

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX072024\  
 Data File : VX042430.D  
 Acq On : 20 Jul 2024 02:11  
 Operator : JC/MD  
 Sample : P3298-06ME 100X  
 Misc : 5.52g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BHB26ME

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: VX042430.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          | 40           | rBV      | 24568          | 36346         | 0.45%           | 0.257%        |
| 2         | 1.368       | 43            | 46          | 63           | rVB      | 63801          | 81104         | 0.99%           | 0.573%        |
| 3         | 1.648       | 88            | 92          | 103          | rVB      | 51550          | 72639         | 0.89%           | 0.513%        |
| 4         | 2.294       | 192           | 198         | 211          | rBV      | 146171         | 234452        | 2.87%           | 1.656%        |
| 5         | 2.441       | 220           | 222         | 223          | rBV      | 168            | 107           | 0.00%           | 0.001%        |
| 6         | 2.508       | 228           | 233         | 235          | rBV2     | 360            | 504           | 0.01%           | 0.004%        |
| 7         | 2.660       | 256           | 258         | 259          | rVB      | 176            | 99            | 0.00%           | 0.001%        |
| 8         | 2.672       | 259           | 260         | 261          | rBV      | 243            | 98            | 0.00%           | 0.001%        |
| 9         | 2.691       | 261           | 263         | 264          | rVV      | 152            | 129           | 0.00%           | 0.001%        |
| 10        | 2.703       | 264           | 265         | 271          | rVV2     | 313            | 469           | 0.01%           | 0.003%        |
| 11        | 2.752       | 271           | 273         | 274          | rVV2     | 213            | 133           | 0.00%           | 0.001%        |
| 12        | 2.788       | 274           | 279         | 285          | rVV4     | 1134           | 2260          | 0.03%           | 0.016%        |
| 13        | 2.941       | 297           | 304         | 316          | rBV      | 5321           | 12763         | 0.16%           | 0.090%        |
| 14        | 3.038       | 318           | 320         | 324          | rBV2     | 114            | 160           | 0.00%           | 0.001%        |
| 15        | 3.081       | 326           | 327         | 329          | rVB      | 195            | 82            | 0.00%           | 0.001%        |
| 16        | 3.099       | 329           | 330         | 332          | rBV2     | 102            | 80            | 0.00%           | 0.001%        |
| 17        | 3.471       | 389           | 391         | 393          | rBV      | 180            | 110           | 0.00%           | 0.001%        |
| 18        | 3.495       | 393           | 395         | 397          | rBV2     | 87             | 90            | 0.00%           | 0.001%        |
| 19        | 3.569       | 404           | 407         | 408          | rBV      | 146            | 127           | 0.00%           | 0.001%        |
| 20        | 3.593       | 410           | 411         | 413          | rVB      | 185            | 85            | 0.00%           | 0.001%        |
| 21        | 3.654       | 419           | 421         | 422          | rBV      | 89             | 80            | 0.00%           | 0.001%        |
| 22        | 3.788       | 441           | 443         | 445          | rBV      | 118            | 87            | 0.00%           | 0.001%        |
| 23        | 3.892       | 458           | 460         | 462          | rBV      | 105            | 100           | 0.00%           | 0.001%        |
| 24        | 4.111       | 495           | 496         | 498          | rBV      | 108            | 96            | 0.00%           | 0.001%        |
| 25        | 4.129       | 498           | 499         | 502          | rVB      | 287            | 160           | 0.00%           | 0.001%        |
| 26        | 4.337       | 531           | 533         | 534          | rBV2     | 122            | 93            | 0.00%           | 0.001%        |
| 27        | 4.471       | 546           | 555         | 576          | rBV2     | 67929          | 239832        | 2.94%           | 1.694%        |
| 28        | 4.922       | 627           | 629         | 633          | rVB      | 230            | 221           | 0.00%           | 0.002%        |
| 29        | 5.056       | 639           | 651         | 670          | rBV      | 92518          | 284720        | 3.49%           | 2.011%        |
| 30        | 5.385       | 701           | 705         | 708          | rBV3     | 337            | 583           | 0.01%           | 0.004%        |
| 31        | 5.532       | 725           | 729         | 731          | rBV2     | 131            | 180           | 0.00%           | 0.001%        |
| 32        | 5.550       | 731           | 732         | 733          | rBV      | 187            | 89            | 0.00%           | 0.001%        |
| 33        | 5.849       | 779           | 781         | 782          | rBV2     | 127            | 130           | 0.00%           | 0.001%        |
| 34        | 5.964       | 789           | 800         | 823          | rBV2     | 248757         | 739601        | 9.06%           | 5.224%        |
| 35        | 6.416       | 872           | 874         | 877          | rVB2     | 182            | 159           | 0.00%           | 0.001%        |
| 36        | 6.598       | 903           | 904         | 905          | rBV      | 134            | 73            | 0.00%           | 0.001%        |

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Integrator: RTE

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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

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

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 6.647  | 910  | 912  | 914  | rVB2 | 104     | 92      | 0.00%   | 0.001%  |
| 38 | 6.672  | 914  | 916  | 918  | rBV  | 144     | 134     | 0.00%   | 0.001%  |
| 39 | 6.757  | 921  | 930  | 953  | rBV  | 227839  | 560730  | 6.87%   | 3.960%  |
| 40 | 7.123  | 982  | 990  | 1002 | rBV  | 80957   | 184644  | 2.26%   | 1.304%  |
| 41 | 7.306  | 1011 | 1020 | 1038 | rBV  | 147510  | 328017  | 4.02%   | 2.317%  |
| 42 | 7.641  | 1071 | 1075 | 1076 | rBB  | 211     | 196     | 0.00%   | 0.001%  |
| 43 | 7.720  | 1087 | 1088 | 1089 | rBV  | 120     | 82      | 0.00%   | 0.001%  |
| 44 | 7.775  | 1093 | 1097 | 1098 | rBV2 | 108     | 124     | 0.00%   | 0.001%  |
| 45 | 7.836  | 1105 | 1107 | 1108 | rBV  | 149     | 154     | 0.00%   | 0.001%  |
| 46 | 7.891  | 1114 | 1116 | 1120 | rVB  | 174     | 110     | 0.00%   | 0.001%  |
| 47 | 7.958  | 1122 | 1127 | 1128 | rBV2 | 450     | 664     | 0.01%   | 0.005%  |
| 48 | 8.196  | 1165 | 1166 | 1167 | rBV  | 283     | 123     | 0.00%   | 0.001%  |
| 49 | 8.324  | 1181 | 1187 | 1204 | rBV  | 76593   | 133903  | 1.64%   | 0.946%  |
| 50 | 8.647  | 1234 | 1240 | 1249 | rBV  | 383476  | 589373  | 7.22%   | 4.163%  |
| 51 | 8.952  | 1285 | 1290 | 1304 | rVB  | 54129   | 83419   | 1.02%   | 0.589%  |
| 52 | 9.104  | 1312 | 1315 | 1320 | rVV2 | 403     | 460     | 0.01%   | 0.003%  |
| 53 | 9.141  | 1320 | 1321 | 1322 | rVB  | 203     | 74      | 0.00%   | 0.001%  |
| 54 | 9.275  | 1336 | 1343 | 1357 | rBV  | 5461809 | 8166785 | 100.00% | 57.682% |
| 55 | 9.385  | 1357 | 1361 | 1378 | rVB  | 224210  | 329603  | 4.04%   | 2.328%  |
| 56 | 9.702  | 1410 | 1413 | 1419 | rVB4 | 1309    | 1971    | 0.02%   | 0.014%  |
| 57 | 9.756  | 1419 | 1422 | 1425 | rVB3 | 486     | 557     | 0.01%   | 0.004%  |
| 58 | 9.787  | 1425 | 1427 | 1430 | rBV3 | 340     | 274     | 0.00%   | 0.002%  |
| 59 | 9.872  | 1439 | 1441 | 1443 | rBV  | 364     | 333     | 0.00%   | 0.002%  |
| 60 | 10.006 | 1457 | 1463 | 1465 | rBV5 | 931     | 1483    | 0.02%   | 0.010%  |
| 61 | 10.055 | 1465 | 1471 | 1487 | rVB  | 462699  | 645407  | 7.90%   | 4.559%  |
| 62 | 10.275 | 1505 | 1507 | 1508 | rBV  | 347     | 260     | 0.00%   | 0.002%  |
| 63 | 10.305 | 1508 | 1512 | 1517 | rVV3 | 2013    | 3357    | 0.04%   | 0.024%  |
| 64 | 10.360 | 1517 | 1521 | 1524 | rVB3 | 993     | 1221    | 0.01%   | 0.009%  |
| 65 | 10.433 | 1531 | 1533 | 1536 | rBV2 | 181     | 180     | 0.00%   | 0.001%  |
| 66 | 10.506 | 1543 | 1545 | 1550 | rVB  | 119     | 117     | 0.00%   | 0.001%  |
| 67 | 10.567 | 1554 | 1555 | 1556 | rBV  | 187     | 110     | 0.00%   | 0.001%  |
| 68 | 10.647 | 1565 | 1568 | 1574 | rVB3 | 561     | 880     | 0.01%   | 0.006%  |
| 69 | 10.744 | 1583 | 1584 | 1590 | rBV  | 72      | 101     | 0.00%   | 0.001%  |
| 70 | 10.848 | 1598 | 1601 | 1604 | rVB2 | 131     | 176     | 0.00%   | 0.001%  |
| 71 | 11.189 | 1652 | 1657 | 1671 | rBV  | 226716  | 298231  | 3.65%   | 2.106%  |
| 72 | 11.281 | 1671 | 1672 | 1676 | rVB3 | 292     | 290     | 0.00%   | 0.002%  |
| 73 | 11.348 | 1681 | 1683 | 1684 | rBV3 | 107     | 101     | 0.00%   | 0.001%  |
| 74 | 11.403 | 1689 | 1692 | 1694 | rBV2 | 127     | 109     | 0.00%   | 0.001%  |
| 75 | 11.591 | 1721 | 1723 | 1724 | rBV  | 152     | 127     | 0.00%   | 0.001%  |
| 76 | 11.634 | 1728 | 1730 | 1731 | rBV  | 147     | 97      | 0.00%   | 0.001%  |

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Instrument :  
 MSVOA\_X  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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

|     |        |      |      |      |      |        |        |       |        |
|-----|--------|------|------|------|------|--------|--------|-------|--------|
| 77  | 11.701 | 1739 | 1741 | 1742 | rBV  | 231    | 91     | 0.00% | 0.001% |
| 78  | 11.732 | 1745 | 1746 | 1747 | rBV  | 131    | 75     | 0.00% | 0.001% |
| 79  | 12.018 | 1788 | 1793 | 1806 | rBV  | 464200 | 596012 | 7.30% | 4.210% |
| 80  | 12.317 | 1837 | 1842 | 1852 | rBV  | 398345 | 515197 | 6.31% | 3.639% |
|     |        |      |      |      |      |        |        |       |        |
| 81  | 12.762 | 1912 | 1915 | 1916 | rBV3 | 294    | 250    | 0.00% | 0.002% |
| 82  | 12.805 | 1921 | 1922 | 1924 | rBV  | 164    | 140    | 0.00% | 0.001% |
| 83  | 13.091 | 1968 | 1969 | 1972 | rVV2 | 151    | 131    | 0.00% | 0.001% |
| 84  | 13.122 | 1972 | 1974 | 1977 | rVV  | 195    | 134    | 0.00% | 0.001% |
| 85  | 13.195 | 1985 | 1986 | 1989 | rBV2 | 124    | 139    | 0.00% | 0.001% |
|     |        |      |      |      |      |        |        |       |        |
| 86  | 13.439 | 2025 | 2026 | 2029 | rVB  | 147    | 112    | 0.00% | 0.001% |
| 87  | 13.487 | 2033 | 2034 | 2037 | rVV  | 129    | 101    | 0.00% | 0.001% |
| 88  | 13.542 | 2041 | 2043 | 2045 | rBV2 | 177    | 156    | 0.00% | 0.001% |
| 89  | 13.744 | 2074 | 2076 | 2077 | rVB  | 237    | 110    | 0.00% | 0.001% |
| 90  | 13.762 | 2077 | 2079 | 2081 | rBV  | 117    | 94     | 0.00% | 0.001% |
|     |        |      |      |      |      |        |        |       |        |
| 91  | 13.884 | 2096 | 2099 | 2101 | rVB  | 233    | 191    | 0.00% | 0.001% |
| 92  | 13.920 | 2101 | 2105 | 2106 | rBV2 | 175    | 217    | 0.00% | 0.002% |
| 93  | 13.975 | 2112 | 2114 | 2116 | rBV  | 177    | 184    | 0.00% | 0.001% |
| 94  | 13.993 | 2116 | 2117 | 2120 | rBV2 | 216    | 234    | 0.00% | 0.002% |
| 95  | 14.067 | 2127 | 2129 | 2131 | rBV2 | 197    | 126    | 0.00% | 0.001% |
|     |        |      |      |      |      |        |        |       |        |
| 96  | 14.134 | 2136 | 2140 | 2147 | rVB3 | 853    | 1359   | 0.02% | 0.010% |
| 97  | 14.237 | 2154 | 2157 | 2158 | rBV2 | 206    | 232    | 0.00% | 0.002% |
| 98  | 14.530 | 2203 | 2205 | 2206 | rBV  | 242    | 149    | 0.00% | 0.001% |
| 99  | 14.823 | 2251 | 2253 | 2259 | rBV3 | 289    | 352    | 0.00% | 0.002% |
| 100 | 15.548 | 2371 | 2372 | 2374 | rBV  | 498    | 304    | 0.00% | 0.002% |

Sum of corrected areas: 14158200



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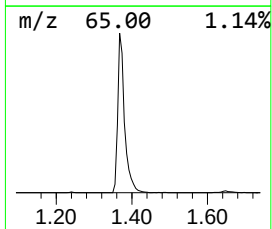
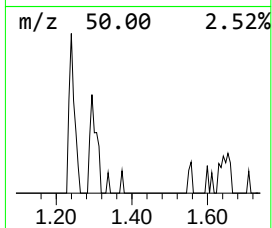
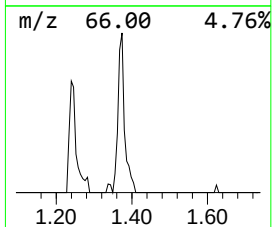
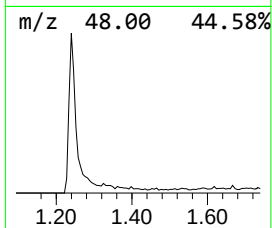
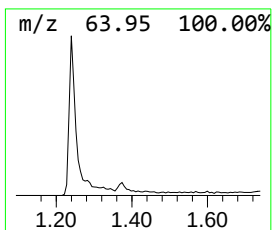
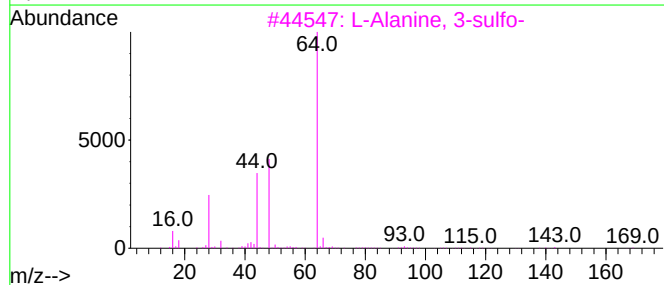
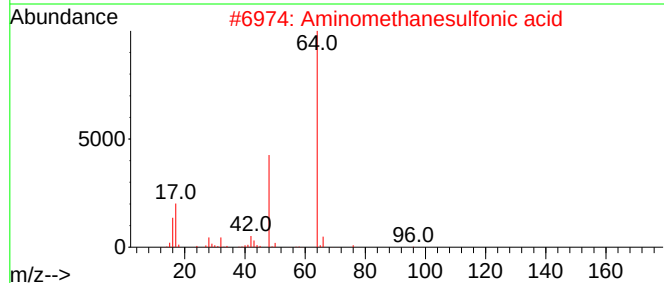
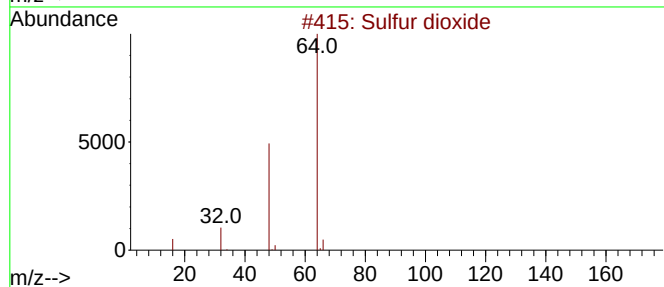
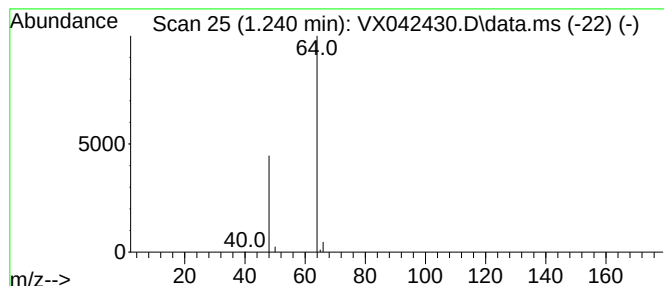
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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

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

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.240 | 3.24 ug/L | 36346 | 1,4-Difluorobenzene | 6.763 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 64   |
| 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 Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide   | 1.240 | 3.2     | ug/L  | 36346    | 1                     | 6.763 | 560730 | 50.0 |