

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX072024\  
 Data File : VX042417.D  
 Acq On : 19 Jul 2024 21:11  
 Operator : JC/MD  
 Sample : P3298-08 100X  
 Misc : 5.23g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BHB28

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\_X\Method\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042417.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         | 1.240       | 22            | 25          | 37           | rBV      | 44768          | 61218         | 8.40%           | 1.022%        |
| 2         | 1.368       | 43            | 46          | 57           | rVB      | 75866          | 91772         | 12.59%          | 1.532%        |
| 3         | 1.648       | 88            | 92          | 102          | rVB      | 50804          | 69392         | 9.52%           | 1.159%        |
| 4         | 2.209       | 182           | 184         | 185          | rBV      | 346            | 135           | 0.02%           | 0.002%        |
| 5         | 2.294       | 192           | 198         | 209          | rBV      | 147876         | 233300        | 31.99%          | 3.895%        |
| 6         | 2.502       | 228           | 232         | 234          | rBV2     | 326            | 526           | 0.07%           | 0.009%        |
| 7         | 2.575       | 243           | 244         | 247          | rBV2     | 184            | 129           | 0.02%           | 0.002%        |
| 8         | 2.654       | 255           | 257         | 260          | rVB      | 226            | 221           | 0.03%           | 0.004%        |
| 9         | 2.782       | 275           | 278         | 287          | rVB3     | 834            | 1451          | 0.20%           | 0.024%        |
| 10        | 2.873       | 291           | 293         | 296          | rBV      | 171            | 136           | 0.02%           | 0.002%        |
| 11        | 2.941       | 299           | 304         | 313          | rVB      | 1563           | 3727          | 0.51%           | 0.062%        |
| 12        | 3.154       | 337           | 339         | 341          | rBV      | 170            | 146           | 0.02%           | 0.002%        |
| 13        | 3.239       | 351           | 353         | 355          | rBV      | 165            | 126           | 0.02%           | 0.002%        |
| 14        | 3.306       | 363           | 364         | 368          | rBV2     | 101            | 147           | 0.02%           | 0.002%        |
| 15        | 3.392       | 377           | 378         | 381          | rVB      | 231            | 205           | 0.03%           | 0.003%        |
| 16        | 3.690       | 425           | 427         | 428          | rBV      | 169            | 114           | 0.02%           | 0.002%        |
| 17        | 3.757       | 436           | 438         | 441          | rBV2     | 107            | 132           | 0.02%           | 0.002%        |
| 18        | 3.825       | 447           | 449         | 453          | rBV      | 167            | 235           | 0.03%           | 0.004%        |
| 19        | 3.995       | 474           | 477         | 479          | rBV      | 112            | 168           | 0.02%           | 0.003%        |
| 20        | 4.068       | 486           | 489         | 492          | rVB2     | 109            | 126           | 0.02%           | 0.002%        |
| 21        | 4.117       | 496           | 497         | 501          | rBV      | 201            | 189           | 0.03%           | 0.003%        |
| 22        | 4.203       | 509           | 511         | 513          | rBV2     | 147            | 141           | 0.02%           | 0.002%        |
| 23        | 4.282       | 522           | 524         | 525          | rBV      | 205            | 171           | 0.02%           | 0.003%        |
| 24        | 4.324       | 529           | 531         | 534          | rVV      | 190            | 179           | 0.02%           | 0.003%        |
| 25        | 4.465       | 546           | 554         | 578          | rBV      | 52547          | 160682        | 22.04%          | 2.683%        |
| 26        | 4.965       | 633           | 636         | 638          | rBV2     | 145            | 186           | 0.03%           | 0.003%        |
| 27        | 5.056       | 638           | 651         | 668          | rBV      | 89432          | 278661        | 38.21%          | 4.652%        |
| 28        | 5.471       | 718           | 719         | 720          | rBV      | 169            | 115           | 0.02%           | 0.002%        |
| 29        | 5.721       | 758           | 760         | 763          | rVB2     | 140            | 156           | 0.02%           | 0.003%        |
| 30        | 5.964       | 789           | 800         | 824          | rBV2     | 249813         | 729210        | 100.00%         | 12.175%       |
| 31        | 6.190       | 835           | 837         | 840          | rBV2     | 247            | 209           | 0.03%           | 0.003%        |
| 32        | 6.251       | 844           | 847         | 850          | rBV2     | 209            | 366           | 0.05%           | 0.006%        |
| 33        | 6.355       | 862           | 864         | 865          | rBV      | 170            | 133           | 0.02%           | 0.002%        |
| 34        | 6.373       | 865           | 867         | 869          | rVB      | 174            | 112           | 0.02%           | 0.002%        |
| 35        | 6.623       | 907           | 908         | 911          | rVB      | 150            | 130           | 0.02%           | 0.002%        |
| 36        | 6.666       | 913           | 915         | 918          | rVB2     | 130            | 135           | 0.02%           | 0.002%        |

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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\_X\Method\SFAMXML070324WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.757  | 921  | 930  | 951  | rBV  | 246496 | 596546 | 81.81% | 9.960%  |
| 38 | 7.123  | 983  | 990  | 1000 | rVB7 | 1547   | 3793   | 0.52%  | 0.063%  |
| 39 | 7.208  | 1000 | 1004 | 1005 | rBV3 | 409    | 499    | 0.07%  | 0.008%  |
| 40 | 7.306  | 1012 | 1020 | 1045 | rVB  | 141272 | 320497 | 43.95% | 5.351%  |
| 41 | 7.769  | 1092 | 1096 | 1097 | rBV2 | 132    | 173    | 0.02%  | 0.003%  |
| 42 | 7.787  | 1097 | 1099 | 1101 | rVB  | 203    | 119    | 0.02%  | 0.002%  |
| 43 | 7.812  | 1101 | 1103 | 1107 | rBV2 | 97     | 150    | 0.02%  | 0.003%  |
| 44 | 7.958  | 1122 | 1127 | 1132 | rBV4 | 623    | 1436   | 0.20%  | 0.024%  |
| 45 | 8.324  | 1182 | 1187 | 1213 | rBV  | 78372  | 138247 | 18.96% | 2.308%  |
| 46 | 8.519  | 1213 | 1219 | 1225 | rVV4 | 399    | 983    | 0.13%  | 0.016%  |
| 47 | 8.647  | 1234 | 1240 | 1256 | rBV  | 376320 | 592089 | 81.20% | 9.885%  |
| 48 | 8.952  | 1285 | 1290 | 1305 | rVV  | 58130  | 87602  | 12.01% | 1.463%  |
| 49 | 9.055  | 1305 | 1307 | 1308 | rVV2 | 244    | 177    | 0.02%  | 0.003%  |
| 50 | 9.116  | 1316 | 1317 | 1320 | rVB2 | 347    | 247    | 0.03%  | 0.004%  |
| 51 | 9.275  | 1338 | 1343 | 1351 | rVB  | 22678  | 33988  | 4.66%  | 0.567%  |
| 52 | 9.385  | 1356 | 1361 | 1381 | rBV  | 223086 | 342823 | 47.01% | 5.724%  |
| 53 | 9.695  | 1410 | 1412 | 1418 | rVV3 | 525    | 840    | 0.12%  | 0.014%  |
| 54 | 9.921  | 1446 | 1449 | 1452 | rBV2 | 113    | 151    | 0.02%  | 0.003%  |
| 55 | 9.964  | 1454 | 1456 | 1457 | rVB2 | 170    | 112    | 0.02%  | 0.002%  |
| 56 | 10.055 | 1465 | 1471 | 1490 | rBV  | 495832 | 691821 | 94.87% | 11.550% |
| 57 | 10.269 | 1505 | 1506 | 1508 | rVB  | 241    | 133    | 0.02%  | 0.002%  |
| 58 | 10.311 | 1508 | 1513 | 1521 | rBV5 | 584    | 1472   | 0.20%  | 0.025%  |
| 59 | 10.372 | 1521 | 1523 | 1526 | rBV  | 216    | 200    | 0.03%  | 0.003%  |
| 60 | 10.500 | 1542 | 1544 | 1546 | rBV2 | 132    | 134    | 0.02%  | 0.002%  |
| 61 | 10.604 | 1560 | 1561 | 1563 | rBV  | 202    | 118    | 0.02%  | 0.002%  |
| 62 | 10.646 | 1565 | 1568 | 1574 | rBV3 | 288    | 373    | 0.05%  | 0.006%  |
| 63 | 10.835 | 1597 | 1599 | 1601 | rBV2 | 174    | 184    | 0.03%  | 0.003%  |
| 64 | 11.055 | 1634 | 1635 | 1638 | rVB2 | 267    | 160    | 0.02%  | 0.003%  |
| 65 | 11.098 | 1638 | 1642 | 1646 | rBV2 | 290    | 548    | 0.08%  | 0.009%  |
| 66 | 11.189 | 1652 | 1657 | 1670 | rBV  | 273319 | 368974 | 50.60% | 6.160%  |
| 67 | 11.384 | 1686 | 1689 | 1694 | rVB2 | 219    | 218    | 0.03%  | 0.004%  |
| 68 | 11.427 | 1694 | 1696 | 1698 | rBV2 | 108    | 117    | 0.02%  | 0.002%  |
| 69 | 11.451 | 1698 | 1700 | 1704 | rVB3 | 325    | 392    | 0.05%  | 0.007%  |
| 70 | 11.494 | 1704 | 1707 | 1713 | rBV2 | 197    | 293    | 0.04%  | 0.005%  |
| 71 | 11.628 | 1727 | 1729 | 1732 | rBV2 | 238    | 310    | 0.04%  | 0.005%  |
| 72 | 11.927 | 1775 | 1778 | 1779 | rBV  | 142    | 117    | 0.02%  | 0.002%  |
| 73 | 11.969 | 1782 | 1785 | 1788 | rBV  | 245    | 341    | 0.05%  | 0.006%  |
| 74 | 12.018 | 1788 | 1793 | 1808 | rBV  | 491997 | 642276 | 88.08% | 10.723% |
| 75 | 12.256 | 1831 | 1832 | 1836 | rVB  | 195    | 139    | 0.02%  | 0.002%  |
| 76 | 12.317 | 1837 | 1842 | 1853 | rVV  | 407382 | 519564 | 71.25% | 8.674%  |

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 MSVOA\_X  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_X\Method\SFAMXML070324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |     |      |       |        |
|-----|--------|------|------|------|------|-----|------|-------|--------|
| 77  | 12.567 | 1881 | 1883 | 1884 | rBV  | 203 | 122  | 0.02% | 0.002% |
| 78  | 12.725 | 1907 | 1909 | 1912 | rVB  | 170 | 142  | 0.02% | 0.002% |
| 79  | 12.756 | 1912 | 1914 | 1918 | rBV3 | 410 | 551  | 0.08% | 0.009% |
| 80  | 12.786 | 1918 | 1919 | 1921 | rBV2 | 149 | 122  | 0.02% | 0.002% |
| 81  | 12.817 | 1921 | 1924 | 1925 | rBV2 | 299 | 295  | 0.04% | 0.005% |
| 82  | 13.042 | 1960 | 1961 | 1968 | rBV2 | 141 | 220  | 0.03% | 0.004% |
| 83  | 13.231 | 1989 | 1992 | 1993 | rBV2 | 102 | 110  | 0.02% | 0.002% |
| 84  | 13.268 | 1996 | 1998 | 1999 | rBV  | 155 | 127  | 0.02% | 0.002% |
| 85  | 13.408 | 2019 | 2021 | 2022 | rBV2 | 227 | 122  | 0.02% | 0.002% |
| 86  | 13.445 | 2023 | 2027 | 2030 | rVV3 | 497 | 561  | 0.08% | 0.009% |
| 87  | 13.512 | 2036 | 2038 | 2039 | rBV  | 234 | 170  | 0.02% | 0.003% |
| 88  | 13.548 | 2042 | 2044 | 2046 | rBV3 | 335 | 311  | 0.04% | 0.005% |
| 89  | 13.683 | 2064 | 2066 | 2067 | rBV2 | 193 | 145  | 0.02% | 0.002% |
| 90  | 13.737 | 2072 | 2075 | 2076 | rBV  | 110 | 121  | 0.02% | 0.002% |
| 91  | 14.012 | 2118 | 2120 | 2121 | rVB  | 197 | 113  | 0.02% | 0.002% |
| 92  | 14.036 | 2121 | 2124 | 2125 | rBV  | 125 | 140  | 0.02% | 0.002% |
| 93  | 14.134 | 2136 | 2140 | 2146 | rVB4 | 883 | 1457 | 0.20% | 0.024% |
| 94  | 14.189 | 2148 | 2149 | 2152 | rBV2 | 219 | 193  | 0.03% | 0.003% |
| 95  | 14.286 | 2163 | 2165 | 2167 | rBV  | 283 | 233  | 0.03% | 0.004% |
| 96  | 14.310 | 2167 | 2169 | 2171 | rVV2 | 173 | 175  | 0.02% | 0.003% |
| 97  | 14.536 | 2204 | 2206 | 2207 | rBV2 | 389 | 305  | 0.04% | 0.005% |
| 98  | 14.652 | 2222 | 2225 | 2226 | rBV2 | 265 | 319  | 0.04% | 0.005% |
| 99  | 14.786 | 2246 | 2247 | 2249 | rBV2 | 332 | 218  | 0.03% | 0.004% |
| 100 | 15.536 | 2368 | 2370 | 2373 | rBV3 | 564 | 791  | 0.11% | 0.013% |

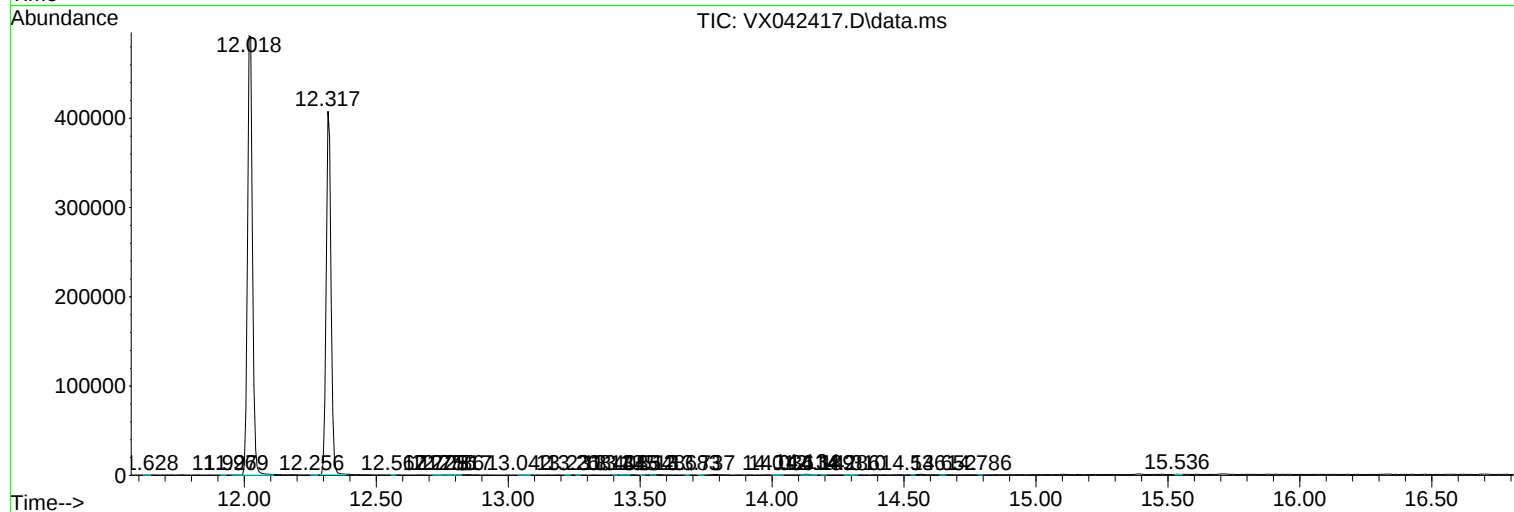
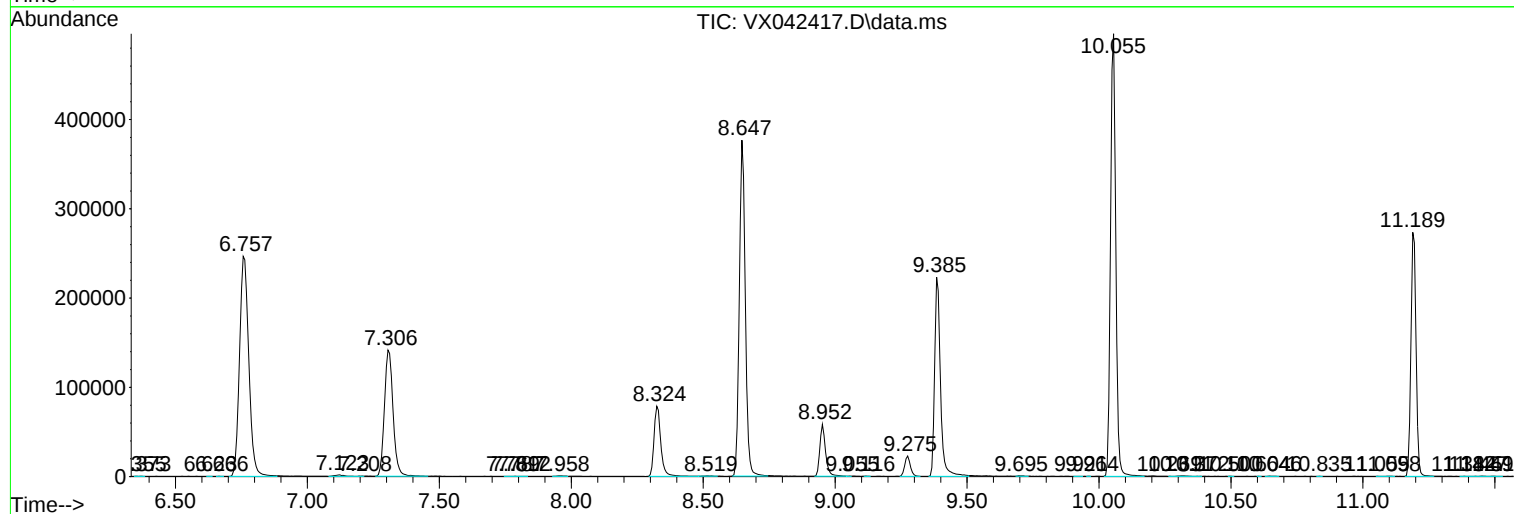
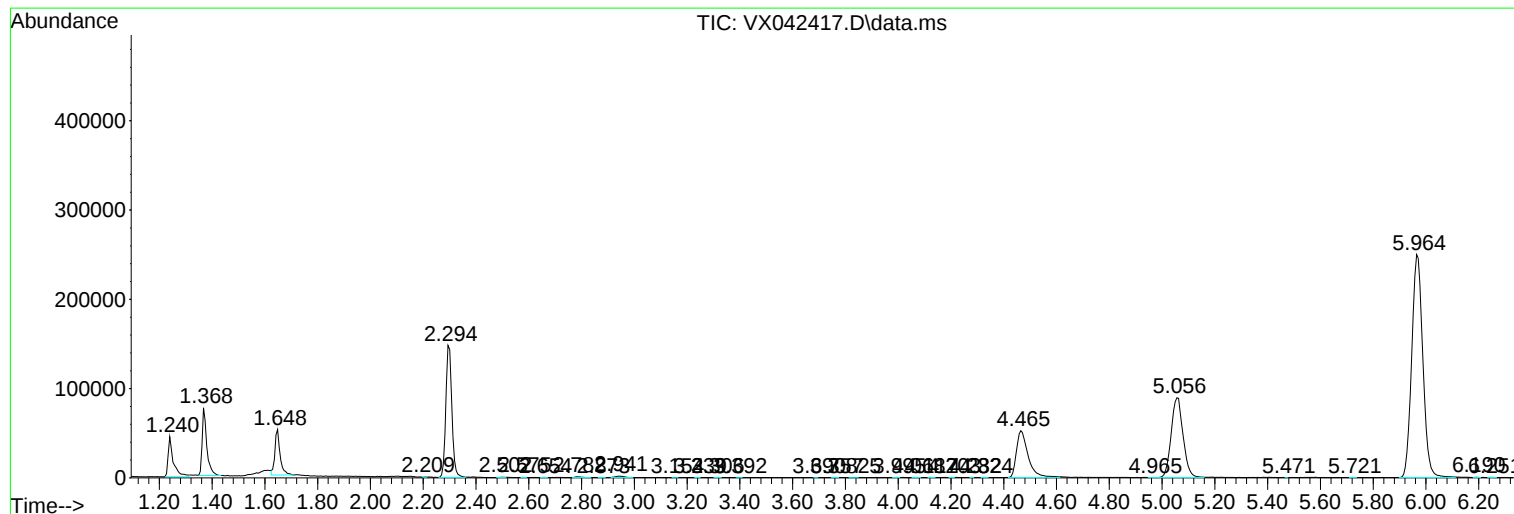
Sum of corrected areas: 5989600

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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



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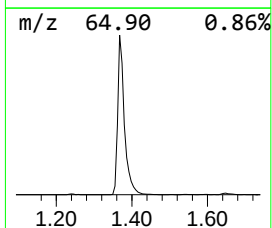
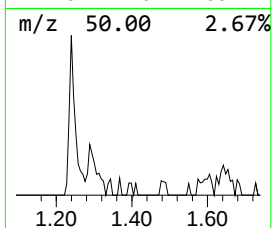
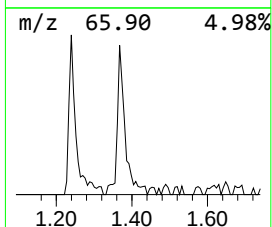
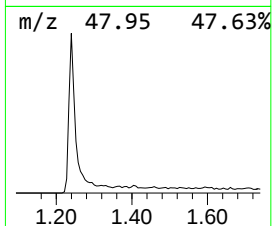
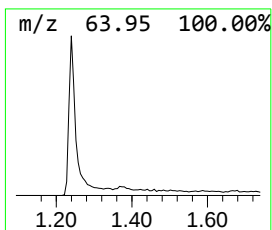
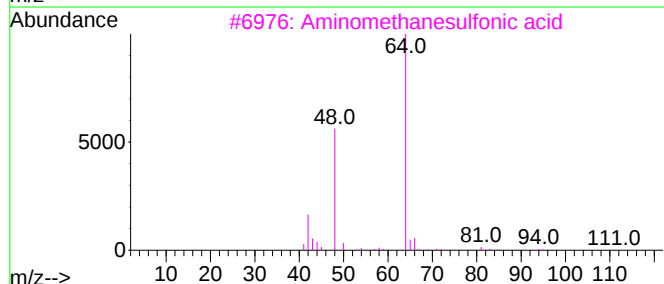
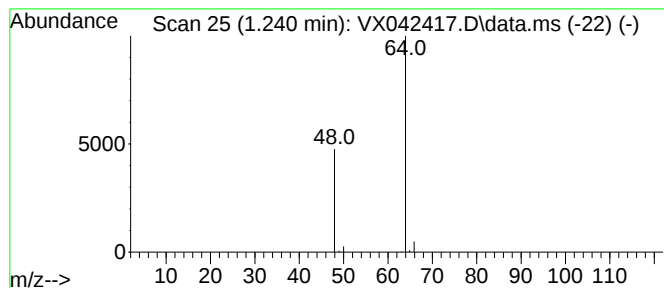
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\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.240 | 5.13 ug/L | 61218 | 1,4-Difluorobenzene | 6.763 |

| 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    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 4    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 5    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.240 | 5.1     | ug/L  | 61218    | 1                     | 6.763 | 596546 | 50.0 |