Supporting Information

Ultrasound-Promoted Synthesis of Novel *N*-Arylamino-3,5'-biquinoline Derivatives: Their Applications in Live-Cell Imaging and in Vitro Anticancer Activity Evaluation

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Experimental Section

General remarks:

All Starting materials were synthesized according to the procedures reported in the literature [32, 33]. A single crystal of compounds **3a** was formed in DCM and MeOH mixture. Elemental analyses for C, H and N were performed using a Heraeus CHN–O–Rapid analyzer. Mass spectra were recorded on a Finnigan-MATT 8430 mass spectrometer operating at an ionization potential of 70 eV. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were obtained using Bruker DRX-300 AVANCE and

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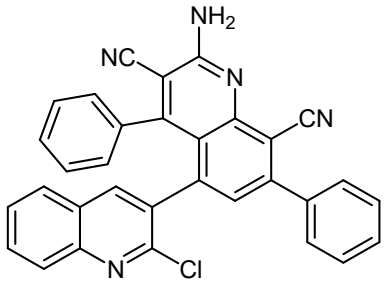
Bruker DRX-500 AVANCE spectrometers. The fluorescence spectra were recorded on PerkinElmer LS 45 fluorescence spectrometer. The absorption spectra were taken via the Rayleigh UV-2601 spectrophotometer. Chemical shifts are reported in parts per million (δ) downfield from an internal tetramethylsilane reference. Coupling constants (J values) are reported in hertz (Hz). IR spectra were recorded as KBr pellets on a NICOLET FT-IR 100 spectrometer; absorbances are reported in cm^{-1}. Melting points were measured on an Electrothermal 9100. All reactions were conducted by the QSONICA Q700 sonicator at an amplitude of 60% and a frequency of 20 kHz. The temperature of the reaction under US irradiation was checked using a mercury laboratory thermometer.

General Procedure for Preparation of Compounds 3a-j.

To a mixture of 2-chloro-3-formyl quinoline derivatives (1.0 mmol), and α,α-dicyanoolefines (2.0 mmol) in EtOH (10 mL), Et_3N (15 mmol %) were added. Then, the mixture was subjected to US irradiation (20 kHz) at 60 °C temperature. The amplitude of the US waves was fixed at 60%. After 30-40 min continuous irradiation, the reaction was completed and a light-yellow solid was isolated by simple filtration [derivatives (**3a**, **3g**, **3h**, **3i**, **3j**) were purified by washing with EtOH twice] and other derivatives (**3b**, **3c**, **3d**, **3e**, **3f**) were purified by recrystallization in DMF.

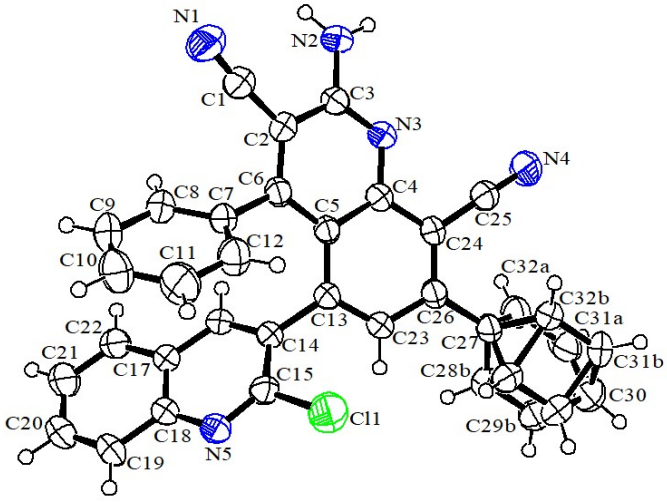
Characteristic data for compounds (3a-3j).

2'-Amino-2-chloro-4',7'-diphenyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3a).



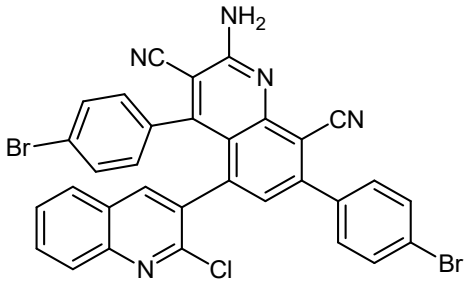
Light yellow solid, m.p = 268-270 °C (dec.), 0.46 g, yield: 91%. IR (KBr) (ν_{max}, cm^{-1}): 3469, 3381, 2223, 1606, 1560, 1546, 1420 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 6.60 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 6.63 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 6.96 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 7.03 (1H, d,

$^3J_{HH}$ = 7.3 Hz, CH of Ph), 7.23 (1H, d, $^3J_{HH}$ = 7.6 Hz, CH of Ph), 7.34 (1H, s, $CH^{6'}$ of quinoline), 7.56 (1H, t, $^3J_{HH}$ = 7.1 Hz, CH of Ph), 7.57- 7.62 (3H, m, CH^6 of quinoline and 2CH of Ph), 7.68 (2H, bs, NH_2), 7.75- 7.79 (4H, m, 2CH of Ph, CH^5 and CH^8 of quinoline), 7.76 (1H, t,$^3J_{HH}$ = 7.6 Hz, CH^7 of quinoline), 8.09 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 98.70, 107.13, 114.98, 117.03, 118.48, 125.91, 127.06, 127.21, 127.28, 127.40, 127.79, 127.81, 128.76, 128.97, 129.09, 129.59, 130.83, 132.14, 135.56, 136.98, 140.26, 140.90, 146.09, 147.71, 149.17, 151.23, 156.61, 156.71. MS (EI, 70 eV) *m/z* (%): 509 (M^{+2}, 47), 508 (M^{+1}, 52), 507 (M^+, 100), 473 (17), 472 (37), 469 (6), 446 (6), 427 (5), 393 (5), 235 (32), 213 (9), 194 (9), 76 (9), 51 (14). Anal. calcd. for $C_{32}H_{18}ClN_5$ (507.98): C, 75.66; H, 3.57; N, 13.79. Found: C, 75.68; H, 3.56; N, 13.78%. Crystal data for **3a** $C_{32}H_{18}ClN_5$ (CCDC 2092629): M_W = 507.96, monoclinic, C 1 2/c 1, a = 27.234(5) Å, b = 8.3608(17) Å, c = 23.028(5) Å, α = 90.0, β = 109.84(3), γ = 90.0, V = 4932.2(19) Å^3, Z = 8, Dc = 1.368 mg/m^3, F (000) = 2096, crystal dimension 0.20 × 0.15 × 0.10 mm, radiation, Mo Kα (λ = 0.71073 Å), 1.9 ≤ 2θ ≤ 25.0, intensity data were collected at 290 K with a Bruker APEX area-detector diffractometer, and employing ω/2θ scanning technique, in the range of -32 ≤ h ≤ 32, -9 ≤ k ≤ 9, -26 ≤ l ≤ 24; the structure was solved by a direct method, all non-hydrogen atoms were positioned and anisotropic thermal parameters refined from 4153 observed reflections with R (into) = 0.0499 by a full-matrix least-squares technique converged to R1 = 0.0668, and wR2 = 0.1571 [I>2sigma(I)].



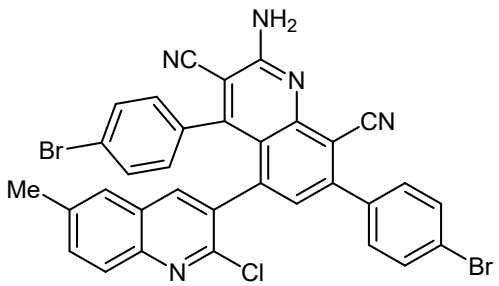
ORTEP diagram of **3a**

2'-Amino-4',7'-bis(4-bromophenyl)-2-chloro-[3,5'-biquinoline]-3',8'-dicarbonitrile (3b).



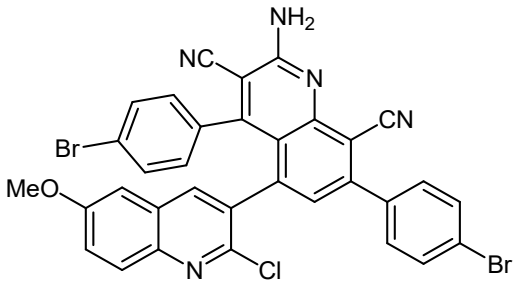
Light yellow solid, m.p = 280-282 °C (dec.), 0.51 g, yield: 82%. IR (KBr) (ν_{max}, cm^{-1}): 3380, 3319, 3229, 2223, 1642, 1590, 1569, 1486, 1426, 1052, 1005, 749 cm^{-1}. ^{1}H NMR (300.13 MHz, DMSO-d_6): 6.80 (1H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 1.7 Hz, CH of Ar), 6.96 (1H, dd, $^3J_{HH}$ = 8.3 Hz, $^4J_{HH}$ = 1.9 Hz, CH of Ar), 7.15 (1H, dd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.7 Hz, CH of Ar), 7.19 (1H, dd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.9 Hz, CH of Ar), 7.37 (1H, s, CH$^{6'}$), 7.66 (1H, t, $^3J_{HH}$ = 7.8 Hz, CH^6 of quinoline), 7.71 (2CH, d, $^3J_{HH}$ = 7.2 Hz, CH of Ar), 7.72 (2H, bs, NH_2), 7.77 (2H, d, $^3J_{HH}$ = 7.8 Hz, CH of Ar), 7.79 (1H, d, $^3J_{HH}$ = 8.0 Hz, CH^8 of quinoline), 7.82 (1H, d, $^3J_{HH}$ = 7.9 Hz, CH^5 of quinoline), 7.84 (1H, t, $^3J_{HH}$ = 8.7 Hz, CH^7 of quinoline), 8.10 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 98.73, 107.20, 114.80, 116.82, 118.37, 122.43, 123.39 , 125.82, 127.23, 127.53, 127.61, 128.22, 129.29, 130.85, 131.18, 131.67, 131.80, 131.95, 134.47, 136.03, 140.19, 140.77, 146.13, 147.63, 148.01, 151.09, 155.43, 156.50. MS (EI, 70 eV) *m/z* (%): 667 (M^{+2}, 28), 666 (M^{+1}, 76), 665 (M^+, 100), 664 (45), 630 (23), 586 (4), 550 (15), 469 (4), 442 (13), 274 (4), 234 (25), 221 (14), 207 (17), 83 (12), 56 (13). Anal. calcd. for $C_{32}H_{16}Br_2ClN_5$ (665.77): C, 57.73; H, 2.42; N, 10.52. Found: C, 57.75; H, 2.41; N, 10.51%.

2'-Amino-4',7'-bis(4-bromophenyl)-2-chloro-6-methyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3c).



Light yellow solid, m.p = 286-288 °C (dec.), 0.55 g, yield: 82%. IR (KBr) (ν_{max}, cm^{-1}): 3440, 3336, 3225, 2220, 1642, 1566, 1490, 1420, 1073, 1004, 837, 824, 803 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 2.51 (3H, s, CH_3), 6.85 (1H, dd, $^3J_{HH}$ = 8.3 Hz, $^4J_{HH}$ = 1.8 Hz, CH of Ar), 6.94 (1H, dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 1.8 Hz, CH of Ar), 7.11 (1H, dd, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.7 Hz, CH of Ar), 7.14 (1H, dd, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.9 Hz, CH of Ar), 7.34 (1H, s, $CH^{6'}$), 7.56 (1H, s, CH^5 of quinoline), 7.61 (1H, dd, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 1.9 Hz, CH^7 of quinoline), 7.70 (2H, d, $^3J_{HH}$ = 8.6 Hz, 2CH of Ar), 7.72 (1H, d, $^3J_{HH}$ = 8.6 Hz, CH^8 of quinoline), 7.74 (2H, bs, NH_2), 7.76 (2H, d, $^3J_{HH}$ = 8.8 Hz, 2CH of Ar), 7.96 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 21.23, 98.77, 107.20, 114.82, 116.85, 118.45, 122.49, 123.41, 125.85, 126.18, 126.35, 127.54, 129.16, 129.20, 131.04, 131.36, 131.60, 131.86, 134.54, 136.08, 137.28, 139.70 140.96, 144.80, 146.74, 148.03, 151.11, 155.51, 156.51. MS (EI, 70 eV) *m/z* (%): 683 (M^{+4}, 19), 682 (M^{+3}, 21), 681 (M^{+2}, 88), 680 (M^{+1}, 80), 679 (M^+, 100), 677 (25), 676 (50), 645 (18), 644 (33), 600 (4), 563 (14), 522 (6), 482 (5), 281 (5), 260 (13), 228 (17), 207 (6), 148 (51), 83 (15), 56 (61), 55 (51), 50 (8). Anal. calcd. for $C_{33}H_{18}Br_2ClN_5$ (679.80): C, 58.31; H, 2.67; N, 10.30. Found: C, 58.33; H, 2.66; N, 10.29%.

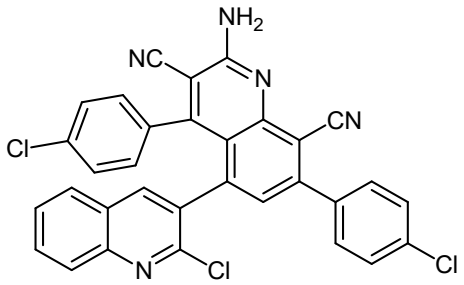
2'-Amino-4',7'-bis(4-bromophenyl)-2-chloro-6-methoxy-[3,5'-biquinoline]-3',8'-dicarbonitrile (3d).



Light yellow solid, m.p = 315-317 °C (dec.), 0.57 g, yield: 82%. IR (KBr) (ν_{max}, cm^{-1}): cm^{-1}. 3392, 2217, 1621, 1590, 1568, 1492, 1457, 1383, 1227, 1073, 1040, 1011, 803 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 3.91 (3H, s, OCH_3), 6.75 (1H, dd, $^3J_{HH}$ = 7.9 Hz, $^4J_{HH}$ = 1.8 Hz, CH of Ar), 6.94 (1H, dd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.1 Hz, CH of Ar), 7.10-7.12 (2H, m, 2CH of Ar), 7.14 (1H, d, $^4J_{HH}$ = 2.8 Hz, CH^5 of quinoline), 7.34 (1H, s, $CH^{6'}$), 7.41 (1H, dd, $^3J_{HH}$ = 9.1 Hz, $^4J_{HH}$ = 2.7 Hz, CH^7 of quinoline),

7.70 (1H, d, $^{3}J_{HH}$ = 8.7 Hz, CH^{8} of quinoline), 7.72 (2H, bs, NH_2), 7.75 (2H, d, $^{3}J_{HH}$ = 8.5 Hz, 2CH of Ar), 7.77 (2H, dd, $^{3}J_{HH}$ = 8.5 Hz, $^{4}J_{HH}$ = 1.8 Hz, 2CH of Ar), 7.92 (1H, s, CH^{4} of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 55.71, 98.73, 105.43, 107.17, 114.83, 116.86, 118.39, 122.53, 123.41, 127.08, 127.43, 128.85, 129.07, 130.17, 130.82, 131.21, 131.59, 131.78, 132.00, 134.53, 136.05, 138.99, 142.15, 144.99, 148.02, 151.11, 155.52, 156.50, 158.08. MS (EI, 70 eV) *m/z* (%): 700 (M^{+4}, 9), 699 (M^{+3}, 23), 698 (M^{+2}, 60), 697 (M^{+1}, 100), 696 (M^{+}, 100), 694 (14), 692 (35), 660 (24), 617 (6), 580 (8), 558 (9), 536 (8), 522 (14), 506 (13), 486 (3), 455 (3), 424 (4), 343 (4), 313 (5), 289 (3), 260 (5), 228 (14), 193 (14), 156 (9), 127(5), 102 (14), 72 (38), 52 (4). Anal. calcd. for $C_{33}H_{18}Br_2ClN_5O$ (695.80): C, 56.97; H, 2.61; N, 10.07. Found: C, 56.99; H, 2.60; N, 10.06%.

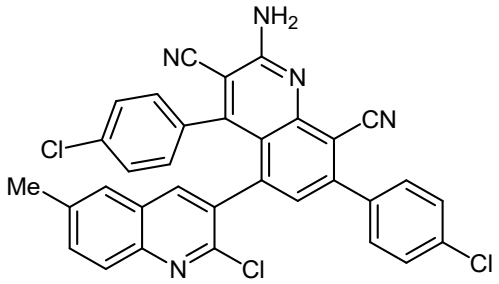
2'-Amino-2-chloro-4',7'-bis(4-chlorophenyl)-[3,5'-biquinoline]-3',8'-dicarbonitrile (3e).



Light yellow solid, m.p = 275-276 °C (dec.), 0.43 g, yield: 75%. IR (KBr) (ν_{max}, cm^{-1}):3467, 2222, 1674, 1625, 1594, 1560, 1543, 1491, 1384, 1092, 1016, 831, 771 cm^{-1}. ^{1}H NMR (300.13 MHz, DMSO-d_6): 6.66 (1H, dd, $^{3}J_{HH}$ = 8.2 Hz, $^{4}J_{HH}$ = 2.2 Hz, 2CH of Ph), 7.02 (2H, dd, $^{3}J_{HH}$ = 8.4 Hz, $^{4}J_{HH}$ = 1.8 Hz, 2CH of Ph), 7.25 (1H, dd, $^{3}J_{HH}$ = 8.2 Hz, $^{4}J_{HH}$ = 2.2 Hz, 2CH of Ph), 7.38 (1H, s, CH$^{6'}$), 7.63 (2H, d, $^{3}J_{HH}$ = 8.6 Hz, 2CH of Ph), 7.65 (1H, t, $^{3}J_{HH}$ = 7.6 Hz, CH^{6} of quinoline), 7.73 (2H, bs, NH_2), 7.75 (1H, t, $^{3}J_{HH}$ = 7.6 Hz, CH^{7} of quinoline), 7.79 (1H, d, $^{3}J_{HH}$ = 7.3 Hz, CH^{8} of quinoline), 7.81 (2H, d, $^{3}J_{HH}$ = 8.6 Hz, 2CH of Ph), 7.84 (1H, d, $^{3}J_{HH}$ = 7.3 Hz, CH^{5} of quinoline), 8.10 (1H, s, CH^{4} of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 99.12, 109.27, 114.70, 116.57, 119.17, 125.75, 126.86, 127.64, 128.01, 128.30, 128.93, 129.26, 130.29, 131.31, 132.24, 133.39, 135.25, 135.65, 136.29, 138.56, 138.91, 140.75, 146.85, 148.23, 148.98, 151.18, 155.42, 155.78. MS (EI, 70 eV) *m/z* (%): 582 (M^{+4}, 16), 580 (M^{+3}, 33), 579 (M^{+2}, 66), 578 (M^{+1}, 88), 577 (M^{+}, 100), 575(61), 558 (11),

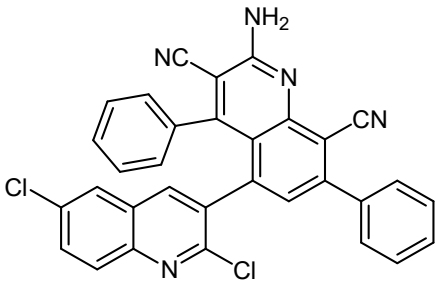
557 (19), 541 (23), 540 (27), 522 (5), 504 (9), 478 (5), 415 (10), 295 (5), 270 (5), 252 (9), 234 (6), 207 (7), 162 (5), 126 (9), 100 (10), 74 (28), 72 (81), 50 (19). Anal. calcd. for $C_{32}H_{16}Cl_3N_5$ (576.87): C, 66.63; H, 2.80; N, 12.14. Found: C, 66.65; H, 2.79; N, 12.13%.

2'-Amino-2-chloro-4',7'-bis(4-chlorophenyl)-6-methyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3f).



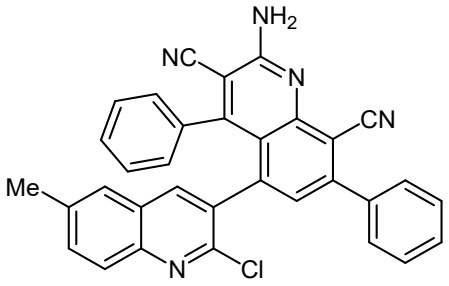
Light yellow solid, m.p = 320-321 °C (dec.), 0.47 g, yield: 80%. IR (KBr) (ν_{max}, cm^{-1}): 3440, 3335, 3219, 2219, 1643, 1562, 1496, 1413, 821, 697 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 2.47 (3H, s, CH_3), 6.65 (1H, dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.1 Hz, CH of Ph), 6.76 (1H, dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.2 Hz, CH of Ph), 6.98 (1H, dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.1 Hz, CH of Ph), 7.25 (1H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.2 Hz, 1CH of Ph), 7.26 (1H, s, $CH^{6'}$), 7.51 (2H, $^3J_{HH}$ = 8.4 Hz, 2CH of Ar), 7.58 (1H, d, $^4J_{HH}$ = 1.1 Hz, CH^5 of quinoline), 7.62 (2H, bs, NH_2), 7.64 (2H, d, $^3J_{HH}$ = 8.6 Hz, 2CH of Ar), 7.68 (1H, dd, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 1.9 Hz, CH^7 of quinoline), 7.96 (1H, d, $^3J_{HH}$ = 8.4 Hz, CH^8 of quinoline), 8.03 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 21.16, 98.84, 107.22, 114.78, 116.83, 118.48, 125.81, 127.60, 127.90, 128.97, 129.04, 130.79, 131.05, 131.32, 131.88, 133.06, 133.65, 134.13, 134.61, 135.67, 137.19, 139.37, 140.89, 144.74, 146.71, 147.92, 151.08, 155.46, 156.48. MS (EI, 70 eV) *m/z* (%): 590 (M^+, 2), 572 (12), 571 (38), 570 (16), 569 (33), 560 (38), 522 (14), 389 (3), 368 (3), 295 (4), 260 (14), 148 (9), 121 (9), 94 (28), 83 (57), 68 (100), 51 (14). Anal. calcd. for $C_{33}H_{18}Cl_3N_5$ (590.89): C, 67.08; H, 3.07; N, 11.85. Found: C, 67.10; H, 3.08; N, 11.86%.

2'-Amino-2,6-dichloro-4',7'-diphenyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3g).



Light yellow solid, m.p = 268-270 °C (dec.), 0.46 g, yield: 85%. IR (KBr) (ν_{max}, cm^{-1}): 3382, 2223, 1648, 1561, 1481, 1420, 1050, 1027, 754, 701 cm^{-1}. ^1H NMR (500.13 MHz, DMSO-d_6): 6.67 (1H, t, $^3J_{HH}$ = 7.0 Hz, CH of Ph), 6.73 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 6.97 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 7.04 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH of Ph), 7.23 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH of Ph), 7.35 (1H, s, $CH^{6'}$), 7.50-7.59 (3H, m, 3CH of Ph), 7.69 (2H, bs, NH_2), 7.73-7.75 (2H, m, CH^7 and CH^8 of quinoline), 7.77-7.79 (2H, m, 2CH of Ph), 7.91 (1H, s, CH^5 of quinoline), 8.01 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 98.76, 107.32, 114.93, 116.98, 118.35, 126.23, 126.73, 127.49, 127.96, 128.73, 128.81, 128.90, 129.21, 129.58, 129.76, 131.51, 133.19, 135.52, 136.93, 139.39, 139.60, 140.40, 144.53, 148.40, 149.18, 151.21, 156.54, 156.62. MS (EI, 70 eV) *m/z* (%): 545 (M^{+4}, 19), 544 (M^{+3}, 40), 543 (M^{+1}, 95), 542 (M^+, 100), 508 (10), 507 (15), 506 (33), 470 (9), 453 (3), 427 (5), 401 (2), 343 (5), 252 (4), 77 (9), 51 (5). Anal. calcd. for $C_{32}H_{17}Cl_2N_5$ (542.42): C, 70.86; H, 3.16; N, 12.91. Found: C, 70.88; H, 3.15; N, 12.90%.

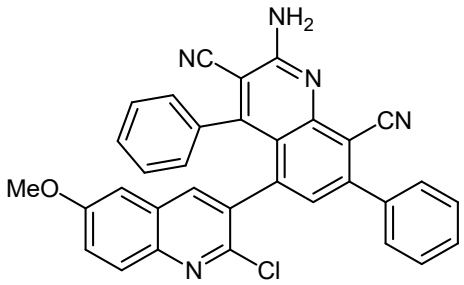
2'-Amino-2-chloro-6-methyl-4',7'-diphenyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3h).



Light yellow solid, m.p = 265-267 °C (dec.), 0.46 g, yield: 88%. IR (KBr) (ν_{max}, cm^{-1}): 3450, 2217, 1638, 1561, 1494, 1418, 1050, 1026, 1001, 703 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 2.46 (3H, s, CH_3), 6.62 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 6.67 (1H, t, $^3J_{HH}$ = 7.6 Hz, CH of Ph), 6.96 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 7.01 (1H, d, $^3J_{HH}$ = 7.3 Hz, CH of Ph), 7.23 (1H, d, $^3J_{HH}$ = 7.5 Hz, CH of

Ph), 7.29 (1H, s, $CH^{6'}$), 7.50-7.57 (3H, m, 3CH of Ph), 7.53 (2H, bs, NH_2), 7.59 (1H, s, CH^5 of quinolone), 7.63 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH^7 of quinoline), 7.65 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH^8 of quinoline), 7.74 (2H, dd, $^3J_{HH}$ = 7.5 Hz, $^4J_{HH}$ = 2.4 Hz, 2CH of Ph), 7.96 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 21.10, 98.68, 107.08, 114.94, 116.98, 118.43, 125.89, 126.23, 126.40, 127.41, 126.75, 127.05, 127.98, 128.70, 128.83, 129.16, 129.46, 129.59, 132.08, 135.46, 136.78, 136.94, 141.00, 144.69, 146.75, 149.08, 151.18, 156.56, 156.69. MS (EI, 70 eV) m/z (%): 523 (M^{+2}, 40), 522 (M^{+1}, 43), 521 (M^+, 100), 487 (10), 486 (36), 460 (3), 442 (4), 242 (19), 221 (5), 187 (2), 161 (2), 111 (3), 83 (8), 56 (7). Anal. calcd. for $C_{33}H_{20}ClN_5$ (521.14): C, 75.93; H, 3.86; N, 13.42. Found: C, 75.95; H, 3.85; N, 13.41%.

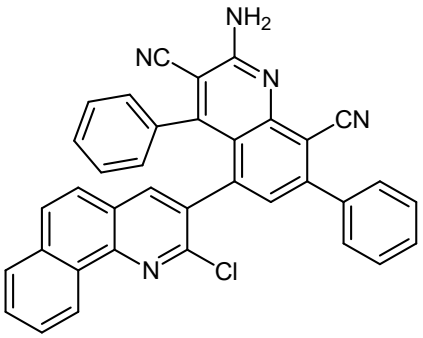
2'-Amino-2-chloro-6-methoxy-4',7'-diphenyl-[3,5'-biquinoline]-3',8'-dicarbonitrile (3i).



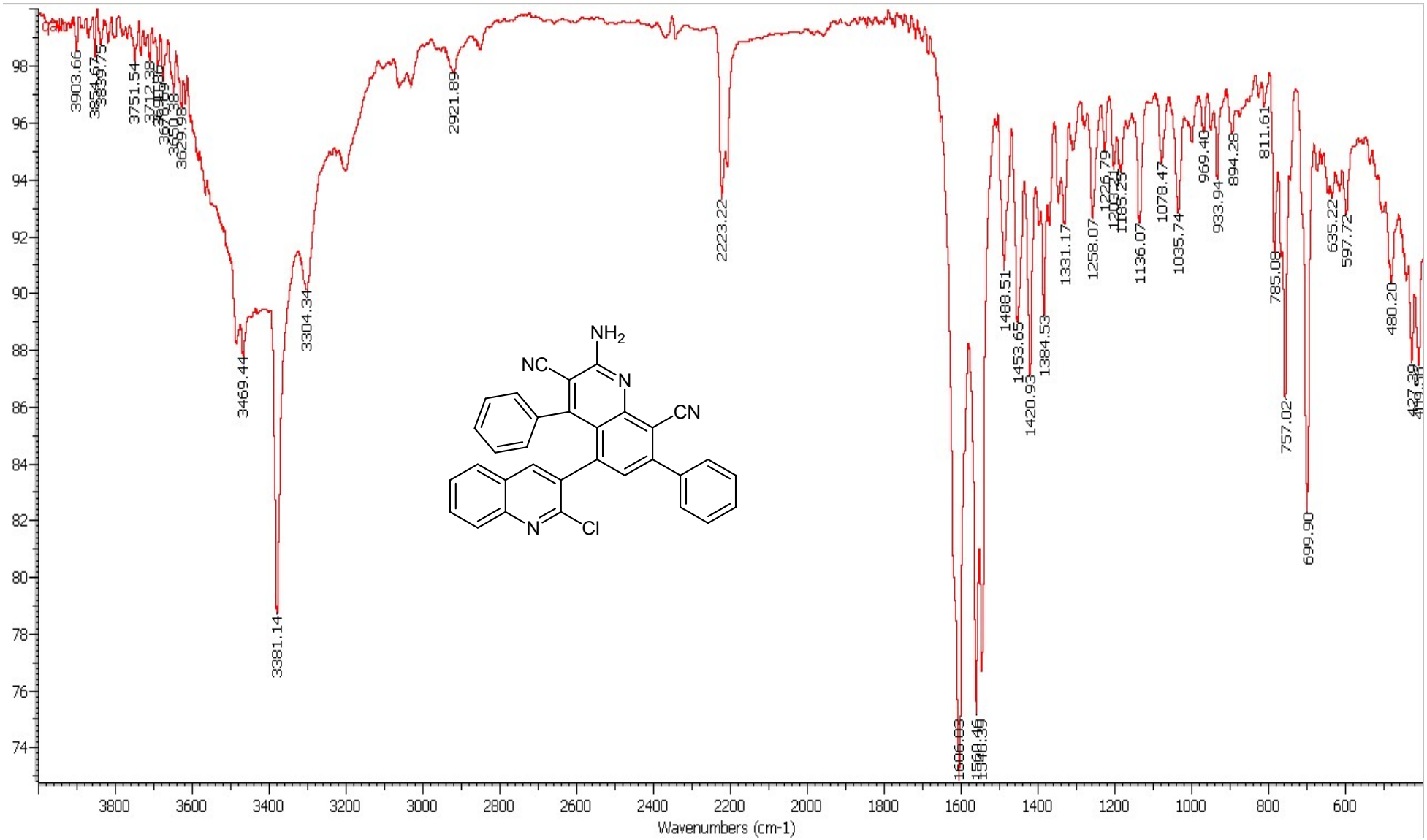
Light yellow solid, m.p = 295-297 °C (dec.), 0.48 g, yield: 90%. IR (KBr) (ν_{max}, cm^{-1}): 3438, 3332, 3213, 2219, 1644, 1620, 1546, 1495, 1415, 1329, 1224, 1024, 839, 699 cm^{-1}. ^{1}H NMR (300.13 MHz, DMSO-d_6): 3.87 (3H, s, OCH_3), 6.64 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 6.75 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 6.95 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 7.03 (1H, d, $^3J_{HH}$ = 7.7 Hz, CH of Ph), 7.13 (1H, d, $^4J_{HH}$ = 2.8 Hz, CH^5 of quinoline), 7.21 (1H, d, $^3J_{HH}$ = 8.0 Hz, CH of Ph), 7.30 (1H, s, $CH^{6'}$), 7.37 (1H, dd, $^3J_{HH}$ = 9.0 Hz, $^4J_{HH}$ = 2.7 Hz, CH^7 of quinoline), 7.50-7.57 (3H, m, 3CH of Ph), 7.65 (2H, bs, NH_2), 7.66 (1H, d, $^3J_{HH}$ = 9.0 Hz, CH^8 of quinoline), 7.75 (2H, dd, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 2.4 Hz, 2CH of Ph), 7.93 (1H, s, CH^4 of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 55.39, 98.66, 105.62 107.09, 114.94, 116.98, 118.40, 122.95, 127.10, 128.72, 127.88, 127.90, 128.06 128.71, 128.82, 129.14, 129.45, 129.61, 132.23, 135.45, 136.95, 141.05, 142.07, 145.03, 149.10, 151.18, 156.56, 156.69, 157.64. MS (EI, 70 eV) *m/z* (%): 539 (M^{+2}, 44), 538 (M^{+1}, 52), 537 (M^+, 100), 518 (9), 502

(14), 503 (38), 459 (18), 430 (9), 250 (2), 229 (19), 188 (4), 83 (4), 66 (3), 50 (2). Anal. calcd. for $C_{33}H_{20}ClN_5O$ (537.14): C, 73.67; H, 3.75; N, 13.02. Found: C, 73.69; H, 3.74; N, 13.01%.

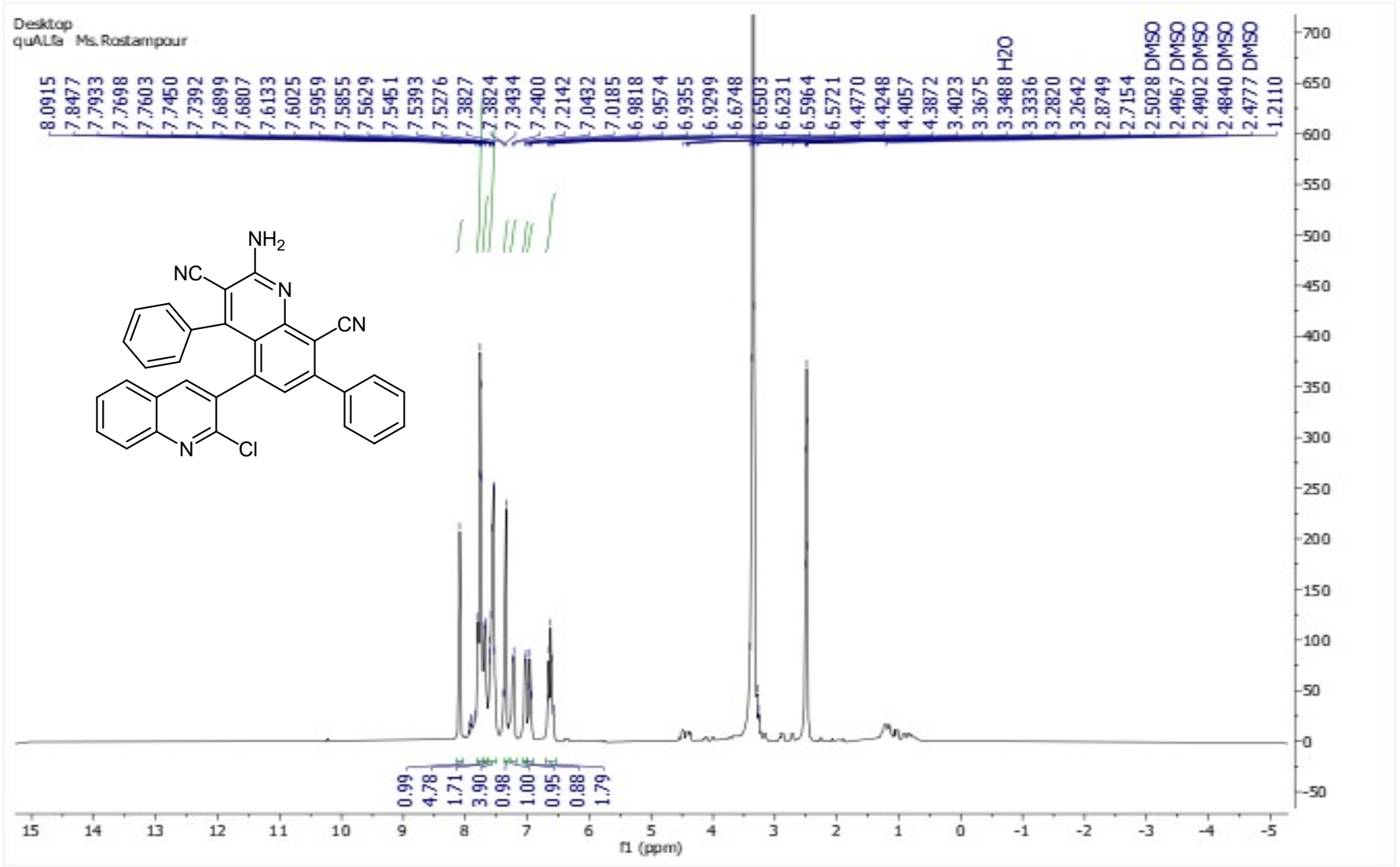
2-Amino-5-(2-chlorobenzo[*h*]quinolin-3-yl)-4,7-diphenylquinoline-3,8-dicarbonitrile (3j).



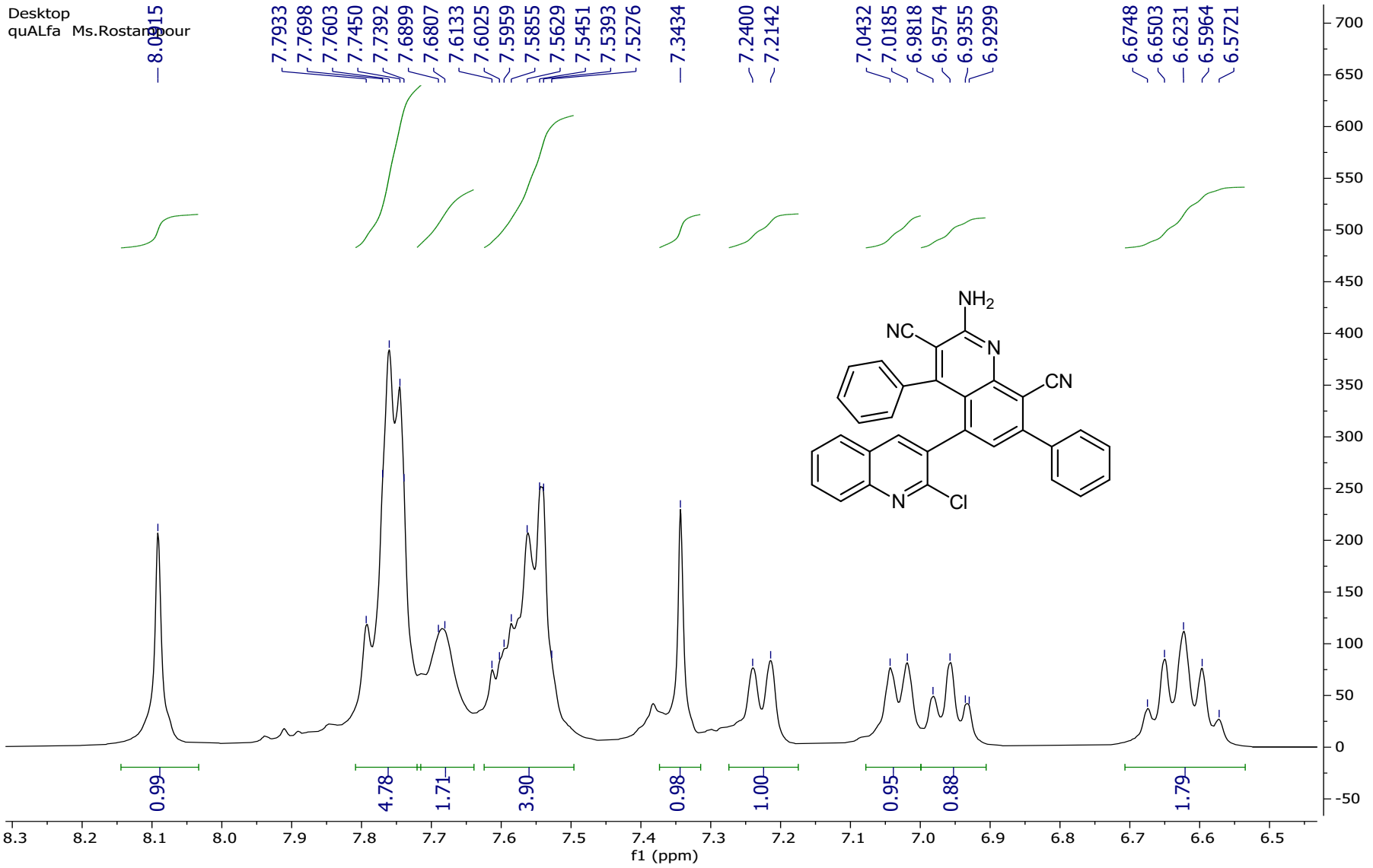
Light yellow solid, m.p = 350 °C (dec.), 0.47 g, yield: 85%. IR (KBr) (ν_{max}, cm^{-1}): 3405, 3340, 3229, 2225, 1636, 1562, 1481, 1419, 1368, 750, 701 cm^{-1}. ^1H NMR (300.13 MHz, DMSO-d_6): 6.45 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH of Ph), 6.66 (1H, t, $^3J_{HH}$ = 7.7 Hz, CH of Ph), 6.88 (1H, t, $^3J_{HH}$ = 7.6 Hz, CH of Ph), 7.05 (1H, d, $^3J_{HH}$ = 7.7 Hz, CH of Ph), 7.25 (1H, d, $^3J_{HH}$ = 7.8 Hz, CH of Ph), 7.37 (1H, s, $CH^{6'}$), 7.52-7.60 (3H, m, 3CH of Ph), 7.65 (1H, d, $^3J_{HH}$ = 8.8 Hz, CH^6 of quinoline), 7.69 (2H, bs, NH_2), 7.71-7.80 (4H, m, 2CH of Ph, CH^8 and CH^9 of quinoline), 7.93 (1H, d, $^3J_{HH}$ = 8.8 Hz, CH^5 of quinoline), 8.03 (1H, dd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 2.5 Hz, CH^7 of quinoline), 8.12 (1H, s, CH^4 of quinoline), 8.84 (1H, dd, $^3J_{HH}$ = 7.9 Hz, $^4J_{HH}$ = 2.7 Hz, CH^{10} of quinoline). ^{13}C NMR (75.46 MHz, DMSO-d_6): 98.71, 107.15, 114.99, 117.06, 118.39, 123.73, 124.12, 124.65, 127.04, 127.39, 127.44, 127.77, 127.93, 128.00, 128.10, 128.79, 128.89, 129.09, 129.21, 129.61, 132.89, 133.46, 135.57, 136.98, 140.24, 140.92, 144.37, 146.85, 149.19, 151.28, 156.63, 156.68. MS (EI, 70 eV) *m/z* (%): 559 (M^{+2}, 13), 558 (M^{+1}, 9), 557 (M^+, 41), 522 (15), 294 (9), 260 (19), 238 (5), 218 (5), 184 (5), 166 (5), 148 (25), 120 (9), 96 (23), 83 (60), 68 (100), 50 (9). Anal. calcd. for $C_{36}H_{20}ClN_5$ (557.14): C, 77.48; H, 3.61; N, 12.55. Found: C, 77.50; H, 3.60; N, 12.54%.



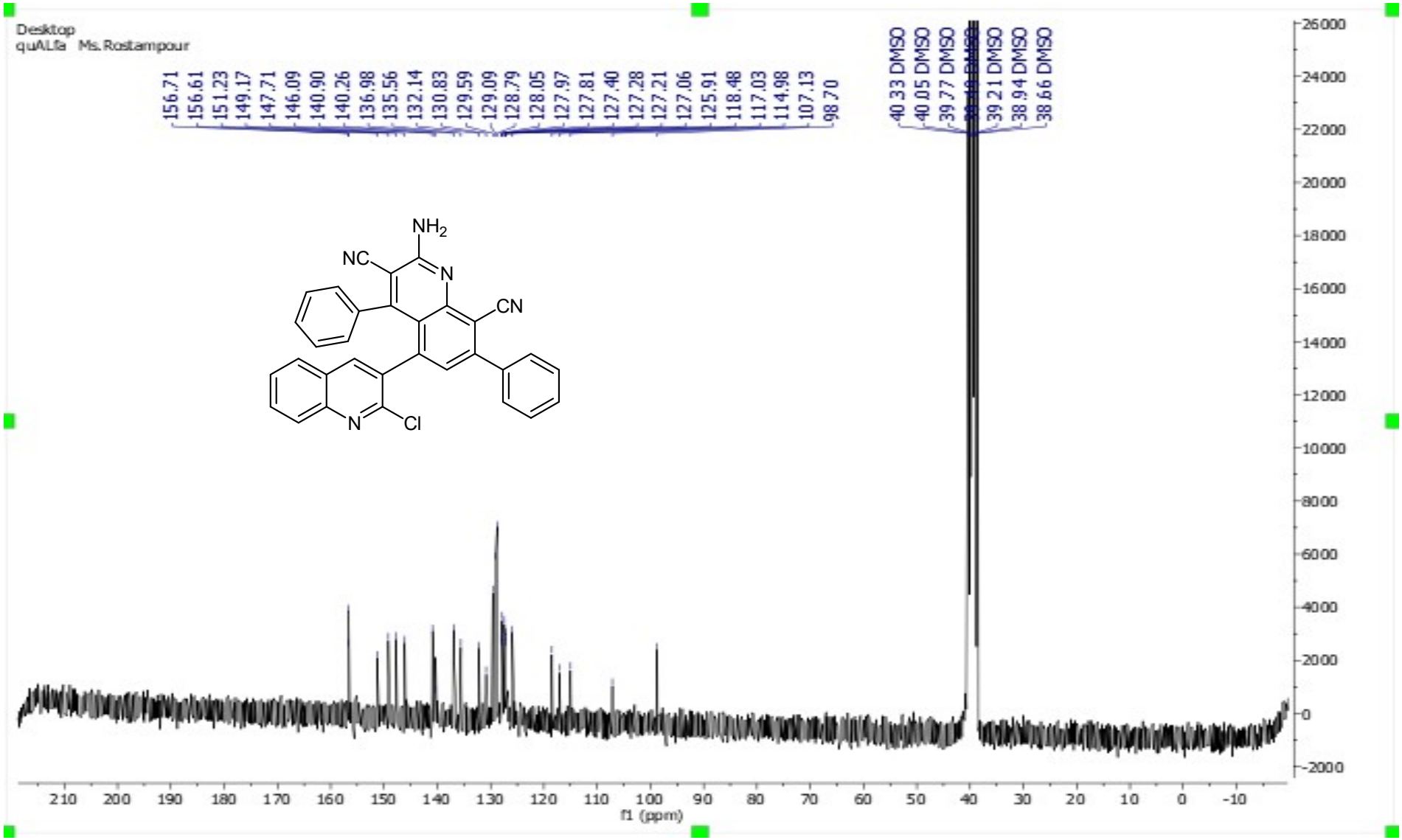
IR Spectrum of **3a**



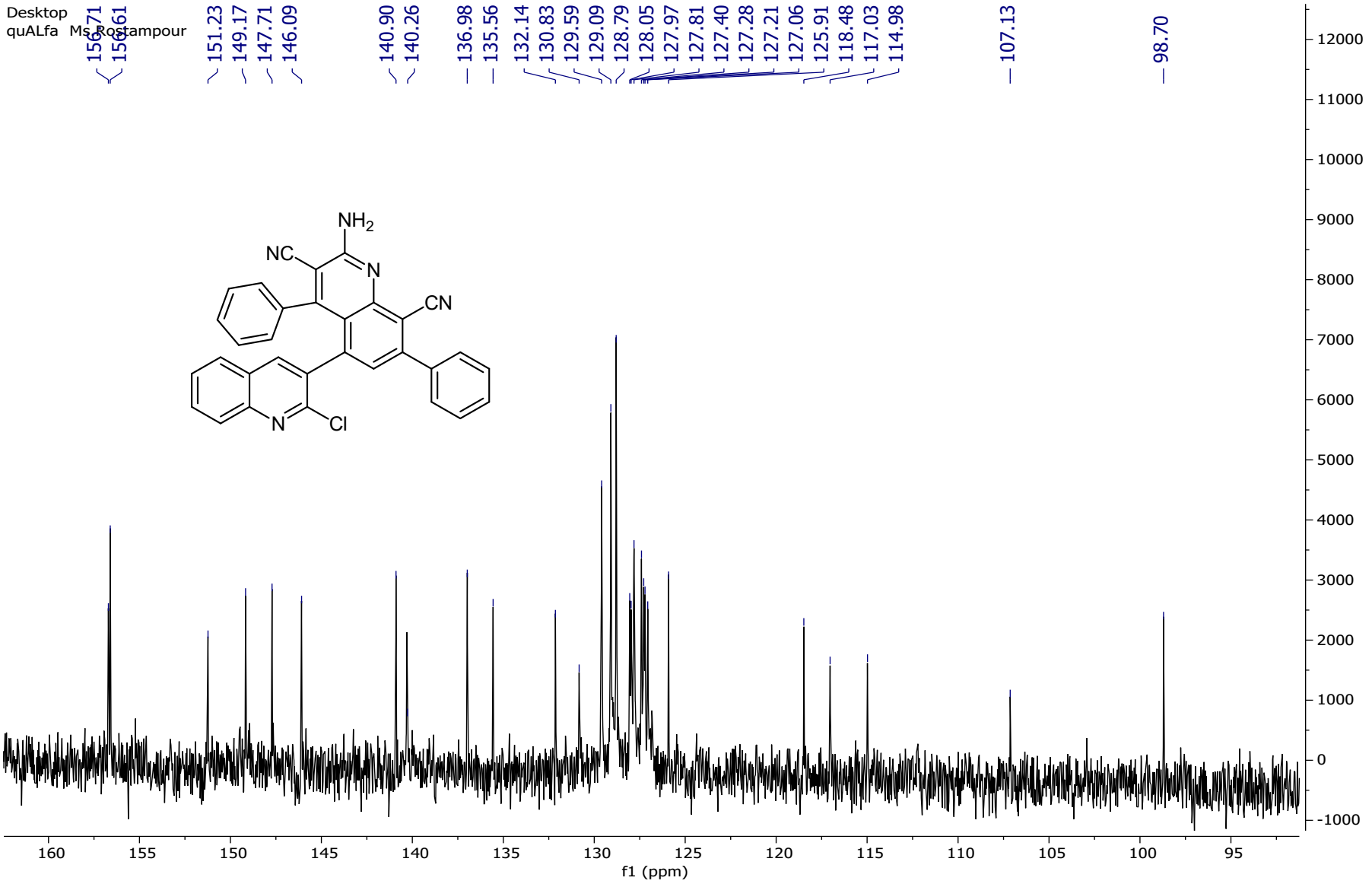
^{1}H NMR Spectrum of **3a**



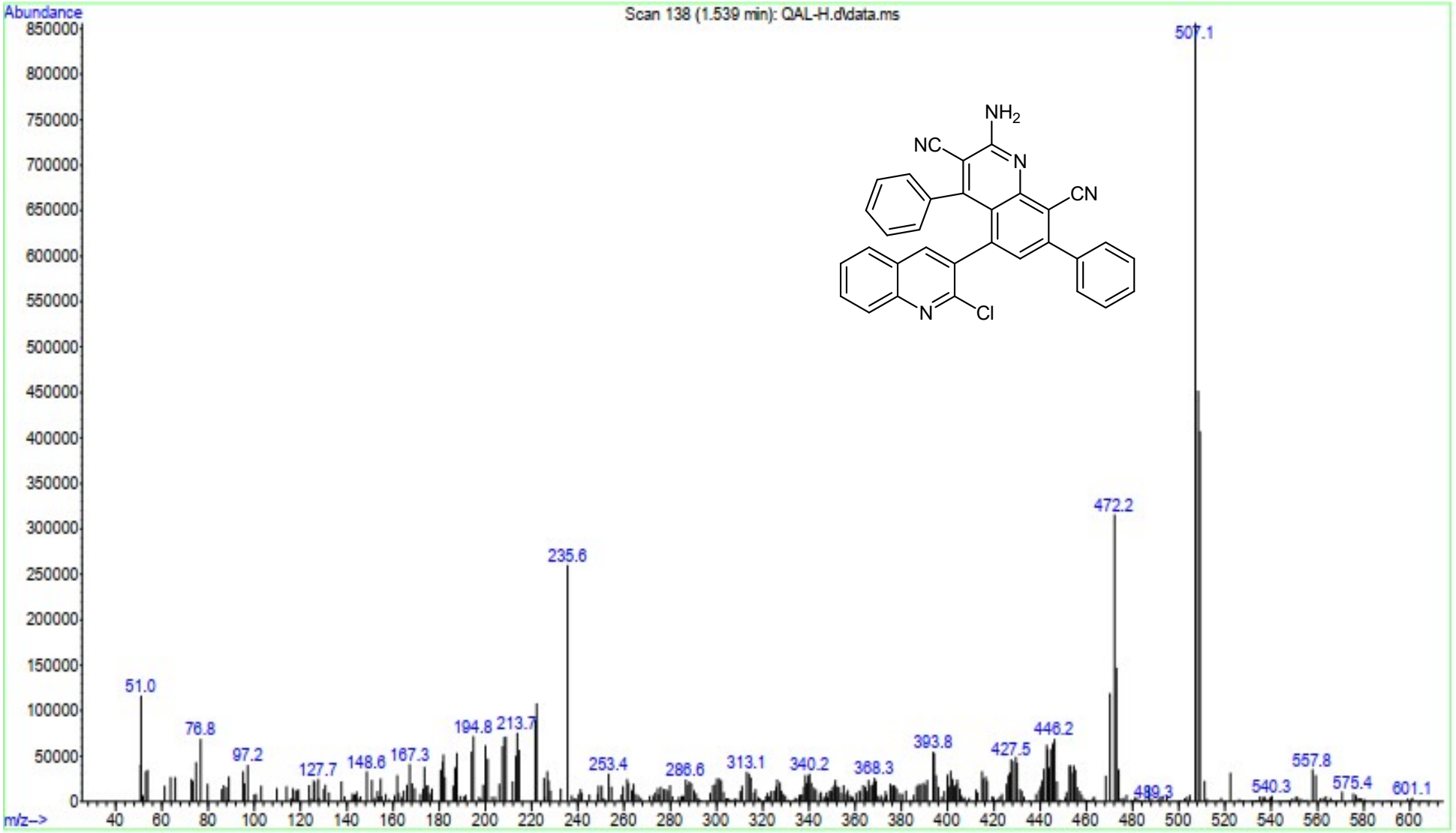
^{1}H NMR Spectrum of **3a**



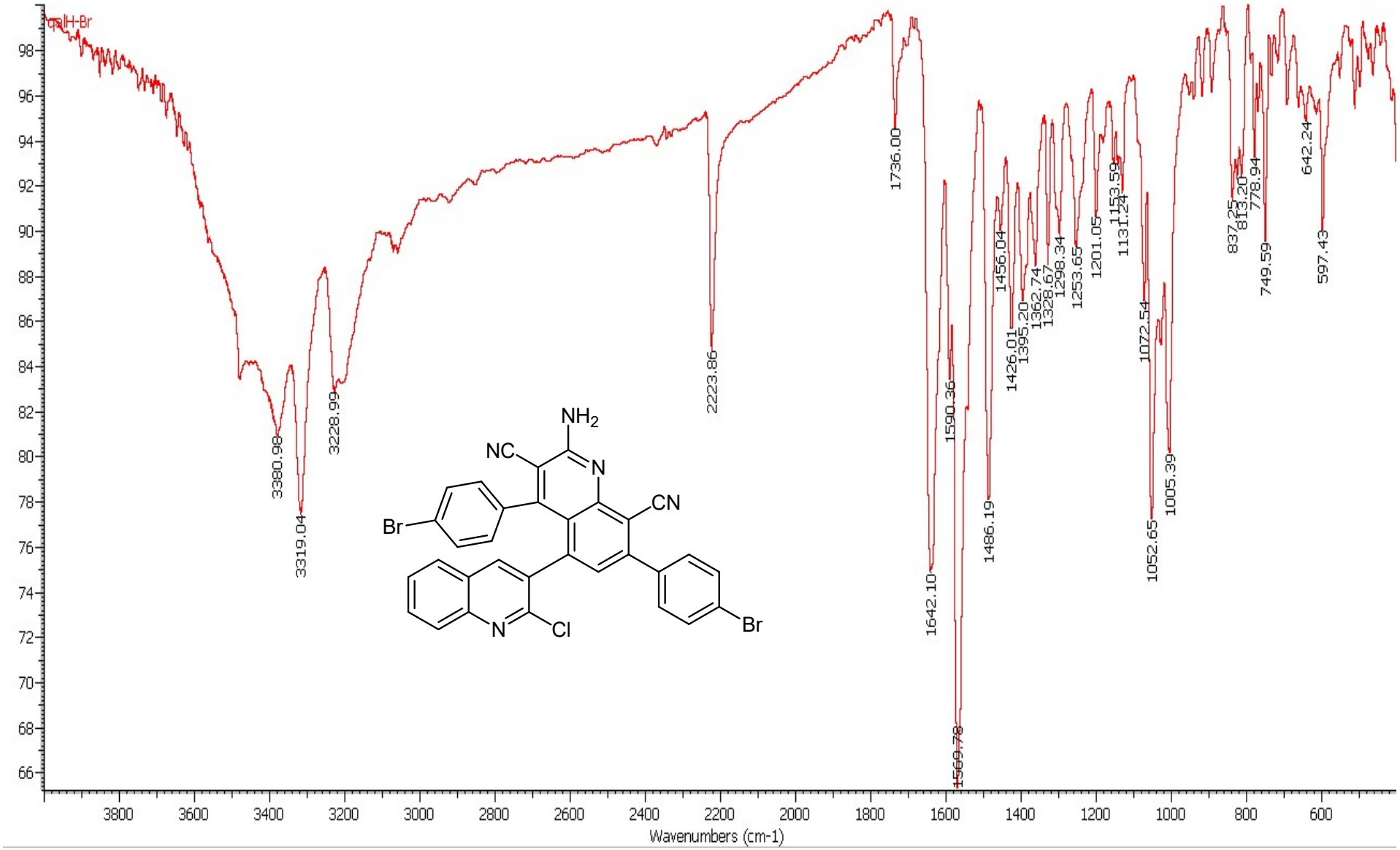
^{13}C NMR spectrum of **3a**



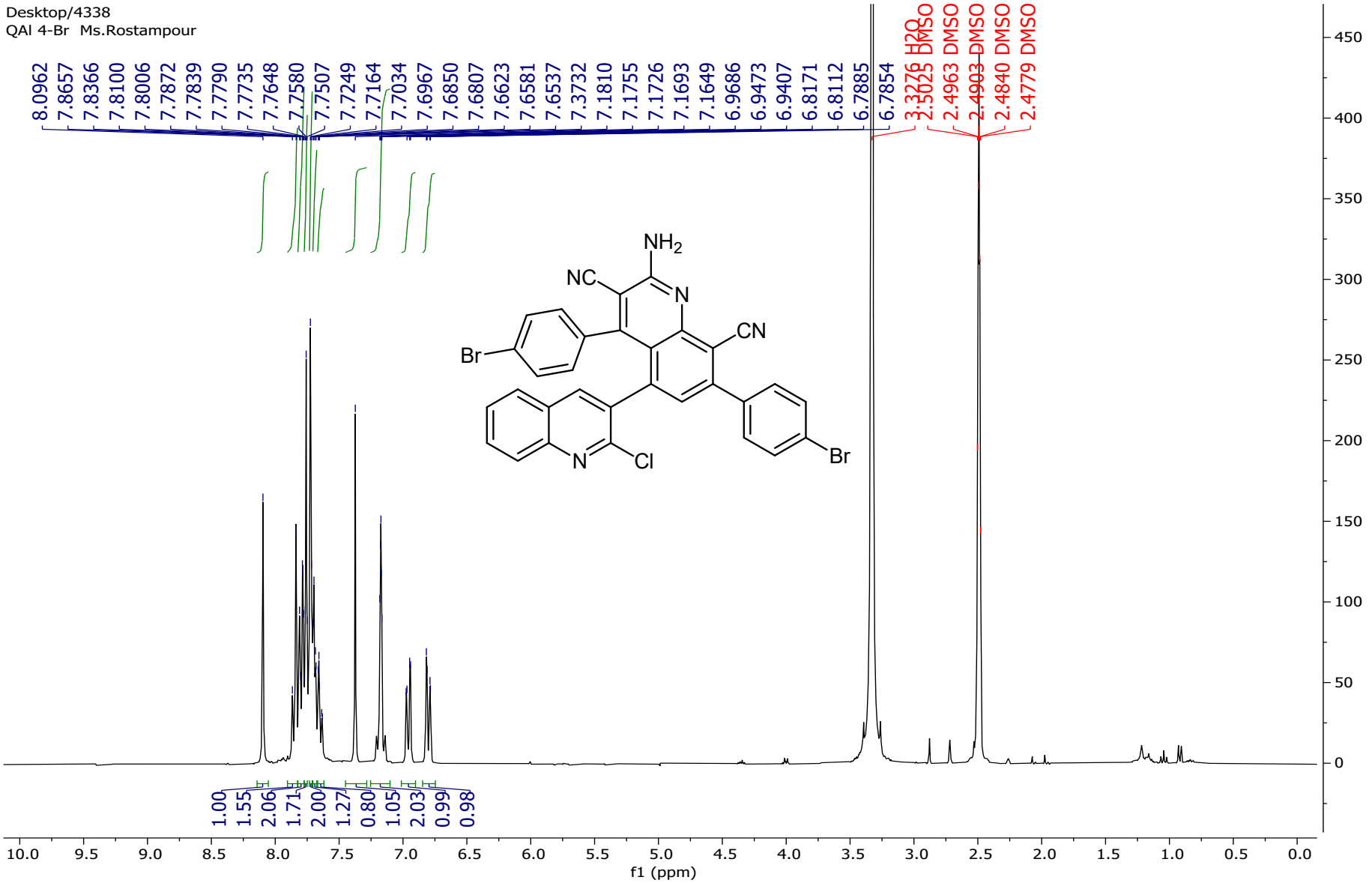
^{13}C NMR spectrum of **3a**



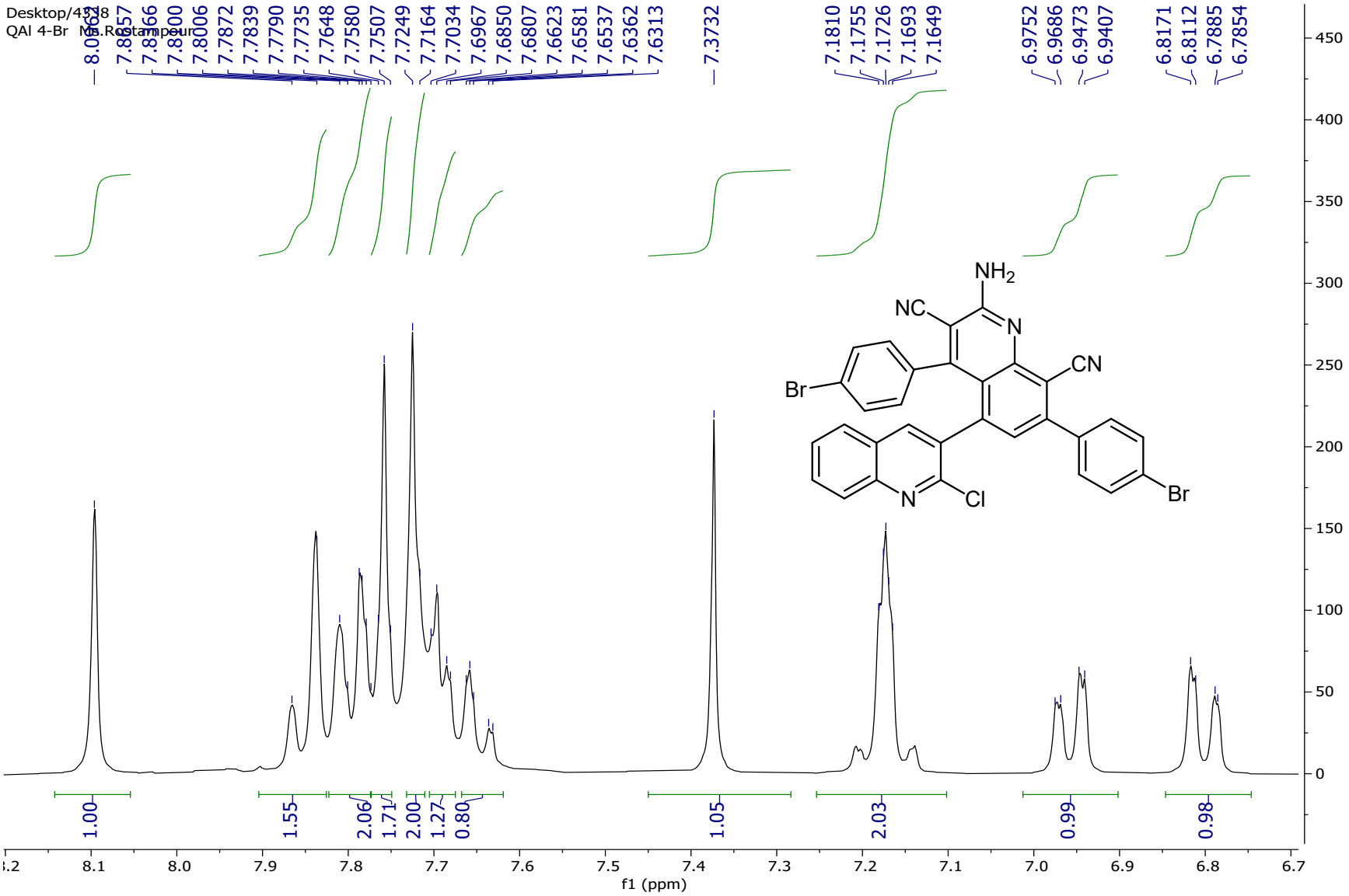
Mass Spectrum of **3a**



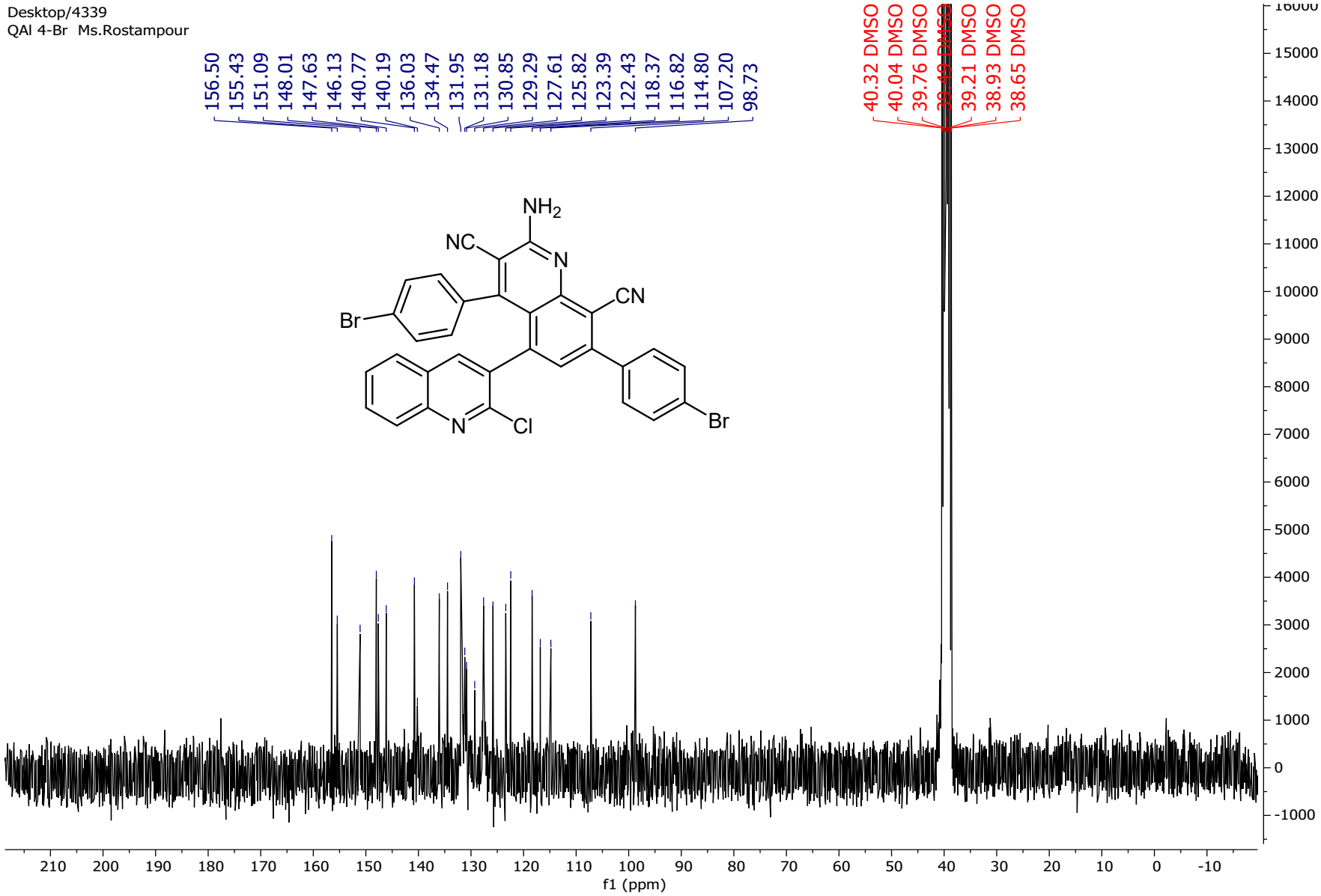
IR Spectrum of **3b**



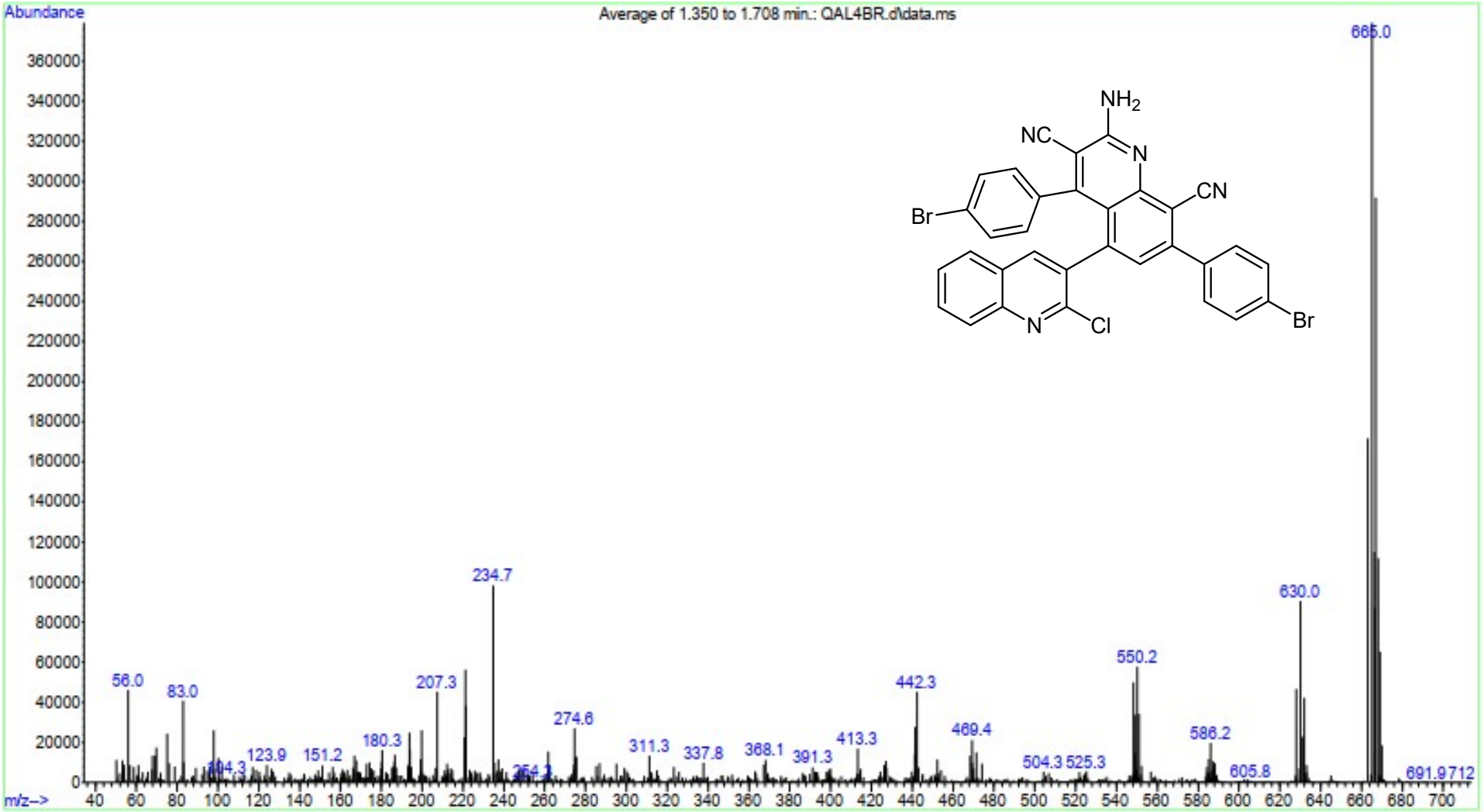
^{1}H NMR Spectrum of **3b**



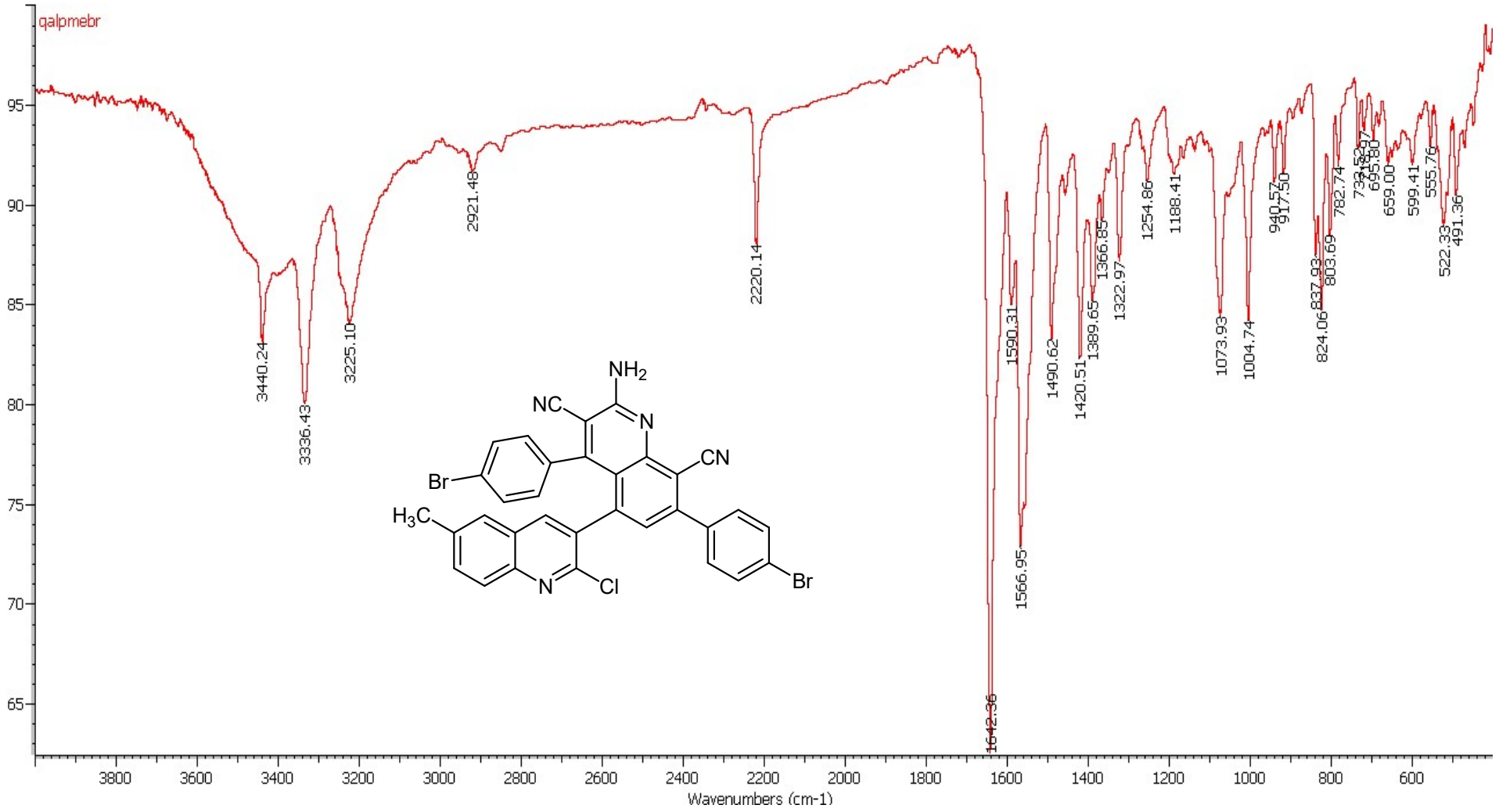
^{1}H NMR Spectrum of **3b**



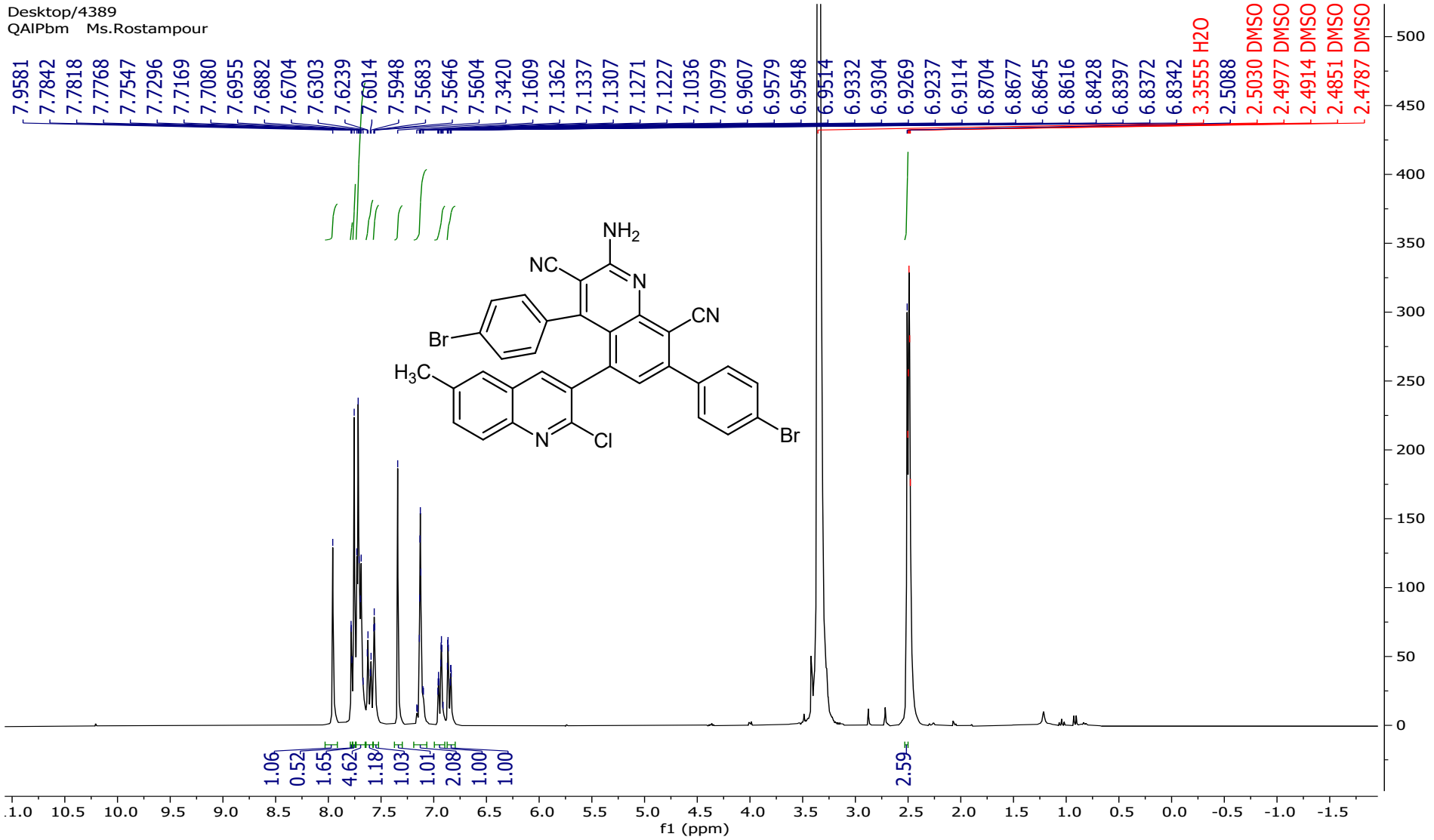
^{13}C NMR Spectrum of **3b**



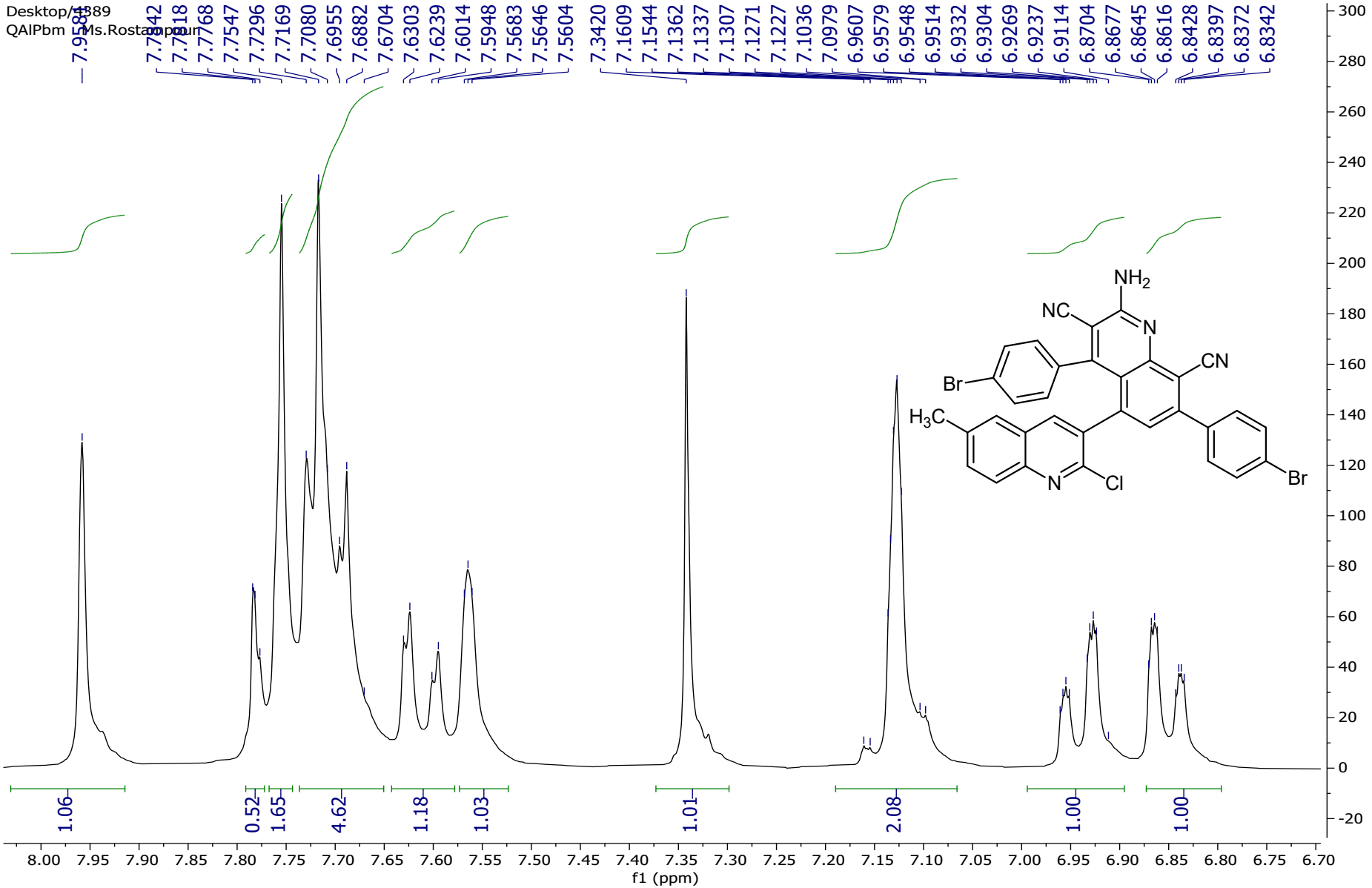
Mass Spectrum of **3b**



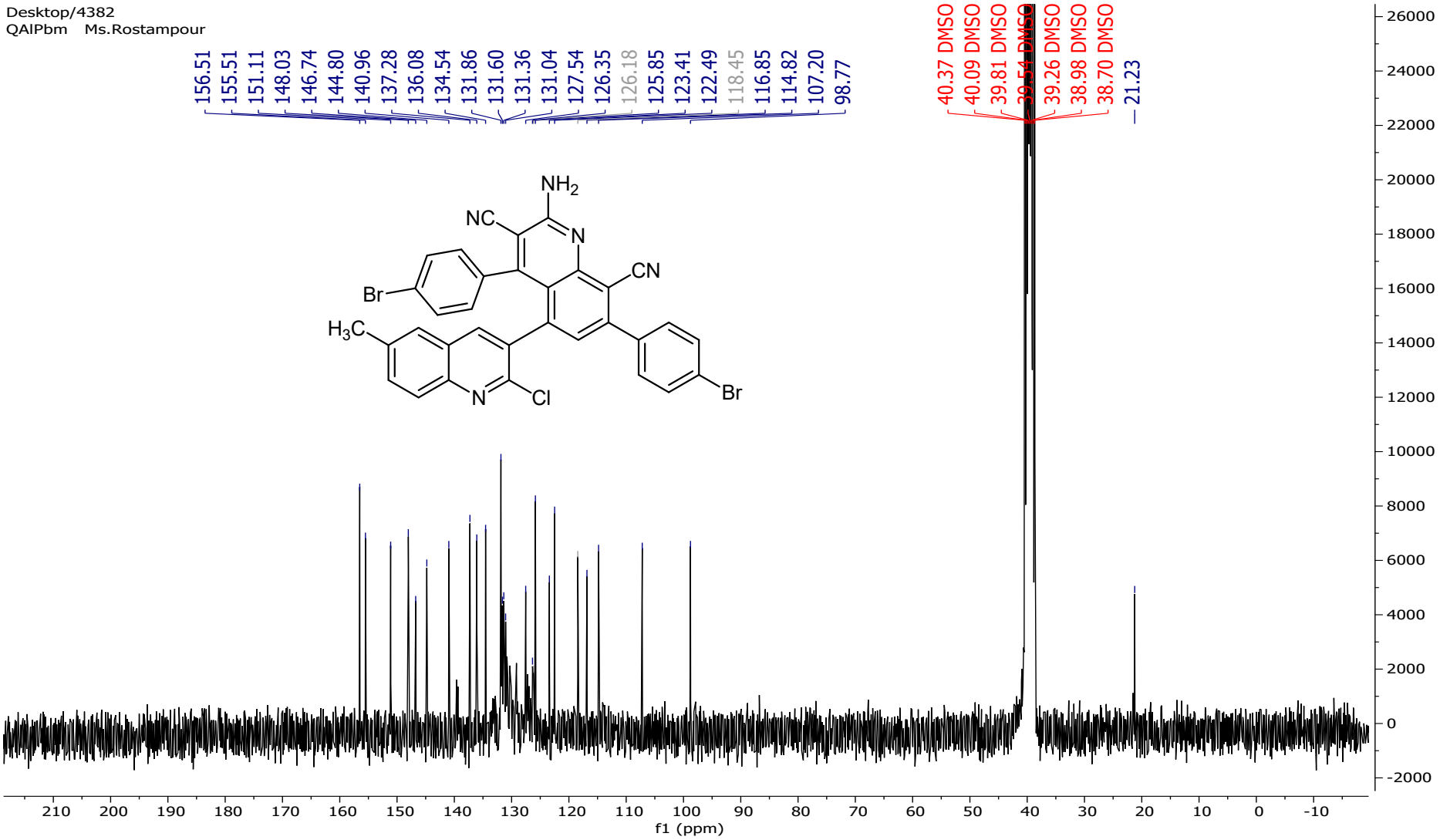
IR Spectrum of **3c**



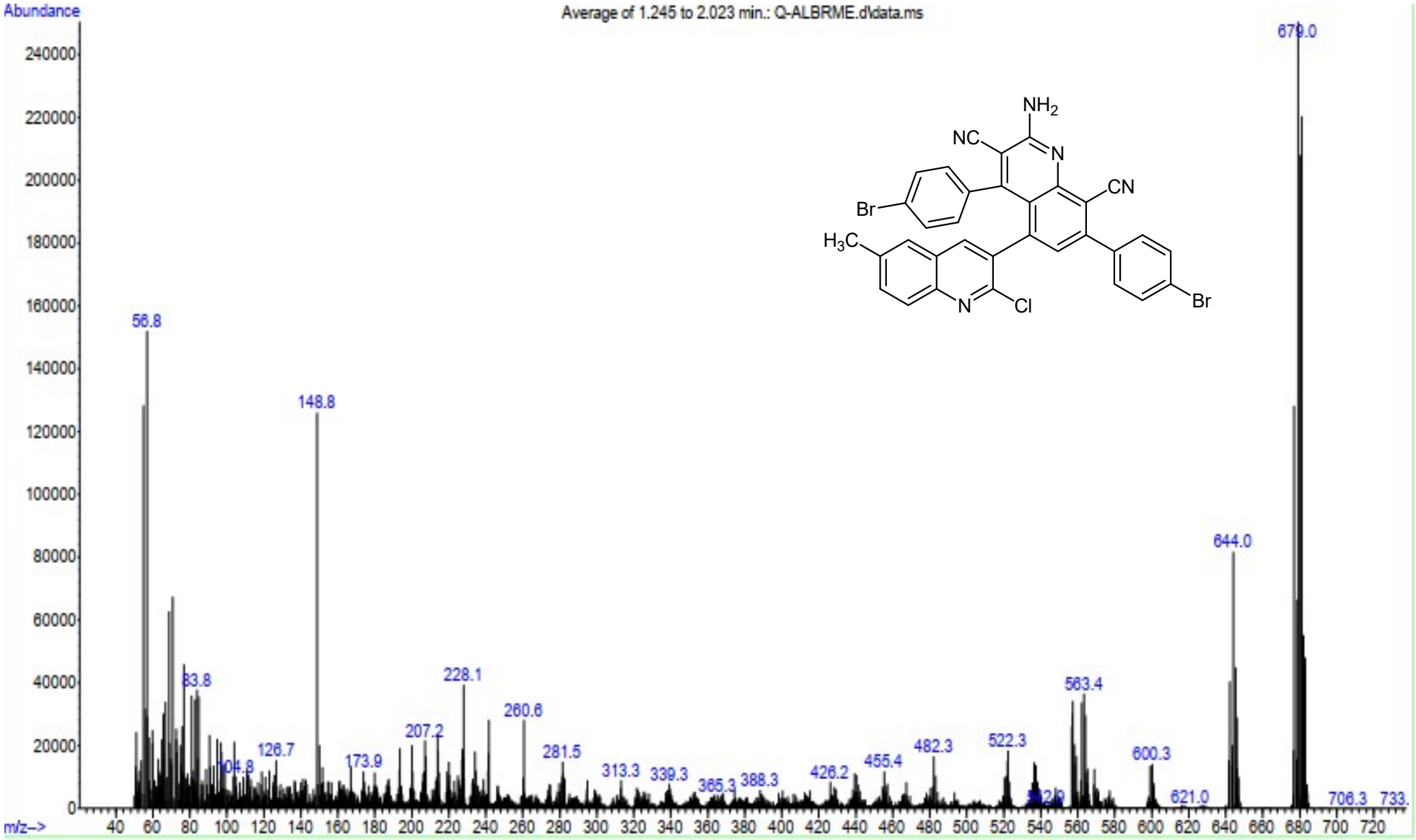
^{1}H NMR Spectrum **3c**



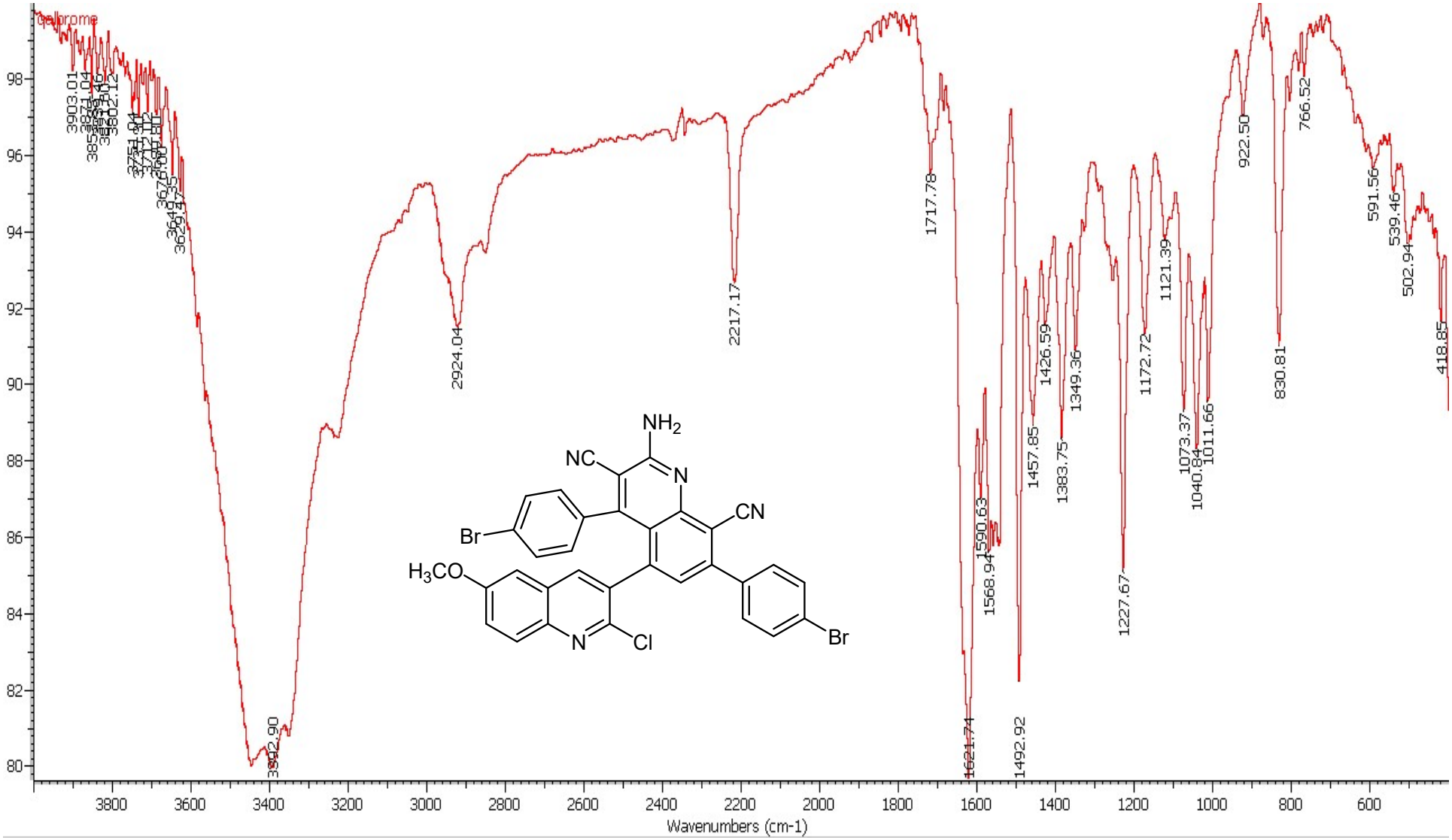
^{1}H NMR Spectrum **3c**



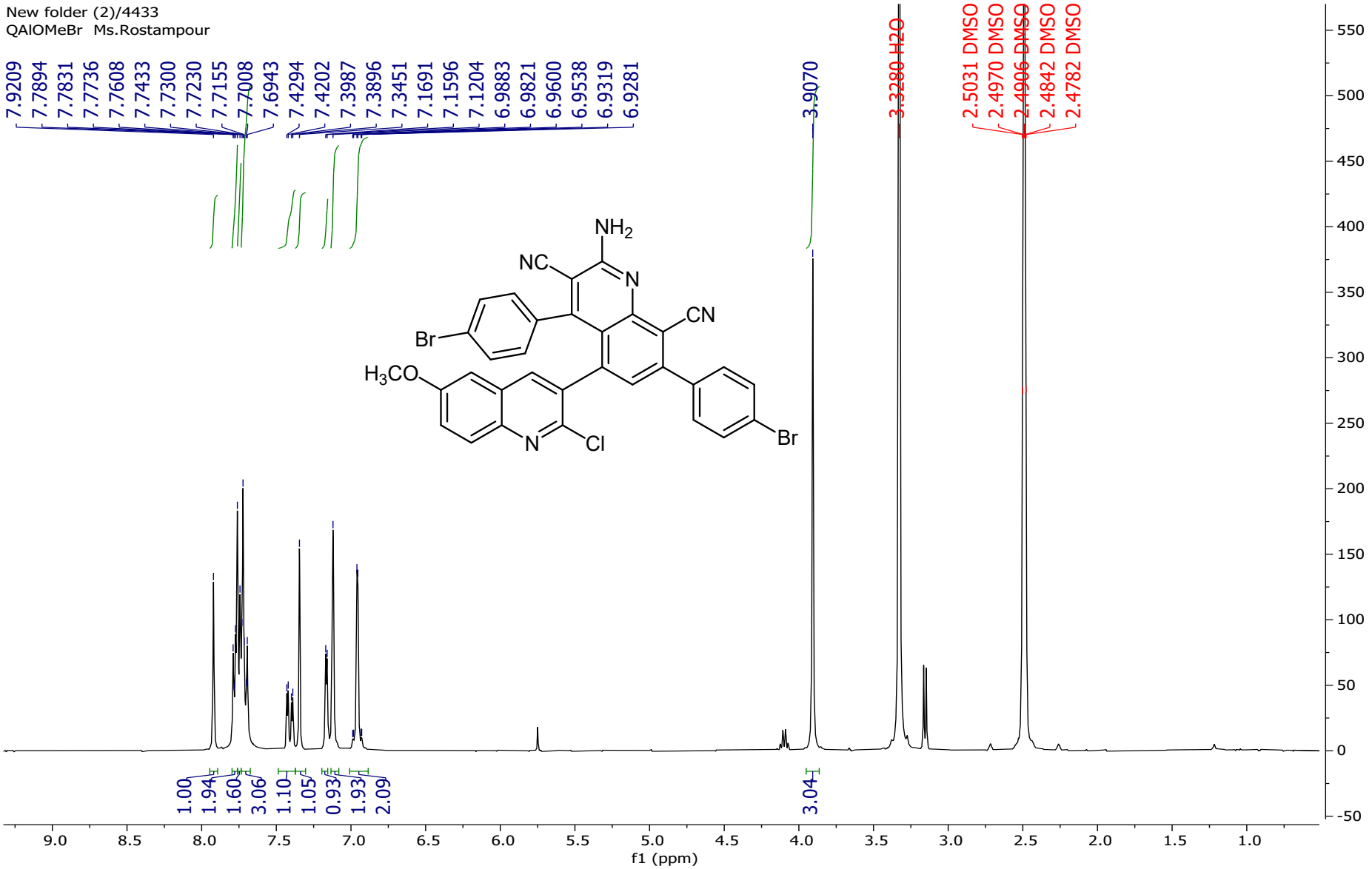
^{13}C NMR Spectrum **3c**



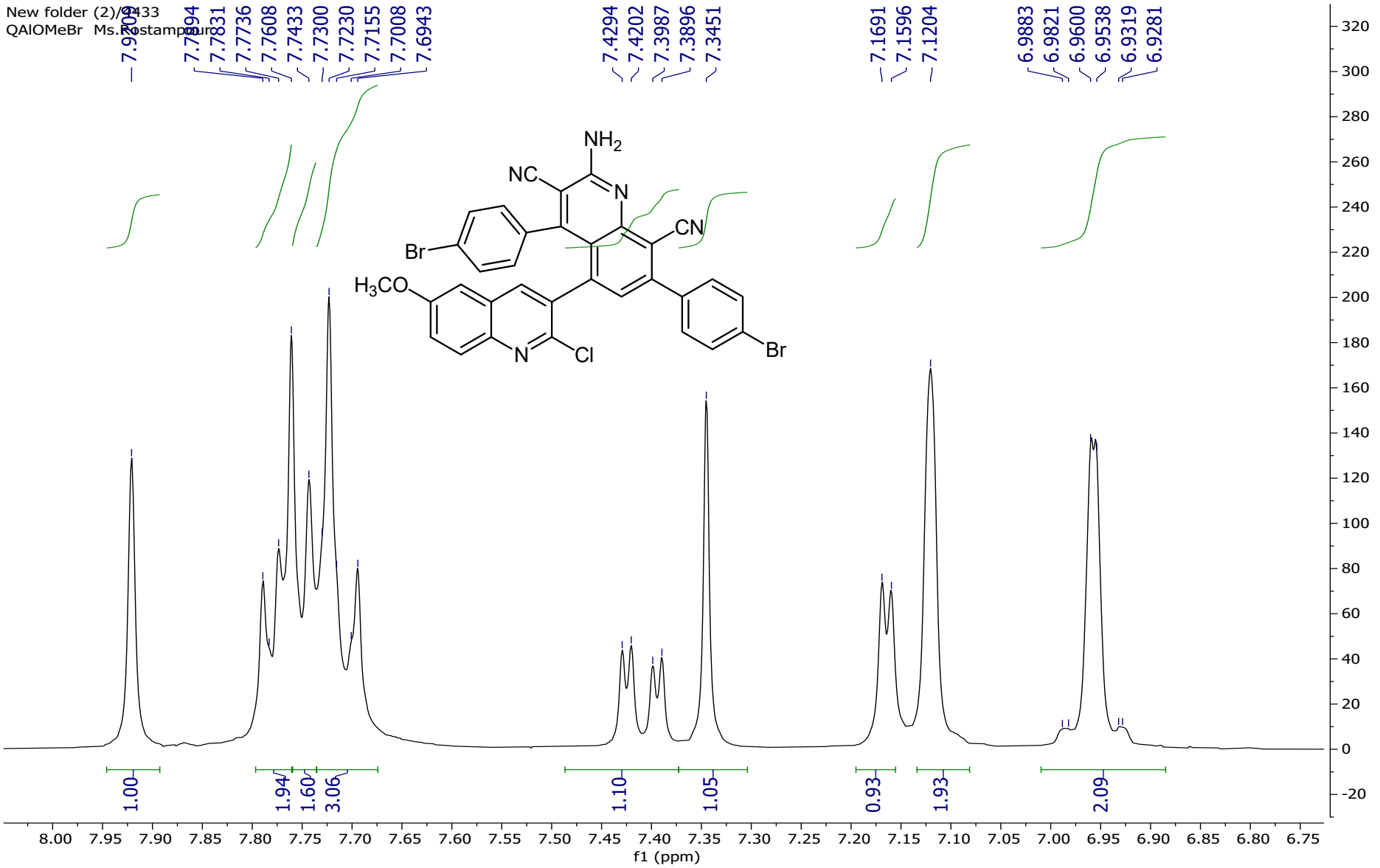
Mass Spectrum of **3c**



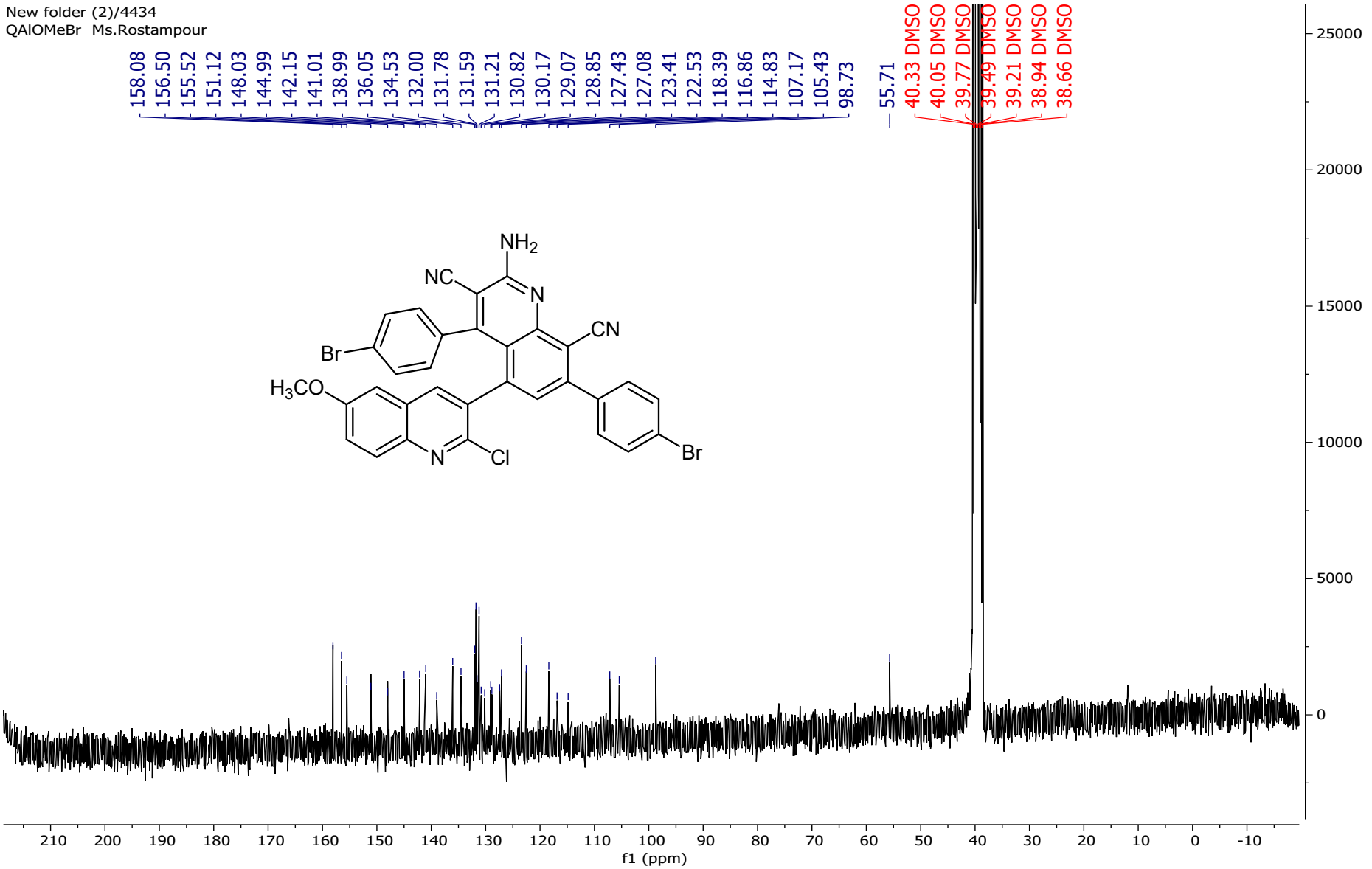
IR Spectrum of **3d**



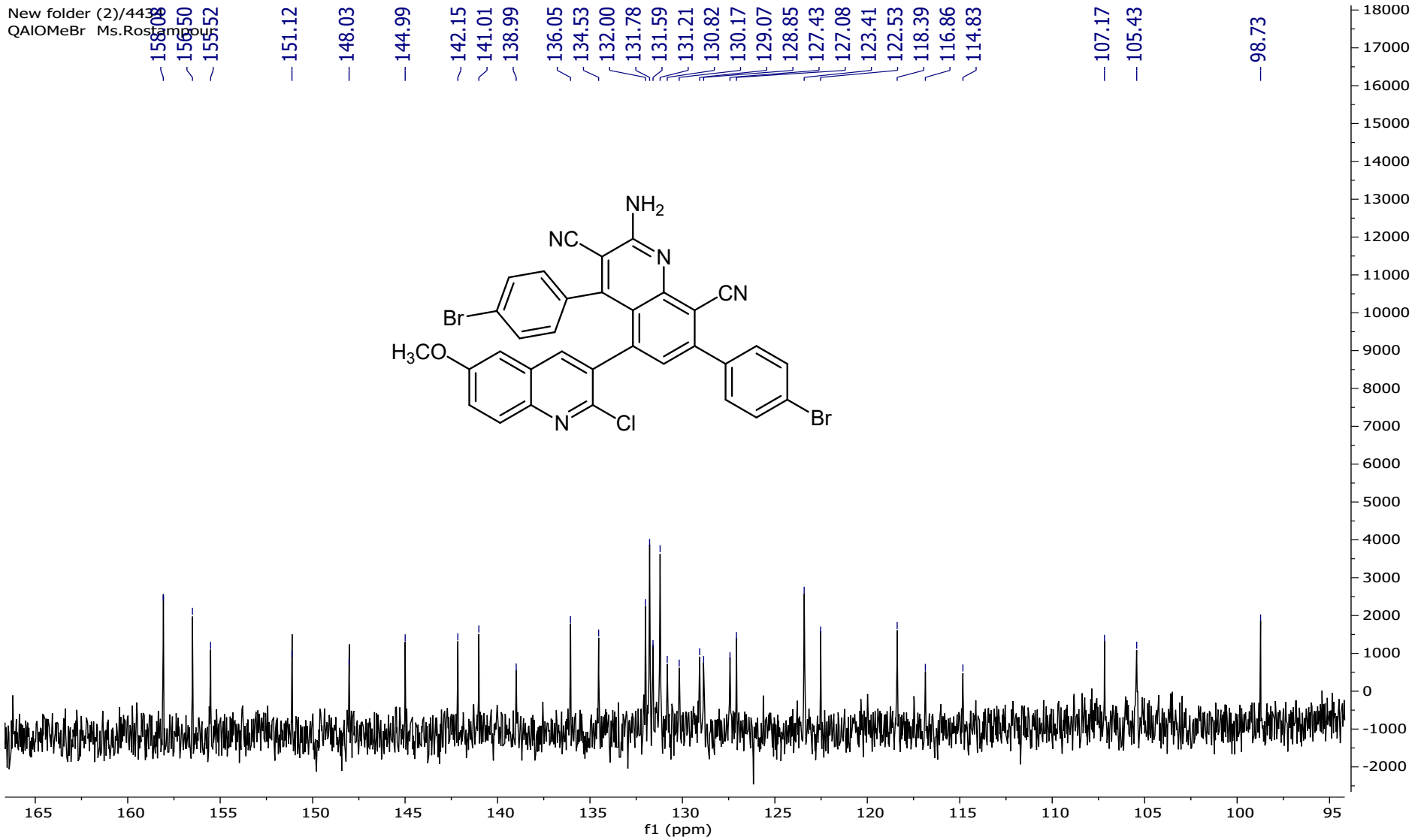
^{1}H NMR Spectrum **3d**



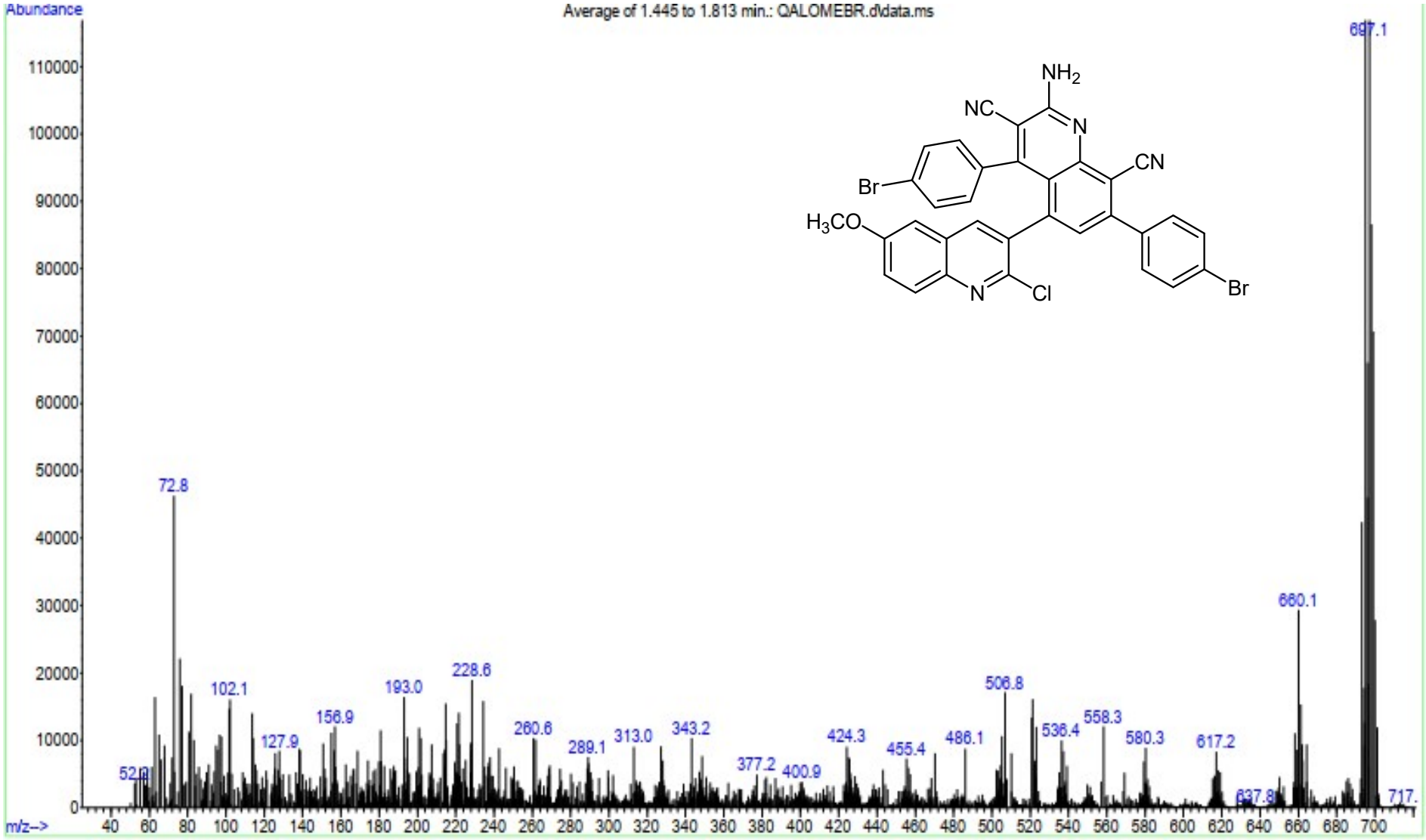
^{1}H NMR Spectrum **3d**



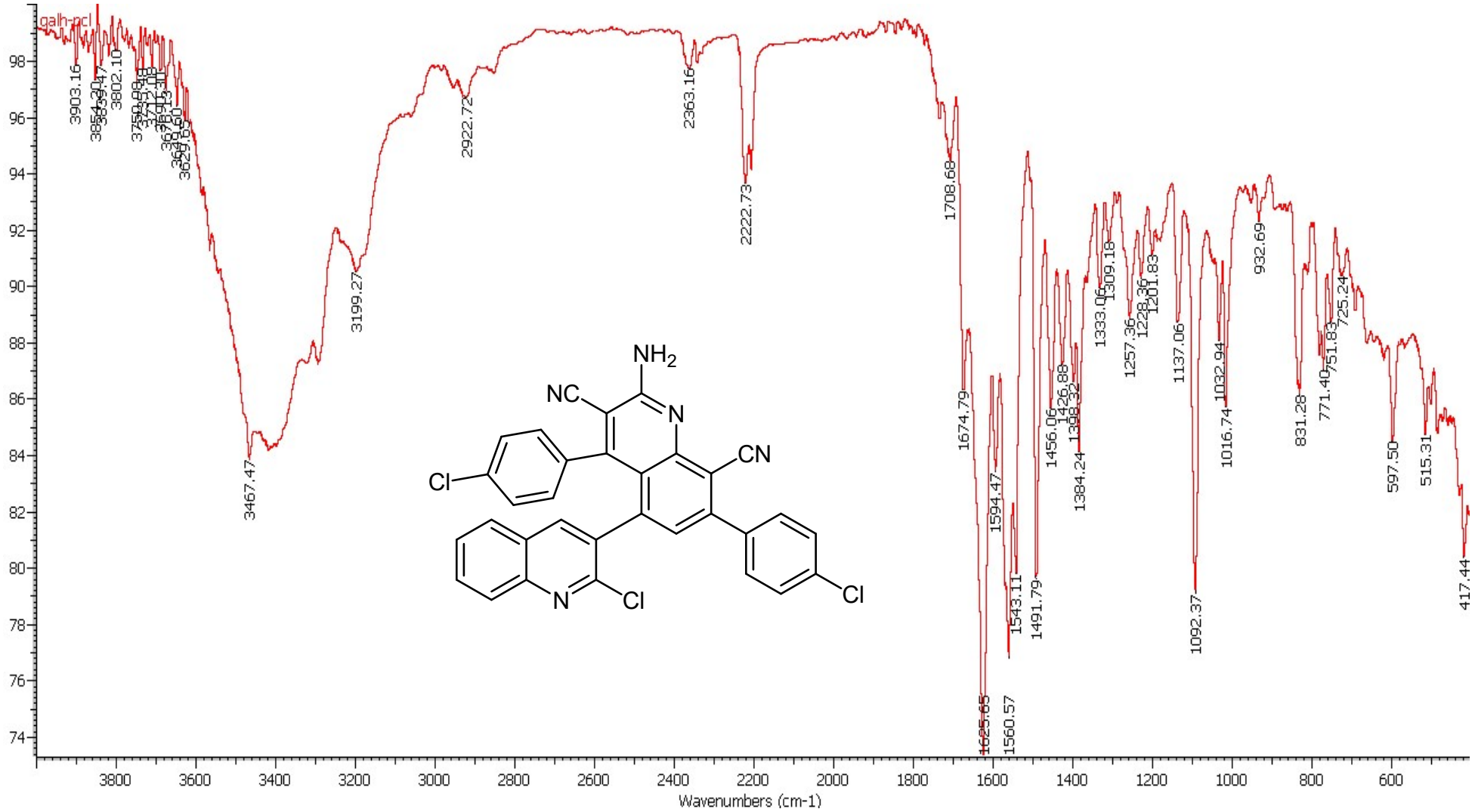
^{13}C NMR Spectrum **3d**



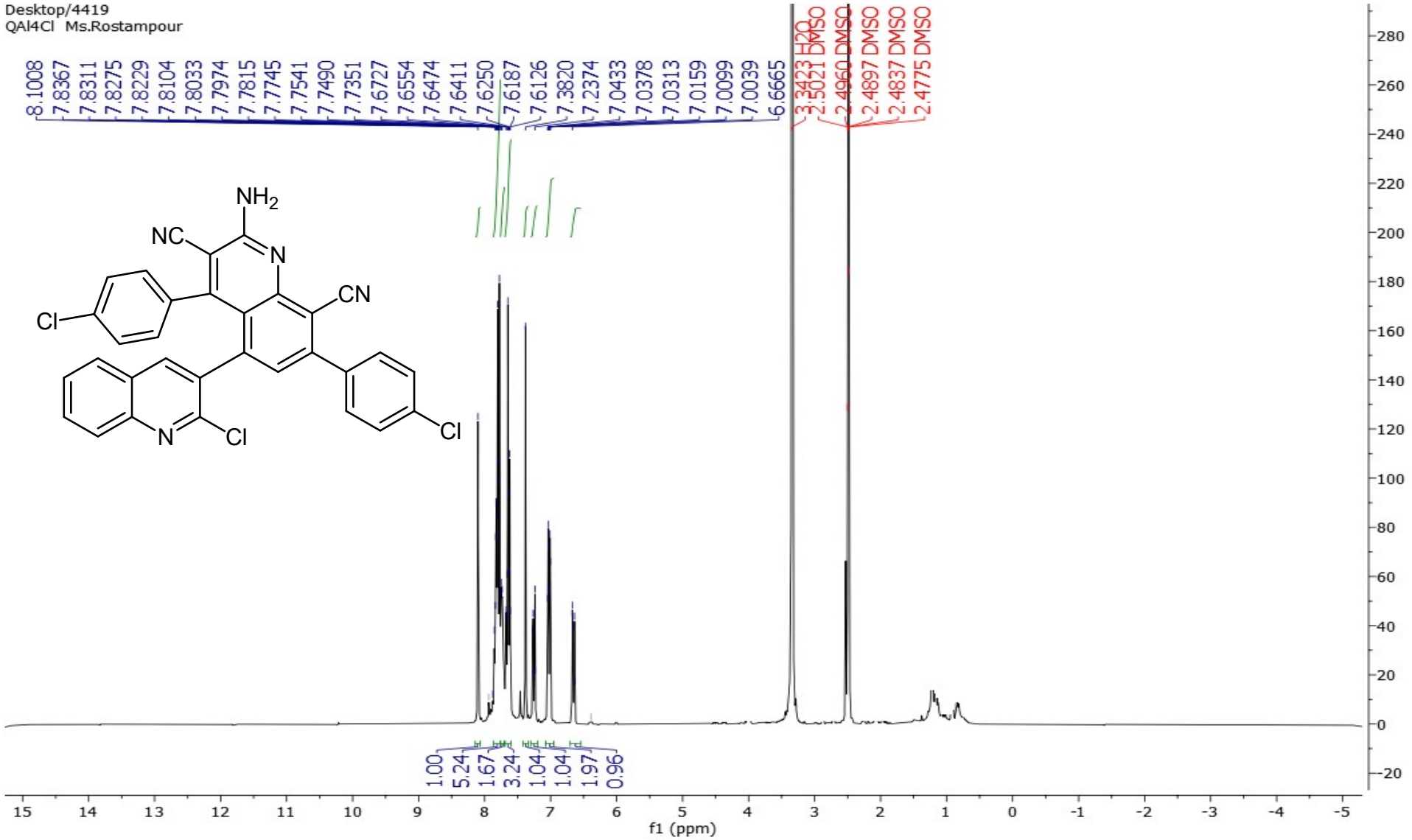
^{13}C NMR Spectrum **3d**



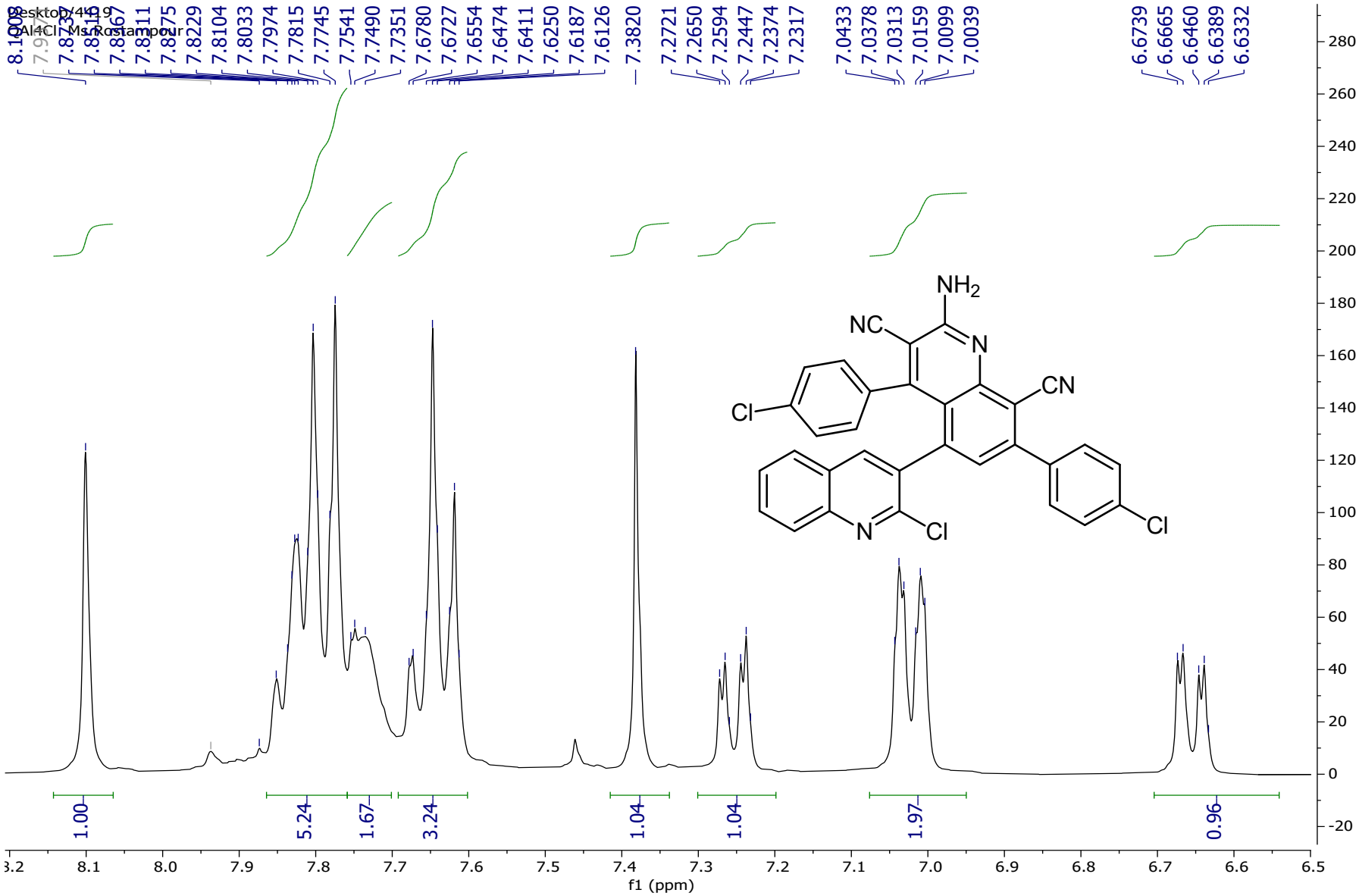
Mass Spectrum of **3d**



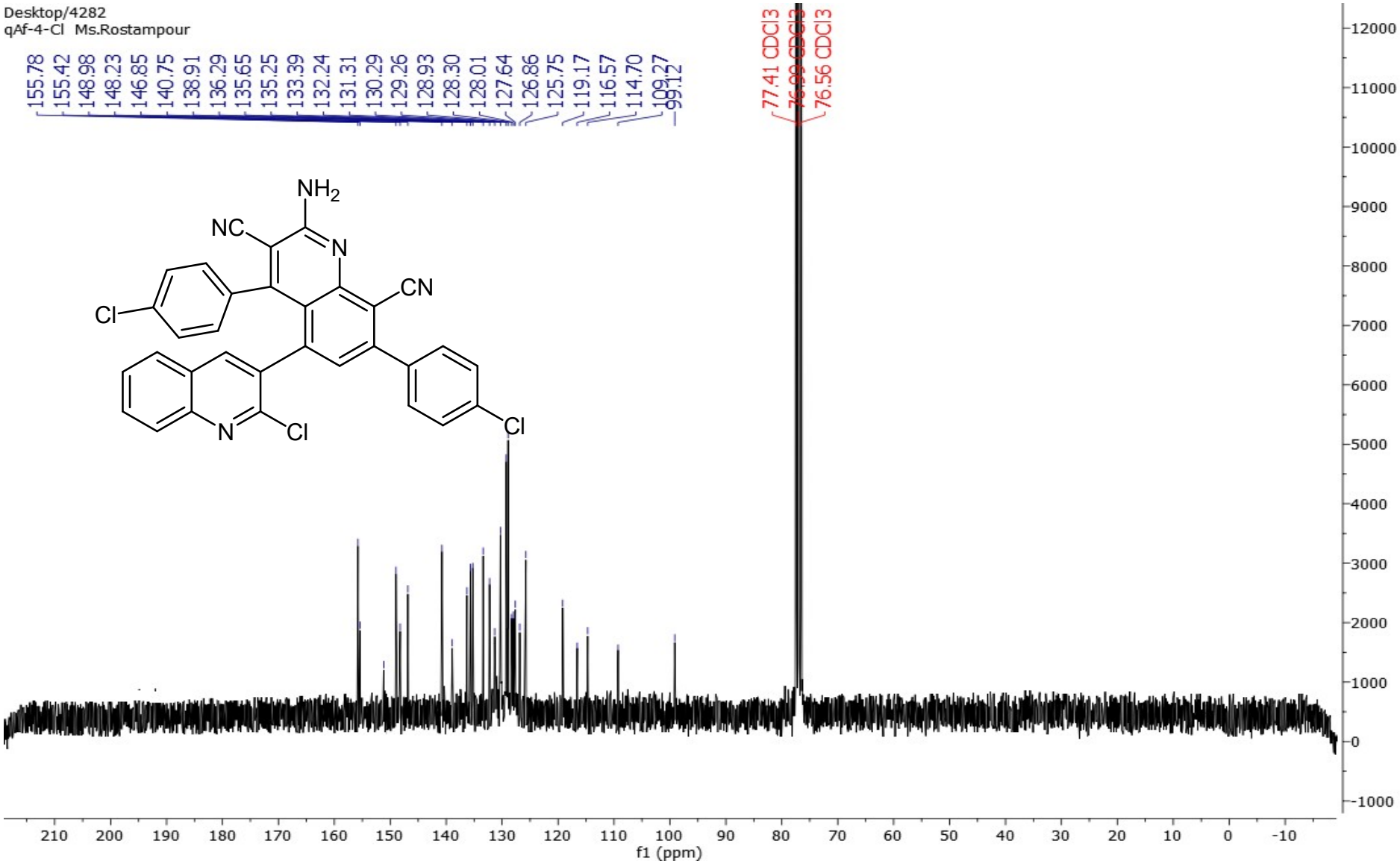
IR Spectrum of **3e**



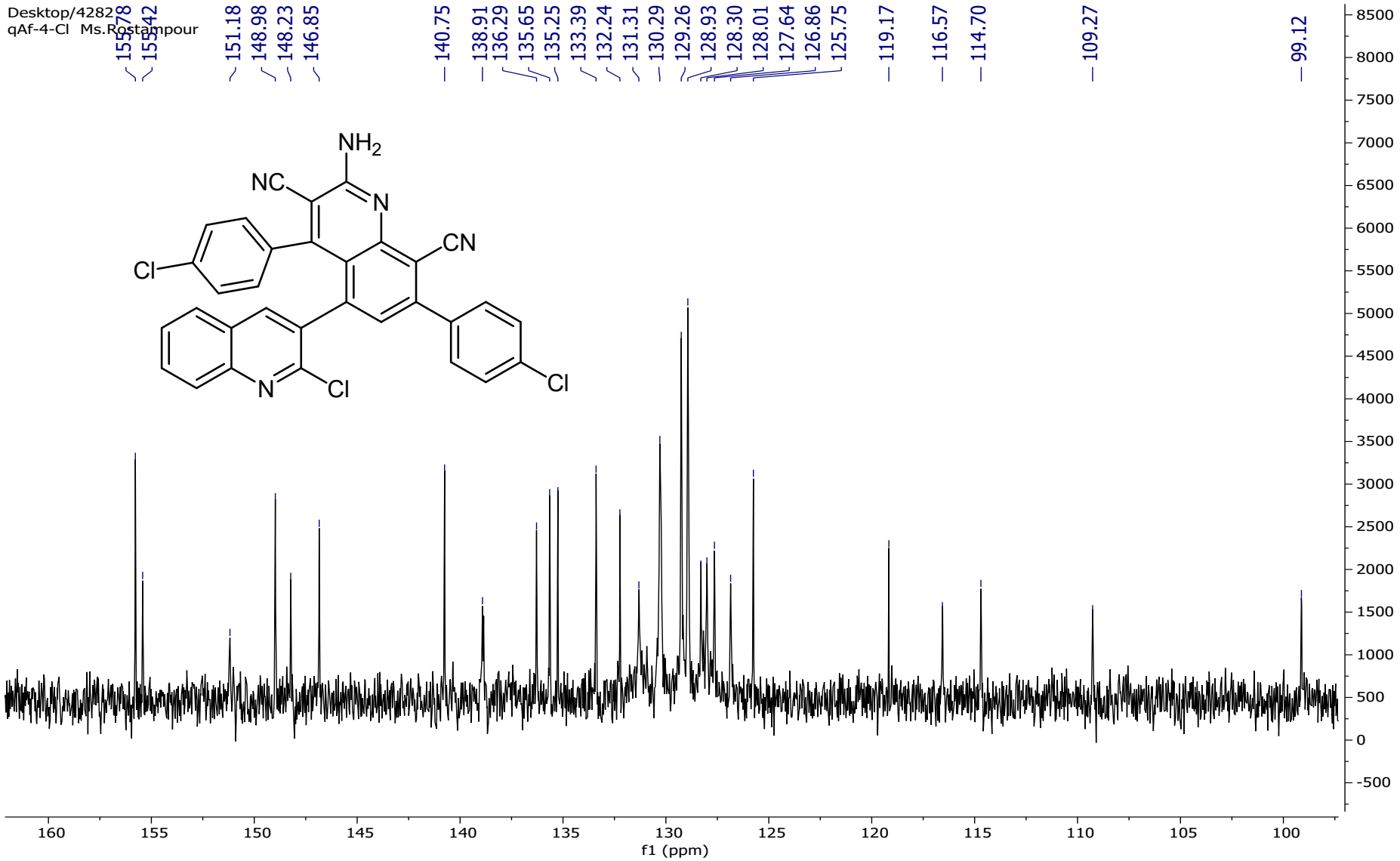
^{1}H NMR Spectrum **3e**



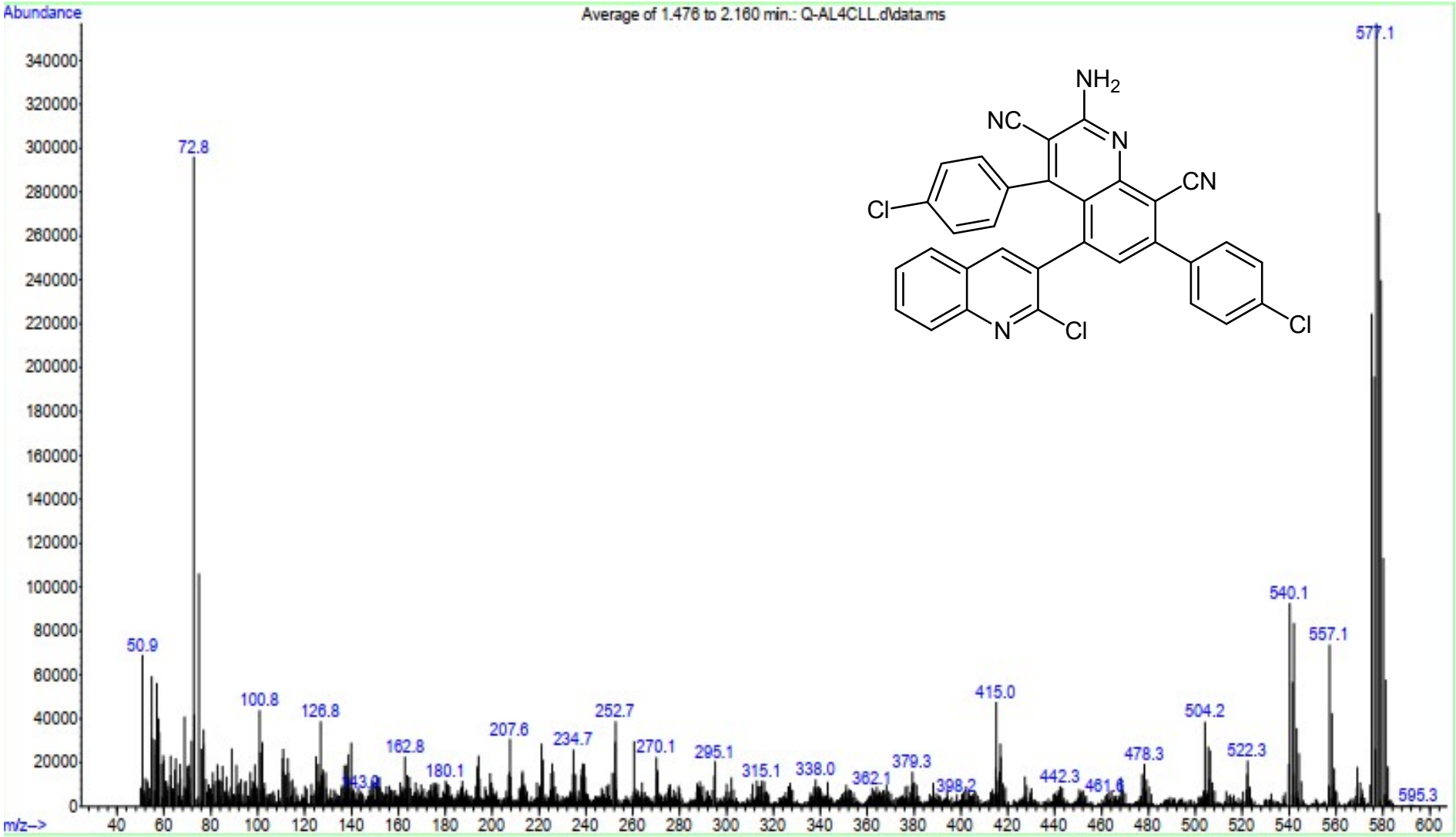
^{1}H NMR Spectrum **3e**



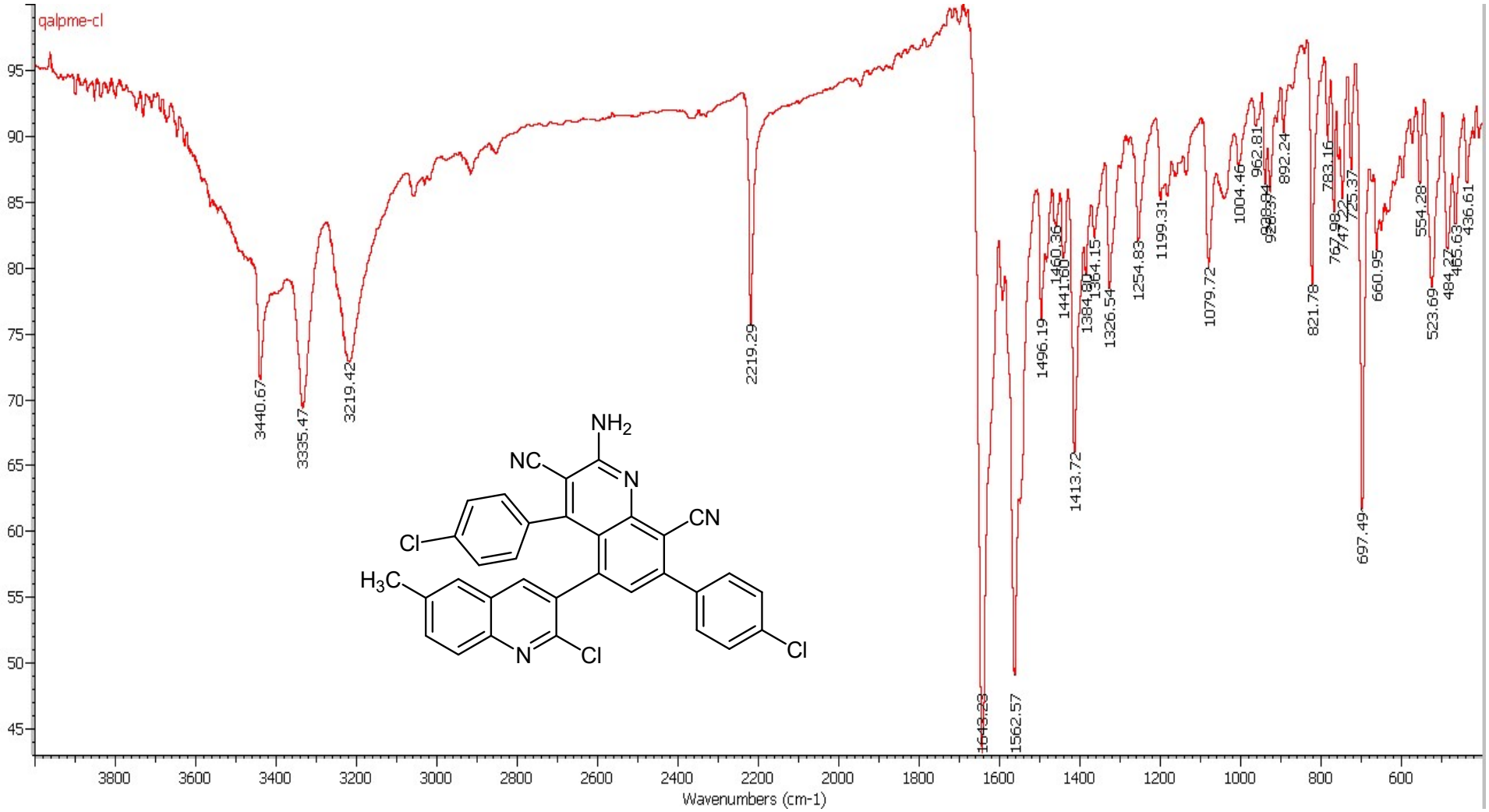
^{13}C NMR Spectrum **3e**



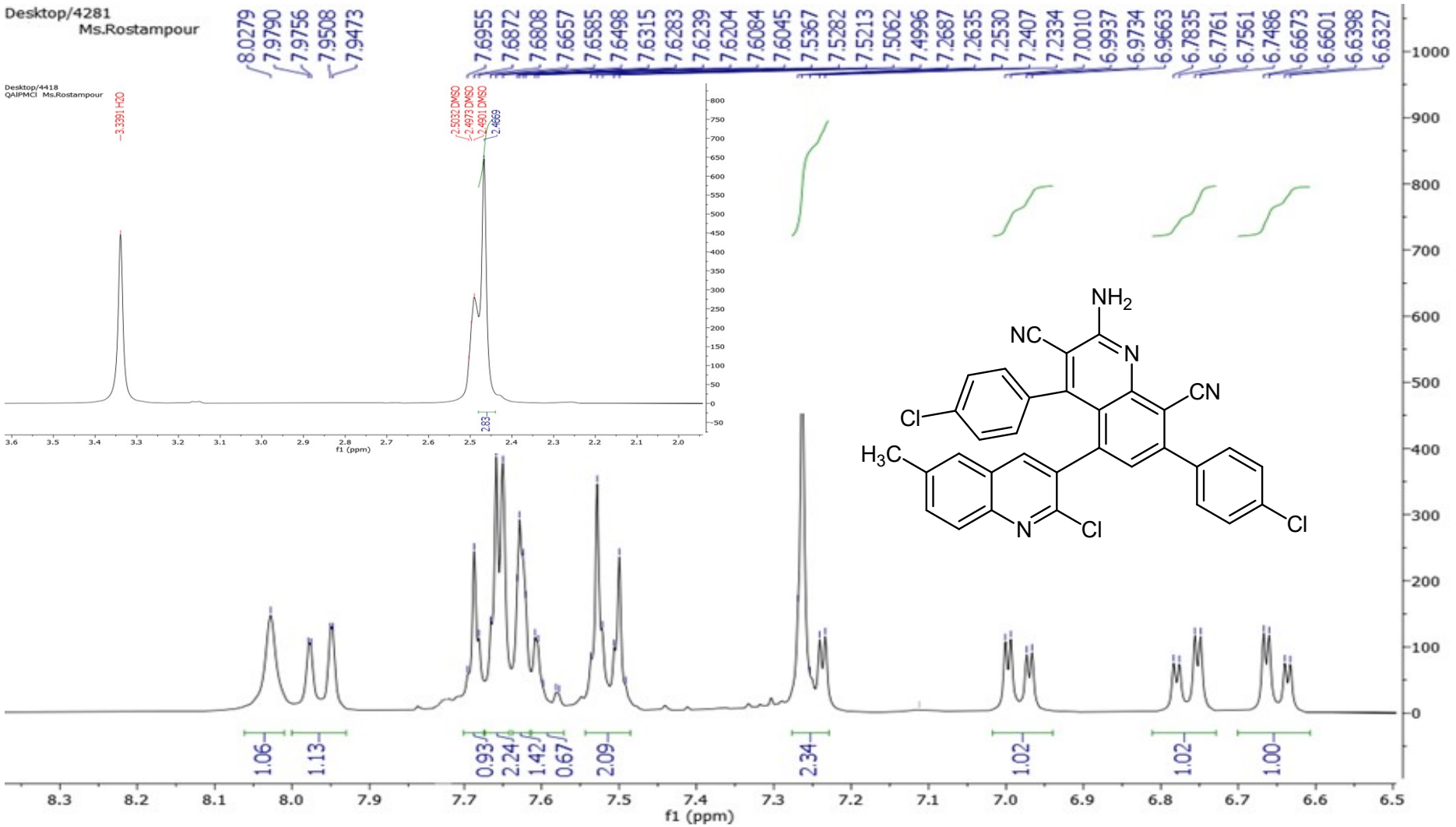
^{13}C NMR Spectrum **3e**



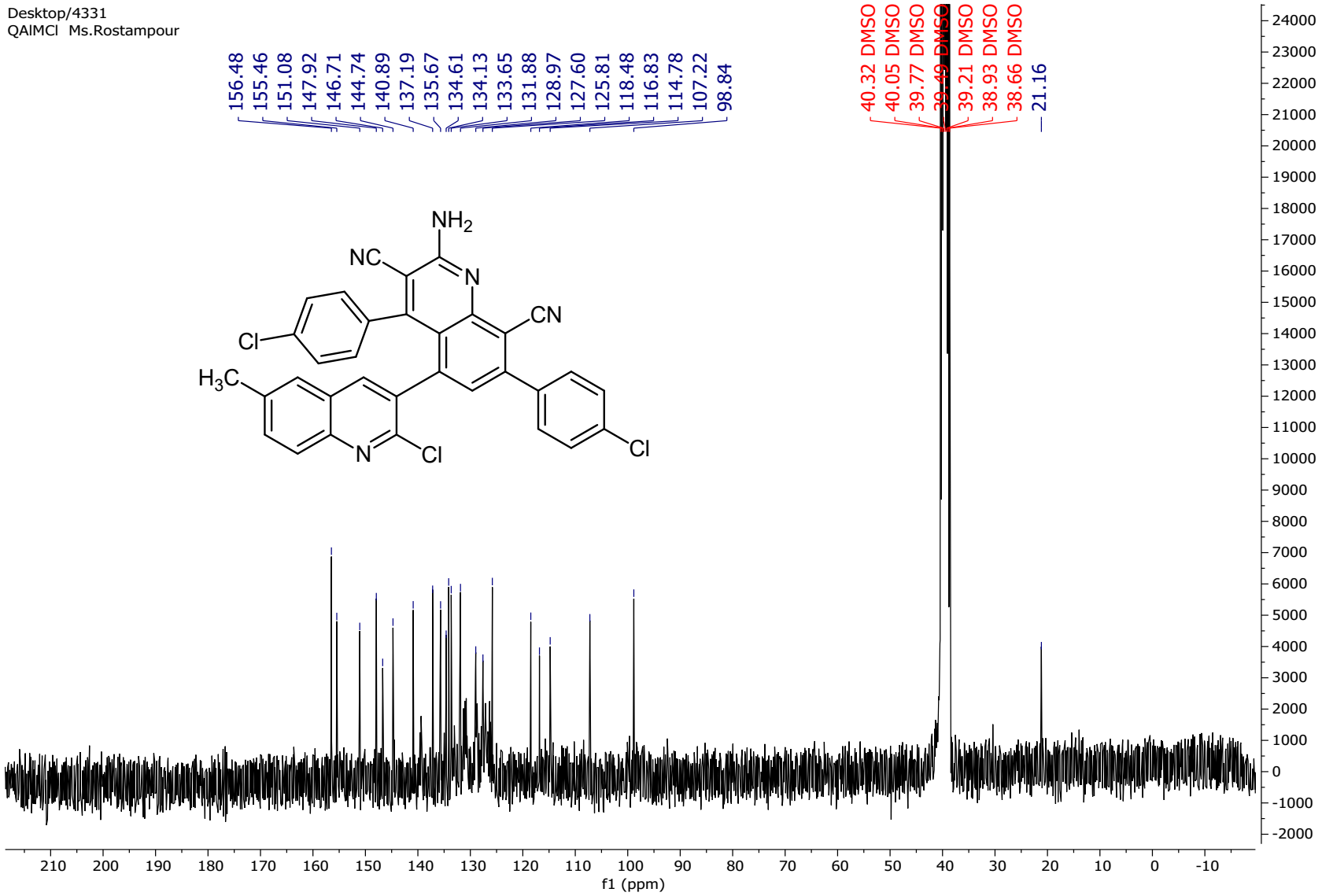
Mass Spectrum of **3e**



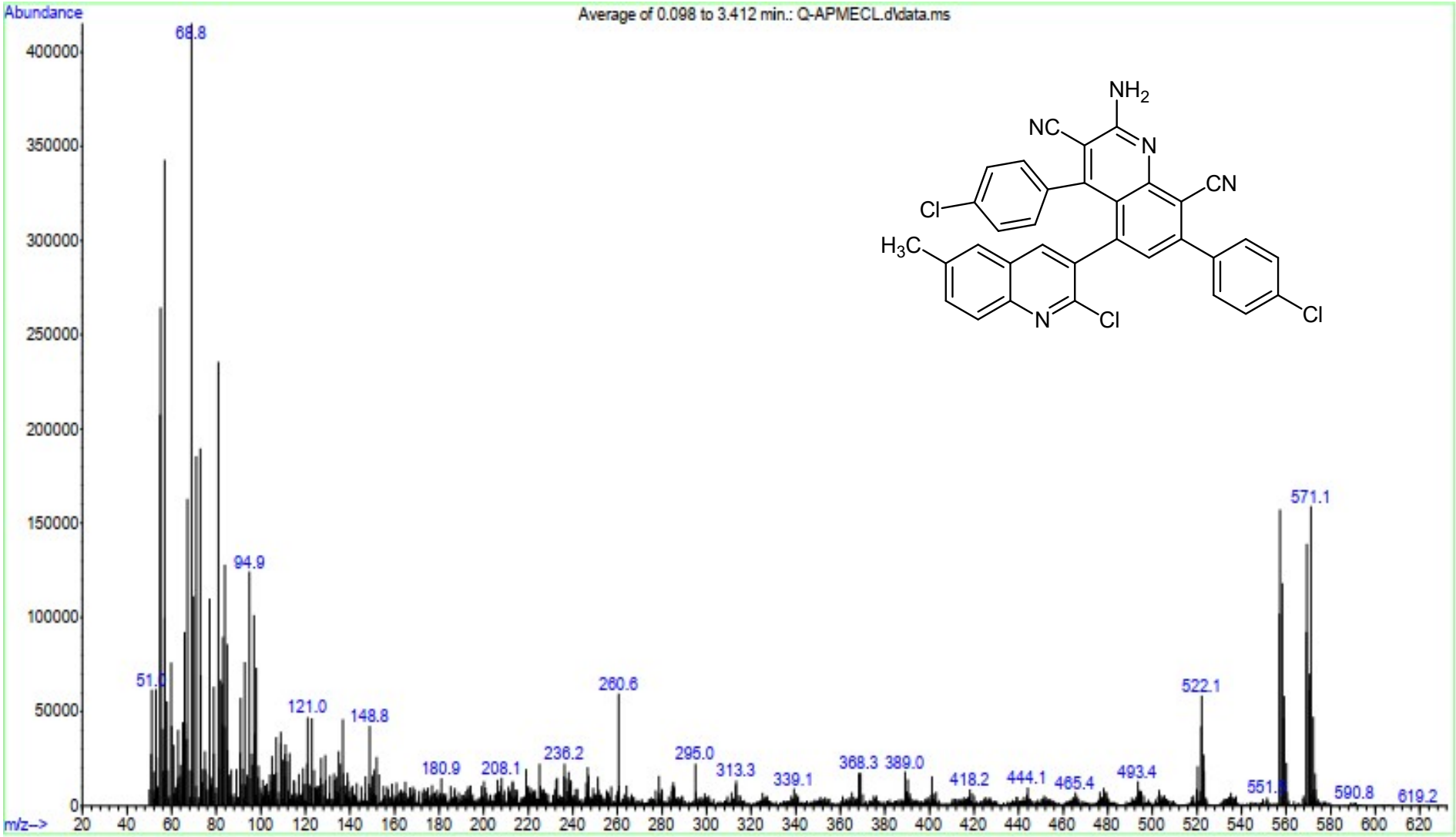
IR Spectrum **3f**



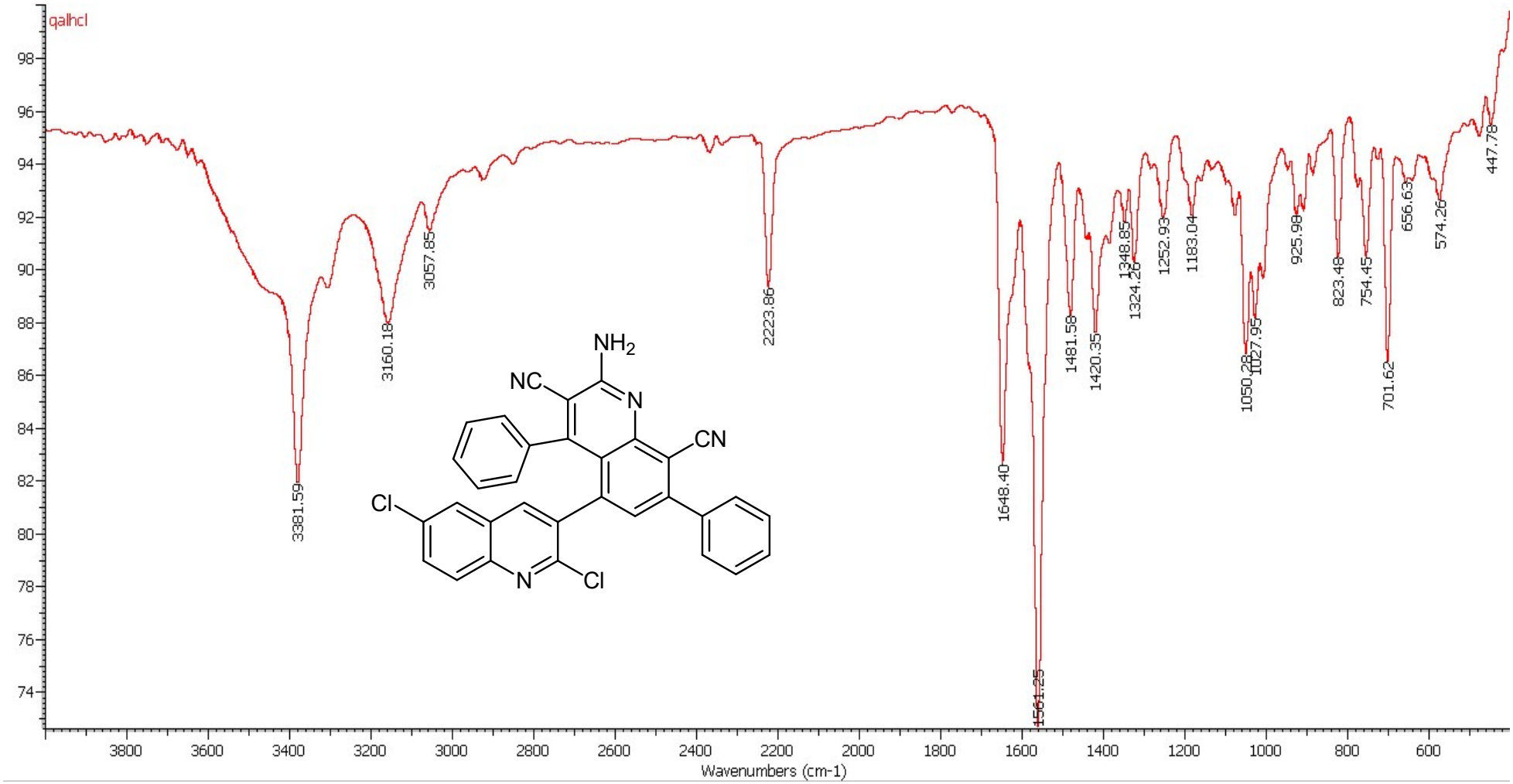
^{1}H NMR Spectrum **3f**



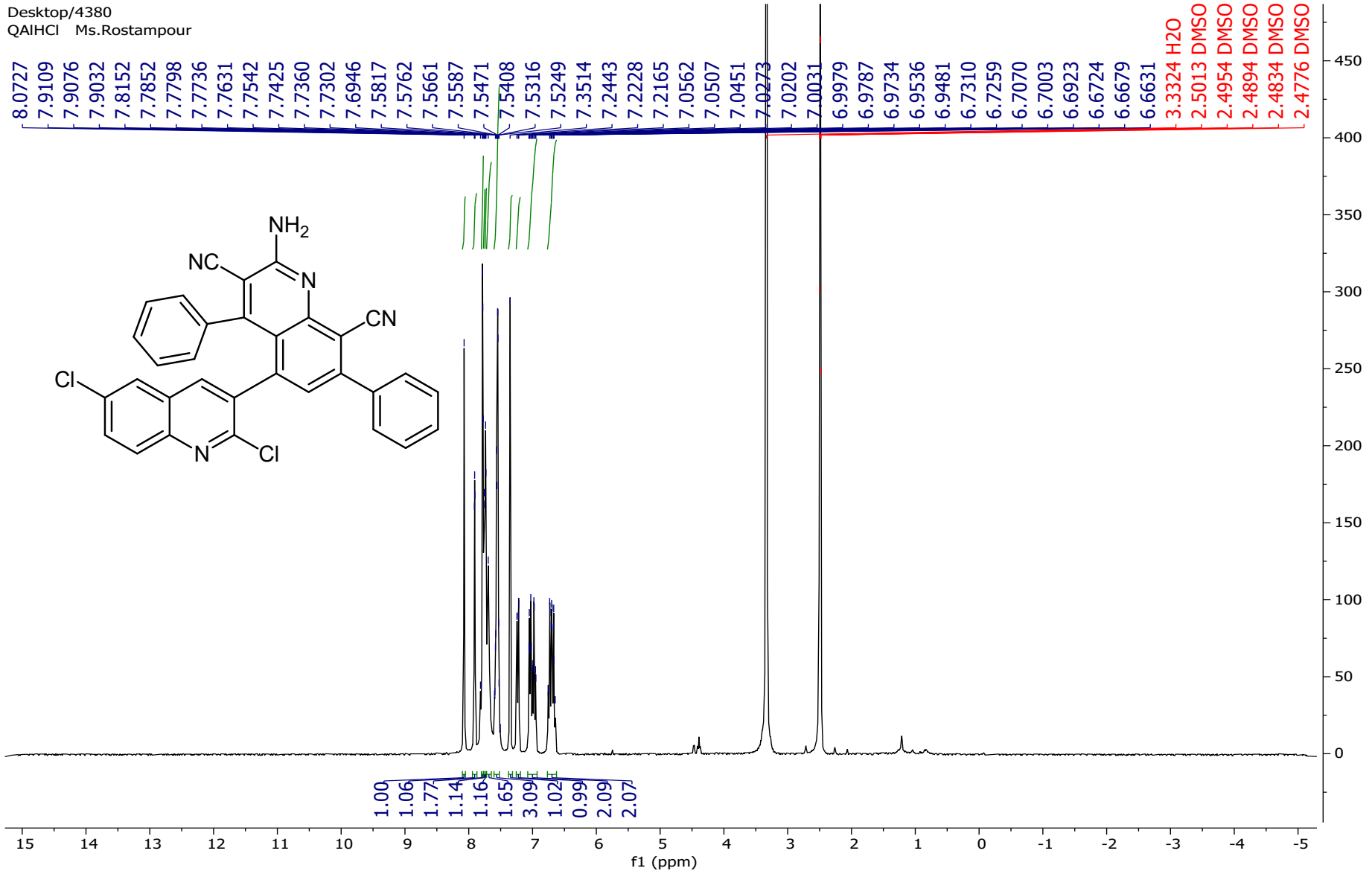
^{13}C NMR Spectrum **3f**



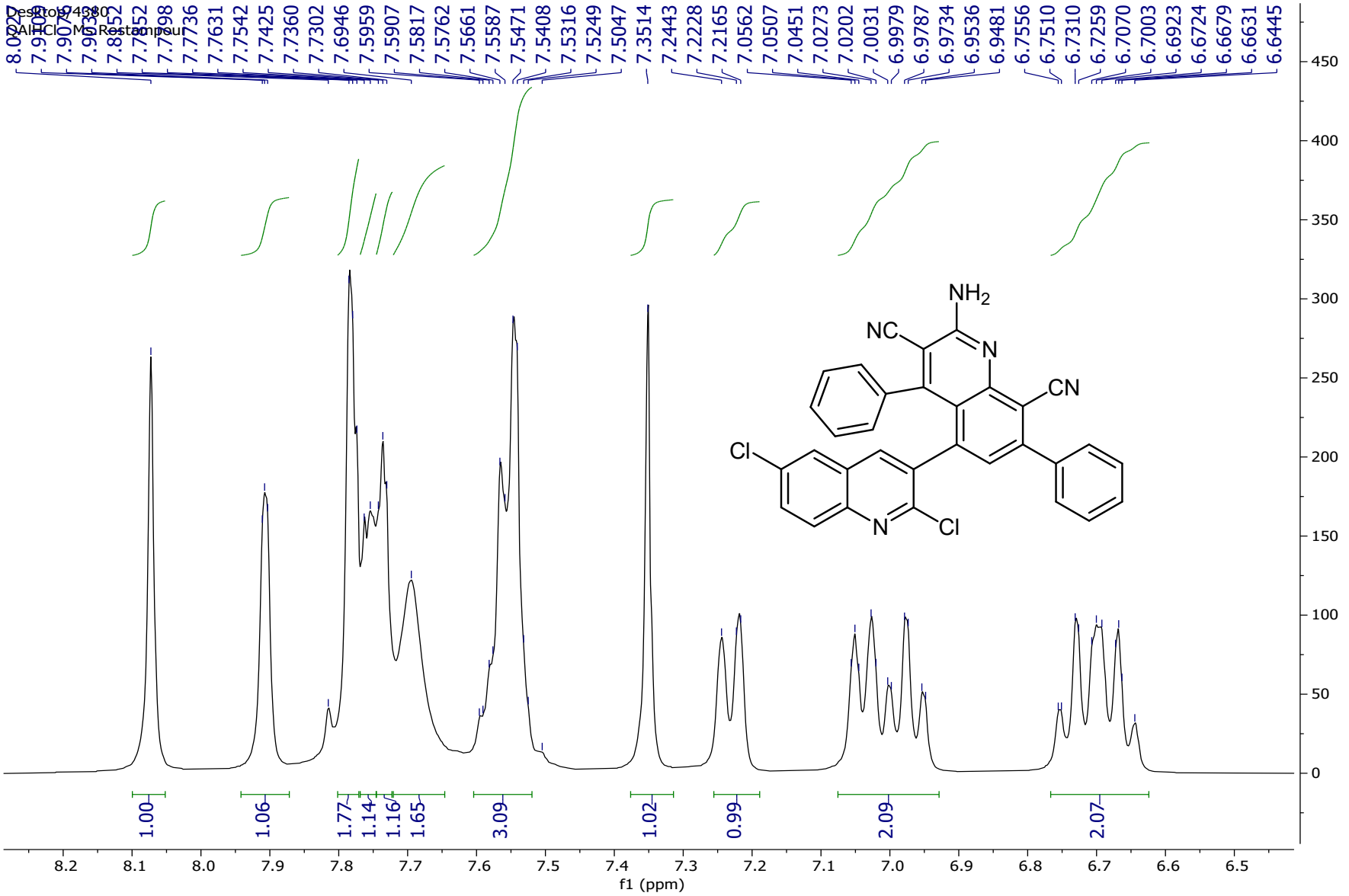
Mass Spectrum **3f**



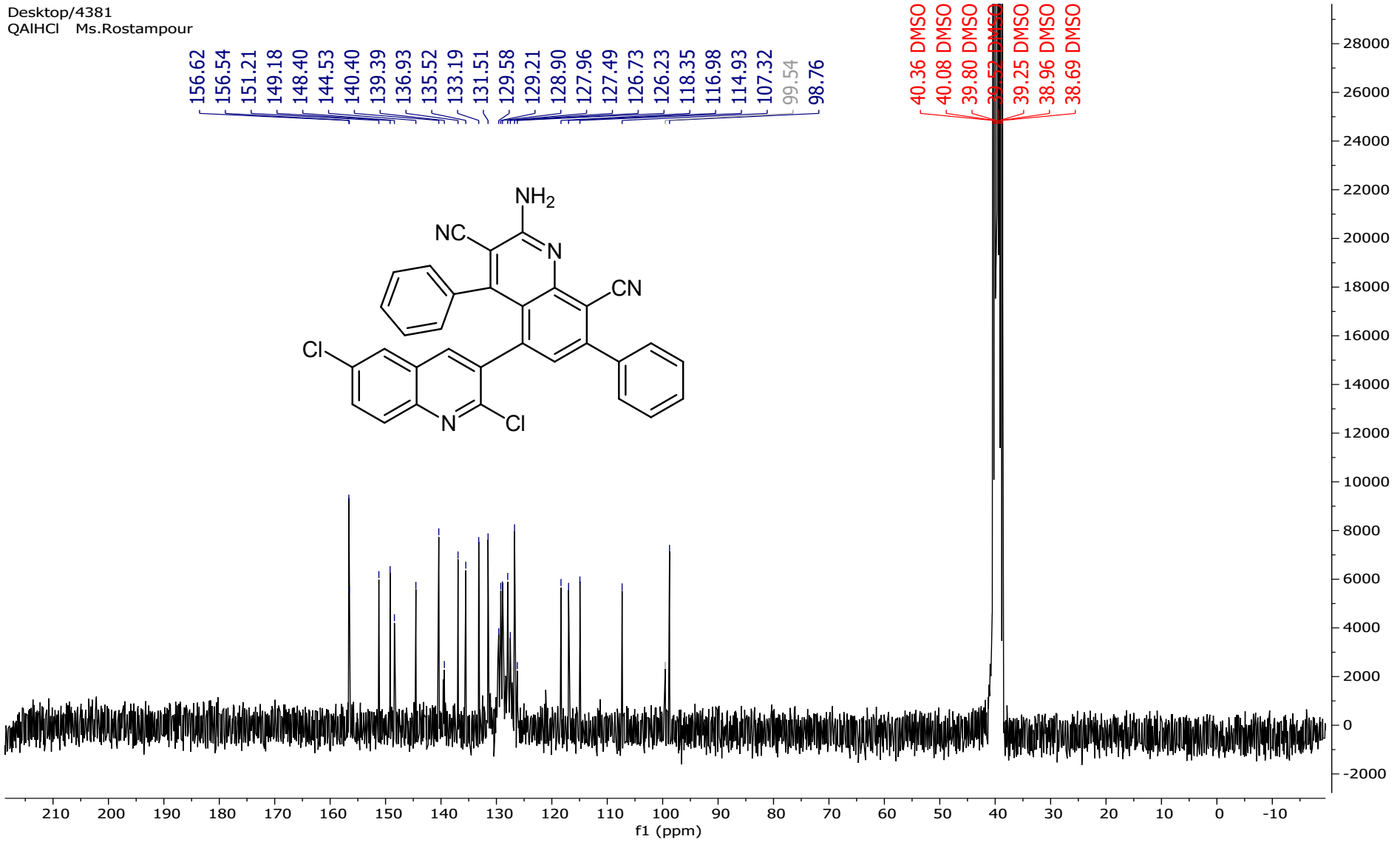
IR Spectrum **3g**



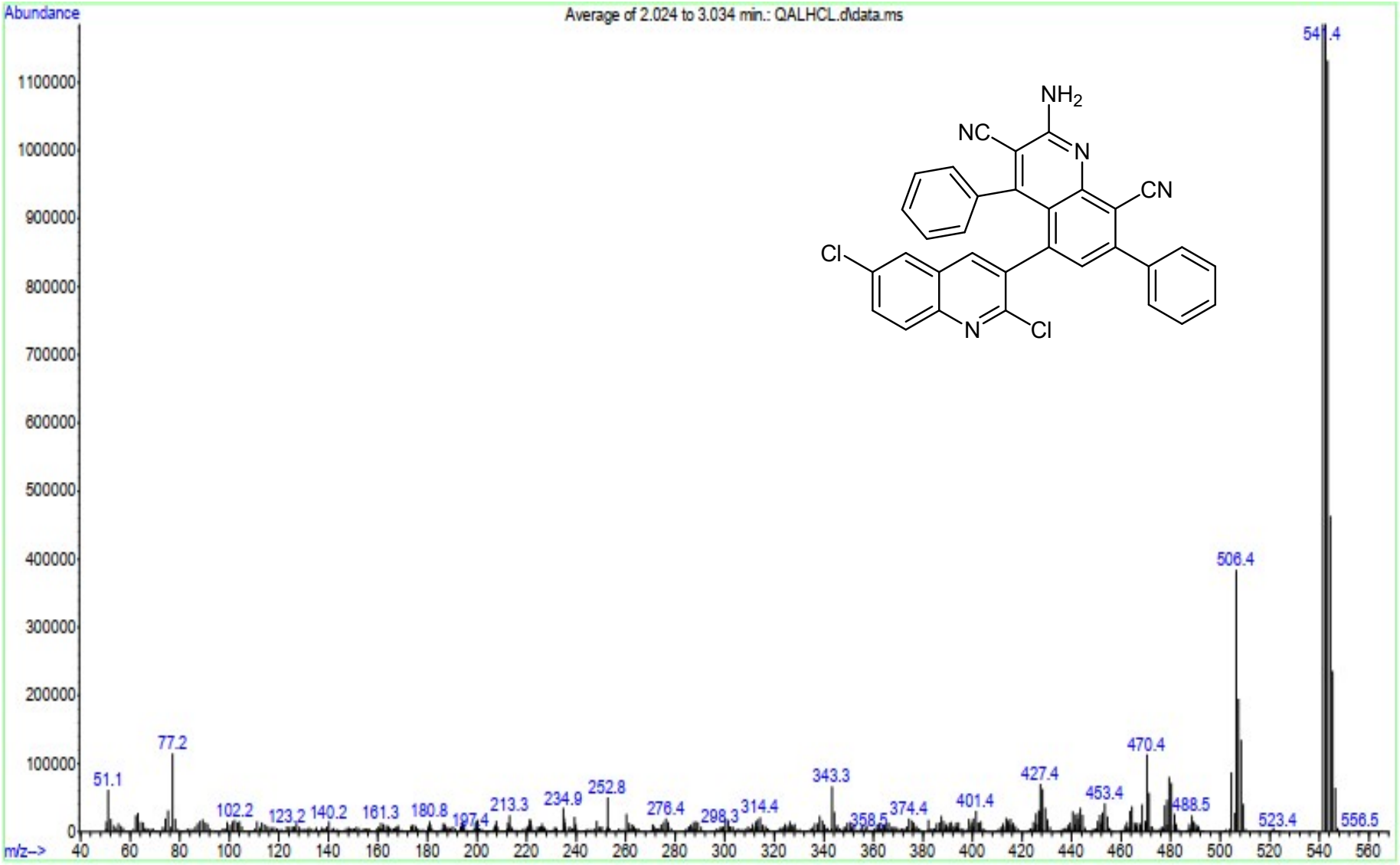
^{1}H NMR Spectrum **3g**



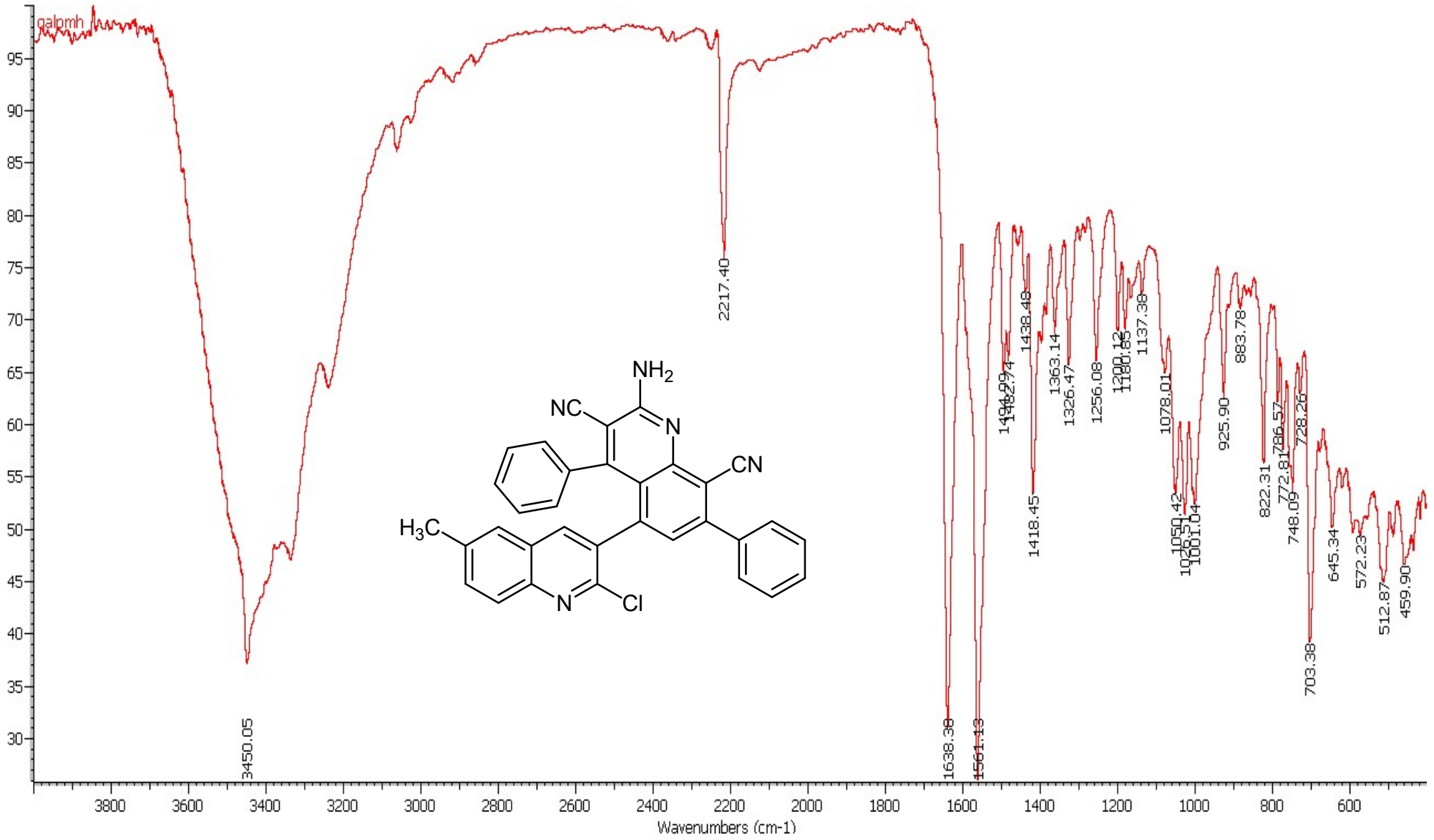
^{1}H NMR Spectrum **3g**



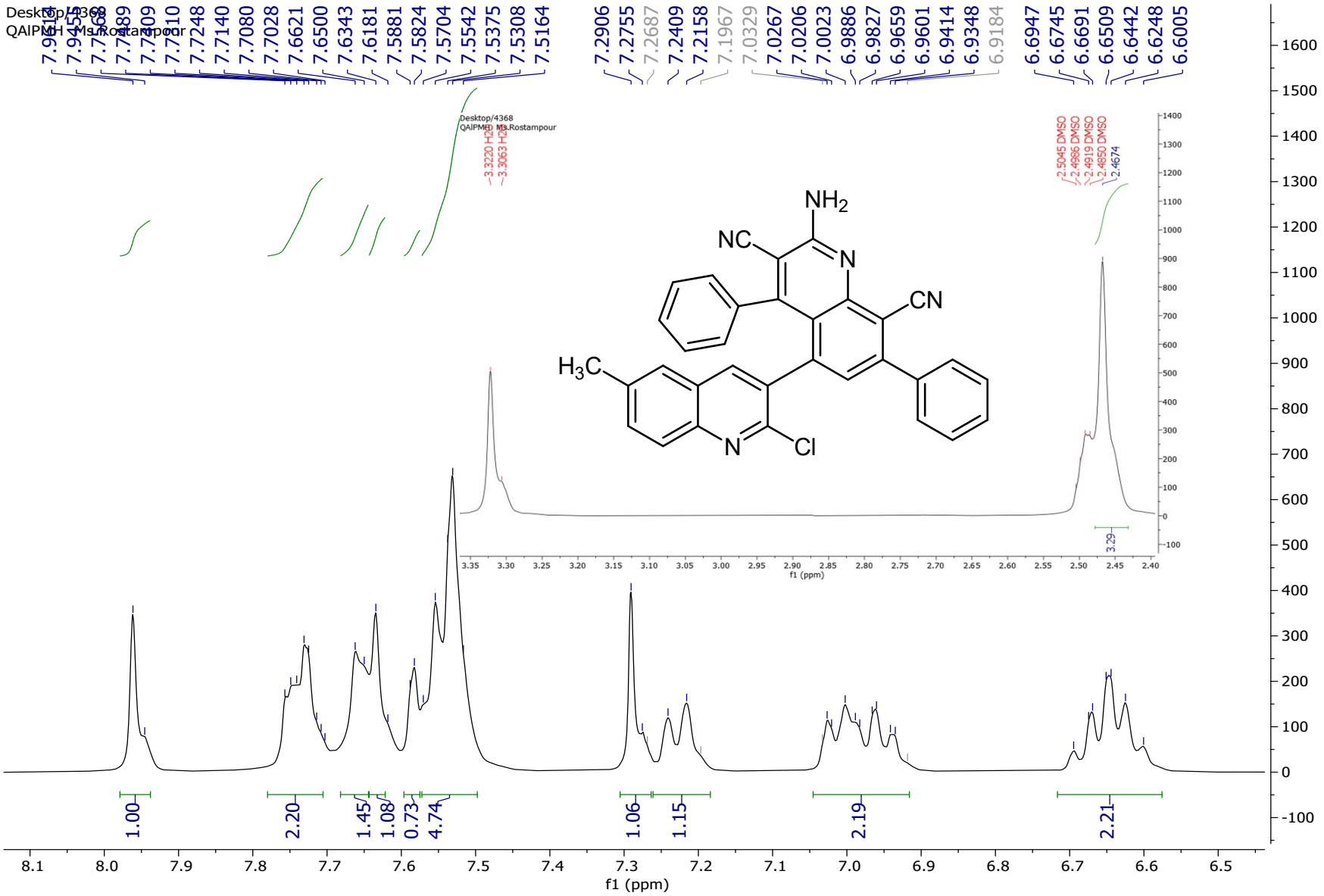
^{13}C NMR Spectrum **3g**



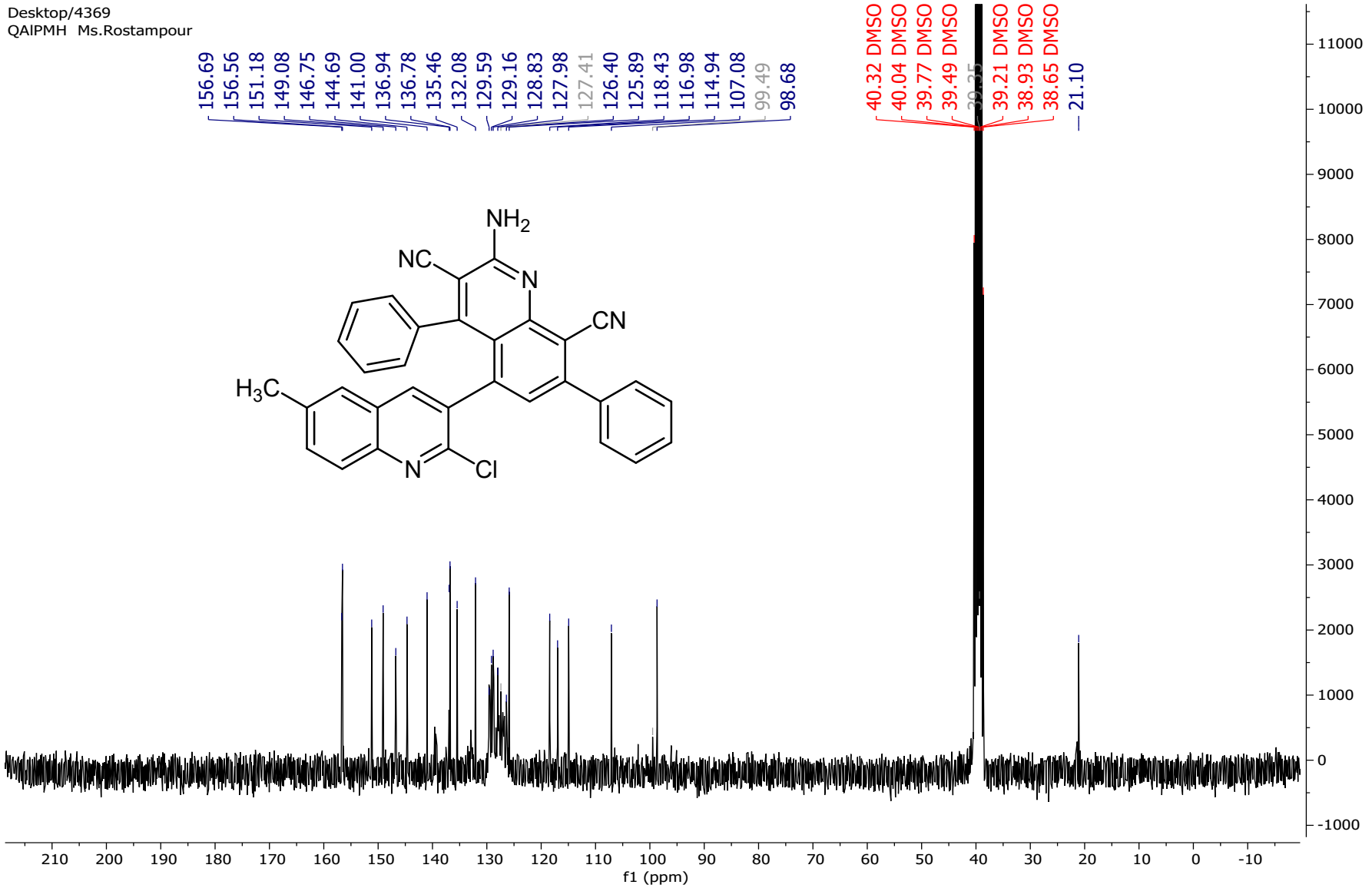
Mass Spectrum **3g**



IR Spectrum **3h**

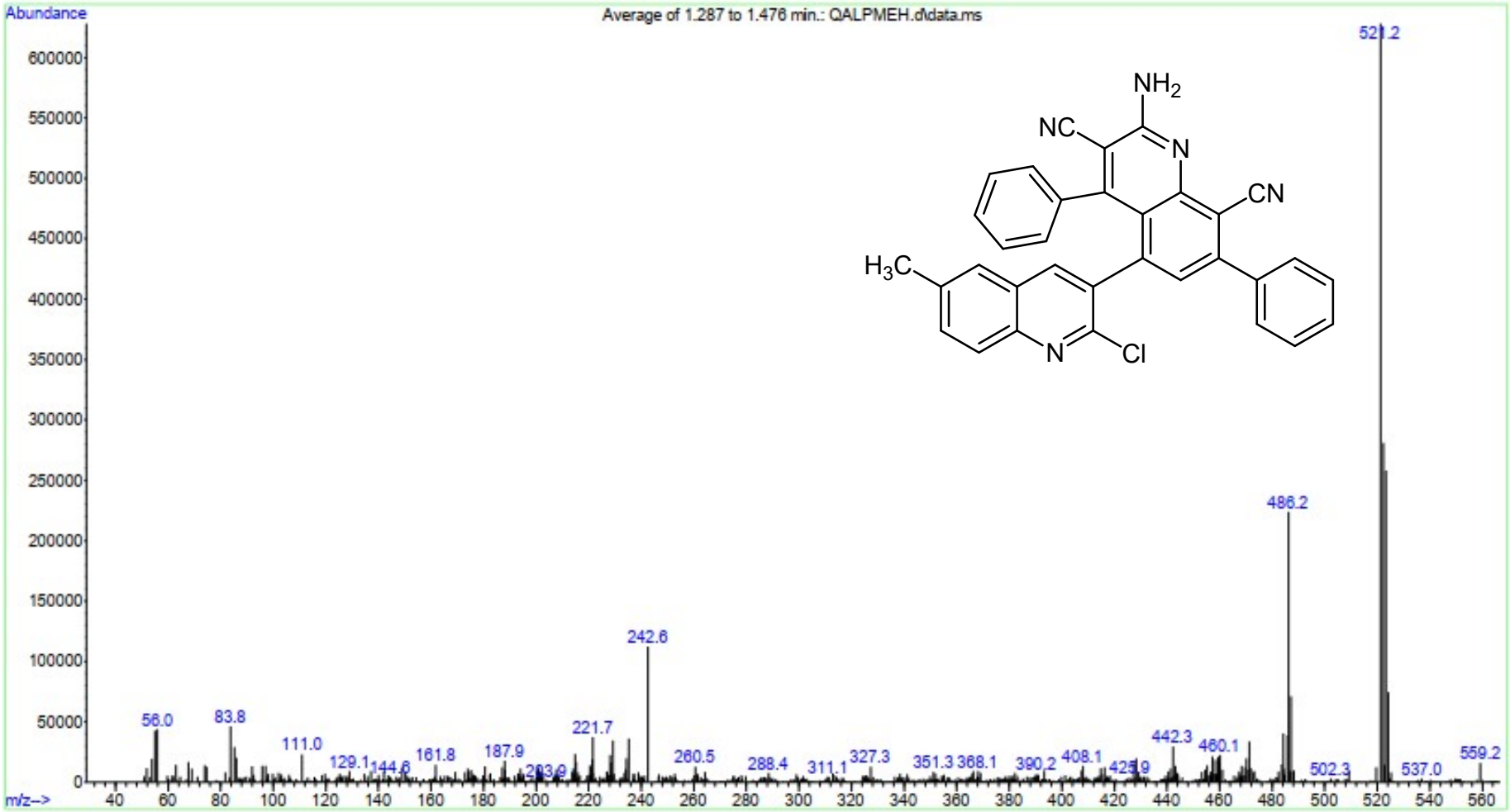


^{1}H NMR Spectrum **3h**

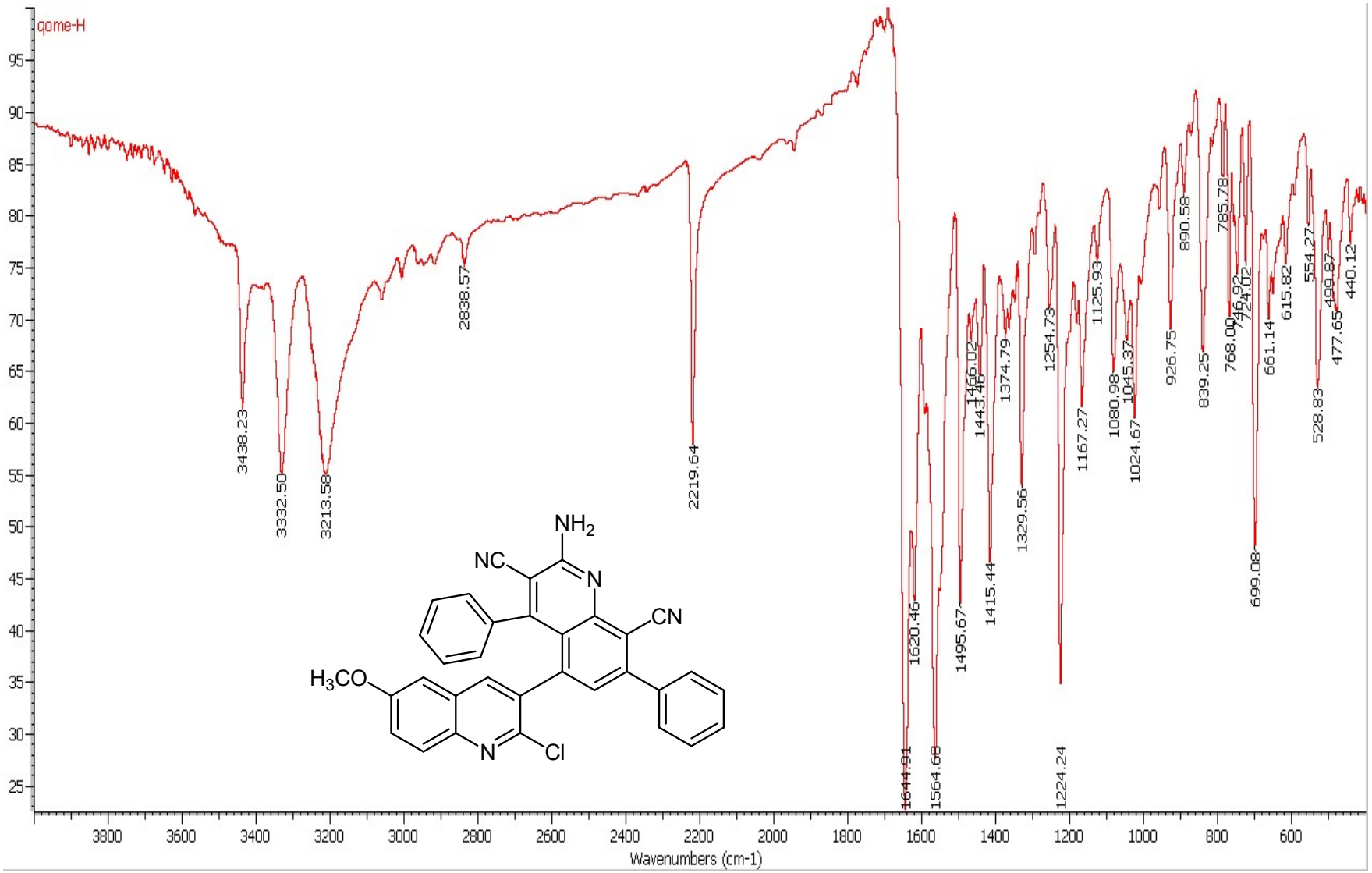


^{13}C NMR Spectrum **3h**

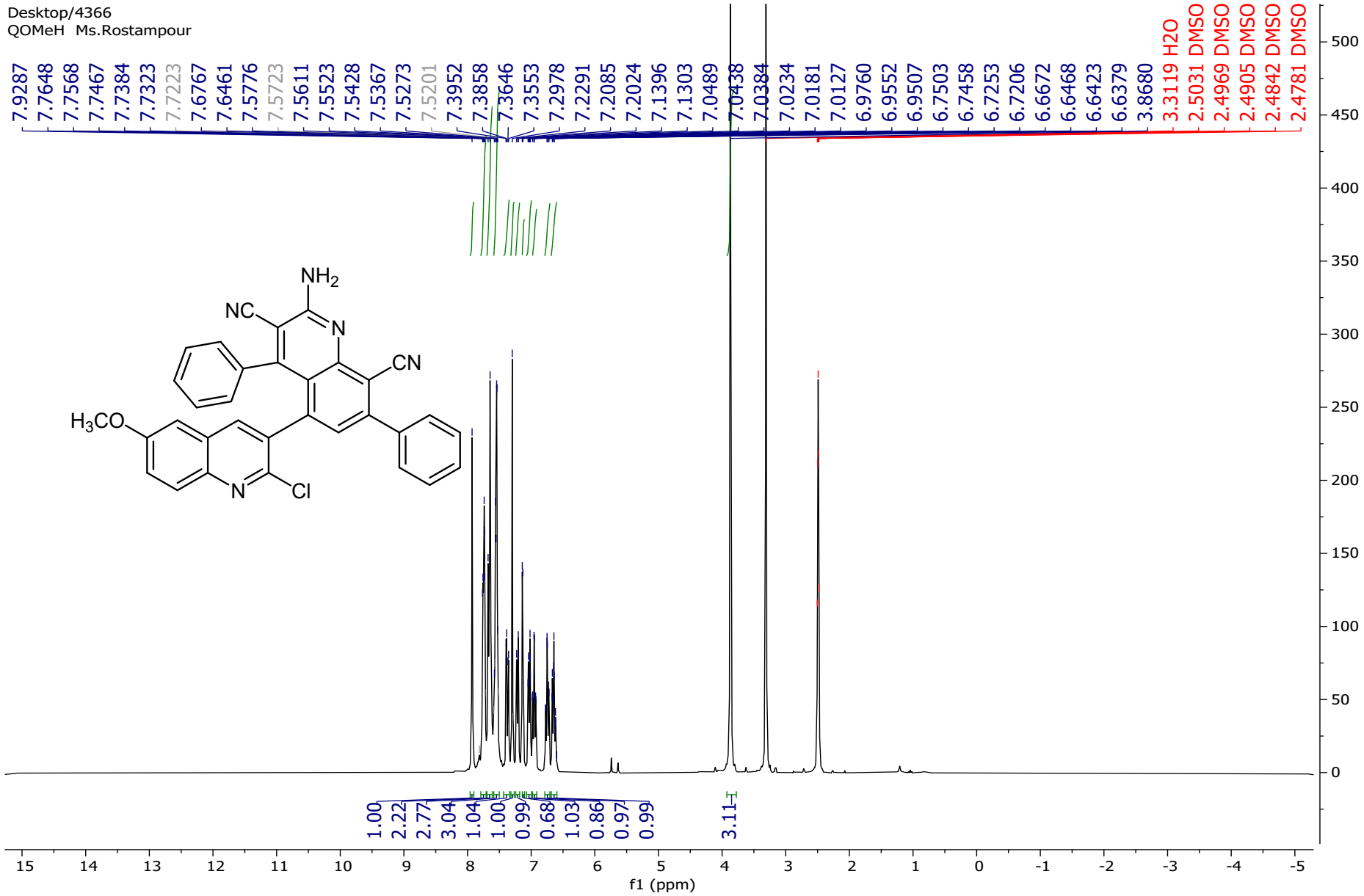
Sample Name:
Misc Info :
Vial Number: 1



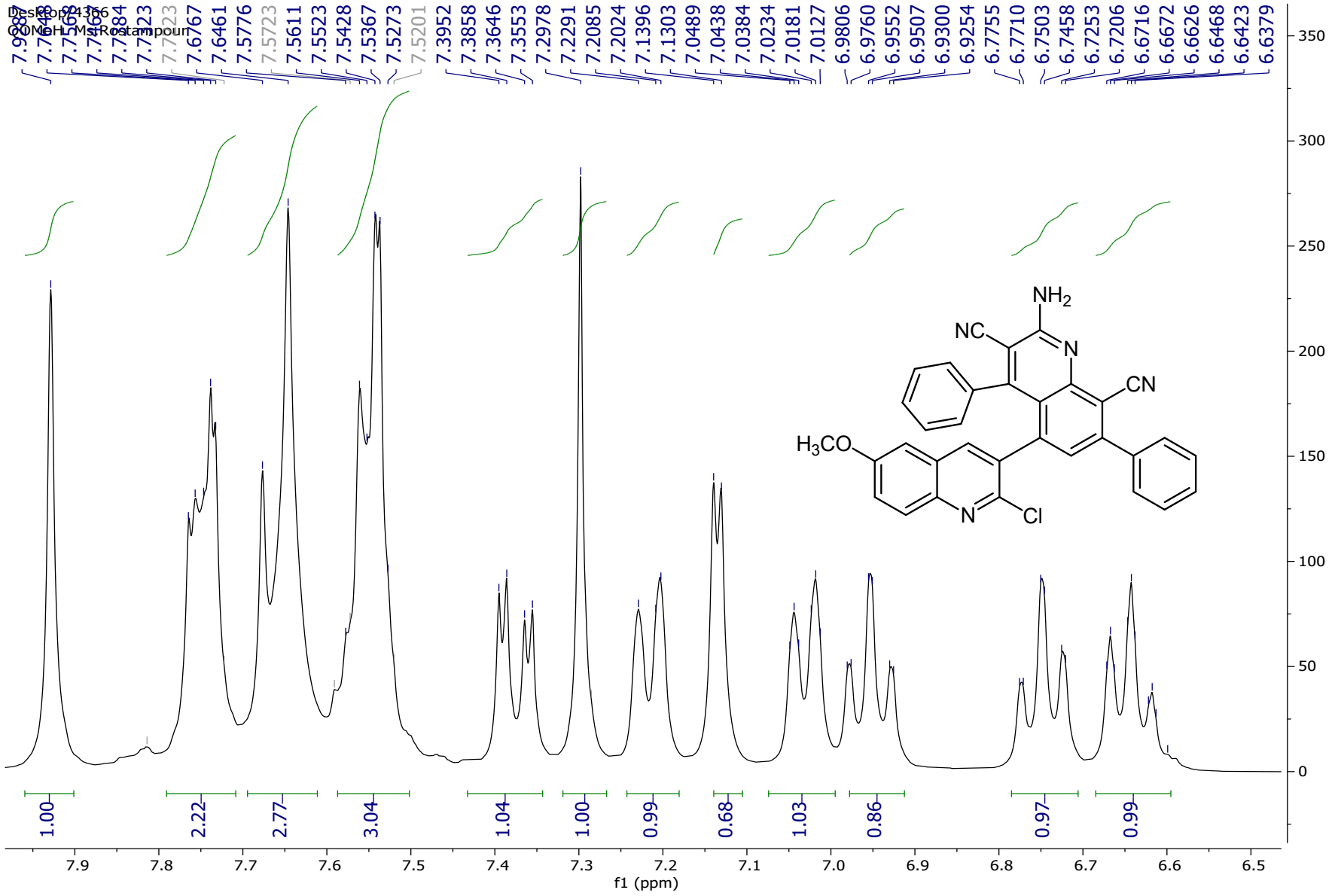
Mass spectrum **3h**



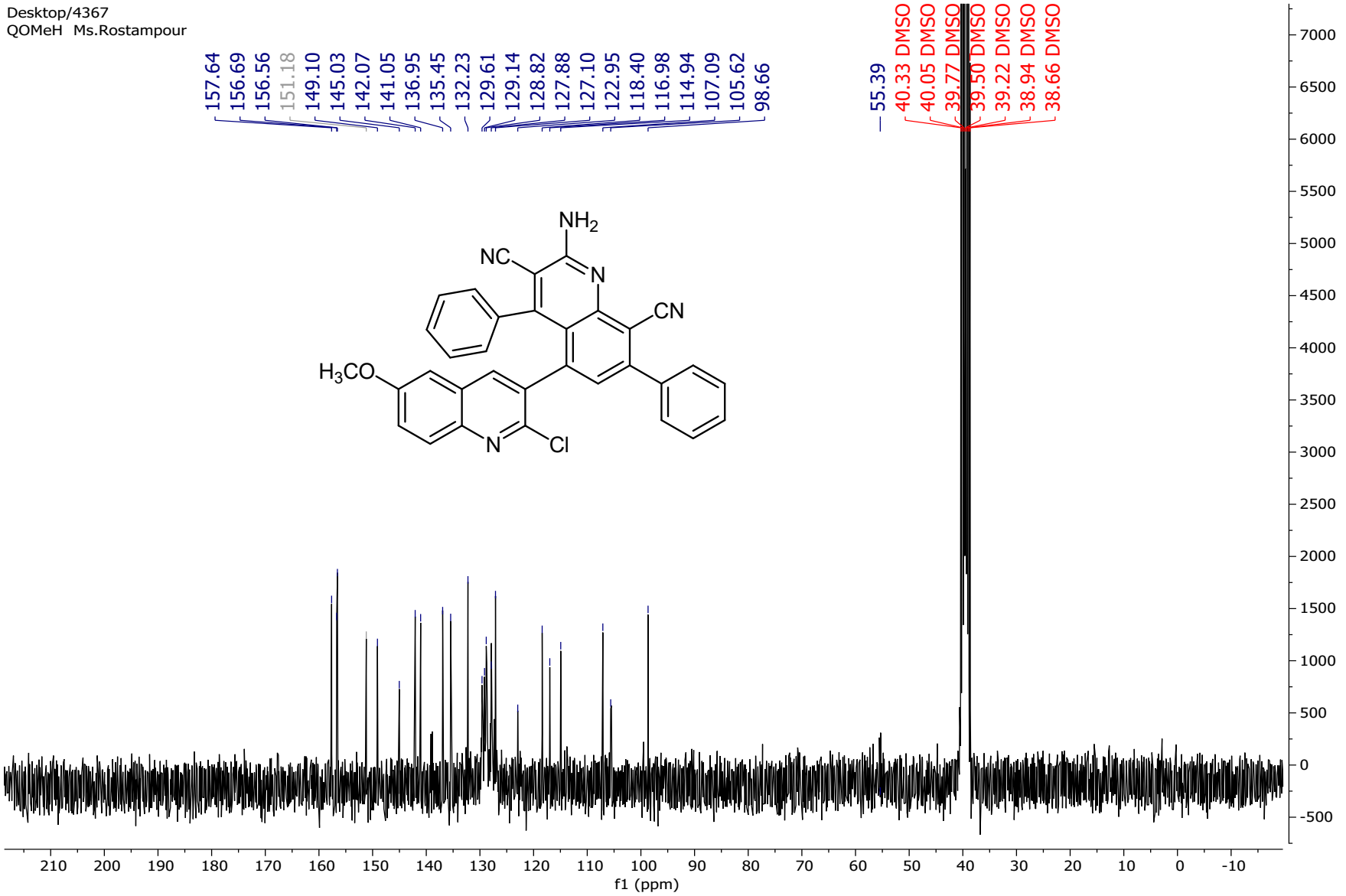
IR Spectrum **3i**


Desktop/4366
QOMeH Ms.Rostampour
7.9287
7.7648
7.7568
7.7467
7.7384
7.7323
7.7223
7.6767
7.6461
7.5776
7.5723
7.5611
7.5523
7.5428
7.5367
7.5273
7.5201
7.3952
7.3858
7.3646
7.3553
7.2978
7.2291
7.2085
7.2024
7.1396
7.1303
7.0489
7.0438
7.0384
7.0234
7.0181
7.0127
6.9760
6.9552
6.9507
6.7503
6.7458
6.7253
6.7206
6.6672
6.6468
6.6423
6.6379
3.8680
3.3119 H2O
2.5031 DMSO
2.4969 DMSO
2.4905 DMSO
2.4842 DMSO
2.4781 DMSO
NH2
NC
N
CN
H3CO
N
Cl
1.00
2.22
2.77
3.04
1.04
1.00
0.99
0.68
1.03
0.86
0.97
0.99
3.11
f1 (ppm)

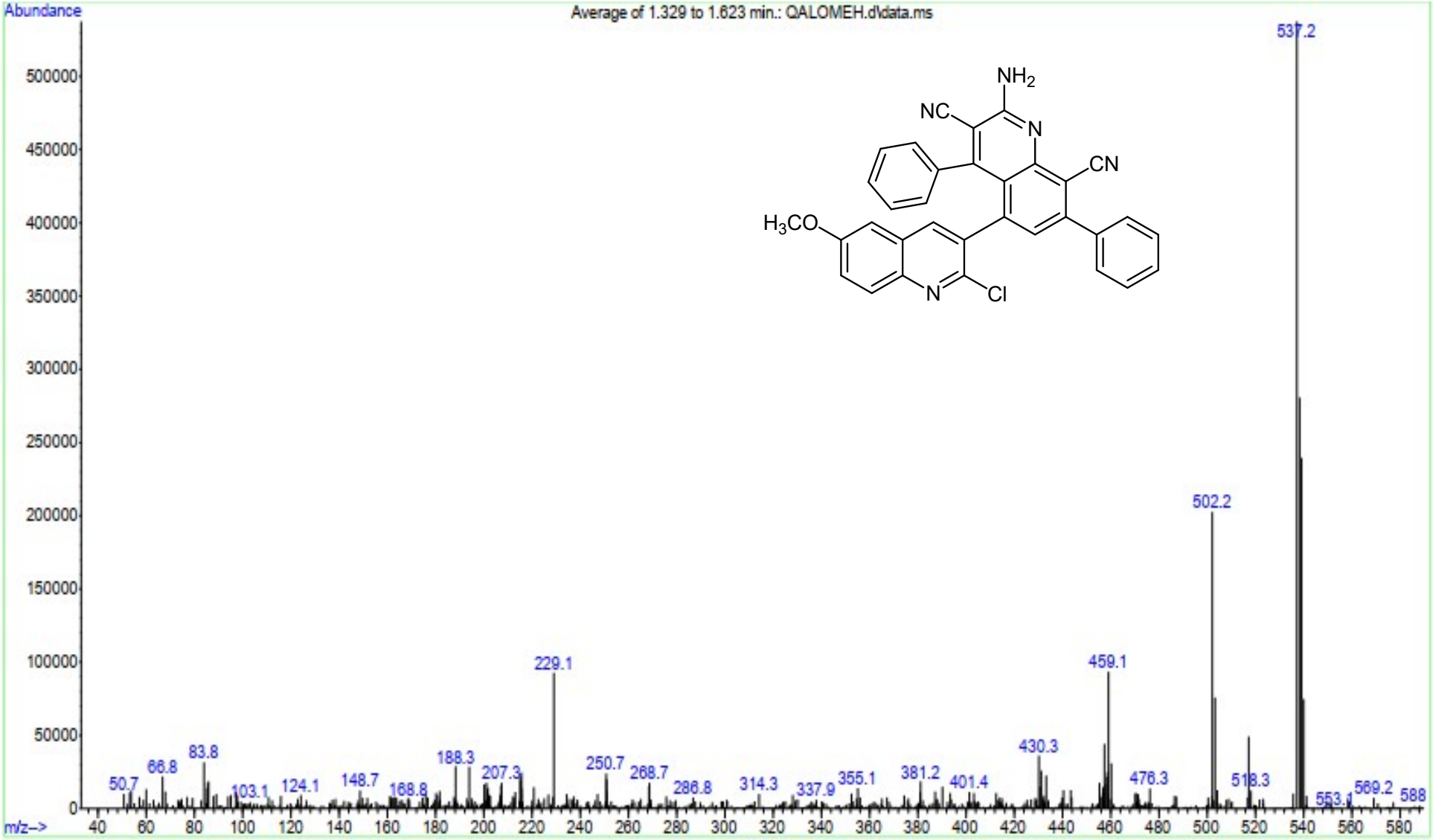
^{1}H NMR Spectrum **3i**



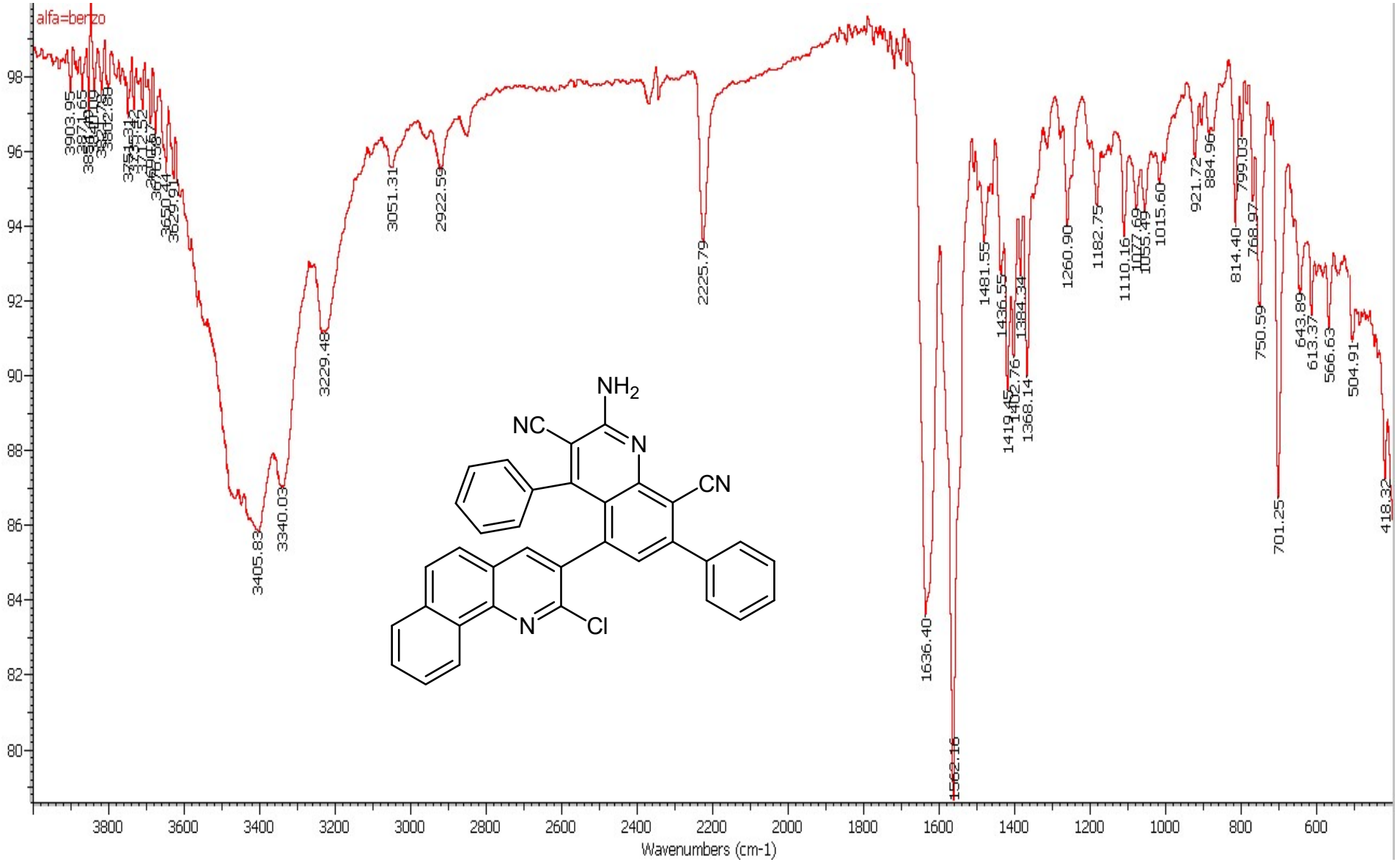
^{1}H NMR Spectrum **3i**



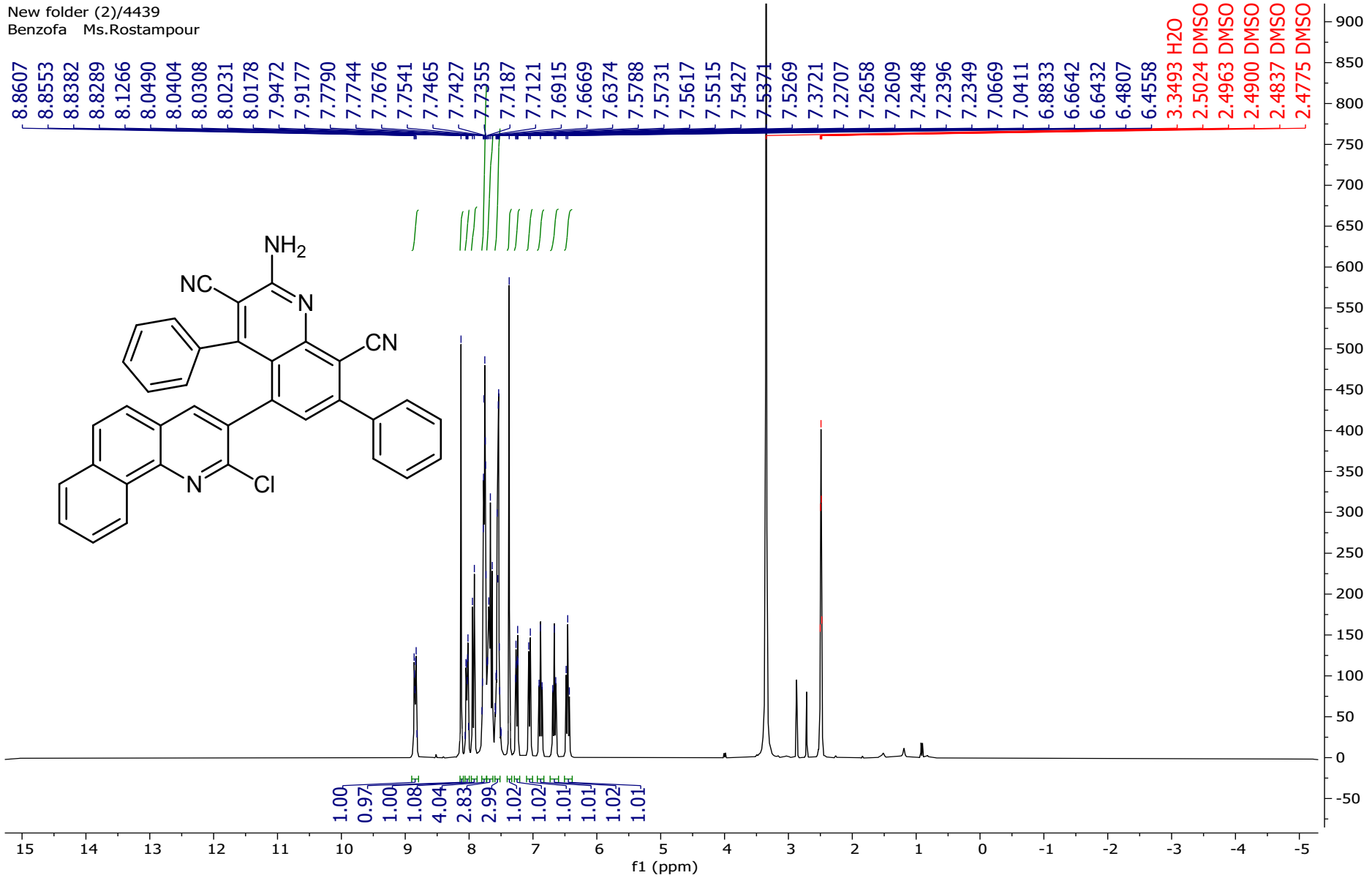
^{13}C NMR Spectrum **3i**



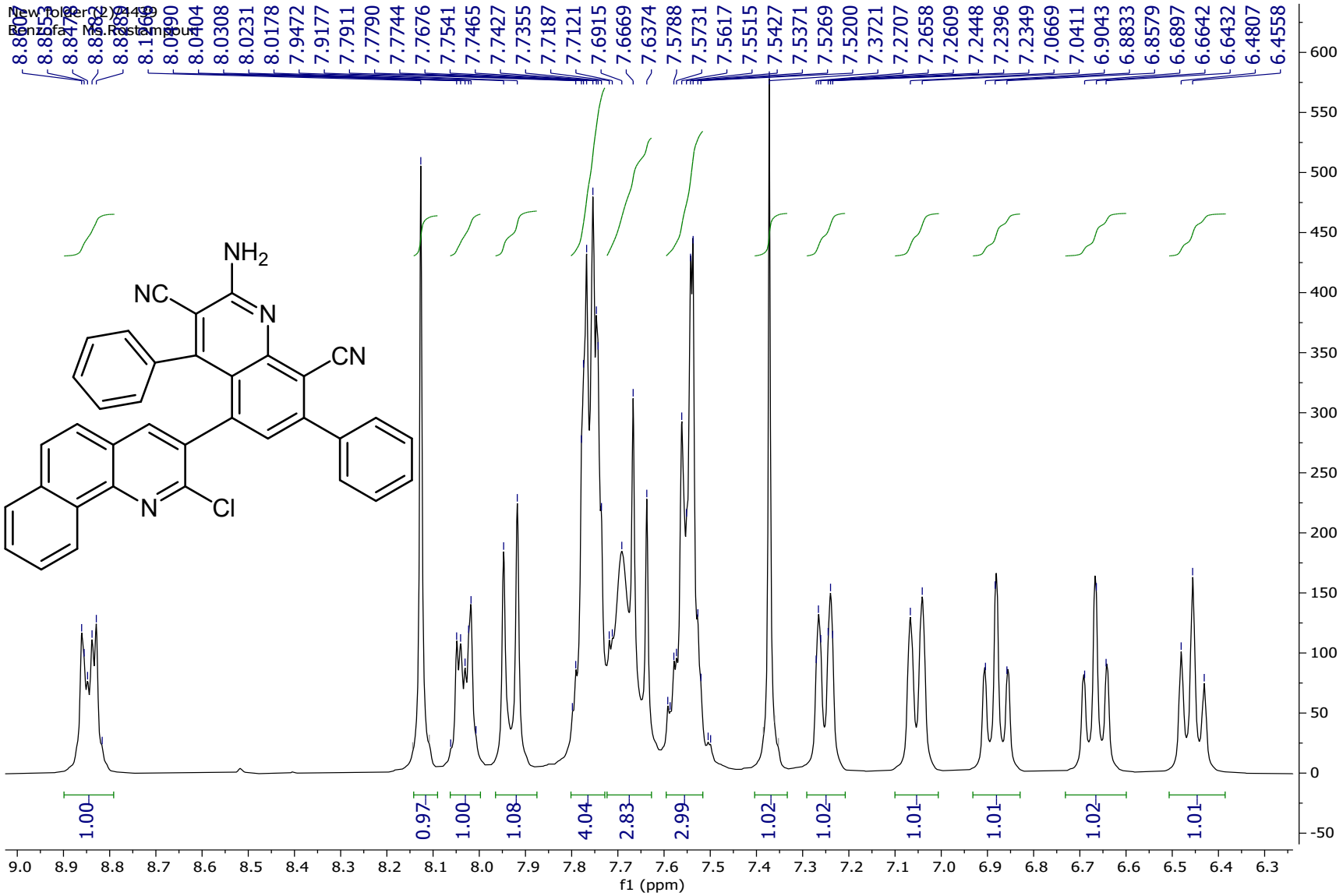
Mass spectrum **3i**



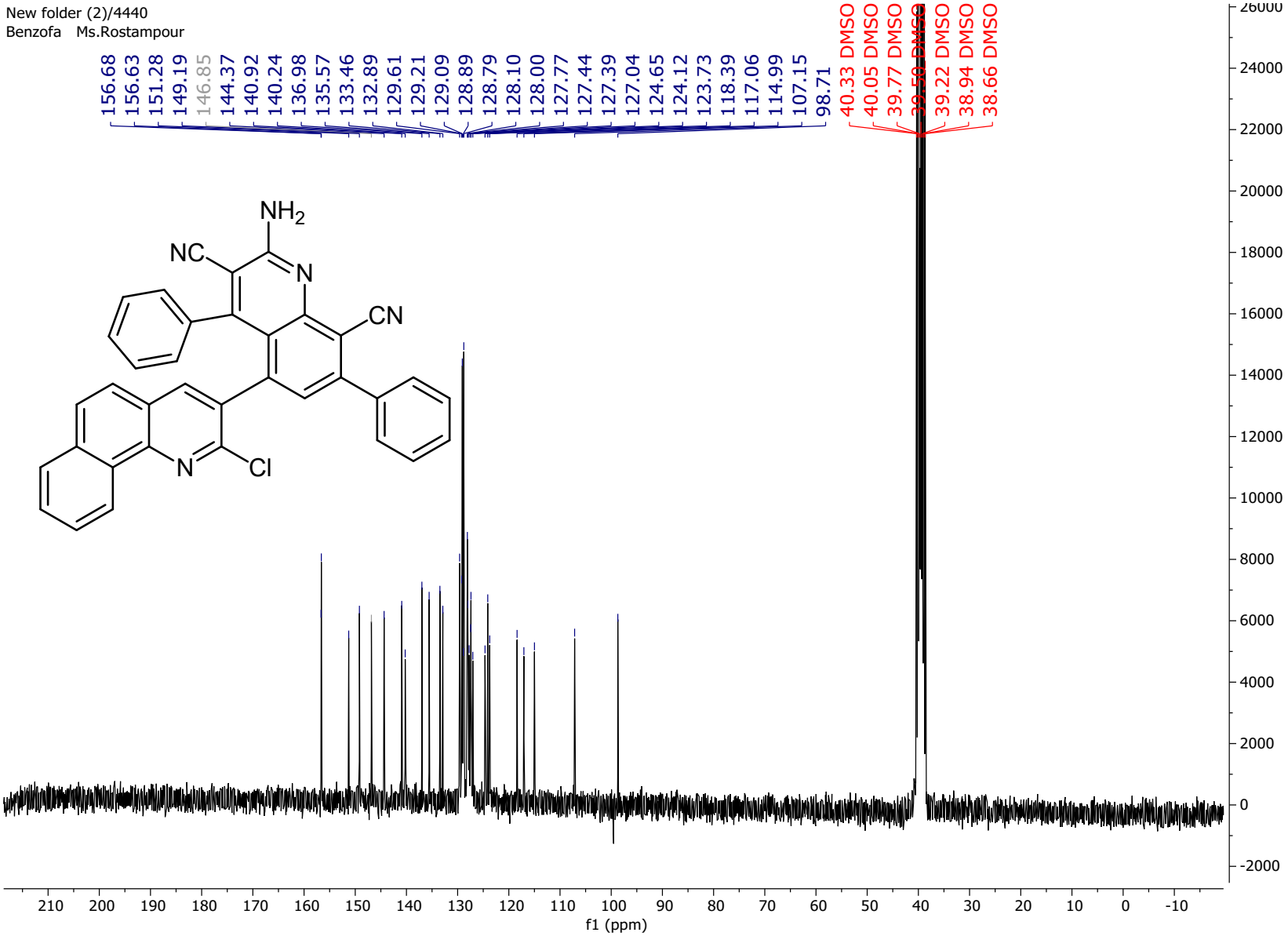
IR Spectrum **3j**



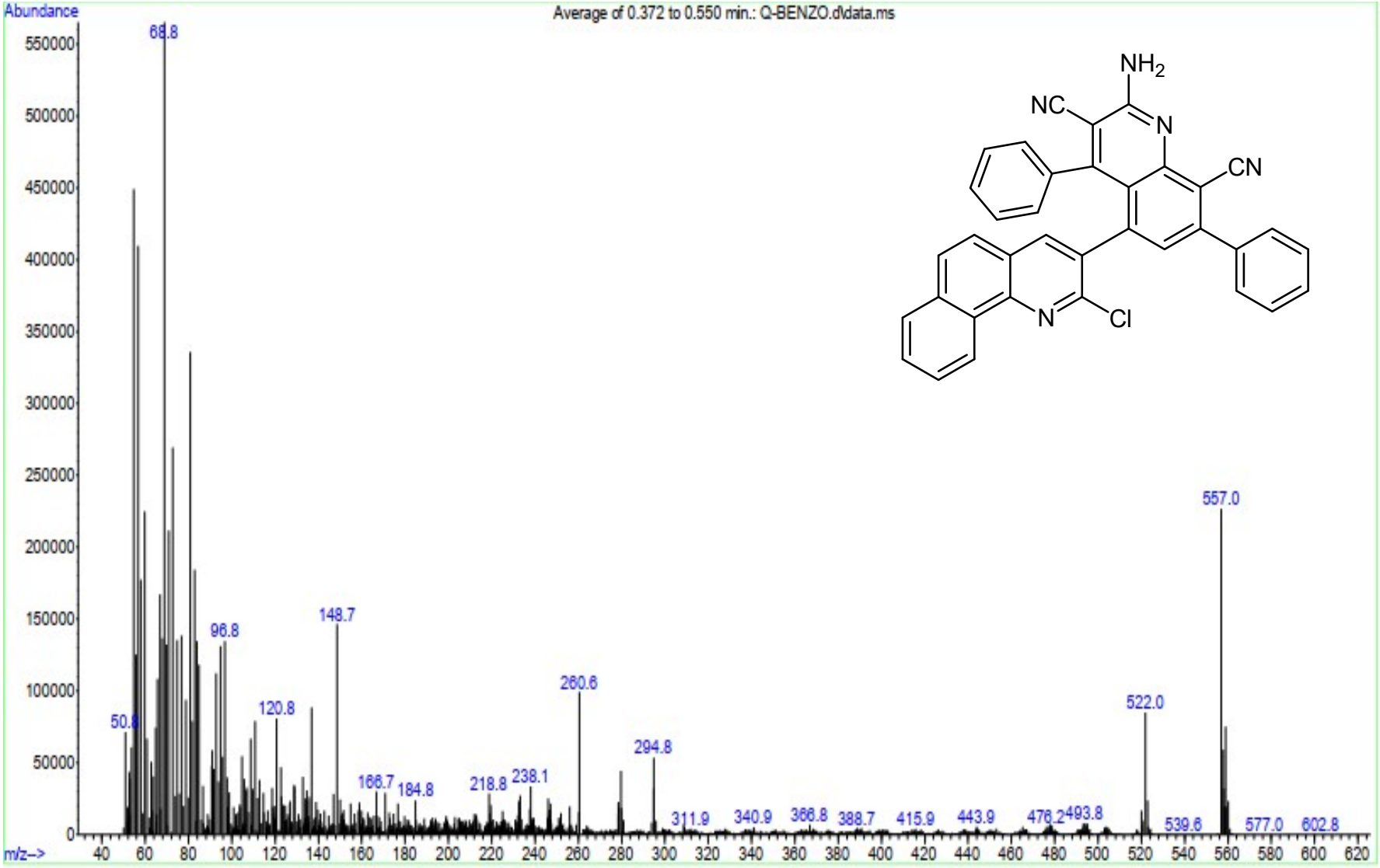
^{1}H NMR Spectrum **3j**



^{1}H NMR Spectrum **3j**



^{13}C NMR spectrum **3j**



Mass spectrum **3j**