Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Copper-catalyzed tandem oxidative synthesis of quinazolinones from 2-aminobenzonitriles and primary alcohols

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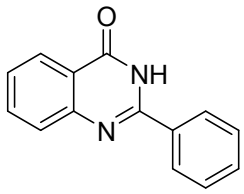
1. General Information

All reagents were purchased from commercial suppliers without further purification. Column chromatography was carried out over 200-300 mesh silica gel. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 500 MHz spectrometer with deuterated dimethyl sulfoxide (DMSO-d_6) or $CDCl_3$ as the solvent and tetramethylsilane (TMS) as an internal standard at room temperature. Chemical shifts are given in δ relative to TMS, and the coupling constants *J* are given in hertz. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight). Melting points were determined using an electrothermal capillary melting point apparatus.

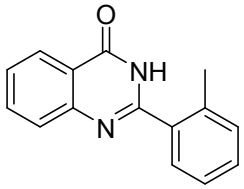
2. General Procedure

To a mixture of 2-aminobenzonitrile **1a** (1 mmol), benzyl alcohol **2a** (1.1 mmol), $Cu(OAc)_2$ (10 mol%), Cs_2CO_3 (1.5 equiv) and DMSO/H_2O (5:1, 2 mL) were added in a 10 mL Schlenk tube. Then the mixture was stirred at 120 ^{o}C for 12 h under air balloon. The progress of the reaction was monitored by TLC. After completion of the reaction, the solution was diluted with ethyl acetate, washed with water, and then the organic layer was separated and dried over anhydrous $MgSO_4$. The solvent was concentrated under reduced pressure and the crude product was purified by column chromatography on silica gel using PE/EtOAc as eluent to afford the pure product **3aa**.

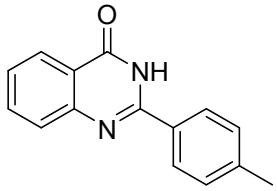
3. Spectra data



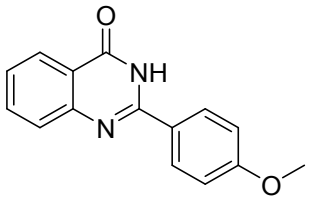
2-Phenylquinazolin-4(3*H*)-one (3aa)[1]: White solid; 87% yield (193 mg); mp 236-237 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.57 (br s, 1H), 8.21–8.17 (m, 3H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.62–7.52 (m, 4H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.4, 152.4, 148.9, 134.7, 132.9, 131.5, 128.7, 127.9, 127.6, 126.7, 126.0, 121.1.



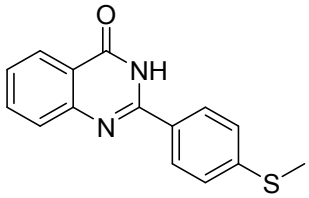
2-(*o*-Tolyl)quinazolin-4(3*H*)-one (3ab)[1]: White solid; 83% yield (196 mg); mp 216–218 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.46 (br s, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.86–7.83 (m, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.58–7.48 (m, 2H), 7.47–7.40 (m, 1H), 7.38 – 7.30 (m, 2H), 2.40 (s, 3H);^{13}C NMR (125 MHz, DMSO-d_6): δ=161.9, 154.5, 148.9, 136.3, 134.6, 134.4, 130.70, 130.1, 129.3, 127.5, 126.8, 126.0, 125.9, 121.2, 19.7.



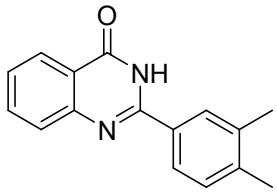
2-(*p*-Tolyl)quinazolin-4(3*H*)-one (3ac)[1]: White solid; 89% yield (212 mg); mp 241-243 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.48 (br s, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 2H), 7.87–7.80 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.4, 152.4, 149.0, 141.6, 134.7, 130.1, 129.4, 127.9, 127.6, 126.6, 126.0, 121.1, 21.2



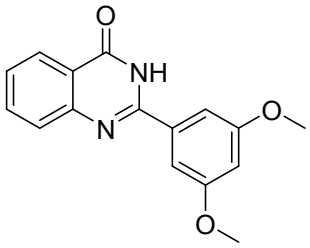
2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (3ad)[1]: White solid; 92% yield (232 mg); mp 248–251 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.42 (br s, 1H), 8.21 (d, *J* = 8.9 Hz, 2H), 8.14 (d, *J* = 6.9 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.5, 162.0, 152.0, 149.1, 134.7, 129.6, 127.5, 126.3126.0, 125.0, 120.9, 114.2, 55.6.



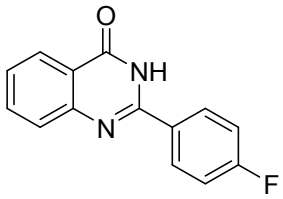
2-(4-Thiomethylphenyl)quinazolin-4(3*H*)-one (3ae)[2]: White solid; 80% yield (214 mg); mp 262–265 °C ^{1}H NMR (500 MHz, DMSO-d_6) δ=12.44 (s, 1H), 8.18 – 8.04 (m, 3H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 2H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ=162.41, 151.95, 148.98 , 143.21, 134.73, 128.83, 128.23, 127.56, 126.54, 126.02, 125.28, 121.07, 14.27.



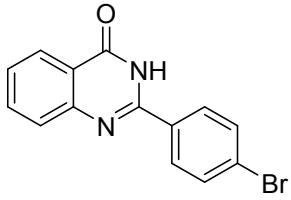
2-(3,4-Dimethylphenyl)quinazolin-4(3*H*)-one (3af)[3]: White solid; 85% yield (212 mg); mp 239–242 °C; ^{1}H NMR (500 MHz, DMSO -d_6) δ=12.36 (br s, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 7.98 (s, 1H), 7.89 (d, *J* = 9.3 Hz, 1H), 7.79 (t, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 7.9 Hz, 1H), 2.29 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ=162.64, 152.72, 149.30, 140.65, 137.01, 134.97, 130.57, 130.11, 129.04, 127.82, 126.75, 126.26, 125.59, 121.33, 19.82, 19.80.



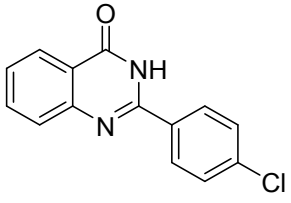
2-(3, 5-Dimethoxyphenyl)quinazolin-4(3*H*)-one (3ag)[4]:White solid; 95% yield (268 mg); mp 248–250 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.49 (br s, 1H), 8.17 (d, *J* = 7.9 Hz, 1H), 7.87–7.82 (m, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 2.2 Hz, 2H), 6.71 (s, 1H), 3.86 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.4, 160.7, 152.0, 148.8, 134.8, 127.8, 126.8, 126.0, 121.2, 105.7, 104.0, 55.7.



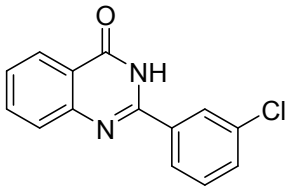
2-(4-Fluorophenyl)quinazolin-4(3*H*)-one (3ah)[1]: Yellow solid; 71% yield (170 mg); mp 284–286 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.58 (br s, 1H), 8.32–8.21 (m, 2H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.85 (t, *J* = 7.4 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=164.2 (d, *J* = 249.4 Hz), 162.4, 151.6, 148.8, 134.8, 130.5 (d, *J* = 7.7 Hz), 129.4, 127.6, 126.8, 126.0, 121.0, 115.8(d, *J* = 21.9 Hz) .



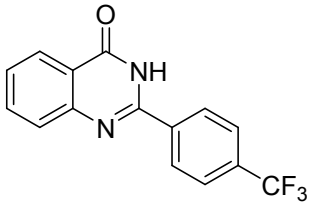
2-(4-Bromophenyl)quinazolin-4(3*H*)-one (3ai)[1]: White solid; 78% yield (234 mg); mp 293-295 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.63 (br s, 1H), 8.15 (m, 3H), 7.85 (t, *J* = 7.5 Hz, 1H), 7.76 (t, *J* = 9.2 Hz, 3H), 7.54 (t, *J* = 7.3 Hz, 1H); ^{13}C NMR (125 MHz, DMSO - d_6): δ=162.3, 151.6, 148.7, 134.9, 132.1, 131.8, 130.0, 127.7, 127.0, 126.1, 125.4, 121.2.



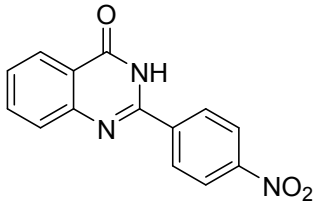
2-(4-Chlorophenyl)quinazolin-4(3*H*)-one (3aj)[1]: White solid; 80% yield (205 mg); mp 298-300 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.62 (br s, 1H), 8.28 – 8.10 (m, 3H), 7.85 (d, *J* = 6.9 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.3, 151.5, 148.8, 136.5, 134.8, 131.7, 129.8, 128.9, 127.7, 127.0, 126.0, 121.2.



2-(3-Chlorophenyl)quinazolin-4(3*H*)-one (3ak)[5]: White solid; 75% yield (192 mg); mp 295-296 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.63 (br s, 1H), 8.25 (s, 1H), 8.21 – 8.12 (m, 2H), 7.86 (t, *J* = 7.5 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.54 – 7.61ppm (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.3, 151.2, 148.7, 134.9, 133.6, 131.3, 130.7, 128.8, 127.8, 127.7, 127.1, 126.6, 126.1, 121.3.

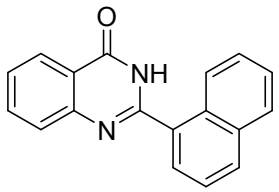


2-(4-(Trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (3al)[2]: White solid; 69% yield (200 mg); mp 284–286 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.75 (br s, 1H), 8.38 (d, *J* = 7.1 Hz, 2H), 8.19 (d, *J* = 7.0 Hz, 1H), 7.90 (m, 3H), 7.79 (d, *J* = 7.3 Hz, 1H), 7.57 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.5, 151.6, 148.9, 137.1, 135.1, 131.7(q, $J_{C\text{-}F}$=31.7), 129.2, 128.1, 127.6, 126.3, 125.9 (q, $J_{C\text{-}F}$ = 3.2 Hz), 124.4(q, $J_{C\text{-}F}$ = 271.5 Hz), 121.7.

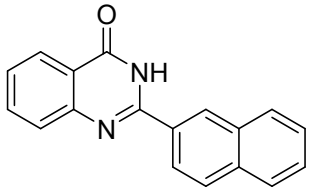


2-(4-Nitrophenyl)quinazolin-4(3*H*)-one (3am)[4]: Brown solid;48% yield (128 mg); mp >300 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.84 (br s, 1H), 8.41 (dd, *J* = 17.8, 8.5 Hz, 4H), 8.19 (d, *J* = 7.7 Hz, 1H), 7.89 (t, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 7.9 Hz,

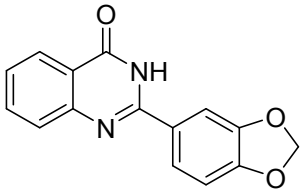
1H), 7.59 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.3, 150.9, 149.2, 148.5, 138.7, 135.0, 129.5, 127.9, 127.5, 126.1, 123.8, 121.4.



2-(Naphthalen-1-yl)quinazolin-4(3*H*)-one (3an)[2]: White solid; 76% yield (206 mg); mp 278-281 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.67 (br s, 1H), 8.23 (d, *J* = 7.8 Hz, 1H), 8.18 (d, *J* = 7.7 Hz, 1H), 8.13 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.87 (t, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.0 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.57 - 7.62 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.1, 153.9, 148.9, 134.7, 133.3, 131.9, 130.6, 130.4, 128.5, 127.9, 127.7, 127.3, 127.0, 126.5, 126.0, 125.4, 125.2, 121.4.

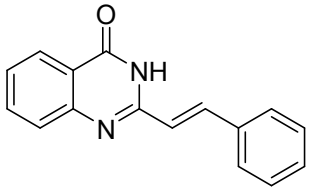


2-(Naphthalen-2-yl)quinazolin-4(3*H*)-one(3ao)[2]: White solid; 72% yield (196 mg); mp 214-216 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.68 (br s, 1H), 8.83 (s, 1H), 8.32 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 8.13 – 7.97 (m, 3H), 7.87 (t, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.65 (s, 2H), 7.55 (t, *J* = 7.1 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.5, 152.5, 148.9, 134.8, 134.3, 132.5, 130.2, 129.1, 128.33, 128.28, 128.1, 127.8, 127.7, 127.1, 126.8, 126.1, 124.7, 121.2.

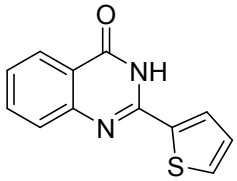


2-(3,4-Methylenedioxyphenyl) quinazolin-4(3H)-one (3ap)[4]: White solid; 90% yield (239 mg); mp 276-278 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.38 (br s, 1H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 7.7 Hz, 2H), 7.75 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 8.1 Hz, 1H), 6.15 (s, 2H); ^{13}C NMR (125

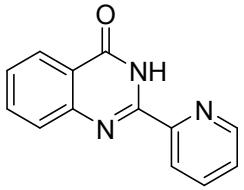
MHz, DMSO-d_6): δ=162.4, 151.8, 150.2, 148.9, 147.9, 134.7, 127.5, 126.7, 126.4, 126.0, 123.0, 120.9, 108.4, 107.7, 102.1.



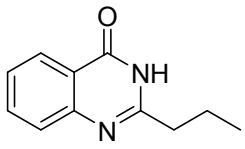
2-Styrylquinazolin-4(3*H*)-one (3aq)[6]: Light yellow solid; 68% yield (169 mg); mp 226-228 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.34 (br s, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 7.96 (d, *J* = 16.2 Hz, 1H), 7.82 (t, *J* = 7.4 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 3H), 7.50 -7.42 (m, 4H), 7.02 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=161.9, 151.6, 149.2, 138.4, 135.2, 134.7, 130.0, 129.3, 127.8, 127.3, 126.4, 126.0, 121.3.



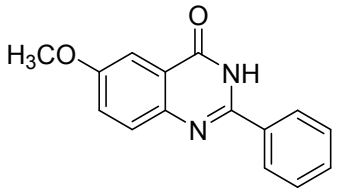
2-(Thiophen-2-yl)quinazolin-4(3*H*)-one (3ar)[2]: White solid; 76% (173 mg); mp 275-276 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.66 (br s, 1H), 8.25 (d, *J* = 4.6 Hz, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 5.0 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.9 Hz, 1H), 7.27–7.23 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.0, 148.8, 148.0, 137.5, 134.9, 132.3, 129.6, 128.7, 127.1, 126.5, 126.2, 121.1



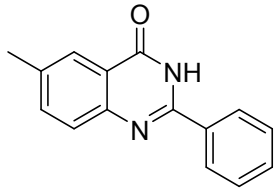
2-(Pyridin-2-yl)quinazolin-4(3*H*)-one (3as)[4]: White solid;43% yield (96 mg); mp 170-173 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=11.86 (br s, 1H), 8.77 (d, *J* = 4.5 Hz, 1H), 8.47 (d, *J* = 7.9 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.09 (td, *J* = 7.8, 1.5 Hz, 1H), 7.91–7.86 (m, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.59 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=160.9, 150.1, 149.2, 148.9, 148.6, 138.2, 134.9, 127.9, 127.4, 126.8, 126.3, 122.3, 122.2.



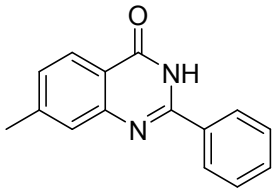
2-Propylquinazolin-4(3H)-one (3at): White solid; 70% yield (132 mg); mp 203-205 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.16 (br s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.74 (m, 1H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 2.58 (t, *J* = 7.5 Hz, 2H), 1.79 – 1.71 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.0, 157.5, 149.1, 134.4, 127.0, 126.1, 125.8, 121.0, 36.5, 20.4, 13.7 ppm.



6-Methoxy-2-phenylquinazolin-4(3*H*)-one (3ba)[1]: Light yellow solid; 86% yield (217 mg); mp 244–246 °C; ^{1}H NMR (500 MHz, DMSO-d_6); δ=12.52 (br s, 1H), 8.17 (d, *J* = 7.0 Hz, 2H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.59–7.52 (m, 4H), 7.45 (dd, *J* = 8.9, 2.8 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.2, 157.9, 150.3, 143.4, 133.0, 131.2, 129.4, 128.8, 127.7, 124.3, 122.0, 106.1, 55.8.

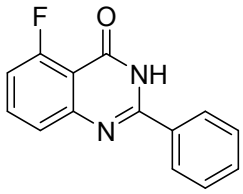


6-Methyl-2-phenylquinazolin-4(3*H*)-one (3ca)[7]: White solid; 80% yield (189 mg); mp 265−268 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ=12.42 (s, 1H), 8.12 (d, *J* = 7.0 Hz, 2H), 7.91 (s, 1H), 7.64 – 7.59 (m, 2H), 7.55 – 7.47 (m, 3H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ=162.31, 151.63, 146.93, 136.45, 136.02, 132.97, 131.38, 128.74, 127.80, 127.55, 125.41, 120.91, 21.01.

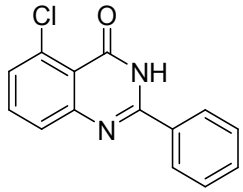


7-Methyl-2-phenylquinazolin-4(3*H*)-one (3da)[2]: White solid; 83% yield (196 mg); mp 229−231 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.46 (br s, 1H), 8.18 (d, *J* = 7.1 Hz, 2H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.52 (m, 4H), 7.35 (d, *J* = 8.0 Hz, 1H), 2.48

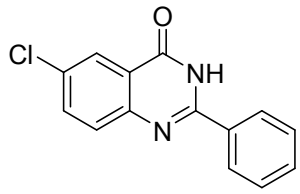
(s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=162.3, 152.5, 149.0, 145.2, 133.0, 131.5, 128.8, 128.2, 127.9, 127.3, 125.9, 118.8, 21.5.



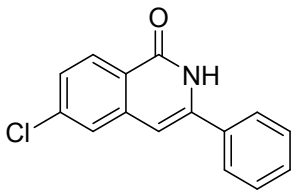
5-Fluoro-2-phenylquinazolin-4(3*H*)-one (3ea)[2]: White solid; 55% yield (132 mg); mp 306–309 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.50 (s, 1H), 8.13 (d, *J* = 7.2 Hz, 2H), 7.75 (m, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.54 – 7.39 (m, 3H), 7.28 – 7.14 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ=162.01, 159.97 (d, *J* = 11.9 Hz), 153.76, 151.29, 135.56 (d, *J* = 10.5 Hz), 132.67, 132.09, 129.04, 128.29, 123.95, 113.29 (d, *J* = 20.5 Hz), 110.84 (d, *J* = 6.0 Hz).



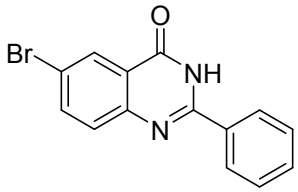
5-Chloro-2-phenylquinazolin-4(3*H*)-one (3fa)[8]: White solid; 70% yield (178 mg); mp 282–285 °C ^{1}H NMR (500 MHz, DMSO-d_6) δ=12.48 (s, 1H), 8.13 (d, *J* = 7.4 Hz, 2H), 7.69 (t, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 6.9 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ=160.53, 153.15, 151.46, 134.50, 132.68, 132.30, 131.84, 129.09, 128.77, 128.01, 128.01, 127.26, 118.12.



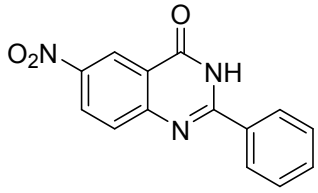
6-Chloro-2-phenylquinazolin-4(3*H*)-one (3ga)[7]: White solid; 72% yield (184 mg); mp 276–278 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.71 (br s, 1H), 8.18 (d, *J* = 6.4 Hz, 2H), 8.09 (s, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.64-7.52 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=161.5, 153.0, 147.7, 134.9, 132.6, 131.8, 130.9, 129.9, 128.8, 128.0, 125.1, 122.4.



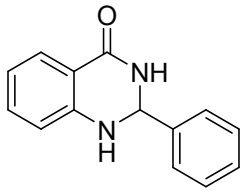
7-Chloro-2-phenylquinazolin-4(3*H*)-one (3ha)[7]: White solid; 78% yield (199 mg); mp 284-286 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.68 (br s, 1H), 8.20 – 8.14 (m, 3H), 7.80 (s, 1H), 7.64–7.52 (m, 4H); ^{13}C NMR (125 MHz, DMSO-d_6): δ= 161.9, 154.0, 150.0, 139.3, 132.6, 131.9, 128.8, 128.1, 127.0, 126.7, 120.0.



6-Bromo-2-phenylquinazolin-4(3*H*)-one (3ia)[8]: White solid;73% yield (219 mg); mp 284−286 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=12.74 (br s, 1H), 8.23 (s, 1H), 8.18 (d, *J* = 7.4 Hz, 2H), 7.98 (d, *J* = 10.0 Hz, 1H), 7.70 (d, *J* = 8.6 Hz, 1H), 7.64–7.50 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=161.4, 153.1, 147.9, 137.6, 132.6, 131.8, 130.0, 128.8, 128.2, 128.0, 122.8, 119.1.

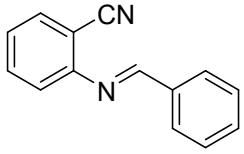


6-Nitro-2-phenylquinazolin-4(3*H*)-one (3ja)[7]: Yellow solid; 46% yield (123 mg); mp 296−298 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ=13.01 (br s, 1H), 8.85 (d, *J* = 2.5 Hz, 1H), 8.57 (dd, *J* = 9.0, 2.6 Hz, 1H), 8.23 (d, *J* = 7.6 Hz, 2H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ= 161.8, 155.9, 153.1, 144.9, 132.5, 132.3, 129.3, 128.9, 128.7, 128.4, 122.2, 121.2.



2-Phenyl-2,3-dihydroquinazolin-4(1*H*)-one (6a)[2]: White solid; mp 216-218 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.28 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 7.3

Hz, 2H), 7.37 (m, 3H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.10 (s, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.67 (t, *J* = 7.4 Hz, 1H), 5.75 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=163.8, 148.0, 141.8, 133.5, 128.6, 128.5, 127.5, 127.0, 117.3, 115.1, 114.6, 66.7.



2-(Benzylideneamino)benzonitrile (7a)[9]: ^{1}H NMR (500 MHz, DMSO) δ 8.73 (s, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.87 (d, *J* = 7.7 Hz, 1H), 7.79 – 7.73 (m, 1H), 7.63 – 7.55 (m, 3H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (125 MHz, DMSO) δ 164.23, 154.04, 135.48, 134.54, 133.38, 132.58, 129.38, 129.12, 126.51, 119.50, 117.43, 106.97.

6. References

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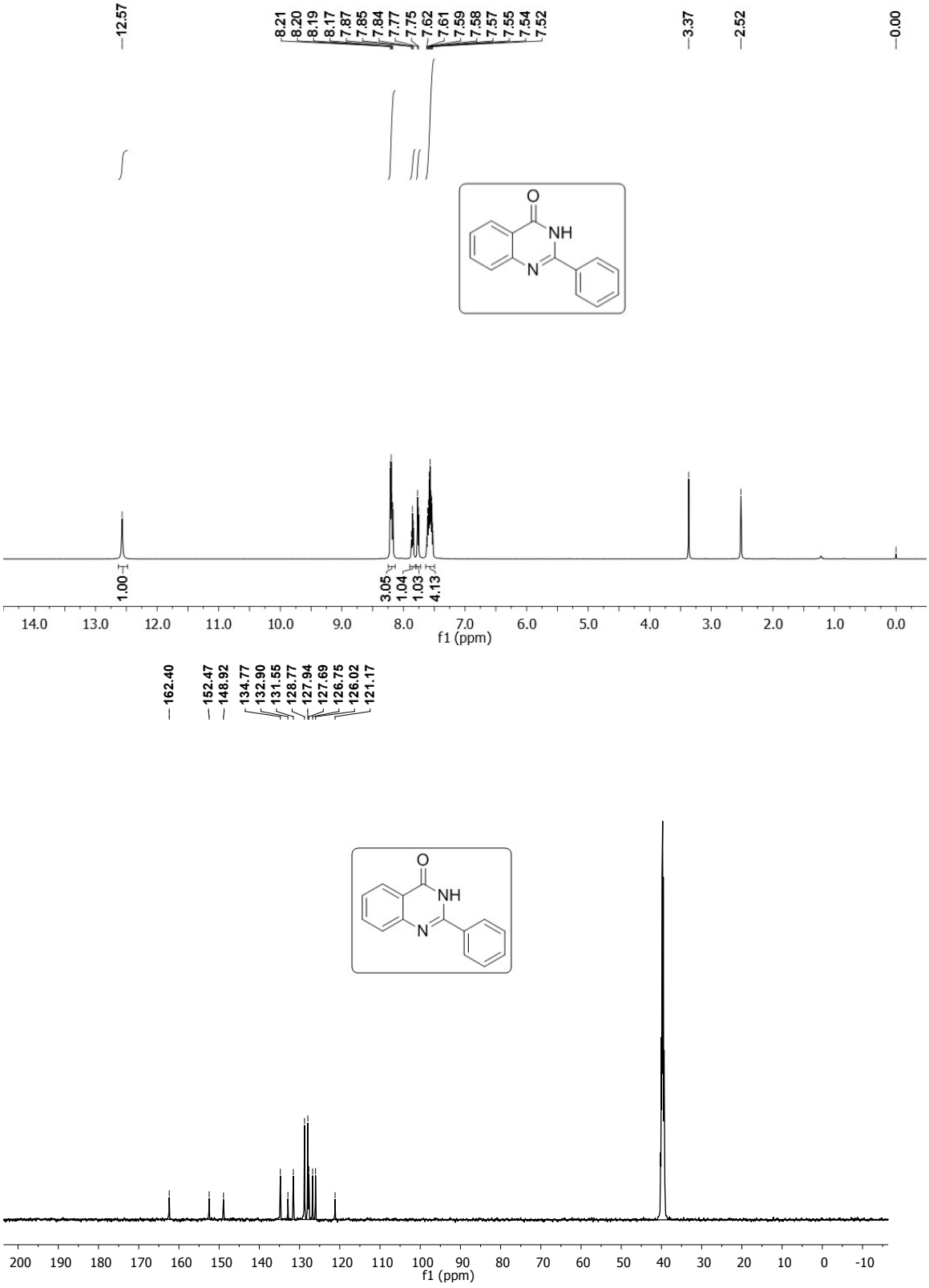
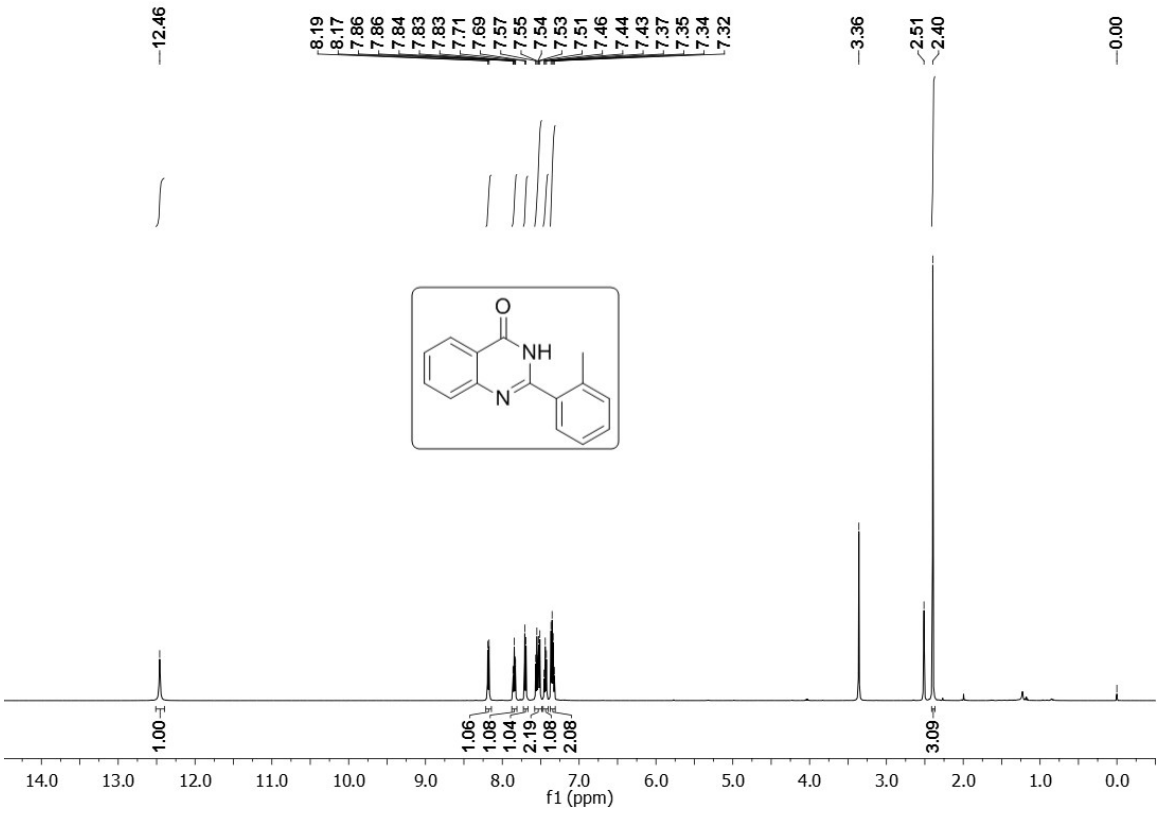
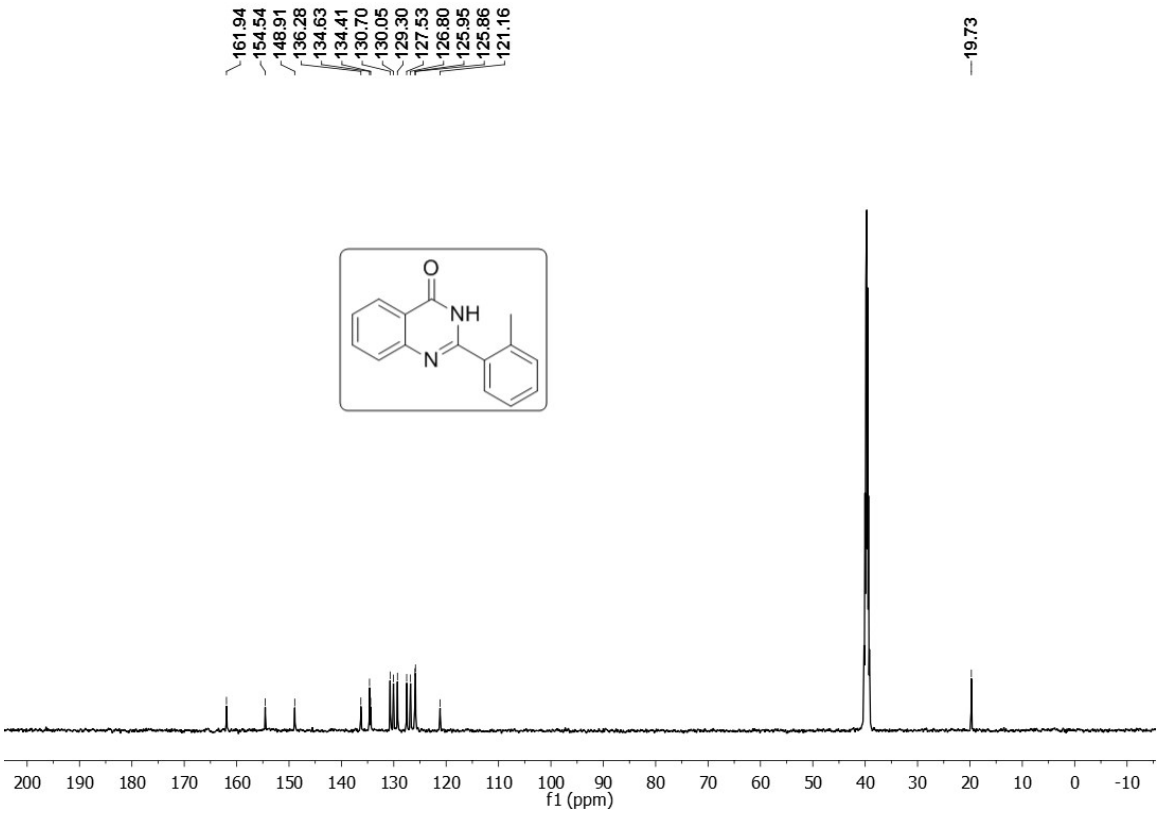
7. ^{1}H NMR and ^{13}C NMR spectra

The ^{1}H and ^{13}C NMR spectra of compounds (3aa)

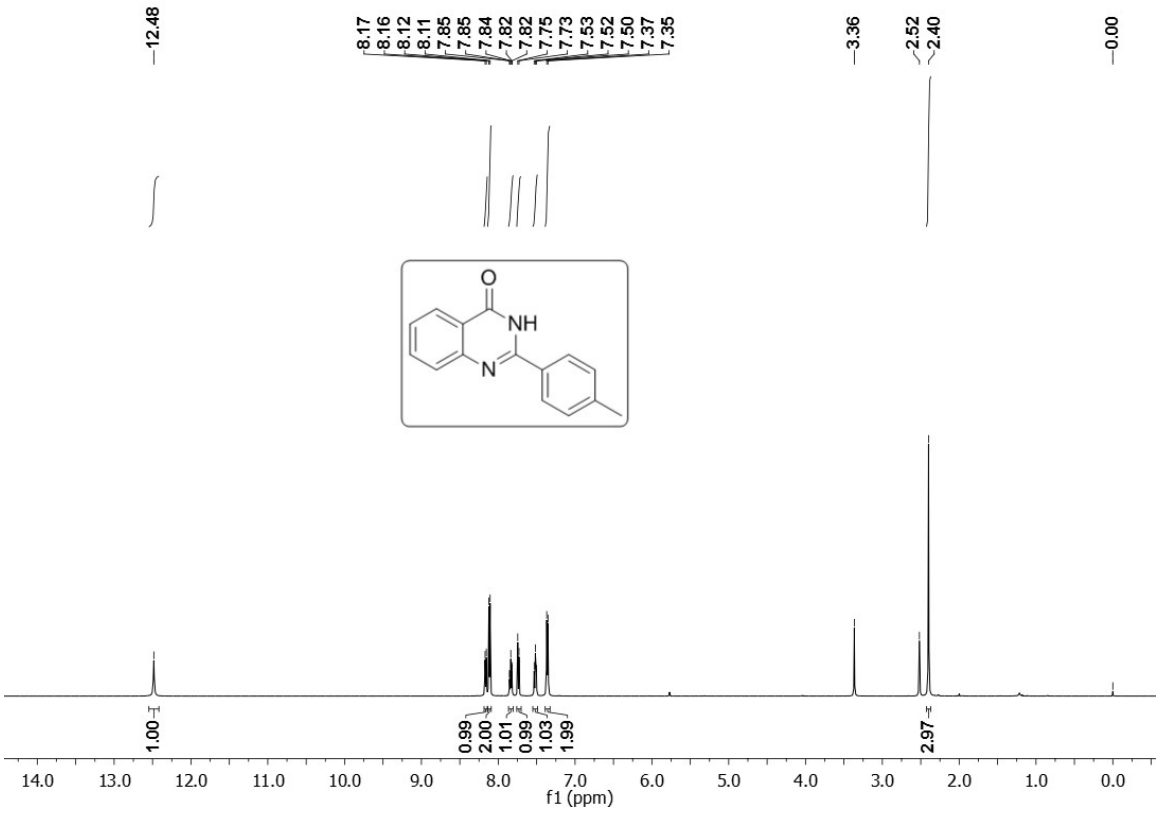


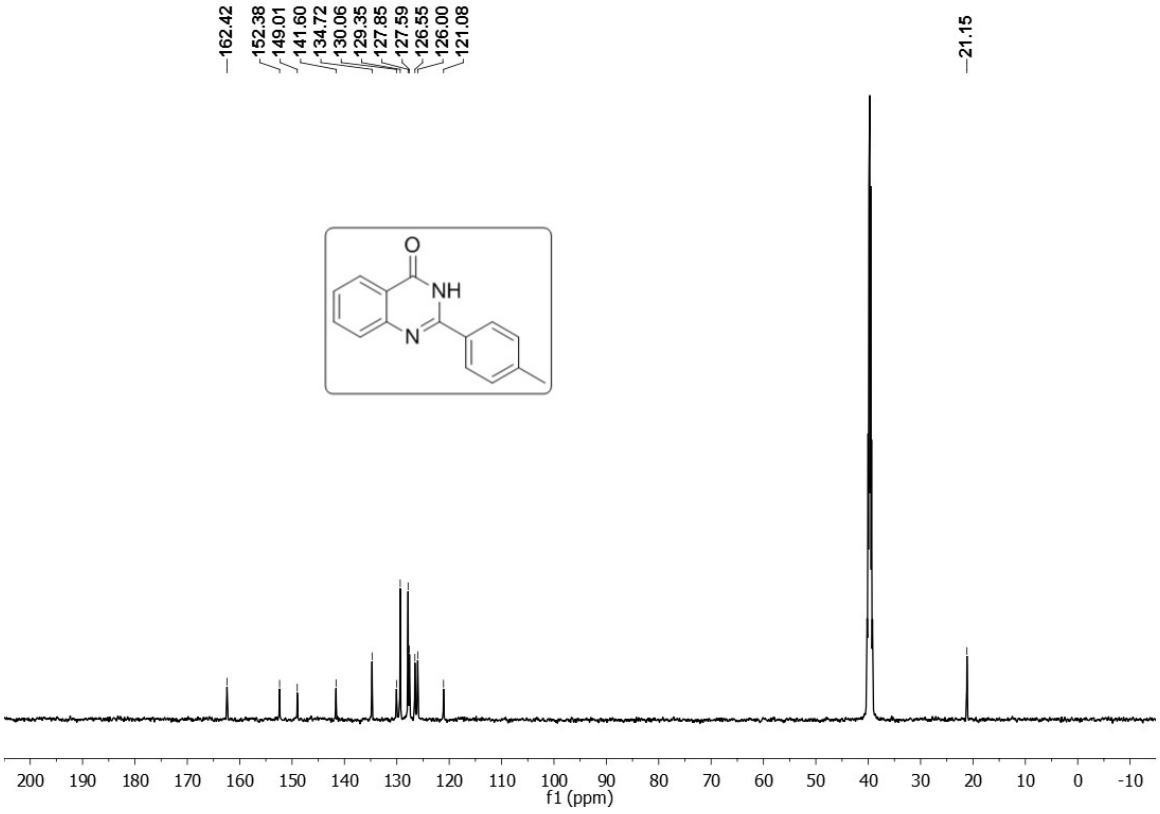
The ^{1}H and ^{13}C NMR spectra of compounds (3ab)



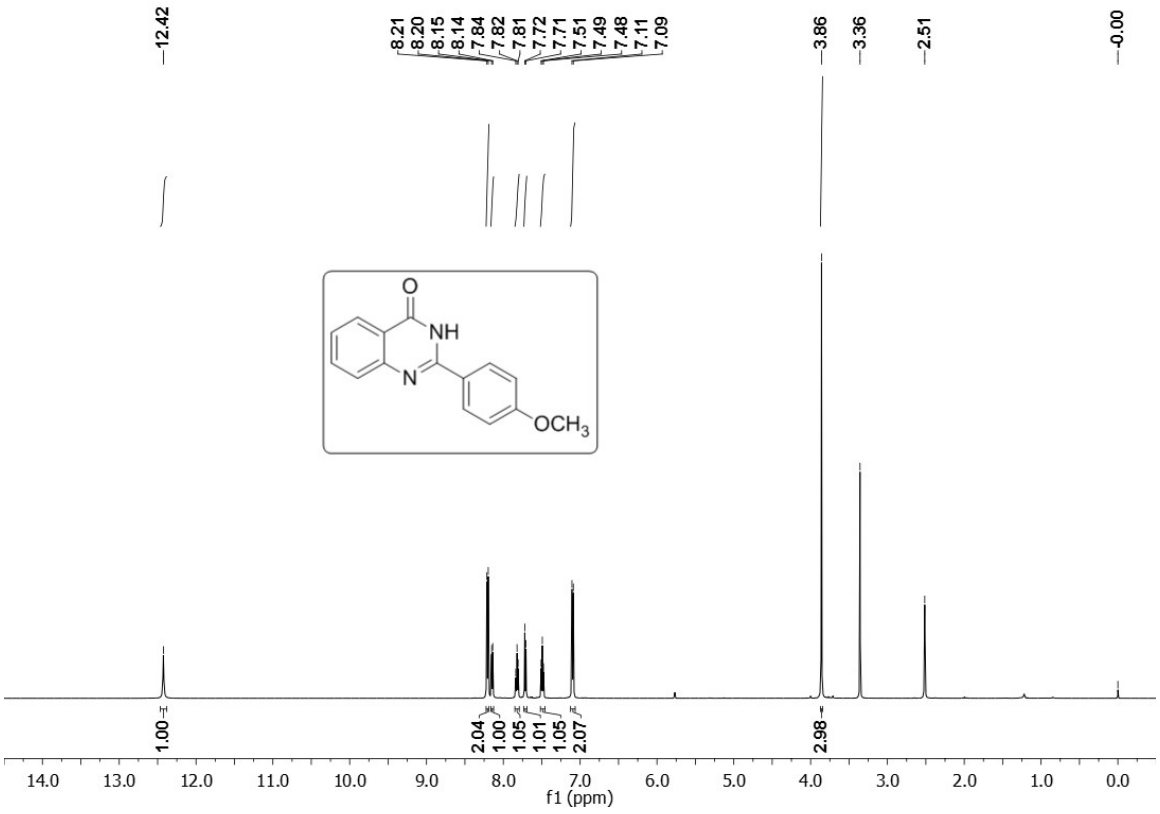


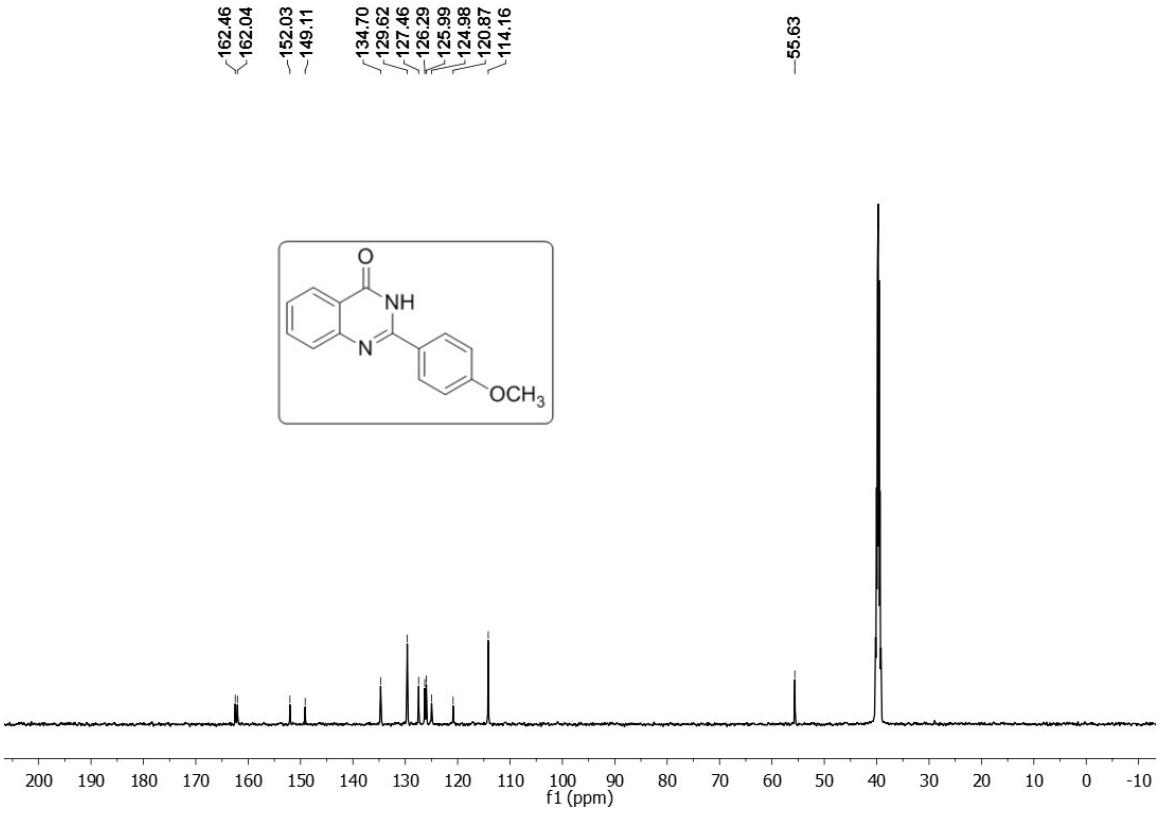
The ^{1}H and ^{13}C NMR spectra of compounds (3ac)



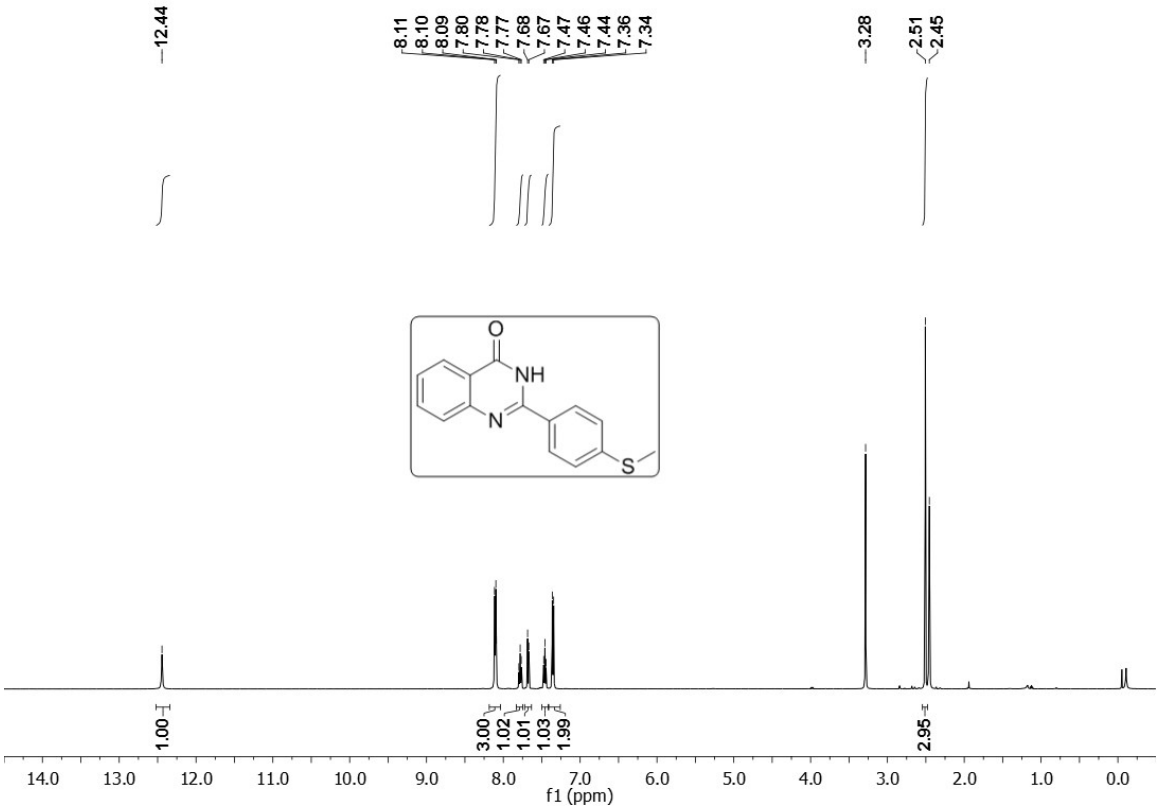


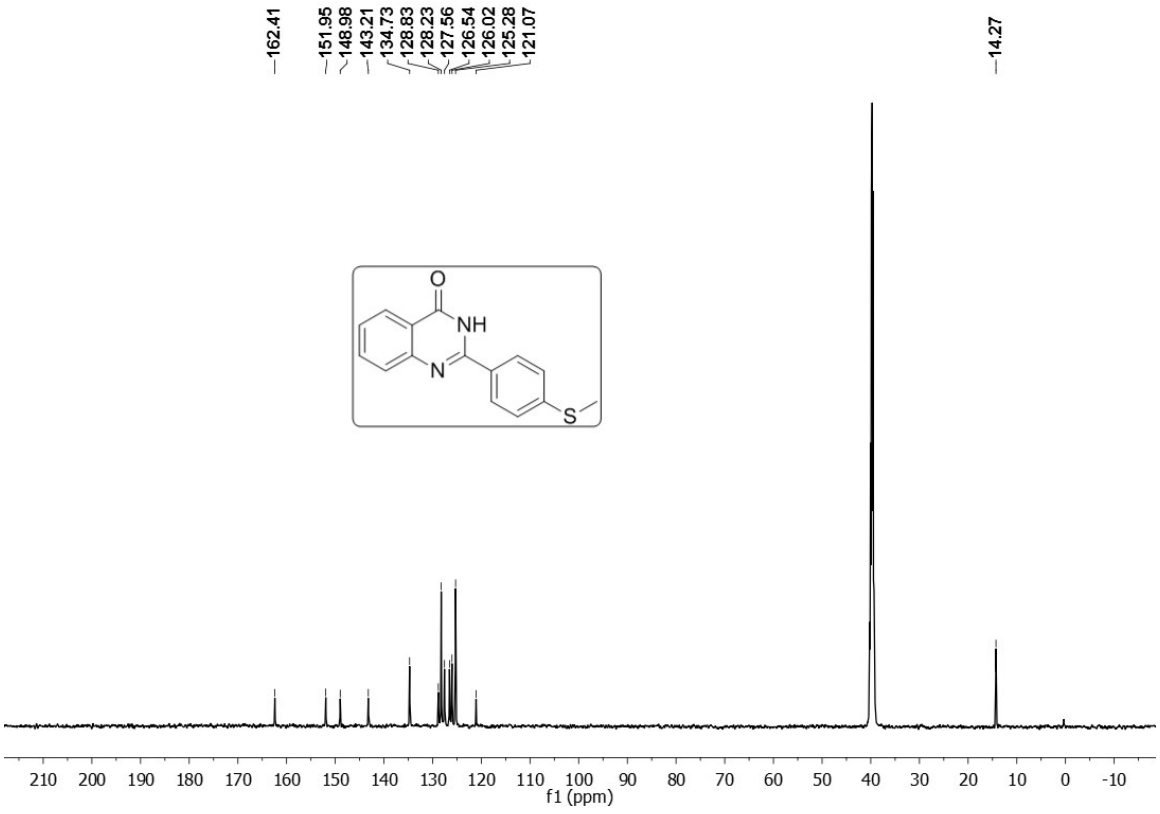
The ^{1}H and ^{13}C NMR spectra of compounds (3ad)



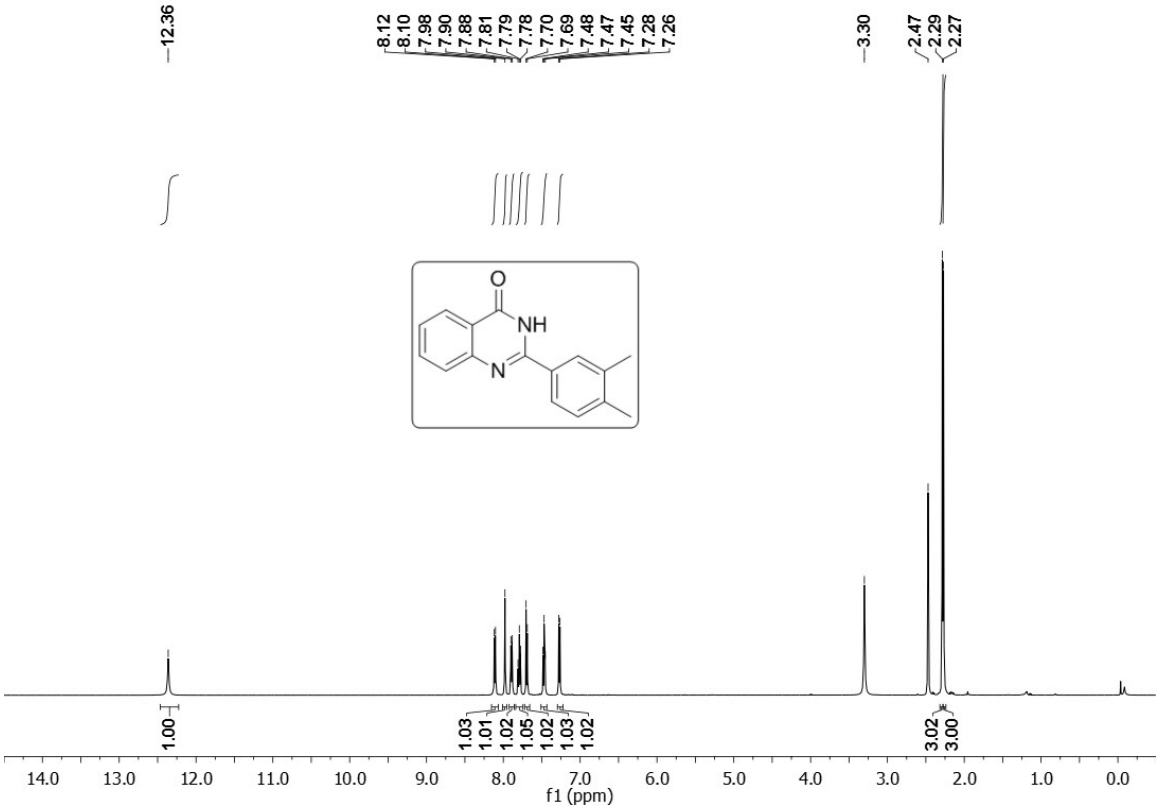


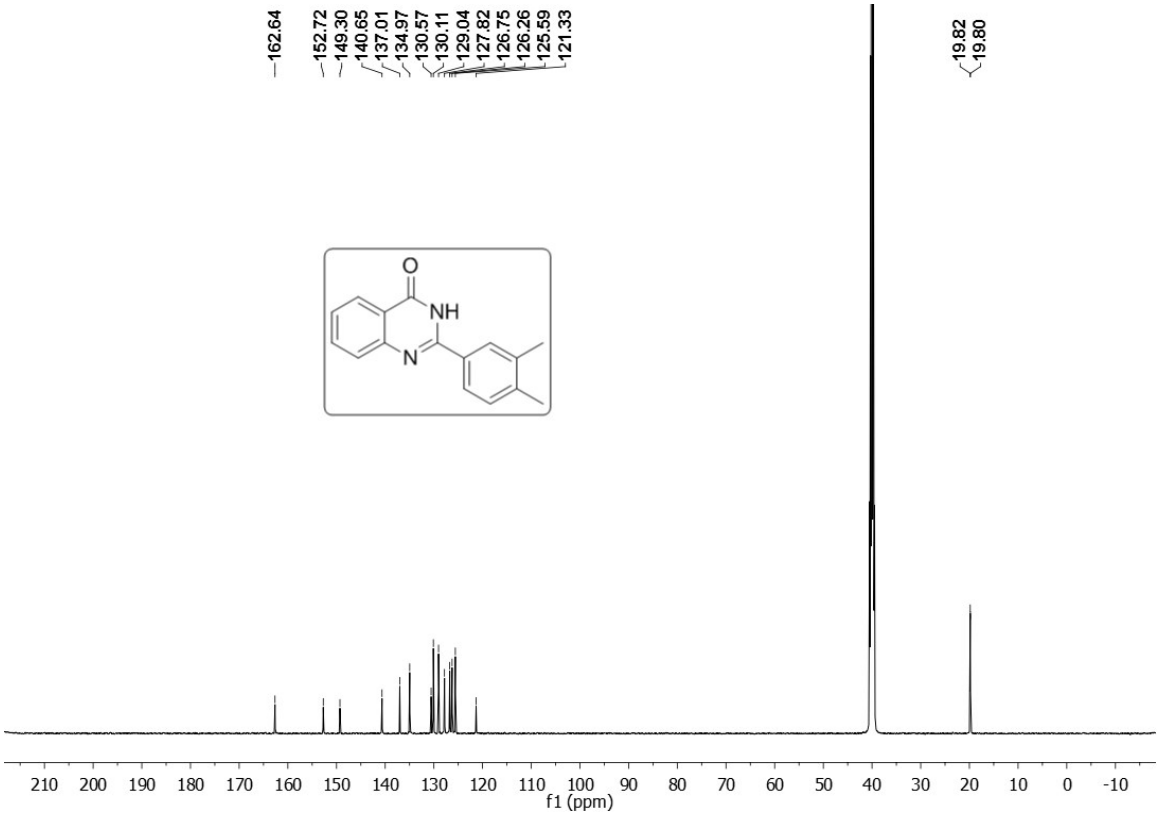
The ^{1}H and ^{13}C NMR spectra of compounds (3ae)



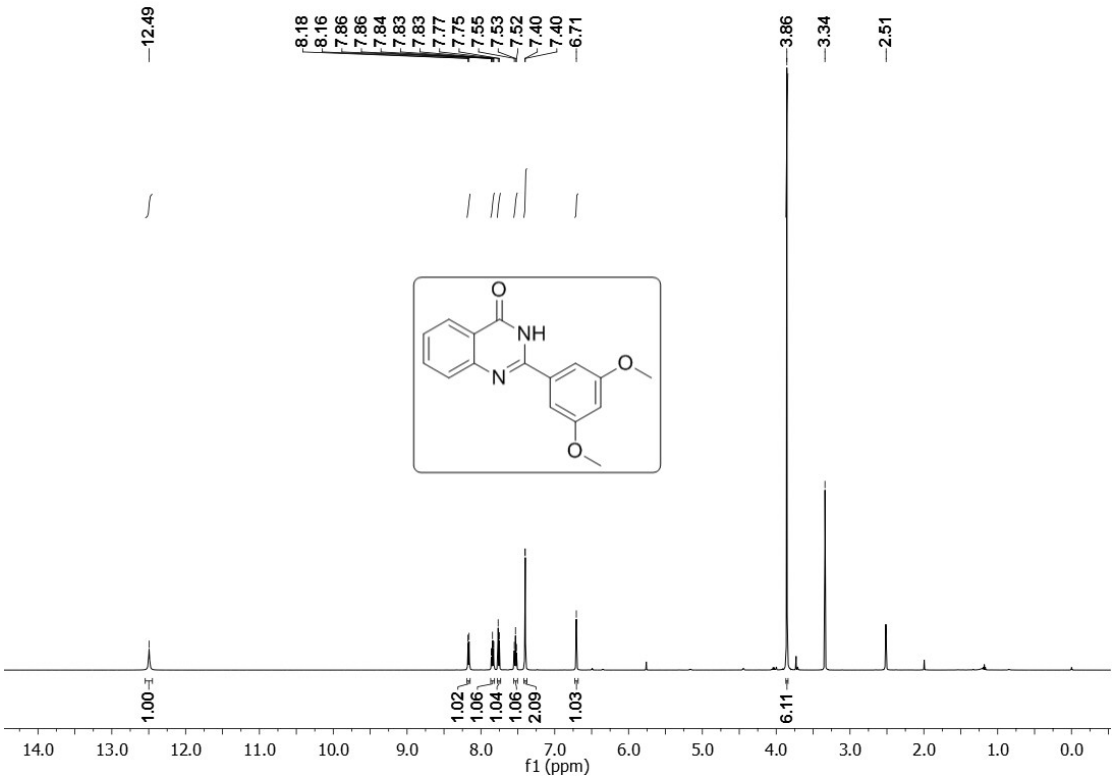


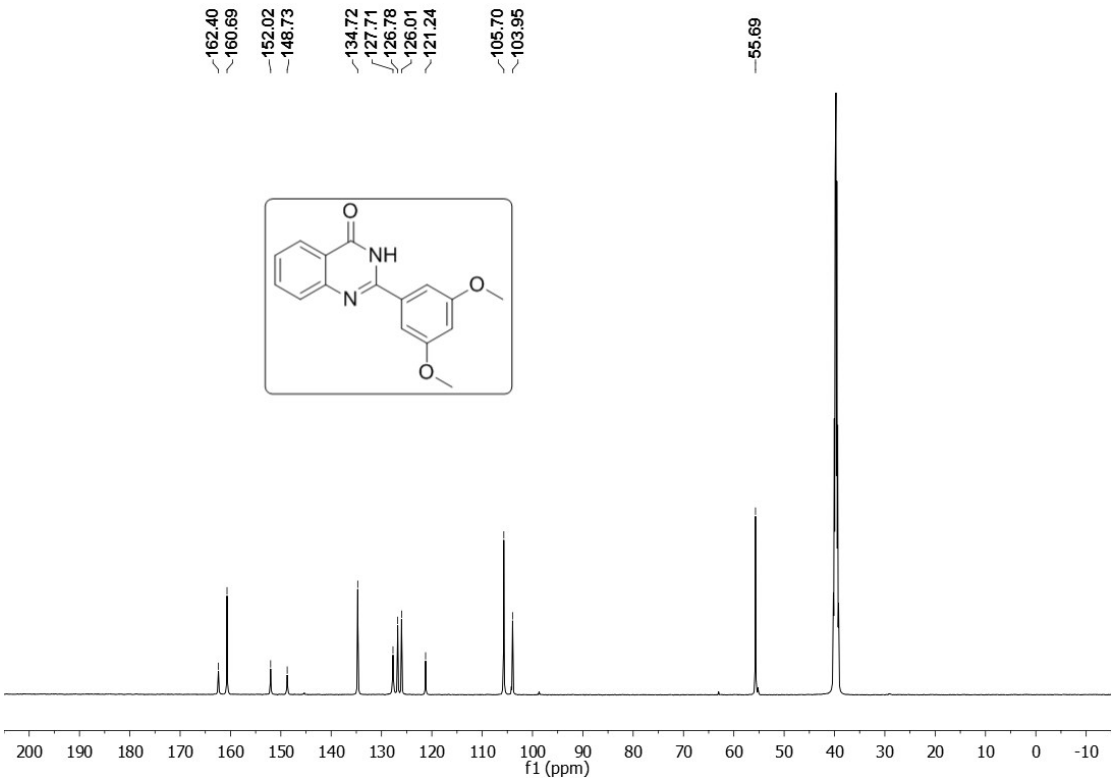
The ^{1}H and ^{13}C NMR spectra of compounds (3af)



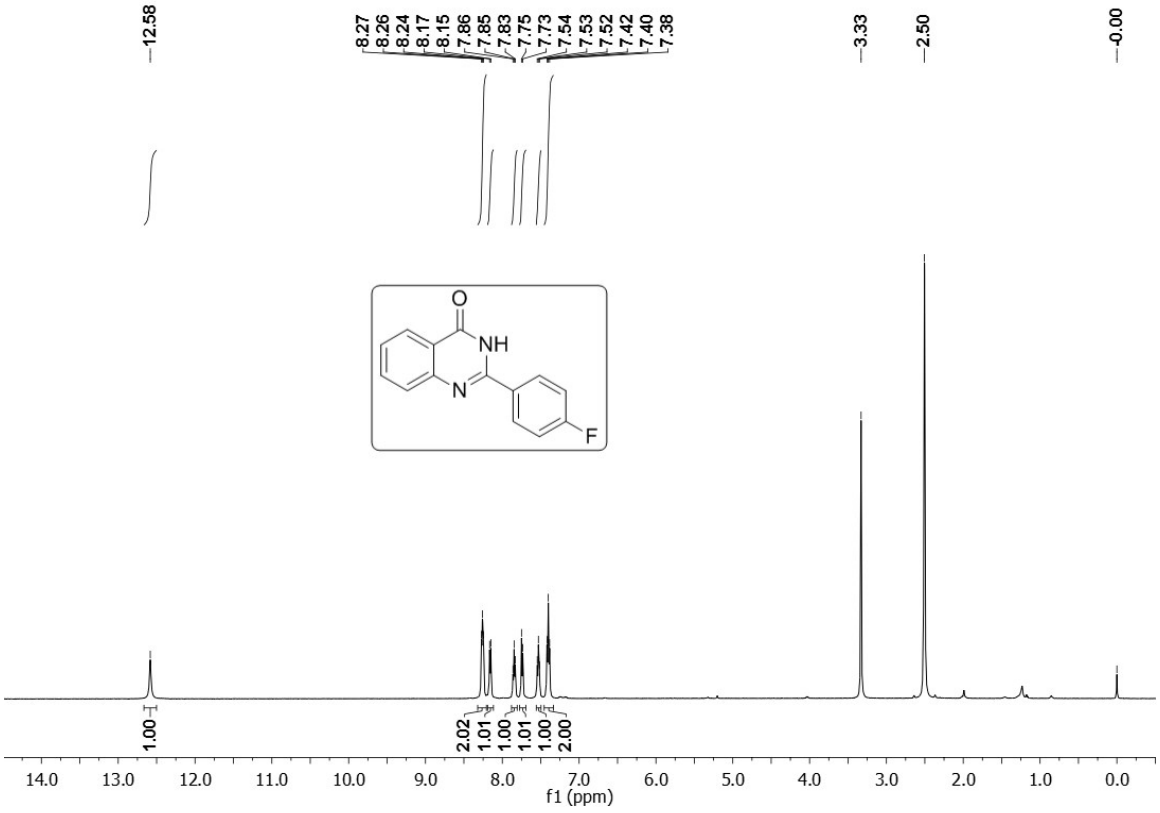


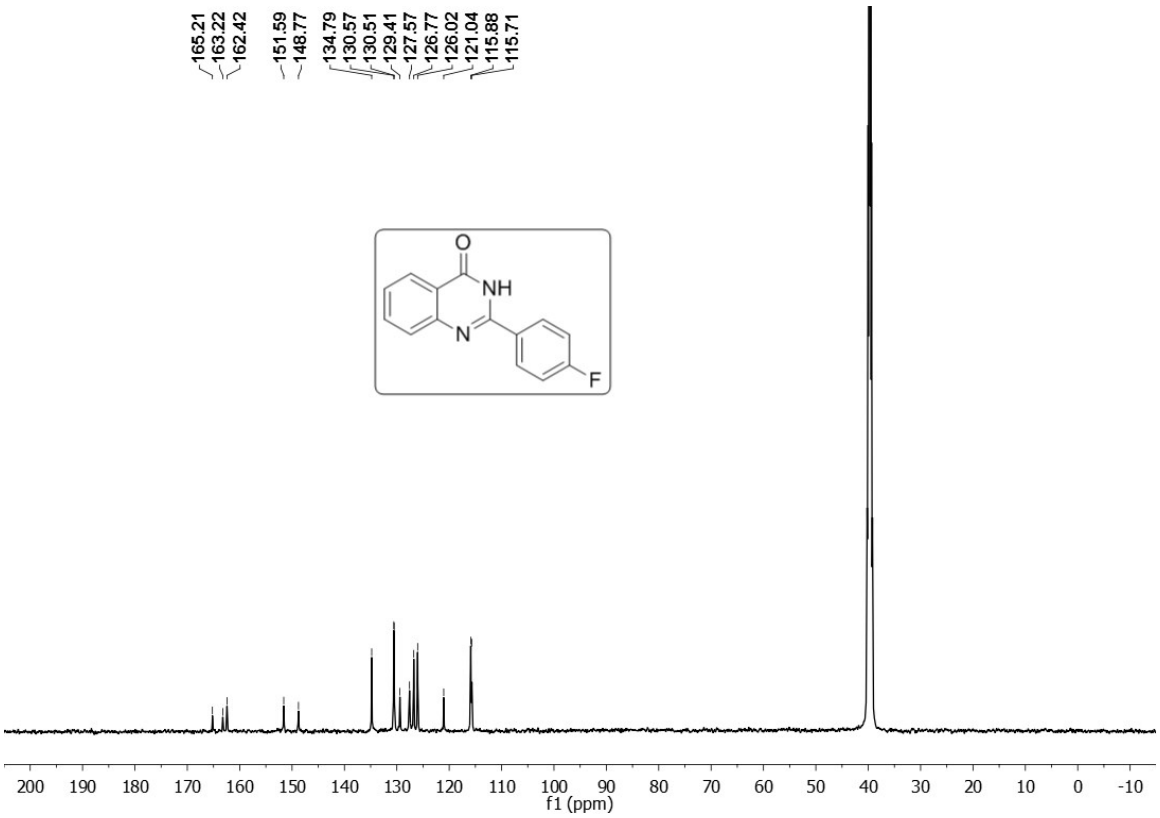
The ^{1}H and ^{13}C NMR spectra of compounds (3ag)



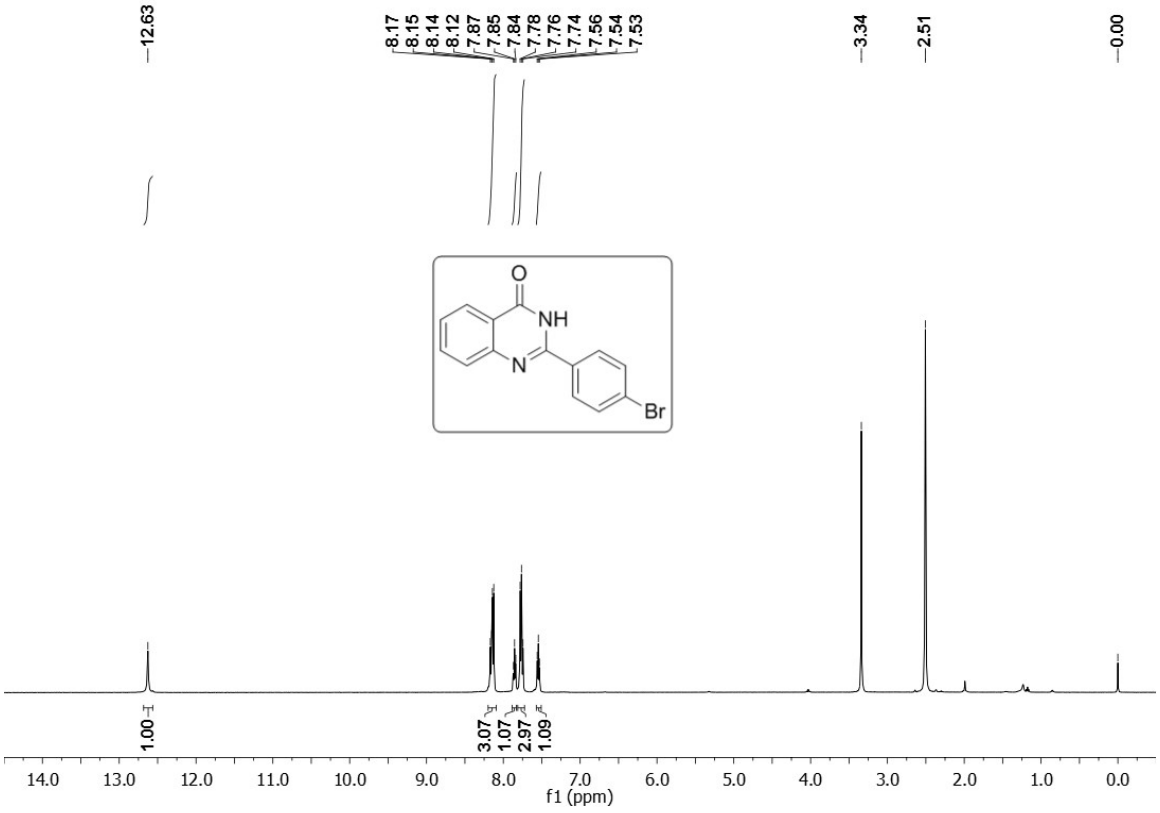


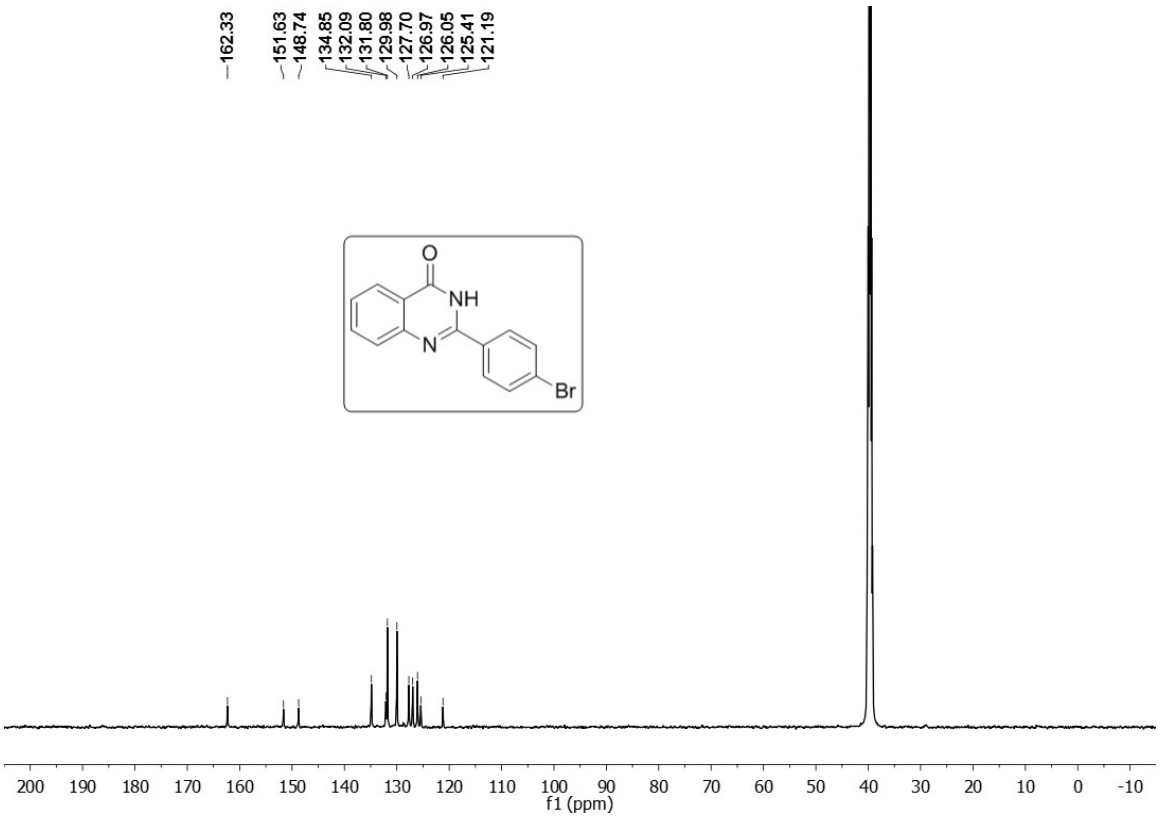
The ^{1}H and ^{13}C NMR spectra of compounds (3ah)



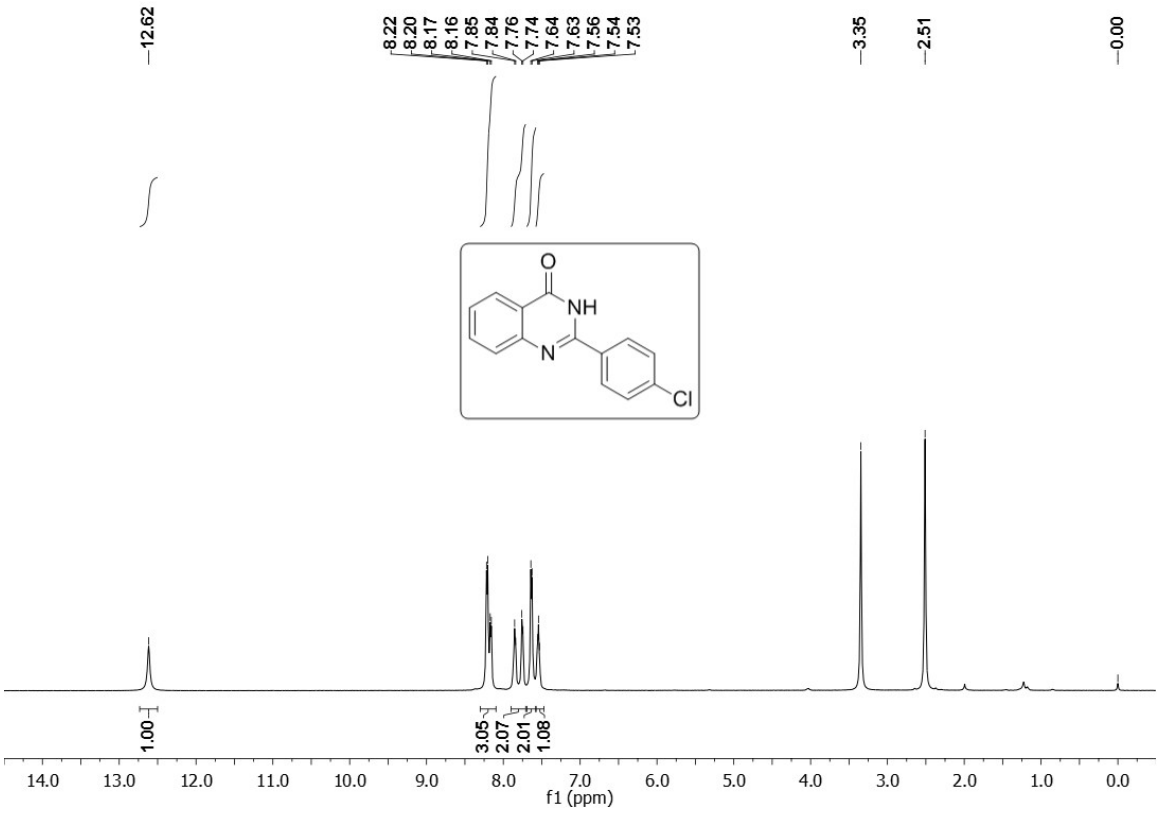


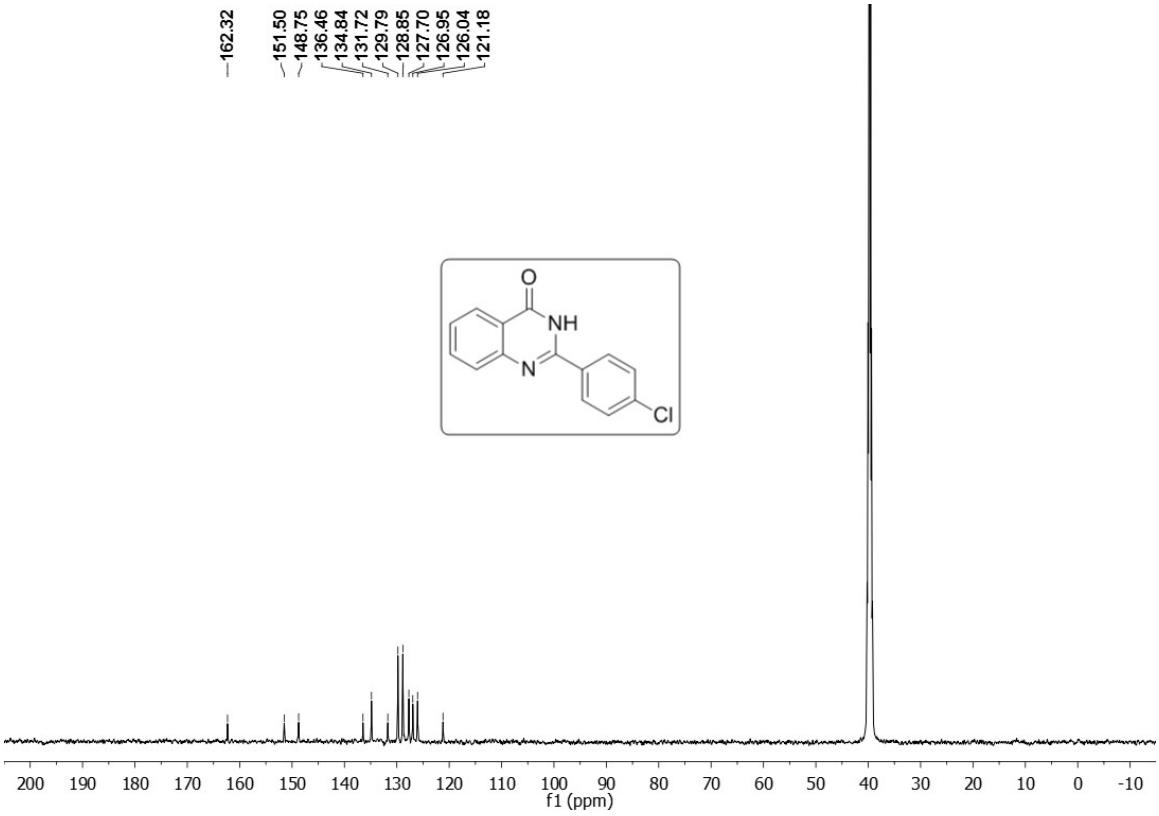
The ^{1}H and ^{13}C NMR spectra of compounds (3ai)



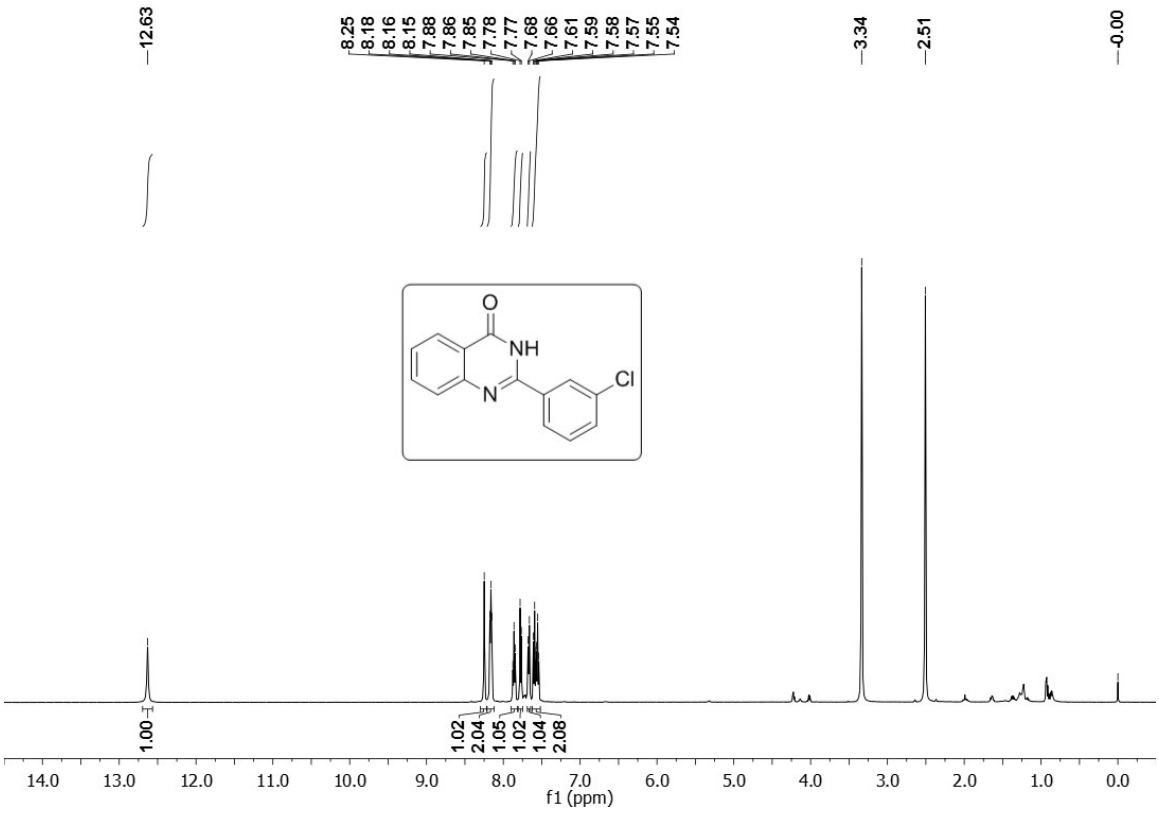


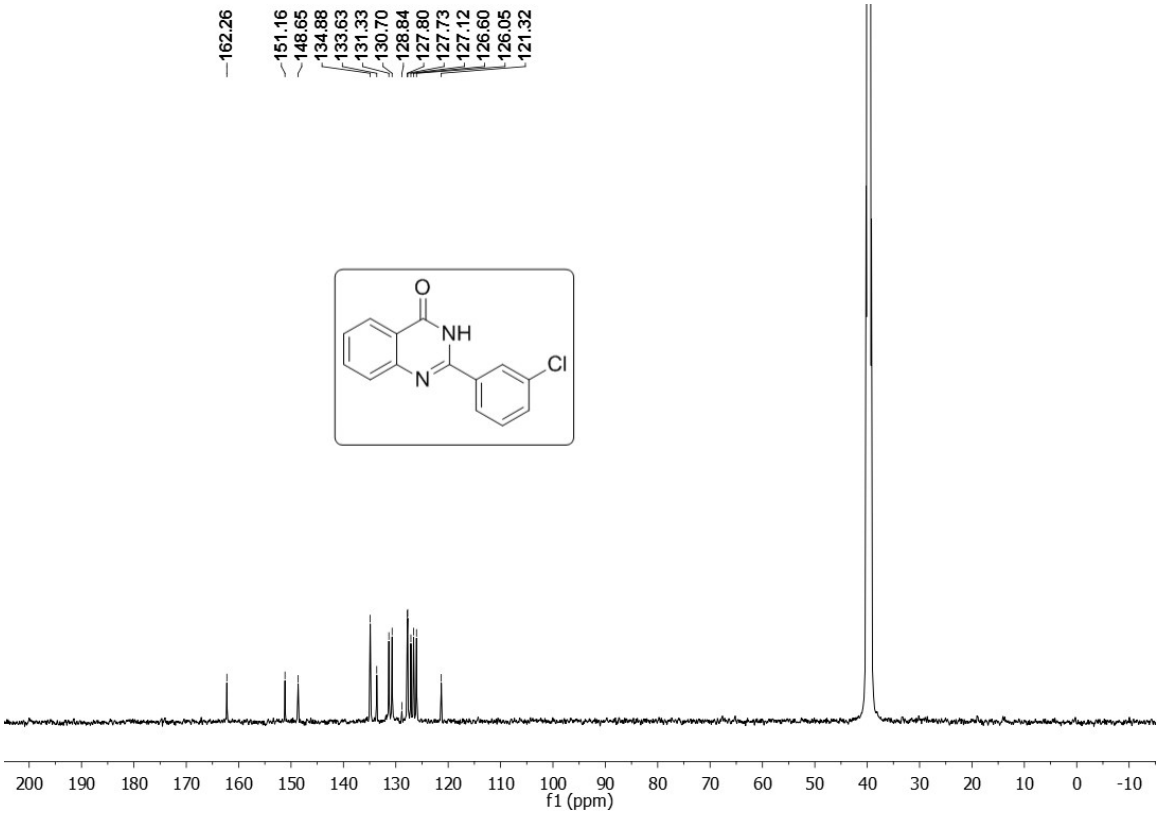
The ^{1}H and ^{13}C NMR spectra of compounds (3aj)



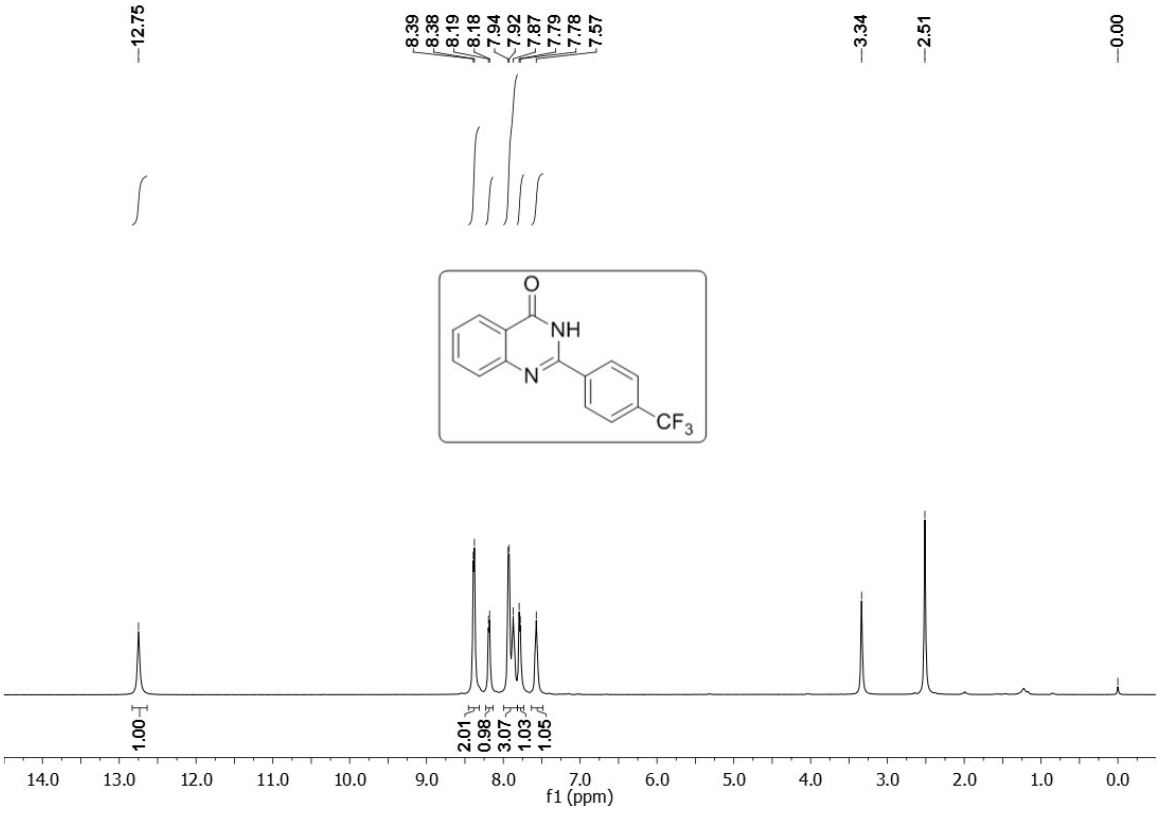


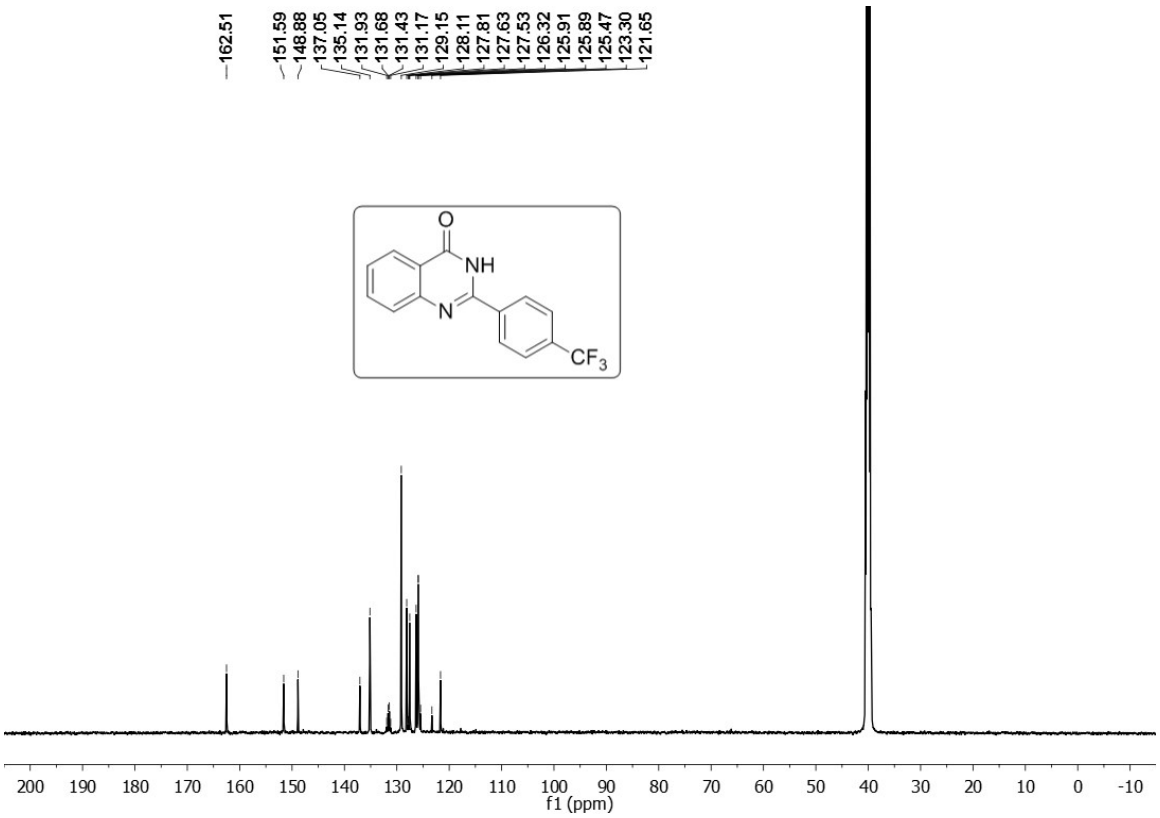
The ^{1}H and ^{13}C NMR spectra of compounds (3ak)



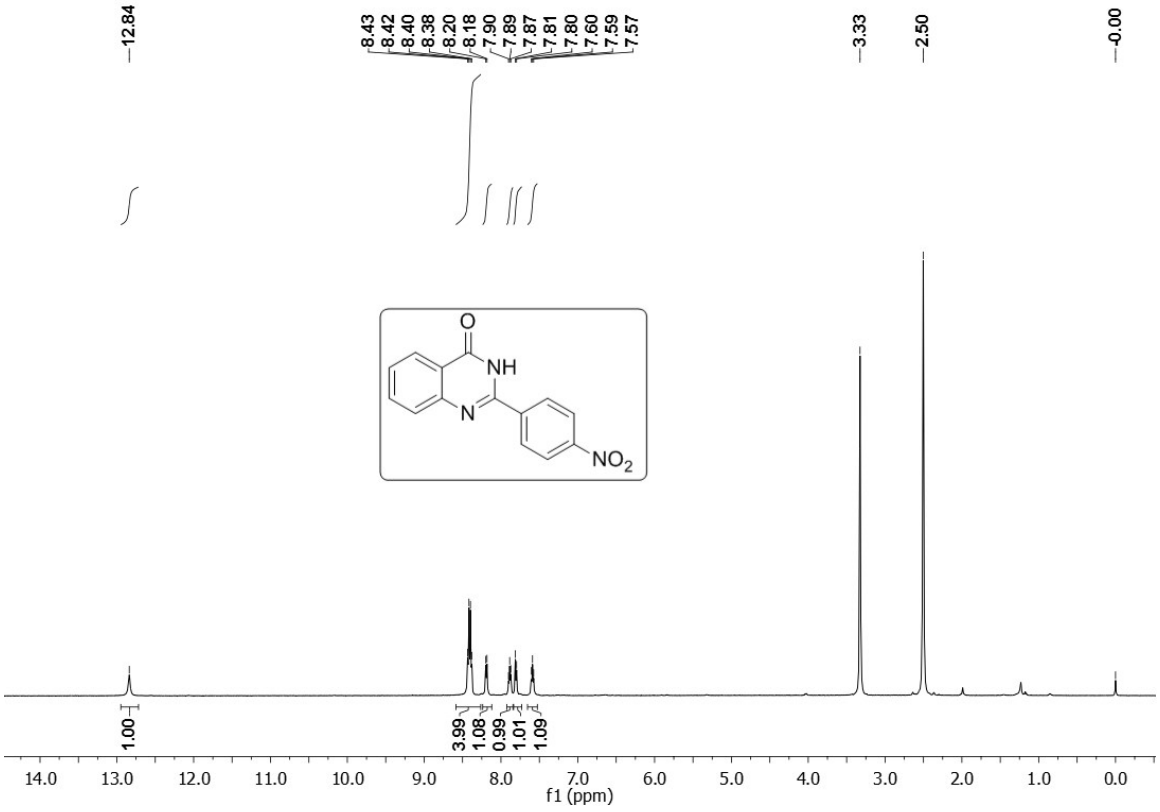


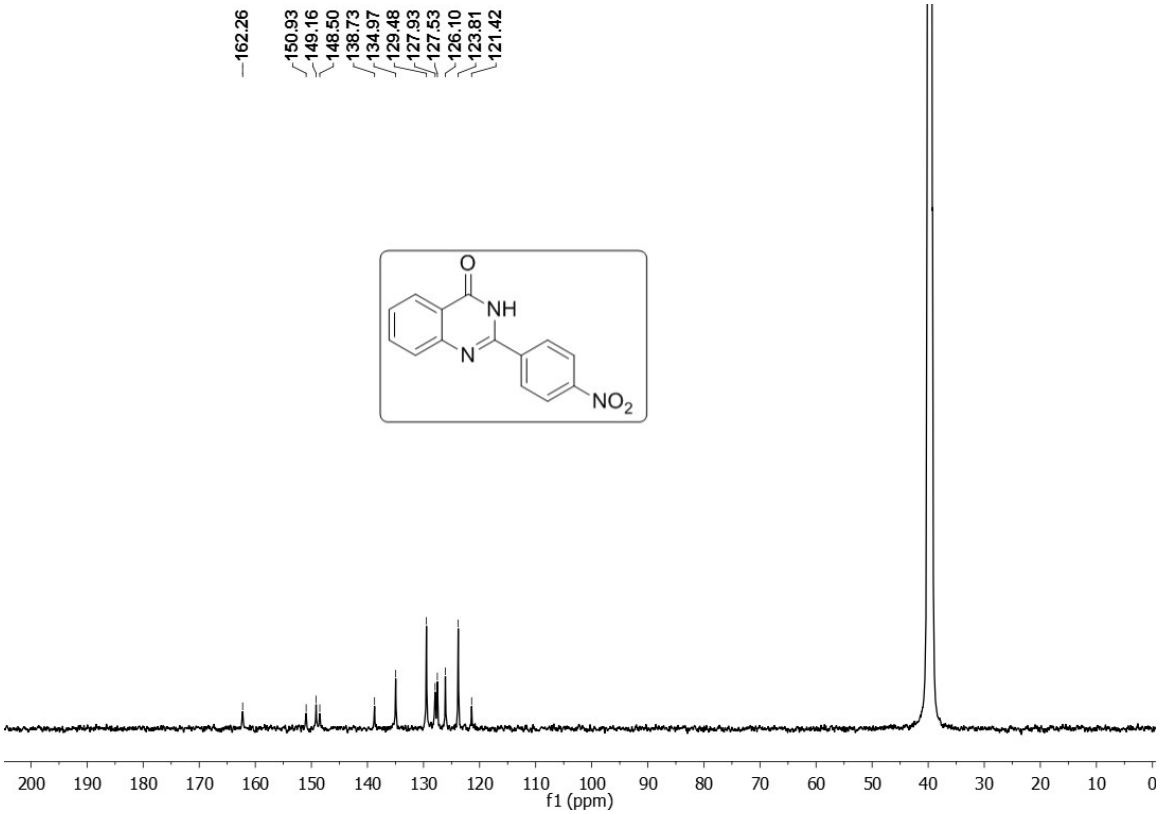
The ^{1}H and ^{13}C NMR spectra of compounds (3al)



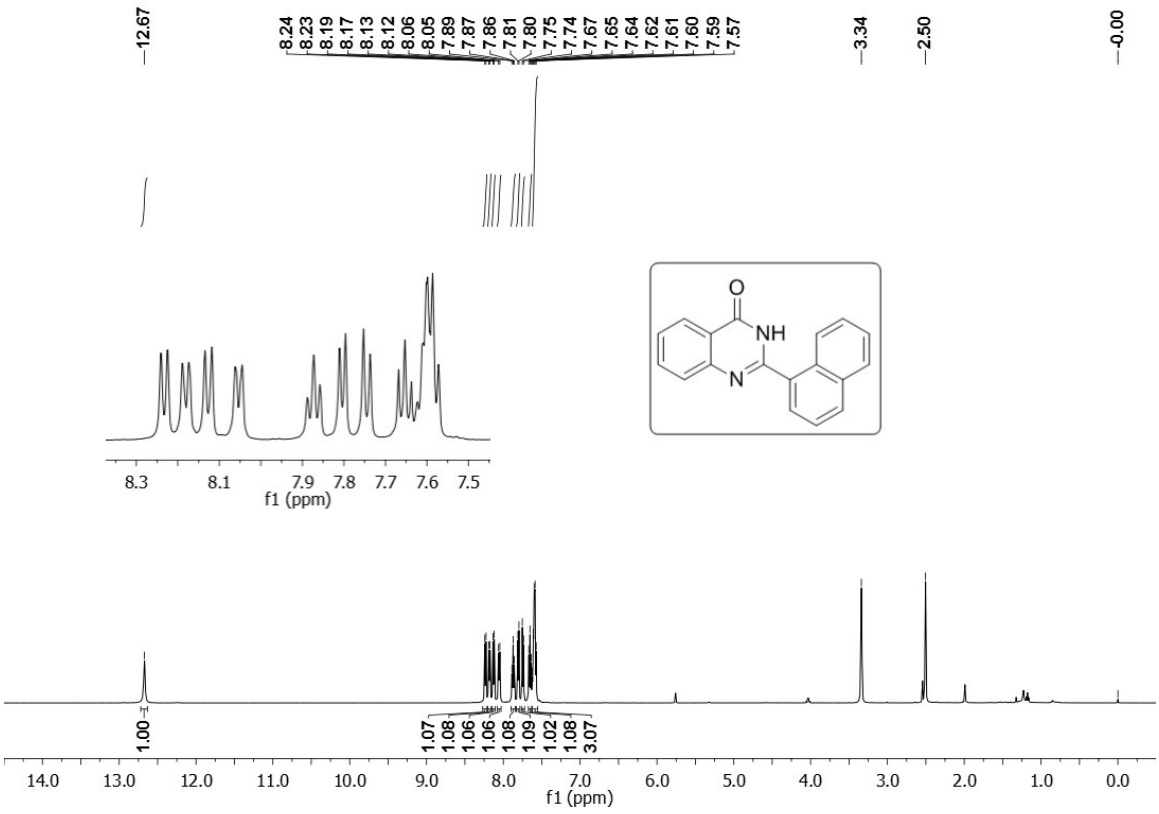


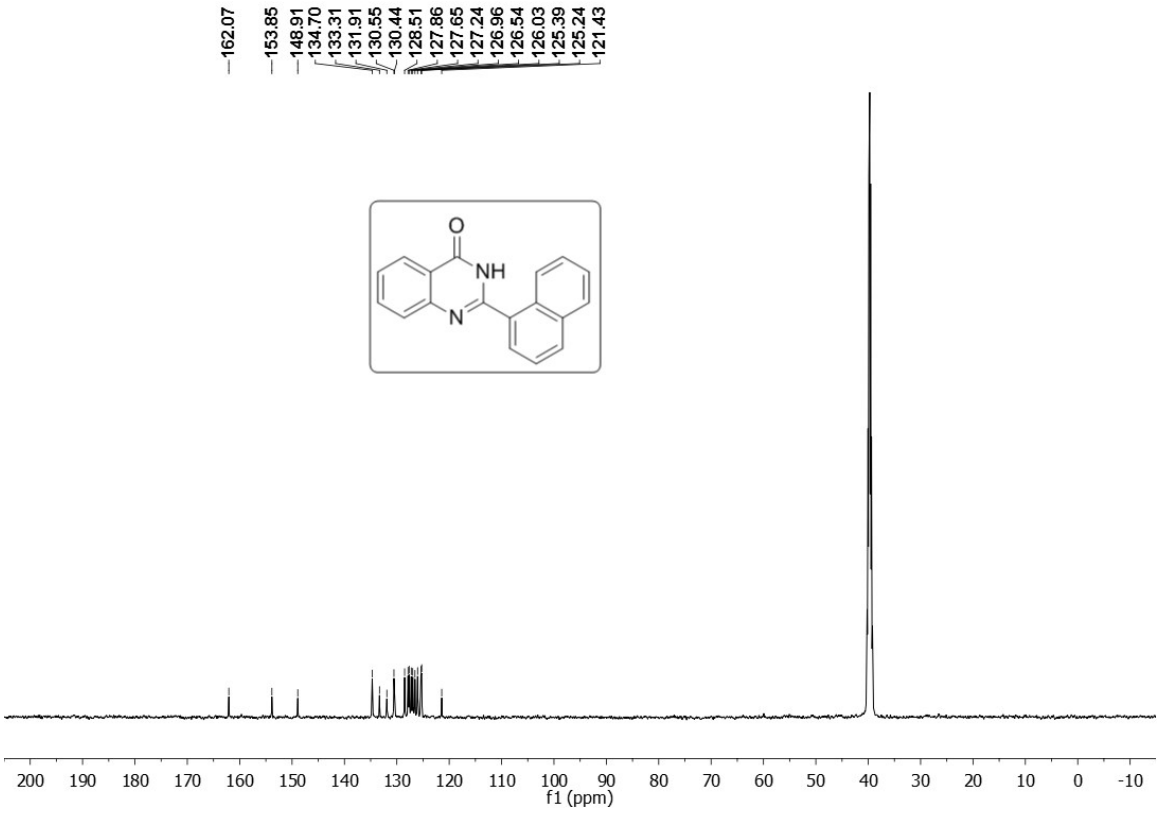
The ^{1}H and ^{13}C NMR spectra of compounds (3am)



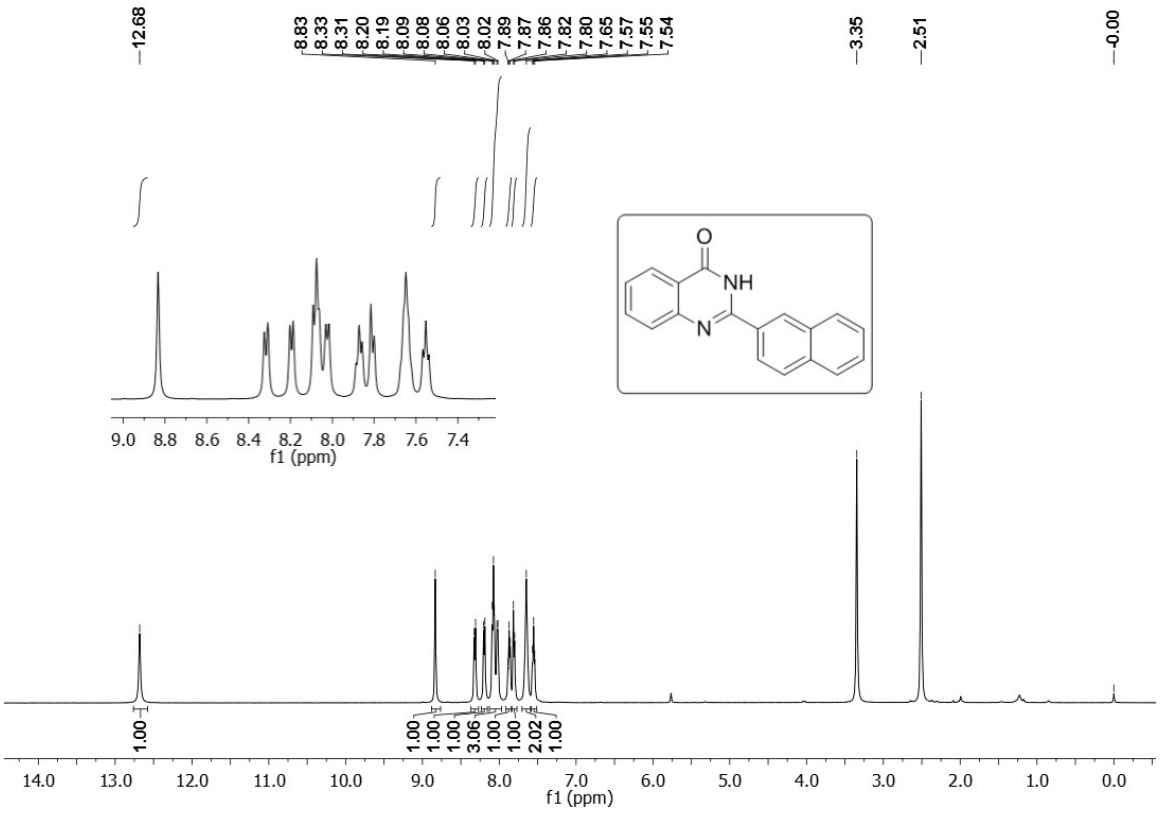


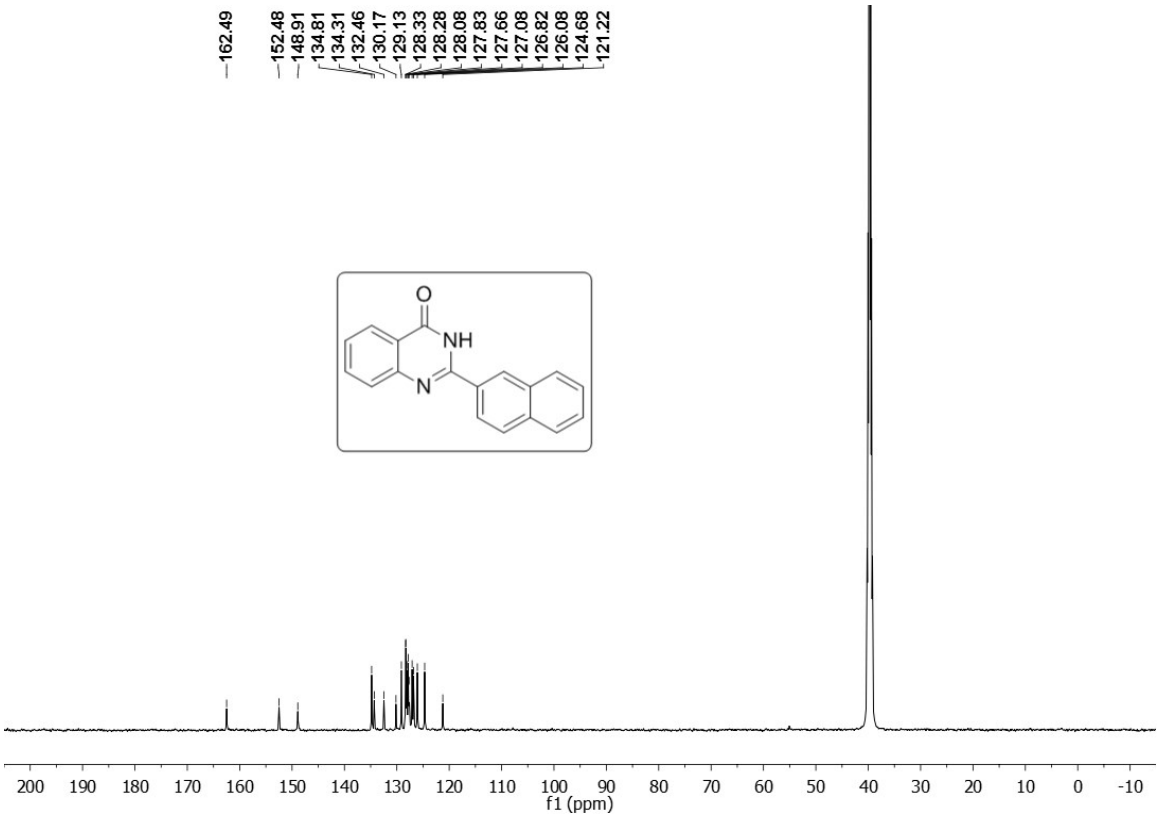
The ^{1}H and ^{13}C NMR spectra of compounds (3an)



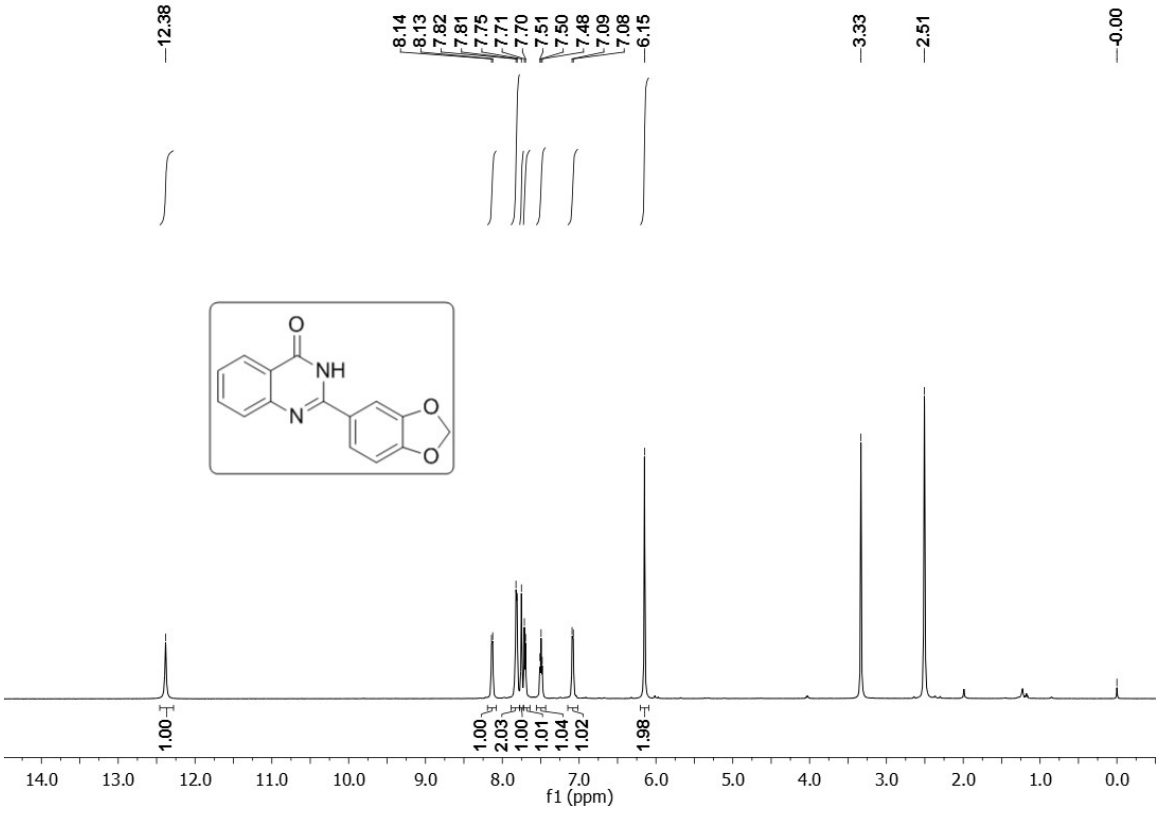


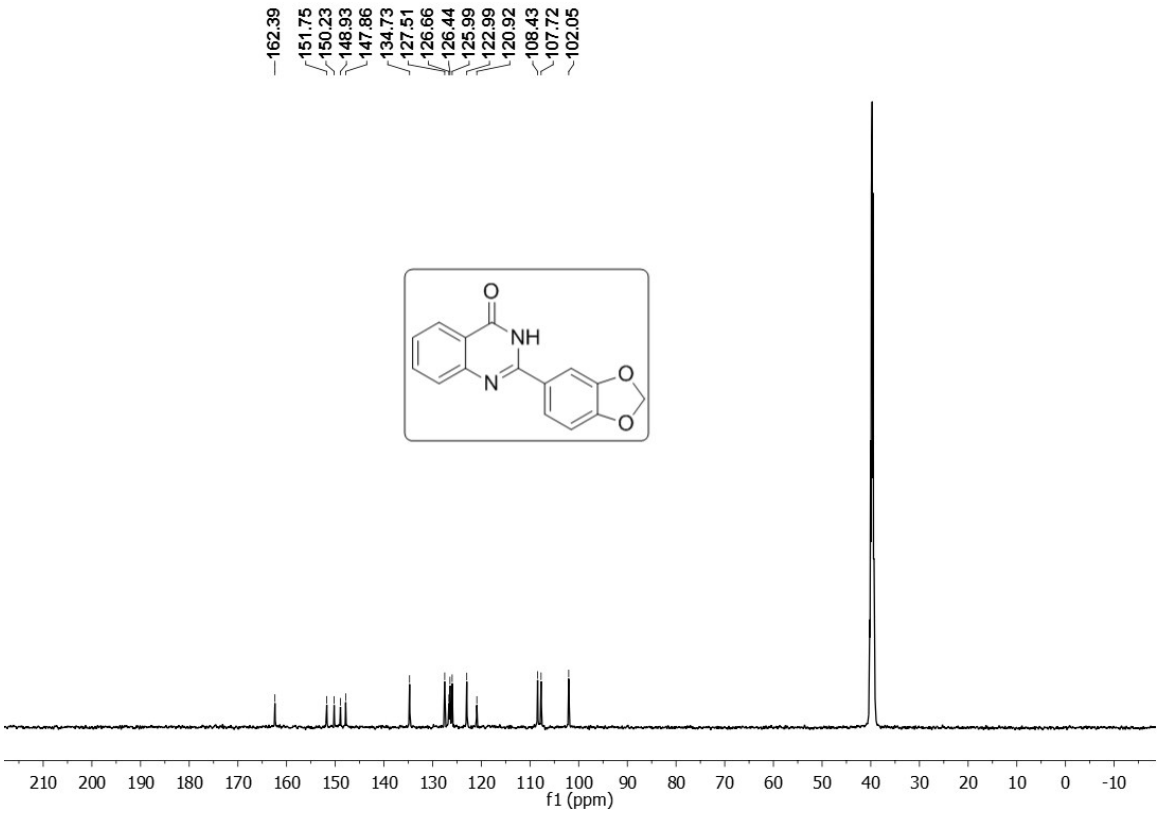
The ^{1}H and ^{13}C NMR spectra of compounds (3ao)



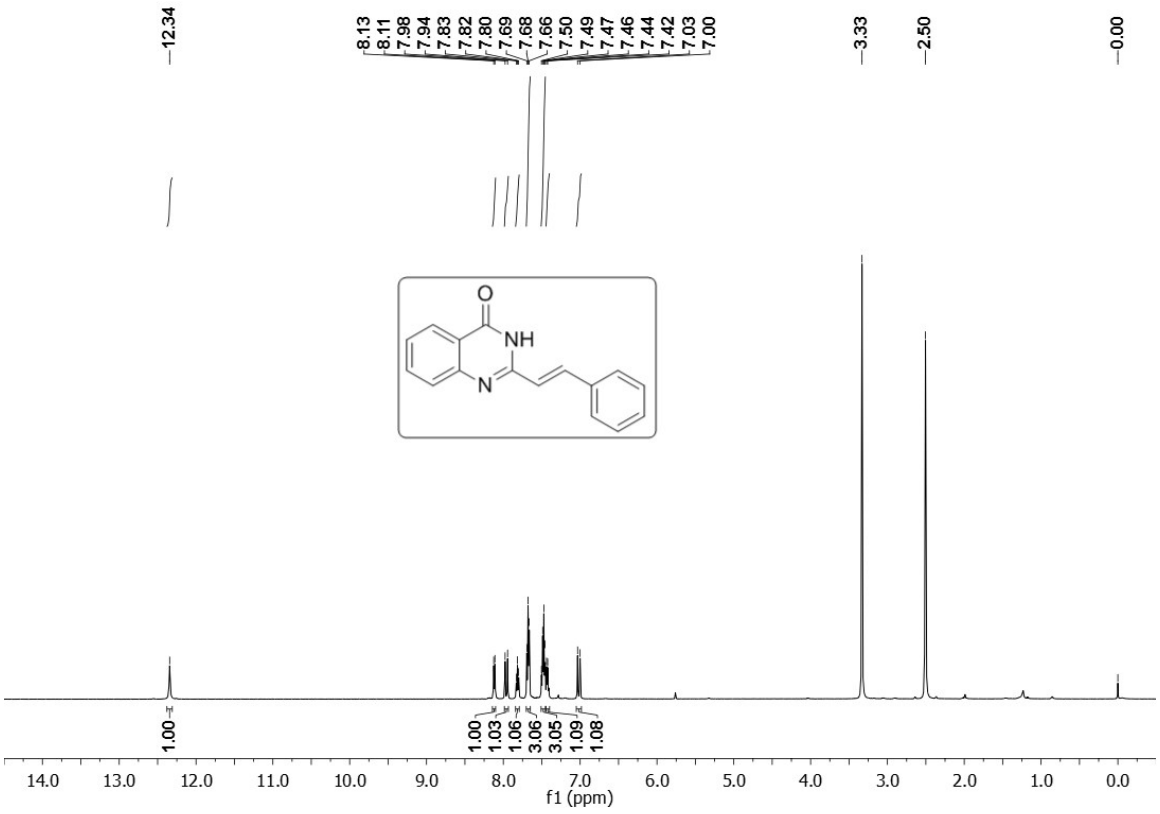


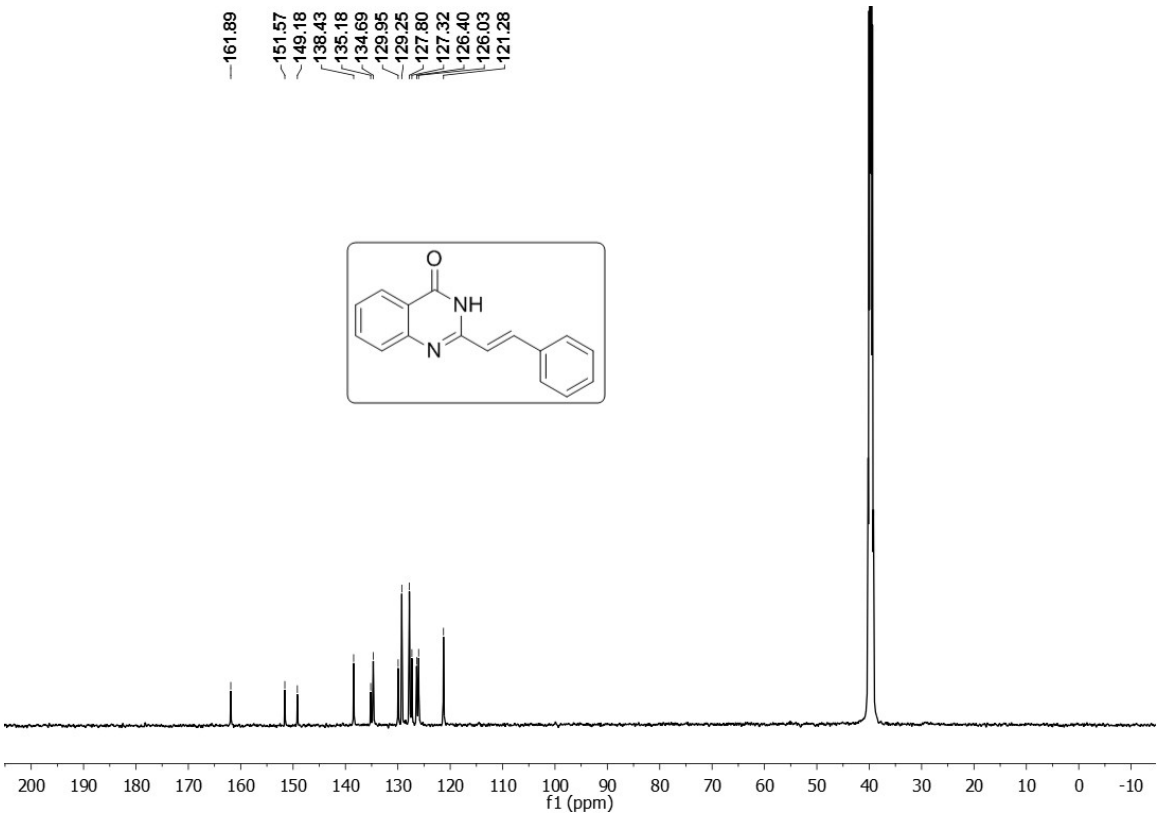
The ^{1}H and ^{13}C NMR spectra of compounds (3ap)



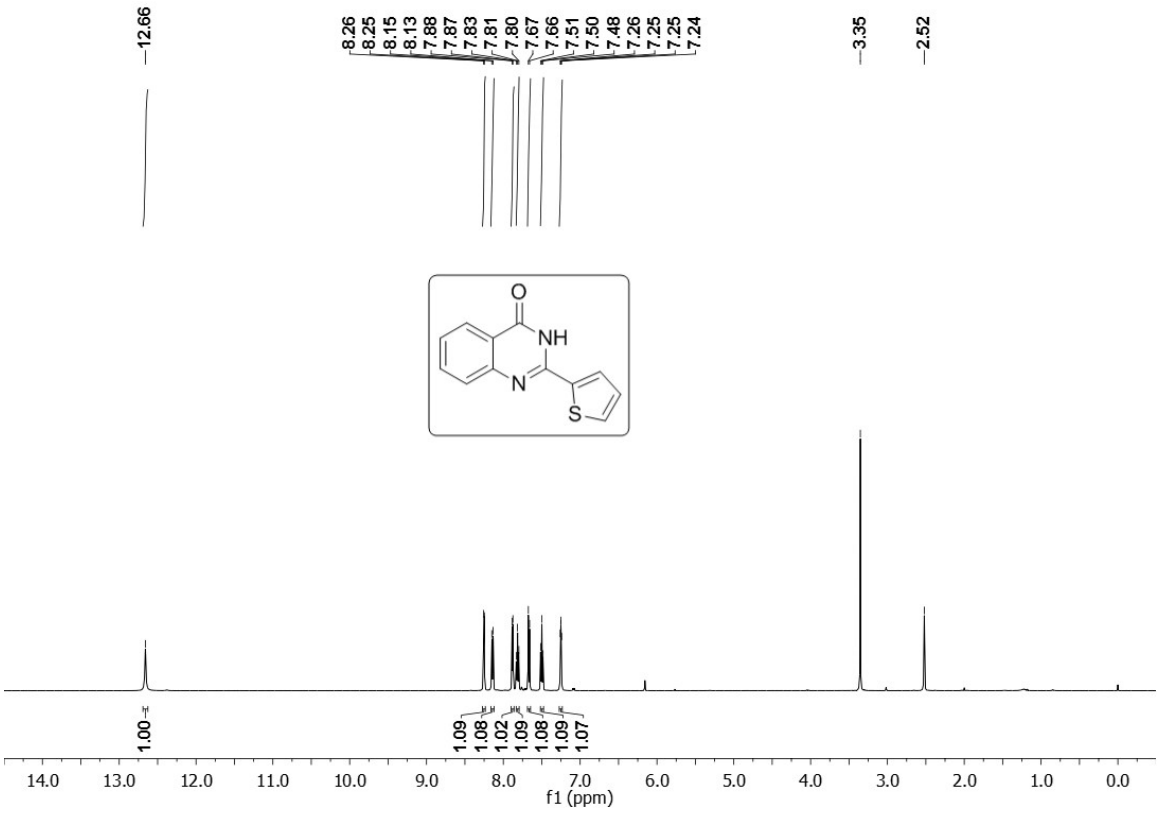


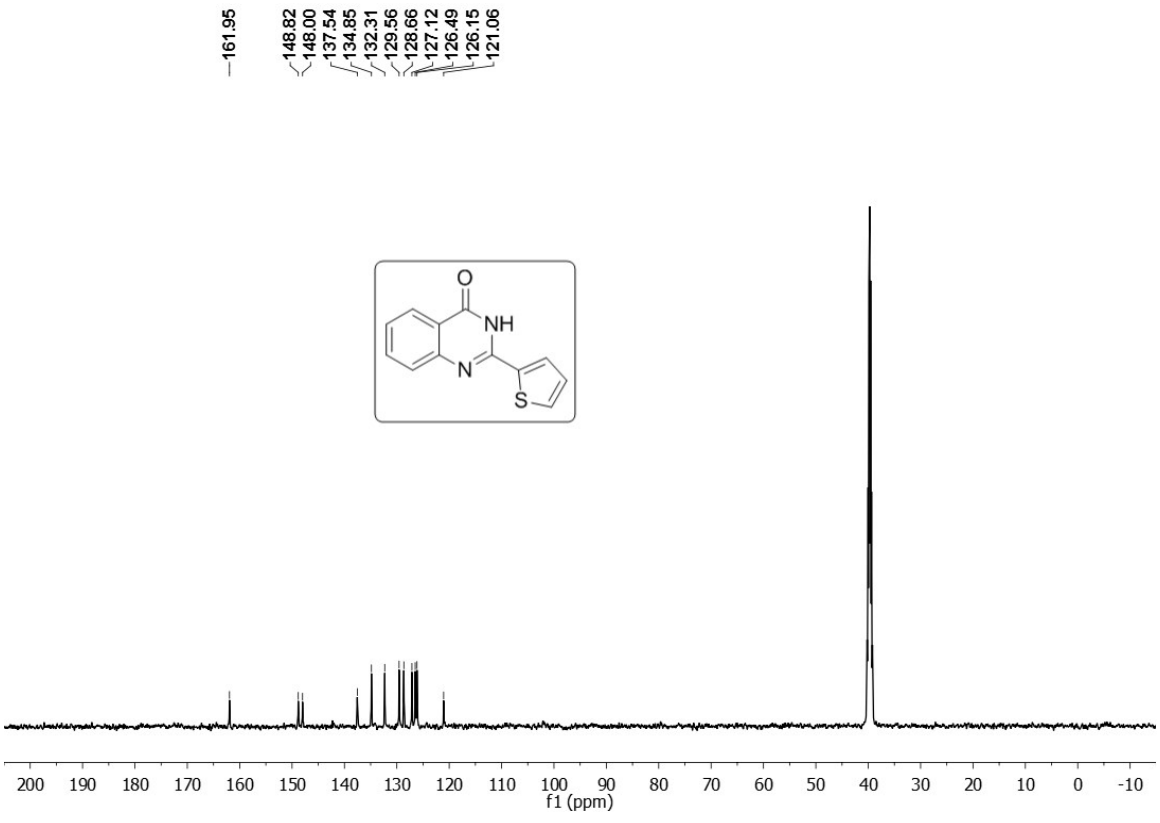
The ^{1}H and ^{13}C NMR spectra of compounds (3aq)



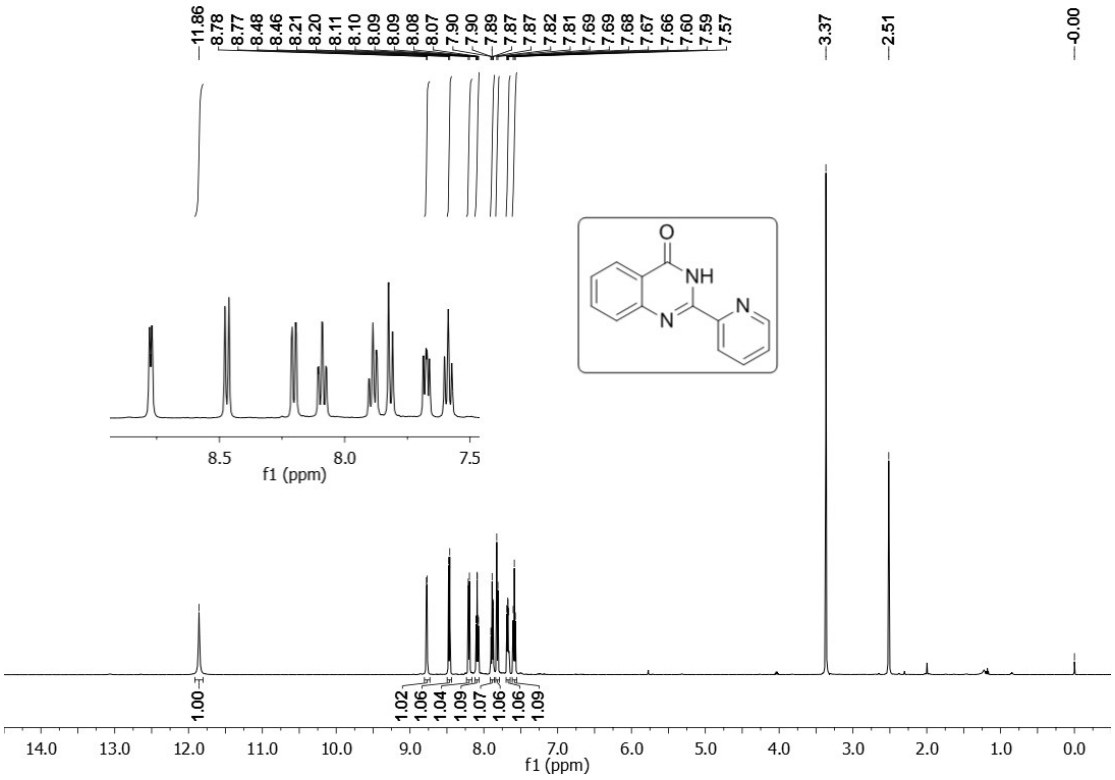


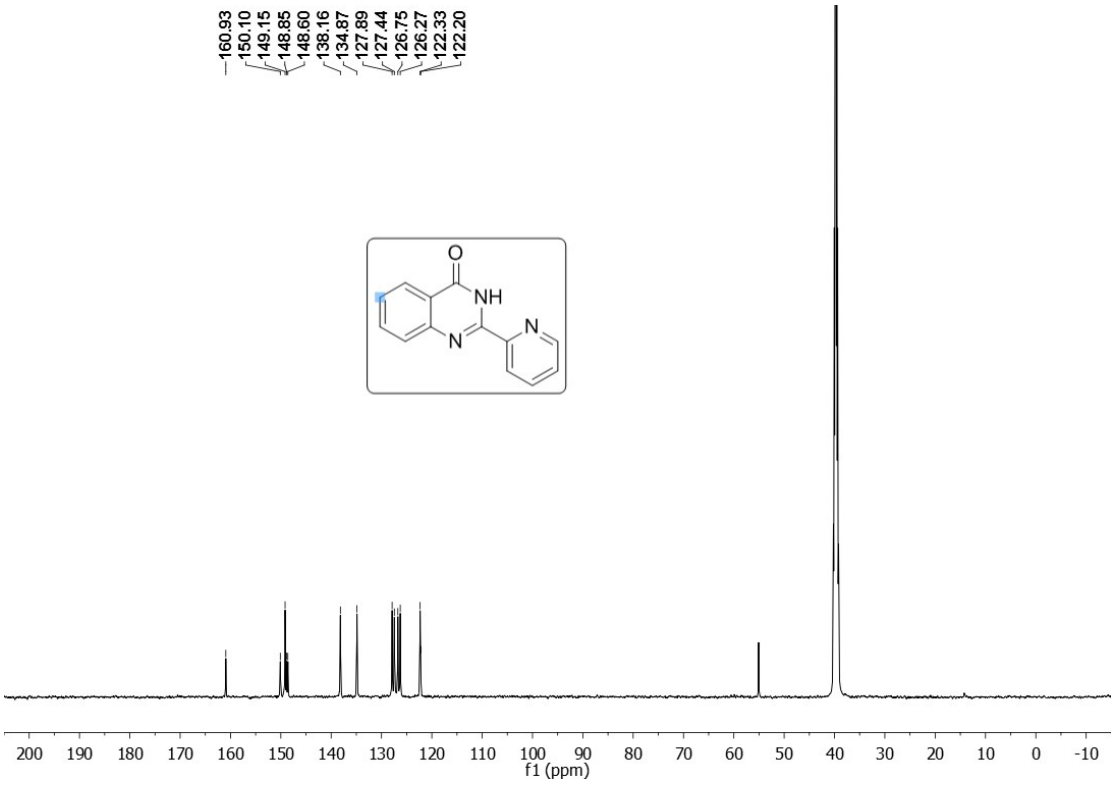
The ^{1}H and ^{13}C NMR spectra of compounds (3ar)



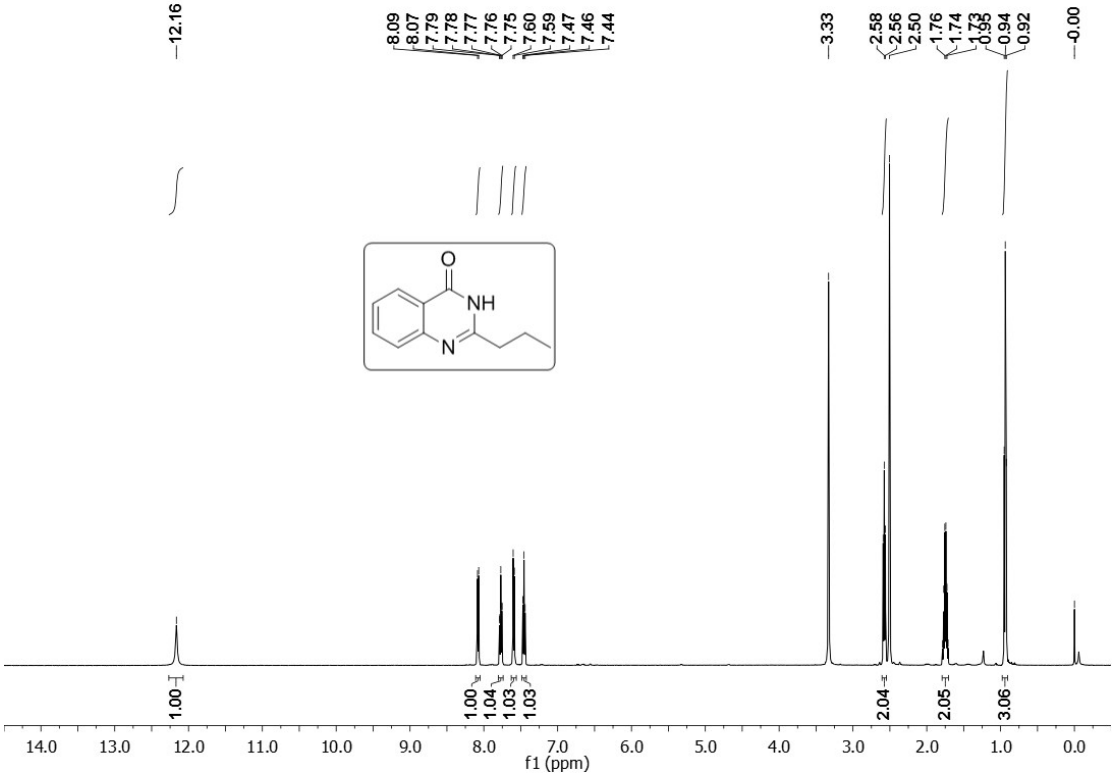


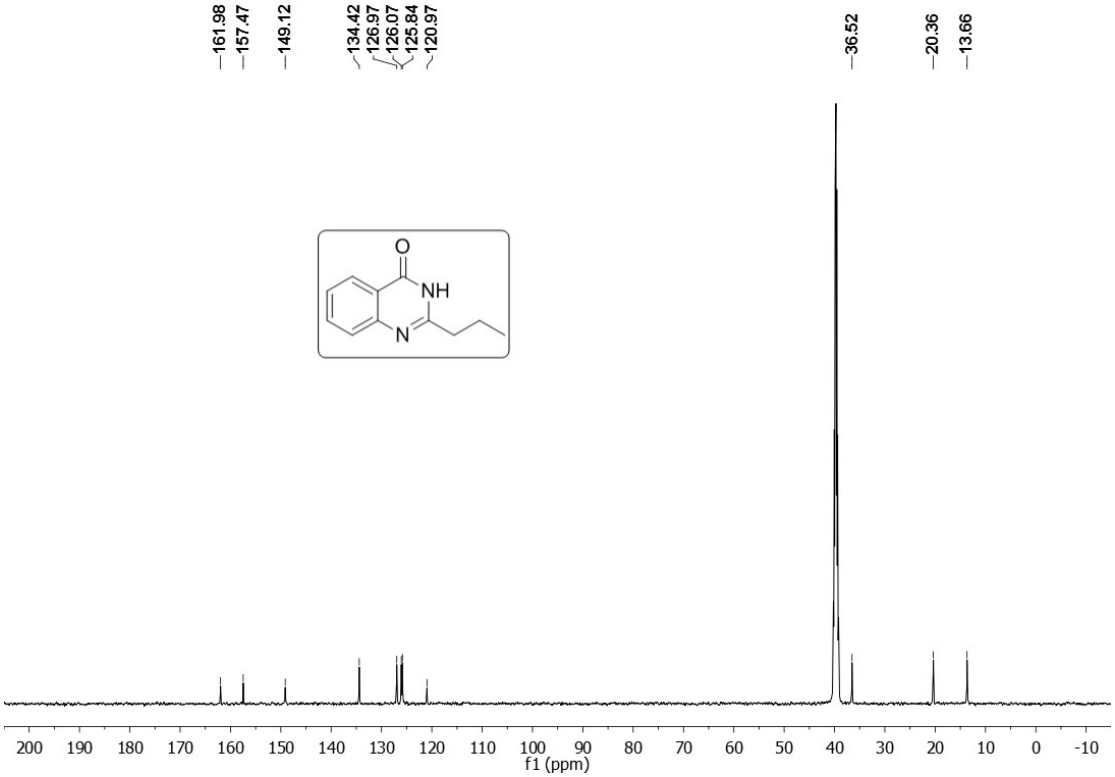
The ^{1}H and ^{13}C NMR spectra of compounds (3as)



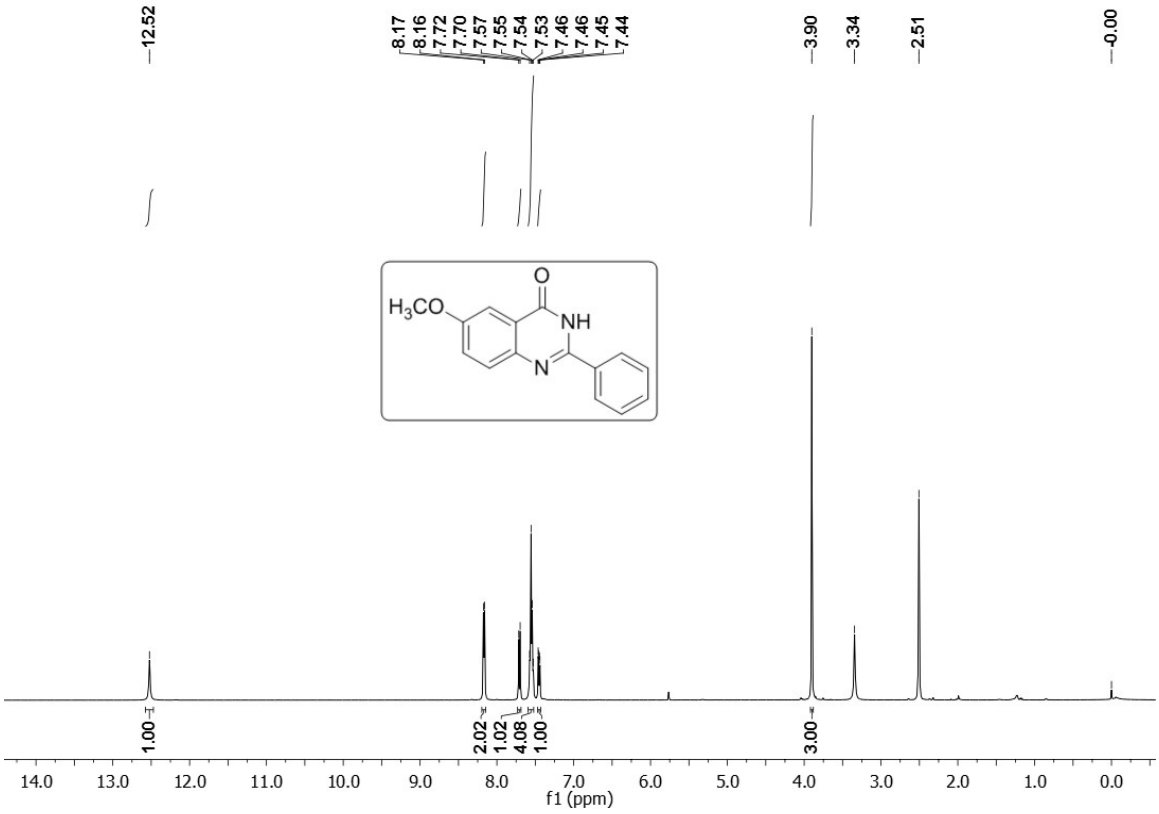


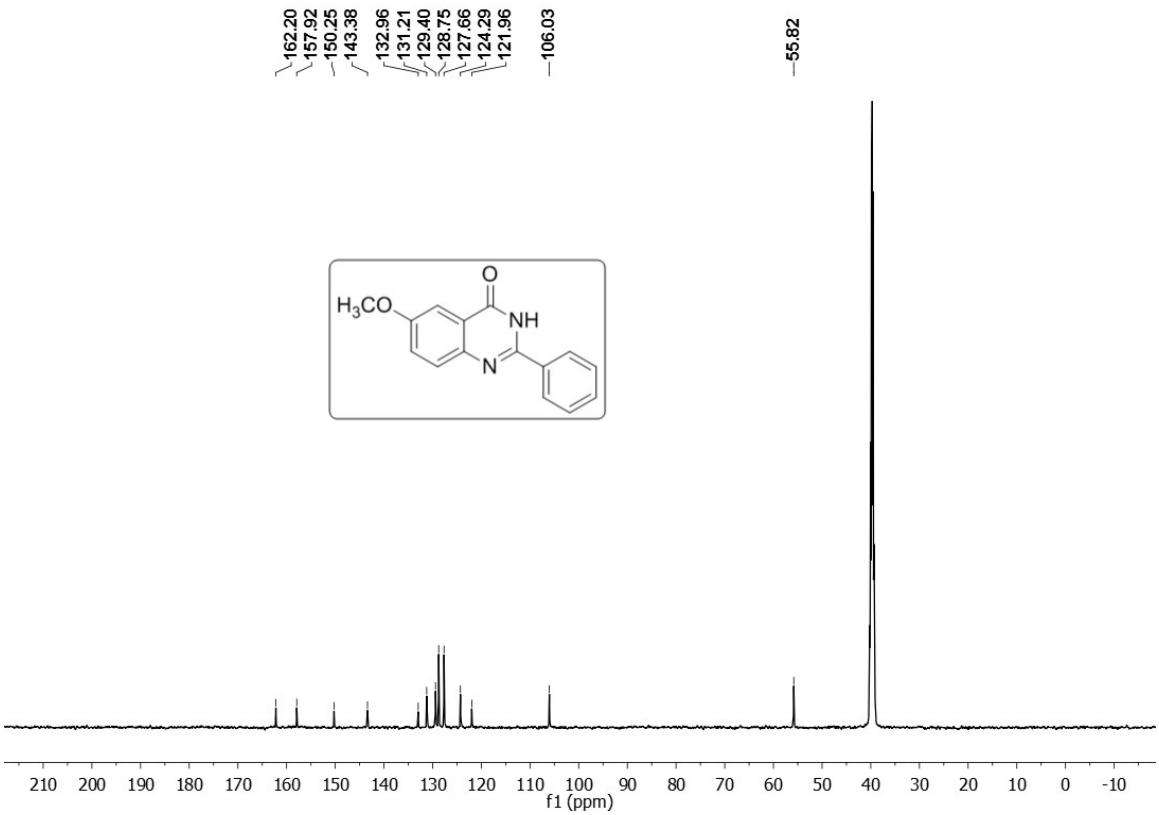
The ^{1}H and ^{13}C NMR spectra of compounds (3at)



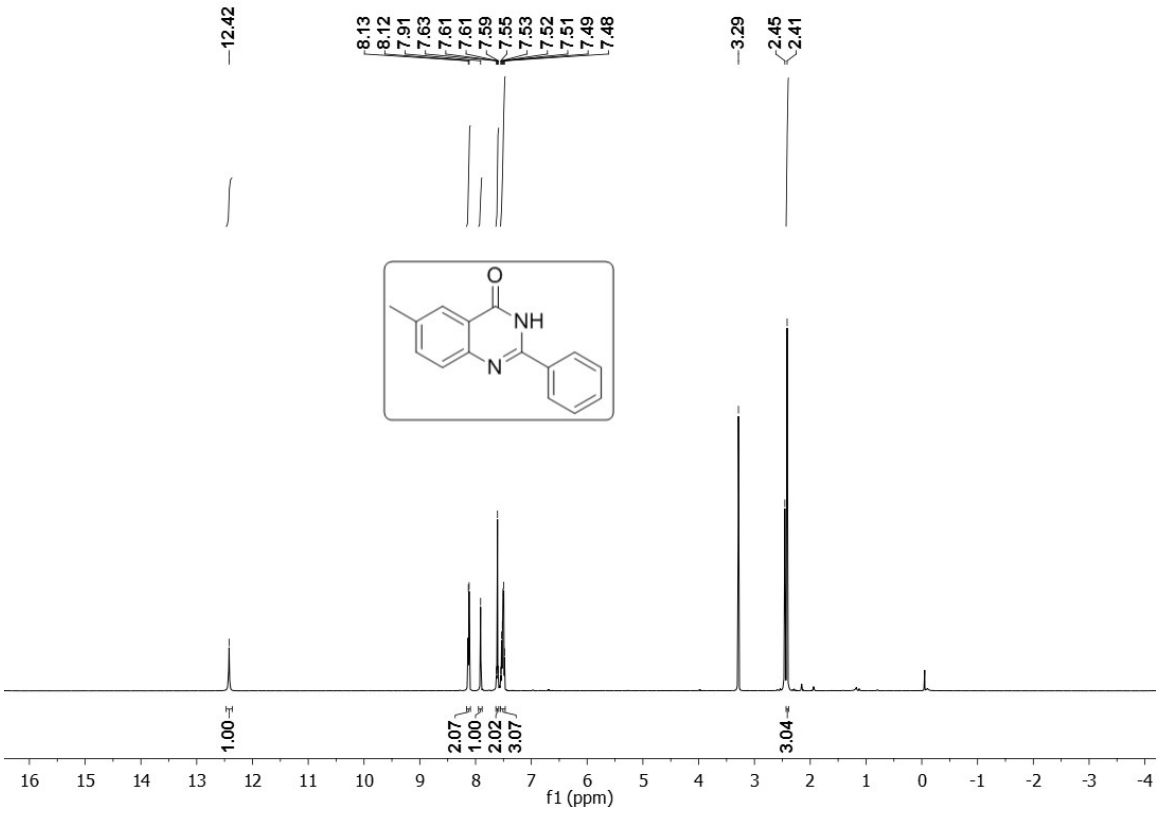


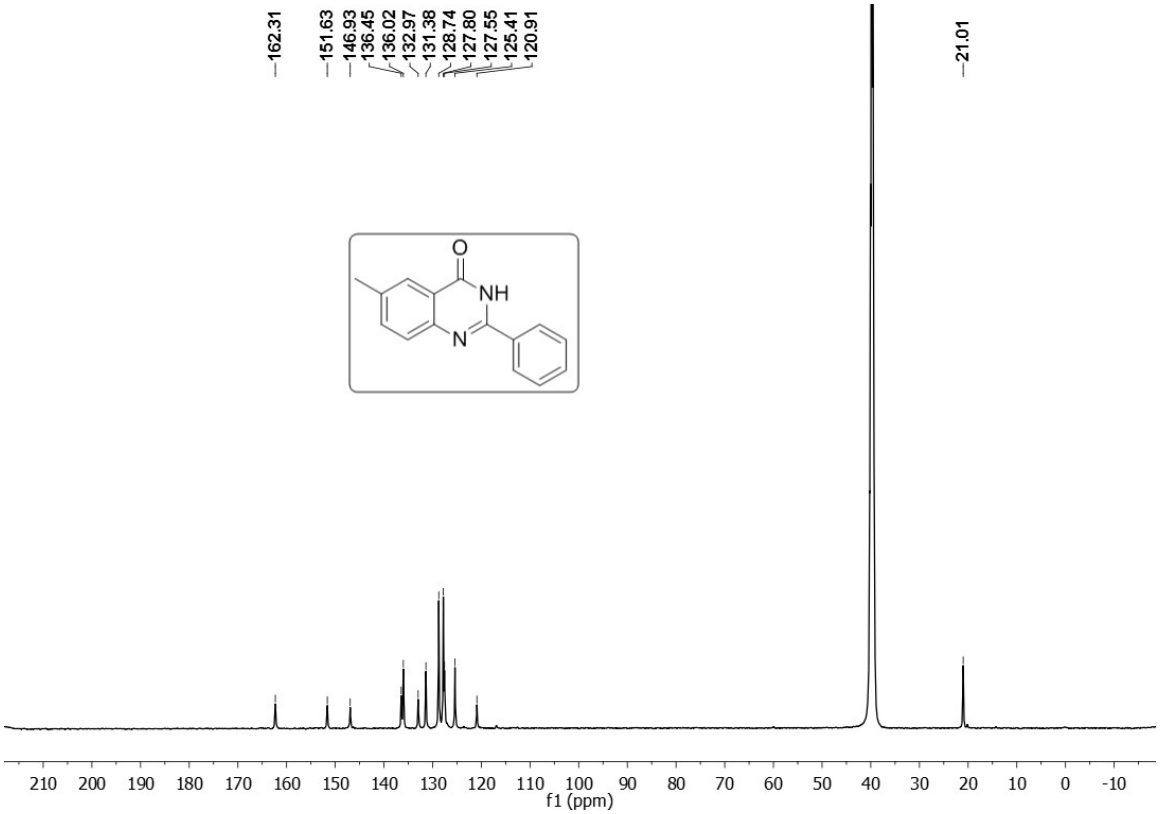
The ^{1}H and ^{13}C NMR spectra of compounds (3ba)



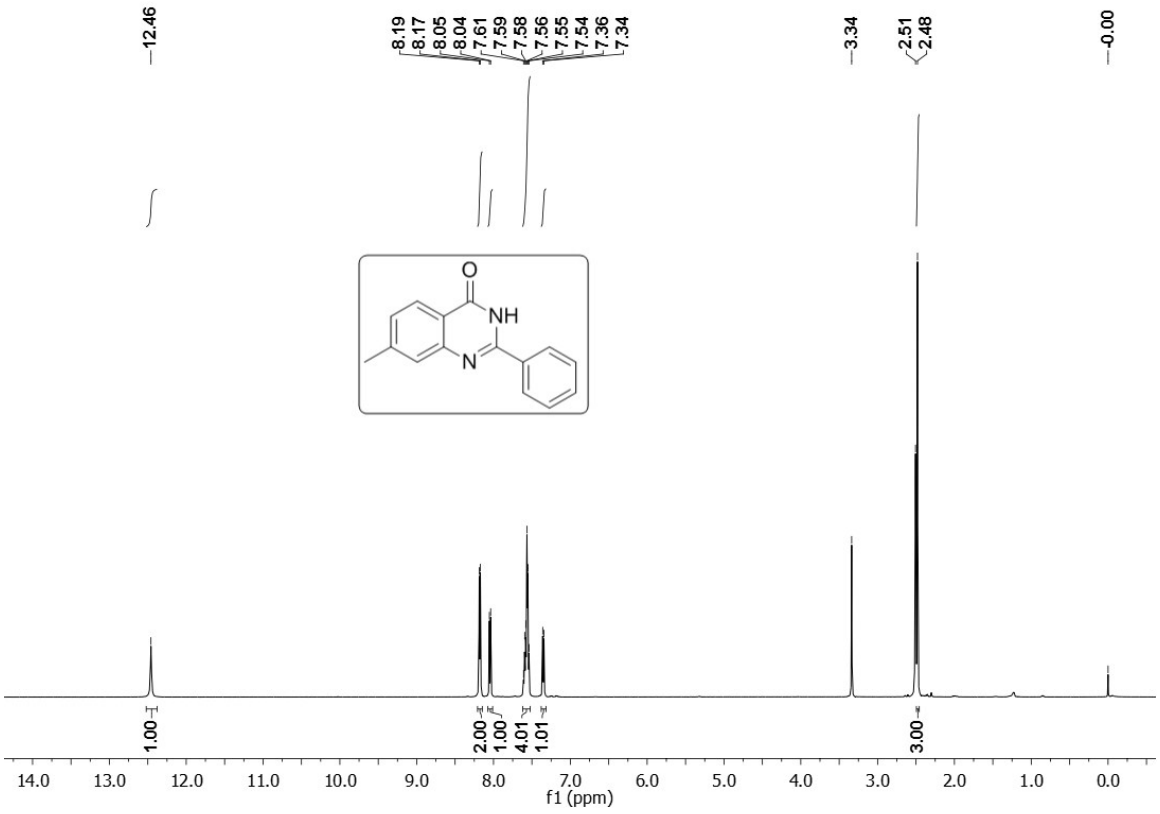


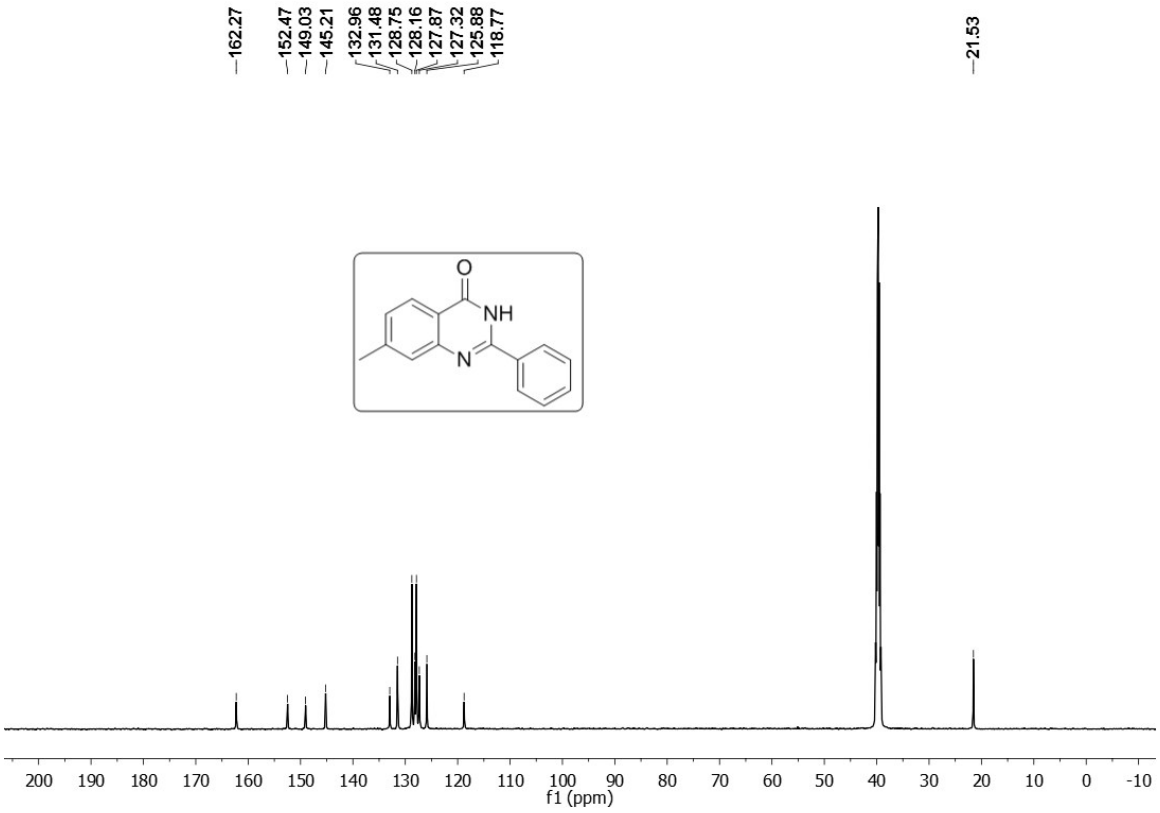
The ^{1}H and ^{13}C NMR spectra of compounds (3ca)



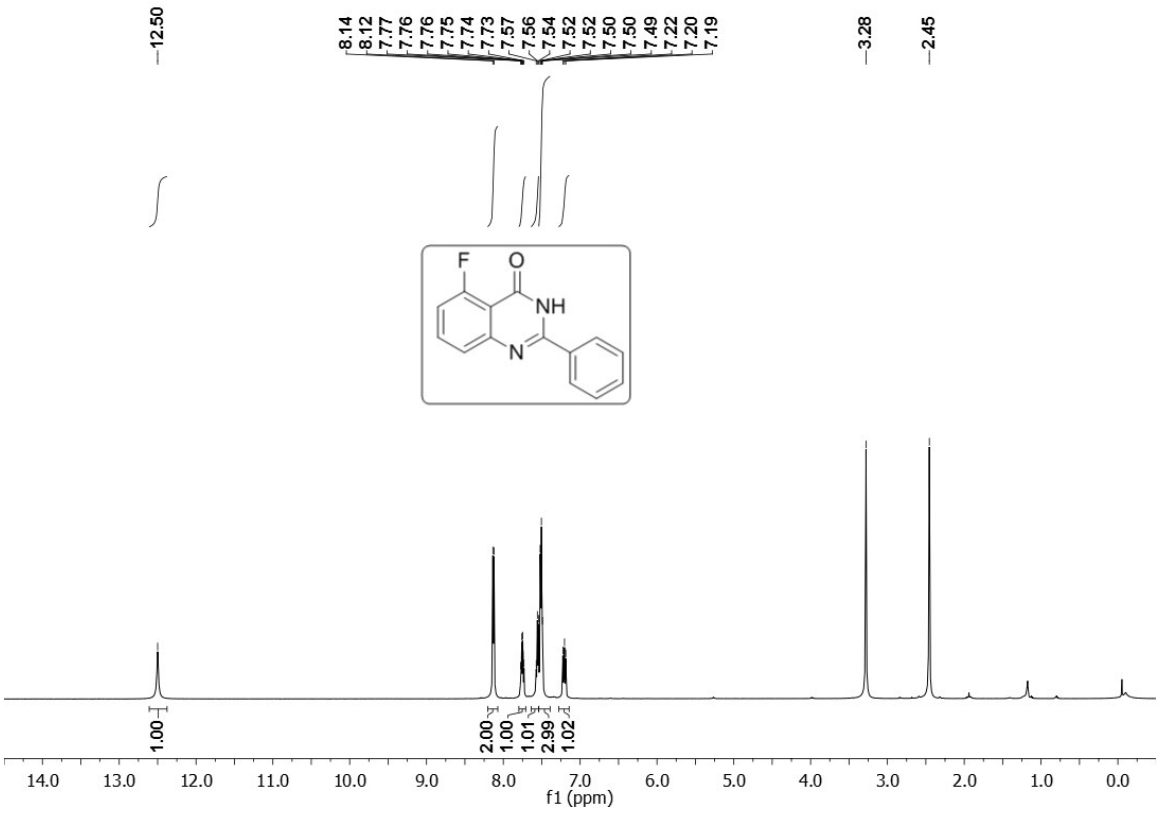


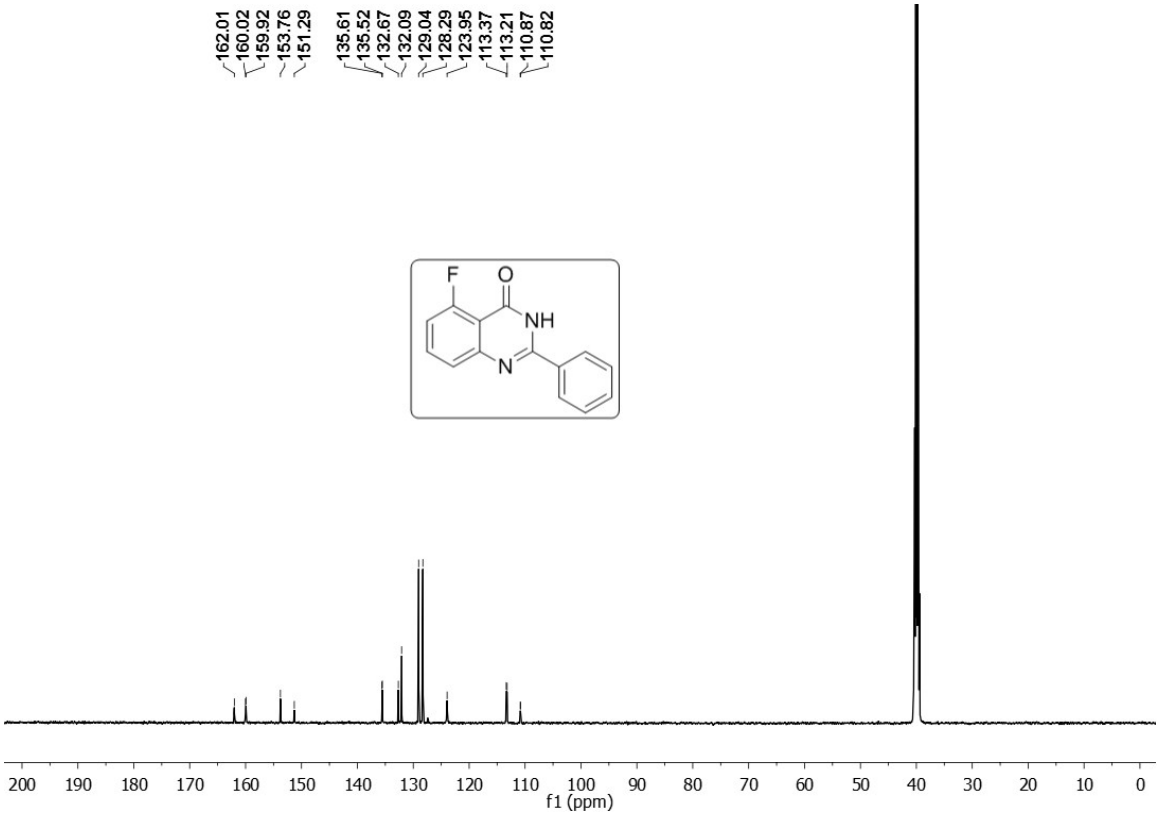
The ^{1}H and ^{13}C NMR spectra of compounds (3da)



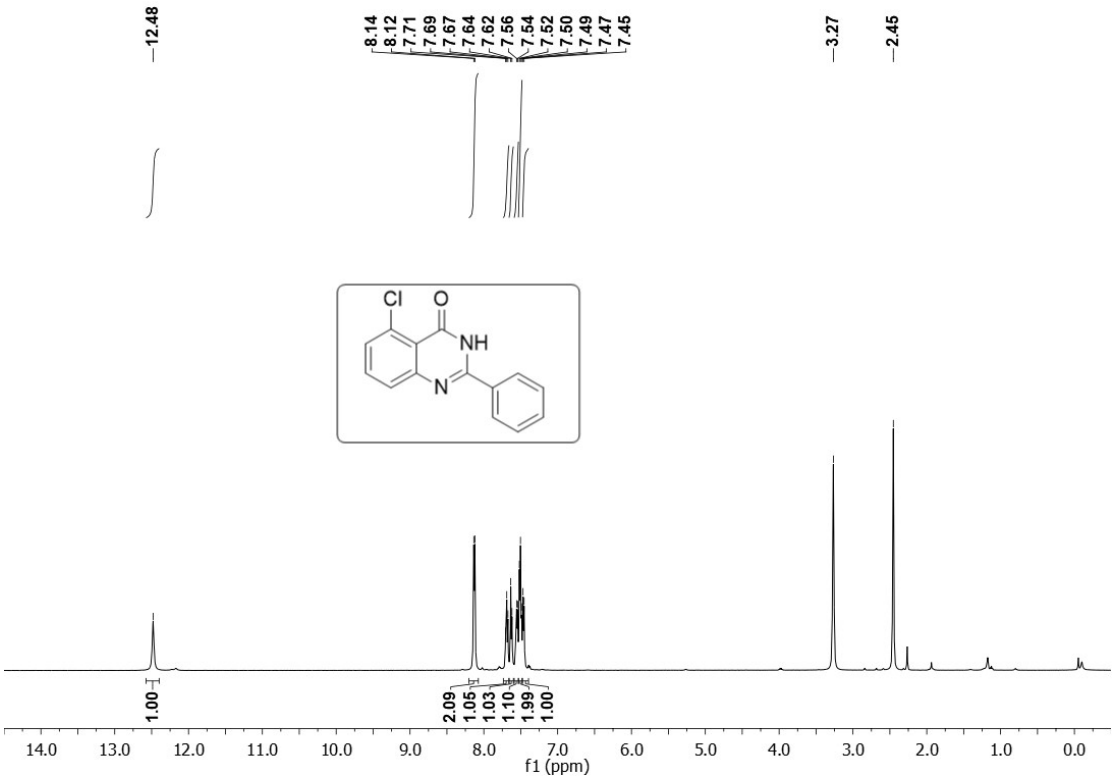


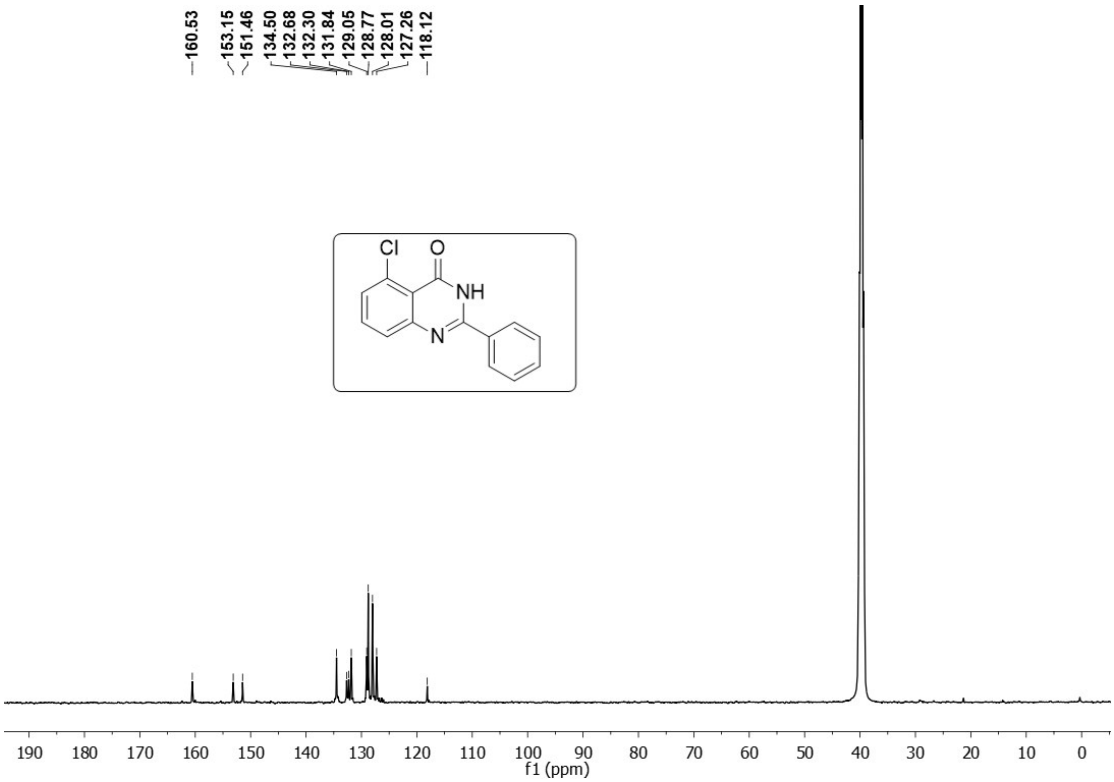
The ^{1}H and ^{13}C NMR spectra of compounds (3ea)



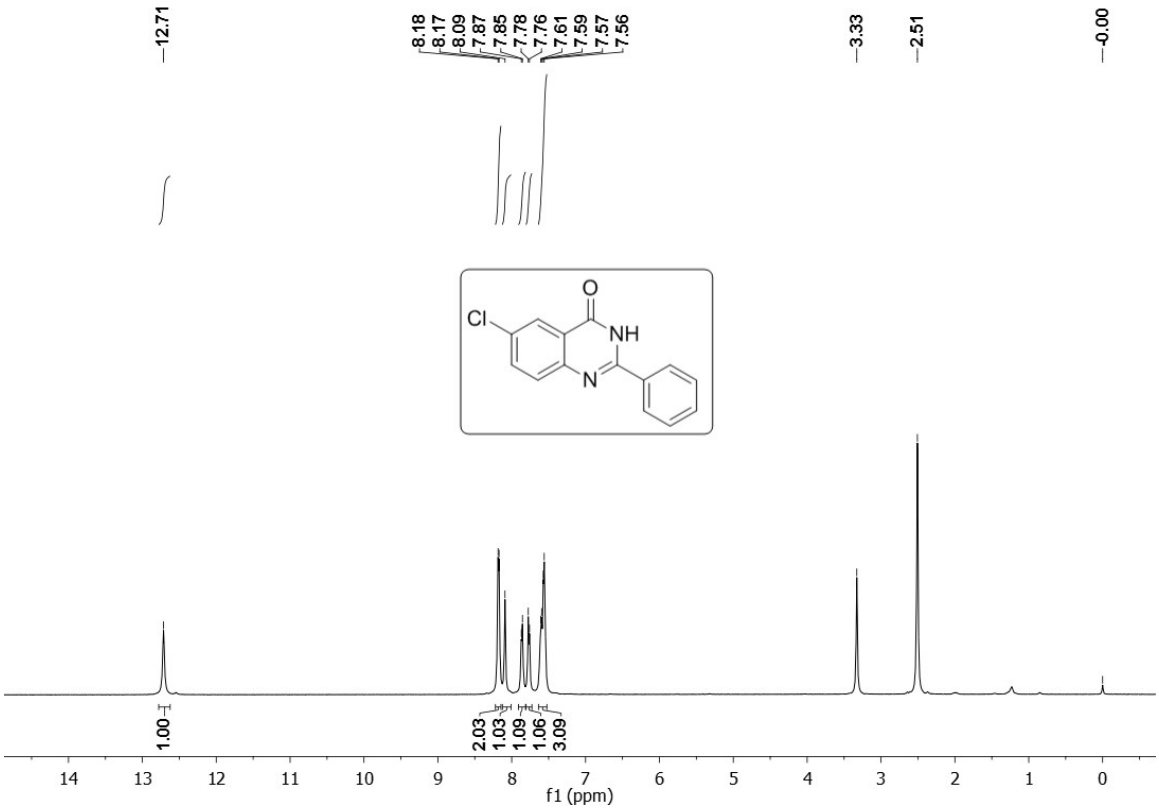


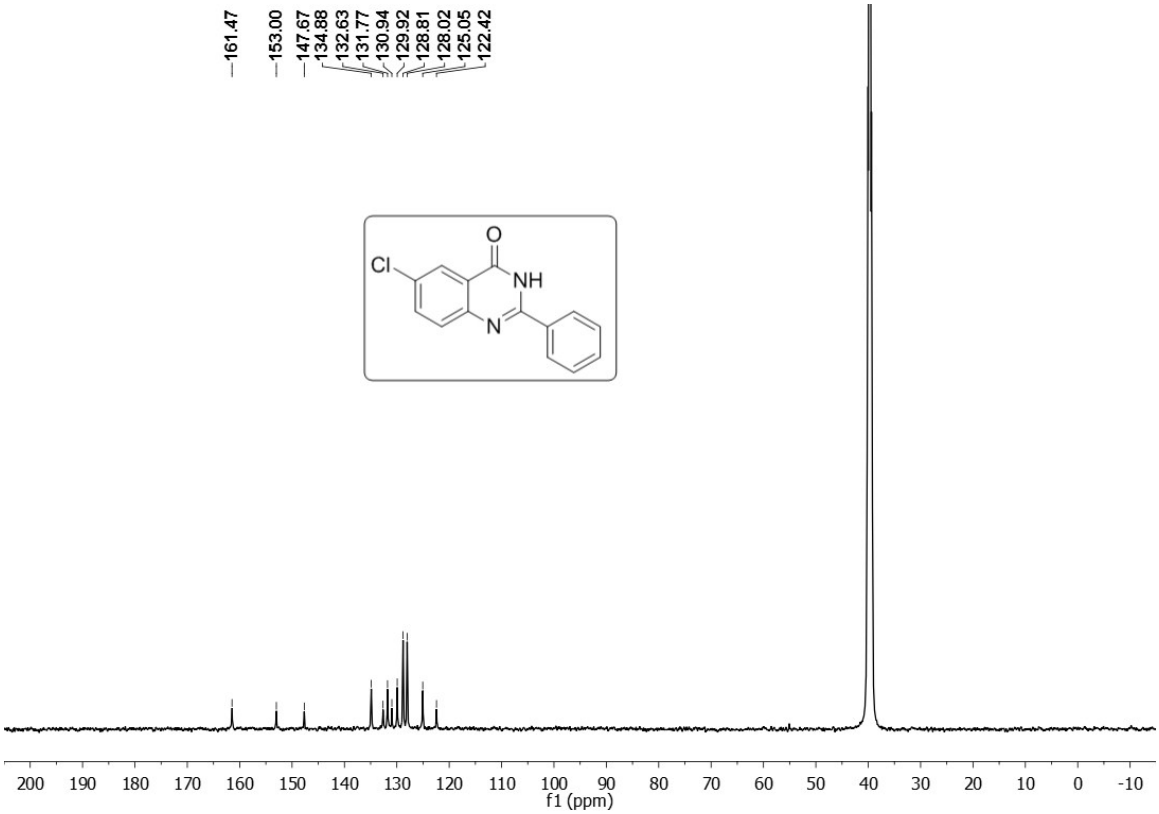
The ^{1}H and ^{13}C NMR spectra of compounds (3fa)



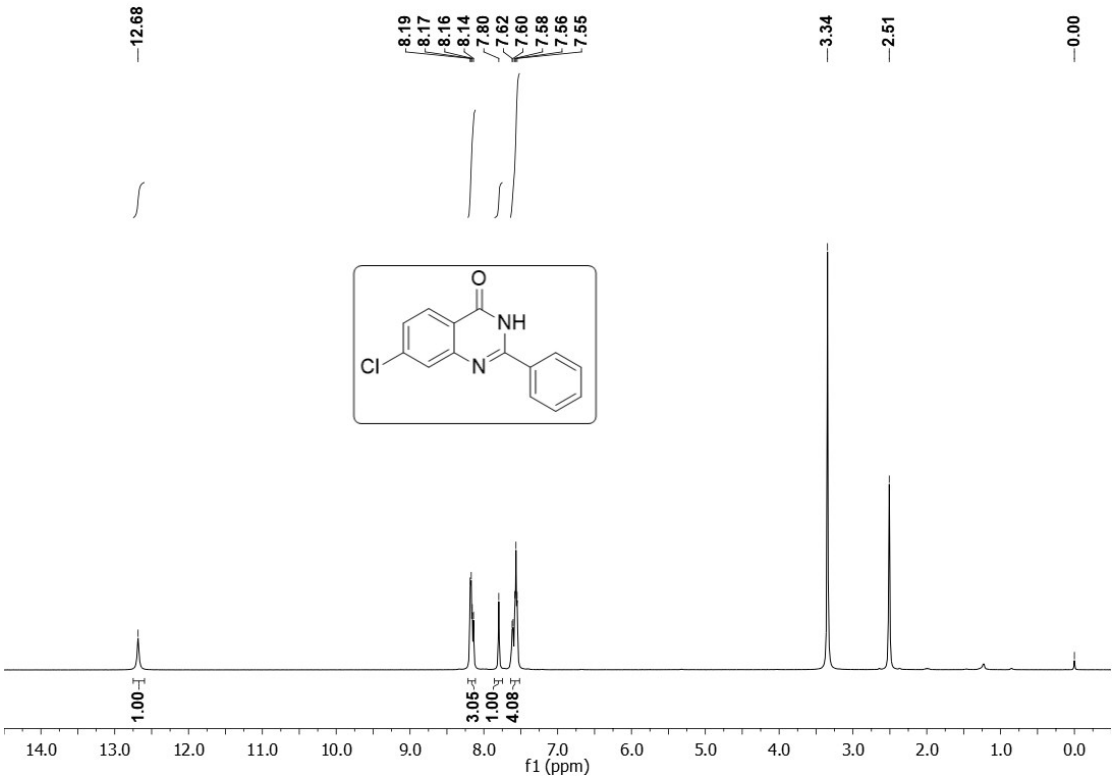


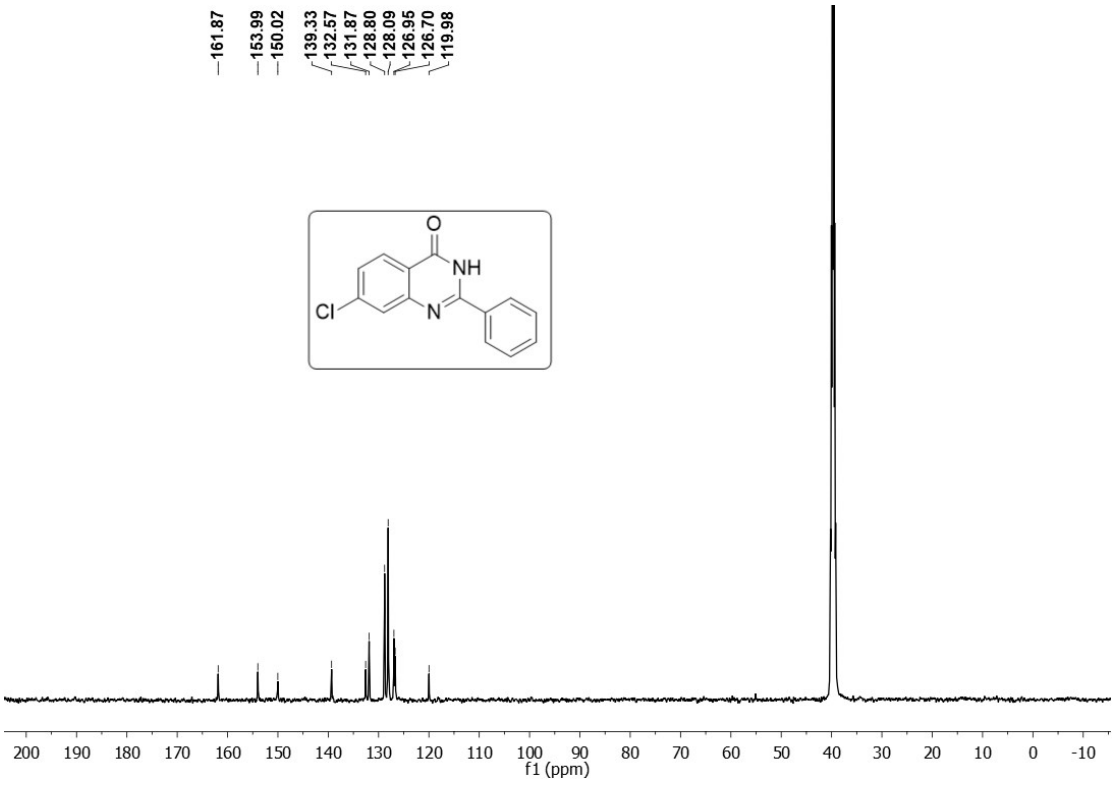
The ^{1}H and ^{13}C NMR spectra of compounds (3ga)



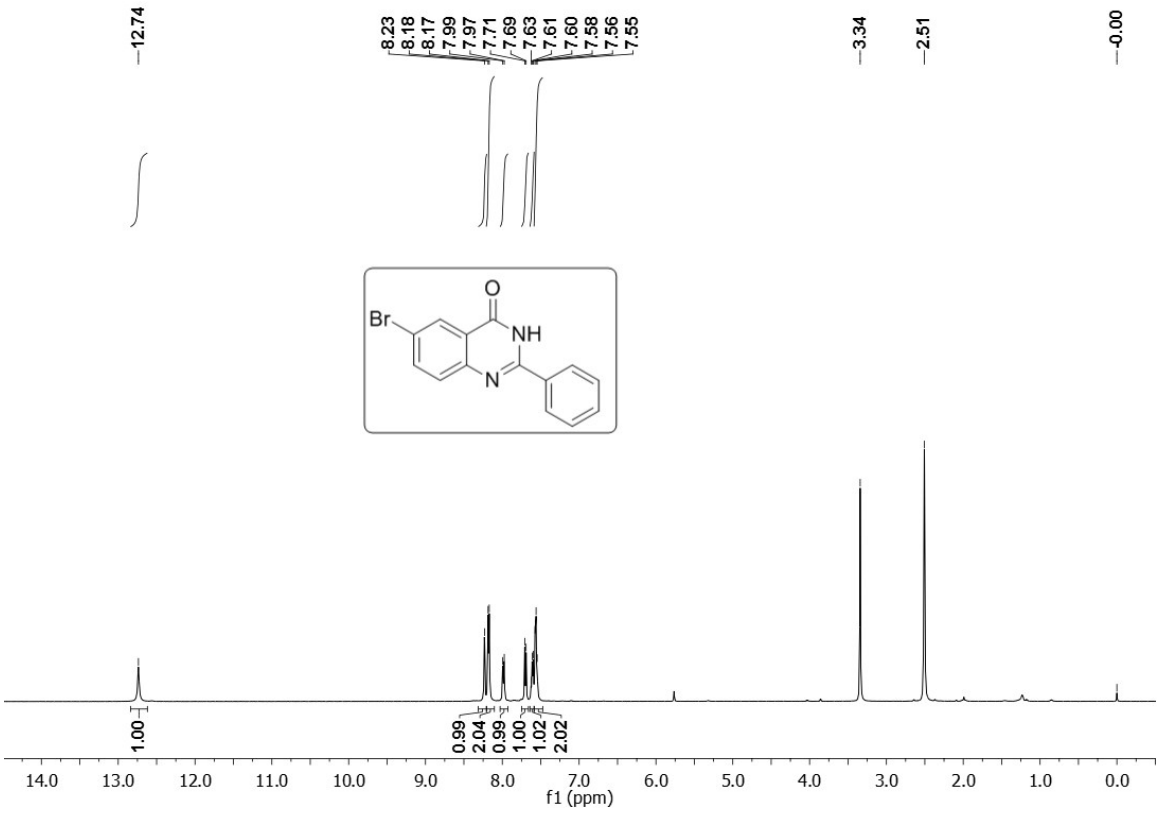


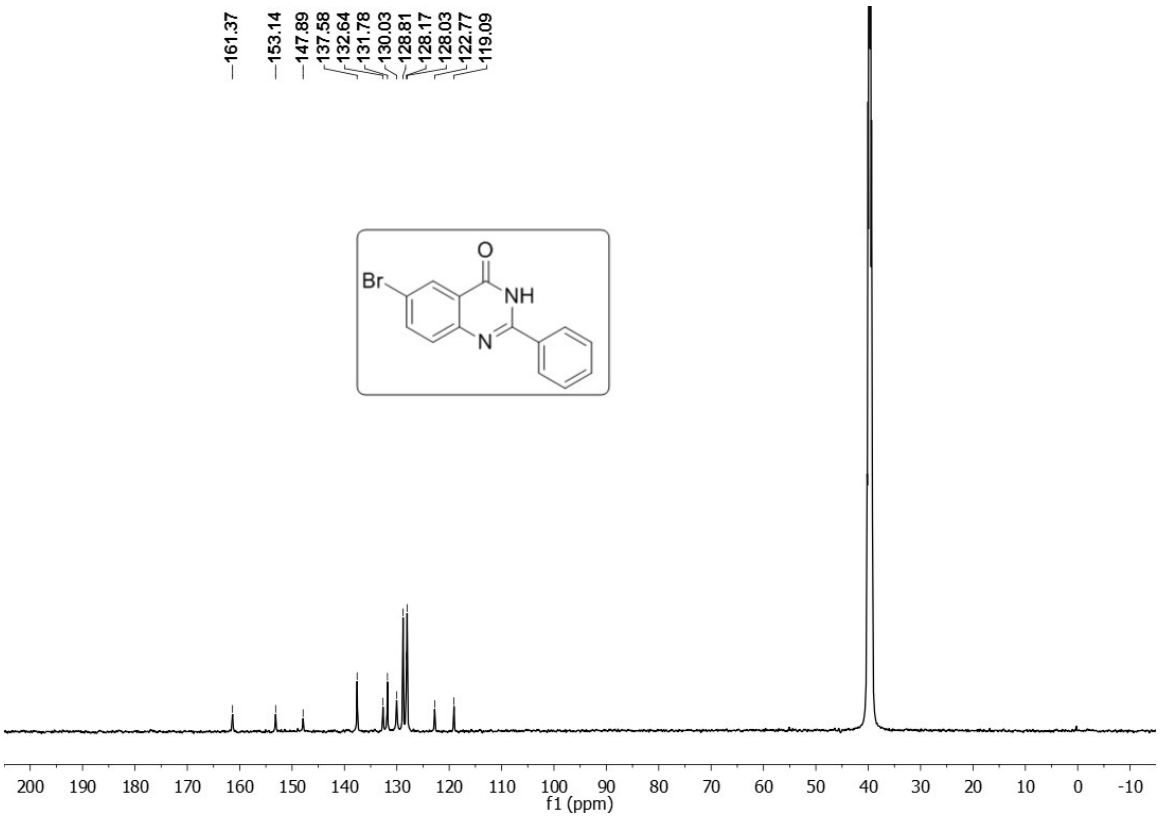
The ^{1}H and ^{13}C NMR spectra of compounds (3ha)



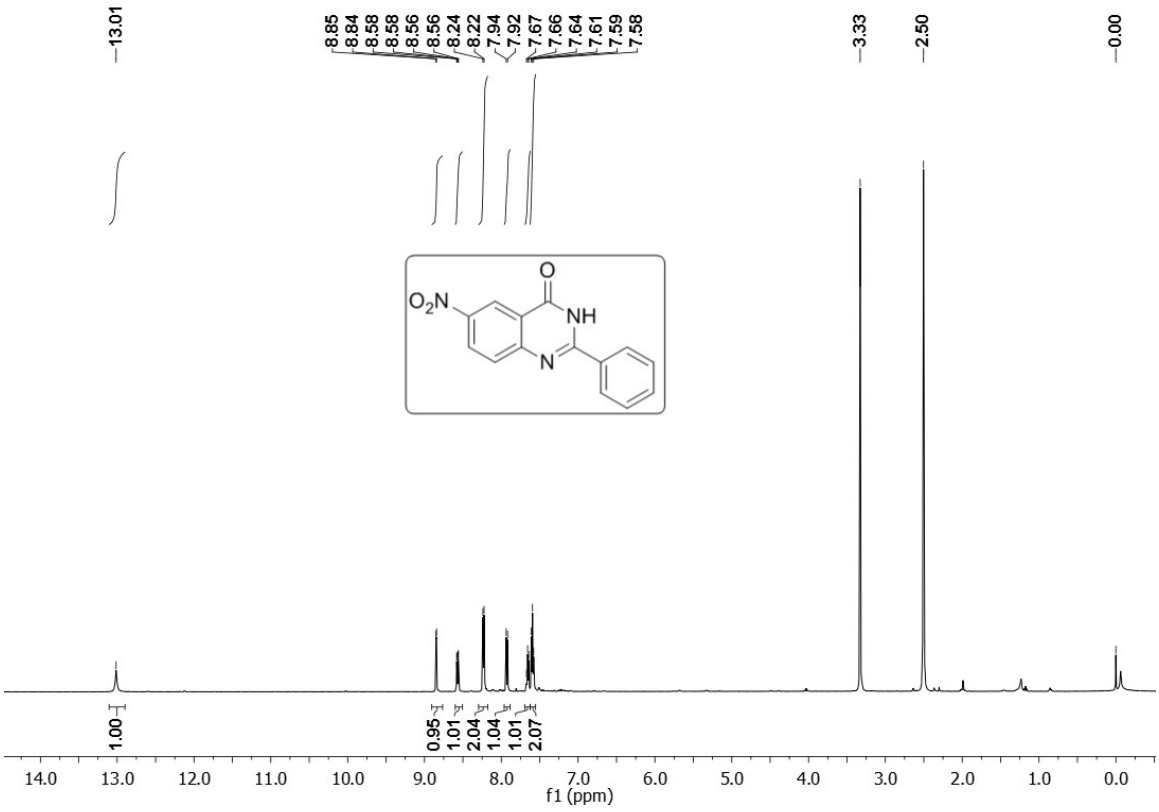


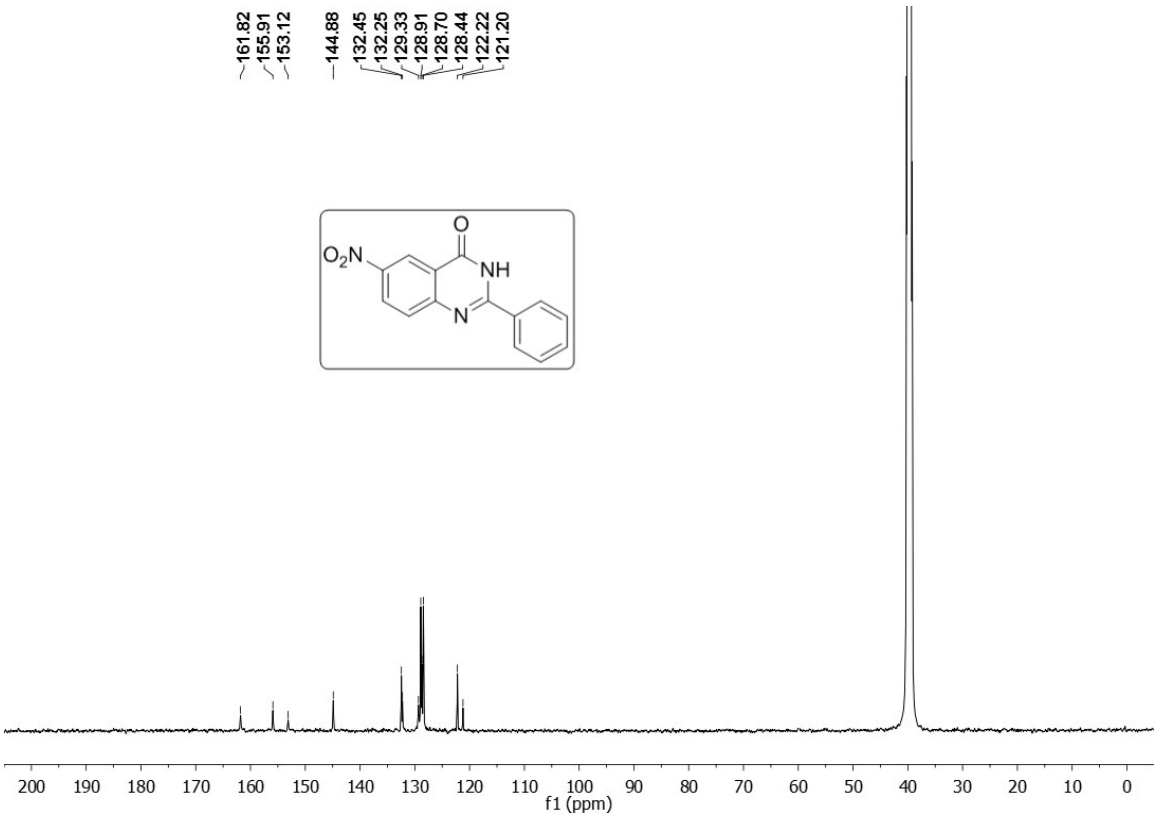
The ^{1}H and ^{13}C NMR spectra of compounds (3ia)



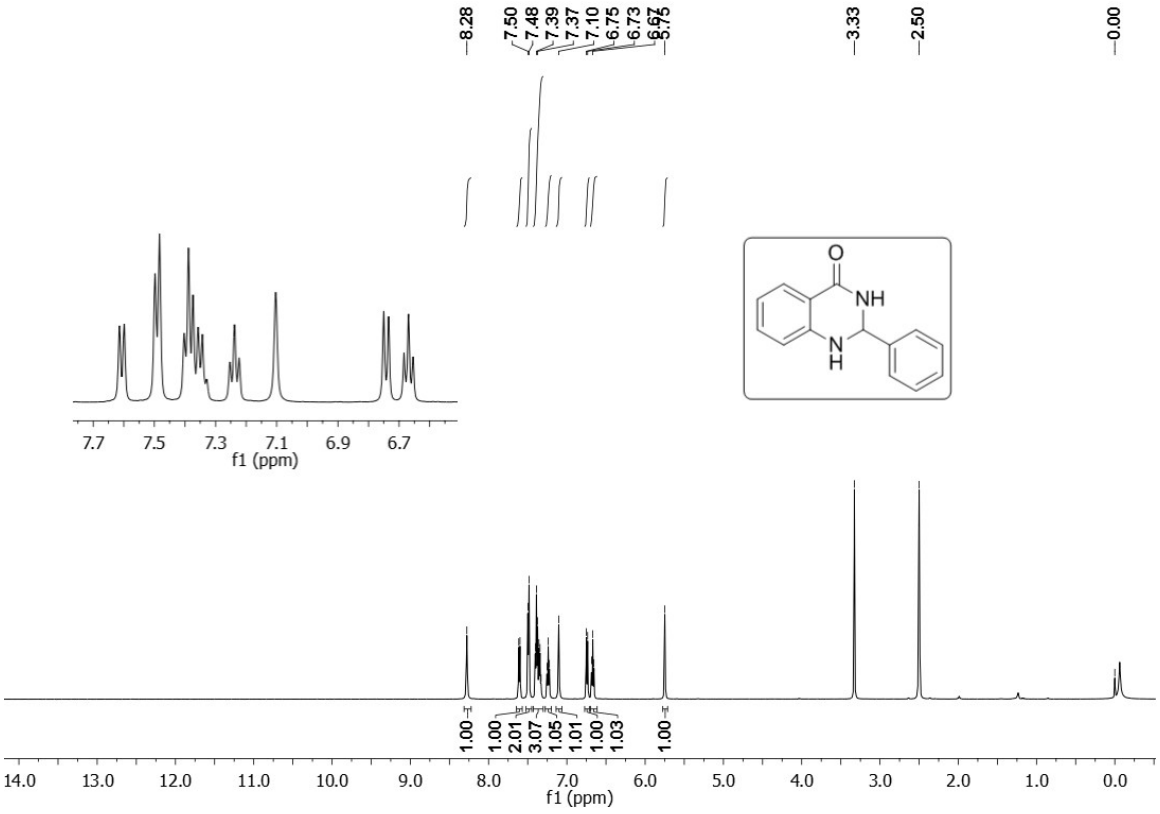


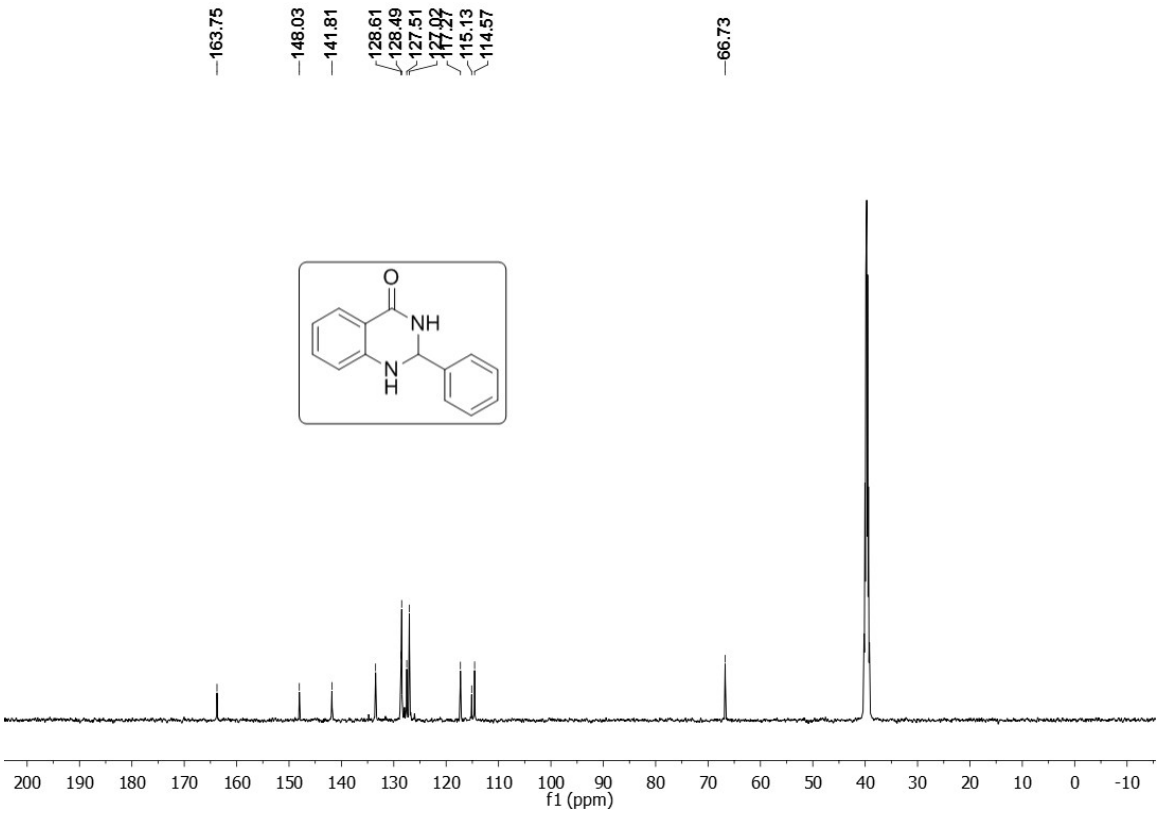
The ^{1}H and ^{13}C NMR spectra of compounds (3ja)





The ^{1}H and ^{13}C NMR spectra of compounds (6a)





The ^{1}H and ^{13}C NMR spectra of compounds (7a)