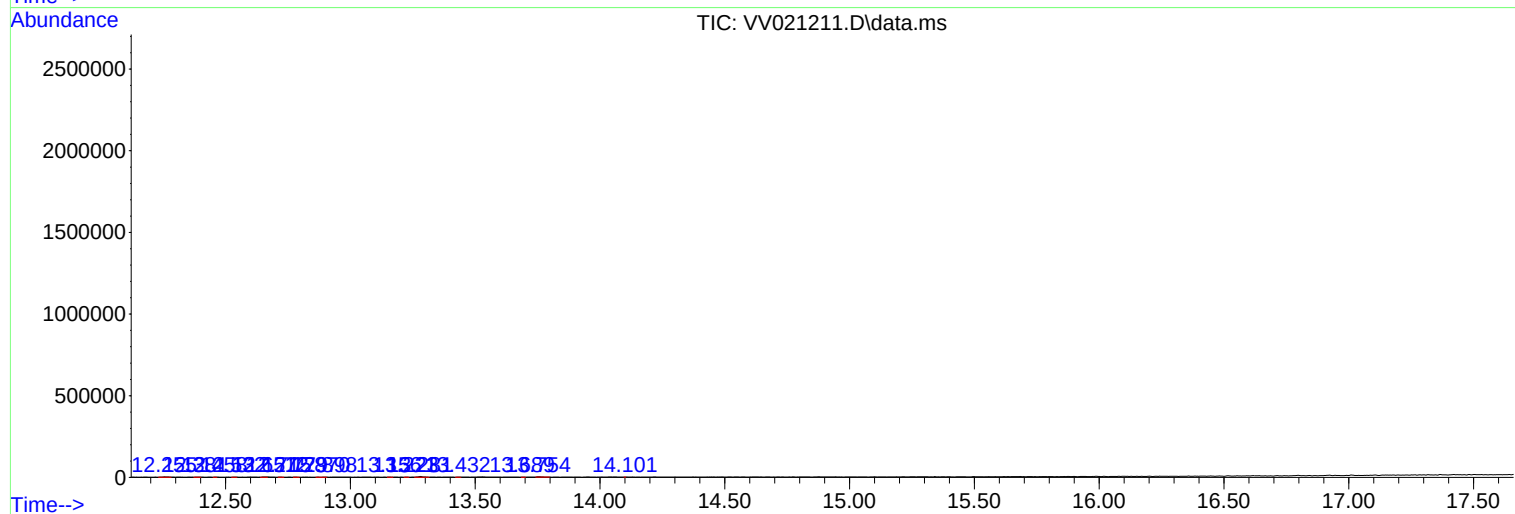
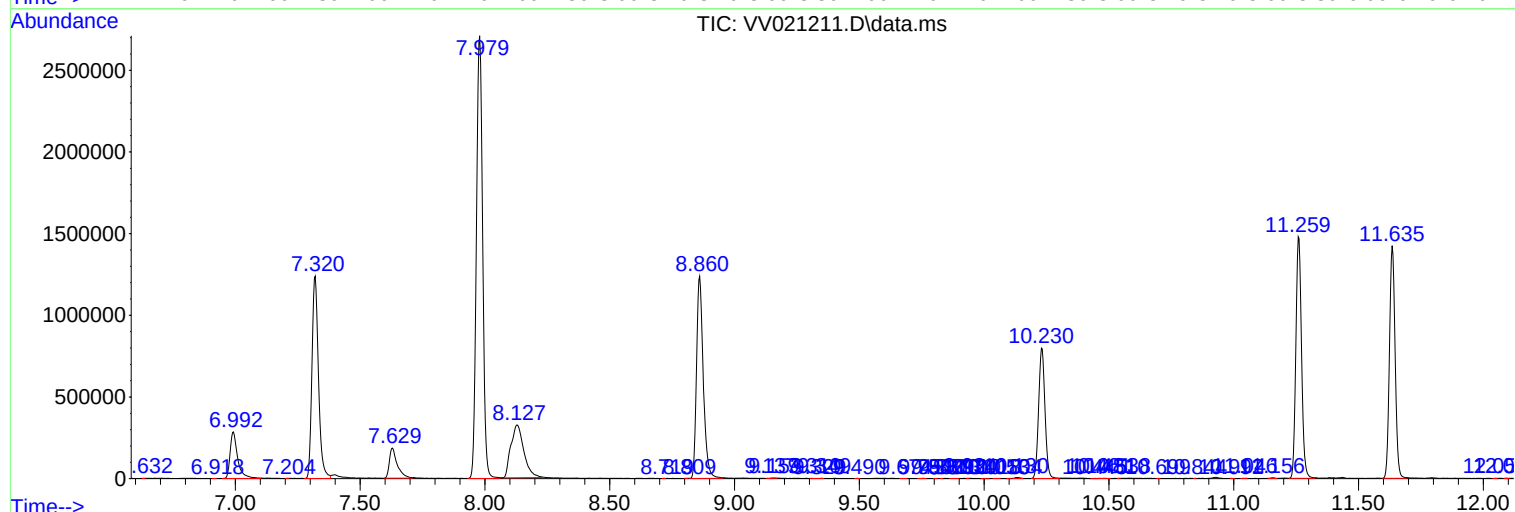
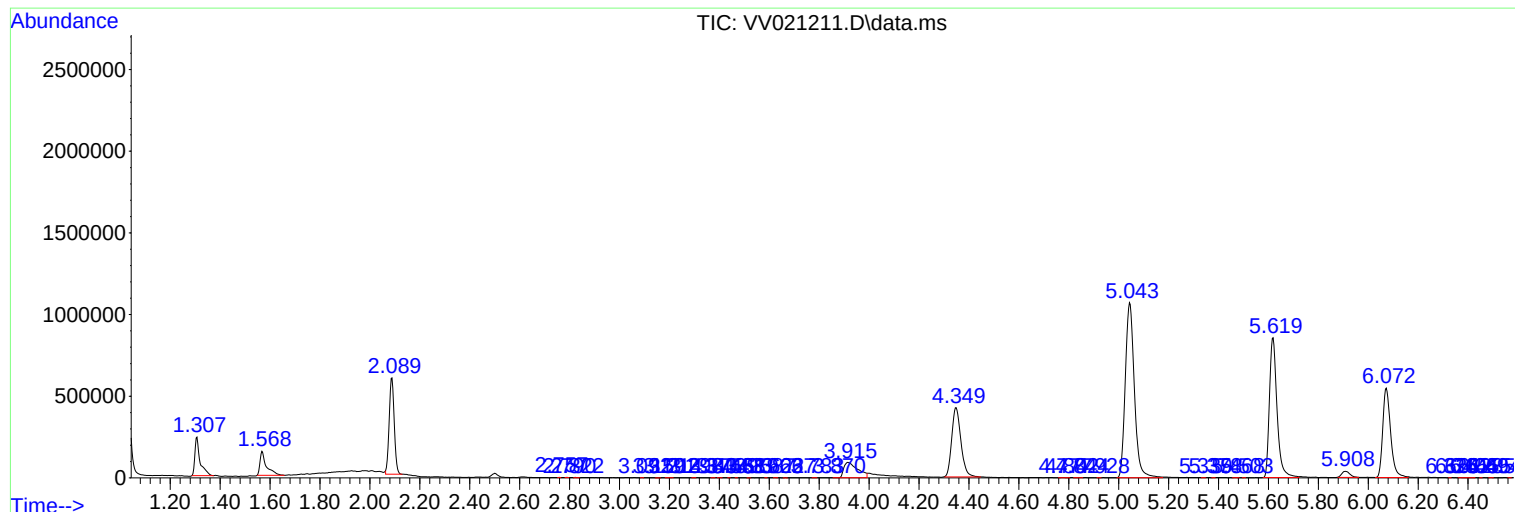
Sum of corrected areas: 26136499

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042821\  
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ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
GB3G4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM042121WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV042821\  
Data File : VV021211.D  
Acq On : 28 Apr 2021 19:23  
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TIC Library : C:\DATABASE\NIST11.L  
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No Library Search Compounds Detected

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TIC Integration Parameters: LSCINT.P

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

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