LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

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_N\methods\82N061722W.M
Title : SW846 8260

Signal : TIC: VN073106.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.328 | 235 | 245 | 255 | rVB | 296727 | 695065 | 2.65% | 0.124% |
| 2 | 4.992 | 520 | 528 | 547 | rVB2 | 535546 | 1928092 | 7.36% | 0.344% |
| 3 | 5.475 | 594 | 610 | 628 | rBV2 | 516504 | 1793386 | 6.85% | 0.320% |
| 4 | 5.992 | 684 | 698 | 712 | rBV | 797536 | 2489162 | 9.51% | 0.444% |
| 5 | 6.775 | 818 | 831 | 845 | rBV2 | 130464 | 452389 | 1.73% | 0.081% |
| 6 | 6.933 | 845 | 858 | 867 | rBV2 | 242458 | 757784 | 2.89% | 0.135% |
| 7 | 7.039 | 867 | 876 | 887 | rVB2 | 167678 | 492118 | 1.88% | 0.088% |
| 8 | 7.751 | 989 | 997 | 1006 | rVB | 123007 | 325120 | 1.24% | 0.058% |
| 9 | 7.998 | 1020 | 1039 | 1047 | rBV6 | 1035598 | 3983135 | 15.21% | 0.710% |
| 10 | 8.086 | 1047 | 1054 | 1065 | rVV | 1019838 | 2589641 | 9.89% | 0.461% |
| 11 | 8.210 | 1066 | 1075 | 1081 | rVV | 1040518 | 2508568 | 9.58% | 0.447% |
| 12 | 8.275 | 1081 | 1086 | 1094 | rVV | 547034 | 1303415 | 4.98% | 0.232% |
| 13 | 8.369 | 1094 | 1102 | 1111 | rVV2 | 289774 | 746950 | 2.85% | 0.133% |
| 14 | 8.486 | 1112 | 1122 | 1128 | rVV2 | 1228967 | 3116312 | 11.90% | 0.555% |
| 15 | 8.557 | 1128 | 1134 | 1140 | rVV | 977833 | 2277576 | 8.70% | 0.406% |
| 16 | 8.627 | 1140 | 1146 | 1157 | rVV | 1400769 | 3188278 | 12.17% | 0.568% |
| 17 | 8.745 | 1159 | 1166 | 1178 | rVB | 1006773 | 2065671 | 7.89% | 0.368% |
| 18 | 8.898 | 1184 | 1192 | 1204 | rBV | 644128 | 1440910 | 5.50% | 0.257% |
| 19 | 9.204 | 1235 | 1244 | 1255 | rVB | 246025 | 590463 | 2.25% | 0.105% |
| 20 | 9.386 | 1260 | 1275 | 1281 | rBV | 6683230 | 17927372 | 68.46% | 3.194% |
| 21 | 9.439 | 1281 | 1284 | 1294 | rVB | 1218852 | 2080600 | 7.95% | 0.371% |
| 22 | 9.569 | 1294 | 1306 | 1311 | rBV2 | 537596 | 1148508 | 4.39% | 0.205% |
| 23 | 9.657 | 1311 | 1321 | 1332 | rVB2 | 2302391 | 5093984 | 19.45% | 0.908% |
| 24 | 9.804 | 1338 | 1346 | 1357 | rBV2 | 2110358 | 4289955 | 16.38% | 0.764% |
| 25 | 9.904 | 1358 | 1363 | 1366 | rBV2 | 177973 | 325974 | 1.24% | 0.058% |
| 26 | 9.951 | 1366 | 1371 | 1375 | rBV | 1140753 | 2030468 | 7.75% | 0.362% |
| 27 | 9.998 | 1375 | 1379 | 1383 | rVV3 | 711493 | 1368247 | 5.22% | 0.244% |
| 28 | 10.039 | 1383 | 1386 | 1395 | rVB | 701112 | 1287361 | 4.92% | 0.229% |
| 29 | 10.133 | 1395 | 1402 | 1406 | rBV2 | 1572040 | 3454186 | 13.19% | 0.615% |
| 30 | 10.180 | 1406 | 1410 | 1417 | rVB | 1144056 | 2134985 | 8.15% | 0.380% |
| 31 | 10.263 | 1417 | 1424 | 1427 | rBV4 | 592864 | 1271248 | 4.85% | 0.227% |
| 32 | 10.369 | 1435 | 1442 | 1447 | rBV2 | 6460757 | 13252777 | 50.61% | 2.361% |
| 33 | 10.410 | 1447 | 1449 | 1458 | rVB2 | 2810649 | 4170703 | 15.93% | 0.743% |
| 34 | 10.498 | 1458 | 1464 | 1467 | rBV | 1073669 | 1962405 | 7.49% | 0.350% |
| 35 | 10.551 | 1467 | 1473 | 1483 | rVB6 | 3292146 | 8941390 | 34.14% | 1.593% |
| 36 | 10.674 | 1484 | 1494 | 1496 | rBV2 | 1498652 | 3045729 | 11.63% | 0.543% |

LSC Area Percent Report

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Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

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_N\methods\82N061722W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 10.716 | 1496 | 1501 | 1509 | rVB | 4855788 | 9036158 | 34.51% | 1.610% |
| 38 | 10.810 | 1509 | 1517 | 1522 | rBV3 | 2668300 | 6015990 | 22.97% | 1.072% |
| 39 | 10.898 | 1528 | 1532 | 1537 | rVB | 1814366 | 2873107 | 10.97% | 0.512% |
| 40 | 10.986 | 1537 | 1547 | 1553 | rBV | 4098430 | 7623777 | 29.11% | 1.358% |
| 41 | 11.092 | 1553 | 1565 | 1572 | rBV | 3097789 | 8044632 | 30.72% | 1.433% |
| 42 | 11.163 | 1572 | 1577 | 1580 | rVV2 | 1594491 | 2747802 | 10.49% | 0.490% |
| 43 | 11.198 | 1580 | 1583 | 1584 | rVV2 | 1386571 | 1781223 | 6.80% | 0.317% |
| 44 | 11.227 | 1584 | 1588 | 1592 | rVV | 4540151 | 7704735 | 29.42% | 1.373% |
| 45 | 11.280 | 1592 | 1597 | 1603 | rVV | 10208557 | 18656628 | 71.24% | 3.324% |
| 46 | 11.333 | 1603 | 1606 | 1610 | rVB2 | 1144114 | 1494161 | 5.71% | 0.266% |
| 47 | 11.386 | 1610 | 1615 | 1620 | rBV3 | 3869042 | 6732570 | 25.71% | 1.200% |
| 48 | 11.433 | 1620 | 1623 | 1627 | rVB2 | 1230177 | 1625899 | 6.21% | 0.290% |
| 49 | 11.486 | 1627 | 1632 | 1640 | rVB | 4710977 | 8498466 | 32.45% | 1.514% |
| 50 | 11.557 | 1640 | 1644 | 1649 | rBV2 | 1766639 | 2939750 | 11.23% | 0.524% |
| 51 | 11.604 | 1649 | 1652 | 1660 | rVB6 | 636710 | 1233811 | 4.71% | 0.220% |
| 52 | 11.680 | 1661 | 1665 | 1668 | rBV2 | 752275 | 1227569 | 4.69% | 0.219% |
| 53 | 11.715 | 1669 | 1671 | 1676 | rVB4 | 567656 | 695906 | 2.66% | 0.124% |
| 54 | 11.774 | 1676 | 1681 | 1684 | rBV | 910002 | 1421022 | 5.43% | 0.253% |
| 55 | 11.815 | 1684 | 1688 | 1691 | rBV | 2275542 | 3336978 | 12.74% | 0.595% |
| 56 | 11.863 | 1691 | 1696 | 1701 | rBV5 | 2515486 | 5046405 | 19.27% | 0.899% |
| 57 | 11.927 | 1702 | 1707 | 1711 | rVV | 5884312 | 10597237 | 40.47% | 1.888% |
| 58 | 11.968 | 1711 | 1714 | 1719 | rVB2 | 5033978 | 8028141 | 30.66% | 1.431% |
| 59 | 12.027 | 1719 | 1724 | 1731 | rBV3 | 1676472 | 3977092 | 15.19% | 0.709% |
| 60 | 12.115 | 1731 | 1739 | 1744 | rVB3 | 2059920 | 5023154 | 19.18% | 0.895% |
| 61 | 12.192 | 1744 | 1752 | 1758 | rBV3 | 9068928 | 20652067 | 78.86% | 3.680% |
| 62 | 12.310 | 1764 | 1772 | 1776 | rVB | 8748897 | 15196663 | 58.03% | 2.708% |
| 63 | 12.392 | 1776 | 1786 | 1788 | rBV3 | 8533928 | 18516899 | 70.71% | 3.299% |
| 64 | 12.421 | 1788 | 1791 | 1802 | rVB4 | 9681290 | 22877774 | 87.36% | 4.077% |
| 65 | 12.515 | 1803 | 1807 | 1809 | rBV4 | 1799337 | 2977571 | 11.37% | 0.531% |
| 66 | 12.674 | 1828 | 1834 | 1839 | rBV3 | 3582148 | 6542388 | 24.98% | 1.166% |
| 67 | 12.757 | 1841 | 1848 | 1852 | rVV4 | 3189233 | 7187874 | 27.45% | 1.281% |
| 68 | 12.833 | 1856 | 1861 | 1869 | rVB3 | 8651007 | 17609405 | 67.24% | 3.138% |
| 69 | 12.915 | 1869 | 1875 | 1880 | rBV3 | 3791370 | 8697613 | 33.21% | 1.550% |
| 70 | 12.992 | 1880 | 1888 | 1894 | rVV4 | 9076049 | 26187517 | 100.00% | 4.666% |
| 71 | 13.045 | 1894 | 1897 | 1902 | rVB4 | 4833249 | 7908123 | 30.20% | 1.409% |
| 72 | 13.133 | 1908 | 1912 | 1916 | rVB4 | 3809358 | 5310574 | 20.28% | 0.946% |
| 73 | 13.180 | 1916 | 1920 | 1923 | rBV3 | 2445777 | 4162010 | 15.89% | 0.742% |
| 74 | 13.221 | 1923 | 1927 | 1935 | rVB2 | 8548559 | 14385918 | 54.93% | 2.563% |
| 75 | 13.351 | 1946 | 1949 | 1954 | rBV2 | 2122088 | 2634581 | 10.06% | 0.469% |
| 76 | 13.404 | 1954 | 1958 | 1961 | rBV2 | 2512428 | 3906635 | 14.92% | 0.696% |

LSC Area Percent Report

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Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

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_N\methods\82N061722W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 13.504 | 1967 | 1975 | 1979 | rBV3 | 7997523 | 16973316 | 64.81% | 3.024% |
| 78 | 13.757 | 2013 | 2018 | 2032 | rVB6 | 3330530 | 10140324 | 38.72% | 1.807% |
| 79 | 13.933 | 2043 | 2048 | 2053 | rBV2 | 9613947 | 17212910 | 65.73% | 3.067% |
| 80 | 13.980 | 2053 | 2056 | 2060 | rVB2 | 2399334 | 3135516 | 11.97% | 0.559% |
| 81 | 14.039 | 2062 | 2066 | 2069 | rBV3 | 1968771 | 3011757 | 11.50% | 0.537% |
| 82 | 14.151 | 2082 | 2085 | 2090 | rVB | 5418857 | 8131510 | 31.05% | 1.449% |
| 83 | 14.262 | 2098 | 2104 | 2109 | rVB4 | 4022905 | 7639392 | 29.17% | 1.361% |
| 84 | 14.327 | 2110 | 2115 | 2120 | rVB8 | 2094564 | 3892445 | 14.86% | 0.694% |
| 85 | 14.380 | 2121 | 2124 | 2126 | rBV3 | 919416 | 1274601 | 4.87% | 0.227% |
| 86 | 14.445 | 2130 | 2135 | 2139 | rBV3 | 6809586 | 12053137 | 46.03% | 2.148% |
| 87 | 14.556 | 2150 | 2154 | 2157 | rBV | 1971393 | 2862489 | 10.93% | 0.510% |
| 88 | 14.609 | 2158 | 2163 | 2169 | rVV3 | 4041853 | 7602543 | 29.03% | 1.355% |
| 89 | 14.792 | 2191 | 2194 | 2198 | rBV3 | 1094088 | 1537106 | 5.87% | 0.274% |
| 90 | 14.851 | 2199 | 2204 | 2210 | rVV3 | 5668449 | 11868324 | 45.32% | 2.115% |
| 91 | 14.915 | 2210 | 2215 | 2220 | rVB4 | 3275474 | 6404439 | 24.46% | 1.141% |
| 92 | 15.033 | 2232 | 2235 | 2238 | rBV3 | 882243 | 1352437 | 5.16% | 0.241% |
| 93 | 15.127 | 2247 | 2251 | 2255 | rVB3 | 2379805 | 3637300 | 13.89% | 0.648% |
| 94 | 15.168 | 2255 | 2258 | 2264 | rBV3 | 976442 | 2028836 | 7.75% | 0.362% |
| 95 | 15.239 | 2264 | 2270 | 2276 | rVB3 | 3131451 | 6526319 | 24.92% | 1.163% |
| 96 | 15.398 | 2292 | 2297 | 2304 | rVB8 | 1511634 | 3032297 | 11.58% | 0.540% |
| 97 | 15.733 | 2346 | 2354 | 2361 | rBV7 | 997439 | 3521214 | 13.45% | 0.627% |
| 98 | 15.809 | 2362 | 2367 | 2372 | rBV6 | 1325269 | 2687315 | 10.26% | 0.479% |
| 99 | 16.250 | 2436 | 2442 | 2448 | rBV5 | 1708279 | 3825110 | 14.61% | 0.682% |
| 100 | 16.721 | 2517 | 2522 | 2533 | rBV6 | 1049408 | 3208757 | 12.25% | 0.572% |

Sum of corrected areas: 561205146

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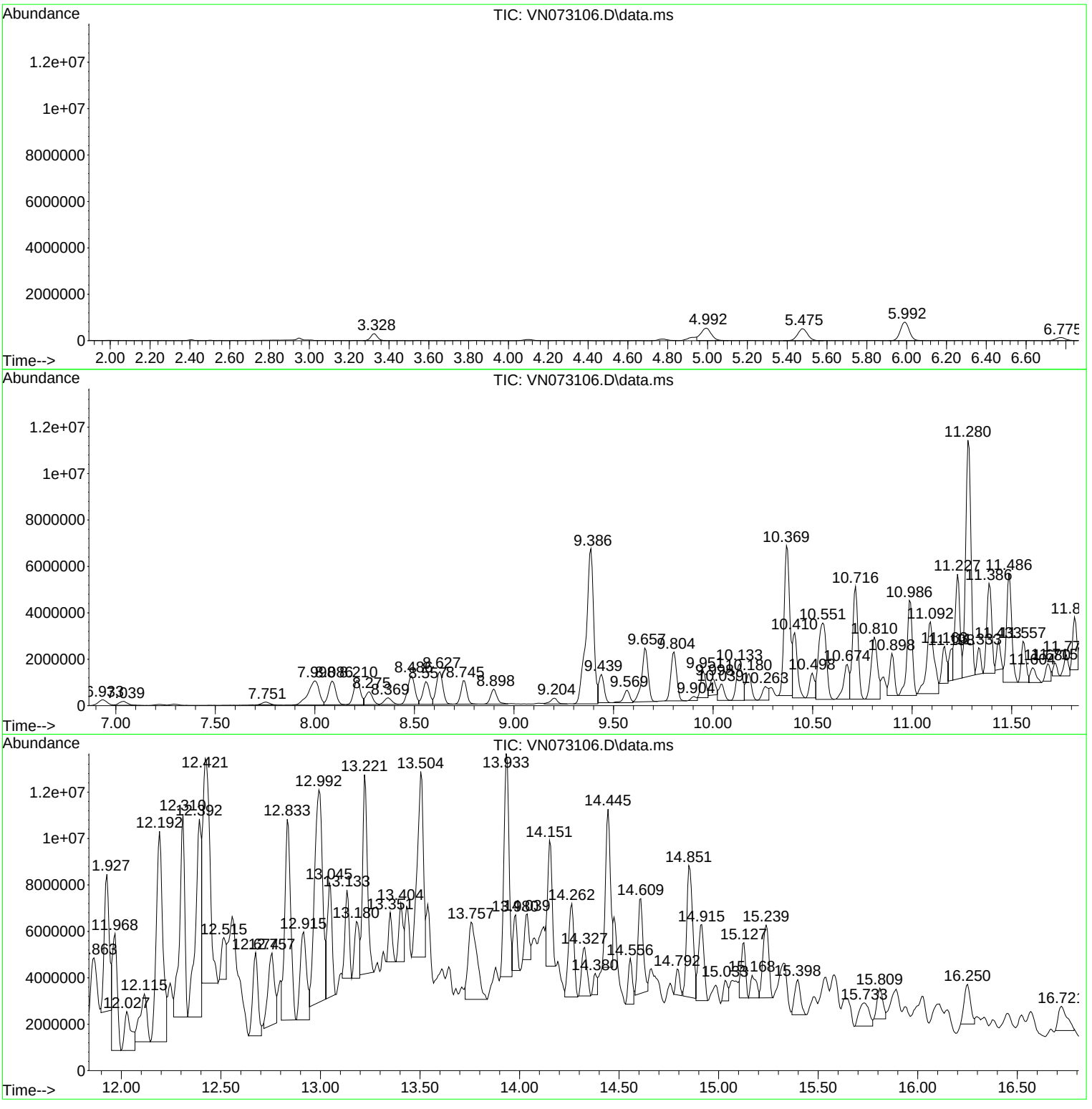
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
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**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

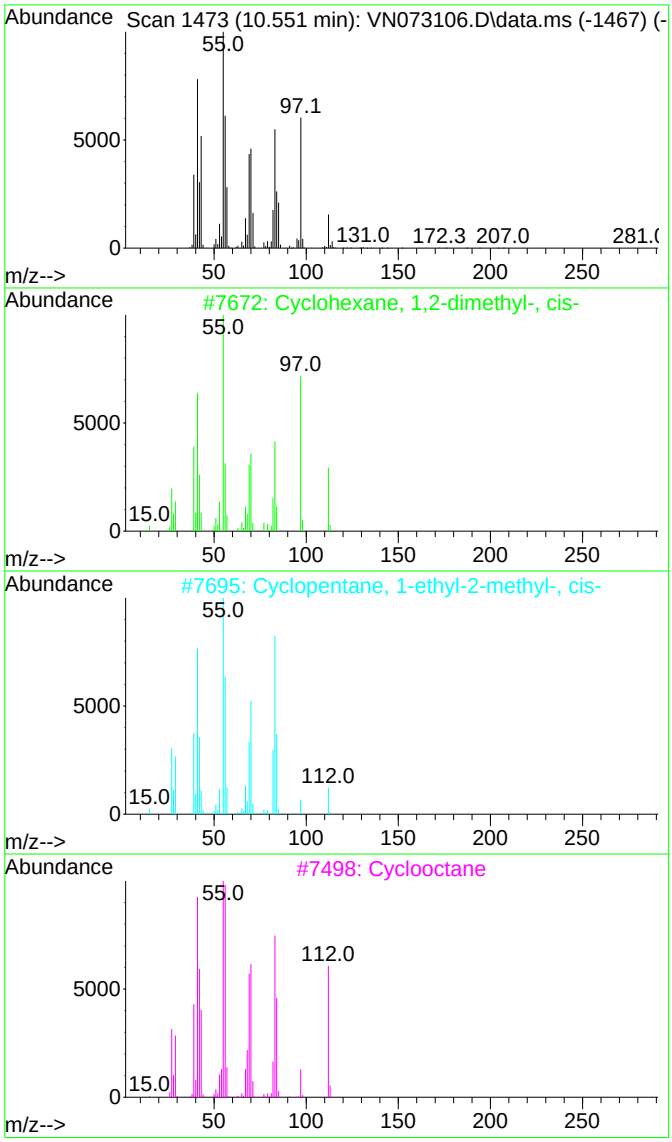
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

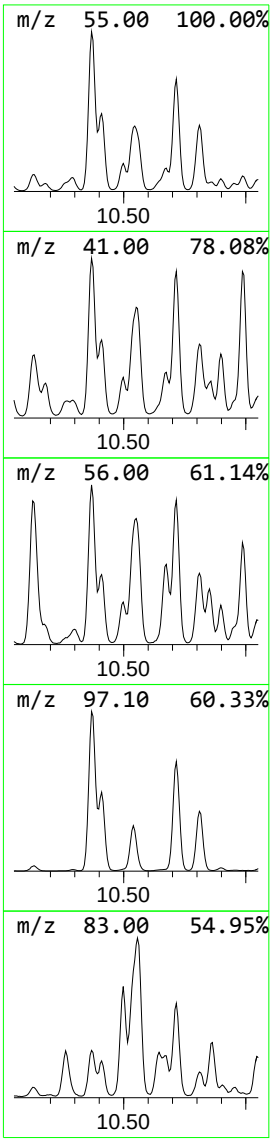
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.551 | 364.19 ug/l | 8941390 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,2-dimethyl-, cis- | 112 | C8H16 | 002207-01-4 | 76 |
| 2 | Cyclopentane, 1-ethyl-2-methyl-,... | 112 | C8H16 | 000930-89-2 | 64 |
| 3 | Cyclooctane | 112 | C8H16 | 000292-64-8 | 62 |
| 4 | 1,2-Cyclohexanedione | 112 | C6H8O2 | 000765-87-7 | 62 |
| 5 | 3-Octene, (Z)- | 112 | C8H16 | 014850-22-7 | 60 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
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ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

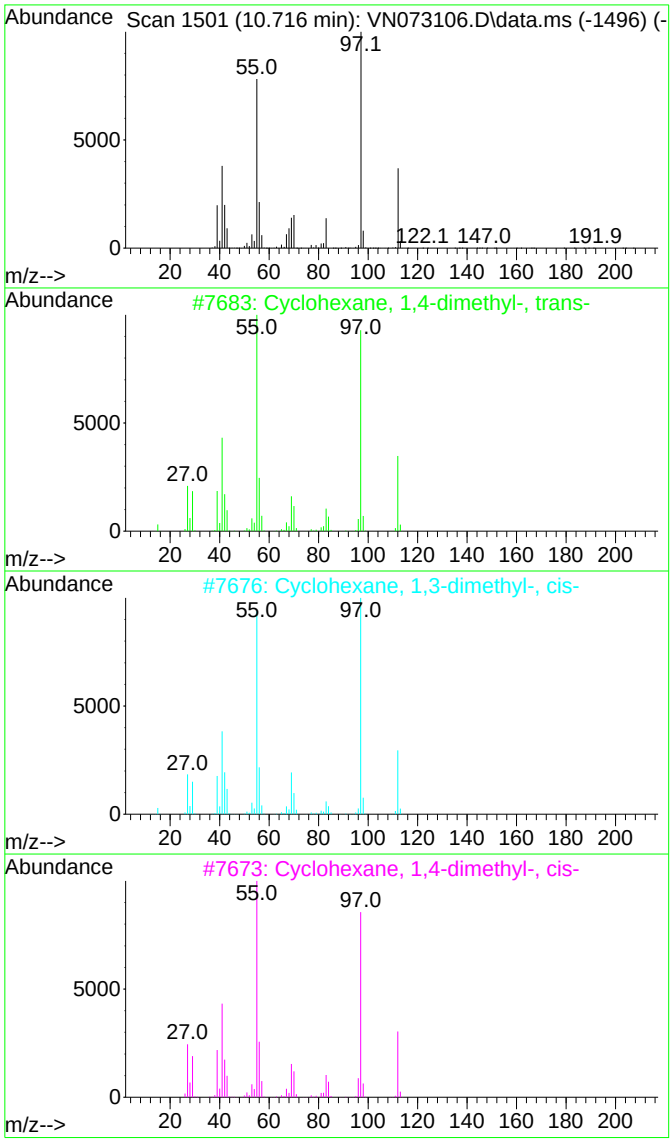
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

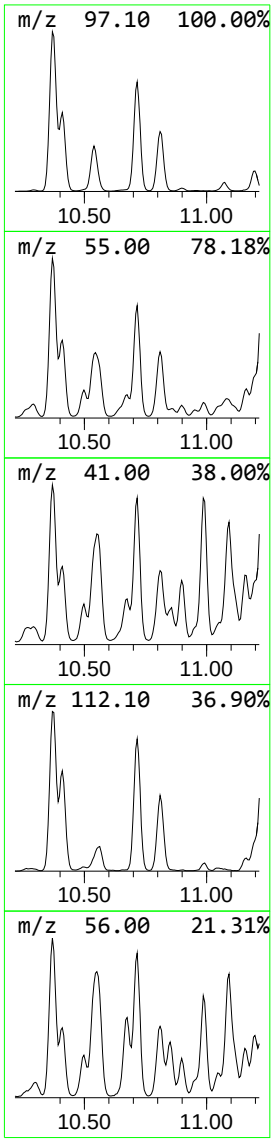
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.716 | 368.05 ug/l | 9036160 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,4-dimethyl-, trans- | 112 | C8H16 | 002207-04-7 | 91 |
| 2 | Cyclohexane, 1,3-dimethyl-, cis- | 112 | C8H16 | 000638-04-0 | 87 |
| 3 | Cyclohexane, 1,4-dimethyl-, cis- | 112 | C8H16 | 000624-29-3 | 87 |
| 4 | Cyclohexane, 1,4-dimethyl- | 112 | C8H16 | 000589-90-2 | 87 |
| 5 | Cyclohexane, 1,3-dimethyl- | 112 | C8H16 | 000591-21-9 | 87 |



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Data File : VN073106.D
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Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

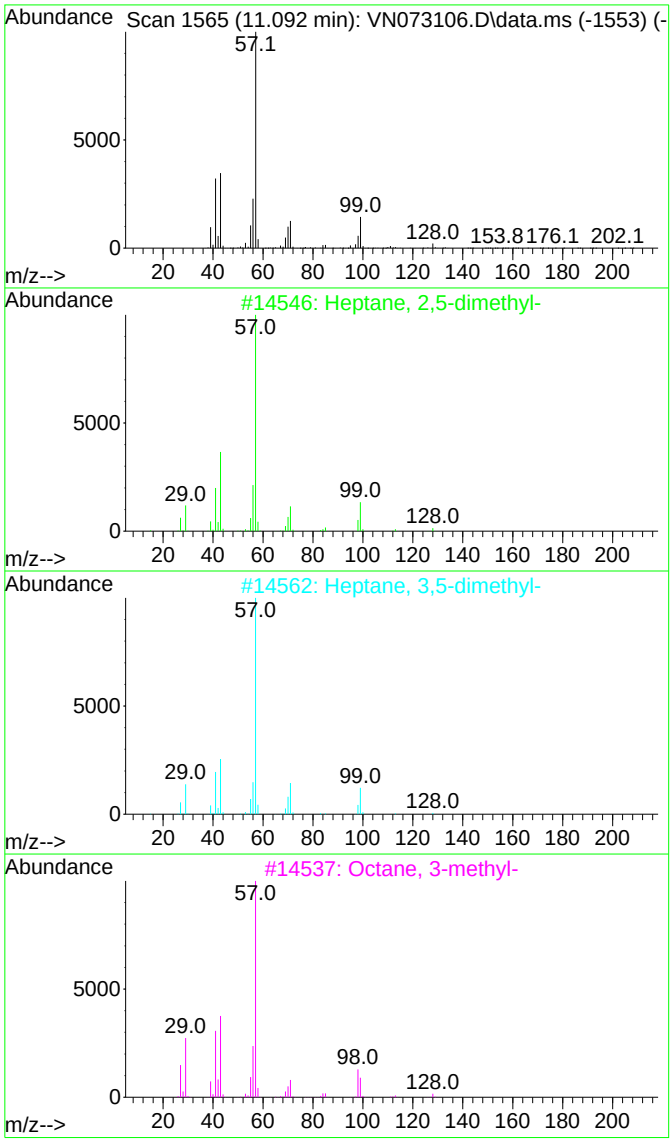
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

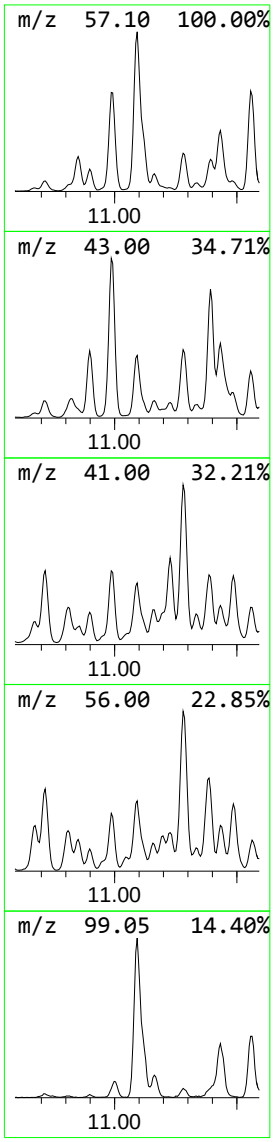
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Heptane, 2,5-dimethyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.092 | 327.67 ug/l | 8044630 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 2,5-dimethyl- | 128 | C9H20 | 002216-30-0 | 91 |
| 2 | Heptane, 3,5-dimethyl- | 128 | C9H20 | 000926-82-9 | 81 |
| 3 | Octane, 3-methyl- | 128 | C9H20 | 002216-33-3 | 80 |
| 4 | Decane, 2,6,6-trimethyl- | 184 | C13H28 | 062108-24-1 | 59 |
| 5 | Decane, 2,5-dimethyl- | 170 | C12H26 | 017312-50-4 | 53 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

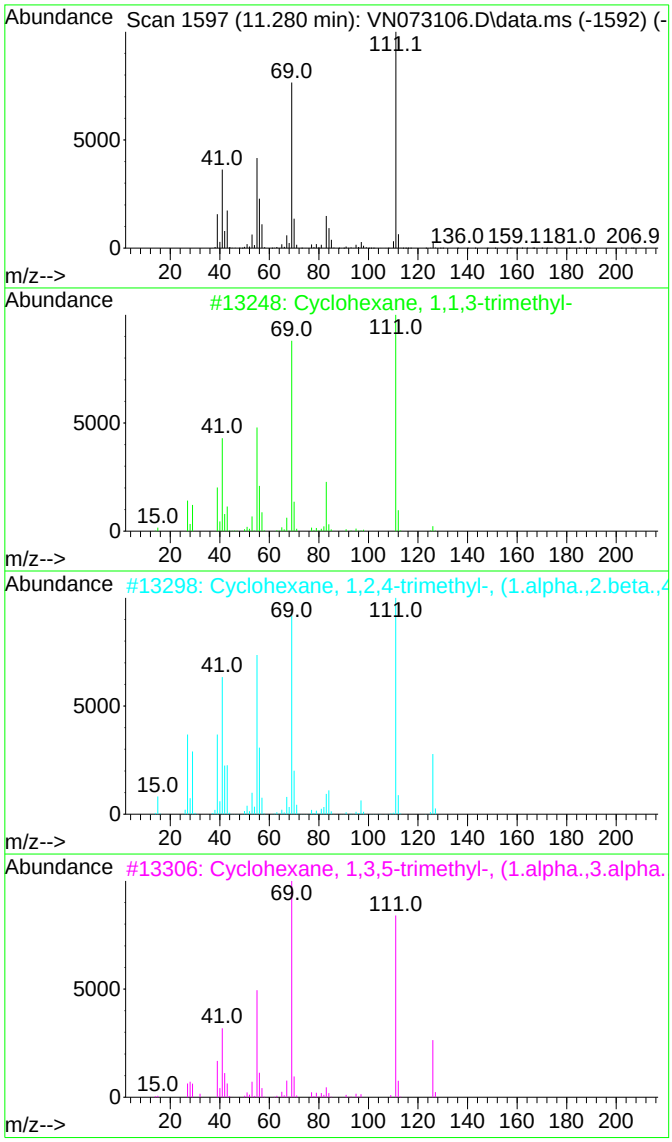
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

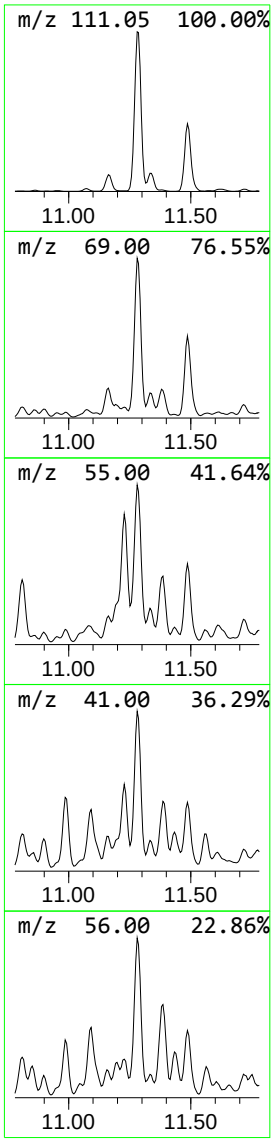
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.280 | 759.90 ug/l | 18656600 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,1,3-trimethyl- | 126 | C9H18 | 003073-66-3 | 87 |
| 2 | Cyclohexane, 1,2,4-trimethyl-, (... | 126 | C9H18 | 007667-60-9 | 78 |
| 3 | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18 | 001795-27-3 | 64 |
| 4 | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18 | 001795-26-2 | 53 |
| 5 | 1,1,4-Trimethylcyclohexane | 126 | C9H18 | 007094-27-1 | 52 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

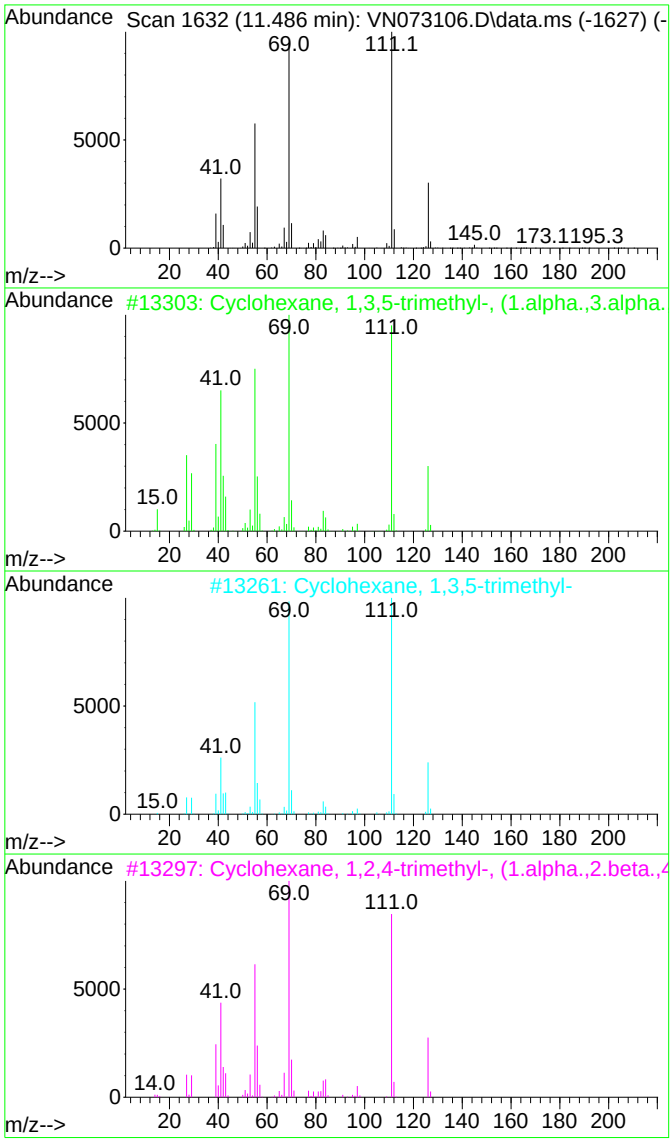
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

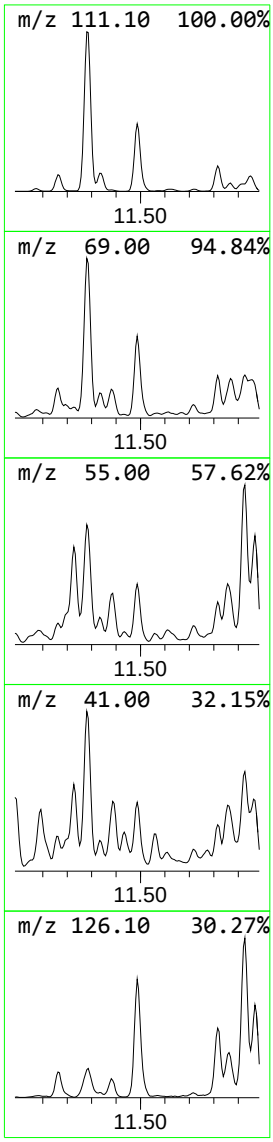
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Cyclohexane, 1,3,5-trimethy... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.486 | 346.15 ug/l | 8498470 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18 | 001795-26-2 | 93 |
| 2 | Cyclohexane, 1,3,5-trimethyl- | 126 | C9H18 | 001839-63-0 | 93 |
| 3 | Cyclohexane, 1,2,4-trimethyl-, (... | 126 | C9H18 | 007667-60-9 | 90 |
| 4 | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18 | 001795-27-3 | 90 |
| 5 | Cyclohexane, 1,2,4-trimethyl- | 126 | C9H18 | 002234-75-5 | 68 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

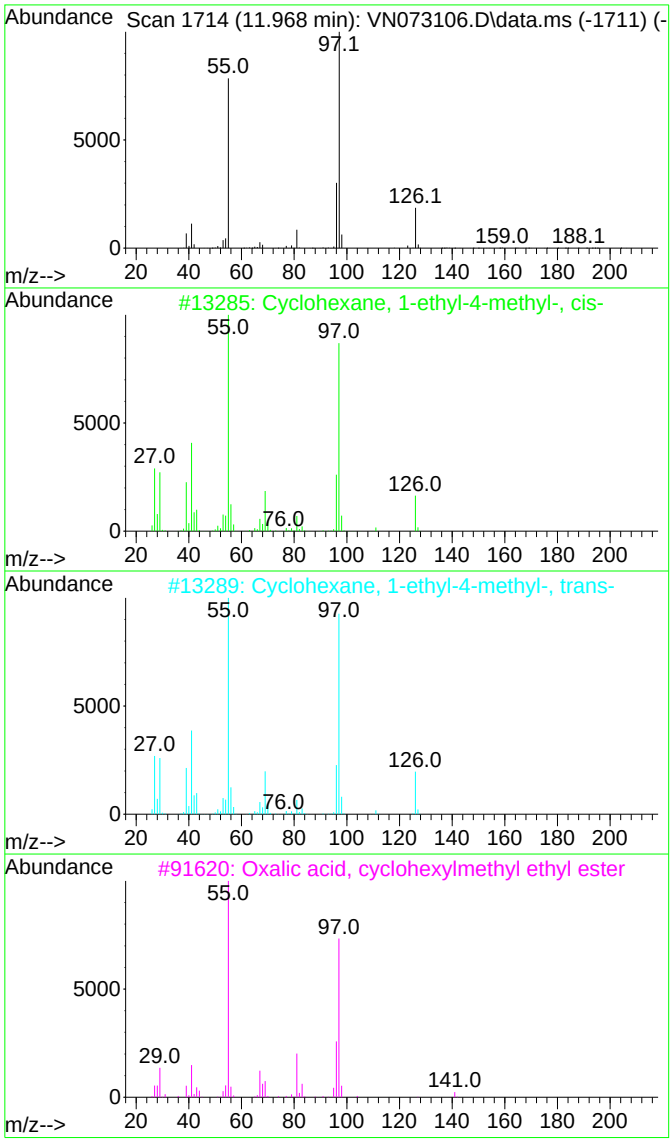
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

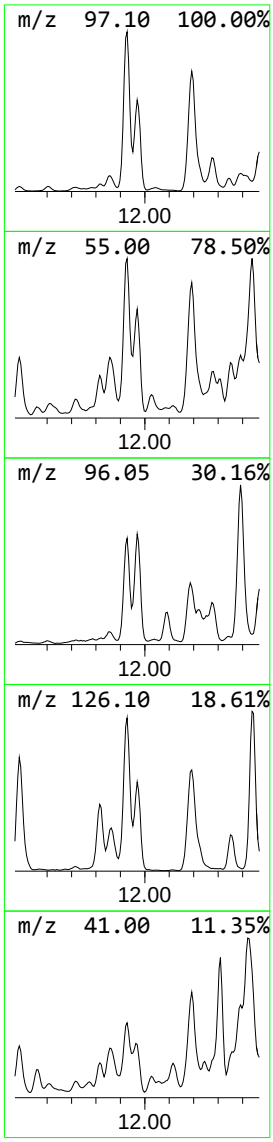
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.968 | 326.99 ug/l | 8028140 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1-ethyl-4-methyl-, ... | 126 | C9H18 | 004926-78-7 | 86 |
| 2 | Cyclohexane, 1-ethyl-4-methyl-, ... | 126 | C9H18 | 006236-88-0 | 72 |
| 3 | Oxalic acid, cyclohexylmethyl et... | 214 | C11H18O4 | 1000309-68-0 | 72 |
| 4 | 1-Ethyl-4-methylcyclohexane | 126 | C9H18 | 003728-56-1 | 72 |
| 5 | cis-1-Ethyl-3-methyl-cyclohexane | 126 | C9H18 | 019489-10-2 | 64 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

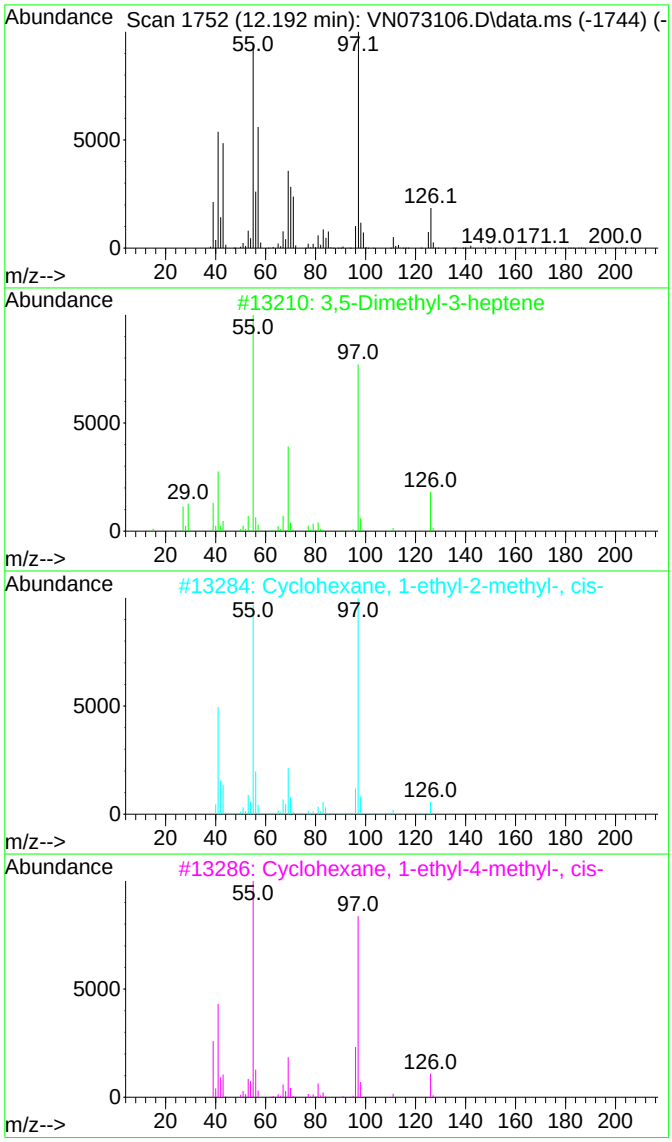
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

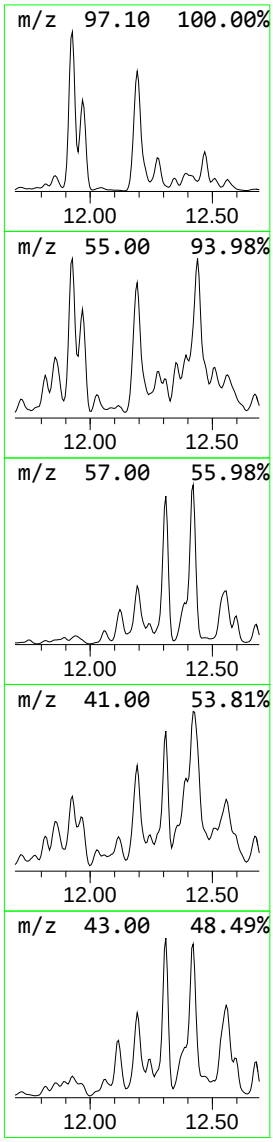
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 3,5-Dimethyl-3-heptene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.192 | 841.18 ug/l | 20652100 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,5-Dimethyl-3-heptene | 126 | C9H18 | 059643-68-4 | 58 |
| 2 | Cyclohexane, 1-ethyl-2-methyl-, ... | 126 | C9H18 | 004923-77-7 | 53 |
| 3 | Cyclohexane, 1-ethyl-4-methyl-, ... | 126 | C9H18 | 004926-78-7 | 52 |
| 4 | Cyclohexane, 1-ethyl-2-methyl-, ... | 126 | C9H18 | 004923-78-8 | 52 |
| 5 | 1-Ethyl-4-methylcyclohexane | 126 | C9H18 | 003728-56-1 | 52 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

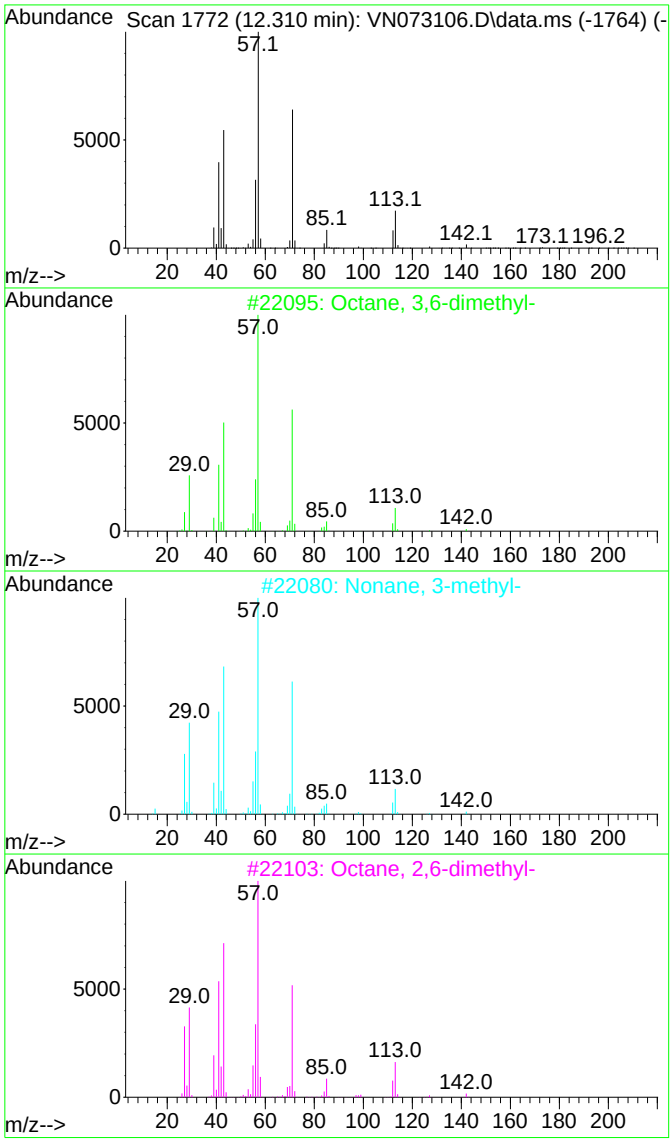
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

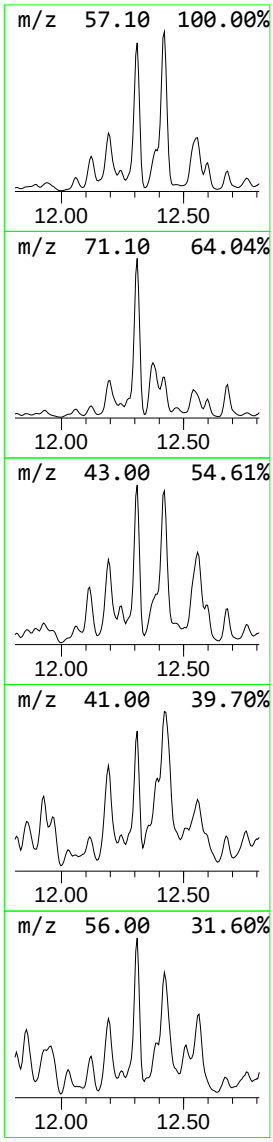
**********

Peak Number 8 Octane, 3,6-dimethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.310 | 618.97 ug/l | 15196700 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane, 3,6-dimethyl- | 142 | C10H22 | 015869-94-0 | 91 |
| 2 | Nonane, 3-methyl- | 142 | C10H22 | 005911-04-6 | 90 |
| 3 | Octane, 2,6-dimethyl- | 142 | C10H22 | 002051-30-1 | 86 |
| 4 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 64 |
| 5 | Butane, 2,2-dimethyl- | 86 | C6H14 | 000075-83-2 | 53 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

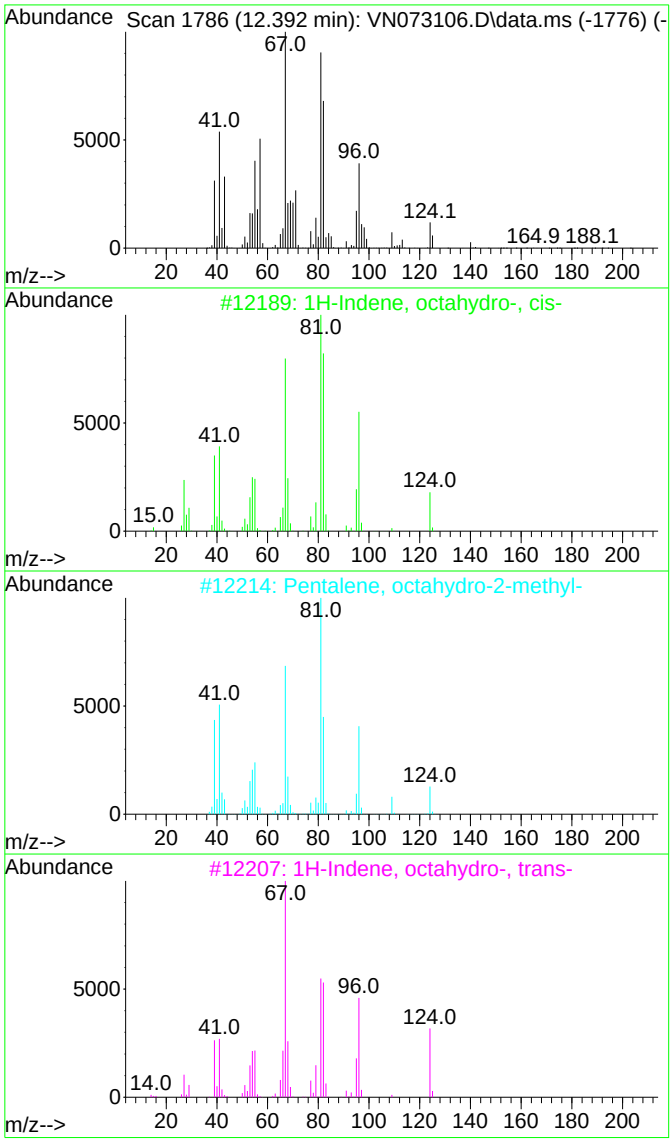
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

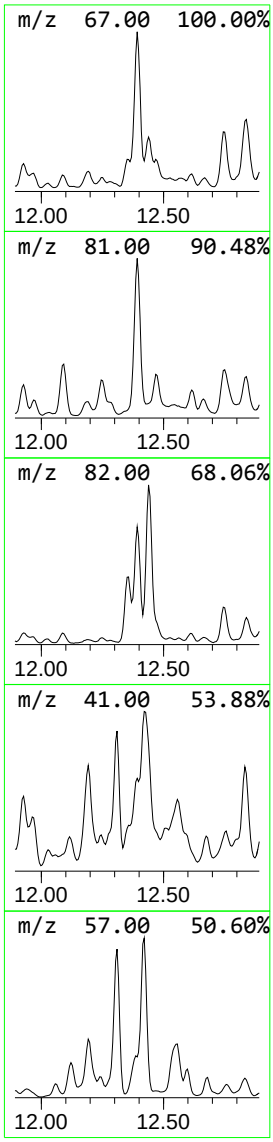
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 1H-Indene, octahydro-, cis- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.392 | 754.21 ug/l | 18516900 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Indene, octahydro-, cis- | 124 | C9H16 | 004551-51-3 | 70 |
| 2 | Pentalene, octahydro-2-methyl- | 124 | C9H16 | 003868-64-2 | 64 |
| 3 | 1H-Indene, octahydro-, trans- | 124 | C9H16 | 003296-50-2 | 53 |
| 4 | 7-Methyl-8-oxabicyclo[4.3.0]nonane | 140 | C9H16O | 1000216-87-6 | 46 |
| 5 | Bicyclo[2.2.1]heptane, 2-ethyl- | 124 | C9H16 | 002146-41-0 | 43 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

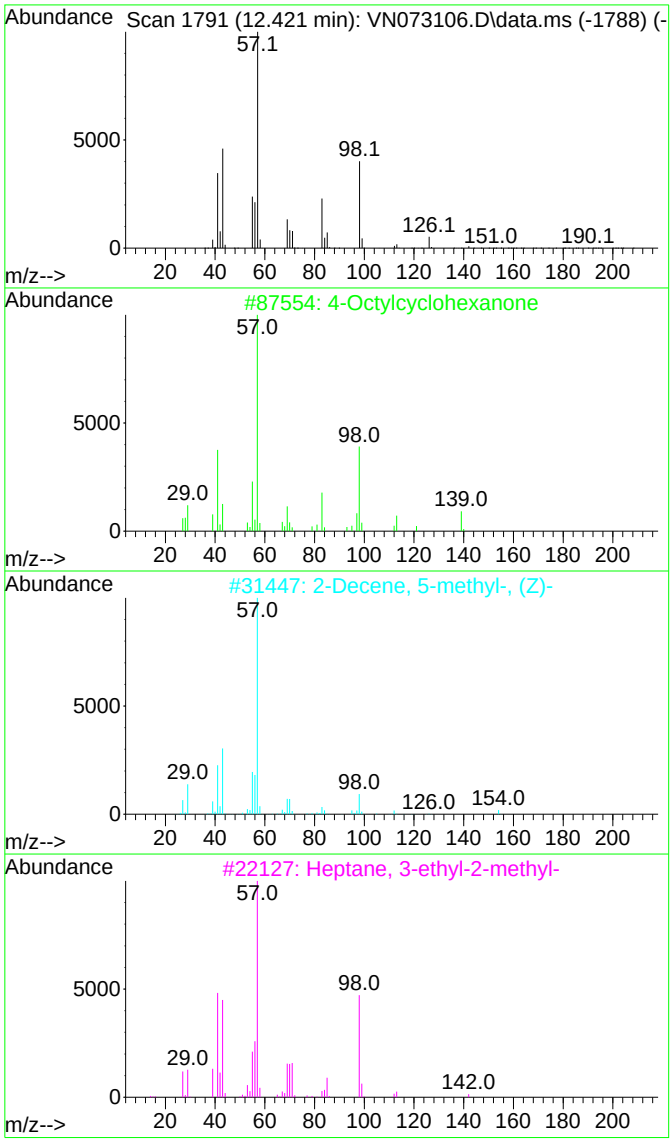
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

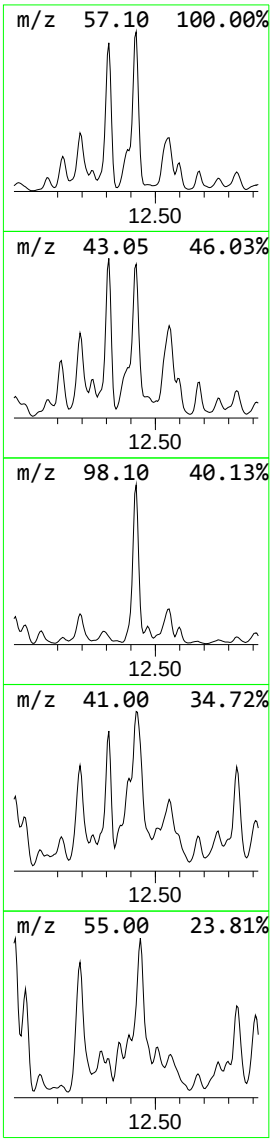
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 4-Octylcyclohexanone Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.421 | 931.83 ug/l | 22877800 | Chlorobenzene-d5 | 11.686 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Octylcyclohexanone | 210 | C14H26O | 1000428-94-1 | 59 |
| 2 | 2-Decene, 5-methyl-, (Z)- | 154 | C11H22 | 074645-86-6 | 45 |
| 3 | Heptane, 3-ethyl-2-methyl- | 142 | C10H22 | 014676-29-0 | 43 |
| 4 | Carbonic acid, heptyl vinyl ester | 186 | C10H18O3 | 1010383-25-4 | 42 |
| 5 | Octane, 2,3-dimethyl- | 142 | C10H22 | 007146-60-3 | 40 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073106.D
Acq On : 25 Jun 2022 13:27
Operator : JC\MD
Sample : N3431-21
Misc : 5.09g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
WC-14B-2-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Cyclohexane, 1,... | 10.551 | 364.2 | ug/l | 8941390 | 3 | 11.686 | 1227570 | 50.0 |
| Cyclohexane, 1,... | 10.716 | 368.1 | ug/l | 9036160 | 3 | 11.686 | 1227570 | 50.0 |
| Heptane, 2,5-di... | 11.092 | 327.7 | ug/l | 8044630 | 3 | 11.686 | 1227570 | 50.0 |
| Cyclohexane, 1,... | 11.280 | 759.9 | ug/l | 18656600 | 3 | 11.686 | 1227570 | 50.0 |
| Cyclohexane, 1,... | 11.486 | 346.1 | ug/l | 8498470 | 3 | 11.686 | 1227570 | 50.0 |
| Cyclohexane, 1-... | 11.968 | 327.0 | ug/l | 8028140 | 3 | 11.686 | 1227570 | 50.0 |
| 3,5-Dimethyl-3-... | 12.192 | 841.2 | ug/l | 20652100 | 3 | 11.686 | 1227570 | 50.0 |
| Octane, 3,6-dim... | 12.310 | 619.0 | ug/l | 15196700 | 3 | 11.686 | 1227570 | 50.0 |
| 1H-Indene, octa... | 12.392 | 754.2 | ug/l | 18516900 | 3 | 11.686 | 1227570 | 50.0 |
| 4-Octylcyclohex... | 12.421 | 931.8 | ug/l | 22877800 | 3 | 11.686 | 1227570 | 50.0 |