LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
Acq On : 19 Nov 2021 19:02
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
VHBLK001

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\SFAMXLM111121WMA.M
Title : VOC Analysis

Signal : TIC: VX025243.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.246 | 22 | 26 | 32 | rBV | 25901 | 41567 | 7.30% | 0.898% |
| 2 | 1.368 | 42 | 46 | 54 | rVB | 92184 | 88531 | 15.55% | 1.913% |
| 3 | 1.666 | 91 | 95 | 105 | rVB | 64132 | 84744 | 14.89% | 1.831% |
| 4 | 2.307 | 194 | 200 | 211 | rVB | 124458 | 203304 | 35.72% | 4.394% |
| 5 | 2.508 | 230 | 233 | 235 | rBV2 | 240 | 243 | 0.04% | 0.005% |
| 6 | 2.733 | 268 | 270 | 272 | rVB | 210 | 137 | 0.02% | 0.003% |
| 7 | 2.794 | 275 | 280 | 284 | rBV5 | 743 | 1303 | 0.23% | 0.028% |
| 8 | 2.947 | 301 | 305 | 310 | rVB4 | 364 | 722 | 0.13% | 0.016% |
| 9 | 2.983 | 310 | 311 | 313 | rBV | 129 | 108 | 0.02% | 0.002% |
| 10 | 3.392 | 376 | 378 | 381 | rVB | 225 | 208 | 0.04% | 0.004% |
| 11 | 3.416 | 381 | 382 | 383 | rBV | 223 | 123 | 0.02% | 0.003% |
| 12 | 3.453 | 386 | 388 | 391 | rVV2 | 138 | 142 | 0.02% | 0.003% |
| 13 | 3.495 | 394 | 395 | 398 | rVB | 147 | 122 | 0.02% | 0.003% |
| 14 | 3.788 | 441 | 443 | 447 | rBV2 | 135 | 167 | 0.03% | 0.004% |
| 15 | 3.983 | 473 | 475 | 477 | rVV | 183 | 123 | 0.02% | 0.003% |
| 16 | 4.233 | 512 | 516 | 519 | rBV2 | 172 | 231 | 0.04% | 0.005% |
| 17 | 4.459 | 542 | 553 | 575 | rVV | 47356 | 135635 | 23.83% | 2.931% |
| 18 | 4.769 | 603 | 604 | 607 | rBV2 | 234 | 222 | 0.04% | 0.005% |
| 19 | 5.062 | 640 | 652 | 670 | rVV | 72944 | 226950 | 39.87% | 4.905% |
| 20 | 5.233 | 678 | 680 | 683 | rVB2 | 166 | 138 | 0.02% | 0.003% |
| 21 | 5.324 | 693 | 695 | 698 | rBV2 | 183 | 169 | 0.03% | 0.004% |
| 22 | 5.440 | 711 | 714 | 716 | rVB | 164 | 156 | 0.03% | 0.003% |
| 23 | 5.471 | 716 | 719 | 721 | rBV2 | 115 | 139 | 0.02% | 0.003% |
| 24 | 5.550 | 730 | 732 | 736 | rVB2 | 247 | 281 | 0.05% | 0.006% |
| 25 | 5.970 | 789 | 801 | 816 | rBV2 | 192557 | 569219 | 100.00% | 12.302% |
| 26 | 6.196 | 833 | 838 | 841 | rVB3 | 138 | 219 | 0.04% | 0.005% |
| 27 | 6.257 | 845 | 848 | 849 | rBV2 | 118 | 136 | 0.02% | 0.003% |
| 28 | 6.269 | 849 | 850 | 853 | rVB | 235 | 156 | 0.03% | 0.003% |
| 29 | 6.464 | 880 | 882 | 884 | rBV2 | 136 | 110 | 0.02% | 0.002% |
| 30 | 6.672 | 912 | 916 | 917 | rVV | 145 | 117 | 0.02% | 0.003% |
| 31 | 6.763 | 920 | 931 | 949 | rVV2 | 159470 | 381711 | 67.06% | 8.250% |
| 32 | 6.879 | 949 | 950 | 952 | rVV | 236 | 168 | 0.03% | 0.004% |
| 33 | 6.903 | 952 | 954 | 956 | rVV2 | 227 | 204 | 0.04% | 0.004% |
| 34 | 6.928 | 956 | 958 | 961 | rVV2 | 170 | 147 | 0.03% | 0.003% |
| 35 | 6.989 | 964 | 968 | 970 | rVV2 | 115 | 190 | 0.03% | 0.004% |
| 36 | 7.111 | 982 | 988 | 997 | rVB4 | 2283 | 5217 | 0.92% | 0.113% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
Acq On : 19 Nov 2021 19:02
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
VHBLK001

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\SFAMXLM111121WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 7.312 | 1012 | 1021 | 1034 | rVB | 115243 | 254991 | 44.80% | 5.511% |
| 38 | 7.476 | 1045 | 1048 | 1054 | rBV3 | 239 | 456 | 0.08% | 0.010% |
| 39 | 7.726 | 1087 | 1089 | 1092 | rBV | 124 | 114 | 0.02% | 0.002% |
| 40 | 7.927 | 1116 | 1122 | 1127 | rVV4 | 936 | 1622 | 0.28% | 0.035% |
| 41 | 8.190 | 1162 | 1165 | 1166 | rBV2 | 102 | 125 | 0.02% | 0.003% |
| 42 | 8.324 | 1181 | 1187 | 1200 | rBV | 83236 | 137509 | 24.16% | 2.972% |
| 43 | 8.415 | 1200 | 1202 | 1205 | rVV2 | 144 | 147 | 0.03% | 0.003% |
| 44 | 8.476 | 1205 | 1212 | 1219 | rVB3 | 595 | 1147 | 0.20% | 0.025% |
| 45 | 8.653 | 1234 | 1241 | 1248 | rVV | 303323 | 474729 | 83.40% | 10.260% |
| 46 | 8.720 | 1248 | 1252 | 1260 | rVB2 | 4219 | 7322 | 1.29% | 0.158% |
| 47 | 8.811 | 1265 | 1267 | 1269 | rVB2 | 212 | 159 | 0.03% | 0.003% |
| 48 | 8.952 | 1284 | 1290 | 1303 | rBV | 62061 | 88150 | 15.49% | 1.905% |
| 49 | 9.177 | 1323 | 1327 | 1329 | rBV2 | 96 | 139 | 0.02% | 0.003% |
| 50 | 9.275 | 1342 | 1343 | 1346 | rBV | 170 | 132 | 0.02% | 0.003% |
| 51 | 9.385 | 1355 | 1361 | 1385 | rVB | 212565 | 301143 | 52.90% | 6.508% |
| 52 | 9.555 | 1385 | 1389 | 1393 | rVB3 | 173 | 244 | 0.04% | 0.005% |
| 53 | 10.055 | 1465 | 1471 | 1489 | rVV | 336889 | 452666 | 79.52% | 9.783% |
| 54 | 10.195 | 1491 | 1494 | 1498 | rVV2 | 397 | 544 | 0.10% | 0.012% |
| 55 | 10.299 | 1508 | 1511 | 1516 | rBV3 | 896 | 1340 | 0.24% | 0.029% |
| 56 | 10.354 | 1518 | 1520 | 1522 | rVB | 141 | 114 | 0.02% | 0.002% |
| 57 | 10.457 | 1534 | 1537 | 1539 | rVB | 180 | 141 | 0.02% | 0.003% |
| 58 | 10.653 | 1564 | 1569 | 1571 | rVB3 | 264 | 418 | 0.07% | 0.009% |
| 59 | 10.915 | 1610 | 1612 | 1613 | rBV | 121 | 124 | 0.02% | 0.003% |
| 60 | 11.122 | 1642 | 1646 | 1652 | rVB | 1699 | 1878 | 0.33% | 0.041% |
| 61 | 11.195 | 1652 | 1658 | 1669 | rBV | 220150 | 283891 | 49.87% | 6.135% |
| 62 | 11.287 | 1669 | 1673 | 1675 | rBV2 | 304 | 337 | 0.06% | 0.007% |
| 63 | 11.378 | 1686 | 1688 | 1693 | rBV2 | 209 | 353 | 0.06% | 0.008% |
| 64 | 11.451 | 1697 | 1700 | 1703 | rBV2 | 230 | 305 | 0.05% | 0.007% |
| 65 | 11.482 | 1703 | 1705 | 1710 | rVB4 | 412 | 487 | 0.09% | 0.011% |
| 66 | 11.665 | 1733 | 1735 | 1736 | rBV2 | 182 | 105 | 0.02% | 0.002% |
| 67 | 11.750 | 1744 | 1749 | 1753 | rBV2 | 1867 | 2079 | 0.37% | 0.045% |
| 68 | 11.847 | 1762 | 1765 | 1767 | rBV | 434 | 384 | 0.07% | 0.008% |
| 69 | 11.939 | 1775 | 1780 | 1782 | rBV3 | 751 | 1002 | 0.18% | 0.022% |
| 70 | 12.024 | 1789 | 1794 | 1805 | rBV | 351375 | 429200 | 75.40% | 9.276% |
| 71 | 12.122 | 1808 | 1810 | 1813 | rVV2 | 596 | 894 | 0.16% | 0.019% |
| 72 | 12.146 | 1813 | 1814 | 1819 | rVB3 | 1028 | 1118 | 0.20% | 0.024% |
| 73 | 12.244 | 1827 | 1830 | 1835 | rBV3 | 596 | 764 | 0.13% | 0.017% |
| 74 | 12.323 | 1837 | 1843 | 1852 | rVV | 322931 | 413686 | 72.68% | 8.941% |
| 75 | 12.414 | 1855 | 1858 | 1863 | rVB2 | 812 | 1362 | 0.24% | 0.029% |
| 76 | 12.591 | 1885 | 1887 | 1890 | rBV2 | 105 | 117 | 0.02% | 0.003% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
Acq On : 19 Nov 2021 19:02
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** VHBLK001

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\SFAMXLM111121WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 12.658 | 1896 | 1898 | 1899 | rBV | 223 | 229 | 0.04% | 0.005% |
| 78 | 12.774 | 1912 | 1917 | 1919 | rBV2 | 158 | 233 | 0.04% | 0.005% |
| 79 | 12.859 | 1925 | 1931 | 1932 | rBV2 | 352 | 512 | 0.09% | 0.011% |
| 80 | 13.018 | 1956 | 1957 | 1960 | rBV2 | 146 | 124 | 0.02% | 0.003% |
| 81 | 13.055 | 1960 | 1963 | 1968 | rVB2 | 293 | 294 | 0.05% | 0.006% |
| 82 | 13.201 | 1985 | 1987 | 1989 | rBV | 183 | 140 | 0.02% | 0.003% |
| 83 | 13.414 | 2020 | 2022 | 2024 | rBV | 158 | 139 | 0.02% | 0.003% |
| 84 | 13.597 | 2047 | 2052 | 2053 | rBV2 | 155 | 202 | 0.04% | 0.004% |
| 85 | 13.695 | 2067 | 2068 | 2072 | rVB | 171 | 135 | 0.02% | 0.003% |
| 86 | 13.743 | 2074 | 2076 | 2077 | rBV2 | 273 | 275 | 0.05% | 0.006% |
| 87 | 13.780 | 2077 | 2082 | 2090 | rVV | 11440 | 15918 | 2.80% | 0.344% |
| 88 | 13.871 | 2094 | 2097 | 2102 | rVB3 | 415 | 612 | 0.11% | 0.013% |
| 89 | 13.926 | 2102 | 2106 | 2108 | rBV | 199 | 174 | 0.03% | 0.004% |
| 90 | 14.128 | 2138 | 2139 | 2145 | rVB3 | 465 | 589 | 0.10% | 0.013% |
| 91 | 14.274 | 2160 | 2163 | 2164 | rBV2 | 192 | 176 | 0.03% | 0.004% |
| 92 | 14.432 | 2187 | 2189 | 2192 | rVB2 | 189 | 164 | 0.03% | 0.004% |
| 93 | 14.579 | 2211 | 2213 | 2214 | rBV | 152 | 107 | 0.02% | 0.002% |
| 94 | 14.640 | 2220 | 2223 | 2227 | rBV3 | 485 | 712 | 0.13% | 0.015% |
| 95 | 14.792 | 2241 | 2248 | 2250 | rBV5 | 309 | 616 | 0.11% | 0.013% |
| 96 | 14.981 | 2278 | 2279 | 2282 | rVB2 | 234 | 185 | 0.03% | 0.004% |
| 97 | 15.213 | 2315 | 2317 | 2321 | rBV2 | 207 | 315 | 0.06% | 0.007% |
| 98 | 15.298 | 2329 | 2331 | 2332 | rBV | 198 | 147 | 0.03% | 0.003% |
| 99 | 15.572 | 2374 | 2376 | 2378 | rBV2 | 148 | 140 | 0.02% | 0.003% |
| 100 | 16.511 | 2526 | 2530 | 2532 | rBV | 343 | 441 | 0.08% | 0.010% |

Sum of corrected areas: 4627076

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
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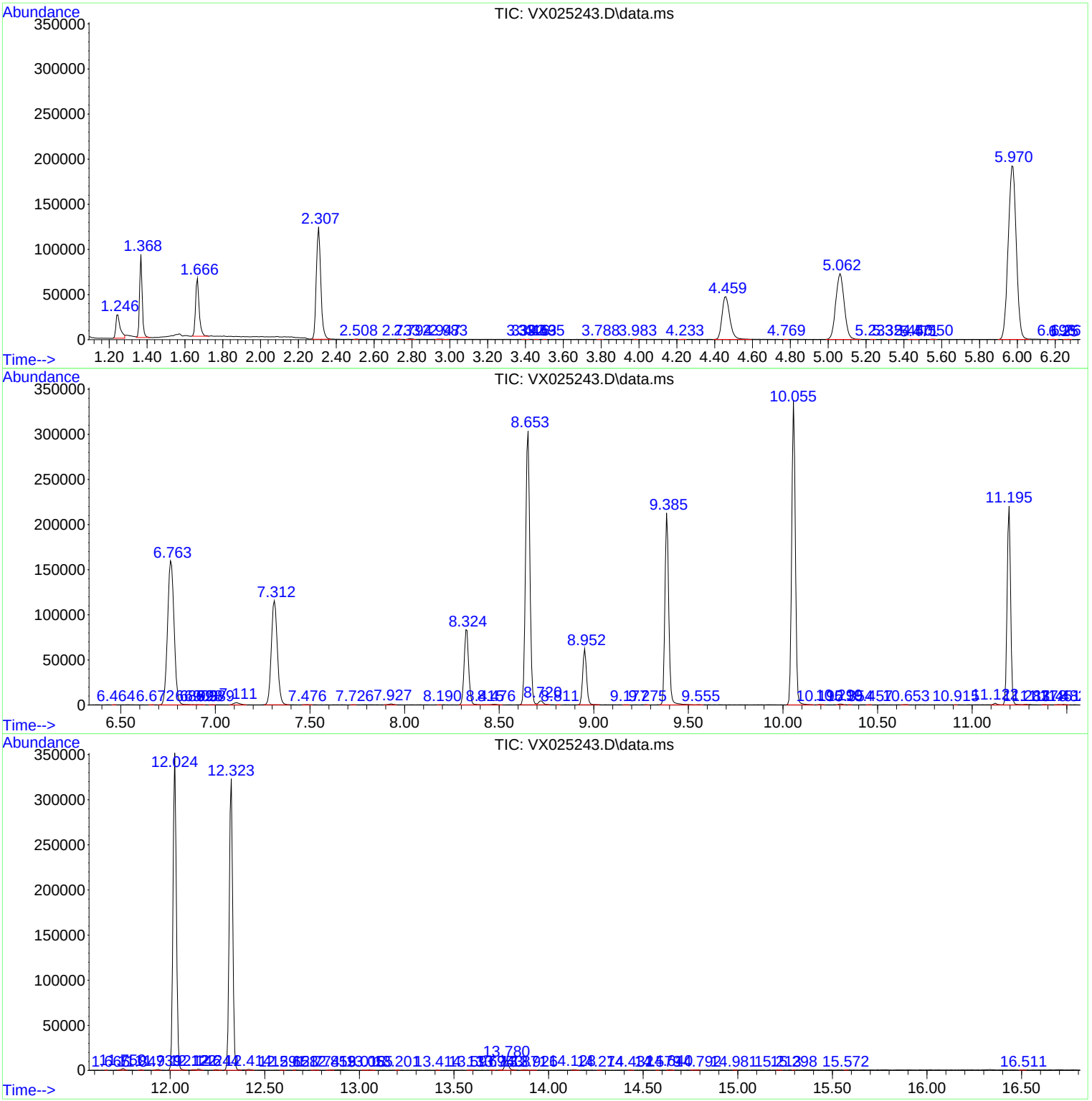
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
Acq On : 19 Nov 2021 19:02
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

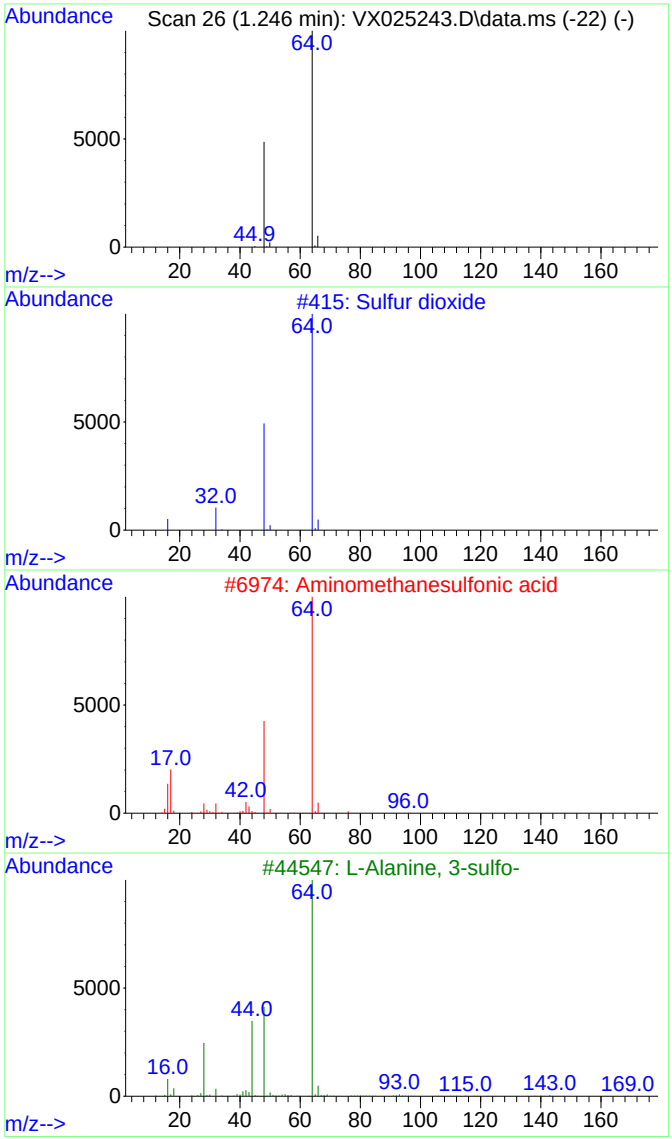
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

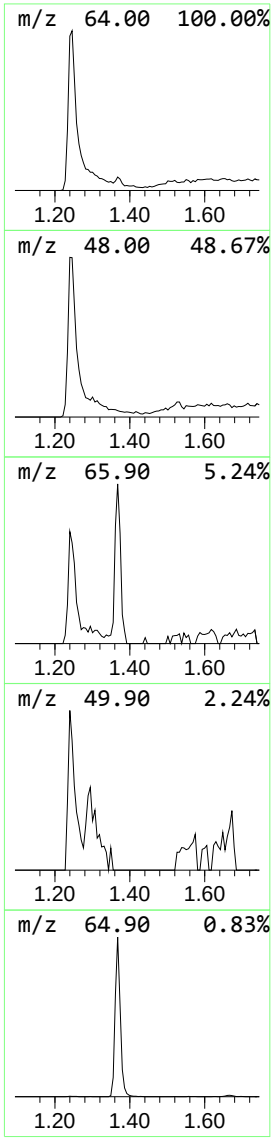
**********

Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.246 | 5.44 ug/L | 41567 | 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 | 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 | 4 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
Data File : VX025243.D
Acq On : 19 Nov 2021 19:02
Operator : JC/MD
Sample : M4677-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Sulfur dioxide | 1.246 | 5.4 | ug/L | 41567 | 1 | 6.763 | 381711 | 50.0 |