LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

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\SFAMXLM112221WMA.M
Title : VOC Analysis

Signal : TIC: VX025584.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.239 | 22 | 25 | 42 | rBV2 | 5050 | 13093 | 3.75% | 0.465% |
| 2 | 1.367 | 43 | 46 | 53 | rVB | 36406 | 41309 | 11.84% | 1.466% |
| 3 | 1.648 | 88 | 92 | 99 | rBV | 22285 | 29520 | 8.46% | 1.048% |
| 4 | 2.282 | 189 | 196 | 205 | rBV | 67758 | 113438 | 32.51% | 4.027% |
| 5 | 2.367 | 207 | 210 | 215 | rVV2 | 728 | 1244 | 0.36% | 0.044% |
| 6 | 2.471 | 226 | 227 | 233 | rBV2 | 198 | 275 | 0.08% | 0.010% |
| 7 | 2.788 | 274 | 279 | 286 | rVB3 | 979 | 2002 | 0.57% | 0.071% |
| 8 | 2.953 | 297 | 306 | 313 | rBV | 6697 | 17546 | 5.03% | 0.623% |
| 9 | 3.129 | 333 | 335 | 339 | rBV2 | 132 | 185 | 0.05% | 0.007% |
| 10 | 4.489 | 548 | 558 | 584 | rVV | 15609 | 70064 | 20.08% | 2.487% |
| 11 | 5.068 | 640 | 653 | 671 | rVB | 40570 | 135128 | 38.73% | 4.797% |
| 12 | 5.690 | 752 | 755 | 760 | rBV2 | 91 | 196 | 0.06% | 0.007% |
| 13 | 5.970 | 790 | 801 | 825 | rBV2 | 119892 | 348941 | 100.00% | 12.387% |
| 14 | 6.373 | 859 | 867 | 877 | rBV6 | 1785 | 5752 | 1.65% | 0.204% |
| 15 | 6.763 | 921 | 931 | 950 | rBV | 88614 | 224789 | 64.42% | 7.979% |
| 16 | 6.903 | 952 | 954 | 957 | rBV3 | 176 | 234 | 0.07% | 0.008% |
| 17 | 7.123 | 983 | 990 | 995 | rBV5 | 1042 | 2842 | 0.81% | 0.101% |
| 18 | 7.214 | 1000 | 1005 | 1012 | rVV3 | 1004 | 2528 | 0.72% | 0.090% |
| 19 | 7.312 | 1013 | 1021 | 1037 | rVV | 65073 | 152928 | 43.83% | 5.429% |
| 20 | 7.866 | 1110 | 1112 | 1115 | rBV | 161 | 170 | 0.05% | 0.006% |
| 21 | 7.964 | 1124 | 1128 | 1131 | rVV4 | 412 | 398 | 0.11% | 0.014% |
| 22 | 8.330 | 1180 | 1188 | 1198 | rBV | 35319 | 62657 | 17.96% | 2.224% |
| 23 | 8.653 | 1234 | 1241 | 1248 | rBV | 171253 | 278680 | 79.86% | 9.892% |
| 24 | 8.720 | 1248 | 1252 | 1258 | rVB | 6635 | 9937 | 2.85% | 0.353% |
| 25 | 8.958 | 1285 | 1291 | 1300 | rBV | 22821 | 38223 | 10.95% | 1.357% |
| 26 | 9.397 | 1357 | 1363 | 1377 | rBV | 91362 | 151359 | 43.38% | 5.373% |
| 27 | 9.543 | 1384 | 1387 | 1391 | rBV | 205 | 278 | 0.08% | 0.010% |
| 28 | 9.714 | 1411 | 1415 | 1419 | rVV2 | 654 | 1008 | 0.29% | 0.036% |
| 29 | 10.061 | 1466 | 1472 | 1485 | rBV | 176903 | 260380 | 74.62% | 9.243% |
| 30 | 10.195 | 1491 | 1494 | 1499 | rBV | 545 | 729 | 0.21% | 0.026% |
| 31 | 10.305 | 1507 | 1512 | 1519 | rBV | 4847 | 6969 | 2.00% | 0.247% |
| 32 | 10.646 | 1564 | 1568 | 1573 | rVB | 1638 | 2276 | 0.65% | 0.081% |
| 33 | 10.963 | 1618 | 1620 | 1623 | rVB2 | 222 | 290 | 0.08% | 0.010% |
| 34 | 11.073 | 1634 | 1638 | 1640 | rBV2 | 124 | 165 | 0.05% | 0.006% |
| 35 | 11.122 | 1642 | 1646 | 1650 | rVV2 | 1439 | 1909 | 0.55% | 0.068% |
| 36 | 11.195 | 1653 | 1658 | 1666 | rBV | 127923 | 162264 | 46.50% | 5.760% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

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\SFAMXLM112221WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 11.280 | 1670 | 1672 | 1674 | rBV2 | 290 | 267 | 0.08% | 0.009% |
| 38 | 11.305 | 1674 | 1676 | 1677 | rVV | 349 | 257 | 0.07% | 0.009% |
| 39 | 11.384 | 1686 | 1689 | 1690 | rBV | 304 | 225 | 0.06% | 0.008% |
| 40 | 11.451 | 1697 | 1700 | 1703 | rBV2 | 875 | 1122 | 0.32% | 0.040% |
| 41 | 11.622 | 1725 | 1728 | 1732 | rBV2 | 252 | 325 | 0.09% | 0.012% |
| 42 | 11.713 | 1741 | 1743 | 1745 | rBV3 | 320 | 341 | 0.10% | 0.012% |
| 43 | 11.750 | 1745 | 1749 | 1756 | rVB2 | 2676 | 3663 | 1.05% | 0.130% |
| 44 | 11.841 | 1762 | 1764 | 1769 | rVB3 | 240 | 322 | 0.09% | 0.011% |
| 45 | 11.939 | 1775 | 1780 | 1781 | rBV2 | 793 | 795 | 0.23% | 0.028% |
| 46 | 11.963 | 1781 | 1784 | 1789 | rVB2 | 1127 | 1453 | 0.42% | 0.052% |
| 47 | 12.024 | 1789 | 1794 | 1802 | rBV | 216783 | 263721 | 75.58% | 9.361% |
| 48 | 12.122 | 1808 | 1810 | 1812 | rBV2 | 493 | 486 | 0.14% | 0.017% |
| 49 | 12.152 | 1812 | 1815 | 1821 | rVB3 | 1473 | 1729 | 0.50% | 0.061% |
| 50 | 12.225 | 1825 | 1827 | 1829 | rBV | 237 | 237 | 0.07% | 0.008% |
| 51 | 12.323 | 1835 | 1843 | 1851 | rBV | 203232 | 259018 | 74.23% | 9.194% |
| 52 | 12.378 | 1851 | 1852 | 1856 | rVB3 | 219 | 174 | 0.05% | 0.006% |
| 53 | 12.426 | 1856 | 1860 | 1863 | rVB3 | 1361 | 1771 | 0.51% | 0.063% |
| 54 | 12.487 | 1865 | 1870 | 1873 | rBV2 | 319 | 398 | 0.11% | 0.014% |
| 55 | 12.664 | 1896 | 1899 | 1903 | rBV3 | 230 | 313 | 0.09% | 0.011% |
| 56 | 12.695 | 1903 | 1904 | 1912 | rVB2 | 297 | 383 | 0.11% | 0.014% |
| 57 | 12.768 | 1912 | 1916 | 1920 | rBV2 | 332 | 410 | 0.12% | 0.015% |
| 58 | 12.890 | 1932 | 1936 | 1939 | rBV | 1186 | 1399 | 0.40% | 0.050% |
| 59 | 12.926 | 1939 | 1942 | 1945 | rBV | 814 | 896 | 0.26% | 0.032% |
| 60 | 12.969 | 1945 | 1949 | 1954 | rBV3 | 1849 | 2455 | 0.70% | 0.087% |
| 61 | 13.170 | 1979 | 1982 | 1985 | rBV4 | 263 | 296 | 0.08% | 0.011% |
| 62 | 13.268 | 1994 | 1998 | 2000 | rBV | 1007 | 1185 | 0.34% | 0.042% |
| 63 | 13.341 | 2008 | 2010 | 2014 | rVB2 | 412 | 460 | 0.13% | 0.016% |
| 64 | 13.384 | 2014 | 2017 | 2021 | rVB2 | 573 | 693 | 0.20% | 0.025% |
| 65 | 13.426 | 2021 | 2024 | 2027 | rBV | 1116 | 1487 | 0.43% | 0.053% |
| 66 | 13.579 | 2046 | 2049 | 2054 | rVV2 | 491 | 729 | 0.21% | 0.026% |
| 67 | 13.621 | 2054 | 2056 | 2059 | rVV | 275 | 268 | 0.08% | 0.010% |
| 68 | 13.664 | 2059 | 2063 | 2065 | rVB2 | 236 | 252 | 0.07% | 0.009% |
| 69 | 13.780 | 2075 | 2082 | 2088 | rVV | 24729 | 33739 | 9.67% | 1.198% |
| 70 | 13.841 | 2088 | 2092 | 2095 | rVV3 | 1242 | 1639 | 0.47% | 0.058% |
| 71 | 13.877 | 2095 | 2098 | 2100 | rVV | 967 | 1261 | 0.36% | 0.045% |
| 72 | 13.926 | 2104 | 2106 | 2109 | rVB2 | 307 | 275 | 0.08% | 0.010% |
| 73 | 13.999 | 2113 | 2118 | 2121 | rBV2 | 326 | 466 | 0.13% | 0.017% |
| 74 | 14.042 | 2121 | 2125 | 2128 | rBV2 | 1770 | 2198 | 0.63% | 0.078% |
| 75 | 14.140 | 2137 | 2141 | 2143 | rVV3 | 570 | 824 | 0.24% | 0.029% |
| 76 | 14.188 | 2146 | 2149 | 2151 | rBV2 | 249 | 281 | 0.08% | 0.010% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

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\SFAMXLM112221WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 14.219 | 2151 | 2154 | 2157 | rVB3 | 594 | 754 | 0.22% | 0.027% |
| 78 | 14.322 | 2169 | 2171 | 2173 | rVB3 | 387 | 339 | 0.10% | 0.012% |
| 79 | 14.371 | 2176 | 2179 | 2182 | rBV | 348 | 490 | 0.14% | 0.017% |
| 80 | 14.432 | 2186 | 2189 | 2194 | rVB2 | 314 | 405 | 0.12% | 0.014% |
| 81 | 14.499 | 2199 | 2200 | 2207 | rVB3 | 663 | 1082 | 0.31% | 0.038% |
| 82 | 14.566 | 2209 | 2211 | 2213 | rBV2 | 363 | 367 | 0.11% | 0.013% |
| 83 | 14.640 | 2219 | 2223 | 2230 | rVB | 8639 | 10864 | 3.11% | 0.386% |
| 84 | 14.780 | 2236 | 2246 | 2253 | rBV | 17670 | 27948 | 8.01% | 0.992% |
| 85 | 14.847 | 2253 | 2257 | 2261 | rVB5 | 1559 | 2154 | 0.62% | 0.076% |
| 86 | 14.938 | 2268 | 2272 | 2275 | rBV4 | 720 | 1274 | 0.37% | 0.045% |
| 87 | 15.121 | 2299 | 2302 | 2305 | rBV4 | 476 | 619 | 0.18% | 0.022% |
| 88 | 15.213 | 2313 | 2317 | 2322 | rVB3 | 5041 | 6948 | 1.99% | 0.247% |
| 89 | 15.267 | 2322 | 2326 | 2331 | rBV6 | 722 | 1380 | 0.40% | 0.049% |
| 90 | 15.481 | 2356 | 2361 | 2369 | rBV5 | 3419 | 6744 | 1.93% | 0.239% |
| 91 | 15.615 | 2378 | 2383 | 2387 | rBV2 | 5863 | 9365 | 2.68% | 0.332% |
| 92 | 15.743 | 2401 | 2404 | 2407 | rVB3 | 621 | 741 | 0.21% | 0.026% |
| 93 | 15.816 | 2411 | 2416 | 2417 | rBV | 1040 | 1384 | 0.40% | 0.049% |
| 94 | 15.993 | 2440 | 2445 | 2450 | rBV3 | 878 | 1138 | 0.33% | 0.040% |
| 95 | 16.090 | 2457 | 2461 | 2466 | rVB3 | 2006 | 3193 | 0.92% | 0.113% |
| 96 | 16.139 | 2467 | 2469 | 2471 | rVV2 | 267 | 222 | 0.06% | 0.008% |
| 97 | 16.206 | 2476 | 2480 | 2482 | rVB2 | 418 | 494 | 0.14% | 0.018% |
| 98 | 16.334 | 2494 | 2501 | 2505 | rBV4 | 1921 | 4014 | 1.15% | 0.142% |
| 99 | 16.438 | 2515 | 2518 | 2519 | rBV2 | 314 | 276 | 0.08% | 0.010% |
| 100 | 16.688 | 2551 | 2559 | 2570 | rVB4 | 2464 | 6984 | 2.00% | 0.248% |

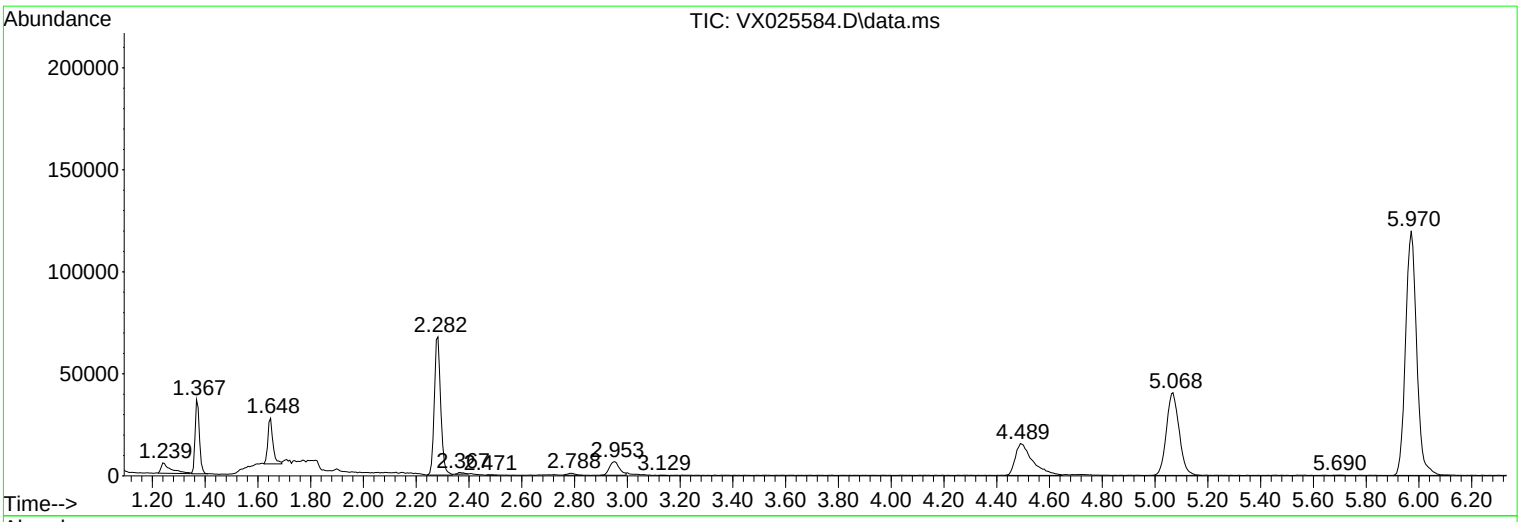
Sum of corrected areas: 2817098

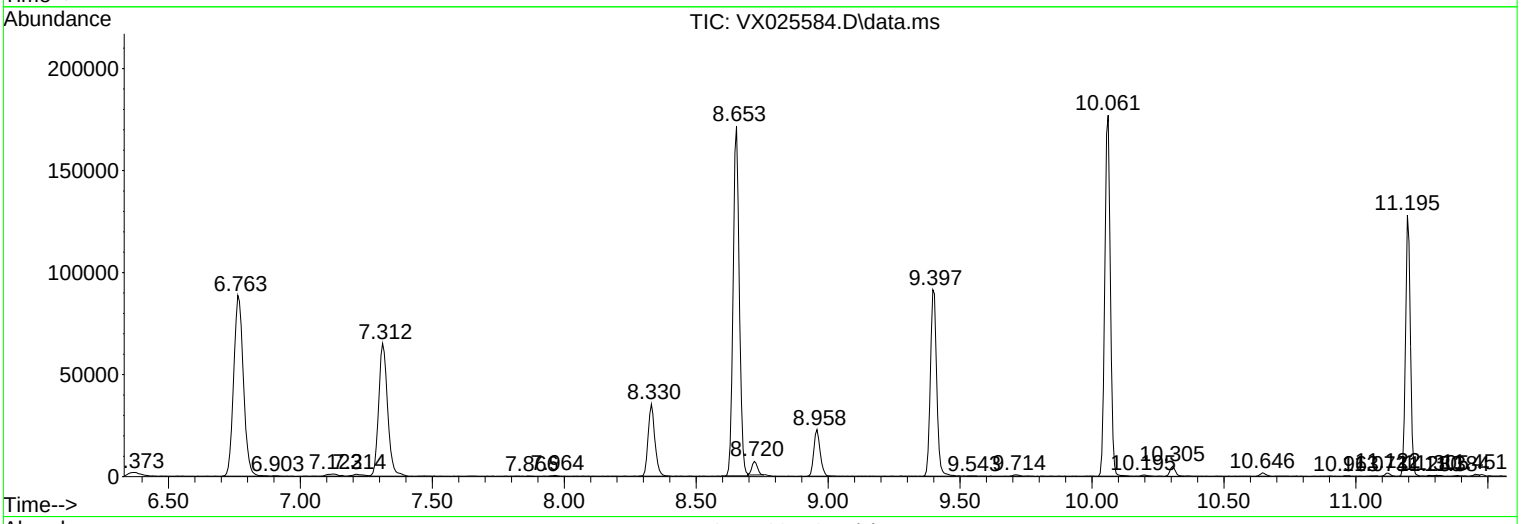
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

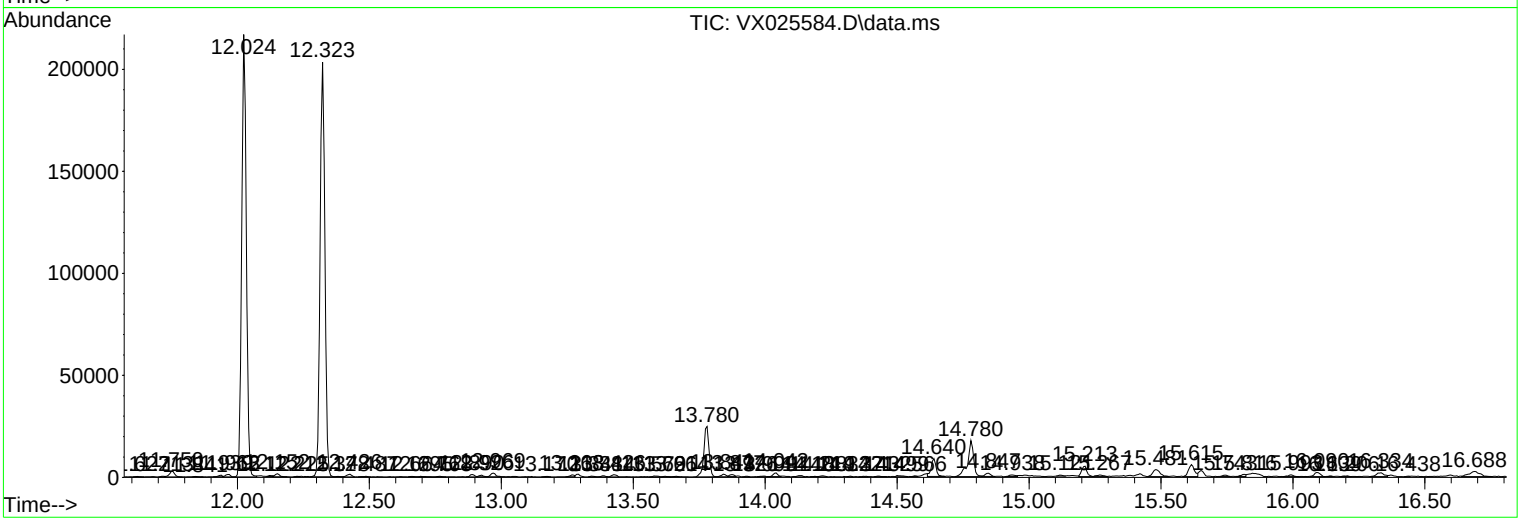
**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

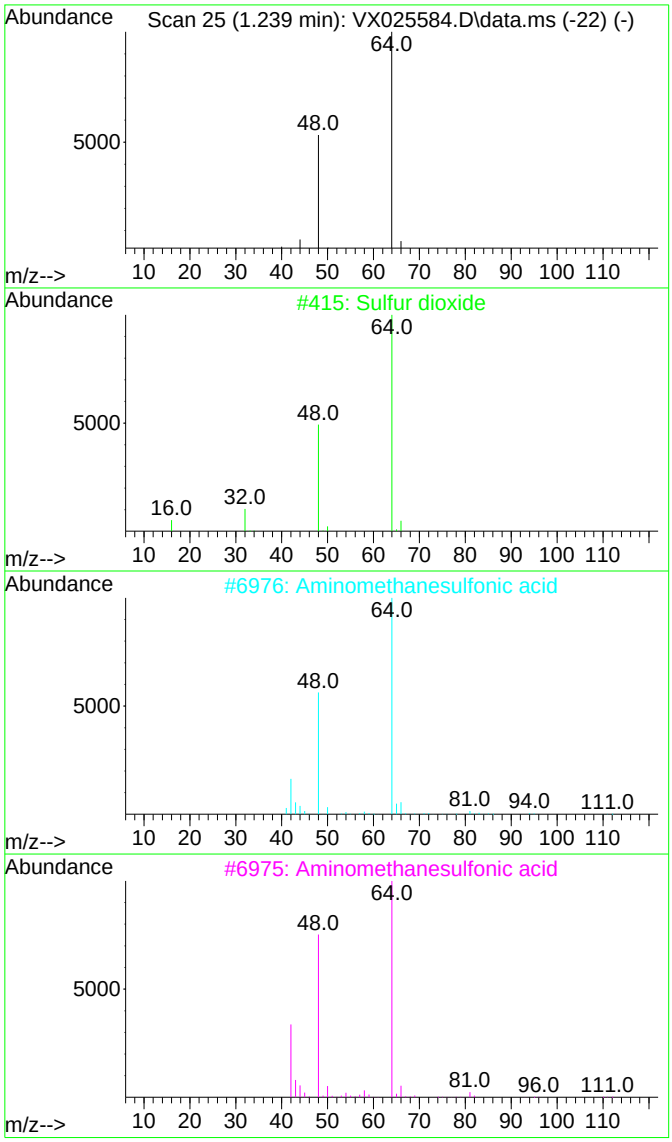
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

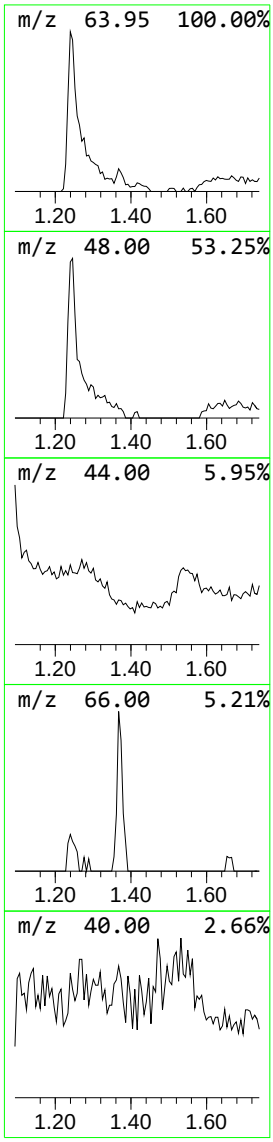
**********

Peak Number 1 Sulfur dioxide Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.239 | 2.91 ug/L | 13093 | 1,4-Difluorobenzene | 6.763 |

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

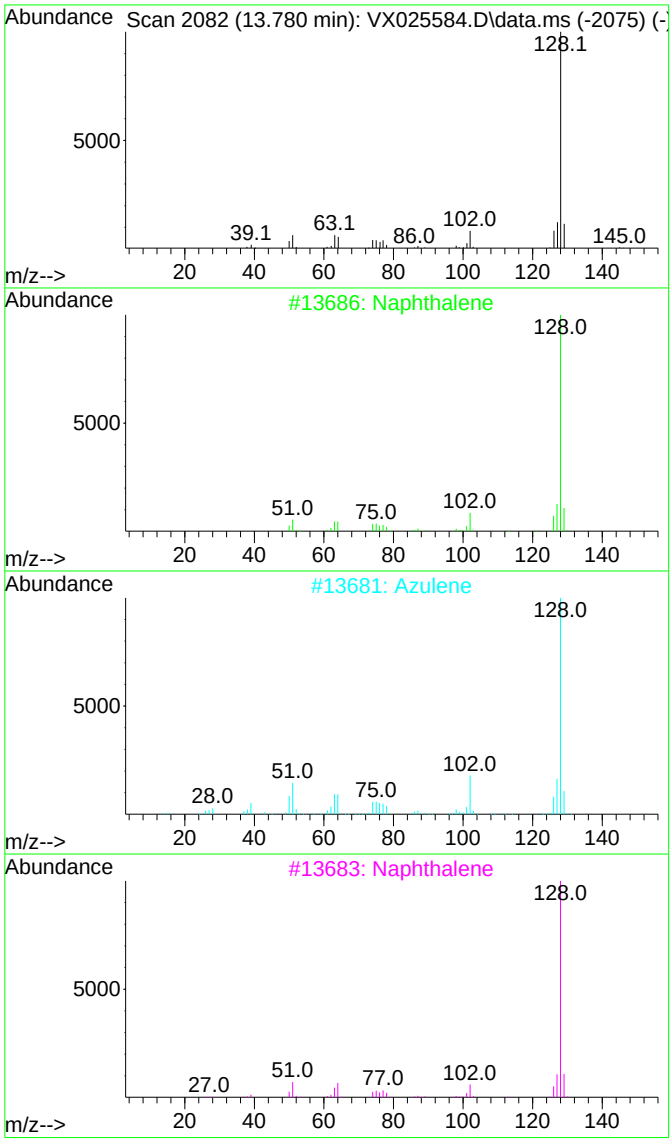
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

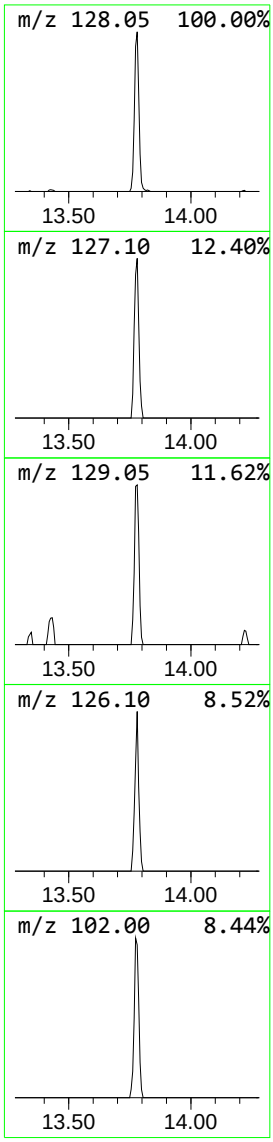
**********

Peak Number 4 Azulene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.780 | 6.40 ug/L | 33739 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene | 128 | C10H8 | 000091-20-3 | 95 |
| 2 | Azulene | 128 | C10H8 | 000275-51-4 | 94 |
| 3 | Naphthalene | 128 | C10H8 | 000091-20-3 | 93 |
| 4 | 1H-Indene, 1-methylene- | 128 | C10H8 | 002471-84-3 | 91 |
| 5 | Azulene | 128 | C10H8 | 000275-51-4 | 90 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

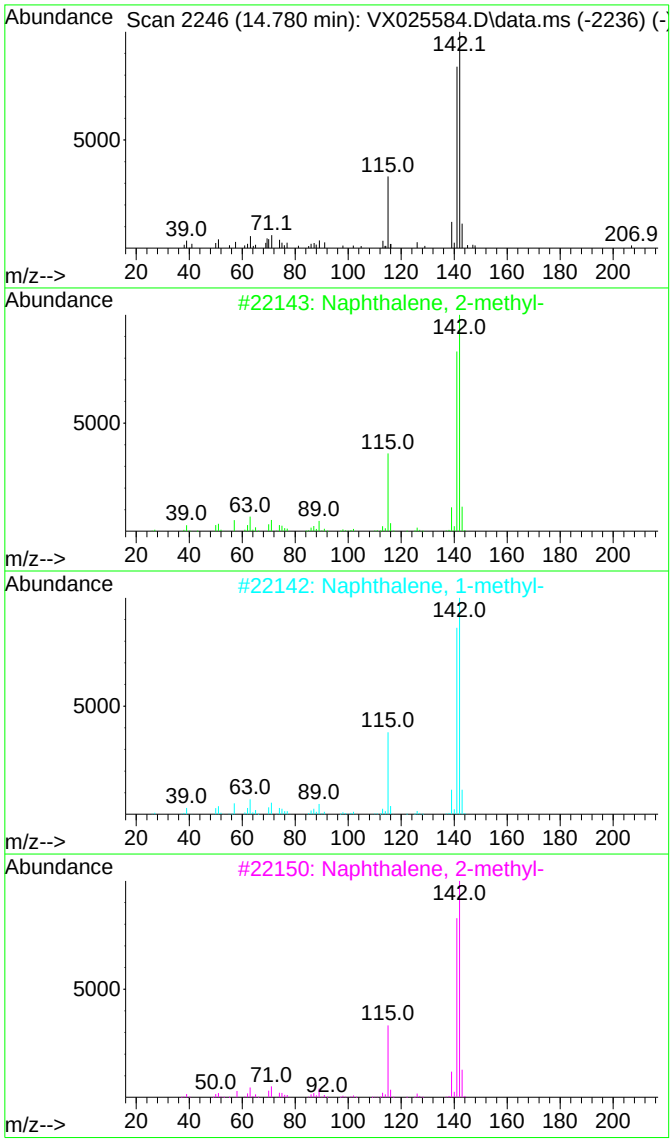
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

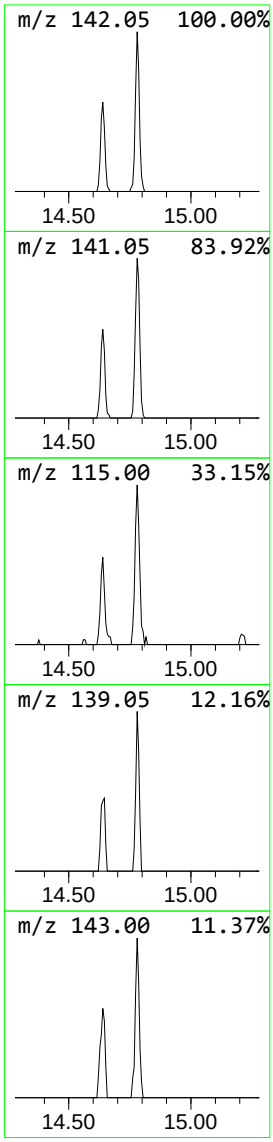
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.780 | 5.30 ug/L | 27948 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 97 |
| 2 | Naphthalene, 1-methyl- | 142 | C11H10 | 000090-12-0 | 97 |
| 3 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 96 |
| 4 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 95 |
| 5 | Naphthalene, 1-methyl- | 142 | C11H10 | 000090-12-0 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025584.D
Acq On : 07 Dec 2021 17:26
Operator : JC/MD
Sample : M4881-11ME
Misc : 5.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
EW9E7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.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 | 1.239 | 2.9 | ug/L | 13093 | 1 | 6.763 | 224789 | 50.0 |
| Azulene | 13.780 | 6.4 | ug/L | 33739 | 3 | 12.024 | 263721 | 50.0 |
| Naphthalene, 2-... | 14.780 | 5.3 | ug/L | 27948 | 3 | 12.024 | 263721 | 50.0 |