Supporting Information for

Preparation of 2, 3-Dihydroquinazolin-4(1*H*)-ones Derivatives in Aqueous Media with *β*-Cyclodextrine-SO_3H as Recyclable Catalyst

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Electronic Supplementary Information

Contents

1. General remarks

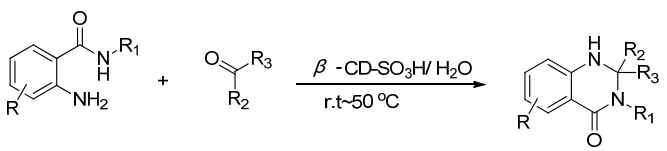
Unless otherwise stated, all the reagents and reactants were purchased from commercial suppliers; melting points were uncorrected and determined on a XT-4 binocular microscope (Beijing Tech Instrument Co., China). The ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a JEOL ECX 500 NMR spectrometer (JEOL Ltd., Japan) at room temperature operating at 500 MHz for ^{1}H-NMR and 125 MHz for ^{13}C-NMR by using $CDCl_3$ or DMSO as solvents and TMS as an internal standard; infrared spectra were recorded in KBr on a IR Pristige-21 spectrometer (Shimadzu corporation, Japan); elemental analysis was performed on an Elemental Vario-III CHN analyzer (Elementar, German). The course of the reactions was monitored by TLC; analytical TLC was performed on silica gel GF 254.

2. General procedure for the preparation of *β*-cyclodextrine-SO_3H

To a well stirred mixture of *β*-cyclodextrine (10.0 g, 4.5 mmol) in CH_2Cl_2 (50 mL), chlorosulfonic acid (2.00 g, 10 mmol) was added slowly at 0 ^{o}C during 3 h. After complication of addition, the resulted mixture was stirred for another 2 h to remove HCl from reaction vessel. Then, the mixture was filtered and washed with methanol (50 mL) and dried at room temperature to obtain sulfonated *β*-cyclodextrine as white powder (10.56 g). The $–SO_3H$ content was measured by titration method and showed 0.52 mequiv./g.

3. General procedure for t he prep aration of 2, 3-Dihydroquin-azolin-4(1*H*)-ones

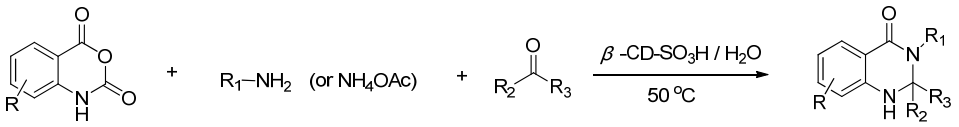
3.1 The method of ring closure reaction.



To a solution of *β*-cyclodextrine-SO_3H (0.1 mmol) in H_2O (10 mL), substituted 2-aminobenzamide (1 mmol) was added and stirred for 5 min at room temperature, Then aldehyde/ keton (1 mmol) was added. The resulted solution was stirred under

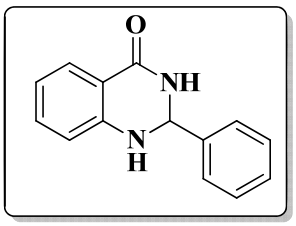
room temperature (or 50 ^{o}C) for 25 min. After completion of the reaction, the precipitated product was filtered, and recrystallized from EtOH. The catalyst β-cyclodextrine-SO_3H remain in filter liquor could be used directly as a catalyst media for next runs.

3.2 The method of one-pot three-component condensation.



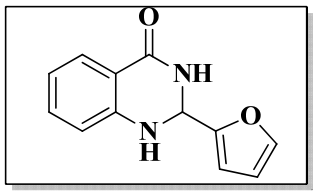
To a solution of β-cyclodextrine-SO_3H (0.15 mmol) in 10 mL H_2O, The amine (1.2 mmol) and substituted isatoic anhydride (1 mmol) were added, respectively. After 5 min later, aldehyde/ keton (1 mmol) was slowly added. The resulted solution was heated under 80 ^{o}C for 30 min. After completion of the reaction, the precipitated product was filtered, and recrystallized from EtOH. The catalyst β-cyclodextrine-SO_3H remain in filter liquor could be used directly as a catalyst media for next runs.

4. Characterization Data of the Products

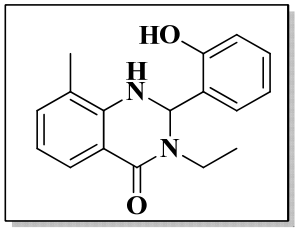


2-Phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 1 and Table 5, entry 1), white solid, m.p. 217-219 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 7.45 Hz, 1H, Ar-H), 7.58-7.60 (m, 2H, Ar-H), 7.43-7.45 (m, 3H, Ar-H), 7.33 (t, J = 7.40 Hz, 1H, Ar-H), 6.90 (t, J = 8.00 Hz, 1H, Ar-H), 6.67 (d, J = 8.05 Hz, 1H, Ar-H), 5.89 (s, 1H, Ar-H), 5.77 (br, 1H, NH), 4.40 (br, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$): 164.8, 147.3, 138.5, 134.1, 130.3, 129.2, 128.8, 127.5, 119.8, 115.7, 114.6, 69.2; Ms (EI, 70 eV): m/z (%) = 223 (29.7), 147 (100), 120 (39.5), 104 (7.7), 92(19.8), 77 (11.4); *Anal. Calcd*. for $C_{14}H_{18}N_2O$: C, 74.98%; H, 5.39%; N, 12.49%. Found: C, 74.95%; H,

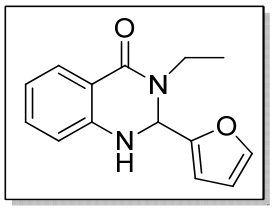
5.42%; N, 12.52%.



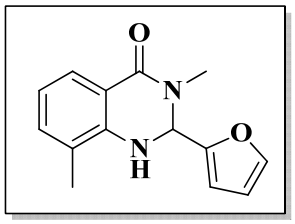
2-(Furan-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 1), white solid, m.p. 166-168 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, J = 8.00 Hz, 1H, Ar-H), 7.39 (d, ^{4}J = 1.15 Hz, 1H, Ar-H), 7.31 (t, J = 7.45 Hz, 1H, Ar-H), 6.87 (t, J = 8.00 Hz, 1H, Ar-H), 6.69 (d, J = 8.00 Hz, 1H, Ar-H), 6.54 (br, 1H, NH), 6.33 (dd, ^{4}J = 1.70 Hz, ^{3}J = 3.45 Hz, 1H, furan-H), 5.90 (s, 1H, Ar-H), 4.68 (br, 1H, NH). ^{13}C NMR (125 MHz, $CDCl_3$): 164.6, 152.1, 146.2, 143.2, 134.1, 128.6, 119.9, 115.8, 115.0, 110.6, 108.4, 62.0; Ms (EI, 70 eV): m/z (%) = 213 (100), 197 (27), 185 (13.4), 147 (18.9), 120 (93.1), 92 (42.4), 65 (14.9); *Anal. Calcd*. for $C_{12}H_{10}N_2O_2$: C, 67.28%; H, 4.71%; N, 13.08%. Found: C 67.32%; H, 4.67%; N, 13.12%.



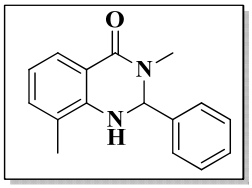
3-Ethyl-2-(2-hydroxyphenyl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2), white solid, m.p. 214-215 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d6): δ 10.11 (br, 1H, OH), 7.55 (d, J = 8.00 Hz, 1H, Ar-H), 7.07-7.10 (m, 2H, ArH), 6.92 (d, J = 6.3 Hz, 1H, Ar-H), 6.85 (d, J = 8.00 Hz, 1H, Ar-H), 6.70 (t, J = 7.45 Hz, 1H, Ar-H), 6.60 (t, J = 8.00 Hz, 1H, Ar-H), 6.18 (d, J = 2.85 Hz, 1H, Ar-H), 6.09 (d, J = 2.85 Hz, 1H, N-H), 3.94 (dq, J = 6.85 Hz, J = 14.30 Hz,1H, -CH-), 2.88 (dq, J = 6.85 Hz, J = 14.60Hz,1H, -CH-), 2.00 (s, 3H, -CH_3), 1.10 (t, J = 6.55 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 162.8, 154.9, 144.9, 134.2, 129.7, 127.4, 126.6, 125.7, 122.4, 119.3, 117.5, 116.1, 115.5, 65.5, 16.7, 13.8; Ms (EI, 70 eV): m/z (%) = 282 (10.8), 281 (6.4), 176 (11.8), 175 (100), 105 (6.3), 77 (4.4), 42 (2.9); *Anal. Calcd*. For $C_{17}H_{18}N_2O_2$: C, 72.32%; H, 6.43%; N, 9.92%. Found: C, 72.35%; H, 6.38%; N, 9.89%.



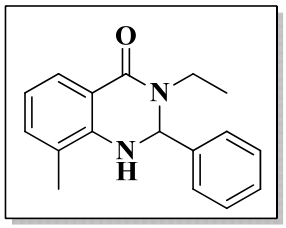
3-Ethyl-2-(furan-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 3 and Table 5, entry 6), white solid, m.p.: 119-120 ^{o}C^{1}H NMR (500 MHz, DMSO-d_6): δ 7.63 (d, J = 6.85 Hz, 1H, Ar-H), 7.57 (s, 1H, Ar-H), 7.34 (brs, 1H, N-H), 7.22 (t, J = 6.85 Hz, 1H, Ar-H), 6.70-6.68 (m, 2H, ArH), 6.35 (s, 1H, NH), 6.22 (d, J = 3.40 Hz, 1H, furan-H), 5.92 (d, J = 2.25 Hz, 1H, furan-H), 3.79 (dq, J = 7.45 Hz, J = 14.30 Hz, 1H, -CH-), 3.06 (dq, J = 7.45 Hz, J = 14.45 Hz, 1H, -CH-), 1.07 (t, J = 6.9 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.2, 154.1, 146.9, 143.5, 133.5, 127.8, 117.8, 115.6, 114.7, 110.8, 108.0, 64.5, 13.8; Ms (EI, 70 eV): m/z (%) = 242 (100), 241 (60.3), 213 (48.4), 198 (20.3), 175 (63.4), 147 (41.8), 130 (14.6), 119 (54.9), 92 (32.3), 77 (9.9), 65 (10.5); *Anal. Calcd*. For $C_{14}H_{14}ClN_2O_2$: C, 69.41%; H, 5.82%; N, 11.56%. Found: C, 69.47%; H, 5.79%; N, 11.58%.



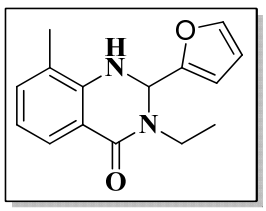
2-(Furan-2-yl)-3,8-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 4 and Table 5, entry 7), white solid, m.p. 182-183 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, J = 8.05 Hz, 1H, Ar-H),7.37 (s, 1H, Ar-H), 7.15 (d, J = 6.90 Hz, 1H, Ar-H), 6.78 (t, J = 7.45 Hz, 1H, Ar-H), 6.25 (t, J = 1.75 Hz, 1H, furan-H),6.18 (m, 1H, Ar-H), 5.75 (br, 1H, NH), 4.60 (br, 1H, NH), 3.12 (s, 3H, -NCH_3), 2.19 (s, 3H, -CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 163.6, 152.0, 143.3, 143.0, 134.3, 126.3, 122.1, 119.2, 116.1, 110.4, 108.0, 67.4, 32.8, 16.4; Ms (EI, 70 eV): m/z (%) = 252 (11), 175 (100), 118 (5.2), 105 (6.7), 77 (6.7), 42 (2.8); *Anal. Calcd*. For $C_{16}H_{16}N_2O$: C, 76.16%; H, 6.39%; N, 11.10%. Found: C, 76.23%; H, 6.43%; N, 11.16%.



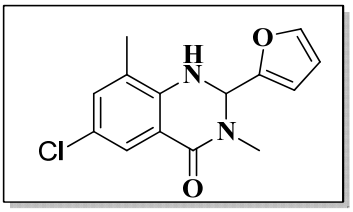
3,8-Dimethyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 5), white solid, m.p. 135-136 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, J = 7.80 Hz, 1H, Ar-H),7.38~7.43 (m, 5H, Ar-H), 7.15 (d, J = 7.30 Hz, 1H, Ar-H), 6.78 (t, J = 7.45 Hz, 1H, Ar-H), 5.75 (s, 1H, Ar-H), 4.33 (br, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$): 164.0, 143.6, 139.7, 134.3, 129.5, 129.1, 126.9, 126.5, 121.5, 118.7, 115.5, 74.1, 32.0, 16.5; Ms (EI, 70 eV): m/z (%) = 242 (100), 213 (8.8), 183 (12.3), 175 (74.2), 133 (11), 105 (56.9), 77 (12.8), 42 (8.8); *Anal. Calcd*. for $C_{14}H_{14}N_2O_2$: C, 69.41%; H, 5.82%; N, 11.56%. Found: C, 69.38%; H, 5.75%; N, 11.49%.



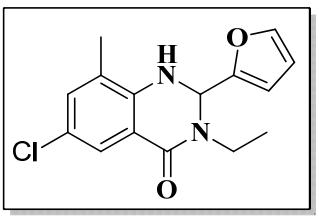
3-Ethyl-8-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 6 and Table 5, entry 2), white solid, m.p. 152-153 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.53 (d, J = 7.45 Hz, 1H, Ar-H), 7.34-7.24 (m, 5H, Ar-H), 6.07 (d, J = 6.85 Hz, 1H, Ar-H), 6.89 (d, J = 3.45 Hz, 1H, Ar-H),6.59 (t, J = 7.45 Hz, 1H, Ar-H), 5.8 (d, J = 3.45 Hz, 1H, N-H), 3.96 (dq, J = 7.45 Hz, J = 14.30 Hz, 1H, -CH-), 2.95 (dq, J = 6.85 Hz, J = 13.75 Hz, 1H, -CH-),, 2.03 (s, 3H, -CH_3), 1.08 (t, J = 6.9 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 162.7, 144.5, 142.3, 134.2, 128.9, 128.6, 125.7, 122.6, 117.3, 115.7, 69.6, 17.2, 13.9; Ms (EI, 70 eV): m/z (%) = 266 (12.3), 237 (4.9), 189 (100), 161 (28), 104 (9.1), 91 (4.6), 77 (6.7); *Anal. Calcd*. For $C_{17}H_{18}N_2O$: C, 76.66%; H, 6.81%; N, 10.52%. Found: C, 76.69%; H, 6.87%; N, 10.60%.



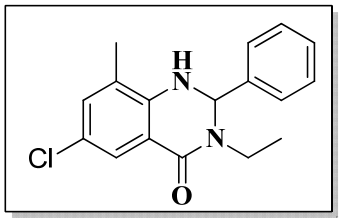
3-Ethyl-2-(furan-2-yl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 7 and Table 5, entry 8); white solid, m.p. 106-107 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.55 (s, 1H, Ar-H), 7.52 (d, J = 7.8 Hz, 1H, Ar-H), 7.13 (d, J = 7.13 Hz, 1H, Ar-H), 6.85 (d, J = 5.15 Hz, 1H, furan-H), 6.63 (d, J = 7.80 Hz, 1H, Ar-H), 6.32 (dd, ^{4}J = 1.85 Hz, ^{3}J = 3.20 Hz 1H, Ar-H), 6.14 (d, J = 3.25 Hz, 1H, Ar-H), 5.88 (d, J = 3.65 Hz, 1H, N-H), 3.88 (dq, J = 7.30 Hz, J = 14.15 Hz, 1H, -CH-), 3.14 (dq, J = 7.30 Hz, J = 14.15 Hz, 1H, -CH-), 2.08 (s, 3H, -CH_3), 1.10 (t, J = 6.9 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 162.5, 154.3, 144.6, 143.2, 134.2, 125.7, 122.9, 117.7, 116.0, 110.7, 107.7, 64.4, 17.2, 13.9; Ms (EI, 70 eV): m/z (%) = 256 (100), 239 (3.1), 227 (25.8), 189 (50.8), 161 (24.3), 133 (11.3), 124 (23.7), 105 (45.6), 91 (4.9), 77 (12.9); *Anal. Calcd*. For $C_{15}H_{16}N_2O_2$: C, 70.29%; H, 6.29%; N, 10.93%. Found: C, 70.35%; H, 6.24%; N, 10.89%.



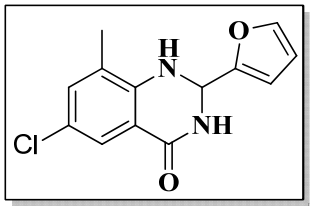
6-Chloro-2-(furan-2-yl)-3,8-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 8 and Table 5, entry 9), white solid, m.p. 155-156 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.56 (d, ^{4}J = 1.85 Hz, 1H, Ar-H), 7.45 (d, ^{3}J = 2.3 Hz, 1H, furan -H), 7.21 (d, ^{4}J = 1.85 Hz, 1H, Ar-H), 7.11 (d, ^{3}J = 3.65 Hz, 1H, furan -H), 6.35 (dd, ^{3}J = 3.65 Hz, ^{4}J = 1.85 Hz, 1H, furan -H), 6.17 (d, ^{3}J = 3.2 Hz, 1H, Ar-H-furan-2-yl), 5.91 (d, ^{3}J = 3.65 Hz, 1H, NH), 3.01 (s, 3H, N-CH_3), 2.10 (s, 3H, -CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.1, 153.4, 143.6, 133.6, 125.9, 124.5, 121.2, 116.5, 110.8, 107.9, 66.0, 32.8, 17.04; Ms (EI, 70 eV): m/z (%) = 276 (18.9), 249 (9.4), 235 (100), 222 (22.1), 194 (10.4), 117 (3.3), 68 (4.05); *Anal. Calcd*. For $C_{14}H_{13}ClN_2O_2$: C, 60.77%; H, 4.74%; N,10.12%. Found: C, 60.81%; H, 4.77%; N, 10.09%.



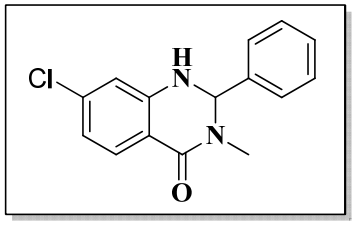
6-Chloro-3-ethyl-2-(furan-2-yl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 9 and Table 5, entry 10), white solid, m.p. 168-170 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.58 (d, ^{4}J = 1.70 Hz, 1H, Ar-H), 7.45 (d, ^{3}J = 2.3 Hz, 1H, furan -H), 7.21 (d, ^{4}J = 2.85 Hz, 1H, Ar-H), 7.08 (d, ^{3}J = 4.05 Hz, 1H, furan -H), 6.34 (dd, ^{3}J = 3.45 Hz, ^{4}J = 1.70 Hz, 1H, furan -H), 6.18 (d, ^{3}J = 3.4 Hz, 1H, Ar-H), 5.92 (d, ^{3}J = 4.00 Hz, 1H, NH), 3.86 (dq, J = 6.85 Hz, J = 14.30 Hz, 1H, -CH-), 3.17 (dq, J = 7.45 Hz, J = 14.30 Hz, 1H, -CH-), 2.09 (s, 3H, -CH_3), 1.09 (t, ^{3}J = 6.85 Hz, 1H, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 161.4, 153.9, 143.5, 133.5, 124.6, 121.1, 117.0, 110.8, 108.0, 64.3, 17.04, 13.86; Ms (EI, 70 eV): m/z (%) = 290 (100), 261 (23.4), 246 (7.8), 223 (49.5), 195 (23.4), 167 (16.1), 139 (42.4), 124 (34.8), 104 (18.9), 77 (12.4); *Anal. Calcd*. For $C_{15}H_{15}ClN_2O_2$: C, 61.97%; H, 5.20%; N, 9.64%. Found: C, 61.95%; H, 5.23%; N, 9.54%.



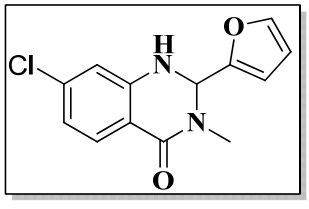
6-Chloro-3-ethyl-8-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 10), white solid, m.p. 228-230 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.46 (d, ^{4}J = 2.30 Hz, 1H, Ar-H), 7.25~7.33 (m, 5H, Ar-H), 7.15 (d, ^{4}J = 2.30 Hz, 1H, Ar-H), 7.14 (d, ^{3}J = 3.70 Hz, 1H, Ar-H),6.34 (dd, ^{3}J = 3.45 Hz, ^{4}J = 1.70 Hz, 1H, furan -H), 5.88 (d, ^{3}J = 4.10 Hz, 1H, NH), 3.94 (dq, J = 7.35 Hz, J = 14.20 Hz, 1H, -CH-), 3.00 (dq, J = 6.85 Hz, J = 13.70 Hz, 1H, -CH-), 2.04 (s, 3H, -CH_3), 1.08 (t, ^{3}J = 7.35 Hz, 1H, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 161.6, 143.4, 141.9, 133.5, 129.0, 128.7, 126.4, 125.6, 124.6, 120.9, 116.7, 69.5, 17.0, 13.9; Ms (EI, 70 eV): m/z (%) = 300 (15.9), 271 (4.4), 223 (100), 195 (26.5), 139 (7.2), 104 (8.7), 77 (7.3); *Anal. Calcd*. For $C_{17}H_{17}ClN_2O$: C, 67.88%; H, 5.70%; N, 9.31%. Found: C, 67.93%; H, 5.73%; N, 9.34%.



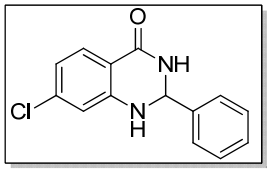
6-Chloro-2-(furan-2-yl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 11), white solid, m.p. 179-180 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.62 (d, J = 3.65 Hz, NH), 7.59 (s, 1H, Ar-H), 7.43 (d, ^{4}J = 2.75 Hz, 1H, Ar-H), 7.21 (d, ^{4}J = 2.75 Hz, 1H, Ar-H), 6.91 (d, J = 3.20 Hz, 1H, furan-H), 6.35 (dd, ^{4}J = 1.85 Hz, ^{3}J = 3.20 Hz, 1H, furan-H), 6.19 (d, J = 3.20 Hz, 1H, NH), 5.72 (d, ^{3}J = 3.65 Hz, 1H, ArH), 2.11 (s, 3H, -CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.9, 155.0, 144.2, 143.4, 133.8, 125.9, 124.5, 121.1, 116.6, 112.9, 110.8, 107.5, 60.2, 17.1; Ms (EI, 70 eV): m/z (%) = 261 (100), 245 (19.6), 195 (98), 168 (56), 139 (53), 96 (29.6), 77 (21.4); *Anal. Calcd*. For $C_{13}H_{11}ClN_2O_2$: C, 59.44%; H, 4.22%; N, 10.66%. Found: C, 59.51%; H, 4.34%; N, 10.67%.



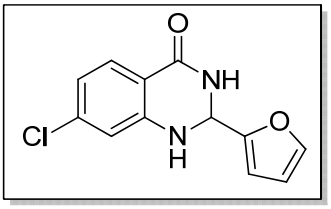
7-Chloro-3-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 12 and Table 5, entry 3), white solid, m.p. 211-213 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.64 (d, ^{3}J = 9.15 Hz, 1H, Ar-H), 7.60 (d, ^{4}J = 1.7 Hz, 1H, Ar-H), 7.31~7.40 (m, 5H, Ar-H), 6.65~6.67 (m, ^{2}H, Ar-H), 5.89 (d, ^{3}J = 1.75 Hz, 1H, NH), 2.83 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.2, 147.9,140.8, 138.3, 129.9, 129.3, 129.2, 126.5, 117.4, 113.6, 113.5, 72.4, 32.5; Ms (EI, 70 eV): m/z (%) = 272 (8.9), 195 (100), 154 (7.0), 126 (6.0), 118 (6.7), 77 (5.7), 42 (4.3); *Anal. Calcd*. For $C_{15}H_{13}ClN_2O$: C, 66.06%; H, 4.80%; N, 10.27%. Found: C, 66.11%; H, 4.82%; N, 10.31%.



7-Chloro-2-(furan-2-yl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 13 and Table 5, entry 11), white solid, m.p. 176-178 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.65 (d, ^{3}J = 2.25 Hz, 1H, Ar-H), 7.63 (br, 1H, NH), 7.61 (s, 1H, ArH), 6.75 (d, ^{3}J = 1.85 Hz, 1H, furan-H), 6.69 (dd, ^{4}J = 1.85 Hz, ^{3}J = 8.85 Hz, 1H, Ar-H), 6.38 (dd, ^{4}J = 1.85 Hz, ^{3}J = 3.25 Hz, 1H, furan-H), 6.26 (d,J = 3.20 Hz, 1H, Ar-H), 5.96 (d, J = 2.70 Hz, 1H, Ar-H), 2.94 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.2, 153.0, 148.0, 143.8, 138.1, 129.8, 117.7, 113.9, 113.8, 110.8, 108.2, 66.2, 32.5; Ms (EI, 70 eV): m/z (%) = 262 (93), 261 (100), 233 (16.5), 204 (18.7), 195 (80.7), 153 (43.6), 139 (19.9), 126 (29.0), 110 (29.3), 90 (7.7), 75 (9.1), 63 (12.3), 42 (18.2); *Anal. Calcd*. For $C_{13}H_{11}ClN_2O_2$: C, 59.44%; H, 4.22%; N, 10.66%. Found: C, 59.47%; H, 4.29%; N, 10.57%.

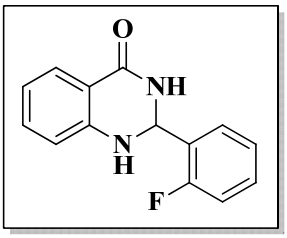


7-Chloro-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 14 and Table 5, entry 4), white solid, m.p. 186-187 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.42 (br s, 1H, NH), 7.60 (d, J = 8.25 Hz,1H, ArH), 7.48 (br s, 1H, NH), 7.46 (s, 1H, ArH), 7.41-7.34 (m, 4H, Ph-H), 6.78 (d, ^{4}J = 2.20 Hz,1H, ArH), 6.69 (dd, ^{4}J = 2.25 Hz, ^{3}J = 8.20 Hz, 1H, ArH), 5.8 (s, 1H, ArH); ^{13}C NMR (125 MHz, DMSO-d_6): 163.2, 149.3, 141.8, 138.3, 129.8, 129.1, 128.9, 127.3, 117.5, 114.1, 113.9, 66.9; Ms (EI, 70 eV): m/z (%) = 258 (22.7), 257 (30.7), 181 (100), 154 (53.1), 126 (23), 104 (12.4), 90 (7.9), 77 (13.5), 63 (8.5), 51 (6.9); *Anal. Calcd*. For *Anal. Calcd*. For $C_{14}H_{11}ClN_2O$: C, 65.00%; H, 4.29%; N, 10.83%. Found: C, 65.06%; H, 4.32%; N, 10.85%.

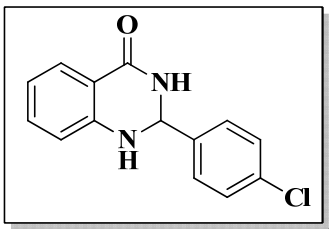


7-Chloro-2-(furan-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 15 and Table 5, entry 5), white solid, m.p. 203-204 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ

8.52 (br s, 1H, NH), 7.63- 7.56 (m, 2H, ArH), 7.48 (d, *J* = 7.35 Hz,1H, ArH), 6.78 (d, *J* = 7.35 Hz,1H, ArH), 6.70 (m, 1H, ArH), 6.38 (d, *J* = 5.0 Hz,1H, furan-H) 6.28 (d, *J* = 5.95 Hz,1H, furan-H) 5.80 (d, *J* = 5.95 Hz,1H, ArH); ^{13}C NMR (125 MHz, DMSO-d_6): 162.9, 154.6, 148.6, 143.5, 138.2, 129.7, 117.6, 114.1, 114.0, 110.8, 107.7, 60.6; Ms (EI, 70 eV): m/z (%) = 248 (51.3), 247 (82.6), 231 (25.0), 219 (11.6), 181 (16.9), 154 (100), 126 (21.2), 90 (10.4), 63 (12.5), 39 (10); *Anal. Calcd*. For *Anal. Calcd*. For $C_{12}H_9ClN_2O_2$: C, 57.96%; H, 3.65%; N, 11.27%. Found: C, 58.02%; H, 3.67%; N, 11.23%.

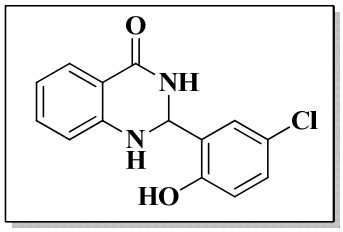


2-(2-Fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 16), white solid, m.p. 219-220 ^{o}C; ^{1}H NMR (500 MHz,DMSO-*d6*): δ 8.25 (br, 1H, N-H), 7.64 (d, *J* = 8.05 Hz, 2H, Ar-H), 7.55 (t, *J* = 7.45 Hz, 1H, Ar-H), 7.40 (q *J* = 5.75 Hz, 1H, Ar-H), 7.20~7.26 (m, 3H, Ar-H), 7.05 (s, 1H, Ar-H), 6.74 (d, *J* = 8.60 Hz, 1H, Ar-H), 6.69 (t, *J* = 7.45 Hz, 1H, Ar-H), 6.04 (br, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$): 164.1, 161.2 (d, $^{1}J_{CF}$=246.4 Hz), 159.2, 148.1, 133.9, 131.1, 128.9(d, $^{2}J_{CF}$=23.8 Hz), 128.0 (d, $^{2}J_{CF}$=23.8 Hz), 124.9 (d, $^{3}J_{CF}$=7.4 Hz), 117.8, 116.0, 115.1 (d, $^{3}J_{CF}$=7.4 Hz), 114.9, 61.3; Ms (EI, 70 eV): m/z (%) = 241 (22.2), 222 (6), 173 (8.4), 147 (100), 120 (54.5), 92 (31), 65 (8); *Anal. Calcd*. for $C_{14}H_{11}FN_2O$: C, 69.41%; H, 4.58%; N, 11.56%. Found: C, 69.37%; H, 4.49%; N, 11.60%.

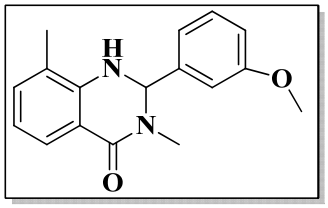


2-(4-Chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 17), white solid, m.p. 205-207 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, *J* = 6.3 Hz, 1H, Ar-H), 7.54 (d, *J* = 8.00 Hz, 2H, Ar-H), 7.40 (d, *J* = 8.05 Hz, 2H, Ar-H), 7.35 (t, *J* = 8.00 Hz, 1H, Ar-H), 6.91 (t, *J* = 8.05 Hz, 1H, Ar-H), 6.68 (d, *J* = 8.0 Hz, 1H, Ar-H), 5.89 (s, 1H,

Ar-H), 5.81 (br, 1H, NH), 4.37 (br, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$): 164.6, 147.0, 137.1, 136.1, 134.2, 129.6, 129.4, 128.9, 128.8, 120.0, 115.6, 114.7,68.5; Ms (EI, 70 eV): m/z (%) = 257 (34.6), 147 (100), 120 (55.4), 92 (24.2), 65 (11.3); *Anal. Calcd*. for $C_{14}H_{11}ClN_2O$: C, 65.00%; H, 4.29%; N, 10.83%. Found: C, 65.12%; H, 4.35%; N, 10.92%.

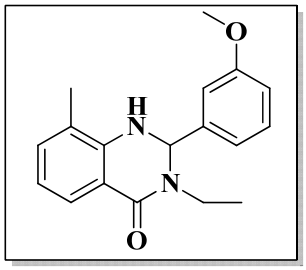


2-(5-Chloro-2-hydroxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 18), white solid, m.p. 182-183 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.57 (br s, 1H, -OH), 8.84 (br s, 1H, -NH), 7.91 (br s, 1H, -NH), 7.91 (d, ^{4}J = 2.25 Hz, 1H, Ar-H), 7.60-7.52 (m, 3H, Ar-H), 7.45 (dd, ^{3}J = 8.6 Hz, ^{4}J = 1.7 Hz, 1H, Ar-H), 7.39-7.36 (m, 2H, Ar-H); ^{13}C NMR (125 MHz, $CDCl_3$): 169.3, 162.2, 159.2, 146.3, 133.4, 132.3, 131.4, 131.3, 128.9, 127.2, 123.0, 121.5, 119.2 61.4; Ms (EI, 70 eV): m/z (%) = 274 (35.6), 147 (100), 120 (53.4), 92 (25.2), 65 (31.3); *Anal. Calcd*. for $C_{14}H_{11}ClN_2O_2$: C, 61.21%; H, 4.04%; N, 10.20%. Found: C, 61.19%; H, 4.24%; N, 10.23%.

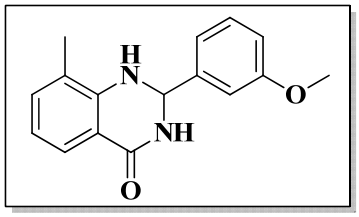


2-(4-Methoxyphenyl)-3,8-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 19, and Table 5, entry 13), white solid, m.p. 122-124 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.52 (d, J = 8.0 Hz,1H,ArH), 7.24 (t, J = 8.00 Hz, 1H, Ar-H), 7.09 (d, J = 6.85 Hz, 1H, ArH), 6.89-6.83 (m, 4H, Ar-H), 6.59 (t, J = 7.45 Hz, 1H, Ar-H), 6.70 (t, J = 7.45 Hz, 1H, Ar-H), 5.78 (d, J = 3.4 Hz, 1H, N-H), 3.69 (s, 3H, OCH_3), 2.95 (s, 3H, NCH_3), 2.03 (s, 3H, $-CH_3$); ^{13}C NMR (125 MHz, $CDCl_3$): 163.3, 159.8, 144.6, 143.2, 134.3, 130.3, 125.6, 122.5, 118.4, 117.2, 115.2, 113.6, 112.6, 71.6, 55.5, 33.1, 17.3; Ms (EI, 70 eV): m/z (%) = 282 (10.8), 176 (11.8), 175 (100), 105 (6.3), 77 (4.4), 42 (2.9); *Anal. Calcd*. For $C_{17}H_{18}N_2O_2$: C, 72.32%; H, 6.43%; N, 9.92%. Found:

C, 72.38%; H, 6.49%; N, 9.88%.

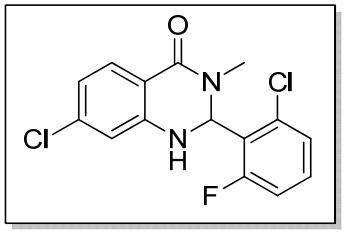


3-Ethyl-2-(3-methoxyphenyl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 20), white solid, m.p. 111-112 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.52 (d, J = 7.3 Hz,1H,ArH), 7.21 (t, J = 7.75 Hz, 1H, Ar-H), 7.07 (d, J = 6.85 Hz, 1H, ArH), 6.93 (brs, 1H, NH),6.86-6.86 (m, 2H, Ar-H),6.83 (d, J = 6.85 Hz, 1H, ArH), 6.58 (t, J = 7.8 Hz, 1H, Ar-H), 5.81 (d, J = 3.65 Hz, 1H, ArH), 3.69 (s, 3H, OCH_3), 2.93 (dq, J = 13.7 Hz, J = 6.85 Hz, 1H, -CH-), 2.03 (s, 3H, -CH_3), 1.09 (t, J = 6.85 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 162.7, 159.7, 144.5, 143.9, 134.2, 129.9, 125.7, 122.6, 118.5, 117.3, 115.2, 113.5, 112.8, 69.5, 55.5, 17.3, 14.0; Ms (EI, 70 eV): m/z (%) = 296 (0.6), 195 (100), 170 (7.5), 154 (7.4), 139 (4.4), 126 (6.7), 75 (3.2), 42 (4.1); *Anal. Calcd*. For $C_{18}H_{20}N_2O_2$: C, 72.95%; H, 6.80%; N, 9.45%. Found: C, 72.93%; H, 6.85%; N, 9.41%.

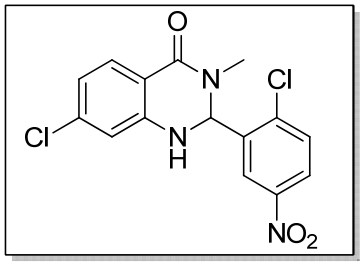


2-(3-Methoxyphenyl)-8-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 21), white solid, m.p. 147-149 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 8.30 (brs, 1H, -NH), 7.60 (d, J = 7.45 Hz,1H,ArH), 7.30-7.22 (m, 2H, Ar-H), 7.13 (brs, 1H, NH), 7.03-7.05 (m, 2H, Ar-H), 6.91 (d, J = 8.0 Hz,1H, ArH), 6.75 (d, J = 8.05 Hz, 1H, Ar-H),6.67 (t, J = 7.45 Hz, 1H, Ar-H), 5.71 (s, 1H, ArH), 3.73 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 164.0, 159.7, 148.3, 143.8, 133.8, 129.9, 127.8, 119.4, 117.6, 115.4, 114.9, 113.0, 66.7, 55.5; Ms (EI, 70 eV): m/z (%) = 254 (2.2), 253 (11.9), 236 (7.6), 209 (33.6), 195 (100), 180 (15.8), 161 (21.7), 119 (19.2), 91 (14.3), 77 (9.5), 65 (8.8), 51 (6.1); *Anal. Calcd*. For $C_{15}H_{14}N_2O_2$: C, 70.85%; H, 5.55%; N, 11.02%.

Found: C, 70.89%; H, 5.58%; N, 10.98%.

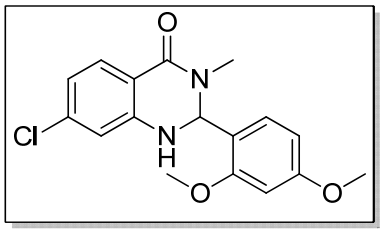


7-Chloro-2-(2-chloro-6-fluorophenyl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 22 and Table 5, entry 12), white solid, m.p. 270-271 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.64 (d, ^{3}J = 8.05 Hz, 1H, Ar-H), 7.56 (br, 1H, N-H), 7.49-7.45 (m, 1H, ArH), 7.42 (d, ^{3}J = 8.05 Hz, 1H, Ar-H), 7.27 (t, J = 8.55 Hz, 1H, Ar-H), 6.65 (dd, ^{4}J = 1.70 Hz, ^{3}J = 8.00 Hz, 1H, ArH), 6.62 (d, ^{4}J = 1.70 Hz, 1H, Ar-H), 6.59 (d, J = 1.70 Hz, 1H, Ar-H),2.73 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 161.2 (d, $^{1}J_{CF}$=246.2 Hz), 147.5, 138.1, 133.7, 132.1, 129.5 (d, $^{3}J_{CF}$=7.4 Hz), 126.8, 125.1(d, $^{2}J_{CF}$=23.8 Hz), 116.8, 116.5, 116.3 (d, $^{2}J_{CF}$=23.6 Hz), 112.5, 112.0, 68.1, 31.1 ; Ms (EI, 70 eV): m/z (%) = 324 (7.6), 195 (100), 170 (7.5), 154 (7.4), 139 (4.4), 126 (6.7), 75 (3.2), 42 (4.1); *Anal. Calcd*. For $C_{15}H_{11}Cl_2FN_2O$: C, 55.41%; H, 3.41%; N, 8.62%. Found: C, 55.43%; H, 3.47%; N, 8.68%.

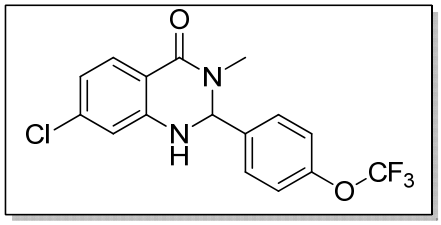


7-Chloro-2-(2-chloro-5-nitrophenyl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 23), white solid, m.p. 207-209 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.83 (s, 1H, ArH), 8.81 (d, ^{4}J = 2.25 Hz, 1H, ArH), 8.38 (dd, ^{4}J = 2.90 Hz, ^{3}J = 8.60 Hz, 1H, ArH), 8.27 (d, J = 4.55 Hz, 1H, Ar-H), 7.93 (d, J = 9.15 Hz, 1H, Ar-H), 7.67 (d, J = 8.0 Hz, 1H, ArH), 7.47 (d, ^{4}J = 1.75 Hz, 1H, Ar-H), 7.41 (dd, ^{4}J = 1.70 Hz, ^{3}J = 8.00 Hz, 1H, ArH), 2.76 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 166.5, 158.1, 149.7, 147.2, 141.6, 135.7, 134.1, 132.4, 131.1, 129.9, 127.7, 126.8, 124.1, 119.7, 26.6; Ms (EI, 70 eV): m/z (%) = 351 (6.0), 321 (4.7), 195 (100), 154 (10), 126 (10.2), 90 (4.2), 63 (4.9), 42 (6.0); *Anal. Calcd*. For $C_{15}H_{11}Cl_2N_3O_3$: C, 51.16%;

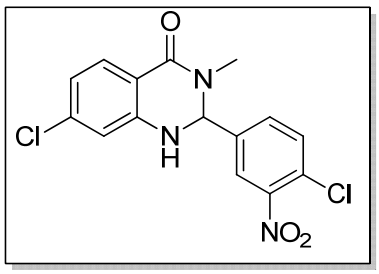
H, 3.15%; N, 11.93%. Found: C, 51.21%; H, 3.09%; N, 11.89%.



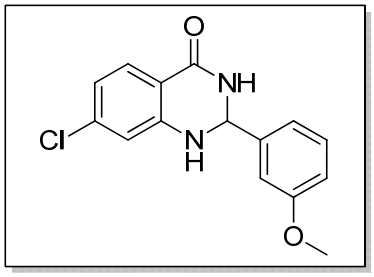
7-Chloro-2-(2,4-dimethoxyphenyl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 24), white solid, m.p. 203-205 ^{o}C;^{1}H NMR (500 MHz, DMSO-d_6): δ7.64 (d, J = 8.60 Hz, 1H, Ar-H), 7.13 (d, J = 1.70 Hz, 1H, Ar-H), 6.90 (d, J = 8.55 Hz, 1H, Ar-H), 6.74 (d, J = 1.75 Hz, 1H, Ar-H), 6.64-6.62 (m, 4H, ArH), 6.46 (dd, ^{4}J = 2.25 Hz, ^{3}J = 8.55 Hz, 1H, ArH), 6.00 (d, J = 2.30 Hz, 1H, Ar-H), 3.81 (s, 3H, OCH_3), 3.73 (s, 3H, OCH_3), 2.81 (s, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.6, 161.3, 158.1, 148.0, 138.0, 129.6, 127.0, 120.0, 117.1, 113.8, 113.4, 105.0, 99.7, 67.5, 56.2, 55.7, 32.3; Ms (EI, 70 eV): m/z (%) = 332 (30.1), 195 (100), 165 (9.7), 149 (24.7), 138 (70.3), 121 (9.0), 77 (6.8), 42 (6.5); *Anal. Calcd*. For $C_{17}H_{17}Cl_1N_2O_3$: C, 61.36%; H, 5.15%; N, 8.42%. Found: C, 61.37%; H, 5.12%; N, 8.45%



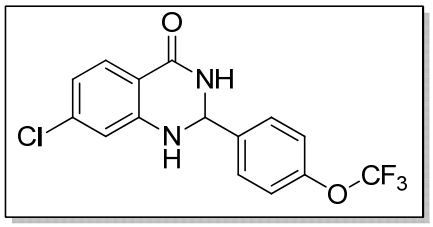
7-Chloro-3-methyl-2-(4-(trifluoromethoxy)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 25 and Table 5, entry 14), white solid, m.p. 189-190 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.65-7.63 (m, 2H, Ar-H + NH), 7.45 (d, J = 8.6 Hz,1H, ArH), 7.41 (d, J = 8.6 Hz,1H, ArH), 6.67 (d, J = 8.6 Hz,1H, ArH), 6.67 (d, J = 1.70 Hz, 1H, ArH), 5.96 (d, J = 1.45 Hz, 1H, ArH), 2.85(s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.1, 148.9, 147.6, 140.2, 138.4, 129.9 (q, $^{1}J_{CF}$=265 Hz), 128.6, 121.9, 117.7, 71.5, 32.5; Ms (EI, 70 eV): m/z (%) = 356 (11.3), 355 (11.3), 197 (3.2), 195 (100), 153 (8.4), 126 (8.7), 69 (3.9), 42 (4.5); *Anal. Calcd*. For $C_{16}H_{12}Cl_2F_3N_2O_2$: C, 53.87%; H, 3.39%; N, 7.85%. Found: C, 53.83%; H, 3.41%; N, 7.87%.



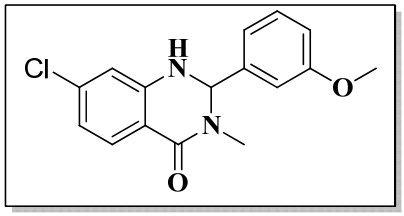
7-Chloro-2-(4-chloro-3-nitrophenyl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 26), white solid, m.p. 248-250 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.0 (br s, 1H, NH), 7.81 (d, J = 8.0 Hz,1H, ArH), 7.74 (s, 1H, ArH), 7.66 (d, J = 8.6 Hz,1H, ArH), 7.56 (dd, ^{4}J = 1.15 Hz, ^{3}J = 8.0 Hz, 1H, ArH), 6.72 (d, J = 8.05 Hz, 1H, ArH), 6.67 (s, 1H, ArH), 6.08 (d, J = 1.75 Hz, 1H, ArH), 2.91 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 161.9, 148.0, 147.2, 141.9, 138.5, 132.8, 131.5, 130.0, 125.7, 124.1, 118.3, 113.9, 113.5, 70.7, 32.7; Ms (EI, 70 eV): m/z (%) = 351 (6.5), 321 (5.7), 195 (100), 154 (10), 126 (10.5), 90 (6.2), 63 (5.9), 42 (6.0); *Anal. Calcd*. For $C_{15}H_{11}Cl_2N_3O_3$: C, 51.16%; H, 3.15%; N, 11.93%. Found: C, 51.12%; H, 3.19%; N, 11.89%.



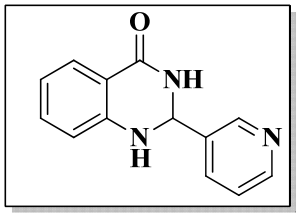
7-Chloro-2-(3-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 27 and Table 5, entry 15), white solid, m.p. 235-237 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.44 (br, 1H, N-H), 7.60 (d, J = 8.00 Hz, 1H, Ar-H), 7.40 (s, 1H, Ar-H), 7.31 (t, J = 8.05 Hz, 1H, Ar-H), 7.04~7.03 (m,2H, Ar-H), 6.93 (d, J = 8.60 Hz, 1H, Ar-H), 6.79 (s, 1H, Ar-H), 6.69 (d, J = 8.00 Hz, 1H, Ar-H), 5.77 (br, 1H, -NH), 3.75 (s, 3H, O-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 163.2, 159.7, 149.2, 143.5, 138.6, 130.1, 129.8, 129.8, 119.3, 117.5, 114.3, 114.1, 113.9, 113.0, 66.6, 55.6; Ms (EI, 70 eV): m/z (%) = 282 (25.1), 281 (30.1), 181 (100), 154 (43.1), 126 (13.8), 108 (11.5), 90 (6.5), 77 (7.3), 63 (7.5); *Anal. Calcd*. For $C_{15}H_{13}ClN_2O_2$: C, 62.40%; H, 4.54%; N, 9.70%. Found: C, 62.37%; H, 4.49%; N, 9.75%.



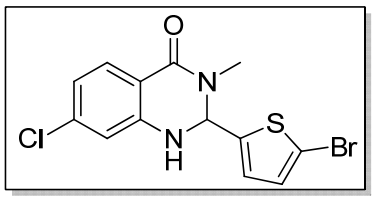
7-Chloro-2-(4-(trifluoromethoxy)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 28 and Table 5, entry 16), white solid: m.p. 210-213 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.46 (br, 1H, N-H), 7.61 (d, J = 9.15 Hz, 2H, Ar-H), 7.40 (d, J = 9.20 Hz, 2H, Ar-H), 6.83 (t, J = 8.05 Hz, 1H, Ar-H), 6.79 (d, ^{4}J = 3.45 Hz, 1H, Ar-H), 6.70 (d, J = 8 Hz, 1H, Ar-H), 6.49 (dd, ^{4}J = 1.75 Hz, ^{3}J = 8.6 Hz, 1H, Ar-H), 5.87 (br, 1H, NH); ^{13}C NMR (125 MHz, DMSO-d_6): 163.1, 152.0, 149.1, 148.9, 141.2, 138.4, 131.1, 129.9 (q, $^{1}J_{CF}$=267 Hz), 129.4, 121.6, 117.7, 115.6, 114.5, 112.8, 66.2; Ms (EI, 70 eV): m/z (%) = 242 (34.2), 211 (47.9), 181 (100), 154 (80.1), 126 (25.0), 99 (6.4), 90 (8.5), 75 (5.3), 63 (12.0); *Anal. Calcd*. For $C_{15}H_{10}ClF_3N_2O_2$: C, 52.57%; H, 2.94%; N, 8.17%. Found: C, 52.61%; H, 2.95%; N, 8.21%.



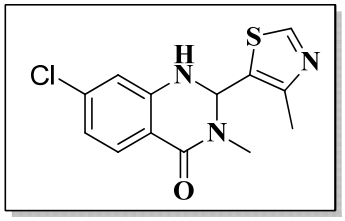
7-Chloro-2-(3-methoxyphenyl)-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 29 and Table 5, entry 17), white solid, m.p. 171-172 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.63 (d, ^{3}J = 9.20 Hz, 1H, Ar-H), 7.58 (d, ^{4}J = 1.70 Hz, 1H, Ph-H), 7.29 (t, J = 8.35 Hz, 1H, Ph-H), 6.91 (dd, ^{4}J = 2.30 Hz, ^{3}J = 8.00 Hz, 1H, ArH), 6.87~6.84 (m, H, Ar-H), 6.67-6.65 (m, 2H, Ar-H), 5.85 (d, J = 2.30 Hz, 1H, N-H), 3.71 (s, 3H, O-CH_3), 2.84 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 162.2, 159.9, 147.9, 142.4, 138.2, 130.5, 129.8, 118.4, 117.5, 114.1, 113.6, 112.7, 72.2, 55.6, 32.5; Ms (EI, 70 eV): m/z (%) = 302 (9.8), 195 (100), 154 (9.8), 126 (4.7), 108 (3.1), 42 (3.7); *Anal. Calcd*. For $C_{16}H_{15}ClN_2O_2$: C, 63.47%; H, 4.99%; N, 9.25%. Found: C, 63.57%; H, 5.03%; N, 9.28%



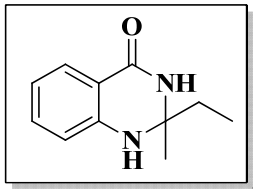
2-(Pyridin-3-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 30), white solid, m.p. 191-193 ^{o}C; ^{1}H NMR (500 MHz,DMSO-*d6*): δ 8.67 (d, ^{4}J = 2.3 Hz, 1H, pyridine-H), 8.56 (dd, ^{4}J = 1.75 Hz, ^{3}J = 4.6 Hz, 1H, pyridine-H), 8.40 (br, 1H, N-H), 7.90 (dd, ^{4}J = 1.70 Hz, ^{3}J = 8.00 Hz, 1H, Ar-H), 7.63 (d, J = 6.3 Hz, 2H, Ar-H), 7.55 (t, J = 7.45 Hz, 1H, Ar-H), 7.40 (q J = 5.75 Hz, 1H, Ar-H), 7.20~7.26 (m, 3H, Ar-H), 7.45 (dd, ^{4}J = 5.15 Hz, ^{3}J = 8.00 Hz, 1H, pyridine-H), 7.27 (t, ^{3}J = 6.85 Hz, Ar-H), 7.18 (s, 1H, Ar-H), 6.77 (d, J = 8.05 Hz, 1H, Ar-H), 6.69 (t, J = 7.45 Hz, 1H, Ar-H), 5.85 (br, 1H, NH); ^{13}C NMR (125 MHz, DMSO-*d6*): 164.1, 150.2, 148.9, 148.2, 137.3, 135.1, 134.0, 127.9, 124.0, 118.0, 115.5, 115.0, 65.1; Ms (EI, 70 eV): m/z (%) = 225 (17.1), 147 (100), 120 (31.5), 92 (22.4), 65 (9.2); *Anal. Calcd*. for $C_{13}H_{11}N_3O$: C, 69.32%; H, 4.92%; N, 18.66%. Found: C 69.43%; H, 5.01%; N, 18.71%.



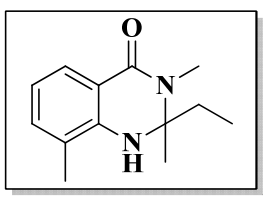
2-(5-Bromothiophen-2-yl)-7-chloro-3-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 31), white solid, m.p. 193-195 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.77 (br, 1H, NH), 8.49 (d, ^{3}J = 4.55 Hz, 1H, thiophen-H), 8.03 (s, 1H, Ar-H), 7.87 (d, J = 8.60 Hz, 1H, Ar-H), 7.78 (d, ^{4}J = 1.70 Hz, 1H, Ar-H), 7.42 (d, J = 1.70 Hz, 1H, ArH), 7.39 (dd, ^{4}J = 1.70 Hz, ^{3}J = 8.00 Hz, 1H, ArH), 2.80 (s, 3H, N-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 166.0, 155.9, 149.4, 143.2, 136.7, 136.1, 131.7, 130.5, 128.5, 126.6, 119.5, 110.6, 26.6; Ms (EI, 70 eV): m/z (%) = 356 (22), 195 (100), 168 (11.1), 153 (24), 139 (7.6), 126 (13.1), 110 (5.7), 82 (6.4), 42 (12.5); *Anal. Calcd*. For $C_{13}H_{10}BrCl_2N_2OS$: C, 43.66%; H, 2.82%; N, 7.83%. Found: C, 43.71%; H, 2.79%; N, 7.85%



7-Chloro-3-methyl-2-(4-methylthiazol-5-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 32), white solid, m.p. 251-253 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.82 (s, 1H, thiazole-H), 7.68 (d, ^{3}J = 8.25 Hz, 1H, Ar-H), 7.62 (d, ^{4}J = 2.30 Hz, 1H, Ar-H), 6.77 (dd, ^{4}J = 1.80 Hz, ^{3}J = 8.25 Hz, 1H, ArH), 6.72 (d, J = 1.80 Hz, 1H, Ar-H), 6.34 (d, ^{3}J = 2.25 Hz, 1H, N-H), 2.80 (s, 3H, N-CH_3) , 2.48 (s, 3H, thiazole-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 161.5, 152.6, 150.9, 147.3, 138.5, 131.2, 129.9, 118.2, 114.1, 113.6, 66.2, 31.5, 15.6; Ms (EI, 70 eV): m/z (%) = 293 (42.7), 235 (5.6), 195 (100), 168 (12.2), 153 (25), 139 (18.8), 126 (16.7), 99 (4.6), 90 (4.4), 42 (10.8); *Anal. Calcd*. For $C_{13}H_{12}ClN_3OS$: C, 53.15%; H, 4.12%; N, 14.30%. Found: C, 53.23%; H, 4.12%; N, 14.33%.

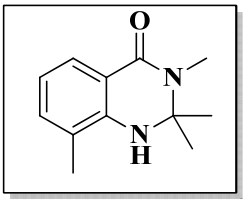


2-Ethyl-2-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 17 and Table 5, entry 18), white solid, m.p. 182-183 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (d, J = 5.7 Hz, 1H, Ar-H), 6.79 (d, J = 6.3 Hz, 1H, Ar-H), 6.62~6.55 (m, 1H, Ar-H), 4.20 (br, 1H, NH), 1.87 (br, 1H, NH), 1.81 (q, J = 5.15 Hz,2H, -CH_2), 1.49 (s, 3H, -CH_3), 0.97 (t, J = 4.55 Hz, 3H, -CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 164.5, 146.1, 134.0, 128.3, 118.5, 114.5, 70.2, 34.88, 27.63, 8.3; Ms (EI, 70 eV): m/z (%) = 190 (2.4), 175 (14.6), 161 (100), 120 (12.6), 92 (12.7), 65 (5.7), 42 (3.9); *Anal. Calcd*. for $C_{11}H_{14}N_2O$: C, 69.45%; H, 7.42%; N, 14.73%. Found: C, 69.51%; H, 7.42%; N, 14.76%.

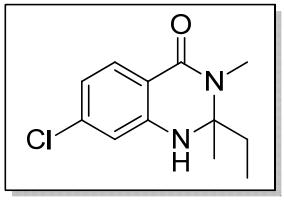


2-Ethyl-2,3,8-trimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 27 and

Table 5, entry 19), white solid, m.p. 161-162 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.48 (d, J = 7.45 Hz, 1H, Ar-H), 7.10 (d, J = 7.45 Hz, 1H, Ar-H), 6.56 (t, J = 7.45 Hz, 1H, Ar-H), 5.67 (s, 1H, Ar-H), 2.93 (s, 3H, NCH_3), 2.11 (s, 3H, CH_3), 1.73-1.84 (m, 2H, CH_2), 1.46 (s, 3H, CH_3), 0.83 (t, J = 7.15 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 163.4, 144.5, 134.3, 125.8, 122.2, 116.7, 114.3, 74.1, 30.7, 27.4, 25.1, 17.4, 8.8; Ms (EI, 70 eV): m/z (%) = 218 (1.5), 203 (12.4), 189 (100), 104 (2.8), 70 (3.1), 56 (14.8); *Anal. Calcd*. For $C_{13}H_{18}N_2O$: C, 71.53%; H, 8.31%; N, 12.83%. Found: C, 71.43%; H, 8.50%; N, 12.78%.

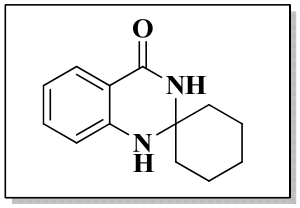


2,2,3,8-Tetramethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3), white solid, m.p. 205-207 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.51 (d, J = 7.45 Hz, 1H, Ar-H), 7.10 (d, J = 6.9 Hz, 1H, Ar-H), 6.60 (t, J = 7.40 Hz, 1H, Ar-H), 5.78 (s, 1H, N-H), 2.91 (s, 3H, NCH_3), 2.12 (s, 3H, CH_3), 1.47 (s, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 163.4, 144.5, 134.3, 125.8, 122.2, 116.7, 114.3, 74.1, 30.7, 27.4, 25.1, 17.4, 8.8; Ms (EI, 70 eV): m/z (%) = 204 (4.8), 189 (100), 105 (4.9), 77 (2.9), 56 (16.7); *Anal. Calcd*. For $C_{16}H_{22}N_2O$: C, 74.38%; H, 8.58%; N, 10.84%. Found: C, 74.42%; H, 8.62%; N, 10.88%.

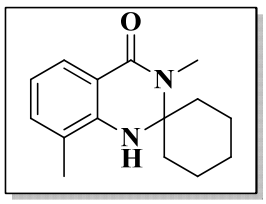


7-Chloro-2-ethyl-2,3-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 47 and Table 5, entry 20), white solid, m.p.: 161-163 ^{o}C^{1}H NMR (500 MHz, DMSO-d_6): δ 7.57 (d, J = 8.30 Hz, 1H, Ar-H), 6.96 (brs, 1H, N-H), 6.67 (d, ^{4}J = 1.75 Hz, 1H, Ar-H), 6.62 (dd, ^{4}J = 1.15 Hz, ^{3}J = 8.60 Hz, 1H, Ar-H), 2.88 (s, 3H, NCH_3), 1.87 (dq, J = 7.40 Hz, J = 14.30 Hz, 1H, -CH-), 1.65 (dq, J = 7.40 Hz, J = 14.85 Hz, 1H, -CH-), 1.42 (s, 3H, CH_3), 0.84 (t, J = 6.9 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6):

162.4, 151.4, 147.7, 138.0, 130.2, 111.5, 113.2, 74.0, 31.4, 27.3, 25.4, 8.6; Ms (EI, 70 eV): m/z (%) = 238 (0.9), 223 (11.1), 212 (32), 210 (12.7), 209 (100), 174 (2.5), 154 (3.1), 126 (2.8), 70 (5.4), 56 (21.3); *Anal. Calcd*. For $C_{12}H_{15}ClN_2O_2$: C, 60.38%; H, 6.33%; N, 11.74%. Found: C, 60.35%; H, 6.37%; N, 11.73%.

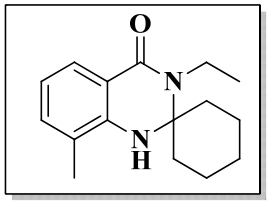


1'*H*-Spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 5 and Table 5, entry 21), white solid, m.p. 225-226 ^{o}C; ^{1}H NMR (500 MHz, DMSO-*d6*): δ 7.93 (br, 1H, N-H), 7.56 (d, J = 7.45 Hz, 1H, Ar-H), 7.22 (t, J = 6.9 Hz, 1H, Ar-H), 6.81 (d, J = 8.00 Hz, 1H, Ar-H), 6.60~6.63 (m, 2H, Ar-H + NH), 1.73~1.76 (m, 2H, cyclohexane-H), 1.54~1.63 (m, 6H, cyclohexane-H), 1.41~1.44 (m, 1H, cyclohexane-H), 1.23~1.28 (m, 1H, cyclohexane-H); ^{13}C NMR (125 MHz, DMSO-*d6*): 163.7, 147.2, 133.6, 127.6, 117.0, 115.0, 114.9, 68.3, 37.6, 25.1, 21.4; Ms (EI, 70 eV): m/z (%) = 216 (18.1), 187 (10.1), 171 (100), 160 (33.3), 120 (10.8), 92 (9.3), 65 (4); *Anal. Calcd*. for $C_{13}H_{16}N_2O$: C, 72.19%; H, 7.46%; N, 12.95%. Found: C, 72.22%; H, 7.57%; N, 13.01%.

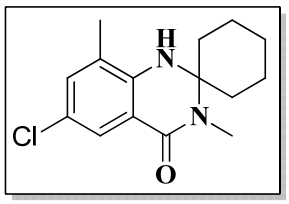


3',8'-Dimethyl-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 6 and Table 5, entry 22), white solid, m.p. 180-181 ^{o}C; ^{1}H NMR (500 MHz,DMSO-d6): δ 7.55 (d, J = 7.45 Hz, 1H, Ar-H), 7.19 (d, J = 6.85 Hz, 1H, Ar-H), 6.72 (t, J = 7.45 Hz, 1H, Ar-H), 5.31 (s, 1H, Ar-H), 2.95 (s, 3H, NCH_3), 2.20 (s, 3H, CH_3), 1.57-1.86 (m, 9H, cyclohexane-H), 1.17-1.20 (m, 1H, cyclohexane-H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.5, 142.6, 133.9, 125.8, 125.7, 118.7, 118.2, 71.3, 32.7, 26.7, 24.9, 22.6, 16.9; Ms (EI, 70 eV): m/z (%) = 244 (21.3), 215 (10.3), 201 (100), 188 (22.5), 160 (14.6), 68 (4.4); *Anal. Calcd*. for $C_{15}H_{20}N_2O$: C, 73.74%; H, 8.25%; N,

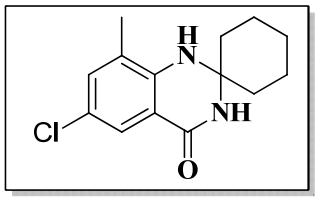
11.47%. Found: C, 73.80%; H, 8.31%; N, 11.43%.



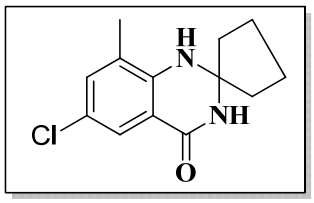
3'-Ethyl-8'-methyl-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 7 and Table 5, entry 23), white solid, m.p. 142-143 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d6): δ 7.55 (d, J = 8.00 Hz, 1H, Ar-H), 7.18 (d, J = 6.9 Hz, 1H, Ar-H), 6.72 (t, J = 7.40 Hz, 1H, Ar-H), 5.29 (s, 1H, N-H), 3.51 (q, J = 6.9 Hz, 2H, CH_2), 2.19 (s, 3H, NCH_3), 1.91-1.95 (m, 2H, cyclohexane-H), 1.72-1.54 (m, 7H, cyclohexane-H), 1.24-1.18 (m, 7H, cyclohexane-H), 1.09 (t, J = 6.85 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$): 163.1, 142.5, 133.8, 125.6, 118.8, 118.4, 71.9, 35.5, 33.8, 24.8, 22.7, 16.9, 16.3; Ms (EI, 70 eV): m/z (%) = 204 (4.8), 189 (100), 105 (4.9), 77 (2.9), 56 (16.7); *Anal. Calcd*. For $C_{12}H_{16}N_2O$: C, 70.56%; H, 7.90%; N, 13.71%. Found: C, 70.53%; H, 7.94%; N, 13.65%.



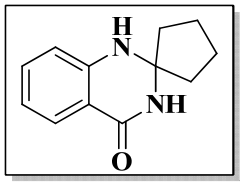
6'-Chloro-3',8'-dimethyl-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 8), white solid, m.p. 166-168 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d6): δ 7.49 (d, ^{4}J = 2.30 Hz, 1H, Ar-H), 7.26 (d, ^{4}J = 2.30 Hz, 1H, Ar-H), 5.52 (br, 1H, N-H), 2.96 (s, 3H, NCH_3), 2.21 (s, 3H, CH_3), 1.85-1.70 (m, 4H, cyclohexane-H), 1.62-1.54 (m, 5H, cyclohexane-H), 1.13-1.22 (m, 1H, cyclohexane-H); ^{13}C NMR (125 MHz, DMSO-d6): 162.4, 141.6, 133.3, 128.9, 124.7, 122.5, 119.4, 71.5, 32.6, 26.5, 24.8, 22.5, 16.7; Ms (EI, 70 eV): m/z (%) = 278 (31), 276 (100), 247 (10.9), 209 (56.4), 167 (14.2), 139 (44), 110 (32.4), 77 (12.2), 42 (11.7); *Anal. Calcd*. For $C_{15}H_{19}ClN_2O$: C, 64.63%; H, 6.87%; N, 10.05%. Found: C, 64.53%; H, 6.92%; N, 10.01%.



6'-Chloro-8'-methyl-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 9), white solid, m.p. 201-202 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.18 (br, 1H, NH), 7.43 (d, ^{4}J = 2.75 Hz 1H, Ar-H), 7.20 (d, ^{4}J = 1.80 Hz, 1H, Ar-H), 5.67 (br, 1H, NH), 2.14 (s, 3H, -CH_3), 1.74-1.52 (m, 8H, cyclohexane-H), 1.40-1.29 (m, 2H, cyclohexane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 162.8, 143.8, 133.6, 126.6, 124.4, 120.9, 116.9, 68.2, 37.2, 25.2, 21.6, 17.2; Ms (EI, 70 eV): m/z (%) = 264 (17.5), 235 (10), 221 (100), 208 (26.2), 168 (6.4), 139 (4.7), 104 (5.3), 77 (4.6); *Anal. Calcd*. For $C_{14}H_{17}ClN_2O$: C, 63.51%; H, 6.47%; N, 10.58%. Found: C, 63.55%; H, 6.52%; N, 10.53%.

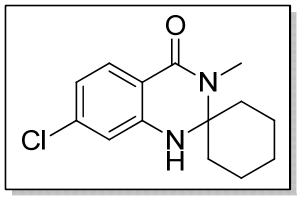


6'-Chloro-8'-methyl-1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 10), white solid, m.p. 198-199 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.32 (br, 1H, NH), 7.42 (d, ^{4}J = 2.30 Hz 1H, Ar-H), 7.19 (d, ^{4}J = 2.25 Hz, 1H, Ar-H), 6.07 (br, 1H, NH), 2.12 (s, 3H, -CH_3), 1.88-1.78 (m, 4H, cyclopentane-H), 1.67-1.64 (m, 4H, cyclopentane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 162.9, 143.8, 133.7, 126.6, 124.5, 121.3, 117.0, 68.2, 37.3, 25.3, 21.7; Ms (EI, 70 eV): m/z (%) = 250 (15.5), 235 (10), 221 (100), 208 (24.2), 168 (6.4), 104 (4.3), 77 (5.6); *Anal. Calcd*. For $C_{13}H_{15}ClN_2O$: C, 62.28%; H, 6.03%; N, 11.17%. Found: C, 62.33%; H, 6.13%; N, 11.12%.

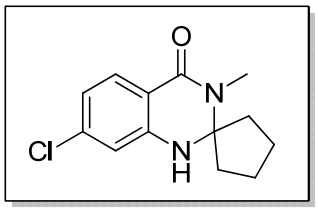


1'*H*-Spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 11 Table 5, entry 24), white solid, m.p. 284-285 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.09 (br, 1H, NH), 7.57 (d, J = 8.00 Hz 1H, Ar-H), 7.22 (t, J = 7.45 Hz, 1H, Ar-H), 6.47 (br, 1H,

NH), 6.68 (d, J = 8.05 Hz 1H, Ar-H), 6.62 (t, J = 7.45 Hz, 1H, Ar-H), 1.81-1.76 (m, 4H, cyclopentane-H), 1.66-1.64 (m, 4H, cyclopentane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 164.0, 148.0, 133.5, 127.7, 117.0, 115.0, 114.8, 77.6, 34.5, 22.4; Ms (EI, 70 eV): m/z (%) = m/z (%) = 202 (11.5), 174 (21.9), 173 (100), 160 (10.5), 146 (4.1), 119 (11.6), 92 (8.4), 65 (4.05); *Anal. Calcd*. For $C_{12}H_{14}ClN_2O$: C, 71.26%; H, 6.98%; N, 13.85%. Found: C, 71.19%; H, 7.03%; N, 13.69%.

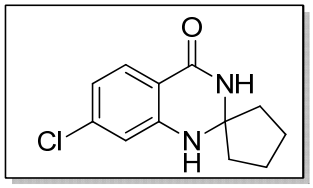


7'-Chloro-3'-methyl-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 12), white solid, m.p. 277-278 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.60 (d, ^{3}J = 8.60 Hz, 1H, Ar-H), 7.04 (d, ^{4}J = 1.70 Hz, 1H, Ar-H), 6.81 (br 1H, N-H), 6.67 (dd, ^{4}J = 2.30 Hz, ^{3}J = 8.55 Hz, 1H, ArH), 2.94 (s, 3H, N-CH_3), 1.83~1.72 (m, 4H, cyclohexane-H), 1.60~1.56 (m, 5H, cyclohexane-H), 1.21~1.12 (m, 5H, cyclohexane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 162.5, 146.8, 137.9, 130.0, 117.5, 114.5, 72.6, 32.9, 26.7, 24.5, 21.6; Ms (EI, 70 eV): m/z (%) = 264 (19.2), 235 (9.5), 221 (100), 208 (22.8), 180 (11.7), 165 (2.8), 68 (5.9), 41 (3.2); *Anal. Calcd*. For $C_{14}H_{17}ClN_2O$: C, 63.51%; H, 6.47%; N, 10.58%. Found: C, 63.54%; H, 6.51%; N, 10.62%.

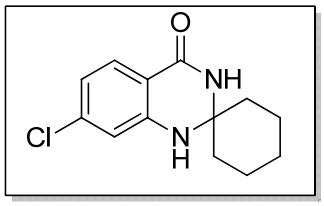


7'-Chloro-3'-methyl-1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 13), white solid, m.p. 213-215 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.60 (d, ^{3}J = 8.60 Hz, 1H, Ar-H), 7.07 (br 1H, N-H), 6.77 (d, ^{4}J = 1.70 Hz, 1H, Ar-H), 6.67 (dd, ^{4}J = 1.70 Hz, ^{3}J = 8.00 Hz, 1H, ArH), 2.90 (s, 3H, N-CH_3), 2.05~1.99 (m, 2H, cyclopentane-H), 1.78~1.62 (m, 6H, cyclopentane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 162.7, 147.7, 137.8, 130.1, 117.5, 114.2, 114.0, 81.7, 36.3, 27.8, 23.3; Ms

(EI, 70 eV): m/z (%) = 250 (15.9), 235 (5.2), 221 (100), 208 (18.7), 194 (15.5), 180 (6.1), 165 (7.9), 126 (5.1), 68 (10.9), 55 (4.2), 41 (3.8); *Anal. Calcd*. For $C_{13}H_{15}ClN_2O$: C, 62.28%; H, 6.03%; N, 11.17%. Found: C, 62.33%; H, 5.97%; N, 11.21%.

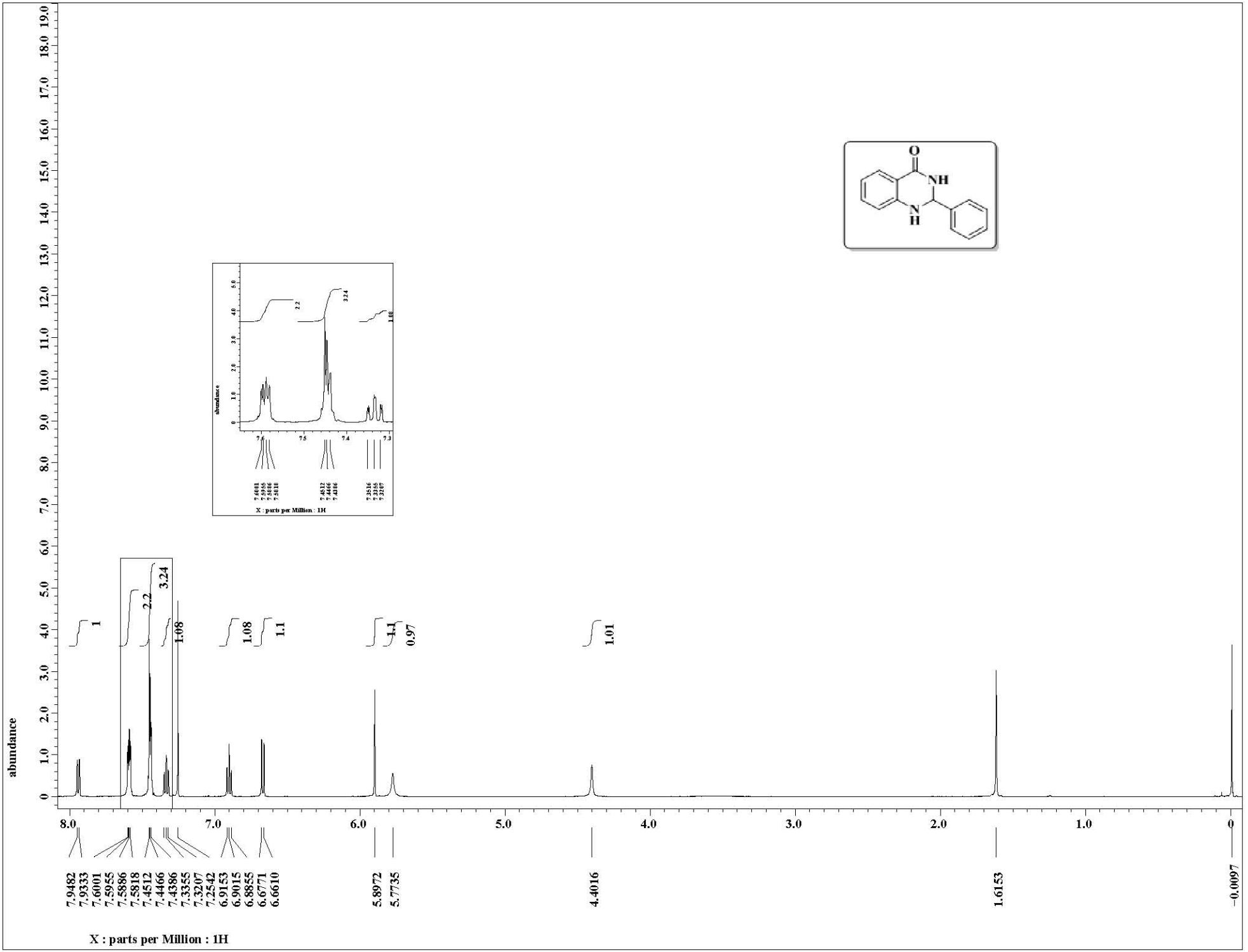


7'-Chloro-1'*H*-spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 14 and Table 5, entry 25), white solid, m.p. 223-224 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.23 (br s, 1H, NH), 7.57 (d, J = 8.25 Hz,1H, ArH), 7.05 (s, 1H, ArH), 6.73 (s, 1H, ArH), 6.65 (d, J = 8.25 Hz, 1H, ArH), 1.80-1.66 (m, 8H, cyclopentane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 163.1, 148.9, 138.0, 129.7, 117.0, 113.9, 113.8, 77.7, 31.6, 22.4; Ms (EI, 70 eV): m/z (%) = 236 (11), 207 (100), 153 (10.9), 126 (8.3), 90 (3.9), 63 (3.6); *Anal. Calcd*. For $C_{12}H_{13}ClN_2O$: C, 60.89%; H, 5.54%; N, 11.84%. Found: C, 60.93%; H, 5.64%; N, 11.90%.



7'-Chloro-1'*H*-spiro[cyclohexane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 15). white solid, m.p. 209-210 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.05 (br s, 1H, NH), 7.55 (d, J = 8.0 Hz,1H, ArH), 6.91 (s, 1H, ArH), 6.86 (d, ^{4}J = 1.75 Hz,1H, ArH), 6.63 (dd, ^{4}J = 2.30 Hz, ^{3}J = 8.60 Hz, 1H, ArH), 1.75-1.73 (m, 2H, cyclohexane-H), 1.60-1.43 (m, 7H, cyclohexane-H), 1.24-1.21 (m, 1H, cyclohexane-H); ^{13}C NMR (125 MHz, DMSO-d_6): 162.8, 148.2, 138.1, 129.6, 116.9, 114.1, 113.6, 68.6, 37.7, 25.0, 21.3; Ms (EI, 70 eV): m/z (%) = 250 (23), 221 (9.8), 209 (31), 207 (100), 154 (10.2), 126 (8.0), 90 (3.2), 63 (3.4), 41 (3.3); *Anal. Calcd*. For *Anal. Calcd*. For $C_{13}H_{15}ClN_2O$: C, 62.28%; H, 6.03%; N, 11.17%. Found: C, 62.34%; H, 5.98%; N, 11.21%.

5 Copies of ^{1}H and ^{13}C NMR Spectras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7.2542
6.9153
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6.8855
6.6771
6.6610
5.8972
5.7735
4.4016
1.6153
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O
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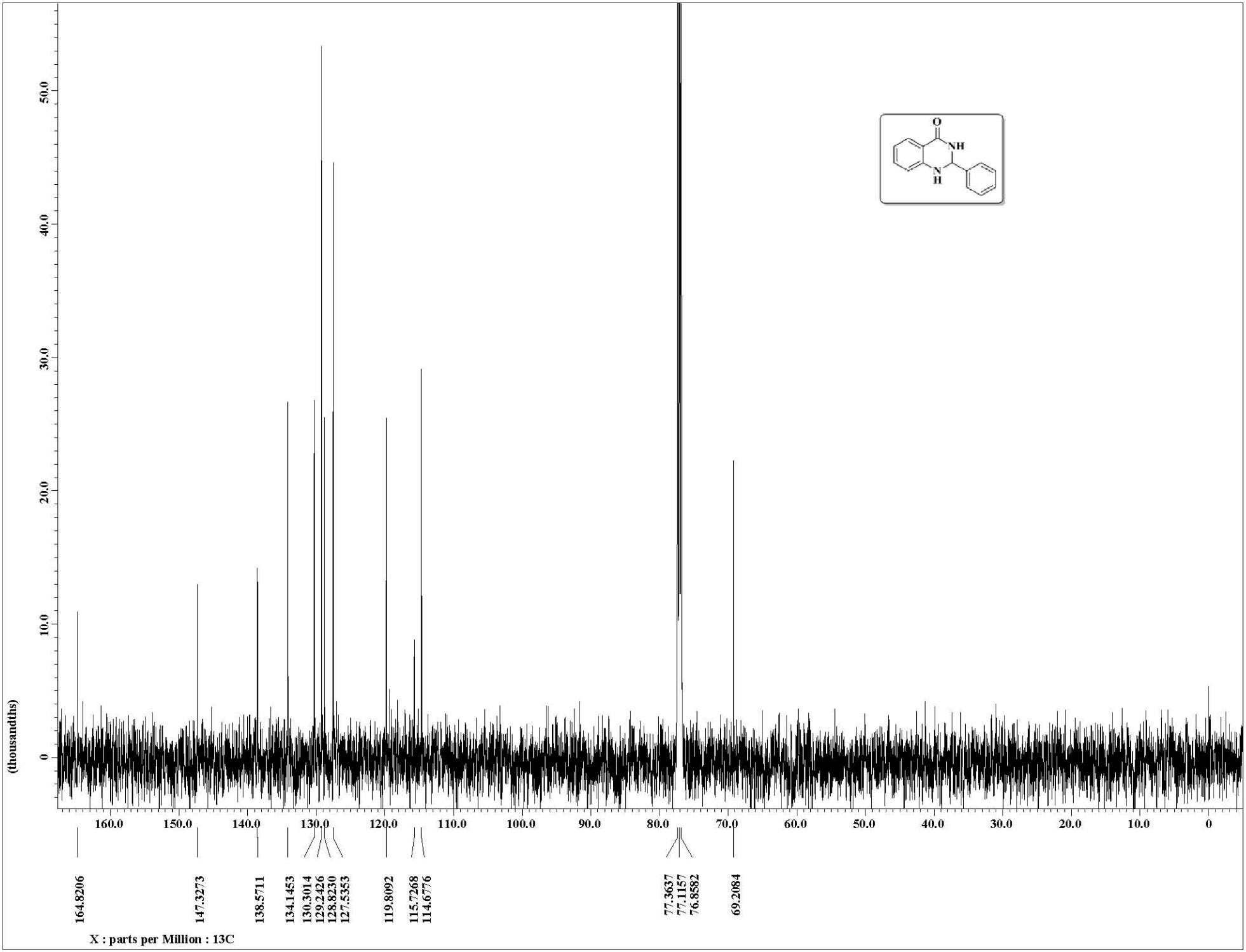
N
H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80.0
70.0
60.0
50.0
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N
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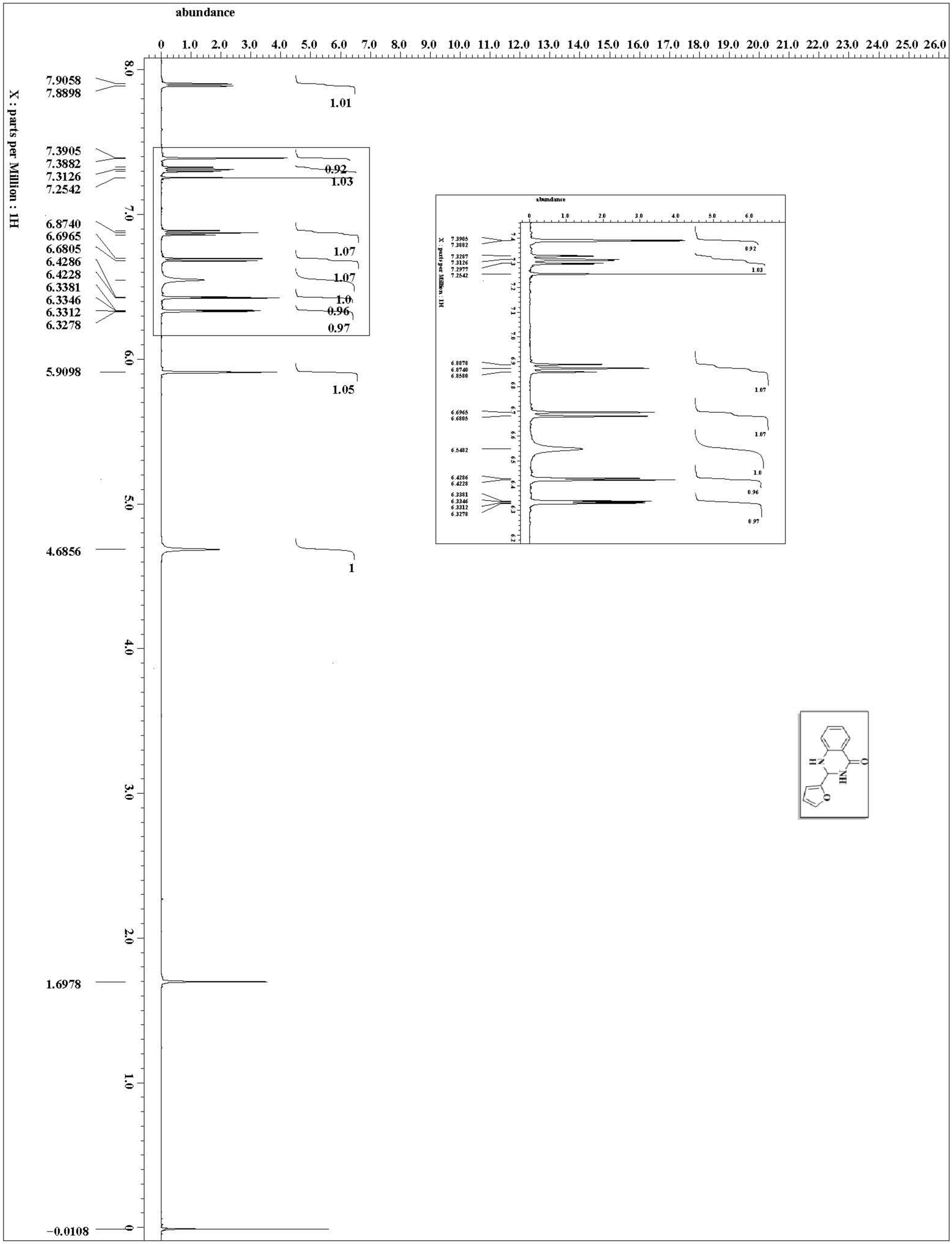
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6.3381
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6.3312
6.3278
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4.6856
1.6978
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0.92
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1.07
1.07
1.0
0.96
0.97
1.05
1
abundance
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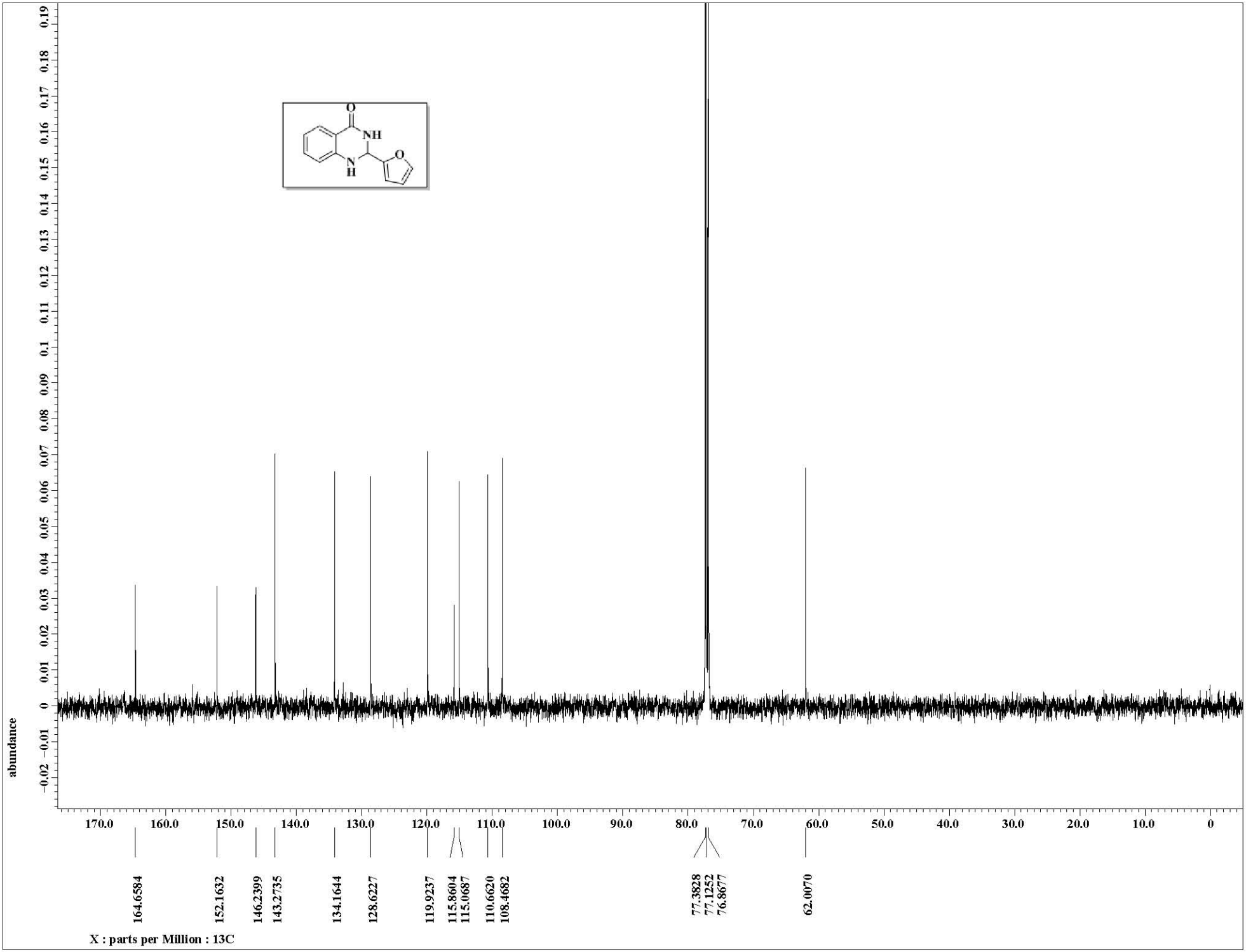
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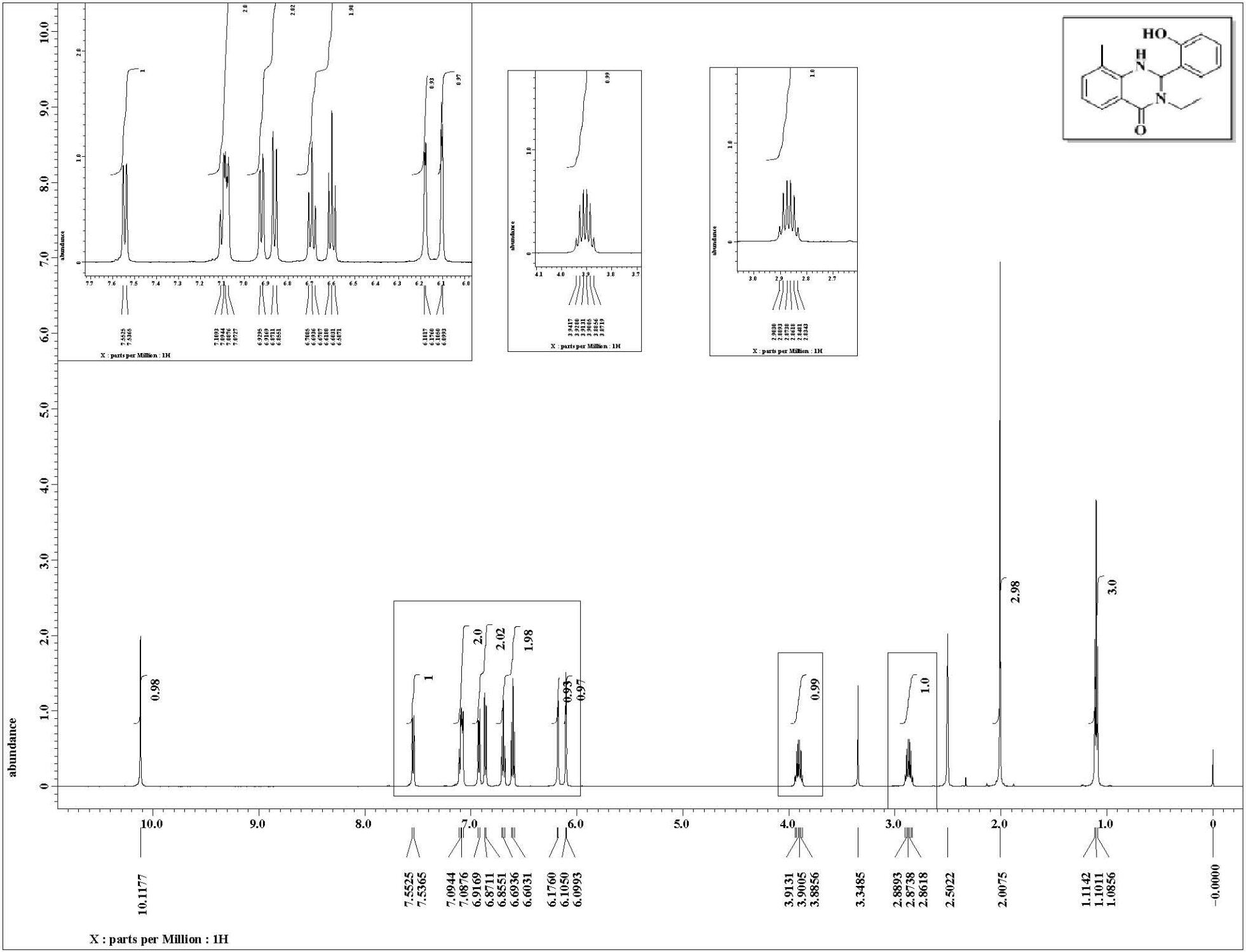
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N
H
N
O
abundance
X : parts per Million : 1H
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3.8856
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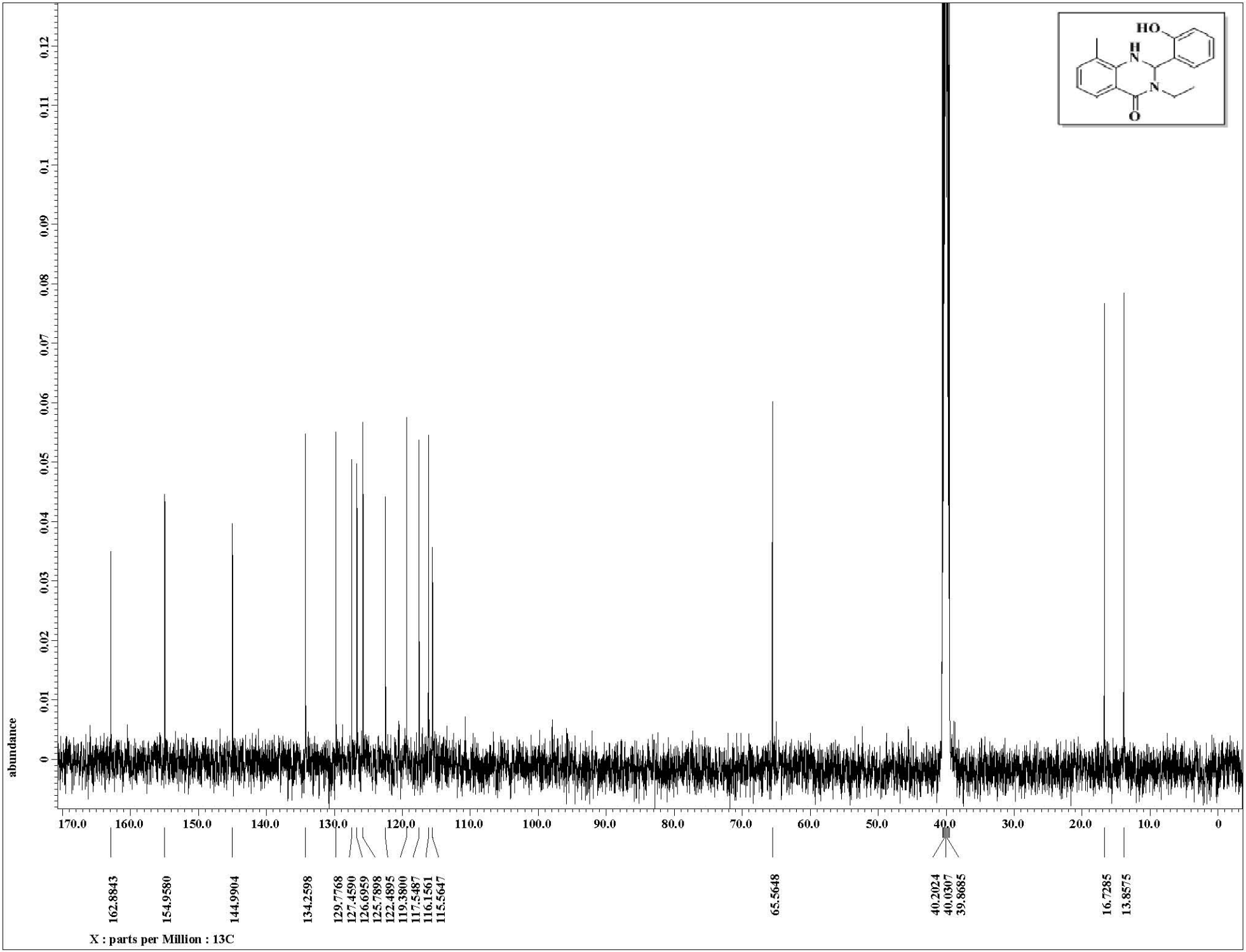
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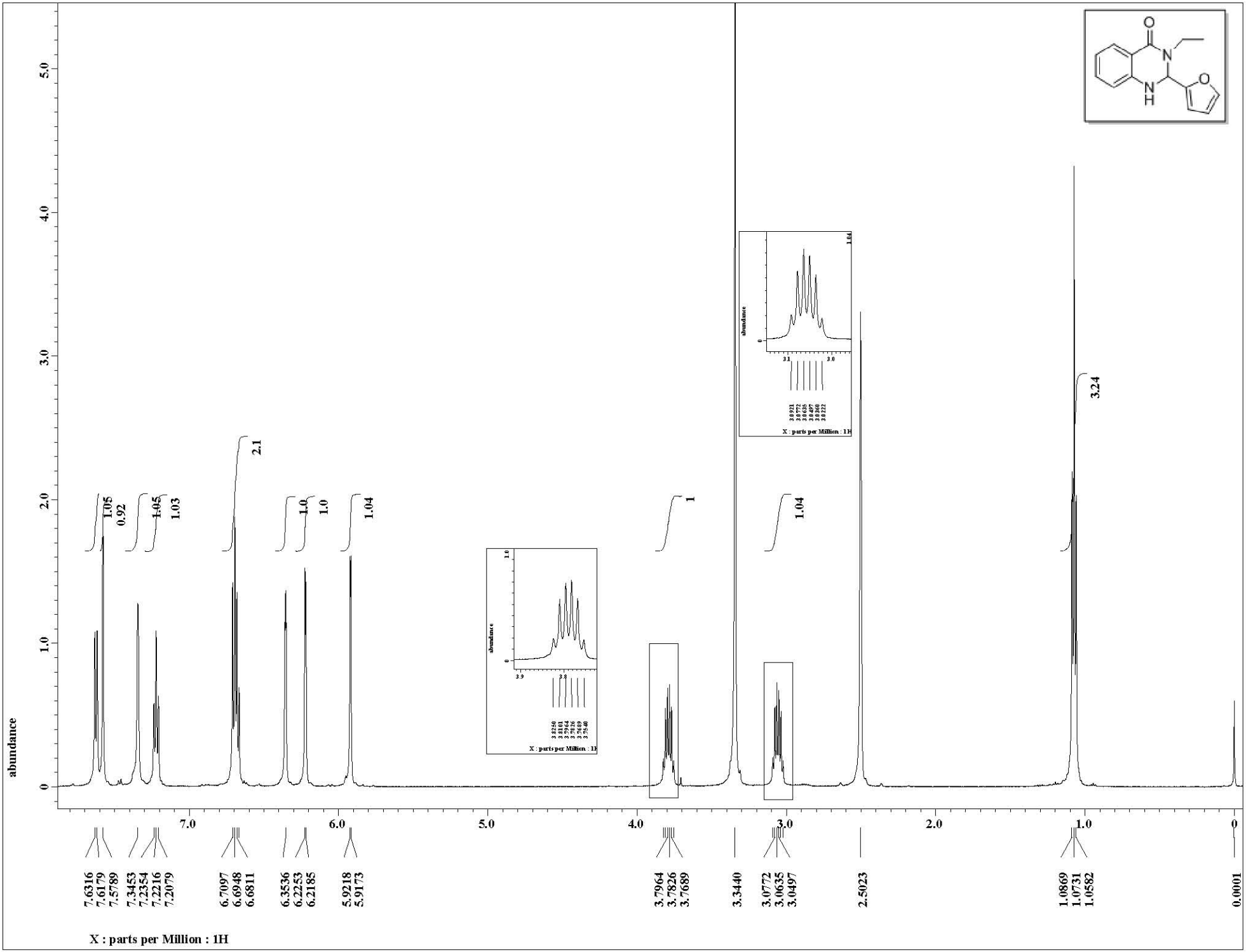
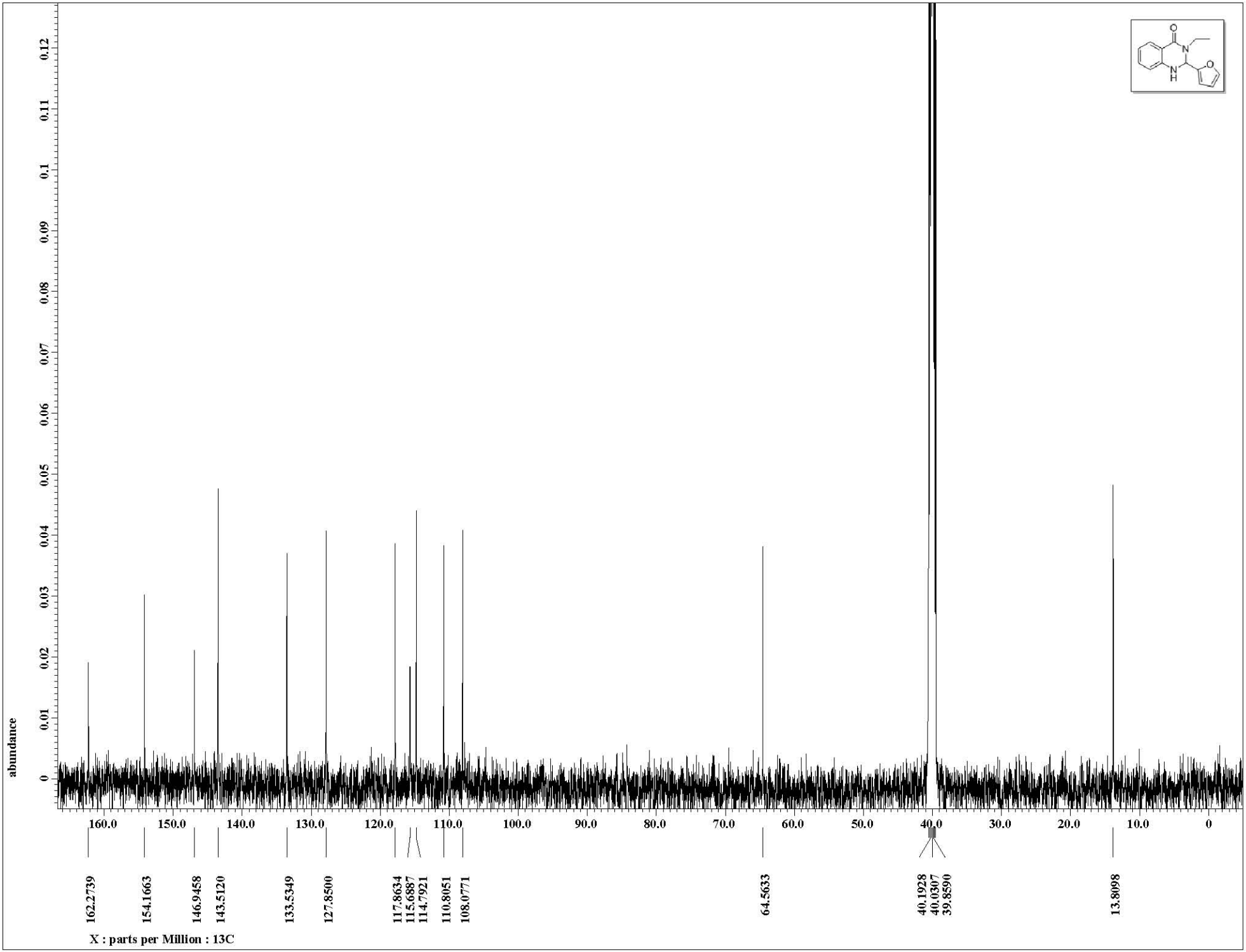
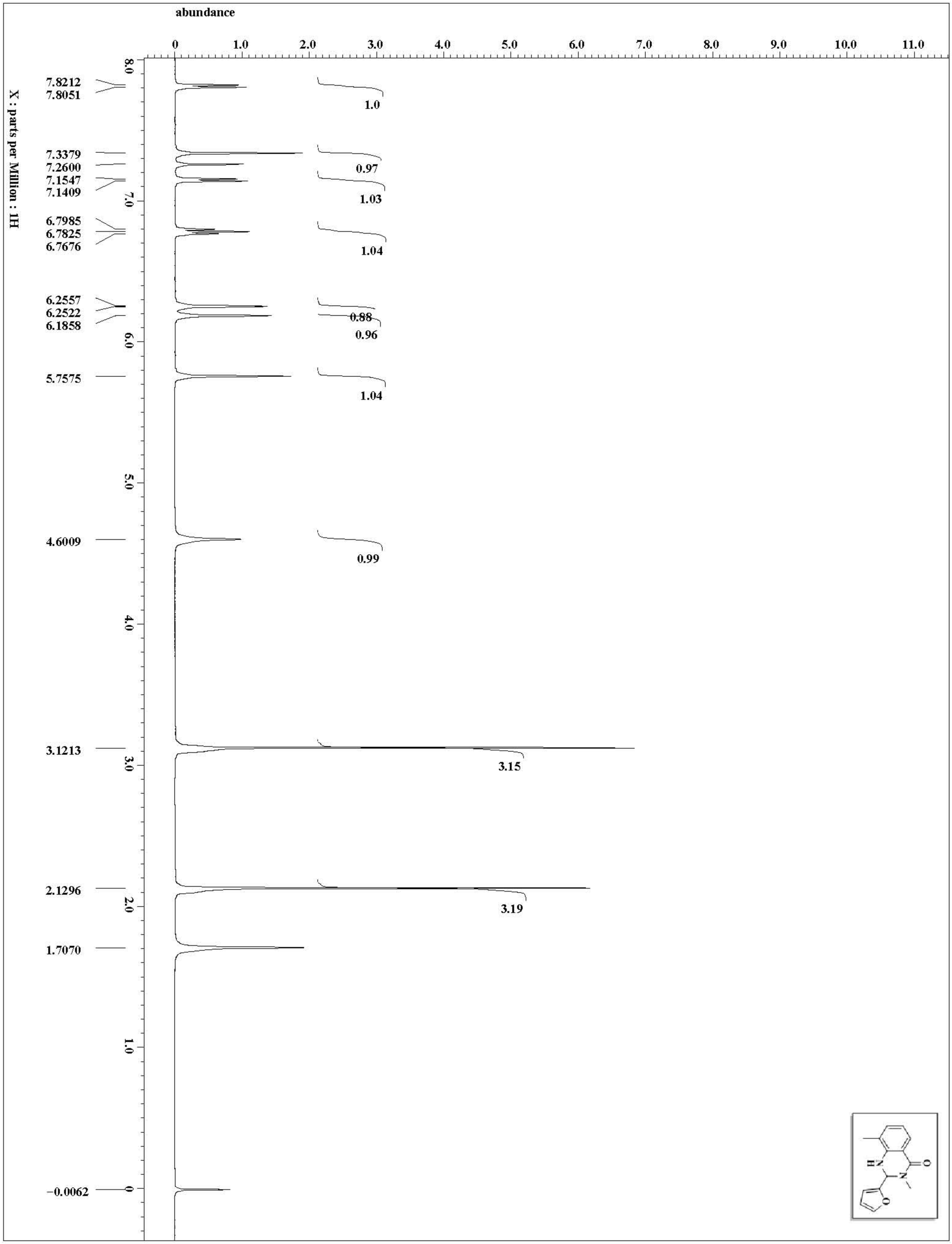
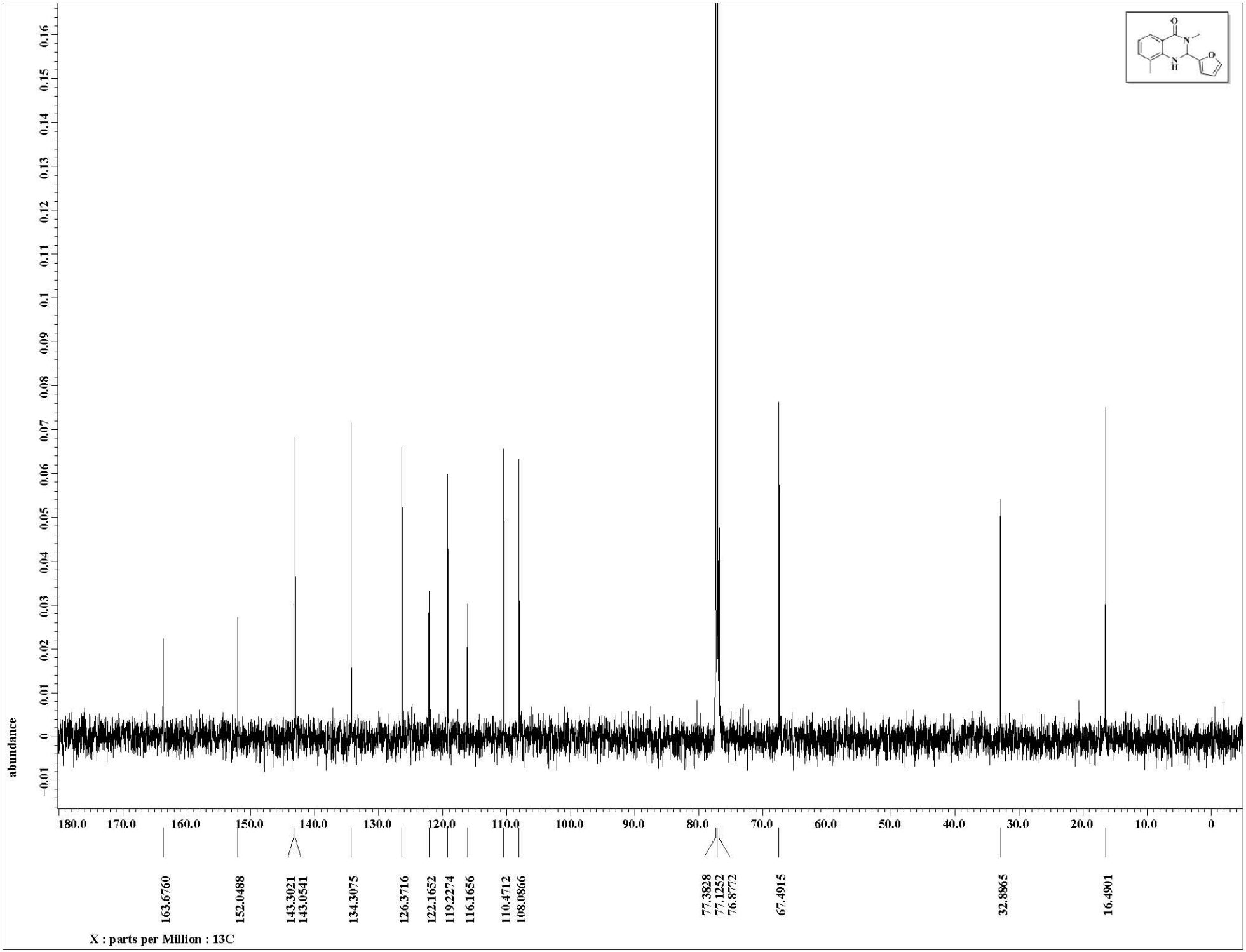
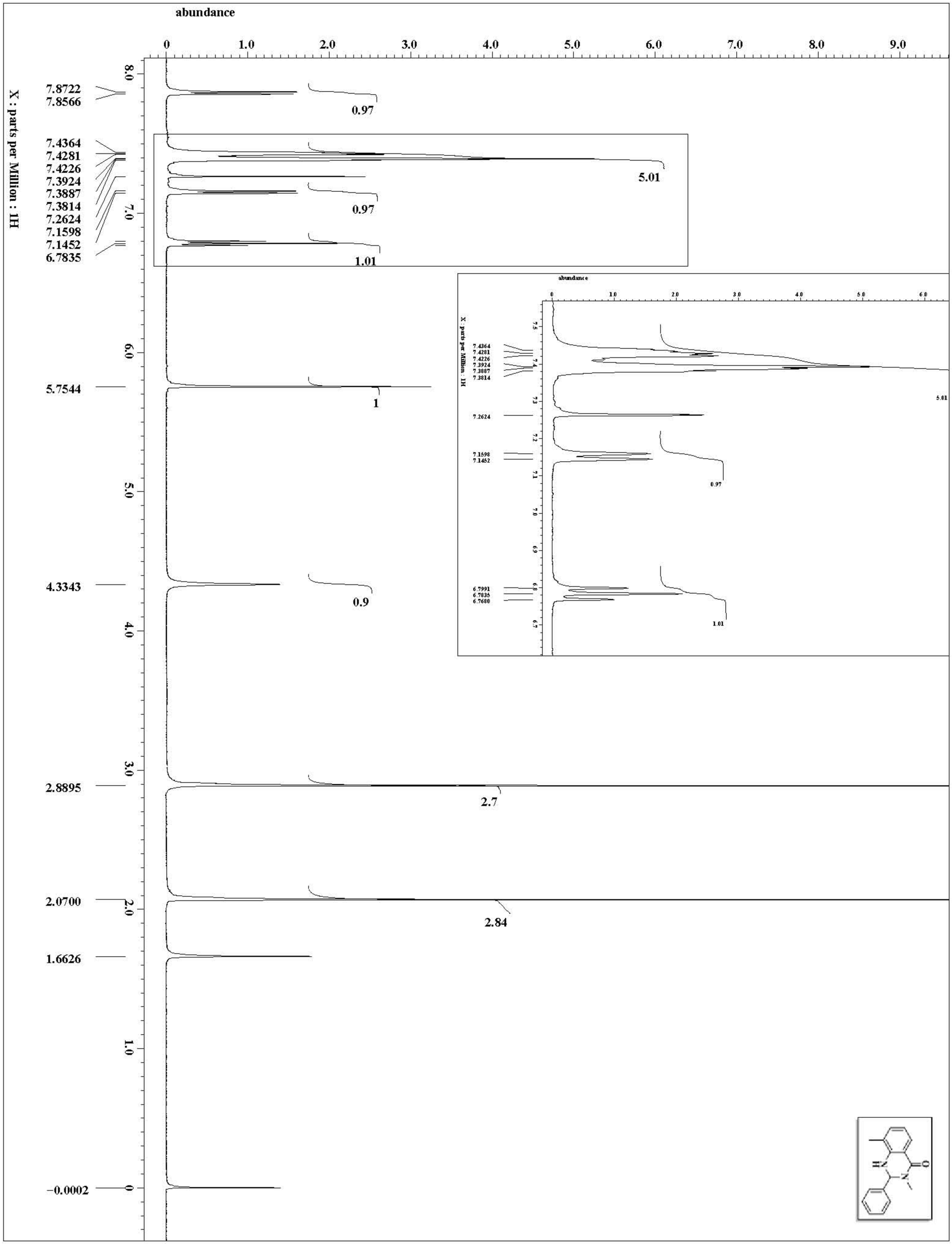
13.8575
X : parts per Million : 13C

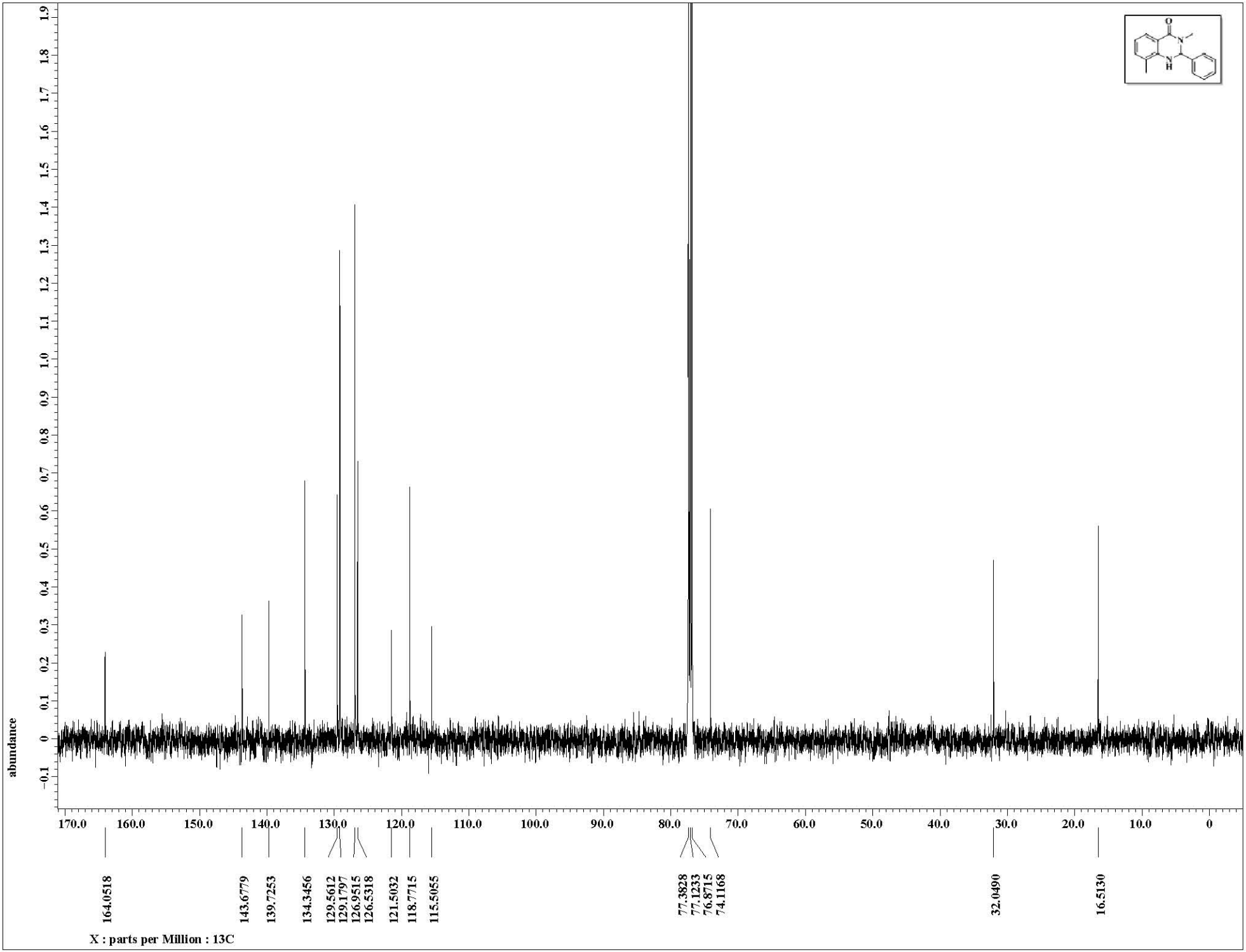

abundance
X : parts per Million : 1H
7.6316
7.6179
7.5789
7.3453
7.2354
7.2216
7.2079
6.7097
6.6948
6.6811
6.3536
6.2253
6.2185
5.9218
5.9173
3.7964
3.7826
3.7689
3.3440
3.0772
3.0635
3.0497
2.5023
1.0869
1.0731
1.0582
0.0001
1.05
0.92
1.05
1.03
2.1
1.0
1.0
1.04
1
1.04
3.24

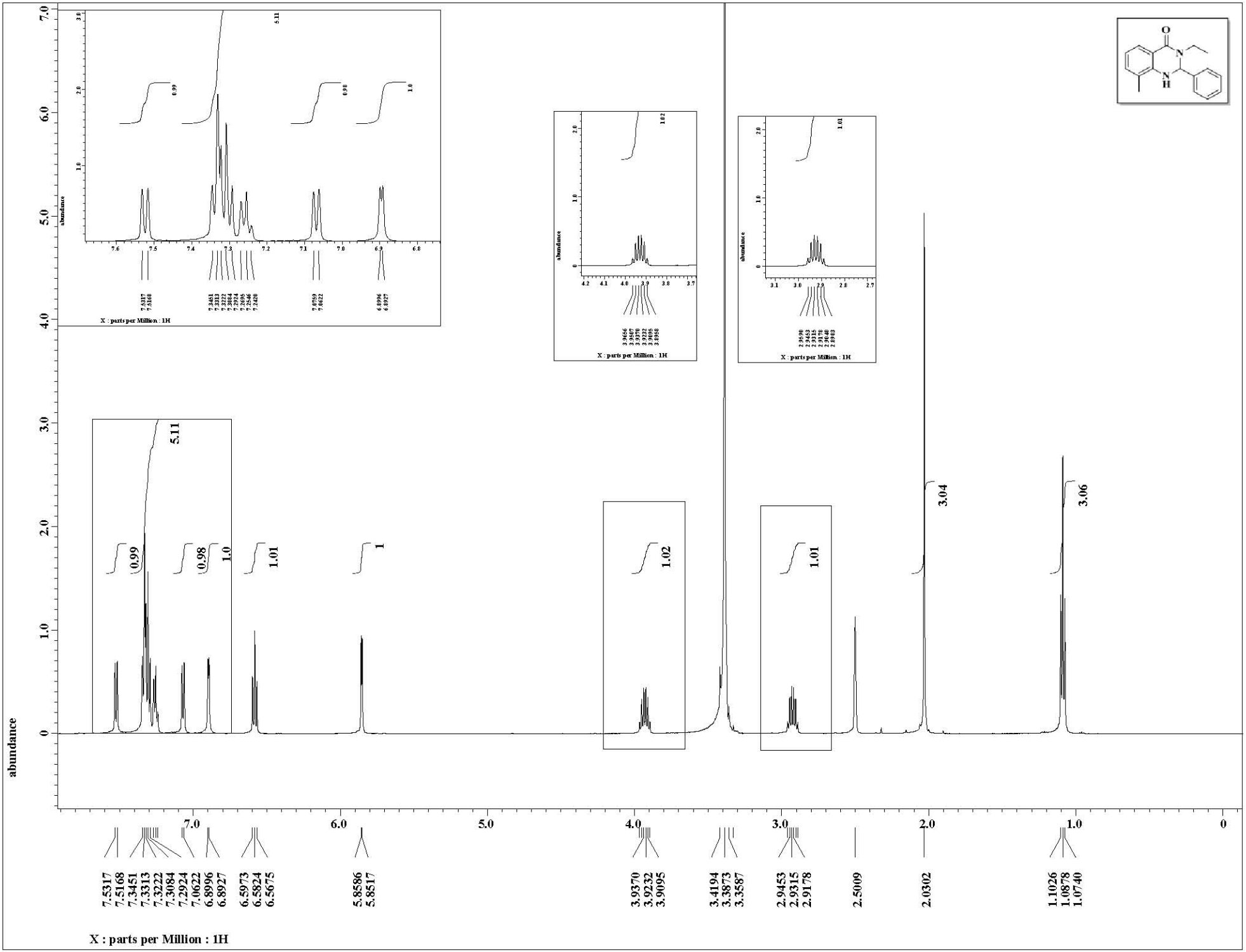

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.2739
154.1663
146.9458
143.5120
133.5349
127.8500
117.8634
115.6887
114.7921
110.8051
108.0771
64.5633
40.1928
40.0307
39.8590
13.8098
X : parts per Million : 13C

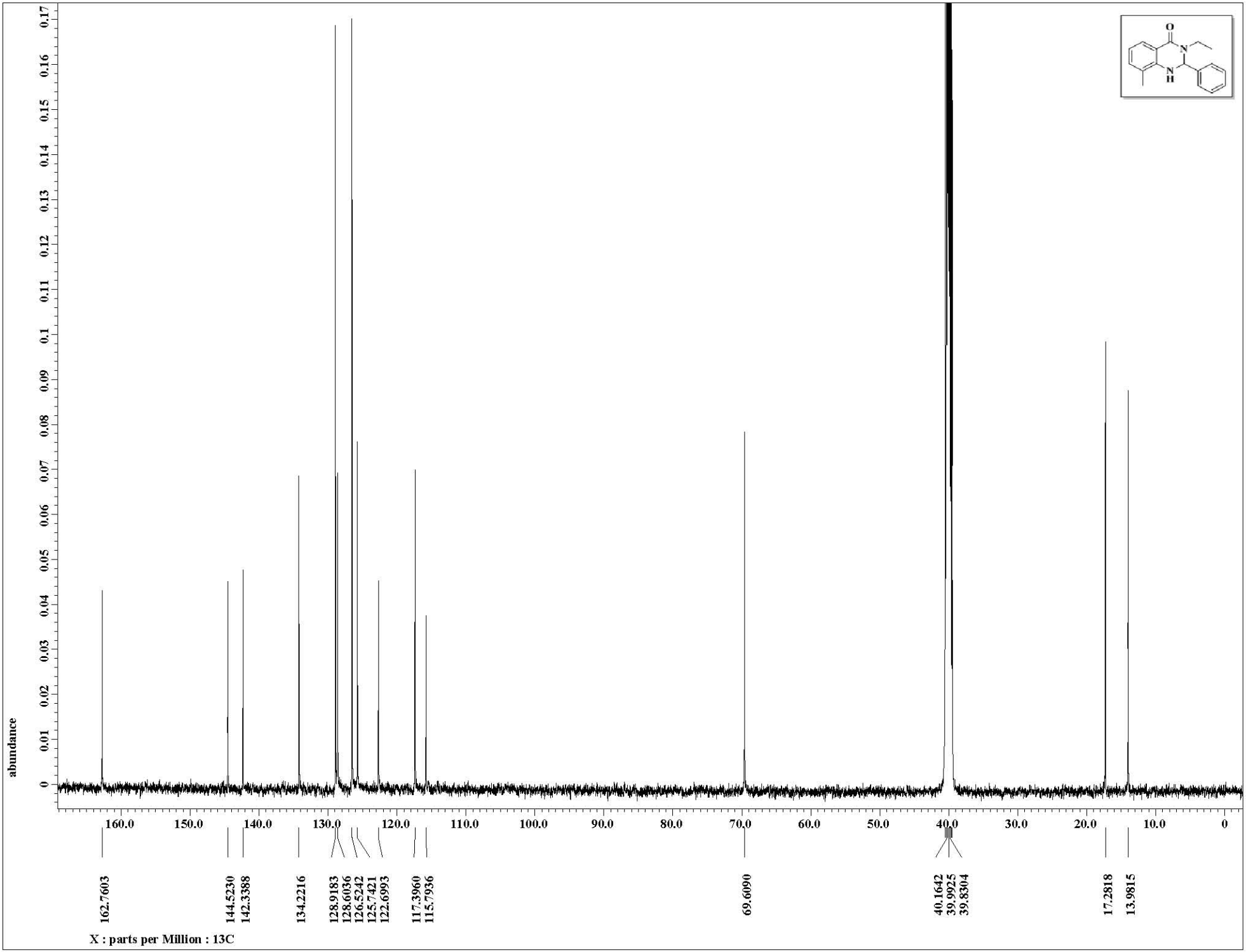

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
X : parts per Million : 1H
7.8212
7.8051
1.0
7.3379
7.2600
7.1547
7.1409
0.97
1.03
6.7985
6.7825
6.7676
1.04
6.2557
6.2522
6.1858
0.88
0.96
5.7575
1.04
4.6009
0.99
3.1213
3.15
2.1296
3.19
1.7070
−0.0062
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
H
N
N
O
O

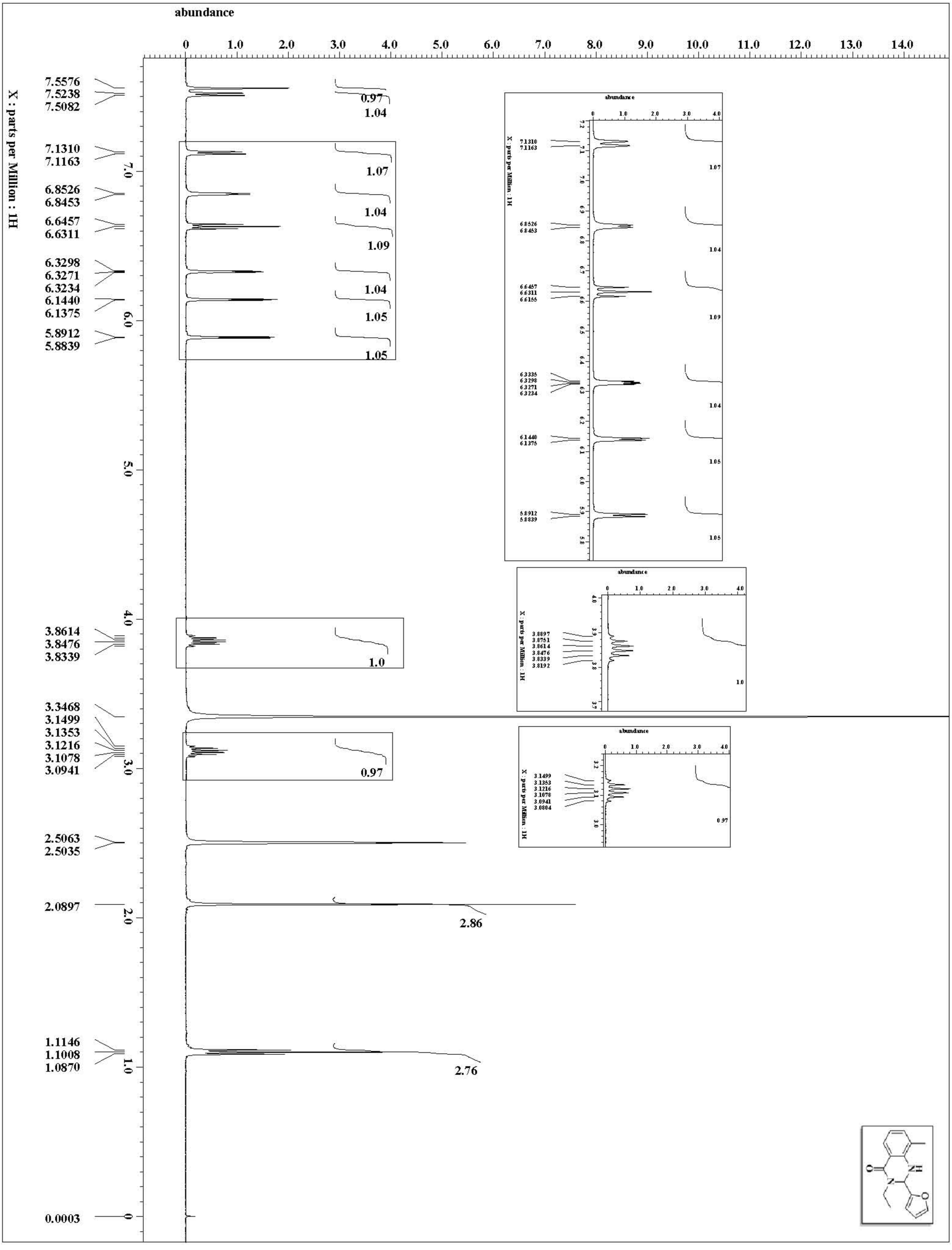

abundance
X : parts per Million : 13C
163.6760
152.0488
143.3021
143.0541
134.3075
126.3716
122.1652
119.2274
116.1656
110.4712
108.0866
77.3828
77.1252
76.8772
67.4915
32.8865
16.4901

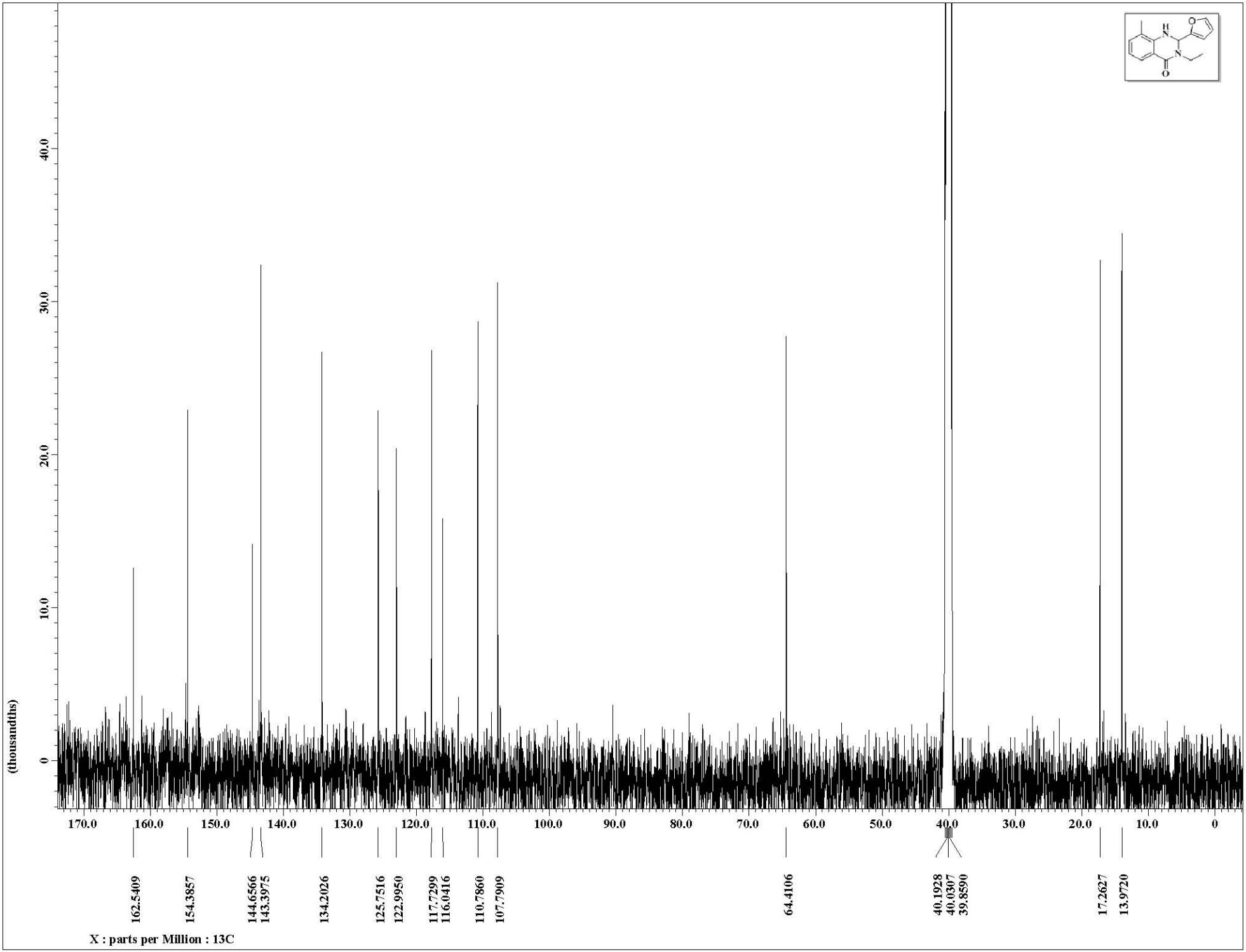

abundance
X : parts per Million : 1H
7.8722
7.8566
7.4364
7.4281
7.4226
7.3924
7.3887
7.3814
7.2624
7.1598
7.1452
6.7835
5.7544
4.3343
2.8895
2.0700
1.6626
−0.0002
0.97
5.01
0.97
1.01
1
0.9
2.7
2.84
6.7991
6.7835
6.7680

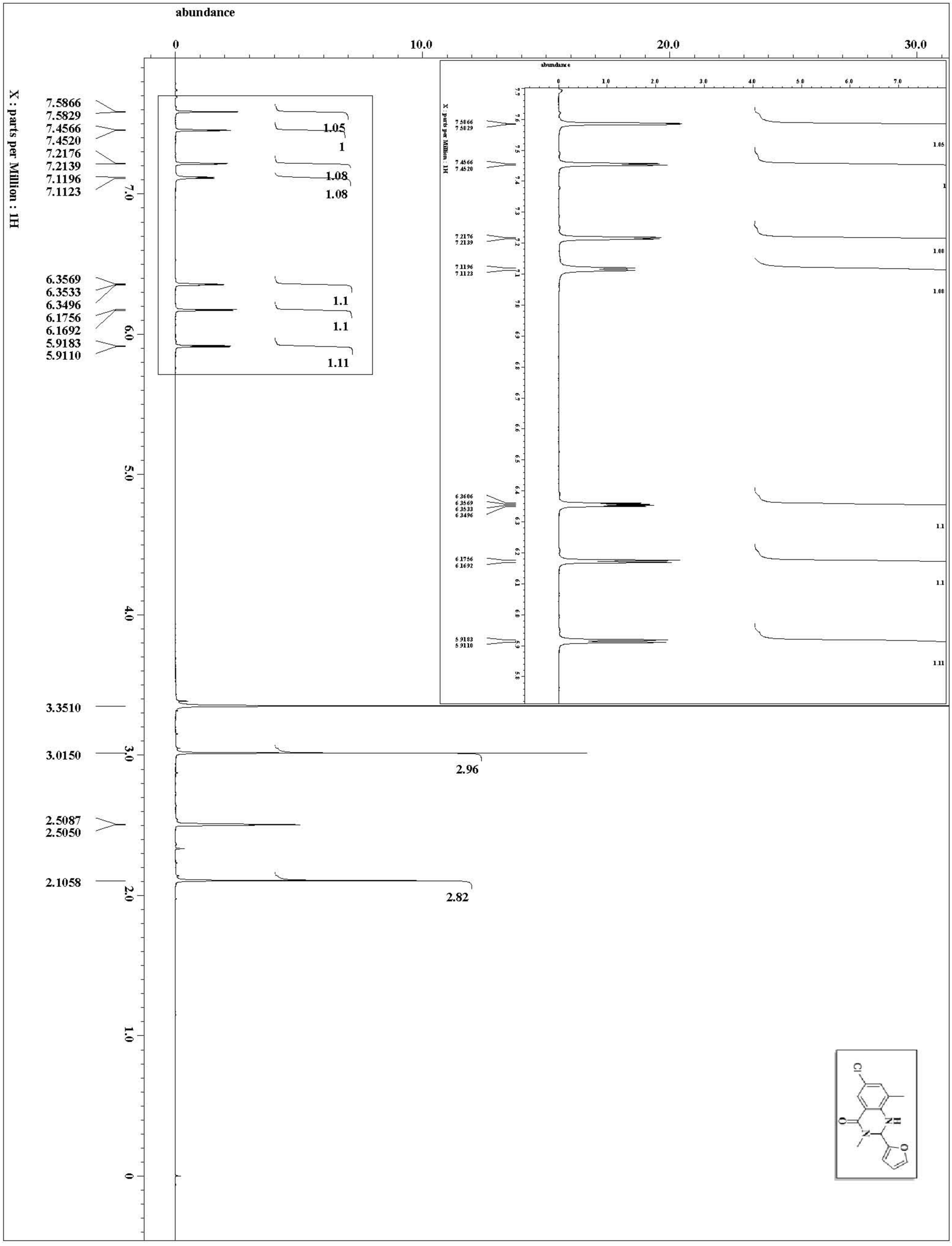

abundance
X : parts per Million : 13C
164.0518
143.6779
139.7253
134.3456
129.5612
129.1797
126.9515
126.5318
121.5032
118.7715
115.5055
77.3828
77.1233
76.8715
74.1168
32.0490
16.5130

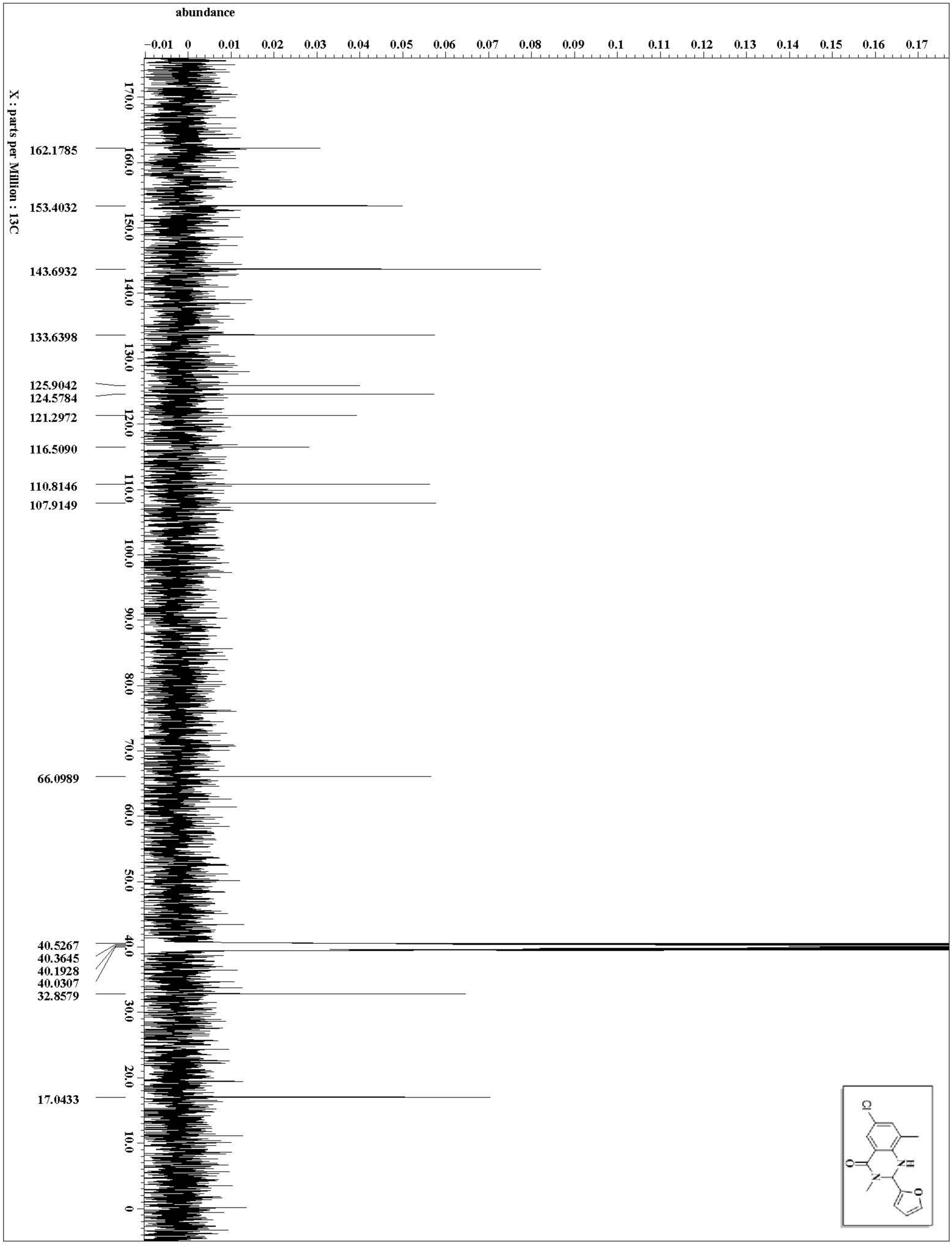

abundance
X : parts per Million : 1H
7.5317
7.5168
7.3451
7.3313
7.3222
7.3084
7.2924
7.0622
6.8996
6.8927
6.5973
6.5824
6.5675
5.8586
5.8517
3.9370
3.9232
3.9095
3.4194
3.3873
3.3587
2.9453
2.9315
2.9178
2.5009
2.0302
1.1026
1.0878
1.0740
5.11
0.99
0.98
1.0
1.01
1
1.02
1.01
3.04
3.06

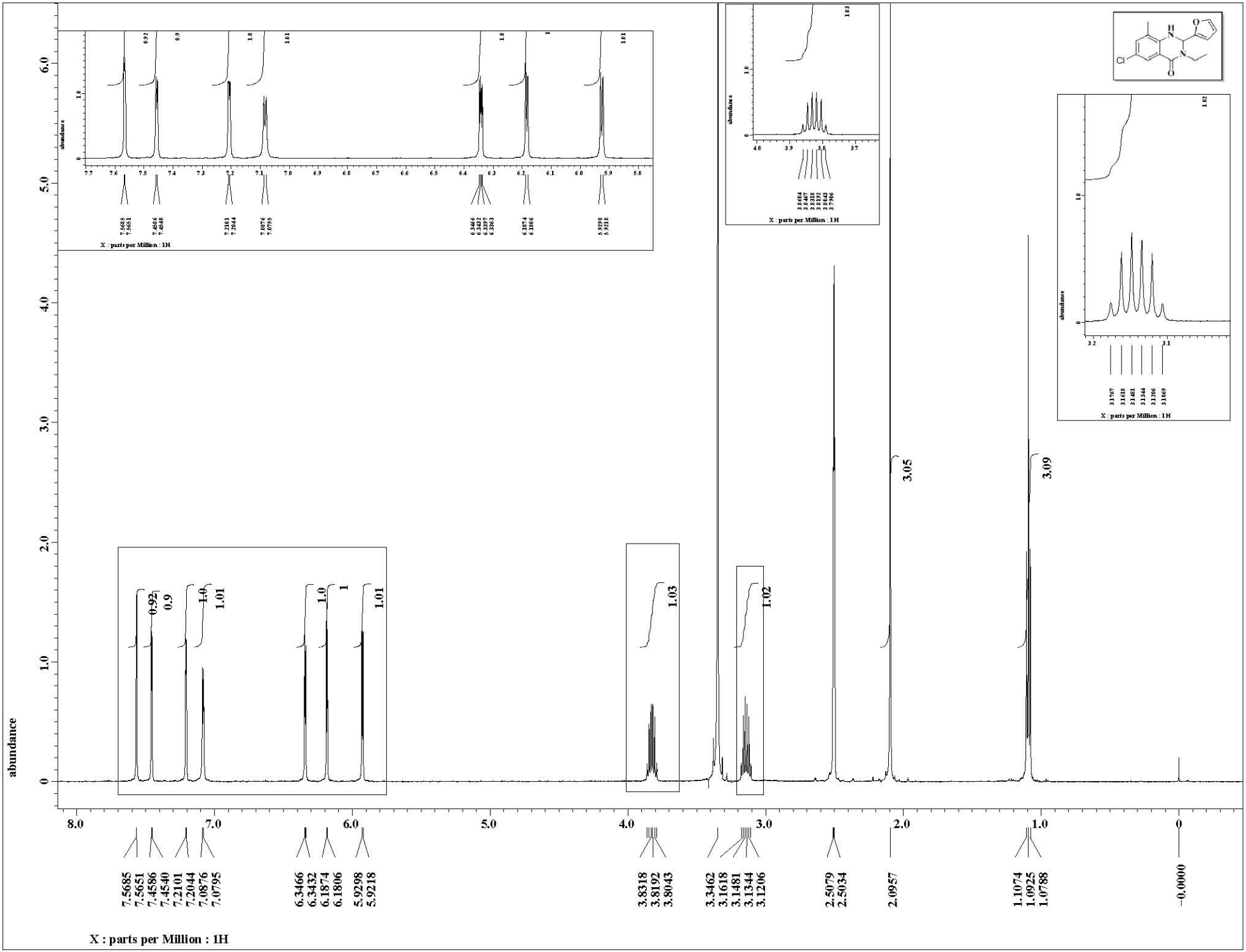

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
0.16
0.17
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.7603
144.5230
142.3388
134.2216
128.9183
128.6036
126.5242
125.7421
122.6993
117.3960
115.7936
69.6090
40.1642
39.9925
39.8304
17.2818
13.9815
X : parts per Million : 13C

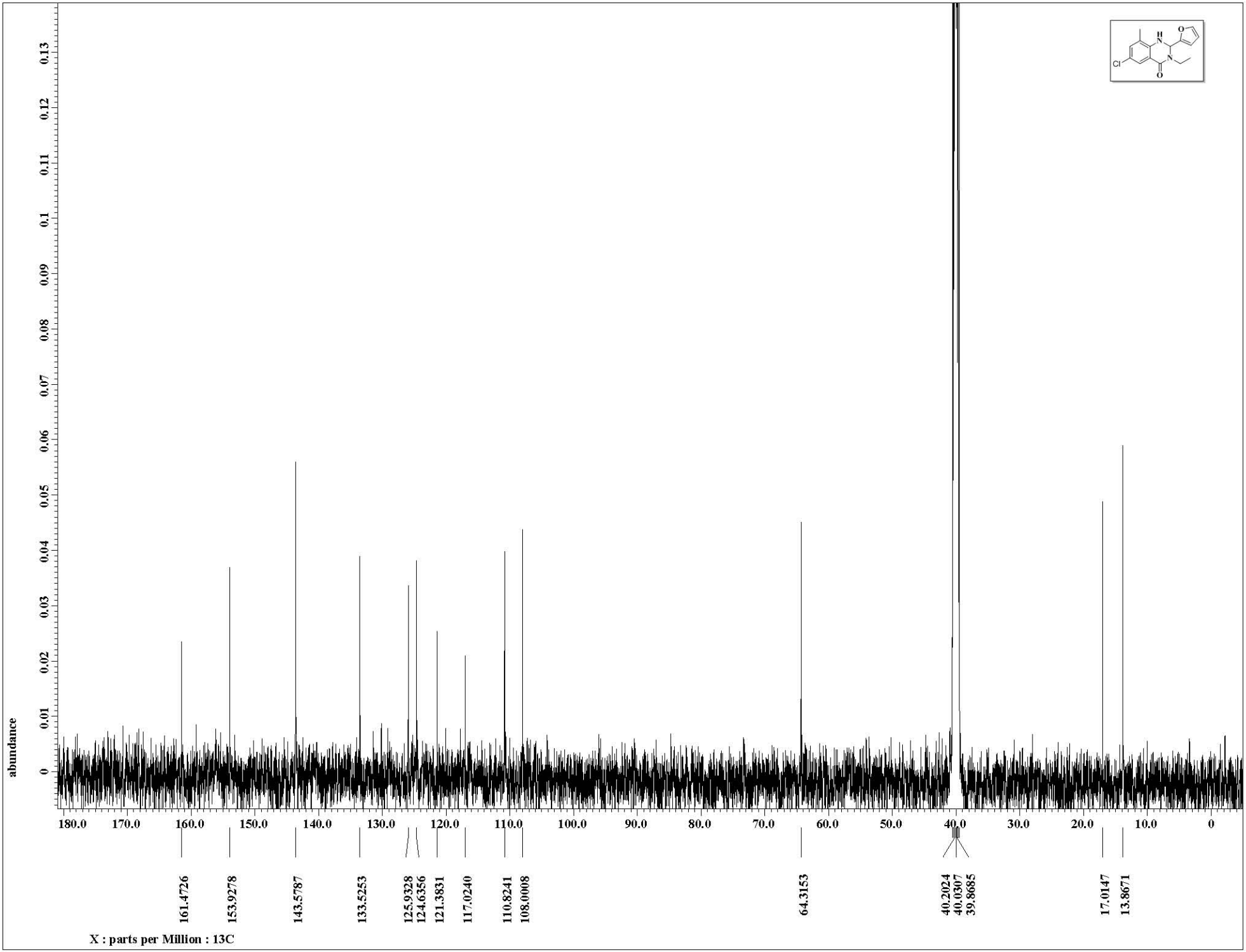

abundance
X : parts per Million : 1H
7.5576
7.5238
7.5082
7.1310
7.1163
6.8526
6.8453
6.6457
6.6311
6.3298
6.3271
6.3234
6.1440
6.1375
5.8912
5.8839
3.8614
3.8476
3.8339
3.3468
3.1499
3.1353
3.1216
3.1078
3.0941
2.5063
2.5035
2.0897
1.1146
1.1008
1.0870
0.0003
0.97
1.04
1.07
1.04
1.09
1.04
1.05
1.05
1.0
0.97
2.86
2.76

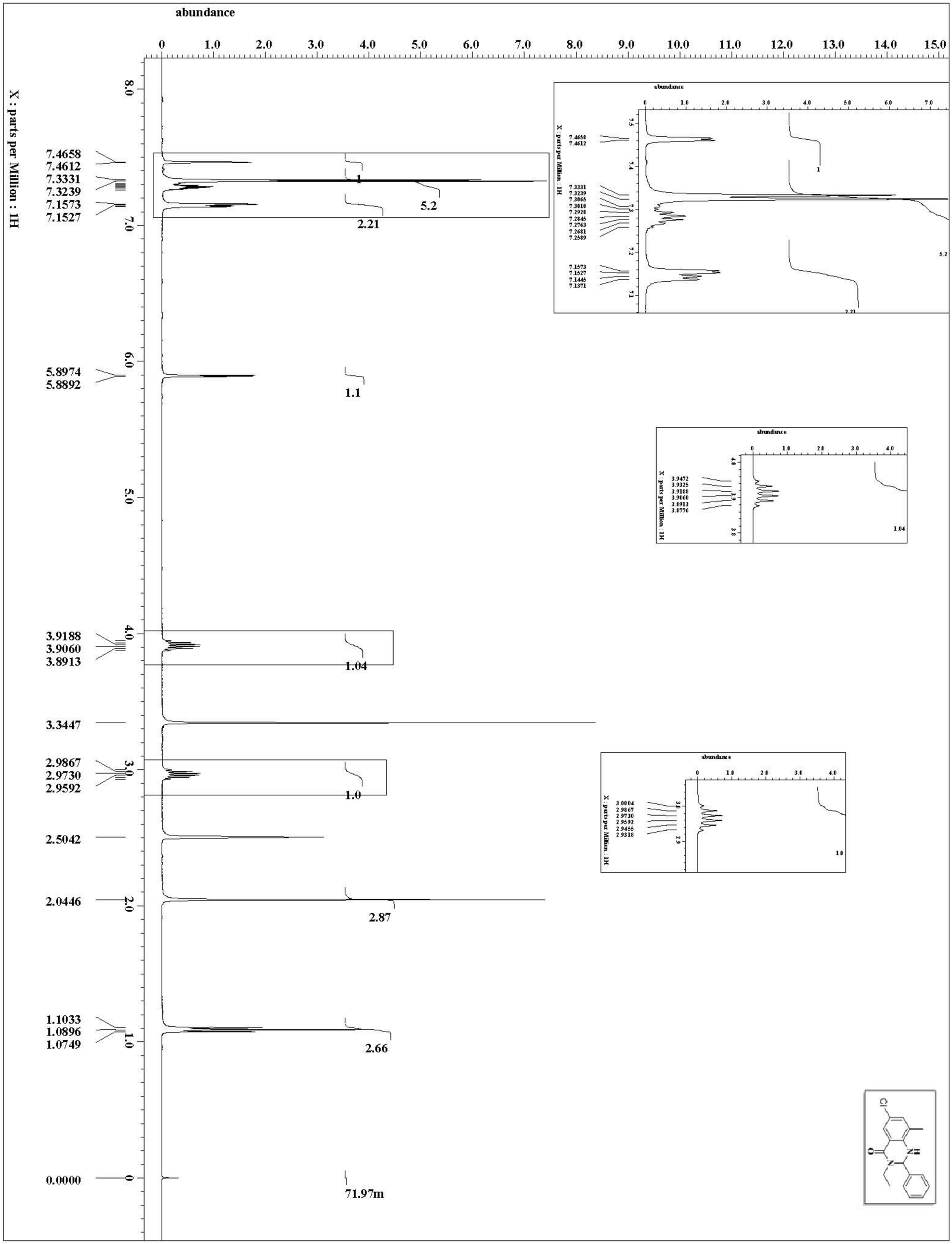

(thousandths)
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.5409
154.3857
144.6566
143.3975
134.2026
125.7516
122.9950
117.7299
116.0416
110.7860
107.7909
64.4106
40.1928
40.0307
39.8590
17.2627
13.9720
X : parts per Million : 13C

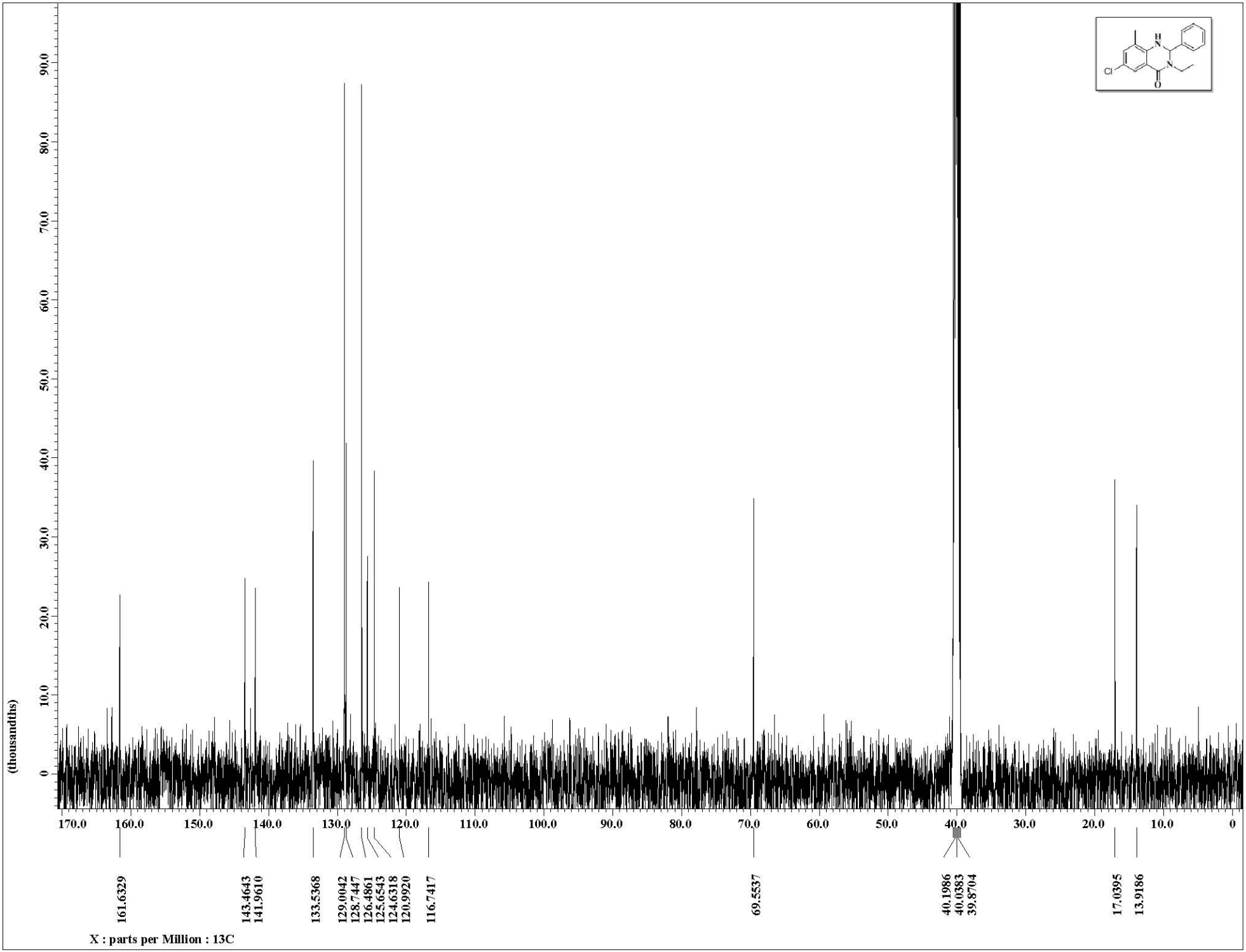

abundance
0
10.0
20.0
30.0
X : parts per Million : 1H
7.5866
7.5829
7.4566
7.4520
7.2176
7.2139
7.1196
7.1123
6.3569
6.3533
6.3496
6.1756
6.1692
5.9183
5.9110
3.3510
3.0150
2.5087
2.5050
2.1058
1.05
1
1.08
1.08
1.1
1.1
1.11
2.96
2.82
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Cl
O
N
H
O

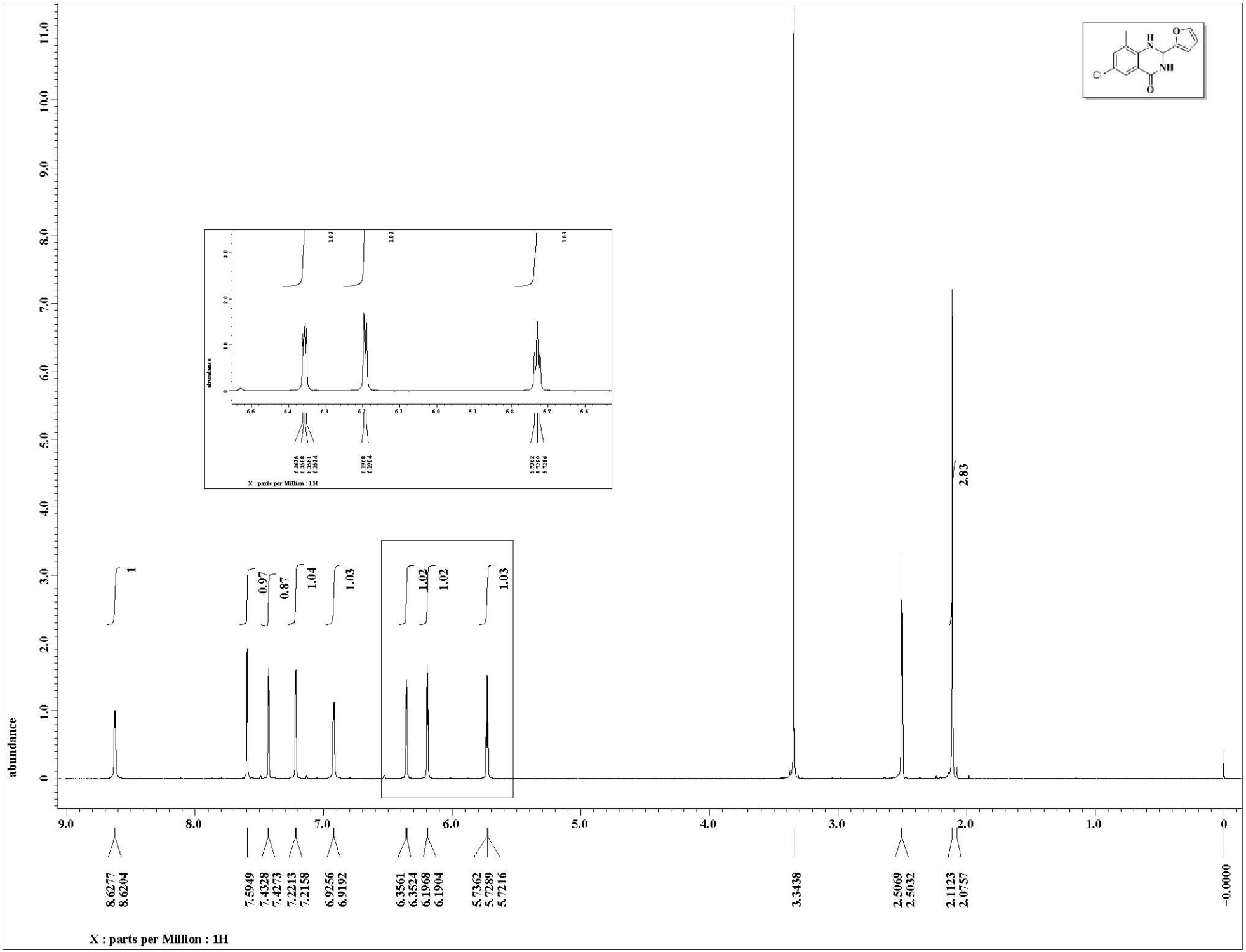

abundance
−0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17
X : parts per Million : 13C
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.1785
153.4032
143.6932
133.6398
125.9042
124.5784
121.2972
116.5090
110.8146
107.9149
66.0989
40.5267
40.3645
40.1928
40.0307
32.8579
17.0433
Cl
O
N
N
O

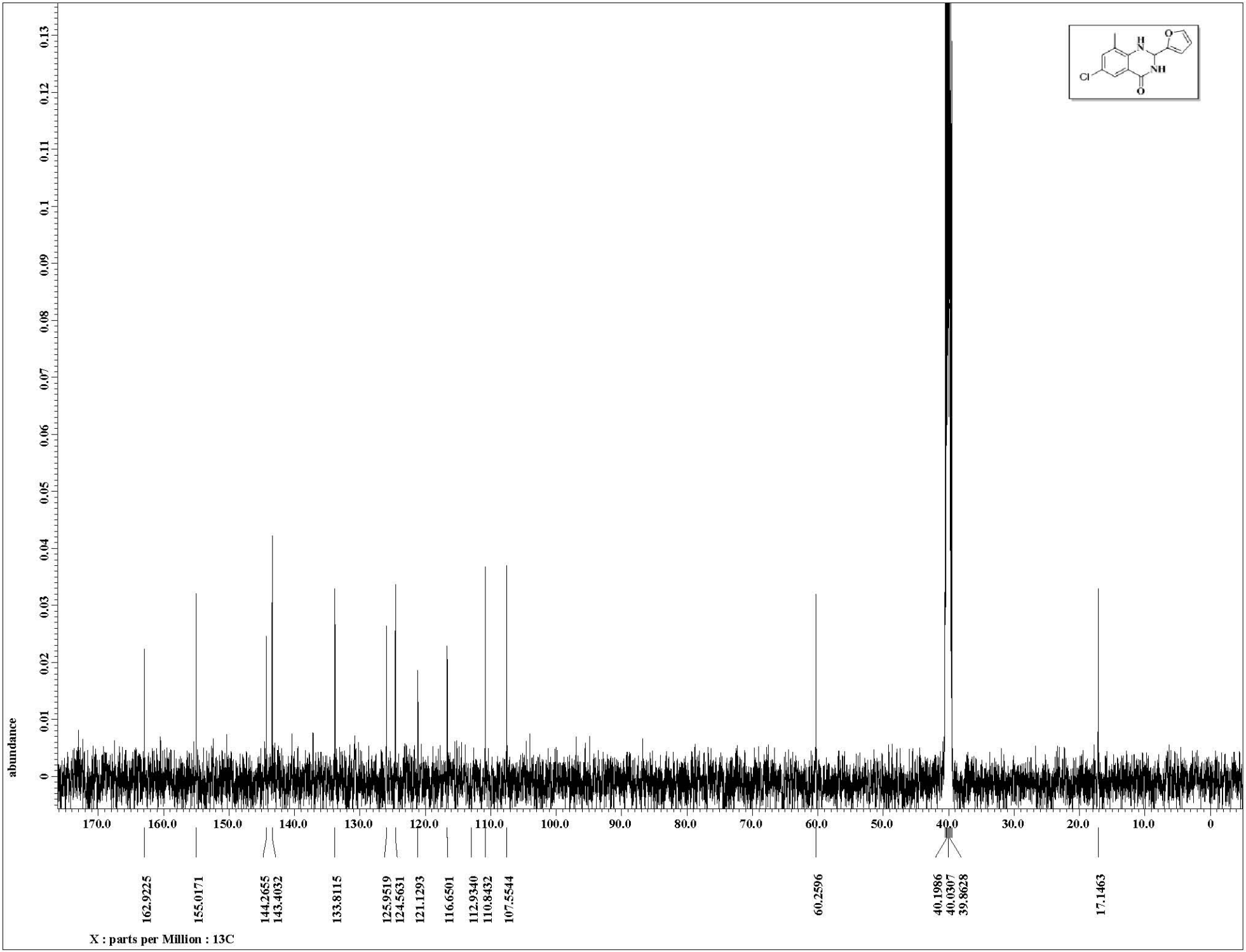

abundance
X : parts per Million : 1H
7.5685
7.5651
7.4586
7.4540
7.2101
7.2044
7.0876
7.0795
6.3466
6.3432
6.1874
6.1806
5.9298
5.9218
3.8318
3.8192
3.8043
3.3462
3.1618
3.1481
3.1344
3.1206
2.5079
2.5034
2.0957
1.1074
1.0925
1.0788
−0.0000
0.92
0.9
1.0
1.01
1
1.03
1.02
3.05
3.09

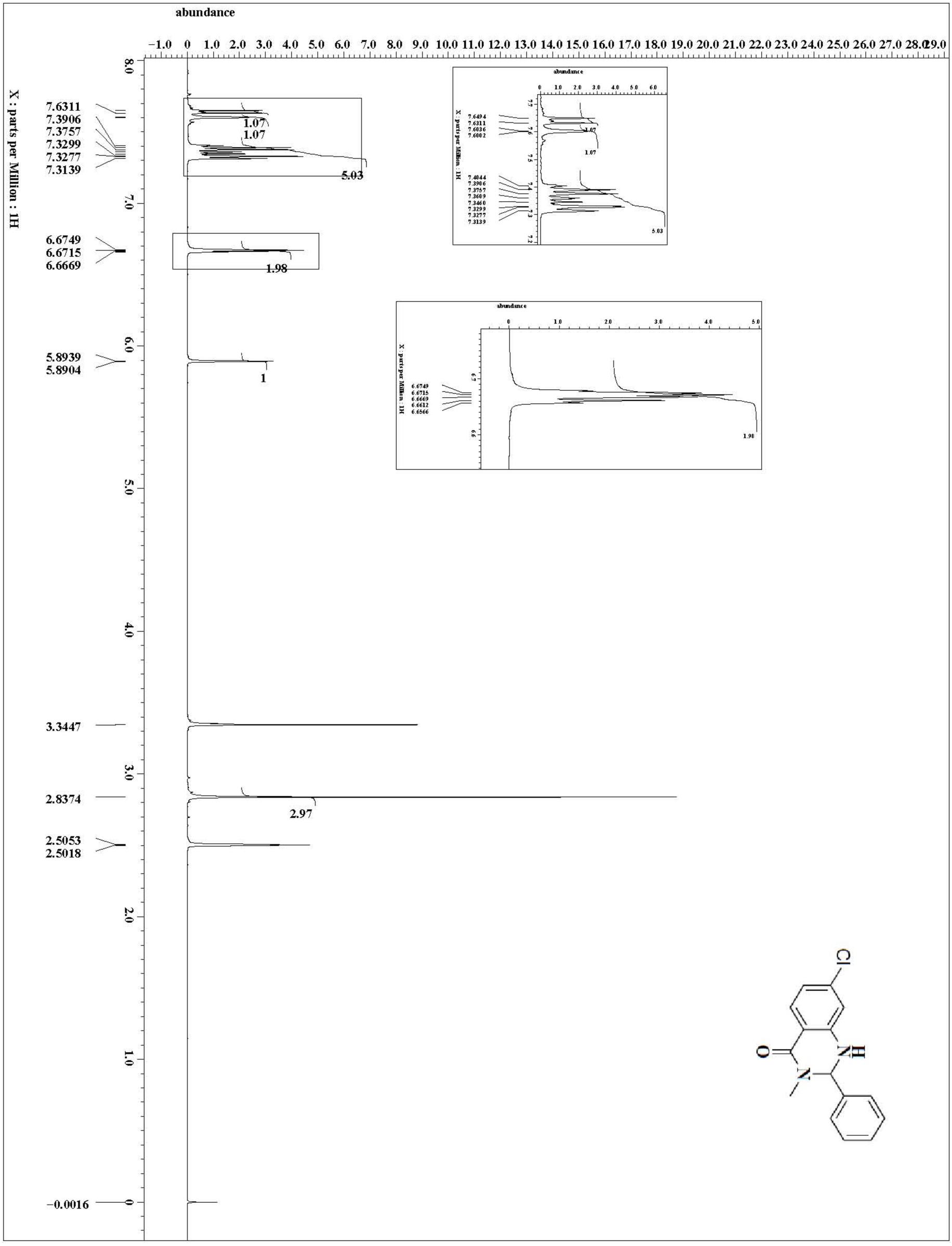

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.4726
153.9278
143.5787
133.5253
125.9328
124.6356
121.3831
117.0240
110.8241
108.0008
64.3153
40.2024
40.0307
39.8685
17.0147
13.8671
X : parts per Million : 13C
Cl
N
H
O
O
N
O

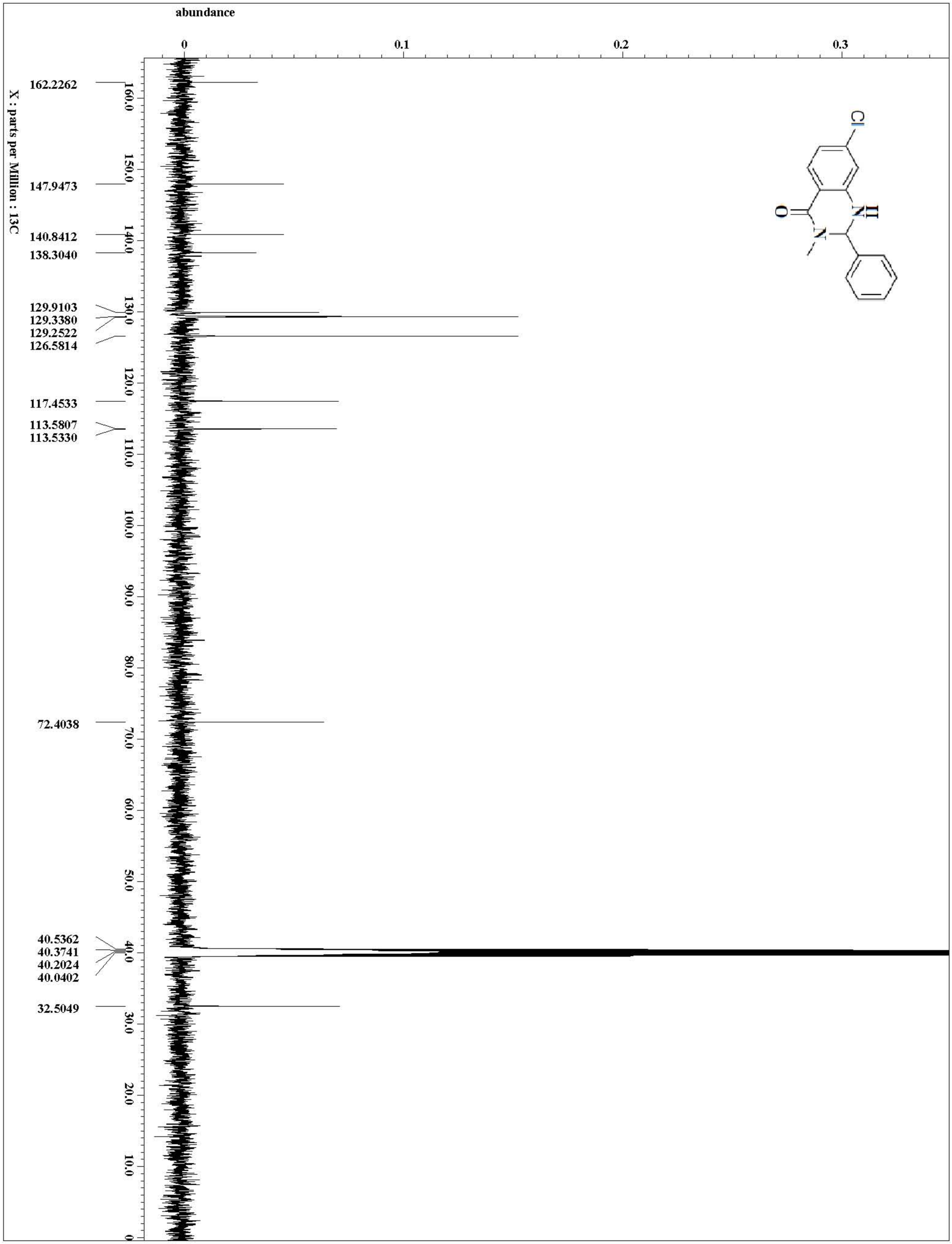

abundance
X : parts per Million : 1H
7.4658
7.4612
7.3331
7.3239
7.1573
7.1527
5.8974
5.8892
3.9188
3.9060
3.8913
3.3447
2.9867
2.9730
2.9592
2.5042
2.0446
1.1033
1.0896
1.0749
0.0000
1
5.2
2.21
1.1
1.04
1.0
2.87
2.66
71.97m
7.4658
7.4612
7.3331
7.3239
7.3065
7.3010
7.2928
7.2845
7.2763
7.2681
7.2589
7.1573
7.1527
7.1445
7.1371
3.9472
3.9325
3.9188
3.9060
3.8913
3.8776
3.0004
2.9867
2.9730
2.9592
2.9455
2.9318

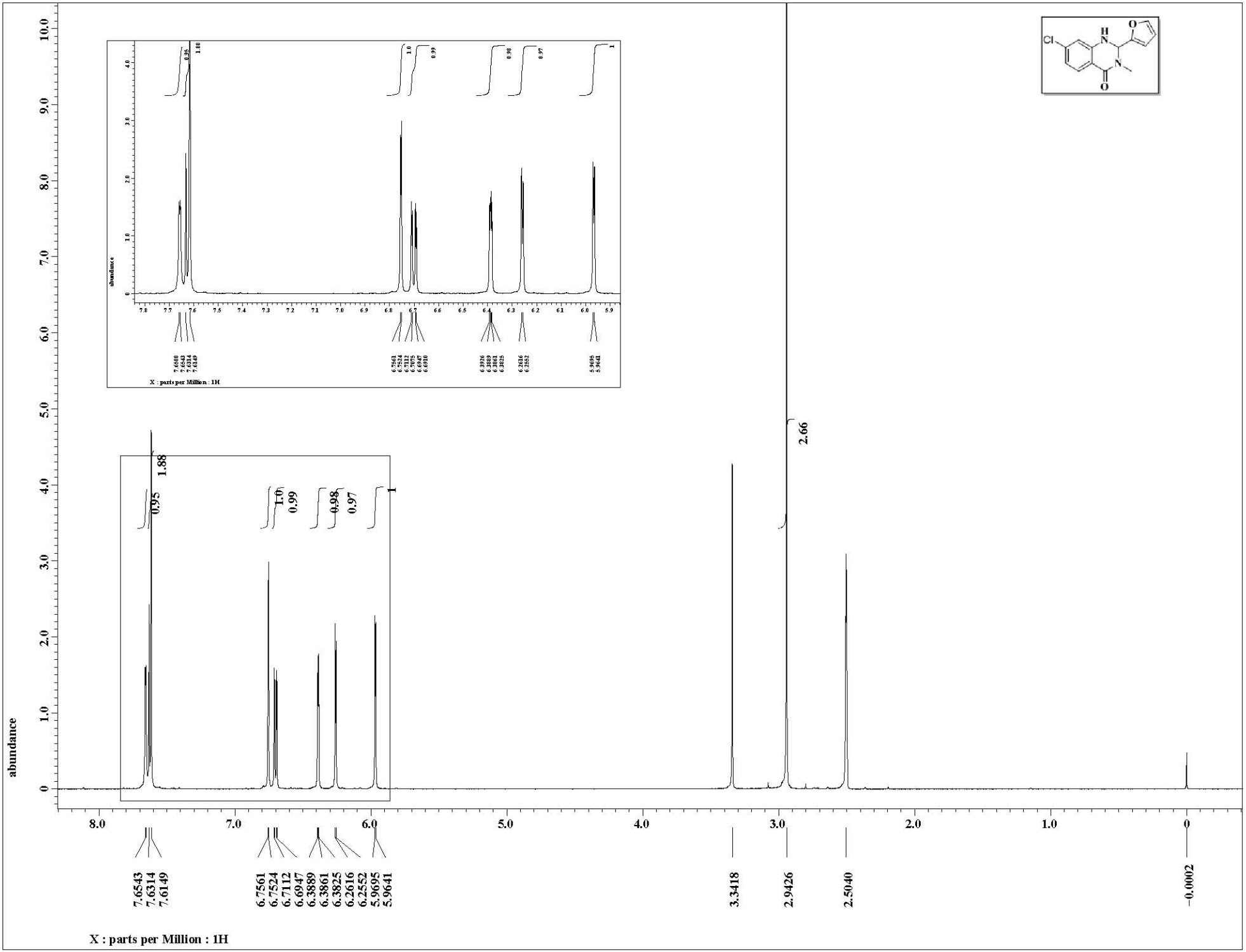

(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.6329
143.4643
141.9610
133.5368
129.0042
128.7447
126.4861
125.6543
124.6318
120.9920
116.7417
69.5537
40.1986
40.0383
39.8704
17.0395
13.9186
X : parts per Million : 13C
Cl
N
H
N
O

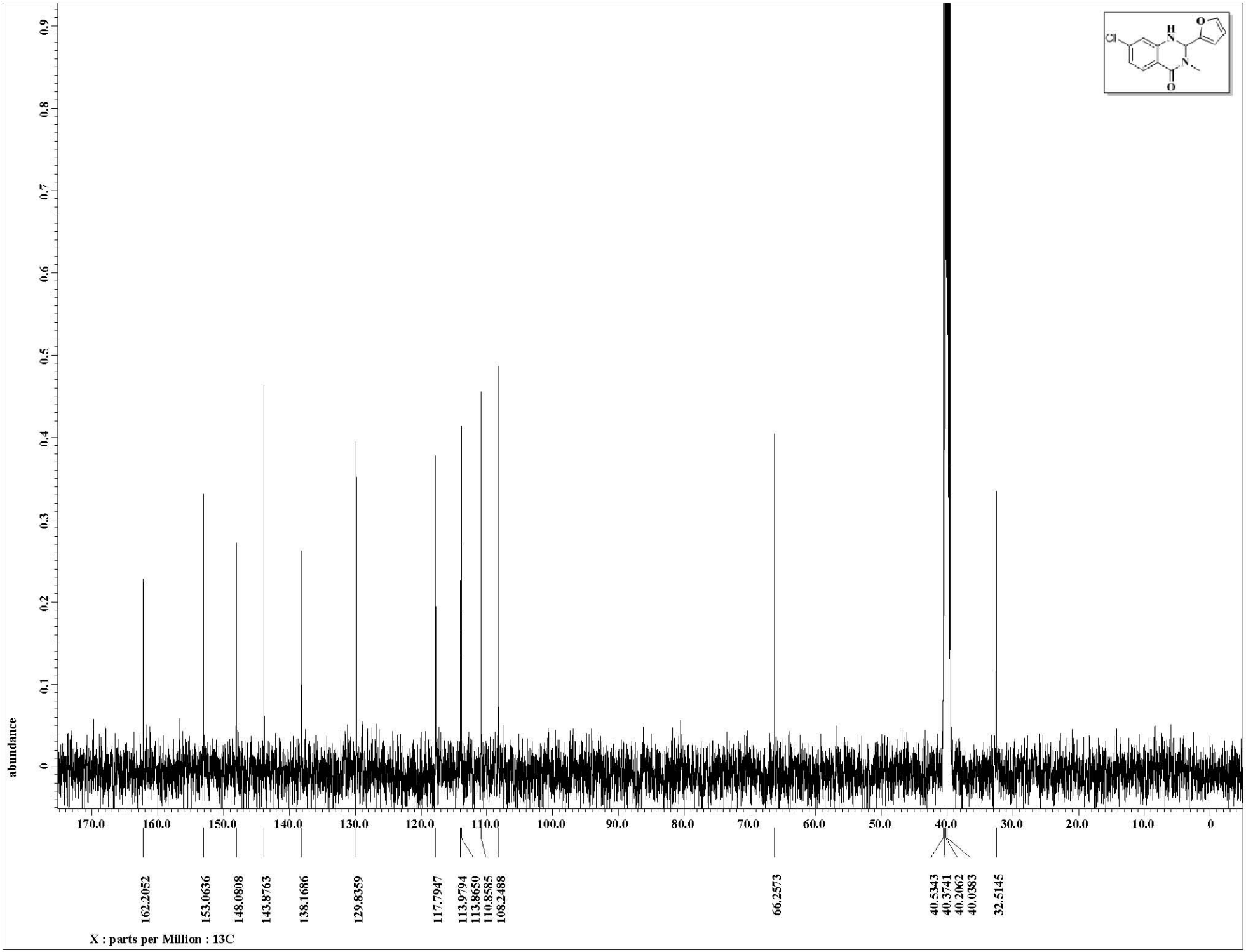

abundance
X : parts per Million : 1H
8.6277
8.6204
7.5949
7.4328
7.4273
7.2213
7.2158
6.9256
6.9192
6.3561
6.3524
6.1968
6.1904
5.7362
5.7289
5.7216
3.3438
2.5069
2.5032
2.1123
2.0757
-0.0000
1
0.97
0.87
1.04
1.03
1.02
1.02
1.03
2.83
Cl
NH
O

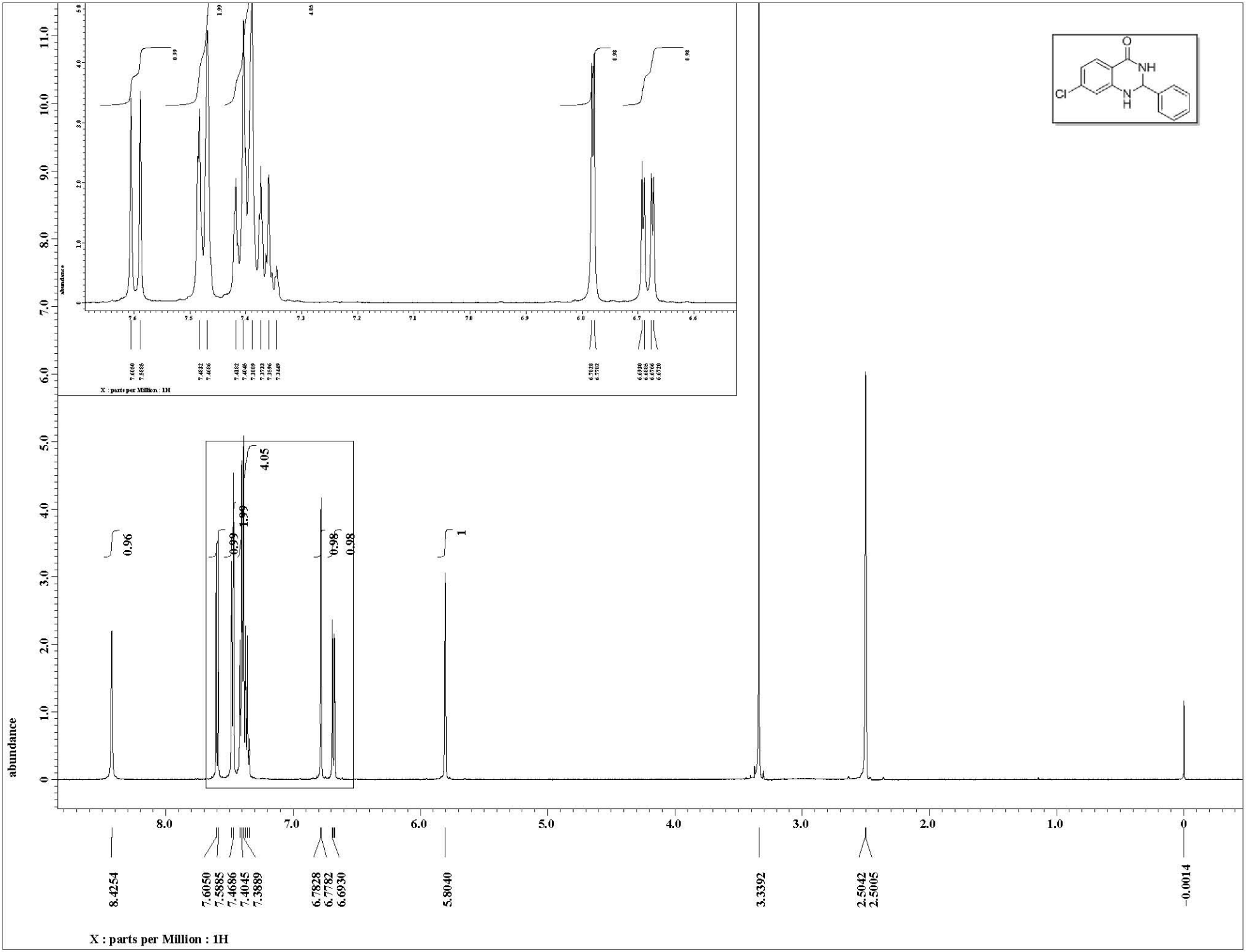

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.9225
155.0171
144.2655
143.4032
133.8115
125.9519
124.5631
121.1293
116.6501
112.9340
110.8432
107.5544
60.2596
40.1986
40.0307
39.8628
17.1463
X : parts per Million : 13C
Cl
NH
NH
O
O

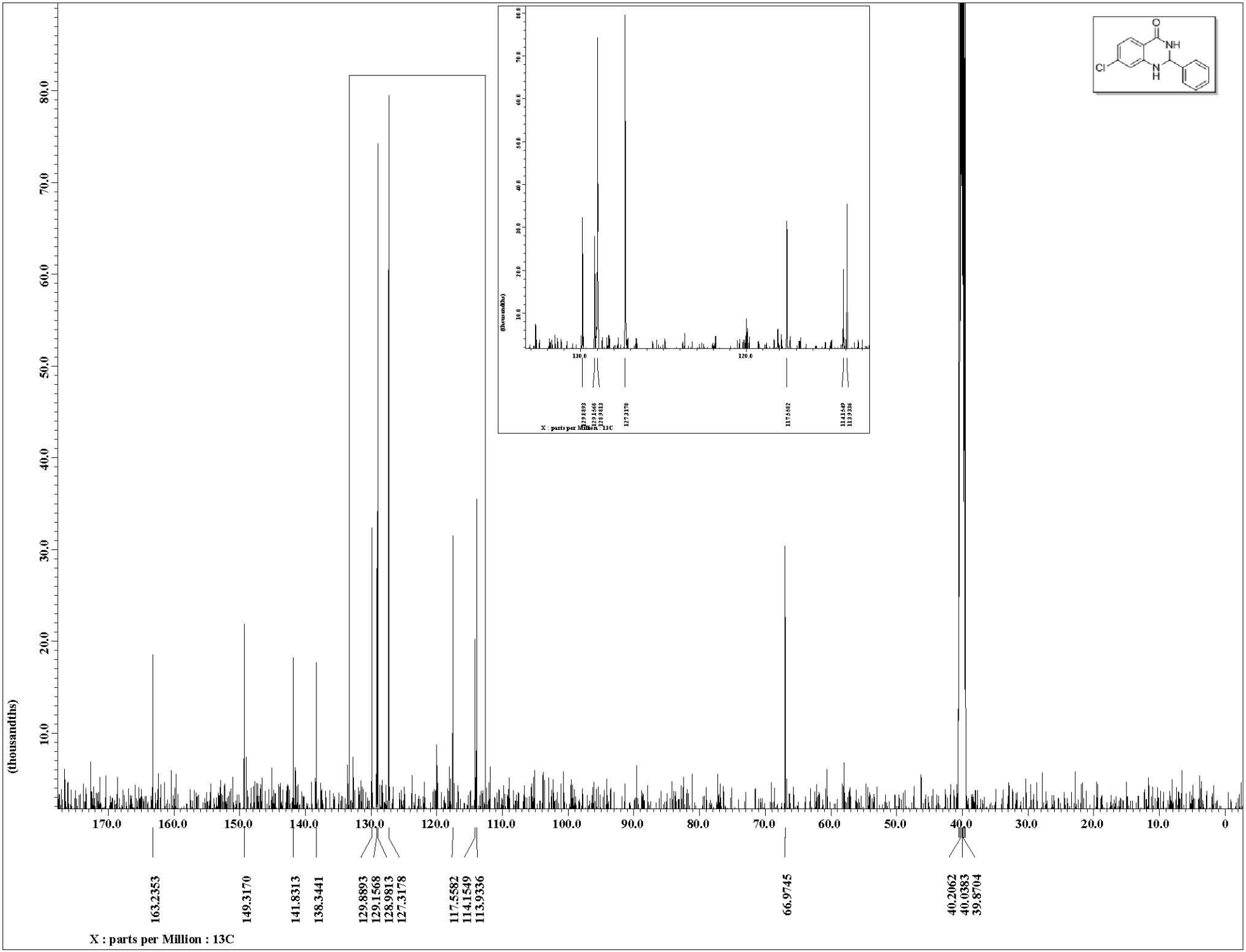

abundance
X : parts per Million : 1H
7.6311
7.3906
7.3757
7.3299
7.3277
7.3139
6.6749
6.6715
6.6669
5.8939
5.8904
3.3447
2.8374
2.5053
2.5018
−0.0016
1.07
1.07
5.03
1.98
1
2.97
Cl
H
N
O
N

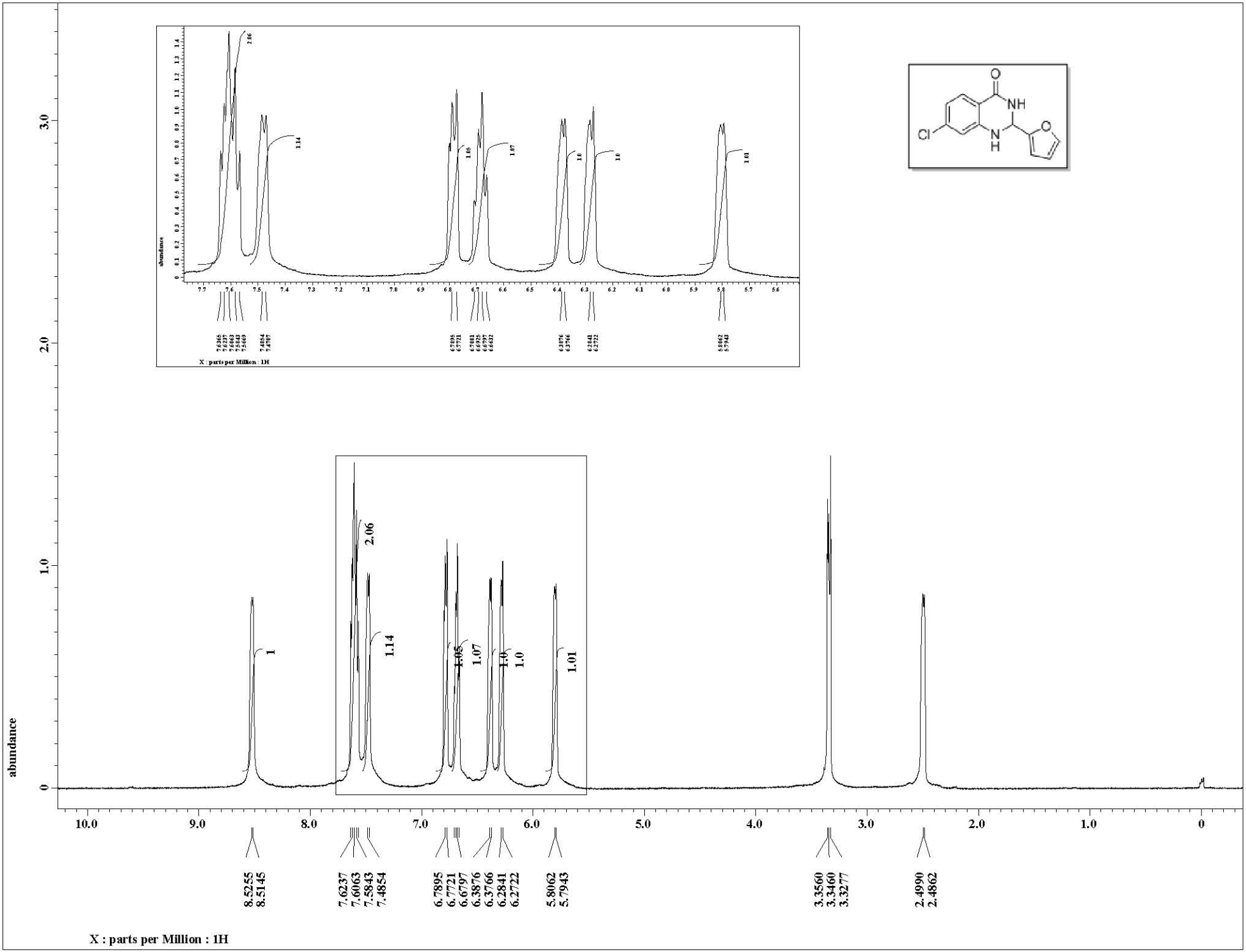

abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.2262
147.9473
140.8412
138.3040
129.9103
129.3380
129.2522
126.5814
117.4533
113.5807
113.5330
72.4038
40.5362
40.3741
40.2024
40.0402
32.5049
Cl
O
N
H
N

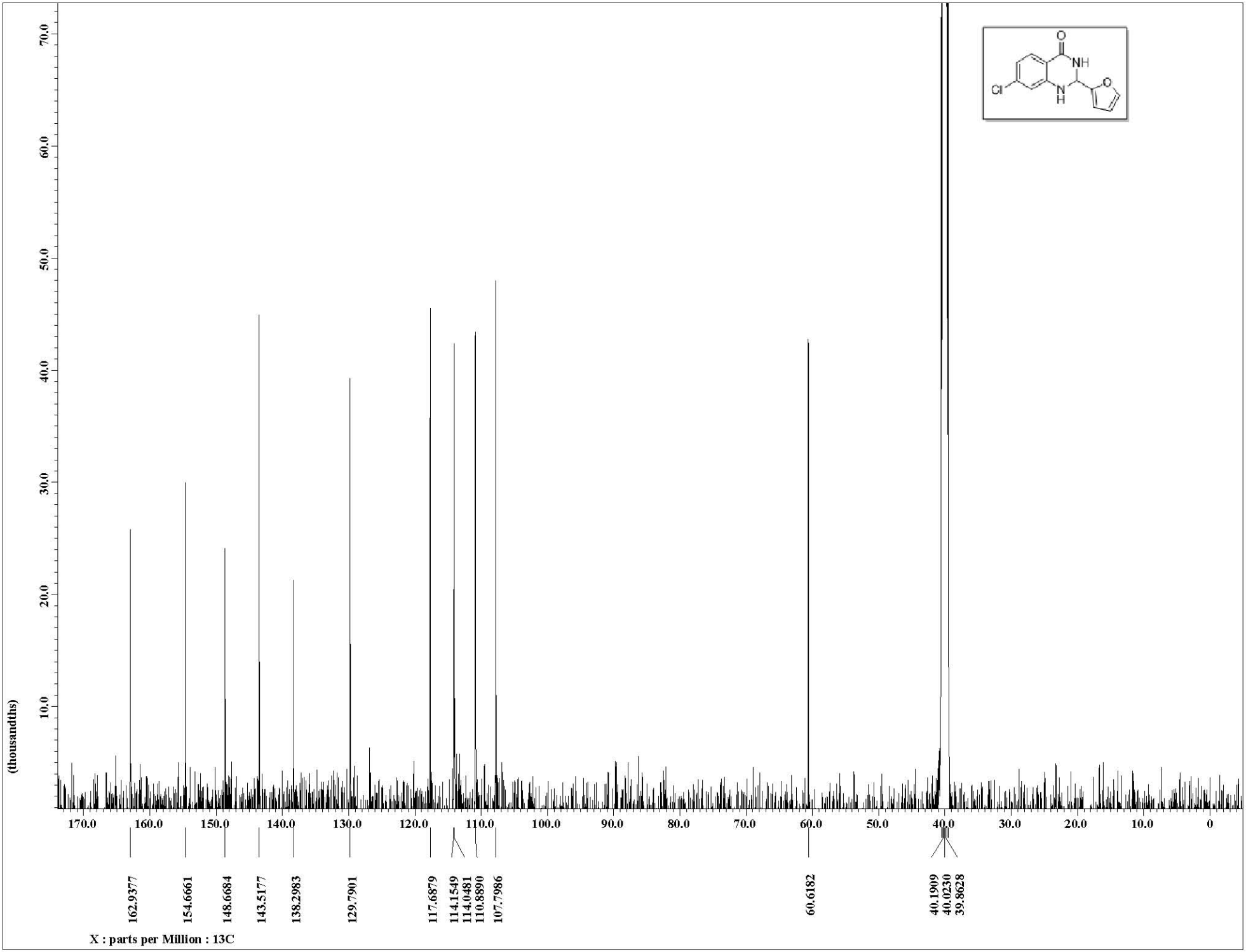

abundance
X : parts per Million : 1H
7.6543
7.6314
7.6149
6.7561
6.7524
6.7112
6.6947
6.3889
6.3861
6.3825
6.2616
6.2552
5.9695
5.9641
3.3418
2.9426
2.5040
-0.0002
2.66
1.88
0.95
1.0
0.99
0.98
0.97
1

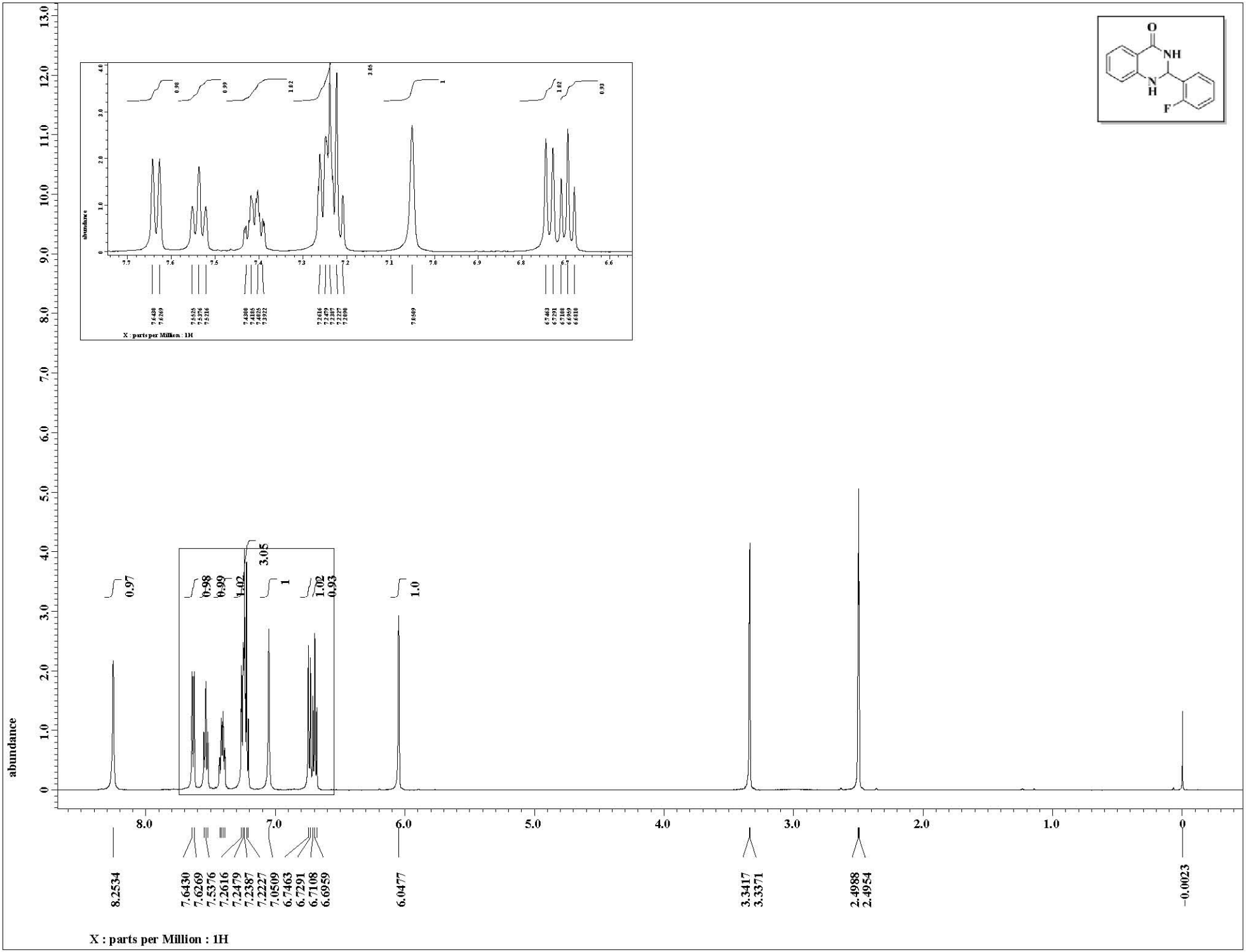

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.2052
153.0636
148.0808
143.8763
138.1686
129.8359
117.7947
113.9794
113.8650
110.8585
108.2488
66.2573
40.5343
40.3741
40.2062
40.0383
32.5145
X : parts per Million : 13C
Cl
H
N
O
N
O

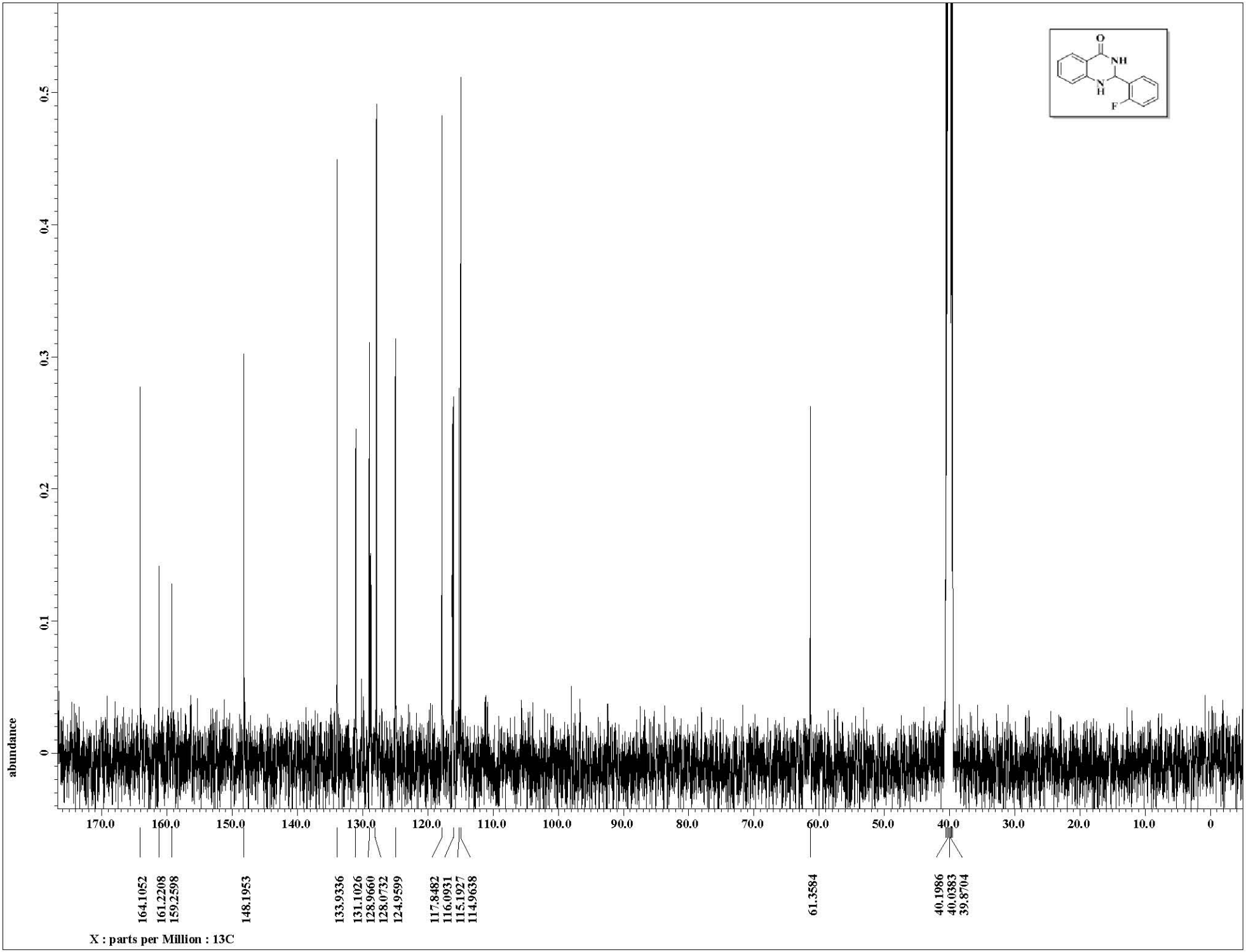

abundance
X : parts per Million : 1H
8.4254
7.6050
7.5885
7.4686
7.4045
7.3889
6.7828
6.7782
6.6930
5.8040
3.3392
2.5042
2.5005
-0.0014
0.96
0.99
1.99
4.05
0.98
0.98
1
Cl
NH
N
H
O

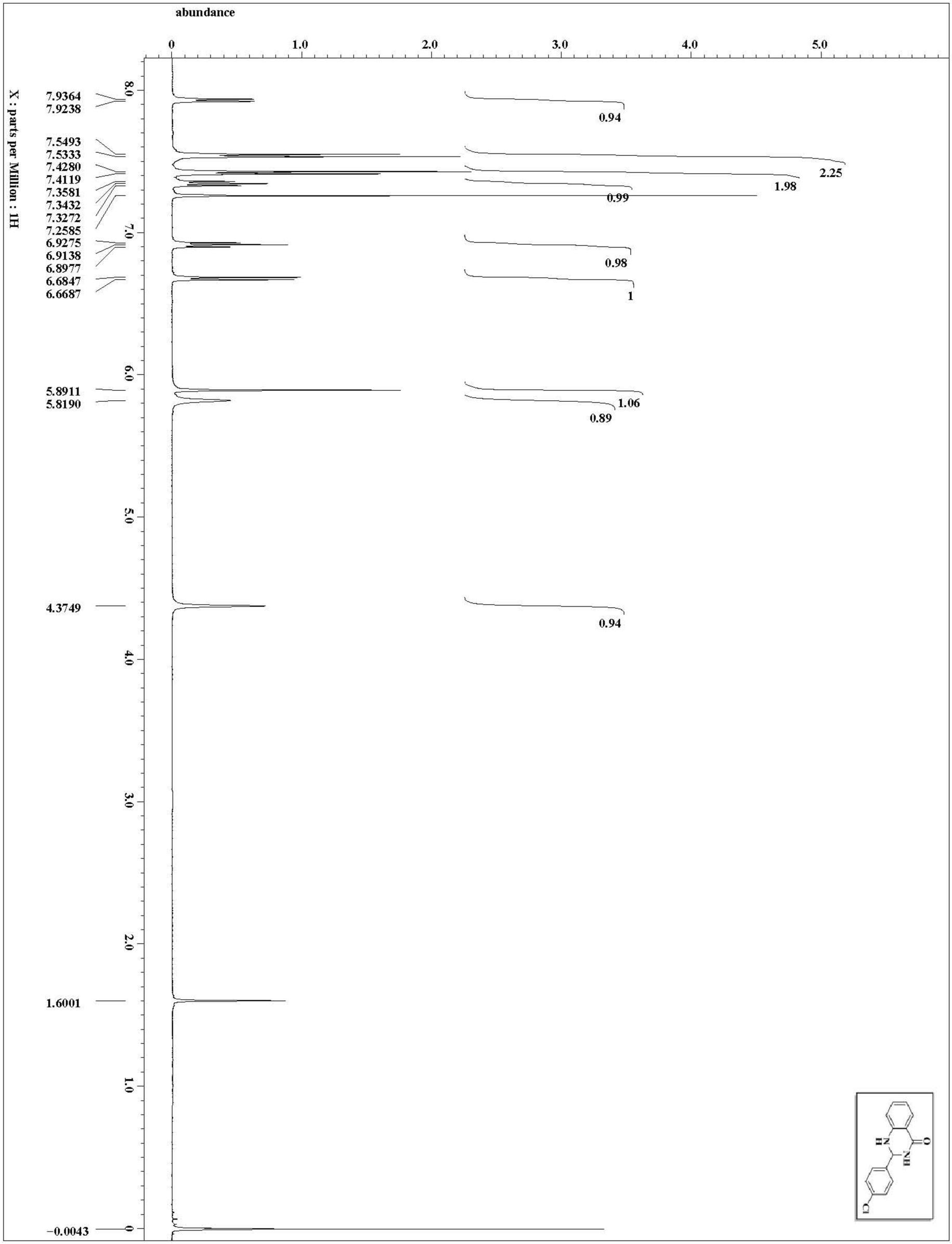

(thousandths)
X : parts per Million : 13C
163.2353
149.3170
141.8313
138.3441
129.8893
129.1568
128.9813
127.3178
117.5582
114.1549
113.9336
66.9745
40.2062
40.0383
39.8704
NH
N
H
Cl
O

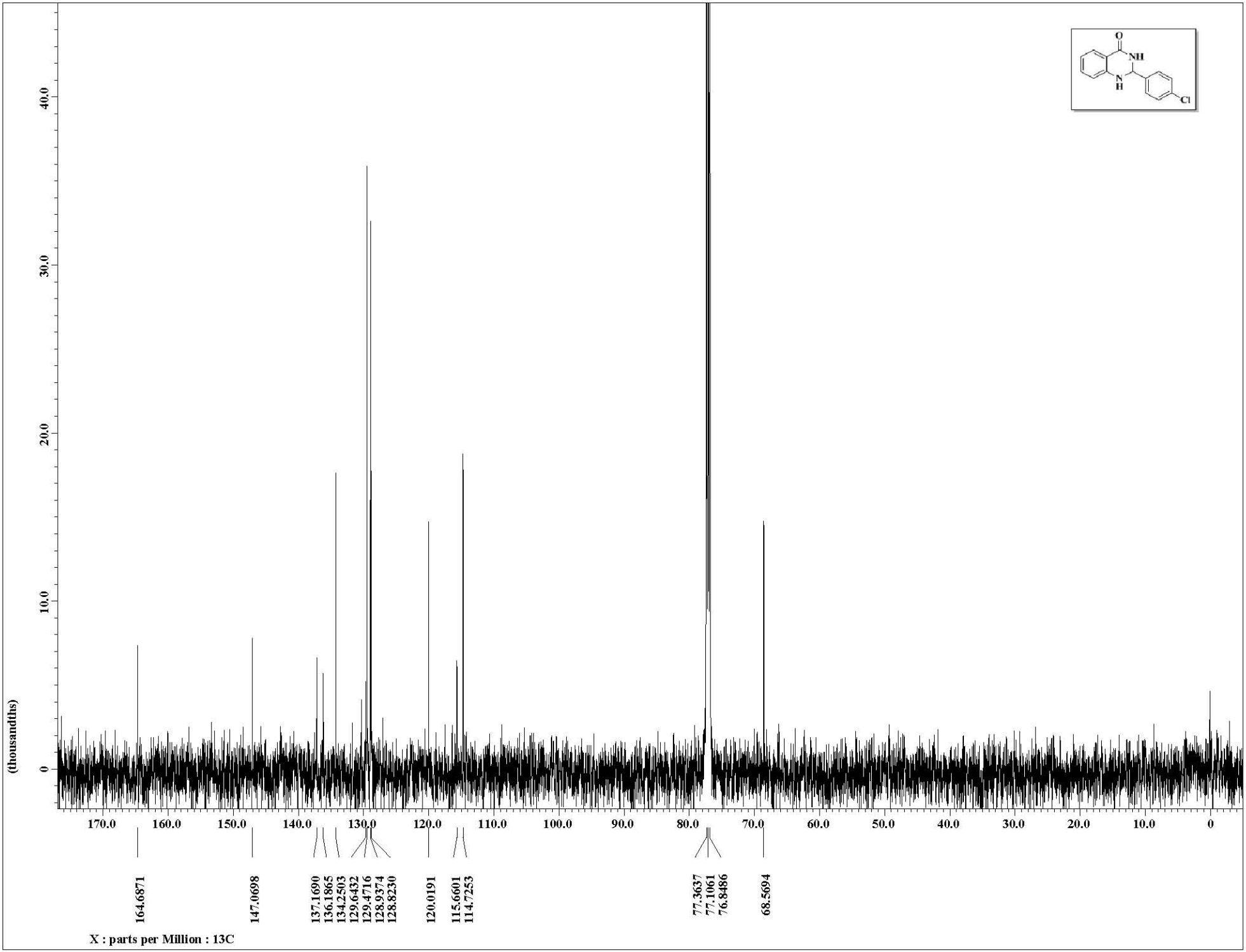

abundance
X : parts per Million : 1H
8.5255
8.5145
7.6237
7.6063
7.5843
7.4854
6.7895
6.7721
6.6797
6.3876
6.3766
6.2841
6.2722
5.8062
5.7943
3.3560
3.3460
3.3277
2.4990
2.4862
1
2.06
1.14
1.05
1.07
1.0
1.0
1.01
NH
N
H
Cl
O

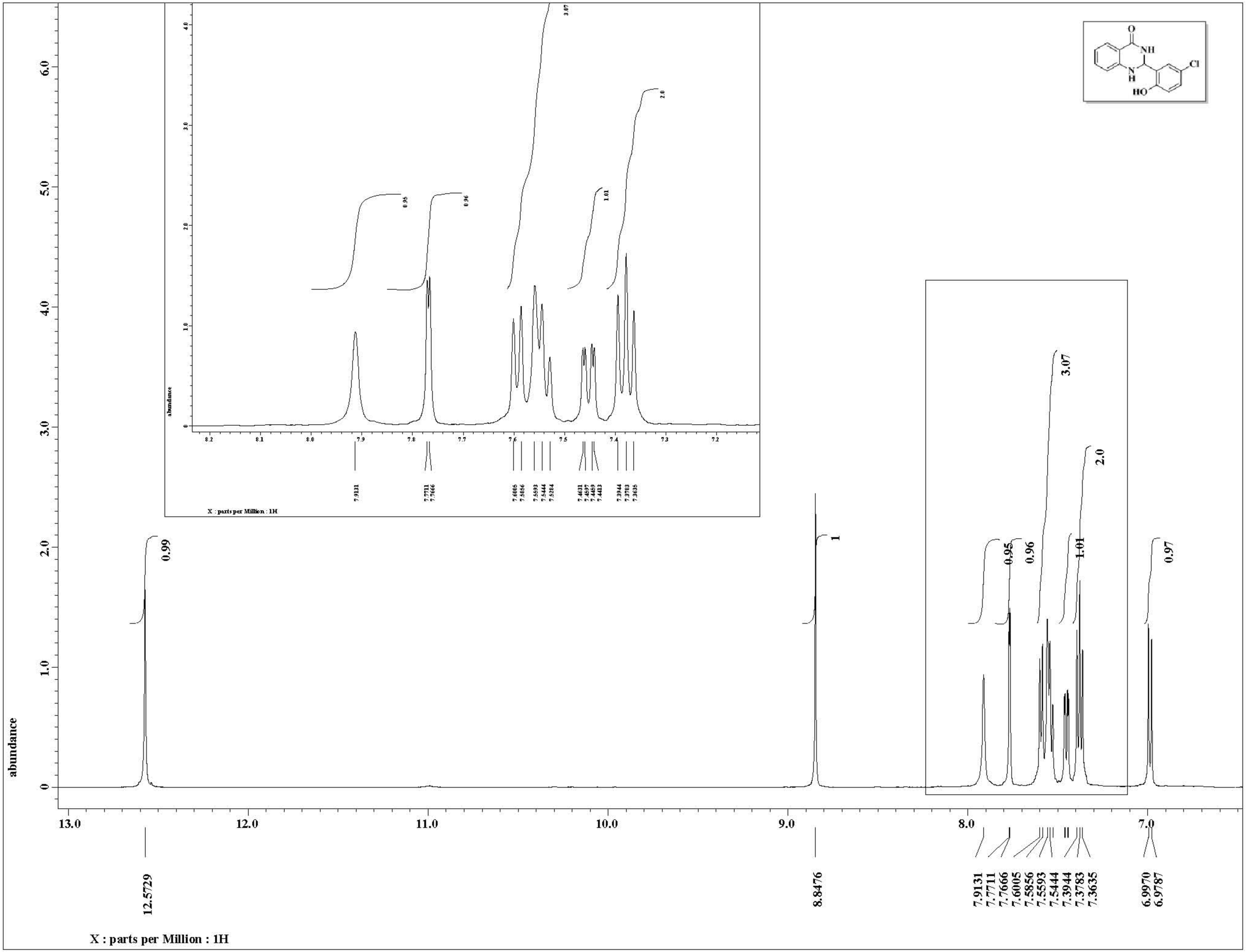

(thousandths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.9377
154.6661
148.6684
143.5177
138.2983
129.7901
117.6879
114.1549
114.0481
110.8890
107.7986
60.6182
40.1909
40.0230
39.8628
X : parts per Million : 13C
O
NH
N
H
Cl
O

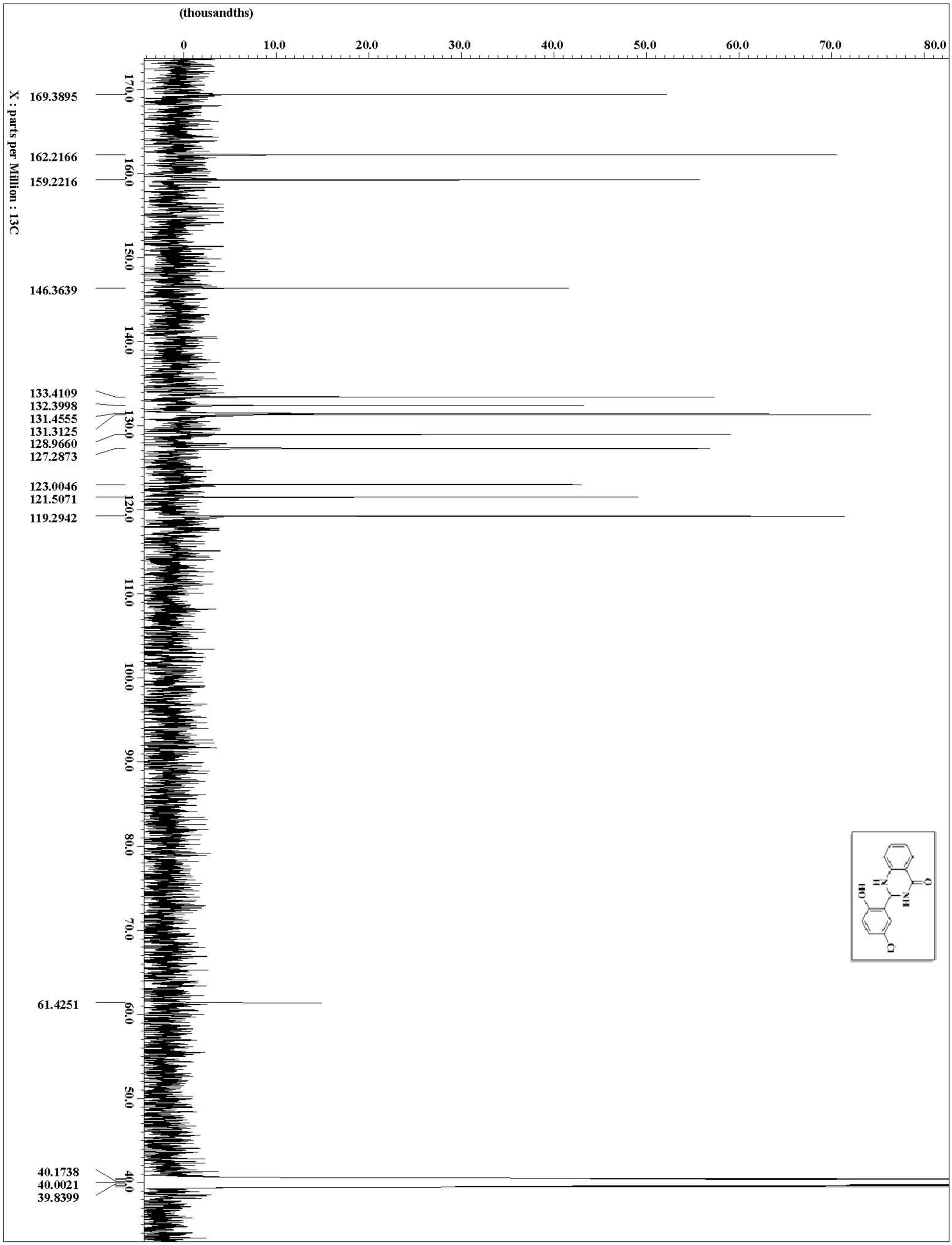

abundance
X : parts per Million : 1H
8.2534
7.6430
7.6269
7.5376
7.2616
7.2479
7.2387
7.2227
7.0509
6.7463
6.7291
6.7108
6.6959
6.0477
3.3417
3.3371
2.4988
2.4954
−0.0023
0.97
0.98
0.99
1.02
3.05
1
1.02
0.93
1.0
O
NH
N
H
F

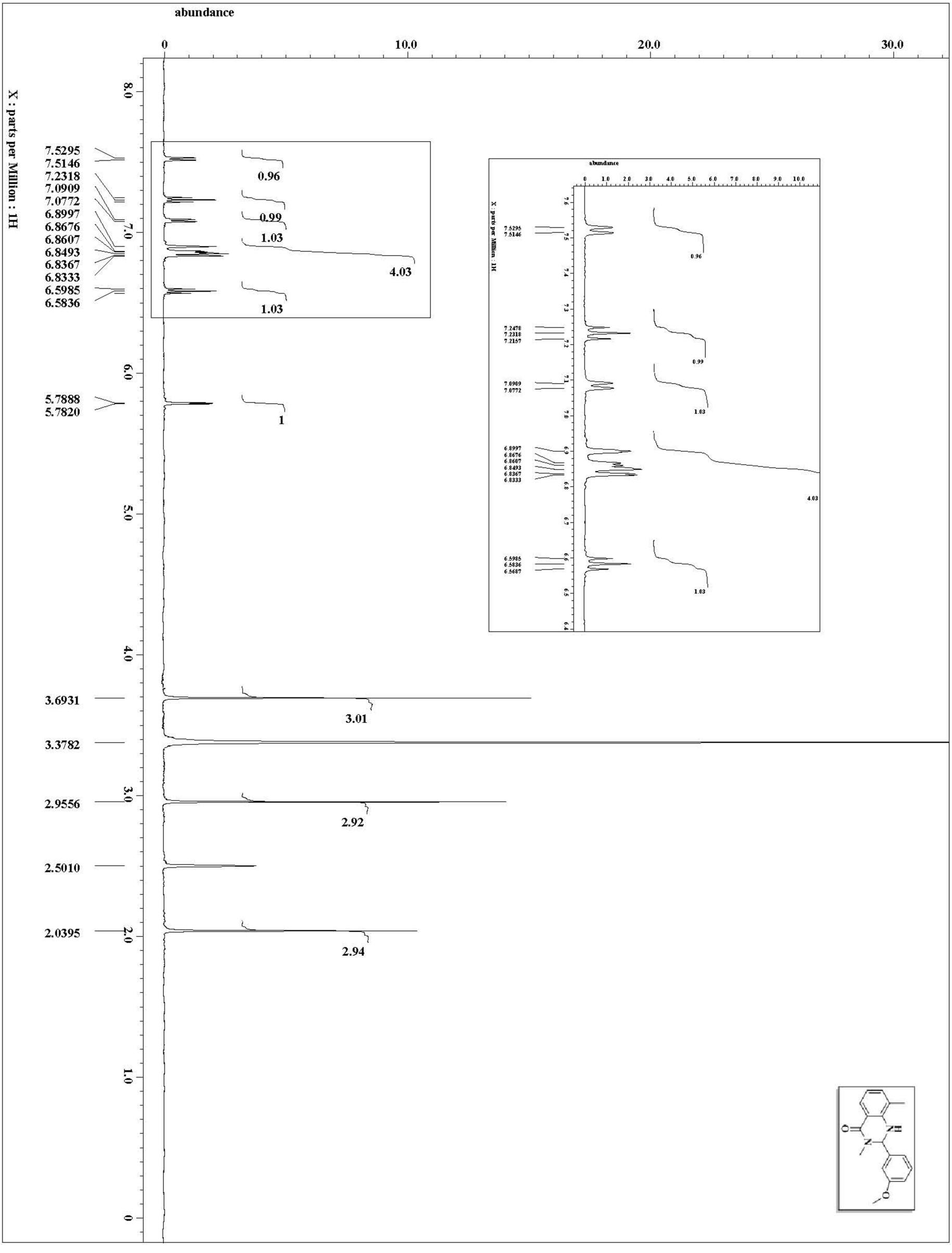

abundance
0
0.1
0.2
0.3
0.4
0.5
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.1052
161.2208
159.2598
148.1953
133.9336
131.1026
128.9660
128.0732
124.9599
117.8482
116.0931
115.1927
114.9638
61.3584
40.1986
40.0383
39.8704
X : parts per Million : 13C
O
NH
N
H
F

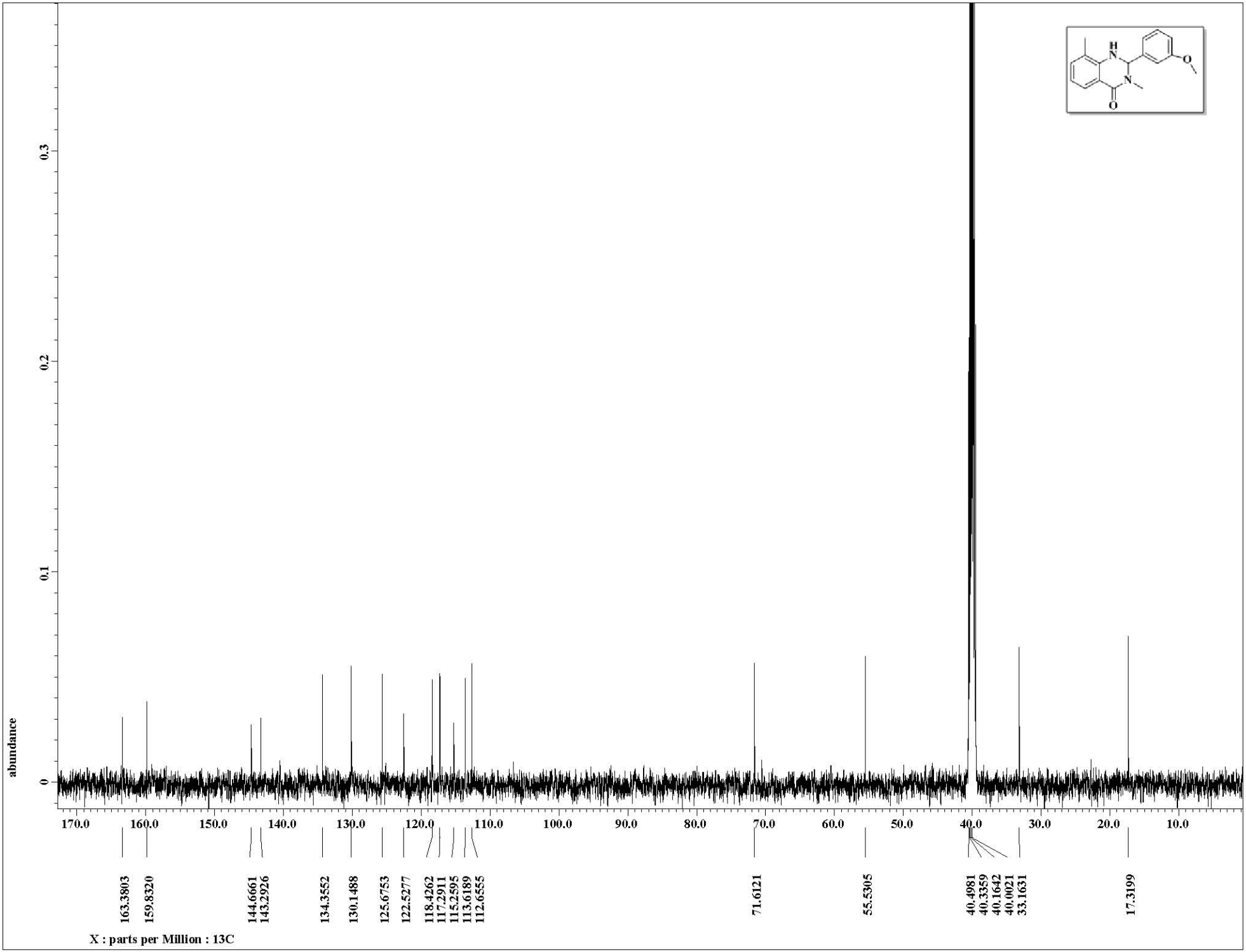

abundance
0
1.0
2.0
3.0
4.0
5.0
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.9364
7.9238
7.5493
7.5333
7.4280
7.4119
7.3581
7.3432
7.3272
7.2585
6.9275
6.9138
6.8977
6.6847
6.6687
5.8911
5.8190
4.3749
1.6001
−0.0043
0.94
2.25
1.98
0.99
0.98
1
1.06
0.89
0.94
O
NH
NH
Cl

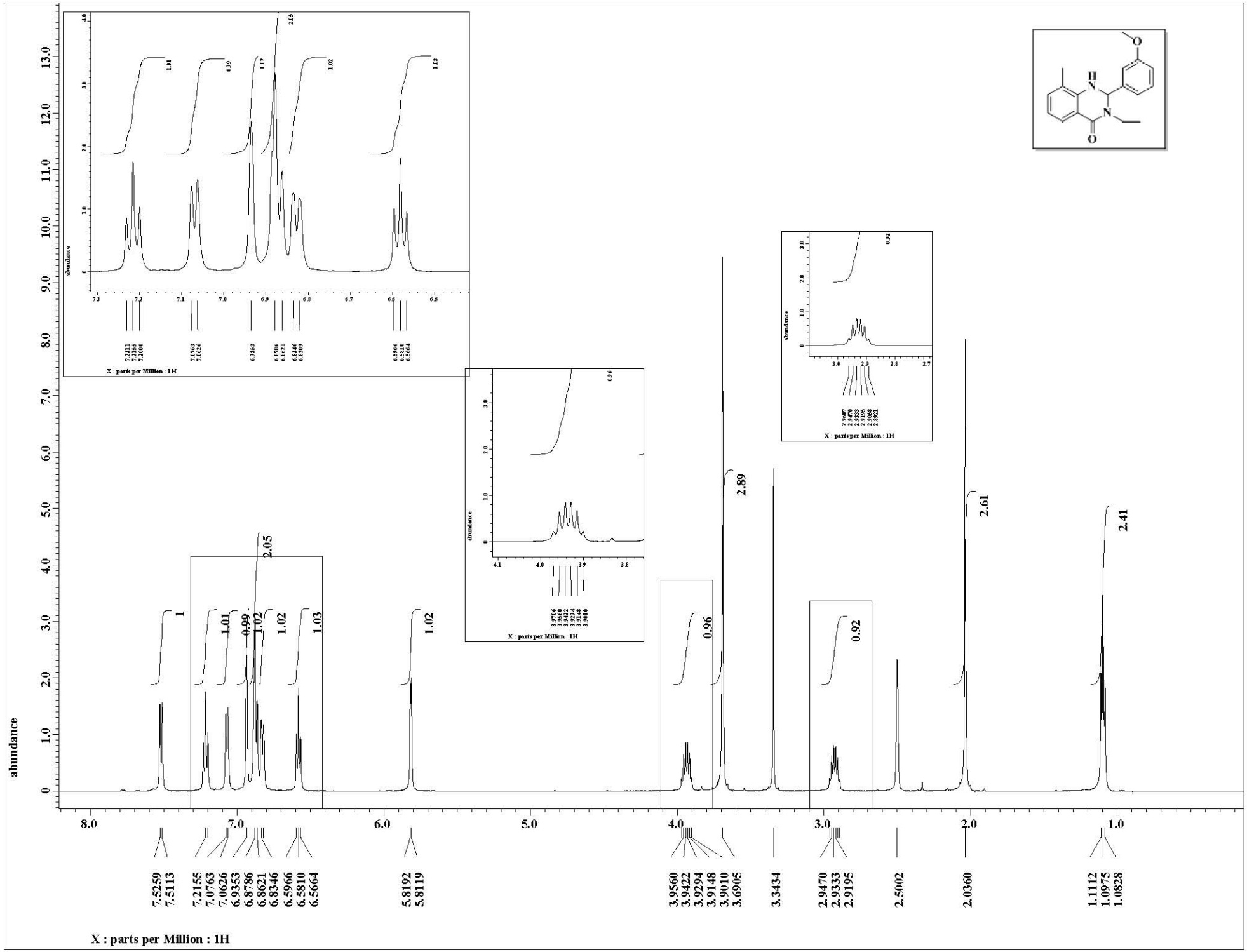

(thousandths)
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.6871
147.0698
137.1690
136.1865
134.2503
129.6432
129.4716
128.9374
128.8230
120.0191
115.6601
114.7253
77.3637
77.1061
76.8486
68.5694
X : parts per Million : 13C
O
NH
N
H
Cl

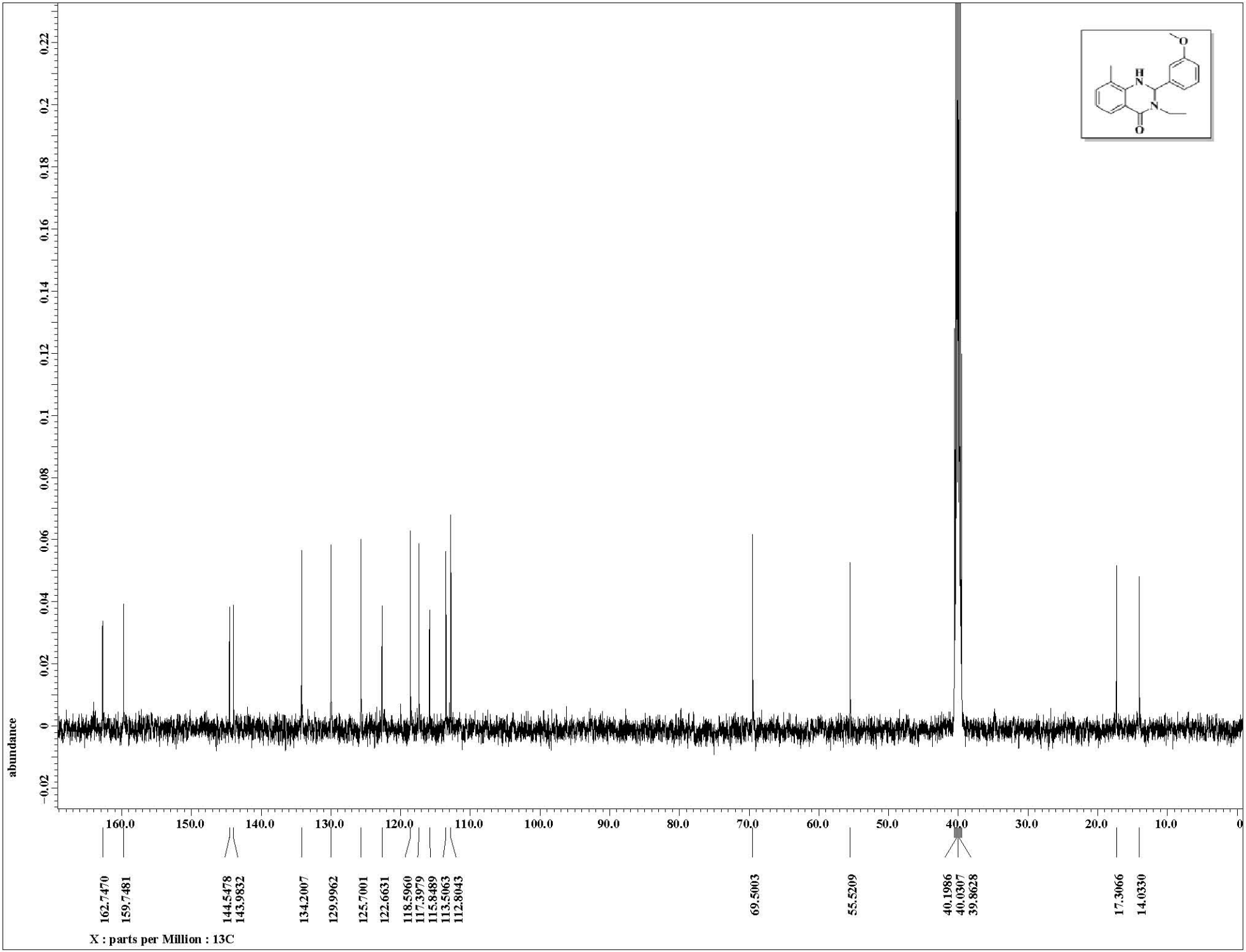

O
NH
N
H
Cl
HO
abundance
X : parts per Million : 1H
12.5729
8.8476
7.9131
7.7711
7.7666
7.6005
7.5856
7.5593
7.5444
7.3944
7.3783
7.3635
6.9970
6.9787
0.99
1
0.95
0.96
1.01
2.0
0.97
3.07

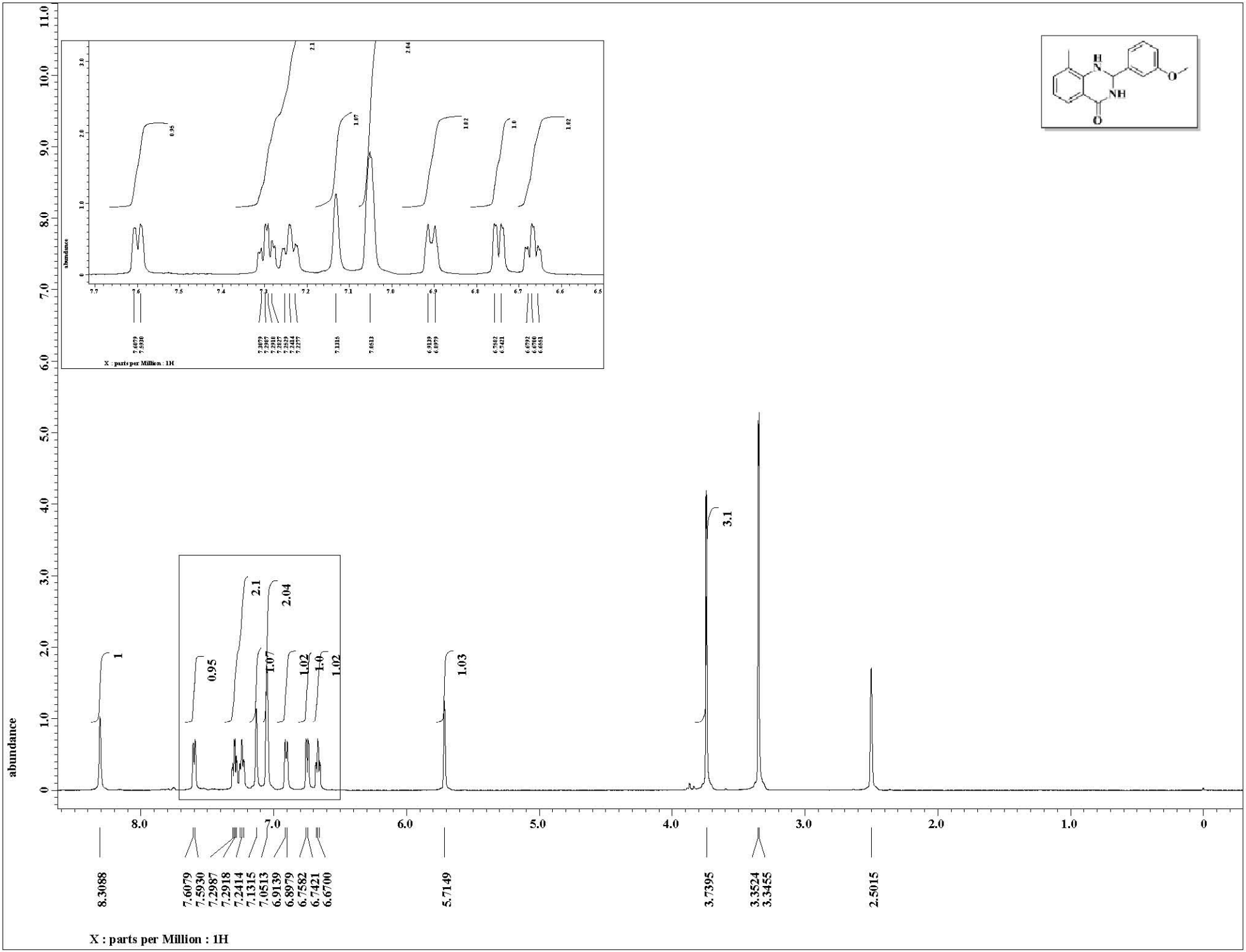

(thousandths)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
X : parts per Million : 13C
169.3895
162.2166
159.2216
146.3639
133.4109
132.3998
131.4555
131.3125
128.9660
127.2873
123.0046
121.5071
119.2942
61.4251
40.1738
40.0021
39.8399
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
HO
N
H
NH
O
Cl

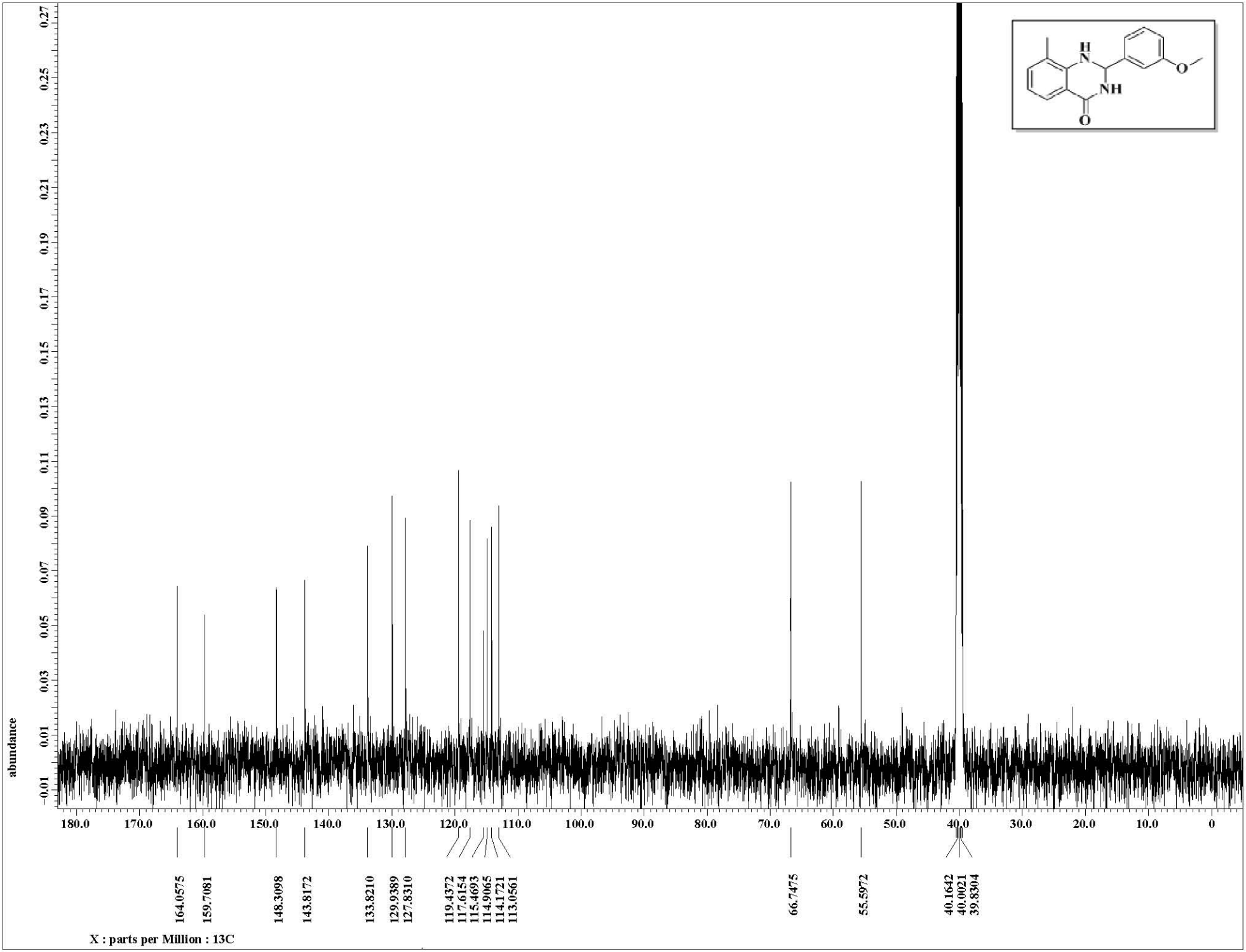

abundance
0
10.0
20.0
30.0
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5295
7.5146
7.2318
7.0909
7.0772
6.8997
6.8676
6.8607
6.8493
6.8367
6.8333
6.5985
6.5836
0.96
0.99
1.03
4.03
1.03
5.7888
5.7820
1
3.6931
3.01
3.3782
2.9556
2.92
2.5010
2.0395
2.94
abundance
X : parts per Million : 1H
7.5295
7.5146
0.96
7.2478
7.2318
7.2157
0.99
7.0909
7.0772
1.03
6.8997
6.8676
6.8607
6.8493
6.8367
6.8333
4.03
6.5985
6.5836
6.5687
1.03

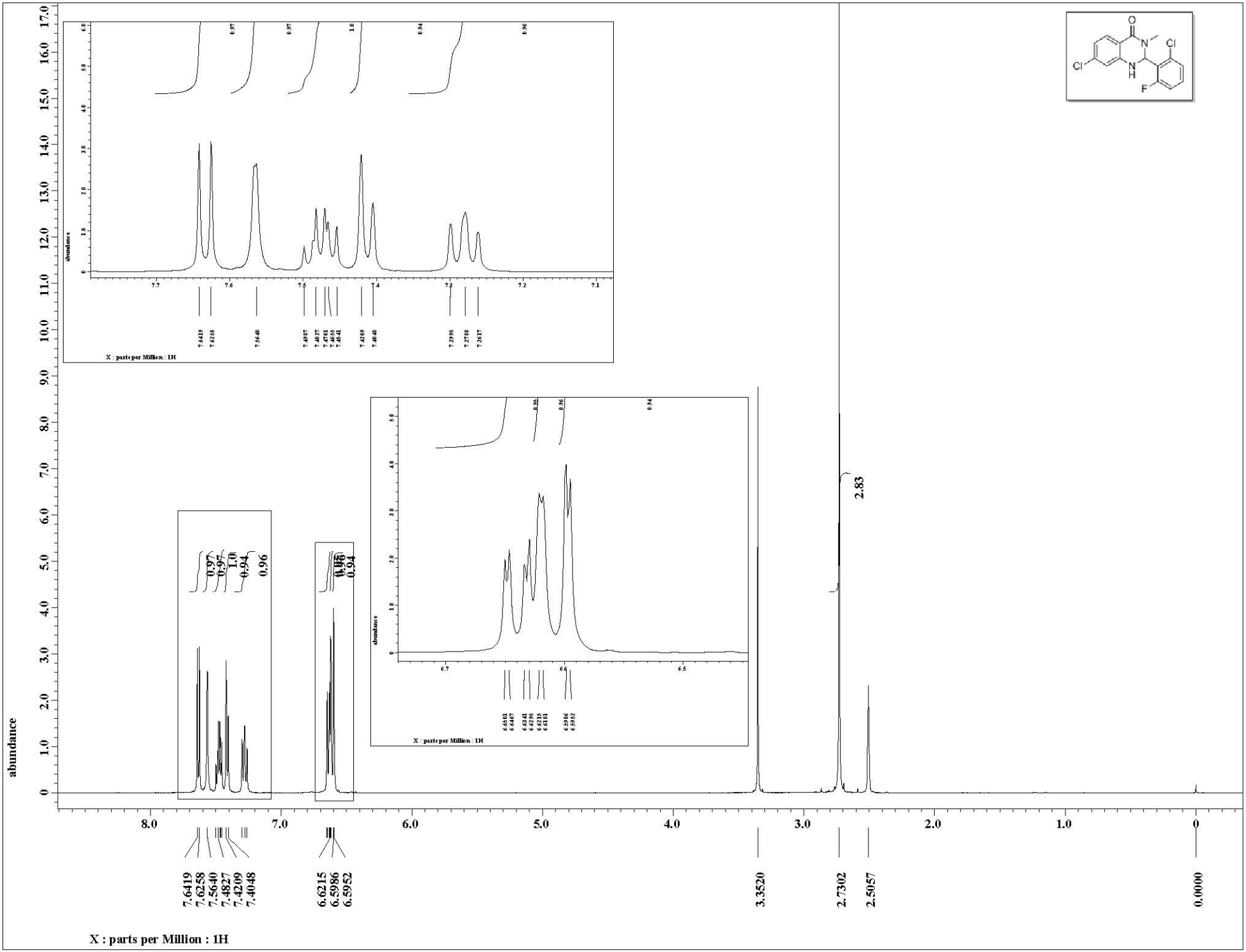

abundance
0
0.1
0.2
0.3
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
163.3803
159.8320
144.6661
143.2926
134.3552
130.1488
125.6753
122.5277
118.4262
117.2911
115.2595
113.6189
112.6555
71.6121
55.5305
40.4981
40.3359
40.1642
40.0021
33.1631
17.3199
X : parts per Million : 13C

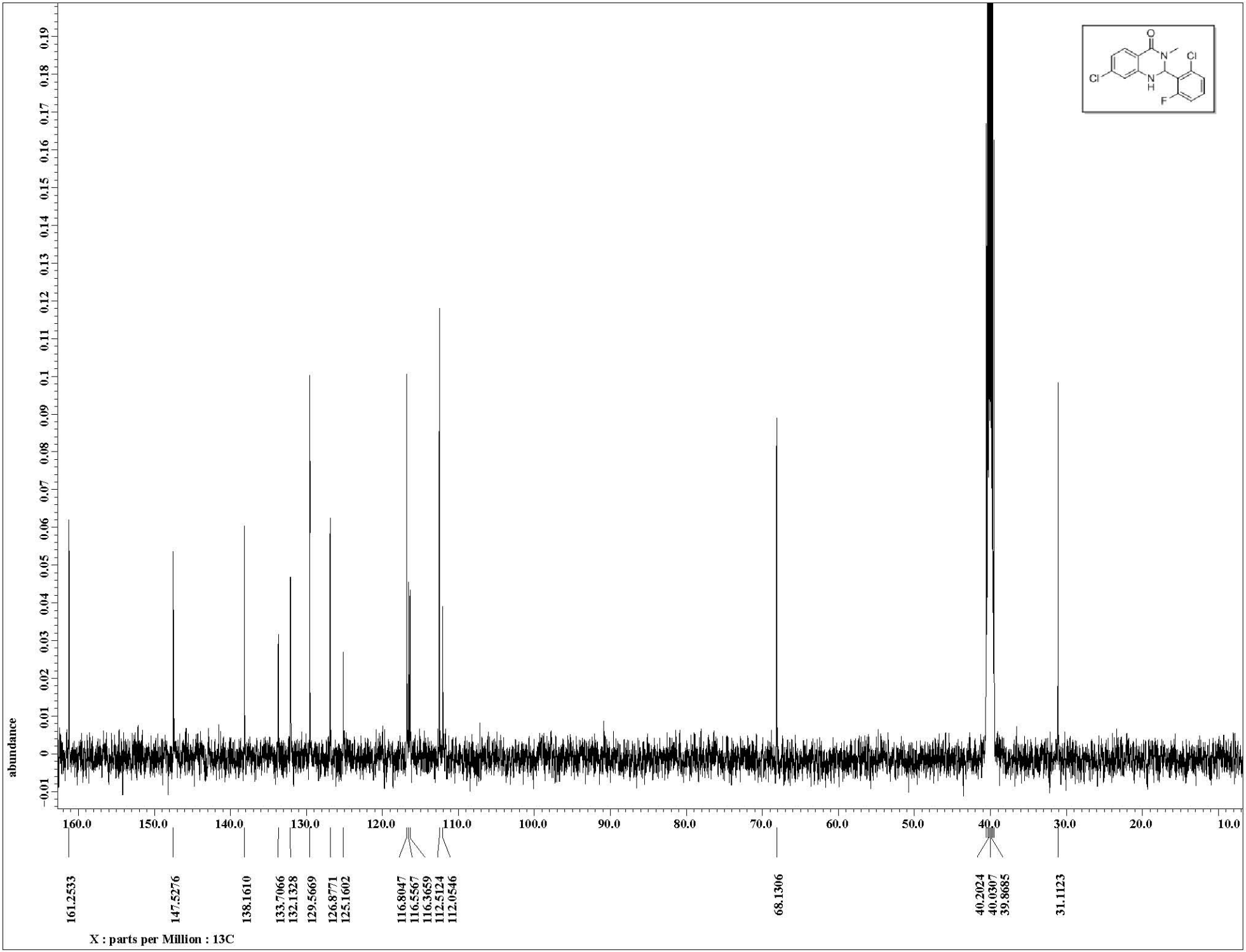

abundance
X : parts per Million : 1H
7.5259
7.5113
7.2155
7.0763
7.0626
6.9353
6.8786
6.8621
6.8346
6.5966
6.5810
6.5664
5.8192
5.8119
3.9560
3.9422
3.9294
3.9148
3.9010
3.6905
3.3434
2.9470
2.9333
2.9195
2.5002
2.0360
1.1112
1.0975
1.0828
1
1.01
0.99
2.05
1.02
1.02
1.03
1.02
0.96
0.92
2.89
2.61
2.41

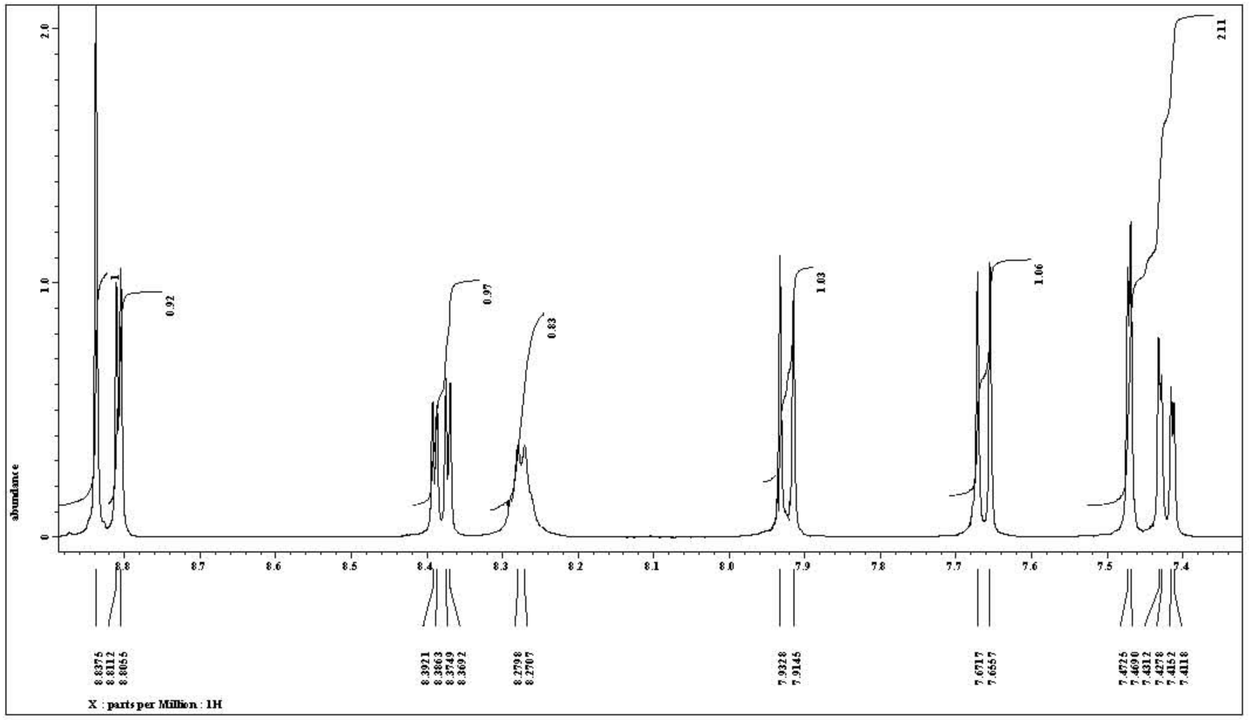

abundance
X : parts per Million : 13C
162.7470
159.7481
144.5478
143.9832
134.2007
129.9962
125.7001
122.6631
118.5960
117.3979
115.8489
113.5063
112.8043
69.5003
55.5209
40.1986
40.0307
39.8628
17.3066
14.0330

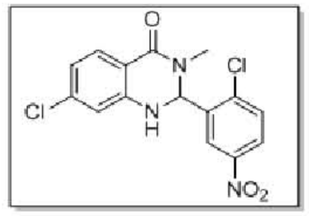

abundance
X : parts per Million : 1H
8.3088
7.6079
7.5930
7.2987
7.2918
7.2414
7.1315
7.0513
6.9139
6.8979
6.7582
6.7421
6.6700
5.7149
3.7395
3.3524
3.3455
2.5015
1
0.95
2.1
2.04
1.07
1.02
1.0
1.02
1.03
3.1

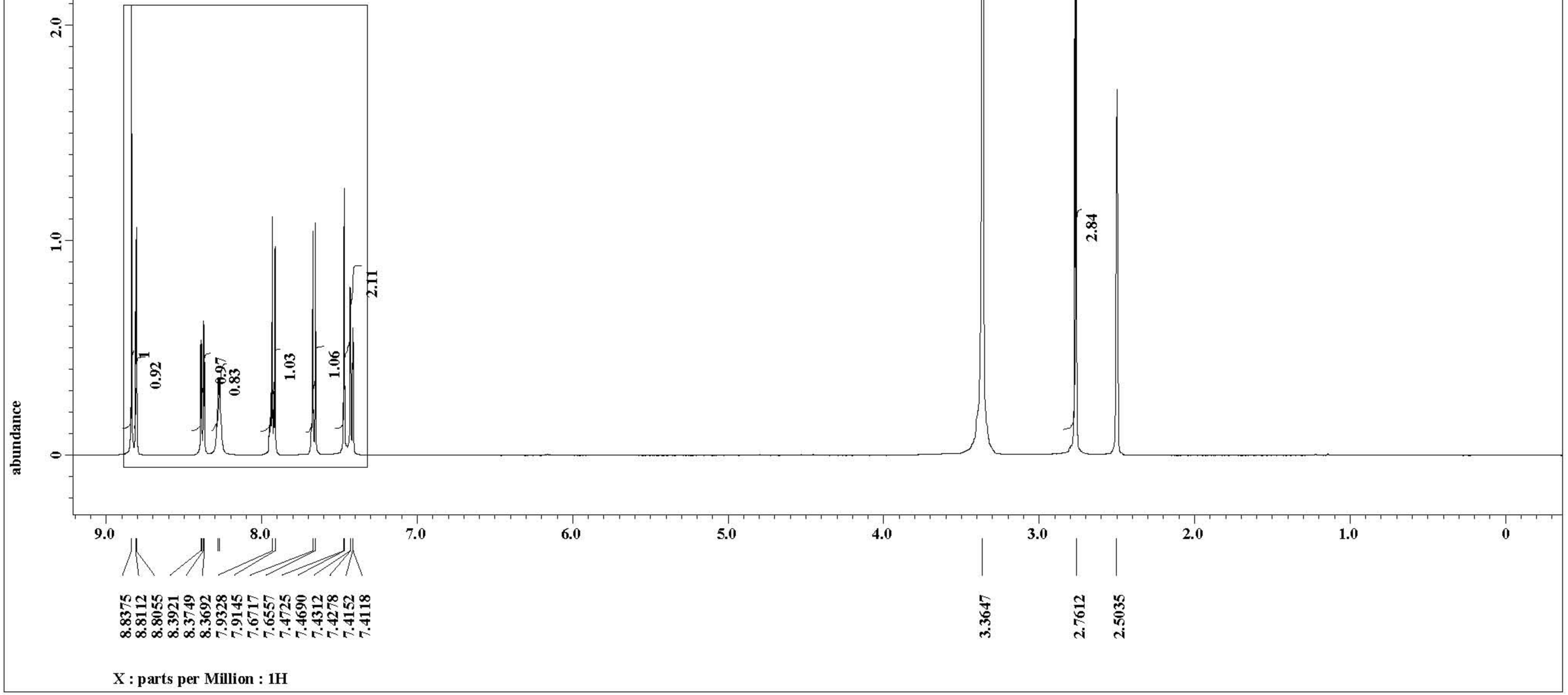

abundance
0.27
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
-0.01
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.0575
159.7081
148.3098
143.8172
133.8210
129.9389
127.8310
119.4372
117.6154
115.4693
114.9065
114.1721
113.0561
66.7475
55.5972
40.1642
40.0021
39.8304
X : parts per Million : 13C
H
N
NH
O
O

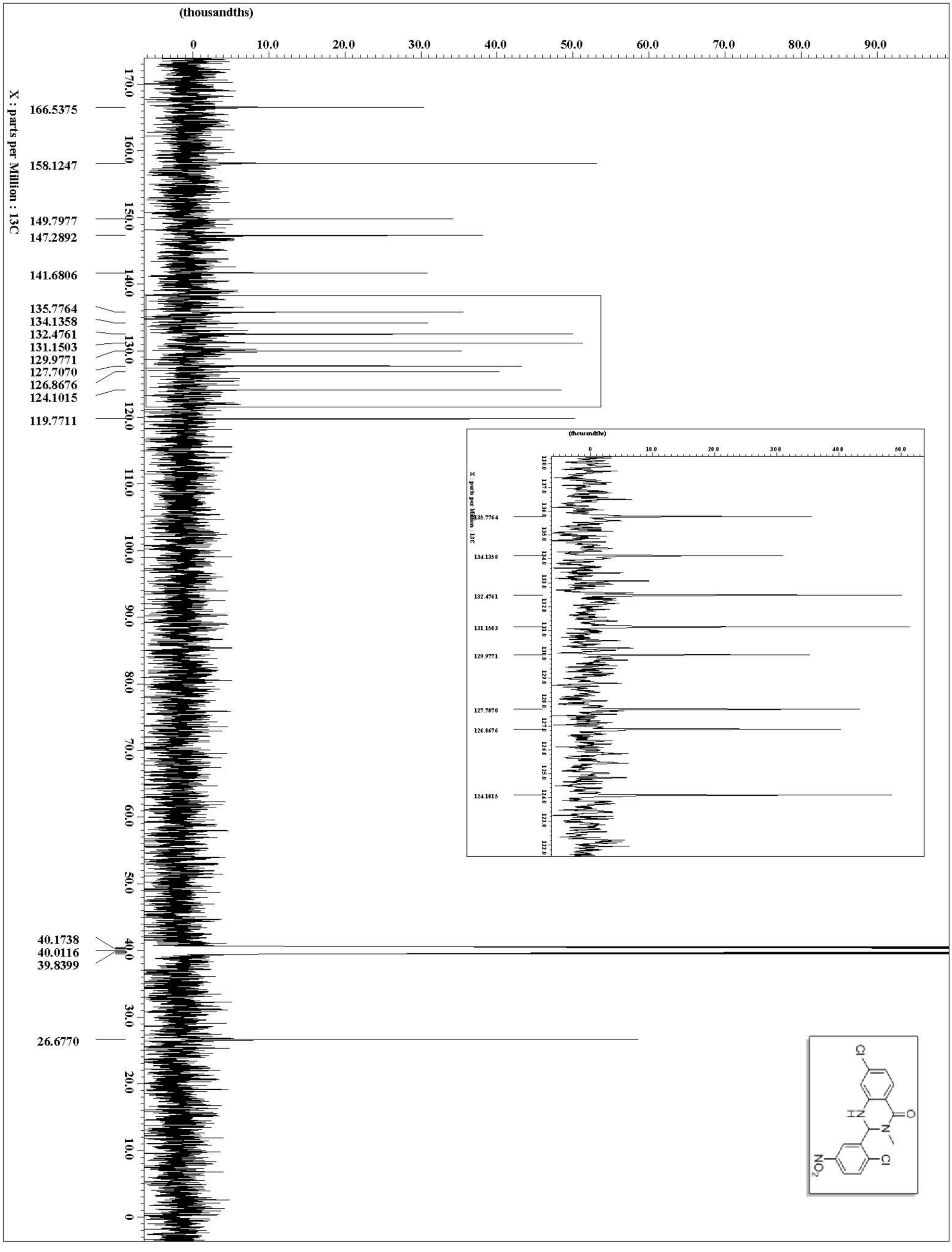

abundance
X : parts per Million : 1H
7.6419
7.6258
7.5640
7.4827
7.4209
7.4048
6.6215
6.5986
6.5952
3.3520
2.7302
2.5057
0.0000
2.83
0.97
0.97
1.0
0.94
0.96
Cl
Cl
F
O
N
H

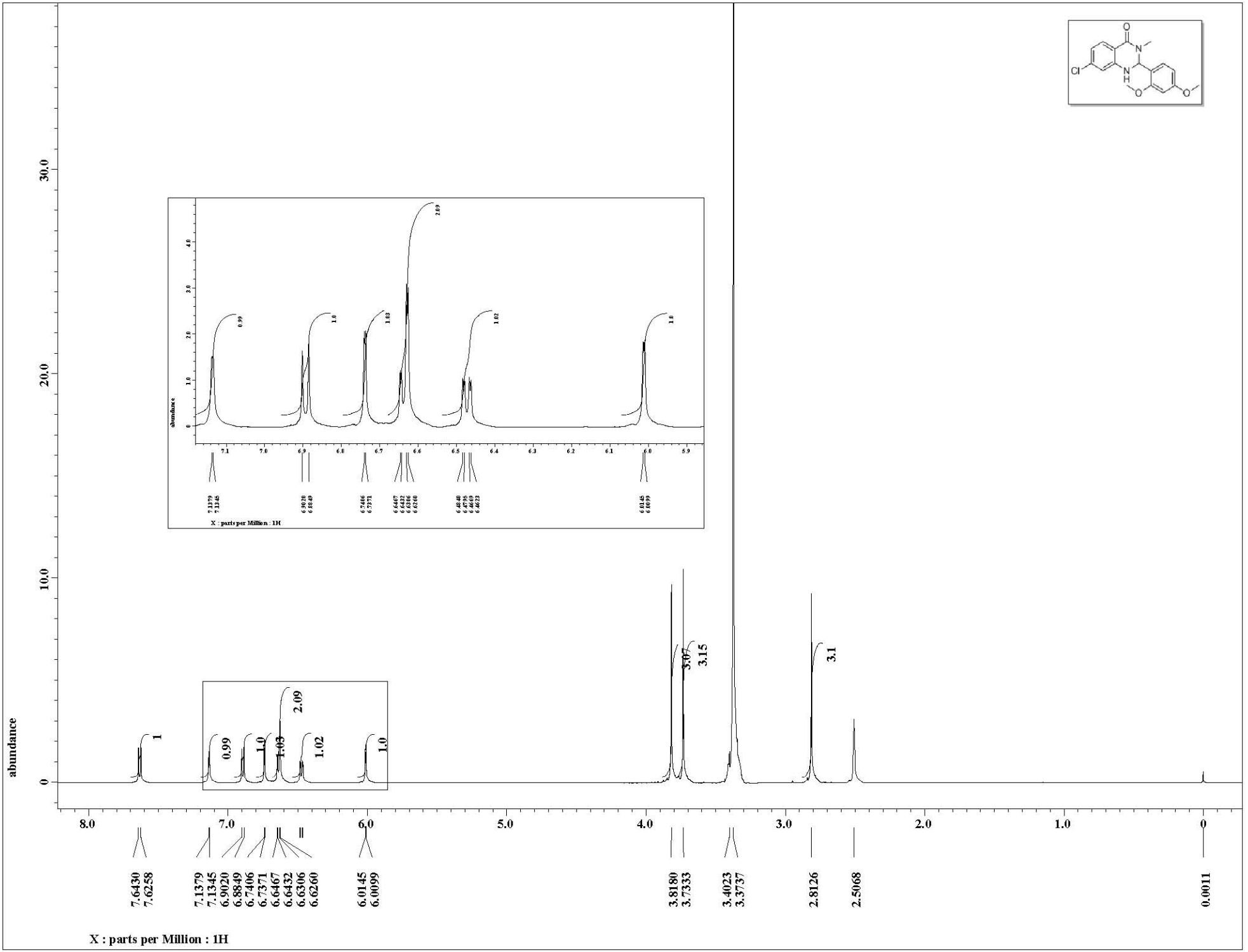

abundance
X : parts per Million : 13C
161.2533
147.5276
138.1610
133.7066
132.1328
129.5669
126.8771
125.1602
116.8047
116.5567
116.3659
112.5124
112.0546
68.1306
40.2024
40.0307
39.8685
31.1123

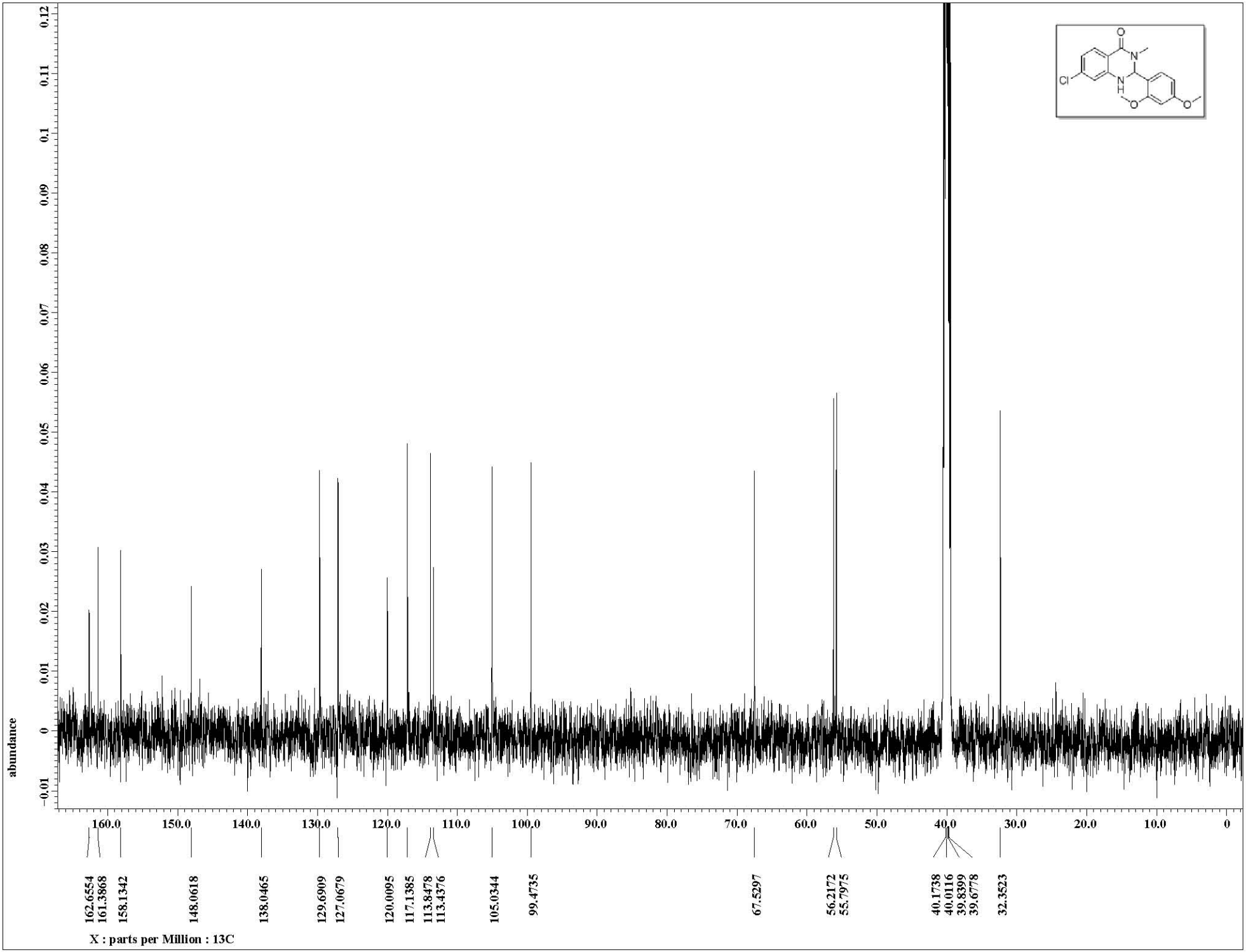

abundance
X : parts per Million : 1H
8.8375
8.8112
8.8055
8.3921
8.3749
8.3692
8.2798
8.2707
7.9328
7.9145
7.6717
7.6557
7.4725
7.4690
7.4312
7.4278
7.4152
7.4118
0.92
0.97
0.83
1.03
1.06
2.11

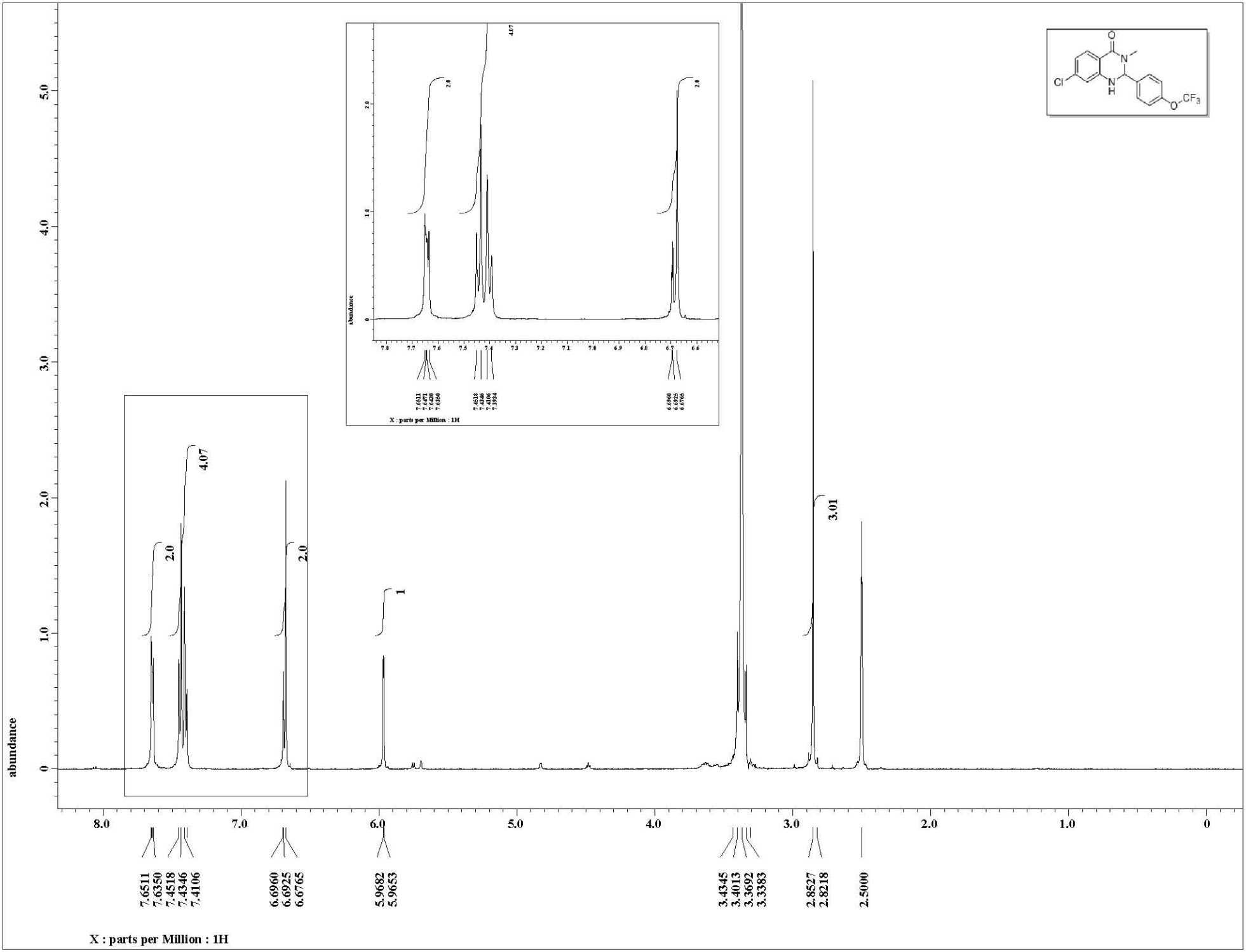

O
N
Cl
Cl
N
H
NO2

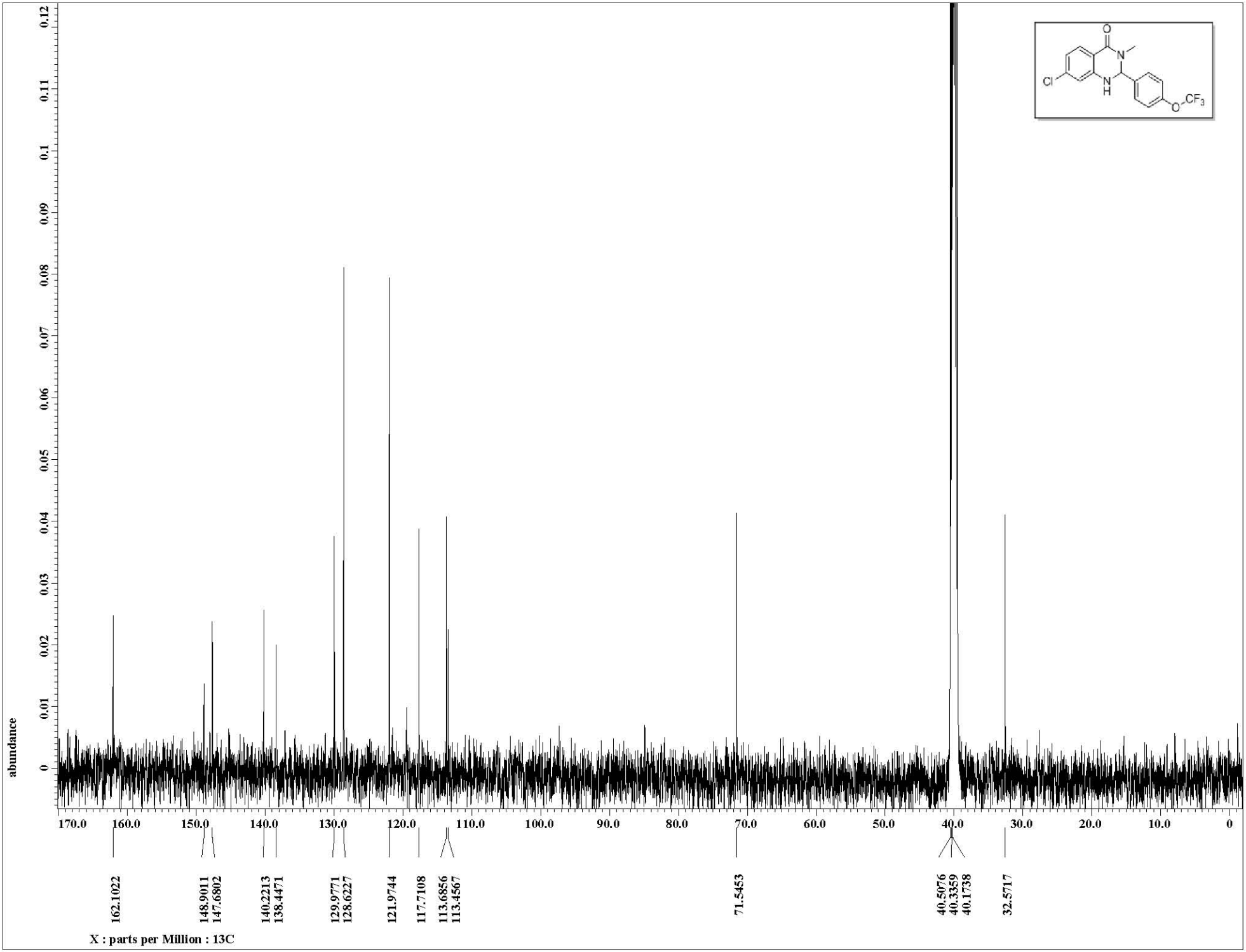

abundance
X : parts per Million : 1H
8.8375
8.8112
8.8055
8.3921
8.3749
8.3692
7.9328
7.9145
7.6717
7.6557
7.4725
7.4690
7.4312
7.4278
7.4152
7.4118
3.3647
2.7612
2.5035
0.92
0.97
0.83
1.03
1.06
2.11
2.84

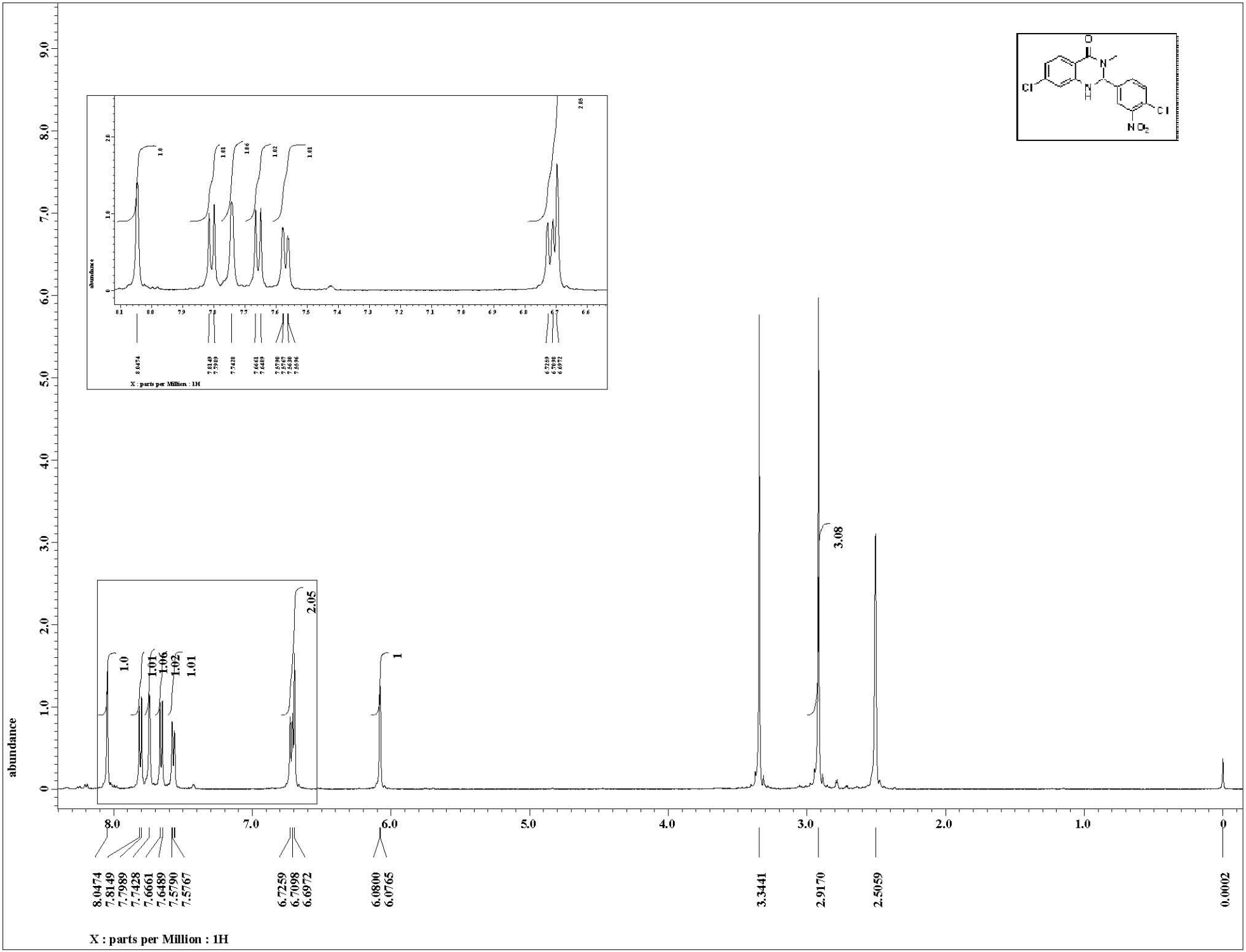

(thousandths)
X : parts per Million : 13C
166.5375
158.1247
149.7977
147.2892
141.6806
135.7764
134.1358
132.4761
131.1503
129.9771
127.7070
126.8676
124.1015
119.7711
40.1738
40.0116
39.8399
26.6770
(thousandths)
X : parts per Million : 13C
135.7764
134.1358
132.4761
131.1503
129.9771
127.7070
126.8676
124.1015
Cl
HN
O
N
Cl
NO2

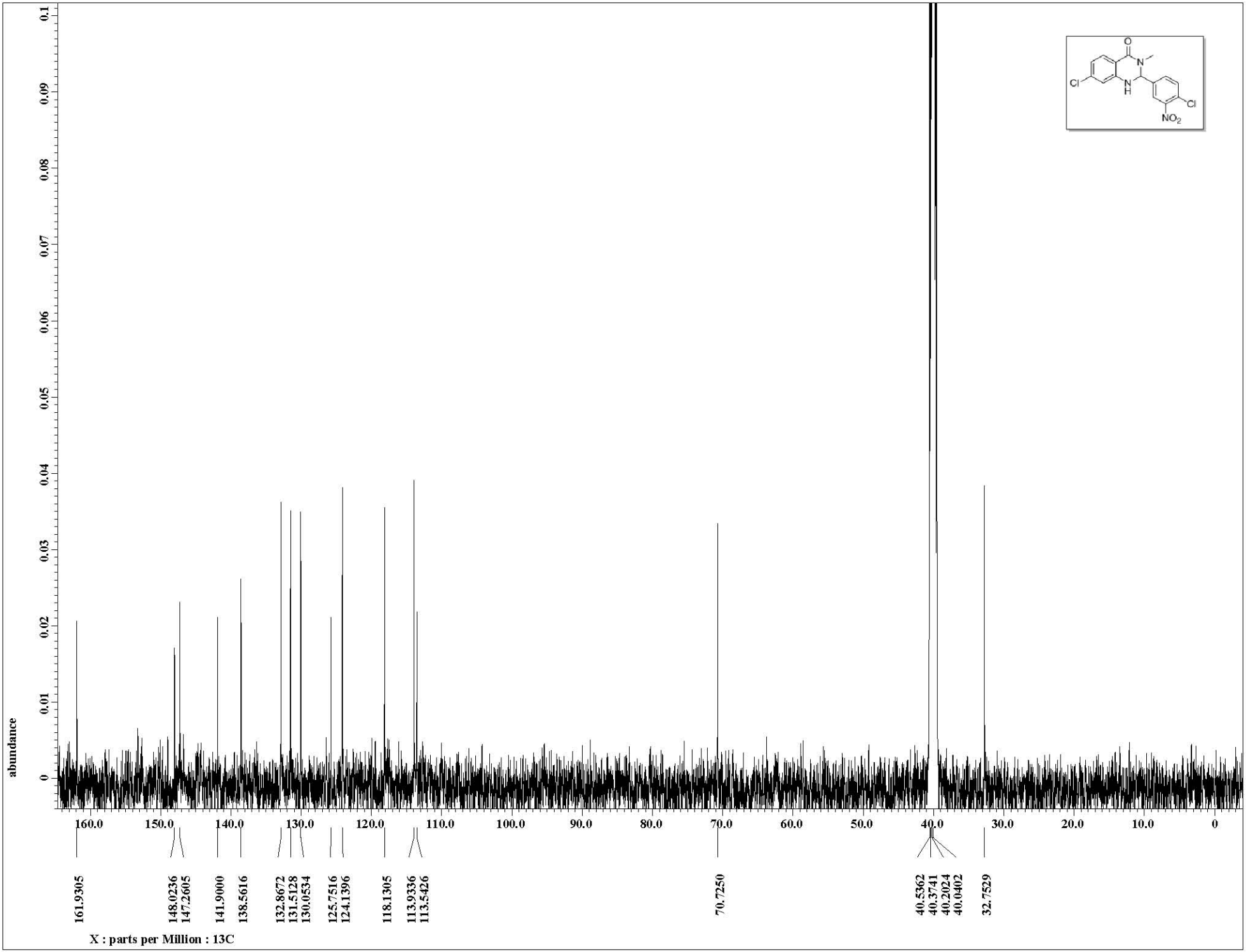

abundance
X : parts per Million : 1H
7.6430
7.6258
7.1379
7.1345
6.9020
6.8849
6.7406
6.7371
6.6467
6.6432
6.6306
6.6260
6.0145
6.0099
3.8180
3.7333
3.4023
3.3737
2.8126
2.5068
0.0011
1
0.99
1.0
1.03
2.09
1.02
1.0
3.07
3.15
3.1

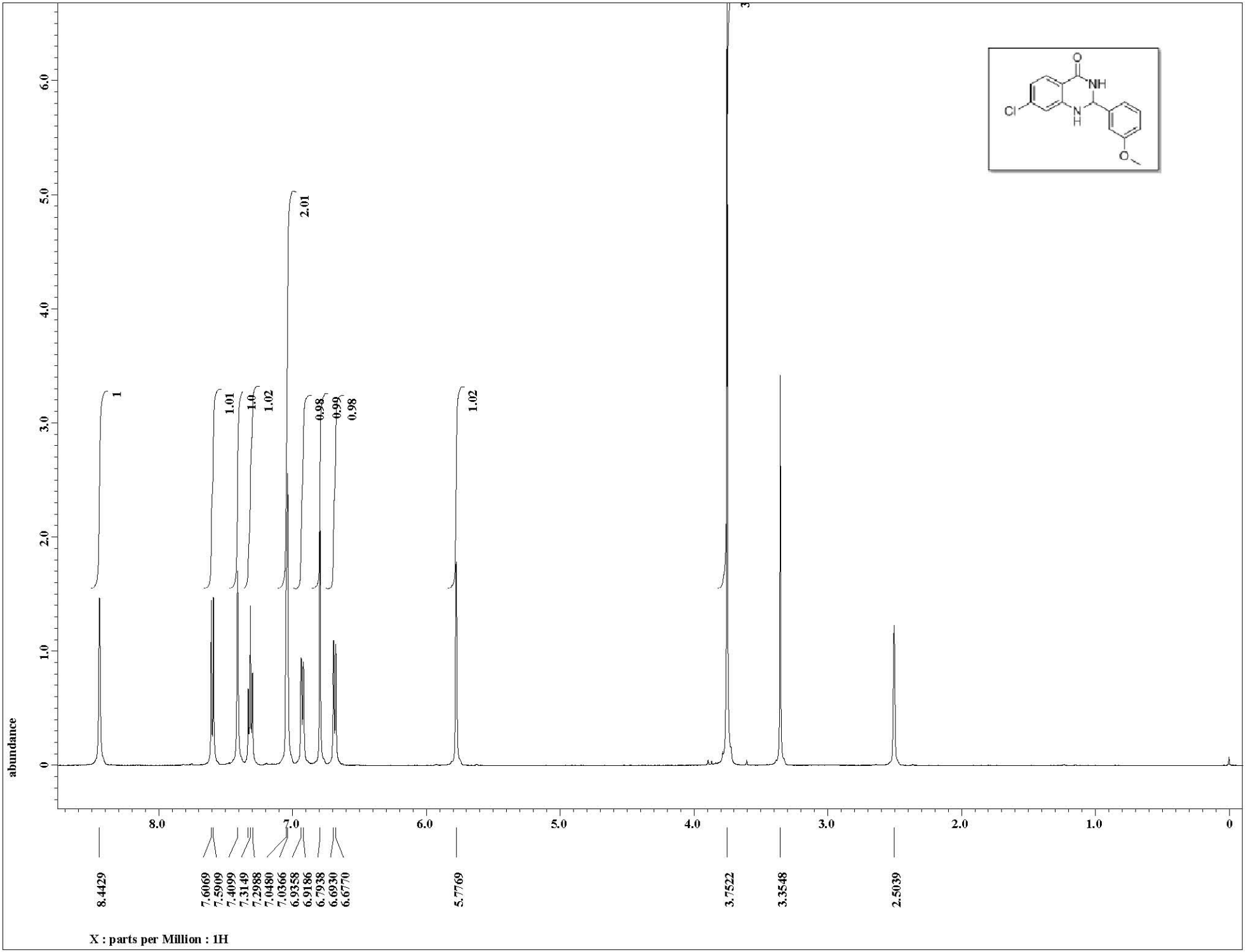

abundance
X : parts per Million : 13C
162.6554
161.3868
158.1342
148.0618
138.0465
129.6909
127.0679
120.0095
117.1385
113.8478
113.4376
105.0344
99.4735
67.5297
56.2172
55.7975
40.1738
40.0116
39.8399
39.6778
32.3523

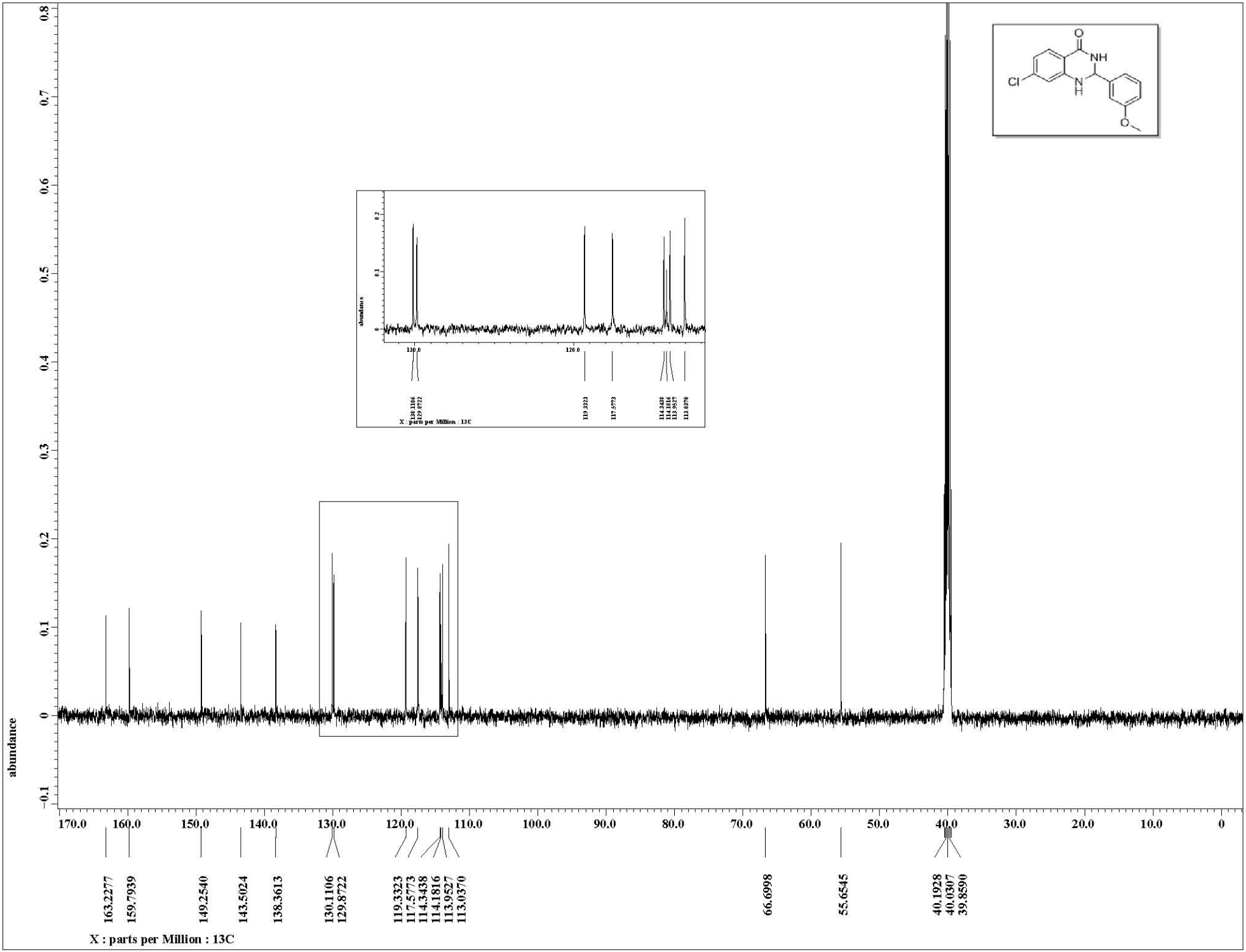

abundance
X : parts per Million : 1H
7.6511
7.6350
7.4518
7.4346
7.4106
6.6960
6.6925
6.6765
5.9682
5.9653
3.4345
3.4013
3.3692
3.3383
2.8527
2.8218
2.5000
2.0
4.07
2.0
1
3.01
Cl
N
H
O
O
CF3

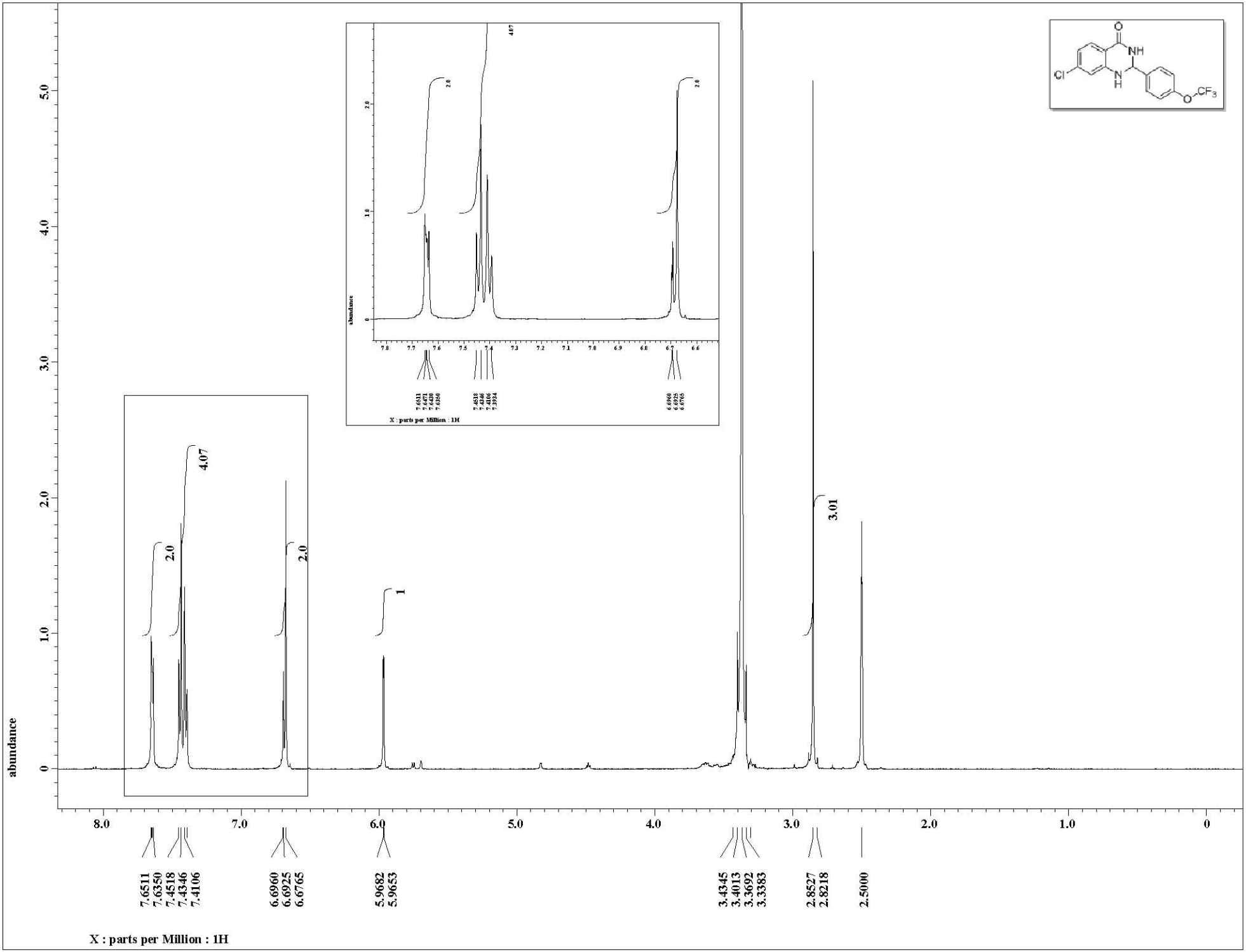

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.1022
148.9011
147.6802
140.2213
138.4471
129.9771
128.6227
121.9744
117.7108
113.6856
113.4567
71.5453
40.5076
40.3359
40.1738
32.5717
X : parts per Million : 13C
Cl
N
H
O
O
CF3

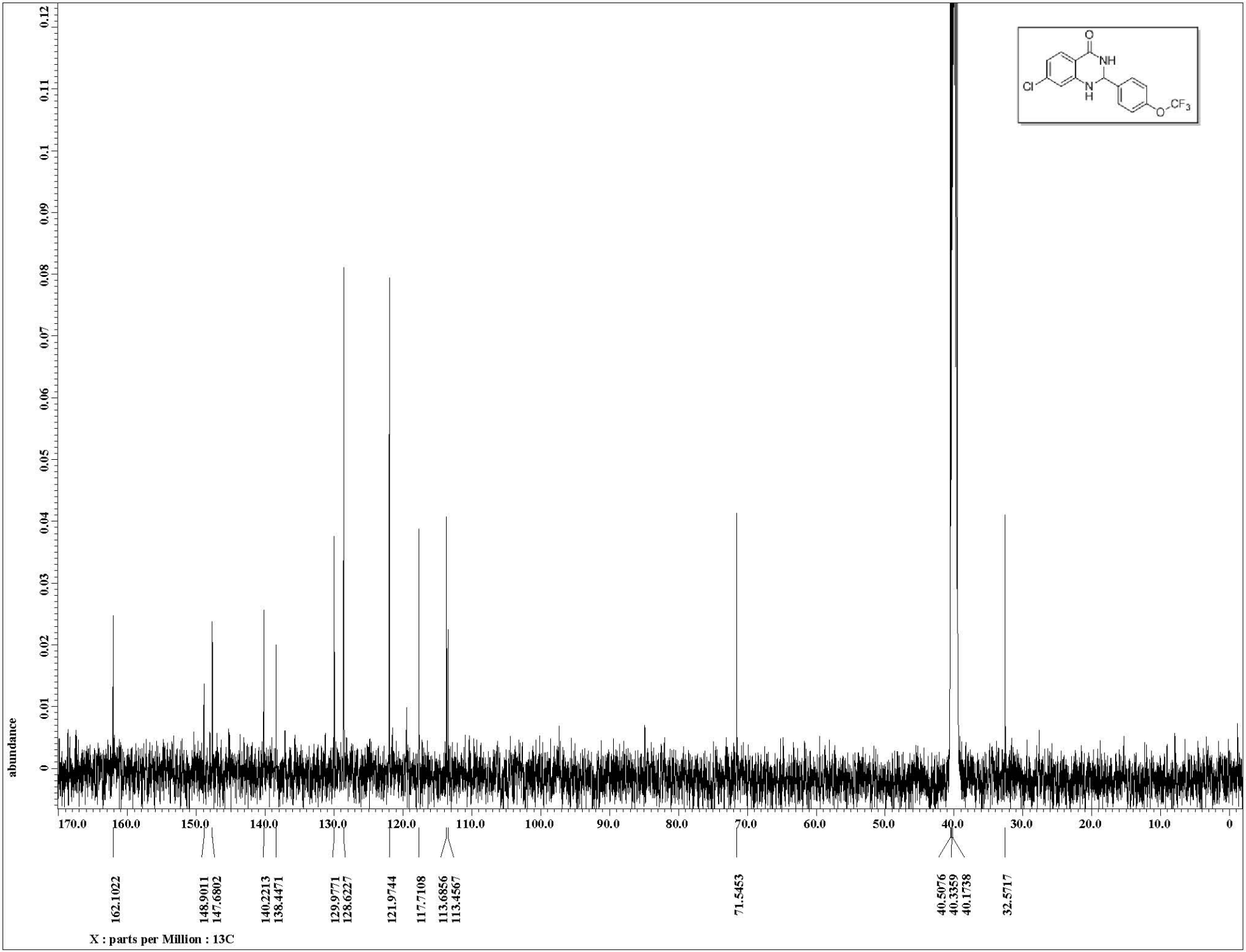

abundance
X : parts per Million : 1H
8.0474
7.8149
7.7989
7.7428
7.6661
7.6489
7.5790
7.5767
6.7259
6.7098
6.6972
6.0800
6.0765
3.3441
2.9170
2.5059
0.0002
1.0
1.01
1.06
1.02
1.01
2.05
1
3.08

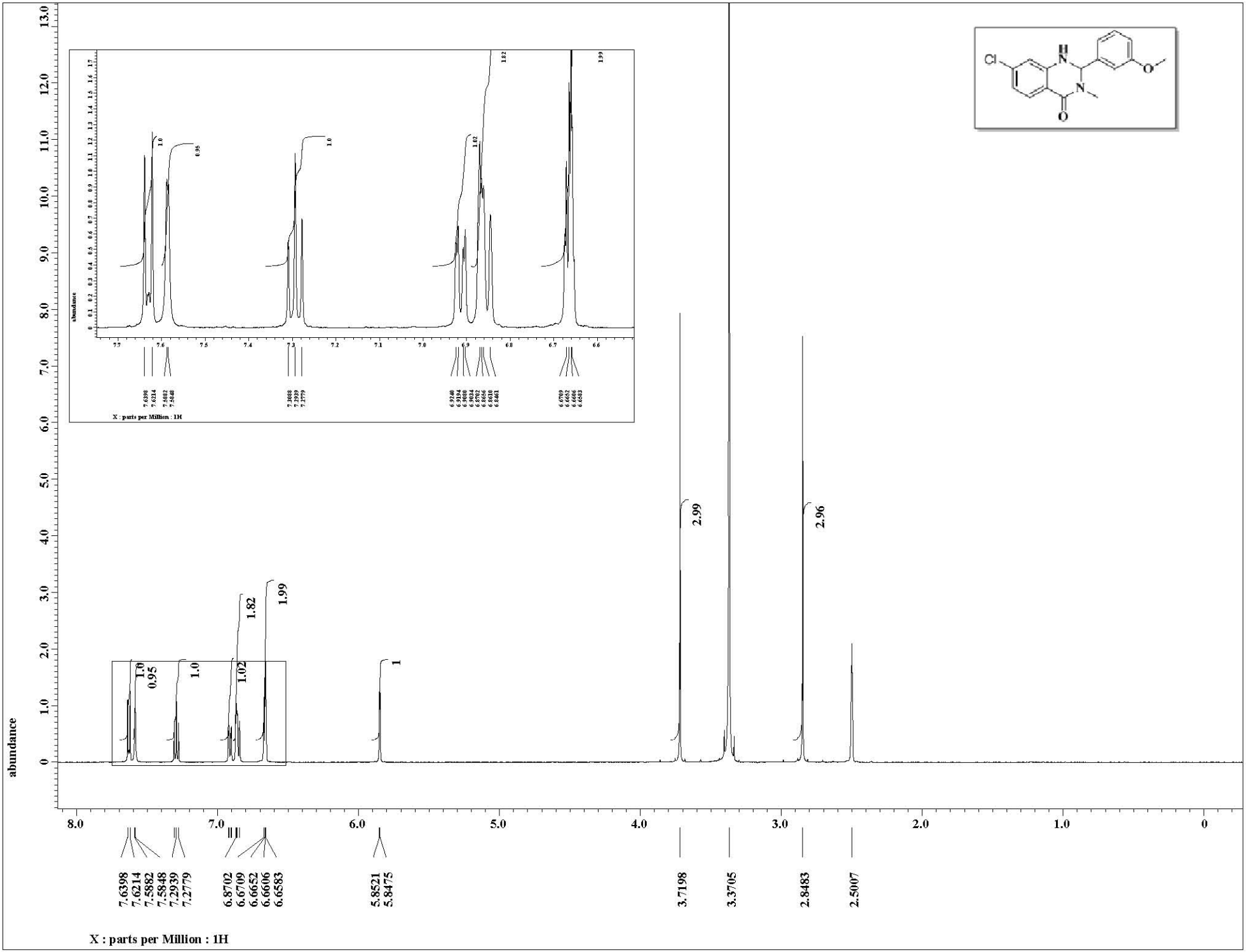

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.9305
148.0236
147.2605
141.9000
138.5616
132.8672
131.5128
130.0534
125.7516
124.1396
118.1305
113.9336
113.5426
70.7250
40.5362
40.3741
40.2024
40.0402
32.7529
X : parts per Million : 13C
O
N
H
Cl
Cl
NO2

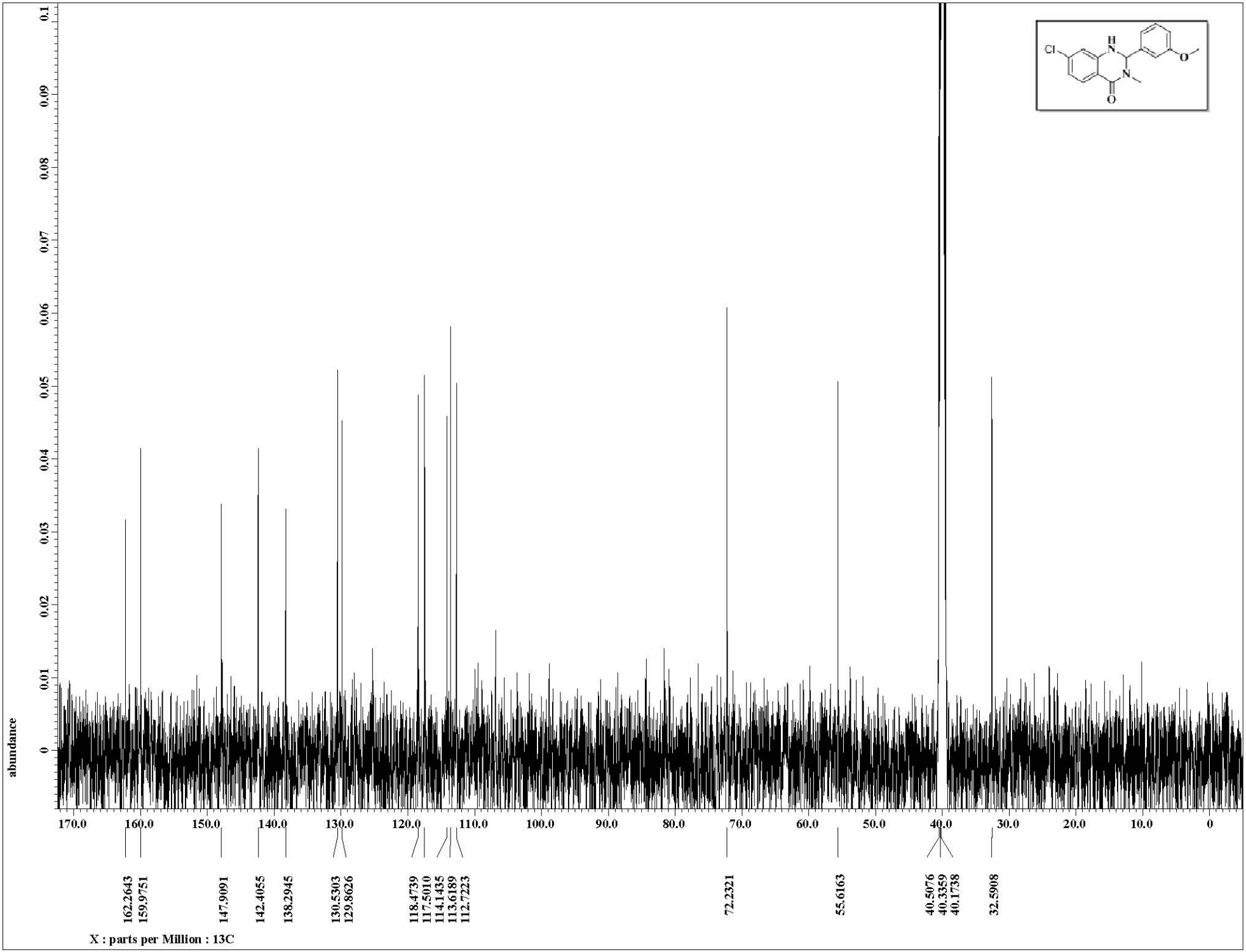

abundance
X : parts per Million : 1H
8.4429
7.6069
7.5909
7.4099
7.3149
7.2988
7.0480
7.0366
6.9358
6.9186
6.7938
6.6930
6.6770
5.7769
3.7522
3.3548
2.5039
1
1.01
1.0
1.02
2.01
0.98
0.99
0.98
1.02
NH
N
H
Cl
O


abundance
X : parts per Million : 13C
163.2277
159.7939
149.2540
143.5024
138.3613
130.1106
129.8722
119.3323
117.5773
114.3438
114.1816
113.9527
113.0370
66.6998
55.6545
40.1928
40.0307
39.8590
Cl
NH
N
H
O
O


abundance
X : parts per Million : 1H
7.6511
7.6350
7.4518
7.4346
7.4106
6.6960
6.6925
6.6765
5.9682
5.9653
3.4345
3.4013
3.3692
3.3383
2.8527
2.8218
2.5000
2.0
4.07
2.0
1
3.01
NH
N
H
Cl
O
CF3


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.1022
148.9011
147.6802
140.2213
138.4471
129.9771
128.6227
121.9744
117.7108
113.6856
113.4567
71.5453
40.5076
40.3359
40.1738
32.5717
X : parts per Million : 13C
O
NH
N
H
Cl
O
CF3


abundance
X : parts per Million : 1H
7.6398
7.6214
7.5882
7.5848
7.2939
7.2779
6.8702
6.6709
6.6652
6.6606
6.6583
5.8521
5.8475
3.7198
3.3705
2.8483
2.5007
1.0
0.95
1.0
1.02
1.82
1.99
1
2.99
2.96
Cl
N
H
O
N
O


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.2643
159.9751
147.9091
142.4055
138.2945
130.5303
129.8626
118.4739
117.5010
114.1435
113.6189
112.7223
72.2321
55.6163
40.5076
40.3359
40.1738
32.5908
X : parts per Million : 13C
Cl
H
N
O
N
O

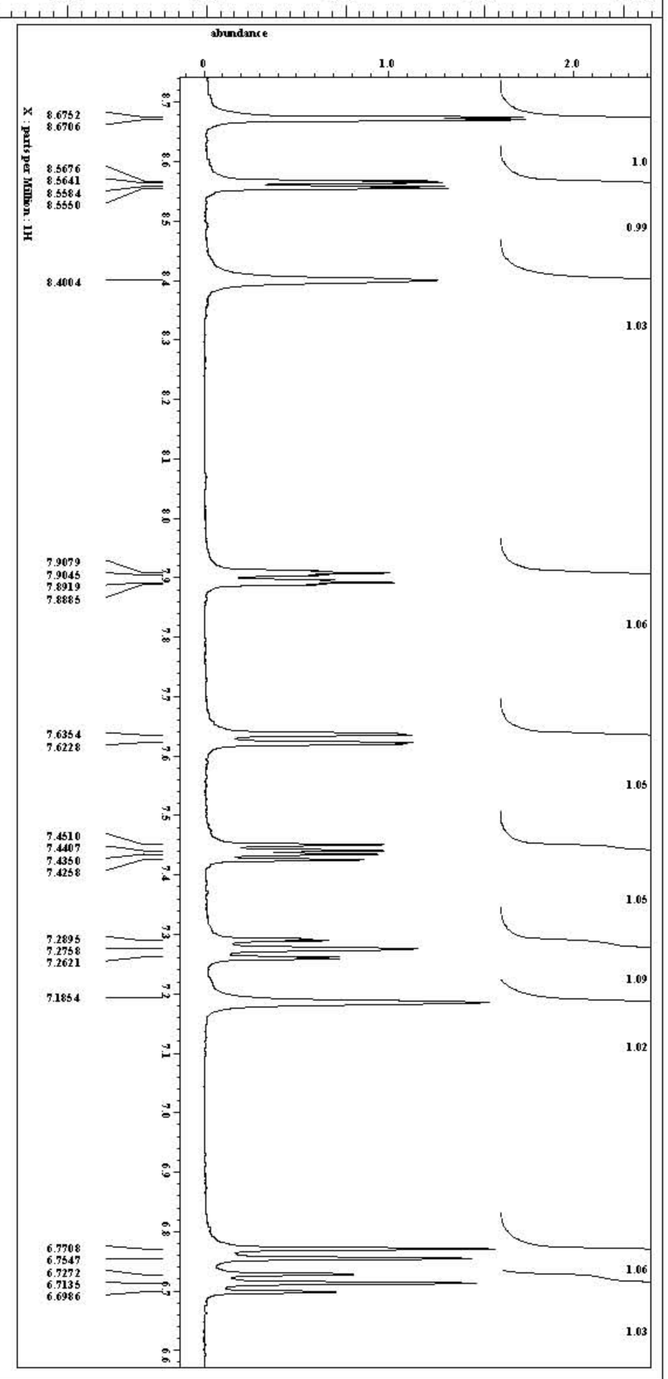
X : parts per Million : 1H

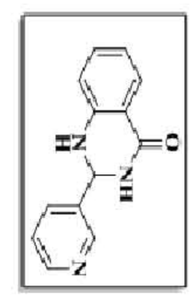
abundance

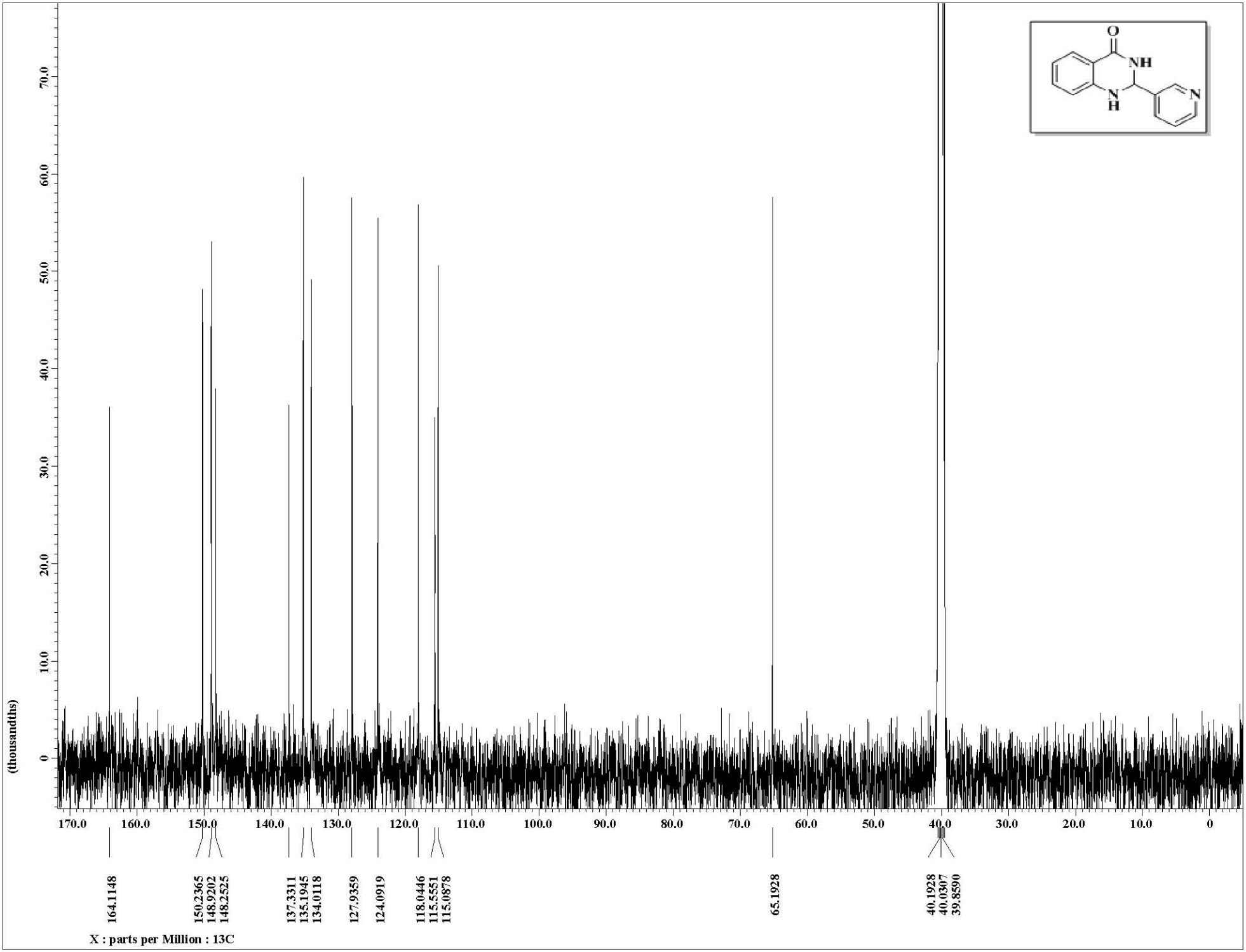
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0

8.6752
8.6706
8.5641
8.5584
8.5550
7.9079
7.8919
7.6354
7.6228
7.4510
7.4407
7.4350
7.4258
7.2758
7.1854
6.7708
6.7547
6.7135
5.8581
3.3890
3.3535
2.5084
2.5049
0.0061

1.0
0.99
1.03
1.06
1.05
1.05
1.09
1.02
1.06
1.03
1.06






(thousandths)
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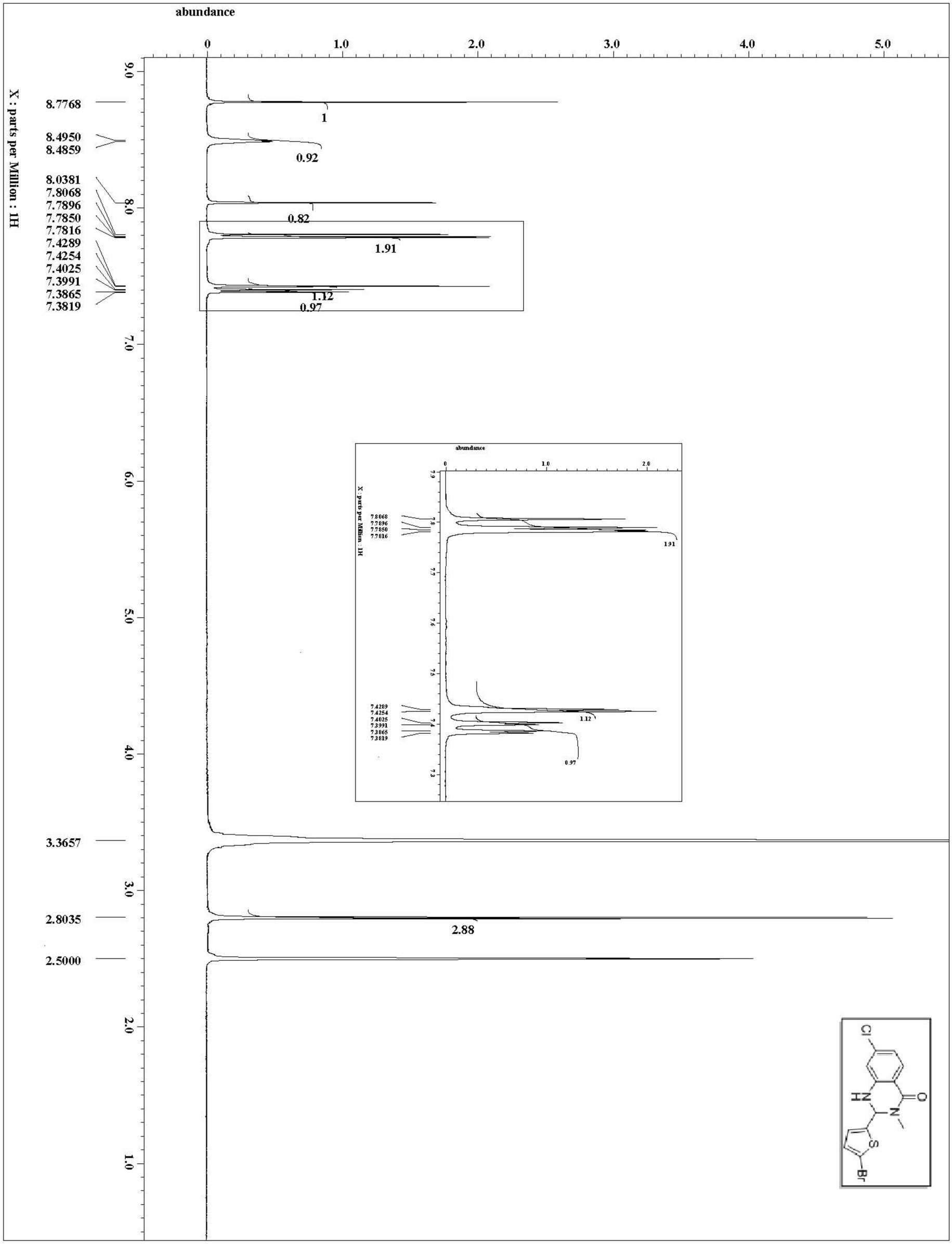
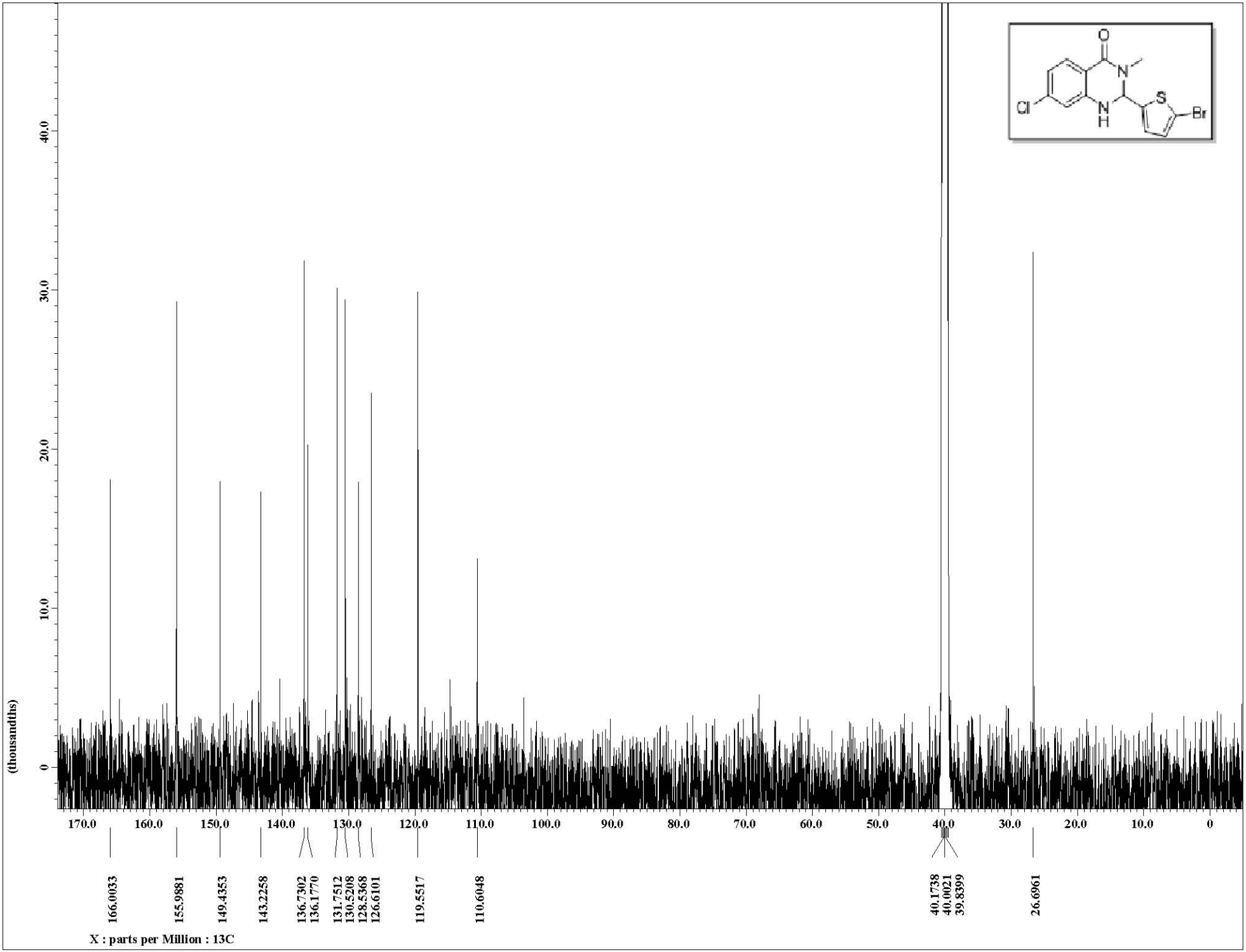
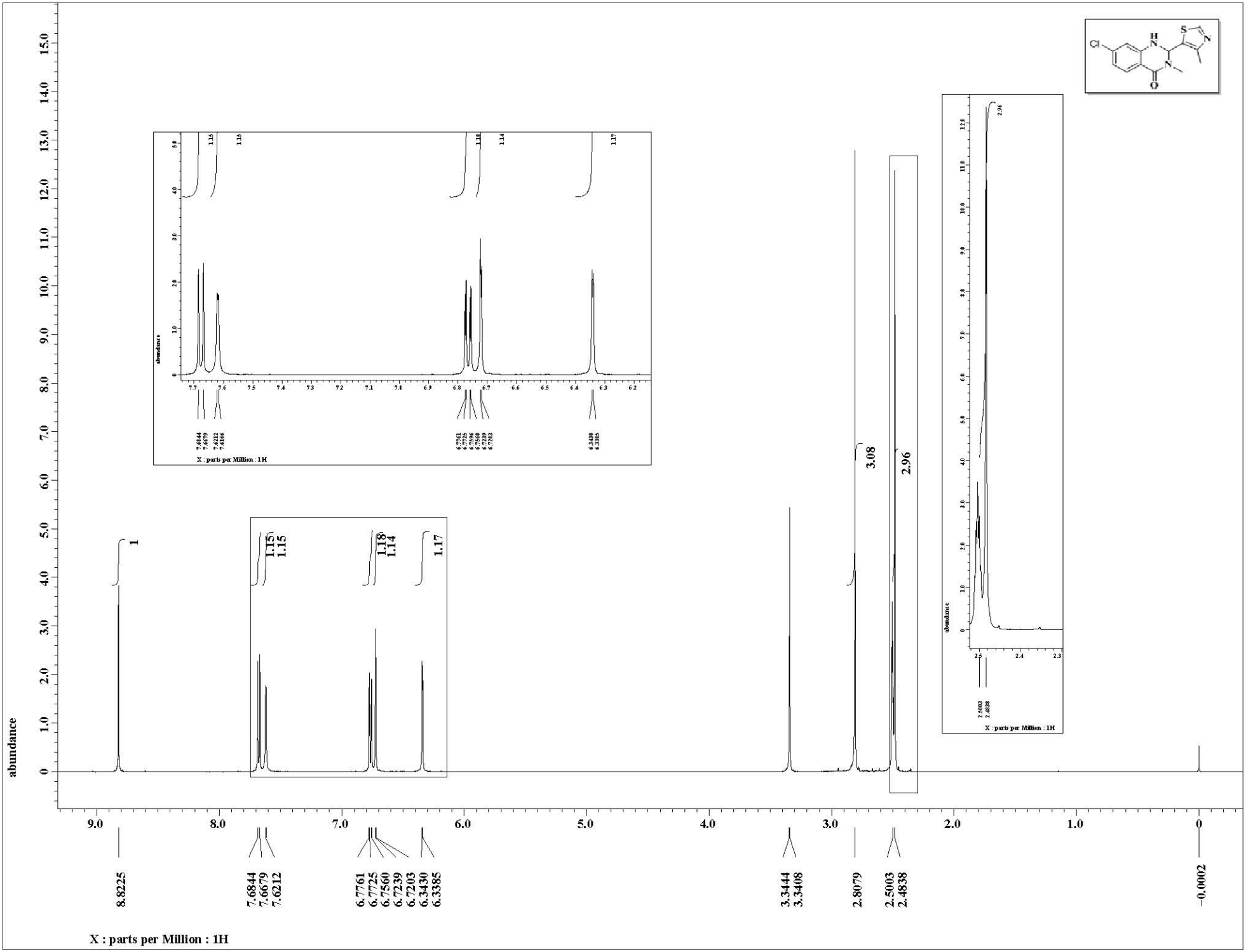
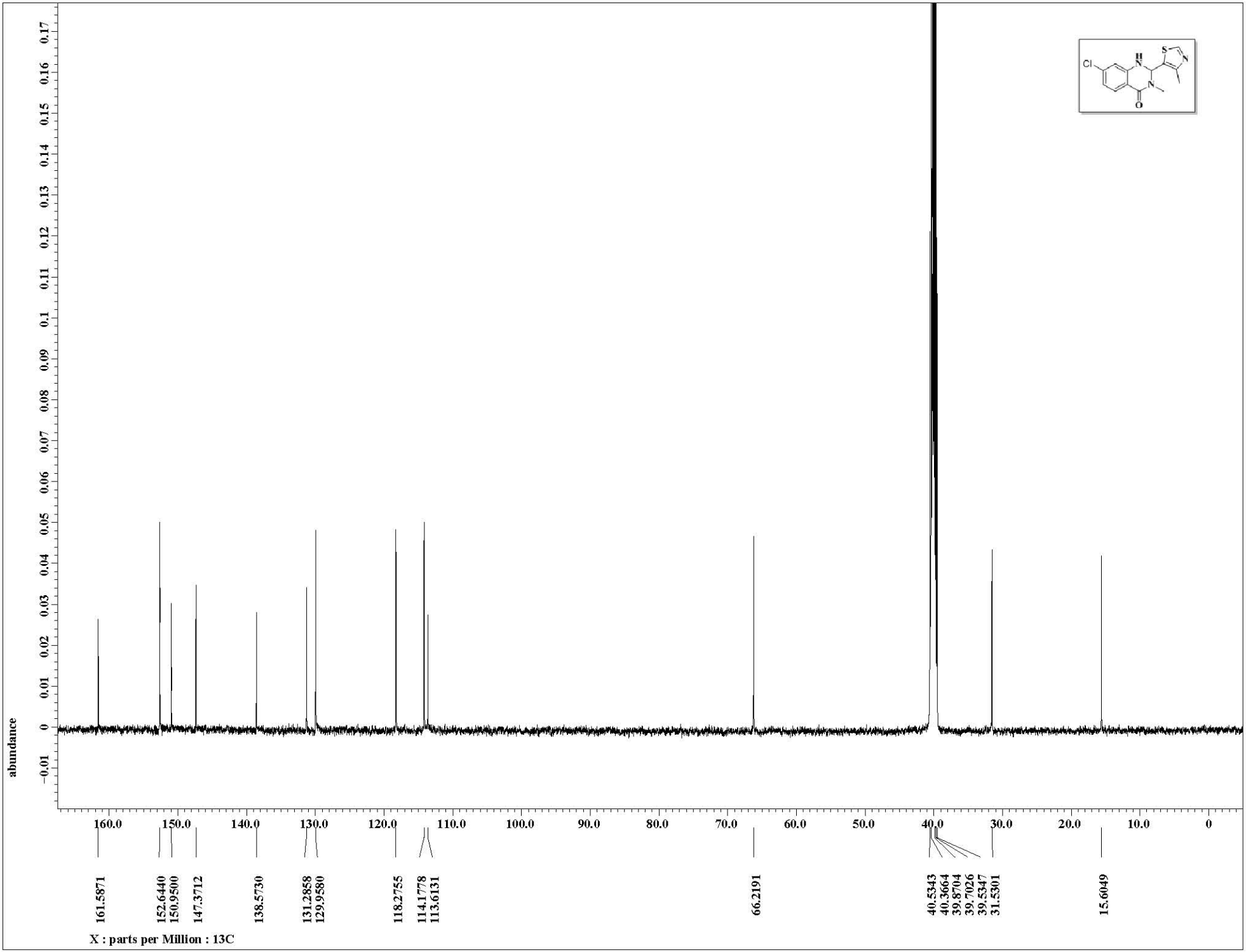
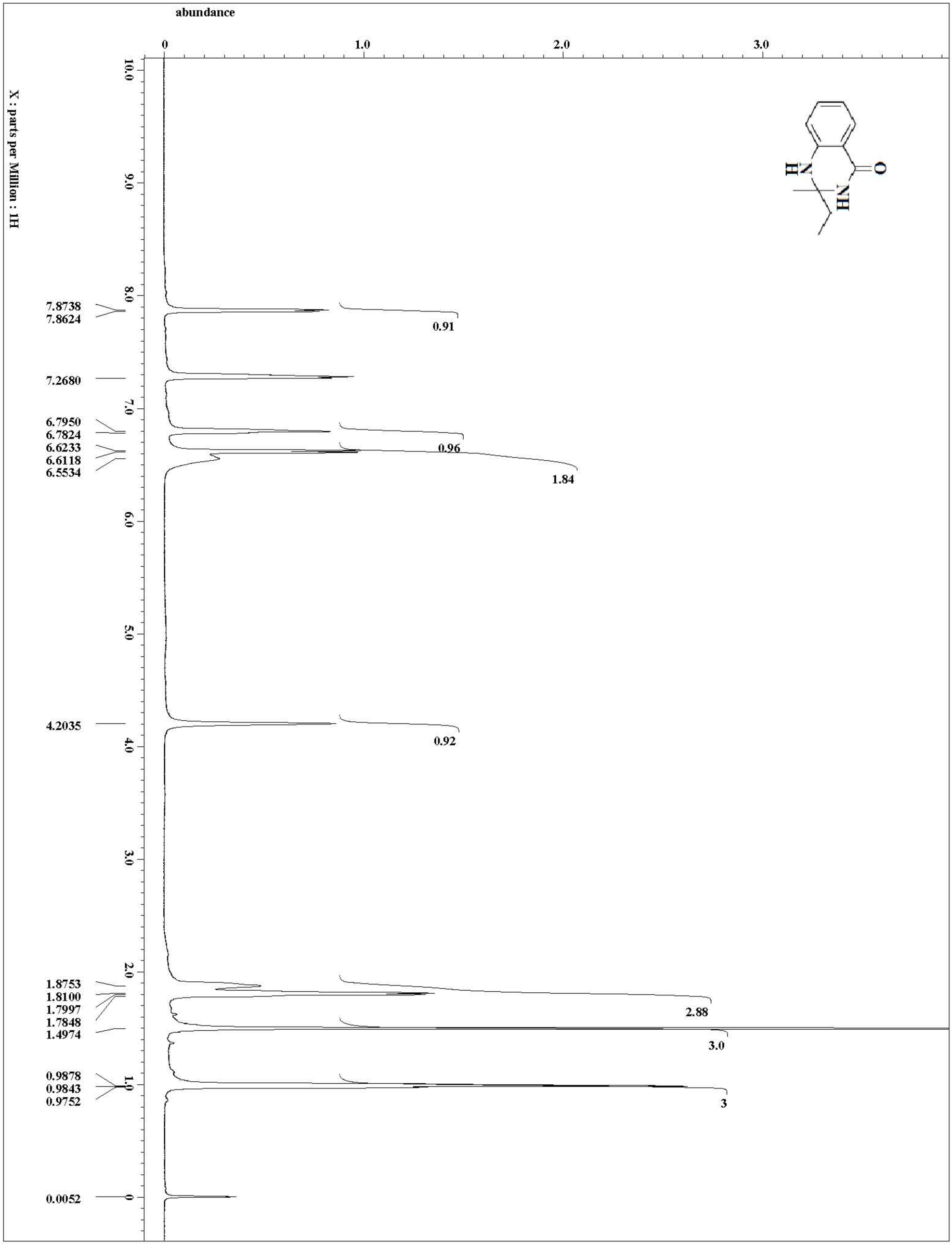
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.1148
150.2365
148.9202
148.2525
137.3311
135.1945
134.0118
127.9359
124.0919
118.0446
115.5551
115.0878
65.1928
40.1928
40.0307
39.8590
X : parts per Million : 13C
O
NH
N
H
N

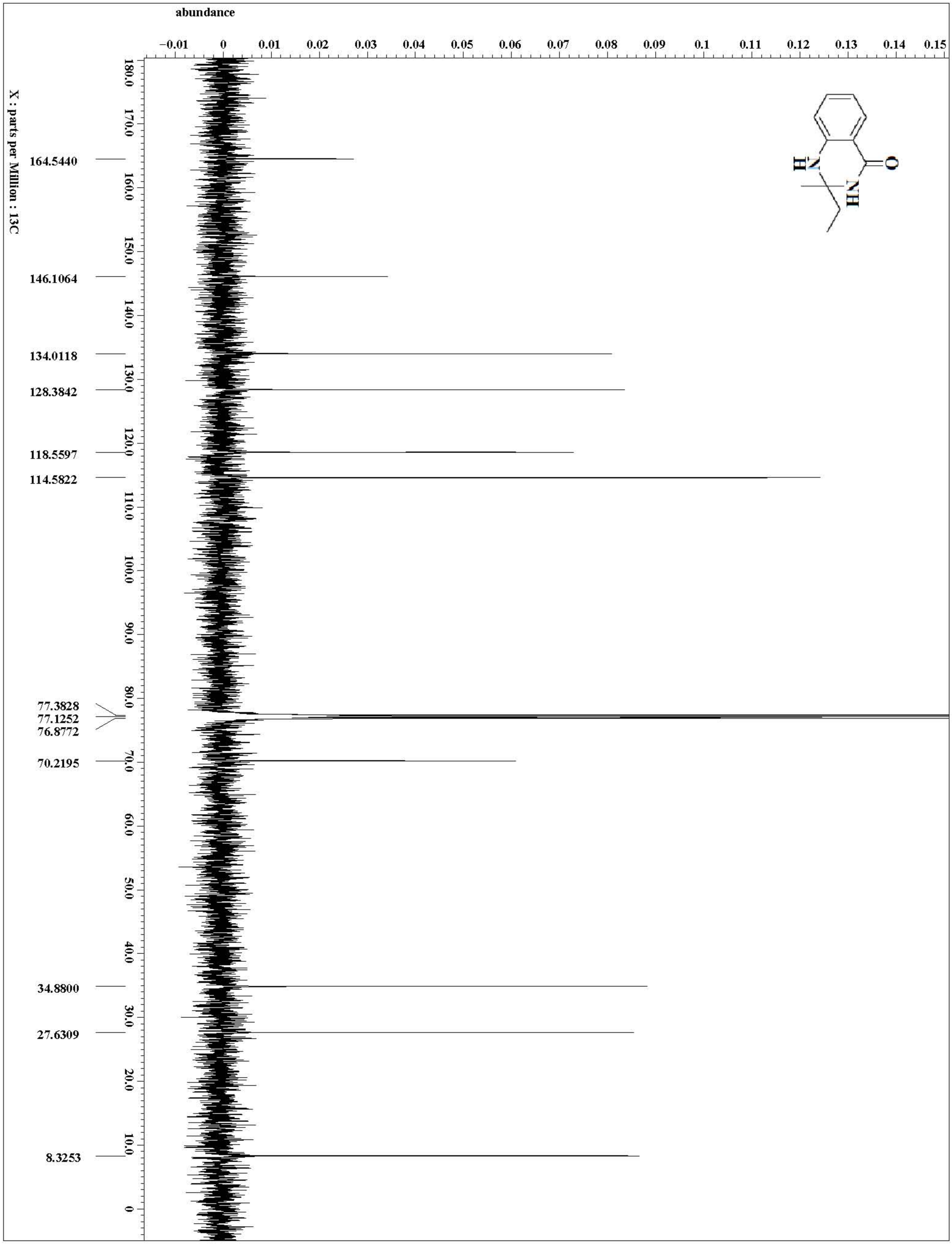

abundance
0
1.0
2.0
3.0
4.0
5.0
X : parts per Million : 1H
8.7768
8.4950
8.4859
8.0381
7.8068
7.7896
7.7850
7.7816
7.4289
7.4254
7.4025
7.3991
7.3865
7.3819
3.3657
2.8035
2.5000
1
0.92
0.82
1.91
1.12
0.97
2.88
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
Cl
N
H
O
N
S
Br

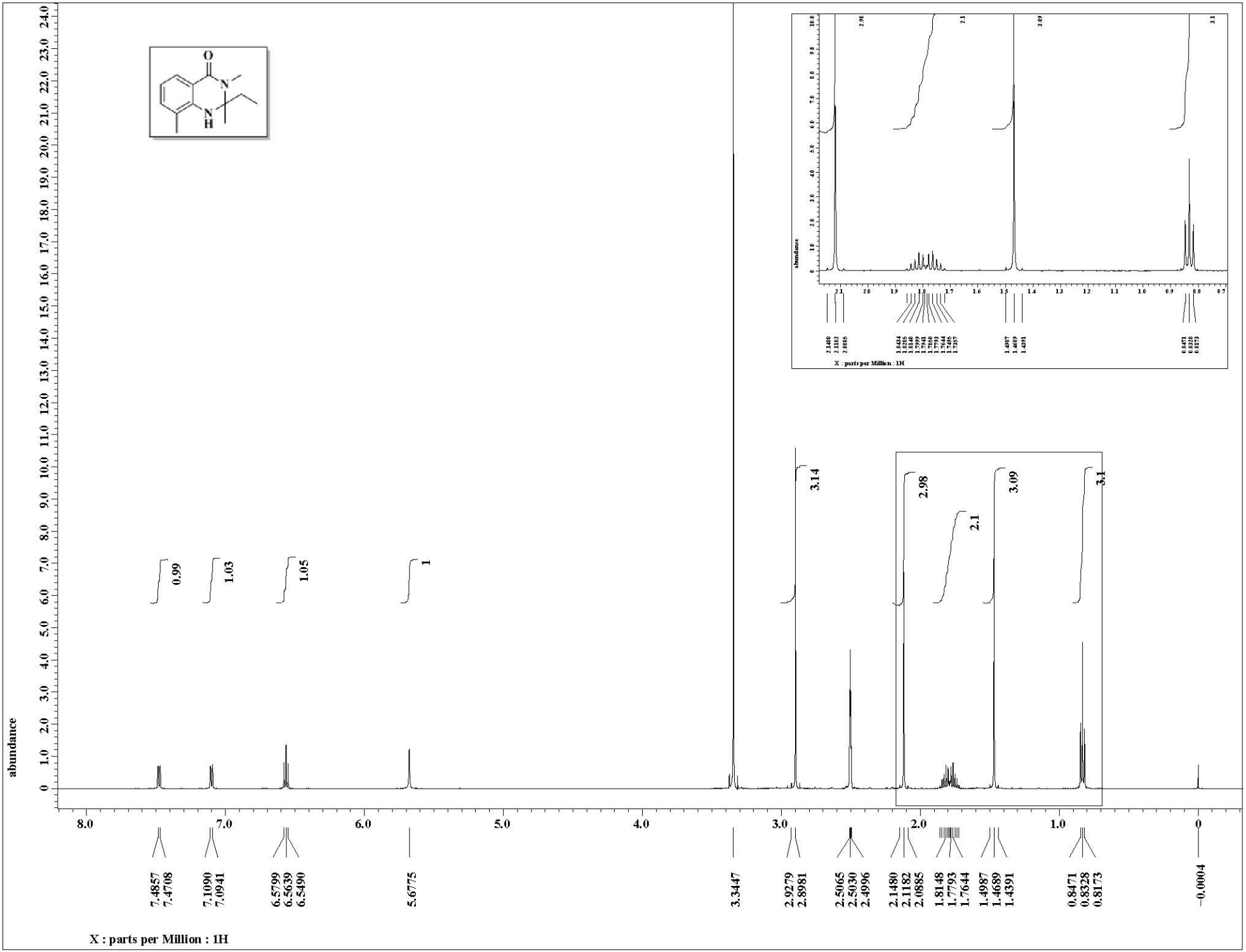

(thousandths)
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.0033
155.9881
149.4353
143.2258
136.7302
136.1770
131.7512
130.5208
128.5368
126.6101
119.5517
110.6048
40.1738
40.0021
39.8399
26.6961
X : parts per Million : 13C
O
N
N
H
S
Cl
Br

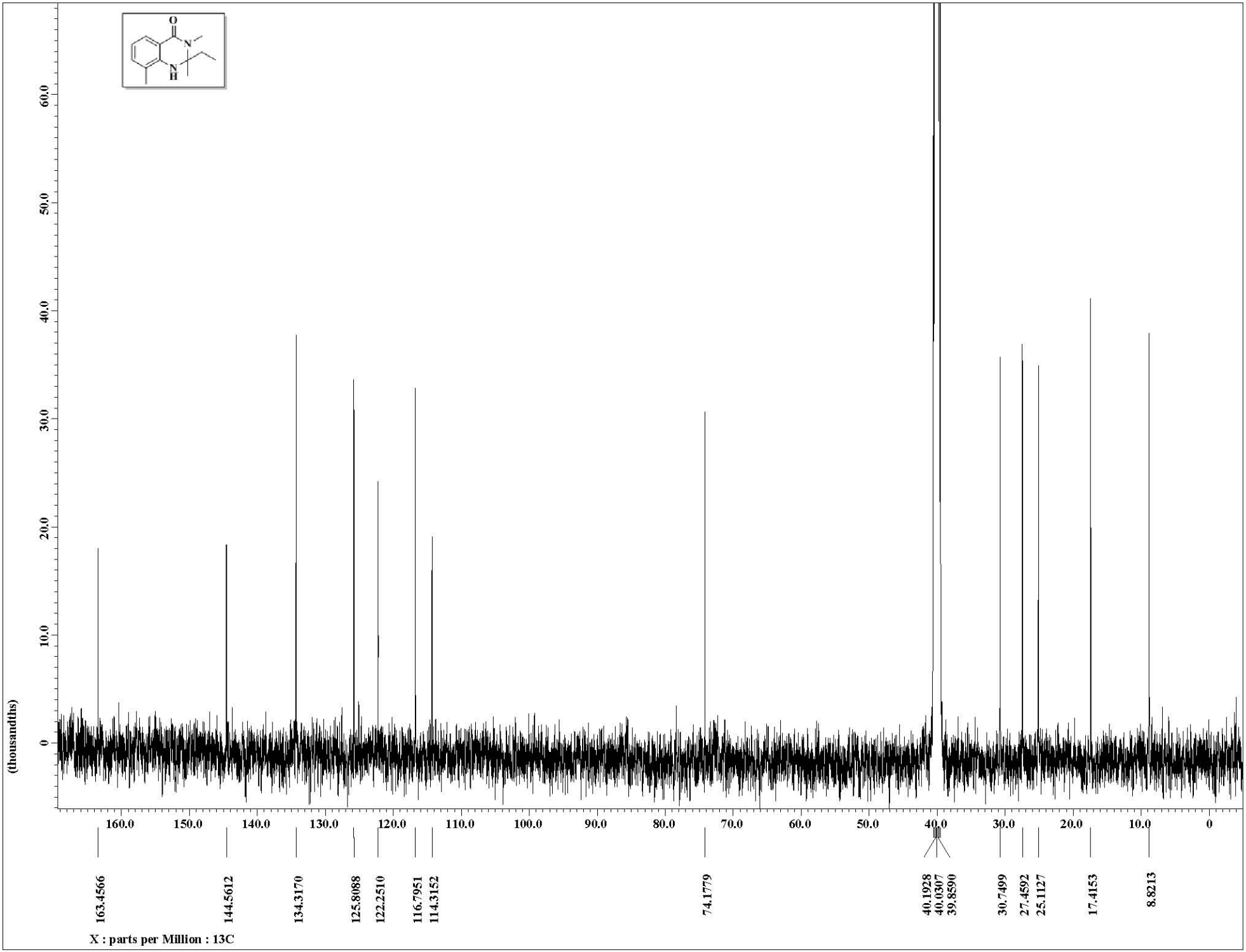

abundance
X : parts per Million : 1H
8.8225
7.6844
7.6679
7.6212
6.7761
6.7725
6.7560
6.7239
6.7203
6.3430
6.3385
3.3444
3.3408
2.8079
2.5003
2.4838
-0.0002
1
1.15
1.15
1.18
1.14
1.17
3.08
2.96

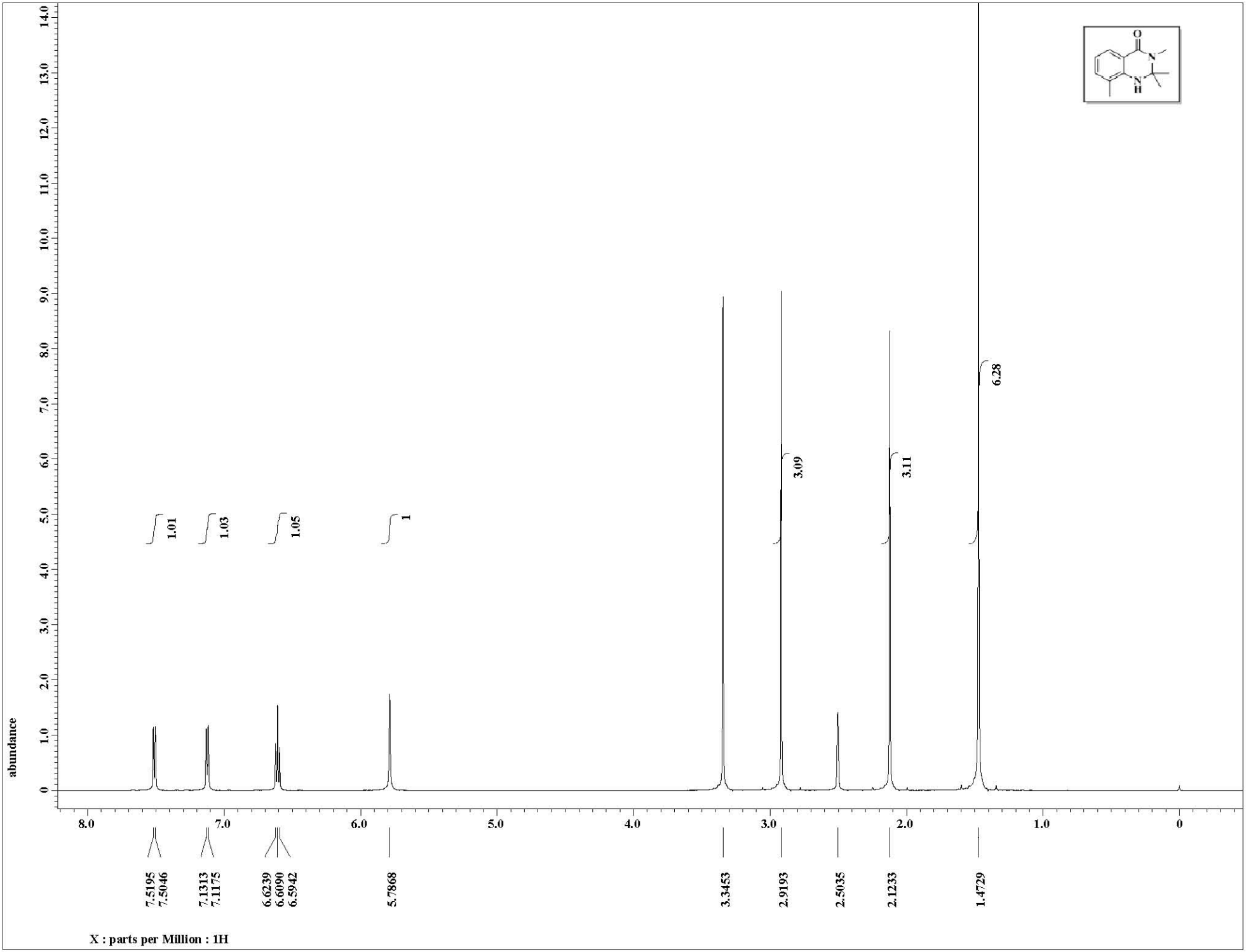

abundance
X : parts per Million : 13C
161.5871
152.6440
150.9500
147.3712
138.5730
131.2858
129.9580
118.2755
114.1778
113.6131
66.2191
40.5343
40.3664
39.8704
39.7026
39.5347
31.5301
15.6049

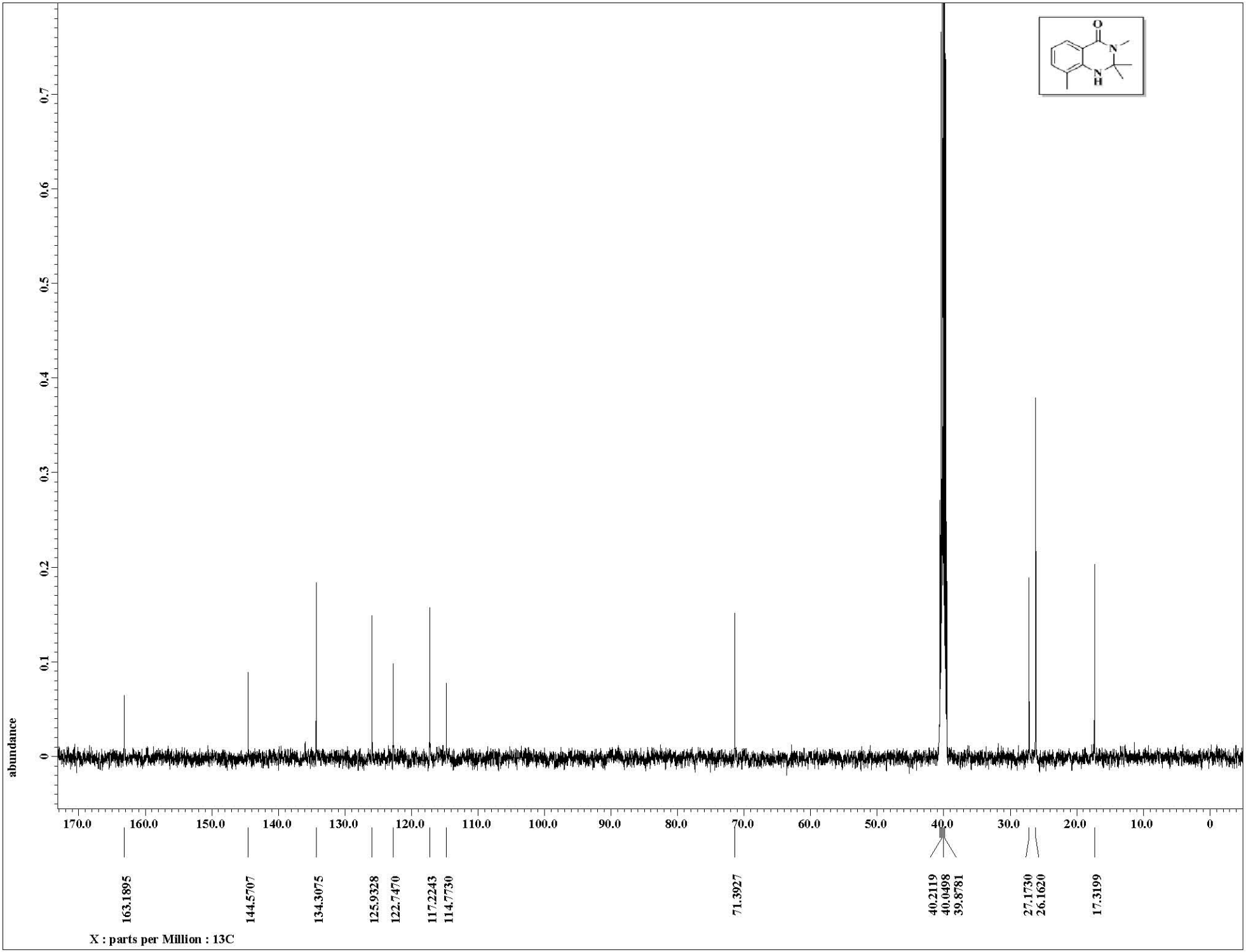

abundance
0
1.0
2.0
3.0
X : parts per Million : 1H
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8738
7.8624
0.91
7.2680
6.7950
6.7824
6.6233
6.6118
6.5534
0.96
1.84
4.2035
0.92
1.8753
1.8100
1.7997
1.7848
1.4974
2.88
3.0
0.9878
0.9843
0.9752
3
0.0052
H
N
HN
O

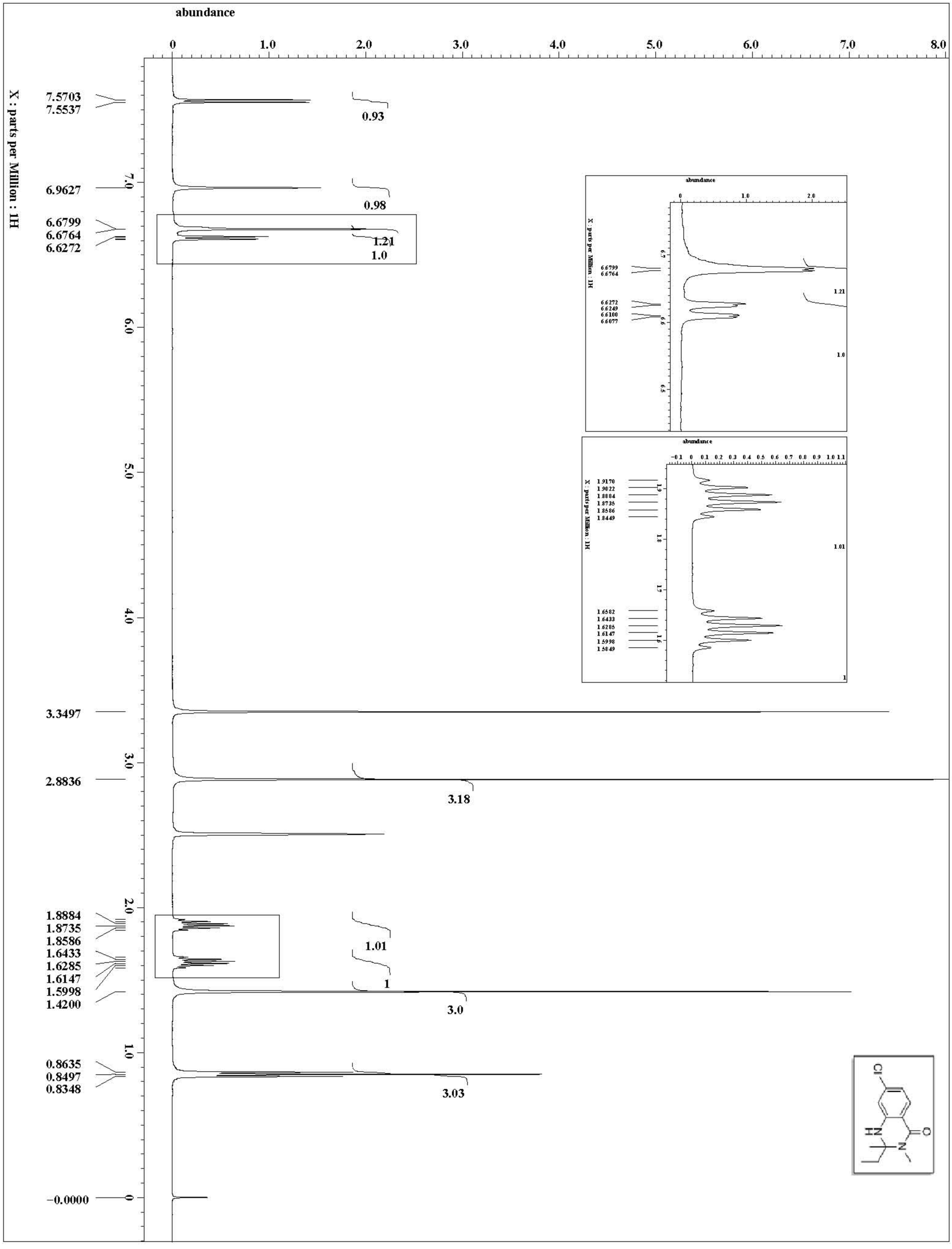

abundance
−0.01
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.5440
146.1064
134.0118
128.3842
118.5597
114.5822
77.3828
77.1252
76.8772
70.2195
34.8800
27.6309
8.3253
H
N
O
NH

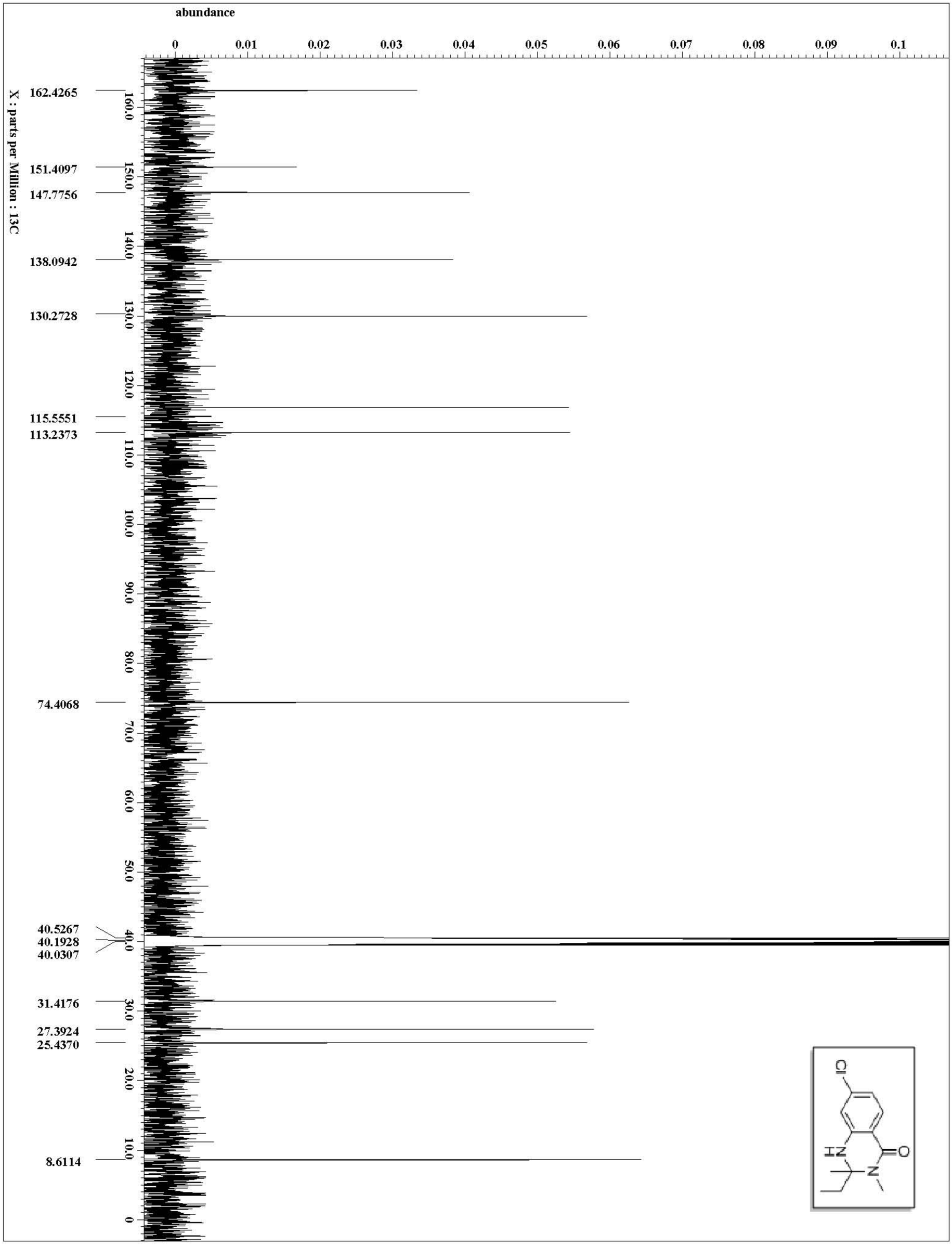

abundance
X : parts per Million : 1H
0.99
1.03
1.05
1
3.14
2.98
2.1
3.09
3.1
7.4857
7.4708
7.1090
7.0941
6.5799
6.5639
6.5490
5.6775
3.3447
2.9279
2.8981
2.5065
2.5030
2.4996
2.1480
2.1182
2.0885
1.8148
1.7793
1.7644
1.4987
1.4689
1.4391
0.8471
0.8328
0.8173
−0.0004

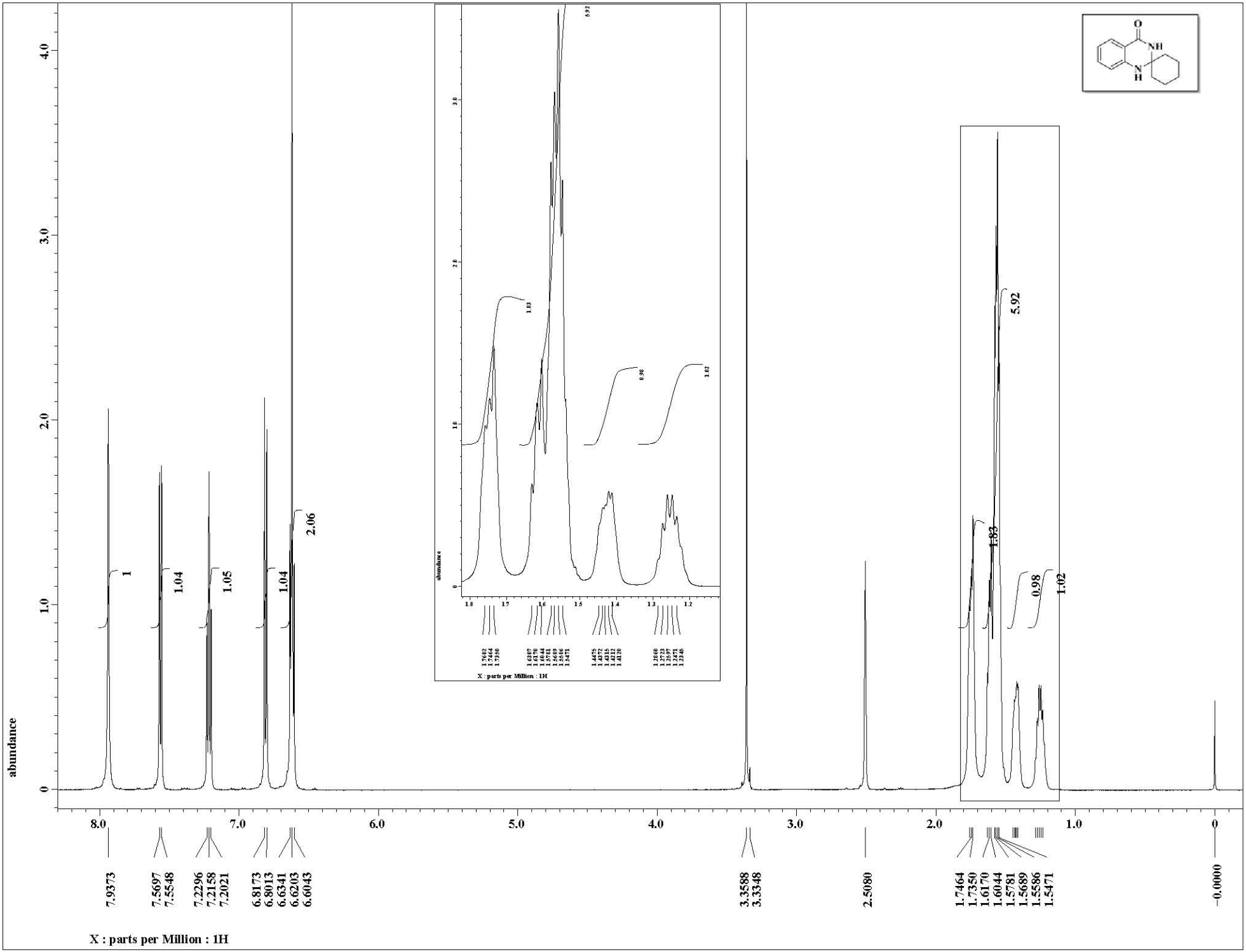

(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.4566
144.5612
134.3170
125.8088
122.2510
116.7951
114.3152
74.1779
40.1928
40.0307
39.8590
30.7499
27.4592
25.1127
17.4153
8.8213
X : parts per Million : 13C

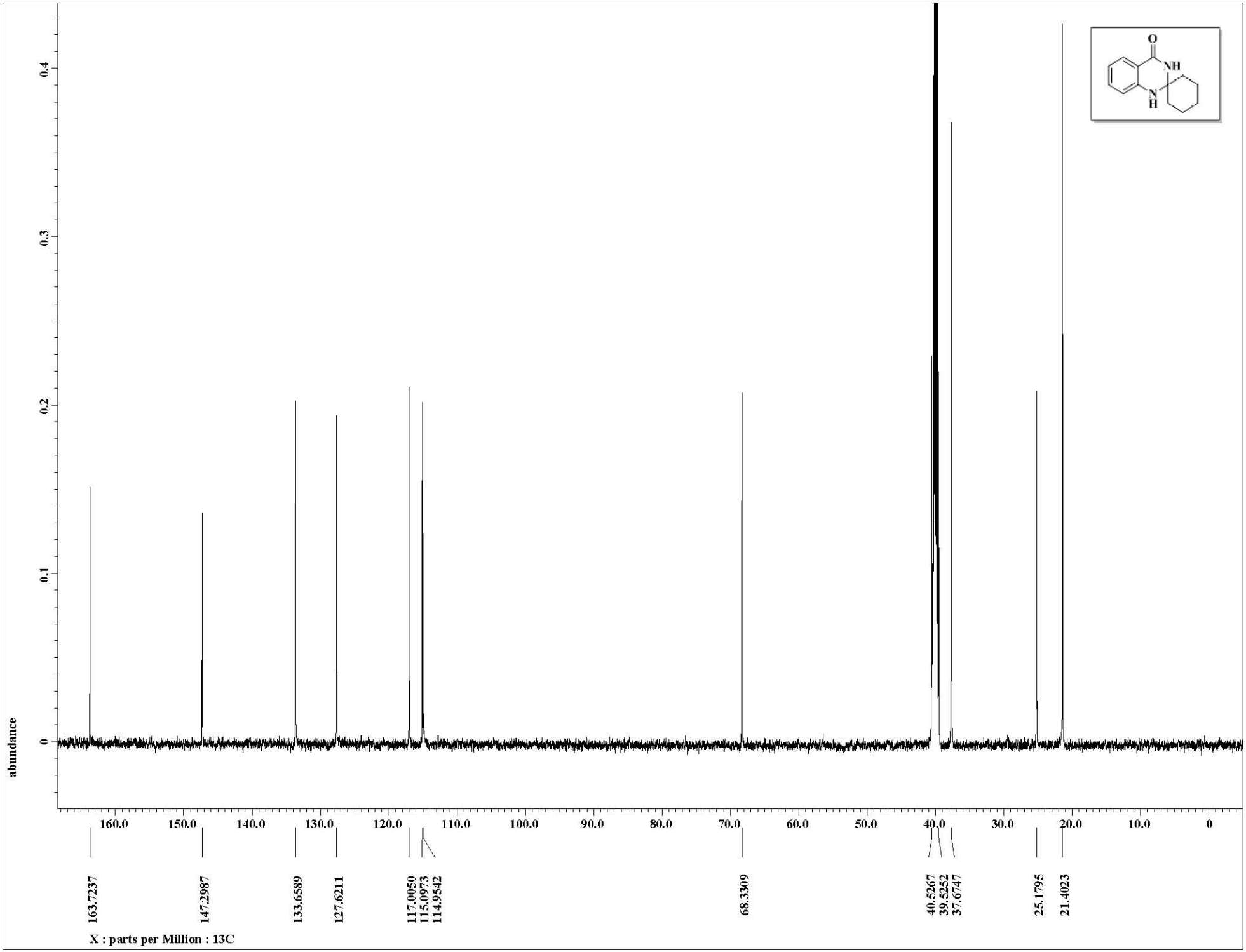

abundance
1.01
1.03
1.05
1
3.09
3.11
6.28
7.5195
7.5046
7.1313
7.1175
6.6239
6.6090
6.5942
5.7868
3.3453
2.9193
2.5035
2.1233
1.4729
X : parts per Million : 1H

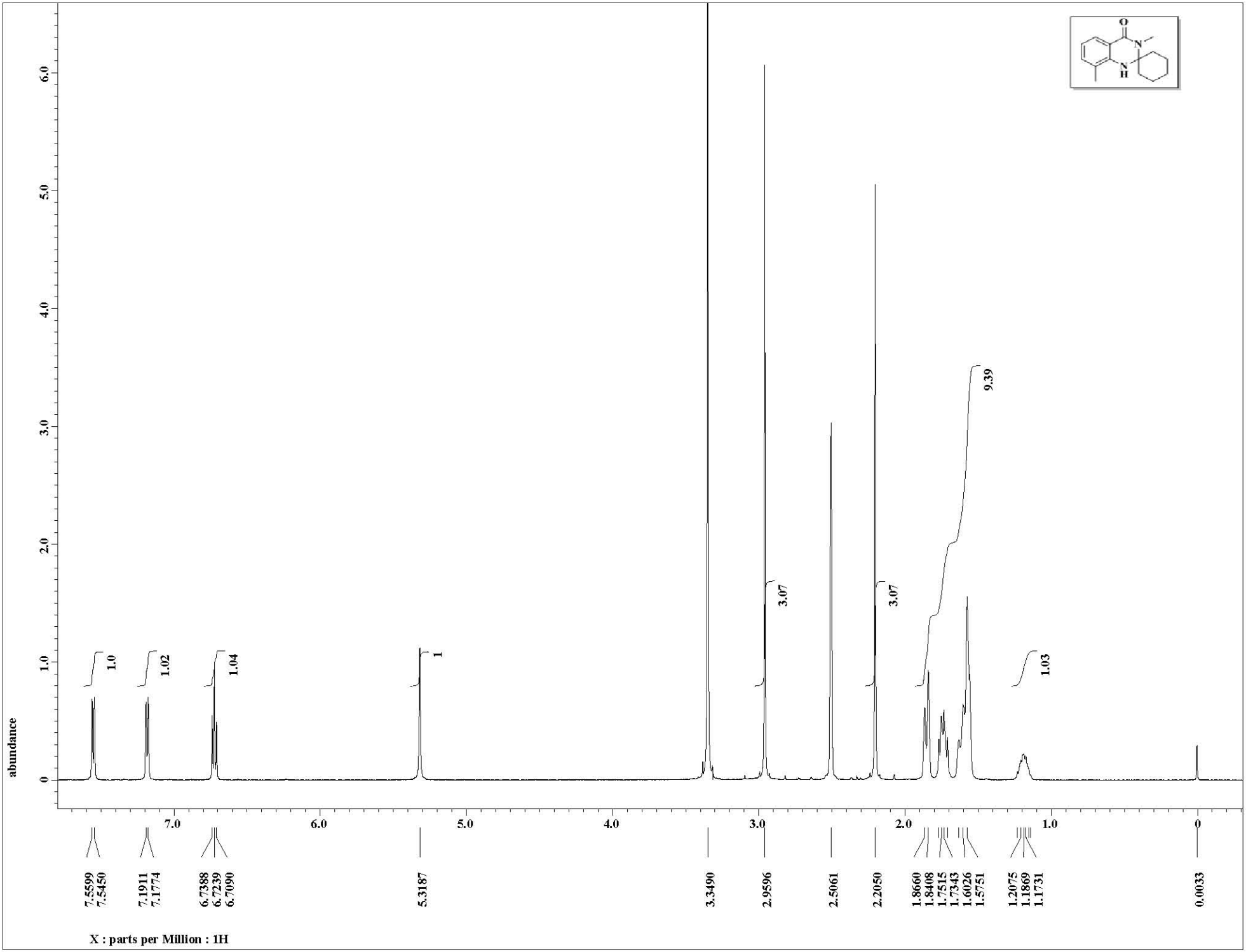

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.1895
144.5707
134.3075
125.9328
122.7470
117.2243
114.7730
71.3927
40.2119
40.0498
39.8781
27.1730
26.1620
17.3199
X : parts per Million : 13C

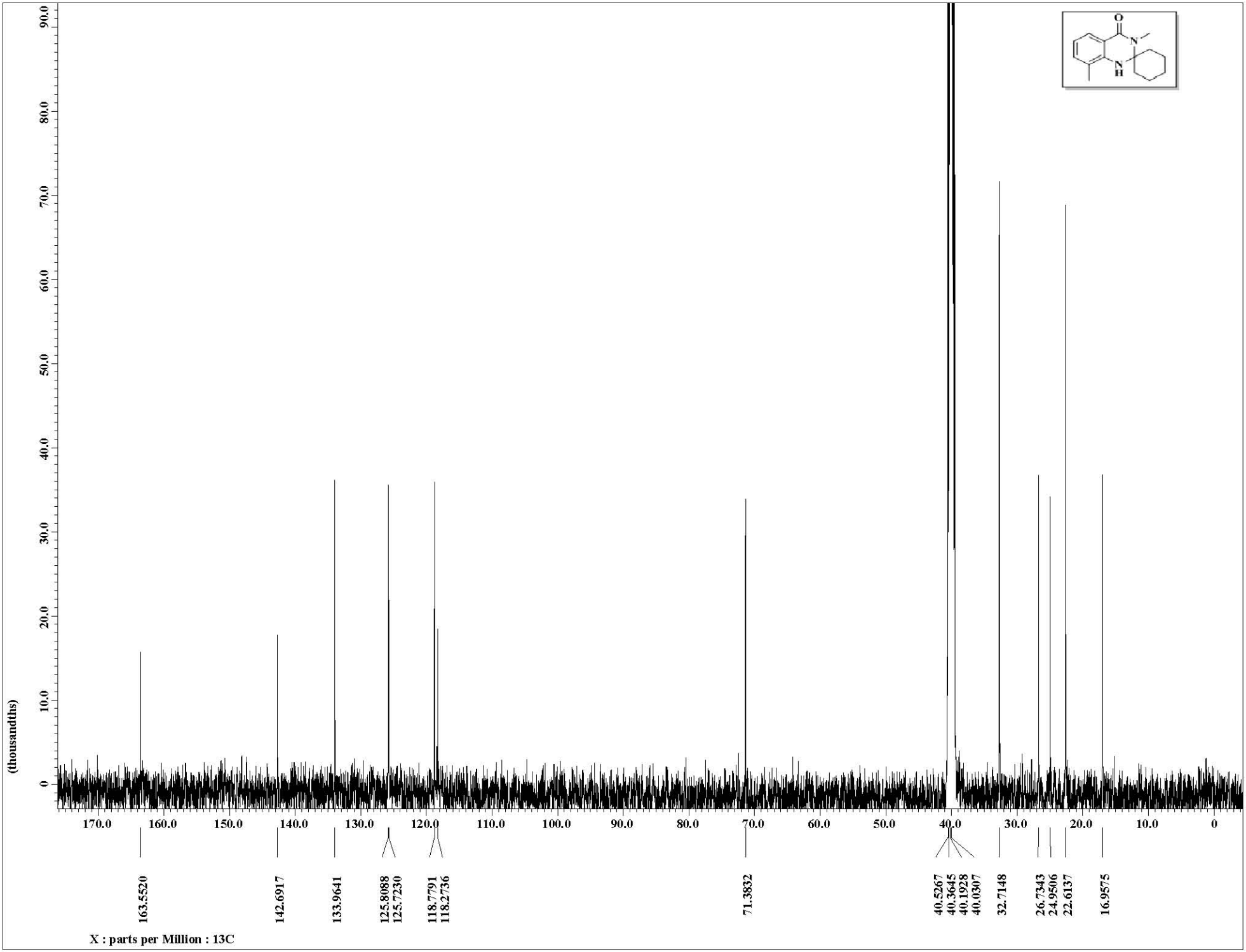

abundance
X : parts per Million : 1H
7.5703
7.5537
6.9627
6.6799
6.6764
6.6272
3.3497
2.8836
1.8884
1.8735
1.8586
1.6433
1.6285
1.6147
1.5998
1.4200
0.8635
0.8497
0.8348
−0.0000
0.93
0.98
1.21
1.0
3.18
1.01
1
3.0
3.03
6.6799
6.6764
6.6272
6.6249
6.6100
6.6077
1.21
1.0
1.9170
1.9022
1.8884
1.8735
1.8586
1.8449
1.6582
1.6433
1.6285
1.6147
1.5998
1.5849
1.01
Cl
HN
O
N

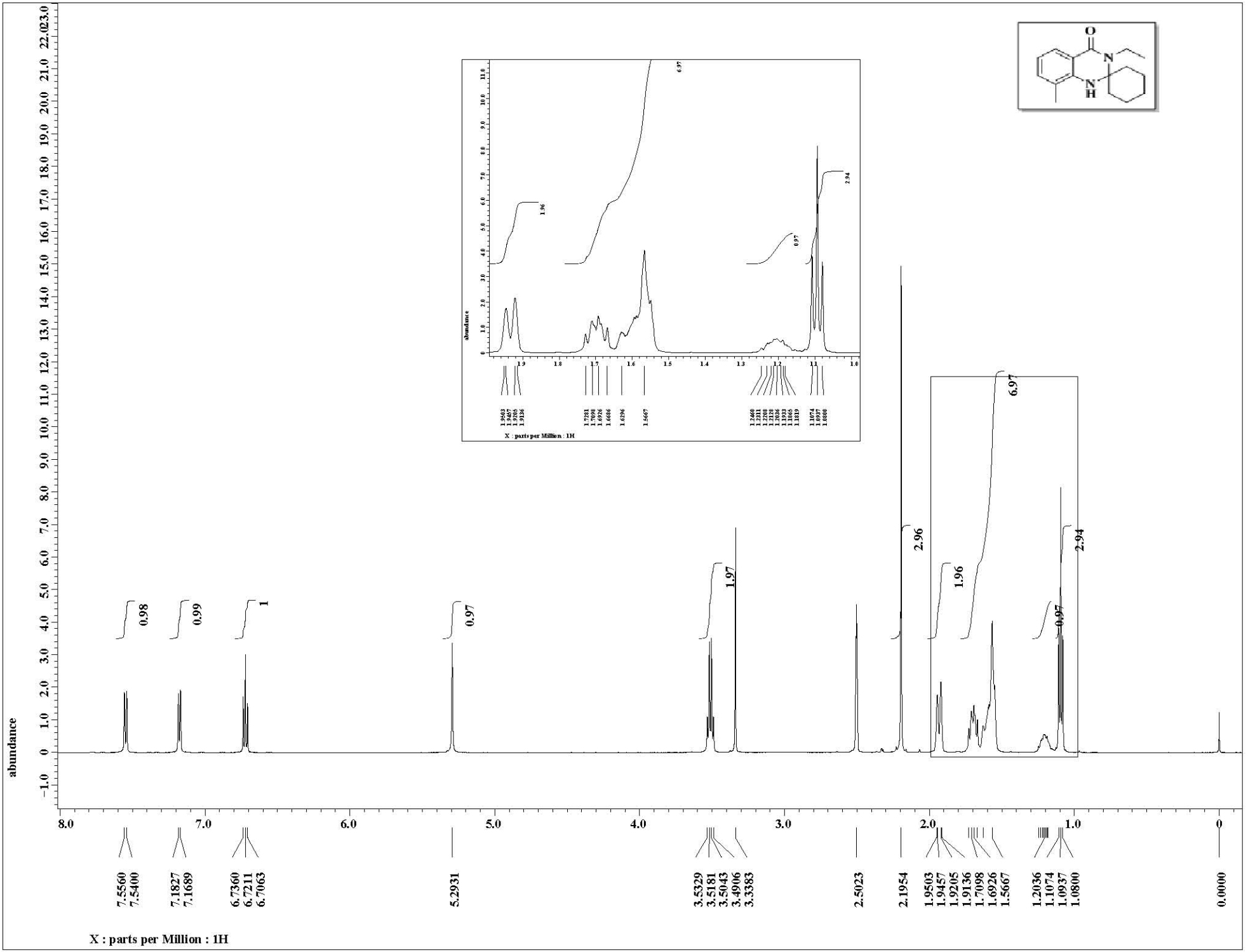

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
X : parts per Million : 13C
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.4265
151.4097
147.7756
138.0942
130.2728
115.5551
113.2373
74.4068
40.5267
40.1928
40.0307
31.4176
27.3924
25.4370
8.6114
O
HN
O
N

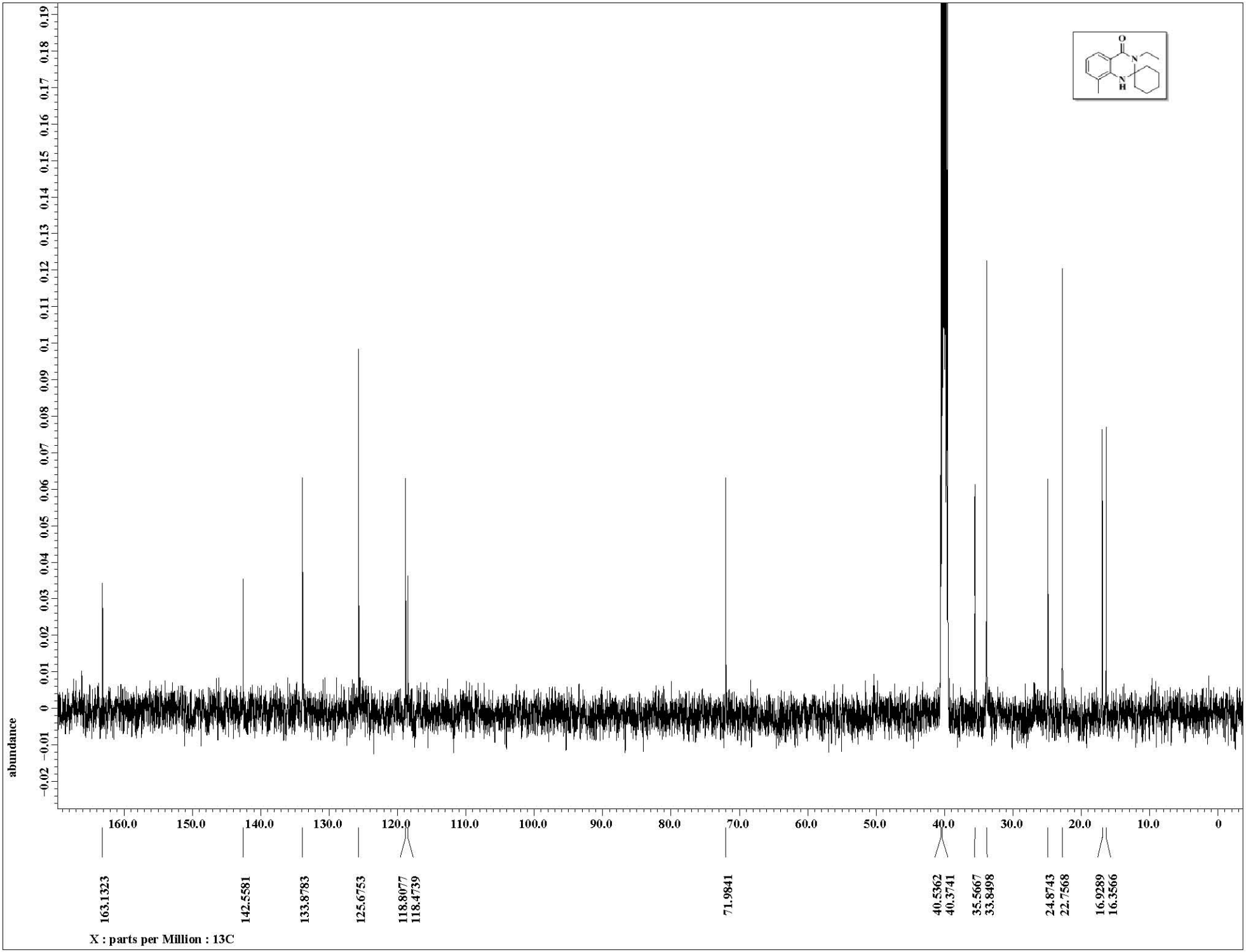

abundance
X : parts per Million : 1H
7.9373
7.5697
7.5548
7.2296
7.2158
7.2021
6.8173
6.8013
6.6341
6.6203
6.6043
3.3588
3.3348
2.5080
1.7464
1.7350
1.6170
1.6044
1.5781
1.5689
1.5586
1.5471
-0.0000
1
1.04
1.05
1.04
2.06
1.83
5.92
0.98
1.02
NH
N
H
O

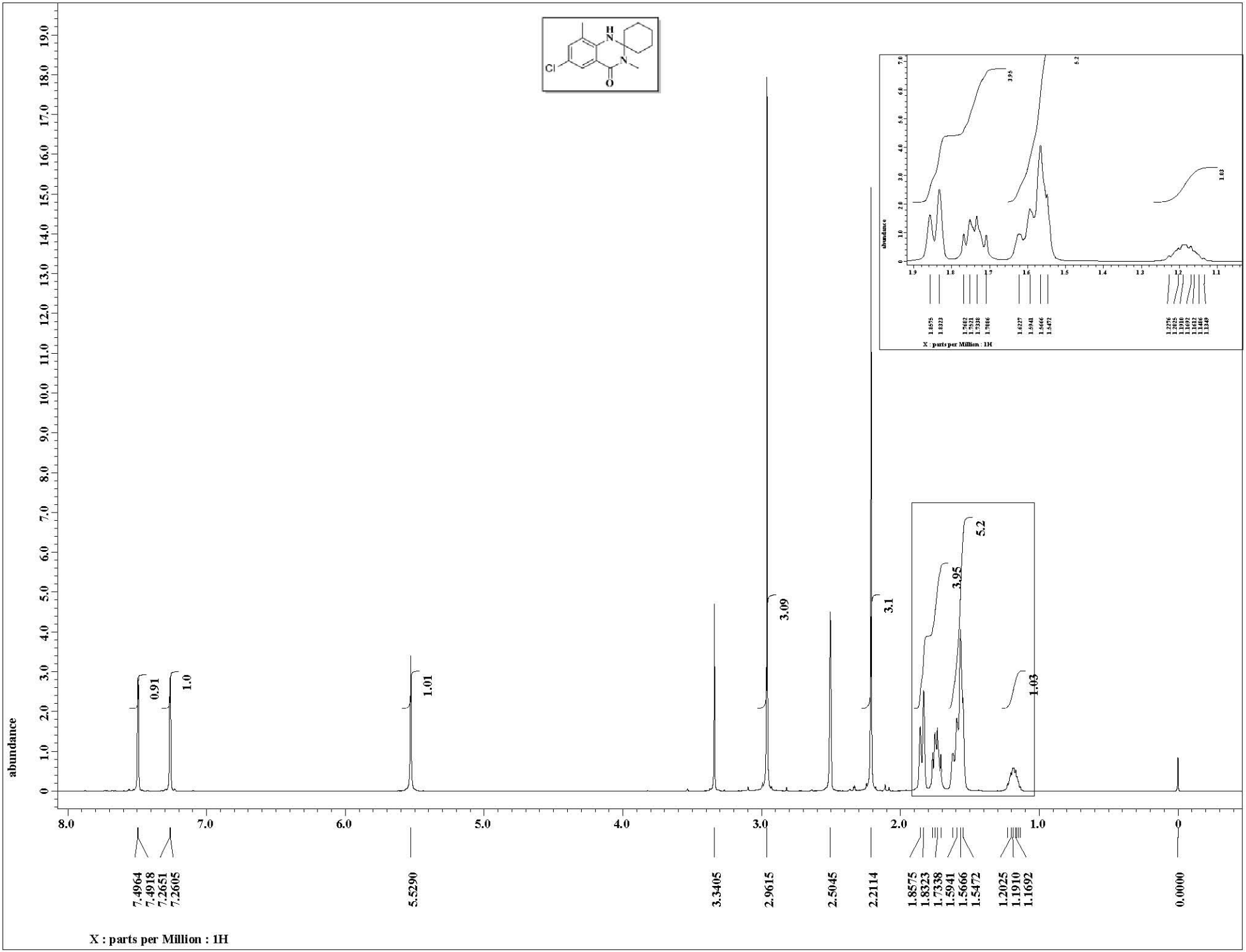

abundance
0
0.1
0.2
0.3
0.4
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.7237
147.2987
133.6589
127.6211
117.0050
115.0973
114.9542
68.3309
40.5267
39.5252
37.6747
25.1795
21.4023
X : parts per Million : 13C
O
NH
N
H

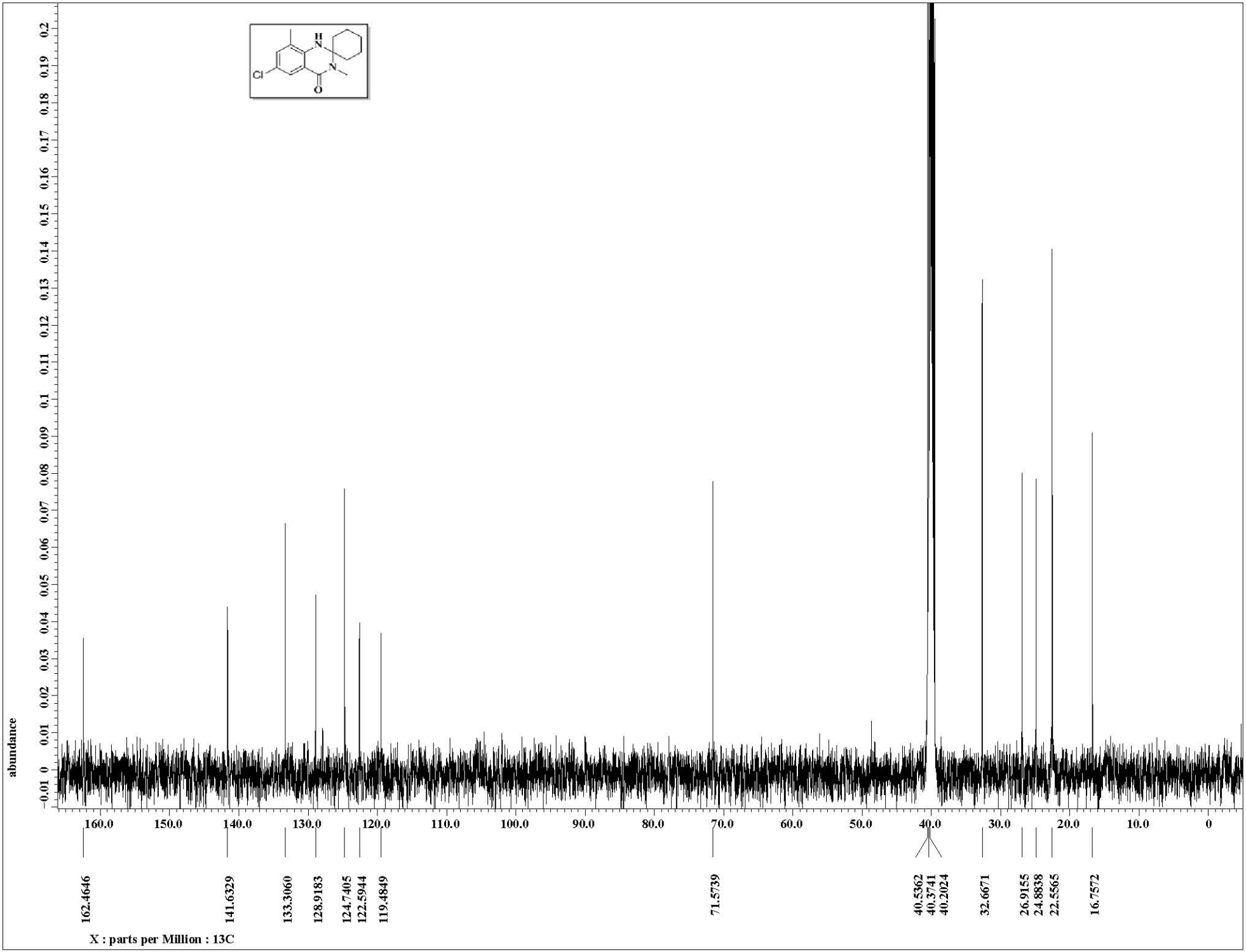

abundance
X : parts per Million : 1H
1.0
1.02
1.04
1
3.07
3.07
9.39
1.03
7.5599
7.5450
7.1911
7.1774
6.7388
6.7239
6.7090
5.3187
3.3490
2.9596
2.5061
2.2050
1.8660
1.8408
1.7515
1.7343
1.6026
1.5751
1.2075
1.1869
1.1731
0.0033

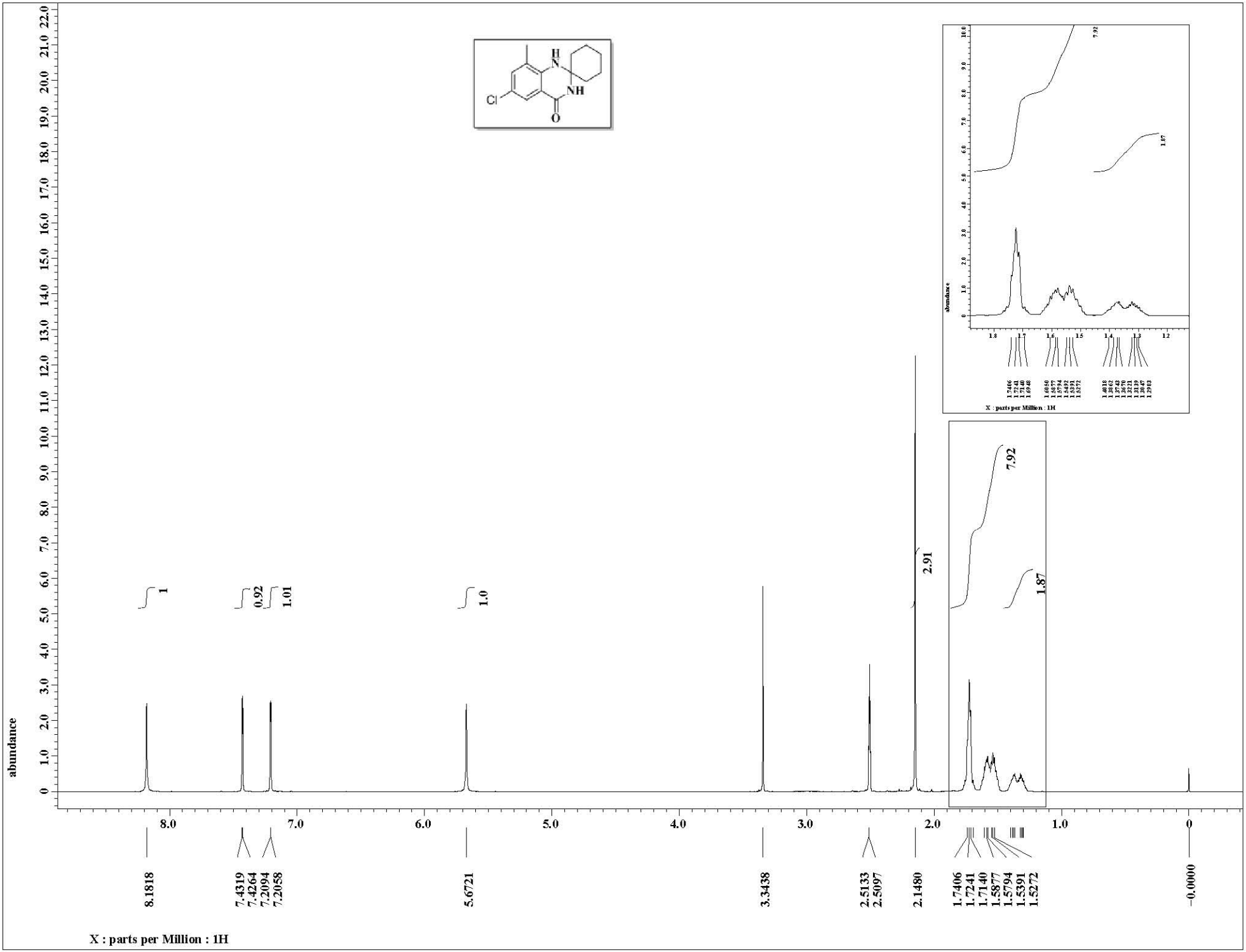

(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.5520
142.6917
133.9641
125.8088
125.7230
118.7791
118.2736
71.3832
40.5267
40.3645
40.1928
40.0307
32.7148
26.7343
24.9506
22.6137
16.9575
X : parts per Million : 13C

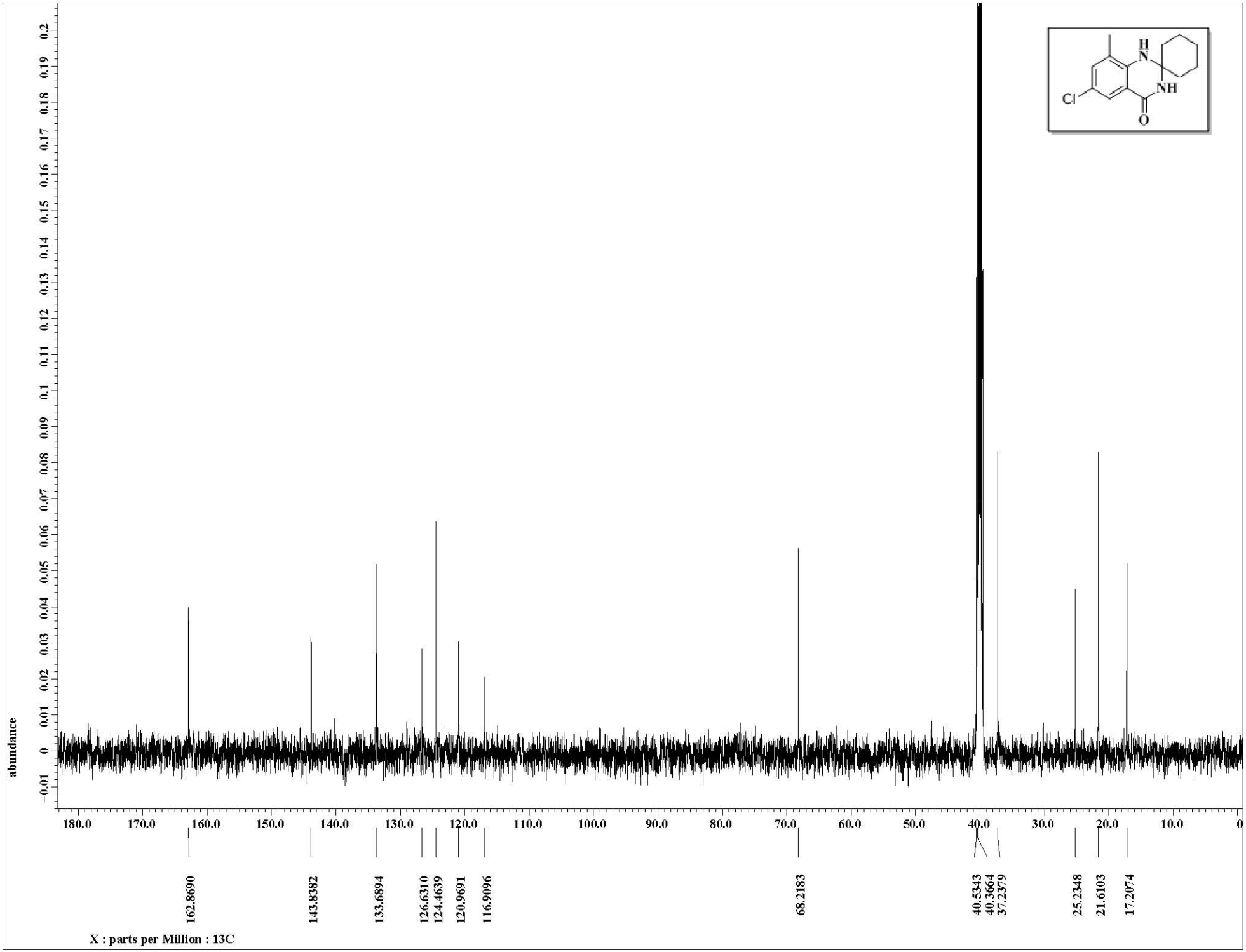

abundance
X : parts per Million : 1H
0.98
0.99
1
0.97
1.97
2.96
1.96
6.97
2.94
7.5560
7.5400
7.1827
7.1689
6.7360
6.7211
6.7063
5.2931
3.5329
3.5181
3.5043
3.4906
3.3383
2.5023
2.1954
1.9503
1.9457
1.9205
1.9136
1.7098
1.6926
1.5667
1.2036
1.1074
1.0937
1.0800
0.0000

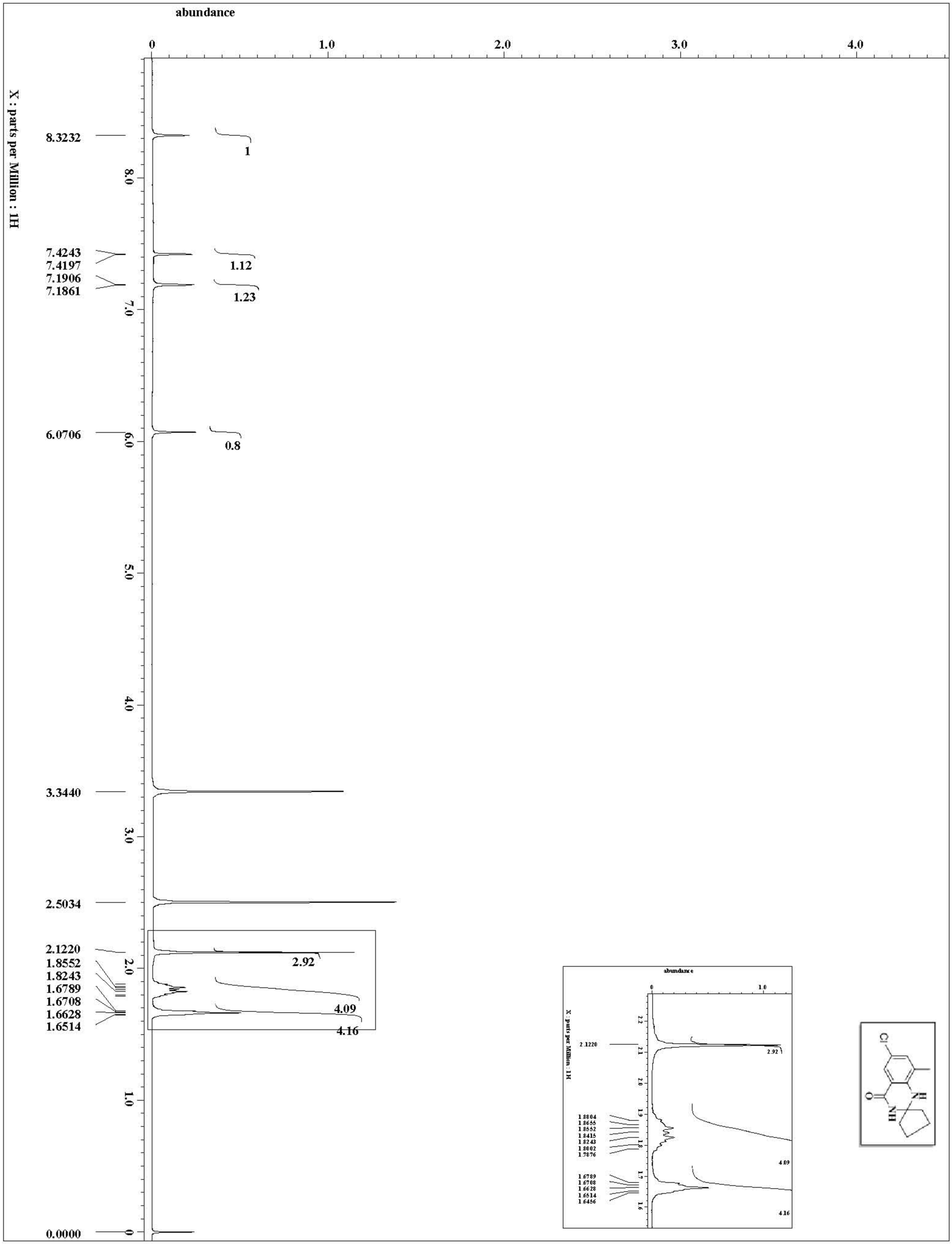

abundance
X : parts per Million : 13C
163.1323
142.5581
133.8783
125.6753
118.8077
118.4739
71.9841
40.5362
40.3741
35.5667
33.8498
24.8743
22.7568
16.9289
16.3566

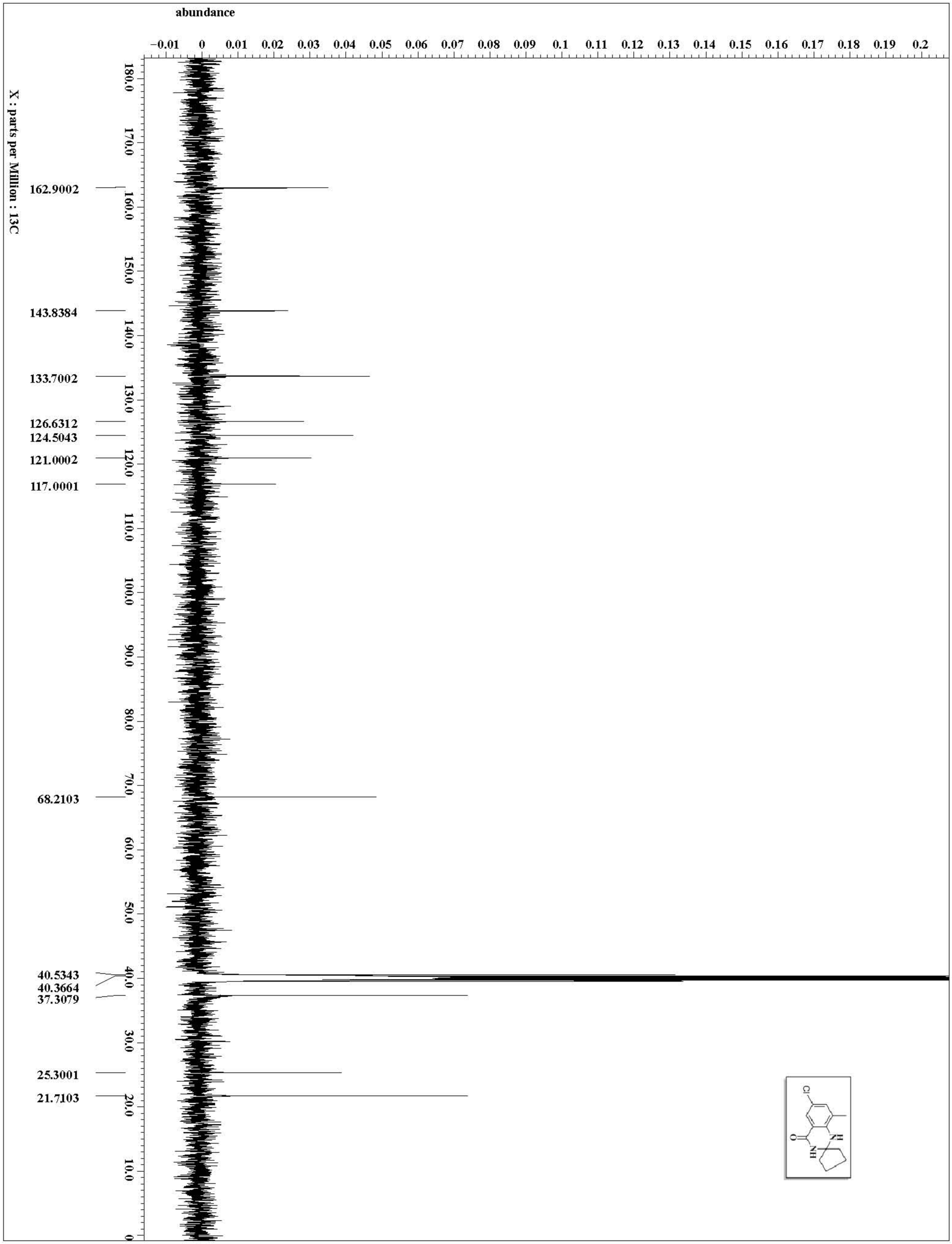

abundance
X : parts per Million : 1H
7.4964
7.4918
7.2651
7.2605
5.5290
3.3405
2.9615
2.5045
2.2114
1.8575
1.8323
1.7338
1.5941
1.5666
1.5472
1.2025
1.1910
1.1692
0.0000
0.91
1.0
1.01
3.09
3.1
3.95
5.2
1.03

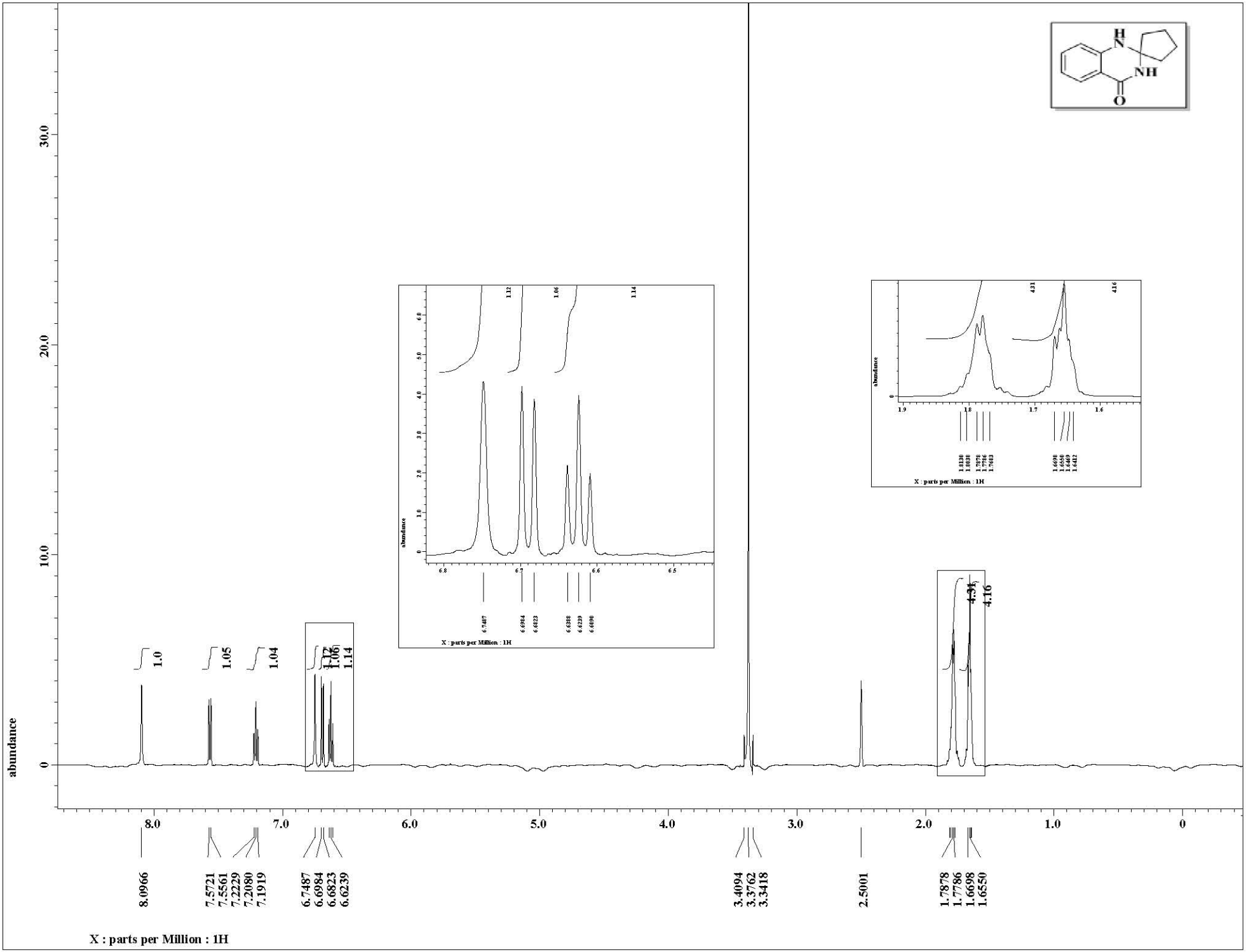

abundance
X : parts per Million : 13C
162.4646
141.6329
133.3060
128.9183
124.7405
122.5944
119.4849
71.5739
40.5362
40.3741
40.2024
32.6671
26.9155
24.8838
22.5565
16.7572

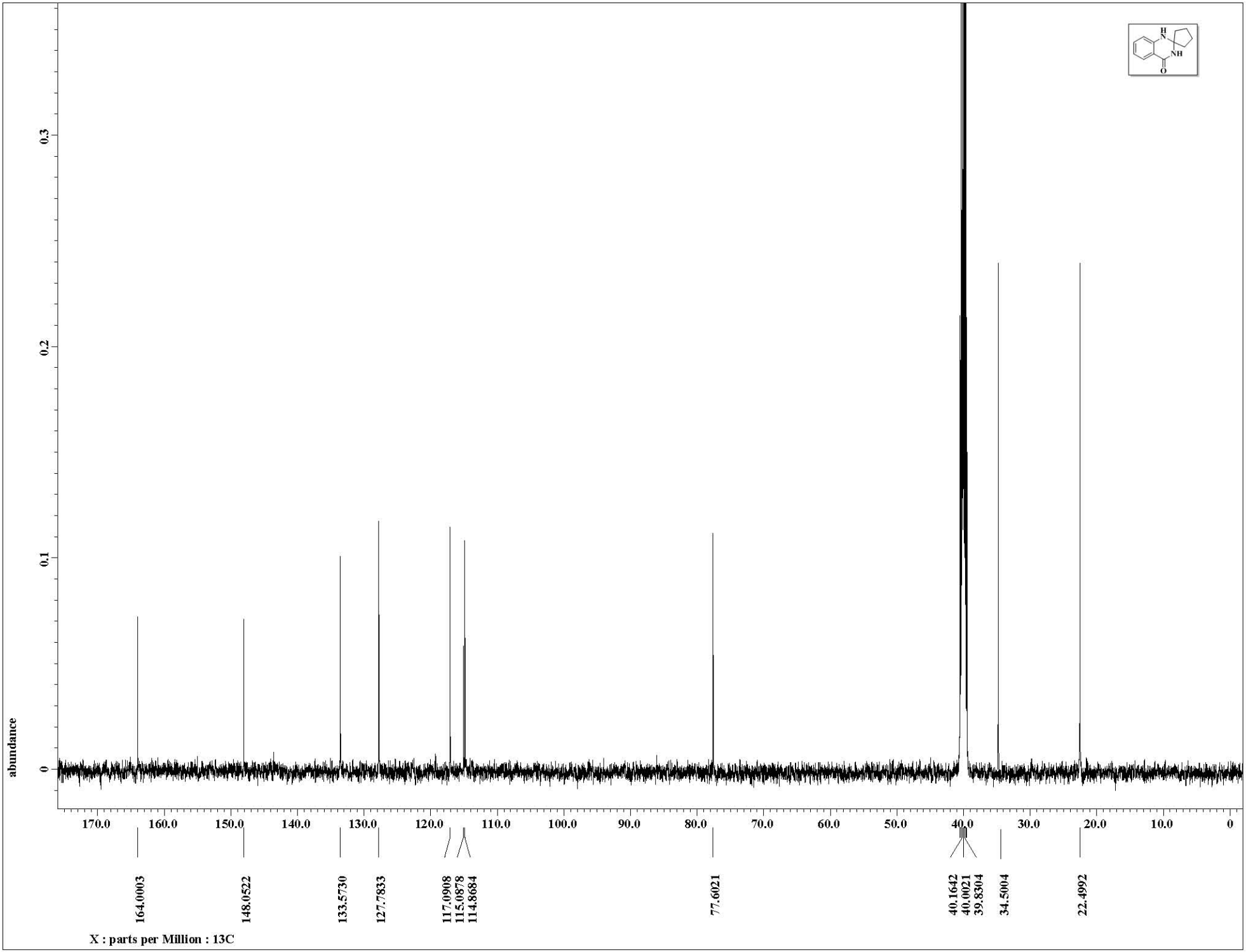

abundance
X : parts per Million : 1H
8.1818
7.4319
7.4264
7.2094
7.2058
5.6721
3.3438
2.5133
2.5097
2.1480
1.7406
1.7241
1.7140
1.5877
1.5794
1.5391
1.5272
-0.0000
1
0.92
1.01
1.0
2.91
1.87
7.92

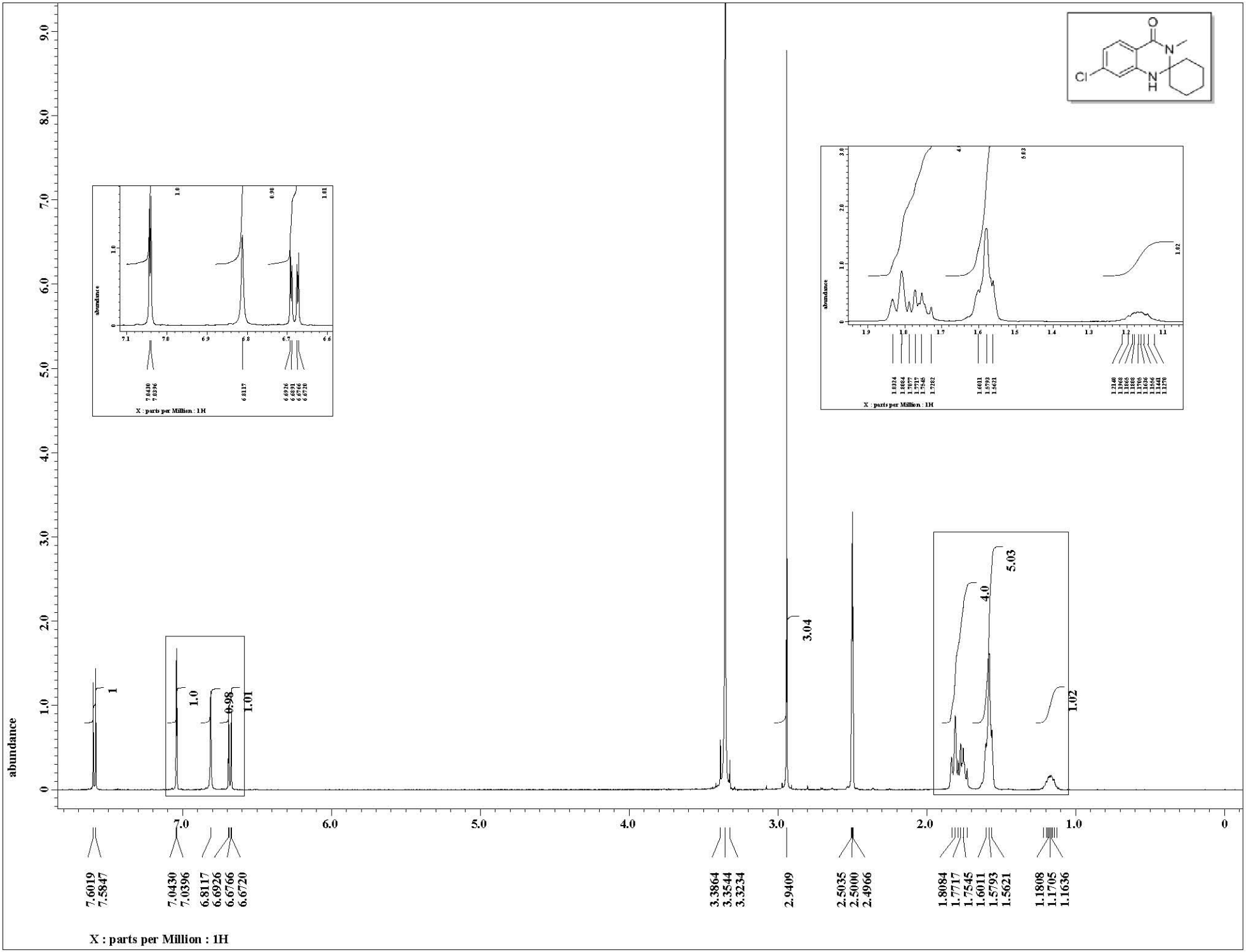

abundance
X : parts per Million : 13C
162.8690
143.8382
133.6894
126.6310
124.4639
120.9691
116.9096
68.2183
40.5343
40.3664
37.2379
25.2348
21.6103
17.2074
Cl
NH
O

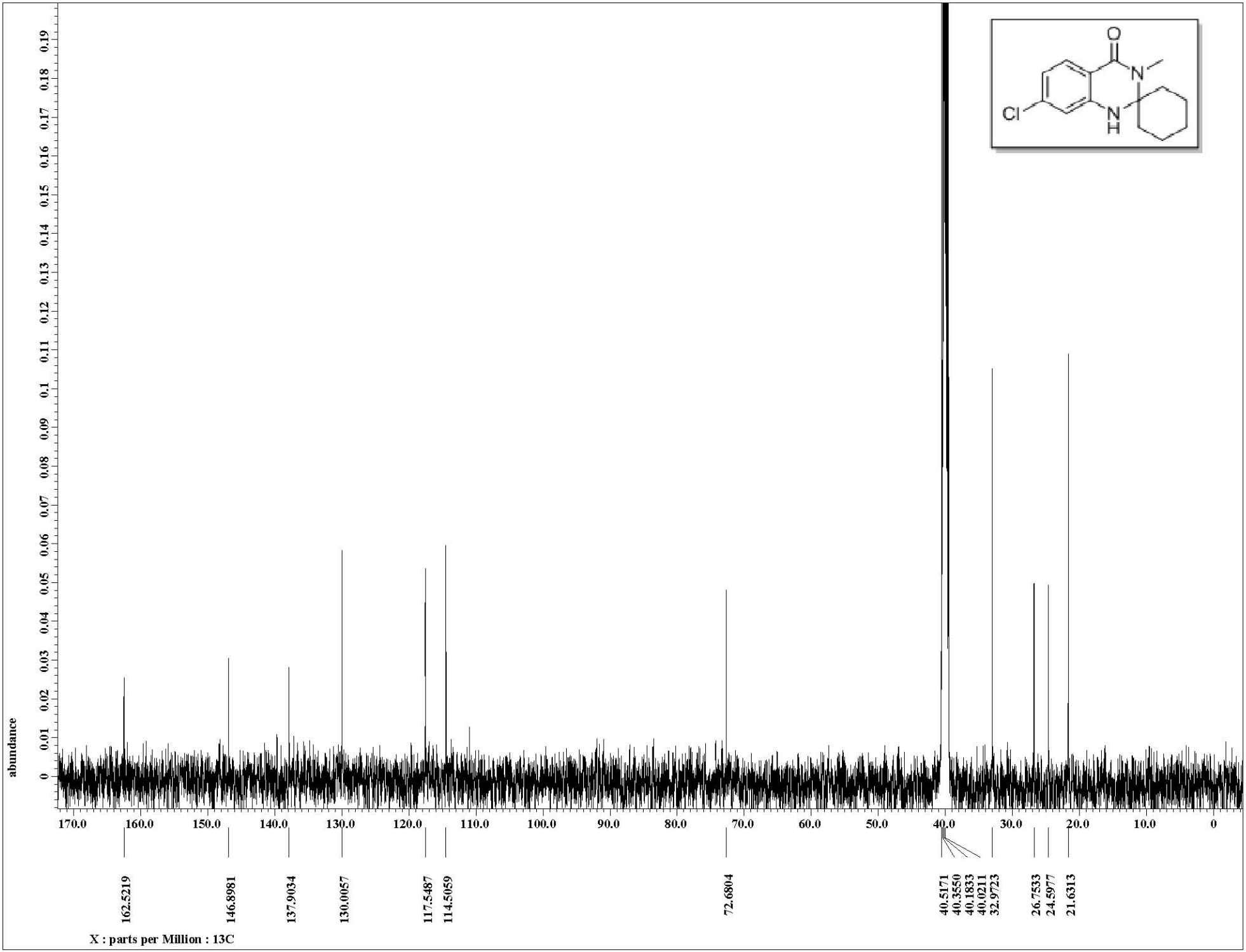

abundance
0
1.0
2.0
3.0
4.0
X : parts per Million : 1H
8.3232
1
7.4243
7.4197
7.1906
7.1861
1.12
1.23
6.0706
0.8
3.3440
2.5034
2.1220
1.8552
1.8243
1.6789
1.6708
1.6628
1.6514
2.92
4.09
4.16
0.0000
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
abundance
X : parts per Million : 1H
2.1220
2.92
1.8804
1.8655
1.8552
1.8415
1.8243
1.8002
1.7876
4.09
1.6789
1.6708
1.6628
1.6514
1.6456
4.16
Cl
H
N
O
NH

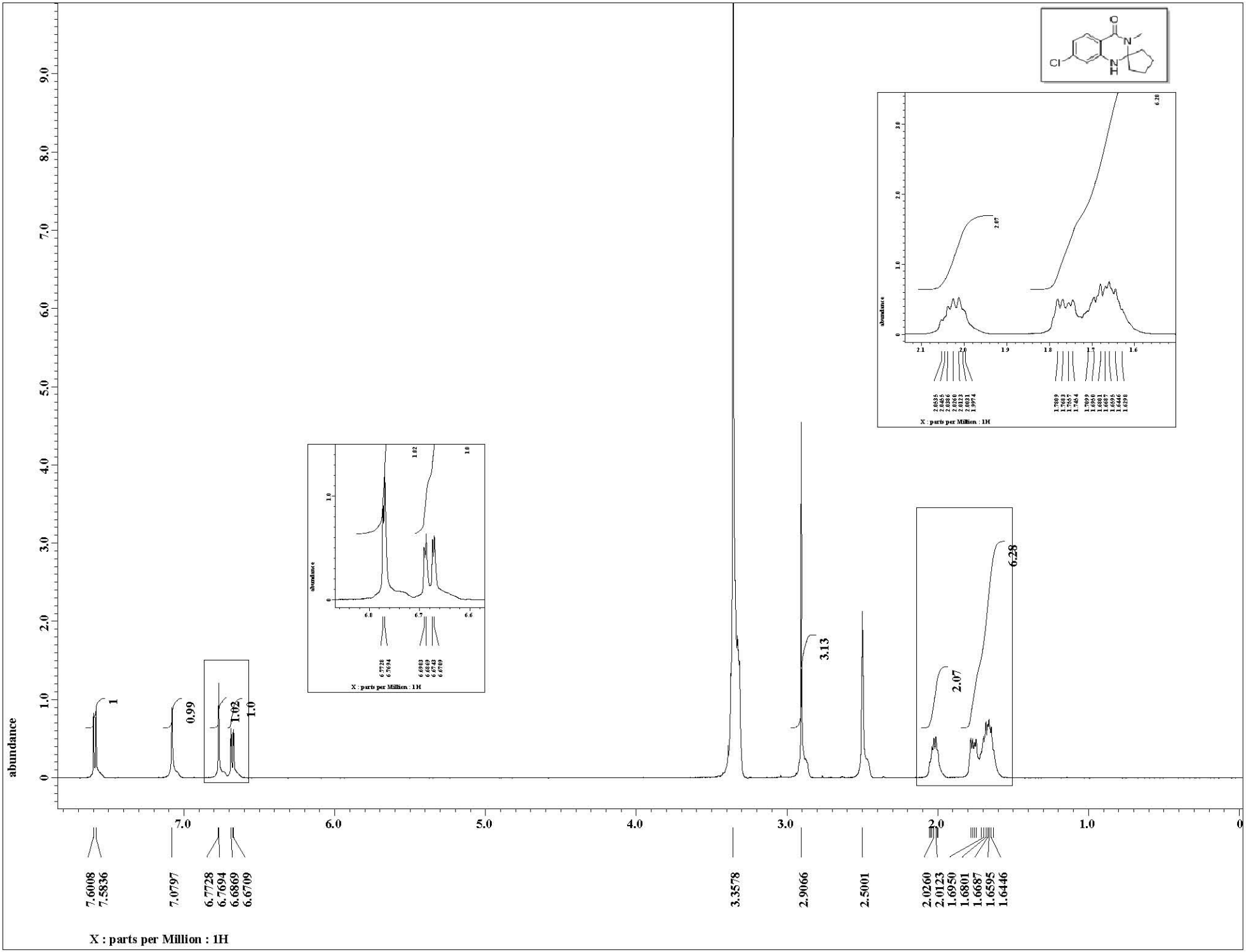

abundance
−0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19 0.2
X : parts per Million : 13C
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
162.9002
143.8384
133.7002
126.6312
124.5043
121.0002
117.0001
68.2103
40.5343
40.3664
37.3079
25.3001
21.7103
Cl
H
N
O
NH

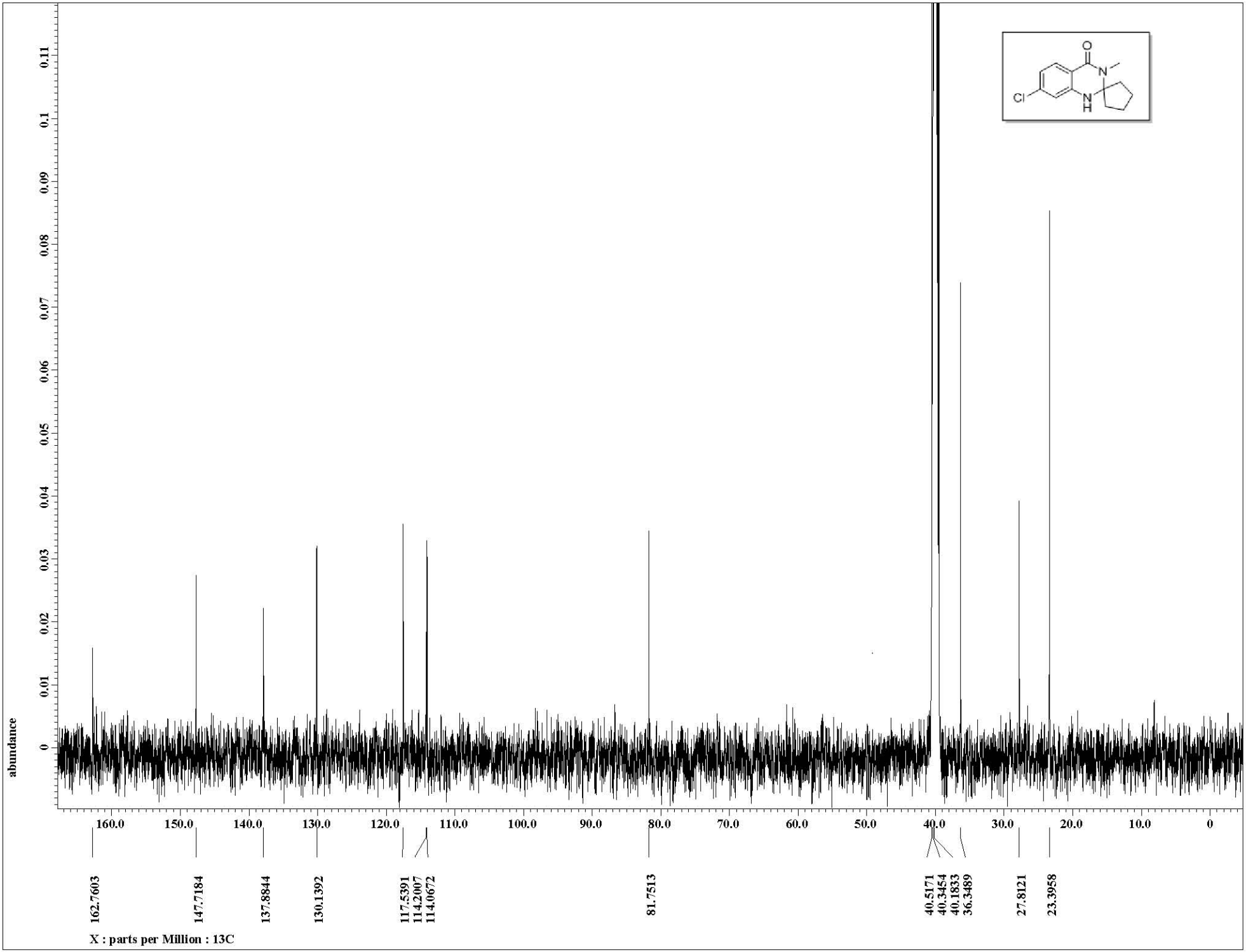

abundance
X : parts per Million : 1H
8.0966
7.5721
7.5561
7.2229
7.2080
7.1919
6.7487
6.6984
6.6823
6.6239
3.4094
3.3762
3.3418
2.5001
1.7878
1.7786
1.6698
1.6550
1.0
1.05
1.04
1.12
1.06
1.14
4.31
4.16

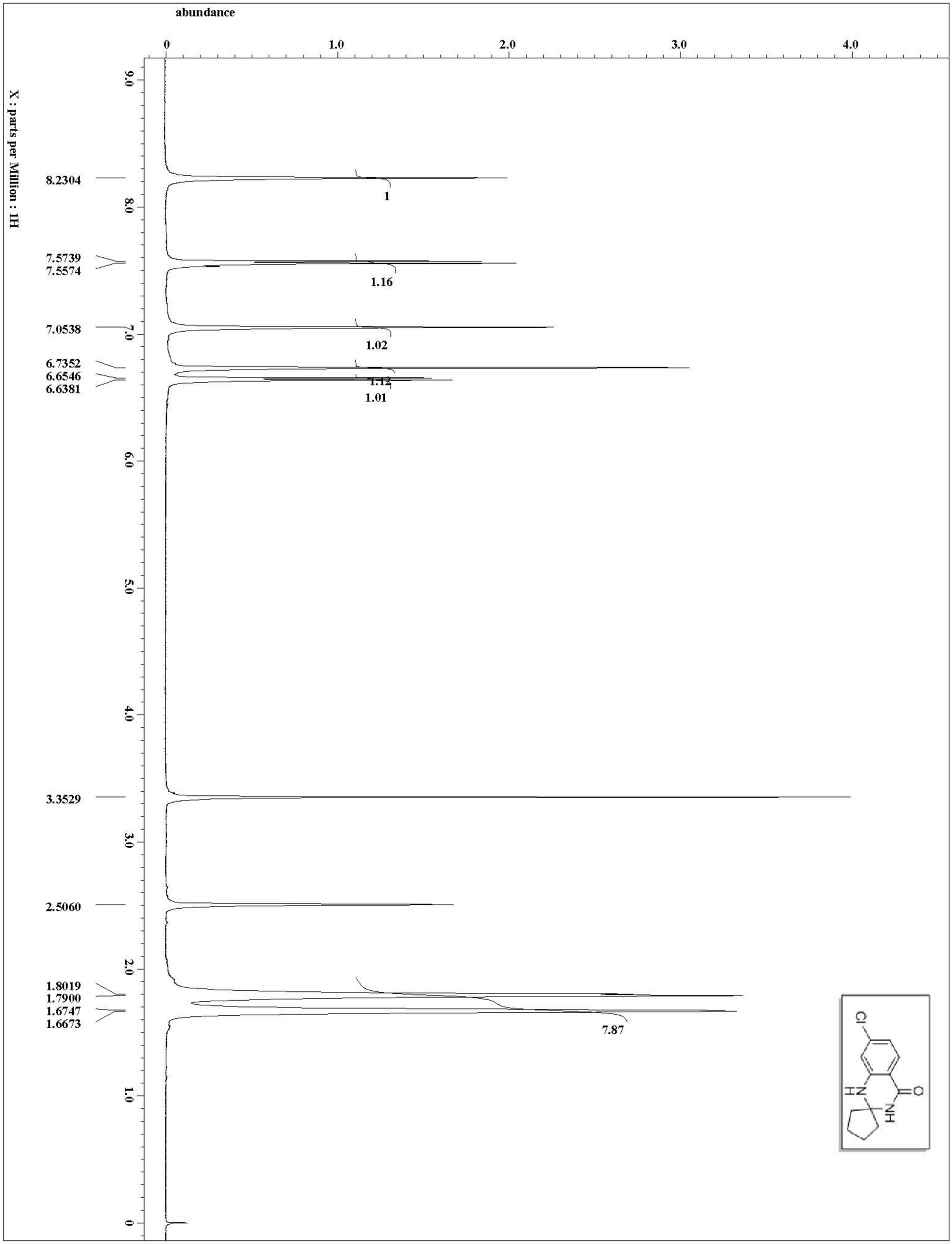

abundance
0
0.1
0.2
0.3
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.0003
148.0522
133.5730
127.7833
117.0908
115.0878
114.8684
77.6021
40.1642
40.0021
39.8304
34.5004
22.4992
X : parts per Million : 13C

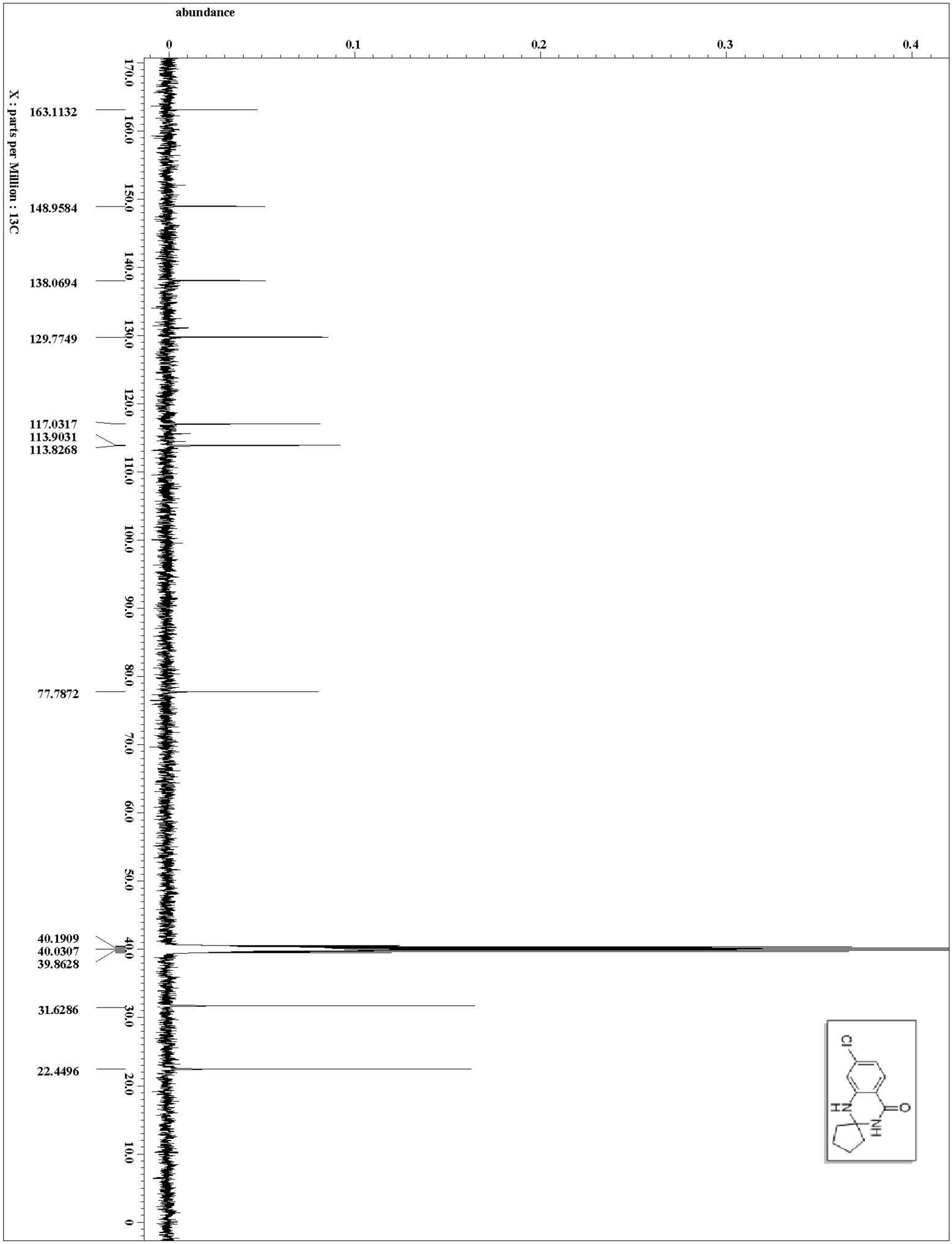

abundance
X : parts per Million : 1H
7.6019
7.5847
7.0430
7.0396
6.8117
6.6926
6.6766
6.6720
3.3864
3.3544
3.3234
2.9409
2.5035
2.5000
2.4966
1.8084
1.7717
1.7545
1.6011
1.5793
1.5621
1.1808
1.1705
1.1636
1
1.0
0.98
1.01
3.04
4.0
5.03
1.02
Cl
N
H
O

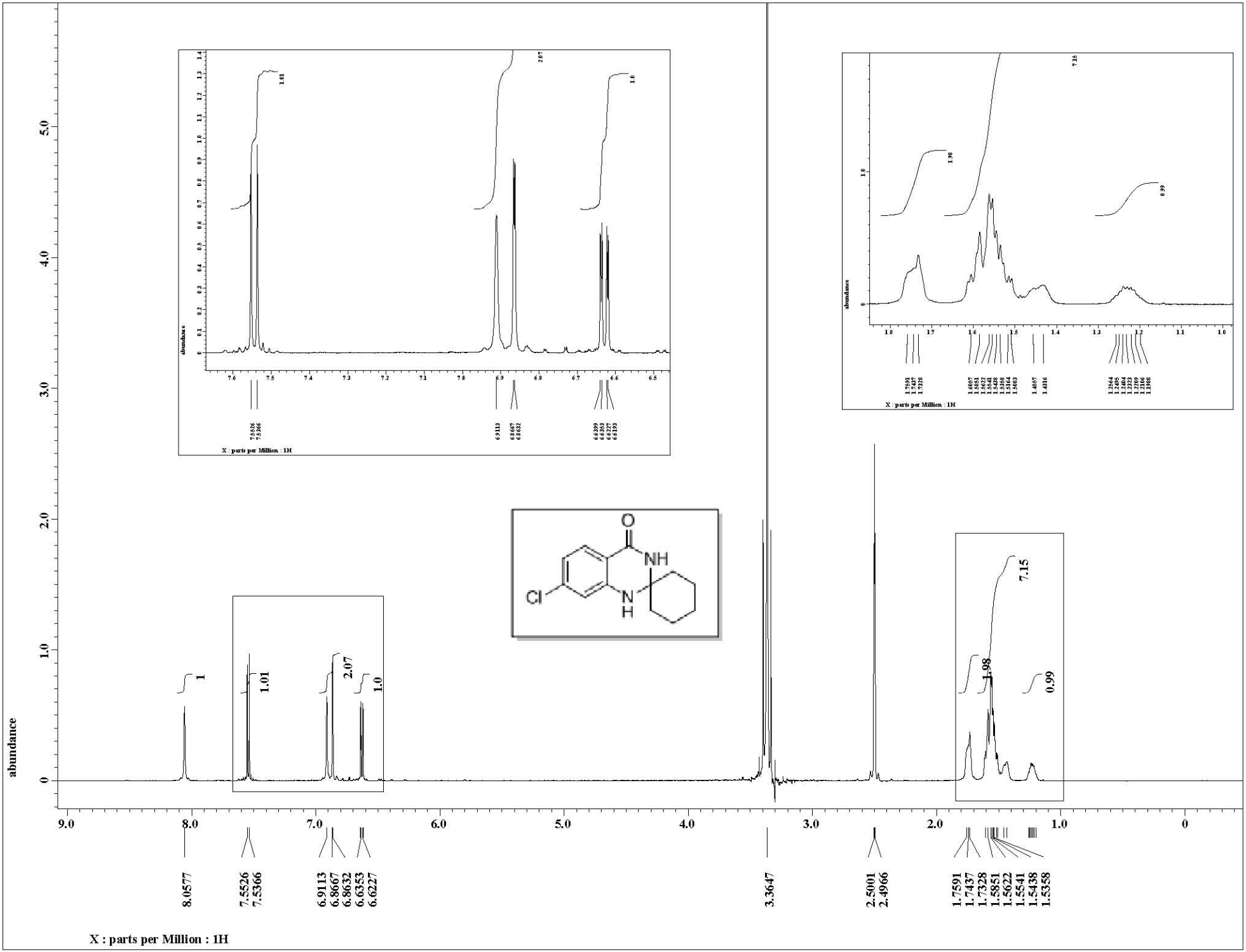

abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
0.16
0.17
0.18
0.19
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
O
N
Cl
N
H
162.5219
146.8981
137.9034
130.0057
117.5487
114.5059
72.6804
40.5171
40.3550
40.1833
40.0211
32.9723
26.7533
24.5977
21.6313
X : parts per Million : 13C

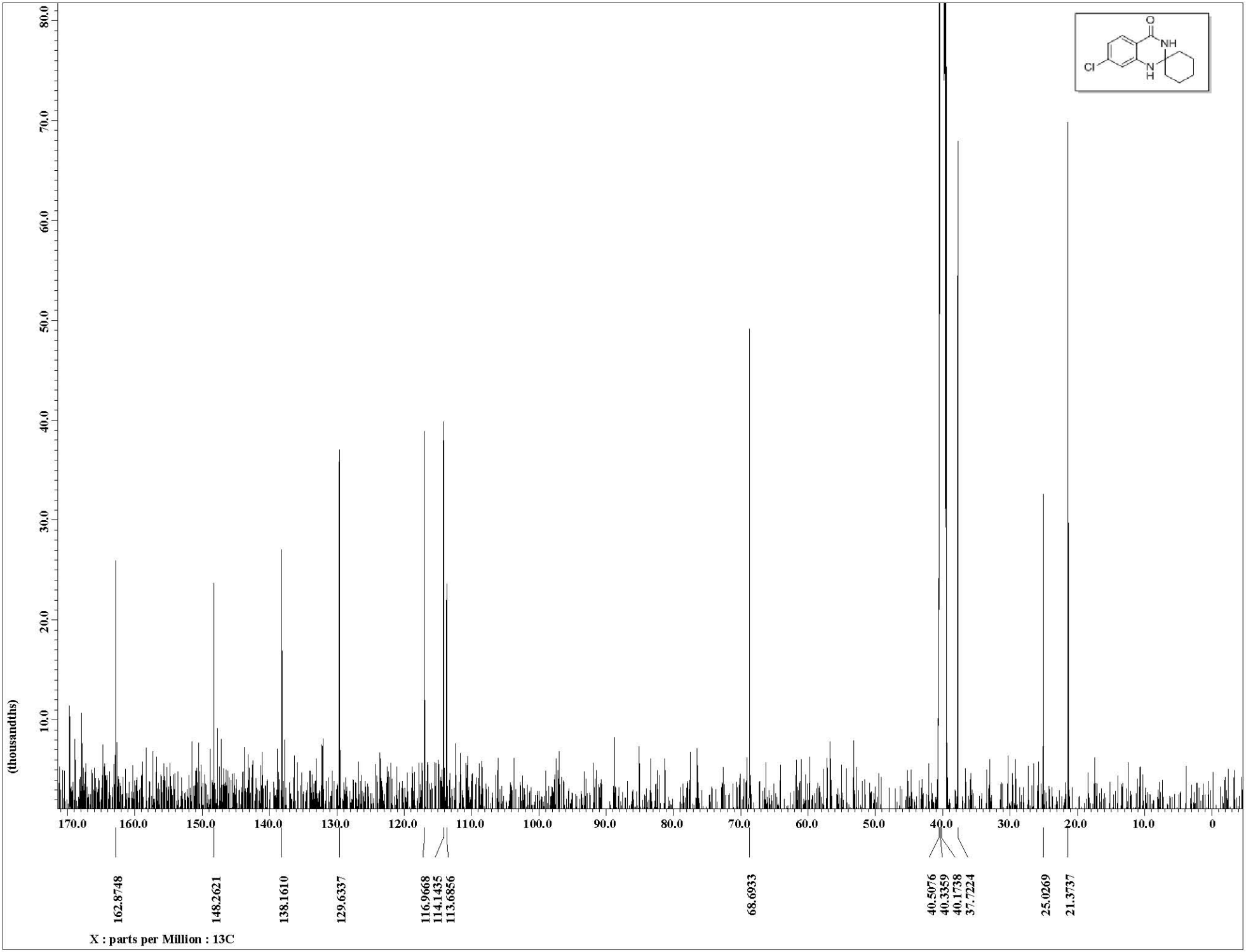

abundance
X : parts per Million : 1H
7.6008
7.5836
7.0797
6.7728
6.7694
6.6869
6.6709
3.3578
2.9066
2.5001
2.0260
2.0123
1.6950
1.6801
1.6687
1.6595
1.6446
1
0.99
1.02
1.0
3.13
2.07
6.28
Cl
O
N
H


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.7603
147.7184
137.8844
130.1392
117.5391
114.2007
114.0672
81.7513
40.5171
40.3454
40.1833
36.3489
27.8121
23.3958
X : parts per Million : 13C
O
N
Cl
N
H


abundance
0
1.0
2.0
3.0
4.0
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2304
7.5739
7.5574
7.0538
6.7352
6.6546
6.6381
3.3529
2.5060
1.8019
1.7900
1.6747
1.6673
1
1.16
1.02
1.12
1.01
7.87
Cl
H
N
O
NH


abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.1132
148.9584
138.0694
129.7749
117.0317
113.9031
113.8268
77.7872
40.1909
40.0307
39.8628
31.6286
22.4496
Cl
HN
NH
O


abundance
X : parts per Million : 1H
O
NH
N
H
Cl
1
1.01
2.07
1.0
1.98
7.15
0.99
8.0577
7.5526
7.5366
6.9113
6.8667
6.8632
6.6353
6.6227
3.3647
2.5001
2.4966
1.7591
1.7437
1.7328
1.5851
1.5622
1.5541
1.5438
1.5358


(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.8748
148.2621
138.1610
129.6337
116.9668
114.1435
113.6856
68.6933
40.5076
40.3359
40.1738
37.7224
25.0269
21.3737
X : parts per Million : 13C
O
NH
N
H
Cl