LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\82X012220W.M
Title : SW846 8260

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.856 | 318 | 323 | 335 | rVB | 812179 | 1661690 | 25.22% | 0.779% |
| 2 | 3.143 | 360 | 370 | 381 | rBV | 742216 | 1686170 | 25.59% | 0.790% |
| 3 | 3.496 | 419 | 428 | 441 | rBV | 535340 | 1209668 | 18.36% | 0.567% |
| 4 | 4.283 | 544 | 557 | 565 | rBV | 321438 | 979946 | 14.87% | 0.459% |
| 5 | 4.374 | 565 | 572 | 584 | rVB | 318170 | 918737 | 13.94% | 0.431% |
| 6 | 5.490 | 738 | 755 | 761 | rBV2 | 241469 | 875496 | 13.29% | 0.410% |
| 7 | 5.594 | 761 | 772 | 779 | rBV | 1354738 | 4160985 | 63.14% | 1.950% |
| 8 | 5.703 | 785 | 790 | 811 | rVB | 963147 | 3144831 | 47.72% | 1.474% |
| 9 | 5.911 | 811 | 824 | 839 | rBV2 | 1966085 | 5724292 | 86.87% | 2.682% |
| 10 | 6.246 | 862 | 879 | 887 | rBV2 | 625479 | 2287924 | 34.72% | 1.072% |
| 11 | 6.337 | 887 | 894 | 903 | rVB2 | 798227 | 2265770 | 34.38% | 1.062% |
| 12 | 6.441 | 903 | 911 | 923 | rVB2 | 639137 | 1806442 | 27.41% | 0.846% |
| 13 | 6.691 | 938 | 952 | 965 | rVB | 1375536 | 3318430 | 50.36% | 1.555% |
| 14 | 6.855 | 969 | 979 | 984 | rBV | 565055 | 1643670 | 24.94% | 0.770% |
| 15 | 6.923 | 984 | 990 | 1002 | rVB2 | 649070 | 1920451 | 29.14% | 0.900% |
| 16 | 7.246 | 1034 | 1043 | 1049 | rBV | 457268 | 1017648 | 15.44% | 0.477% |
| 17 | 7.447 | 1065 | 1076 | 1088 | rVB2 | 2474950 | 6162032 | 93.51% | 2.887% |
| 18 | 7.569 | 1088 | 1096 | 1100 | rBV2 | 698632 | 1416943 | 21.50% | 0.664% |
| 19 | 7.630 | 1100 | 1106 | 1115 | rVB | 858302 | 1735109 | 26.33% | 0.813% |
| 20 | 7.727 | 1115 | 1122 | 1133 | rVB | 489512 | 1036819 | 15.73% | 0.486% |
| 21 | 7.837 | 1133 | 1140 | 1148 | rVB2 | 741726 | 1555603 | 23.61% | 0.729% |
| 22 | 8.044 | 1165 | 1174 | 1186 | rVB3 | 572122 | 2125137 | 32.25% | 0.996% |
| 23 | 8.166 | 1186 | 1194 | 1198 | rBV2 | 801575 | 1753235 | 26.61% | 0.822% |
| 24 | 8.245 | 1203 | 1207 | 1212 | rVB2 | 646035 | 963762 | 14.63% | 0.452% |
| 25 | 8.337 | 1216 | 1222 | 1225 | rBV | 2665757 | 4512948 | 68.49% | 2.115% |
| 26 | 8.373 | 1225 | 1228 | 1234 | rVB2 | 1773137 | 2746541 | 41.68% | 1.287% |
| 27 | 8.495 | 1243 | 1248 | 1257 | rBV | 3008996 | 5484379 | 83.23% | 2.570% |
| 28 | 8.569 | 1257 | 1260 | 1269 | rVB4 | 461397 | 990471 | 15.03% | 0.464% |
| 29 | 8.660 | 1269 | 1275 | 1279 | rBV3 | 2091716 | 4321955 | 65.59% | 2.025% |
| 30 | 8.703 | 1279 | 1282 | 1292 | rVB2 | 1540744 | 3152582 | 47.84% | 1.477% |
| 31 | 8.831 | 1292 | 1303 | 1307 | rBV | 968593 | 2051157 | 31.13% | 0.961% |
| 32 | 8.873 | 1307 | 1310 | 1313 | rBV | 481194 | 715337 | 10.86% | 0.335% |
| 33 | 8.965 | 1320 | 1325 | 1332 | rBV2 | 2214787 | 3915179 | 59.41% | 1.835% |
| 34 | 9.032 | 1332 | 1336 | 1342 | rVV3 | 1082370 | 2022793 | 30.70% | 0.948% |

LSC Area Percent Report

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Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\82X012220W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.160 | 1348 | 1357 | 1362 | rBV3 | 1022008 | 2048013 | 31.08% | 0.960% |
| 36 | 9.215 | 1362 | 1366 | 1370 | rVV2 | 1046900 | 1600765 | 24.29% | 0.750% |
| 37 | 9.343 | 1382 | 1387 | 1391 | rBV | 526620 | 715548 | 10.86% | 0.335% |
| 38 | 9.440 | 1397 | 1403 | 1407 | rBV | 1499769 | 2291105 | 34.77% | 1.074% |
| 39 | 9.550 | 1417 | 1421 | 1428 | rVV2 | 1799311 | 3621460 | 54.96% | 1.697% |
| 40 | 9.617 | 1428 | 1432 | 1436 | rVB | 1269326 | 1680382 | 25.50% | 0.787% |
| 41 | 9.672 | 1436 | 1441 | 1445 | rBV2 | 1023806 | 1917131 | 29.09% | 0.898% |
| 42 | 9.715 | 1445 | 1448 | 1457 | rVB7 | 583225 | 1439715 | 21.85% | 0.675% |
| 43 | 9.812 | 1457 | 1464 | 1470 | rBV3 | 862080 | 1795517 | 27.25% | 0.841% |
| 44 | 9.873 | 1470 | 1474 | 1479 | rBV2 | 906652 | 1994428 | 30.27% | 0.935% |
| 45 | 9.916 | 1479 | 1481 | 1483 | rVV3 | 623339 | 774453 | 11.75% | 0.363% |
| 46 | 9.952 | 1483 | 1487 | 1493 | rVB | 3669663 | 5467840 | 82.98% | 2.562% |
| 47 | 10.062 | 1497 | 1505 | 1509 | rVB | 3445315 | 4795919 | 72.78% | 2.247% |
| 48 | 10.111 | 1509 | 1513 | 1517 | rBV | 1420494 | 1904412 | 28.90% | 0.892% |
| 49 | 10.245 | 1530 | 1535 | 1540 | rVB4 | 403664 | 811056 | 12.31% | 0.380% |
| 50 | 10.324 | 1540 | 1548 | 1552 | rBV5 | 716598 | 1864997 | 28.30% | 0.874% |
| 51 | 10.367 | 1552 | 1555 | 1558 | rVB2 | 593116 | 793867 | 12.05% | 0.372% |
| 52 | 10.410 | 1558 | 1562 | 1573 | rVB6 | 968591 | 2443417 | 37.08% | 1.145% |
| 53 | 10.635 | 1594 | 1599 | 1603 | rBV2 | 1300864 | 1791404 | 27.19% | 0.839% |
| 54 | 10.721 | 1608 | 1613 | 1618 | rBV2 | 854921 | 1500902 | 22.78% | 0.703% |
| 55 | 10.830 | 1623 | 1631 | 1635 | rBV2 | 1781581 | 3094669 | 46.96% | 1.450% |
| 56 | 10.910 | 1639 | 1644 | 1647 | rVV3 | 1114989 | 1633630 | 24.79% | 0.765% |
| 57 | 11.013 | 1655 | 1661 | 1665 | rBV2 | 693192 | 1223719 | 18.57% | 0.573% |
| 58 | 11.080 | 1668 | 1672 | 1675 | rBV | 597603 | 749736 | 11.38% | 0.351% |
| 59 | 11.135 | 1675 | 1681 | 1683 | rVV2 | 2300807 | 3491373 | 52.98% | 1.636% |
| 60 | 11.160 | 1683 | 1685 | 1692 | rVB2 | 1675673 | 2318152 | 35.18% | 1.086% |
| 61 | 11.239 | 1692 | 1698 | 1701 | rBV | 1503732 | 1880222 | 28.53% | 0.881% |
| 62 | 11.355 | 1713 | 1717 | 1728 | rVB | 2427443 | 3127287 | 47.46% | 1.465% |
| 63 | 11.531 | 1742 | 1746 | 1751 | rVB3 | 579493 | 986356 | 14.97% | 0.462% |
| 64 | 11.678 | 1763 | 1770 | 1775 | rBV5 | 589478 | 1194967 | 18.13% | 0.560% |
| 65 | 11.763 | 1781 | 1784 | 1787 | rVB | 769290 | 792746 | 12.03% | 0.371% |
| 66 | 11.940 | 1811 | 1813 | 1817 | rVB | 731487 | 790044 | 11.99% | 0.370% |
| 67 | 11.989 | 1817 | 1821 | 1824 | rBV4 | 567701 | 937087 | 14.22% | 0.439% |
| 68 | 12.074 | 1829 | 1835 | 1840 | rBV2 | 1621504 | 2725617 | 41.36% | 1.277% |
| 69 | 12.141 | 1840 | 1846 | 1850 | rBV3 | 1573621 | 2864345 | 43.47% | 1.342% |
| 70 | 12.220 | 1857 | 1859 | 1867 | rVB2 | 856757 | 1107376 | 16.80% | 0.519% |
| 71 | 12.300 | 1867 | 1872 | 1877 | rBV | 2467180 | 3367098 | 51.10% | 1.578% |

LSC Area Percent Report

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Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\82X012220W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 12.361 | 1877 | 1882 | 1884 | rBV | 1496799 | 1972466 | 29.93% | 0.924% |
| 73 | 12.470 | 1890 | 1900 | 1904 | rBV3 | 558645 | 1412138 | 21.43% | 0.662% |
| 74 | 12.513 | 1904 | 1907 | 1915 | rVB | 1575569 | 2093719 | 31.77% | 0.981% |
| 75 | 12.665 | 1928 | 1932 | 1935 | rVV | 5570544 | 6589626 | 100.00% | 3.088% |
| 76 | 12.696 | 1935 | 1937 | 1941 | rVV | 838263 | 932881 | 14.16% | 0.437% |
| 77 | 12.751 | 1941 | 1946 | 1954 | rVB3 | 2249030 | 3958262 | 60.07% | 1.855% |
| 78 | 12.897 | 1967 | 1970 | 1974 | rVB2 | 825284 | 950186 | 14.42% | 0.445% |
| 79 | 12.970 | 1978 | 1982 | 1987 | rVV | 3206016 | 4357694 | 66.13% | 2.042% |
| 80 | 13.013 | 1987 | 1989 | 1995 | rVB2 | 789014 | 1195258 | 18.14% | 0.560% |
| 81 | 13.074 | 1995 | 1999 | 2008 | rVB4 | 1144115 | 2082974 | 31.61% | 0.976% |
| 82 | 13.220 | 2020 | 2023 | 2027 | rVV | 2143613 | 2359090 | 35.80% | 1.105% |
| 83 | 13.263 | 2027 | 2030 | 2034 | rVB2 | 563655 | 710721 | 10.79% | 0.333% |
| 84 | 13.312 | 2034 | 2038 | 2040 | rBV2 | 895159 | 1262246 | 19.16% | 0.591% |
| 85 | 13.342 | 2040 | 2043 | 2049 | rVV3 | 3593655 | 5178736 | 78.59% | 2.427% |
| 86 | 13.421 | 2053 | 2056 | 2061 | rVB | 1249620 | 1522494 | 23.10% | 0.713% |
| 87 | 13.476 | 2061 | 2065 | 2073 | rVB3 | 731022 | 1453856 | 22.06% | 0.681% |
| 88 | 13.556 | 2073 | 2078 | 2081 | rBV2 | 1119411 | 1533191 | 23.27% | 0.718% |
| 89 | 13.598 | 2081 | 2085 | 2088 | rBV | 1701613 | 2214424 | 33.60% | 1.038% |
| 90 | 13.635 | 2088 | 2091 | 2096 | rVB3 | 1896121 | 2632971 | 39.96% | 1.234% |
| 91 | 13.720 | 2101 | 2105 | 2110 | rVB2 | 1729807 | 2788949 | 42.32% | 1.307% |
| 92 | 13.976 | 2140 | 2147 | 2152 | rBV2 | 1147332 | 1901600 | 28.86% | 0.891% |
| 93 | 14.025 | 2152 | 2155 | 2158 | rVV | 637362 | 839134 | 12.73% | 0.393% |
| 94 | 14.055 | 2158 | 2160 | 2168 | rVB4 | 404973 | 718663 | 10.91% | 0.337% |
| 95 | 14.129 | 2168 | 2172 | 2176 | rBV | 1434284 | 1747950 | 26.53% | 0.819% |
| 96 | 14.269 | 2190 | 2195 | 2204 | rBV | 1307014 | 2212277 | 33.57% | 1.037% |
| 97 | 14.372 | 2209 | 2212 | 2217 | rVV | 519503 | 700947 | 10.64% | 0.328% |
| 98 | 14.427 | 2217 | 2221 | 2225 | rVB | 938463 | 1102673 | 16.73% | 0.517% |
| 99 | 14.689 | 2261 | 2264 | 2268 | rVV | 1031771 | 1282606 | 19.46% | 0.601% |
| 100 | 14.836 | 2283 | 2288 | 2292 | rBV | 697980 | 880551 | 13.36% | 0.413% |

Sum of corrected areas: 213409170

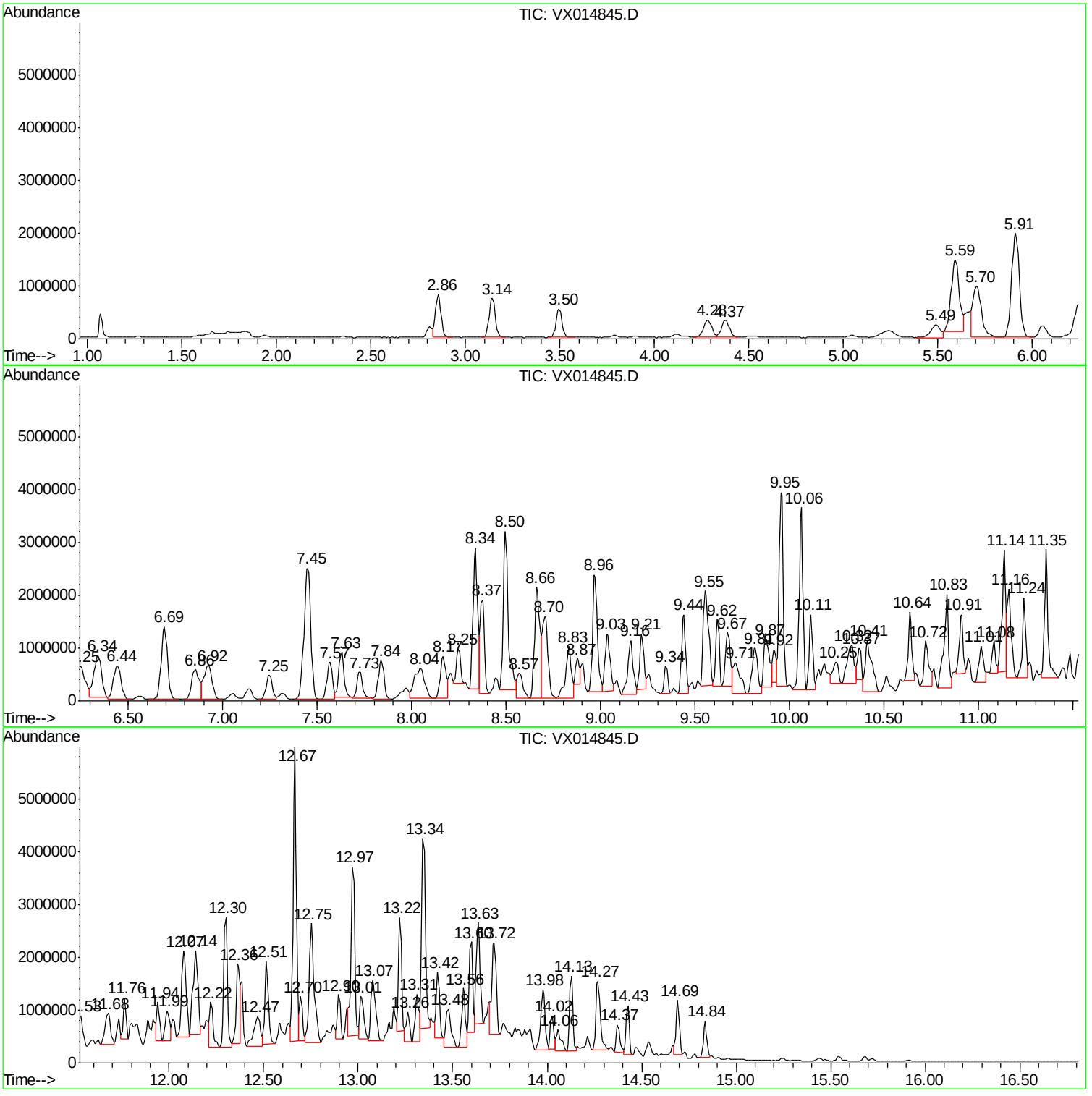
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
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**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

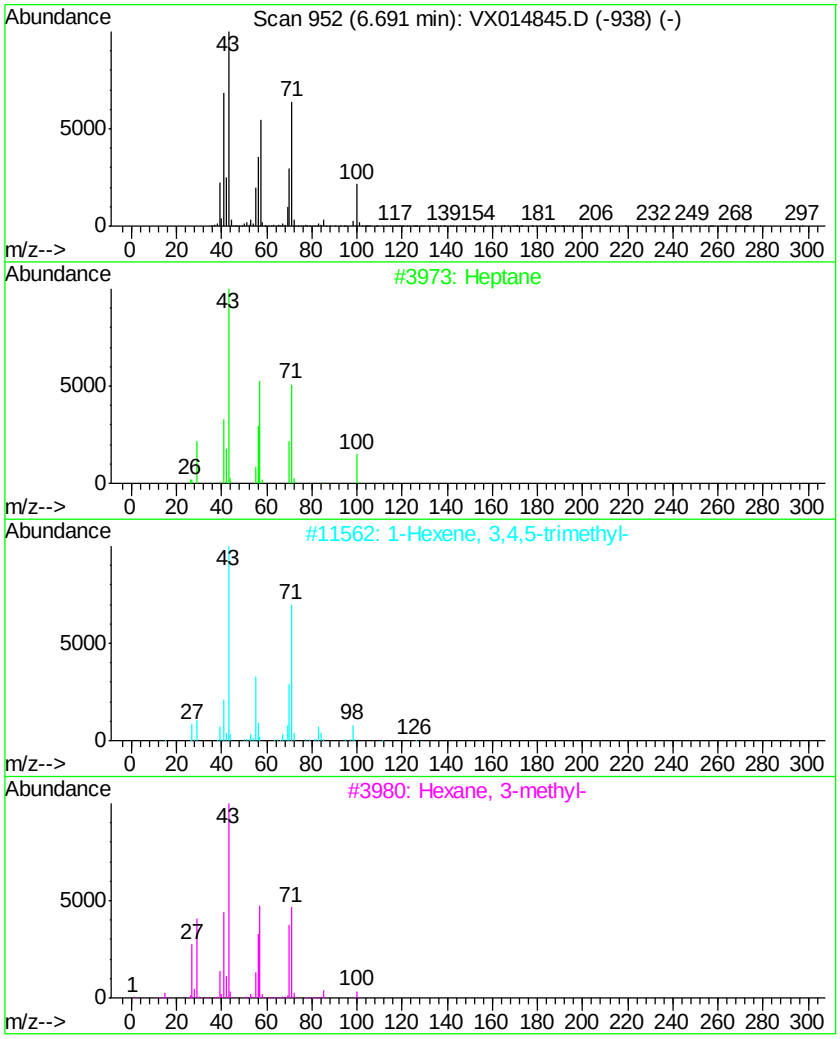
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

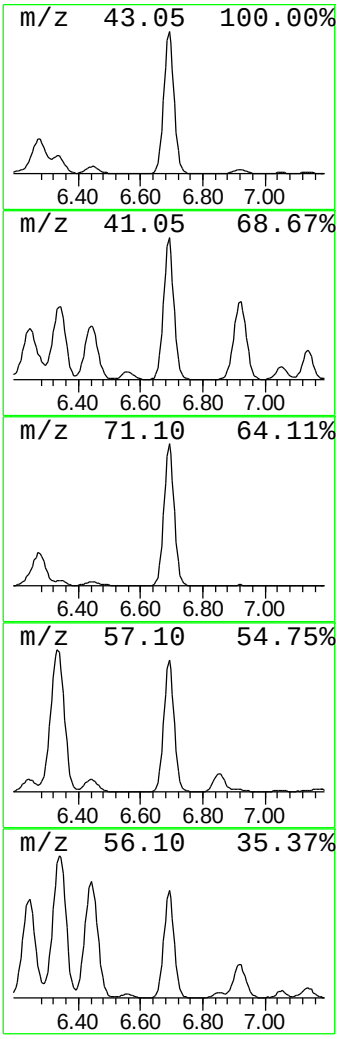
**********

Peak Number 1 Heptane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.69 | 100.95 ug/l | 3318430 | 1,4-Difluorobenzene | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane | 100 | C7H16 | 000142-82-5 | 90 |
| 2 | 1-Hexene, 3,4,5-trimethyl- | 126 | C9H18 | 056728-10-0 | 47 |
| 3 | Hexane, 3-methyl- | 100 | C7H16 | 000589-34-4 | 47 |
| 4 | Ethanedioic acid, bis(3-methylbu... | 230 | C12H22O4 | 002051-00-5 | 47 |
| 5 | Pentane, 1-bromo- | 150 | C5H11Br | 000110-53-2 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
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**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

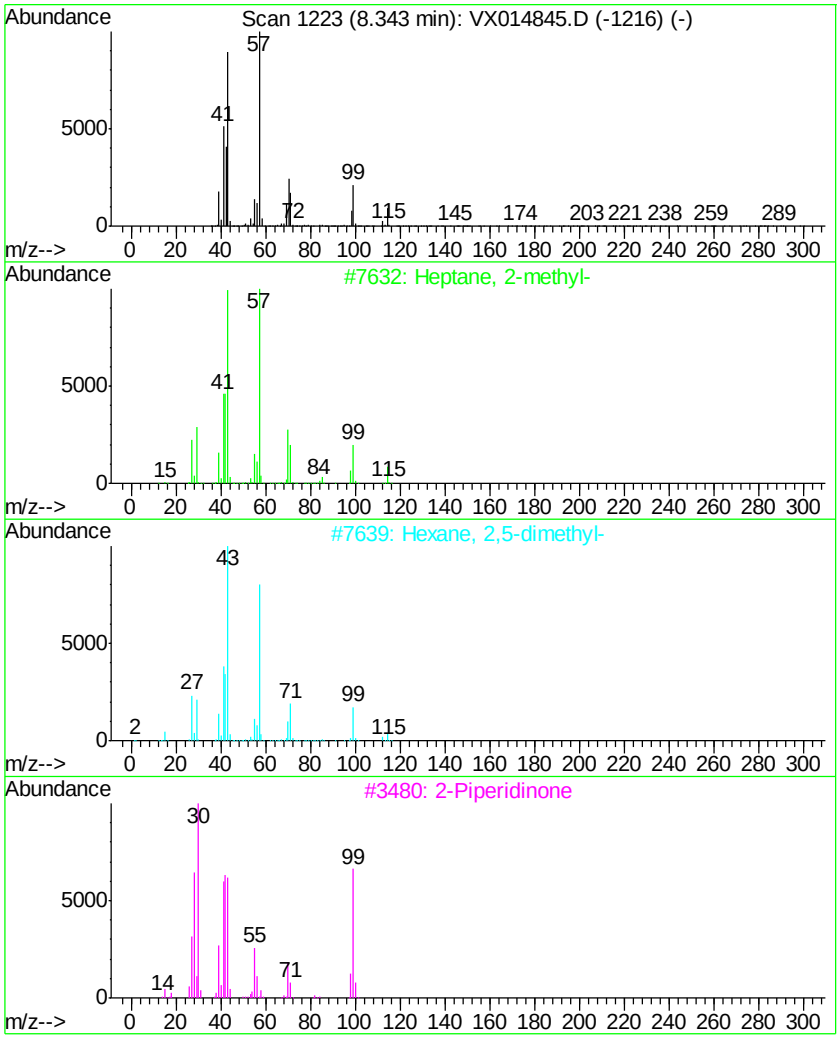
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

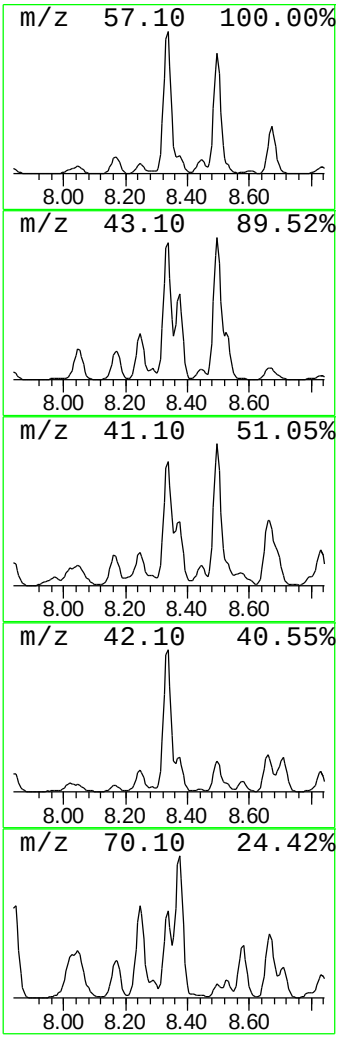
**********

Peak Number 2 Heptane, 2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.34 | 137.28 ug/l | 4512950 | 1,4-Difluorobenzene | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 2-methyl- | 114 | C8H18 | 000592-27-8 | 94 |
| 2 | Hexane, 2,5-dimethyl- | 114 | C8H18 | 000592-13-2 | 58 |
| 3 | 2-Piperidinone | 99 | C5H9NO | 000675-20-7 | 53 |
| 4 | 1-Pyrrolidinecarboxaldehyde | 99 | C5H9NO | 003760-54-1 | 38 |
| 5 | Heptane, 2,5-dimethyl- | 128 | C9H20 | 002216-30-0 | 38 |



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**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

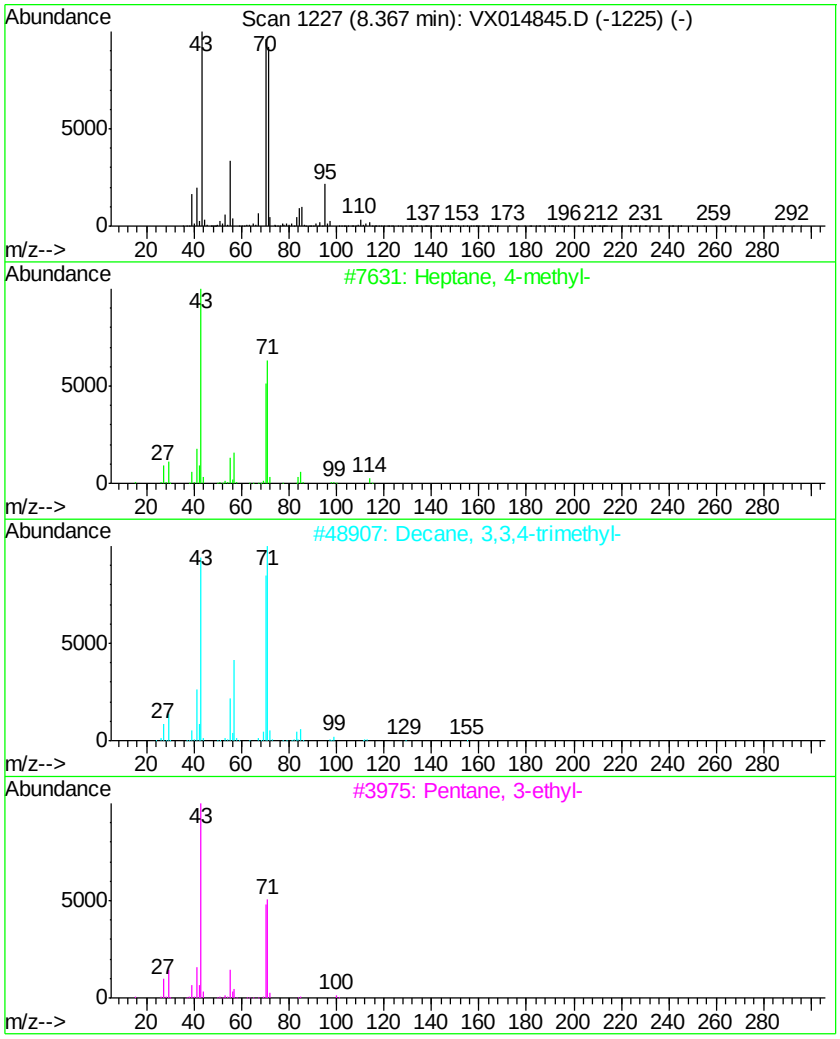
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

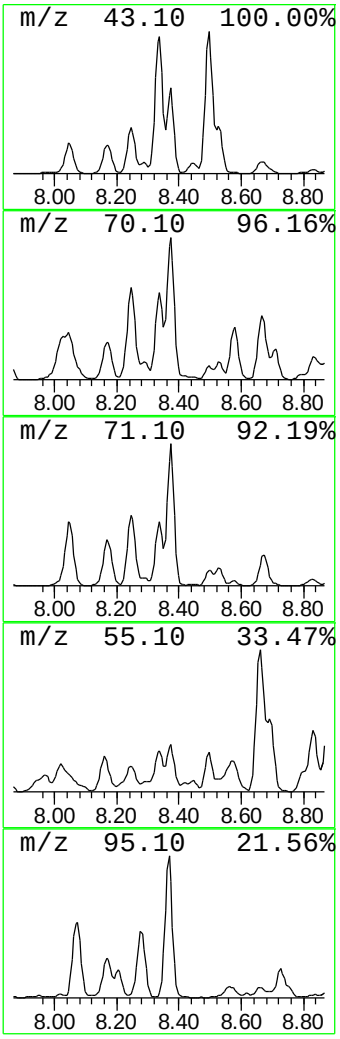
**********

Peak Number 3 Heptane, 4-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.37 | 83.55 ug/l | 2746540 | 1,4-Difluorobenzene | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 4-methyl- | 114 | C8H18 | 000589-53-7 | 78 |
| 2 | Decane, 3,3,4-trimethyl- | 184 | C13H28 | 049622-18-6 | 72 |
| 3 | Pentane, 3-ethyl- | 100 | C7H16 | 000617-78-7 | 64 |
| 4 | Pentane, 2,3,3-trimethyl- | 114 | C8H18 | 000560-21-4 | 59 |
| 5 | Hexane, 2,3-dimethyl- | 114 | C8H18 | 000584-94-1 | 59 |



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Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

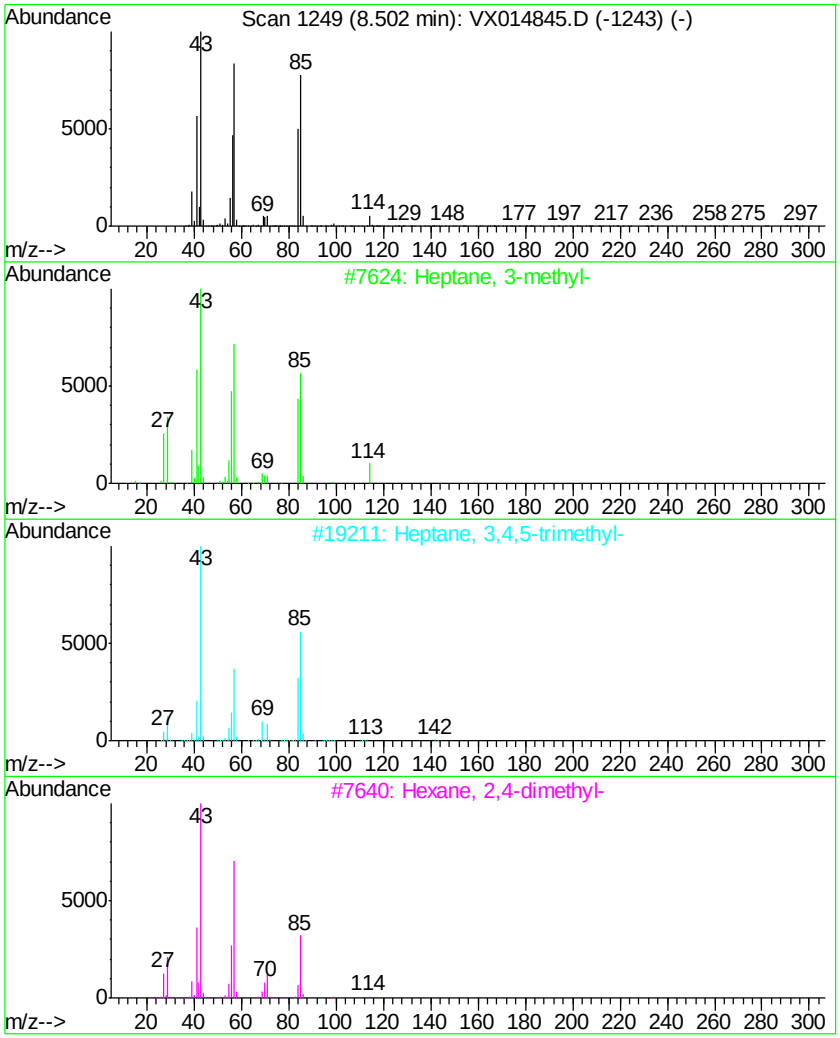
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

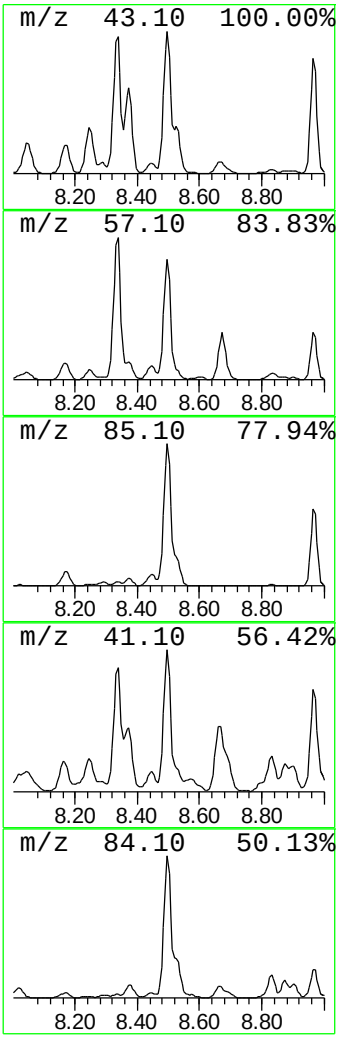
**********

Peak Number 4 Heptane, 3-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.50 | 143.99 ug/l | 5484380 | Chlorobenzene-d5 | 10.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 3-methyl- | 114 | C8H18 | 000589-81-1 | 94 |
| 2 | Heptane, 3,4,5-trimethyl- | 142 | C10H22 | 020278-89-1 | 74 |
| 3 | Hexane, 2,4-dimethyl- | 114 | C8H18 | 000589-43-5 | 72 |
| 4 | Butanoic acid, 2-methyl-, 2-meth... | 186 | C11H22O2 | 083783-88-4 | 64 |
| 5 | Pentane, 3-ethyl-2,4-dimethyl- | 128 | C9H20 | 001068-87-7 | 59 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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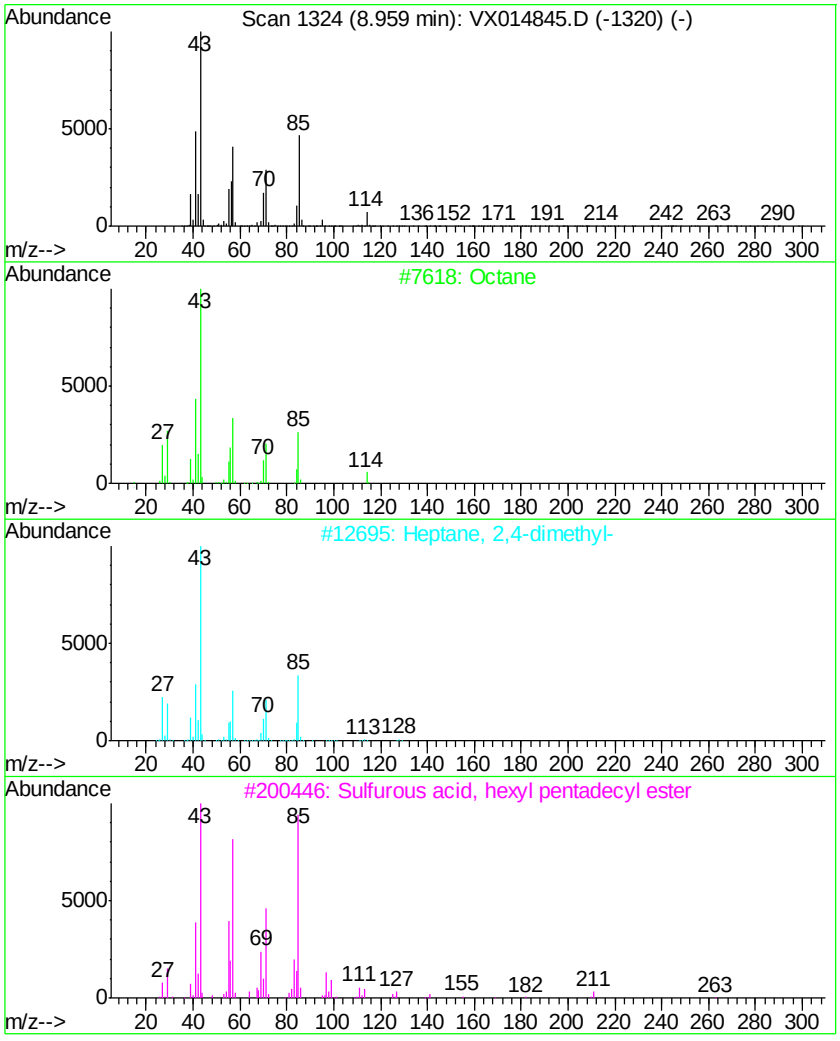
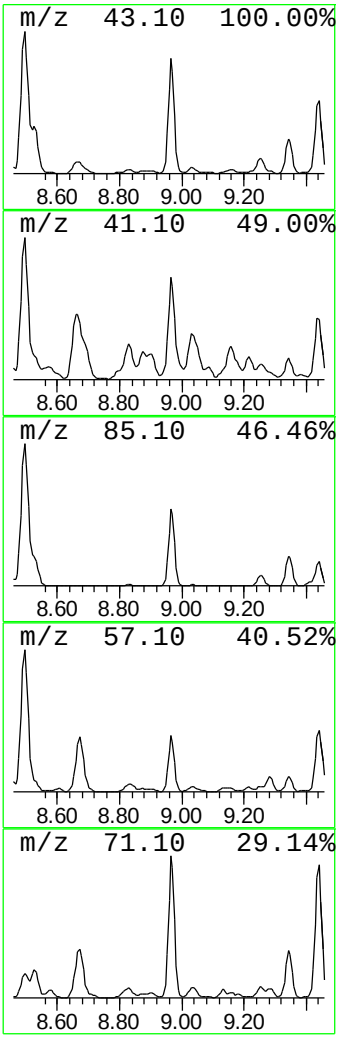
Peak Number 5 Octane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.96 | 102.79 ug/l | 3915180 | Chlorobenzene-d5 | 10.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane | 114 | C8H18 | 000111-65-9 | 93 |
| 2 | Heptane, 2,4-dimethyl- | 128 | C9H20 | 002213-23-2 | 64 |
| 3 | Sulfurous acid, hexyl pentadecyl... | 376 | C21H44O3S | 1000309-13-7 | 53 |
| 4 | Hexane, 2,3,5-trimethyl- | 128 | C9H20 | 001069-53-0 | 53 |
| 5 | Hexane, 2,4-dimethyl- | 114 | C8H18 | 000589-43-5 | 53 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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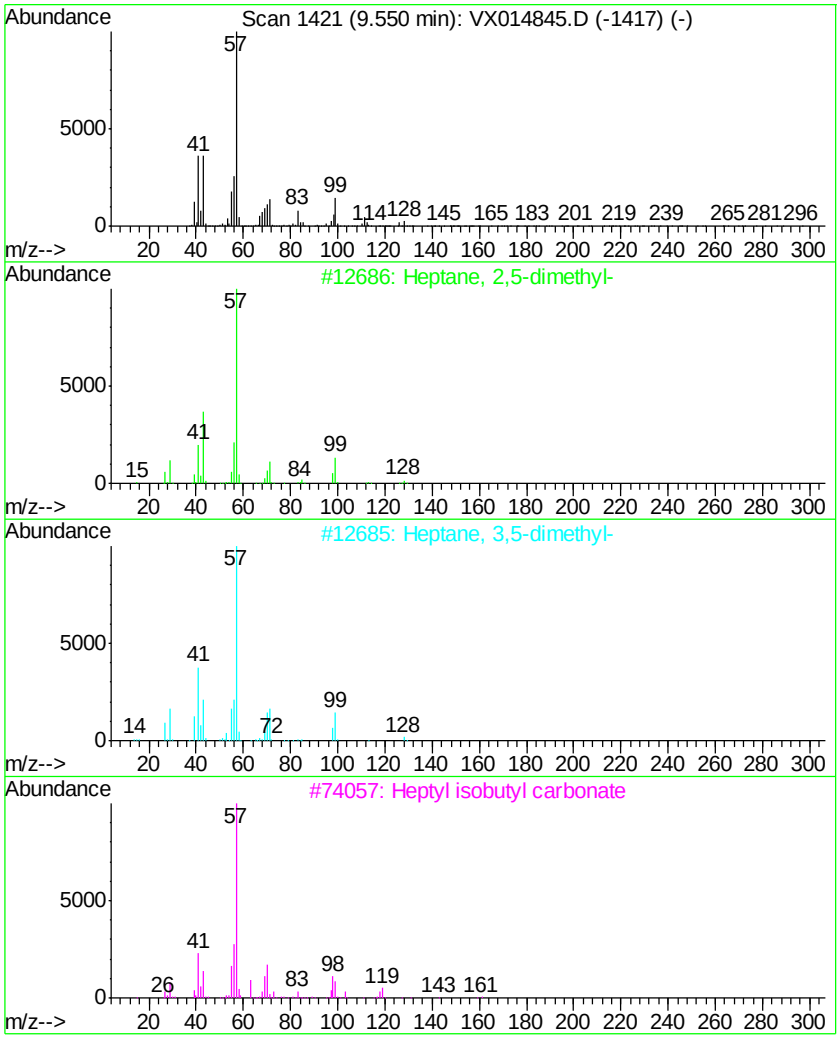
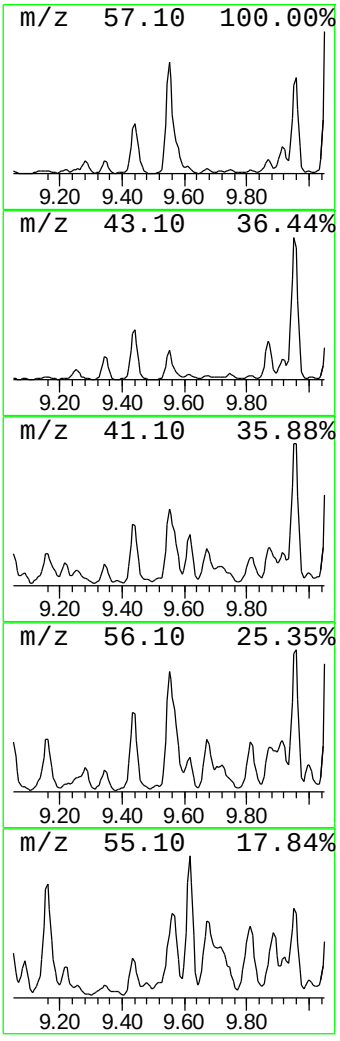
Peak Number 6 Heptane, 2,5-dimethyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.55 | 95.08 ug/l | 3621460 | Chlorobenzene-d5 | 10.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 2,5-dimethyl- | 128 | C9H20 | 002216-30-0 | 87 |
| 2 | Heptane, 3,5-dimethyl- | 128 | C9H20 | 000926-82-9 | 68 |
| 3 | Heptyl isobutyl carbonate | 216 | C12H24O3 | 959068-08-7 | 59 |
| 4 | Octane, 3-methyl- | 128 | C9H20 | 002216-33-3 | 58 |
| 5 | Decane, 2,5-dimethyl- | 170 | C12H26 | 017312-50-4 | 53 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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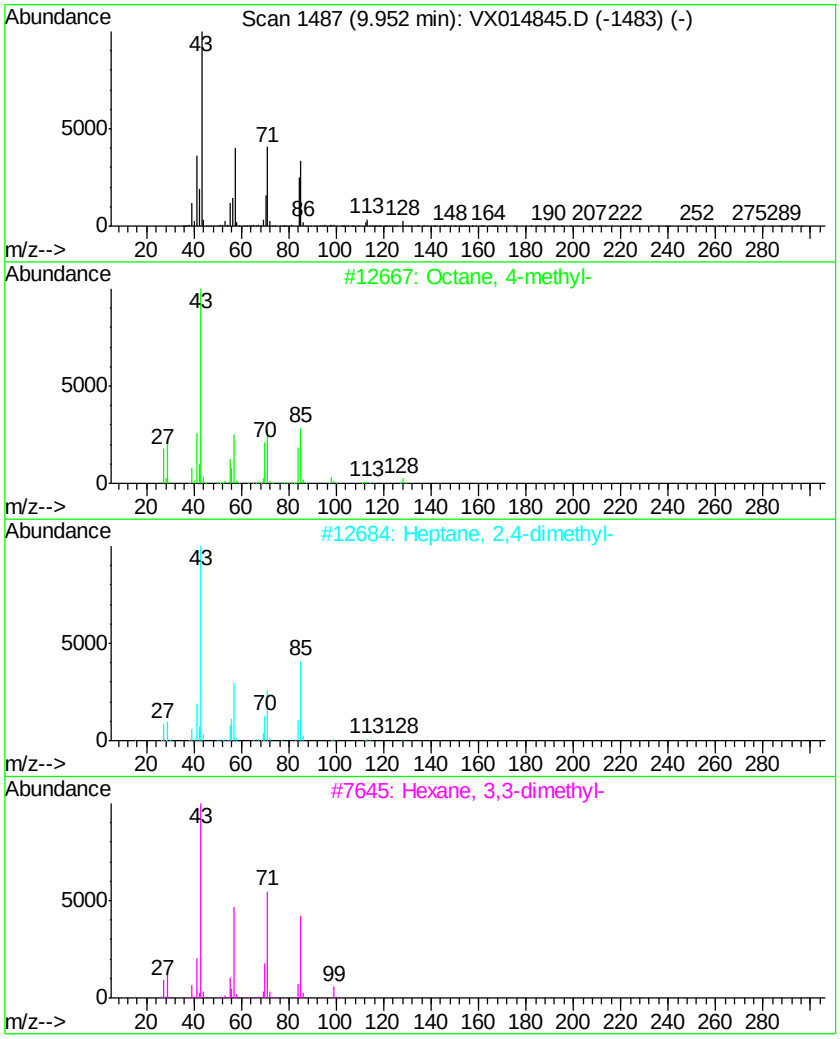
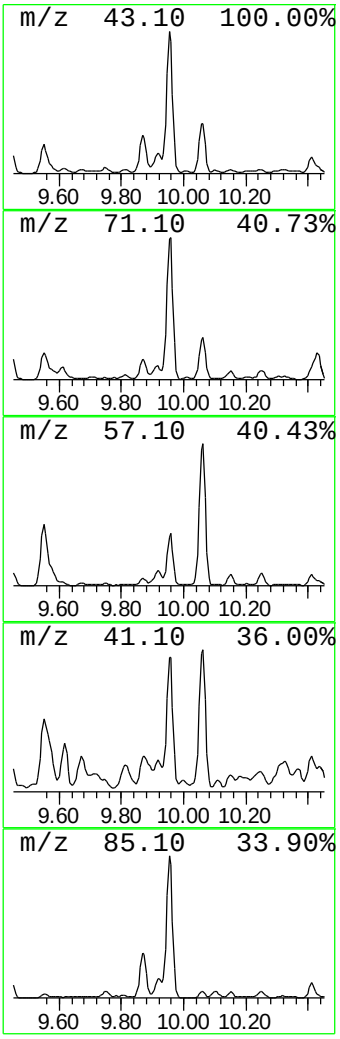
Peak Number 7 Octane, 4-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.95 | 143.56 ug/l | 5467840 | Chlorobenzene-d5 | 10.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane, 4-methyl- | 128 | C9H20 | 002216-34-4 | 80 |
| 2 | Heptane, 2,4-dimethyl- | 128 | C9H20 | 002213-23-2 | 72 |
| 3 | Hexane, 3,3-dimethyl- | 114 | C8H18 | 000563-16-6 | 59 |
| 4 | Hexane, 2,3,5-trimethyl- | 128 | C9H20 | 001069-53-0 | 52 |
| 5 | Heptane, 3,4,5-trimethyl- | 142 | C10H22 | 020278-89-1 | 49 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

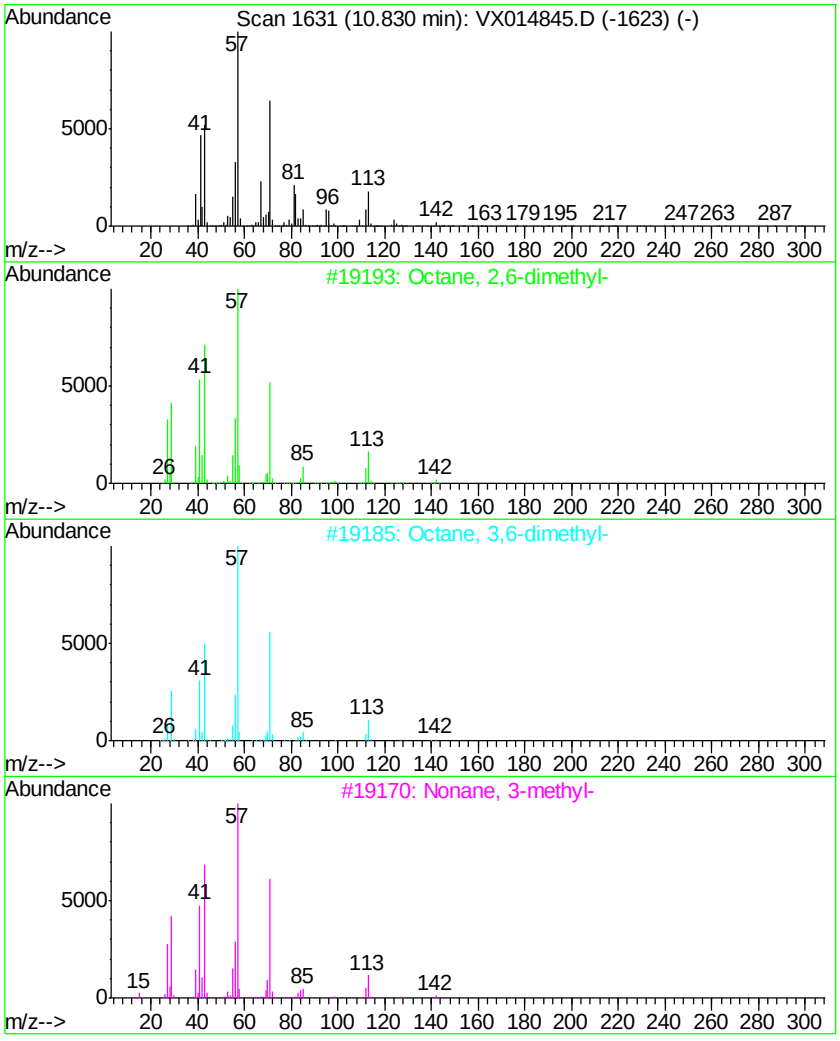
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

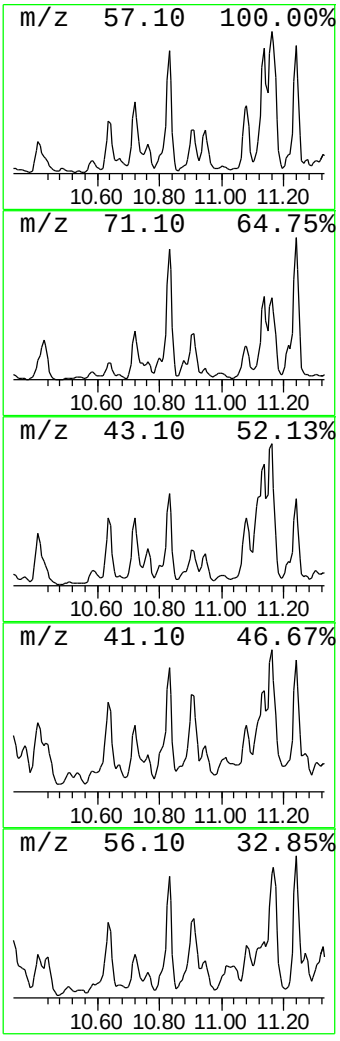
**********

Peak Number 8 Octane, 2,6-dimethyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.83 | 81.25 ug/l | 3094670 | Chlorobenzene-d5 | 10.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane, 2,6-dimethyl- | 142 | C10H22 | 002051-30-1 | 76 |
| 2 | Octane, 3,6-dimethyl- | 142 | C10H22 | 015869-94-0 | 76 |
| 3 | Nonane, 3-methyl- | 142 | C10H22 | 005911-04-6 | 76 |
| 4 | Sulfurous acid, 2-ethylhexyl non... | 320 | C17H36O3S | 1000309-19-2 | 50 |
| 5 | Decane, 3-methyl- | 156 | C11H24 | 013151-34-3 | 47 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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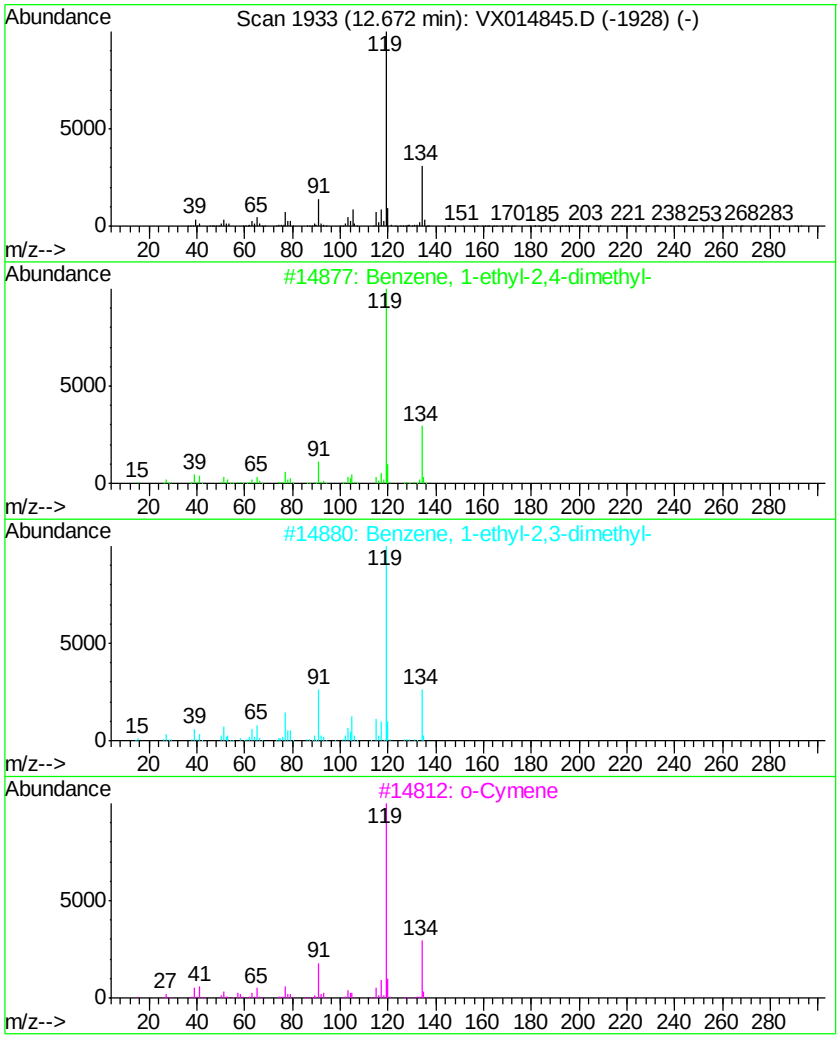
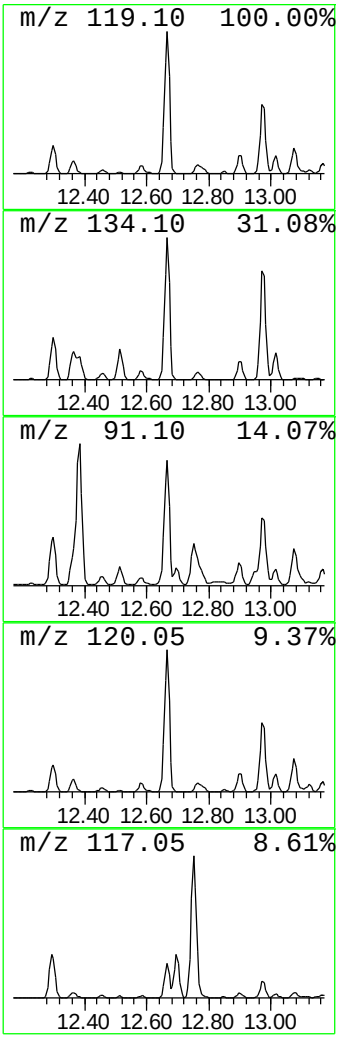
Peak Number 9 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.67 | 120.88 ug/l | 6589630 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-ethyl-2,4-dimethyl- | 134 | C10H14 | 000874-41-9 | 97 |
| 2 | Benzene, 1-ethyl-2,3-dimethyl- | 134 | C10H14 | 000933-98-2 | 96 |
| 3 | o-Cymene | 134 | C10H14 | 000527-84-4 | 95 |
| 4 | Benzene, 2-ethyl-1,3-dimethyl- | 134 | C10H14 | 002870-04-4 | 95 |
| 5 | Benzene, 2-ethyl-1,4-dimethyl- | 134 | C10H14 | 001758-88-9 | 95 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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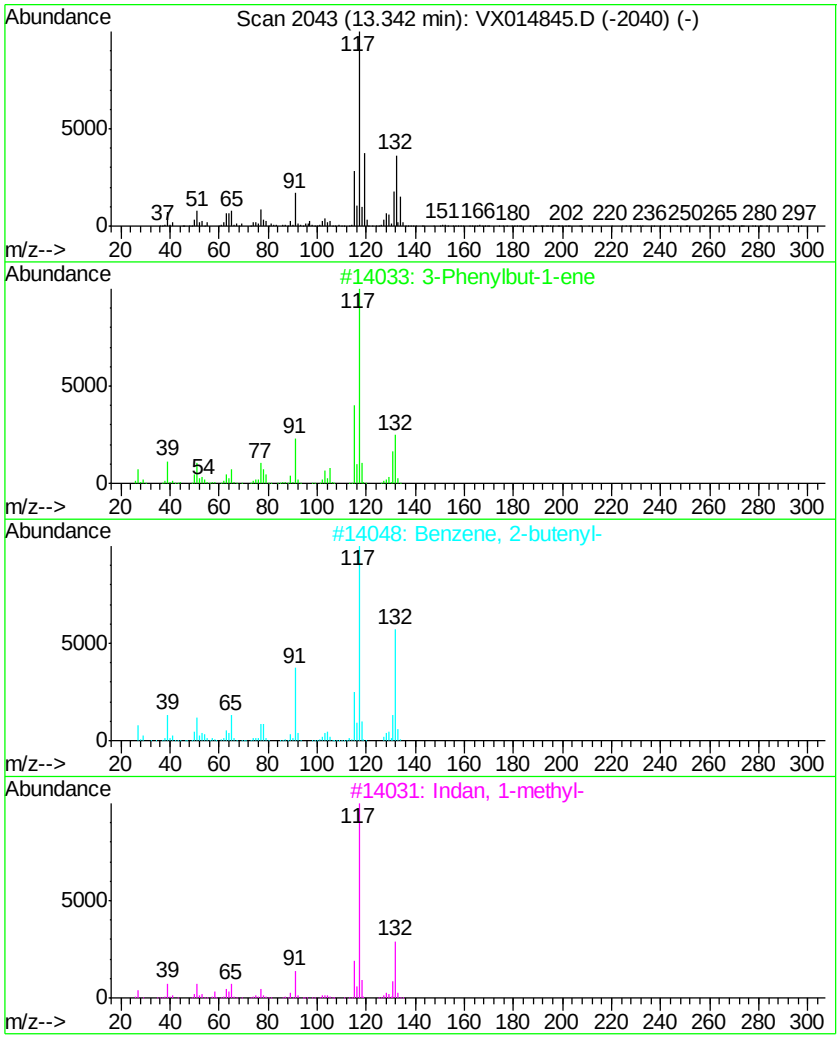
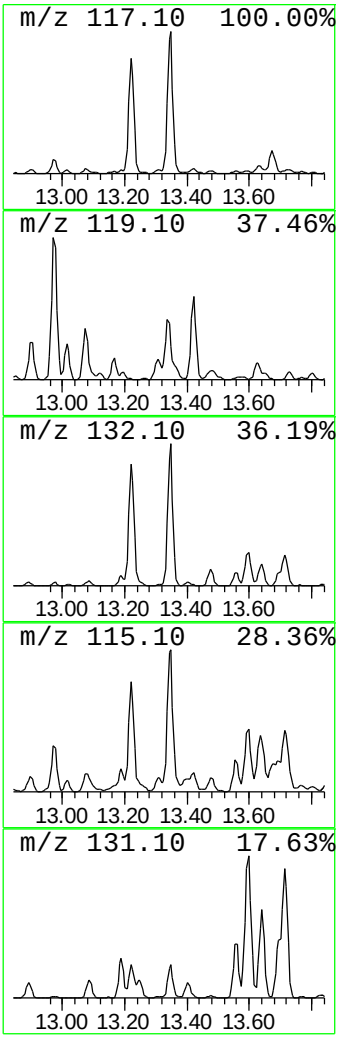
Peak Number 10 3-Phenylbut-1-ene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.34 | 95.00 ug/l | 5178740 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Phenylbut-1-ene | 132 | C10H12 | 000934-10-1 | 81 |
| 2 | Benzene, 2-butenyl- | 132 | C10H12 | 001560-06-1 | 81 |
| 3 | Indan, 1-methyl- | 132 | C10H12 | 000767-58-8 | 81 |
| 4 | 1-Phenyl-1-butene | 132 | C10H12 | 000824-90-8 | 76 |
| 5 | 1H-Indene, 2,3-dihydro-4-methyl- | 132 | C10H12 | 000824-22-6 | 76 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014845.D
Acq On : 06 Feb 2020 14:14
Operator : JC/SP
Sample : L1346-05
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Heptane | 6.69 | 101.0 | ug/l | 3318430 | 2 | 6.85 | 1643670 | 50.0 |
| Heptane, 2-methyl- | 8.34 | 137.3 | ug/l | 4512950 | 2 | 6.85 | 1643670 | 50.0 |
| Heptane, 4-methyl- | 8.37 | 83.5 | ug/l | 2746540 | 2 | 6.85 | 1643670 | 50.0 |
| Heptane, 3-methyl- | 8.50 | 144.0 | ug/l | 5484380 | 3 | 10.11 | 1904410 | 50.0 |
| Octane | 8.96 | 102.8 | ug/l | 3915180 | 3 | 10.11 | 1904410 | 50.0 |
| Heptane, 2,5-dime... | 9.55 | 95.1 | ug/l | 3621460 | 3 | 10.11 | 1904410 | 50.0 |
| Octane, 4-methyl- | 9.95 | 143.6 | ug/l | 5467840 | 3 | 10.11 | 1904410 | 50.0 |
| Octane, 2,6-dimet... | 10.83 | 81.3 | ug/l | 3094670 | 3 | 10.11 | 1904410 | 50.0 |
| Benzene, 1-ethyl-... | 12.67 | 120.9 | ug/l | 6589630 | 4 | 12.07 | 2725620 | 50.0 |
| 3-Phenylbut-1-ene | 13.34 | 95.0 | ug/l | 5178740 | 4 | 12.07 | 2725620 | 50.0 |