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Supporting Information

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Supporting Information

Regio- and Chemoselective Synthesis of 4,6-Dithia-1,2,9-triazaspiro[4.4]non-2-en-8-ones through an Ultrasound-Promoted One-Pot Sequential Pseudo-Five-Component Reaction

Abdolali Alizadeh,* Ebrahim Amir Chelebari, Reza Rezaiyehraad

Department of Chemistry, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran

aalizadeh@modares.ac.ir

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Experimental Section:

General remarks:

The starting materials were supplied by Merck or Aldrich Companies. Melting point of the chemicals was evaluated by an Electrothermal 9100 apparatus. IR spectra were recorded on a NICOLET FT-IR 100 spectrometer. ^{1}H NMR (500.13 MHz) and ^{13}C NMR (125.77 MHz) spectra were also obtained on a Bruker DRX-500 AVANCE instrument in DMSO-d_6. Mass spectra were recorded with an Agilent Technologies 5975C VL MSD mass spectrometer at 70 eV. Elemental analysis was reached by a Heraeus CHN–O–Rapid analyzer.

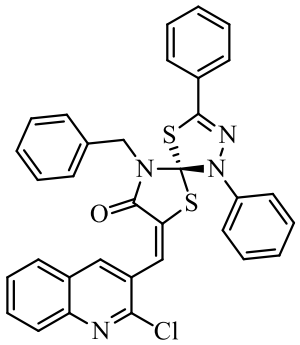
*Corresponding author, Tel.: +98 21 8800663; fax: +98 21 88006544; e-mail: aalizadeh@modares.ac.ir

General preparation procedure for compound 7a:

A mixture of benzylamine (1 mmol, 0.107 g), CS_2 (1.2 mmol, 0.076 g), and ethyl bromoacetate (1.2 mmol, 0.167 g) in acetonitrile (8 mL) was sonicated at a frequency of 20 KHz for 20 minutes. Then, 2-chloroquinoline-3-carbaldehyde (1 mmol, 0.192 g) was added to the reaction media along with Et_3N (1 mmol, 0.101 g). The reaction mixture was ultrasonicated for another 50 minutes. Afterward, hydrazonoyl chloride (1 mmol, 0.231 g) was added and the resulting mixture was treated with ultrasound irradiation for another 20 minutes. The completion of each step was checked by TLC. The yellow precipitates were finally filtered by a sintered glass and washed several times with acetonitrile. Other derivatives **7b-f** were synthesized similarly.

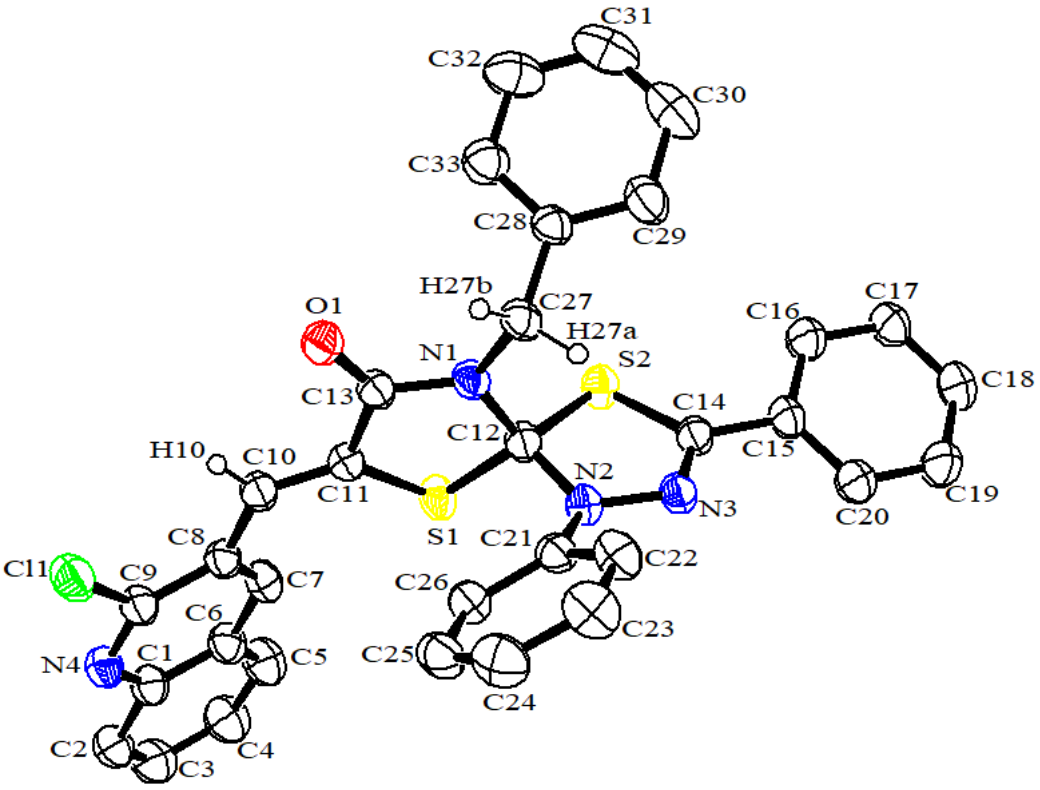
Characteristic data for compounds (7a-f).

(5*R*,7*Z*)-9-Benzyl-7-[(2-chloroquinolin-3-yl)methylene]-1,3-diphenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7a).



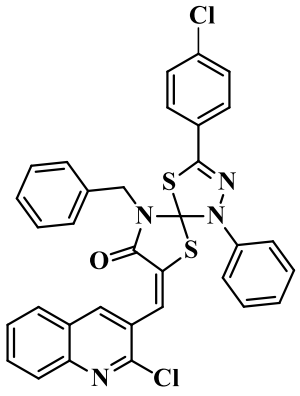
Yellow powder, m.p. = 180-182 °C, 0.47 g, yield: 80%. IR (KBr) (ν_{max}, cm^{-1}): 1698 (C=O), 1580 and 1595 (C=N), 1489 and 1559 (Ar), 747 (C-Cl), 590 (C-S). Anal. calcd. for $C_{33}H_{23}ClN_4OS_2$ (590.10): C, 67.05; H, 3.92; N, 9.48 %. Found C, 67.01; H, 3.94; N, 9.50 %. MS (EI, 70 eV): *m/z* (%): 554 (57), 463 (7), 420 (21), 360 (13), 227 (22), 194 (86), 165 (24), 91 (100), 64 (36). ^{1}H NMR (500.13 MHz, DMSO-d_6): 4.80 (1H, d, $^2J_{HH}$ = 15.8 Hz, CH_2), 4.93 (1H, d, $^2J_{HH}$ = 15.8 Hz, CH_2), 7.10 (1H, t, $^3J_{HH}$ = 7.4 Hz, CH_{para} of Ph), 7.19 (2H, d, $^3J_{HH}$ = 8.0 Hz, CH_{ortho} of Ph), 7.22 (2H, d, $^3J_{HH}$ = 7.2 Hz, CH_{ortho} of Bn), 7.23

(1H, t, $^{3}J_{HH}$ = 7.2 Hz, CH_{para} of Bn), 7.27 (2H, t, $^{3}J_{HH}$ = 7.5 Hz, CH_{meta} of Ph), 7.30 (2H, t, $^{3}J_{HH}$ = 7.5 Hz, CH_{meta} of Bn), 7.49-7.50 (3H, m, 2CH_{meta} and CH_{para} of Ph), 7.61 (2H, d, $^{3}J_{HH}$ = 6.8 Hz, CH_{ortho} of Ph), 7.65 (1H, t, $^{3}J_{HH}$ = 7.6 Hz, CH^{7} of quinoline), 7.82 (1H, t, $^{3}J_{HH}$ = 8.0 Hz, CH^{6} of quinoline), 7.84 (1H, s, CH), 7.93 (1H, d, $^{3}J_{HH}$ = 8.4 Hz, CH^{5} of quinoline), 8.12 (1H, d, $^{3}J_{HH}$ = 8.2 Hz, CH^{8} of quinoline), 8.28 (1H, s, CH^{4} of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 47.04 (CH_2), 106.39 (C^{5}_{spiro}), 120.55 (CH_{para} of Ph), 120.73 (CH_{ortho} of Ph), 125.44 (CH), 126.57 (CH_{meta} of Ph), 126.71 ($CH^{6'}$ of quinoline), 127.01 ($CH^{5'}$ of quinoline), 128.02 ($C^{3'}$ of quinoline), 128.08 (CH_{para} of Bn), 128.50 ($CH^{8'}$ of quinoline), 128.54 (CH_{meta} of Ph), 128.75 (CH_{ortho} of Bn), 128.85 ($C^{4a'}$ of quinoline), 129.14 ($CH^{7'}$ of quinoline), 129.49 (CH_{meta} of Bn), 129.65 (CH_{ortho} of Ph), 130.14 (C_{ipso} of Ph), 131.05 (CH_{para} of Ph), 132.40 ($CH^{4'}$ of quinoline), 135.69 (C_{ipso} of Bn), 137.93 (C_{ipso} of Ph), 140.62 (C^{7}), 143.25 (C^{3}), 146.38 ($C^{8a'}$ of quinoline), 149.89 ($C^{2'}$ of quinoline), 163.71 (C^{8}=O). Crystal data for **7a** $C_{33}H_{23}ClN_4OS_2$ (CCDC 2231969): M_W = 591.12, triclinic, P -1, a = 10.616(2) Å, b = 12.030(2) Å, c = 13.452(3) Å, α = 66.95(2), β = 67.94(3), γ = 69.09(3), V = 1420.0(7) Å^3, Z = 2, Dc = 1.382 mg/m^3, F (000) = 612, crystal dimension 0.2 × 0.15 × 0.1 mm, radiation, Mo Kα (λ = 0.71073 Å), $1.711 \leq 2\theta \leq 26.361$, intensity data were collected at 290 K with a Bruker APEX area-detector diffractometer, and employing $\omega/2\theta$ scanning technique, in the range of $-11 \leq h \leq 13$, $-15 \leq k \leq 14$, $-16 \leq l \leq 15$; the structure was solved by a direct method, all non-hydrogen atoms were positioned and anisotropic thermal parameters refined from 5373 observed reflections with R (into) = 0.0638 by a full-matrix least-squares technique converged to R1 = 0.0601, and wR2 = 0.1670 [I>2sigma(I)].



The ORTEP diagram of **7a**

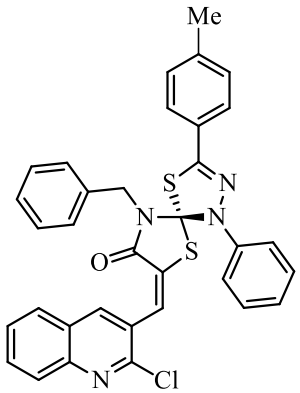
(5*R*,7*Z*)-9-Benzyl-3-(4-chlorophenyl)-7-[(2-chloroquinolin-3-yl)methylene]-1-phenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7b).



Yellow powder, m.p. = 202-204 °C, 0.50 g, yield: 80%. IR (KBr) (ν_{max}, cm^{-1}): 1685 (C=O), 1577 and 1596 (C=N), 1492 and 1560 (Ar), 744 and 828 (C-Cl), 699 (C-S). Anal. calcd. for $C_{33}H_{22}Cl_2N_4OS_2$ (624.06): C, 63.36; H, 3.54; N, 8.96 %. Found C, 63.40; H, 3.52; N, 8.94 %. MS (EI, 70 eV): *m/z* (%): 588 (5), 454 (3), 360 (10), 255 (5), 228 (68), 165 (7), 137 (6), 91 (100), 51 (25). ^{1}H NMR (500.13 MHz,

DMSO-d_6): 4.78 (1H, d, $^2J_{HH}$ = 16.1 Hz, CH_2), 4.92 (1H, d, $^2J_{HH}$ = 16.1 Hz, CH_2), 7.10 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH_{para} of Ph), 7.18 (2H, d, $^3J_{HH}$ = 8.0 Hz, CH_{ortho} of Ph), 7.22 (2H, t, $^3J_{HH}$ = 6.4 Hz, CH_{meta} of Ph), 7.22 (1H, t, $^3J_{HH}$ = 6.4 Hz, CH_{para} of Bn), 7.26 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH_{ortho} of Bn), 7.29 (2H, t, $^3J_{HH}$ = 7.6 Hz, CH_{meta} of Bn), 7.54 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH_{meta} of Ar), 7.60 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH_{ortho} of Ar), 7.64 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH^7 of quinoline), 7.82 (1H, t, $^3J_{HH}$ = 7.9 Hz, CH^6 of quinoline), 7.84 (1H, s, CH), 7.93 (1H, d, $^3J_{HH}$ = 8.4 Hz, CH^5 of quinoline), 8.11 (1H, d, $^3J_{HH}$ = 8.2 Hz, CH^8 of quinoline), 8.27 (1H, s, CH^4 of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 47.02 (CH_2), 106.59 (C^5_{spiro}), 120.65 (CH_{para} of Ph), 120.69 (CH_{ortho} of Ph), 125.50 (CH), 126.67 ($CH^{6'}$ of quinoline), 126.99 ($CH^{5'}$ of quinoline), 128.04 (CH_{para} of Bn), 128.08 ($C^{3'}$ of quinoline), 128.19 (CH_{meta} of Ar), 128.49 ($CH^{8'}$ of quinoline), 128.56 (CH_{meta} of Ph), 128.74 (CH_{ortho} of Bn), 129.02 ($C^{4a'}$ of quinoline), 129.12 ($CH^{7'}$ of quinoline), 129.49 (CH_{meta} of Bn), 129.69 (CH_{ortho} of Ar), 132.40 ($CH^{4'}$ of quinoline), 135.45 (C_{ipso}-Cl), 135.63 (C_{ipso} of Bn), 137.92 (C_{ipso} of Ph), 140.46 (C^7),142.04 (C^3), 146.38 ($C^{8a'}$ of quinoline), 149.86 ($C^{2'}$ of quinoline), 163.68 (C^8=O).

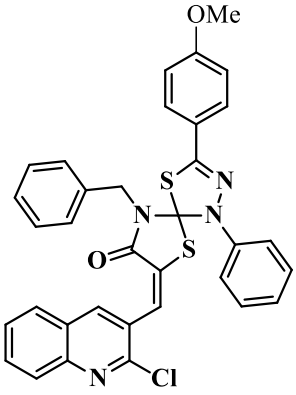
(5*R*,7*Z*)-9-Benzyl-7-[(2-chloroquinolin-3-yl)methylene]-3-(4-methylphenyl)-1-phenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7c).



Yellow powder, dec. = 170-172 °C, 0.45 g, yield: 75%. IR (KBr) (ν_{max}, cm^{-1}): 1704 (C=O), 1488 and 1593 (C=N), 1370 and 1562 (Ar), 816 (C-Cl), 691 (C-S). Anal. calcd. for $C_{34}H_{25}ClN_4OS_2$ (604.12): C, 67.48; H, 4.16; N, 9.26 %. Found C, 67.50; H, 4.18; N, 9.22 %. MS (EI, 70 eV): *m/z* (%): 568 (2), 396

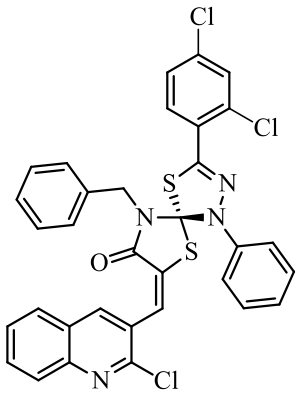
(3), 357 (8), 244 (8), 208 (88), 183 (7), 140 (7), 91 (100), 65 (13). ^{1}H NMR (500.13 MHz, DMSO-d_6): 2.57 (3H, s, CH_3), 4.81 (1H, d, $^{2}J_{HH}$ = 15.7 Hz, CH_2), 4.94 (1H, d, $^{2}J_{HH}$ = 15.7 Hz, CH_2), 7.11 (1H, t, $^{3}J_{HH}$ = 7.4 Hz, CH_{para} of Ph), 7.19 (2H, d, $^{3}J_{HH}$ = 8.5 Hz, CH_{ortho} of Ph), 7.22 (2H, t, $^{3}J_{HH}$ = 6.7 Hz, CH_{meta} of Bn), 7.23 (1H, t, $^{3}J_{HH}$ = 6.7 Hz, CH_{para} of Bn), 7.24 (2H, d, $^{3}J_{HH}$ = 6.7 Hz, CH_{ortho} of Bn), 7.28 (2H, t, $^{3}J_{HH}$ = 7.8 Hz, CH_{meta} of Ph), 7.32 (2H, d, $^{3}J_{HH}$ = 8.1 Hz CH of Ar), 7.52 (2H, d, $^{3}J_{HH}$ = 7.9 Hz, CH of Ar), 7.68 (1H, t, $^{3}J_{HH}$ = 7.6 Hz, CH^{7} of quinoline), 7.85 (1H, t, $^{3}J_{HH}$ = 7.8 Hz, CH^{6} of quinoline), 7.85 (1H, s, CH), 7.97 (1H, d, $^{3}J_{HH}$ = 8.5 Hz, CH^{5} of quinoline), 8.18 (1H, d, $^{3}J_{HH}$ = 8.5 Hz, CH^{8} of quinoline), 8.34 (1H, s, CH^{4} of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 21.55 (CH_3), 47.07 (CH_2), 105.40 (C^{5}_{spiro}), 119.39 (CH_{ortho} of Ph), 121.50 (CH_{para} of Ph), 124.34 (CH), 126.28 (CH of Ar), 126.77 ($CH^{6'}$ of quinoline), 127.32 ($CH^{5'}$ of quinoline), 127.50 (C_{ipso} of Ar), 127.66 ($C^{4a'}$ of quinoline), 127.85 (CH_{para} of Bn), 127.90 ($C^{3'}$ of quinoline), 128.35 (CH_{meta} of Ph), 128.40 ($CH^{8'}$ of quinoline), 128.48 ($CH^{7'}$ of quinoline), 128.96 (CH_{ortho} of Bn), 128.99 (CH_{meta} of Bn), 129.57 (CH of Ar), 131.35 ($CH^{4'}$ of quinoline), 135.20 (C_{ipso} of Bn), 137.32 (C_{ipso} of Ph), 140.69 (C^{7}), 140.71 (C_{ipso}-Me), 143.17 (C^{3}), 146.61 ($C^{8a'}$ of quinoline), 150.64 ($C^{2'}$ of quinoline), 163.76 (C^{8}=O).

(5*R*,7*Z*)-9-Benzyl-7-[(2-chloroquinolin-3-yl)methylene]-3-(4-methoxyphenyl)-1-phenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7d).



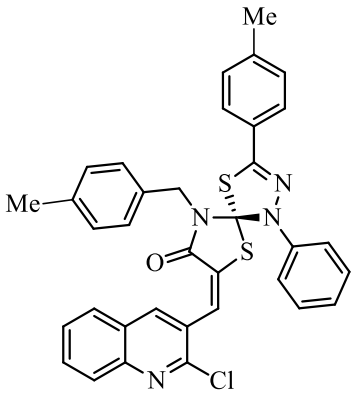
Yellow powder, m.p. = 145-147 °C, 0.47 g, yield: 77%. IR (KBr) (ν_{max}, cm^{-1}): 1689 (C=O), 1579 and 1602 (C=N), 1489 and 1561 (Ar), 751 (C-Cl), 698 (C-S). Anal. calcd. for $C_{34}H_{25}ClN_4O_2S_2$ (620.11): C, 65.74; H, 4.06; N, 9.02 %. Found C, 65.75; H, 4.04; N, 9.03 %. MS (EI, 70 eV): *m/z* (%): 584 (5), 396 (5), 360 (22), 224 (93), 183 (12), 133 (14), 91 (100), 65 (13). ^{1}H NMR (500.13 MHz, DMSO-d_6): 3.82 (3H, s, OCH_3), 4.81 (1H, d, $^2J_{HH}$ = 15.7 Hz, CH_2), 4.95 (1H, d, $^2J_{HH}$ = 15.8 Hz, CH_2), 7.05 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH of Ar), 7.10 (1H, t, $^3J_{HH}$ = 7.5 Hz, CH_{para} of Ph), 7.19 (2H, d, $^3J_{HH}$ = 8.2 Hz, CH_{ortho} of Ph), 7.20-7.31 (7H, m, 5CH of Bn and 2CH_{meta} of Ph), 7.56 (2H, d, $^3J_{HH}$ = 8.7 Hz, CH of Ar), 7.67 (1H, t, $^3J_{HH}$ = 7.4 Hz, CH^7 of quinoline), 7.85 (1H, t, $^3J_{HH}$ = 7.4 Hz, CH^6 of quinoline), 7.84 (1H, s, CH), 7.96 (1H, d, $^3J_{HH}$ = 8.4 Hz, CH^5 of quinoline), 8.16 (1H, d, $^3J_{HH}$ = 8.5 Hz, CH^8 of quinoline), 8.32 (1H, s, CH^4 of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 47.05 (CH_2), 55.94 (OCH_3), 106.44 (C^5_{spiro}), 115.08 (CH of Ar), 120.44 (CH_{para} of Ph), 120.73 (CH_{ortho} of Ph), 122.58 (C_{ipso} of Ar), 125.30 (CH), 126.74 ($CH^{6'}$ of quinoline), 127.05 ($CH^{5'}$ of quinoline), 128.01 (CH_{para} of Bn), 128.08 ($C^{3'}$ of quinoline), 128.24 (CH of Ar), 128.47 (CH_{meta} of Ph), 128.53 ($CH^{8'}$ of quinoline), 128.77 (CH_{ortho} of Bn), 128.96 ($C^{4a'}$ of quinoline), 129.18 ($CH^{7'}$ of quinoline), 129.46 (CH_{meta} of Bn), 132.43 ($CH^{4'}$ of quinoline), 135.76 (C_{ipso} of Bn), 137.97 (C_{ipso} of Ph), 140.80 (C^7), 143.80 (C^3), 146.39 ($C^{8a'}$ of quinoline), 149.88 ($C^{2'}$ of quinoline), 161.52 (C_{ipso}-OMe), 163.79 (C^8=O).

(5*R*,7*Z*)-9-Benzyl-7-[(2-chloroquinolin-3-yl)methylene]-3-(2,4-dichlorophenyl)-1-phenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7e).

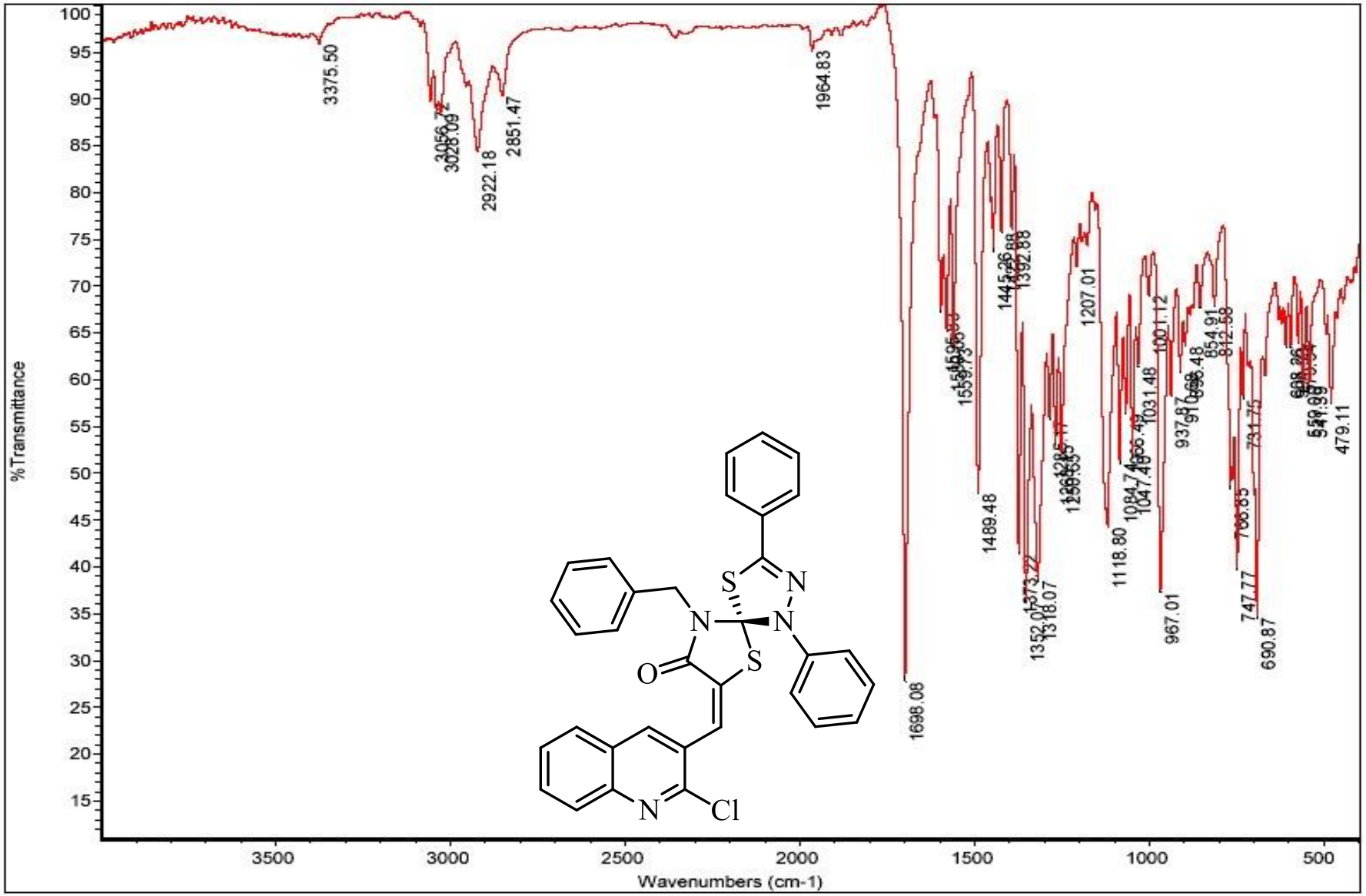


Yellow powder, m.p. = 178-180 °C, 0.48 g, yield: 73%. IR (KBr) (ν_{max}, cm^{-1}): 1686 (C=O), 1596 and 1539 (C=N), 1566 and 1494 (Ar), 735 and 758 and 776 (C-Cl), 696 (C-S). Anal. calcd. for $C_{33}H_{21}Cl_3N_4OS_2$ (660.02): C, 60.05; H, 3.21; N, 8.49 %. Found C, 60.03; H, 3.22; N, 8.50 %. MS (EI, 70 eV): *m/z* (%): 396 (15), 360 (67), 299 (9), 255 (21), 228 (52), 183 (26), 137 (21), 91 (100), 65 (20). ^{1}H NMR (500.13 MHz, DMSO-d_6): 4.79 (1H, d, $^2J_{HH}$ = 15.5 Hz, CH_2), 4.90 (1H, d, $^2J_{HH}$ = 15.7 Hz, CH_2), 7.10 (1H, t, $^3J_{HH}$ = 8.1 Hz, CH_{para} of Ph), 7.17 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH_{ortho} of Ph), 7.20 (2H, t, $^3J_{HH}$ = 8.0 Hz, CH_{meta} of Ph), 7.26 (2H, t, $^3J_{HH}$ = 7.5 Hz, CH_{meta} of Bn), 7.31 (2H, d, $^3J_{HH}$ = 7.8 Hz, CH_{ortho} of Bn), 7.48 (1H, d, $^3J_{HH}$ = 7.5 Hz, CH of Ar), 7.53 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH_{para} of Bn), 7.60 (1H, d, $^3J_{HH}$ = 7.7 Hz, CH of Ar), 7.66 (1H, t, $^3J_{HH}$ = 6.9 Hz, CH^7 of quinoline), 7.84 (1H, s, CH of Ar), 7.84 (1H, t, $^3J_{HH}$ = 7.2 Hz, CH^6 of quinoline), 7.88 (1H, s, CH), 7.95 (1H, d, $^3J_{HH}$ = 8.6 Hz, CH^5 of quinoline), 8.15 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH^8 of quinoline), 8.32 (1H, s, CH^4 of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 46.95 (CH_2), 105.79 ($C^5{}_{spiro}$), 120.32 (CH_{ortho} of Ph), 120.72 (CH_{para} of Ph), 125.33 (CH), 126.72 ($CH^{6'}$ of quinoline), 127.04 ($CH^{5'}$ of quinoline), 128.02 (CH_{para} of Bn), 128.08 ($C^{3'}$ of quinoline), 128.32 (CH of Ar), 128.51 (C_{ipso} of Ar), 128.65 ($CH^{8'}$ of quinoline), 128.67 (CH_{ortho} of Bn and CH_{meta} of Ph), 128.93 ($C^{4a'}$ of quinoline), 129.17 ($CH^{7'}$ of quinoline), 129.49 (CH_{meta} of Bn), 130.90 (CH of Ar), 131.23 (CH of Ar), 131.48 (C_{ipso}-2-Cl), 132.27 (C_{ipso}-4-Cl), 132.42 ($CH^{4'}$ of quinoline), 135.63 (C_{ipso} of Bn), 137.94 (C_{ipso} of Ph), 140.03 (C^3), 140.44 (C^7), 146.41 ($C^{8a'}$ of quinoline), 149.88 ($C^{2'}$ of quinoline), 163.45 (C^8=O).

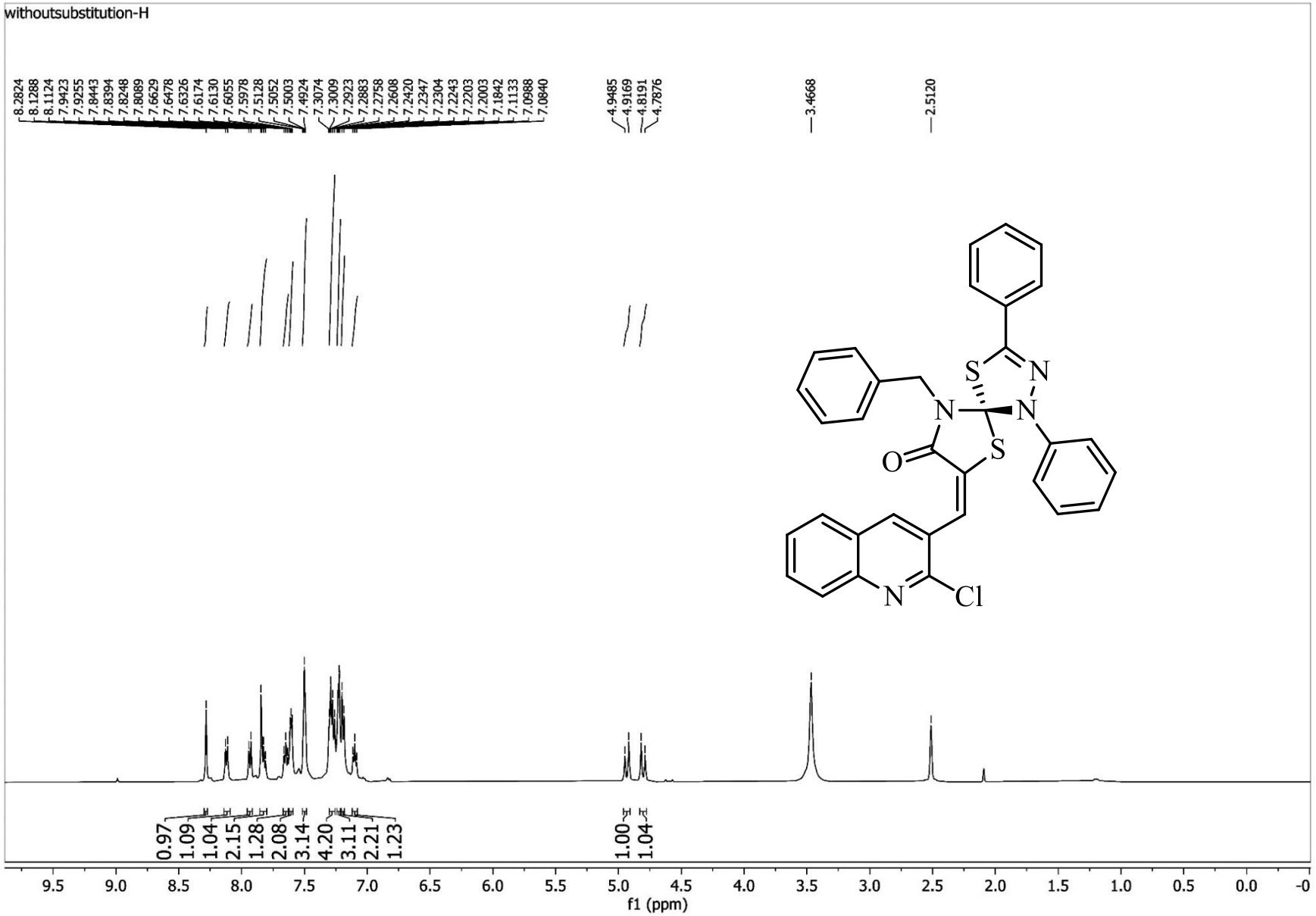
(5*R*,7*Z*)-7-[(2-Chloroquinolin-3-yl)methylene]-9-(4-methylbenzyl)-3-(4-methylphenyl)-1-phenyl-4,6-dithia-1,2,9-triazaspiro[4.4]non-2-en-8-one (7f).



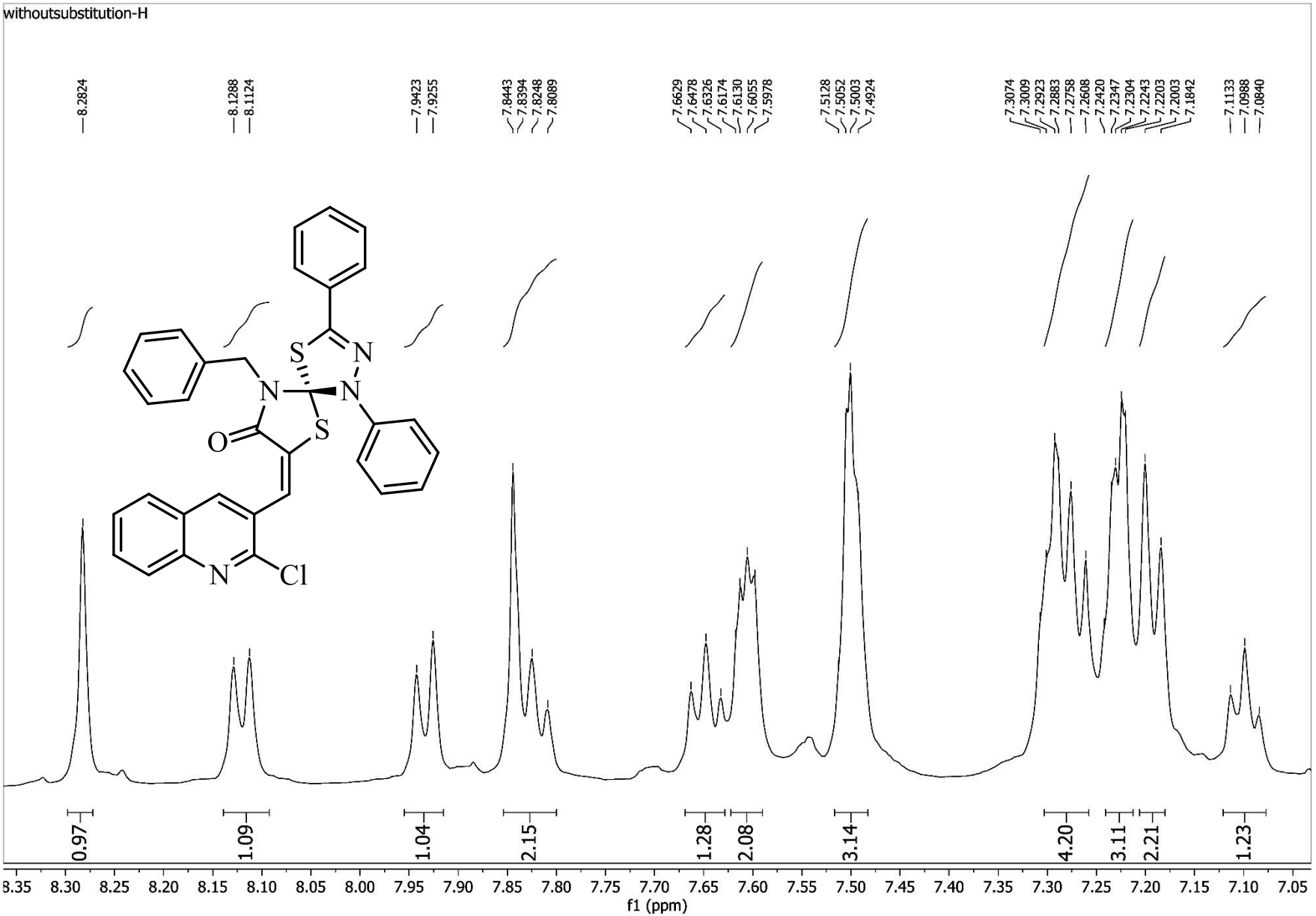
Yellow powder, m.p. = 150-152 °C, 0.51 g, yield: 83%. IR (KBr) (ν_{max}, cm^{-1}): 1682 (C=O), 1595 and 1639 (C=N), 1492 and 1575 (Ar), 744 (C-Cl), 590 (C-S). Anal. calcd. for $C_{35}H_{27}ClN_4OS_2$ (618.13): C, 67.89; H, 4.40; N, 9.05 %. Found C, 67.85; H, 4.43; N, 9.06 %. MS (EI, 70 eV): *m/z* (%): 410 (5), 371 (15), 332 (6), 244 (20), 208 (77), 183 (7), 135 (18), 91 (100), 65 (18). ^{1}H NMR (500.13 MHz, DMSO-d_6): 2.23 (3H, s, Me of Bn), 2.37 (3H, s, Me of Ar), 4.74 (1H, d, $^2J_{HH}$ = 15.6 Hz, CH_2), 4.89 (1H, d, $^2J_{HH}$ = 15.6 Hz, CH_2), 7.03 (2H, d, $^3J_{HH}$ = 7.8 Hz, CH_{ortho} of Ph), 7.10 (1H, t, $^3J_{HH}$ = 7.4 Hz, CH_{para} of Ph), 7.17 (2H, d, $^3J_{HH}$ = 7.7 Hz, CH_{meta} of Bn), 7.18 (2H, d, $^3J_{HH}$ = 7.7 Hz, CH_{ortho} of Bn), 7.28 (2H, t, $^3J_{HH}$ = 7.2 Hz, CH_{meta} of Ph), 7.31 (2H, d, $^3J_{HH}$ = 8.5 Hz, CH of Ar), 7.50 (2H, d, $^3J_{HH}$ = 8.3 Hz, CH of Ar), 7.67 (1H, t, $^3J_{HH}$ = 7.0 Hz, CH^7 of quinoline), 7.83 (1H, s, CH), 7.85 (1H, t, $^3J_{HH}$ = 7.0 Hz, CH^6 of quinoline), 7.96 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH^5 of quinoline), 8.16 (1H, d, $^3J_{HH}$ = 6.7 Hz, CH^8 of quinoline), 8.31 (1H, s, CH^4 of quinoline). ^{13}C NMR (125.77 MHz, DMSO-d_6): 21.15 (Me of Bn), 21.48 (Me of Ar), 46.85 (CH_2), 106.38 (C^5_{spiro}), 120.45 (CH_{para} of Ph), 120.75 (CH_{ortho} of Ph), 125.35 (CH), 126.76 ($CH^{6'}$ of quinoline), 127.05 ($CH^{5'}$ of quinoline), 127.44 (C_{ipso} of Ar), 128.08 ($C^{3'}$ of quinoline), 128.50 (CH_{ortho} of Bn), 128.52 ($CH^{8'}$ of quinoline), 128.95 ($C^{4a'}$ of quinoline), 129.18 ($CH^{7'}$ of quinoline), 129.30 (CH_{meta} of Ph), 129.45 (CH_{meta} of Bn), 130.18 (CH of Ar), 132.42 ($CH^{4'}$ of quinoline), 137.18 (C_{ipso}-*Me* of Bn), 137.97 (C_{ipso} of Ph), 140.69 (C^7), 141.05 (C_{ipso}-*Me* of Ar), 143.39 (C^3), 146.40 ($C^{8a'}$ of quinoline), 149.87 ($C^{2'}$ of quinoline), 163.74 (C^8).



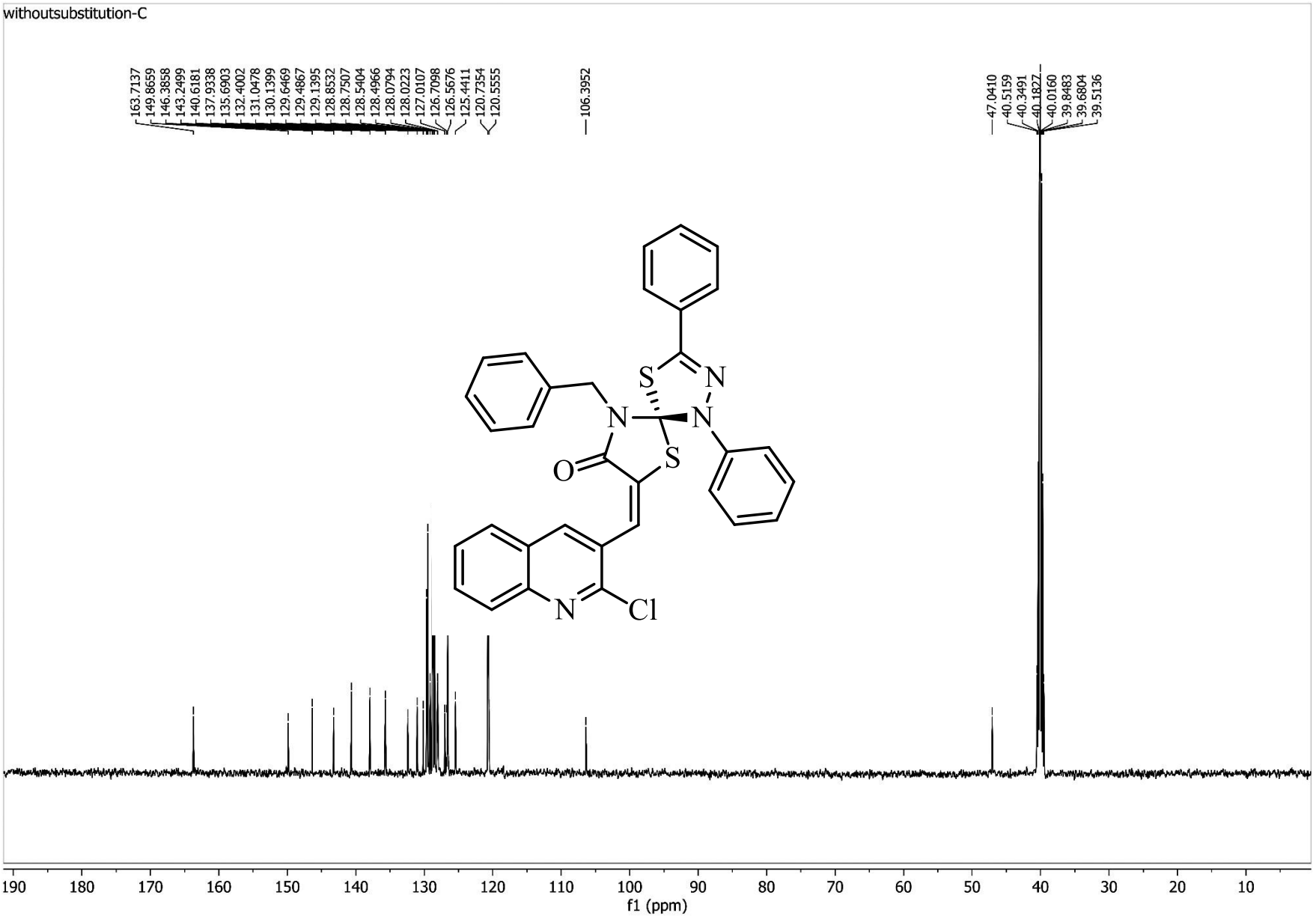
IR Spectrum of **7a**



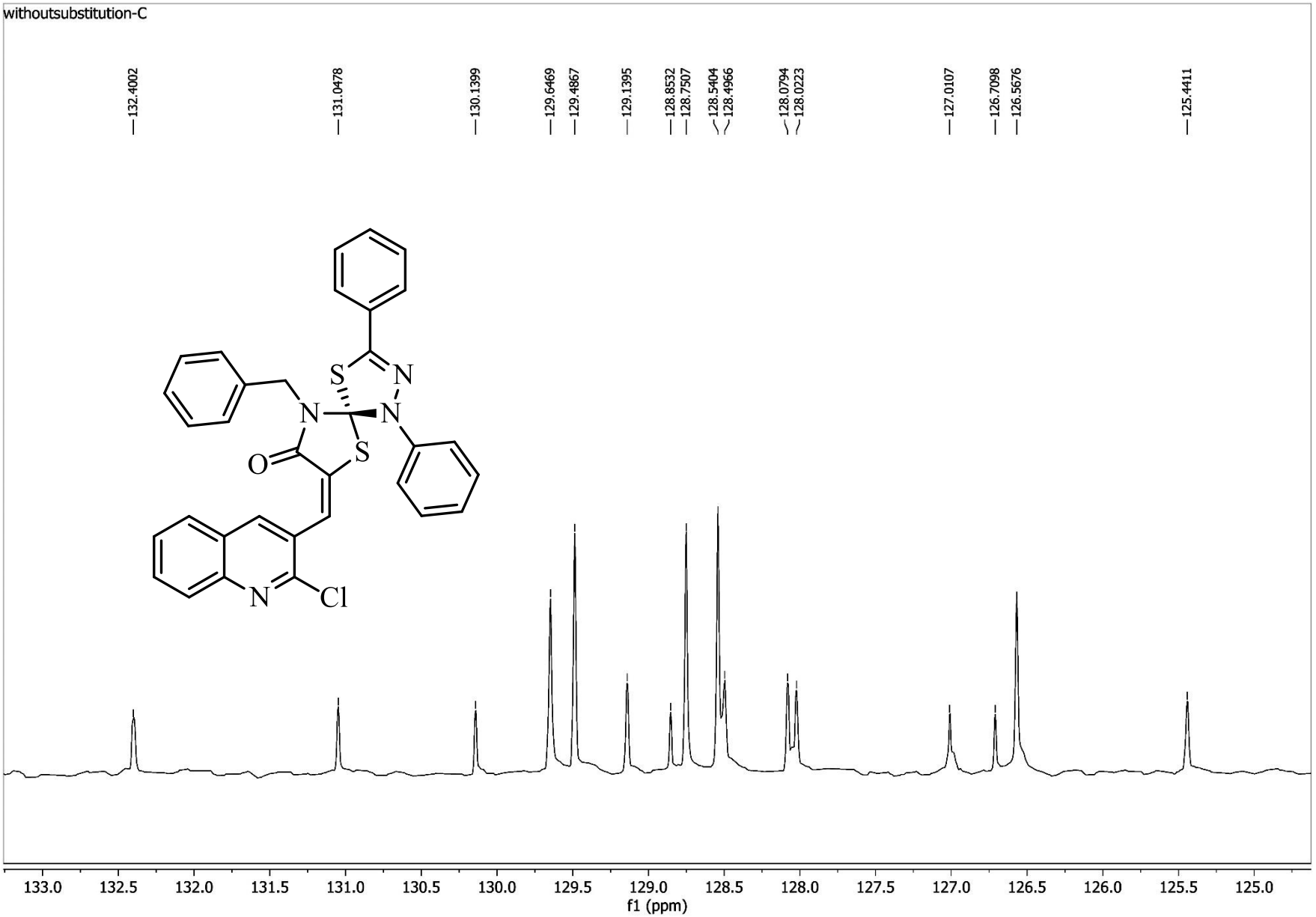
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7a**



Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7a**

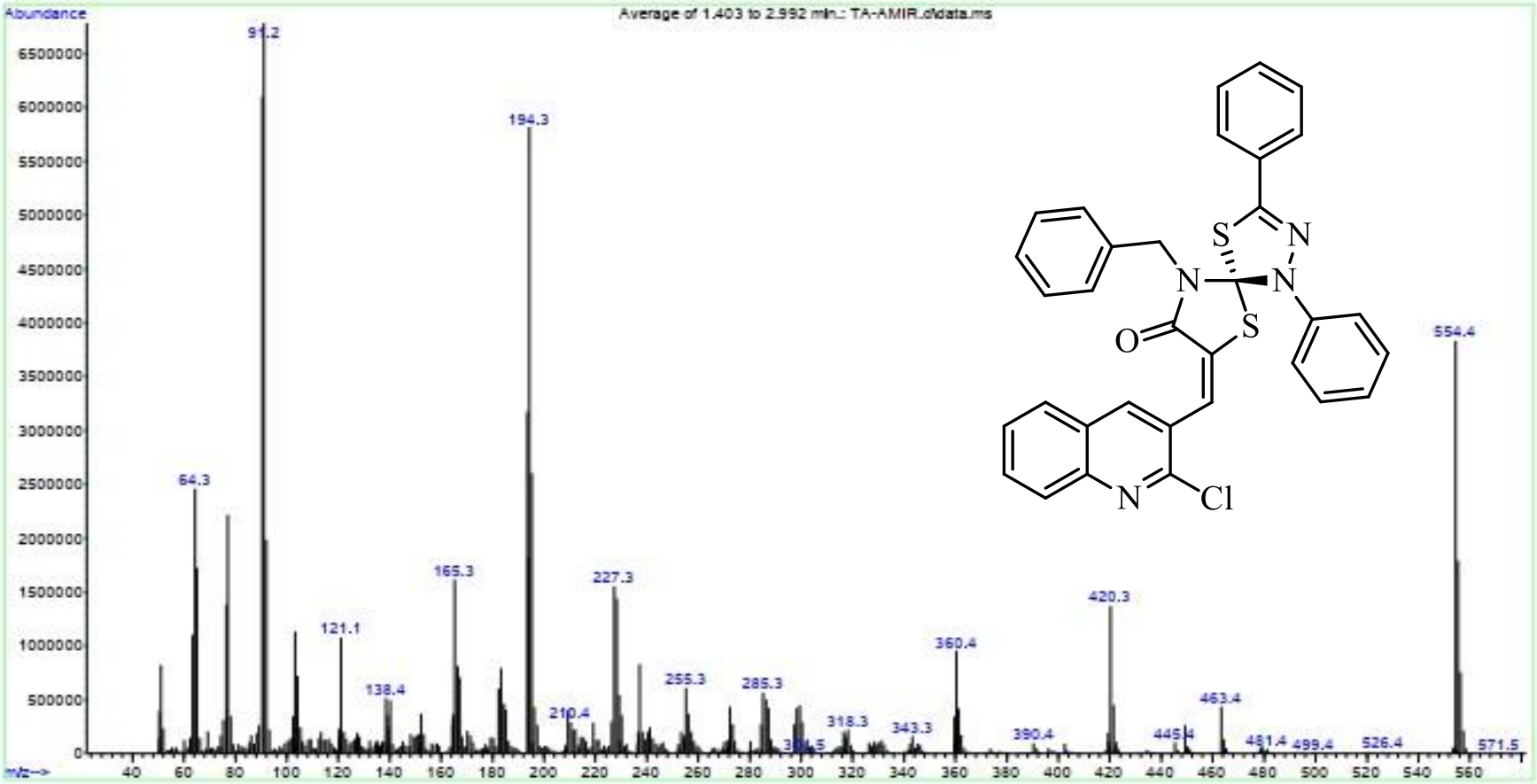


^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7a**

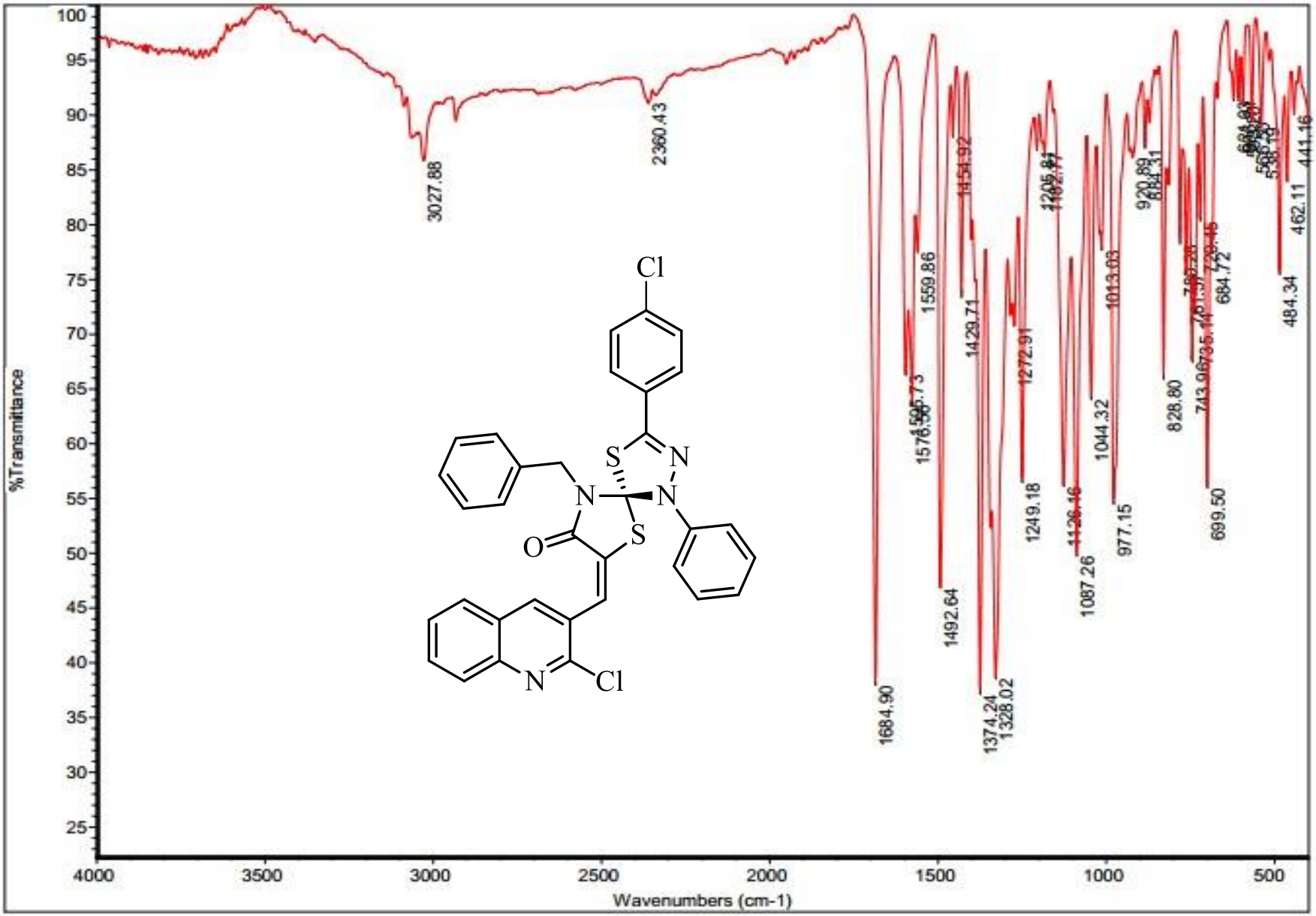


Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7a**

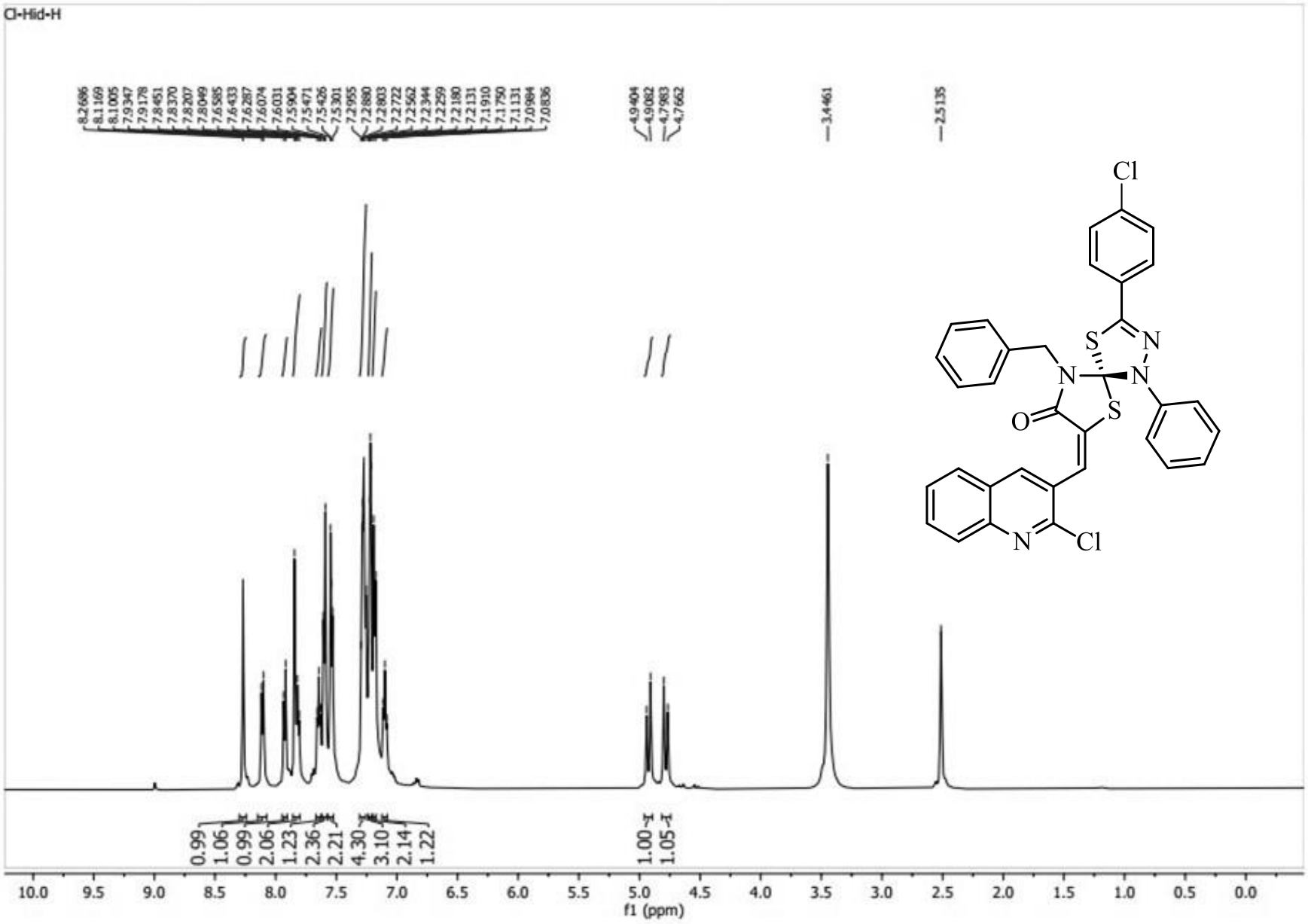
File :C:\MSDCHEM\3\DATA\Snapshot\TA-AMIR.d
Operator :
Acquired : 27 Jul 2021 11:25 using AcqMethod default.m
Instrument : DIRECT PROBE
Sample Name:
Misc Info :
Vial Number: 1



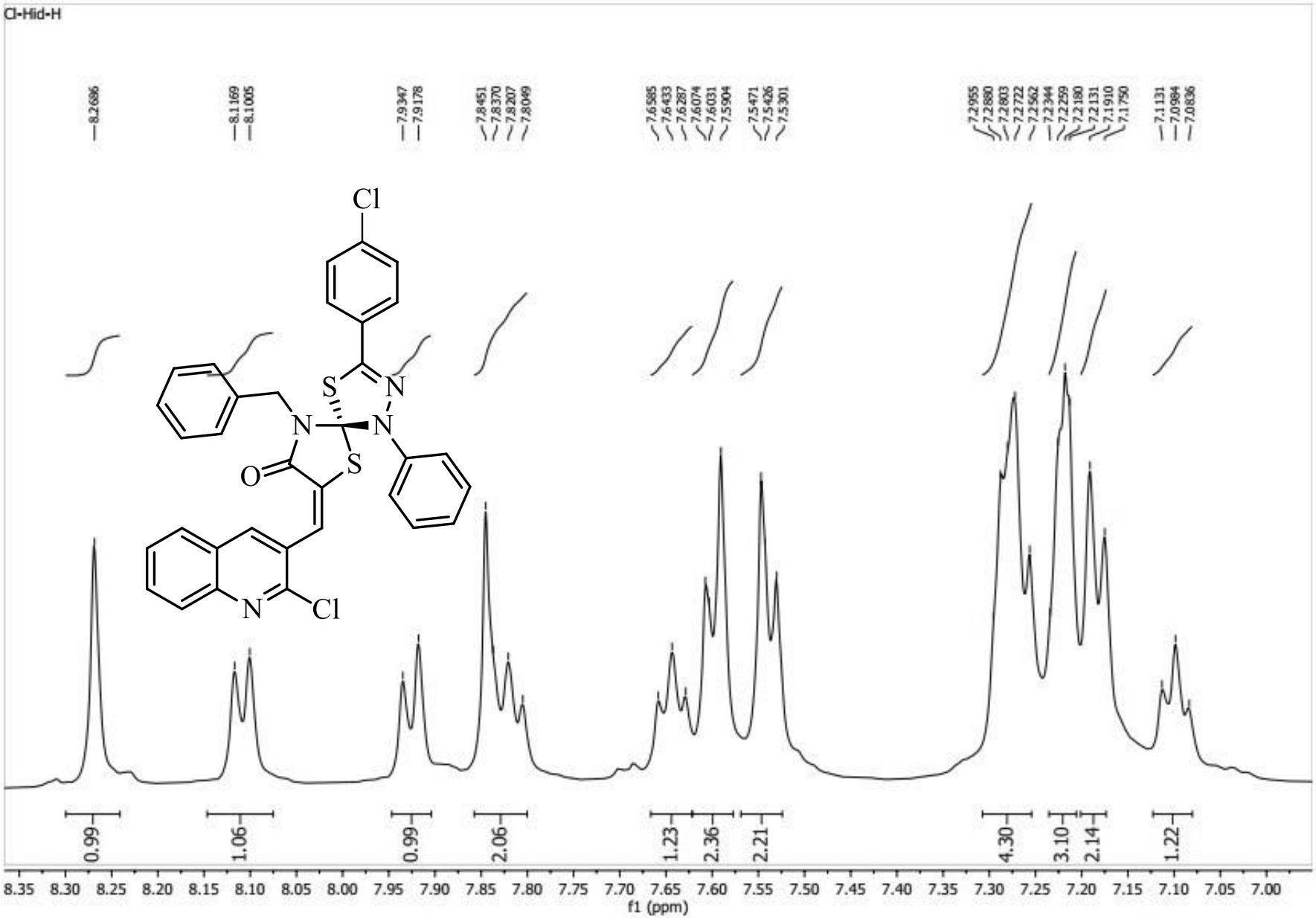
Mass Spectrum of **7a**



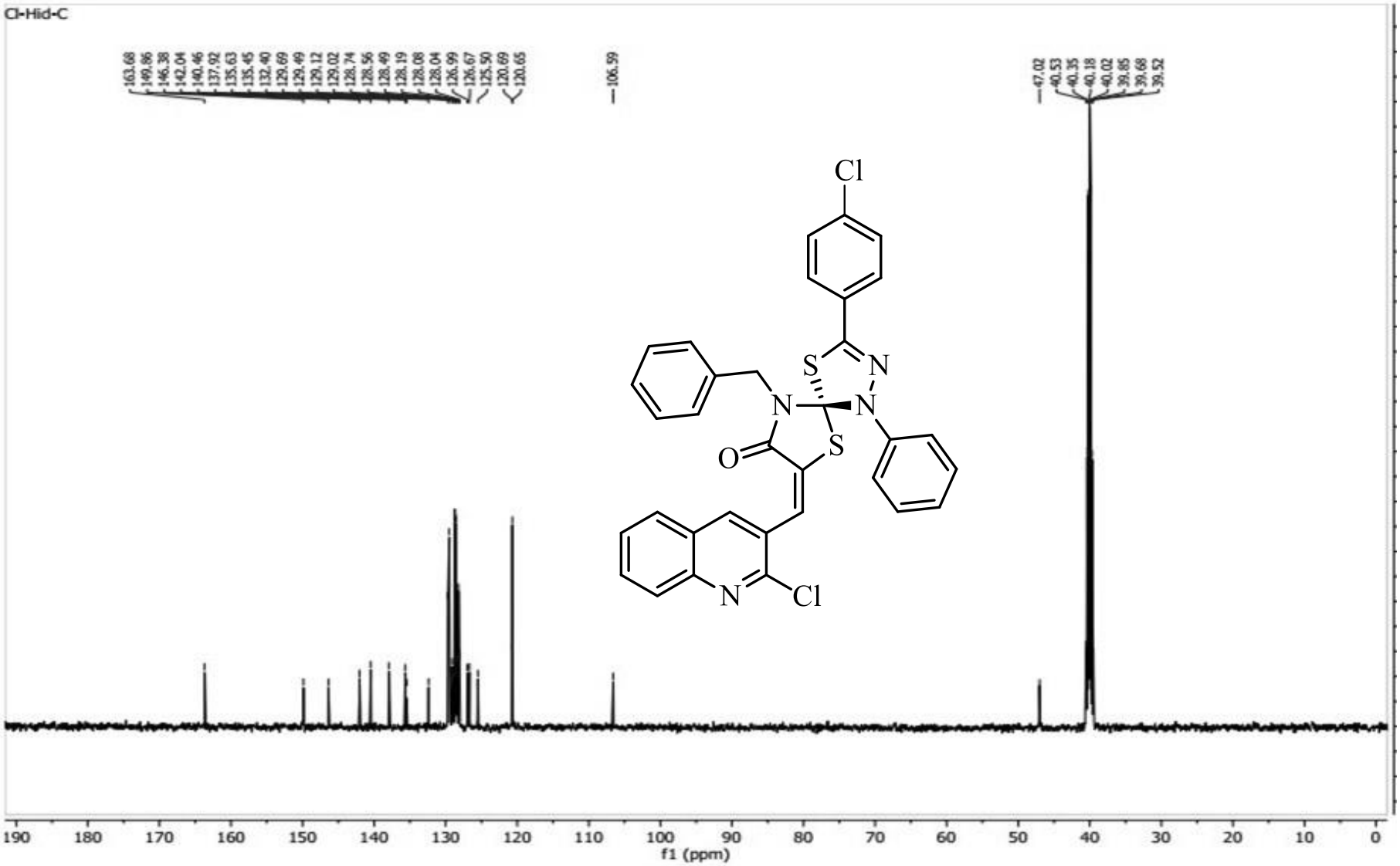
IR Spectrum of **7b**



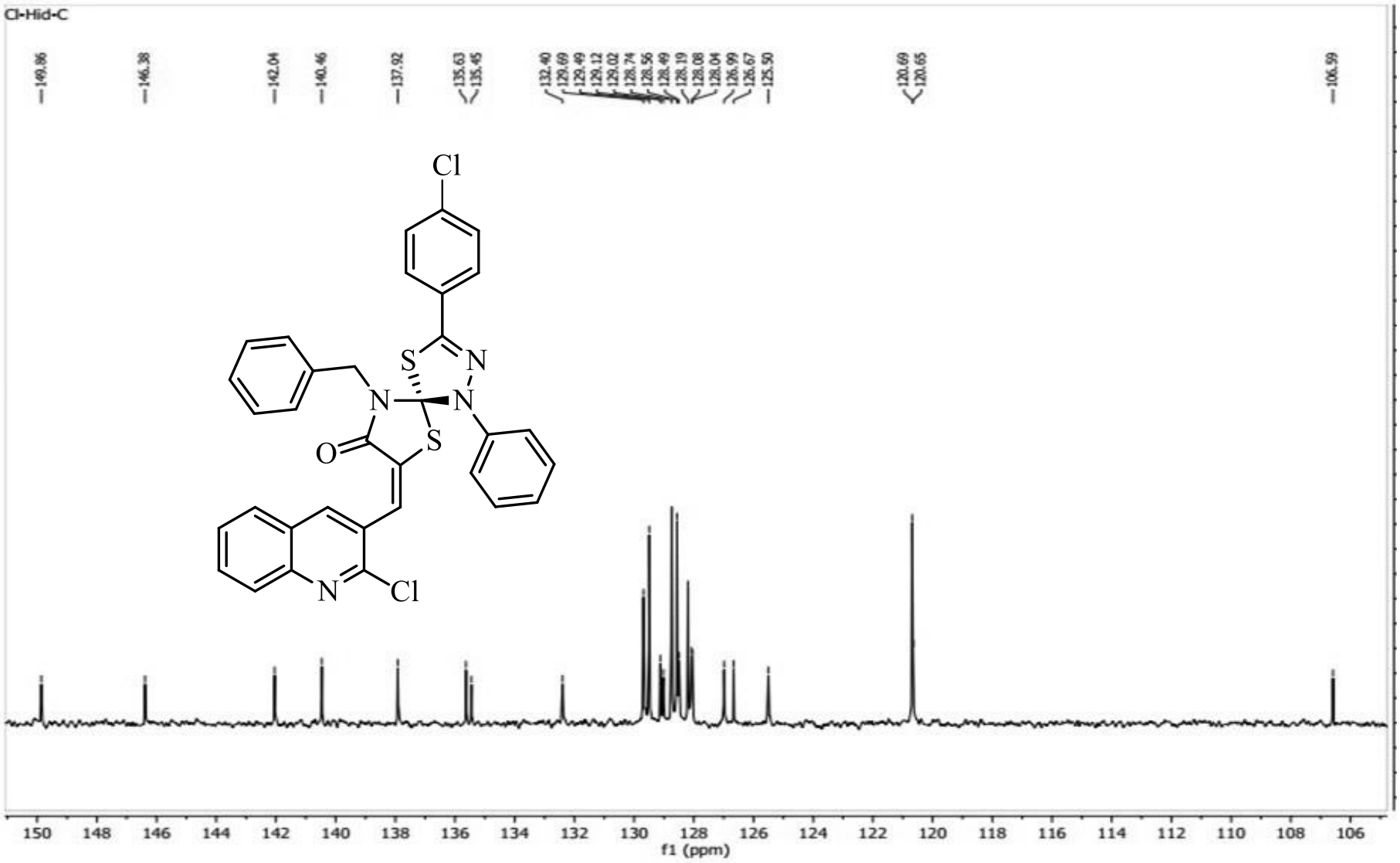
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7b**



Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7b**



^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7b**



Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7b**

File :C:\MSDCHEM\3\DATA\Snapshot\140109304.D
Operator :
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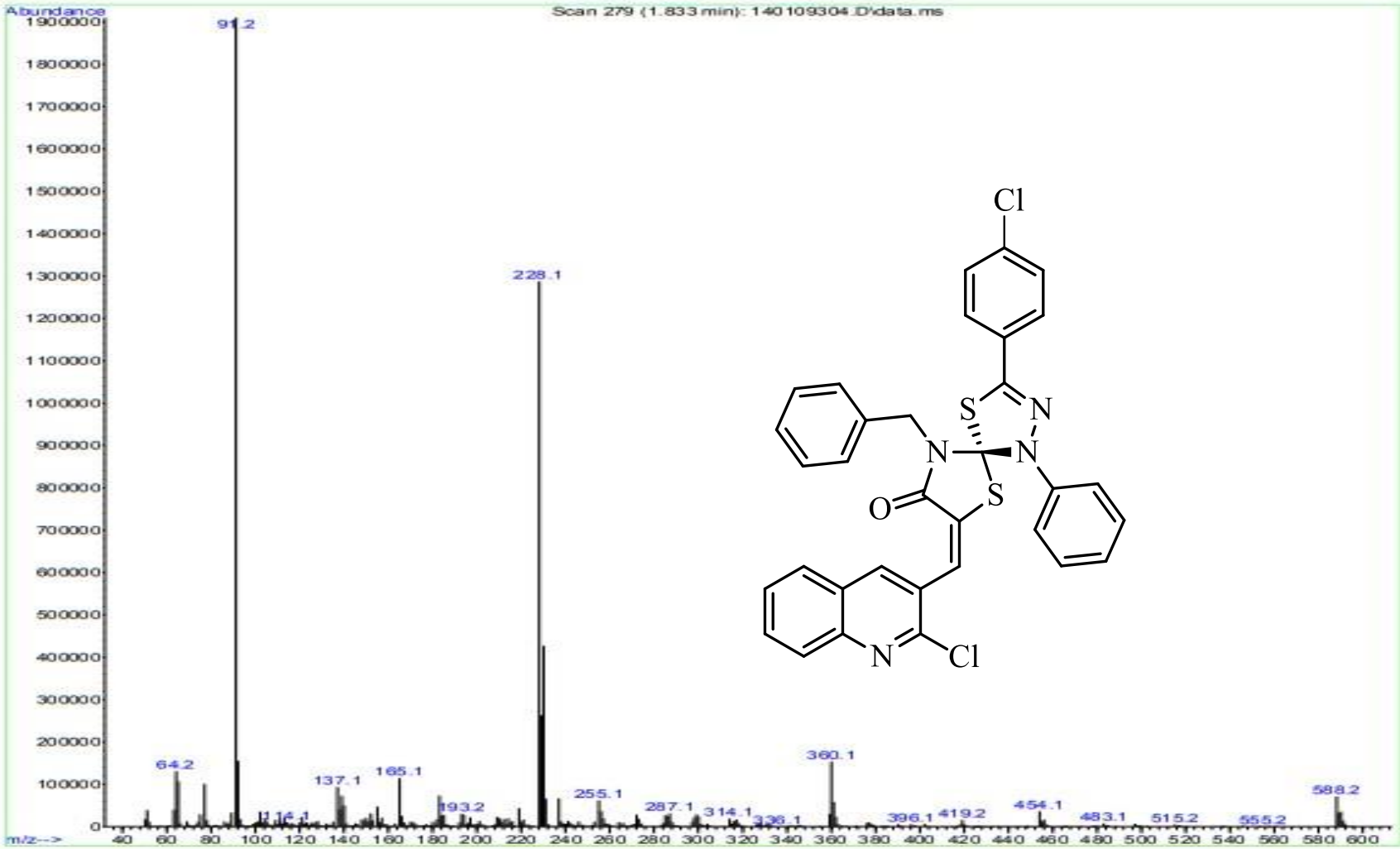
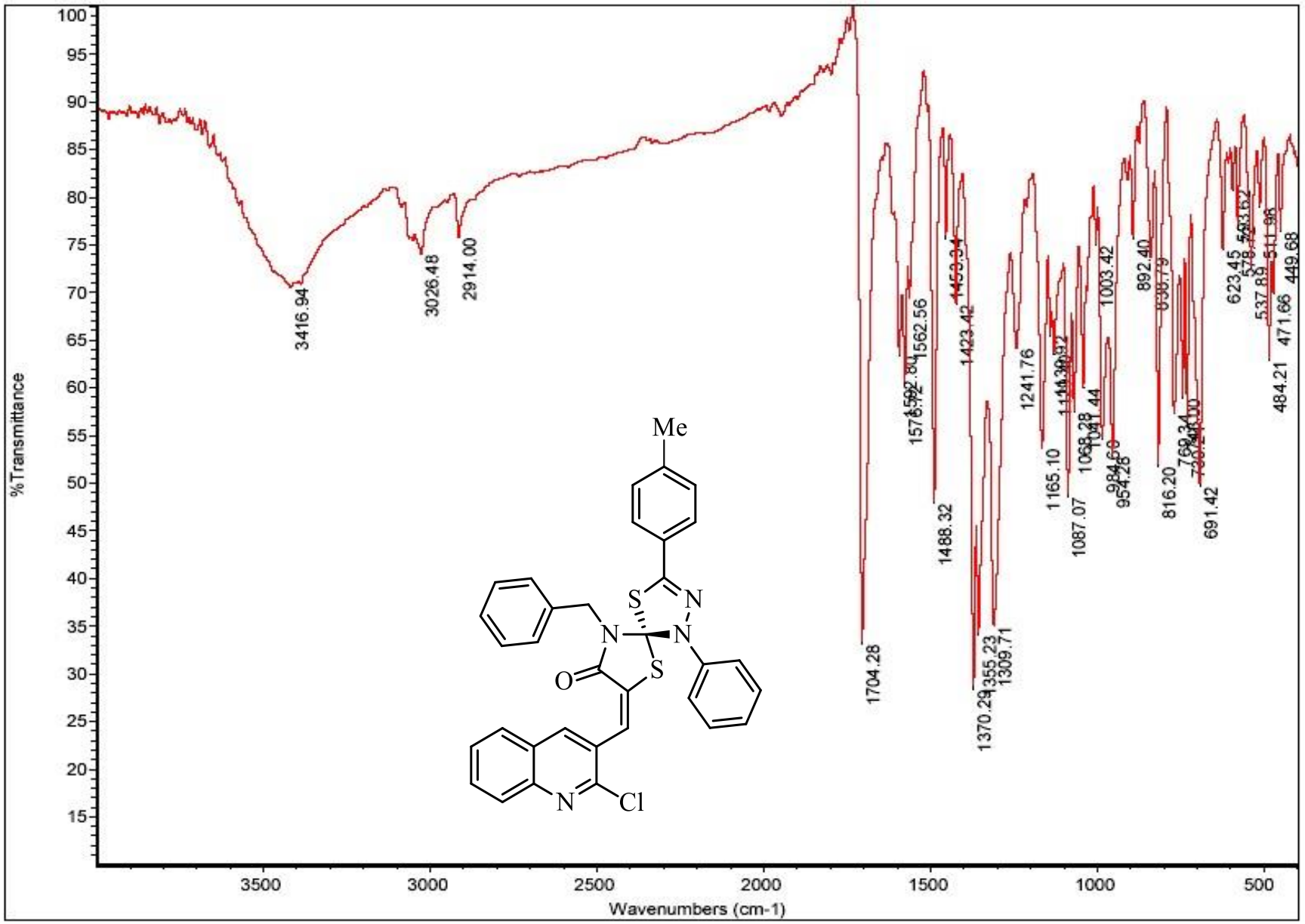
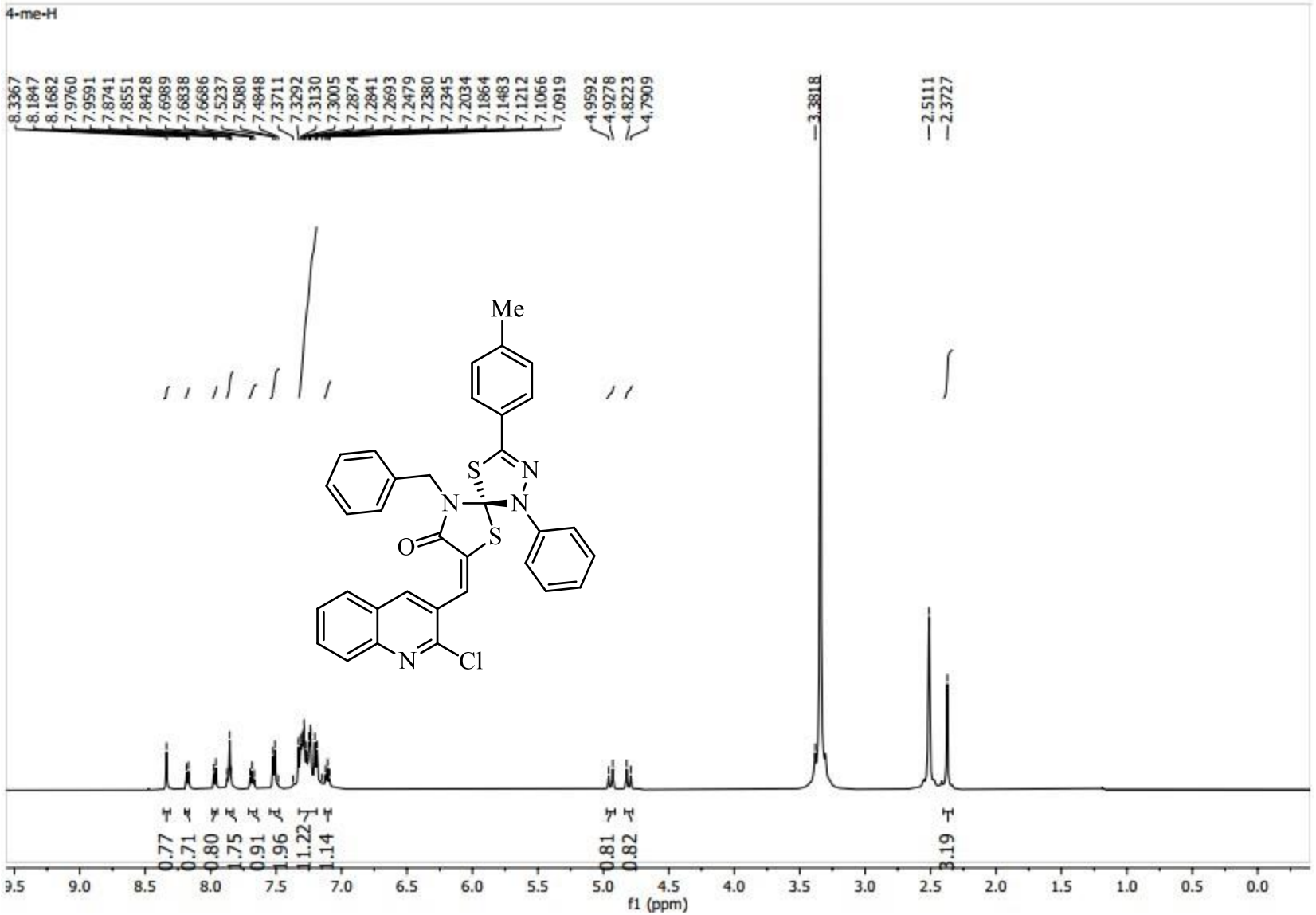
Instrument : MSD
Sample Name: B
Misc Info :
Vial Number: 1



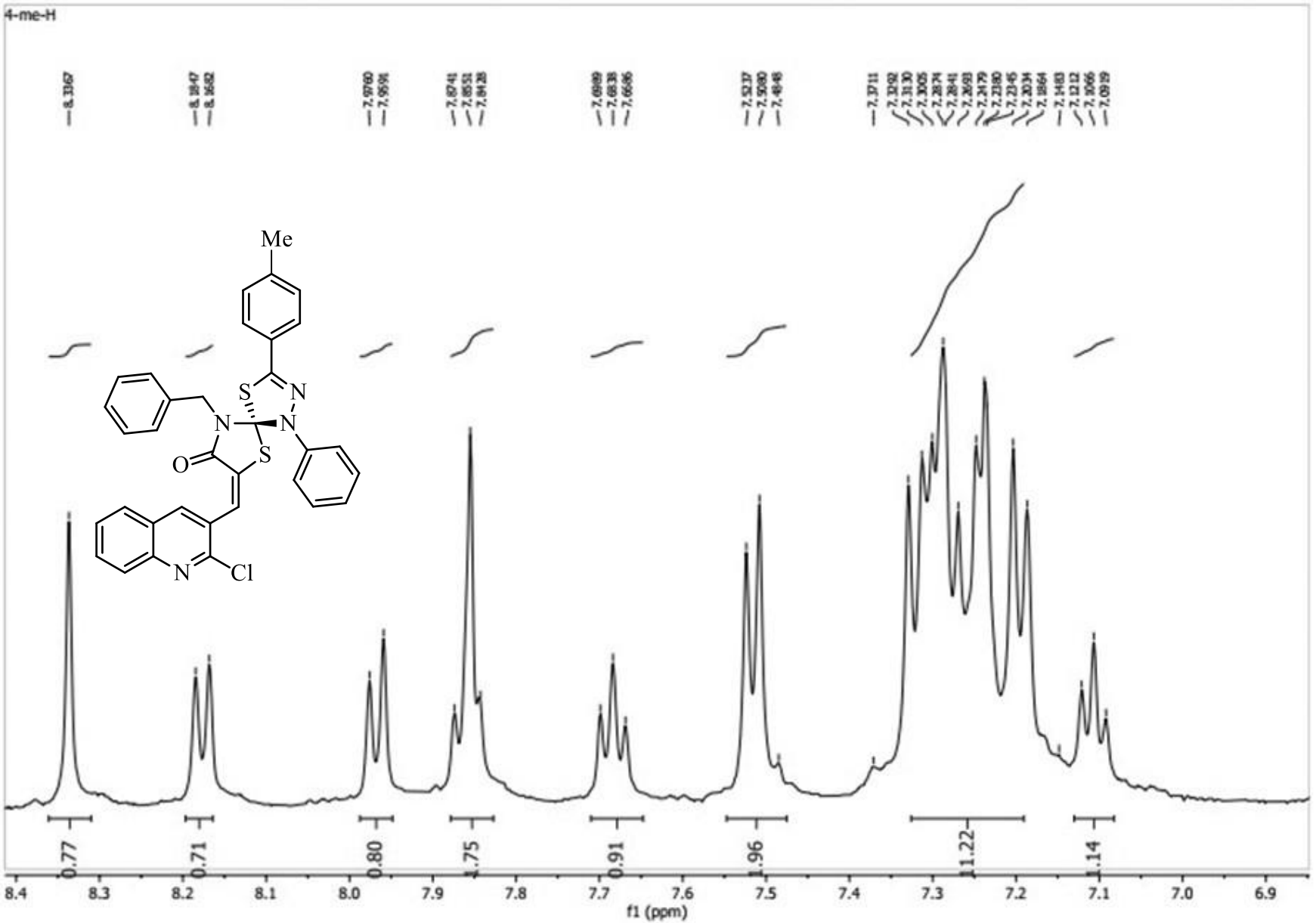
Mass Spectrum of **7b**



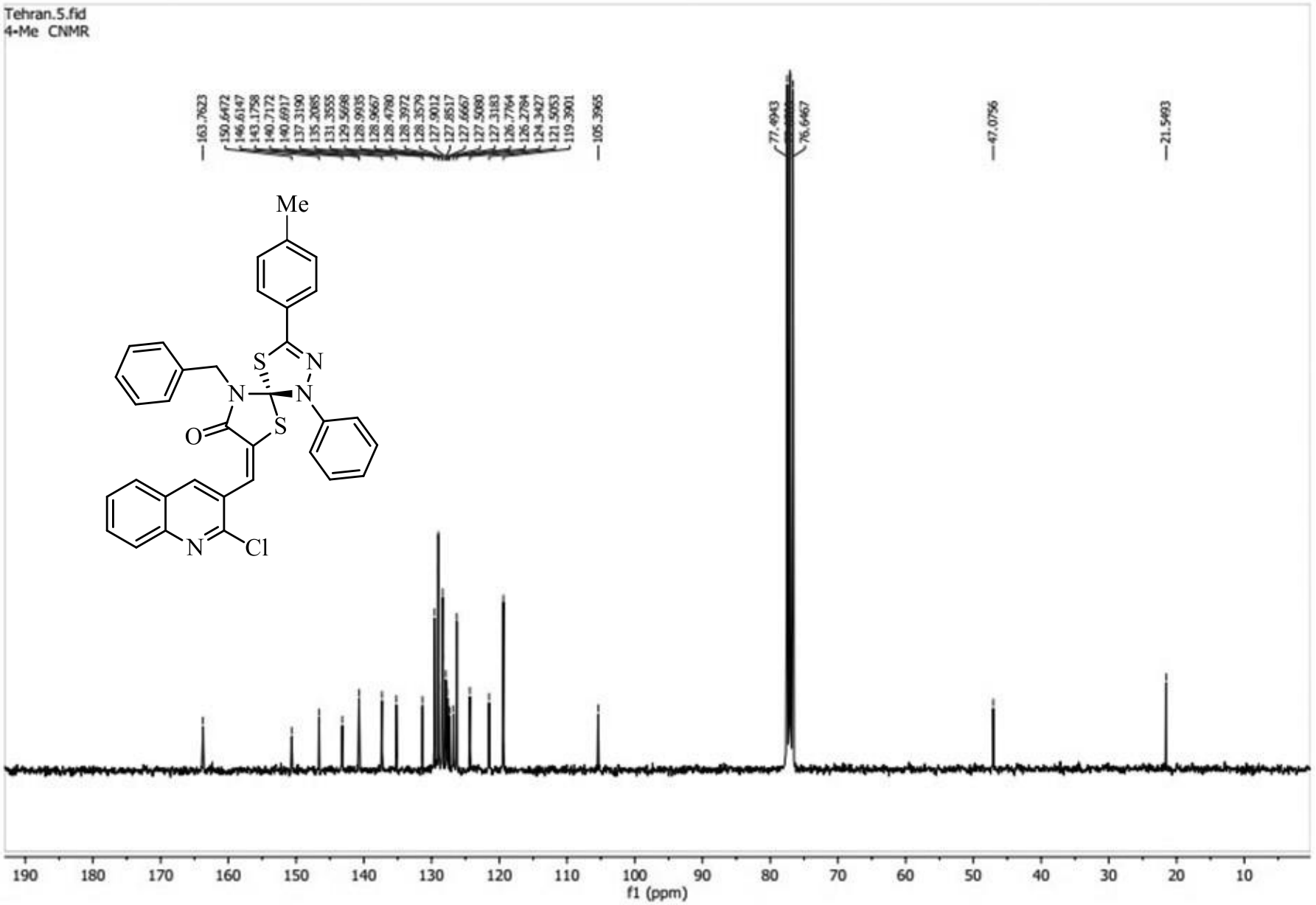
IR Spectrum of **7c**



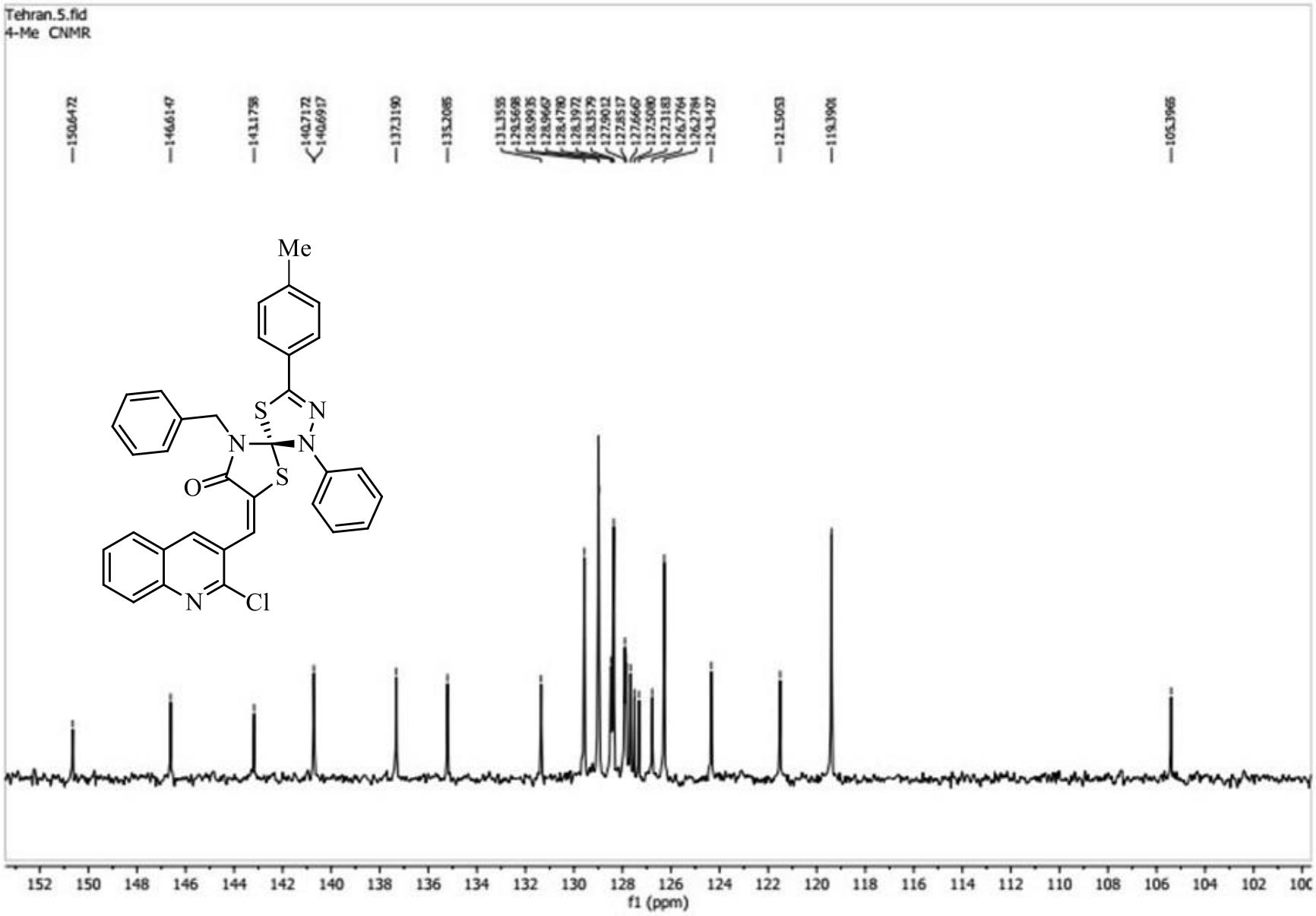
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7c**



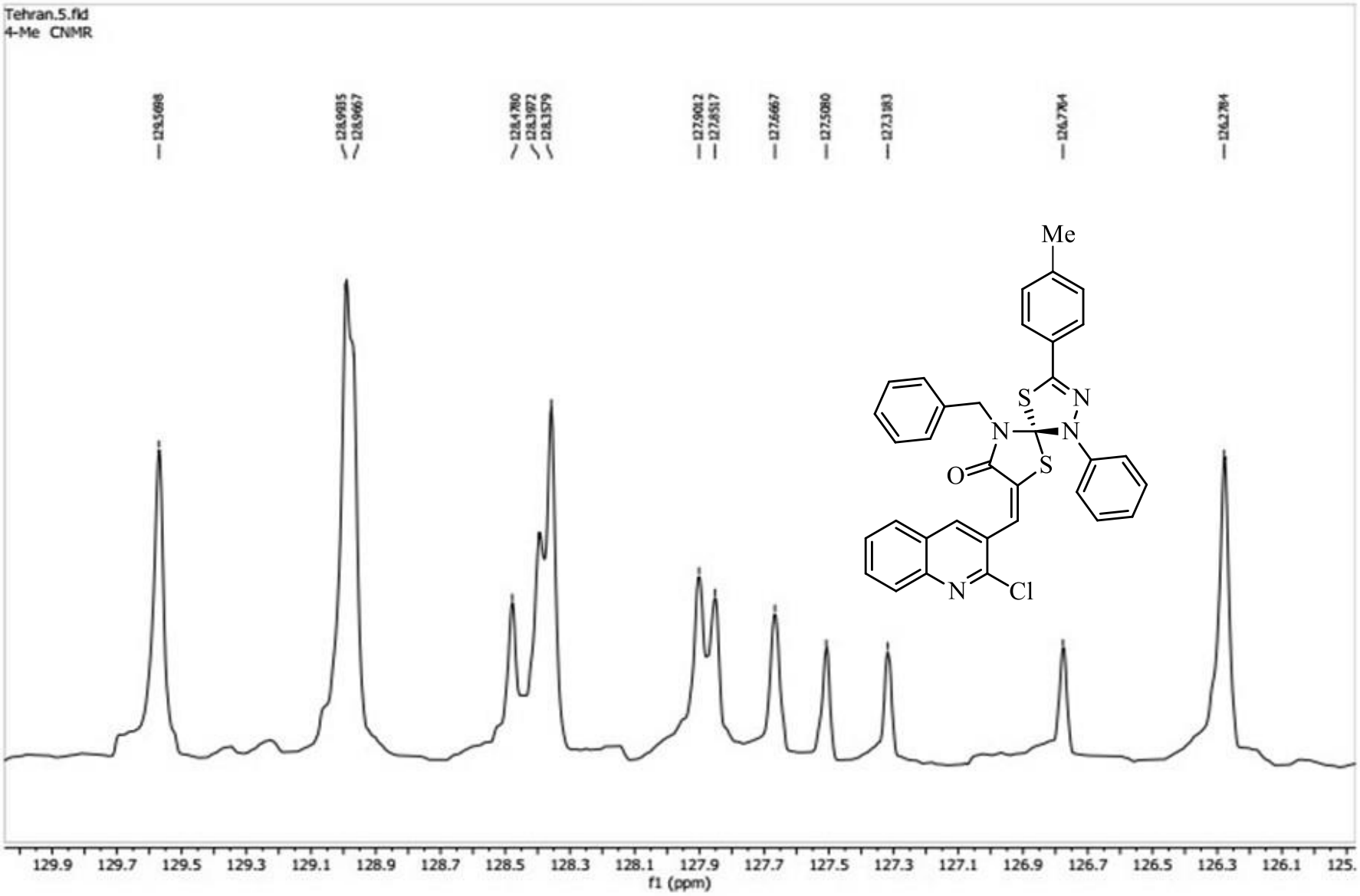
Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7c**



^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7c**

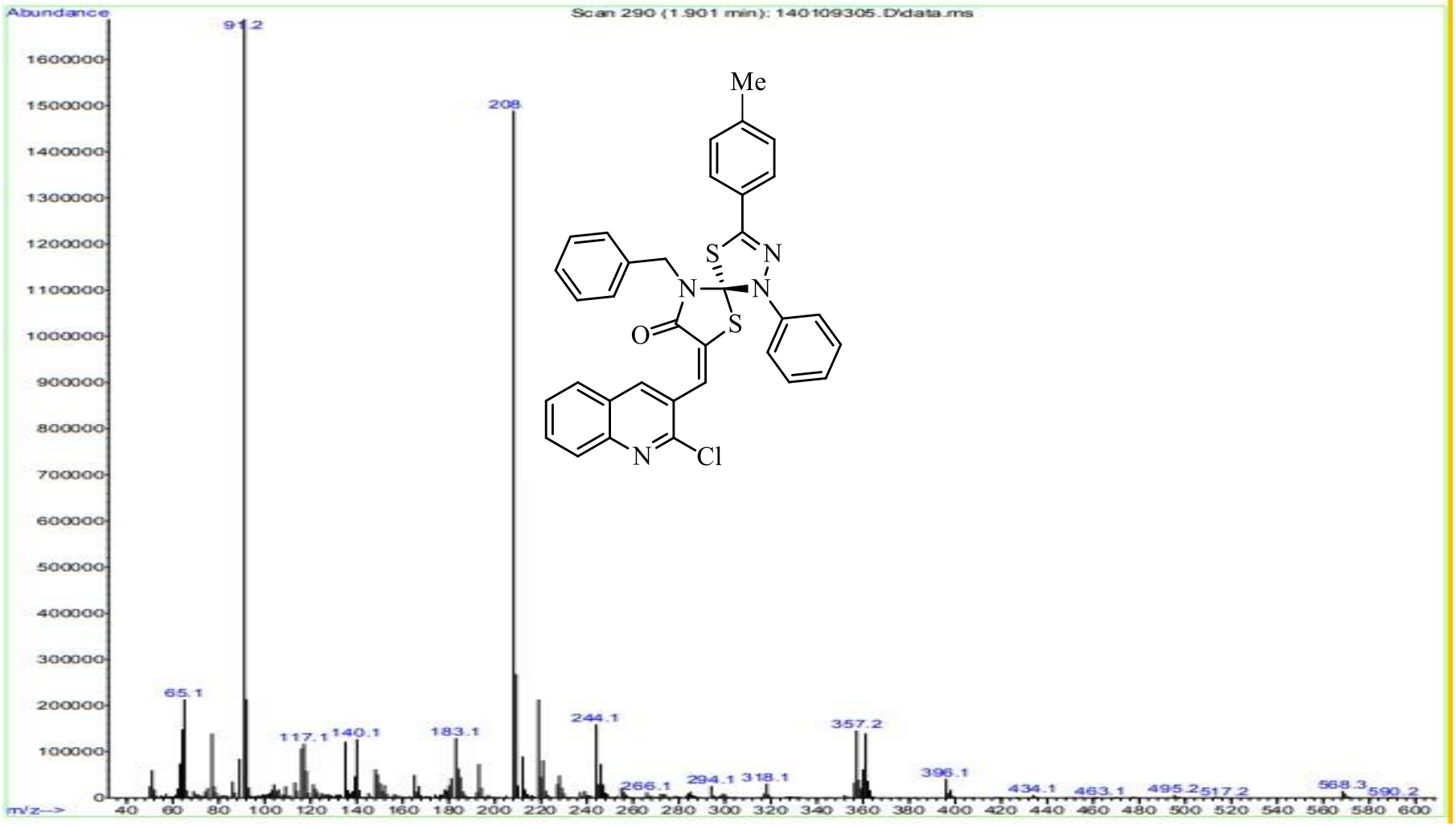


Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7c**

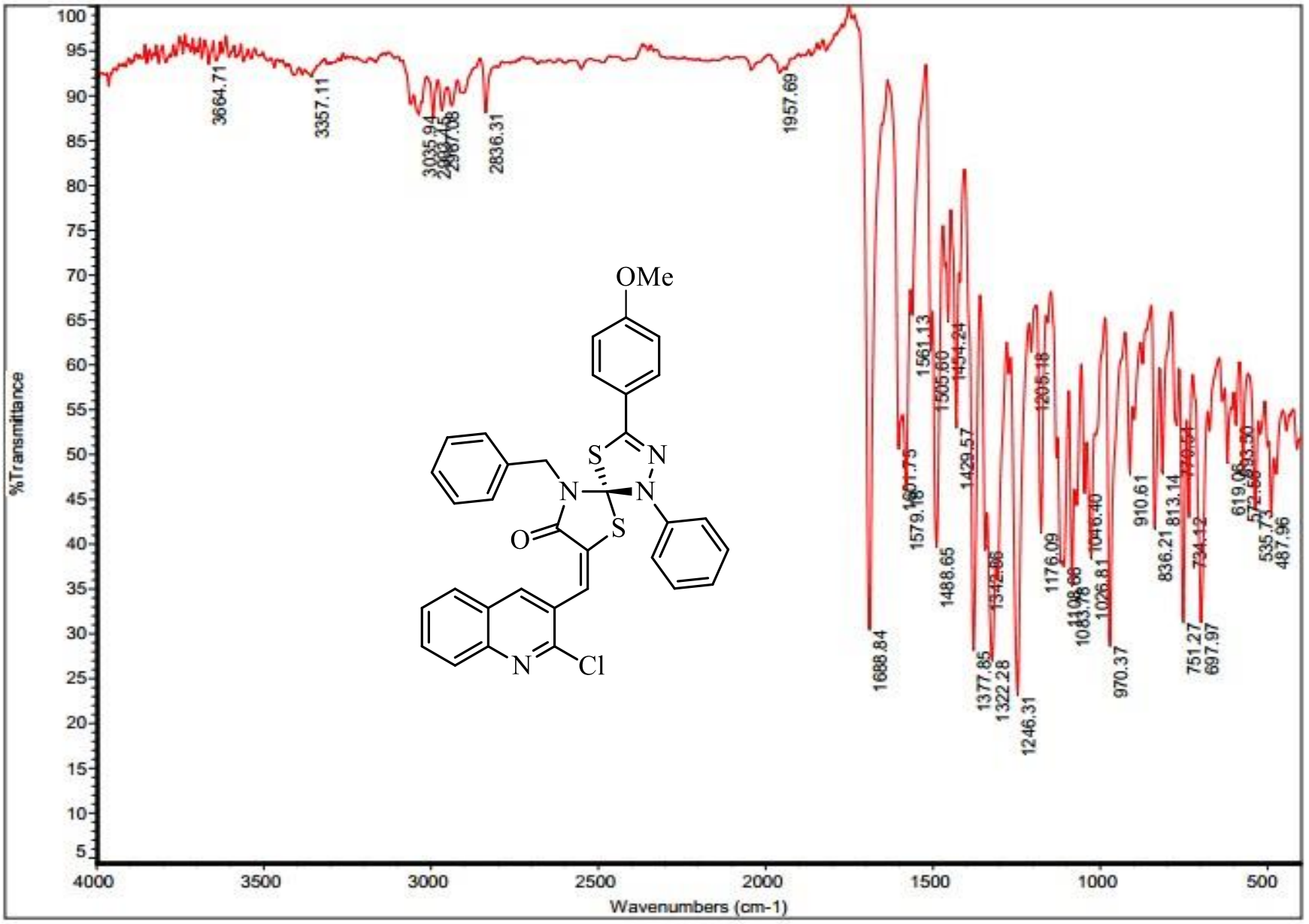


Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7c**

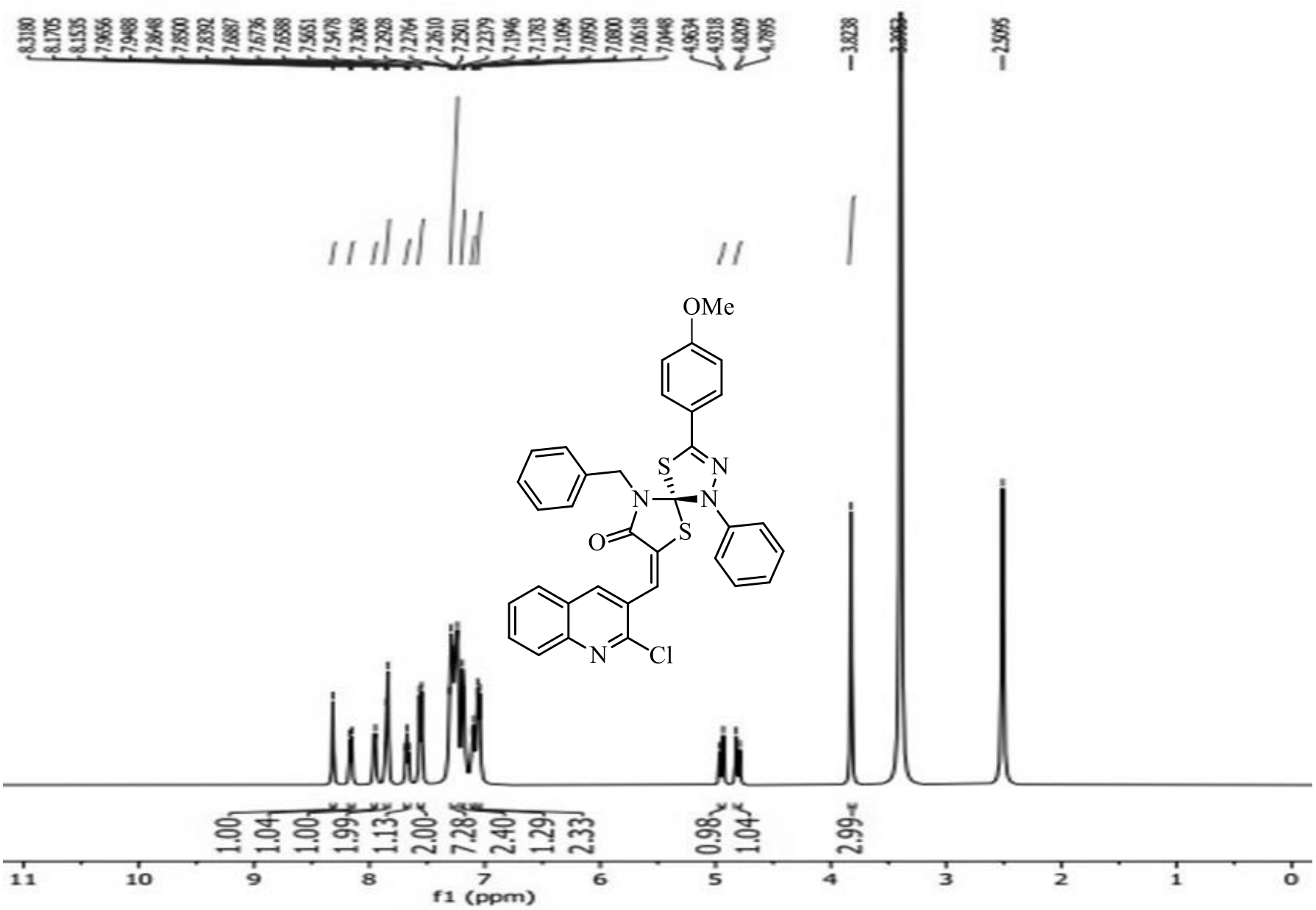
File :C:\MSDCHEM\3\DATA\Snapshot\140109305.D
Operator :
Acquired : 3 Jan 2007 2:35 using AcqMethod tast.M
Instrument : MSD
Sample Name: C
Misc Info :
Vial Number: 1



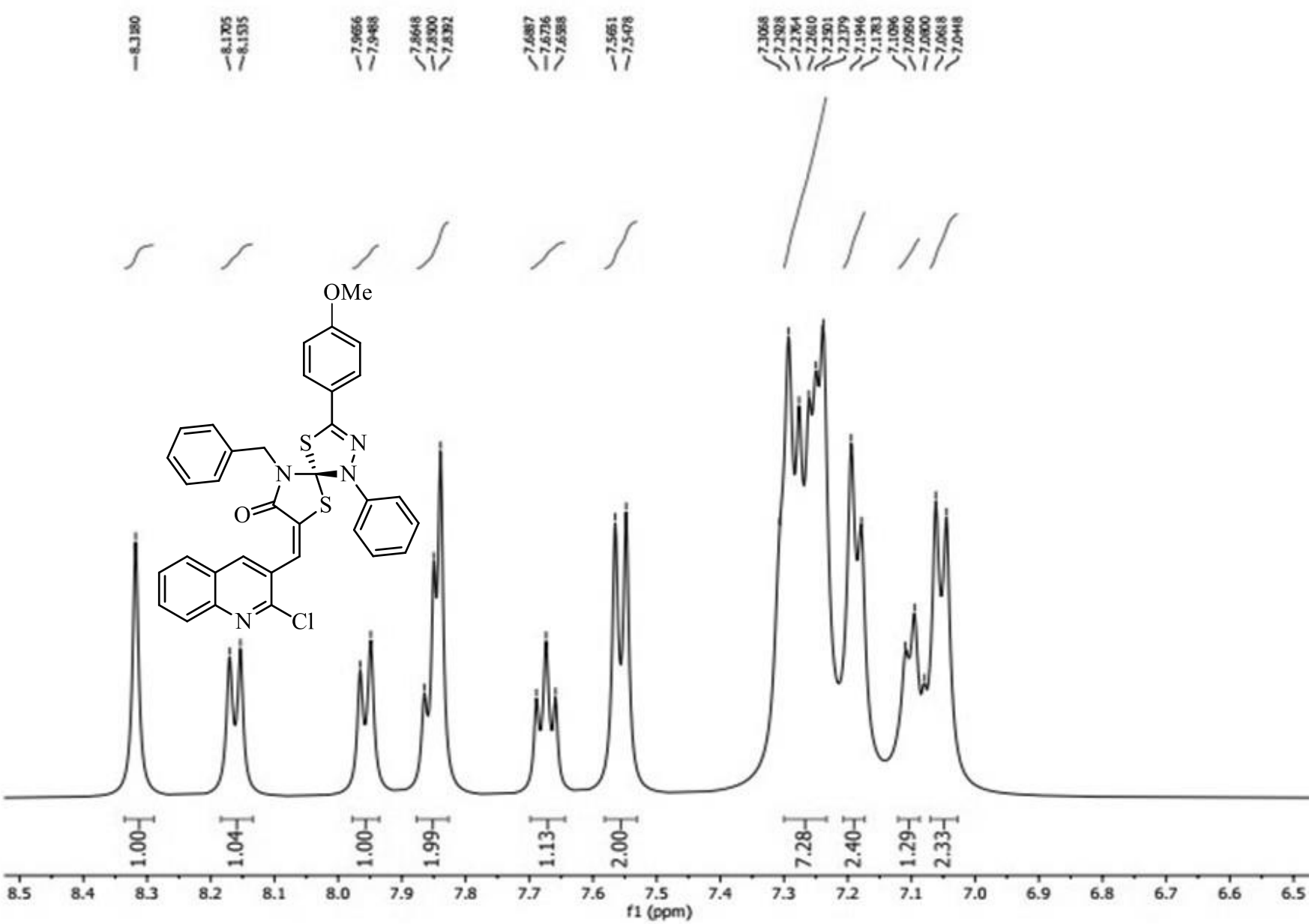
Mass Spectrum of **7c**



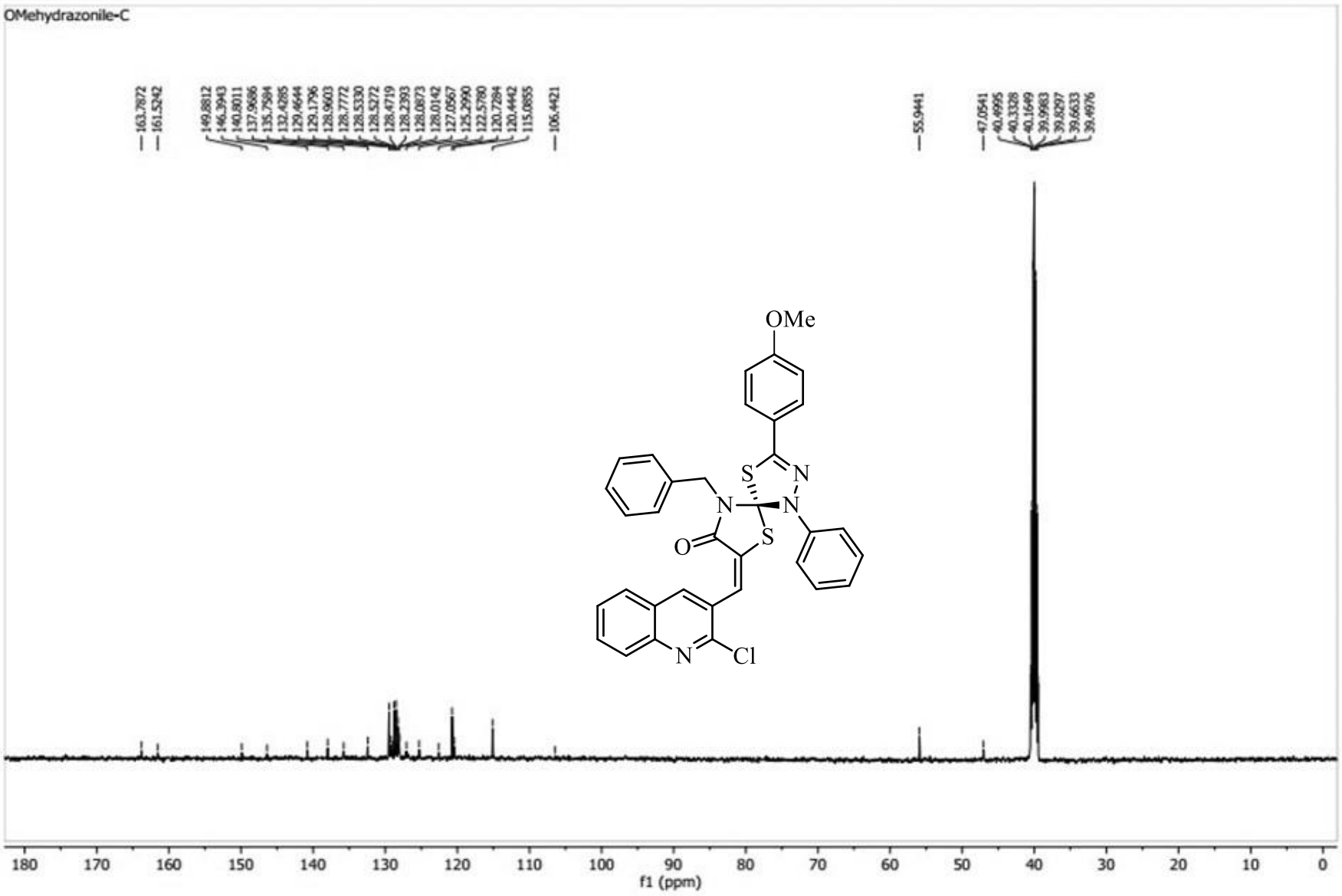
IR Spectrum of **7d**



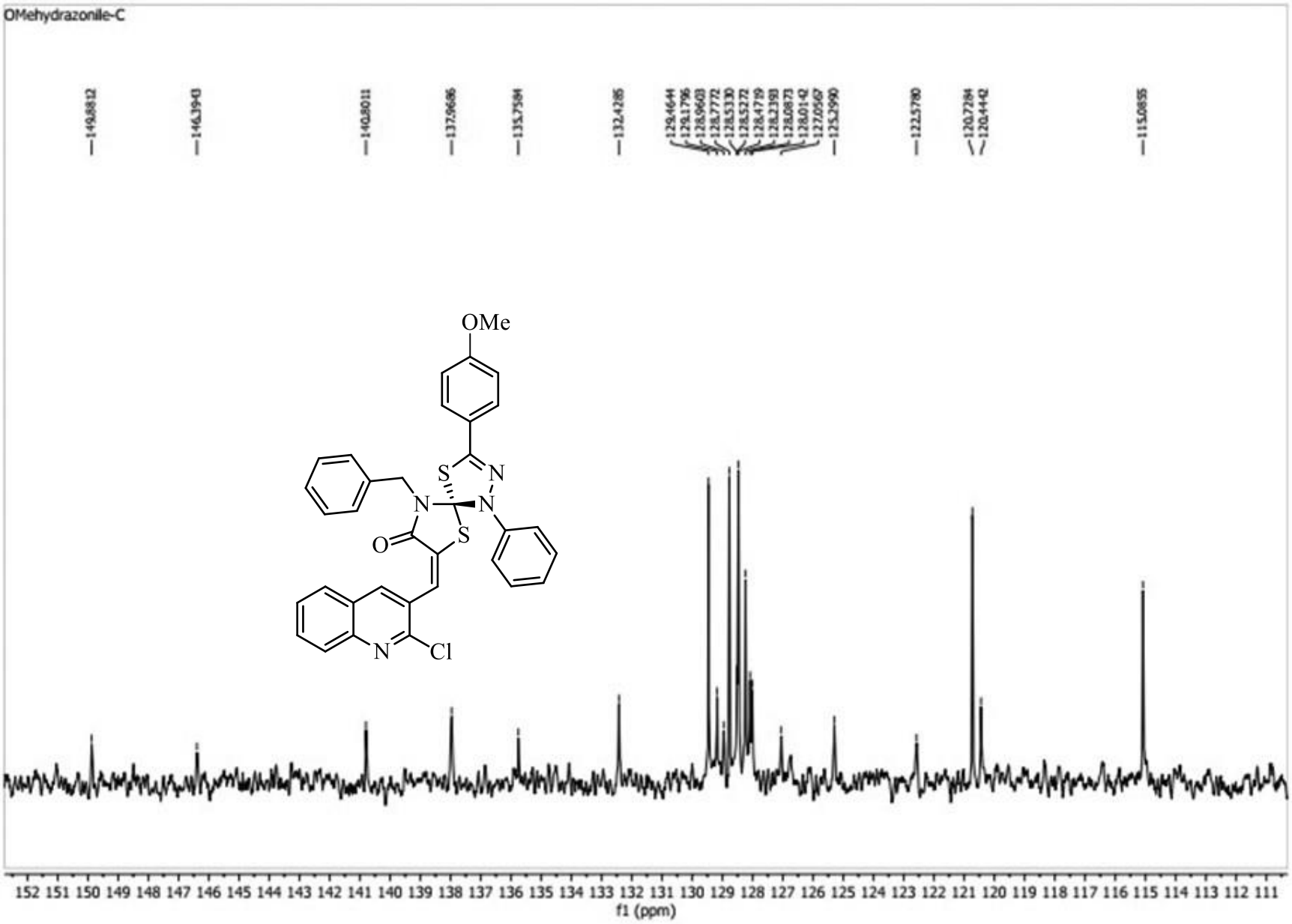
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7d**



Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7d**

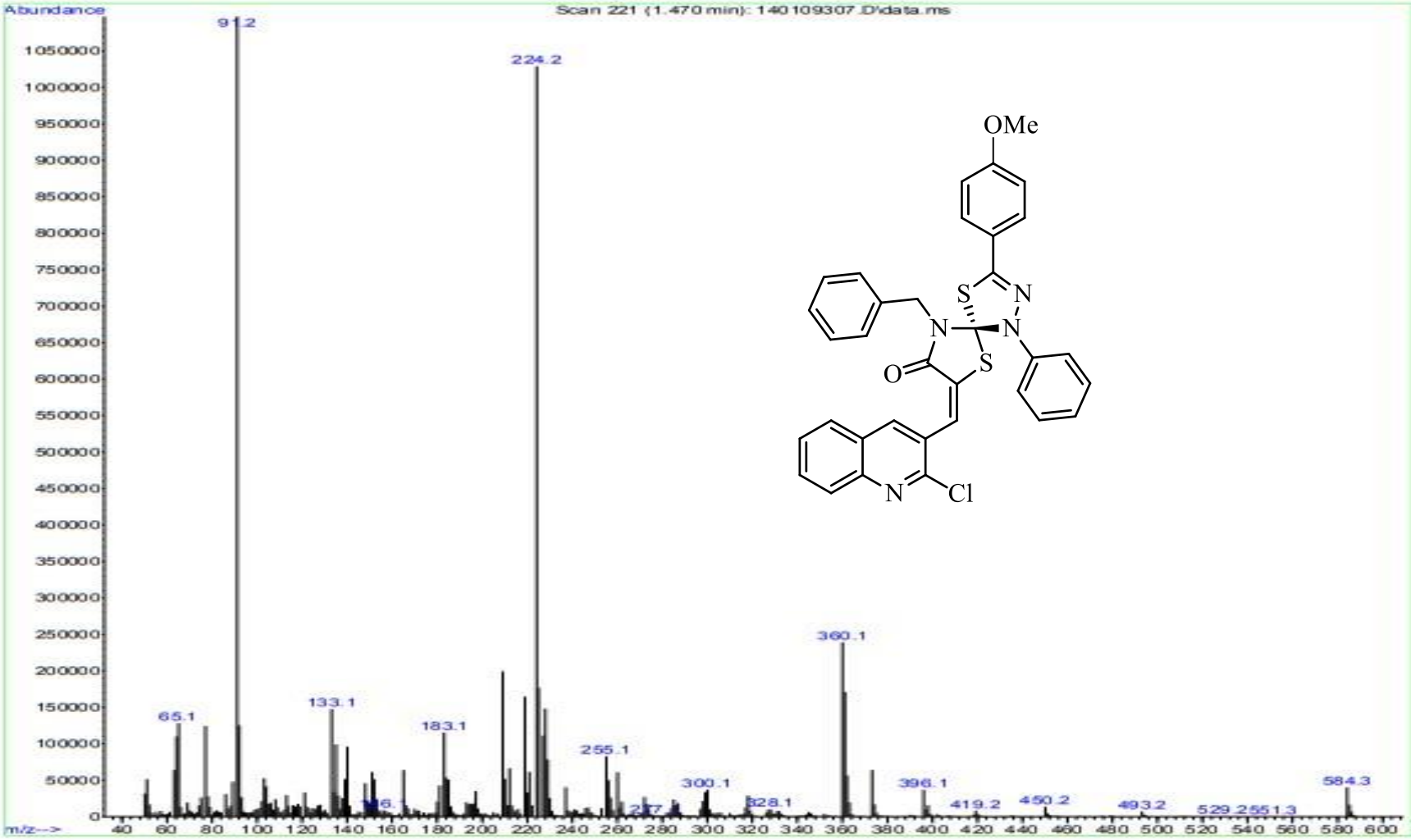


^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7d**

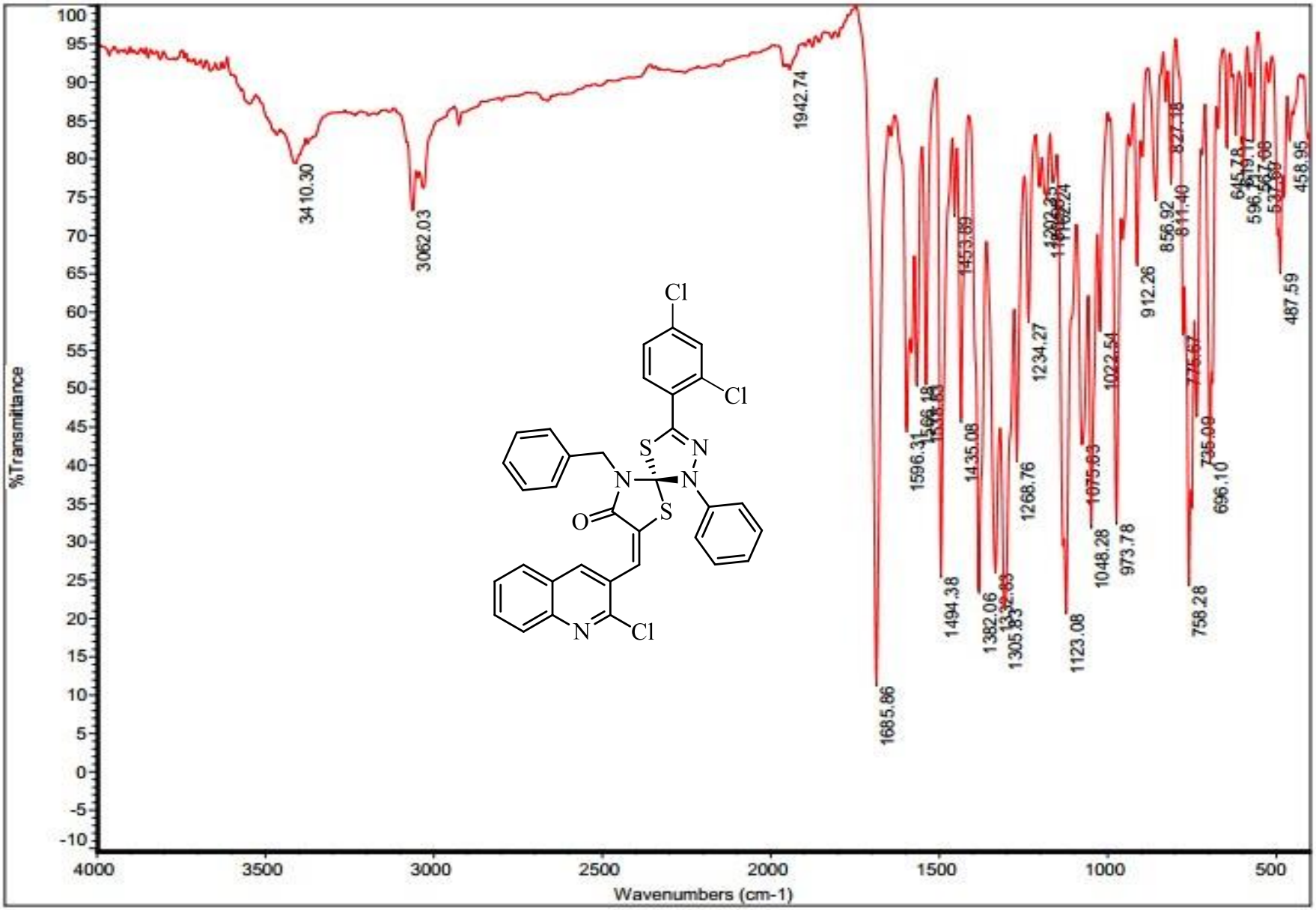


Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7d**

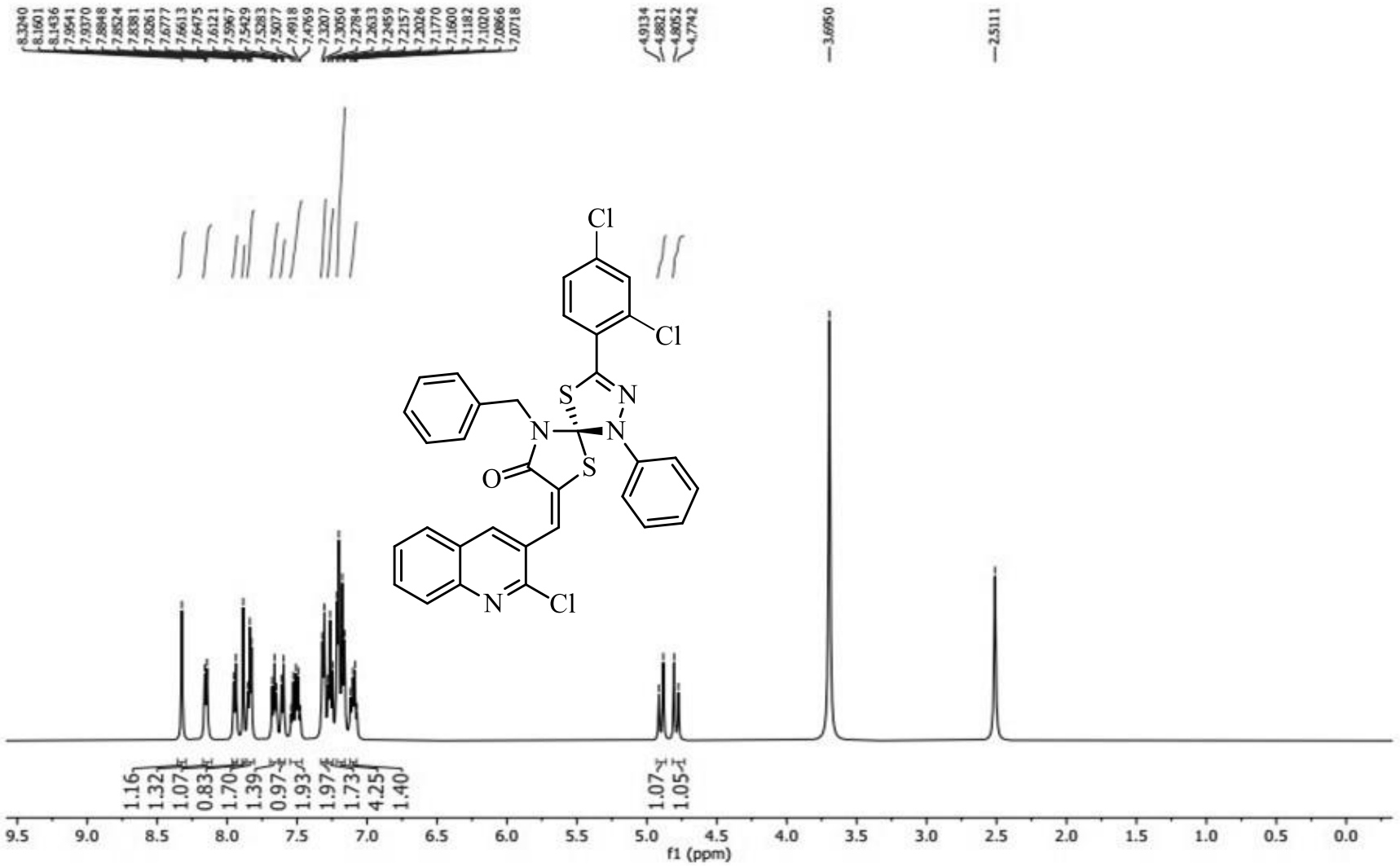
File :C:\MSDCHEM\3\DATA\Snapshot\140109307.D
Operator :
Acquired : 3 Jan 2007 3:07 using AcqMethod tast.M
Instrument : MSD
Sample Name: E
Misc Info :
Vial Number: 1



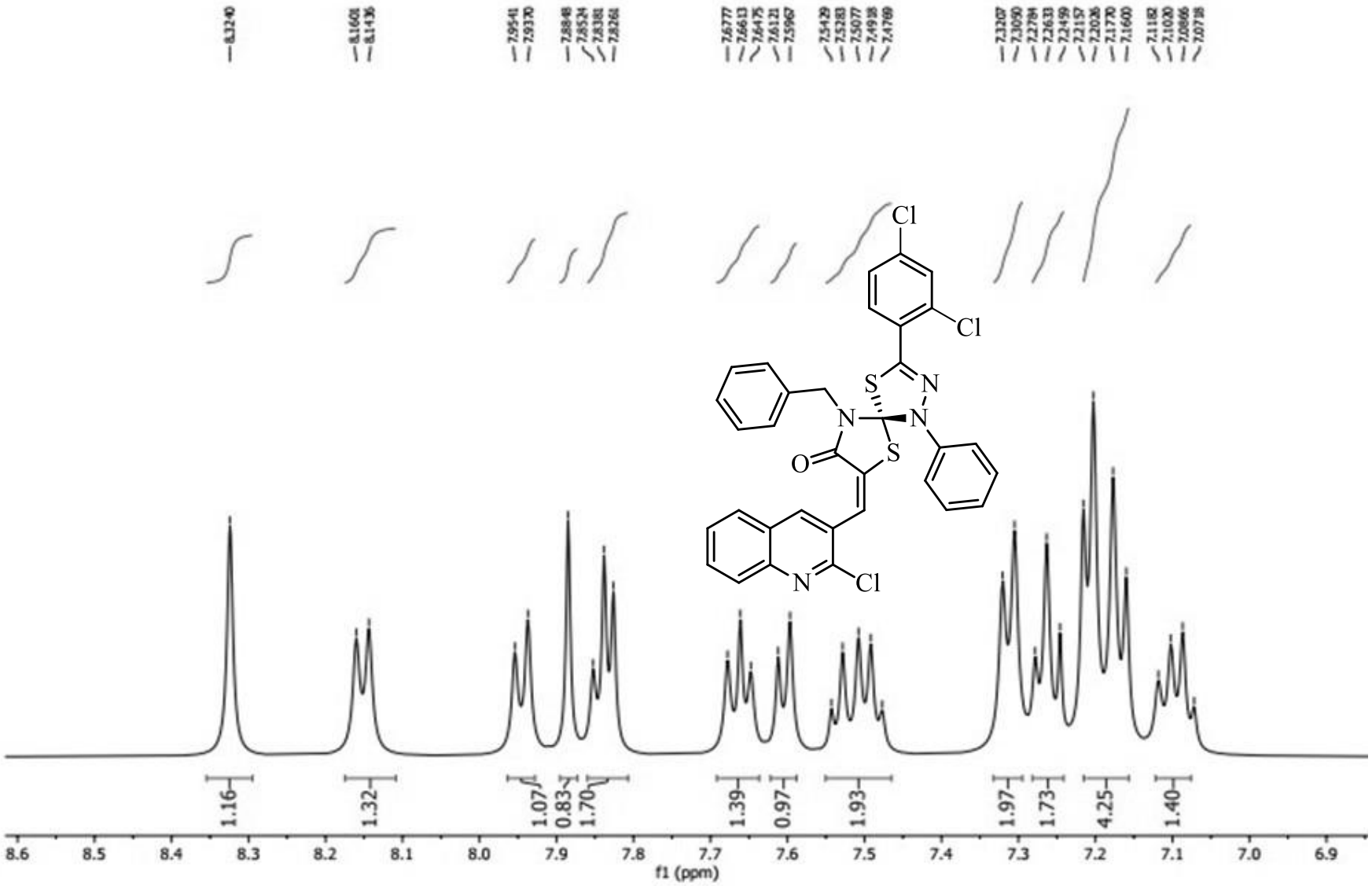
Mass Spectrum of **7d**



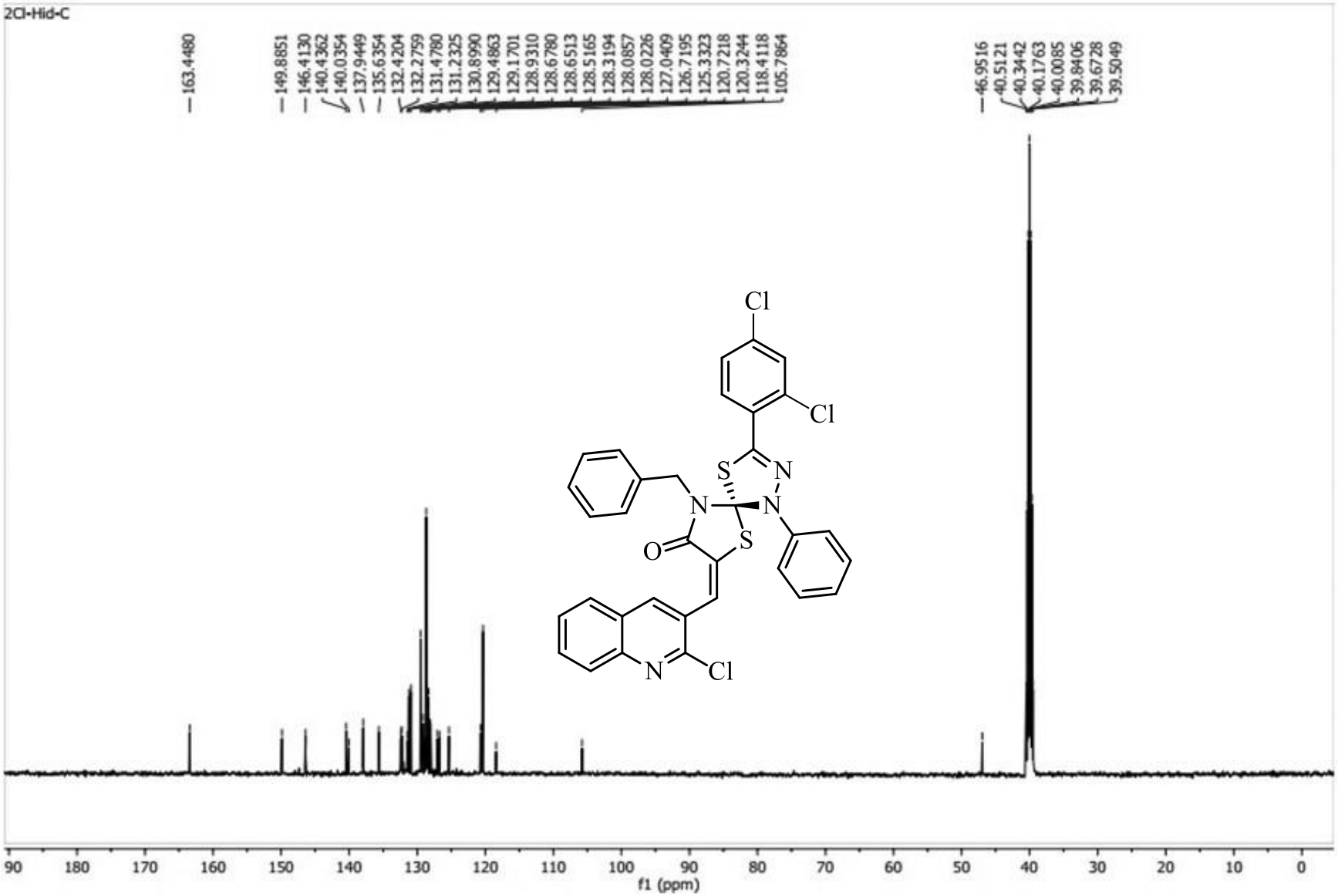
IR Spectrum of **7e**



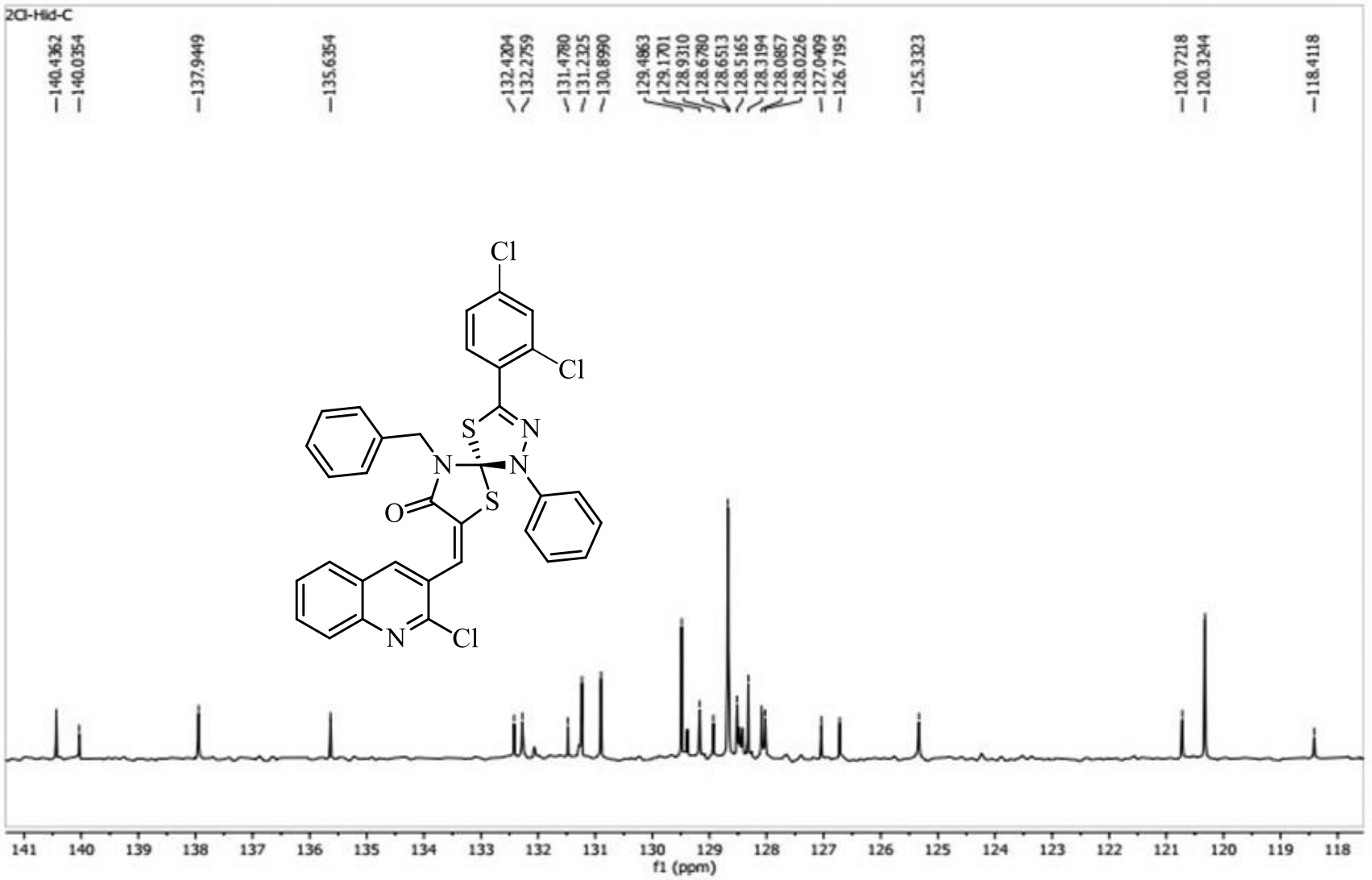
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7e**



Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7e**

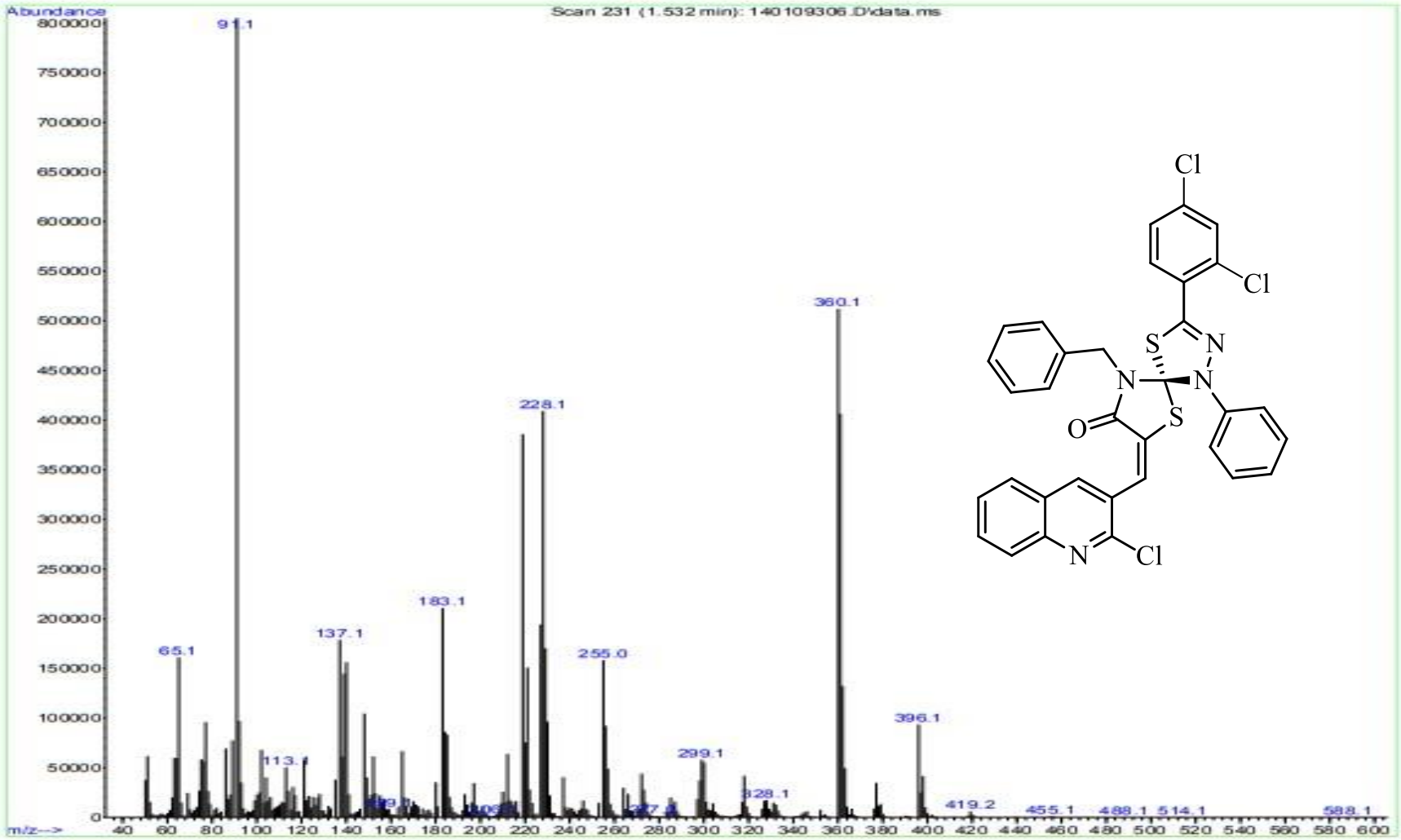


^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7e**

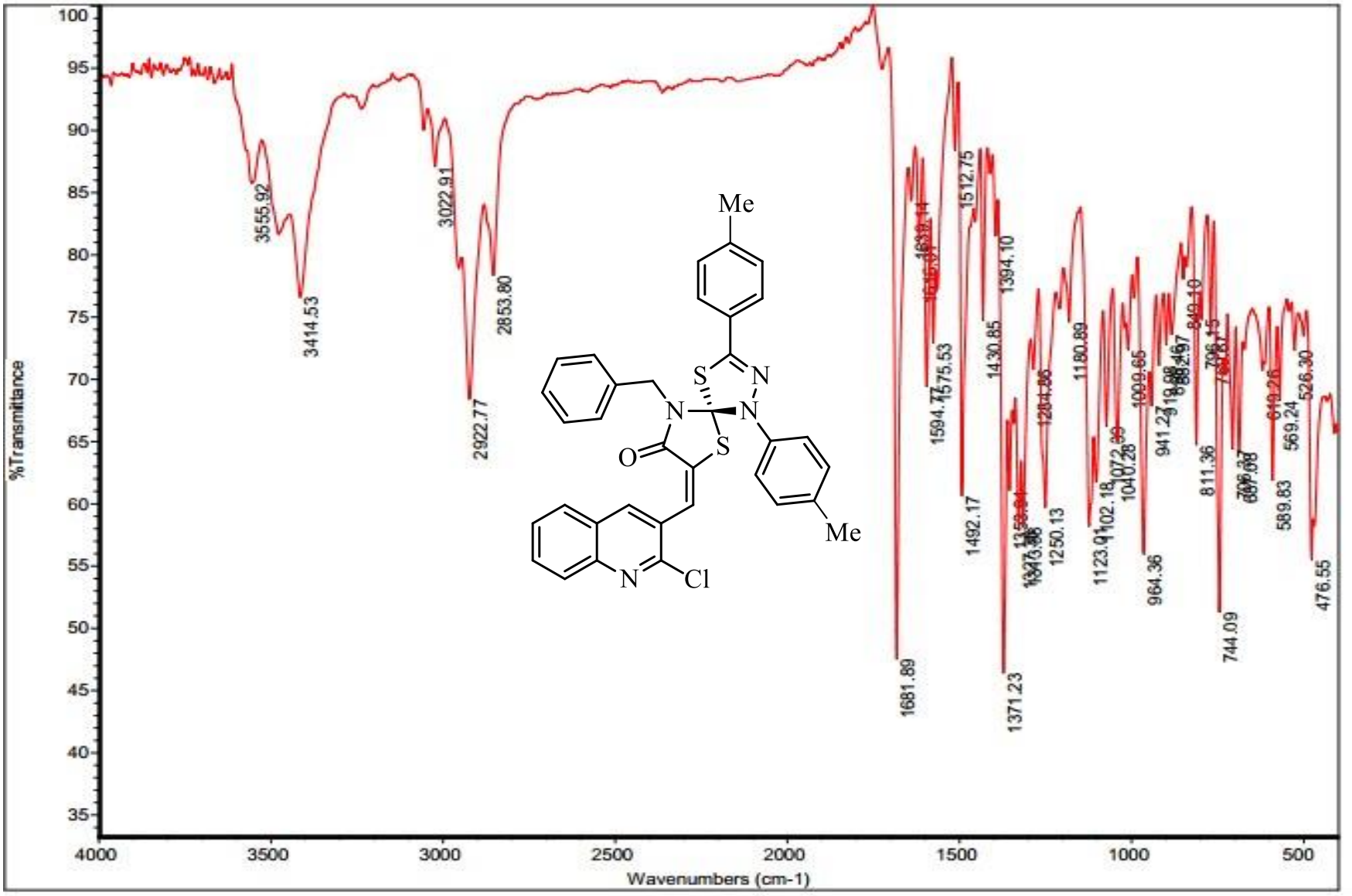


Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7e**

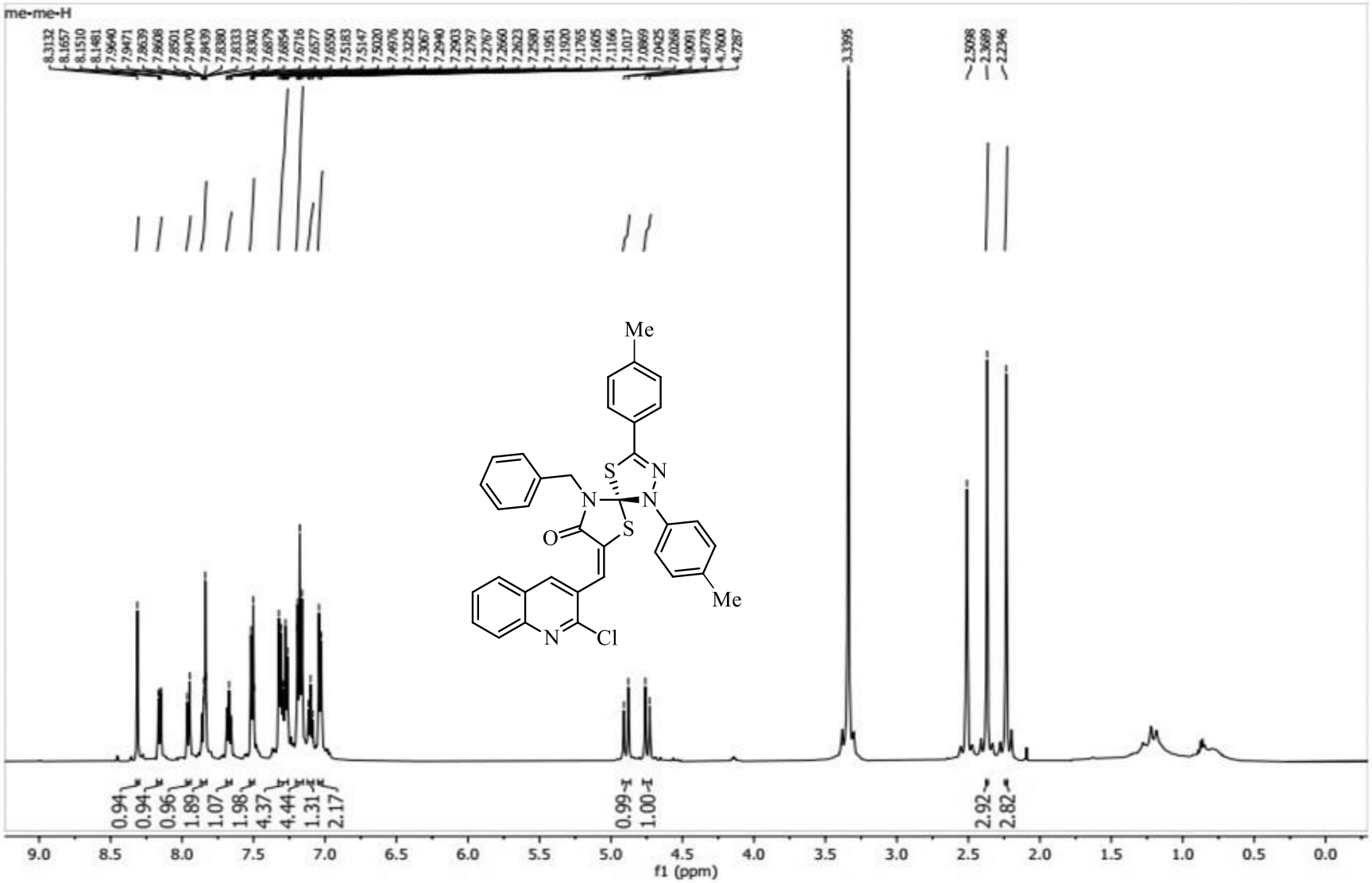
File :C:\MSDCHEM\3\DATA\Snapshot\140109306.D
Operator :
Acquired : 3 Jan 2007 2:53 using AcqMethod tast.M
Instrument : MSD
Sample Name: D
Misc Info :
Vial Number: 1



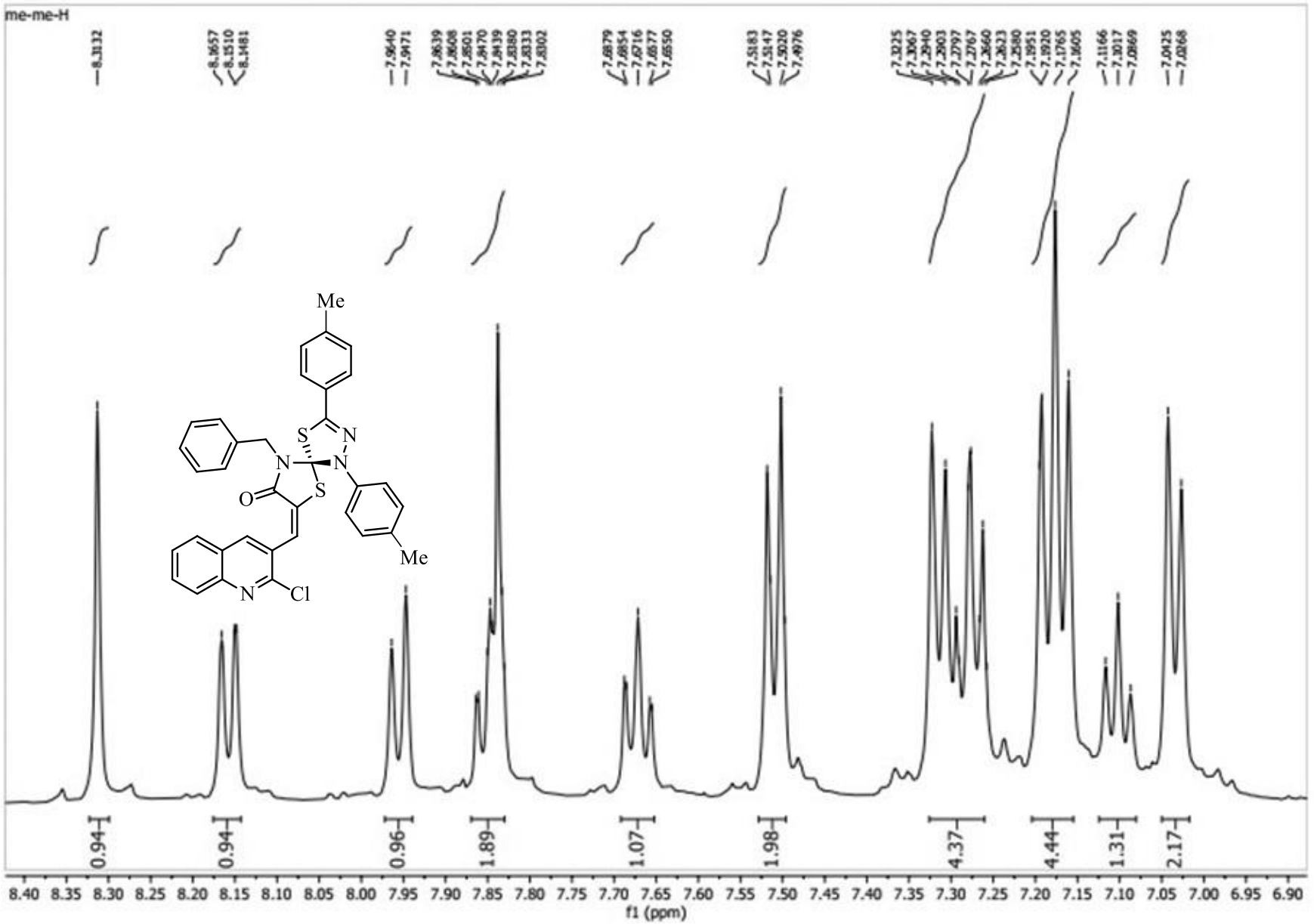
Mass Spectrum of **7e**



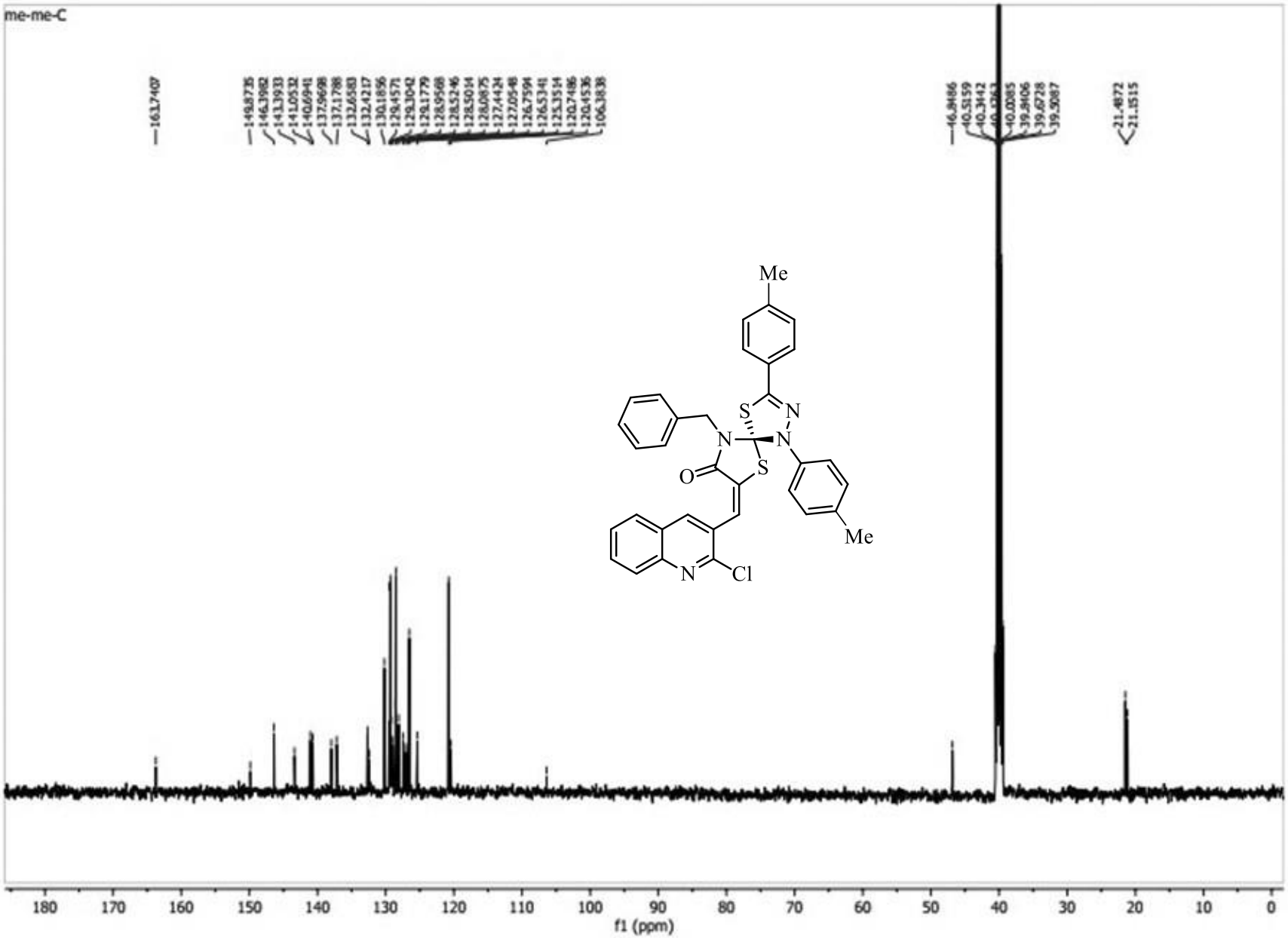
IR Spectrum of **7f**



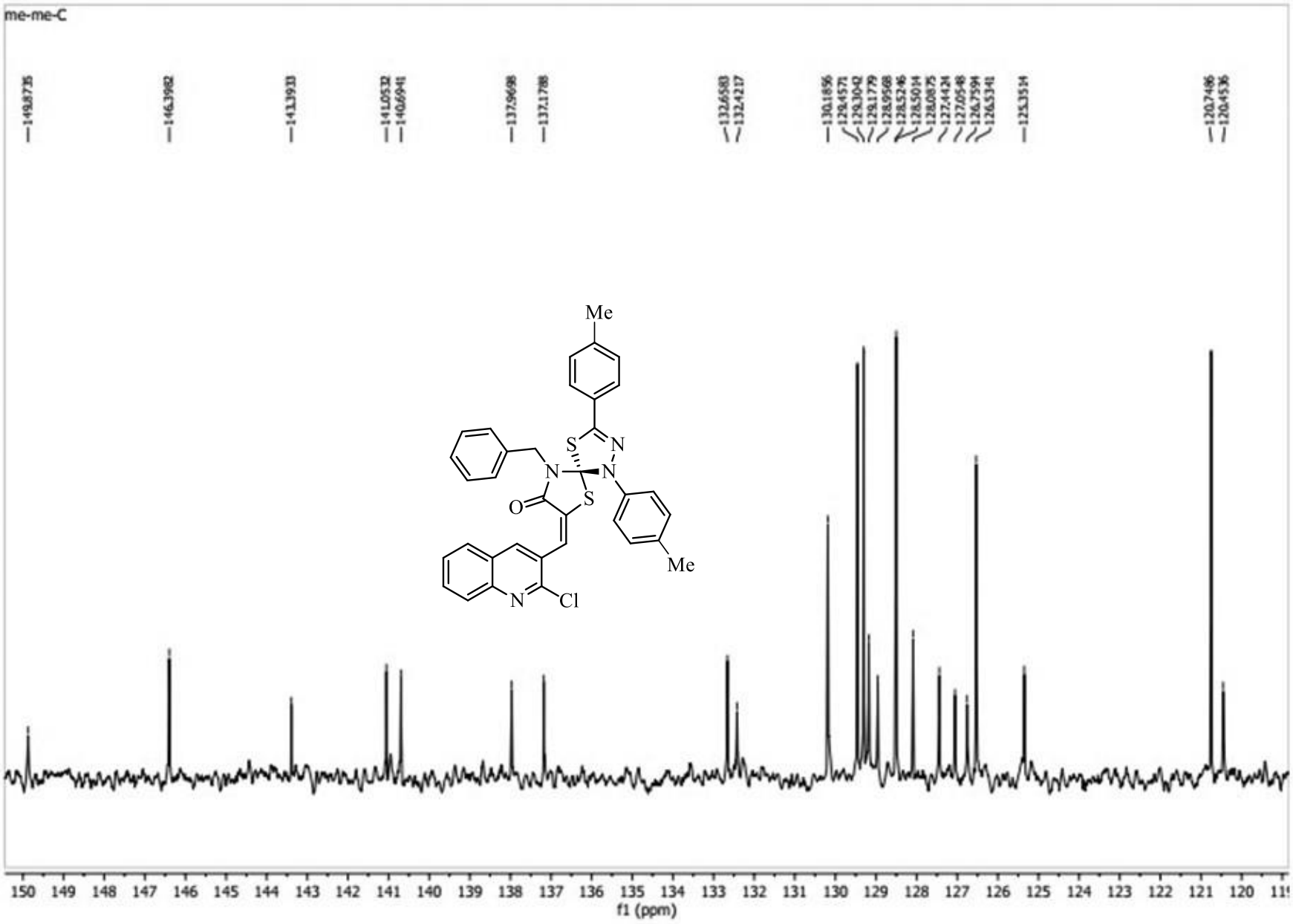
^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7f**



Expand of ^{1}H NMR (500 MHz, DMSO-d_6) Spectrum of **7f**

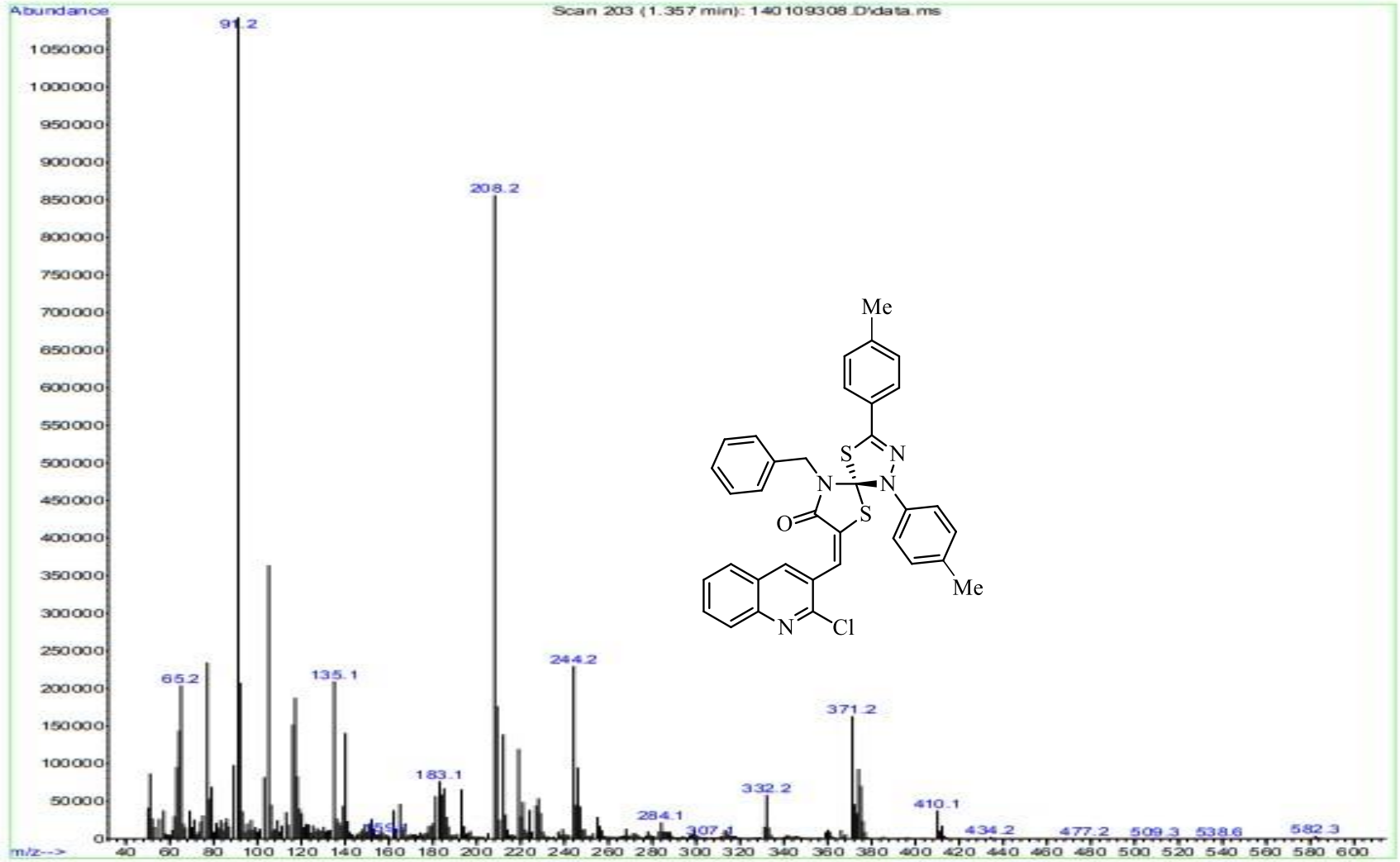


^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7f**



Expand of ^{13}C NMR (125 MHz, DMSO-d_6) Spectrum of **7f**

File :C:\MSDCHEM\3\DATA\Snapshot\140109308.D
Operator :
Acquired : 3 Jan 2007 3:18 using AcqMethod tast.M
Instrument : MSD
Sample Name: R
Misc Info :
Vial Number: 1



Mass Spectrum of **7f**