LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
Acq On : 27 Jul 2024 03:45
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

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\SFAMXLM072624WMA.M
Title : VOC Analysis

Signal : TIC: VX042630.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.264 | 26 | 29 | 40 | rVB2 | 7850 | 10301 | 2.50% | 0.425% |
| 2 | 1.374 | 43 | 47 | 63 | rBV2 | 24461 | 75163 | 18.21% | 3.105% |
| 3 | 2.282 | 190 | 196 | 204 | rBV | 33172 | 58636 | 14.21% | 2.422% |
| 4 | 2.532 | 235 | 237 | 239 | rBV | 169 | 153 | 0.04% | 0.006% |
| 5 | 2.605 | 247 | 249 | 250 | rBV2 | 313 | 272 | 0.07% | 0.011% |
| 6 | 2.861 | 290 | 291 | 293 | rBV | 286 | 140 | 0.03% | 0.006% |
| 7 | 2.947 | 297 | 305 | 316 | rBV2 | 4352 | 11119 | 2.69% | 0.459% |
| 8 | 3.075 | 320 | 326 | 334 | rBV | 12716 | 24571 | 5.95% | 1.015% |
| 9 | 3.178 | 342 | 343 | 349 | rVB | 236 | 404 | 0.10% | 0.017% |
| 10 | 3.245 | 352 | 354 | 357 | rBV | 141 | 158 | 0.04% | 0.007% |
| 11 | 3.325 | 363 | 367 | 368 | rBB | 180 | 204 | 0.05% | 0.008% |
| 12 | 3.483 | 391 | 393 | 396 | rBB | 189 | 232 | 0.06% | 0.010% |
| 13 | 3.605 | 410 | 413 | 416 | rBV2 | 329 | 355 | 0.09% | 0.015% |
| 14 | 3.672 | 420 | 424 | 426 | rBB2 | 186 | 217 | 0.05% | 0.009% |
| 15 | 3.703 | 426 | 429 | 431 | rBV | 231 | 265 | 0.06% | 0.011% |
| 16 | 3.800 | 443 | 445 | 446 | rBV | 217 | 151 | 0.04% | 0.006% |
| 17 | 3.928 | 465 | 466 | 469 | rBV | 238 | 189 | 0.05% | 0.008% |
| 18 | 4.056 | 484 | 487 | 489 | rVB | 167 | 188 | 0.05% | 0.008% |
| 19 | 4.251 | 517 | 519 | 522 | rBV | 205 | 217 | 0.05% | 0.009% |
| 20 | 4.404 | 540 | 544 | 546 | rBV2 | 193 | 354 | 0.09% | 0.015% |
| 21 | 4.495 | 552 | 559 | 574 | rBV2 | 10877 | 38144 | 9.24% | 1.576% |
| 22 | 4.946 | 630 | 633 | 635 | rBV | 209 | 223 | 0.05% | 0.009% |
| 23 | 5.050 | 640 | 650 | 652 | rBV | 25748 | 53254 | 12.90% | 2.200% |
| 24 | 5.391 | 701 | 706 | 708 | rBV3 | 290 | 481 | 0.12% | 0.020% |
| 25 | 5.544 | 728 | 731 | 733 | rBV | 255 | 279 | 0.07% | 0.012% |
| 26 | 5.617 | 742 | 743 | 746 | rBV | 206 | 194 | 0.05% | 0.008% |
| 27 | 5.702 | 756 | 757 | 760 | rBV | 207 | 197 | 0.05% | 0.008% |
| 28 | 5.763 | 766 | 767 | 771 | rVB | 178 | 158 | 0.04% | 0.007% |
| 29 | 5.818 | 774 | 776 | 780 | rVB | 179 | 195 | 0.05% | 0.008% |
| 30 | 5.958 | 790 | 799 | 816 | rBV4 | 75840 | 218385 | 52.91% | 9.021% |
| 31 | 6.160 | 830 | 832 | 838 | rBV2 | 509 | 764 | 0.19% | 0.032% |
| 32 | 6.245 | 843 | 846 | 848 | rBV | 175 | 214 | 0.05% | 0.009% |
| 33 | 6.263 | 848 | 849 | 852 | rVV2 | 202 | 173 | 0.04% | 0.007% |
| 34 | 6.294 | 852 | 854 | 856 | rVB | 277 | 202 | 0.05% | 0.008% |
| 35 | 6.336 | 857 | 861 | 862 | rBV2 | 236 | 292 | 0.07% | 0.012% |
| 36 | 6.440 | 876 | 878 | 880 | rVB | 202 | 135 | 0.03% | 0.006% |

LSC Area Percent Report

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Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

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\SFAMXLM072624WMA.M
Title : VOC Analysis

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | 6.495 | 885 | 887 | 891 | rBV | 340 | 400 | 0.10% | 0.017% |
| 38 | 6.531 | 891 | 893 | 896 | rVB2 | 201 | 221 | 0.05% | 0.009% |
| 39 | 6.757 | 922 | 930 | 947 | rBV | 145676 | 354930 | 85.99% | 14.661% |
| 40 | 7.080 | 982 | 983 | 985 | rBV | 211 | 189 | 0.05% | 0.008% |
| 41 | 7.306 | 1013 | 1020 | 1032 | rBV | 42593 | 94310 | 22.85% | 3.896% |
| 42 | 7.562 | 1058 | 1062 | 1063 | rBV | 209 | 224 | 0.05% | 0.009% |
| 43 | 7.739 | 1088 | 1091 | 1092 | rBV | 211 | 246 | 0.06% | 0.010% |
| 44 | 7.793 | 1096 | 1100 | 1101 | rBV2 | 310 | 289 | 0.07% | 0.012% |
| 45 | 7.903 | 1116 | 1118 | 1121 | rBV | 220 | 180 | 0.04% | 0.007% |
| 46 | 7.970 | 1125 | 1129 | 1133 | rBV2 | 207 | 280 | 0.07% | 0.012% |
| 47 | 8.269 | 1176 | 1178 | 1179 | rBV2 | 172 | 145 | 0.04% | 0.006% |
| 48 | 8.330 | 1182 | 1188 | 1199 | rVV | 20615 | 37130 | 9.00% | 1.534% |
| 49 | 8.476 | 1211 | 1212 | 1215 | rBV | 243 | 244 | 0.06% | 0.010% |
| 50 | 8.580 | 1227 | 1229 | 1233 | rVB | 257 | 185 | 0.04% | 0.008% |
| 51 | 8.647 | 1233 | 1240 | 1247 | rBV | 105930 | 169102 | 40.97% | 6.985% |
| 52 | 8.952 | 1283 | 1290 | 1301 | rBV | 14328 | 23552 | 5.71% | 0.973% |
| 53 | 9.214 | 1330 | 1333 | 1334 | rBV2 | 233 | 269 | 0.07% | 0.011% |
| 54 | 9.275 | 1339 | 1343 | 1347 | rVV | 3088 | 4149 | 1.01% | 0.171% |
| 55 | 9.397 | 1358 | 1363 | 1376 | rBV | 38484 | 83513 | 20.23% | 3.450% |
| 56 | 9.647 | 1402 | 1404 | 1405 | rBV2 | 388 | 318 | 0.08% | 0.013% |
| 57 | 9.708 | 1412 | 1414 | 1419 | rBV2 | 1123 | 1380 | 0.33% | 0.057% |
| 58 | 9.830 | 1431 | 1434 | 1437 | rBV3 | 716 | 924 | 0.22% | 0.038% |
| 59 | 9.872 | 1437 | 1441 | 1444 | rBV2 | 1108 | 1324 | 0.32% | 0.055% |
| 60 | 10.012 | 1459 | 1464 | 1465 | rBV3 | 2103 | 2801 | 0.68% | 0.116% |
| 61 | 10.055 | 1466 | 1471 | 1485 | rVB | 293365 | 412745 | 100.00% | 17.049% |
| 62 | 10.403 | 1524 | 1528 | 1533 | rVB4 | 1088 | 1744 | 0.42% | 0.072% |
| 63 | 10.561 | 1550 | 1554 | 1555 | rBV | 200 | 177 | 0.04% | 0.007% |
| 64 | 10.762 | 1585 | 1587 | 1590 | rBV | 253 | 265 | 0.06% | 0.011% |
| 65 | 10.811 | 1593 | 1595 | 1597 | rVB | 214 | 164 | 0.04% | 0.007% |
| 66 | 10.860 | 1602 | 1603 | 1605 | rBV | 189 | 139 | 0.03% | 0.006% |
| 67 | 10.921 | 1611 | 1613 | 1615 | rVB | 277 | 153 | 0.04% | 0.006% |
| 68 | 11.110 | 1639 | 1644 | 1646 | rBV2 | 223 | 304 | 0.07% | 0.013% |
| 69 | 11.195 | 1652 | 1658 | 1667 | rBV | 77343 | 103115 | 24.98% | 4.259% |
| 70 | 11.354 | 1682 | 1684 | 1685 | rBV | 167 | 142 | 0.03% | 0.006% |
| 71 | 11.494 | 1705 | 1707 | 1710 | rBV2 | 200 | 315 | 0.08% | 0.013% |
| 72 | 11.585 | 1719 | 1722 | 1723 | rBV | 280 | 279 | 0.07% | 0.012% |
| 73 | 11.713 | 1742 | 1743 | 1747 | rVB | 265 | 226 | 0.05% | 0.009% |
| 74 | 11.756 | 1747 | 1750 | 1753 | rBV | 276 | 348 | 0.08% | 0.014% |
| 75 | 11.799 | 1754 | 1757 | 1759 | rBV | 671 | 646 | 0.16% | 0.027% |
| 76 | 12.024 | 1788 | 1794 | 1806 | rBV | 274631 | 355564 | 86.15% | 14.687% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
Acq On : 27 Jul 2024 03:45
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

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\SFAMXLM072624WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 12.219 | 1824 | 1826 | 1828 | rBV | 321 | 333 | 0.08% | 0.014% |
| 78 | 12.323 | 1837 | 1843 | 1854 | rBV | 103928 | 141461 | 34.27% | 5.843% |
| 79 | 12.628 | 1890 | 1893 | 1895 | rBV | 149 | 176 | 0.04% | 0.007% |
| 80 | 12.658 | 1896 | 1898 | 1900 | rVB | 262 | 185 | 0.04% | 0.008% |
| 81 | 13.110 | 1970 | 1972 | 1974 | rBV | 344 | 311 | 0.08% | 0.013% |
| 82 | 13.201 | 1985 | 1987 | 1990 | rBV3 | 430 | 469 | 0.11% | 0.019% |
| 83 | 13.414 | 2020 | 2022 | 2025 | rBV2 | 288 | 367 | 0.09% | 0.015% |
| 84 | 13.591 | 2049 | 2051 | 2052 | rBV2 | 169 | 154 | 0.04% | 0.006% |
| 85 | 13.719 | 2070 | 2072 | 2075 | rVB2 | 356 | 297 | 0.07% | 0.012% |
| 86 | 13.780 | 2079 | 2082 | 2083 | rBV2 | 506 | 440 | 0.11% | 0.018% |
| 87 | 13.884 | 2096 | 2099 | 2102 | rBV | 264 | 336 | 0.08% | 0.014% |
| 88 | 14.000 | 2117 | 2118 | 2120 | rBV | 129 | 137 | 0.03% | 0.006% |
| 89 | 14.323 | 2168 | 2171 | 2172 | rBV2 | 229 | 199 | 0.05% | 0.008% |
| 90 | 14.432 | 2186 | 2189 | 2192 | rBV3 | 667 | 841 | 0.20% | 0.035% |
| 91 | 14.530 | 2203 | 2205 | 2208 | rBV | 377 | 366 | 0.09% | 0.015% |
| 92 | 14.713 | 2234 | 2235 | 2238 | rBV | 269 | 256 | 0.06% | 0.011% |
| 93 | 14.823 | 2251 | 2253 | 2254 | rBV | 298 | 273 | 0.07% | 0.011% |
| 94 | 15.231 | 2315 | 2320 | 2327 | rVB2 | 36989 | 52949 | 12.83% | 2.187% |
| 95 | 15.347 | 2337 | 2339 | 2342 | rVB | 468 | 378 | 0.09% | 0.016% |
| 96 | 15.554 | 2372 | 2373 | 2378 | rBV3 | 434 | 617 | 0.15% | 0.025% |
| 97 | 15.731 | 2397 | 2402 | 2410 | rVB2 | 16168 | 24248 | 5.87% | 1.002% |
| 98 | 15.853 | 2421 | 2422 | 2424 | rBV | 400 | 357 | 0.09% | 0.015% |
| 99 | 15.963 | 2437 | 2440 | 2445 | rVB5 | 1743 | 2784 | 0.67% | 0.115% |
| 100 | 16.091 | 2456 | 2461 | 2466 | rBV2 | 29043 | 43797 | 10.61% | 1.809% |

Sum of corrected areas: 2420941

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
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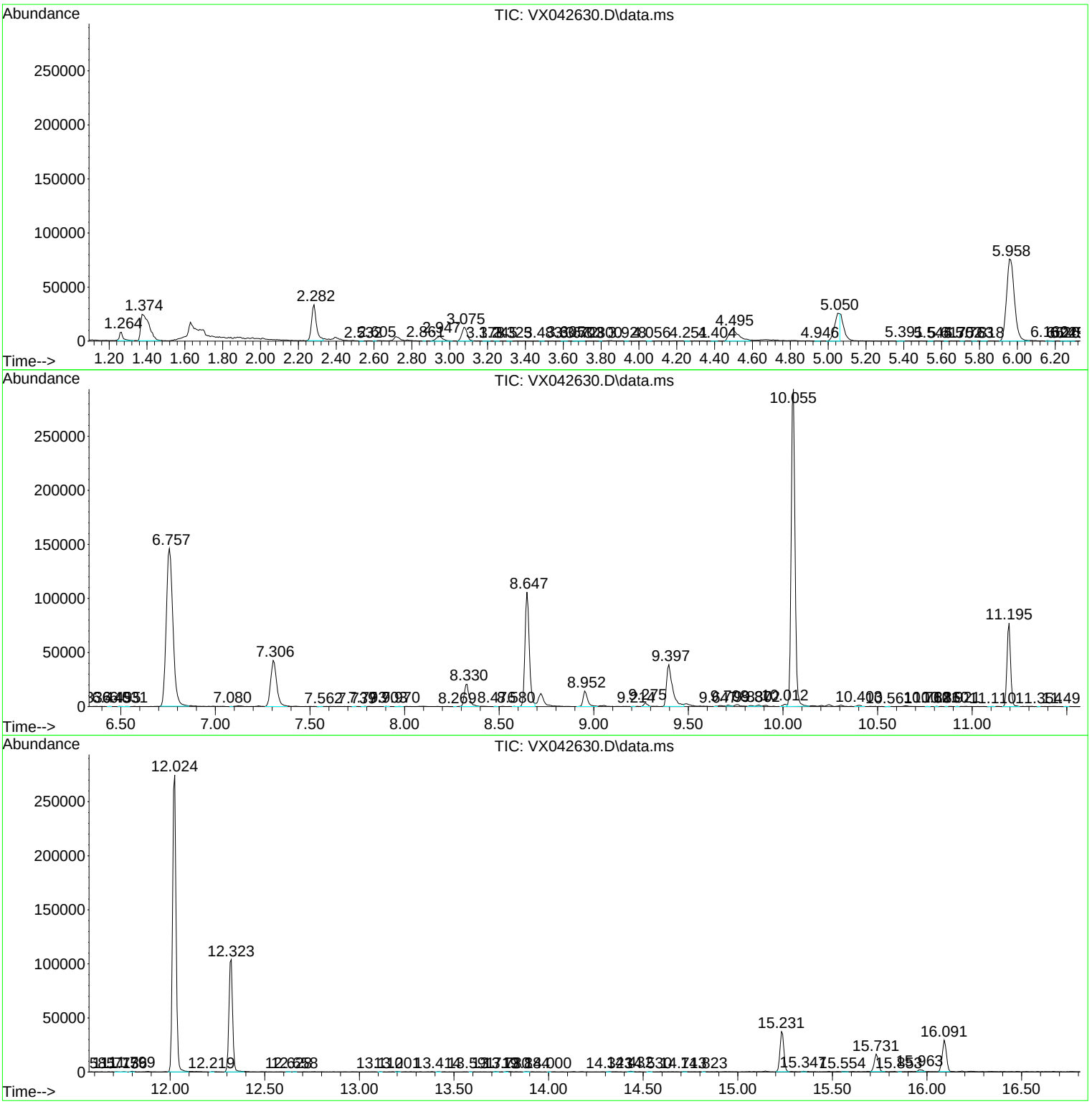
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
Acq On : 27 Jul 2024 03:45
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Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

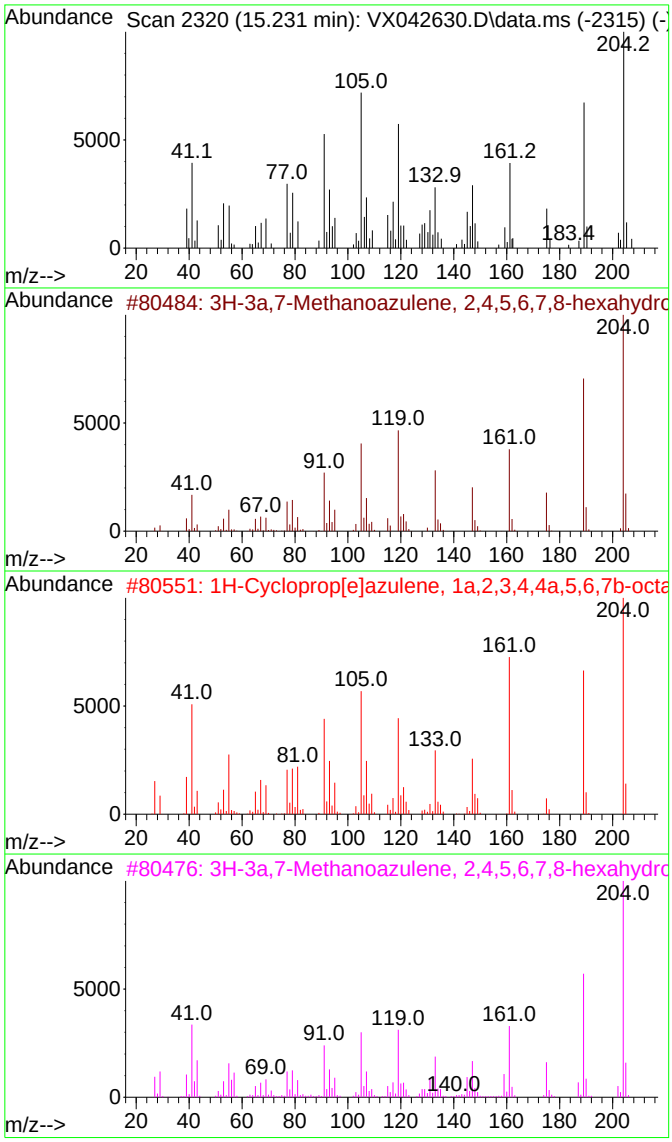
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

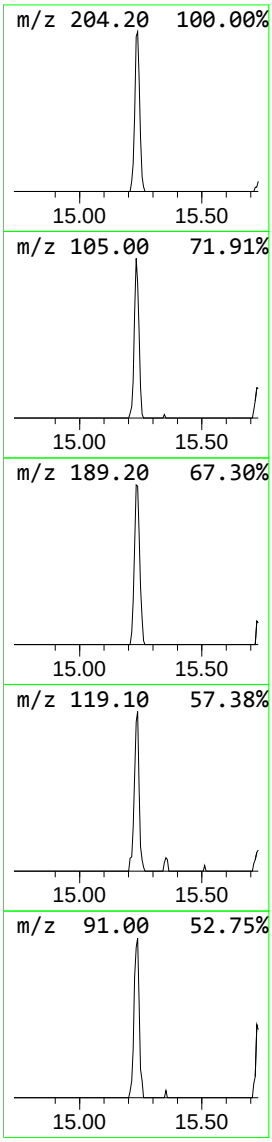
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 3H-3a,7-Methanoazulene, 2,4... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.231 | 7.45 ug/L | 52949 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3H-3a,7-Methanoazulene, 2,4,5,6,... | 204 | C15H24 | 002387-78-2 | 95 |
| 2 | 1H-Cycloprop[e]azulene, 1a,2,3,4... | 204 | C15H24 | 000489-40-7 | 93 |
| 3 | 3H-3a,7-Methanoazulene, 2,4,5,6,... | 204 | C15H24 | 002387-78-2 | 93 |
| 4 | 1,2,4,8-Tetramethylbicyclo[6.3.0... | 204 | C15H24 | 137235-51-9 | 90 |
| 5 | (4aS,9aR)-3,5,5,9-Tetramethyl-2,... | 204 | C15H24 | 053111-25-4 | 90 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
Acq On : 27 Jul 2024 03:45
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

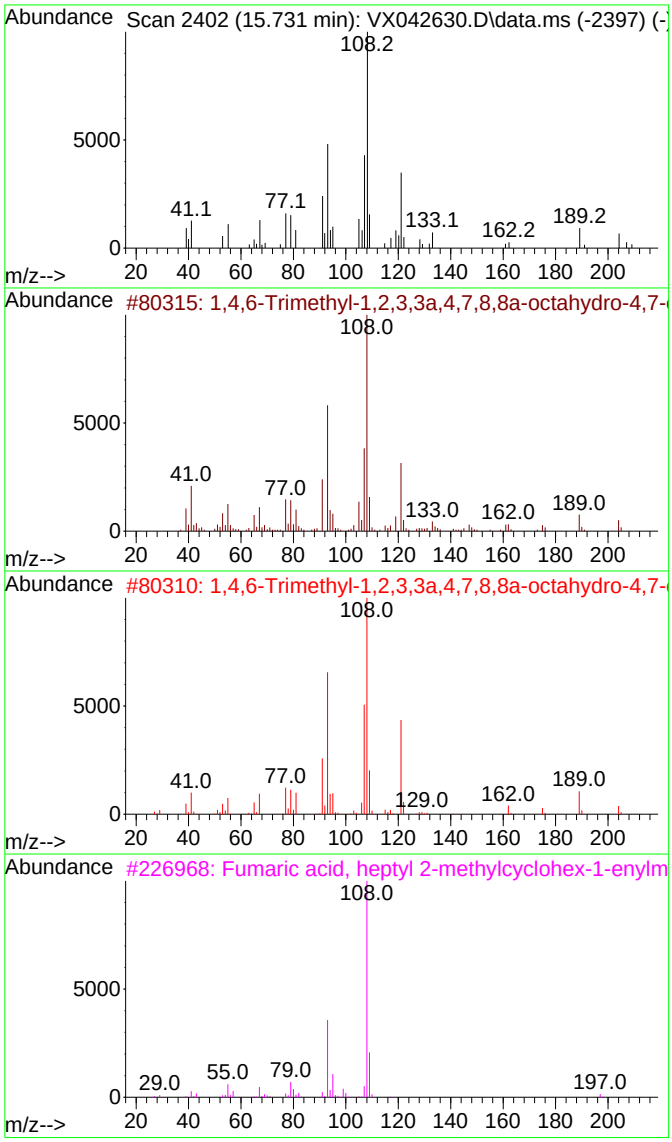
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

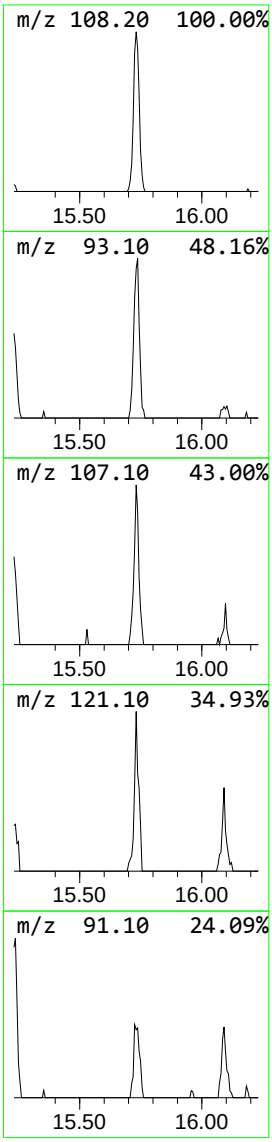
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 1,4,6-Trimethyl-1,2,3,3a,4,... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.731 | 3.41 ug/L | 24248 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4,6-Trimethyl-1,2,3,3a,4,7,8,8... | 204 | C15H24 | 065128-08-7 | 98 |
| 2 | 1,4,6-Trimethyl-1,2,3,3a,4,7,8,8... | 204 | C15H24 | 065128-08-7 | 91 |
| 3 | Fumaric acid, heptyl 2-methylcyc... | 322 | C19H30O4 | 1000345-15-9 | 53 |
| 4 | Fumaric acid, di(2-methylcyclohe... | 332 | C20H28O4 | 1000345-16-5 | 53 |
| 5 | Mephenesin | 182 | C10H14O3 | 000059-47-2 | 50 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
Acq On : 27 Jul 2024 03:45
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

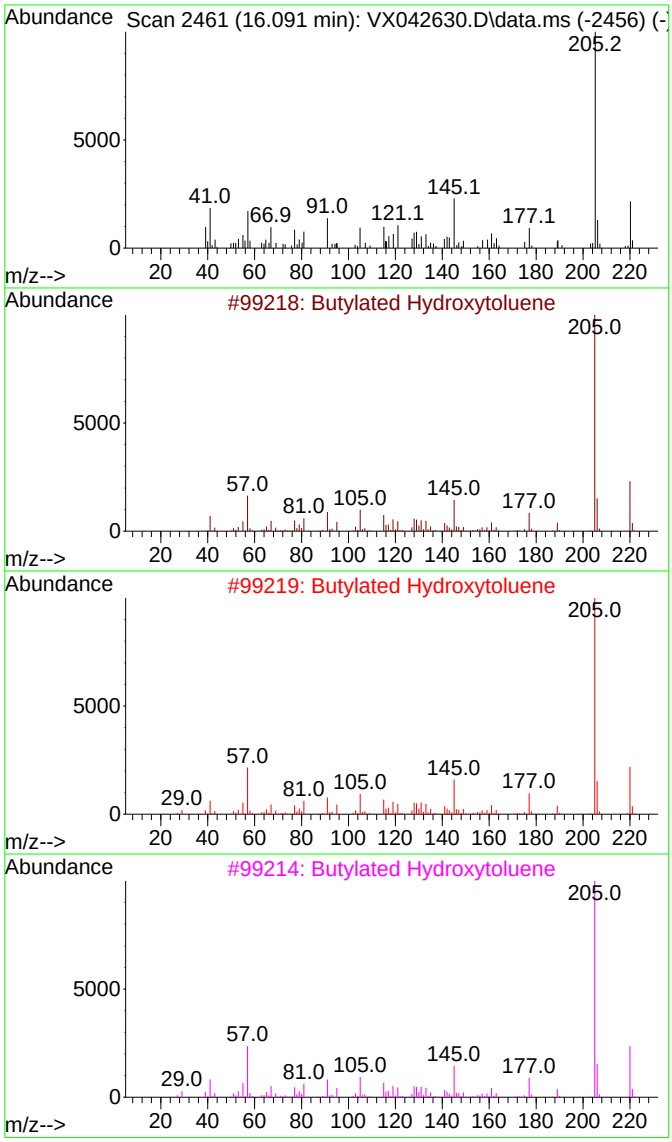
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

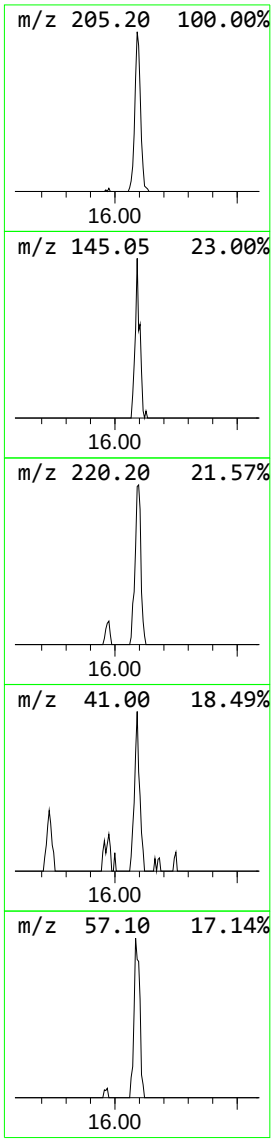
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Butylated Hydroxytoluene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.091 | 6.16 ug/L | 43797 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 98 |
| 2 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 97 |
| 3 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 95 |
| 4 | Phenol, 2,6-bis(1,1-dimethylethy... | 277 | C17H27NO2 | 001918-11-2 | 91 |
| 5 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042630.D
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Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 40 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
BHB19ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.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 |
| 3H-3a,7-Methano... | 15.231 | 7.5 | ug/L | 52949 | 3 | 12.024 | 355564 | 50.0 |
| 1,4,6-Trimethyl... | 15.731 | 3.4 | ug/L | 24248 | 3 | 12.024 | 355564 | 50.0 |
| Butylated Hydro... | 16.091 | 6.2 | ug/L | 43797 | 3 | 12.024 | 355564 | 50.0 |