

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV092524\  
 Data File : VV037508.D  
 Acq On : 25 Sep 2024 09:06  
 Operator : SY/MD  
 Sample : VV0925MBL01  
 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK210

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\SFAMVLM082624WMA.M  
 Title : VOC Analysis

Signal : TIC: VV037508.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         | 1.175       | 34            | 42          | 62           | rBV      | 49251          | 96906         | 3.59%           | 0.481%        |
| 2         | 1.278       | 67            | 74          | 89           | rVV      | 361590         | 395129        | 14.63%          | 1.960%        |
| 3         | 1.532       | 145           | 153         | 168          | rVB      | 315701         | 369969        | 13.70%          | 1.836%        |
| 4         | 2.056       | 306           | 316         | 335          | rBV      | 635022         | 934219        | 34.60%          | 4.635%        |
| 5         | 3.436       | 741           | 745         | 747          | rBV      | 721            | 628           | 0.02%           | 0.003%        |
| 6         | 3.455       | 747           | 751         | 754          | rVV3     | 936            | 679           | 0.03%           | 0.003%        |
| 7         | 3.490       | 760           | 762         | 765          | rBV3     | 953            | 603           | 0.02%           | 0.003%        |
| 8         | 3.555       | 777           | 782         | 785          | rVV4     | 846            | 844           | 0.03%           | 0.004%        |
| 9         | 3.789       | 846           | 855         | 886          | rBV      | 113815         | 345217        | 12.78%          | 1.713%        |
| 10        | 4.133       | 960           | 962         | 964          | rBV2     | 1051           | 580           | 0.02%           | 0.003%        |
| 11        | 4.236       | 978           | 994         | 1023         | rBV      | 432782         | 1109643       | 41.09%          | 5.505%        |
| 12        | 4.654       | 1116          | 1124        | 1126         | rBV5     | 635            | 631           | 0.02%           | 0.003%        |
| 13        | 4.715       | 1140          | 1143        | 1145         | rBV3     | 815            | 559           | 0.02%           | 0.003%        |
| 14        | 4.732       | 1145          | 1148        | 1151         | rVV4     | 973            | 769           | 0.03%           | 0.004%        |
| 15        | 4.748       | 1151          | 1153        | 1159         | rVB3     | 909            | 745           | 0.03%           | 0.004%        |
| 16        | 4.944       | 1199          | 1214        | 1249         | rBV2     | 1045617        | 2700375       | 100.00%         | 13.397%       |
| 17        | 5.265       | 1311          | 1314        | 1318         | rVB5     | 1010           | 722           | 0.03%           | 0.004%        |
| 18        | 5.365       | 1342          | 1345        | 1348         | rBV5     | 1070           | 793           | 0.03%           | 0.004%        |
| 19        | 5.442       | 1366          | 1369        | 1373         | rVB5     | 1203           | 798           | 0.03%           | 0.004%        |
| 20        | 5.484       | 1377          | 1382        | 1383         | rBV4     | 1041           | 833           | 0.03%           | 0.004%        |
| 21        | 5.526       | 1383          | 1395        | 1432         | rBV      | 807870         | 1678559       | 62.16%          | 8.328%        |
| 22        | 5.831       | 1478          | 1490        | 1504         | rVB10    | 8130           | 21742         | 0.81%           | 0.108%        |
| 23        | 5.979       | 1524          | 1536        | 1564         | rBV      | 590717         | 1228969       | 45.51%          | 6.097%        |
| 24        | 6.211       | 1606          | 1608        | 1612         | rVB3     | 935            | 520           | 0.02%           | 0.003%        |
| 25        | 6.355       | 1651          | 1653        | 1660         | rVB5     | 1144           | 1199          | 0.04%           | 0.006%        |
| 26        | 6.481       | 1689          | 1692        | 1697         | rBV5     | 716            | 709           | 0.03%           | 0.004%        |
| 27        | 6.664       | 1744          | 1749        | 1750         | rBV2     | 804            | 591           | 0.02%           | 0.003%        |
| 28        | 6.728       | 1765          | 1769        | 1772         | rBV3     | 1024           | 781           | 0.03%           | 0.004%        |
| 29        | 6.764       | 1778          | 1780        | 1784         | rVB4     | 822            | 491           | 0.02%           | 0.002%        |
| 30        | 6.805       | 1789          | 1793        | 1795         | rBV4     | 1163           | 849           | 0.03%           | 0.004%        |
| 31        | 6.844       | 1799          | 1805        | 1808         | rBV2     | 824            | 681           | 0.03%           | 0.003%        |
| 32        | 6.905       | 1814          | 1824        | 1853         | rBV      | 325685         | 615187        | 22.78%          | 3.052%        |
| 33        | 7.236       | 1915          | 1927        | 1962         | rBV      | 1227395        | 2155624       | 79.83%          | 10.695%       |
| 34        | 7.548       | 2014          | 2024        | 2047         | rBV      | 204186         | 384430        | 14.24%          | 1.907%        |
| 35        | 7.728       | 2078          | 2080        | 2086         | rVB4     | 1348           | 1064          | 0.04%           | 0.005%        |
| 36        | 7.780       | 2093          | 2096        | 2099         | rBV4     | 838            | 749           | 0.03%           | 0.004%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 37 | 7.979  | 2156 | 2158 | 2162 | rBV4 | 673     | 508     | 0.02%  | 0.003%  |
| 38 | 8.021  | 2163 | 2171 | 2214 | rBV2 | 333678  | 747718  | 27.69% | 3.710%  |
| 39 | 8.436  | 2294 | 2300 | 2303 | rBV6 | 1353    | 1634    | 0.06%  | 0.008%  |
| 40 | 8.500  | 2317 | 2320 | 2323 | rBV5 | 747     | 582     | 0.02%  | 0.003%  |
| 41 | 8.670  | 2370 | 2373 | 2377 | rVB5 | 1060    | 669     | 0.02%  | 0.003%  |
| 42 | 8.693  | 2377 | 2380 | 2385 | rBV4 | 548     | 691     | 0.03%  | 0.003%  |
| 43 | 8.725  | 2385 | 2390 | 2395 | rBV5 | 865     | 957     | 0.04%  | 0.005%  |
| 44 | 8.776  | 2395 | 2406 | 2435 | rBV  | 1236827 | 2043717 | 75.68% | 10.140% |
| 45 | 9.014  | 2476 | 2480 | 2484 | rBV7 | 1037    | 942     | 0.03%  | 0.005%  |
| 46 | 9.082  | 2498 | 2501 | 2509 | rVB9 | 2443    | 2582    | 0.10%  | 0.013%  |
| 47 | 9.201  | 2536 | 2538 | 2542 | rBV3 | 974     | 816     | 0.03%  | 0.004%  |
| 48 | 9.329  | 2572 | 2578 | 2583 | rBV7 | 751     | 981     | 0.04%  | 0.005%  |
| 49 | 9.477  | 2619 | 2624 | 2626 | rBV4 | 2167    | 1683    | 0.06%  | 0.008%  |
| 50 | 9.657  | 2676 | 2680 | 2686 | rVB6 | 1477    | 1497    | 0.06%  | 0.007%  |
| 51 | 9.693  | 2690 | 2691 | 2696 | rVB3 | 748     | 478     | 0.02%  | 0.002%  |
| 52 | 9.751  | 2705 | 2709 | 2714 | rBV5 | 1024    | 1165    | 0.04%  | 0.006%  |
| 53 | 9.802  | 2720 | 2725 | 2727 | rBV2 | 619     | 492     | 0.02%  | 0.002%  |
| 54 | 9.870  | 2739 | 2746 | 2754 | rVV9 | 3284    | 5772    | 0.21%  | 0.029%  |
| 55 | 9.969  | 2772 | 2777 | 2786 | rBV7 | 972     | 1325    | 0.05%  | 0.007%  |
| 56 | 10.146 | 2820 | 2832 | 2859 | rVV  | 650917  | 1058716 | 39.21% | 5.253%  |
| 57 | 10.313 | 2879 | 2884 | 2885 | rBV3 | 1237    | 873     | 0.03%  | 0.004%  |
| 58 | 10.394 | 2906 | 2909 | 2914 | rBV5 | 1019    | 1026    | 0.04%  | 0.005%  |
| 59 | 10.474 | 2926 | 2934 | 2945 | rVV8 | 2939    | 5273    | 0.20%  | 0.026%  |
| 60 | 10.522 | 2947 | 2949 | 2952 | rVB3 | 1197    | 591     | 0.02%  | 0.003%  |
| 61 | 10.567 | 2959 | 2963 | 2966 | rBV2 | 860     | 766     | 0.03%  | 0.004%  |
| 62 | 10.744 | 3013 | 3018 | 3021 | rBV5 | 1430    | 1280    | 0.05%  | 0.006%  |
| 63 | 10.780 | 3026 | 3029 | 3035 | rVB8 | 1511    | 1442    | 0.05%  | 0.007%  |
| 64 | 10.853 | 3044 | 3052 | 3061 | rBV9 | 3755    | 6741    | 0.25%  | 0.033%  |
| 65 | 10.982 | 3090 | 3092 | 3096 | rVB3 | 930     | 631     | 0.02%  | 0.003%  |
| 66 | 11.127 | 3126 | 3137 | 3142 | rBV5 | 6783    | 11014   | 0.41%  | 0.055%  |
| 67 | 11.178 | 3142 | 3153 | 3189 | rVV  | 1243215 | 2037136 | 75.44% | 10.107% |
| 68 | 11.403 | 3221 | 3223 | 3228 | rVB5 | 1172    | 891     | 0.03%  | 0.004%  |
| 69 | 11.477 | 3241 | 3246 | 3247 | rBV2 | 786     | 675     | 0.02%  | 0.003%  |
| 70 | 11.551 | 3255 | 3269 | 3294 | rBV  | 1231501 | 1967317 | 72.85% | 9.760%  |
| 71 | 11.950 | 3387 | 3393 | 3394 | rBV3 | 681     | 644     | 0.02%  | 0.003%  |
| 72 | 11.992 | 3402 | 3406 | 3408 | rBV3 | 685     | 588     | 0.02%  | 0.003%  |
| 73 | 12.005 | 3408 | 3410 | 3416 | rVB4 | 931     | 920     | 0.03%  | 0.005%  |
| 74 | 12.037 | 3416 | 3420 | 3426 | rBV6 | 1107    | 1261    | 0.05%  | 0.006%  |
| 75 | 12.217 | 3471 | 3476 | 3478 | rBV5 | 689     | 612     | 0.02%  | 0.003%  |
| 76 | 12.249 | 3483 | 3486 | 3488 | rBV2 | 1083    | 727     | 0.03%  | 0.004%  |

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 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 VBLK210

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\SFAMVLM082624WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 12.316 | 3504 | 3507 | 3509 | rBV3 | 1082  | 728   | 0.03% | 0.004% |
| 78  | 12.471 | 3551 | 3555 | 3558 | rBV4 | 866   | 691   | 0.03% | 0.003% |
| 79  | 12.487 | 3558 | 3560 | 3563 | rBV3 | 918   | 518   | 0.02% | 0.003% |
| 80  | 12.545 | 3574 | 3578 | 3581 | rBV4 | 1132  | 957   | 0.04% | 0.005% |
| 81  | 12.587 | 3581 | 3591 | 3604 | rVV4 | 8585  | 15728 | 0.58% | 0.078% |
| 82  | 12.824 | 3663 | 3665 | 3668 | rVB3 | 1092  | 569   | 0.02% | 0.003% |
| 83  | 12.857 | 3672 | 3675 | 3679 | rBV3 | 731   | 582   | 0.02% | 0.003% |
| 84  | 12.995 | 3715 | 3718 | 3722 | rVB4 | 921   | 780   | 0.03% | 0.004% |
| 85  | 13.024 | 3722 | 3727 | 3730 | rBV3 | 1241  | 1161  | 0.04% | 0.006% |
| 86  | 13.201 | 3774 | 3782 | 3793 | rBV5 | 16340 | 29524 | 1.09% | 0.146% |
| 87  | 13.275 | 3802 | 3805 | 3808 | rBV3 | 1354  | 902   | 0.03% | 0.004% |
| 88  | 13.358 | 3828 | 3831 | 3833 | rBV2 | 1281  | 835   | 0.03% | 0.004% |
| 89  | 13.439 | 3847 | 3856 | 3878 | rBV  | 51064 | 95192 | 3.53% | 0.472% |
| 90  | 13.551 | 3889 | 3891 | 3894 | rBV4 | 749   | 499   | 0.02% | 0.002% |
| 91  | 13.680 | 3921 | 3931 | 3948 | rBV3 | 19943 | 34490 | 1.28% | 0.171% |
| 92  | 13.783 | 3960 | 3963 | 3968 | rVB4 | 1035  | 719   | 0.03% | 0.004% |
| 93  | 13.866 | 3985 | 3989 | 3992 | rBV3 | 573   | 553   | 0.02% | 0.003% |
| 94  | 13.918 | 4003 | 4005 | 4009 | rVB3 | 934   | 488   | 0.02% | 0.002% |
| 95  | 14.133 | 4068 | 4072 | 4077 | rBV5 | 812   | 945   | 0.03% | 0.005% |
| 96  | 14.178 | 4081 | 4086 | 4087 | rBV4 | 905   | 735   | 0.03% | 0.004% |
| 97  | 14.390 | 4150 | 4152 | 4154 | rBV3 | 863   | 506   | 0.02% | 0.003% |
| 98  | 14.609 | 4217 | 4220 | 4225 | rVB6 | 1178  | 1111  | 0.04% | 0.006% |
| 99  | 14.651 | 4231 | 4233 | 4238 | rVB5 | 962   | 676   | 0.03% | 0.003% |
| 100 | 15.516 | 4500 | 4502 | 4506 | rBV5 | 1645  | 916   | 0.03% | 0.005% |

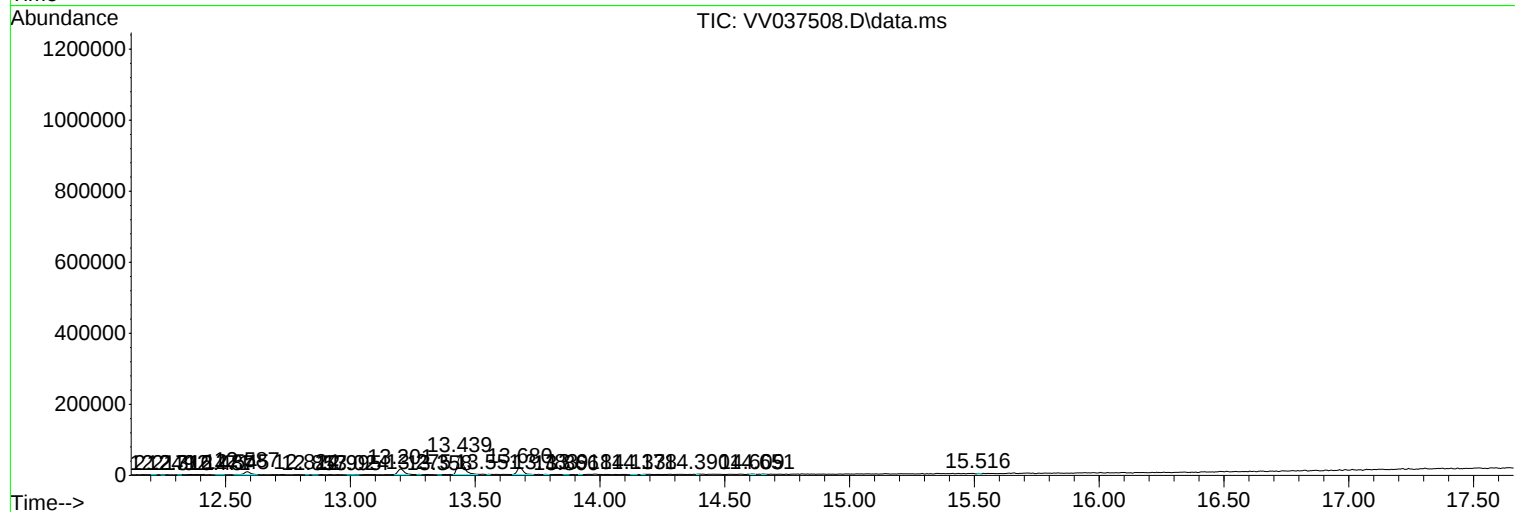
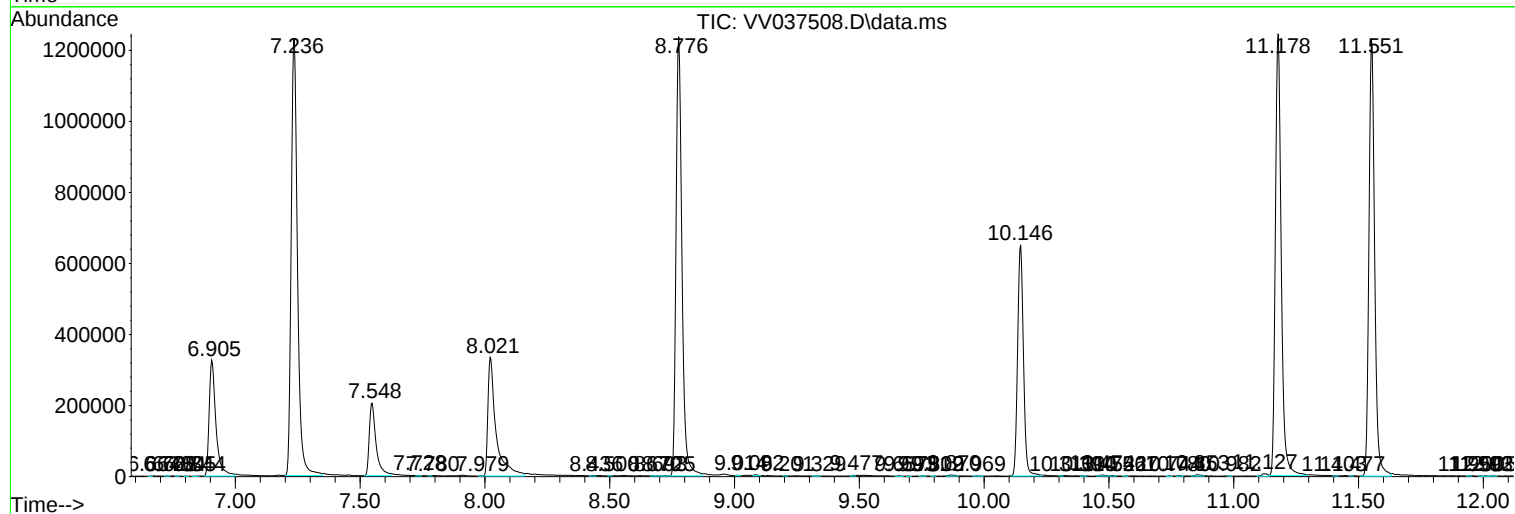
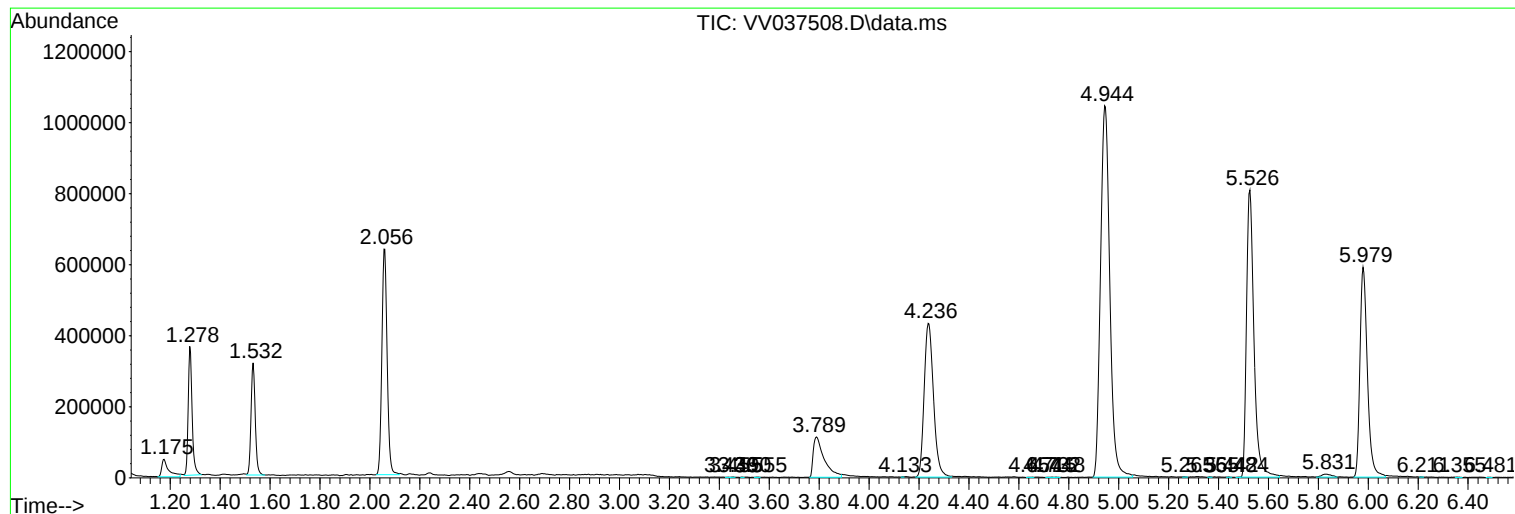
Sum of corrected areas: 20155925

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Instrument :  
MSVOA\_V  
ClientSampleId :  
VBLK210

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM082624WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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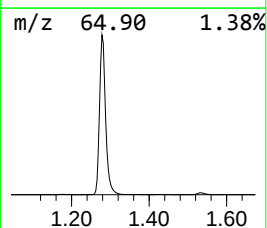
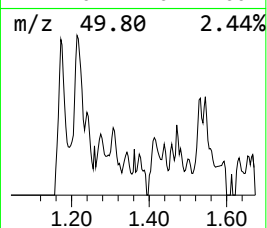
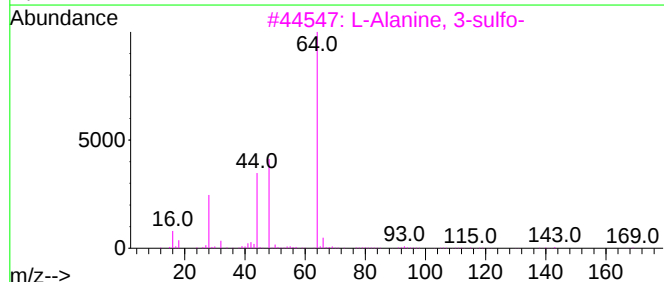
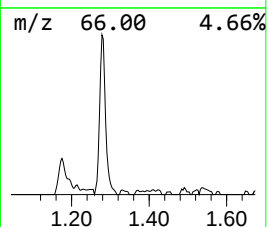
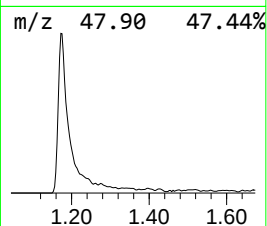
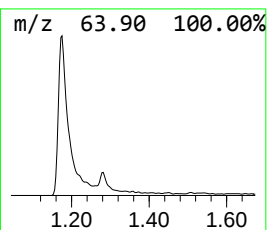
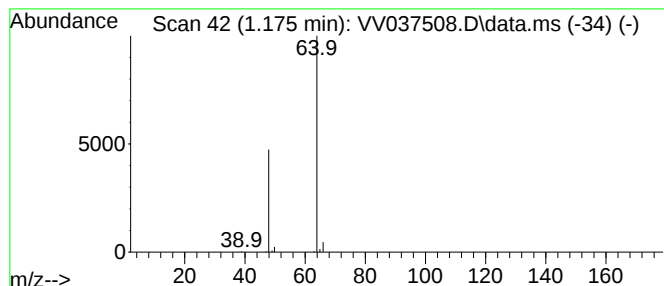
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM082624WMA.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.175 | 2.89 ug/L | 96906 | 1,4-Difluorobenzene | 5.526 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 83   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                  |       |         |       |          | #                     | RT    | Resp    | Conc |
| Sulfur dioxide   | 1.175 | 2.9     | ug/L  | 96906    | 1                     | 5.526 | 1678560 | 50.0 |