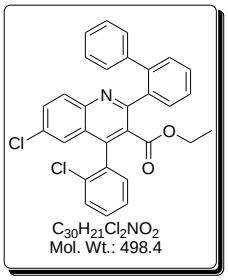
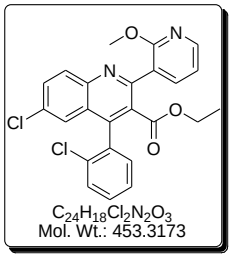
A convenient and efficient C-OH bond activation, $PdCl_2(PPh_3)_2$ catalyzed, C-C bond formation of tautomerizable quinolinones with the aid of BOP reagent and boronic acids

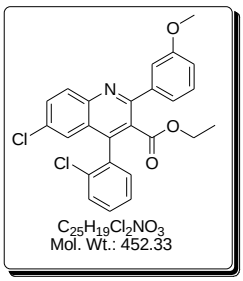
Yadavalli Suneel Kumar[a], C. Dasaradhan[a], Kamalakannan Prabakaran[a], Fazlur-Rahman Nawaz Khan[a*,b*] Euh Duck Jeong[b*], Eun Hyuk Chung[b], Hyun Gyu Kim[b]



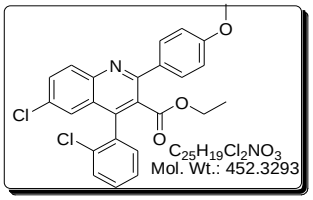
White solid, m.p 120- 122 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 - 8.03 (d, *J* = 8.96 Hz, 1H), 7.67 - 7.62 (m, 2H), 7.51 - 7.47 (m, 4H), 7.41 - 7.38 (t, *J* = 7.48 Hz, 1H), 7.34 - 7.30 (t, *J* = 7.43 Hz, 1H), 7.26 - 7.27 (d, *J* = 1.97 Hz , 1H), 7.18 - 7.16 (m, 2H), 7.14 - 7.12 (m , 4H), 3.66 - 3.61 (q, *J* = 7.11 Hz, 2H), 0.61 - 0.58 (t, *J* = 7.13 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12, 158.36, 145.86, 143.89, 140.69, 140.19, 138.75, 134.41, 133.66, 133.29, 131.58, 131.30, 130.42, 130.00, 129.86, 129.48, 129.44, 129.07, 129.04, 128.14, 127.95, 127.28, 126.65, 126.57, 125.76, 124.87, 61.03, 12.90; IR (v, cm^{-1}) 2997.38, 2960.73, 2926.01, 2854.65, 1726.29, 1612.49, 1546.91, 1479.40, 1450.47, 1402.25, 1384.89, 1334.74, 1261.45, 1226.73, 1184.29, 1163.08, 1145.72, 1130.29, 1099.43, 1008.77, 825.53, 752.24, 744.52, 534.28; LC-MS: m/z calcd. for $C_{30}H_{21}Cl_2NO_2$ 498.4 found 500.0 [M+2].



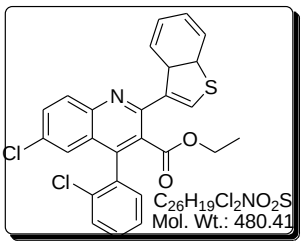
White solid, m.p 115- 118 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 - 8.24 (dd, *J* = 5.04, 1.83 Hz, 1H), 8.16 - 8.14 (d, *J* = 8.84 Hz, 1H), 8.03 - 8.00 (dd, *J* = 7.28, 1.82 Hz, 1H), 7.73 - 7.70 (dd, *J* = 8.99, 2.14 Hz, 1H), 7.581 - 7.56 (d, *J* = 7.96 Hz, 1H), 7.49 - 7.45 (dt, *J* = 7.51, 1.20 Hz, 1H), 7.43 - 7.39 (dt, *J* = 7.36, 0.70 Hz, 1H), 7.35 - 7.35 (d, *J* = 2.17 Hz, 1H), 7.31 - 7.29 (dd, *J* = 7.36, 1.28 Hz, 1H), 7.10 - 7.07 (t, *J* = 6.15 Hz, 1H), 3.87 (s, 3H), 3.86 - 3.83 (q, *J* = 3.09 Hz, 2H), 0.80 - 0.76 (t, *J* = 7.12 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 159.7, 156.4, 146.1, 144.1, 141.0, 133.9, 133.7, 133.4, 131.7, 131.5, 131.1, 130.5, 129.7, 129.6, 126.8, 125.9, 124.9, 121.0, 115.6, 113.6, 61.5, 55.4, 13.4; LC-MS: m/z calcd. for $C_{24}H_{18}Cl_2N_2O_3$ 453.3 found 455.0 [M+2].



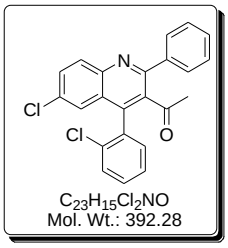
White solid m.p 121- 124 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 - 8.16 (d, *J* = 8.63Hz, 1H), 7.72 - 7.69 (dd, *J* = 8.95, 2.27 Hz, 1H), 7.58 - 7.56 (dd, *J* = 7.93, 0.81Hz, 1H), 7.49 - 7.45 (td, *J* = 7.44, 1.55 Hz, 1H), 7.42 - 7.36 (m, 2H), 7.34 - 7.29 (m, 4H), 7.01 - 6.98 (qd, *J* = 7.98, 1.36 Hz, 1H), 3.92 - 3.86 (q, *J* = 6.96 Hz, 2H), 3.86 (s, 3H), 0.84 - 0.81 (t, *J* = 7.13 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.39, 159.73, 156.39, 146.07, 144.05, 141.03, 133.93, 133.73, 133.43,131.72, 131.56, 131.07, 130.47, 129.74, 129.57, 127.89, 126.80, 125.90, 124.85, 121.02, 115.56, 113.63, 61.49, 55.38, 13.40; IR (v. cm^{-1}), 3132.40, 2995.45, 2929.87, 2833.43, 1730.15, 1606.70, 1583.56, 1573.91, 1550.77, 1490.97, 1469.76, 1450.47, 1435.04, 1396.46, 1346.31, 1288.45, 1244.09, 1226.73, 1213.23, 1170.79, 1112.93, 1087.85, 1053.13, 1020.34, 754.17; LC-MS: m/z calcd. for $C_{25}H_{19}Cl_2NO_3$ 452.3 found 454.0 [M+2].



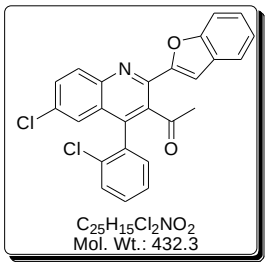
White solid, m.p 140- 142 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 - 8.13 (d, *J* = 8.94 Hz, 1H), 7.75 - 7.73 (d, *J* = 2.13 Hz, 2H), 7.71 - 7.68 (dd, *J* = 8.99, 2.33Hz, 1H), 7.59 - 7.56 (dd, *J* = 7.98, 0.72 Hz, 1H), 7.49 - 7.45 (td, *J* = 7.45, 1.73 Hz, 1H), 7.42 - 7.38 (td, *J* = 7.44, 1.12 Hz, 1H), 7.32 - 7.29 (m, 2H), 7.01 - 6.99 (d, *J* = 8.82 Hz, 2H), 3.95 - 3.89 (q, *J* = 7.12 Hz, 2H), 3.86 (s, 3H), 0.88 - 0.84 (t, *J* = 7.13 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 160.6, 156.0, 146.2, 143.9, 134.1, 133.8, 133.1, 132.2, 131.6, 131.4, 131.1, 130.4, 130.1, 129.7, 127.7, 126.8, 125.6, 124.8, 114.0, 61.4, 55.4, 13.5



Off white solid, m.p 160- 162 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 - 8.18 (d, *J* = 9.02 Hz, 1H), 8.15 - 8.13 (dd, *J* = 7.09, 1.32 Hz, 1H), 7.92 - 7.89 (dd, *J* = 6.90, 2.11 Hz, 1H), 7.77 (s, 1H), 7.75 - 7.72 (dd, *J* = 8.98, 2.30 Hz, 1H), 7.59 - 7.58 (d, *J* = 7.73 Hz, 1H), 7.50 - 7.34 (m, 6H), 3.83 - 3.81 (q, *J* = 2.93 Hz, 2H), 0.75 - 0.72 (t, *J* = 7.14 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 151.5, 146.1, 144.1, 140.1, 138.1, 135.1, 133.8, 133.7, 133.6, 131.8, 131.4, 131.0, 130.5, 129.7, 128.7, 127.5, 126.8, 125.9, 124.9, 124.9, 124.7, 123.8, 122.5, 61.5, 13.3.; IR (v, cm^{-1}) 3089 ,2978 ,2864,1722 ,1597, 1564, 1545, 1489, 1469, 1431, 1402, 1313, 1300, 1221, 1128, 1088, 1009, 835, 759.

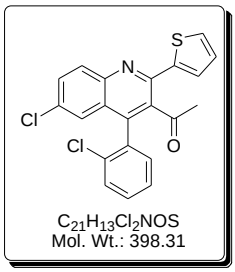


White solid, m.p 111- 114 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.195 - 8.173 (d, *J* = 8.96 Hz, 1H), 7.733 - 7.688 (m, 3H), 7.562 - 7.539 (dd, *J* = 1.41, 1.41 Hz, 1H), 7.505 - 7.402 (m, 5H), 7.340 - 7.317 (dd, *J* = 7.59, 1.40 Hz, 1H), 7.309 - 7.303 (d, *J* = 2.17 Hz, 1H), 1.938 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.68, 155.58, 145.92, 142.20, 139.53, 135.43, 133.49, 133.43, 133.05, 131.90, 131.54, 131.48, 130.54, 129.82, 129.42, 129.12, 128.84, 126.96, 126.11, 124.82, 31.77.; IR (v, cm^{-1}), 3224.98, 3091.89, 3059.10, 2995.45, 2958.80, 2922.16, 2852.72, 1697.36, 1639.49, 1627.92, 1548.84, 1483.26, 1467.83, 1444.68, 1431.18, 1394.53, 1342.46, 1226.73, 1195.87, 1180.44, 1130.29, 1097.50, 1078.21, 1055.06, 1033.85, 972.12, 921.97, 827.46, 794.67, 765.74, 754.17, 732.95, 721.38.; LC-MS: m/z calcd. for $C_{23}H_{15}Cl_2NO$ 392.3 found 394.0 [M+2].

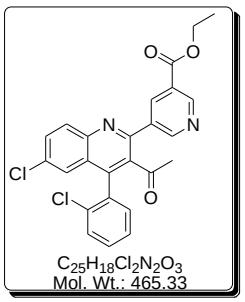


Light yellow solid, m.p 196- 199 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.175 - 8.152 (d, *J* = 9.02 Hz, 1H), 7.723 - 7.706 (dd, *J* = 6.69, 2.27 Hz, 1H), 7.700 - 7.688 (t, *J* = 2.35 Hz, 1H), 7.631 - 7.629 (d, *J* = 0.8 Hz, 1H), 7.603 - 7.581 (dd, *J* = 7.89, 0.91 Hz, 1H), 7.544 – 7.524 (d, *J* = 7.92 Hz, 1H), 7.509 - 7.486 (dd, *J* = 7.97, 1.65 Hz, 1H), 7.471 - 7.430 (dt, *J* = 7.41, 1.27, Hz, 1H), 7.387 - 7.346 (dt, *J* = 7.18, 1.14 Hz, 1H), 7.321 - 7.311 (dd, *J* = 3.06, 1.68 Hz, 1H), 7.302 - 7.293 (t, *J* = 1.85 Hz, 1H), 7.273 - 7.261 (d, *J* = 4.72 Hz, 1H), 2.325 (s, 3H).; ^{13}C NMR (100 MHz , $CDCl_3$) δ 202.90, 155.53, 153.67, 145.92, 144.75, 141.86, 133.98, 133.86, 133.36, 132.90, 132.23, 131.73, 131.42, 130.84, 129.94, 128.30, 127.22, 126.39, 125.92, 124.67, 123.64, 122.11, 111.78, 108.67, 31.79.; IR (v, Cm^{-1}), 3130.47, 3055.24, 2924.09, 2854.65, 1705.07, 1612.49, 1546.91, 1471.69, 1425.40, 1384.89, 1352.10, 1328.95, 1257.59, 1197.79, 1161.15, 1132.21,

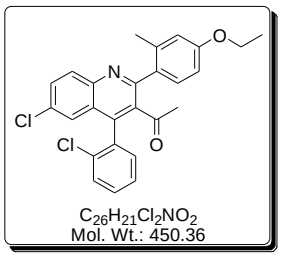
1087.85, 1055.06, 912.33, 819.75, 769.60, 748.38, 540.07.; LC-MS: m/z calcd. for $C_{25}H_{15}Cl_2NO_2$ 432.3 found 434.0 [M+2].



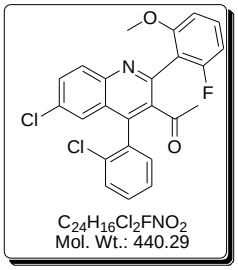
White solid, m.p 125- 128 °C**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.146 - 8.123 (d, *J* = 9Hz, 1H), 7.695 - 7.673 (m, 1H), 7.593 - 7.582 (d, *J* = 4.52 Hz, 1H), 7.563 - 7.543 (d, *J* = 7.75 Hz, 1H), 7.488 - 7.411 (m, 3H), 7.334 - 7.313 (dd, *J* = 7.38, 1.08 Hz, 1H), 7.270 - 7.265 (t, *J* = 1.88 Hz, 1H), 2.076 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.35, 150.04, 145.90, 141.76, 140.60, 135.06, 133.31, 133.20, 133.08, 132.03, 131.47, 131.32, 130.61, 129.83, 128.39, 126.99, 126.94, 126.50, 125.97, 124.68, 31.78.; IR (v, cm^{-1}), 3111.18, 3076.46, 2958.80, 2924.09, 2852.72, 1705.07, 1564.27, 1548.84, 1467.83, 1433.11, 1384.89, 1352.10, 1321.24, 1195.87, 1170.79, 1097.50, 1080.14, 1056.99, 1031.92, 1014.56, 970.19, 866.04, 844.82, 833.25, 808.17, 792.74, 763.81, 746.45.; LC-MS: m/z calcd. for $C_{21}H_{13}Cl_2NOS$ 398.3 found 400.0 [M+2].



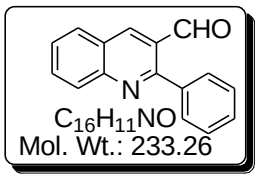
Half white solid, m.p 151- 154 °C**,** ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.326 - 9.322 (d, *J* = 1.67 Hz, 1H), 9.082 - 9.077 (d, *J* = 2.13 Hz, 1H), 8.661 - 8.652 (t, *J* = 2.00 Hz, 1H), 8.206 - 8.184 (d, *J* = 9.45 Hz, 1H), 7.778 - 7.750 (dd, *J* = 8.99, 2.16 Hz, 1H), 7.619 - 7.60 (d, *J* = 7.6 Hz, 1H), 7.546 - 7.504 (dt, *J* = 7.47, 1.56 Hz, 1H), 7.483 - 7.444 (dt, *J* = 7.47, 1.00 Hz, 1H), 7.366 - 7.361 (d, *J* = 1.93 Hz, 1H), 7.326 - 7.305 (dd, *J* = 7.48, 1.25 Hz, 1H), 4.484 - 4.431 (q, *J* = 7.11 Hz, 2H), 2.048 (s, 3H), 1.453 - 1.418 (t, *J* = 7.09 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.01, 164.77, 153.09, 151.71, 151.09, 146.01, 142.58, 137.46, 135.35, 135.15, 134.36, 133.12, 133.09, 132.08, 131.89, 131.59, 131.00, 130.06, 127.36, 126.19, 126.17, 124.83, 61.70, 31.91, 14.28.; IR (v, cm^{-1}) δ 3072.60, 2980.02, 2910.58, 2852.72, 1720.50, 1705.07, 1602.85, 1560.41, 1546.91, 1469.76, 1456.26, 1421.54, 1392.61, 1361.74, 1271.09, 1224.80, 1186.22, 1128.36, 1112.93, 1099.43, 1080.14, 1022.27, 831.32, 767.67, 738.74, 661.58, 557.43, 516.92.; LC-MS: m/z calcd. for $C_{25}H_{18}Cl_2N_2O_3$ 465.3 found 467.0 [M+1].



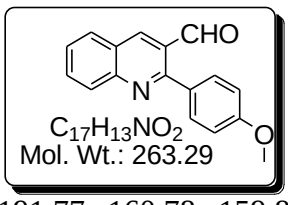
White solid, m.p 132- 135 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.159 - 8.137 (d, *J* = 8.97 Hz, 1H), 7.714 - 7.687 (dd, *J* = 8.96, 1.83 Hz, 1H), 7.563 - 7.543(d, *J* = 7.76 Hz, 1H), 7.479 - 7.400 (m, 2H), 7.339 - 7.322 (m, 2H), 7.230 - 7.209 (d, *J* = 8.4 Hz, 1H), 4.089 - 4.037 (q, *J* = 7.04 Hz, 2H), 1.886 (s, 3H), 2.282 (s, 3H), 1.442 - 1.408 (t, *J* = 6.97 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.66, 159.35, 156.13, 145.53, 141.48, 137.99, 136.31, 133.38, 133.18, 132.95, 131.66, 131.22, 131.08, 130.52, 130.36, 129.67, 126.85, 125.86, 124.61, 116.77, 111.52, 63.26, 31.03, 20.08, 14.66.; IR (v, cm^{-1}) δ 3053.32, 3037.89, 2980.02, 2924.09, 2899.01, 2881.65, 1703.14, 1608.63, 1568.13, 1548.84, 1502.55, 1465.90, 1435.04, 1388.75, 1350.17, 1338.60, 1294.24, 1244.09, 1193.94, 1170.79, 1124.50, 1114.86, 1078.21, 1055.06, 962.48, 879.54, 852.54, 833.25, 808.17, 790.81, 759.95.; LC-MS: m/z calcd. for $C_{26}H_{21}Cl_2NO_2$ 450.4 found 452.2 [M+1].



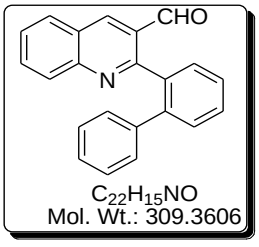
.Light yellow solid, m.p 80- 83 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.198 - 8.167 (dd, *J* = 8.92, 3.49 Hz, 1H), 7.715 - 7.693 (d, *J* = 8.90 Hz, 1H), 7.612 -7.660 (dd, *J* = 13.01, 7.97 Hz, 1H), 7.512 - 7.475 (t, *J* = 7.51 Hz, 1H), 7.430 - 7.413 (d, *J* = 6.85 Hz, 1H), 7.393 - 7.270 (m, 3H), 6.872 - 6.727 (m, 2H), 3.752 (s, 3H), 1.911 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.72, 159.26, 158.44, 158.37, 157.49, 157.42, 149.26, 146.14, 146.01, 141.19, 141.09, 136.94, 136.77, 133.88, 133.76, 133.73, 133.57, 133.44, 133.29, 132.14, 131.92, 131.61, 131.29, 131.08, 130.98, 130.91, 130.81, 130.69, 130.04, 129.95, 127.54, 127.07, 126.41, 126.15, 124.80, 124.78, 117.06, 116.98, 116.88, 116.79, 108.94, 108.72, 108.43, 108.21, 107.03, 107.00, 106.49, 106.47, 56.10, 55.83, 30.34, 29.92.; IR (v, cm^{-1}), 3116.97, 3072.60, 3008.95, 2956.87, 2926.01, 2839.22, 1699.29, 1616.35, 1579.70, 1552.70, 1471.69, 1436.97, 1384.89, 1354.03, 1276.88, 1240.23, 1197.79, 1083.99, 1035.77, 931.62, 833.25, 785.03, 744.52, 686.66. LC-MS: m/z calcd. for $C_{24}H_{16}Cl_2FNO_2$ 440.3 found 442.0 [M+2].



Off White solid, m.p 110- 112 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.191 (s, 1H), 8.867 (s, 1H), 8.236 - 8.214 (d, *J* = 8.8 Hz, 1H), 8.042 - 8.024 (d, *J* = 7.2 Hz, 1H), 7.090 - 7.867 (t, *J* = 8.0 Hz, 1H), 7.705 - 7.625 (m, 3H), 7.582 - 7.561 (m, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.73, 160.50, 149.78, 138.3, 137.90, 132.84, 130.41, 129.76, 129.63, 129.58, 128.92, 127.80, 127.68, 126.55.; IR (v, cm^{-1}), 3053.32, 3028.24, 2927.94, 2862.36, 2746.63, 1693.50, 1676.14, 1656.85, 1614.42, 1583.56, 1575.84, 1554.63, 1487.12, 1454.33, 1384.89, 1371.39, 1157.29, 1122.57, 1076.28, 1008.77, 821.68, 775.38, 754.17, 713.66, 704.02, 613.36, 457.13.; LC-MS: m/z calcd. for $C_{16}H_{11}NO$ 233.3 found 234.0 [M+1].

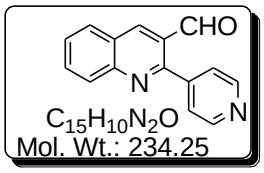


.White solid, m.p 132- 134 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.83 (s, 1H), 8.25 - 8.22 (t, *J* = 5.8 Hz, 1H), 7.87 - 7.84 (t, *J* = 5.2 Hz, 1H), 8.00 - 7.99 (d , *J* = 5.6 Hz, 1H), 7.65 - 7.59 (m, 3H), 7.10 - 7.08 (m, 2H), 3.901 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.77, 160.78, 159.86, 149.71, 138.20, 132.52, 131.77, 130.23, 129.50, 129.42, 127.69, 127.23, 126.20, 114.27, 55.47.; IR (v, cm^{-1}) δ 3049.46, 2970.38, 2939.52, 2854.65, 2843.07, 1691.57, 1656.85, 1604.77, 1583.56, 1552.70, 1516.05, 1487.12, 1454.33, 1384.89, 1371.39, 1296.16, 1257.59, 1174.65, 1155.36, 1111.00, 1035.77, 1020.34, 842.89, 788.89, 752.24, 736.81, 549.71, 487.99.; LC-MS: m/z calcd. for $C_{17}H_{13}NO_2$ 263.3 found 264.1 . [M+1].

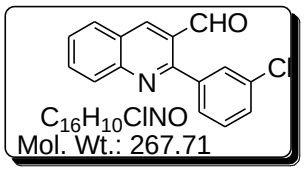


White solid, m.p 97- 99 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.55 (s, 1H), 8.39 (s, 1H), 8.13 - 8.12 (d, *J* = 4.0 Hz, 1H), 7.81 - 7.73 (m, 2H), 7.640 - 7.61 (t, *J* = 4.4 Hz, 1H), 7.52 - 7.45 (m, 3H), 7.41 - 7.39 (d, *J* = 7.8 Hz, 1H), 6.99 - 6.95 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.78, 159.65, 148.48, 140.70, 138.45, 135.75, 135.35, 131.31, 129.71, 128.83, 128.72, 128.66, 128.39, 128.37, 127.21, 126.98, 126.31, 126.29, 126.17, 125.33; IR (v, cm^{-1}) δ 3057.17, 3043.67, 3026.31, 2852.72, 2723.49, 1693.50, 1658.78,

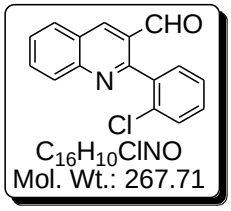
1616.35, 1585.49, 1556.55, 1490.97, 1479.40, 1450.47, 1436.97, 1384.89, 1367.53, 1276.88, 1153.43, 1124.50, 1107.14, 1018.41, 1008.77, 920.05, 825.53, 756.10, 748.38, 700.16, 513.07; LC-MS: m/z calcd. for $C_{22}H_{15}NO$ 309.4 found 310.1[M+1].



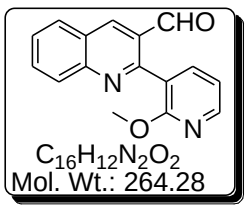
Off White solid, m.p 130-132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.89 (s, 1H), 8.84 - 8.83 (d, *J* = 5.6 Hz, 2H), 8.24 -8.21 (d, *J* = 8.8 Hz, 1H), 8.07 - 8.05 (d, *J* = 8.4 Hz, 1H), 7.95 - 7.91 (t, *J* = 7.7 Hz, 1H), 7.72 - 7.68 (t, *J* = 7.6 Hz, 1H), 7.62 - 7.61 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.23, 157.50, 150.19, 149.59, 145.52, 139.09, 133.17, 129.79, 129.54, 128.31, 127.40, 126.77, 124.58; IR (v, cm^{-1}), 3045.60, 3024.38, 2993.52, 2872.01, 2758.21, 1689.64, 1616.35, 1598.99, 1579.70, 1544.98, 1489.05, 1409.96, 1394.53, 1375.25, 1186.22, 1161.15, 1120.64, 835.18, 786.96, 758.02, 721.38, 698.23, 540.07, 462.92; LC-MS: m/z calcd. for $C_{15}H_{10}N_2O$ 234.3 found 235.1 [M+1].



Off White solid, m.p 125- 127 °C**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 8.87 (s, 1H), 8.22 - 8.20 (d, *J* = 8.4 Hz, 1H), 8.06 - 8.04 (d, *J* = 8Hz, 1H), 7.91 - 7.87 (t, *J* = 7.6 Hz, 1H), 7.70 - 7.66 (t, *J* = 7.6 Hz, 1H), 7.61 - 7.59 (t, *J* = 4 Hz, 1H), 7.54 - 7.52 (t , *J* = 3.6 Hz, 1H), 7.50 -7.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.60, 158.20, 149.84, 137.74, 137.04, 133.28, 132. 88, 131.61, 130.84, 129.81, 129.79, 129.74, 128.07, 127.90, 127.63, 126.99; IR (v, cm^{-1}), 3068.75, 2873.94, 1693.50, 1616.35, 1587.42, 1554.63, 1494.83, 1452.40, 1435.04, 1384.89, 1371.39, 1159.22, 1124.50, 1064.71, 823.60, 765.74, 756.10, 709.80.

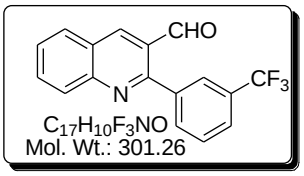


Pale yellow solid, m.p 102- 104 °C**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 8.86 (s, 1H), 8.22 - 8.20 (d, *J* = 8.4 Hz, 1H), 8.04 - 8.02 (d, *J* = 8.4 Hz, 1H), 7.92 - 7.88 (t, *J* = 7.2 Hz, 1H), 7.76 - 7.75 (d, *J* = 5.6 Hz, 1H), 7.68 - 7.64 (t ,*J* = 7.6 Hz, 1H), 7.53 - 7.48 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.04, 158.85, 149.70, 139.69, 138.72, 135.11, 133.08, 130.25, 130.02, 129.78, 129.70, 129.65, 128.66, 128.02, 127.65, 126.68; IR (v, cm^{-1}) δ 3064.89, 3030.17, 2918.30, 2866.22, 1689.64, 1616.35, 1581.63, 1556.55, 1490.97, 1477.47, 1448.54, 1396.46, 1384.89, 1367.53, 1155.36, 839.03, 779.24, 758.02, 738.74, 690.52; LC-MS: m/z calcd. for $C_{16}H_{10}ClNO$ 267.7 found 268.0 [M+1].

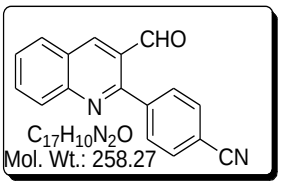


Off White solid, mp 177- 179 °C**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.79 (s, 1H), 8.36 - 8.35 (dd, *J* = 5.00, 2.0 Hz, 1H), 8.19 - 8.17 (d, *J* = 8.4 Hz, 1H), 8.03 - 8.01 (dd, *J* = 7.29, 2.0 Hz, 2H), 7.88 - 7.84 (dt, *J* = 8.38, 1.6 Hz, 1H), 7.66 - 7.62 (td , *J* = 8.04, 0.8 Hz, 1H), 7.17 - 7.14 (dd, *J* = 7.24, *4.8* Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.34, 160.87, 155.64, 149.77, 148.37, 139.99, 137.05, 132.18, 129.35, 129.28, 128.01, 127.48, 126.53, 121.44, 117.59, 53.40; IR (v, cm^{-1}), 3059.10, 2953.02, 2924.09, 2852.72, 1737.86, 1695.43, 1616.35, 1587.42, 1554.63, °1492.90, 1462.04, 1446.61, 1402.25, 1371.39,

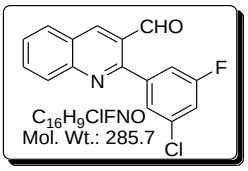
1298.09, 1257.59, 1224.80, 1157.29, 1109.07, 1070.49, 1012.63, 806.25, 788.89, 767.6; LC-MS: m/z calcd. for $C_{16}H_{12}N_2O_2$ 264.28 found 265.1 [M+1].



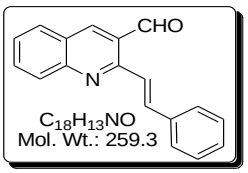
White solid, m.p 112- 114℃, ^{1}H NMR (400 MHz,$CDCl_3$) δ 10.17 (s, 1H), 8.93 (s, 1H), 8.31 (s, 1H), 8.07 - 8.03 (m, *J* = 4.00, 2H), 7.94 - 7.92 (d, *J* = 8.00 Hz, 1H), 7.86 - 7.82 (m, *J* = 8.00 Hz, 2H), 7.73- 7.69 (m, *J* = 8.40 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 158.5, 149.2, 139.5, 138.2, 133.8, 133.5, 131.7, 131.4, 129.7, 129.5, 129.4, 128.4, 127.6, 127.2, 127.2, 126.8, 126.5.; IR (v, cm^{-1}) 3123, 3074, 2925, 2874, 1695, 1687, 1619, 1585., 1487, 1460, 1431, 1384. 1342, 1325, 1255, 1173, 1151, 1113, 1097, 1078, 932, 854, 810, 759, 754, 704, 652, 478.; LC-MS: m/z calcd. for $C_{17}H_{10}F_3NO$ 301.26 found 302.1 [M+1]..



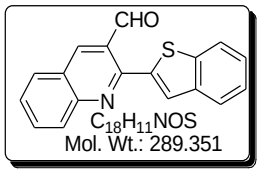
White solid, m.p 145- 147℃**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.85 (s, 1H), 8.22 - 8.20 (d, *J* = 7.20 Hz, 1H), 8.02 - 8.00 (d, *J* = 6 Hz, 1H), 7.91 - 7.86 (t, *J* = 8.8 Hz, 1H), 7.83 - 7.80 (d , *J* = 8.4 Hz, 1H), 7.77 - 7.75 (d, *J* = 8.40 Hz, 1H), 7.71 - 7.64 (t, *J* = 6.80 Hz, 1H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 157.9, 149.3, 139.9, 133.6, 133.1, 132.6, 131.1, 129.7, 129.6, 128.6, 128.1, 127.6, 126.8, 113.5.; IR (v, cm^{-1}) 3179, 3126, 2228, 1703, 1691, 1620, 1550, 1489, 1384, 852, 817, 754.



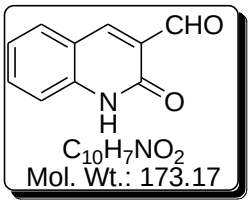
White solid, m.p 145- 147℃**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.88 (s, 1H), 8.22 - 8.20 (d, *J* = 8.40 Hz,1H), 8.06 - 8.04 (d, *J* = 8.00 Hz, 1H), 7.94 - 7.91 (t, *J* = 8.40 Hz, 1H), 7.71 - 7.67 (t, *J* = 8.00 Hz, 1H), 7.48 (s, 1H), 7.33 -7.27 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 149.6, 139.2, 133.3, 129.8, 129.7, 128.3, 127.5, 126.8, 126.4, 117.5, 117.2, 116.1, 115.8.; IR (v, cm^{-1}) 3132, 3082, 3057, 3013, 1701, 1618, 1605, 1578, 1558, 1400, 1371, 1089, 862.; LC-MS: m/z calcd. for $C_{16}H_{19}ClFNO$ 285.7 found 286.0[M+1]. .



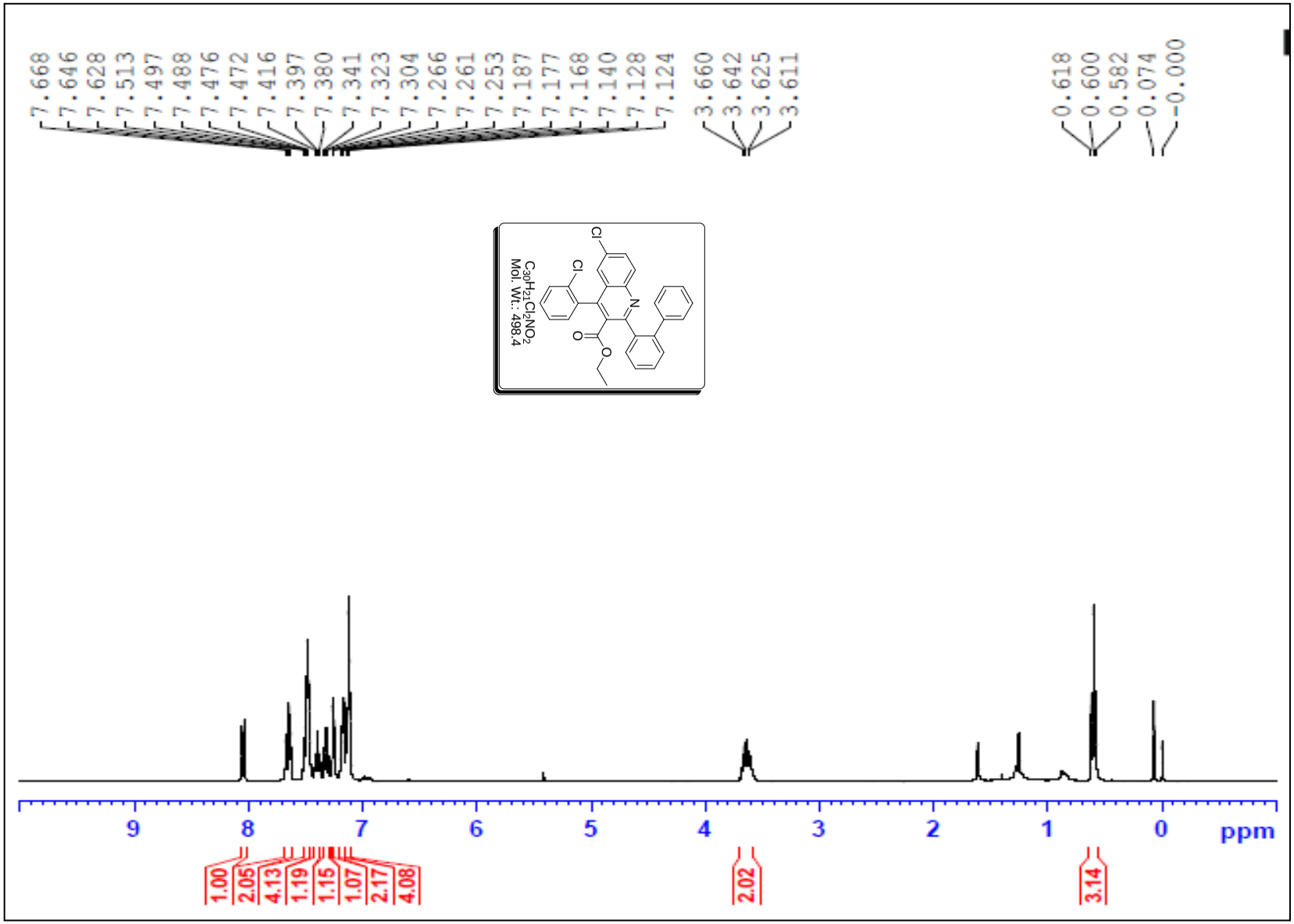
White solid, m.p 123- 128℃**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.43 (s, 1H), 8.61 (s, 1H), 8.33 - 8.29 (d, *J* = 15.6 Hz, 1H), 8.16 - 8.14 (d, *J* = 8.40 Hz, 1H), 8.11 - 8.07 (d, *J* = 15.6 Hz, 1H), 7.95 - 7.93 (d, *J* = 8.00 Hz, 1H), 7.88 - 7.84 (t, *J* = 7.20 Hz, 1H), 7.73 - 7.71 (d, *J* = 7.60 Hz, 2H), 7.60 - 7.57 (t, *J* = 7.60 Hz, 1H), 7.44 - 7.40 (t, *J* = 7.2 Hz 2H), 7.37 - 7.33 (t, *J* = 7.20 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 154.5, 149.7, 143.9, 138.1, 136.8, 133.1, 129.6, 129.1, 128.9, 127.9, 127.3, 127.2, 126.5, 123.9; IR (v, cm^{-1}) 3095, 3030, 2922, 2760, 1693, 1633, 1610, 1587, 1550, 1489, 1431, 1400, 1384, 1373, 1182, 1109, 985, 786, 763, 752, 711, 688; LC-MS: m/z calcd. for $C_{18}H_{13}NO$ 259.3 found 260.1[M+1]. .



White solid, m.p 128- 130℃**,** ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.81 (s, 1H), 8.22 - 8.19 (d, *J* = 8.80 Hz, 1H), 8.01 - 7.99 (d, *J* = 8.40 Hz, 1H), 7.95 - 7.93 (t, *J* = 4.00 Hz, 1H), 7.90 - 7.86 (m, 2H), 7.58 (s, 1H), 7.45 - 7.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.9, 152.9, 149.4, 141.1, 141.1, 139.9, 138.5, 132.7, 129.4, 129.2, 127.7, 127.6, 126.2, 125.6, 124.6, 124.4, 122.3; IR (v, cm^{-1}) 3065, 2957, 2922, 2853, 1692, 1614, 1578, 1556, 1491, 1393, 1373, 1111, 1014, 916, 862, 800, 744.5; LC-MS: m/z calcd. for $C_{18}H_{11}NOS$ 289.35 found 290.0 [M+1].



Pale yellow, m.p > 250℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.27(s, 1H), 10.28 (s, 1H), 8.54 (s, 1H), 7.96 – 7.93 (d, *J* = 8.64 Hz, 1H), 7.69 – 7.67 (d, *J* = 8.44 Hz, 1H), 7.39 – 7.38 (t, *J* = 7.84 Hz, 1H), 7.29 – 7.27 (t, *J* = 7.87 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.7, 161.4, 142.4, 141.1, 133.7, 130.9, 125.6, 122.6, 118.1, 115.4.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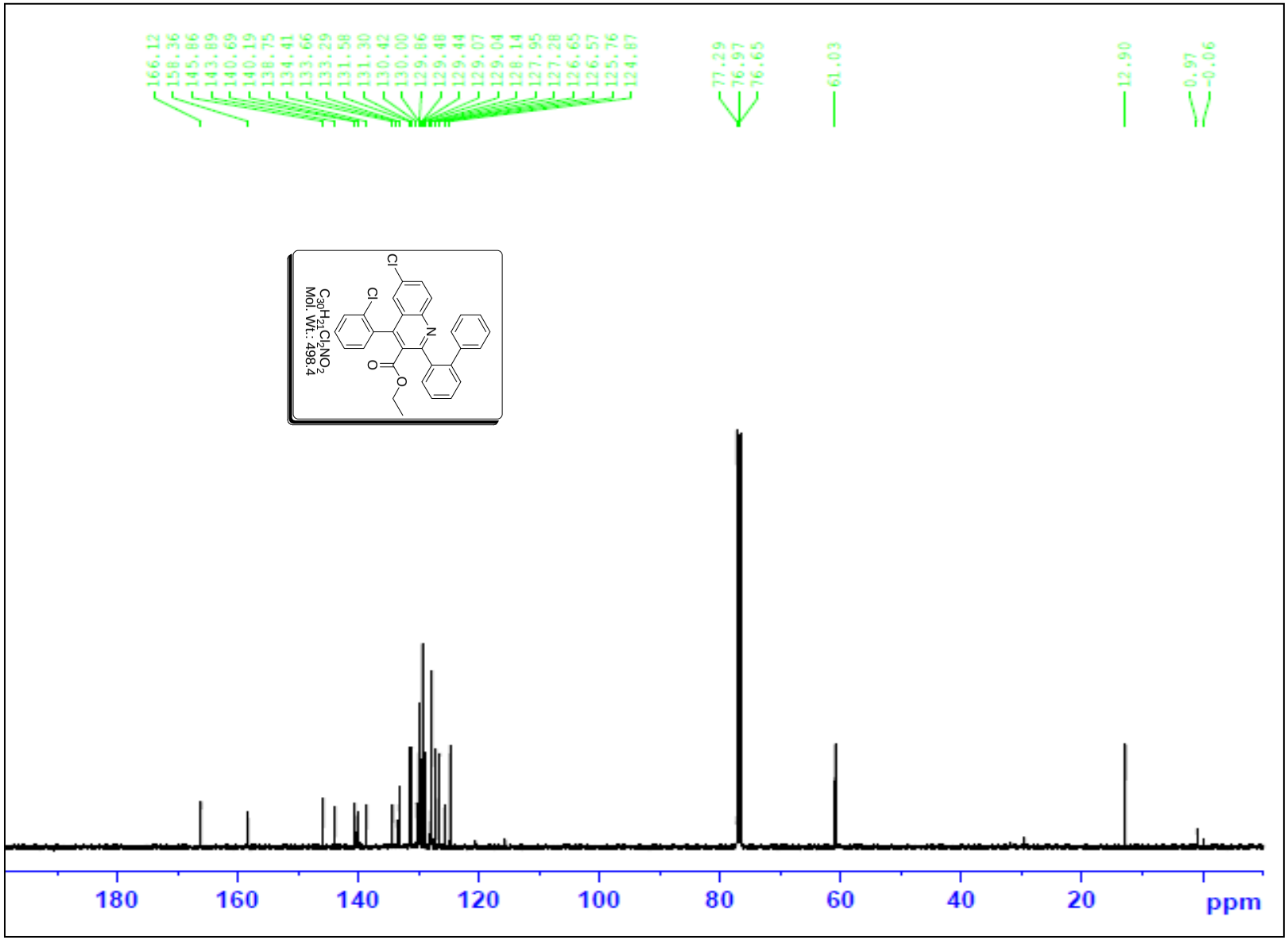
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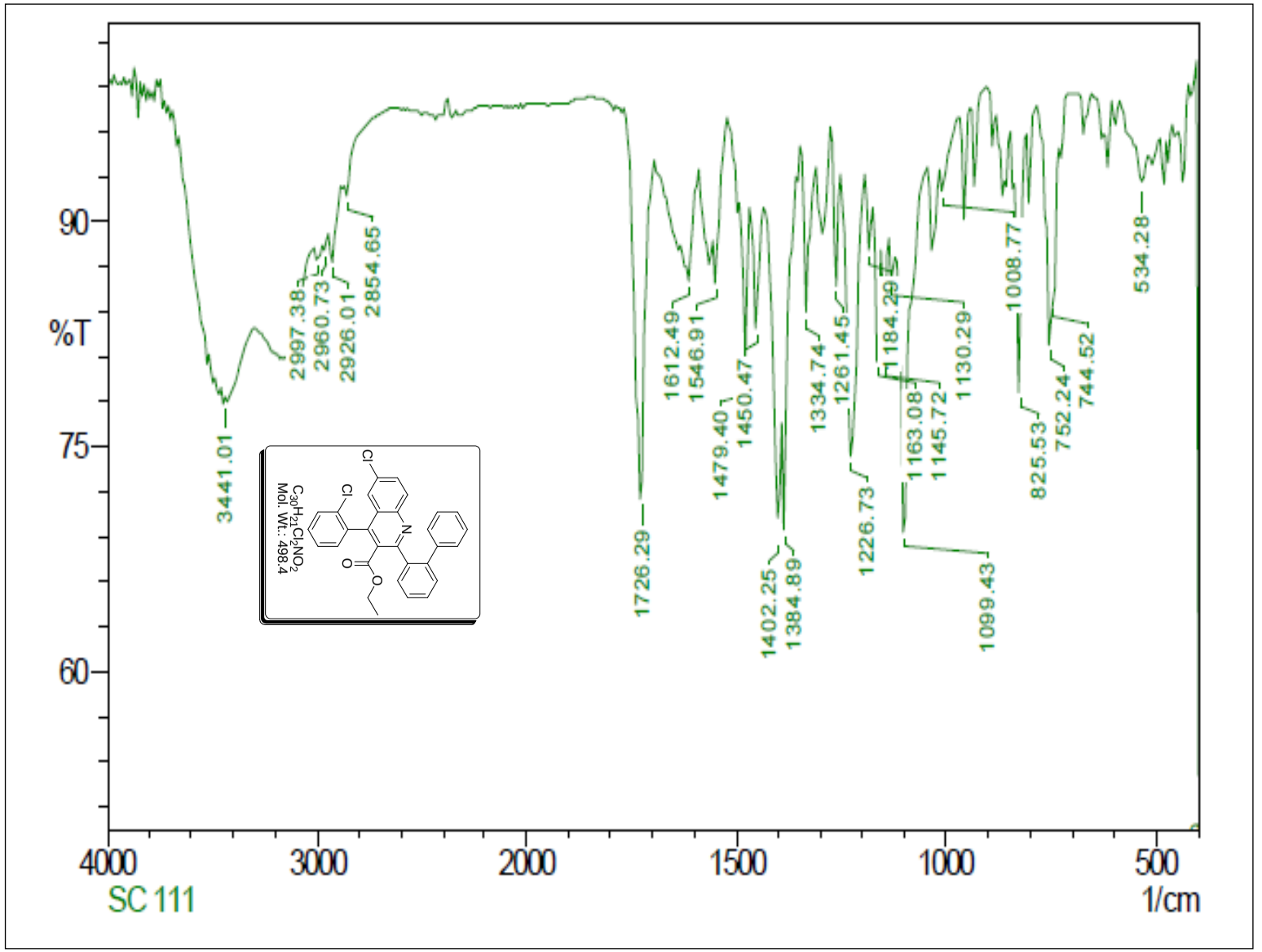
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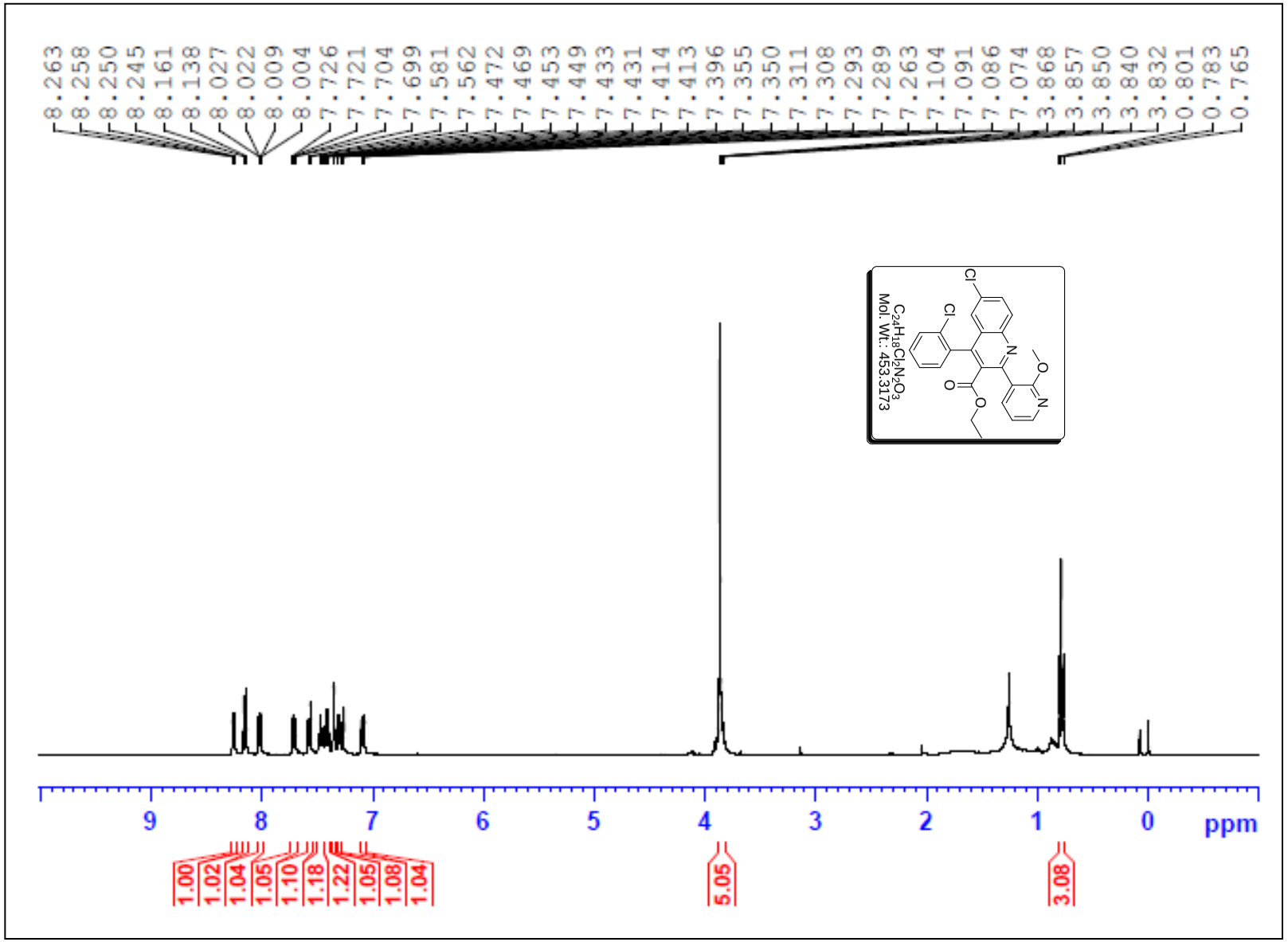
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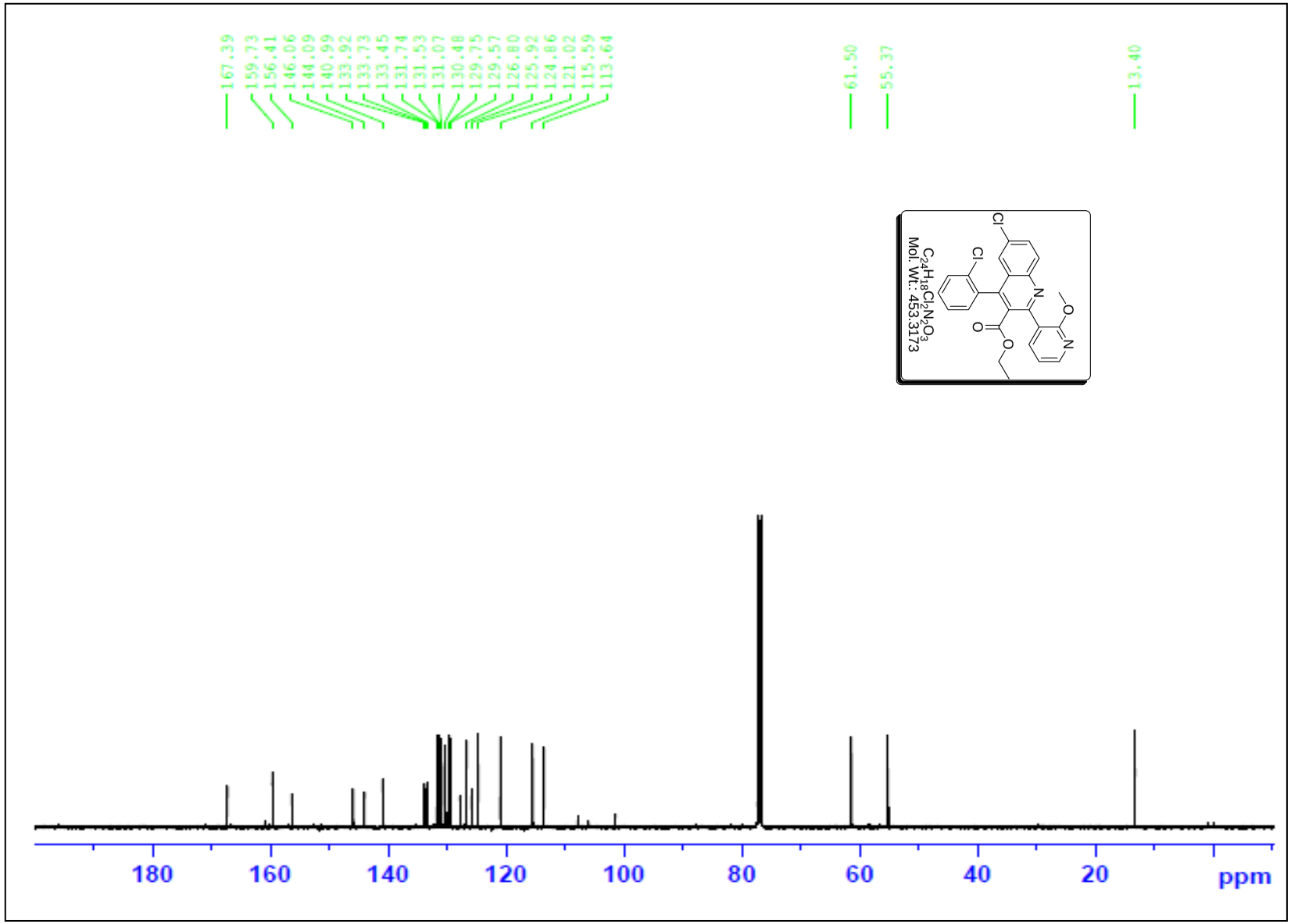
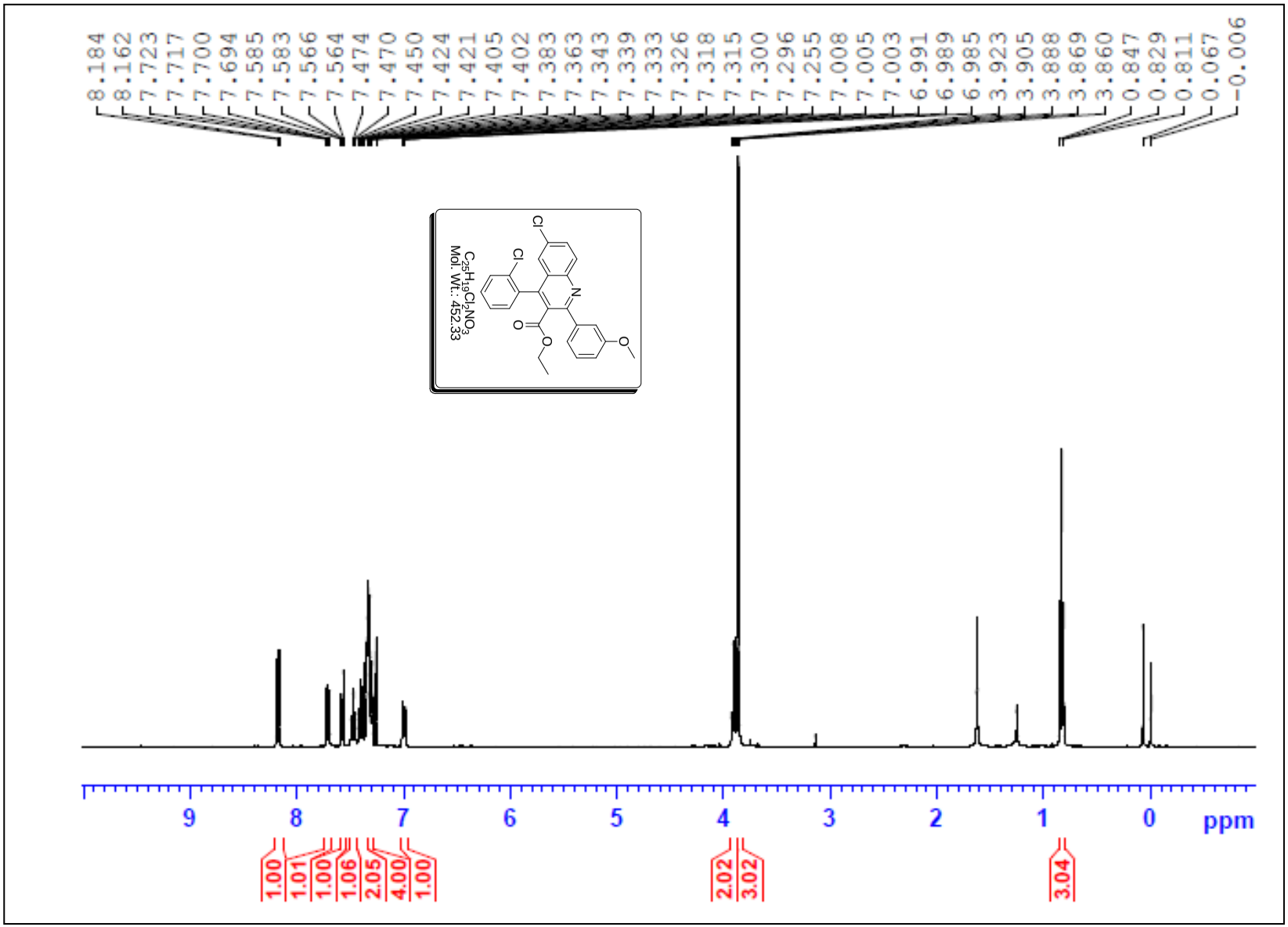
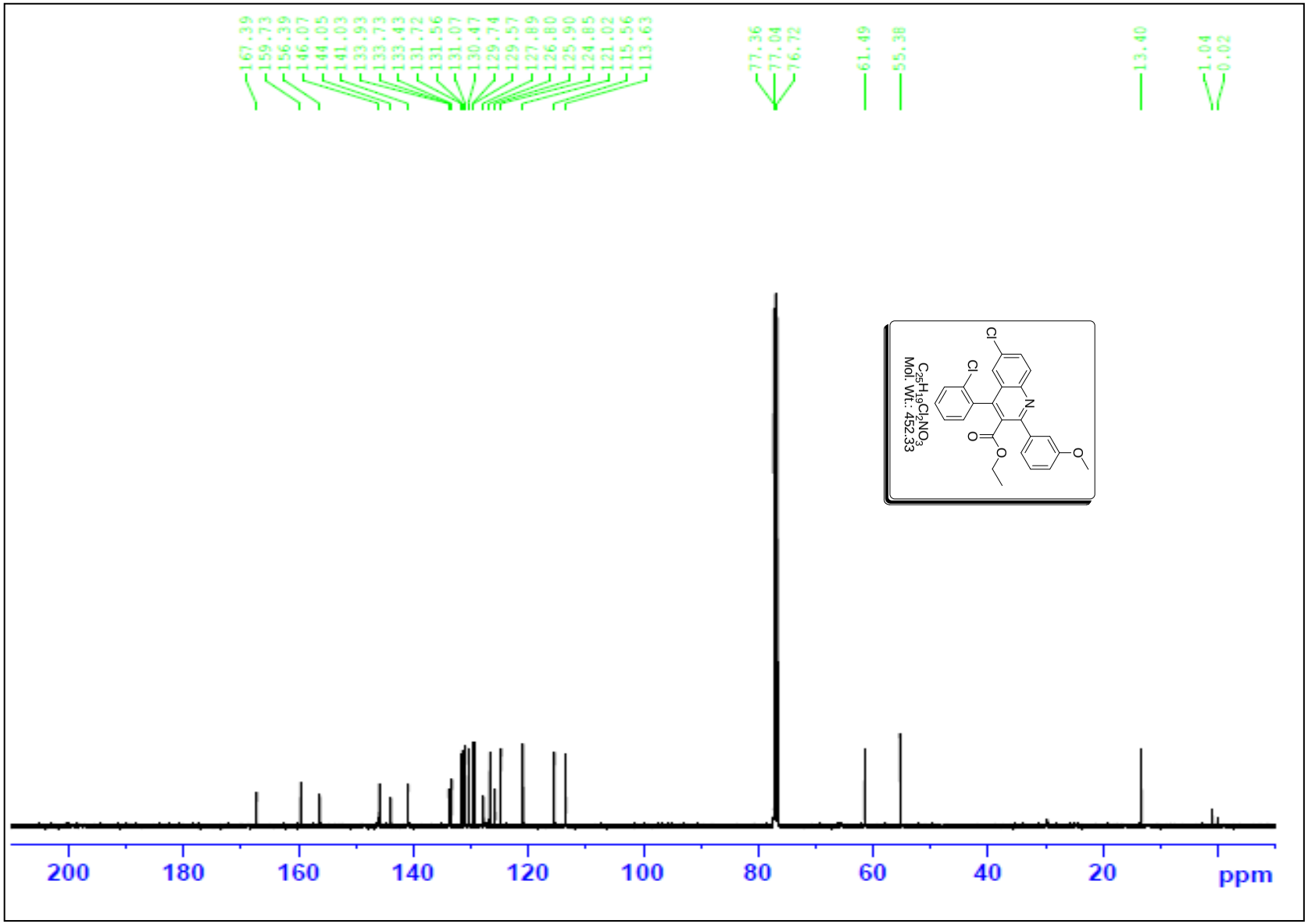
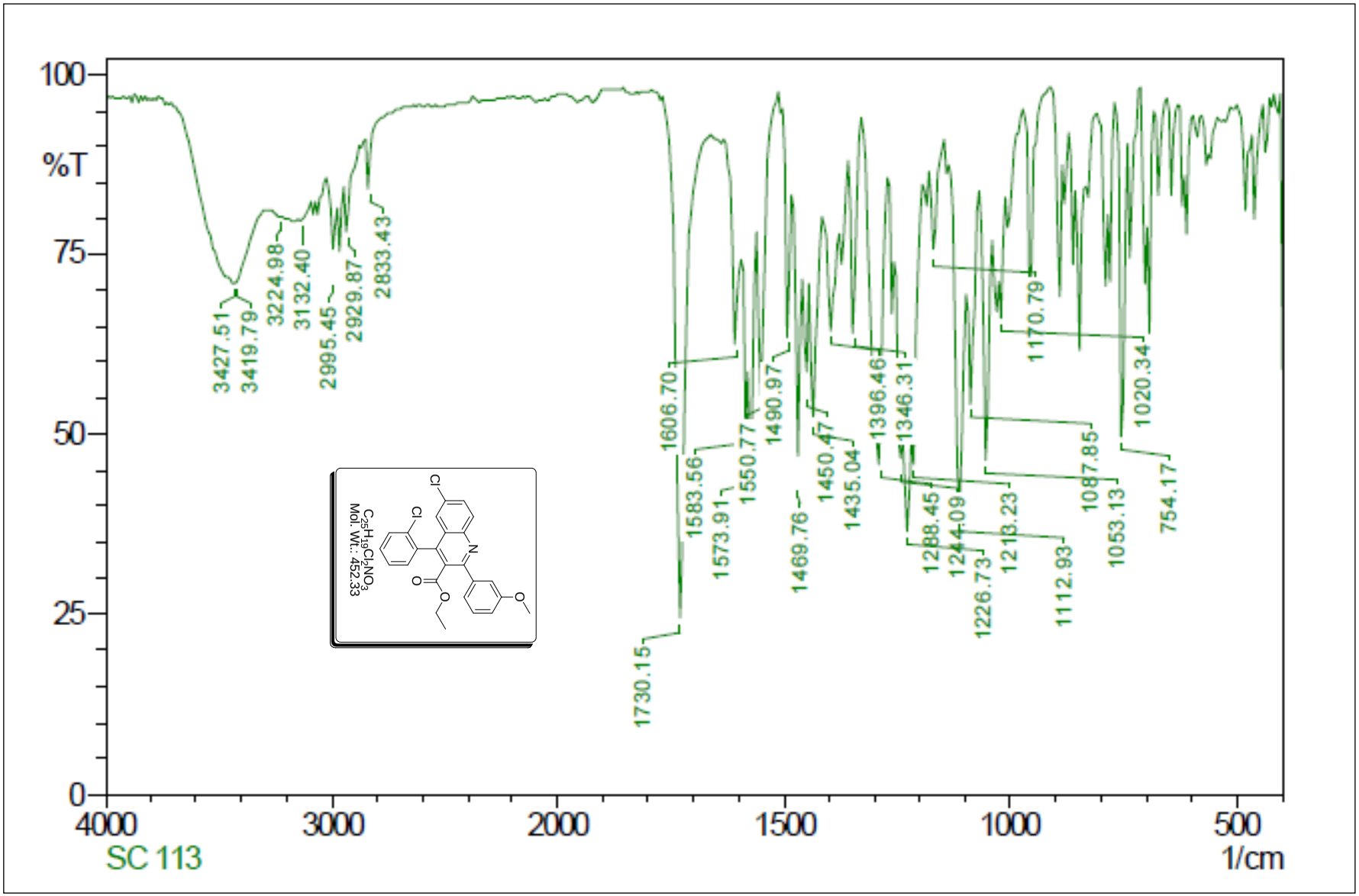
5.05
3.08

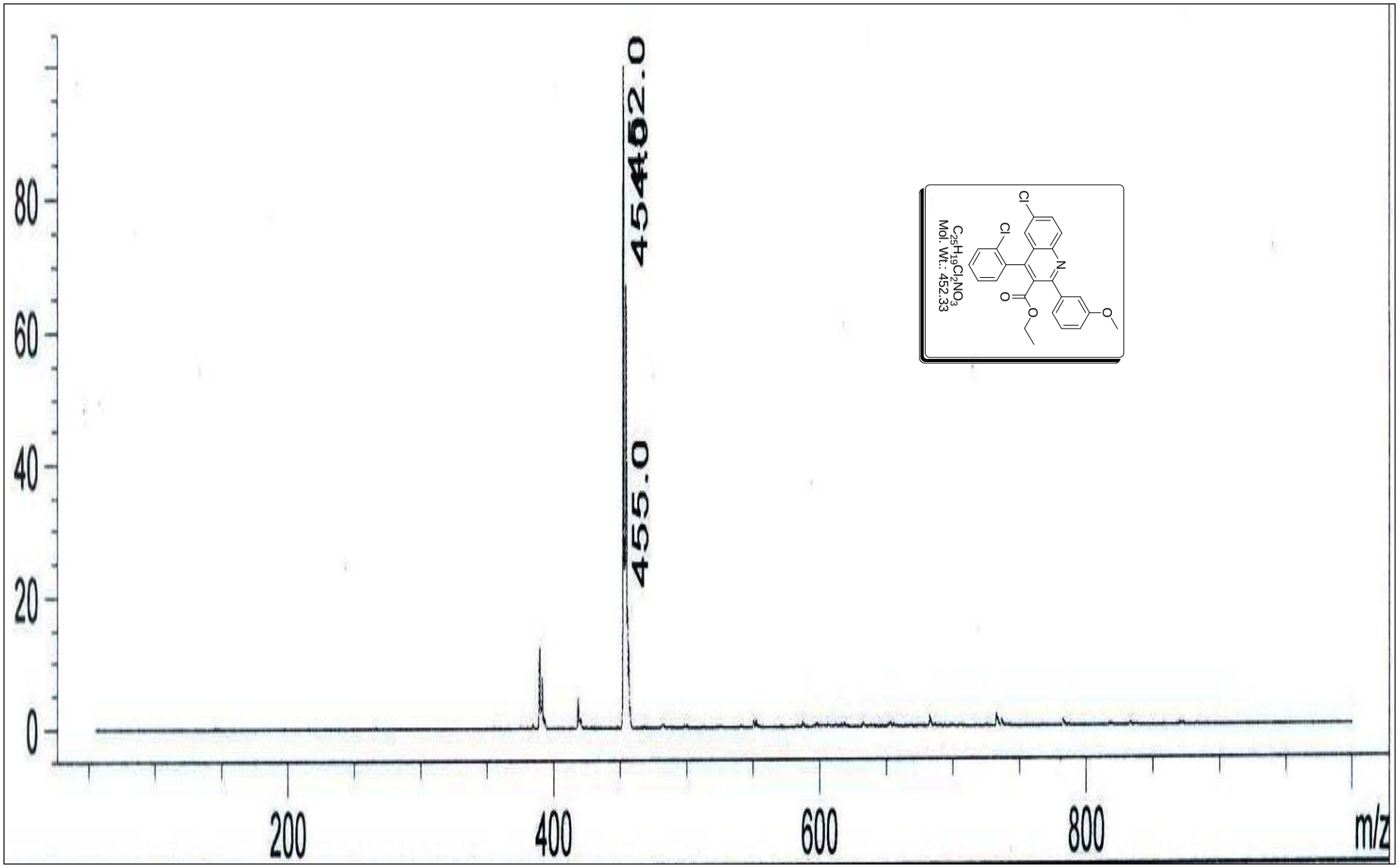

167.39
159.73
156.41
146.06
144.09
140.99
133.92
133.73
133.45
131.74
131.53
131.07
130.48
129.75
129.57
126.80
125.92
124.86
121.02
115.59
113.64
61.50
55.37
13.40
Cl
Cl
N
O
O
O
N
C24H18Cl2N2O3
Mol. Wt.: 453.3173
180
160
140
120
100
80
60
40
20
ppm

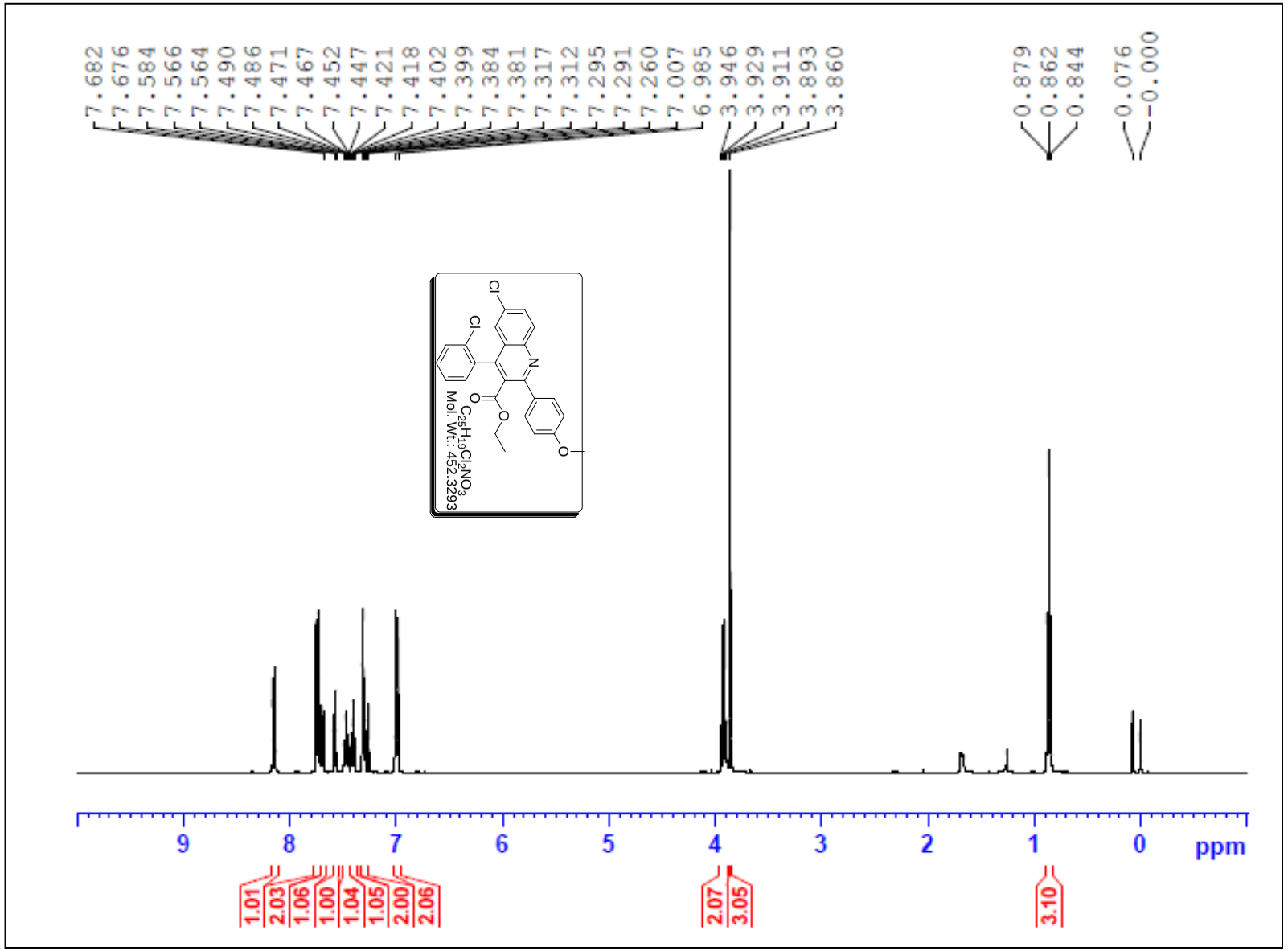
O
N
N
Cl
O
Cl
O
C24H18Cl2N2O3
Mol. Wt.: 453.3173
456.0
454603.0
800
600
400
200
40
30
20
10
0

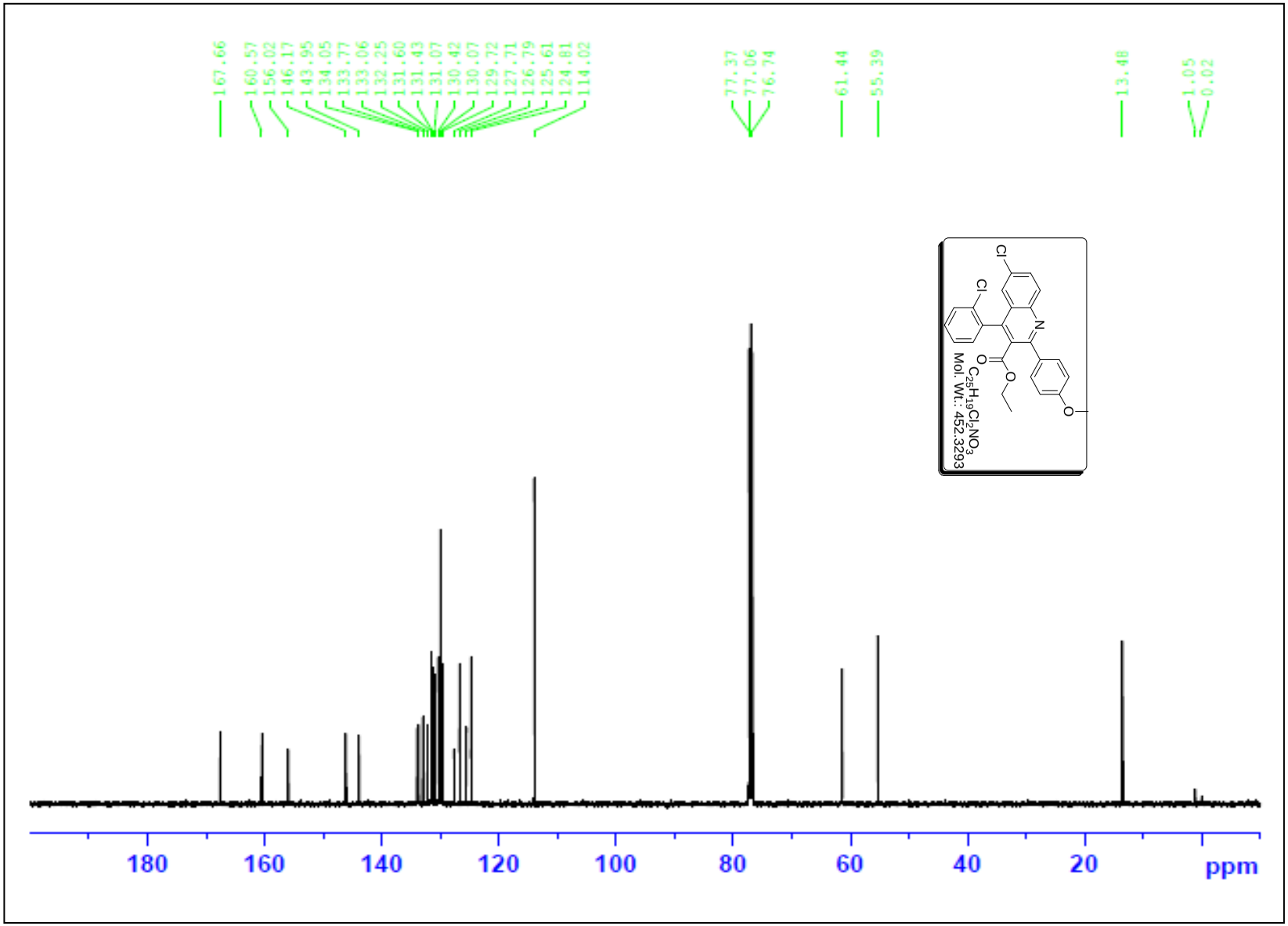

8.184
8.162
7.723
7.717
7.700
7.694
7.585
7.583
7.566
7.564
7.474
7.470
7.450
7.424
7.421
7.405
7.402
7.383
7.363
7.343
7.339
7.333
7.326
7.318
7.315
7.300
7.296
7.255
7.008
7.005
7.003
6.991
6.989
6.985
3.923
3.905
3.888
3.869
3.860
0.847
0.829
0.811
0.067
-0.006
C25H19Cl2NO3
Mol. Wt.: 452.33
Cl
Cl
N
O
O
O
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.06
2.05
4.00
1.00
2.02
3.02
3.04

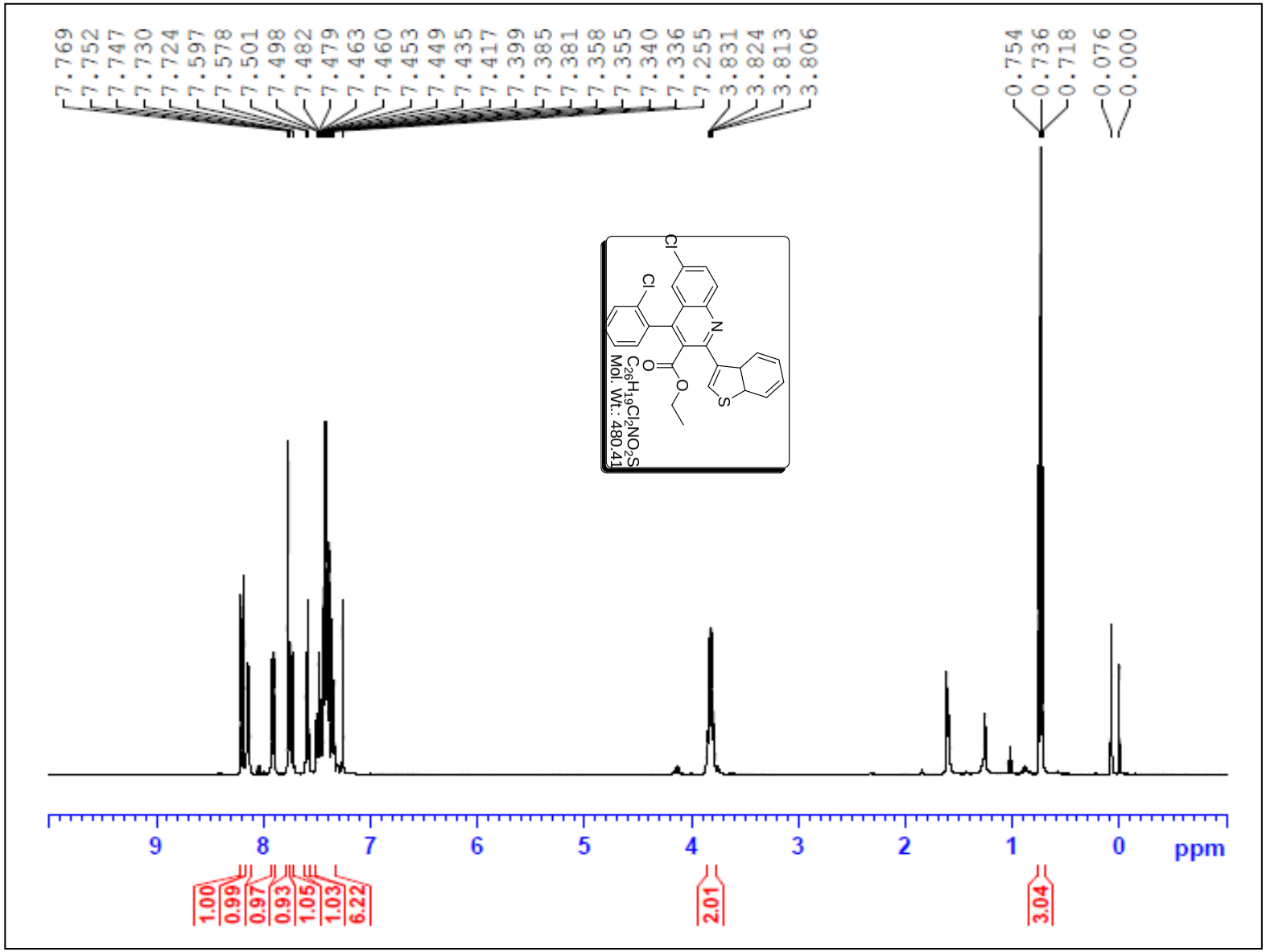

167.39
159.73
156.39
146.07
144.05
141.03
133.93
133.73
133.43
131.72
131.56
131.07
130.47
129.74
129.57
127.89
126.80
125.90
124.85
121.02
115.56
113.63
77.36
77.04
76.72
61.49
55.38
13.40
1.04
0.02
Cl
Cl
N
O
O
O
C25H19Cl2NO3
Mol. Wt.: 452.33
200
180
160
140
120
100
80
60
40
20
ppm

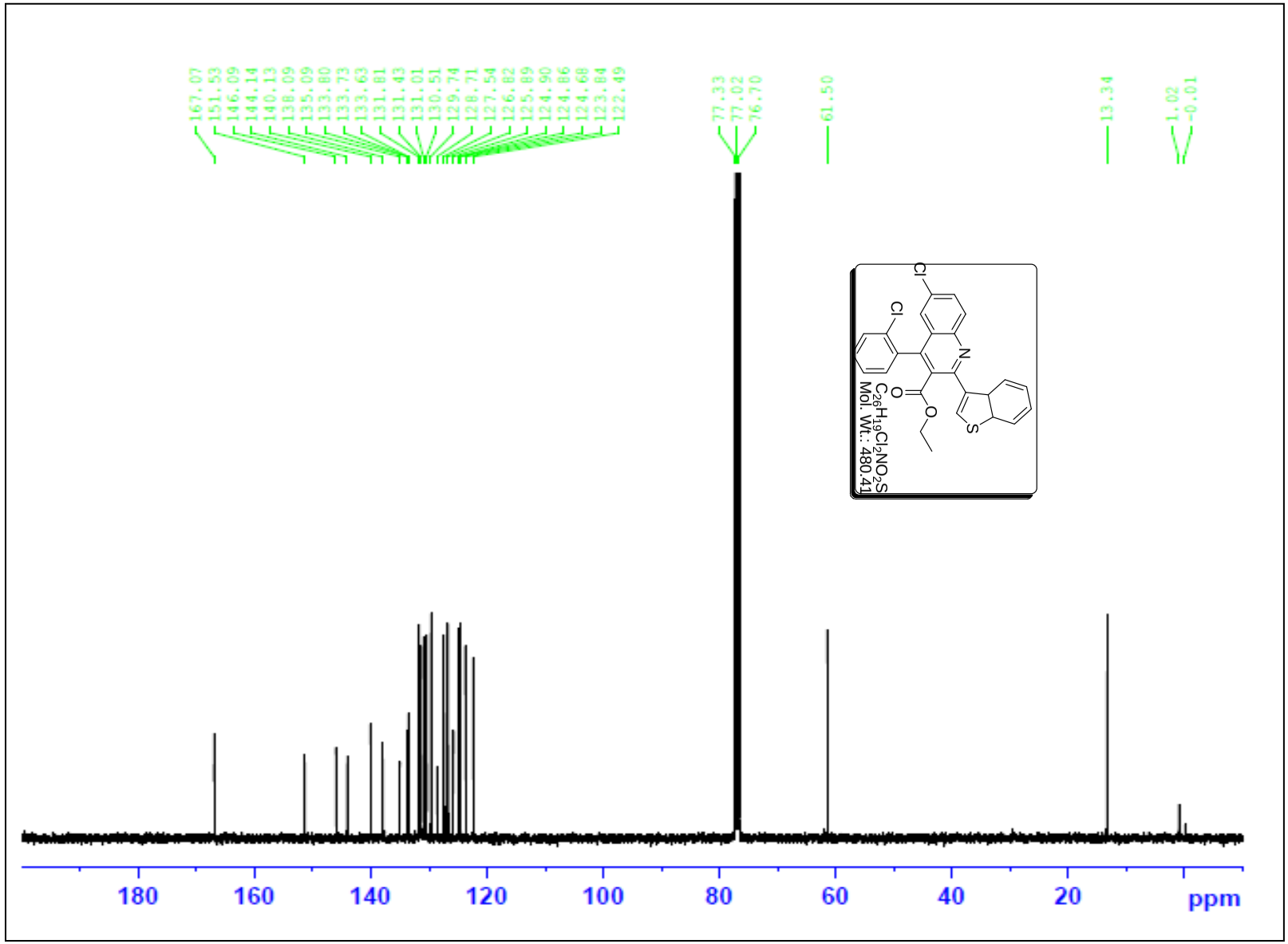

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC 113
3427.51
3419.79
3224.98
3132.40
2995.45
2929.87
2833.43
1730.15
1606.70
1583.56
1573.91
1550.77
1490.97
1469.76
1450.47
1435.04
1396.46
1346.31
1288.45
1244.09
1226.73
1213.23
1170.79
1112.93
1087.85
1053.13
1020.34
754.17
Cl
Cl
N
O
O
O
C25H19Cl2NO3
Mol. Wt.: 452.33

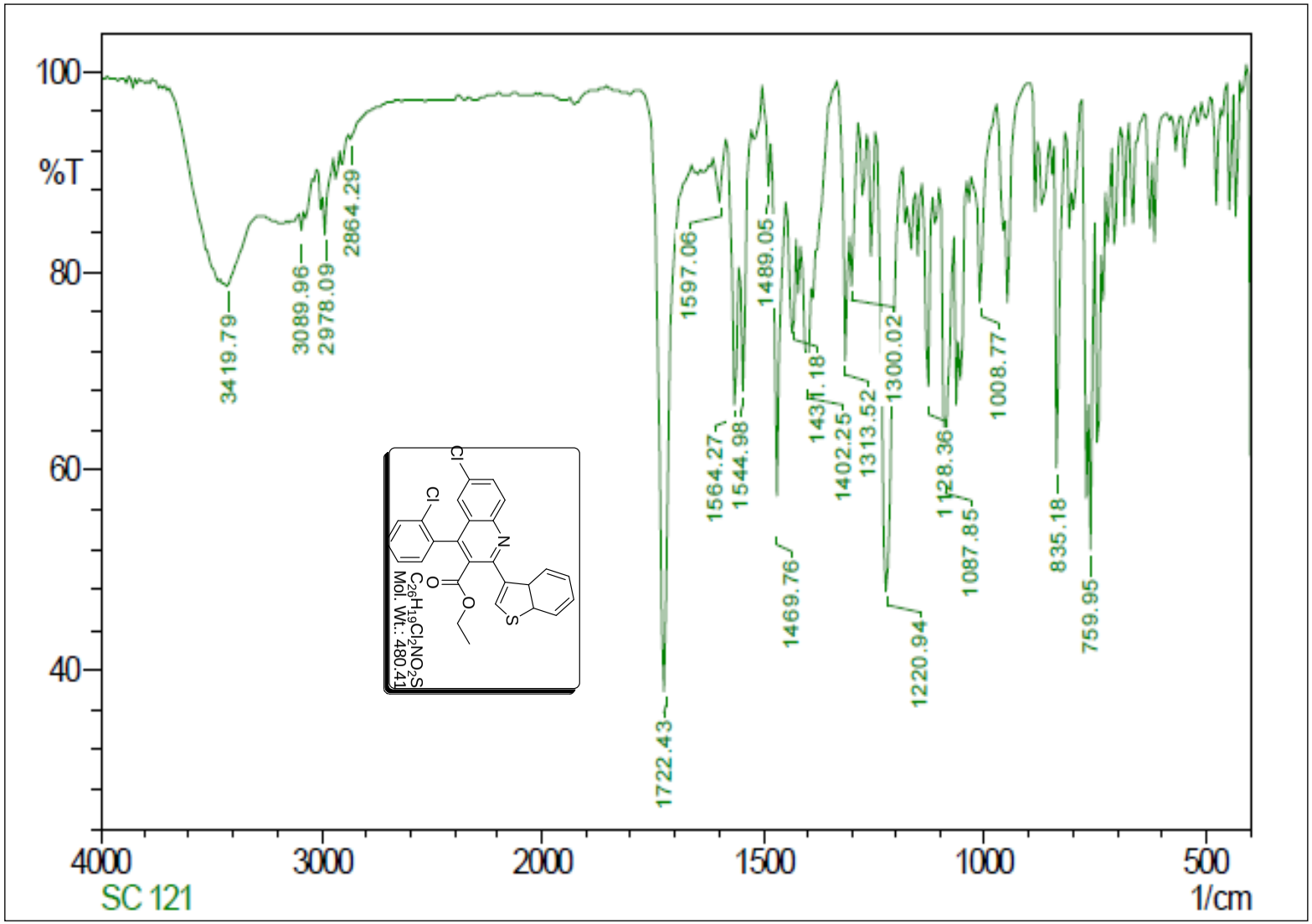

454.0
452.0
455.0
80
60
40
20
0
200
400
600
800
m/z
Cl
Cl
N
O
O
O
C25H19Cl2NO3
Mol. Wt.: 452.33


7.682
7.676
7.584
7.566
7.564
7.490
7.486
7.471
7.467
7.452
7.447
7.421
7.418
7.402
7.399
7.384
7.381
7.317
7.312
7.295
7.291
7.260
7.007
6.985
3.946
3.929
3.911
3.893
3.860
0.879
0.862
0.844
0.076
-0.000
Cl
Cl
N
O
O
O
C25H19Cl2NO3
Mol. Wt.: 452.3293
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.03
1.06
1.00
1.04
1.05
2.00
2.06
2.07
3.05
3.10

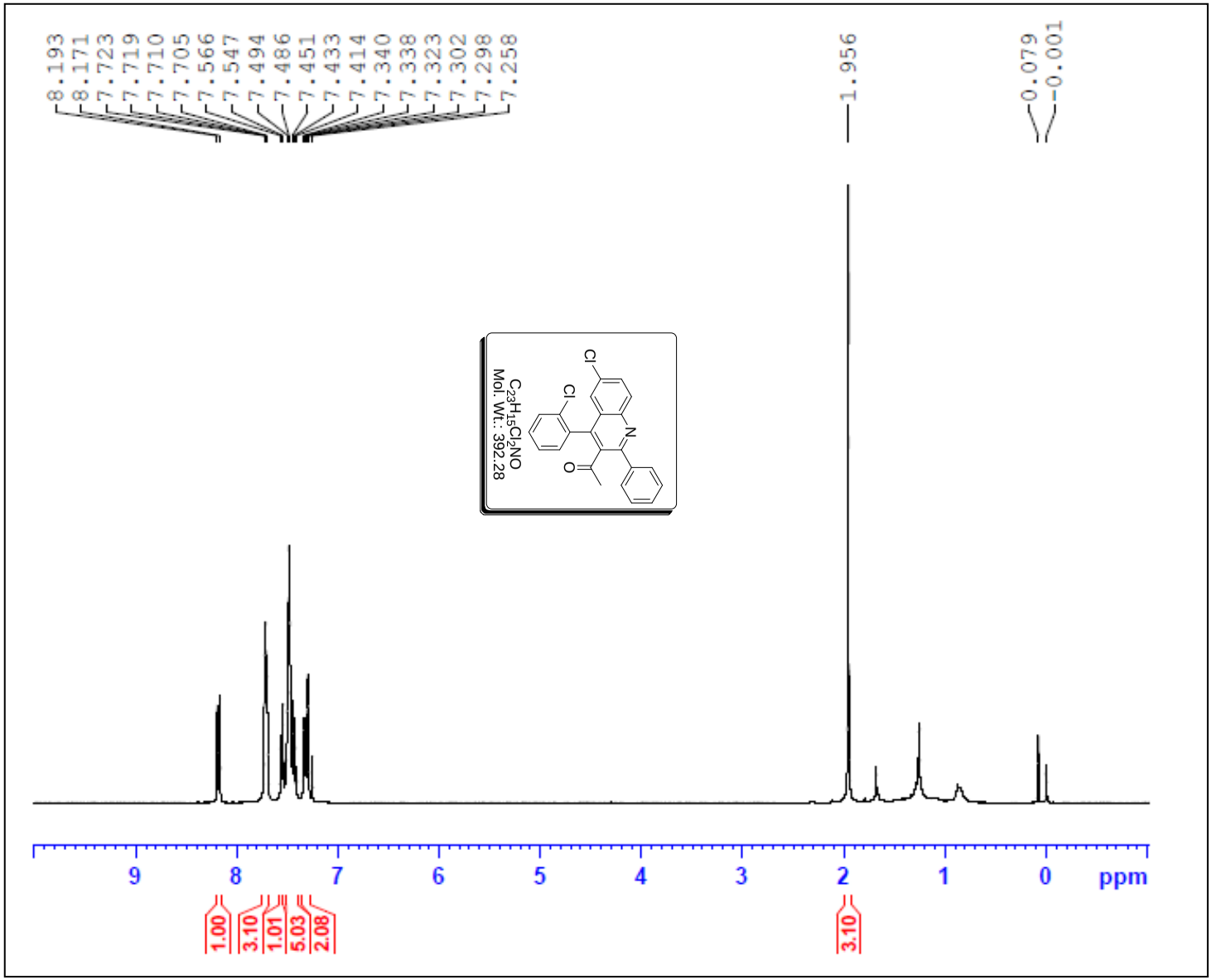

167.66
160.57
156.02
146.17
143.95
134.05
133.77
133.06
132.25
131.60
131.43
131.07
130.42
130.07
129.72
127.71
126.79
125.61
124.81
114.02
77.37
77.06
76.74
61.44
55.39
13.48
1.05
0.02
Cl
Cl
N
O
O
O
$C_{25}H_{19}Cl_2NO_3$
Mol. Wt.: 452.3293
180
160
140
120
100
80
60
40
20
ppm

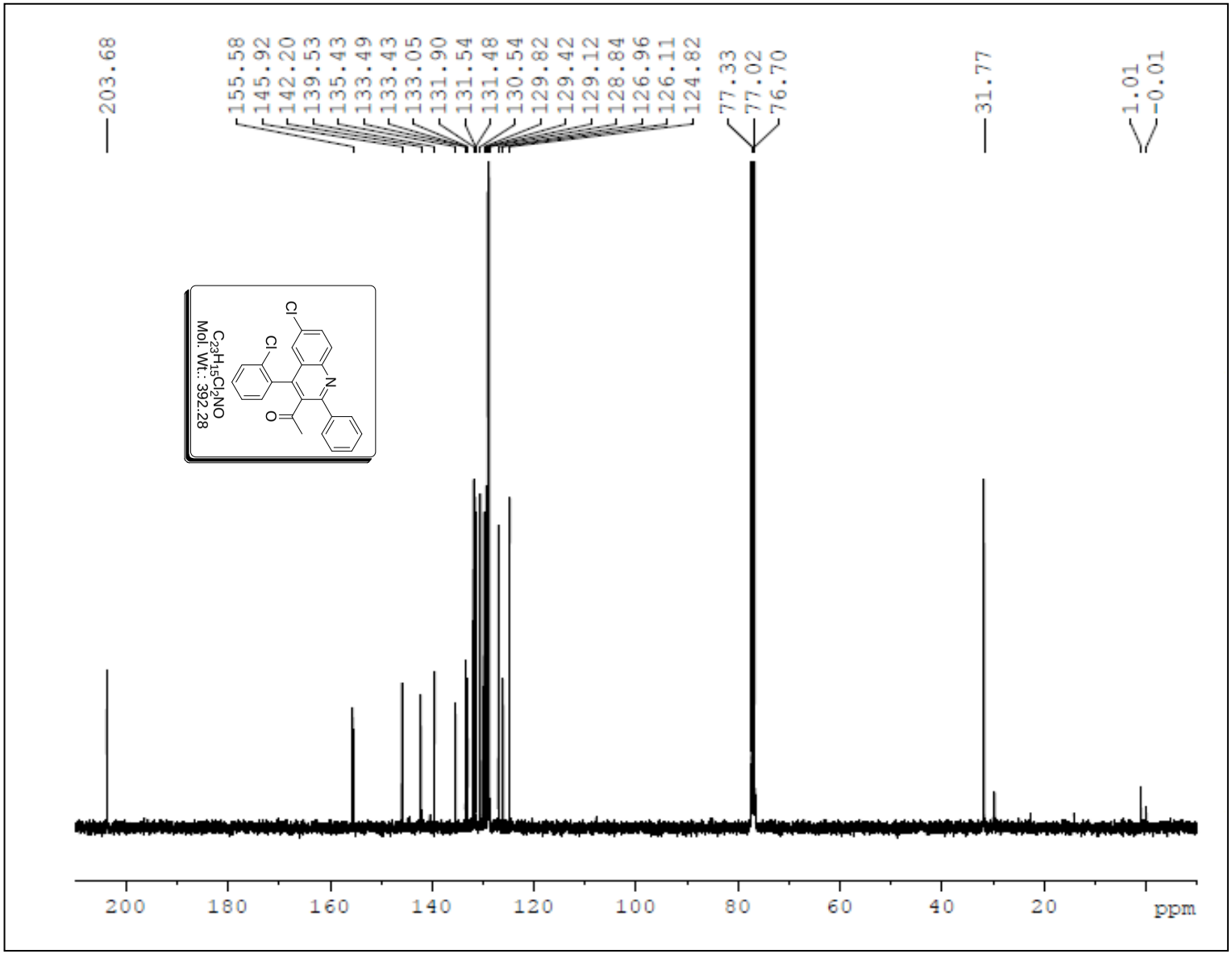

7.769
7.752
7.747
7.730
7.724
7.597
7.578
7.501
7.498
7.482
7.479
7.463
7.460
7.453
7.449
7.435
7.417
7.399
7.385
7.381
7.358
7.355
7.340
7.336
7.255
3.831
3.824
3.813
3.806
0.754
0.736
0.718
0.076
0.000
Cl
Cl
N
O
O
S
C26H19Cl2NO2S
Mol. Wt.: 480.41
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.99
0.97
0.93
1.05
1.03
6.22
2.01
3.04

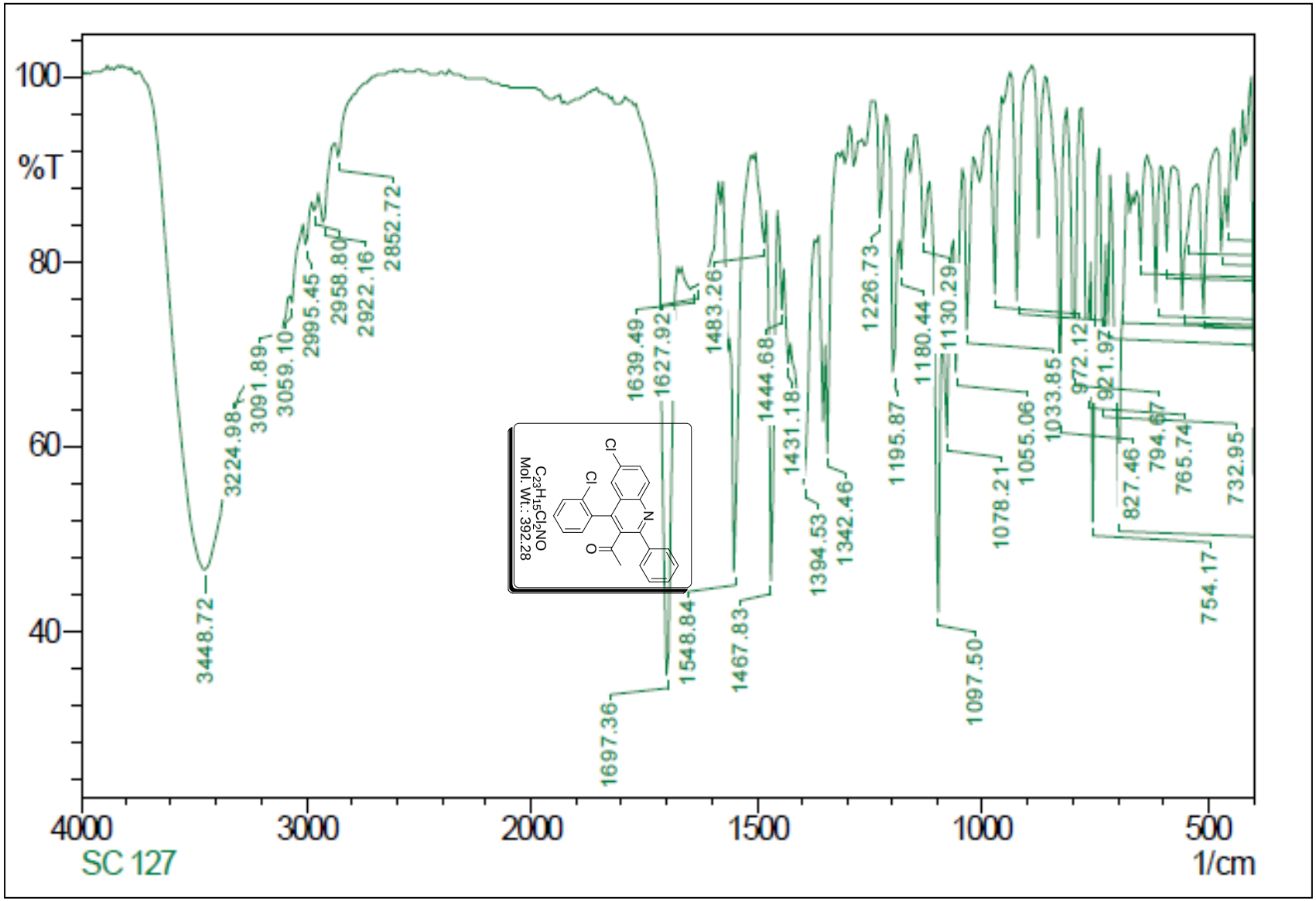

167.07
151.53
146.09
144.14
140.13
138.09
135.09
133.80
133.73
133.63
131.81
131.43
131.01
130.51
129.74
128.71
127.54
126.82
125.89
124.90
124.86
124.60
123.84
122.49
77.33
77.02
76.70
61.50
13.34
1.02
-0.01
Cl
Cl
N
O
O
S
C26H19Cl2NO2S
Mol. Wt.: 480.41
180
160
140
120
100
80
60
40
20
ppm

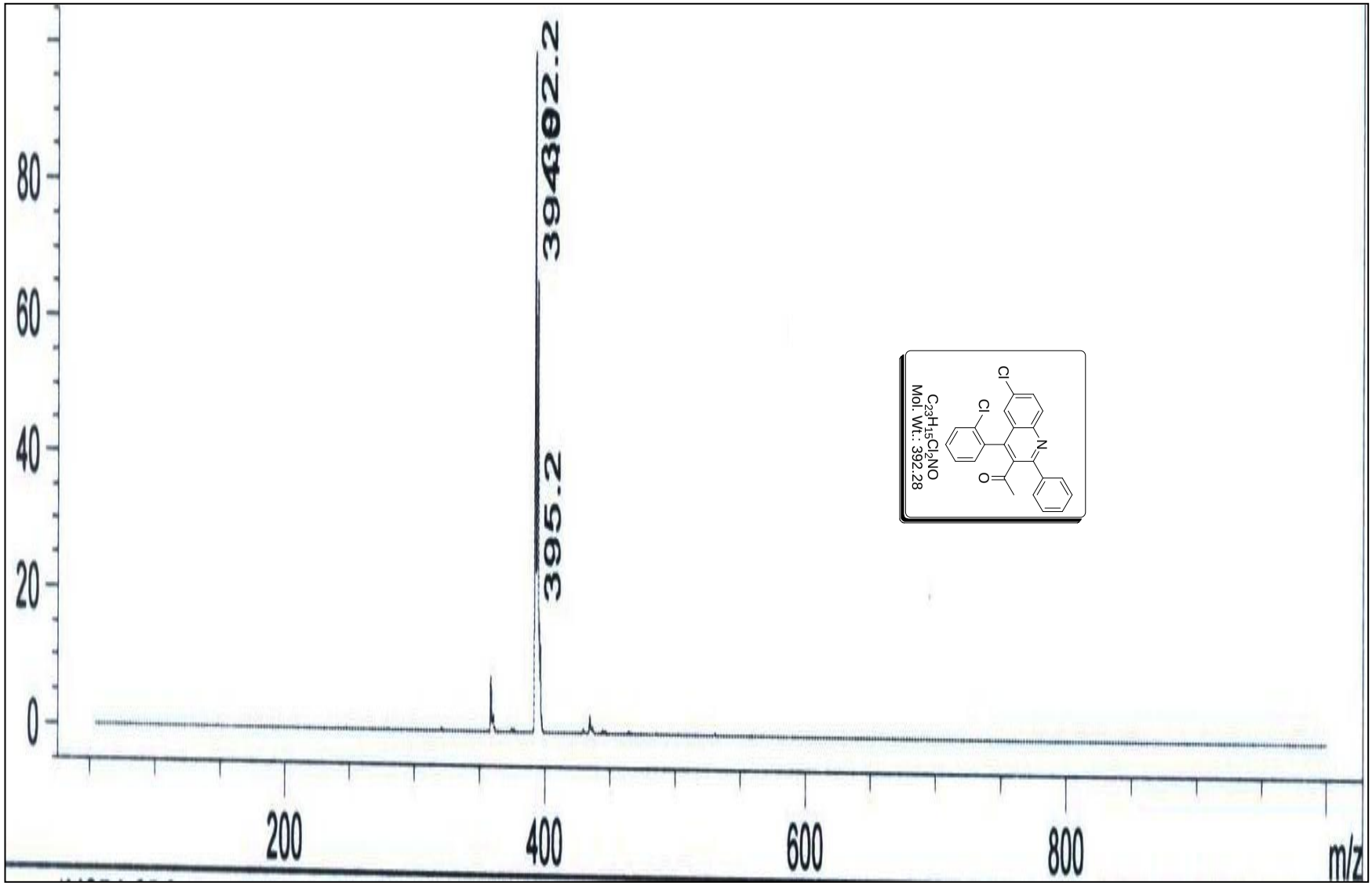

100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
SC 121
3419.79
3089.96
2978.09
2864.29
1722.43
1597.06
1564.27
1544.98
1489.05
1469.76
1437.18
1402.25
1313.52
1300.02
1220.94
1128.36
1087.85
1008.77
835.18
759.95
Cl
Cl
N
O
O
S
C26H19Cl2NO2S
Mol. Wt.: 480.41

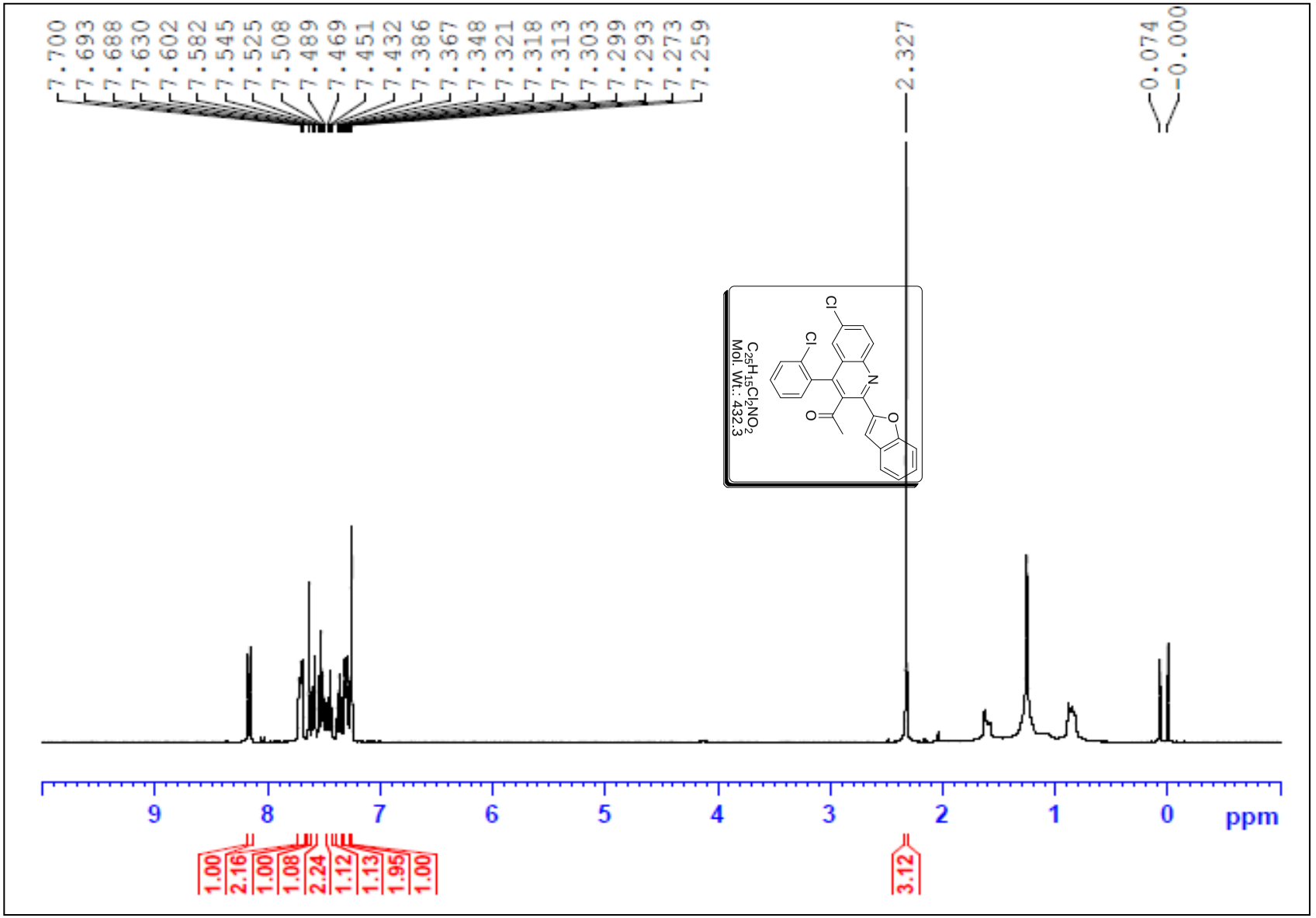
m/z
800
600
400
200
480.0
479.0
482.0
60
50
40
30
20
10
0
N
S
Cl
Cl
O
O
C26H19Cl2NO2S
Mol. Wt.: 480.41

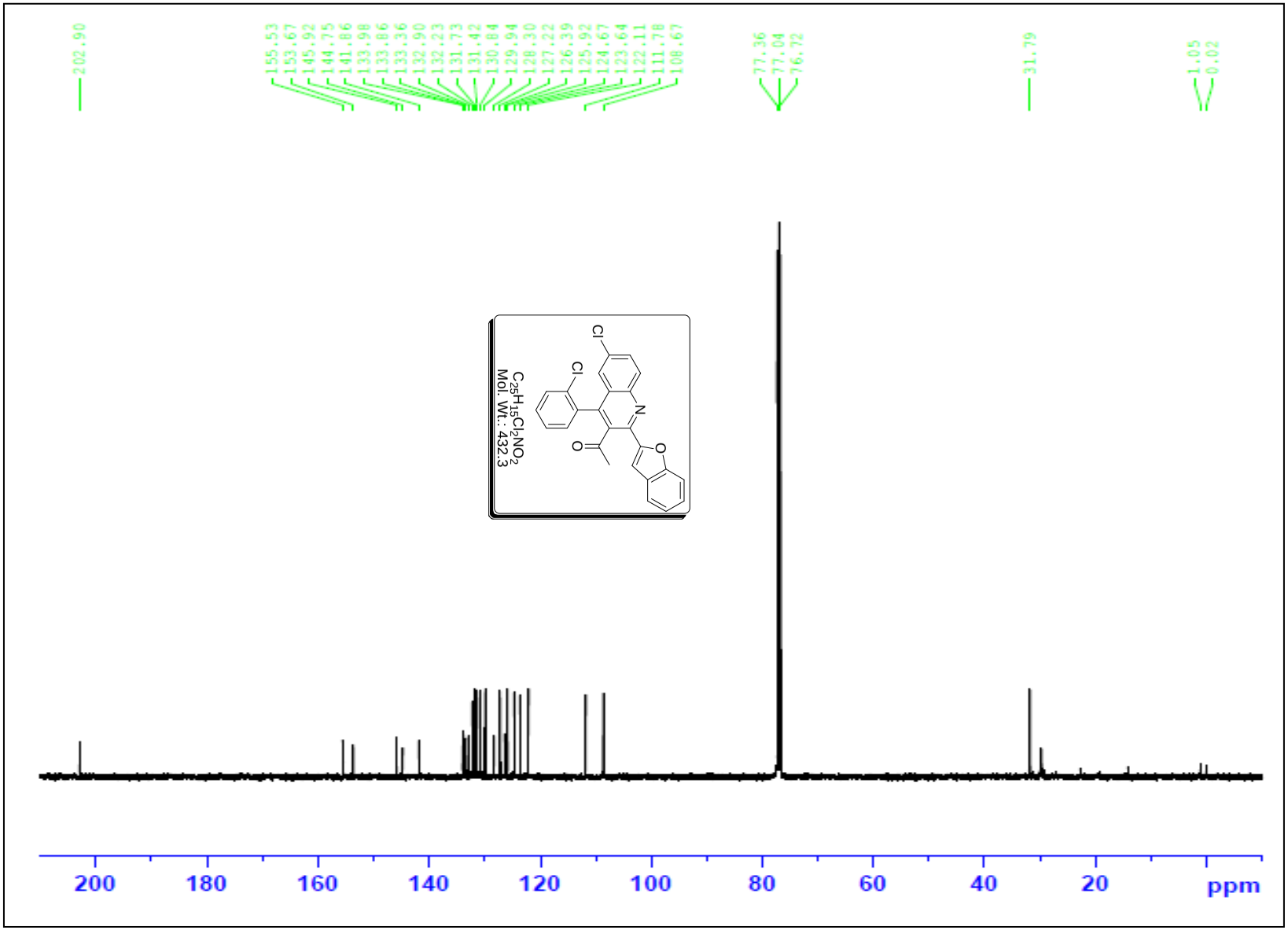

8.193
8.171
7.723
7.719
7.710
7.705
7.566
7.547
7.494
7.486
7.451
7.433
7.414
7.340
7.338
7.323
7.302
7.298
7.258
1.956
0.079
0.001
Cl
Cl
N
O
C23H15Cl2NO
Mol. Wt.: 392.28
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.10
1.01
5.03
2.08
3.10

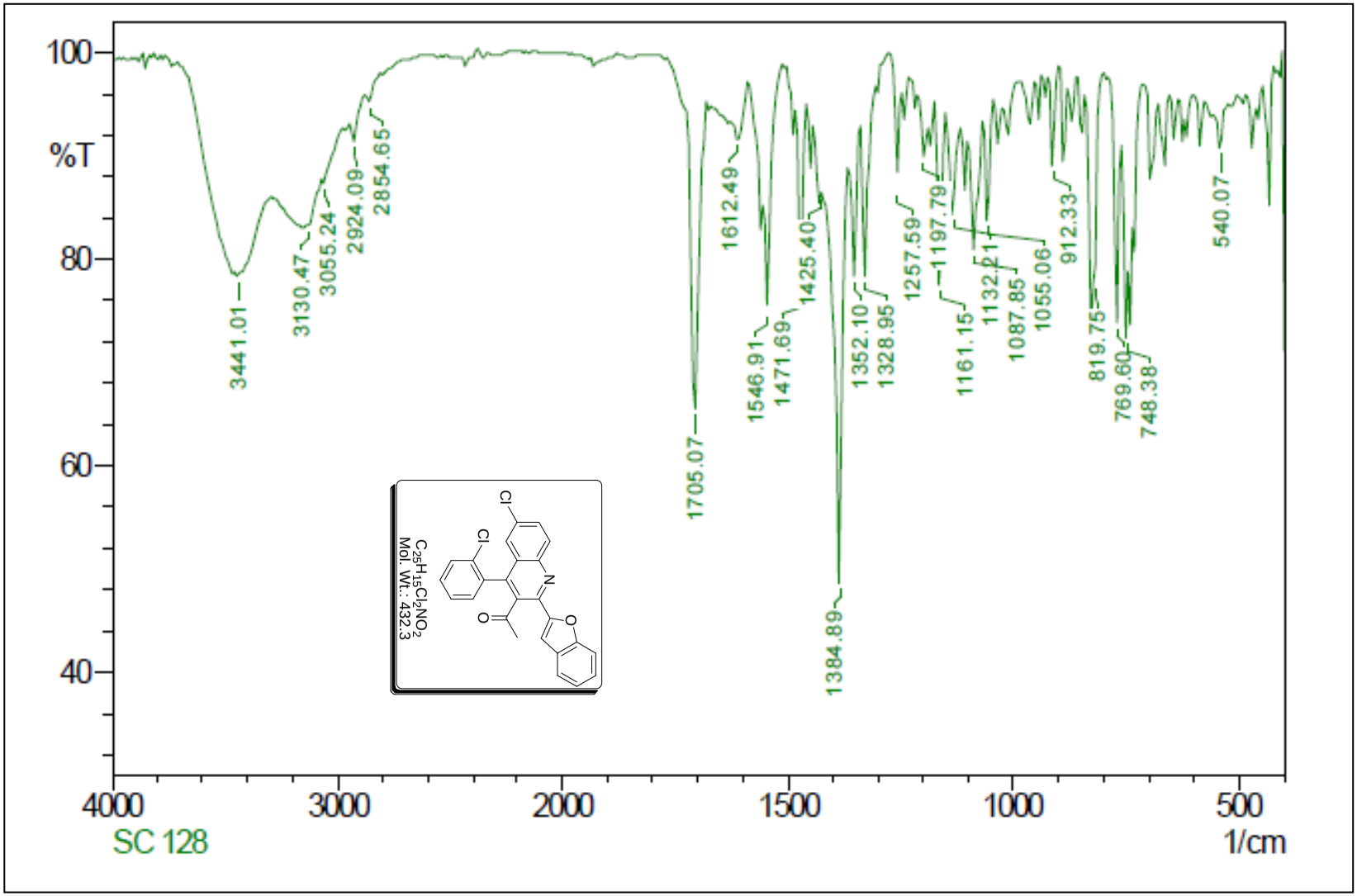

203.68
155.58
145.92
142.20
139.53
135.43
133.49
133.43
133.05
131.90
131.54
131.48
130.54
129.82
129.42
129.12
128.84
126.96
126.11
124.82
77.33
77.02
76.70
31.77
1.01
-0.01
Cl
Cl
N
O
C23H15Cl2NO
Mol. Wt.: 392.28
200
180
160
140
120
100
80
60
40
20
ppm


100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
SC 127
3448.72
3224.98
3091.89
3059.10
2995.45
2958.80
2922.16
2852.72
1697.36
1639.49
1627.92
1548.84
1483.26
1467.83
1444.68
1431.18
1394.53
1342.46
1226.73
1195.87
1180.44
1130.29
1097.50
1078.21
1055.06
1033.85
972.12
921.97
827.46
794.67
765.74
754.17
732.95
Cl
Cl
N
O
C23H15Cl2NO
Mol.Wt.: 392.28

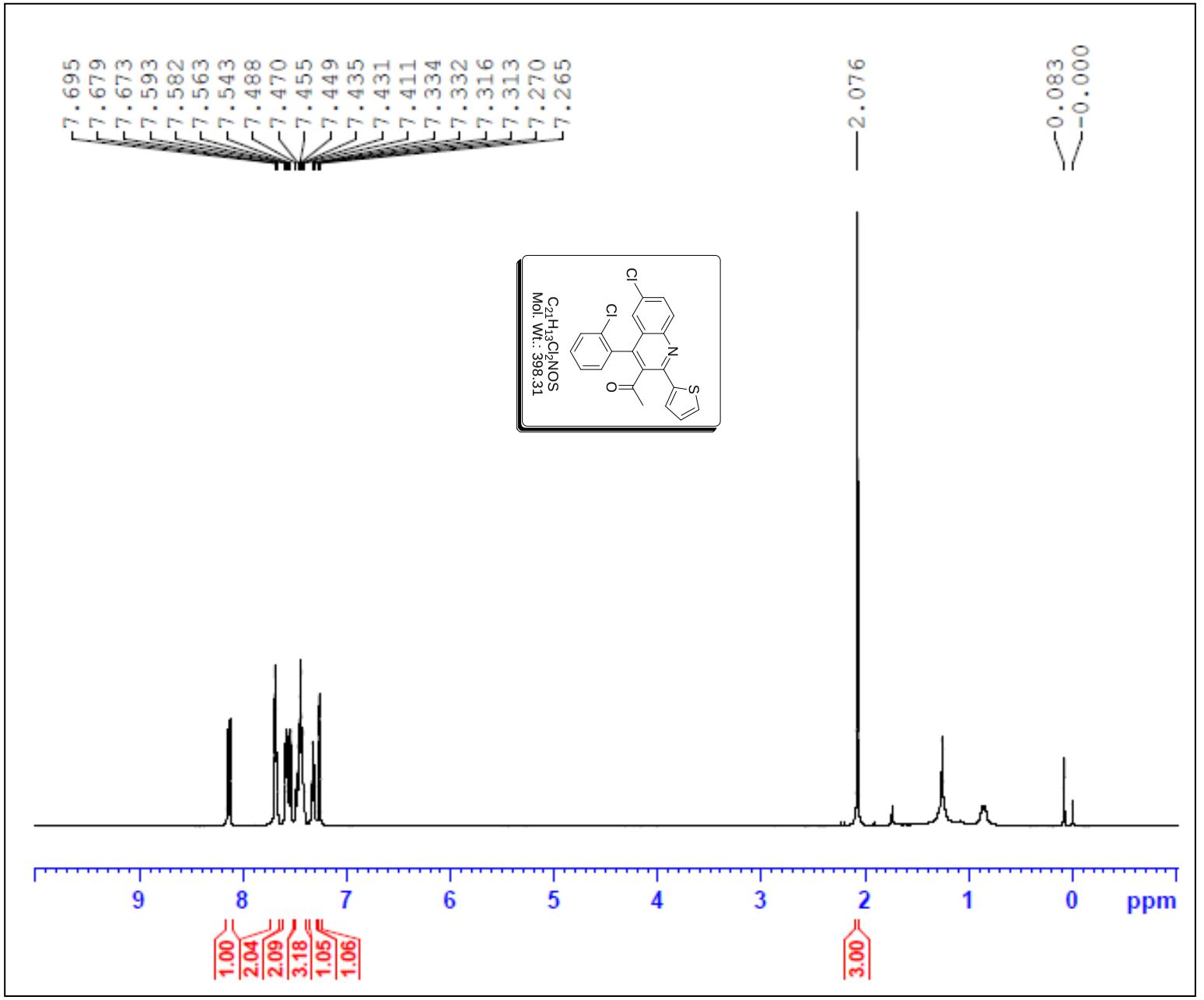

394302.2
395.2
80
60
40
20
0
200
400
600
800
m/z
Cl
Cl
N
O
$C_{23}H_{15}Cl_2NO$
Mol. Wt.: 392.28

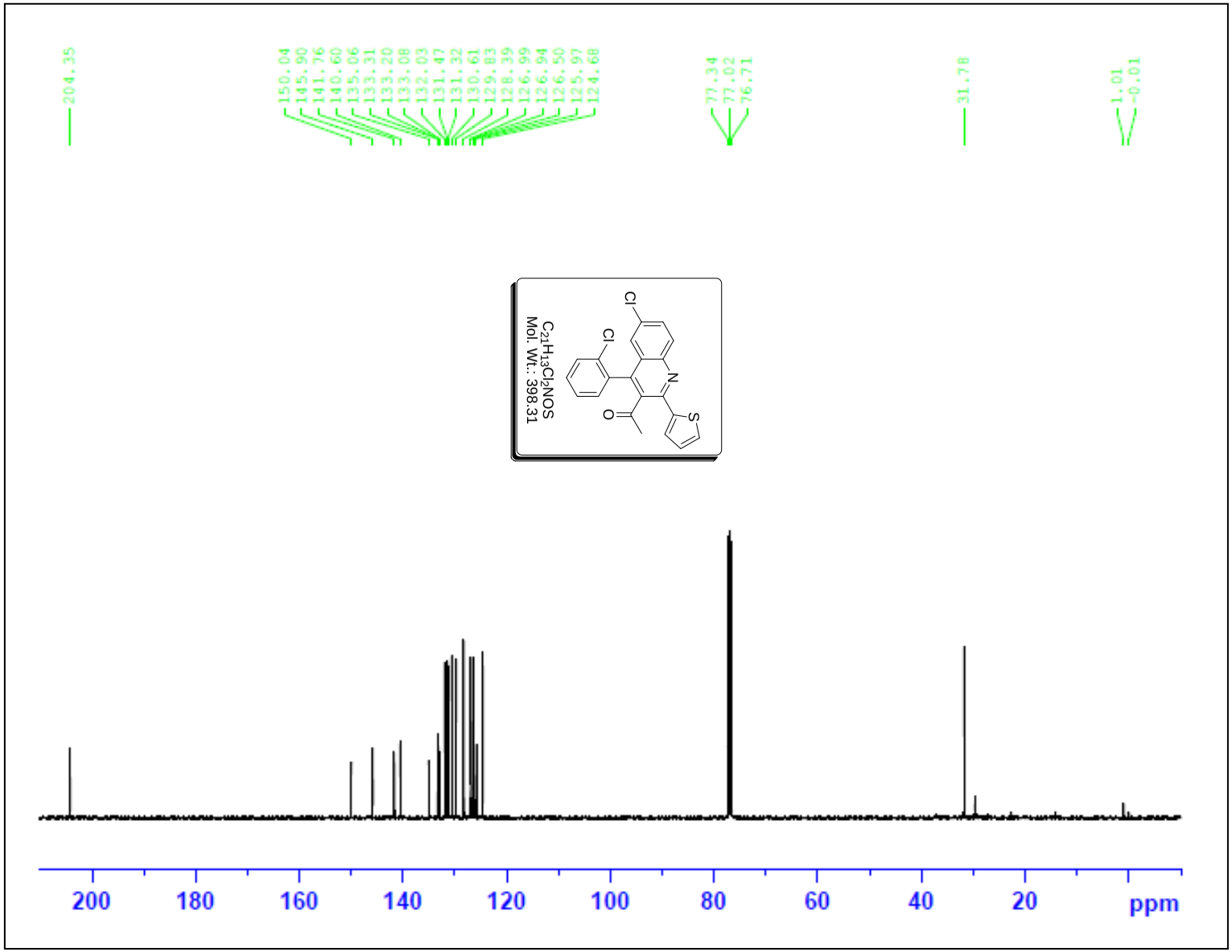

7.700
7.693
7.688
7.630
7.602
7.582
7.545
7.525
7.508
7.489
7.469
7.451
7.432
7.386
7.367
7.348
7.321
7.318
7.313
7.303
7.299
7.293
7.273
7.259
2.327
0.074
0.000
Cl
Cl
N
O
O
C25H15Cl2NO2
Mol. Wt.: 432.3
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.16
1.00
1.08
2.24
1.12
1.13
1.95
1.00
3.12

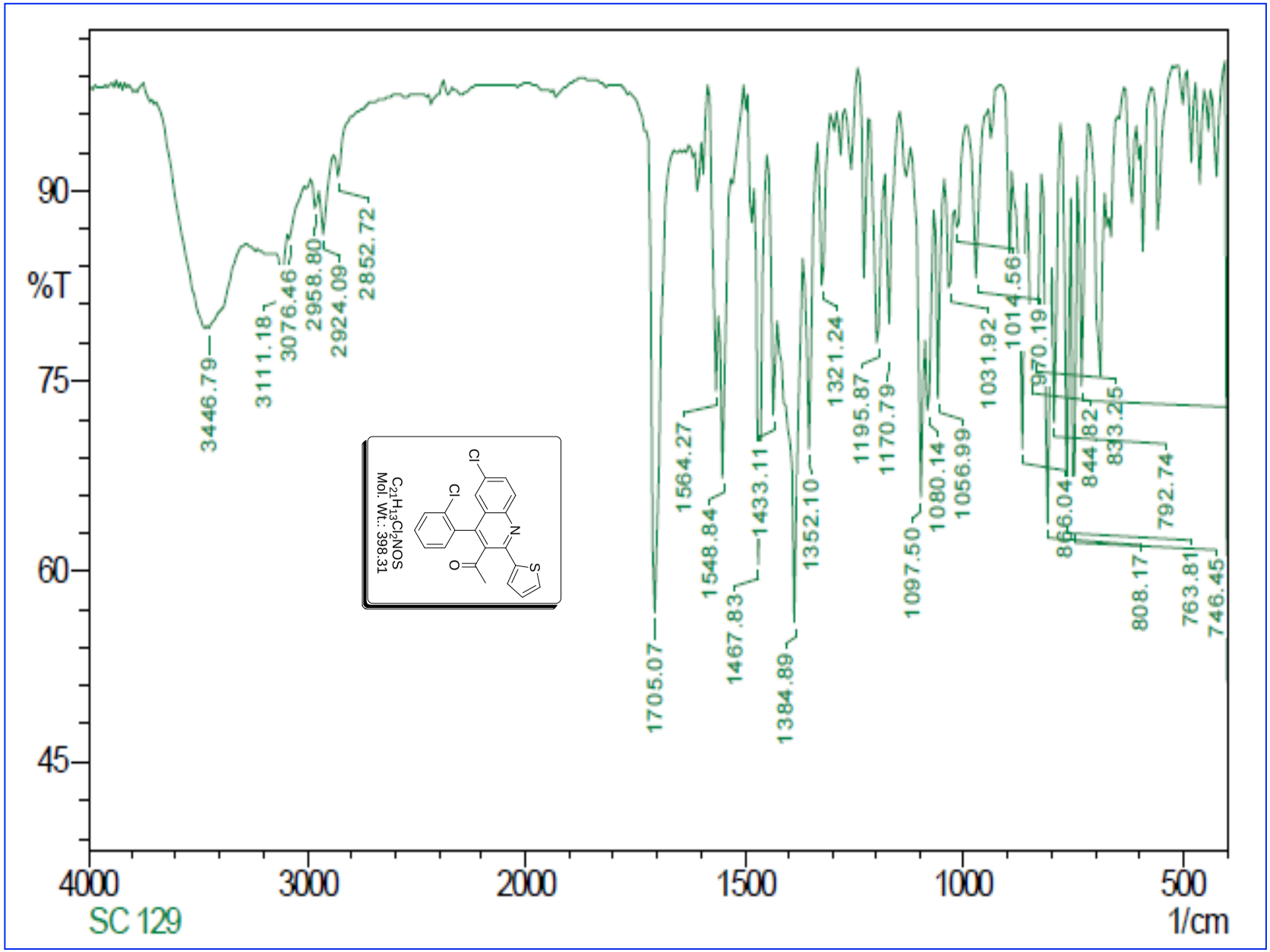

202.90
155.53
153.67
145.92
144.75
141.86
133.98
133.86
133.36
132.90
132.23
131.73
131.42
130.84
129.94
128.30
127.22
126.39
125.92
124.67
123.64
122.11
111.78
108.67
77.36
77.04
76.72
31.79
1.05
0.02
Cl
Cl
N
O
O
C25H15Cl2NO2
Mol. Wt.: 432.3
200
180
160
140
120
100
80
60
40
20
ppm

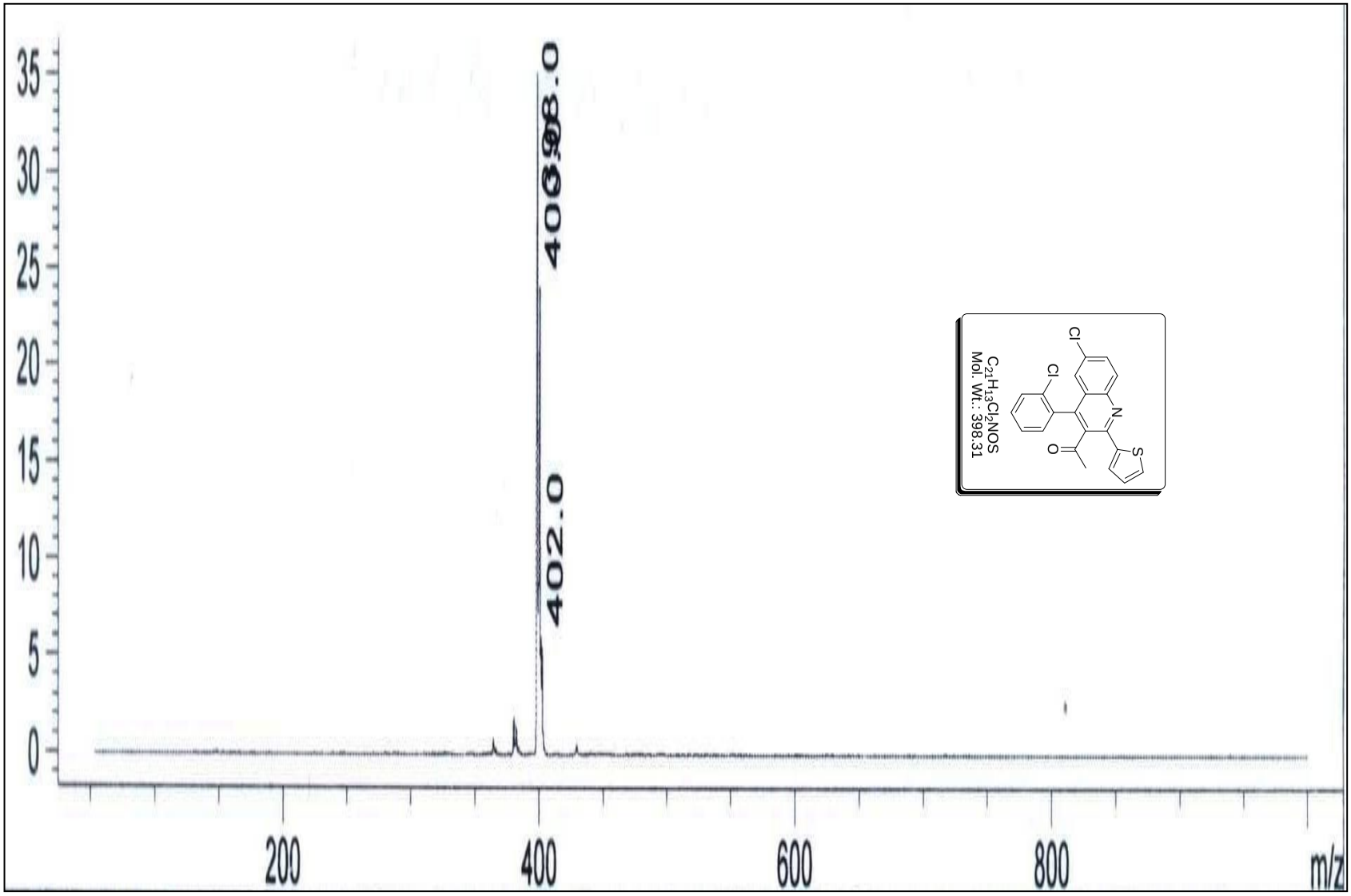

100
%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
SC 128
3441.01
3130.47
3055.24
2924.09
2854.65
1705.07
1612.49
1546.91
1471.69
1425.40
1384.89
1352.10
1328.95
1257.59
1197.79
1161.15
1132.21
1087.85
1055.06
912.33
819.75
769.60
748.38
540.07
Cl
Cl
N
O
O
C25H15Cl2NO2
Mol. Wt.: 432.3

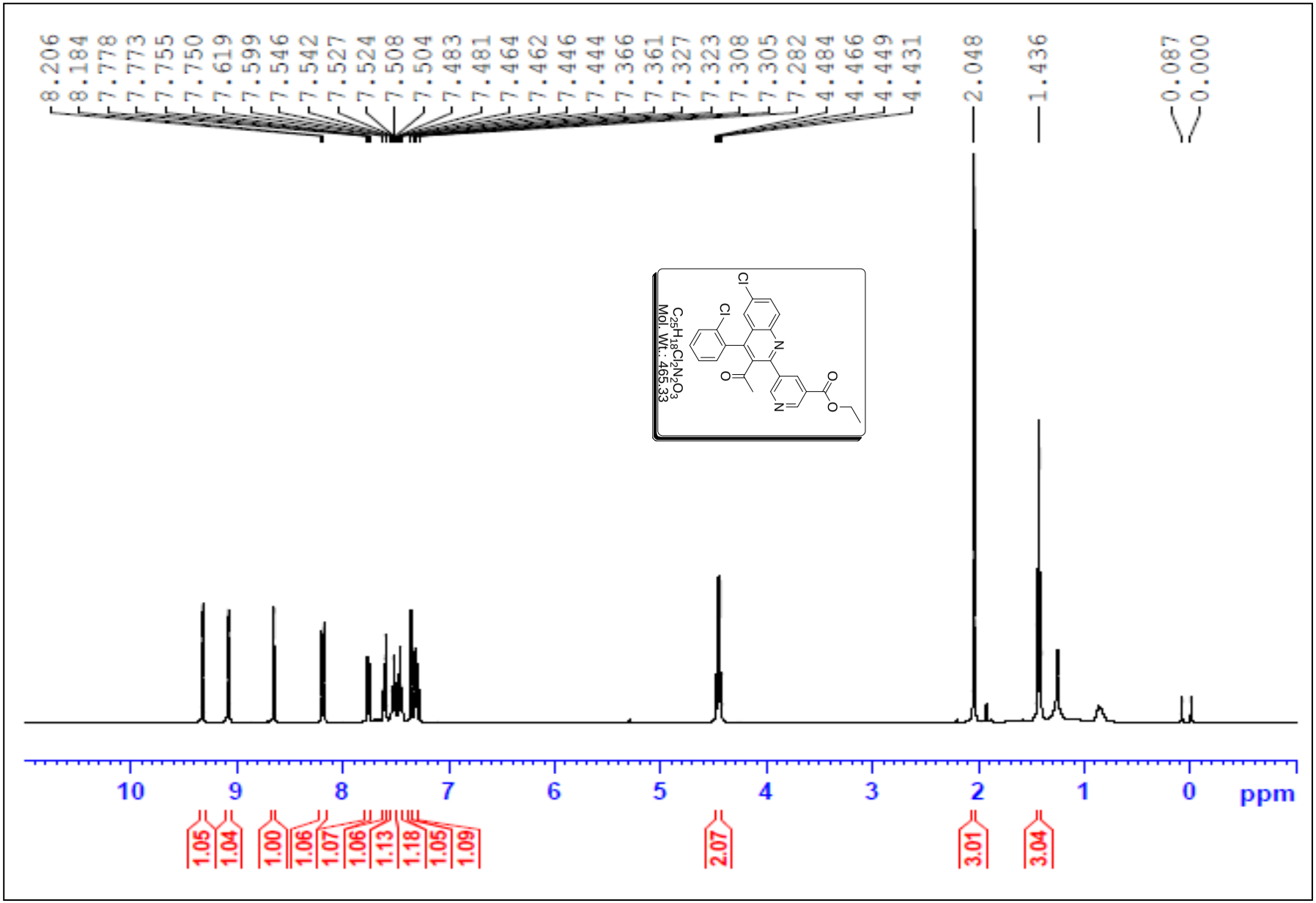
O
N
Cl
Cl
O
C25H15Cl2NO2
Mol. Wt.: 432.3
435.0
m/z
200
400
600
800
0
20
40
60
80

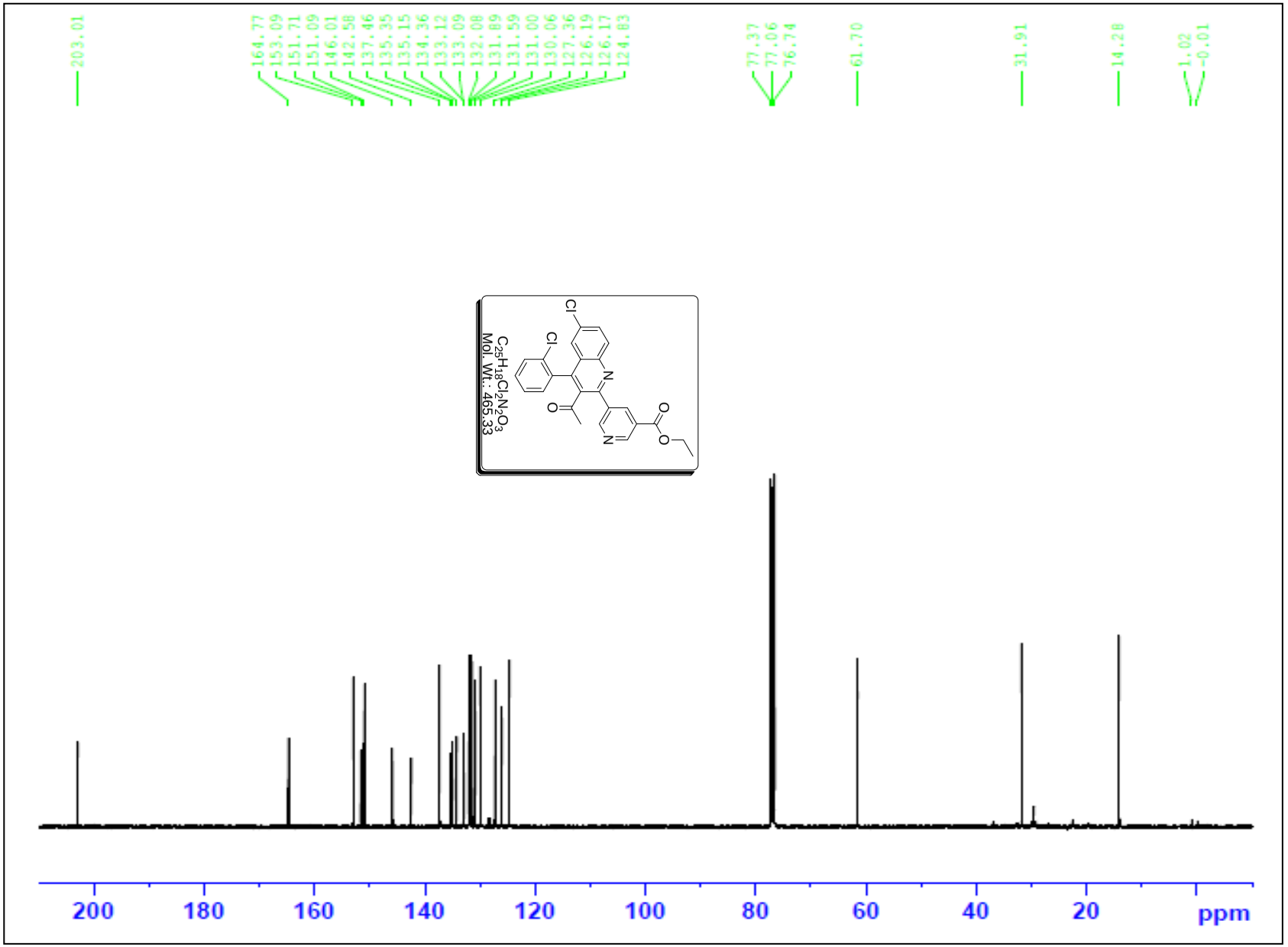

7.695
7.679
7.673
7.593
7.582
7.563
7.543
7.488
7.470
7.455
7.449
7.435
7.431
7.411
7.334
7.332
7.316
7.313
7.270
7.265
2.076
0.083
0.000
C21H13Cl2NOS
Mol. Wt.: 398.31
Cl
Cl
N
O
S
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.04
2.09
3.18
1.05
1.06
3.00

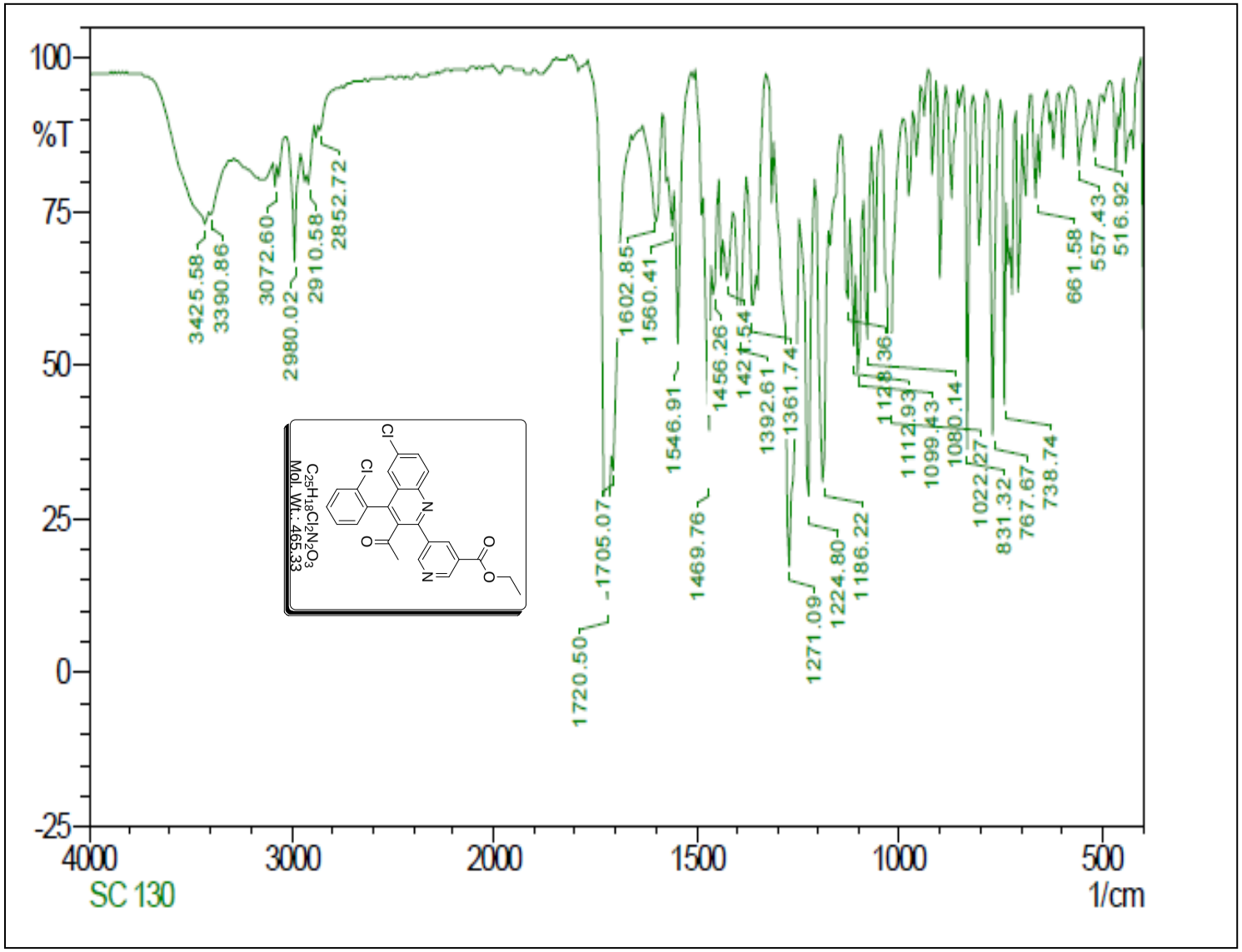

204.35
150.04
145.90
141.76
140.60
135.06
133.31
133.20
133.08
132.03
131.47
131.32
130.61
129.83
128.39
126.99
126.94
126.50
125.97
124.68
77.34
77.02
76.71
31.78
1.01
-0.01
C21H13Cl2NOS
Mol. Wt.: 398.31
Cl
Cl
N
O
S
200
180
160
140
120
100
80
60
40
20
ppm


%T
90
75
60
45
4000
3000
2000
1500
1000
500
1/cm
SC 129
3446.79
3111.18
3076.46
2958.80
2924.09
2852.72
1705.07
1564.27
1548.84
1467.83
1433.11
1384.89
1352.10
1321.24
1195.87
1170.79
1097.50
1080.14
1056.99
1031.92
1014.56
970.19
866.04
844.82
833.25
808.17
792.74
763.81
746.45
C21H13Cl2NOS
Mol. Wt.: 398.31
Cl
Cl
N
S
O

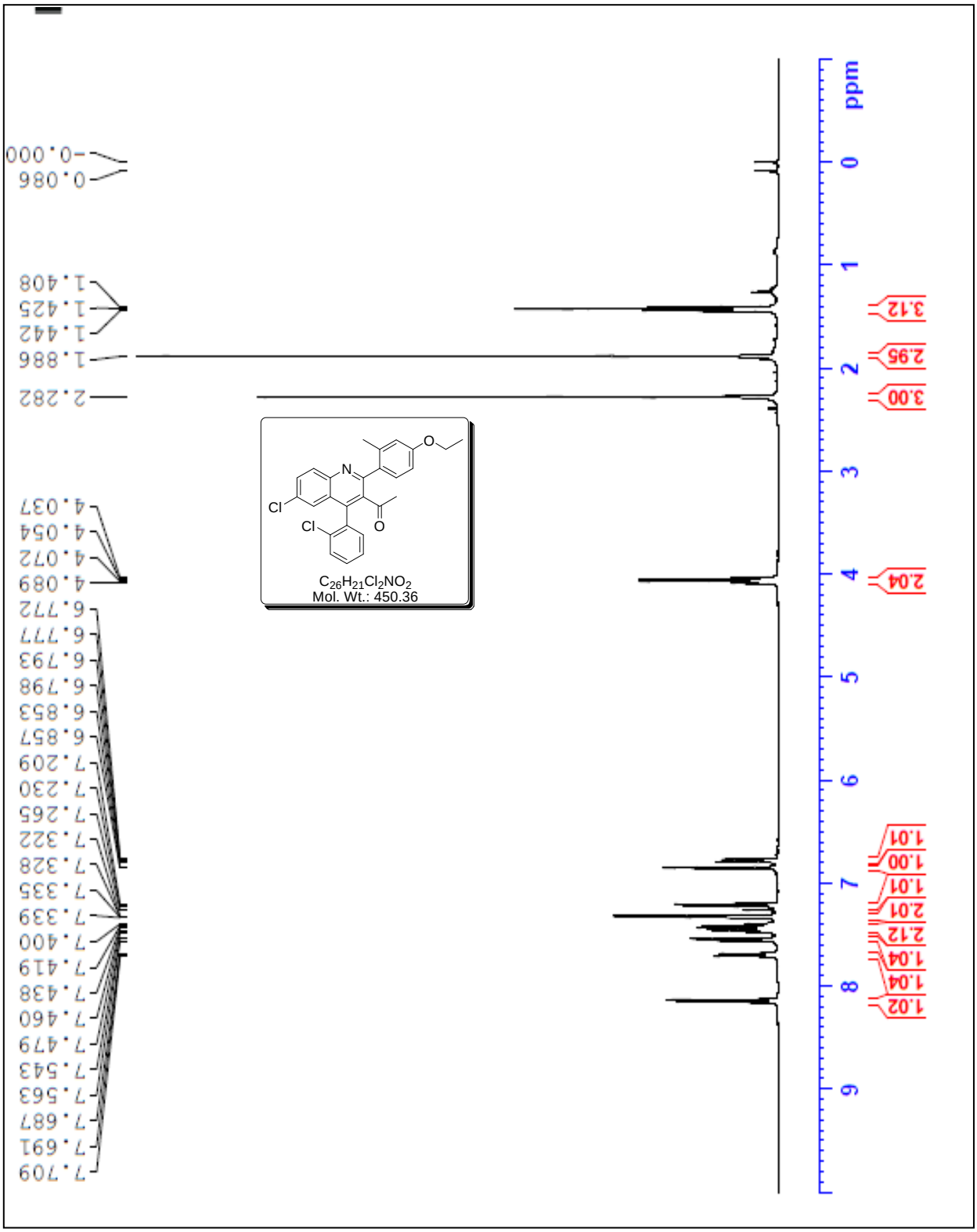

35
30
25
20
15
10
5
0
402.0
200
400
600
800
m/z
Cl
Cl
N
O
S
$C_{21}H_{13}Cl_2NOS$
Mol. Wt.: 398.31

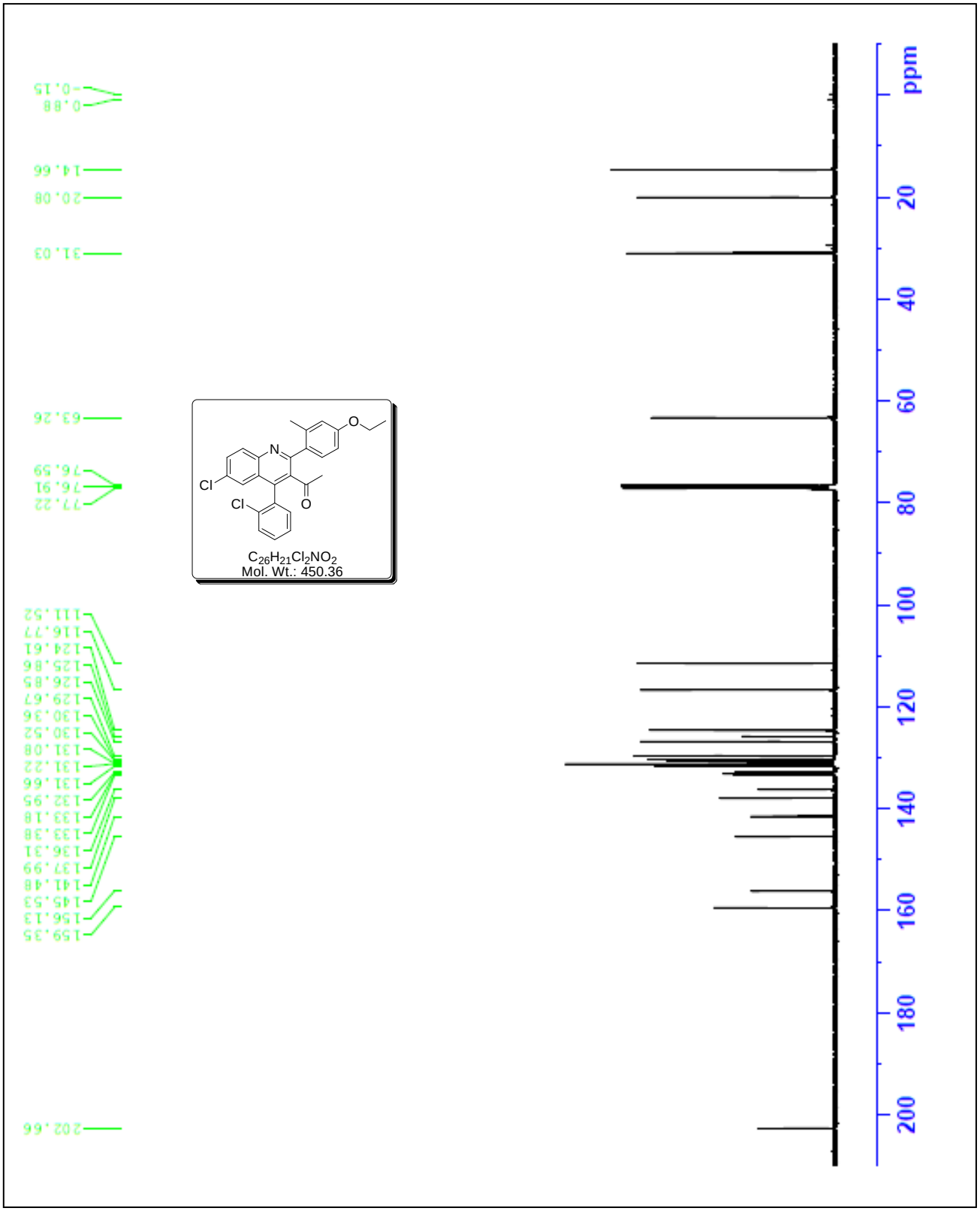

8.206
8.184
7.778
7.773
7.755
7.750
7.619
7.599
7.546
7.542
7.527
7.524
7.508
7.504
7.483
7.481
7.464
7.462
7.446
7.444
7.366
7.361
7.327
7.323
7.308
7.305
7.282
4.484
4.466
4.449
4.431
2.048
1.436
0.087
0.000
Cl
Cl
N
O
N
O
O
C25H18Cl2N2O3
Mol. Wt.: 465.33
10
9
8
7
6
5
4
3
2
1
0
ppm
1.05
1.04
1.00
1.06
1.07
1.06
1.13
1.18
1.05
1.09
2.07
3.01
3.04

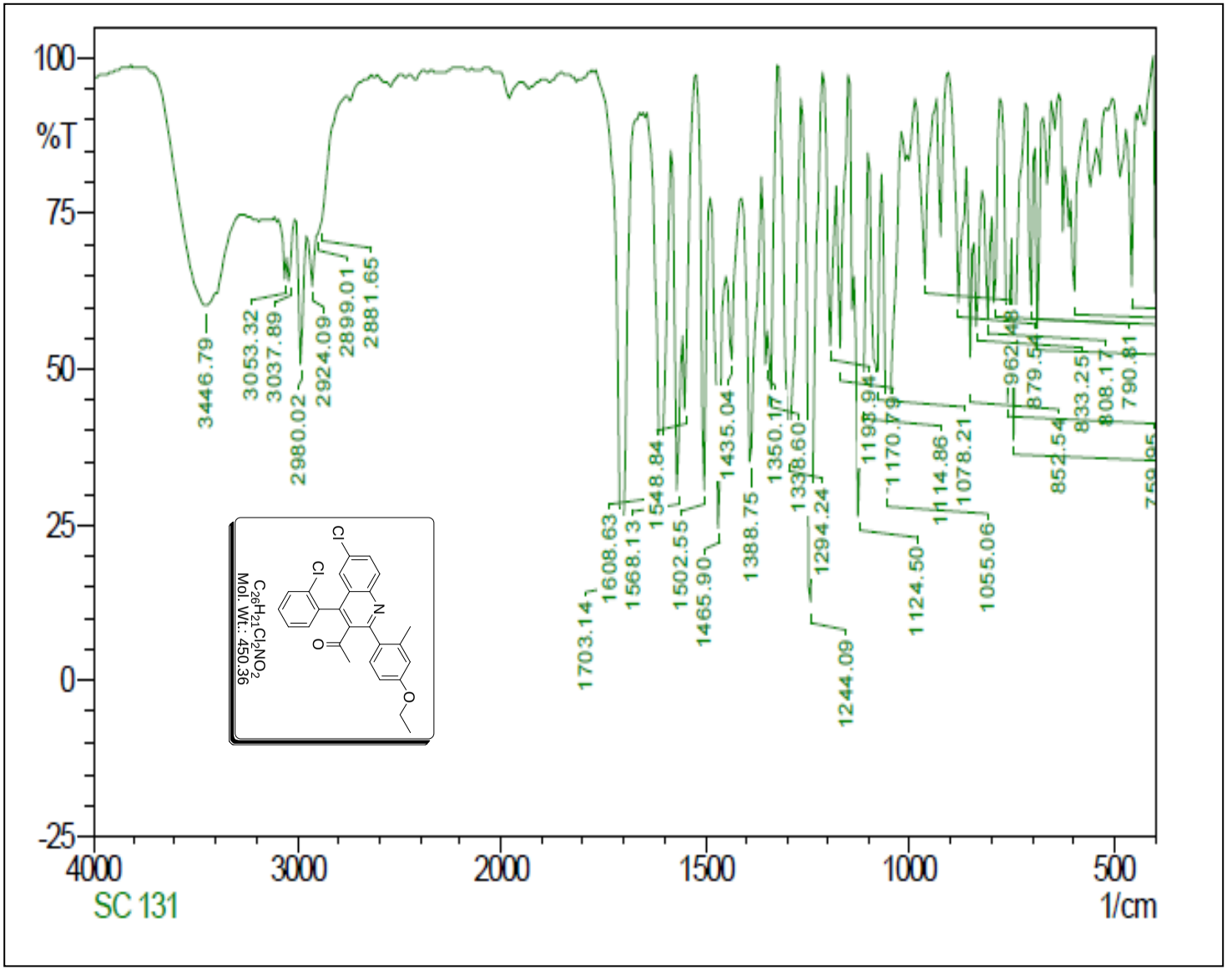

203.01
164.77
153.09
151.71
151.09
146.01
142.58
137.46
135.35
135.15
134.36
133.12
133.09
132.08
131.89
131.59
131.00
130.06
127.36
126.19
126.17
124.83
77.37
77.06
76.74
61.70
31.91
14.28
1.02
-0.01
Cl
Cl
N
O
N
O
O
C25H18Cl2N2O3
Mol. Wt.: 465.33
200
180
160
140
120
100
80
60
40
20
ppm

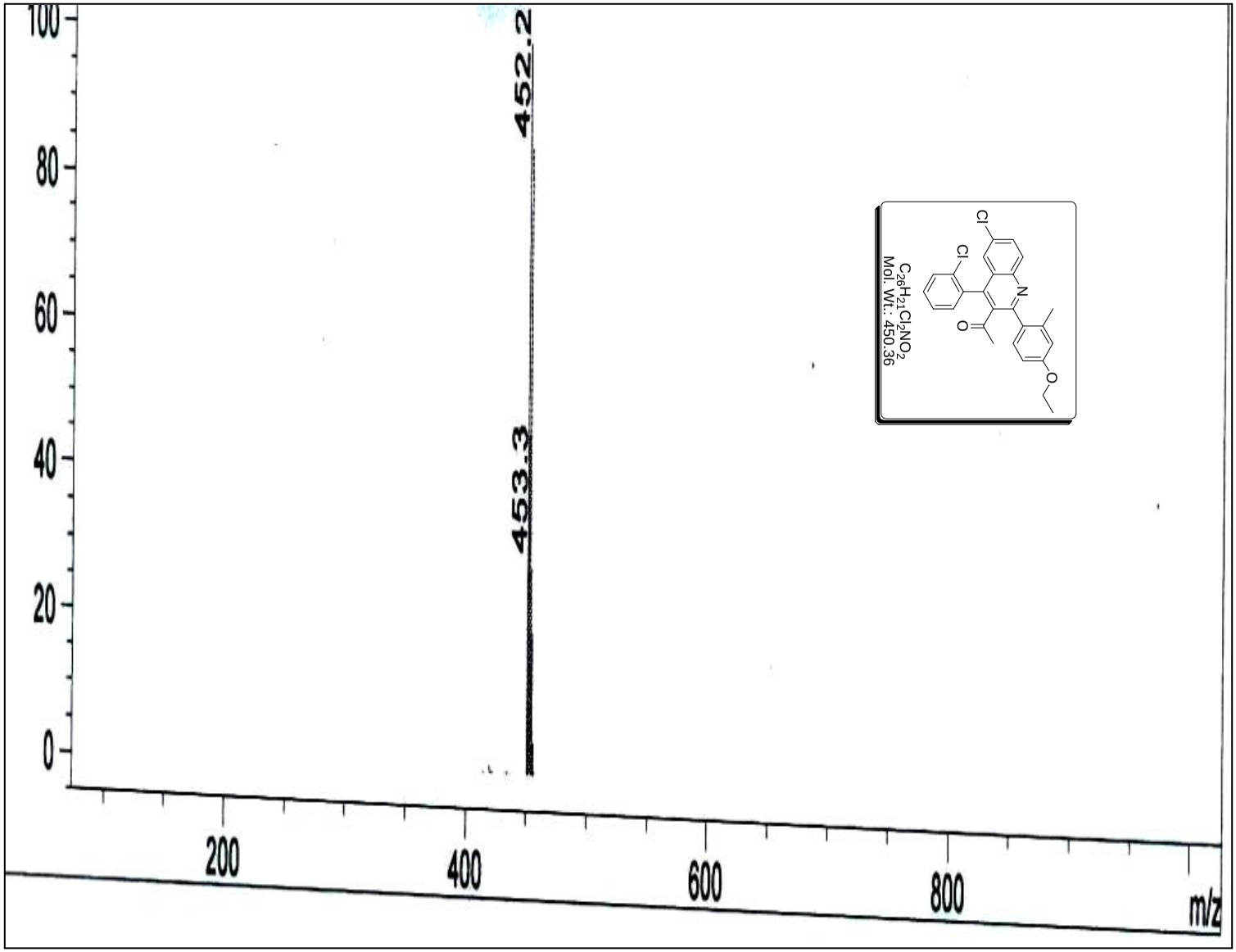

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC 130
3425.58
3390.86
3072.60
2980.02
2910.58
2852.72
1720.50
1705.07
1602.85
1560.41
1546.91
1469.76
1456.26
1421.54
1392.61
1361.74
1271.09
1224.80
1186.22
1128.36
1112.93
1099.43
1080.14
1022.27
831.32
767.67
738.74
661.58
557.43
516.92
Cl
Cl
N
N
O
O
O
C25H18Cl2N2O3
Mol. Wt.: 465.33

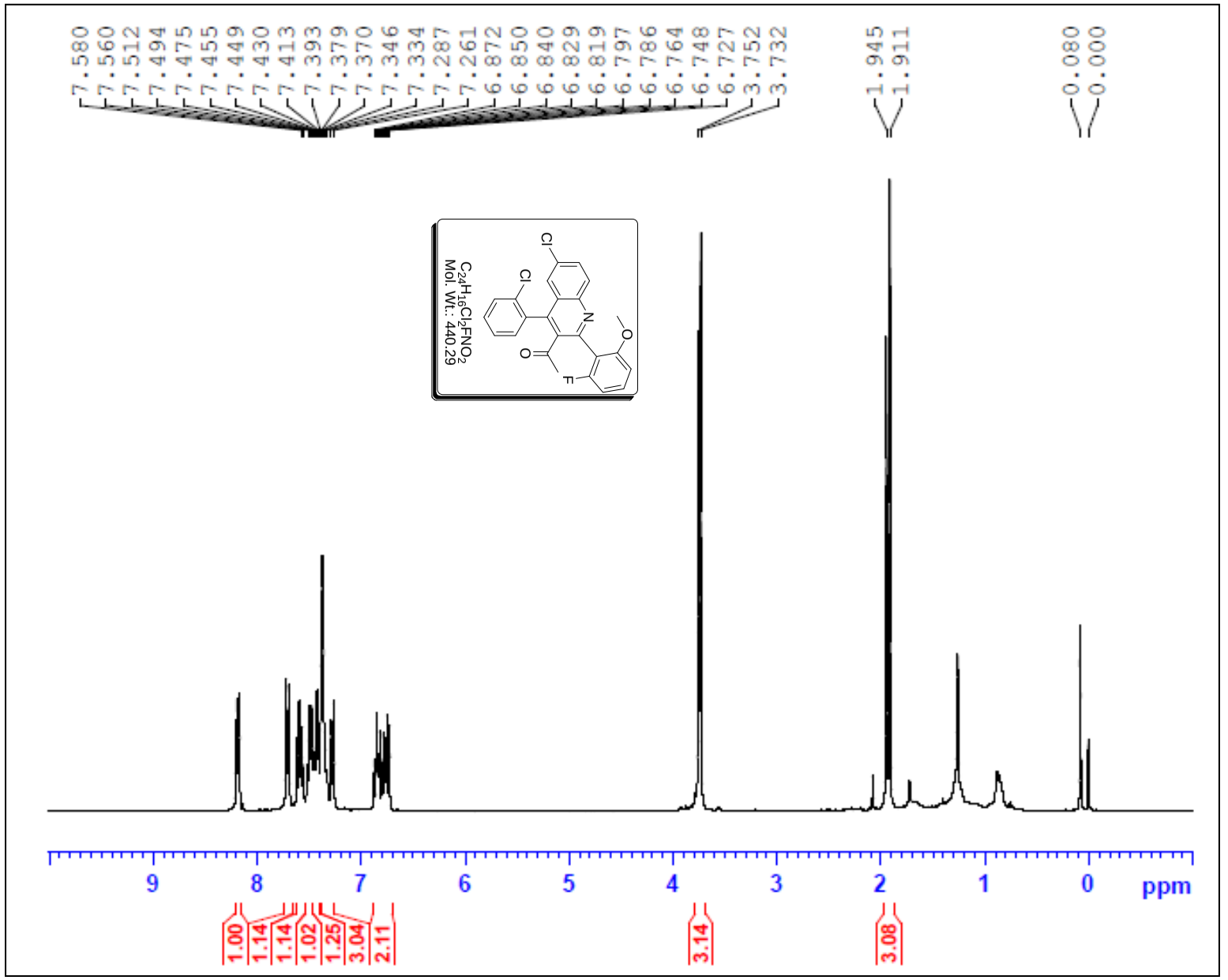
m/z
800
600
400
200
100
80
60
40
20
0
468.0
467.0
O
O
N
N
Cl
Cl
O
$C_{25}H_{18}Cl_2N_2O_3$
Mol. Wt.: 465.33

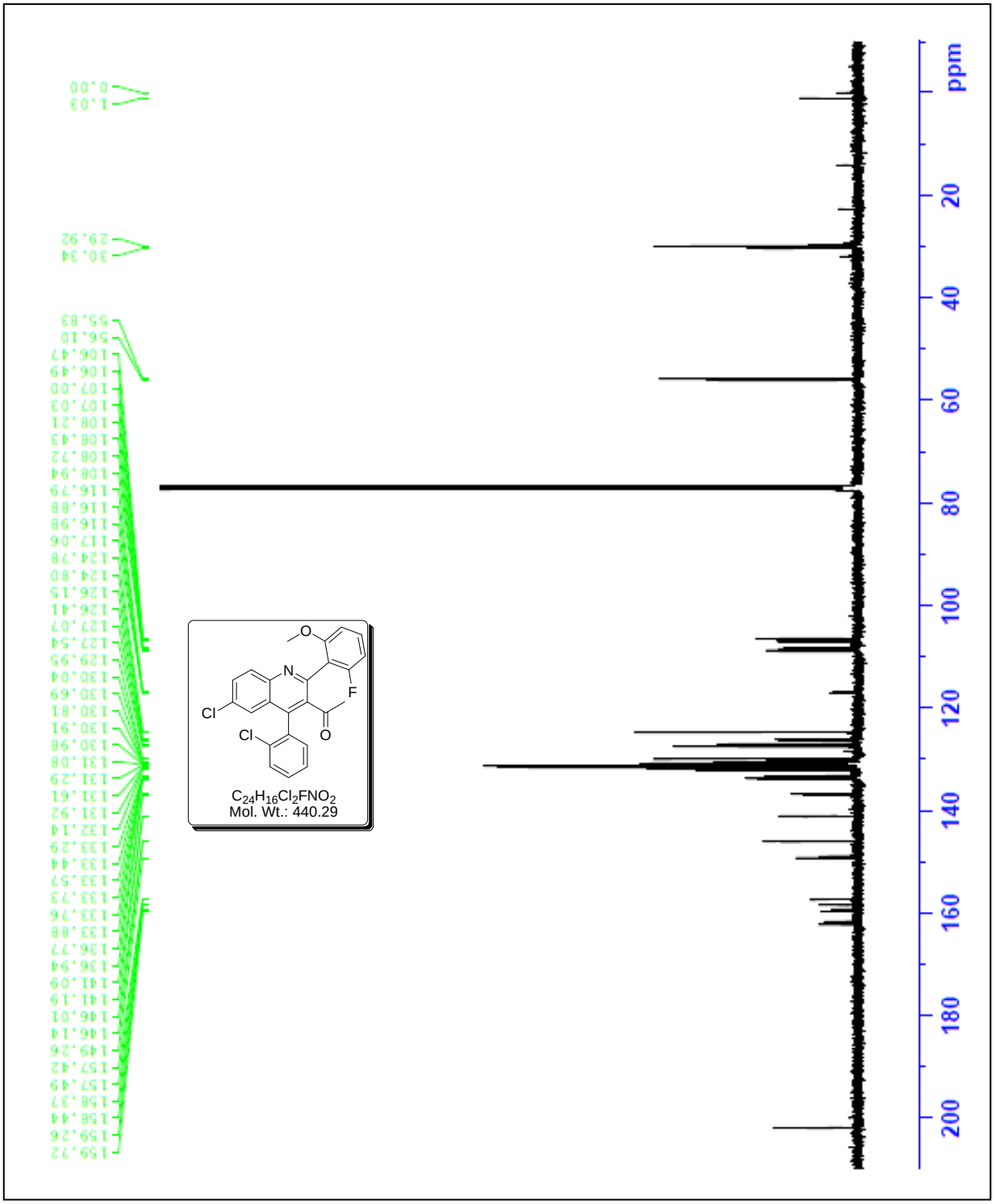

ppm
0
1
2
3
4
5
6
7
8
9
3.12
2.95
3.00
2.04
1.02
1.04
1.04
2.12
2.01
1.01
1.00
1.01
0.000
0.086
1.408
1.425
1.442
1.886
2.282
4.037
4.054
4.072
4.089
6.772
6.777
6.793
6.798
6.853
6.857
7.209
7.230
7.265
7.322
7.328
7.335
7.339
7.400
7.419
7.438
7.460
7.479
7.543
7.563
7.687
7.691
7.709
Cl
Cl
N
O
O
C26H21Cl2NO2
Mol. Wt.: 450.36

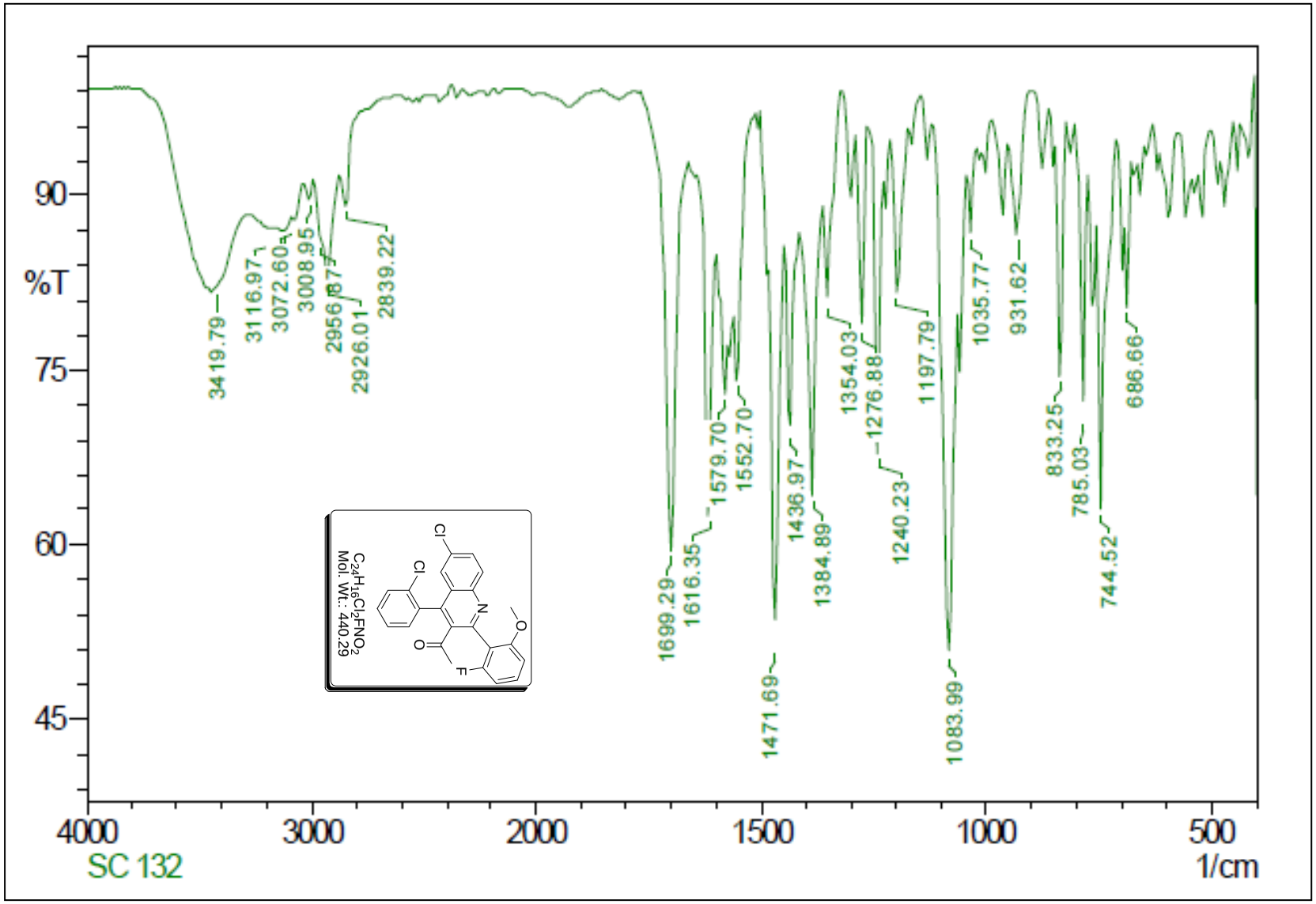

-0.15
0.88
14.66
20.08
31.03
63.26
76.59
76.91
77.22
111.52
116.77
124.61
125.86
126.85
129.67
130.36
130.52
131.08
131.22
131.66
132.95
133.18
133.38
136.31
137.99
141.48
145.53
156.13
159.35
202.66
O
N
Cl
Cl
O
C26H21Cl2NO2
Mol. Wt.: 450.36
ppm
20
40
60
80
100
120
140
160
180
200

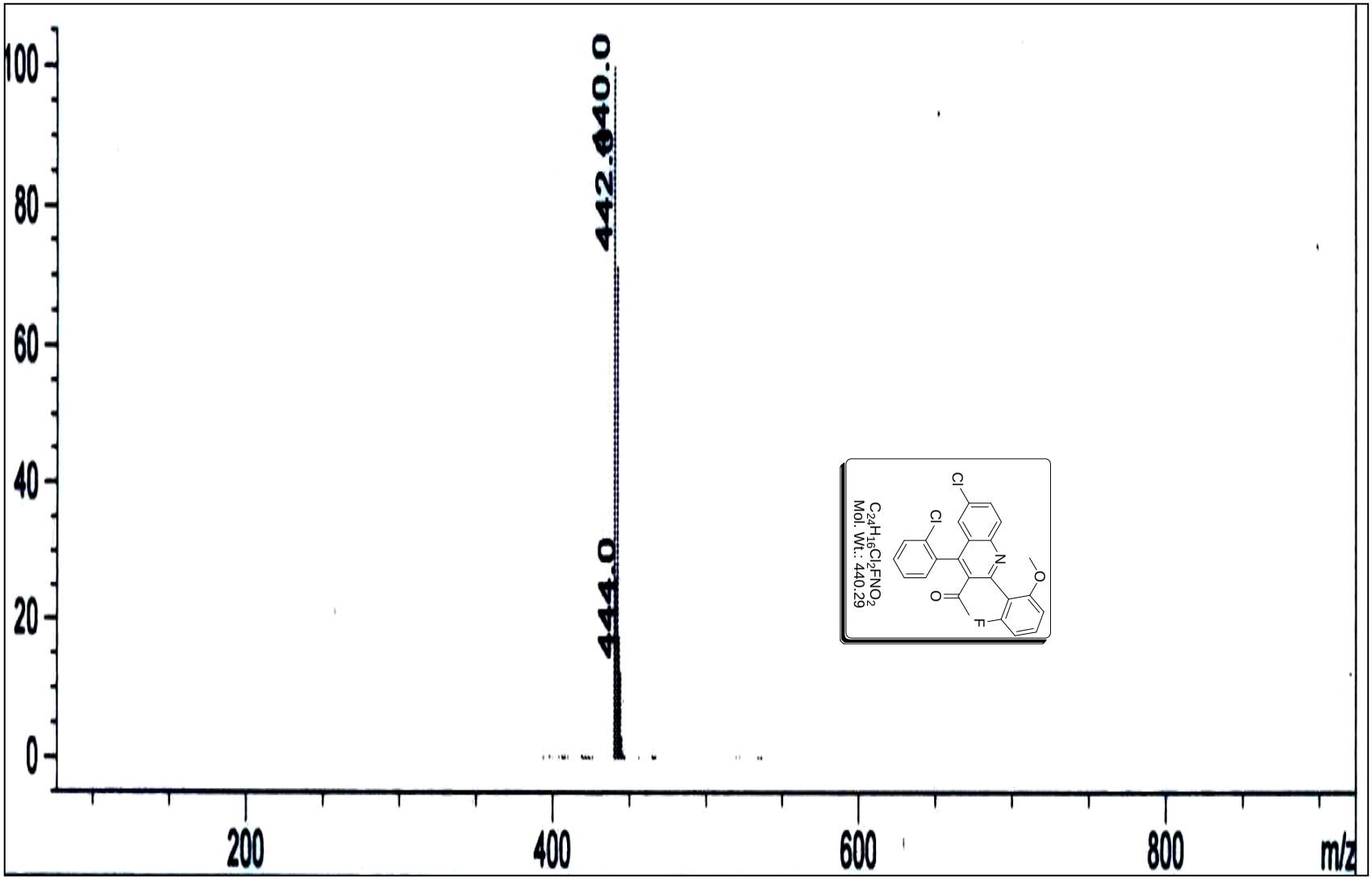

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC 131
3446.79
3053.32
3037.89
2980.02
2924.09
2899.01
2881.65
1703.14
1608.63
1568.13
1548.84
1502.55
1465.90
1435.04
1388.75
1350.17
1338.60
1294.24
1244.09
1198.94
1170.79
1124.50
1114.86
1078.21
1055.06
962.48
879.54
852.54
833.25
808.17
790.81
Cl
Cl
N
O
O
C26H21Cl2NO2
Mol. Wt.: 450.36


100
80
60
40
20
0
452.2
453.3
200
400
600
800
m/z
Cl
Cl
N
O
O
C26H21Cl2NO2
Mol. Wt.: 450.36

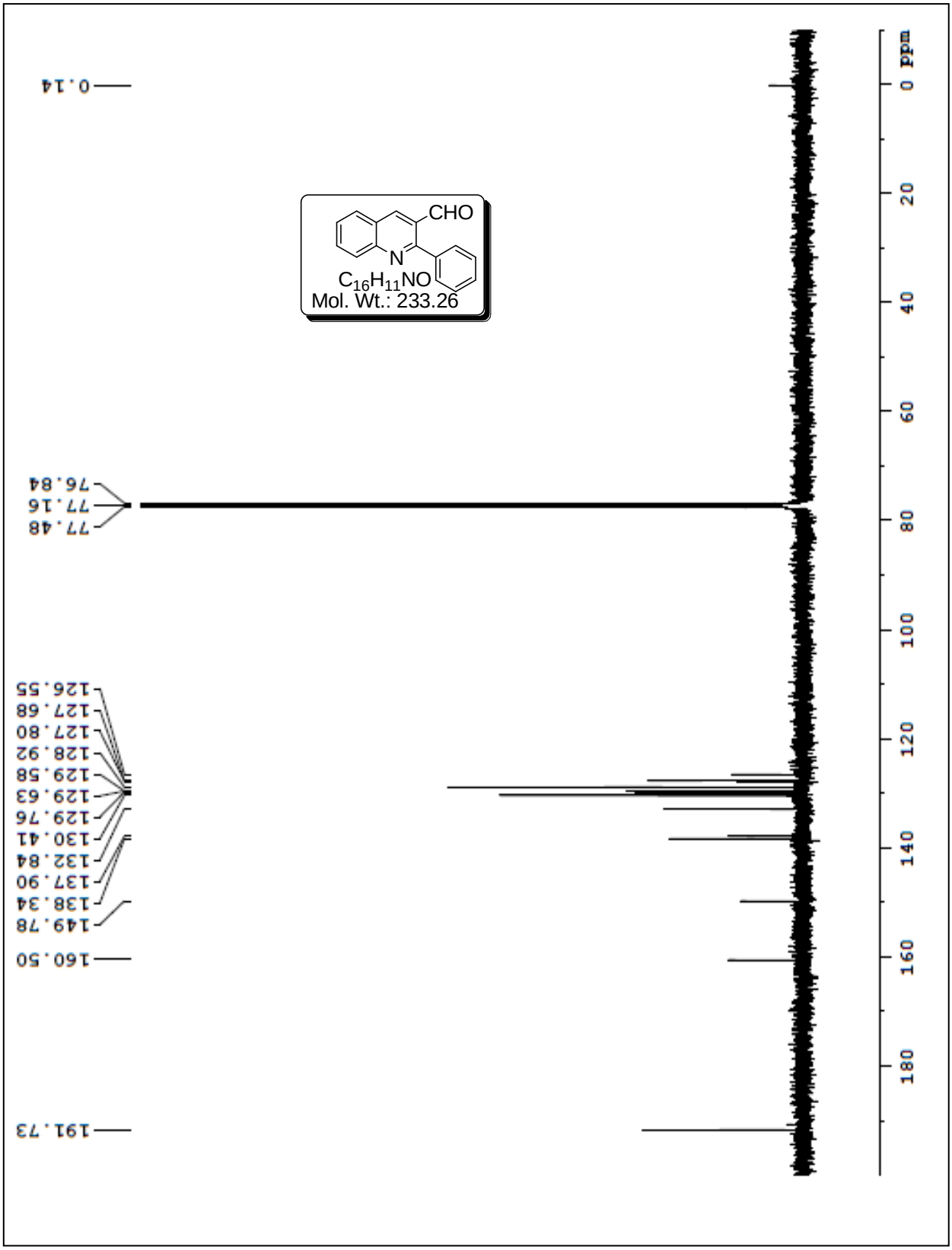

7.580
7.560
7.512
7.494
7.475
7.455
7.449
7.430
7.413
7.393
7.379
7.370
7.346
7.334
7.287
7.261
6.872
6.850
6.840
6.829
6.819
6.797
6.786
6.764
6.748
6.727
3.752
3.732
1.945
1.911
0.080
0.000
C24H16Cl2FNO2
Mol. Wt.: 440.29
Cl
Cl
N
O
O
F
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.14
1.14
1.02
1.25
3.04
2.11
3.14
3.08

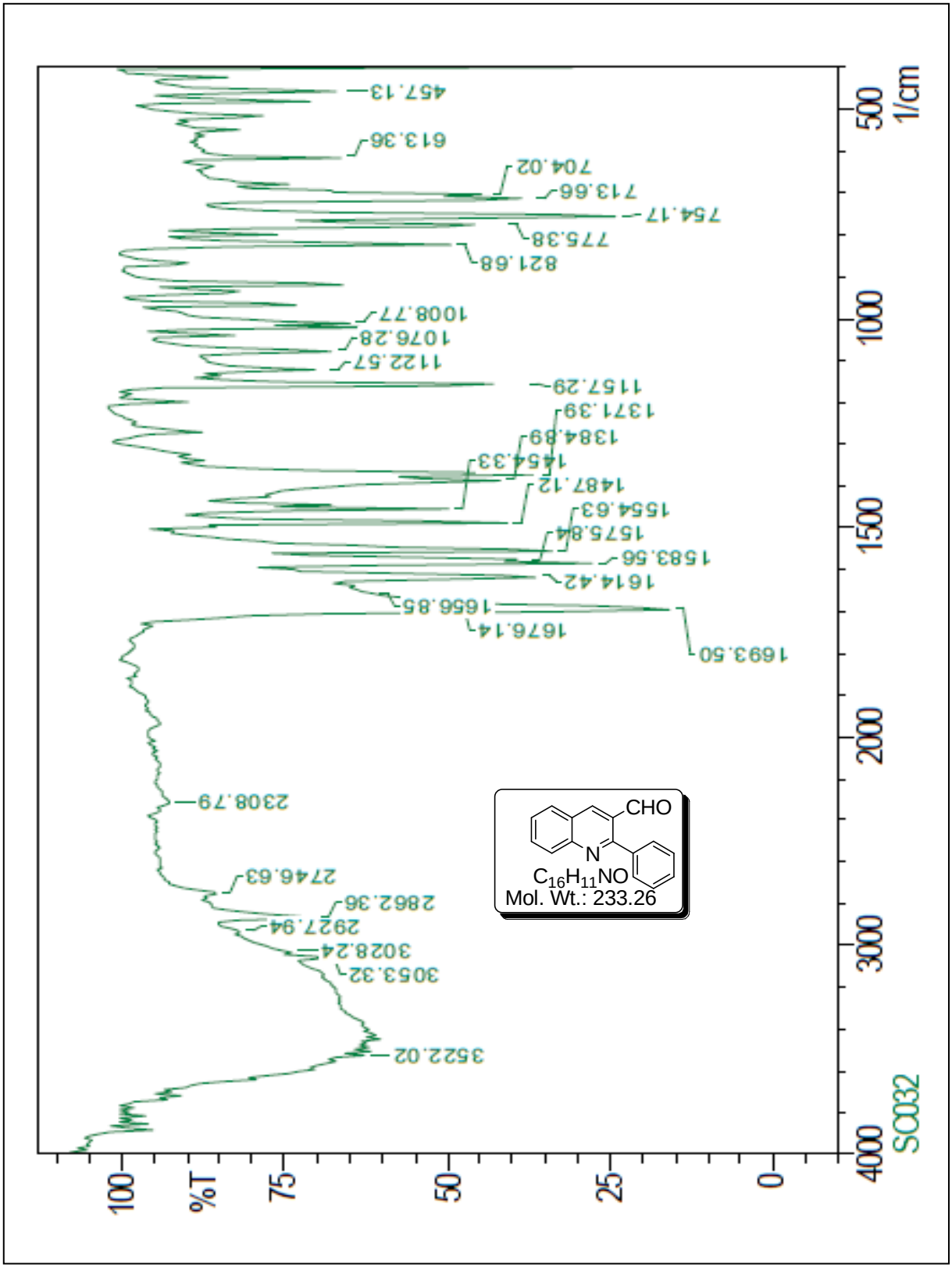

ppm
200
180
160
140
120
100
80
60
40
20
0.00
1.03
29.92
30.34
55.83
56.10
106.47
106.49
107.00
107.03
108.21
108.43
108.72
108.94
116.79
116.88
116.98
117.06
124.78
124.80
126.15
126.41
127.07
127.54
129.95
130.04
130.69
130.81
130.91
130.98
131.08
131.29
131.61
131.92
132.14
133.29
133.44
133.57
133.73
133.76
133.88
136.77
136.94
141.09
141.19
146.01
146.14
149.26
157.42
157.49
158.37
158.44
159.26
159.72
O
N
F
Cl
Cl
O
C24H16Cl2FNO2
Mol. Wt.: 440.29

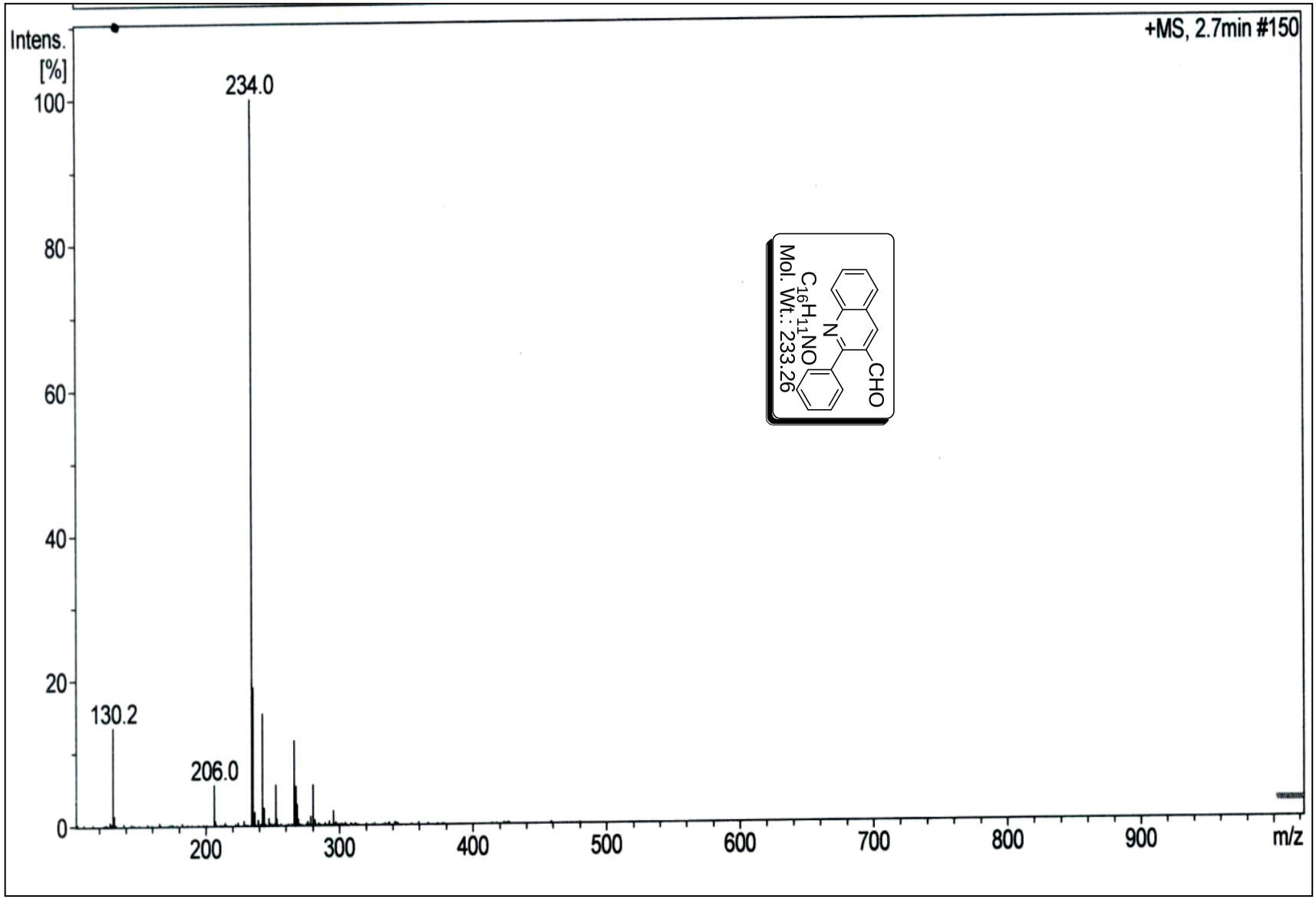

%T
90
75
60
45
4000
3000
2000
1500
1000
500
1/cm
SC 132
3419.79
3116.97
3072.60
3008.95
2956.87
2926.01
2839.22
1699.29
1616.35
1579.70
1552.70
1471.69
1436.97
1384.89
1354.03
1276.88
1240.23
1197.79
1083.99
1035.77
931.62
833.25
785.03
744.52
686.66
Cl
Cl
N
O
O
F
C24H16Cl2FNO2
Mol. Wt.: 440.29

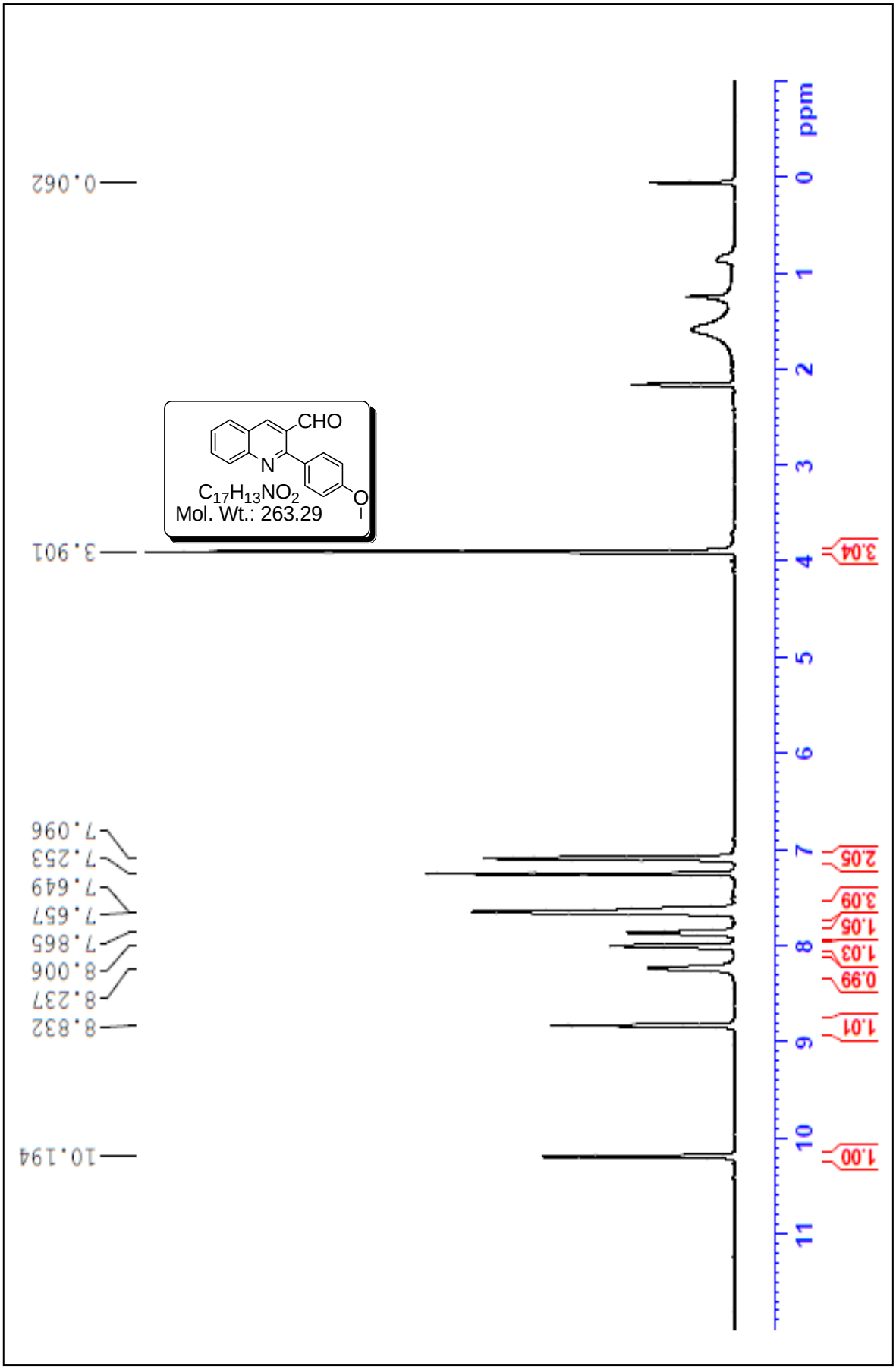

100
80
60
40
20
0
442.0
440.0
444.0
200
400
600
800
m/z
C24H16Cl2FNO2
Mol. Wt.: 440.29
Cl
Cl
N
O
O
F

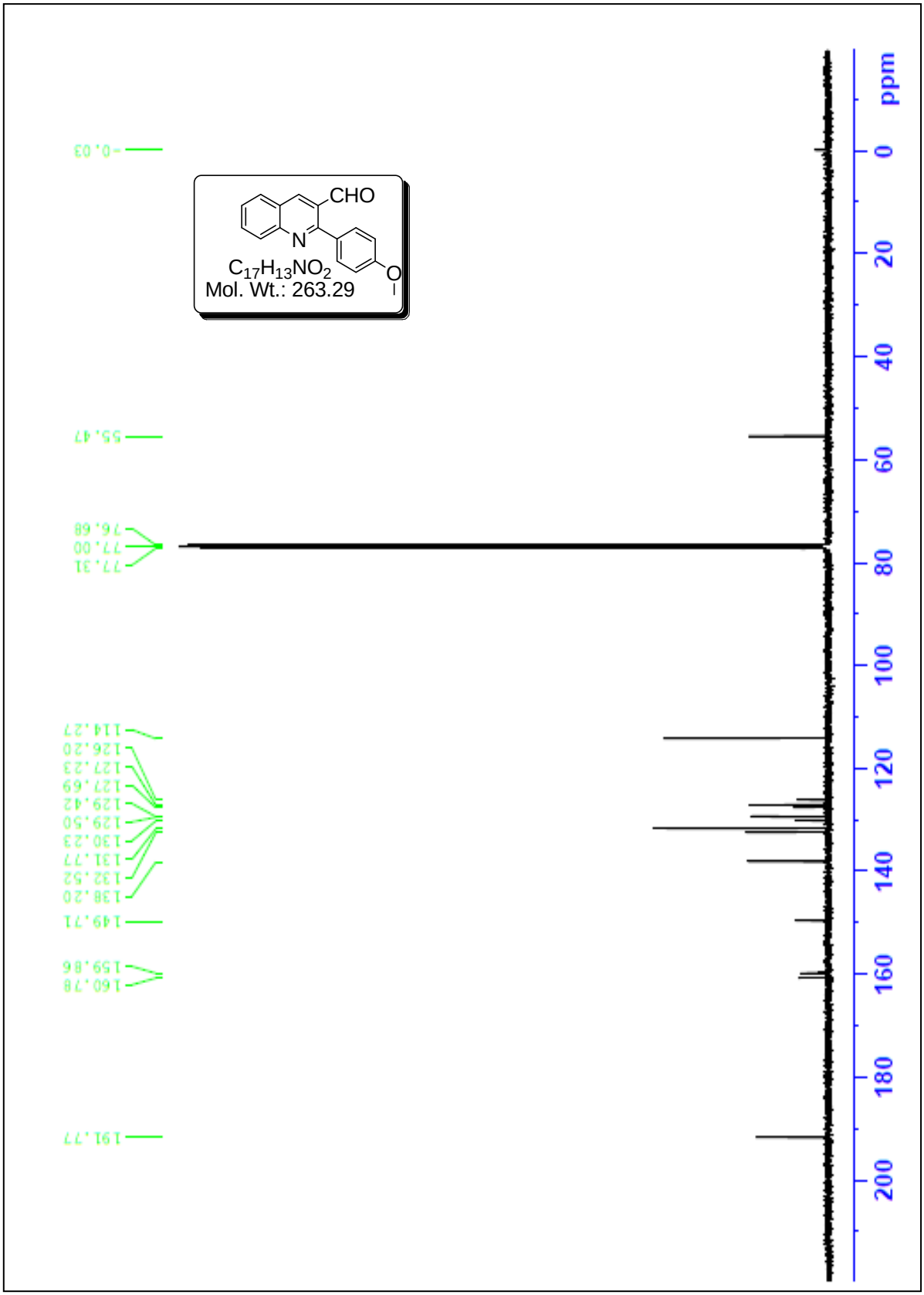
0.000
10.191
8.867
8.236
8.214
8.042
8.024
7.889
7.690
7.650
7.564
7.264
CHO
N
C16H11NO
Mol. Wt.: 233.26
ppm
1
2
3
4
5
6
7
8
9
10
11
0.75
3.23
3.14
1.13
1.06
1.04
1.01
1.00

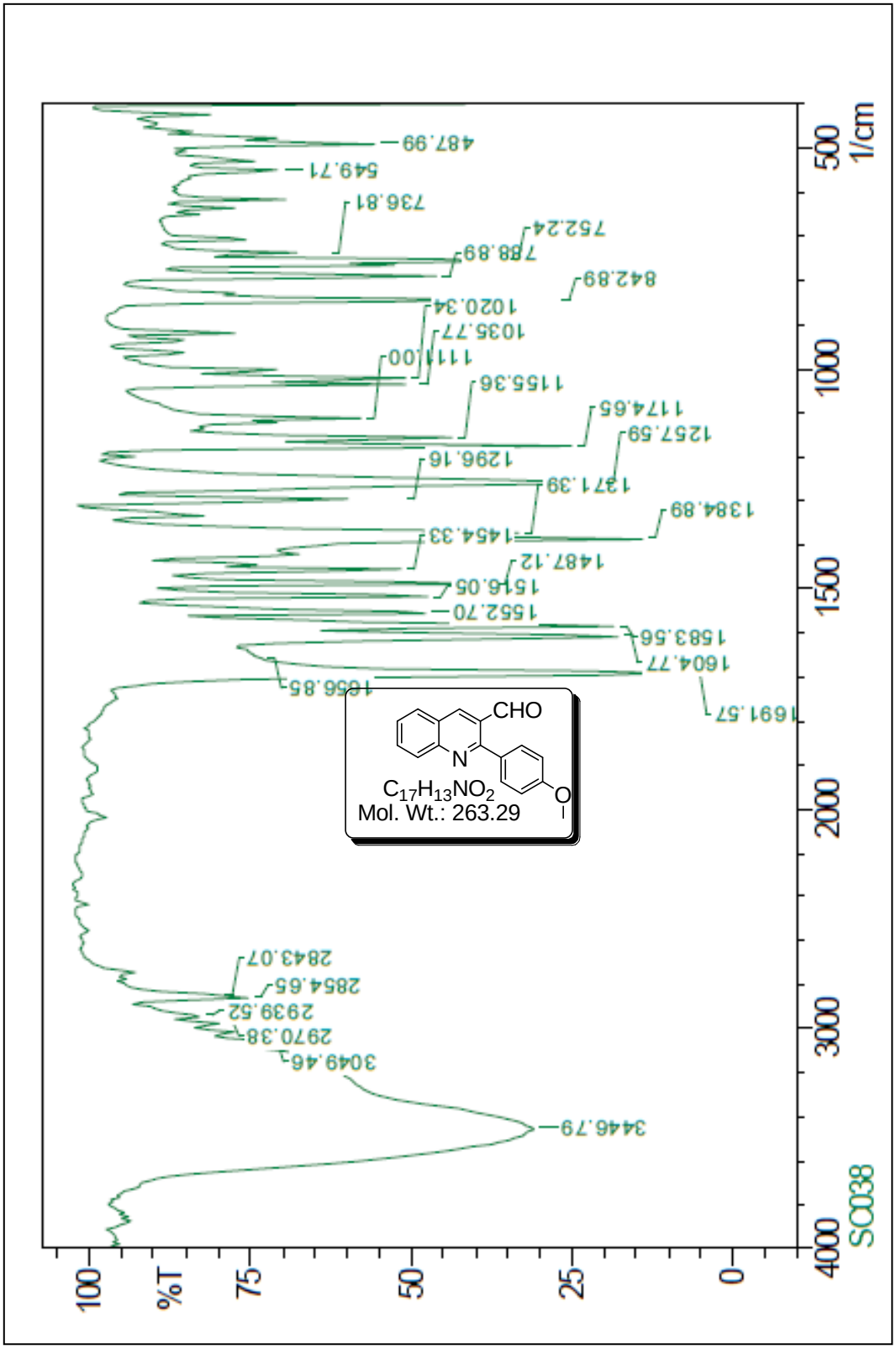

CHO
N
$C_{16}H_{11}NO$
Mol. Wt.: 233.26
0.14
76.84
77.16
77.48
126.55
127.68
127.80
128.92
129.58
129.63
129.76
130.41
132.84
137.90
138.34
149.78
160.50
191.73
0 ppm
20
40
60
80
100
120
140
160
180

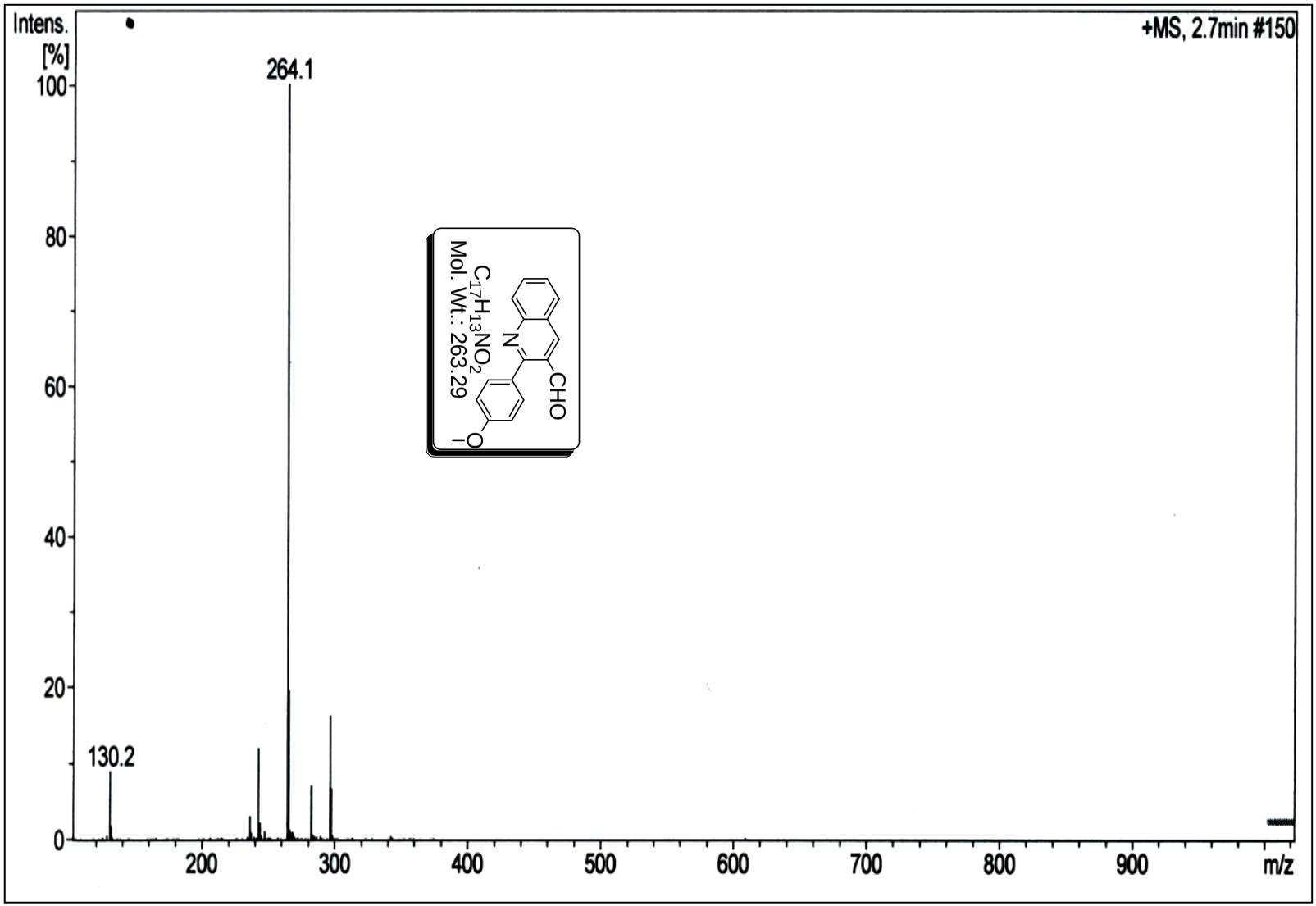

457.13
613.36
704.02
713.66
754.17
775.38
821.68
1008.77
1076.28
1122.57
1157.29
1371.39
1384.89
1454.33
1487.12
1554.63
1575.84
1583.56
1614.42
1656.85
1676.14
1693.50
2308.79
2746.63
2862.36
2927.94
3028.24
3053.32
3522.02
CHO
N
C16H11NO
Mol. Wt.: 233.26
100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC032

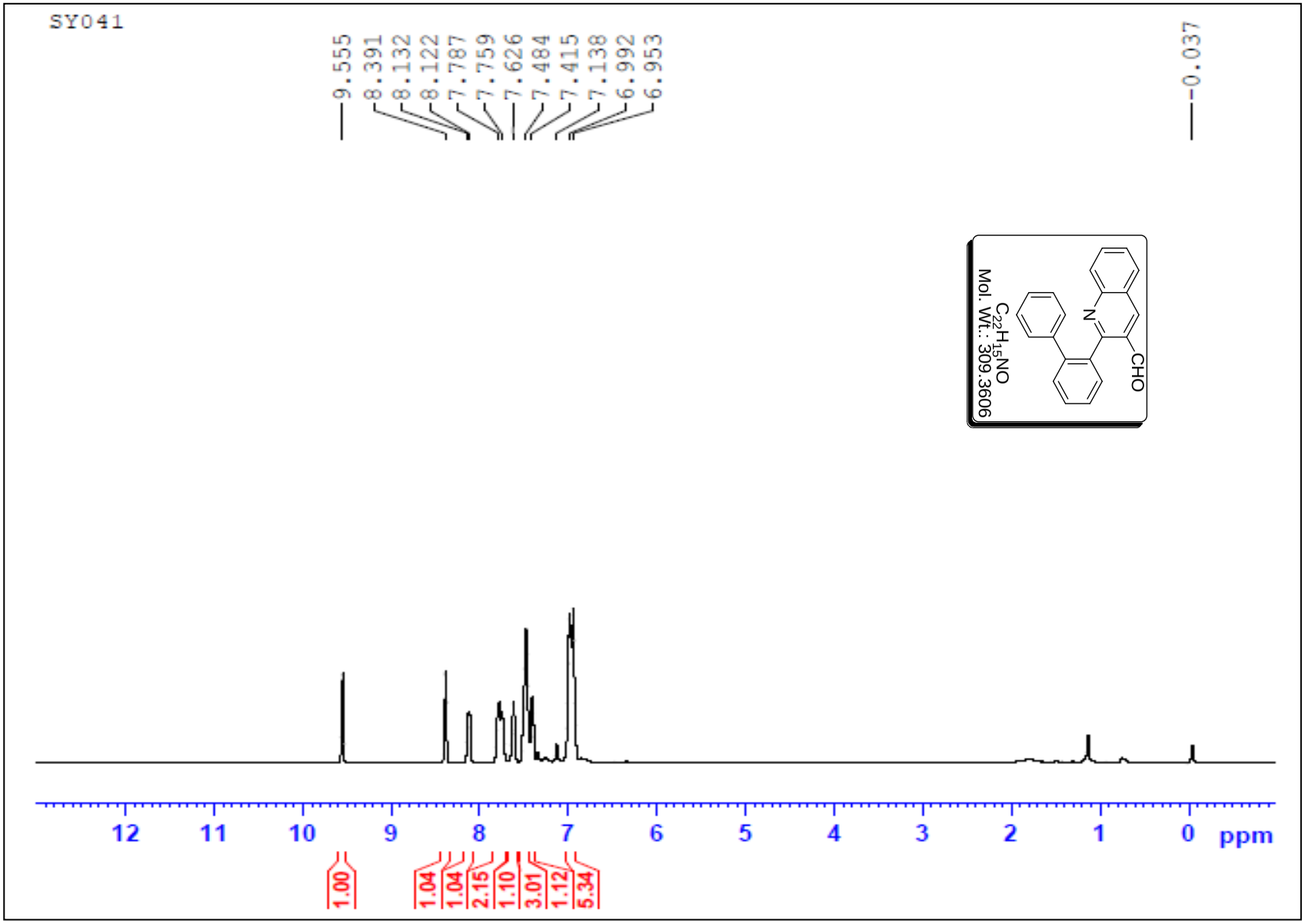

+MS, 2.7min #150
Intens.
[%]
100
80
60
40
20
0
234.0
130.2
206.0
200
300
400
500
600
700
800
900
m/z
C16H11NO
Mol. Wt.: 233.26
N
CHO

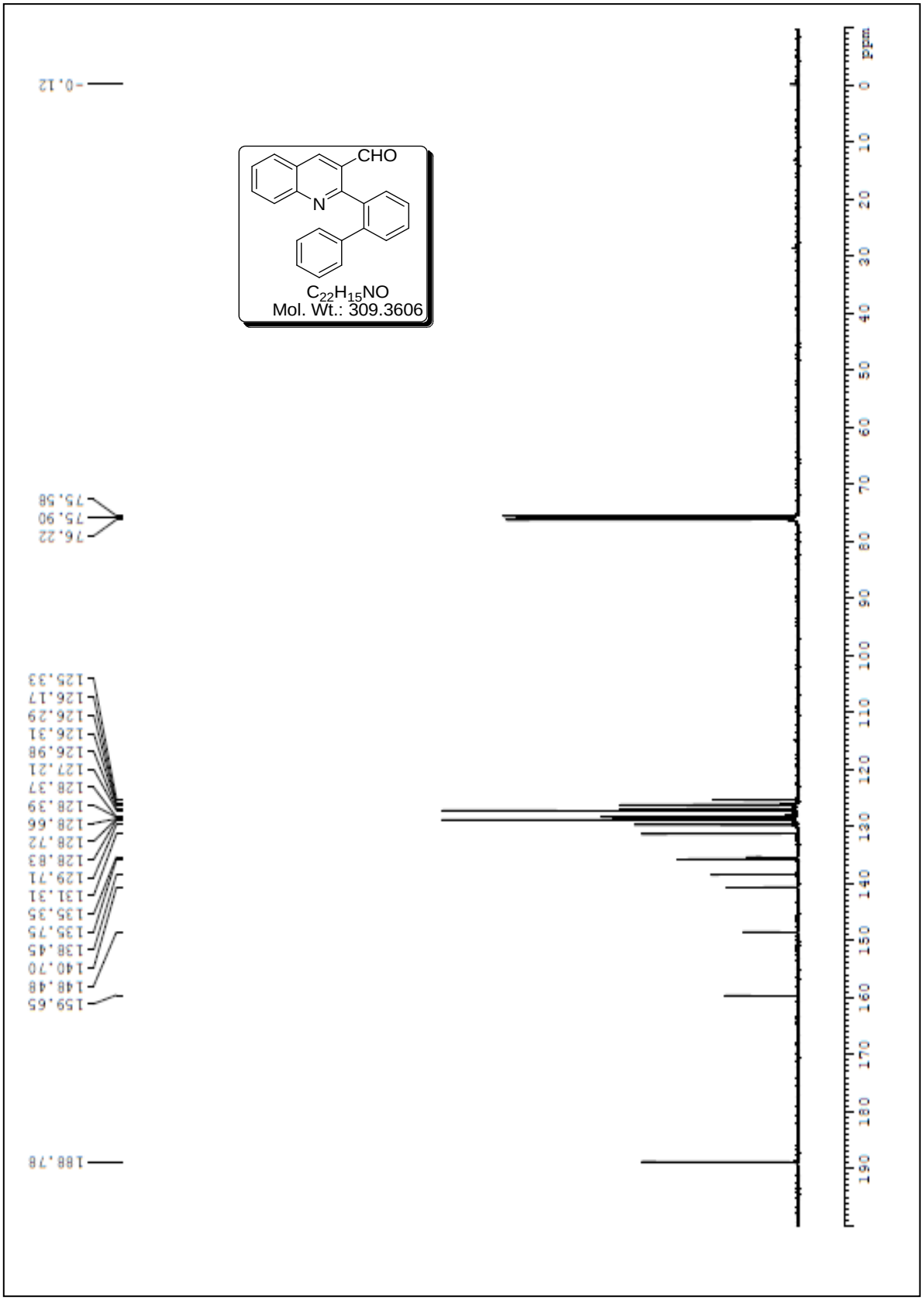

CHO
N
O
$C_{17}H_{13}NO_2$
Mol. Wt.: 263.29
ppm
0
1
2
3
4
5
6
7
8
9
10
11
0.062
3.901
7.096
7.253
7.649
7.657
7.865
8.006
8.237
8.832
10.194
3.04
2.05
3.09
1.05
1.03
0.99
1.01
1.00

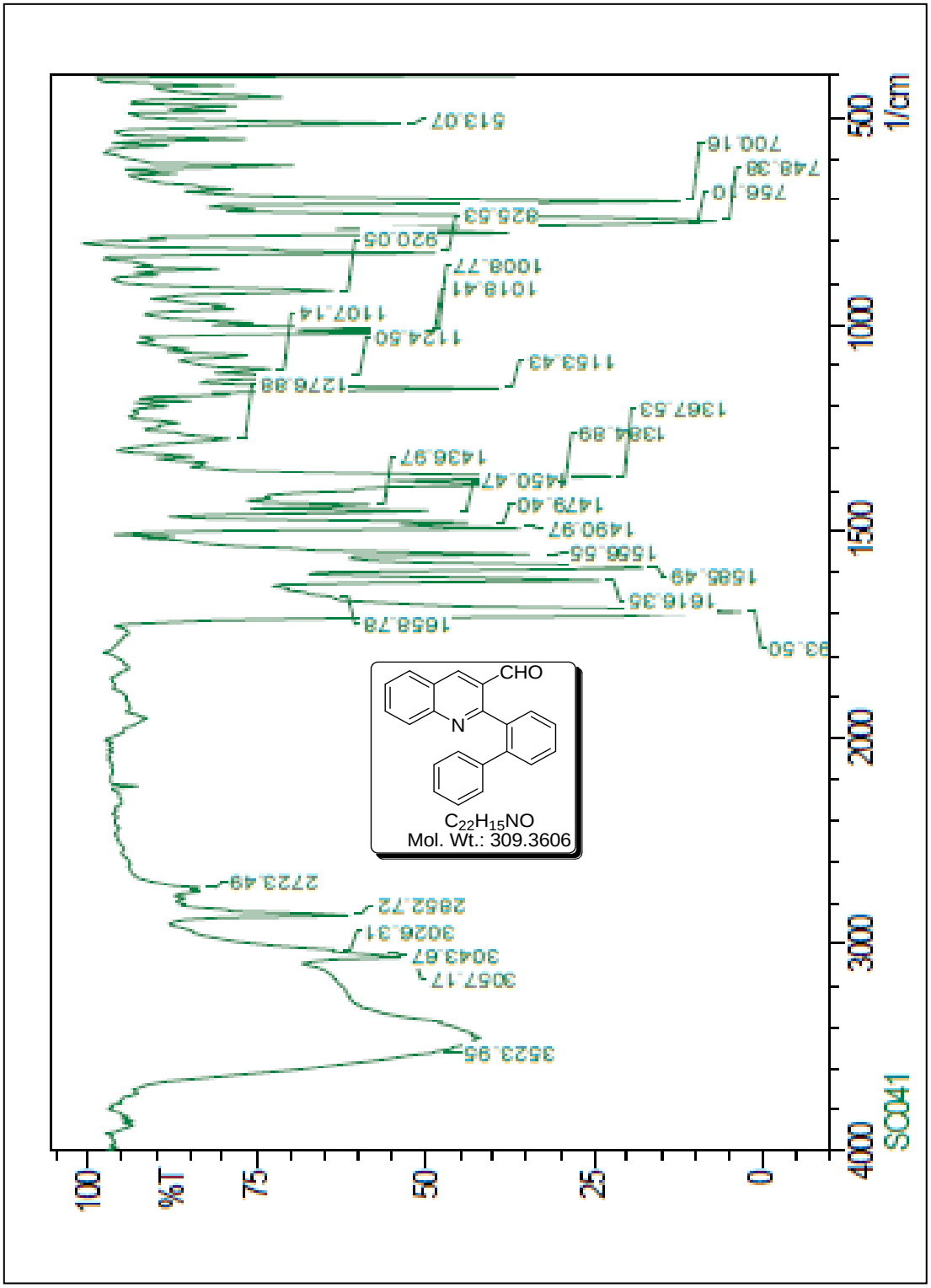

CHO
N
O
$C_{17}H_{13}NO_2$
Mol. Wt.: 263.29
ppm
0
20
40
60
80
100
120
140
160
180
200
-0.03
55.47
76.68
77.00
77.31
114.27
126.20
127.23
127.69
129.42
129.50
130.23
131.77
132.52
138.20
149.71
159.86
160.78
191.77

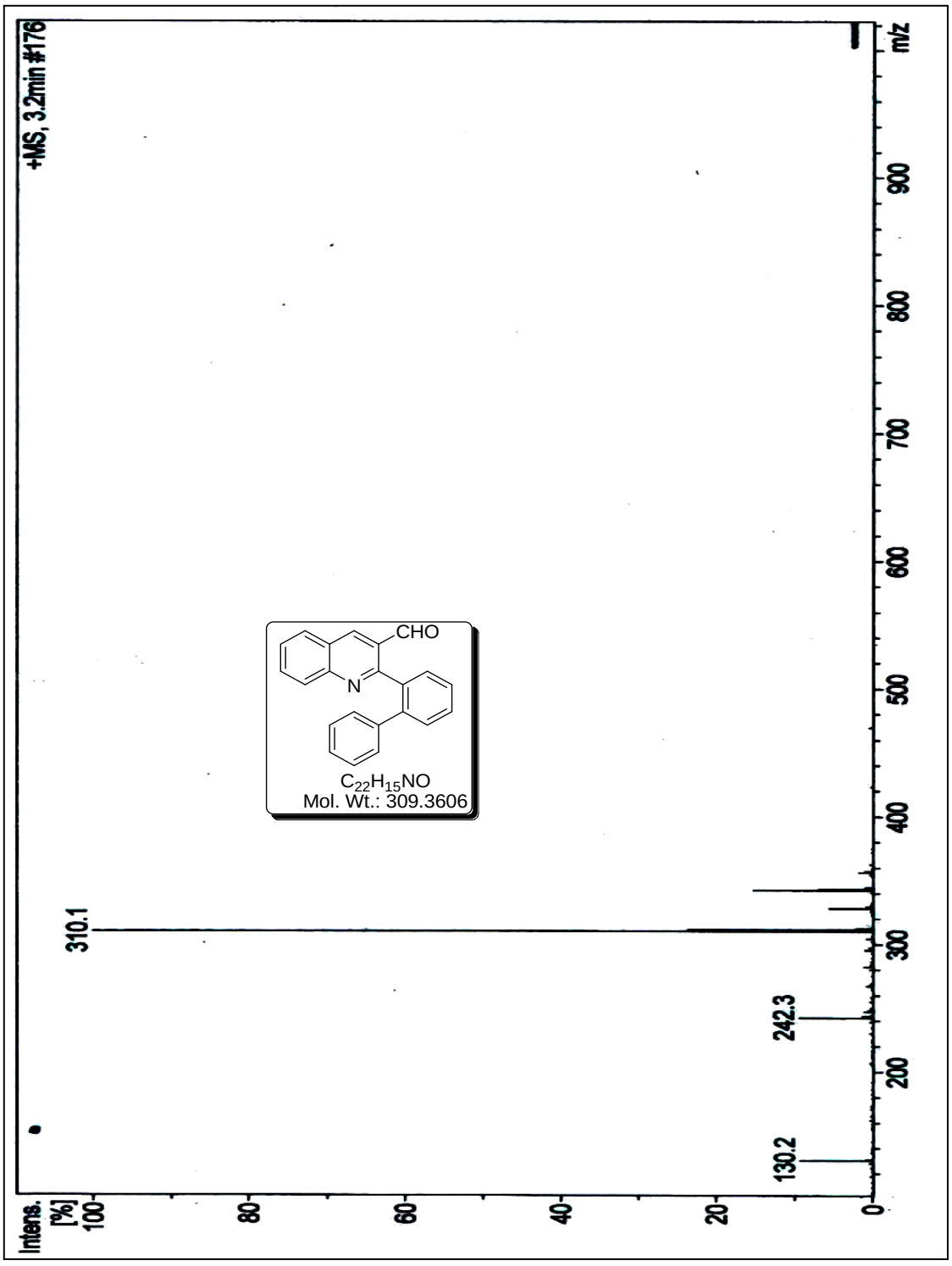

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC038
3446.79
3049.46
2970.38
2939.52
2854.65
2843.07
1656.85
1691.57
1604.77
1583.56
1552.70
1516.05
1487.12
1454.33
1384.89
1371.39
1296.16
1257.59
1174.65
1155.36
1111.00
1035.77
1020.34
842.89
788.89
752.24
736.81
549.71
487.99
CHO
N
O
C17H13NO2
Mol. Wt.: 263.29

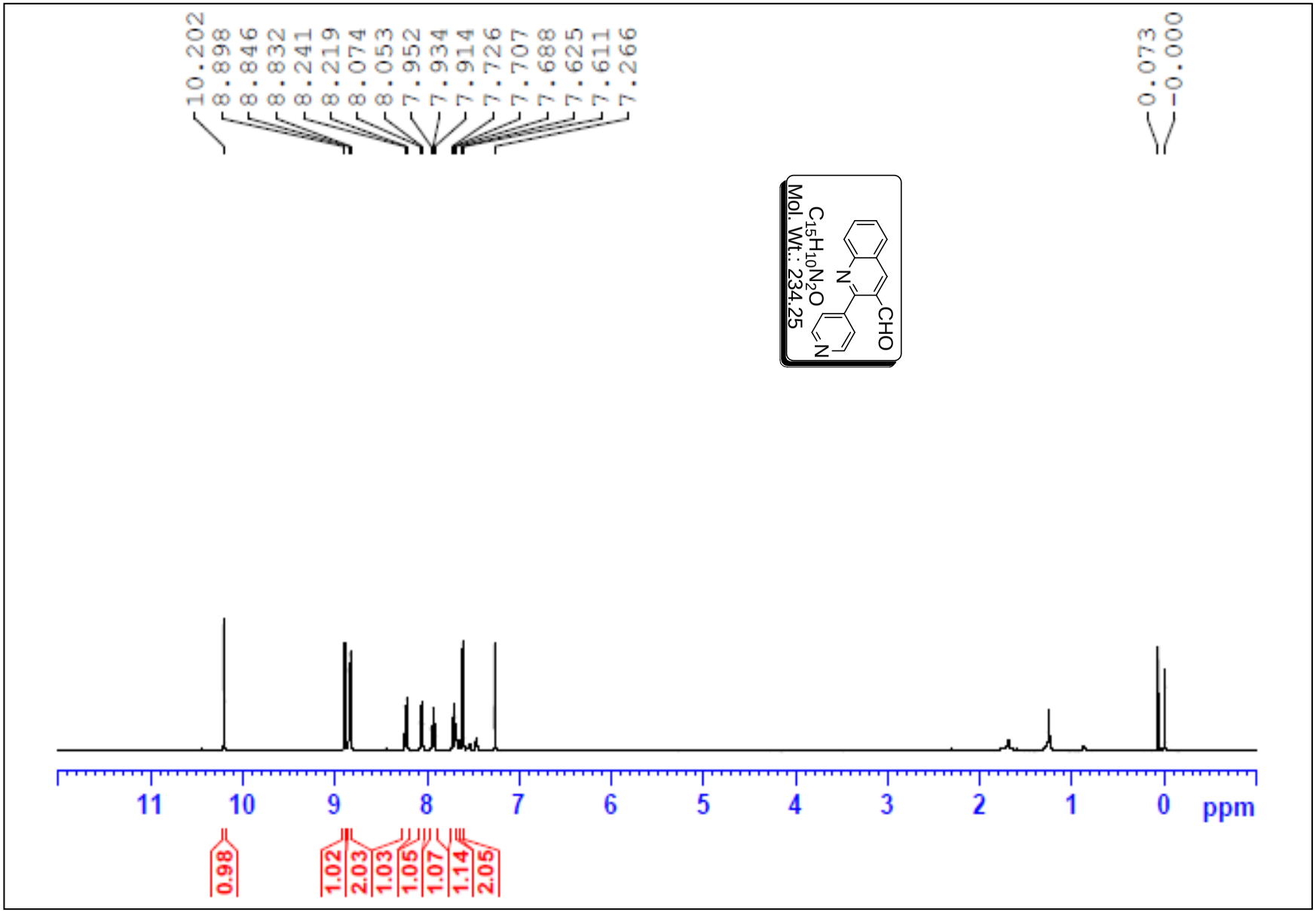

Intens.
[%]
+MS, 2.7min #150
264.1
130.2
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z
C17H13NO2
Mol. Wt.: 263.29
N
CHO
O

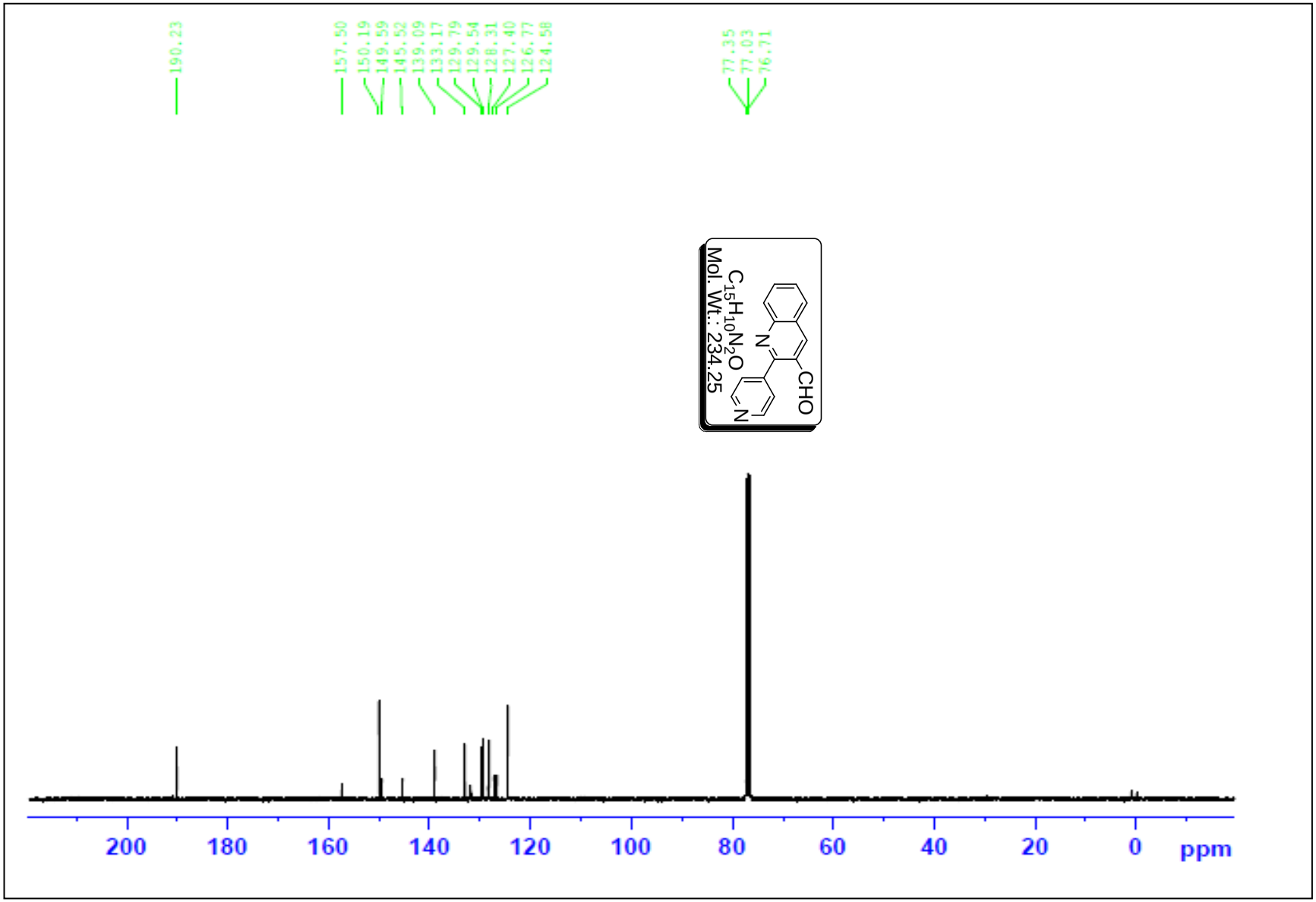

SY041
9.555
8.391
8.132
8.122
7.787
7.759
7.626
7.484
7.415
7.138
6.992
6.953
0.037
$C_{22}H_{15}NO$
Mol. Wt.: 309.3606
N
CHO
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
1.04
2.15
1.10
3.01
1.12
5.34

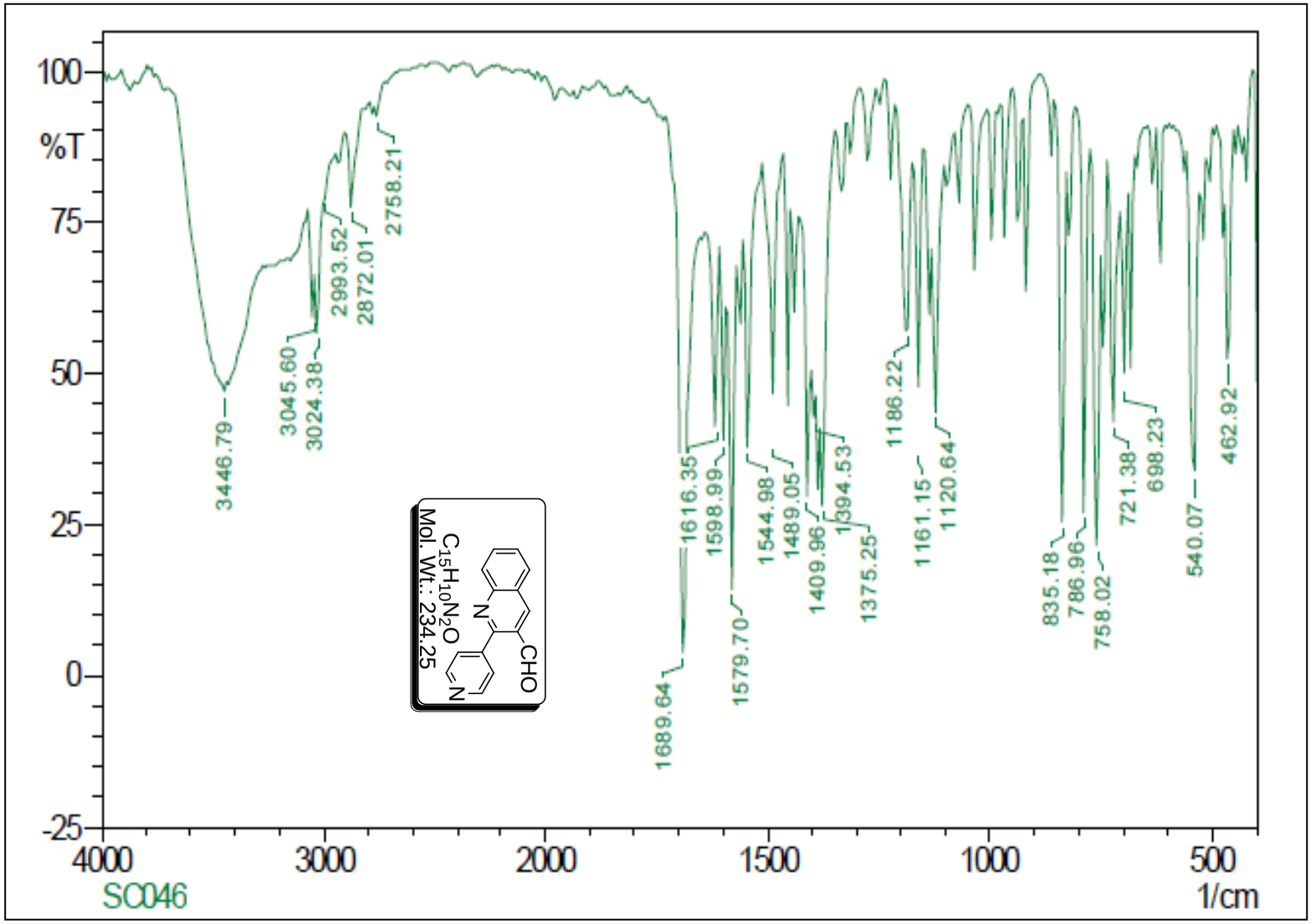

CHO
N
$C_{22}H_{15}NO$
Mol. Wt.: 309.3606
-0.12
75.58
75.90
76.22
125.33
126.17
126.29
126.31
126.98
127.21
128.37
128.39
128.66
128.72
128.83
129.71
131.31
135.35
135.75
138.45
140.70
148.48
159.65
188.78
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

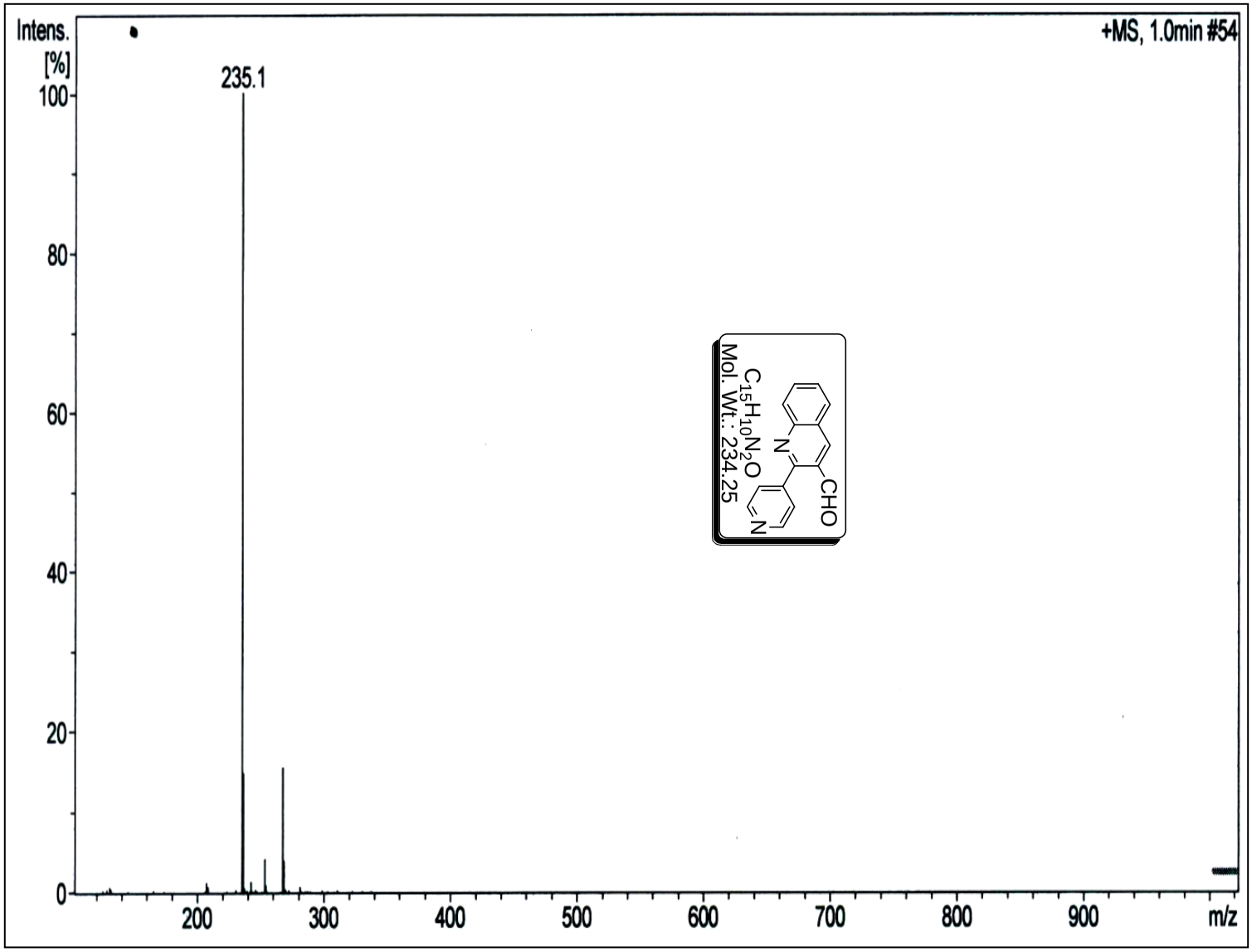

513.07
700.16
748.38
756.10
825.53
920.05
1008.77
1018.41
1107.14
1124.50
1153.43
1276.88
1367.53
1384.89
1436.97
1450.47
1479.40
1490.97
1556.55
1585.49
1616.35
1658.78
33.50
CHO
N
C22H15NO
Mol. Wt.: 309.3606
2723.49
2852.72
3026.31
3043.87
3057.17
3523.95
100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC041

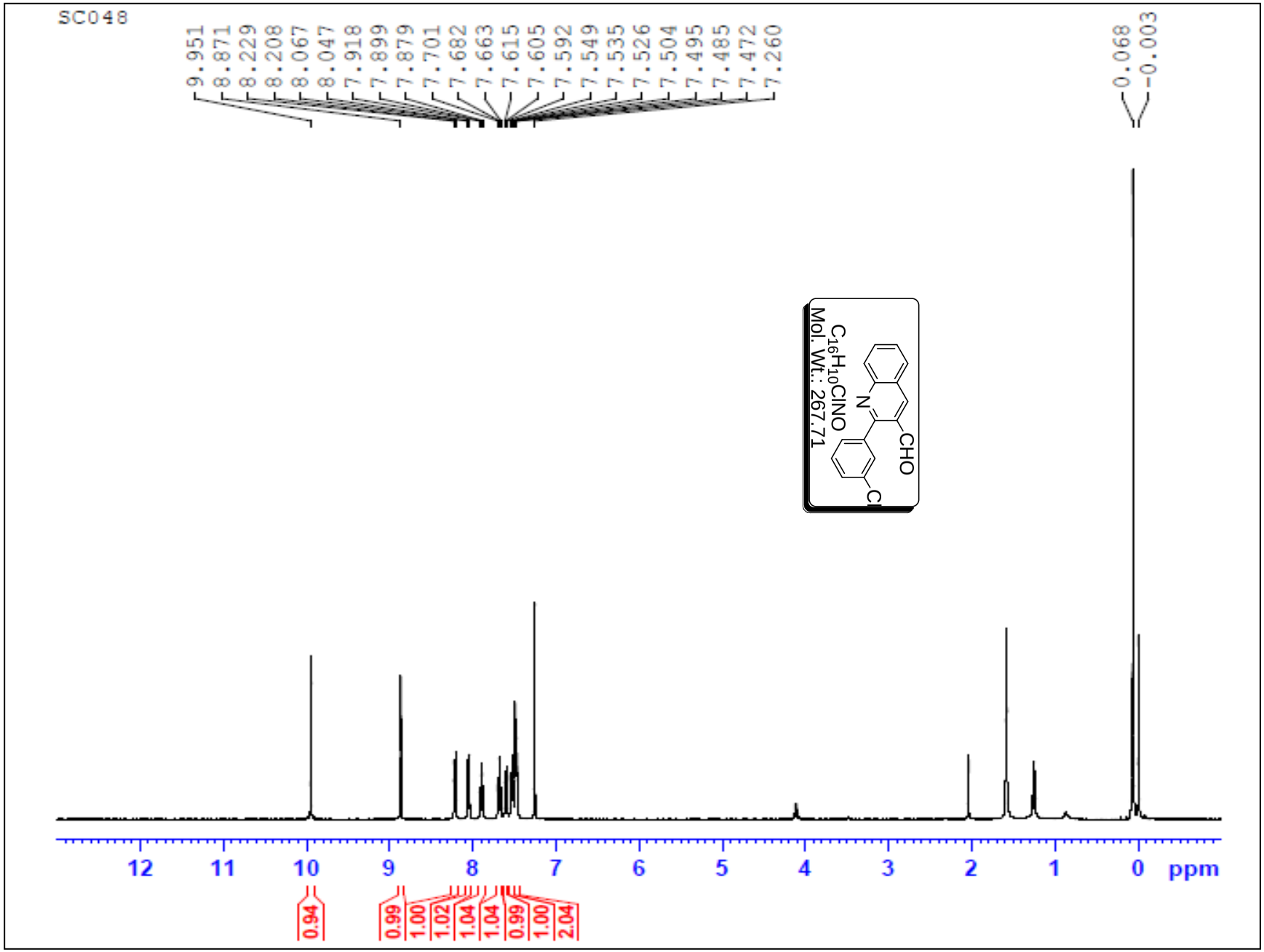

+MS, 3.2min #176
Intens.
[%]
100
80
60
40
20
0
310.1
242.3
130.2
200
300
400
500
600
700
800
900
m/z
CHO
N
C22H15NO
Mol. Wt.: 309.3606

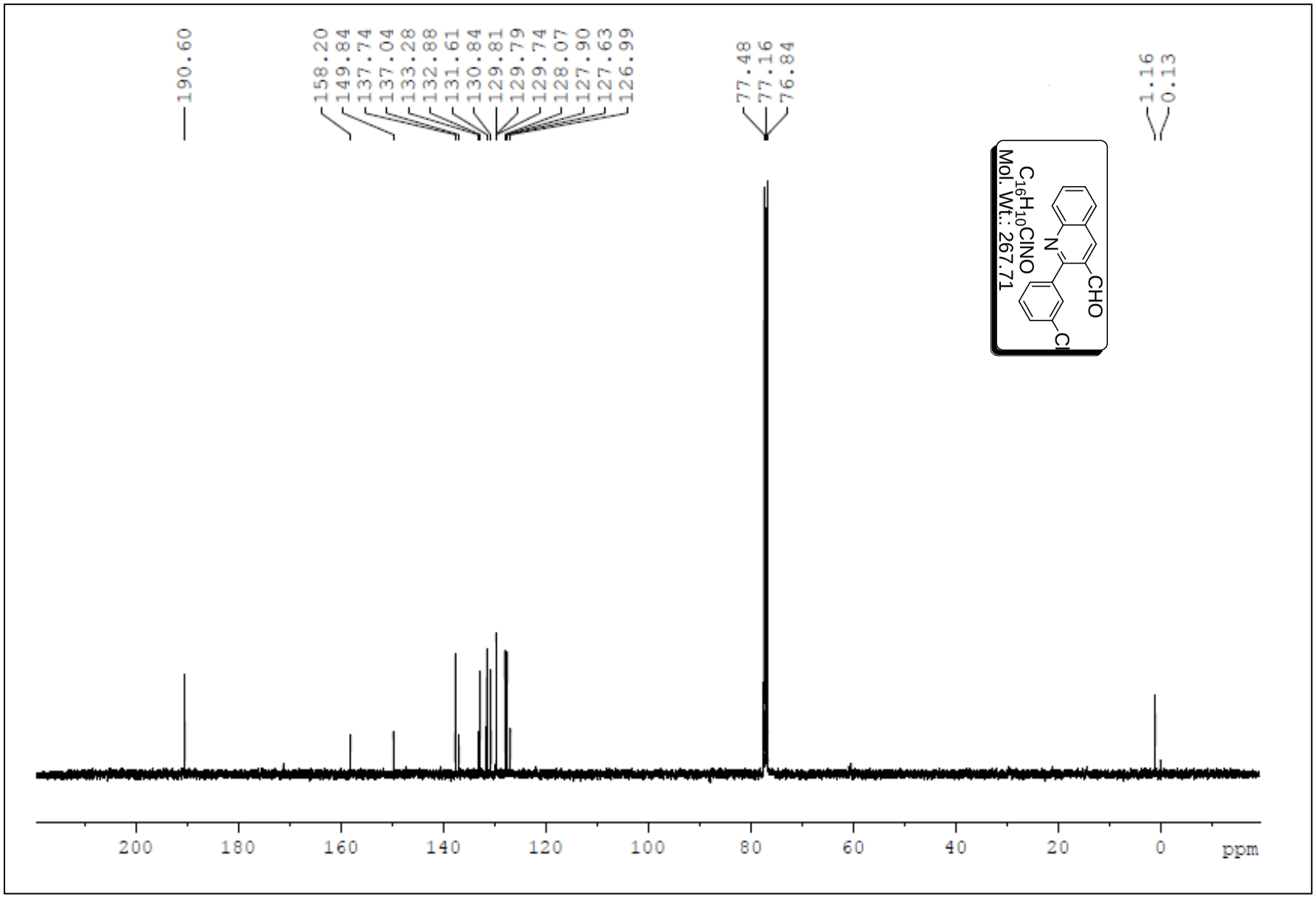

10.202
8.898
8.846
8.832
8.241
8.219
8.074
8.053
7.952
7.934
7.914
7.726
7.707
7.688
7.625
7.611
7.266
0.073
-0.000
C15H10N2O
Mol. Wt.: 234.25
N
N
CHO
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.02
2.03
1.03
1.05
1.07
1.14
2.05

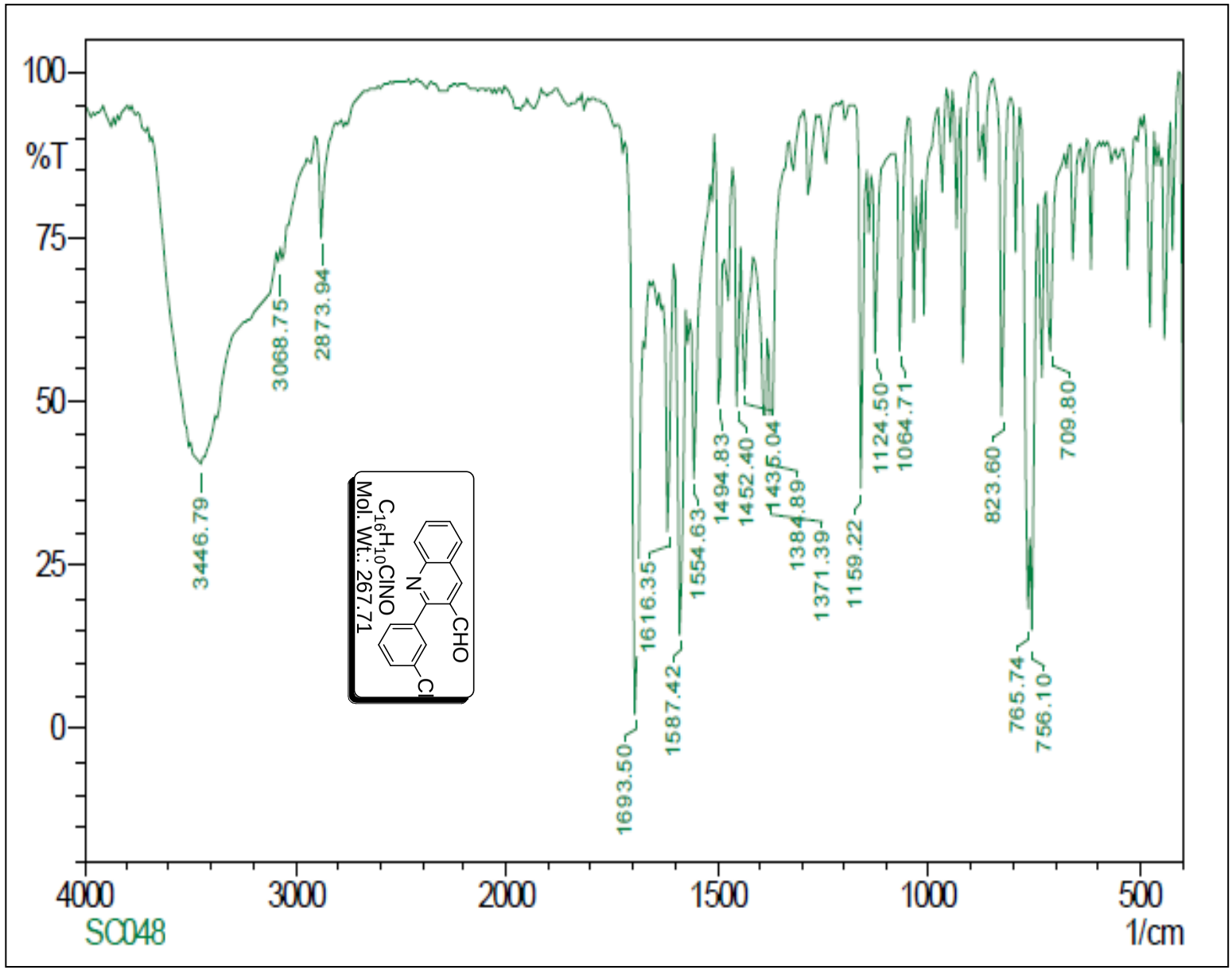

190.23
157.50
150.19
149.59
145.52
139.09
133.17
129.79
129.54
128.31
127.40
126.77
124.58
77.35
77.03
76.71
C15H10N2O
Mol. Wt.: 234.25
N
N
CHO
200
180
160
140
120
100
80
60
40
20
0
ppm

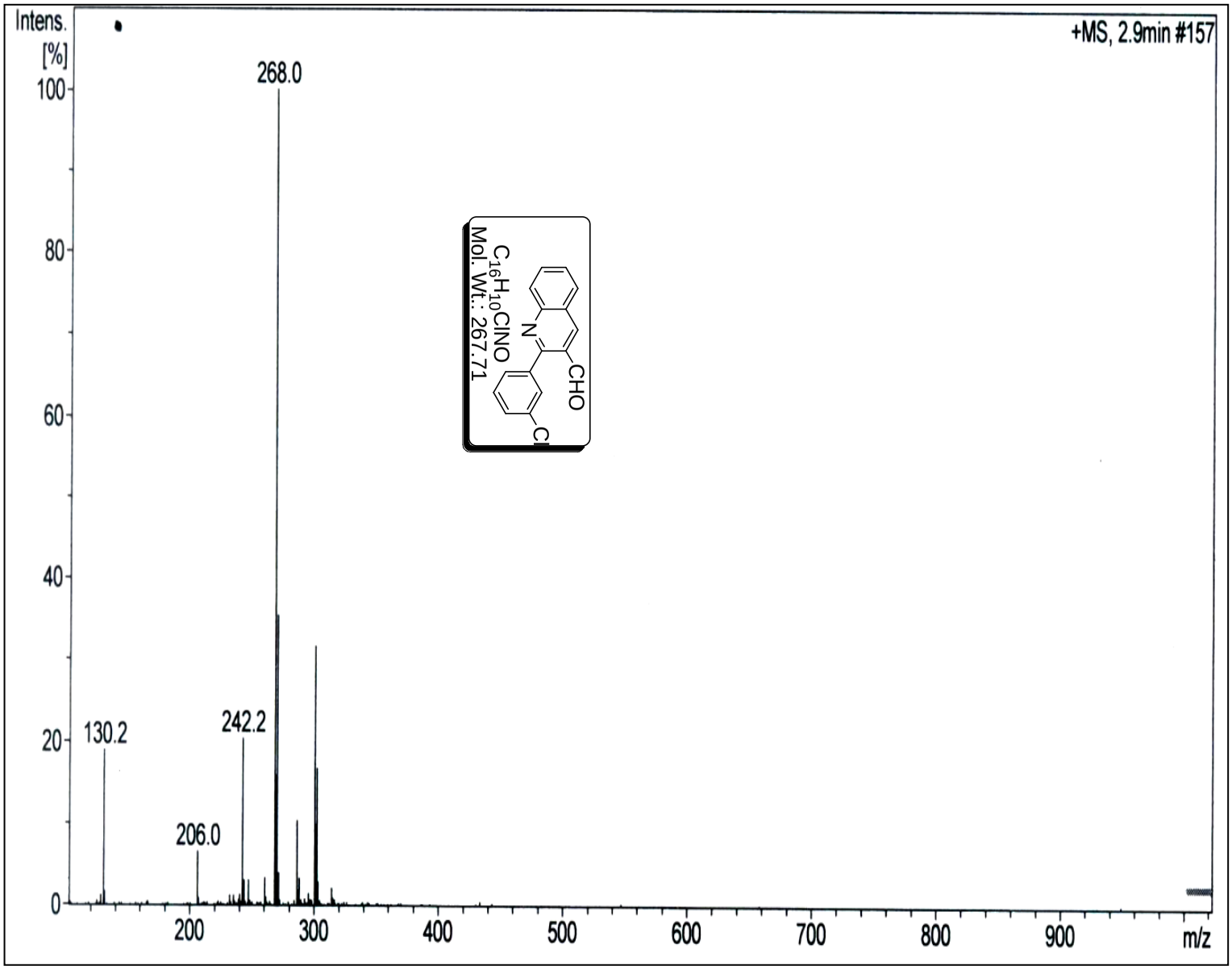

100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC046
3446.79
3045.60
3024.38
2993.52
2872.01
2758.21
1689.64
1616.35
1598.99
1579.70
1544.98
1489.05
1409.96
1394.53
1375.25
1186.22
1161.15
1120.64
835.18
786.96
758.02
721.38
698.23
540.07
462.92
C15H10N2O
Mol. Wt.: 234.25
N
N
CHO

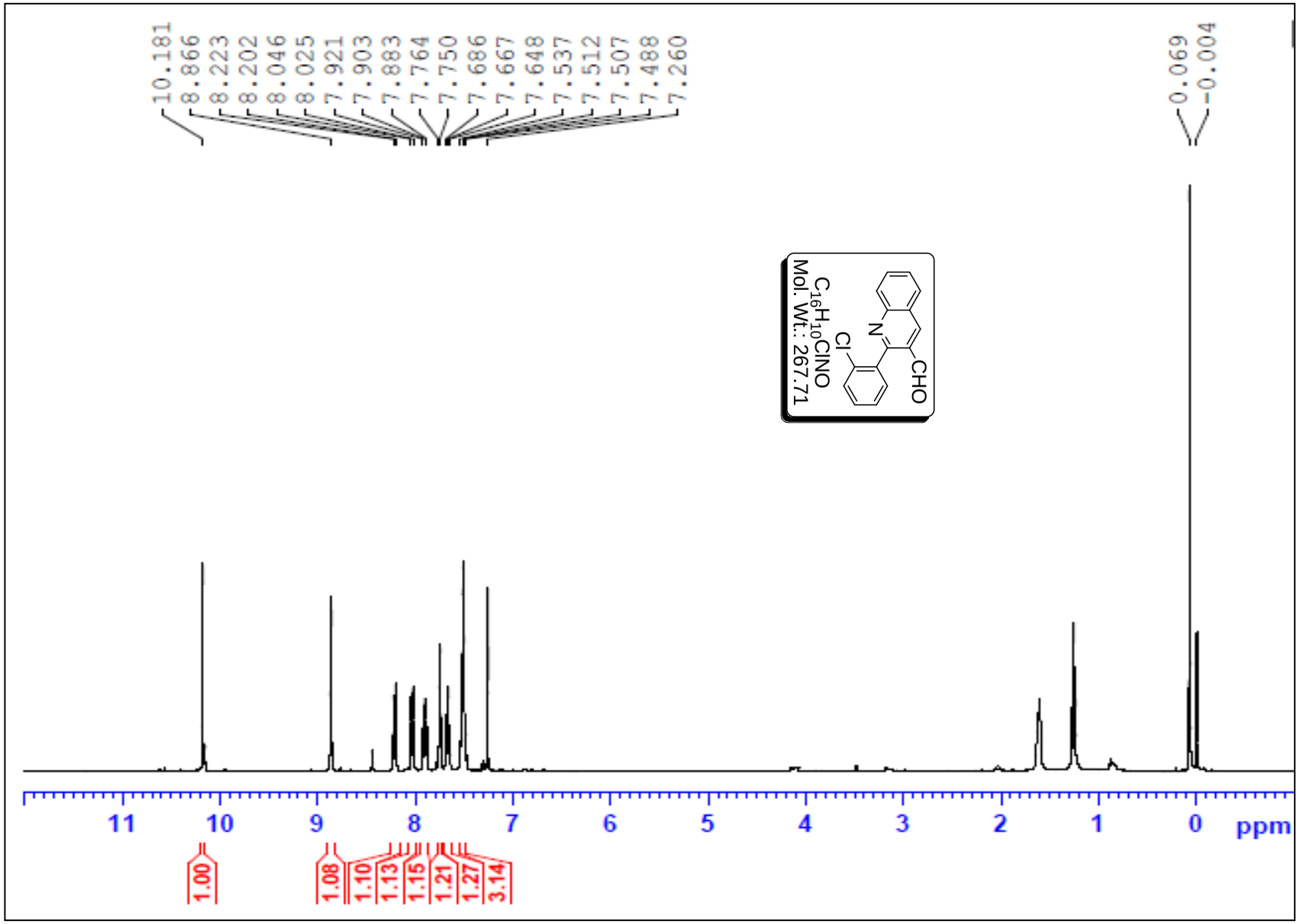

Intens.
[%]
+MS, 1.0min #54
235.1
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z
C15H10N2O
Mol. Wt.: 234.25
N
N
CHO

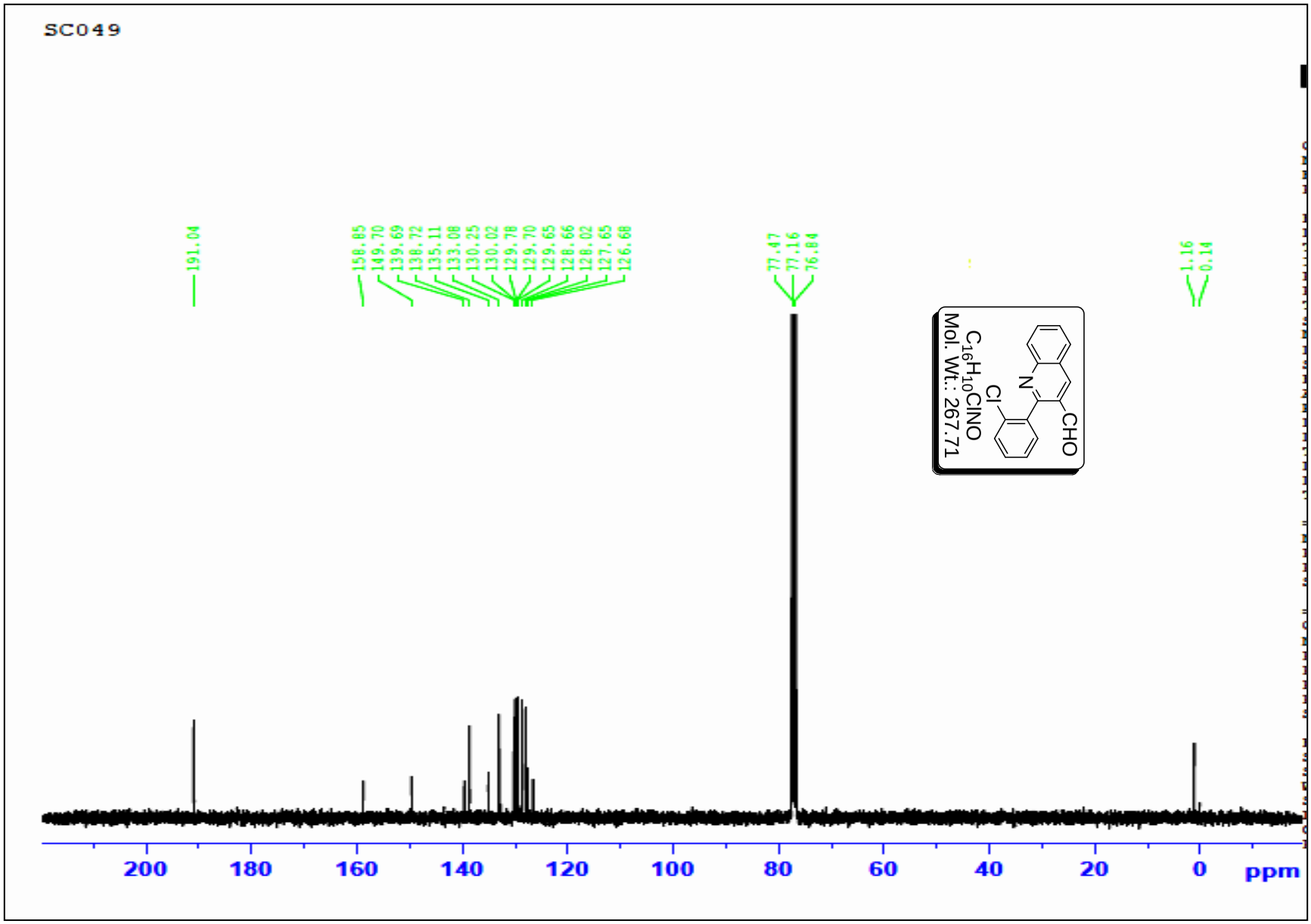

SC048
9.951
8.871
8.229
8.208
8.067
8.047
7.918
7.899
7.879
7.701
7.682
7.663
7.615
7.605
7.592
7.549
7.535
7.526
7.504
7.495
7.485
7.472
7.260
0.068
-0.003
C16H10ClNO
Mol. Wt.: 267.71
N
CHO
Cl
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
0.99
1.00
1.02
1.04
1.04
0.99
1.00
2.04

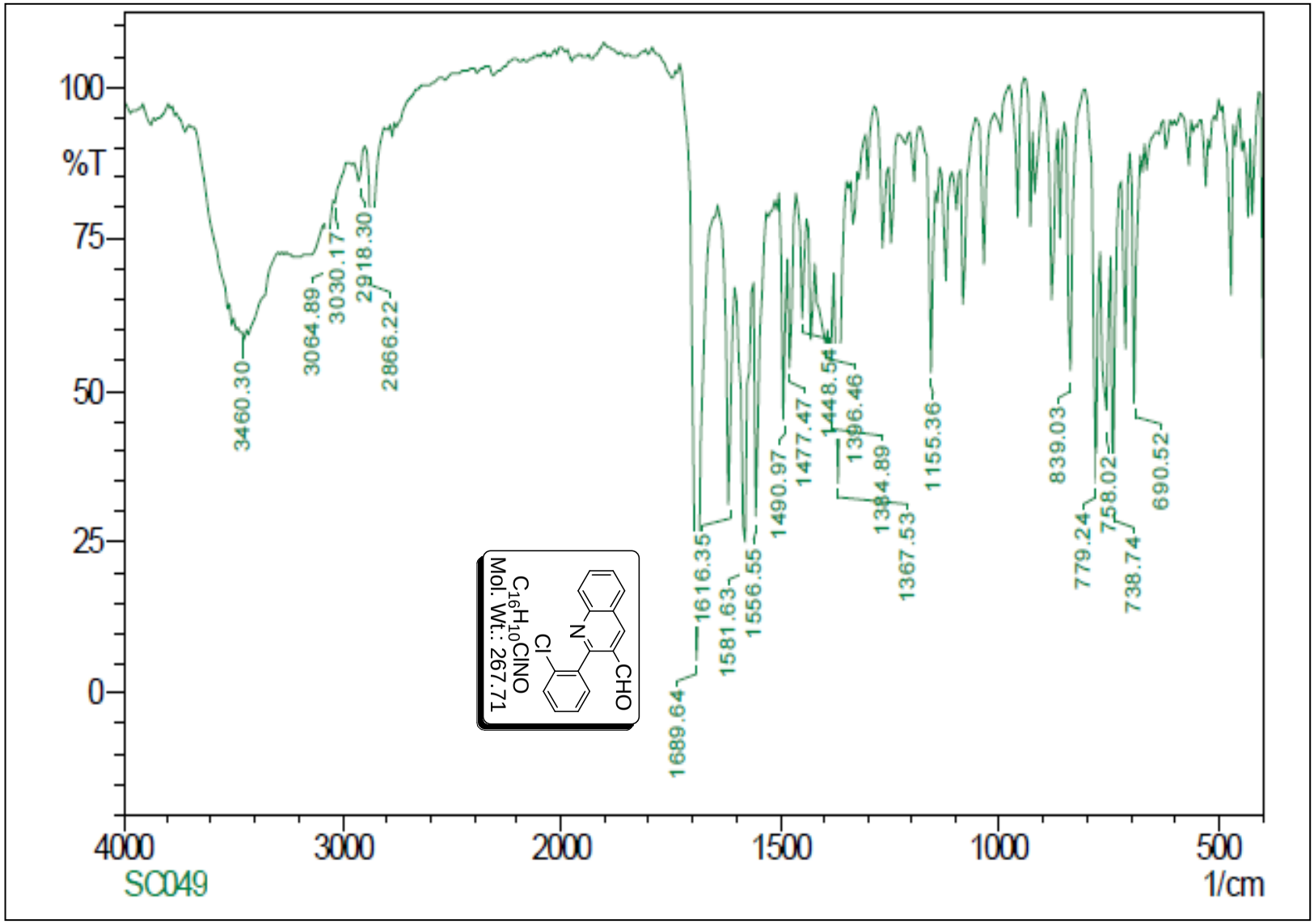

190.60
158.20
149.84
137.74
137.04
133.28
132.88
131.61
130.84
129.81
129.79
129.74
128.07
127.90
127.63
126.99
77.48
77.16
76.84
1.16
0.13
C16H10ClNO
Mol. Wt.: 267.71
N
CHO
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

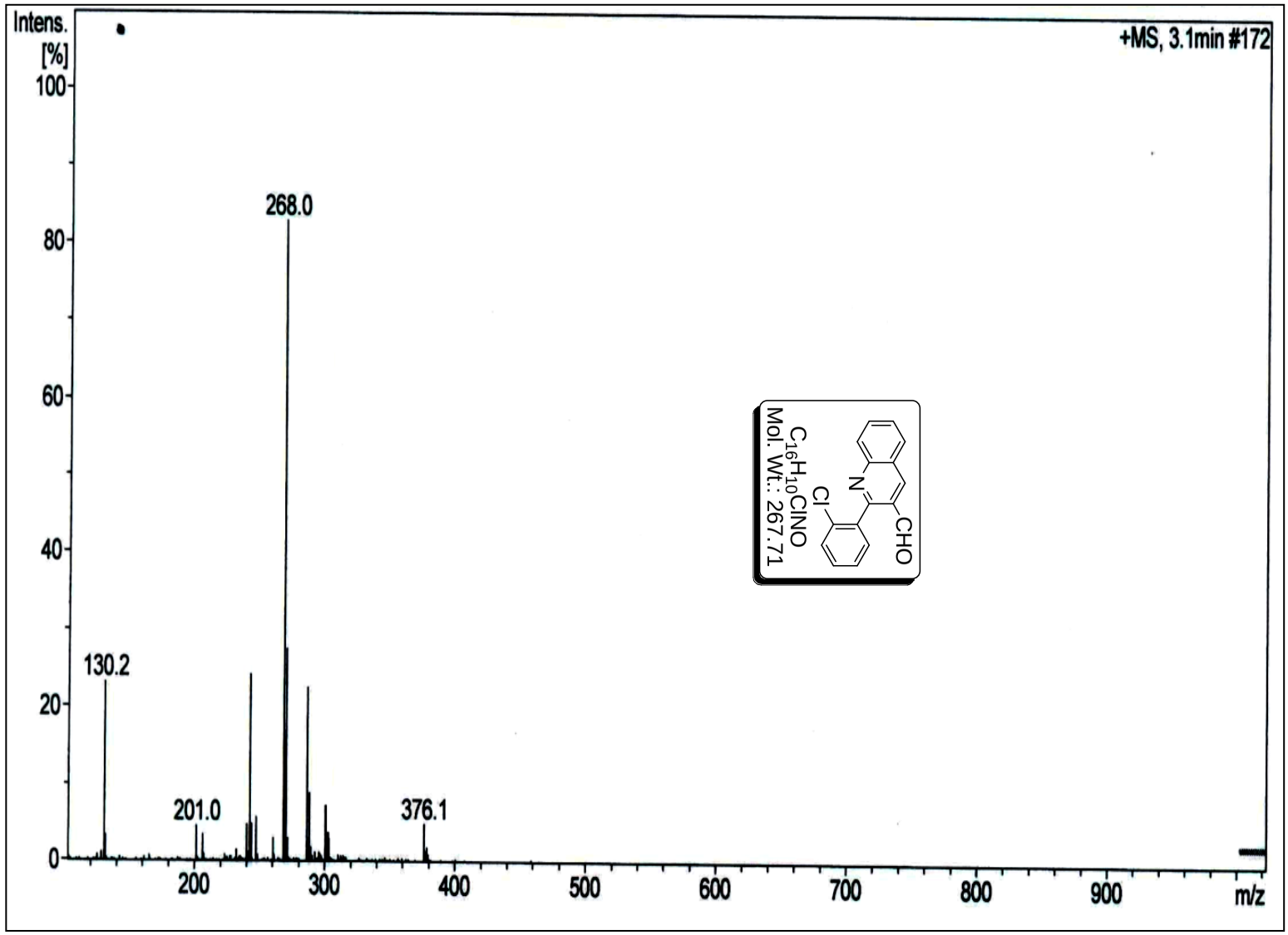

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC048
3446.79
3068.75
2873.94
1693.50
1616.35
1587.42
1554.63
1494.83
1452.40
1435.04
1384.89
1371.39
1159.22
1124.50
1064.71
823.60
765.74
756.10
709.80
C16H10ClNO
Mol. Wt.: 267.71
N
CHO
Cl

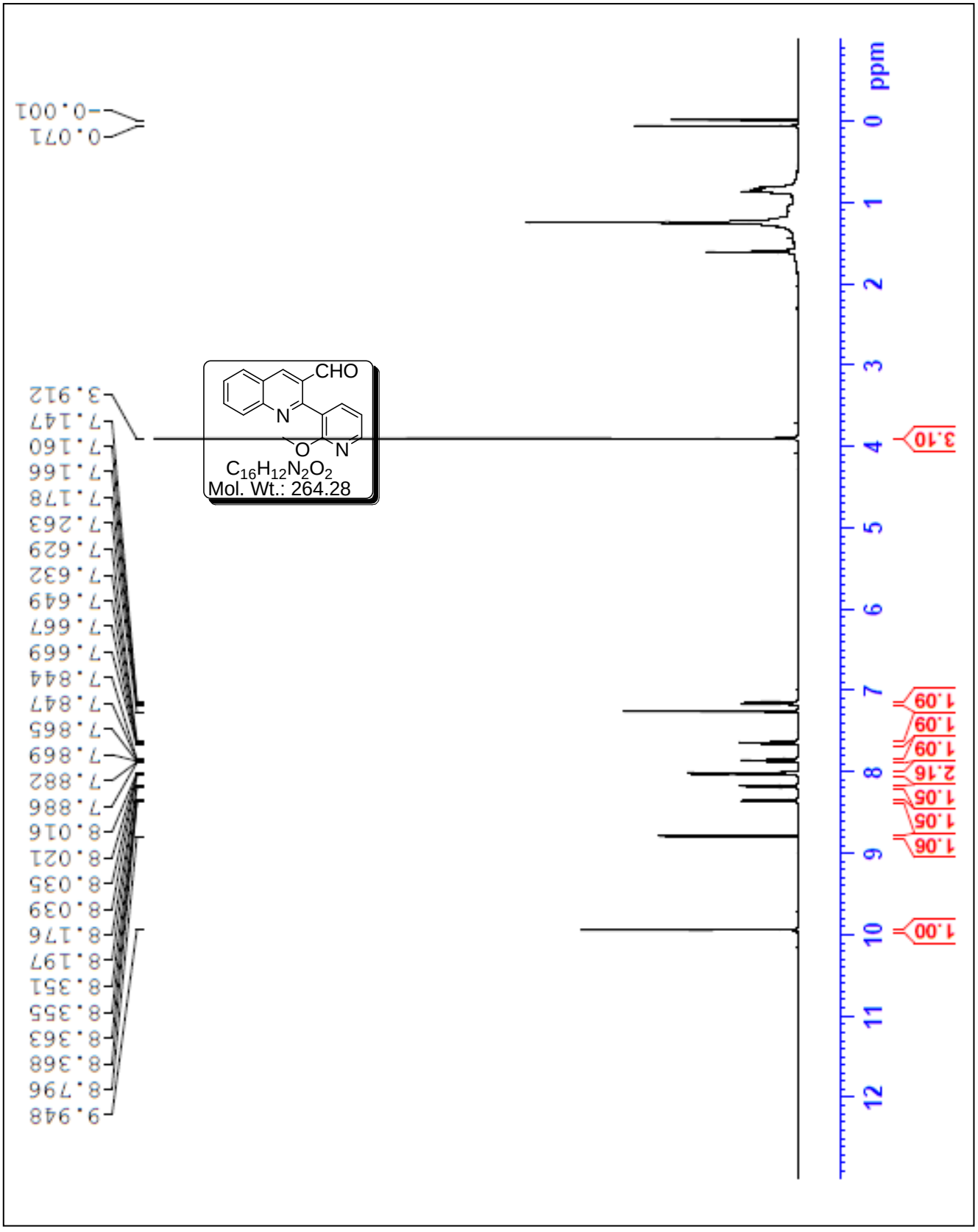

Intens.
[%]
+MS, 2.9min #157
268.0
130.2
242.2
206.0
C16H10ClNO
Mol. Wt.: 267.71
CHO
N
Cl
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z

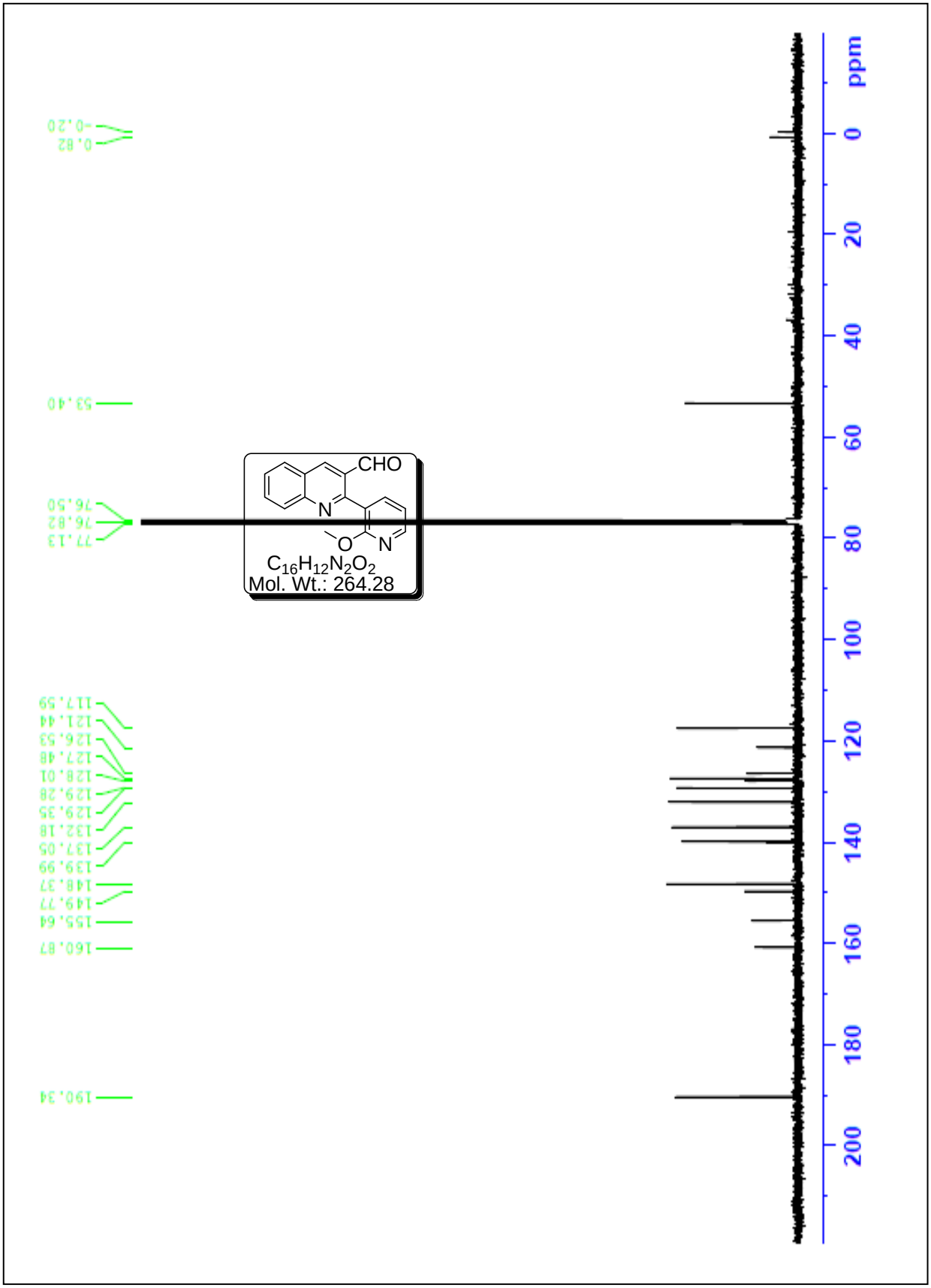

10.181
8.866
8.223
8.202
8.046
8.025
7.921
7.903
7.883
7.764
7.750
7.686
7.667
7.648
7.537
7.512
7.507
7.488
7.260
0.069
-0.004
C16H10ClNO
Mol. Wt.: 267.71
Cl
N
CHO
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.08
1.10
1.13
1.15
1.21
1.27
3.14

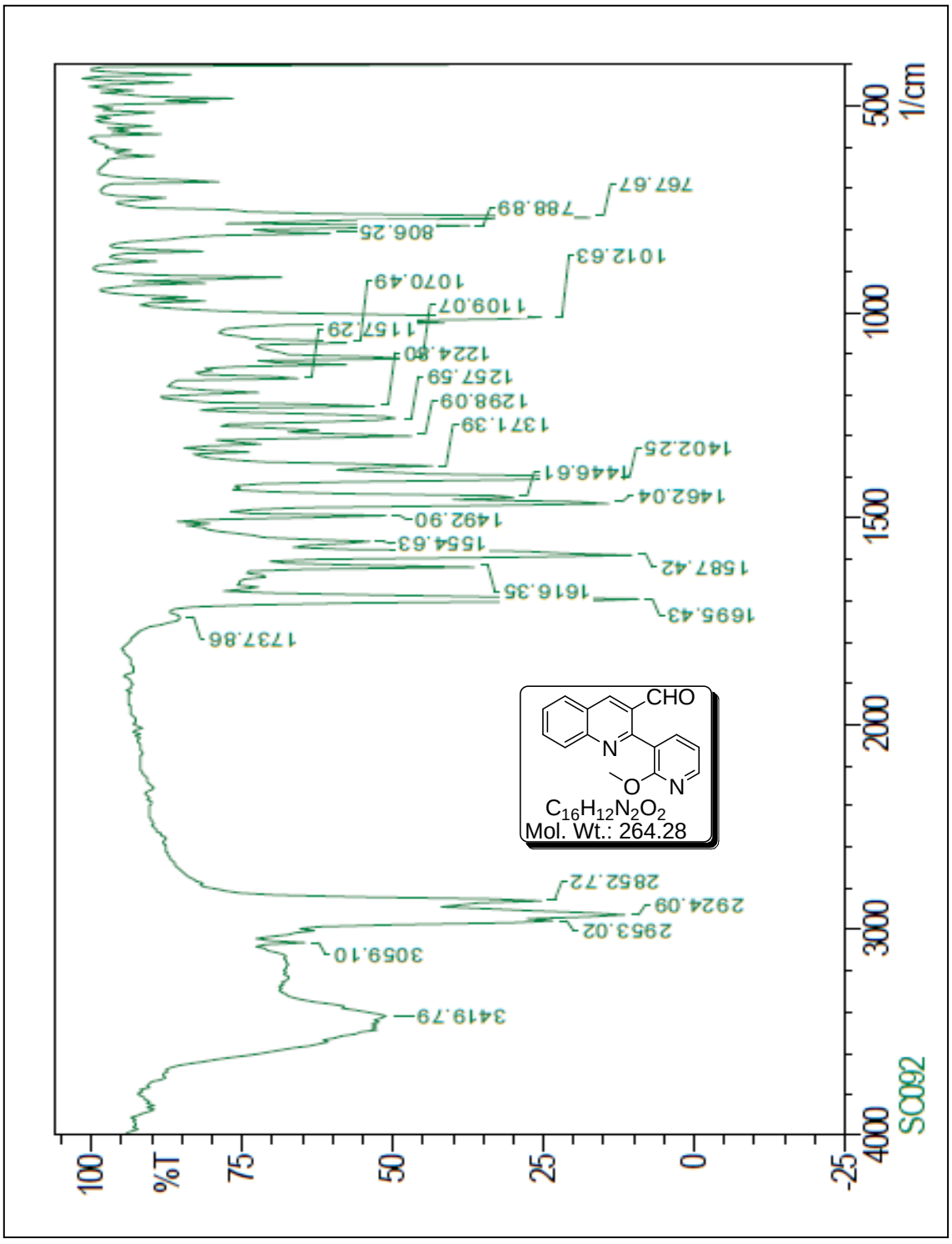

SC049
191.04
158.85
149.70
139.69
138.72
135.11
133.08
130.25
130.02
129.78
129.70
129.65
128.66
128.02
127.65
126.68
77.47
77.16
76.84
1.16
0.14
C16H10ClNO
Mol. Wt.: 267.71
Cl
N
CHO
200
180
160
140
120
100
80
60
40
20
0
ppm

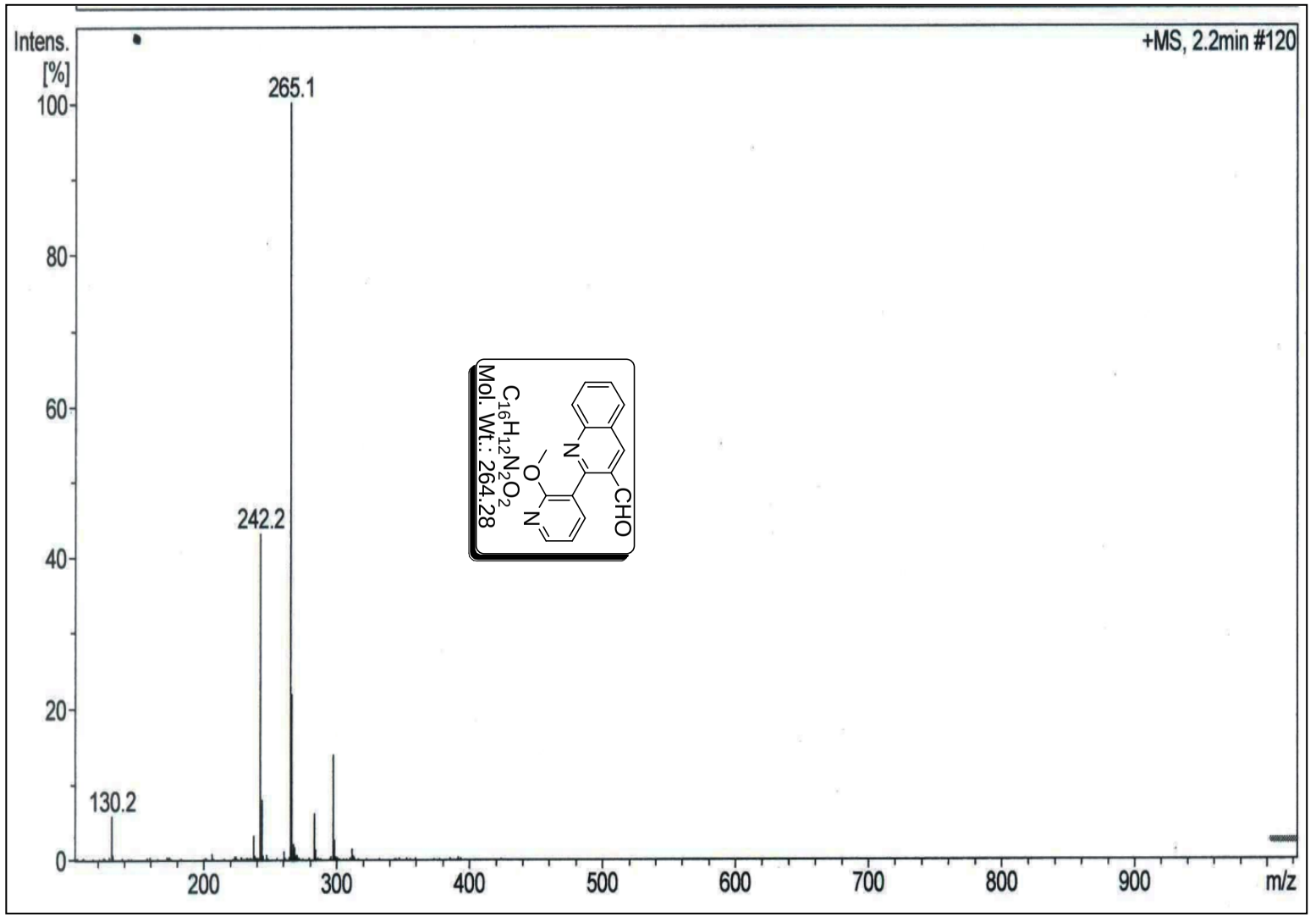

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SO049
3460.30
3064.89
3030.17
2918.30
2866.22
1689.64
1616.35
1581.63
1556.55
1490.97
1477.47
1448.54
1396.46
1384.89
1367.53
1155.36
839.03
779.24
758.02
738.74
690.52
C16H10ClNO
Mol. Wt.: 267.71
Cl
N
CHO

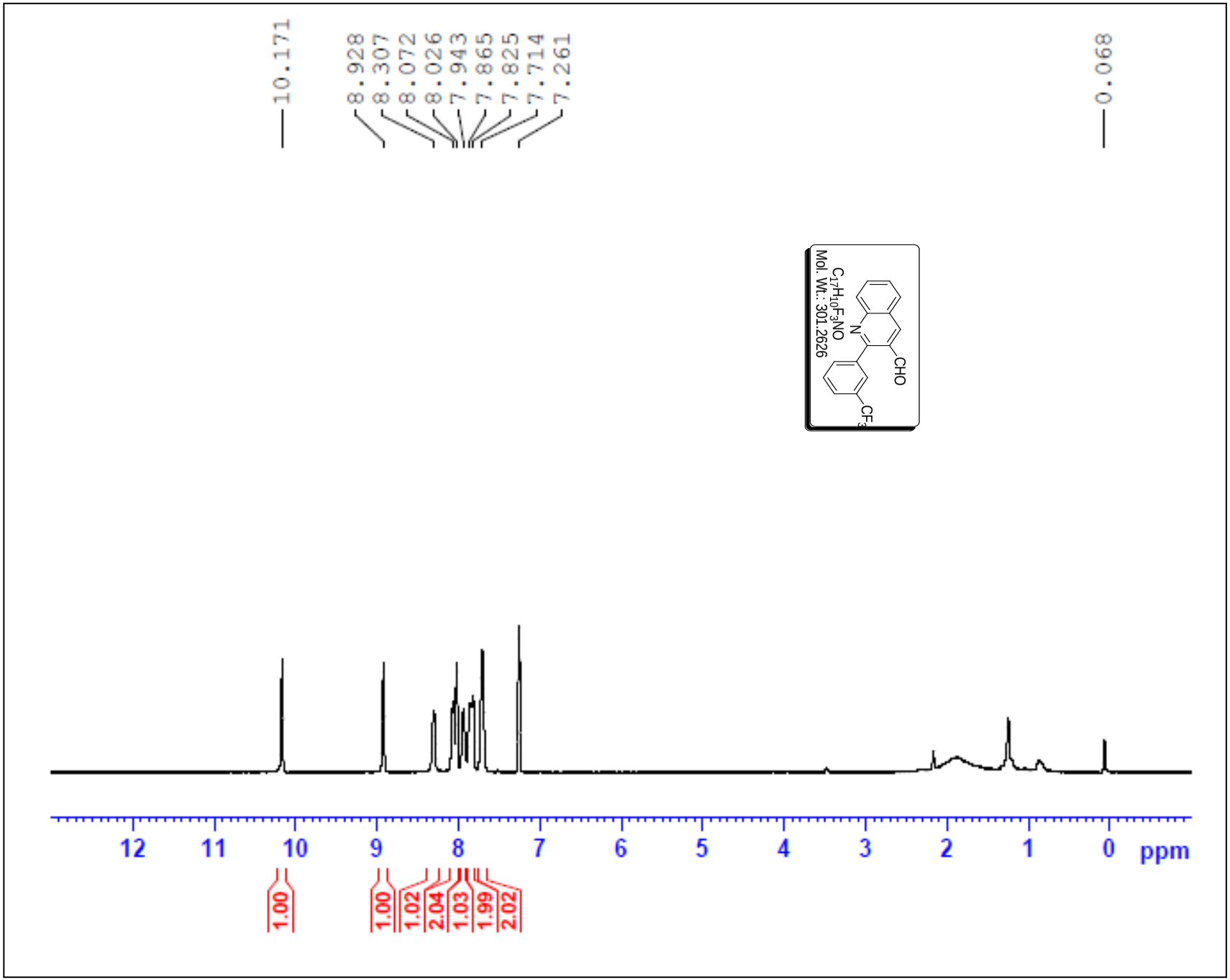

Intens.
[%]
100
80
60
40
20
0
+MS, 3.1min #172
268.0
130.2
201.0
376.1
200
300
400
500
600
700
800
900
m/z
C16H10ClNO
Mol. Wt.: 267.71
Cl
N
CHO

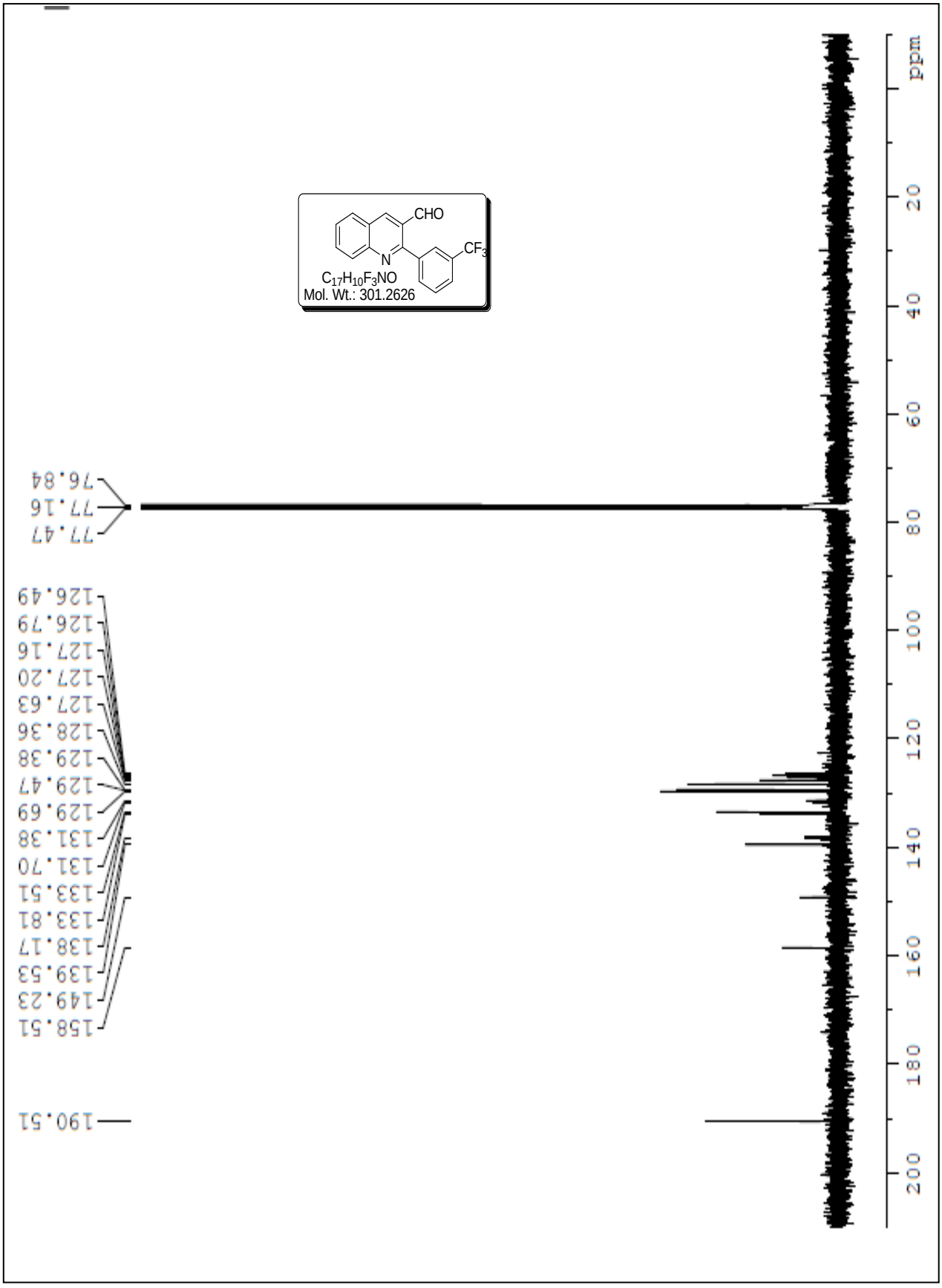

CHO
N
O
N
C16H12N2O2
Mol. Wt.: 264.28
ppm
0
1
2
3
4
5
6
7
8
9
10
11
12
3.10
1.09
1.09
1.09
2.16
1.05
1.05
1.06
1.00
-0.001
0.071
3.912
7.147
7.160
7.166
7.178
7.263
7.629
7.632
7.649
7.667
7.669
7.844
7.847
7.865
7.869
7.882
7.886
8.016
8.021
8.035
8.039
8.176
8.197
8.351
8.355
8.363
8.368
8.796
9.948

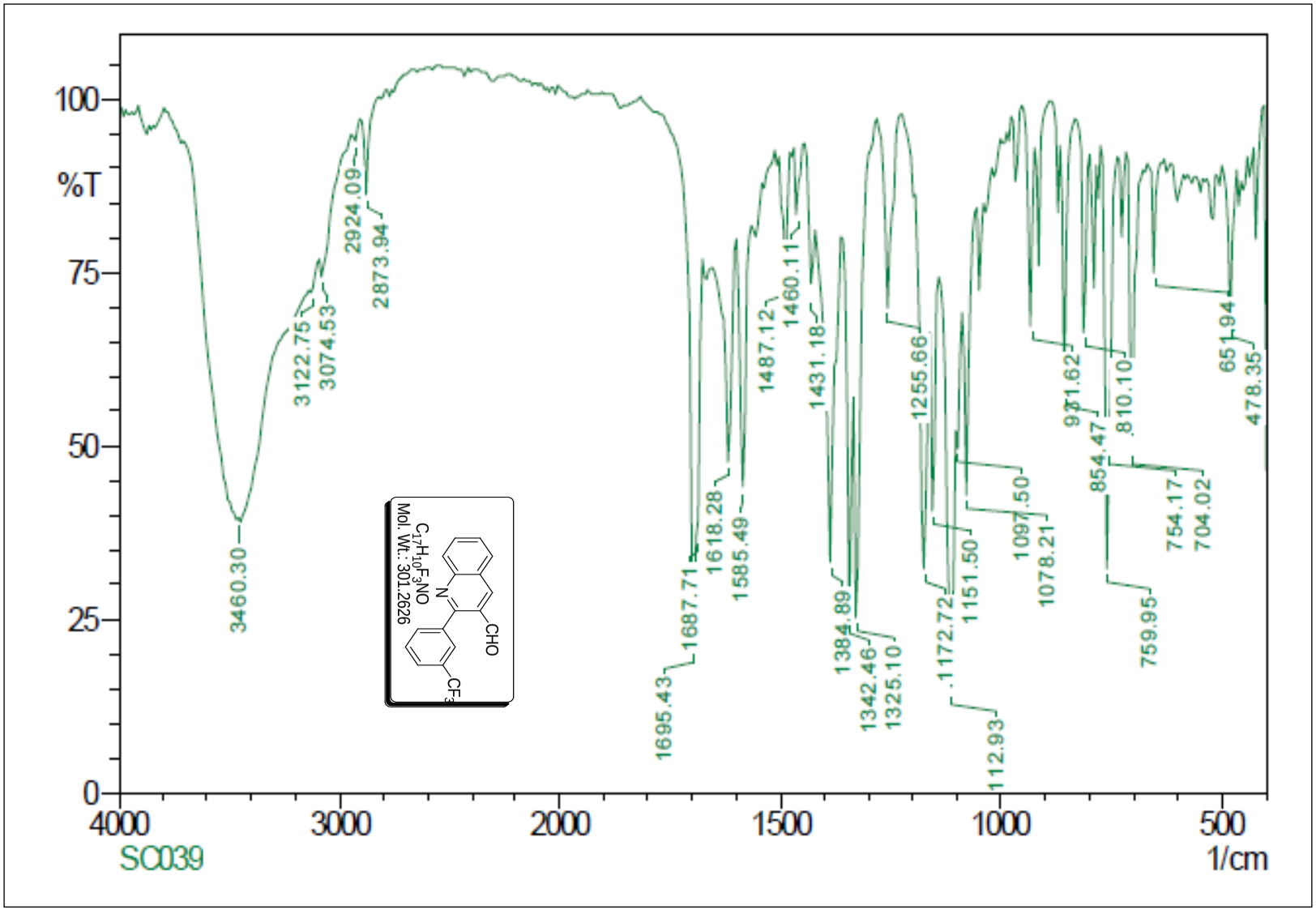

CHO
N
O
N
C16H12N2O2
Mol. Wt.: 264.28
ppm
0
20
40
60
80
100
120
140
160
180
200

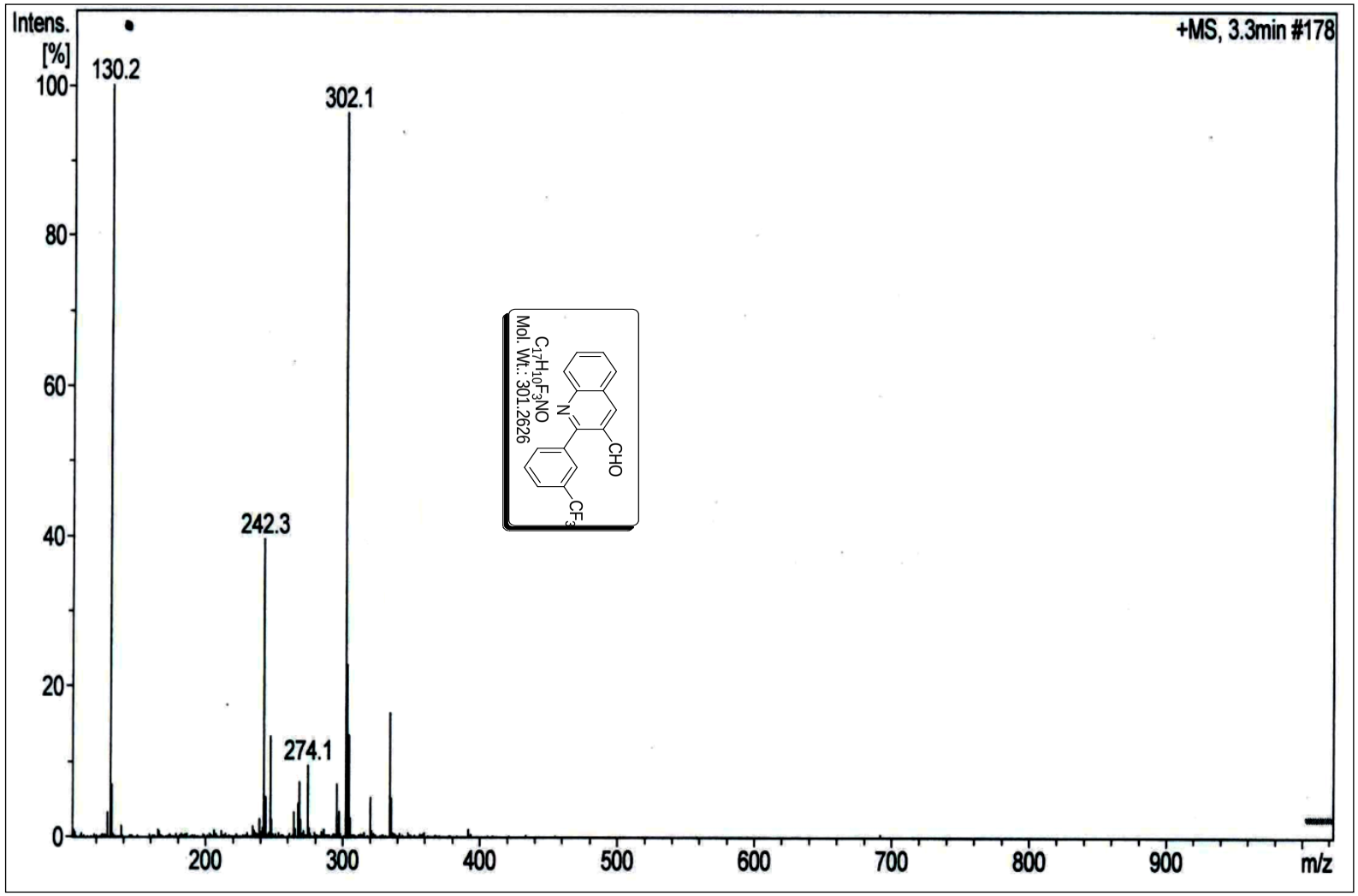

767.67
788.89
806.25
1012.63
1070.49
1109.07
1157.29
1224.80
1257.59
1298.09
1371.39
1402.25
1446.61
1462.04
1492.90
1554.63
1587.42
1616.35
1695.43
1737.86
2852.72
2924.09
2953.02
3059.10
3419.79
CHO
N
O
N
$C_{16}H_{12}N_2O_2$
Mol. Wt.: 264.28
100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC092

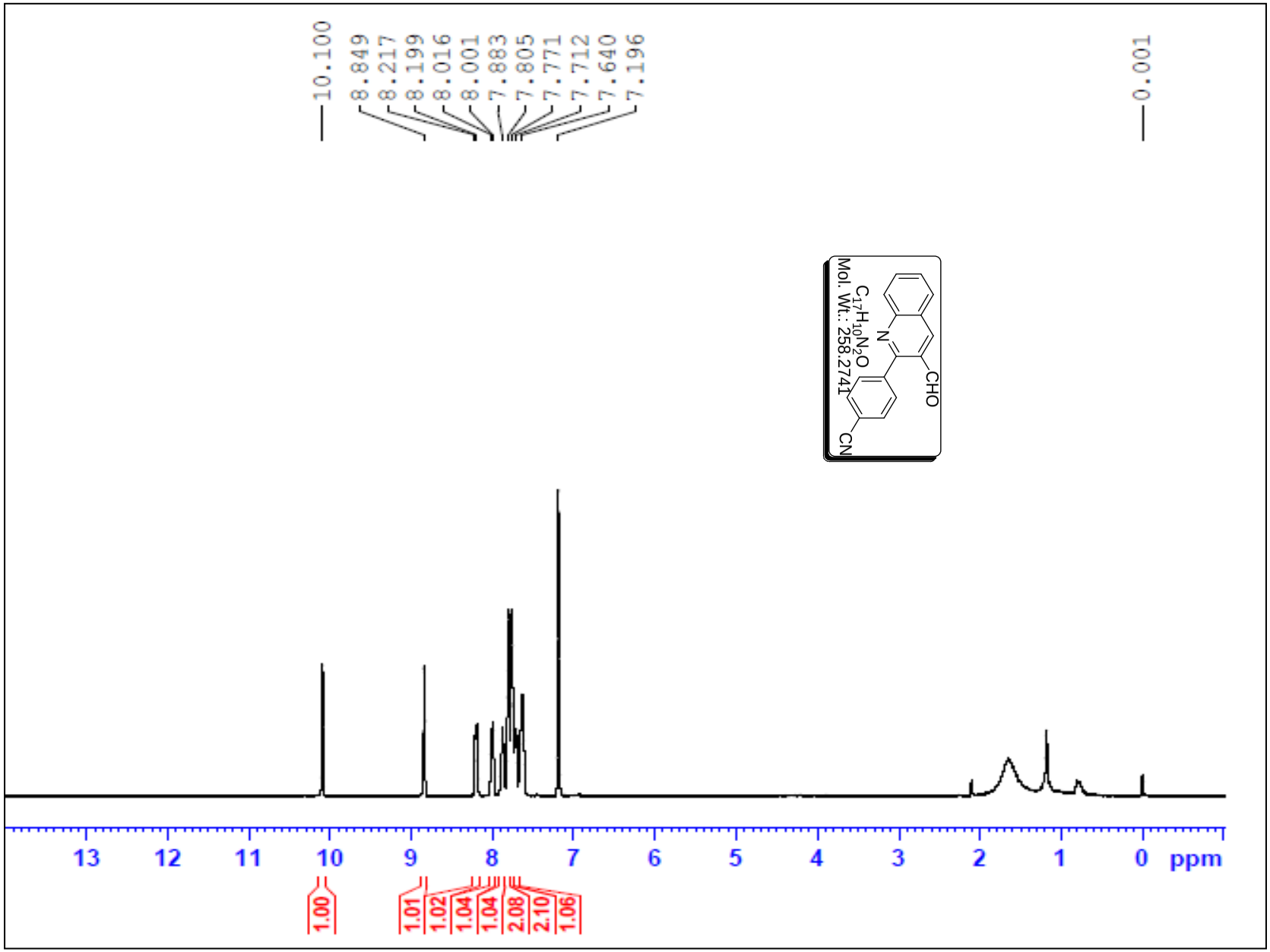

Intens.
[%]
+MS, 2.2min #120
265.1
242.2
130.2
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z
C16H12N2O2
Mol. Wt.: 264.28
CHO
N
O
N

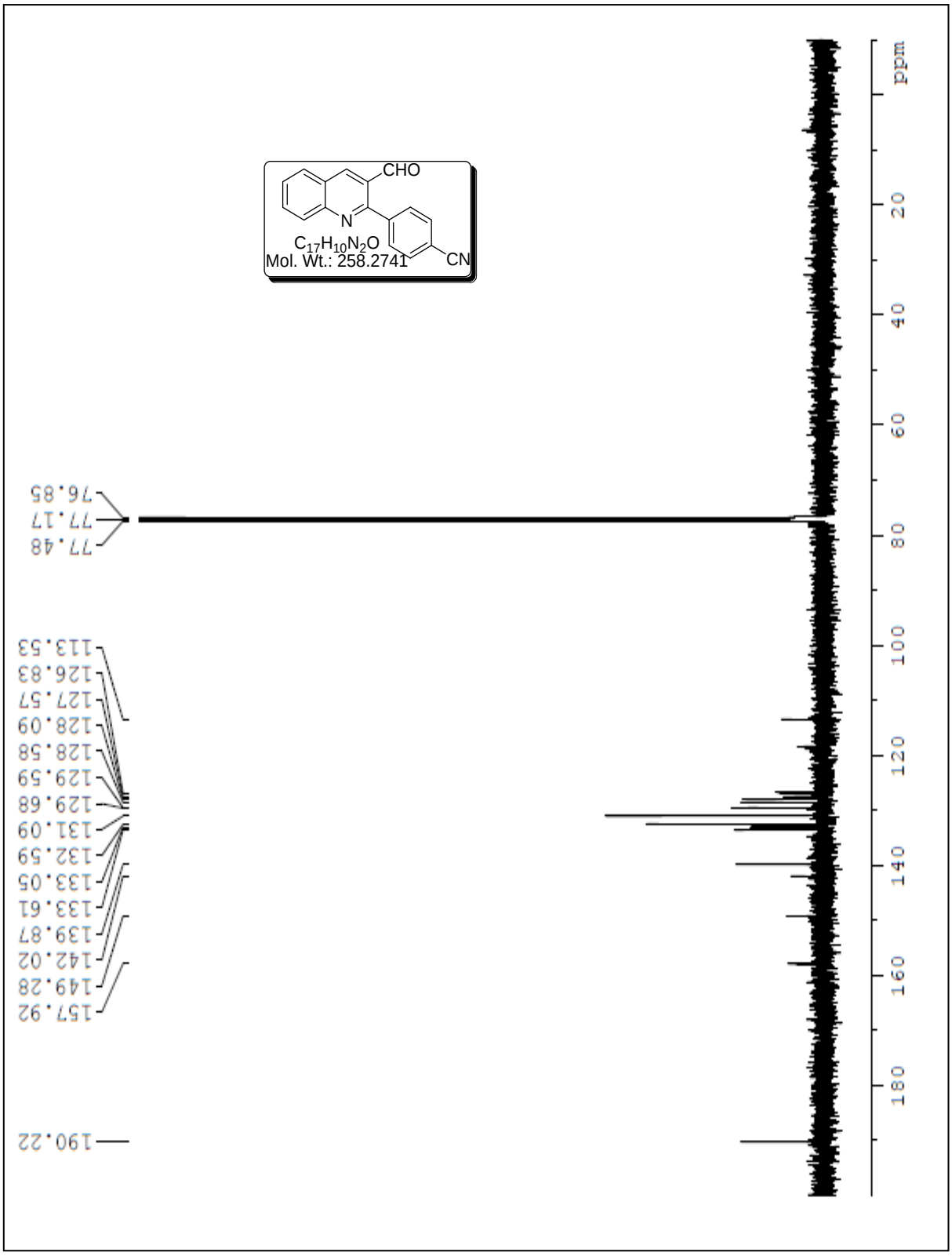

10.171
8.928
8.307
8.072
8.026
7.943
7.865
7.825
7.714
7.261
0.068
C17H10F3NO
Mol. Wt.: 301.2626
N
CHO
CF3
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.02
2.04
1.03
1.99
2.02

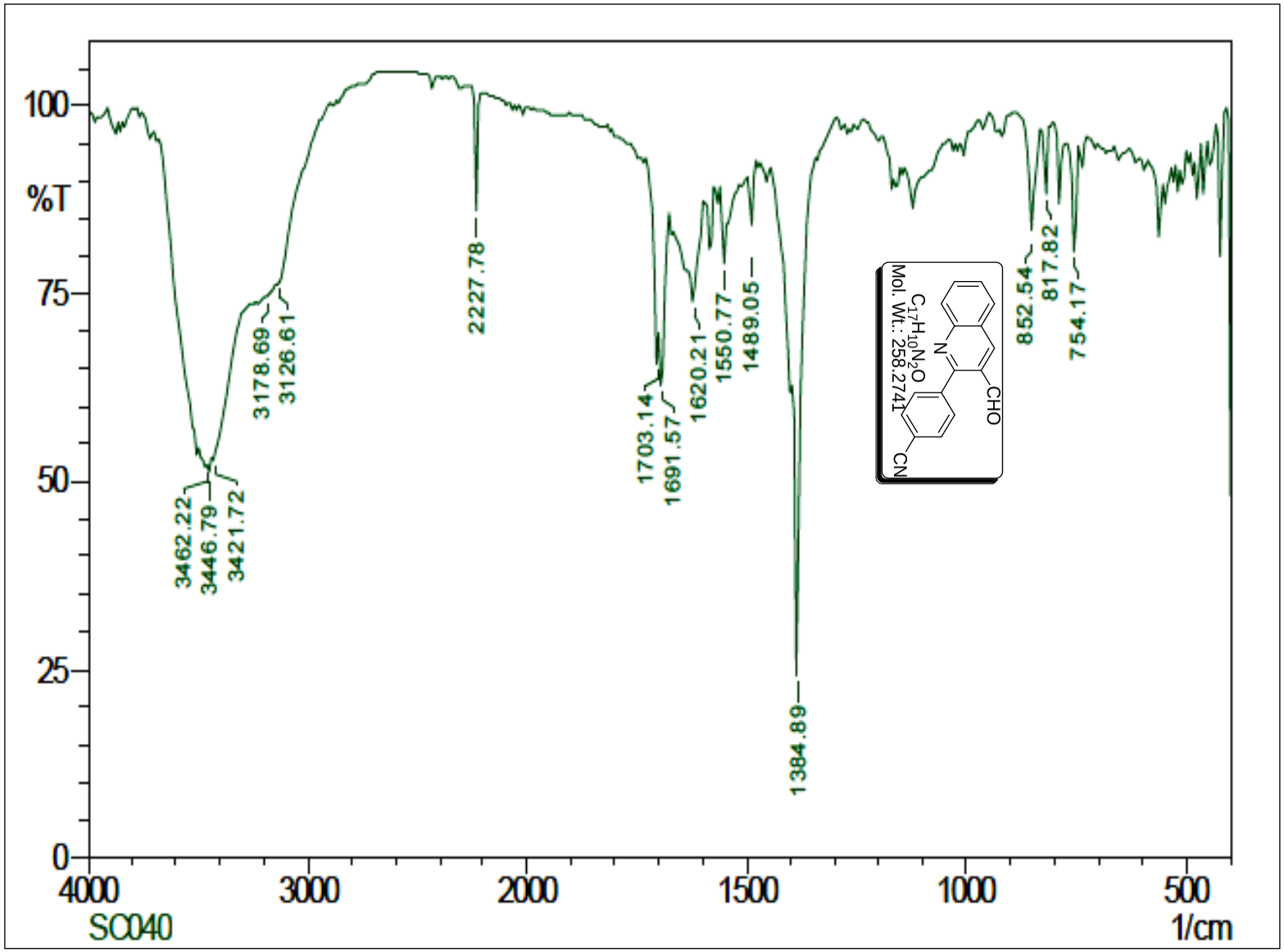

CHO
CF3
N
C17H10F3NO
Mol. Wt.: 301.2626
ppm
20
40
60
80
100
120
140
160
180
200
76.84
77.16
77.47
126.49
126.79
127.16
127.20
127.63
128.36
129.38
129.47
129.69
131.38
131.70
133.51
133.81
138.17
139.53
149.23
158.51
190.51

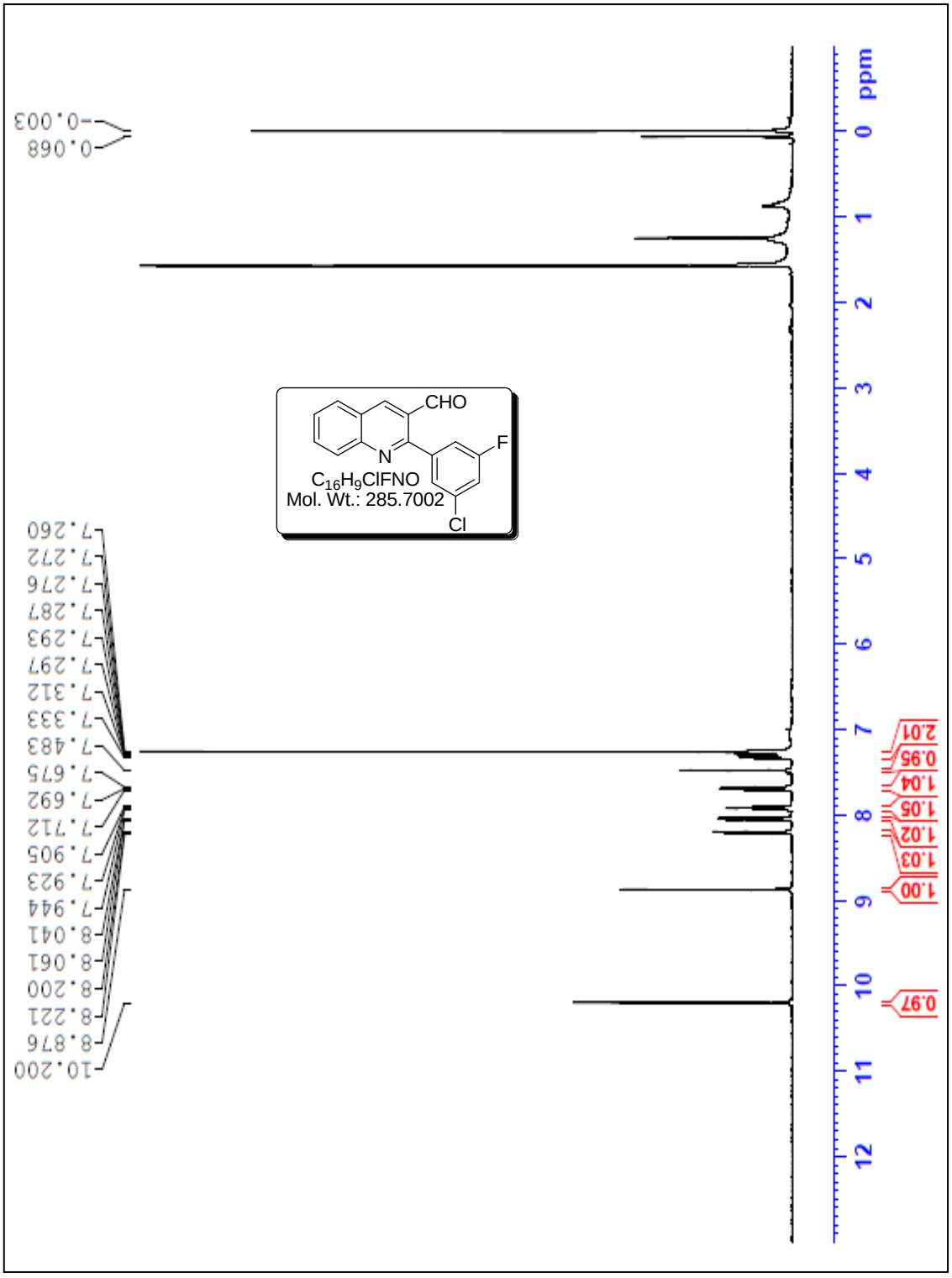

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC039
3460.30
3122.75
3074.53
2924.09
2873.94
1695.43
1687.71
1618.28
1585.49
1487.12
1460.11
1431.18
1384.89
1342.46
1325.10
1255.66
1172.72
1151.50
1112.93
1097.50
1078.21
971.62
854.47
810.10
759.95
754.17
704.02
651.94
478.35
C17H10F3NO
Mol. Wt.: 301.2626
N
CHO
CF3


Intens.
[%]
+MS, 3.3min #178
130.2
302.1
242.3
274.1
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z
C17H10F3NO
Mol. Wt.: 301.2626
N
CHO
CF3

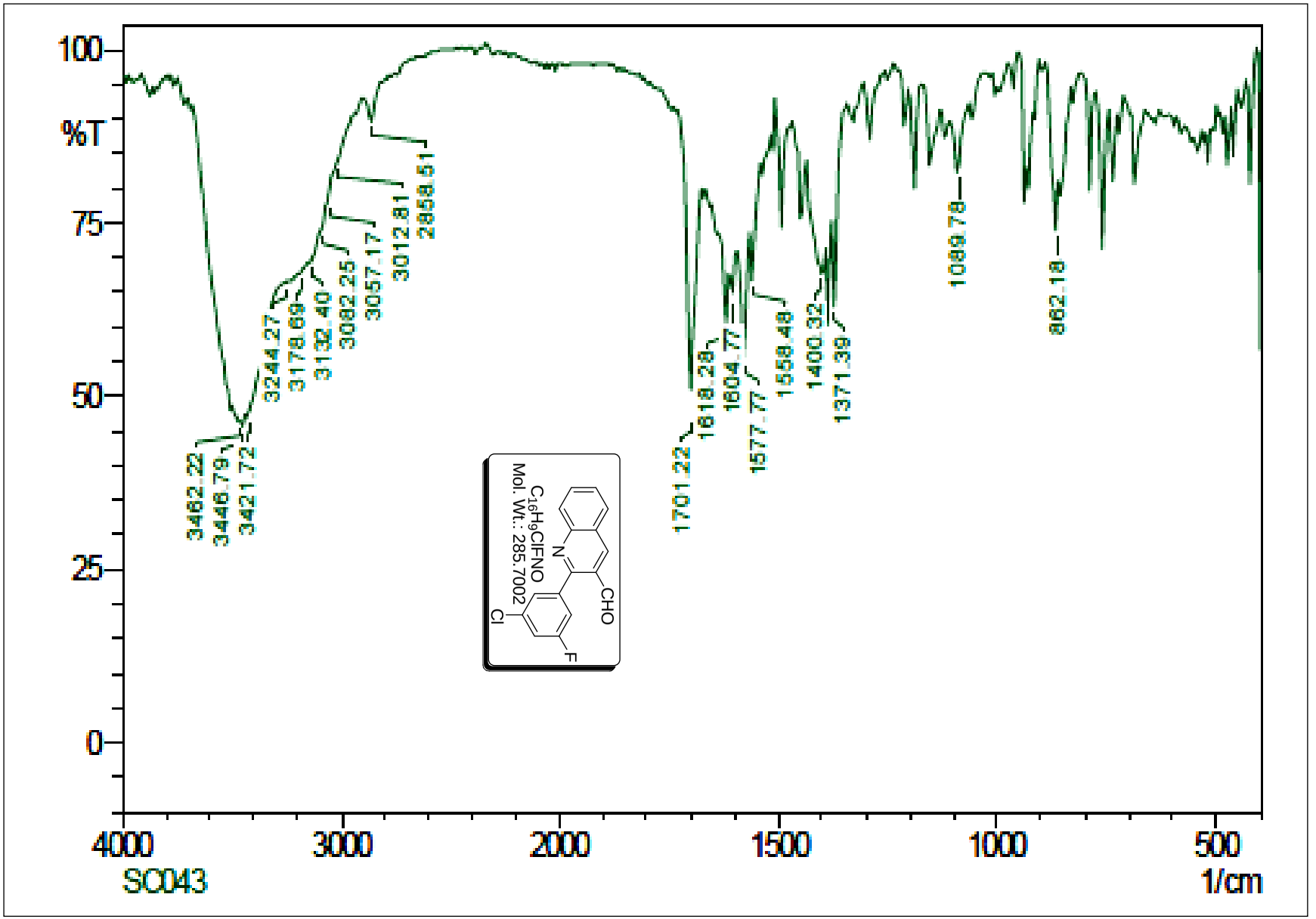

10.100
8.849
8.217
8.199
8.016
8.001
7.883
7.805
7.771
7.712
7.640
7.196
0.001
C17H10N2O
Mol. Wt.: 258.2741
N
CHO
CN
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.02
1.04
1.04
2.08
2.10
1.06

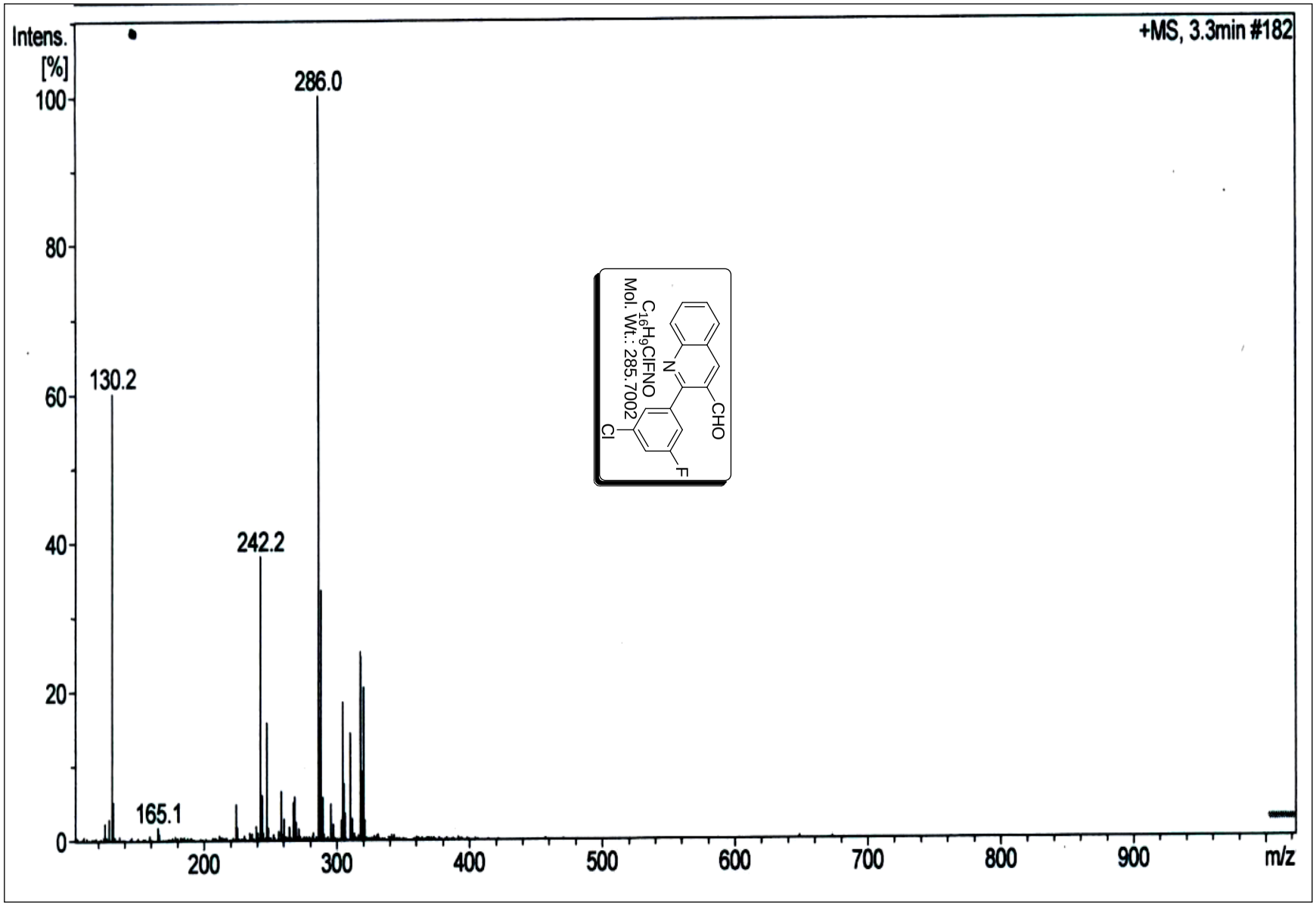

CHO
N
CN
$C_{17}H_{10}N_2O$
Mol. Wt.: 258.2741
ppm
20
40
60
80
100
120
140
160
180
190.22
157.92
149.28
142.02
139.87
133.61
133.05
132.59
131.09
129.68
129.59
128.58
128.09
127.57
126.83
113.53
77.48
77.17
76.85

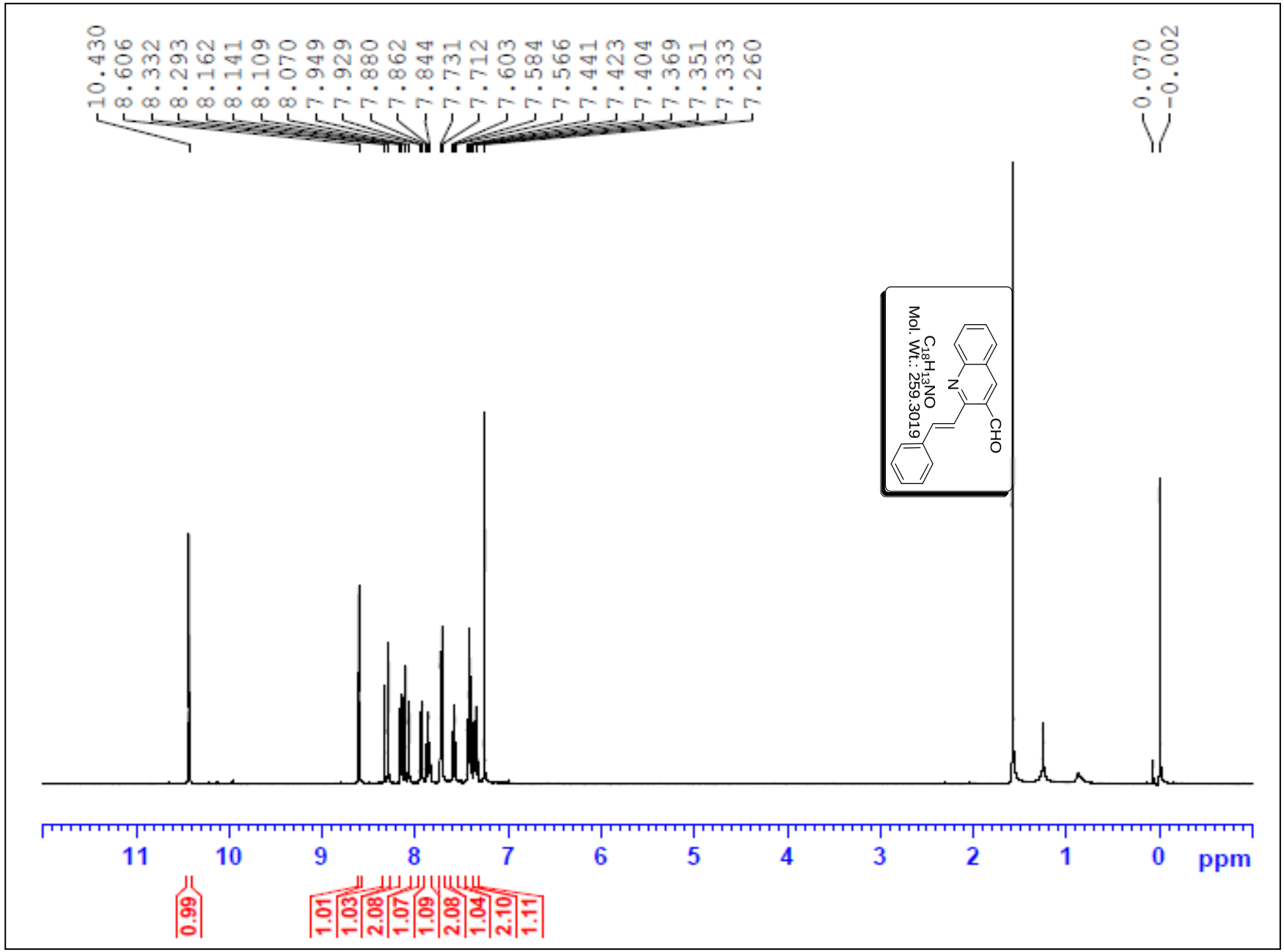

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC040
3462.22
3446.79
3421.72
3178.69
3126.61
2227.78
1703.14
1691.57
1620.21
1550.77
1489.05
1384.89
852.54
817.82
754.17
C17H10N2O
Mol. Wt.: 258.2741
N
CHO
CN

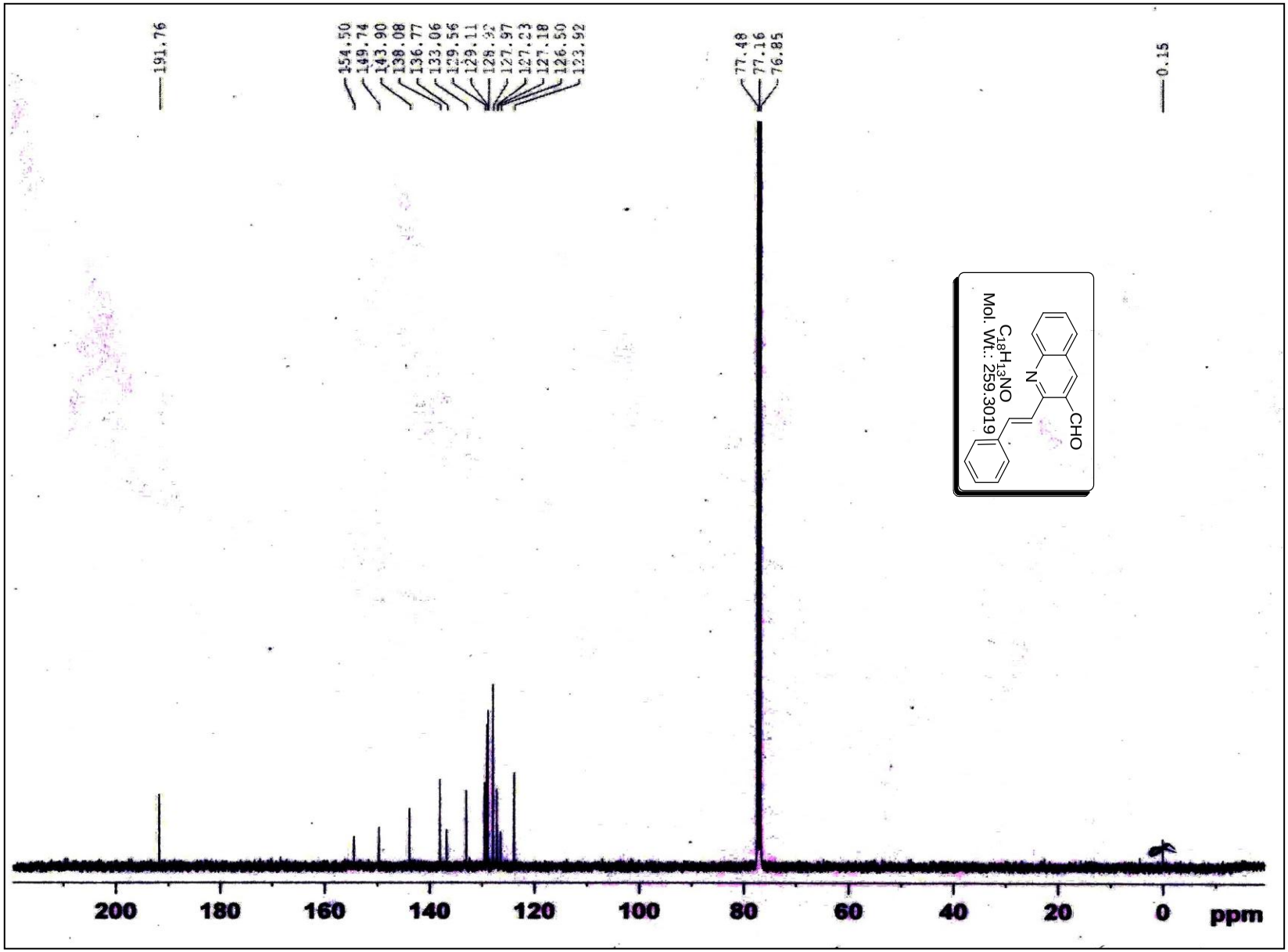

CHO
N
F
Cl
C16H9ClFNO
Mol. Wt.: 285.7002
ppm
0 1 2 3 4 5 6 7 8 9 10 11 12
0.003
0.068
7.260
7.272
7.276
7.287
7.293
7.297
7.312
7.333
7.483
7.675
7.692
7.712
7.905
7.923
7.944
8.041
8.061
8.200
8.221
8.876
10.200
2.01
0.95
1.04
1.05
1.02
1.03
1.00
0.97

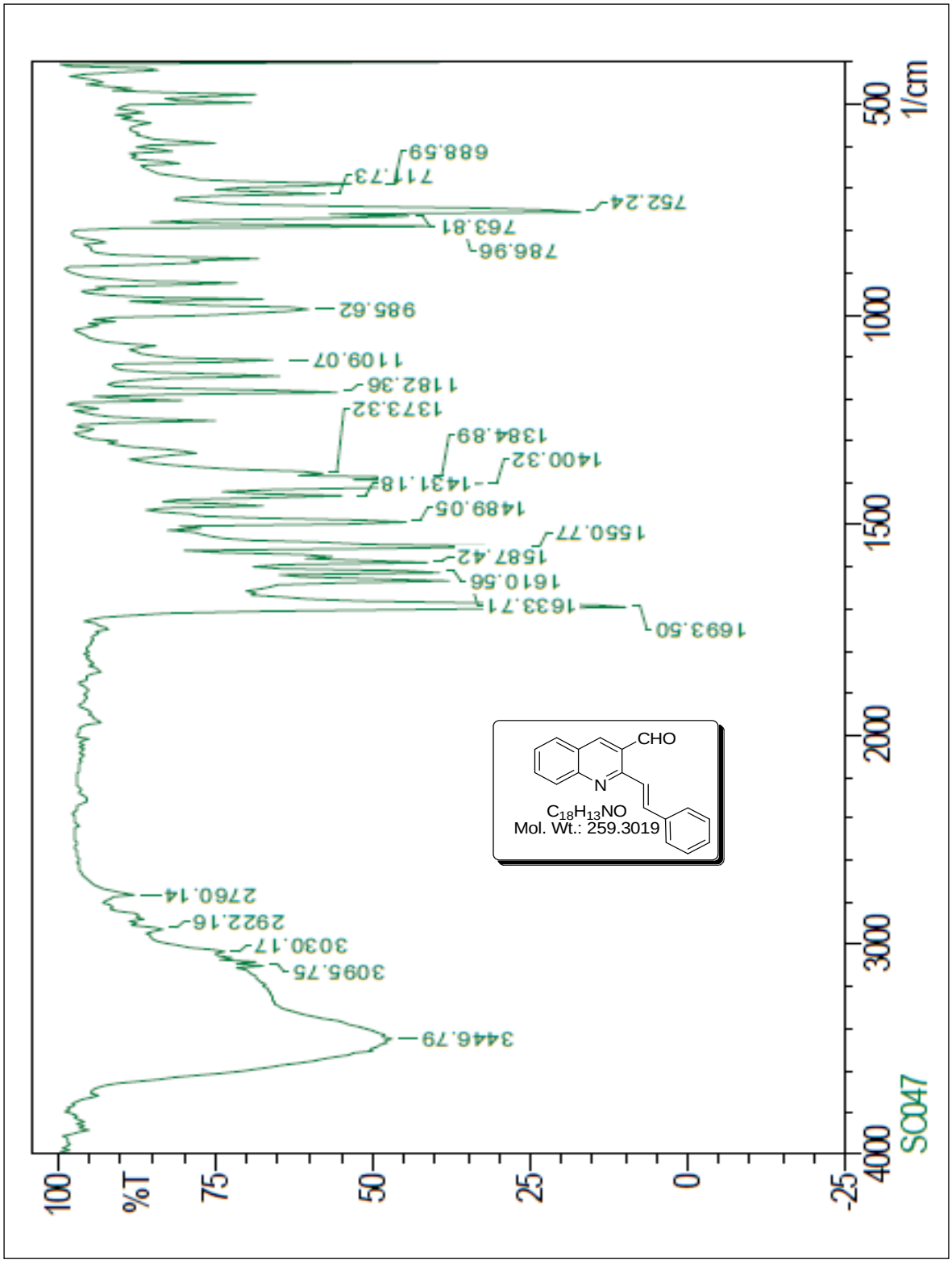
0.15
76.84
77.16
77.48
115.86
116.08
117.22
117.47
126.39
126.82
127.52
128.34
129.67
129.83
133.31
139.16
149.62
190.48
CHO
N
F
Cl
C16H9ClFNO
Mol. Wt.: 285.7002
ppm
0
20
40
60
80
100
120
140
160
180
200

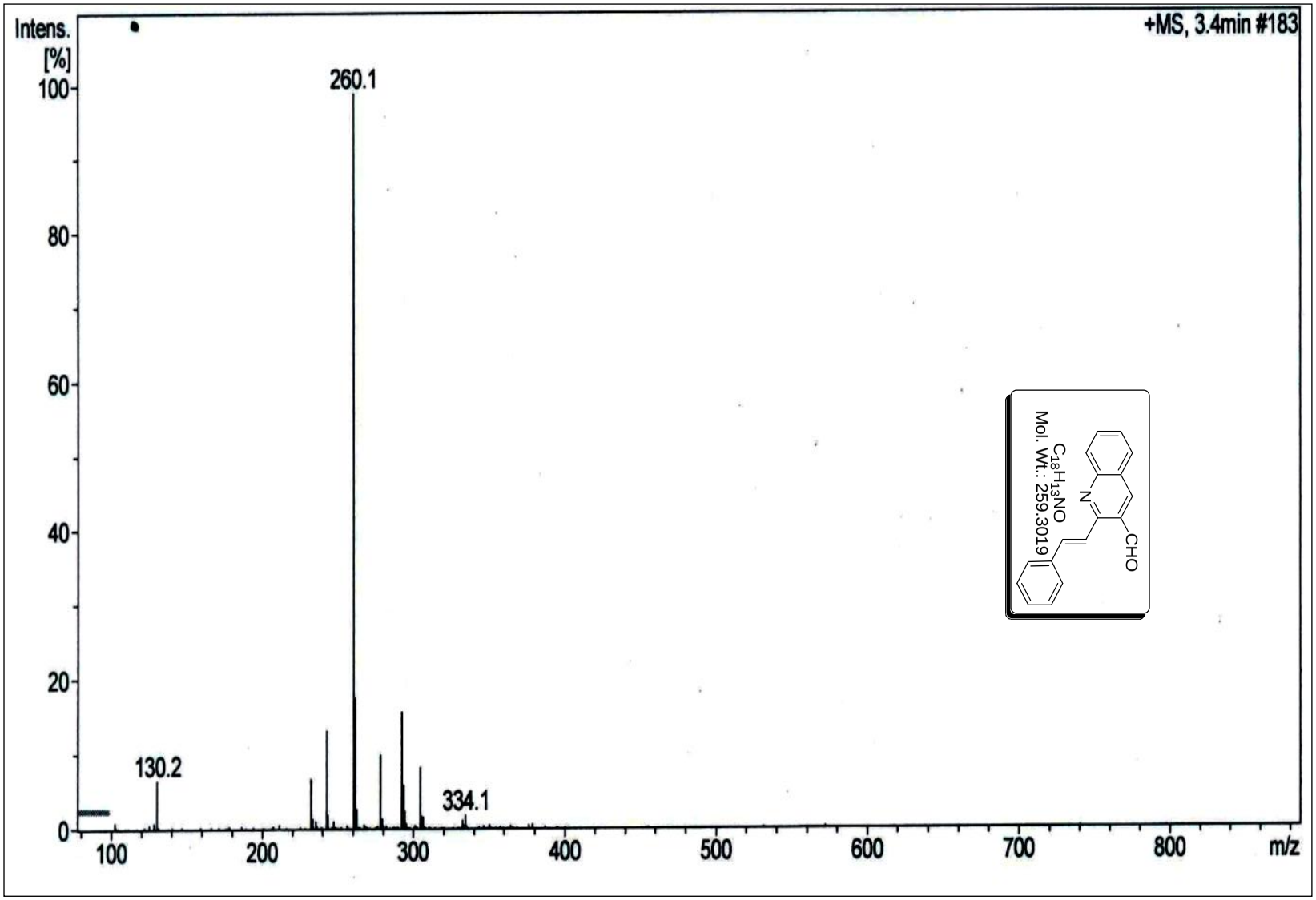

100
%T
75
50
25
0
4000
3000
2000
1500
1000
500
1/cm
SC043
3462.22
3446.79
3421.72
3244.27
3178.69
3132.40
3082.25
3057.17
3012.81
2958.51
1701.22
1618.28
1604.77
1577.77
1558.48
1400.32
1371.39
1089.78
862.18
C16H9ClFNO
Mol. Wt.: 285.7002
N
CHO
Cl
F

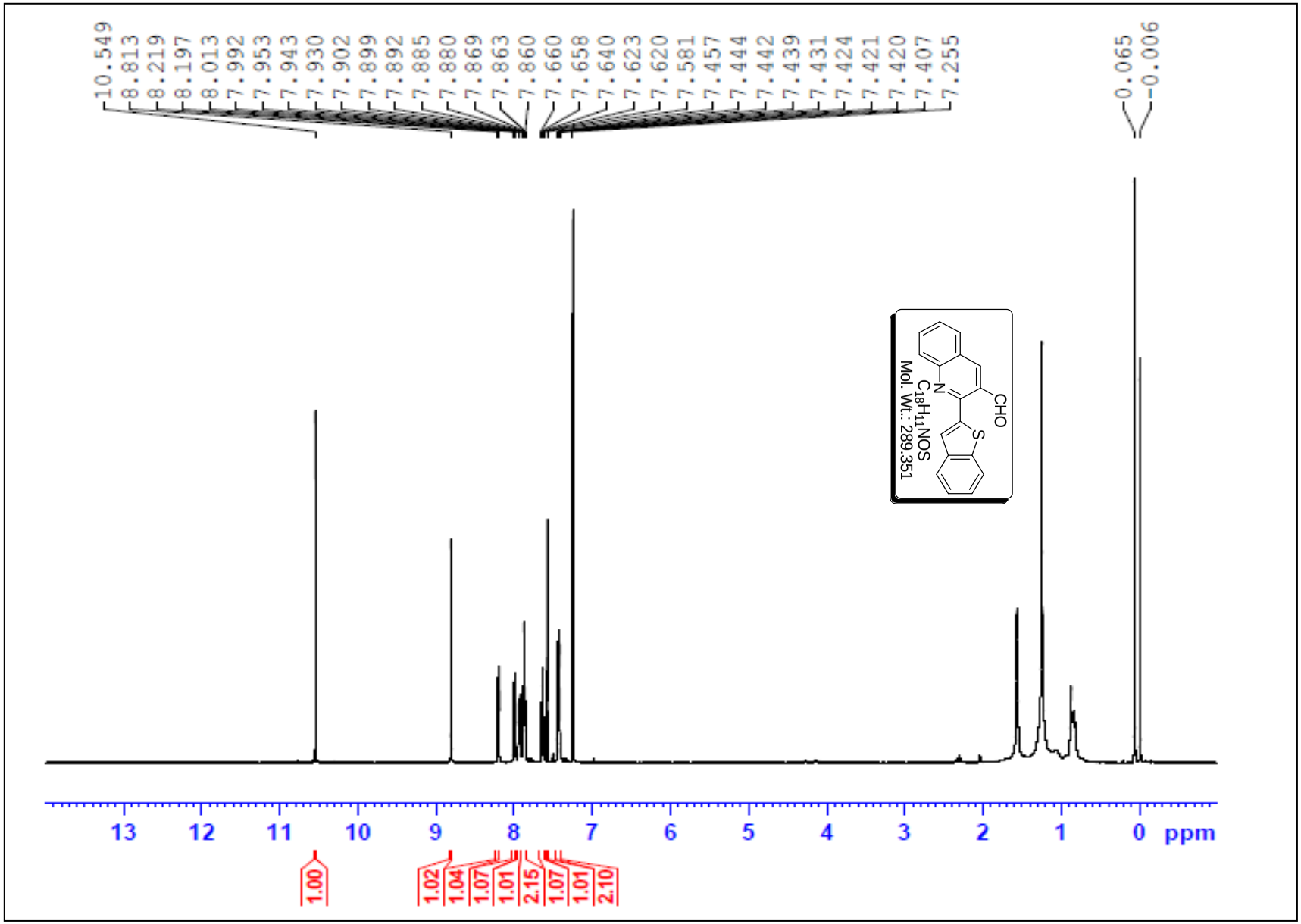

+MS, 3.3min #182
Intens.
[%]
100
80
60
40
20
0
286.0
130.2
242.2
165.1
200
300
400
500
600
700
800
900
m/z
C16H9ClFNO
Mol. Wt.: 285.7002
N
CHO
Cl
F

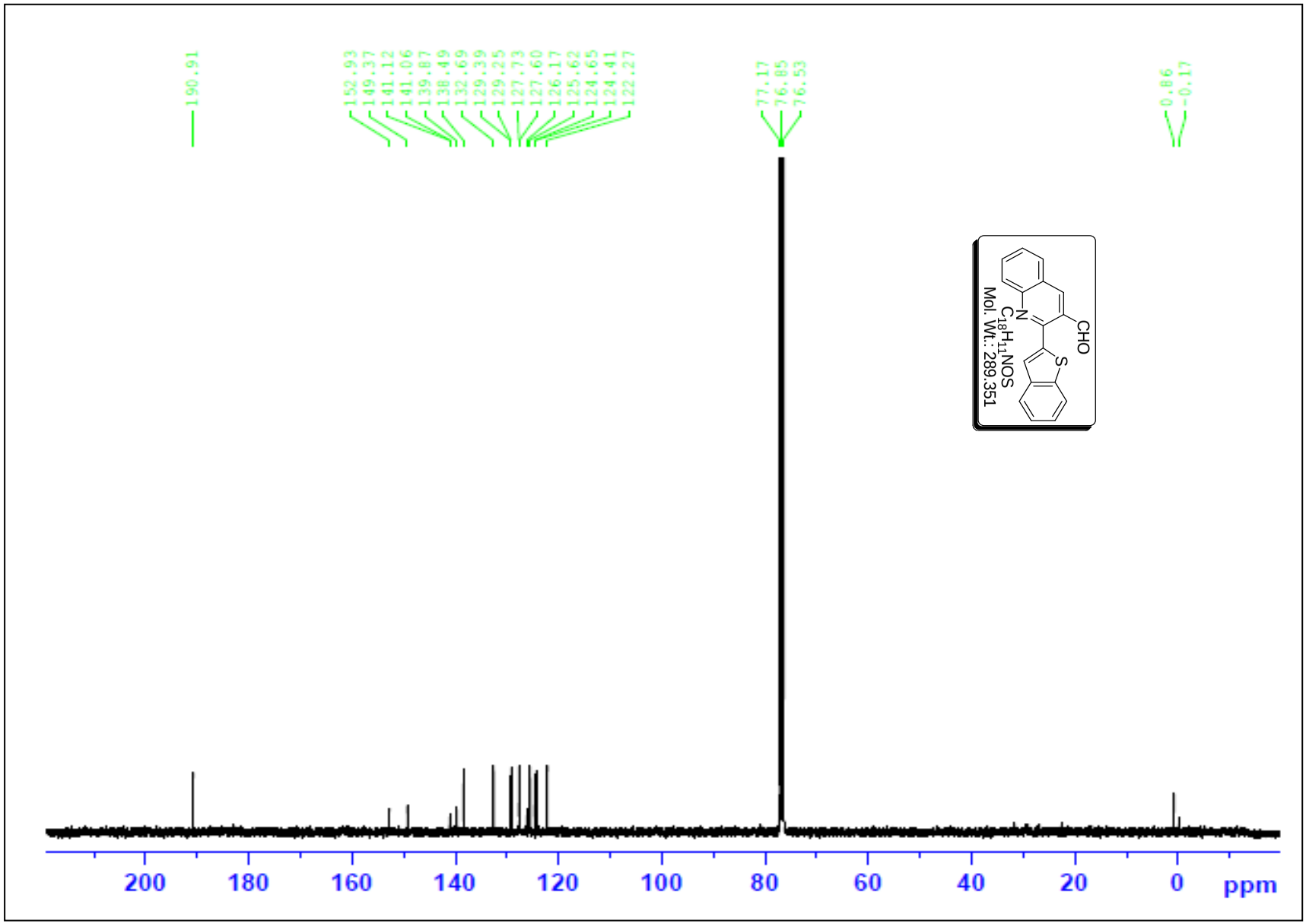

10.430
8.606
8.332
8.293
8.162
8.141
8.109
8.070
7.949
7.929
7.880
7.862
7.844
7.731
7.712
7.603
7.584
7.566
7.441
7.423
7.404
7.369
7.351
7.333
7.260
0.070
-0.002
C18H13NO
Mol. Wt.: 259.3019
N
CHO
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.01
1.03
2.08
1.07
1.09
2.08
1.04
2.10
1.11

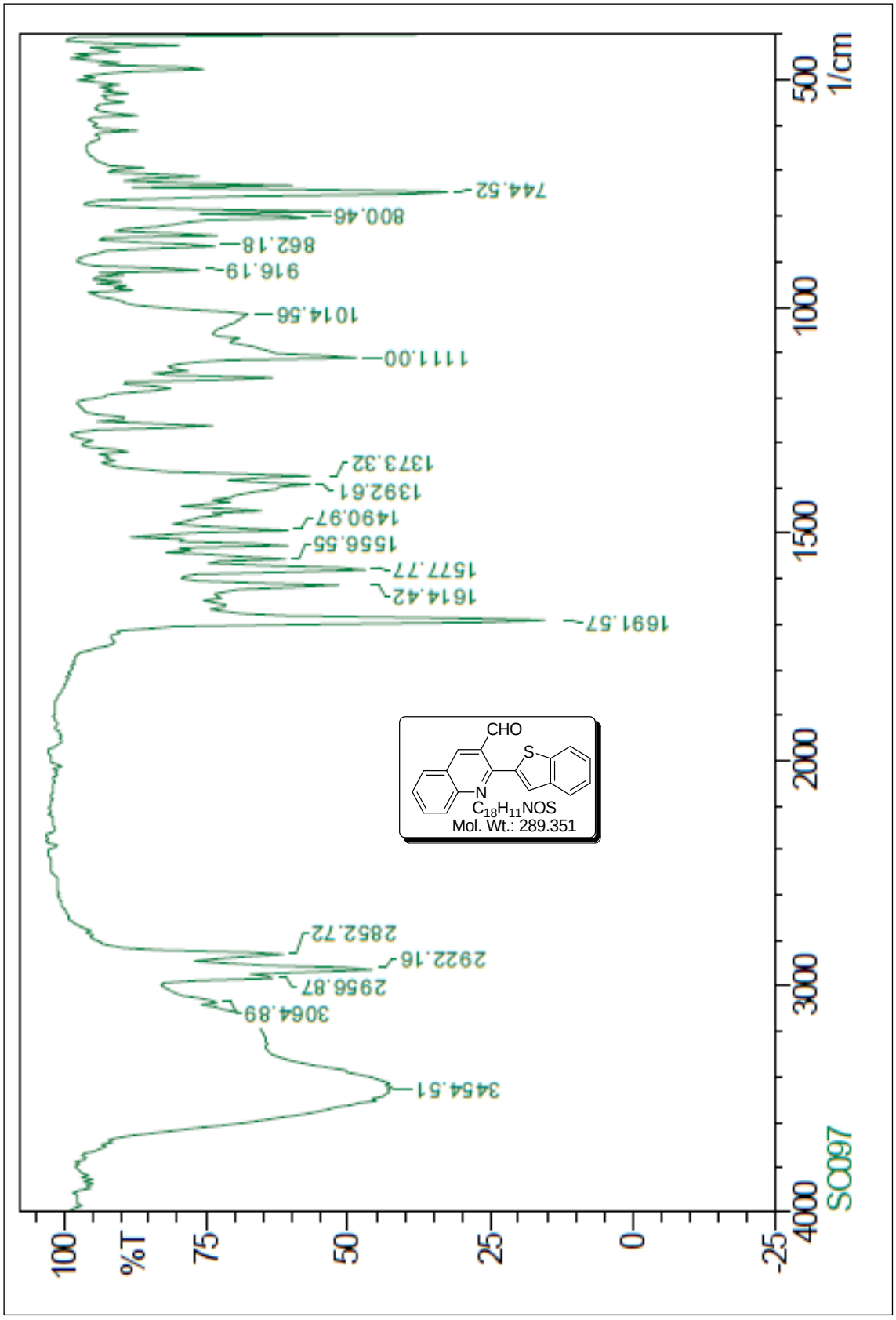

191.76
154.50
149.74
143.90
138.08
136.77
133.06
129.56
129.11
128.32
127.97
127.23
127.18
126.50
123.92
77.48
77.16
76.85
0.15
$C_{18}H_{13}NO$
Mol. Wt.: 259.3019
N
CHO
200
180
160
140
120
100
80
60
40
20
0
ppm

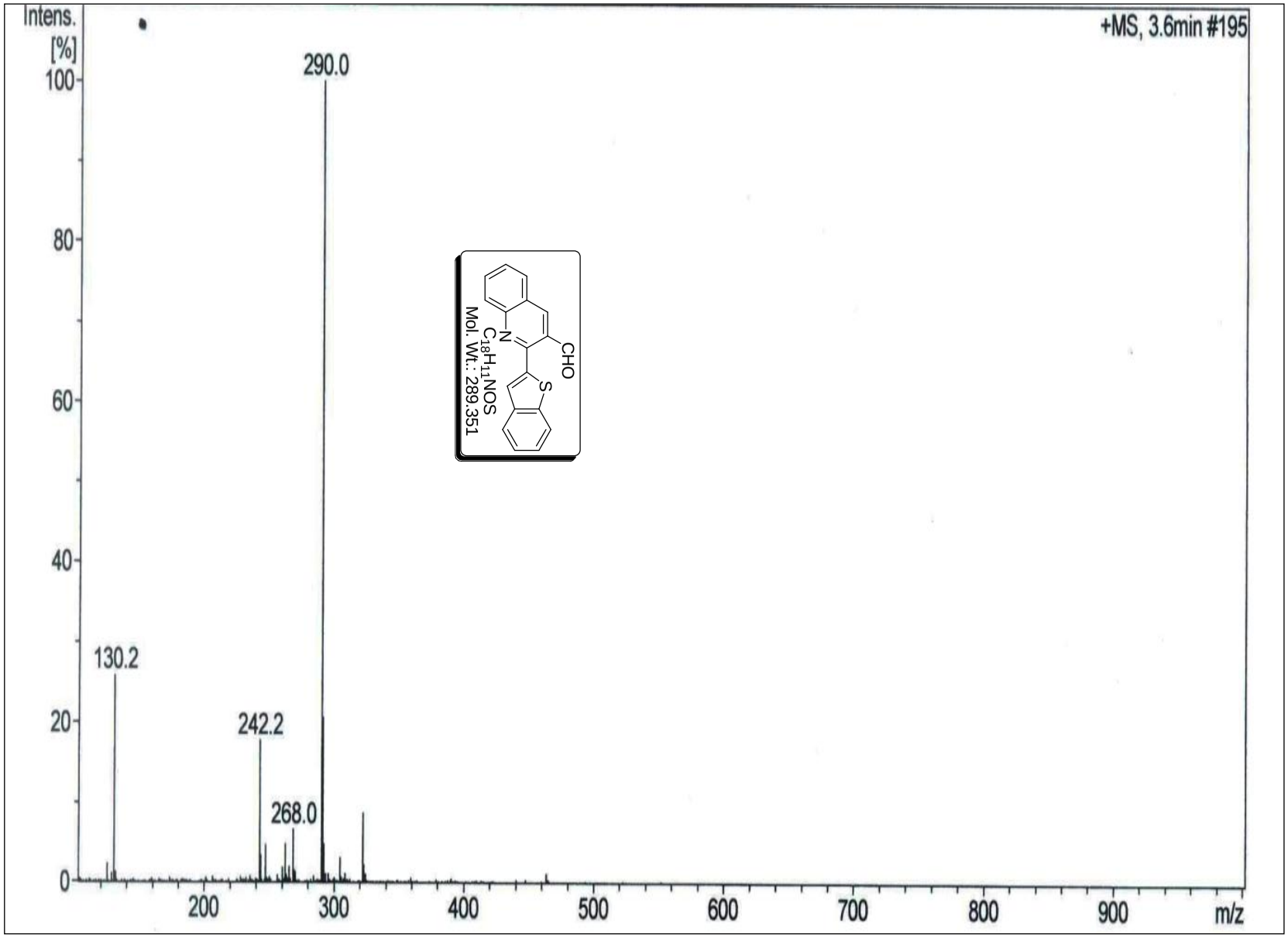

3446.79
3095.75
3030.17
2922.16
2760.14
1693.50
1633.71
1610.56
1587.42
1550.77
1489.05
1431.18
1400.32
1384.89
1373.32
1182.36
1109.07
985.62
786.96
763.81
752.24
711.73
688.59
CHO
N
C18H13NO
Mol. Wt.: 259.3019
100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC047

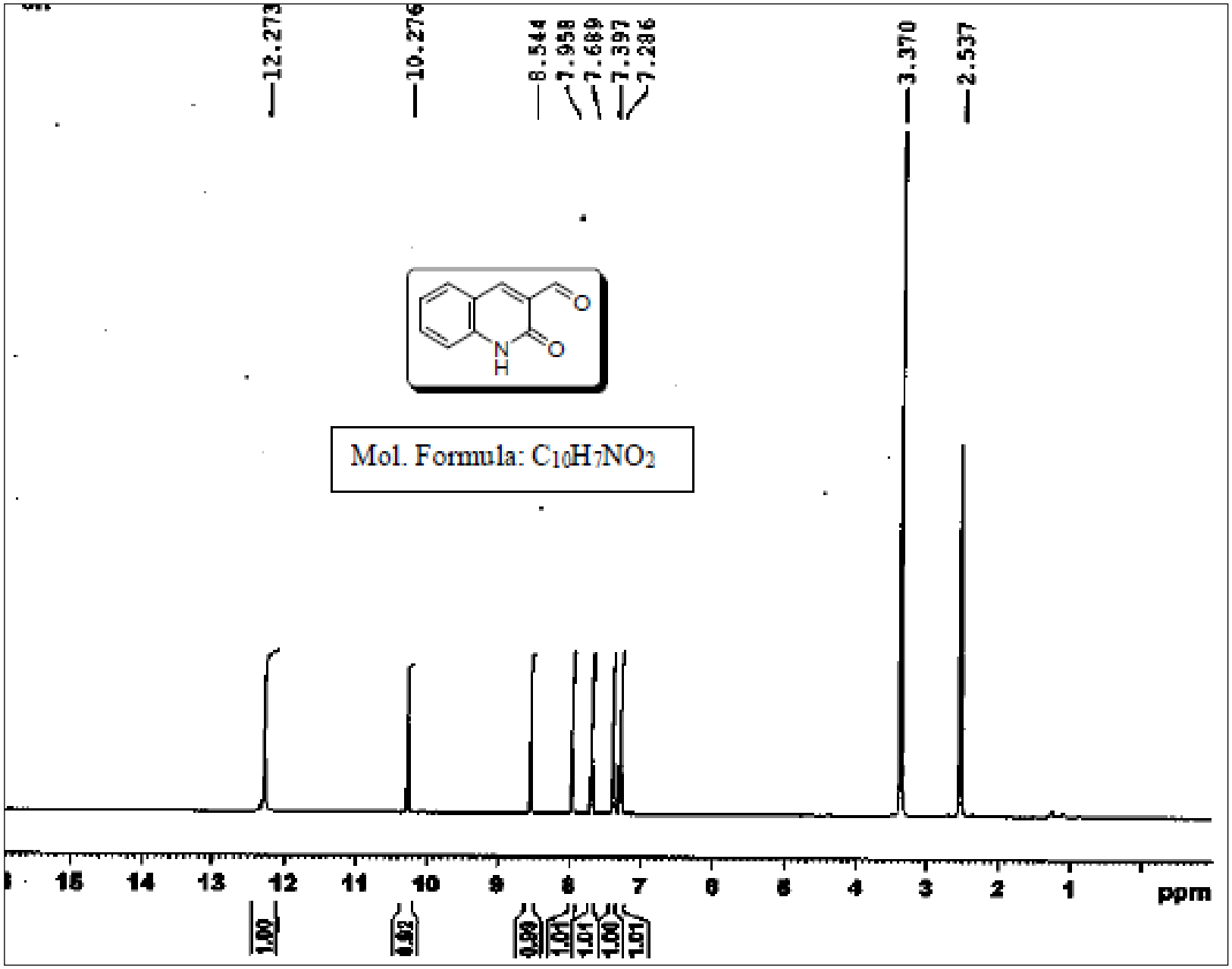

Intens.
[%]
+MS, 3.4min #183
260.1
130.2
334.1
100
80
60
40
20
0
100
200
300
400
500
600
700
800
m/z
C18H13NO
Mol. Wt.: 259.3019
N
CHO

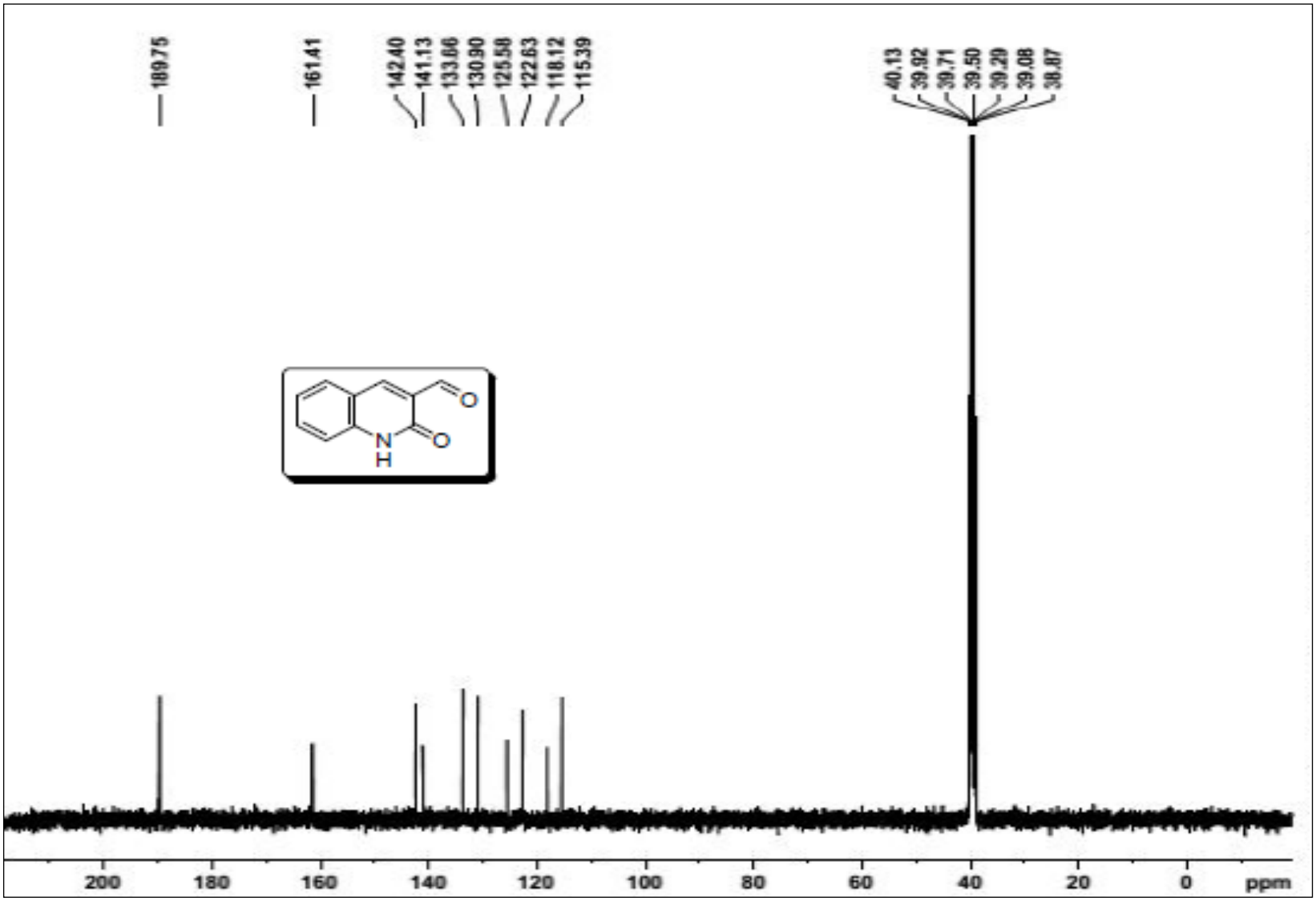

10.549
8.813
8.219
8.197
8.013
7.992
7.953
7.943
7.930
7.902
7.899
7.892
7.885
7.880
7.869
7.863
7.860
7.660
7.658
7.640
7.623
7.620
7.581
7.457
7.444
7.442
7.439
7.431
7.424
7.421
7.420
7.407
7.255
0.065
-0.006
N
CHO
S
C18H11NOS
Mol. Wt.: 289.351
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
1.04
1.07
1.01
2.15
1.07
1.01
2.10

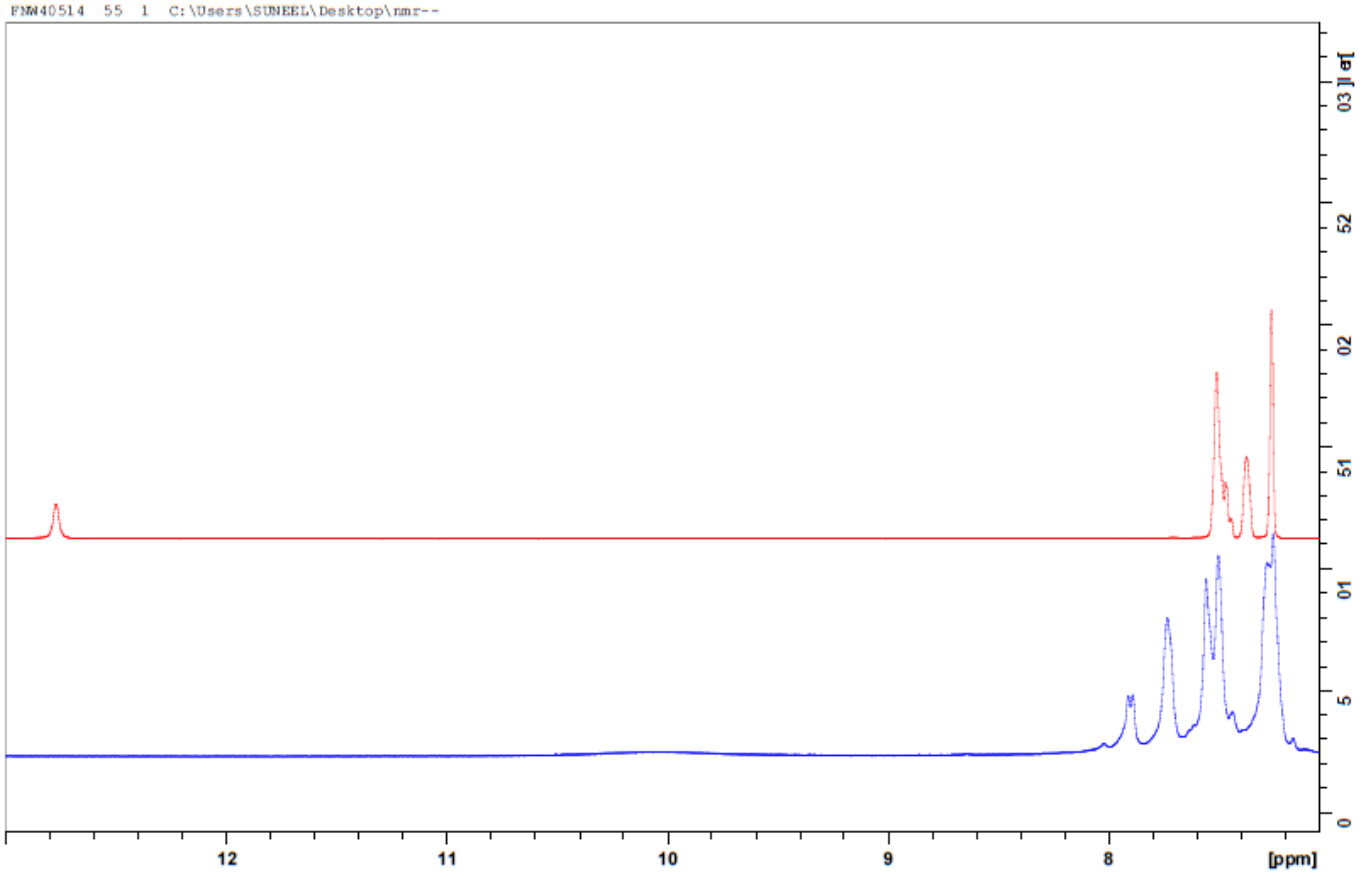

190.91
152.93
149.37
141.12
141.06
139.87
138.49
132.69
129.39
129.25
127.73
127.60
126.17
125.62
124.65
124.41
122.27
77.17
76.85
76.53
0.86
-0.17
N
S
CHO
C18H11NOS
Mol. Wt.: 289.351
200
180
160
140
120
100
80
60
40
20
0
ppm

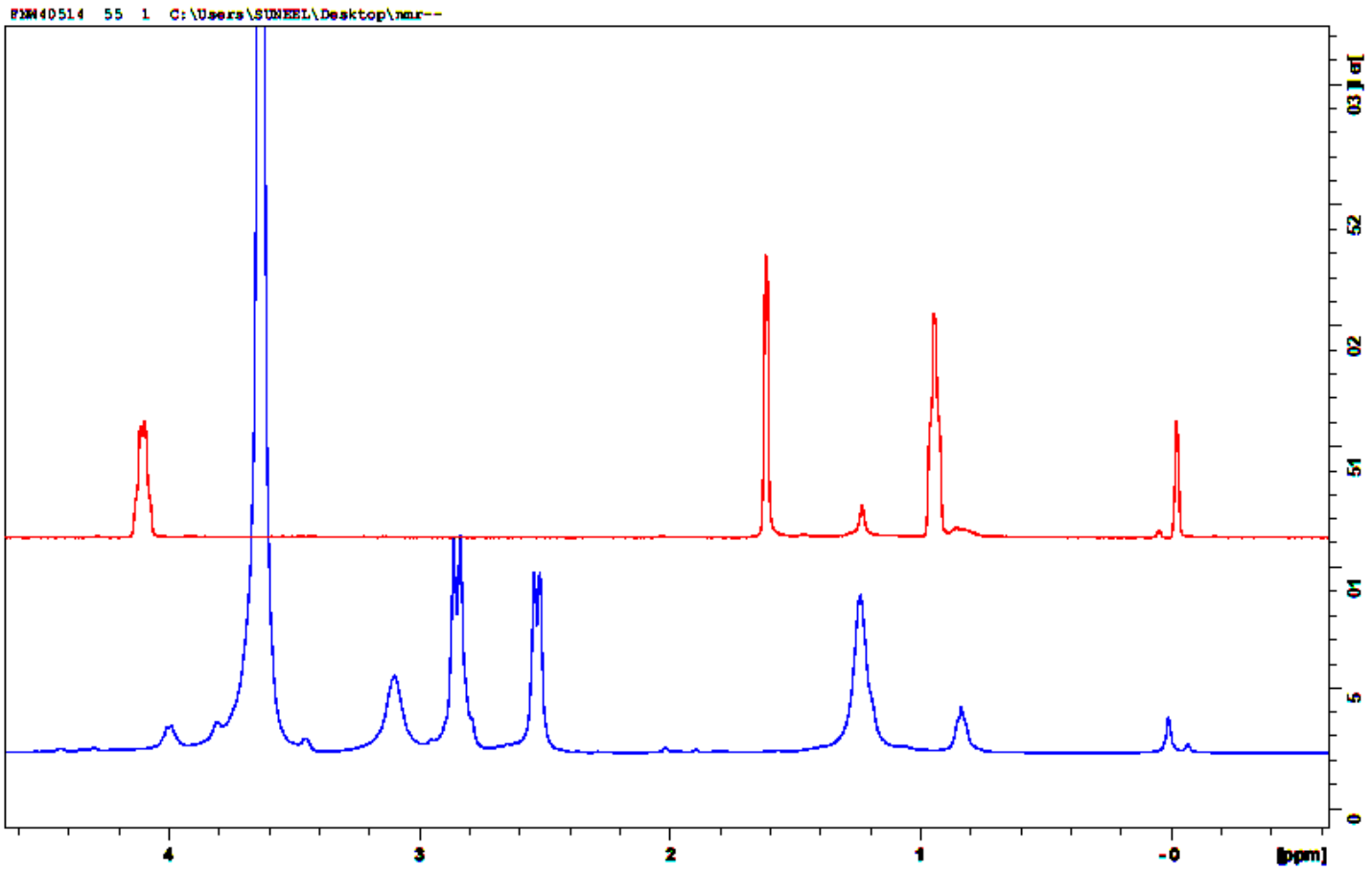

744.52
800.46
862.18
916.19
1014.56
1111.00
1373.32
1392.61
1490.97
1556.55
1577.77
1614.42
1691.57
2852.72
2922.16
2956.87
3064.89
3454.51
CHO
S
N
C18H11NOS
Mol. Wt.: 289.351
100
%T
75
50
25
0
-25
4000
3000
2000
1500
1000
500
1/cm
SC097

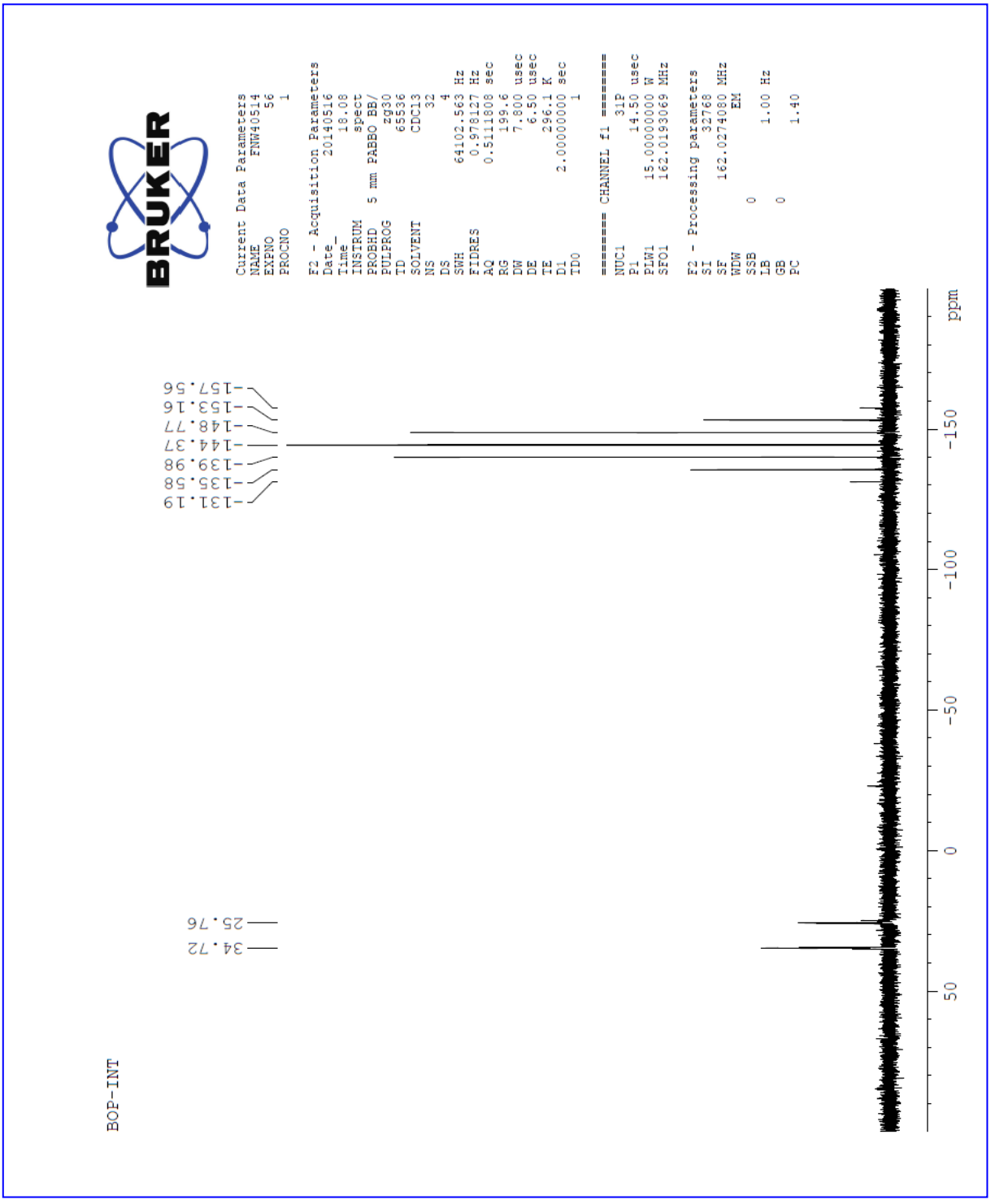

Intens.
[%]
+MS, 3.6min #195
290.0
130.2
242.2
268.0
CHO
N
S
C18H11NOS
Mol. Wt.: 289.351
100
80
60
40
20
0
200
300
400
500
600
700
800
900
m/z


12.273
10.276
8.544
7.958
7.689
7.397
7.286
3.370
2.537
O
O
N
H
Mol. Formula: $C_{10}H_7NO_2$
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
0.98
1.01
1.01
1.00
1.01


189.75
161.41
142.40
141.13
133.66
130.90
125.58
122.63
118.12
115.39
40.13
39.92
39.71
39.50
39.29
39.08
38.87
O
N
H
O
200
180
160
140
120
100
80
60
40
20
0
ppm


FNW40514 55 1 C:\Users\SUNEEL\Desktop\nmr--
12
11
10
9
8
[ppm]
0
5
01
51
02
52
03


PNM40514 55 1 C:\Users\SUNEEL\Desktop\nmr--
4
3
2
1
-0
[ppm]



The Overlap ^{1}H NMR spectra of the starting material (red spectrum) and the phosphonium salt intermediate (blue spectrum) and the P NMR of the phosphonium salt intermediate