LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025646.D
Acq On : 09 Dec 2021 01:42
Operator : JC/MD
Sample : M4975-11
Misc : 5.91g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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: VX025646.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 | 31 | rBV2 | 4199 | 7282 | 1.48% | 0.190% |
| 2 | 1.374 | 43 | 47 | 52 | rVB | 53257 | 62954 | 12.79% | 1.640% |
| 3 | 1.538 | 68 | 74 | 75 | rBV3 | 2828 | 4356 | 0.89% | 0.113% |
| 4 | 1.648 | 88 | 92 | 98 | rBV | 34232 | 39776 | 8.08% | 1.036% |
| 5 | 2.282 | 190 | 196 | 206 | rBV | 99111 | 160878 | 32.69% | 4.191% |
| 6 | 2.946 | 300 | 305 | 316 | rBV | 6065 | 13875 | 2.82% | 0.361% |
| 7 | 3.117 | 332 | 333 | 334 | rBV | 433 | 227 | 0.05% | 0.006% |
| 8 | 3.221 | 348 | 350 | 352 | rBV | 331 | 224 | 0.05% | 0.006% |
| 9 | 3.392 | 376 | 378 | 381 | rVB | 579 | 393 | 0.08% | 0.010% |
| 10 | 3.532 | 400 | 401 | 402 | rBV | 267 | 106 | 0.02% | 0.003% |
| 11 | 3.587 | 408 | 410 | 412 | rBV | 379 | 274 | 0.06% | 0.007% |
| 12 | 3.605 | 412 | 413 | 414 | rBV | 279 | 126 | 0.03% | 0.003% |
| 13 | 3.702 | 428 | 429 | 430 | rBV | 260 | 113 | 0.02% | 0.003% |
| 14 | 3.751 | 435 | 437 | 438 | rBV | 318 | 252 | 0.05% | 0.007% |
| 15 | 3.824 | 448 | 449 | 450 | rBV | 251 | 118 | 0.02% | 0.003% |
| 16 | 4.117 | 495 | 497 | 498 | rBV | 372 | 292 | 0.06% | 0.008% |
| 17 | 4.489 | 549 | 558 | 589 | rBV2 | 20366 | 97694 | 19.85% | 2.545% |
| 18 | 4.916 | 626 | 628 | 630 | rVB | 343 | 216 | 0.04% | 0.006% |
| 19 | 5.068 | 641 | 653 | 672 | rVB | 57719 | 194244 | 39.47% | 5.060% |
| 20 | 5.970 | 789 | 801 | 817 | rBV2 | 171618 | 492122 | 100.00% | 12.820% |
| 21 | 6.312 | 855 | 857 | 858 | rVB | 271 | 136 | 0.03% | 0.004% |
| 22 | 6.769 | 922 | 932 | 949 | rBV | 121630 | 318452 | 64.71% | 8.296% |
| 23 | 7.129 | 982 | 991 | 1000 | rBV8 | 3356 | 9238 | 1.88% | 0.241% |
| 24 | 7.312 | 1013 | 1021 | 1033 | rVB | 92653 | 214555 | 43.60% | 5.589% |
| 25 | 7.446 | 1041 | 1043 | 1044 | rBV | 250 | 208 | 0.04% | 0.005% |
| 26 | 7.629 | 1071 | 1073 | 1076 | rBV | 240 | 250 | 0.05% | 0.007% |
| 27 | 7.677 | 1079 | 1081 | 1082 | rBV2 | 215 | 139 | 0.03% | 0.004% |
| 28 | 7.744 | 1090 | 1092 | 1093 | rBV | 550 | 366 | 0.07% | 0.010% |
| 29 | 7.763 | 1093 | 1095 | 1099 | rVB2 | 332 | 319 | 0.06% | 0.008% |
| 30 | 7.805 | 1101 | 1102 | 1104 | rBV | 247 | 191 | 0.04% | 0.005% |
| 31 | 7.933 | 1122 | 1123 | 1126 | rBV | 472 | 325 | 0.07% | 0.008% |
| 32 | 8.019 | 1135 | 1137 | 1138 | rBV | 304 | 186 | 0.04% | 0.005% |
| 33 | 8.116 | 1150 | 1153 | 1155 | rBV2 | 592 | 723 | 0.15% | 0.019% |
| 34 | 8.183 | 1162 | 1164 | 1166 | rBV | 421 | 291 | 0.06% | 0.008% |
| 35 | 8.330 | 1182 | 1188 | 1199 | rBV | 53308 | 97947 | 19.90% | 2.552% |
| 36 | 8.482 | 1210 | 1213 | 1214 | rBV | 236 | 206 | 0.04% | 0.005% |

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Sample : M4975-11
Misc : 5.91g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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 | 8.653 | 1234 | 1241 | 1249 | rBV | 236243 | 392754 | 79.81% | 10.232% |
| 38 | 8.720 | 1249 | 1252 | 1264 | rVB2 | 3254 | 6924 | 1.41% | 0.180% |
| 39 | 8.897 | 1280 | 1281 | 1282 | rBV | 484 | 261 | 0.05% | 0.007% |
| 40 | 8.915 | 1282 | 1284 | 1285 | rVV | 440 | 355 | 0.07% | 0.009% |
| 41 | 8.958 | 1285 | 1291 | 1302 | rVB2 | 34791 | 62221 | 12.64% | 1.621% |
| 42 | 9.073 | 1308 | 1310 | 1313 | rVB | 374 | 234 | 0.05% | 0.006% |
| 43 | 9.098 | 1313 | 1314 | 1315 | rBV | 241 | 138 | 0.03% | 0.004% |
| 44 | 9.275 | 1337 | 1343 | 1351 | rVB | 84748 | 122715 | 24.94% | 3.197% |
| 45 | 9.397 | 1357 | 1363 | 1377 | rBV | 126248 | 211373 | 42.95% | 5.506% |
| 46 | 9.573 | 1390 | 1392 | 1393 | rBV | 347 | 191 | 0.04% | 0.005% |
| 47 | 9.714 | 1410 | 1415 | 1418 | rBV2 | 1163 | 1795 | 0.36% | 0.047% |
| 48 | 9.768 | 1422 | 1424 | 1426 | rVV | 270 | 199 | 0.04% | 0.005% |
| 49 | 9.811 | 1429 | 1431 | 1434 | rBV2 | 299 | 345 | 0.07% | 0.009% |
| 50 | 9.854 | 1437 | 1438 | 1439 | rBV | 365 | 217 | 0.04% | 0.006% |
| 51 | 9.890 | 1442 | 1444 | 1446 | rBV | 311 | 322 | 0.07% | 0.008% |
| 52 | 9.982 | 1458 | 1459 | 1460 | rBV | 287 | 128 | 0.03% | 0.003% |
| 53 | 10.061 | 1465 | 1472 | 1482 | rBV | 244328 | 368619 | 74.90% | 9.603% |
| 54 | 10.348 | 1517 | 1519 | 1520 | rVB | 260 | 161 | 0.03% | 0.004% |
| 55 | 10.451 | 1534 | 1536 | 1537 | rBV | 316 | 189 | 0.04% | 0.005% |
| 56 | 10.470 | 1537 | 1539 | 1543 | rVV | 442 | 379 | 0.08% | 0.010% |
| 57 | 10.567 | 1553 | 1555 | 1556 | rVB | 292 | 135 | 0.03% | 0.004% |
| 58 | 10.787 | 1589 | 1591 | 1593 | rBV | 315 | 323 | 0.07% | 0.008% |
| 59 | 10.884 | 1605 | 1607 | 1611 | rBV | 337 | 409 | 0.08% | 0.011% |
| 60 | 10.969 | 1620 | 1621 | 1622 | rVB | 341 | 125 | 0.03% | 0.003% |
| 61 | 11.043 | 1631 | 1633 | 1635 | rBV | 416 | 340 | 0.07% | 0.009% |
| 62 | 11.116 | 1643 | 1645 | 1648 | rVB2 | 1167 | 1236 | 0.25% | 0.032% |
| 63 | 11.201 | 1653 | 1659 | 1665 | rBV | 164998 | 222386 | 45.19% | 5.793% |
| 64 | 11.311 | 1675 | 1677 | 1678 | rBV | 433 | 429 | 0.09% | 0.011% |
| 65 | 11.475 | 1703 | 1704 | 1708 | rVB2 | 470 | 537 | 0.11% | 0.014% |
| 66 | 11.579 | 1719 | 1721 | 1722 | rBV2 | 260 | 196 | 0.04% | 0.005% |
| 67 | 11.750 | 1746 | 1749 | 1754 | rVB3 | 1212 | 1807 | 0.37% | 0.047% |
| 68 | 11.786 | 1754 | 1755 | 1756 | rBV | 329 | 172 | 0.03% | 0.004% |
| 69 | 11.817 | 1759 | 1760 | 1763 | rBV | 309 | 387 | 0.08% | 0.010% |
| 70 | 11.878 | 1769 | 1770 | 1772 | rVB | 242 | 118 | 0.02% | 0.003% |
| 71 | 11.908 | 1774 | 1775 | 1776 | rBV | 287 | 136 | 0.03% | 0.004% |
| 72 | 12.024 | 1789 | 1794 | 1805 | rBV | 300573 | 364328 | 74.03% | 9.491% |
| 73 | 12.183 | 1818 | 1820 | 1821 | rVB | 377 | 207 | 0.04% | 0.005% |
| 74 | 12.323 | 1838 | 1843 | 1850 | rVB | 278030 | 350206 | 71.16% | 9.123% |
| 75 | 12.567 | 1881 | 1883 | 1884 | rBV | 265 | 184 | 0.04% | 0.005% |
| 76 | 12.628 | 1890 | 1893 | 1896 | rBV2 | 386 | 577 | 0.12% | 0.015% |

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ALS Vial : 36 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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 | 12.707 | 1904 | 1906 | 1907 | rBV | 397 | 248 | 0.05% | 0.006% |
| 78 | 12.872 | 1931 | 1933 | 1935 | rBV | 316 | 181 | 0.04% | 0.005% |
| 79 | 13.274 | 1998 | 1999 | 2001 | rBV | 317 | 211 | 0.04% | 0.005% |
| 80 | 13.384 | 2016 | 2017 | 2019 | rBV | 235 | 194 | 0.04% | 0.005% |
| 81 | 13.463 | 2028 | 2030 | 2031 | rBV | 385 | 304 | 0.06% | 0.008% |
| 82 | 13.518 | 2038 | 2039 | 2040 | rVB | 360 | 132 | 0.03% | 0.003% |
| 83 | 13.567 | 2045 | 2047 | 2048 | rVB | 365 | 153 | 0.03% | 0.004% |
| 84 | 13.676 | 2063 | 2065 | 2068 | rBV | 383 | 393 | 0.08% | 0.010% |
| 85 | 13.762 | 2078 | 2079 | 2084 | rBV | 357 | 413 | 0.08% | 0.011% |
| 86 | 13.957 | 2109 | 2111 | 2115 | rVB | 452 | 342 | 0.07% | 0.009% |
| 87 | 14.066 | 2126 | 2129 | 2130 | rBV2 | 353 | 307 | 0.06% | 0.008% |
| 88 | 14.518 | 2201 | 2203 | 2206 | rVB | 451 | 366 | 0.07% | 0.010% |
| 89 | 14.566 | 2210 | 2211 | 2216 | rBV | 439 | 637 | 0.13% | 0.017% |
| 90 | 14.810 | 2250 | 2251 | 2252 | rVB | 395 | 145 | 0.03% | 0.004% |
| 91 | 15.304 | 2331 | 2332 | 2336 | rBV | 325 | 293 | 0.06% | 0.008% |
| 92 | 15.511 | 2365 | 2366 | 2369 | rBV | 356 | 212 | 0.04% | 0.006% |
| 93 | 16.097 | 2458 | 2462 | 2465 | rBV2 | 469 | 822 | 0.17% | 0.021% |
| 94 | 16.688 | 2557 | 2559 | 2561 | rBV | 472 | 458 | 0.09% | 0.012% |

Sum of corrected areas: 3838623

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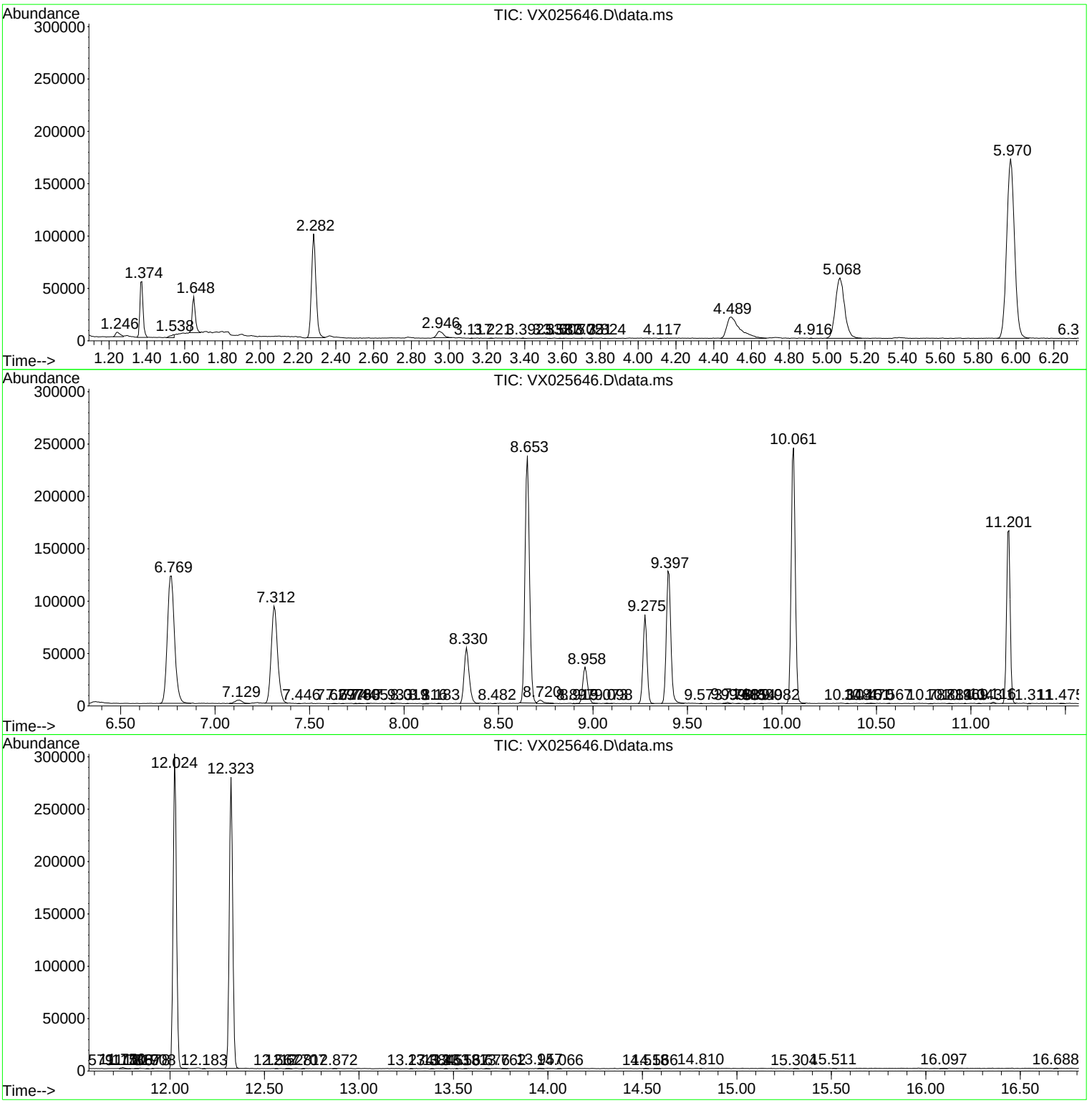
**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025646.D
Acq On : 09 Dec 2021 01:42
Operator : JC/MD
Sample : M4975-11
Misc : 5.91g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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

No Library Search Compounds Detected

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Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
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**Instrument :**
MSVOA_X
**ClientSampleId :**
BGKT5

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 |