Electronic Supplementary Material (ESI) for RSC Advances.

PIDA-mediated Intramolecular Oxidative C-N Bond Formation for the Direct Synthesis of Quinoxalines from Enaminones

Hong Zhang,[a] Jinhai Shen, [a] Zhenhui Yang,[a] and Xiuling Cui[a]*

*Engineering Research Center of Molecular Medicine of Ministry of Education, Key Laboratory of Fujian Molecular Medicine, Key Laboratory of Xiamen Marine and Gene Drugs, School of Biomedical Sciences, Huaqiao University, Xiamen 361021, P. R. China, *e-mail: cuixl@hqu.edu.cn*

Contents

1. General information:

Unless otherwise stated, all commercial materials and solvents were used directly without further purification. Melting points were determined in open glass capillaries and were uncorrected. ^{1}H NMR spectra were recorded on 400 MHz spectrometers, and ^{13}C NMR spectra were recorded on a 100 MHz spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ and DMSO-d_6 as an internal standard at room temperature. ^{13}C NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm) and DMSO-d_6 (δ = 39.5 ppm). High-resolution mass spectra (HRMS) were equipped with an ESI source and a TOF detector. Column chromatography was performed on silica gel (70-230 mesh ASTM) using the reported eluents. Thin-layer chromatography (TLC) was carried out on 4×15 cm plates with a layer thickness of 0.2 mm (silica gel 60 F_{254}). The *N*-(2-acetaminophenyl)enaminones **1** were prepared according to the literatures.[1-2]

2. General Procedure for the Preparation of Quinoxalines **2**

A mixture of *N*-(2-acetaminophenyl) enaminones **1** (0.2 mmol), PIDA (71 mg, 0.22 mmol), PhCOOH (25 mg, 0.2 mmol) in toluene (2 mL) was stirred at 80 ^{o}C under air atmosphere for 12 h (monitored by TLC). After evaporation of toluene, H_2O was added and the resultant was extracted with EtOAc (3×10 mL). The combined EtOAc extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 10 % EtOAc in PE) to give **2**.

3. Chemical transformations of product **2a**:

The compounds **3a** and **4a** were prepared according to the literatures.[3] A

suspension of **2a** (62 mg, 0.2 mmol) in EtOH (2 mL) was heated at 50 ^{O}C, then KBH_4 was added (23 mg, 0.4 mmol). This mixture was stirred at 50 ^{O}C for 3 h (monitored by TLC). After evaporation of EtOH, H_2O was added and the resultant was extracted with EtOAc (3×10 mL). The combined EtOAc extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 10 % EtOAc in PE) to give **3a**.

A suspension of **2a** (62 mg, 0.2 mmol) in EtOH (2 mL) was heated at 50 ^{O}C, then KBH_4 was added (23 mg, 0.4 mmol). This mixture was stirred at 50 ^{O}C for 3 h (monitored by TLC). After evaporation of EtOH, concentrated H_2SO_4 (0.5 mL) was added and stirred at 0 ^{O}C for 5 h (monitored by TLC). Then the solution was poured slowly in water at 0 ^{O}C. The final mixture was extracted with CH_2Cl_2 (3×10 mL). The combined CH_2Cl_2 extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 6 % EtOAc in PE) to give **4a**.

4. Preparation of 1-(2-Benzoyl-3-phenylquinoxalin-1(2H)-yl)ethan-1-one 5a

A mixture of *N*-(2-acetaminophenyl) enaminones **1a** (178 mg, 0.5 mmol), PIDA (177 mg, 0.55mmol), PhCOOH (61 mg, 0.5 mmol) in toluene (5 mL) was stirred at 80 ^{O}C under air atmosphere for 2 h. After evaporation of toluene, H_2O was added and the resultant was extracted with EtOAc (3×15 mL). The combined EtOAc extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 10 % EtOAc in PE) to give **5a**.

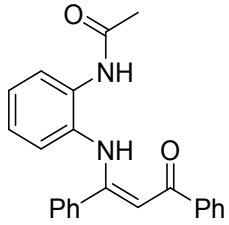
Reference

1. Y. Zheng, C. Yang, D. Zhang-Negrerie, Y. Du, K. Zhao, *Tetrahedron Letters*, **2013**, 54, 6157.

2. X. Li, Y. Du, Z. Liang, X. Li, Y. Pan, K. Zhao, *Organic Letters*, **2009**, 11, 2643.

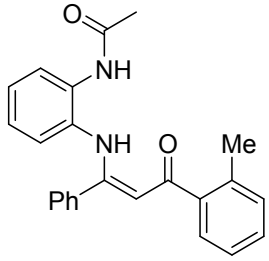
3. Nicole V, Pierre M. *Bulletin de la Societe Chimique de France*, **1977**, (11-12, Pt. 2), 1245.

5. Characterization of the products



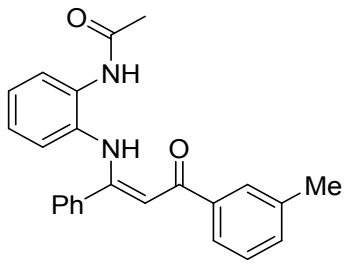
(*Z*)-*N*-(2-((3-oxo-1,3-diphenylprop-1-en-1-yl)amino)phenyl)acetamide **(1a)**

289 mg, 80 % yield; Yellow solid; mp: 177-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 8.19 (s, 1H), 7.91 (dd, *J* = 18.2, 7.7 Hz, 3H), 7.44 (dt, *J* = 24.8, 7.2 Hz, 3H), 7.35 – 7.20 (m, 5H), 7.01 (t, *J* = 7.7 Hz, 1H), 6.76 (t, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 7.9 Hz, 1H), 6.18 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.1, 169.1, 162.8, 139.6, 135.2, 131.6, 131.4, 131.2, 129.8, 128.4, 128.4, 128.0, 127.2, 125.9, 125.5, 124.5, 123.4, 97.7, 24.3. HRMS m/z (ESI) calcd for $C_{23}H_{21}N_2O_2$ $(M + H)^+$ 357.1598, found 357.1598.



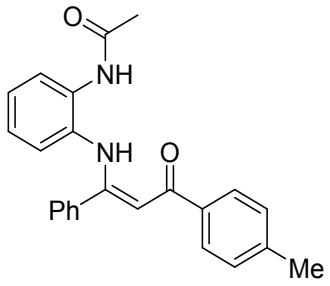
(*Z*)-*N*-(2-((3-oxo-1-phenyl-3-(*o*-tolyl)prop-1-en-1-yl)amino)phenyl)acetamide **(1b)**

281 mg, 76 % yield; Yellow solid; mp: 188-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.55 (s, 1H), 8.08 (s, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.37 – 7.13 (m, 8H), 7.01 (t, *J* = 7.7 Hz, 1H), 6.78 (t, *J* = 7.4 Hz, 1H), 6.52 (d, *J* = 7.8 Hz, 1H), 5.85 (s, 1H), 2.53 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.0, 169.1, 162.1, 141.1, 136.0, 135.0, 131.6, 131.3, 131.1, 129.8, 129.6, 128.4, 128.0, 127.6, 125.7, 125.5, 125.4, 124.7, 123.8, 101.5, 24.2, 20.4. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_2$ $(M + H)^+$ 371.1754, found 371.1755.



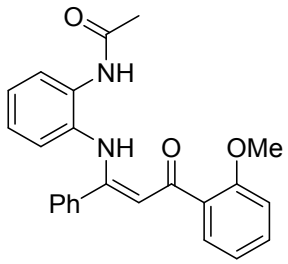
(*Z*)-*N*-(2-((3-oxo-1-phenyl-3-(*m*-tolyl)prop-1-en-1-yl)amino)phenyl)acetamide **(1c)**

278 mg, 75 % yield; Yellow solid; mp: 170-171 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 8.10 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 5.6 Hz, 2H), 7.37 – 7.21 (m, 7H), 7.05 – 6.98 (m, 1H), 6.77 (t, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 7.9 Hz, 1H), 6.18 (s, 1H), 2.38 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 169.0, 162.7, 139.6, 138.1, 135.3, 132.3, 131.6, 131.1, 129.8, 128.4, 128.3, 128.0, 127.9, 125.9, 125.6, 124.4, 124.4, 123.3, 97.8, 24.4, 21.4. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_2$ $(M + H)^+$ 371.1754, found 371.1754.



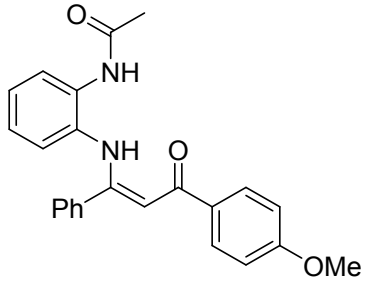
(*Z*)-*N*-(2-((3-oxo-1-phenyl-3-(*p*-tolyl)prop-1-en-1-yl)amino)phenyl)acetamide **(1d)**

307 mg, 83 % yield; Yellow solid; mp: 151-153 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.59 (s, 1H), 8.28 (s, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 2H), 7.34 – 7.16 (m, 7H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.75 (t, *J* = 7.5 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 1H), 6.16 (s, 1H), 2.38 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 169.1, 162.4, 142.0, 136.9, 135.3, 131.6, 131.1, 129.7, 129.1, 128.3, 128.0, 127.3, 125.8, 125.4, 124.3, 123.3, 97.7, 24.3, 21.4. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_2$ $(M + H)^+$ 371.1754, found 371.1752.



(*Z*)-*N*-(2-((3-(2-methoxyphenyl)-3-oxo-1-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1e)**

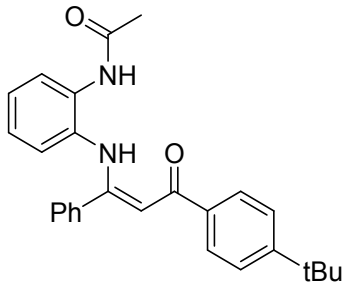
250 mg, 65 % yield; Yellow solid; mp: 220-222 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.22 (s, 1H), 9.87 (s, 1H), 7.63 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.49 – 7.32 (m, 7H), 7.12 (d, *J* = 8.3 Hz, 1H), 7.06 – 6.95 (m, 2H), 6.82 (t, *J* = 7.6 Hz, 1H), 6.40 (d, *J* = 8.0 Hz, 1H), 6.10 (s, 1H), 3.84 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 189.7, 169.4, 159.9, 157.5, 136.2, 134.9, 132.5, 131.5, 130.4, 130.2, 130.1, 129.0, 128.5, 126.6, 125.7, 125.5, 124.8, 120.9, 112.6, 103.0, 56.2, 23.6. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_3$ $(M + H)^+$ 387.1703, found 387.1703.



(*Z*)-*N*-(2-((3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1f)**

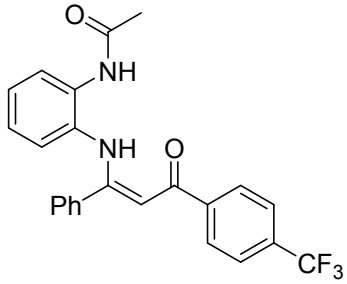
273 mg, 71 % yield; Yellow solid; mp: 172-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.54 (s, 1H), 8.16 (s, 1H), 7.93 (d, *J* = 8.7 Hz, 3H), 7.37 – 7.20 (m, 5H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.75 (t, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 7.9 Hz, 1H), 6.15 (s, 1H), 3.84 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 169.0, 162.4, 162.2, 135.4, 132.2, 131.7, 131.1, 129.7, 129.3, 128.4, 128.0, 125.9,

125.4, 124.3, 123.1, 113.6, 97.5, 55.3, 24.4. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_3$ $(M + H)^+$ 387.1703, found 387.1703.



(*Z*)-*N*-(2-((3-(4-(*tert*-butyl)phenyl)-3-oxo-1-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1g)**

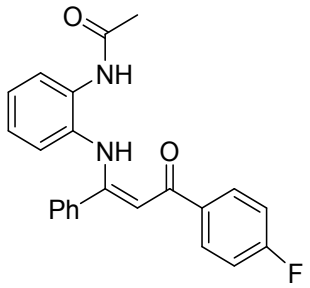
306 mg, 74 % yield; Yellow solid; mp: 238-240 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.60 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.85 (s, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.24 (m, 5H), 7.03 (dd, *J* = 11.4, 4.1 Hz, 1H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 7.8 Hz, 1H), 6.22 (s, 1H), 2.27 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 168.8, 162.6, 155.2, 136.8, 135.4, 131.9, 131.0, 129.9, 128.5, 128.0, 127.2, 126.1, 125.7, 125.4, 124.4, 123.0, 97.8, 34.9, 31.2, 31.2, 31.2, 24.5. HRMS m/z (ESI) calcd for $C_{27}H_{29}N_2O_2$ $(M + H)^+$ 413.2224, found 413.2224.



(*Z*)-*N*-(2-((3-oxo-1-phenyl-3-(4-(trifluoromethyl)phenyl)prop-1-en-1yl)amino)phenyl)-acetamide **(1h)**

295 mg, 70 % yield; Yellow solid; mp: 200-201 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 9.93 (s, 1H), 8.23 (d, *J* = 8.1 Hz, 2H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.45 – 7.32 (m, 4H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.48 (d, *J* = 7.9 Hz, 1H), 6.27 (s, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz,

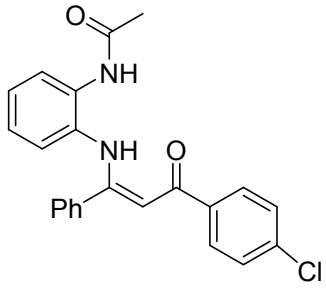
DMSO-d_6) δ 183.5, 165.9, 159.2, 139.7, 132.3, 131.0, 128.5, 128.1 (q, *J* = 31.8 Hz), 126.9, 125.5, 125.2, 125.0, 123.0, 122.5, 122.4 (q, *J* = 3.8 Hz), 122.3, 122.0, 121.0 (q, *J* = 272.9 Hz), 93.8, 20.1; ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.3. HRMS m/z (ESI) calcd for $C_{24}H_{20}F_3N_2O_2$ $(M + H)^+$ 425.1471, found 425.1471.



(*Z*)-*N*-(2-((3-(4-fluorophenyl)-3-oxo-1-phenylprop-1-en-1yl)amino)phenyl)acetamide

(1i)

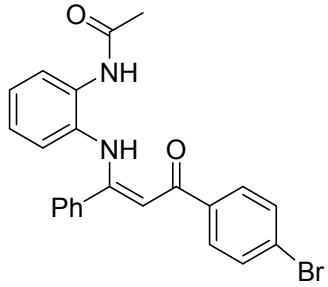
318 mg, 85 % yield; Yellow solid; mp: 154-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.60 (s, 1H), 8.15 (s, 1H), 8.00 – 7.90 (m, 2H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.21 (m, 5H), 7.07 (t, *J* = 8.6 Hz, 2H), 7.01 (t, *J* = 7.7 Hz, 1H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 7.9 Hz, 1H), 6.11 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.5, 169.1, 164.8 (d, *J* = 252.2 Hz), 162.9, 135.8 (d, *J* = 2.8 Hz), 135.1, 131.5, 131.3, 129.9, 129.6 (d, *J* = 8.9 Hz), 128.4, 127.9, 125.9, 125.6, 124.6, 123.6, 115.3 (d, *J* = 21.7 Hz), 97.2, 24.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.1; HRMS m/z (ESI) calcd for $C_{23}H_{20}FN_2O_2$ $(M + H)^+$ 375.1503, found 375.1503.



(*Z*)-*N*-(2-((3-(4-chlorophenyl)-3-oxo-1-phenylprop-1-en-1yl)amino)phenyl)acetamide

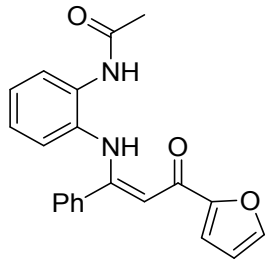
(1j)

311 mg, 80 % yield; Yellow solid; mp: 186-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 8.01 (s, 1H), 7.88 (t, *J* = 8.2 Hz, 3H), 7.42 – 7.23 (m, 7H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 7.9 Hz, 1H), 6.11 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.6, 169.0, 163.2, 137.9, 137.7, 135.0, 131.6, 131.0, 130.0, 128.7, 128.6, 128.5, 127.9, 126.0, 125.8, 124.6, 123.5, 97.2, 24.3. HRMS m/z (ESI) calcd for $C_{23}H_{20}ClN_2O_2$ $(M + H)^+$ 391.1208, found 391.1208.



(*Z*)-*N*-(2-((3-(4-bromophenyl)-3-oxo-1-phenylprop-1-en-1yl)amino)phenyl)acetamide **(1k)**

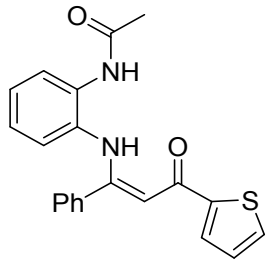
326 mg, 75 % yield; Yellow solid; mp: 199-201 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.45 (s, 1H), 9.88 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 6.9 Hz, 2H), 7.44 – 7.33 (m, 4H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.44 (d, *J* = 8.0 Hz, 1H), 6.20 (s, 1H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 187.4, 169.4, 162.2, 138.7, 135.9, 134.6, 132.0, 131.8, 130.3, 129.8, 128.9, 128.7, 126.5, 125.8, 125.8, 125.7, 125.2, 97.1, 23.6. HRMS m/z (ESI) calcd for $C_{23}H_{20}BrN_2O_2$ $(M + H)^+$ 435.0703, found 435.0705.



(*Z*)-*N*-(2-((3-(furan-2-yl)-3-oxo-1-phenylprop-1-en-1-yl)amino)phenyl)acetamide **(1l)**

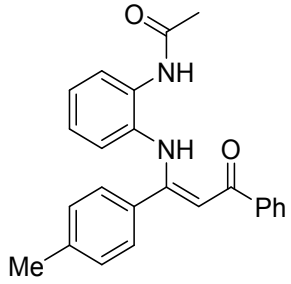
252 mg, 73 % yield; Yellow solid; mp: 208-210 °C; ^{1}H NMR (400 MHz, DMSO-d_6)

δ 12.08 (s, 1H), 9.89 (s, 1H), 7.90 (s, 1H), 7.46 (d, *J* = 6.6 Hz, 2H), 7.42 – 7.30 (m, 5H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.83 (t, *J* = 7.5 Hz, 1H), 6.67 (dd, *J* = 3.3, 1.6 Hz, 1H), 6.43 (d, *J* = 7.9 Hz, 1H), 6.06 (s, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.6, 165.9, 157.8, 150.5, 143.0, 132.4, 131.3, 128.2, 126.8, 125.5, 125.0, 123.0, 122.2, 122.2, 121.5, 111.6, 109.3, 93.8, 20.1. HRMS m/z (ESI) calcd for $C_{21}H_{19}N_2O_3$ $(M + H)^+$ 347.1390, found 347.1390.



(*Z*)-*N*-(2-((3-oxo-1-phenyl-3-(thiophen-2-yl)prop-1-en-1-yl)amino)phenyl)acetamide **(1m)**

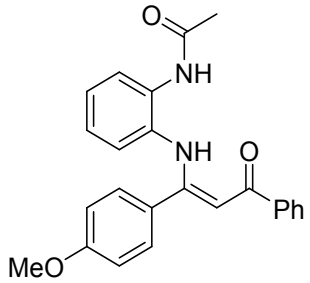
250 mg, 69 % yield; Yellow solid; mp: 196-198 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.25 (s, 1H), 8.06 – 7.81 (m, 2H), 7.67 (d, *J* = 3.4 Hz, 1H), 7.54 (d, *J* = 4.8 Hz, 1H), 7.40 – 7.21 (m, 5H), 7.13 – 7.08 (m, 1H), 7.03 (t, *J* = 7.7 Hz, 1H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 7.8 Hz, 1H), 6.07 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 169.0, 162.5, 146.3, 135.1, 131.7, 131.4, 131.1, 130.0, 129.0, 128.5, 128.0, 128.0, 126.0, 125.7, 124.5, 123.2, 97.6, 24.4. HRMS m/z (ESI) calcd for $C_{21}H_{19}N_2O_2S$ $(M + H)^+$ 363.1162, found 363.1162.



(*Z*)-*N*-(2-((3-oxo-3-phenyl-1-(*p*-tolyl)prop-1-en-1-yl)amino)phenyl)acetamide **(1n)**

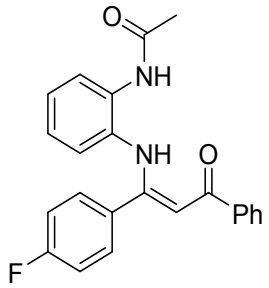
311 mg, 84 % yield; Yellow solid; mp: 174-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ

12.64 (s, 1H), 8.04 (s, 1H), 8.00 – 7.89 (m, 3H), 7.51 – 7.36 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.10 – 6.98 (m, 3H), 6.79 (t, *J* = 7.5 Hz, 1H), 6.56 (d, *J* = 7.9 Hz, 1H), 6.18 (s, 1H), 2.31 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 169.0, 163.1, 140.2, 139.6, 132.3, 131.8, 131.4, 131.1, 129.2, 128.4, 127.9, 127.2, 126.0, 125.6, 124.4, 123.1, 97.5, 24.4, 21.3. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_2$ $(M + H)^+$ 371.1754, found 371.1754.



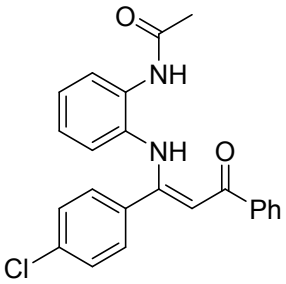
(*Z*)-*N*-(2-((1-(4-methoxyphenyl)-3-oxo-3-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1o)**

294 mg, 76 % yield; Yellow solid; mp: 211-212 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.43 (s, 1H), 9.86 (s, 1H), 8.06 – 7.96 (m, 2H), 7.58 – 7.42 (m, 5H), 7.38 (d, *J* = 7.5 Hz, 1H), 7.05 – 6.98 (m, 1H), 6.96 – 6.83 (m, 3H), 6.47 (d, *J* = 7.8 Hz, 1H), 6.20 (s, 1H), 3.76 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 185.0, 165.9, 158.0, 157.4, 136.4, 131.5, 128.4, 128.2, 126.9, 125.4, 124.5, 124.1, 123.0, 122.3, 122.2, 121.4, 110.9, 93.6, 52.2, 20.2. HRMS m/z (ESI) calcd for $C_{24}H_{23}N_2O_3$ $(M + H)^+$ 387.1703, found 387.1702.



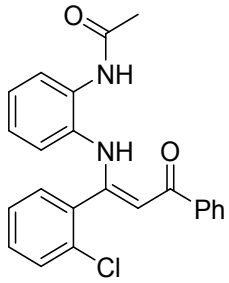
(*Z*)-*N*-(2-((1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1p)**

307 mg, 82 % yield; Yellow solid; mp: 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.60 (s, 1H), 8.38 (s, 1H), 7.92 (d, *J* = 7.2 Hz, 2H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.44 (dt, *J* = 27.2, 7.2 Hz, 3H), 7.26 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.91 (t, *J* = 8.6 Hz, 2H), 6.78 (t, *J* = 7.4 Hz, 1H), 6.45 (d, *J* = 7.8 Hz, 1H), 6.12 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.1, 169.2, 163.3 (d, *J* = 250.9 Hz), 161.5, 139.5, 131.6, 131.5, 131.4, 131.2 (d, *J* = 3.2 Hz), 130.1 (d, *J* = 8.5 Hz), 128.4, 127.2, 125.8, 125.6, 124.7, 123.8, 115.5 (d, *J* = 21.8 Hz), 97.6, 24.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.8; HRMS m/z (ESI) calcd for $C_{23}H_{20}FN_2O_2$ $(M + H)^+$ 375.1503, found 375.1503.



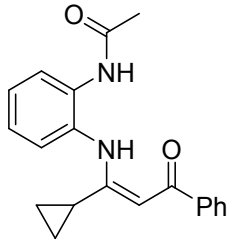
(*Z*)-*N*-(2-((1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1q)**

326 mg, 84 % yield; Yellow solid; mp: 185-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.57 (s, 1H), 8.28 (s, 1H), 7.92 (d, *J* = 7.5 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.31 – 7.14 (m, 4H), 7.03 (t, *J* = 7.7 Hz, 1H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.46 (d, *J* = 7.9 Hz, 1H), 6.13 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 169.2, 161.2, 139.4, 135.9, 133.6, 131.6, 131.5, 131.4, 129.4, 128.7, 128.4, 127.2, 125.8, 125.6, 124.8, 123.8, 97.7, 24.2. HRMS m/z (ESI) calcd for $C_{23}H_{20}ClN_2O_2$ $(M + H)^+$ 391.1208, found 391.1207.



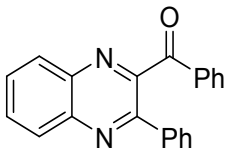
(*Z*)-*N*-(2-((1-(2-chlorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)amino)phenyl)-acetamide **(1r)**

300 mg, 77 % yield; Yellow solid; mp: 226-228 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 9.83 (s, 1H), 8.04 – 7.90 (m, 2H), 7.61 – 7.33 (m, 7H), 7.32 – 7.21 (m, 1H), 7.01 (t, *J* = 7.1 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.45 (d, *J* = 7.6 Hz, 1H), 6.06 (s, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 185.1, 166.1, 155.0, 136.0, 131.6, 131.3, 128.6, 128.4, 128.0, 127.8, 127.7, 126.7, 125.5, 124.4, 124.1, 123.7, 122.6, 121.8, 120.1, 93.9, 20.0. HRMS m/z (ESI) calcd for $C_{23}H_{20}ClN_2O_2$ $(M + H)^+$ 391.1208, found 391.1208.



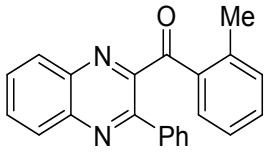
(*Z*)-*N*-(2-((1-cyclopropyl-3-oxo-3-phenylprop-1-en-1-yl)amino)phenyl)acetamide **(1s)**

205 mg, 64 % yield; Yellow solid; mp: 157-158 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.04 (s, 1H), 9.67 (s, 1H), 7.93 (d, *J* = 6.7 Hz, 2H), 7.52 – 7.40 (m, 5H), 7.31 – 7.19 (m, 2H), 5.69 (s, 1H), 2.06 (s, 3H), 1.72 – 1.51 (m, 1H), 1.11 – 0.76 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 184.2, 165.8, 164.8, 136.8, 130.0, 129.5, 127.8, 125.2, 123.9, 123.4, 123.1, 122.9, 122.7, 84.1, 20.1, 10.1, 6.7. HRMS m/z (ESI) calcd for $C_{20}H_{21}N_2O_2$ $(M + H)^+$ 321.1598, found 321.1598.



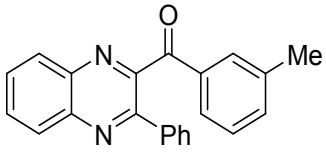
phenyl(3-phenylquinoxalin-2-yl)methanone (2a)

55.9 mg, 90 % yield; White solid; mp: 154-155 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.3, 0.8 Hz, 1H), 8.16 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.84 (dt, *J* = 23.2, 7.2 Hz, 2H), 7.70 (dd, *J* = 4.0, 3.1 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.42 – 7.34 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 152.7, 151.2, 142.1, 139.6, 137.2, 135.5, 134.0, 131.4, 130.5, 130.4, 129.6, 129.4, 129.4, 129.0, 128.6, 128.6. HRMS m/z (ESI) calcd for $C_{21}H_{15}N_2O$ $(M + H)^+$ 311.1179, found 311.1177.



(3-phenylquinoxalin-2-yl)(*o*-tolyl)methanone **(2b)**

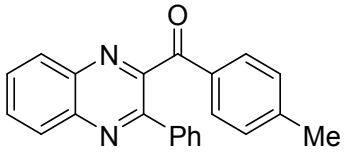
44.7 mg, 69 % yield; Pale yellow solid; mp: 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.84 (dt, *J* = 15.0, 7.1 Hz, 2H), 7.74 – 7.65 (m, 2H), 7.50 (d, *J* = 7.7 Hz, 1H), 7.46 – 7.35 (m, 4H), 7.31 – 7.25 (m, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 2.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 152.8, 152.4, 142.0, 141.3, 139.8, 137.5, 134.8, 132.8, 132.8, 132.3, 131.3, 130.4, 129.5, 129.5, 129.4, 129.0, 128.6, 125.5, 21.8. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O$ $(M + H)^+$ 325.1335, found 325.1335.



(3-phenylquinoxalin-2-yl)(*m*-tolyl)methanone **(2c)**

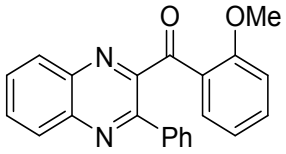
43.6 mg, 67 % yield; White solid; mp: 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ

8.27 (dd, *J* = 8.3, 1.0 Hz, 1H), 8.20 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.92 – 7.80 (m, 3H), 7.80 – 7.71 (m, 3H), 7.50 – 7.33 (m, 5H), 2.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 152.7, 151.4, 142.0, 139.6, 138.5, 137.2, 135.5, 134.9, 131.3, 130.7, 130.3, 129.5, 129.4, 129.4, 129.0, 128.6, 128.5, 127.9, 21.2. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O$ $(M + H)^+$ 325.1335, found 325.1338.



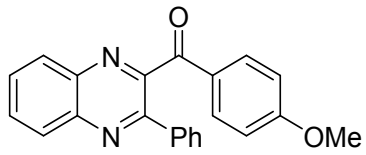
(3-phenylquinoxalin-2-yl)(*p*-tolyl)methanone **(2d)**

53.9 mg, 83 % yield; White solid; mp: 137-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.3, 1.1 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.89 – 7.77 (m, 4H), 7.75 – 7.67 (m, 2H), 7.42 – 7.34 (m, 3H), 7.26 (d, *J* = 7.9 Hz, 2H), 2.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.6, 152.7, 151.5, 145.2, 142.0, 139.6, 137.3, 133.1, 131.2, 130.6, 130.3, 129.5, 129.4, 129.4, 129.4, 129.0, 128.6, 21.8. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O$ $(M + H)^+$ 325.1335, found 325.1334.



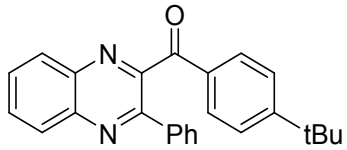
(2-methoxyphenyl)(3-phenylquinoxalin-2-yl)methanone **(2e)**

60.0 mg, 88 % yield; White solid; mp: 145-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 8.3, 0.8 Hz, 1H), 8.10 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.96 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.88 – 7.69 (m, 4H), 7.57 – 7.47 (m, 1H), 7.43 – 7.33 (m, 3H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 159.4, 153.9, 152.0, 141.8, 139.7, 137.6, 135.4, 131.6, 130.6, 129.9, 129.3, 129.3, 129.3, 129.3, 128.5, 126.0, 121.1, 112.0, 55.6. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O_2$ $(M + H)^+$ 341.1285, found 341.1285.



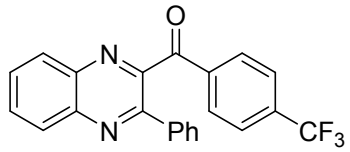
(4-methoxyphenyl)(3-phenylquinoxalin-2-yl)methanone **(2f)**

63.0 mg, 93 % yield; White solid; mp: 132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.1 Hz, 1H), 8.15 (d, *J* = 8.2 Hz, 1H), 7.92 (d, *J* = 8.7 Hz, 2H), 7.88 – 7.76 (m, 2H), 7.72 (dd, *J* = 6.2, 2.4 Hz, 2H), 7.44 – 7.33 (m, 3H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 164.3, 152.7, 151.6, 142.0, 139.6, 137.3, 132.9, 131.2, 130.3, 129.5, 129.4, 129.3, 129.0, 128.6, 128.6, 114.0, 55.5. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O_2$ $(M + H)^+$ 341.1285, found 341.1286.



(4-(tert-butyl)phenyl)(3-phenylquinoxalin-2-yl)methanone **(2g)**

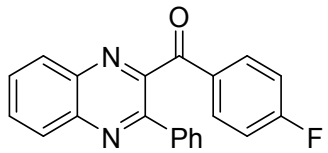
45.9 mg, 63 % yield; White solid; mp: 151-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.3, 0.9 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.95 – 7.77 (m, 4H), 7.76 – 7.69 (m, 2H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.45 – 7.33 (m, 3H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.5, 158.0, 152.9, 151.4, 142.0, 139.5, 137.3, 133.0, 131.3, 130.6, 130.3, 129.5, 129.4, 129.4, 129.1, 128.6, 125.7, 35.3, 31.0, 31.0, 31.0. HRMS m/z (ESI) calcd for $C_{25}H_{23}N_2O$ $(M + H)^+$ 367.1805, found 367.1804.



(3-phenylquinoxalin-2-yl)(4-(trifluoromethyl)phenyl)methanone **(2h)**

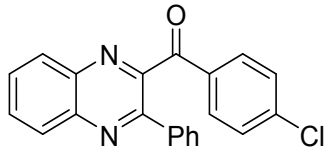
44.1 mg, 58 % yield; White solid; mp: 148-149 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.9 Hz, 1H), 8.18 – 8.14 (m, 1H), 8.09 (d, *J* = 8.2 Hz, 2H), 7.94 – 7.81 (m, 2H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.67 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.47 – 7.36 (m, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ 192.8, 153.0, 150.2, 142.3, 139.5, 138.3, 137.1, 135.1 (q, *J* = 32.7 Hz), 131.8, 130.8, 130.7, 129.8, 129.5, 129.5, 129.1, 128.8, 125.7 (q, *J* = 3.7 Hz), 123.5 (q, *J* = 272.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.2; HRMS m/z (ESI) calcd for $C_{22}H_{14}F_3N_2O$ $(M + H)^+$ 379.1053, found 379.1052.



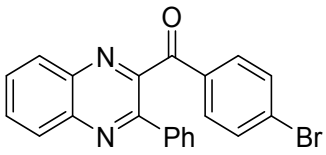
(4-fluorophenyl)(3-phenylquinoxalin-2-yl)methanone **(2i)**

43.9 mg, 67 % yield;White solid; mp: 165-166 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.5, 0.9 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.04 – 7.95 (m, 2H), 7.85 (dtd, *J* = 15.1, 7.1, 1.3 Hz, 2H), 7.72 – 7.64 (m, 2H), 7.44 – 7.35 (m, 3H), 7.18 – 7.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 166.3 (d, *J* = 257.1 Hz), 152.8, 150.8, 142.1, 139.5, 137.2, 133.2 (d, *J* = 9.6 Hz), 132.0 (d, *J* = 2.8 Hz), 131.5, 130.5, 129.6, 129.5, 129.4, 129.0, 128.7, 116.0 (d, *J* = 22.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.9; HRMS m/z (ESI) calcd for $C_{21}H_{14}FN_2O$ $(M + H)^+$ 329.1085, found 329.1079.



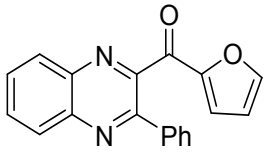
(4-chlorophenyl)(3-phenylquinoxalin-2-yl)methanone **(2j)**

50.1 mg, 73 % yield; White solid; mp: 161-163 °C; ^1H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 8.07 – 8.00 (m, 3H), 7.99 – 7.93 (m, 1H), 7.69 – 7.60 (m, 4H), 7.50 – 7.41 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 189.6, 149.2, 147.6, 138.5, 136.6, 135.8, 133.9, 130.9, 129.2, 129.1, 128.1, 126.6, 126.2, 126.1, 126.1, 125.9, 125.6. HRMS m/z (ESI) calcd for $C_{21}H_{14}ClN_2O$ $(M + H)^+$ 345.0789, found 345.0786.



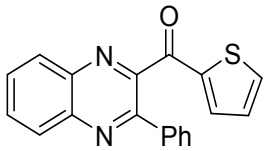
(4-bromophenyl)(3-phenylquinoxalin-2-yl)methanone **(2k)**

41.0 mg, 53 % yield; White solid; mp:167-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.3 Hz, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.93 – 7.79 (m, 4H), 7.73 – 7.57 (m, 4H), 7.40 (d, *J* = 4.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.9, 152.8, 150.6, 142.2, 139.6, 137.1, 134.4, 132.1, 131.9, 131.6, 130.6, 129.7, 129.6, 129.5, 129.4, 129.1, 128.8. HRMS m/z (ESI) calcd for $C_{21}H_{14}BrN_2O$ $(M + H)^+$ 389.0284, found 389.0284.



furan-2-yl(3-phenylquinoxalin-2-yl)methanone **(2l)**

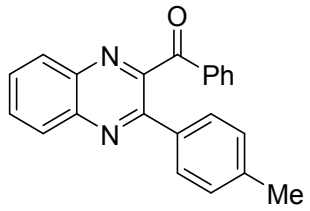
25.1 mg, 42 % yield; Brown solid; mp: 153-154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 15.3, 8.0 Hz, 2H), 7.93 – 7.80 (m, 2H), 7.72 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.67 (s, 1H), 7.49 – 7.39 (m, 3H), 7.30 (d, *J* = 3.5 Hz, 1H), 6.58 (dd, *J* = 3.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.2, 152.8, 151.7, 149.8, 148.3, 142.3, 139.7, 137.2, 131.7, 130.5, 129.6, 129.5, 129.4, 129.0, 128.7, 122.4, 112.8. HRMS m/z (ESI) calcd for $C_{19}H_{13}N_2O_2$ $(M + H)^+$ 301.0972, found 301.0968.



(3-phenylquinoxalin-2-yl)(thiophen-2-yl)methanone **(2m)**

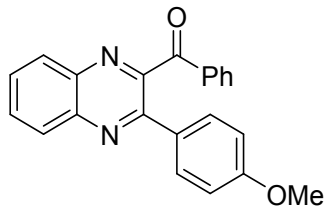
27.0 mg, 43 % yield;White solid; mp: 137-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 13.6, 8.2 Hz, 2H), 7.92 – 7.76 (m, 4H), 7.73 (dd, *J* = 6.2, 2.7 Hz, 2H), 7.48 – 7.39 (m, 3H), 7.17 (t, *J* = 4.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.8,

152.8, 150.2, 142.5, 142.3, 139.4, 137.4, 136.4, 136.2, 131.6, 130.5, 129.6, 129.4, 129.4, 129.0, 128.7, 128.5. HRMS m/z (ESI) calcd for $C_{19}H_{13}N_2OS$ (M + H) $^+$ 317.0743, found 317.0743.



phenyl(3-(*p*-tolyl)quinoxalin-2-yl)methanone **(2n)**

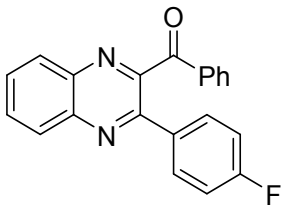
28.6 mg, 44 % yield; White solid; mp: 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 8.00 – 7.91 (m, 2H), 7.82 (dtd, *J* = 16.5, 7.0, 1.3 Hz, 2H), 7.65 – 7.56 (m, 3H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 152.7, 151.2, 142.1, 139.7, 139.5, 135.6, 134.4, 134.0, 131.3, 130.5, 130.2, 129.4, 129.4, 129.4, 129.0, 128.7, 21.3. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O$ (M + H) $^+$ 325.1335, found 325.1333.



(3-(4-methoxyphenyl)quinoxalin-2-yl)(phenyl)methanone **(2o)**

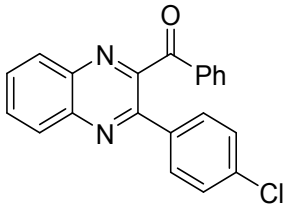
41.5 mg, 61 % yield; Pale yellow solid; mp: 144-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.3 Hz, 2H), 7.89 – 7.84 (m, 1H), 7.82 – 7.76 (m, 1H), 7.71 – 7.65 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 6.95 – 6.87 (m, 2H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.3, 160.9, 152.2, 151.2, 142.2, 139.4, 135.6, 134.1, 131.3, 130.6, 130.5, 130.1, 129.6, 129.4, 129.3, 128.7, 114.3, 55.3. HRMS m/z (ESI) calcd for $C_{22}H_{17}N_2O_2$ (M +

H)$^+$ 341.1285, found 341.1286.



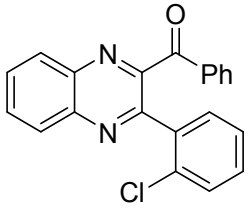
(3-(4-fluorophenyl)quinoxalin-2-yl)(phenyl)methanone **(2p)**

46.2 mg, 70 % yield; White solid; mp: 97-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.85 (dt, *J* = 15.1, 7.1 Hz, 2H), 7.70 (dd, *J* = 8.4, 5.4 Hz, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.08 (t, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 163.6 (d, *J* = 250.3 Hz), 151.6, 151.0, 142.0, 139.6, 135.4, 134.2, 133.4 (d, *J* = 3.3 Hz), 131.5, 131.1 (d, *J* = 8.6 Hz), 130.6, 130.5, 129.4, 129.4, 128.8, 115.9 (d, *J* = 21.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.1; HRMS m/z (ESI) calcd for $C_{21}H_{14}FN_2O$ (M + H)$^+$ 329.1085, found 329.1085.



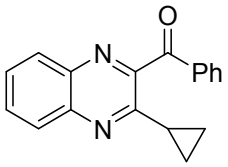
(3-(4-chlorophenyl)quinoxalin-2-yl)(phenyl)methanone **(2q)**

48.7 mg, 71 % yield; White solid; mp: 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.2 Hz, 1H), 8.15 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.99 – 7.92 (m, 2H), 7.90 – 7.79 (m, 2H), 7.69 – 7.59 (m, 3H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 151.5, 150.9, 142.0, 139.6, 135.9, 135.7, 135.4, 134.2, 131.6, 130.6, 130.5, 130.4, 129.4, 129.4, 128.9, 128.8. HRMS m/z (ESI) calcd for $C_{21}H_{14}ClN_2O$ (M + H)$^+$ 345.0789, found 345.0791.



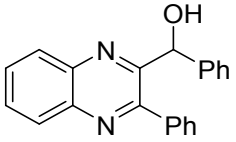
(3-(2-chlorophenyl)quinoxalin-2-yl)(phenyl)methanone **(2r)**

42.8 mg, 62 % yield; White solid; mp: 128-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 16.9, 8.1 Hz, 2H), 8.04 (d, *J* = 7.7 Hz, 2H), 7.94 – 7.80 (m, 2H), 7.69 – 7.56 (m, 2H), 7.55 – 7.29 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 152.2, 150.4, 141.8, 139.6, 136.9, 135.0, 133.6, 132.1, 131.7, 131.4, 131.0, 130.8, 130.4, 129.7, 129.4, 129.4, 128.2, 127.2. HRMS m/z (ESI) calcd for $C_{21}H_{14}ClN_2O$ $(M + H)^+$ 345.0789, found 345.0788.



(3-cyclopropylquinoxalin-2-yl)(phenyl)methanone **(2s)**

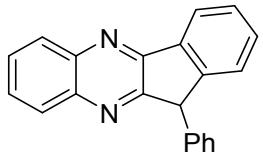
19.3 mg, 35 % yield; White solid; mp: 74-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.3, 1.1 Hz, 1H), 8.03 – 7.95 (m, 3H), 7.80 – 7.74 (m, 1H), 7.72 – 7.62 (m, 2H), 7.51 (t, *J* = 7.8 Hz, 2H), 2.34 – 2.24 (m, 1H), 1.39 – 1.32 (m, 2H), 1.11 – 1.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 156.6, 151.0, 142.4, 139.0, 135.8, 134.2, 130.9, 130.7, 129.4, 129.0, 128.7, 128.6, 14.5, 11.8. HRMS m/z (ESI) calcd for $C_{18}H_{15}N_2O$ $(M + H)^+$ 275.1179, found 275.1178.



phenyl(3-phenylquinoxalin-2-yl)methanol (**3a**)

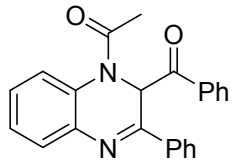
52.9 mg, 85% yield; White solid; mp: 147-148 °C; ^{1}H NMR (400 MHz, CDCl3) δ

8.33 – 8.06 (m, 2H), 7.92 – 7.71 (m, 2H), 7.54 – 7.34 (m, 3H), 7.32 – 7.21 (m, 2H), 7.19 – 7.00 (m, 3H), 6.80 (d, J = 7.0 Hz, 2H), 6.13 (d, J = 7.0 Hz, 1H), 5.59 (d, J = 7.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl3) δ 154.4, 154.2, 141.6, 141.2, 139.6, 137.6, 130.4, 130.2, 129.4, 129.2, 128.8, 128.6, 128.6, 128.3, 127.8, 127.6, 72.9. HRMS m/z (ESI) calcd for C21H17N2O (M + H) + 313.1335, found 313.1335.



11-phenyl-11*H*-indeno[1,2-*b*]quinoxaline (**4a**)

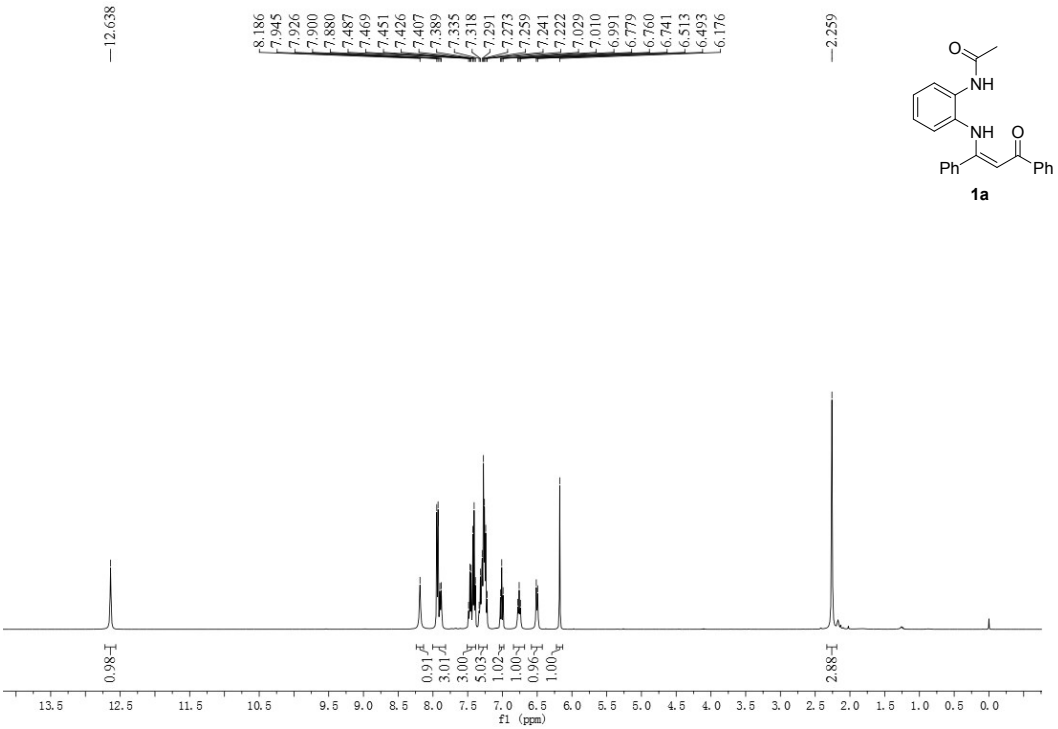
31.1 mg, 53 % yield; Light brown solid; mp: 169-170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.0 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 1H), 7.78 – 7.62 (m, 2H), 7.60 – 7.41 (m, 3H), 7.35 – 7.21 (m, 3H), 7.18 (d, *J* = 6.9 Hz, 2H), 5.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 154.4, 148.2, 142.4, 141.7, 139.2, 137.4, 131.6, 129.5, 129.1, 128.9, 128.8, 128.7, 128.7, 128.6, 127.4, 126.2, 122.5, 52.6. HRMS m/z (ESI) calcd for $C_{21}H_{15}N_2$ $(M + H)^+$ 295.1230, found 295.1232.

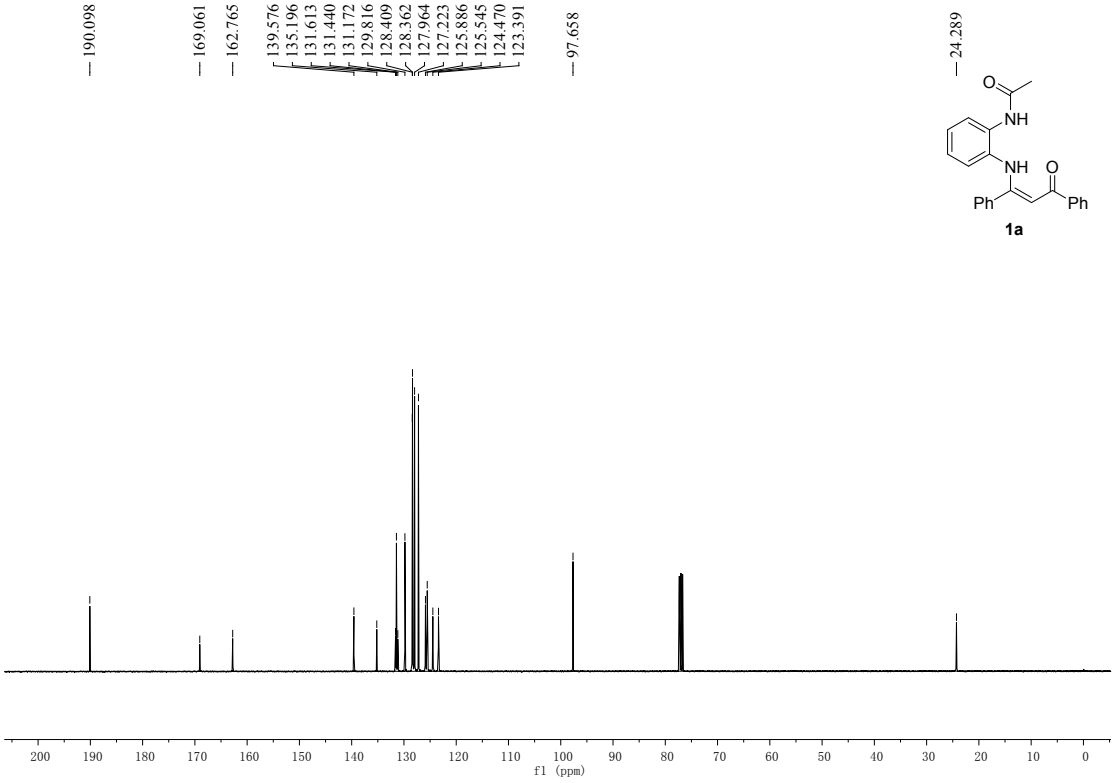


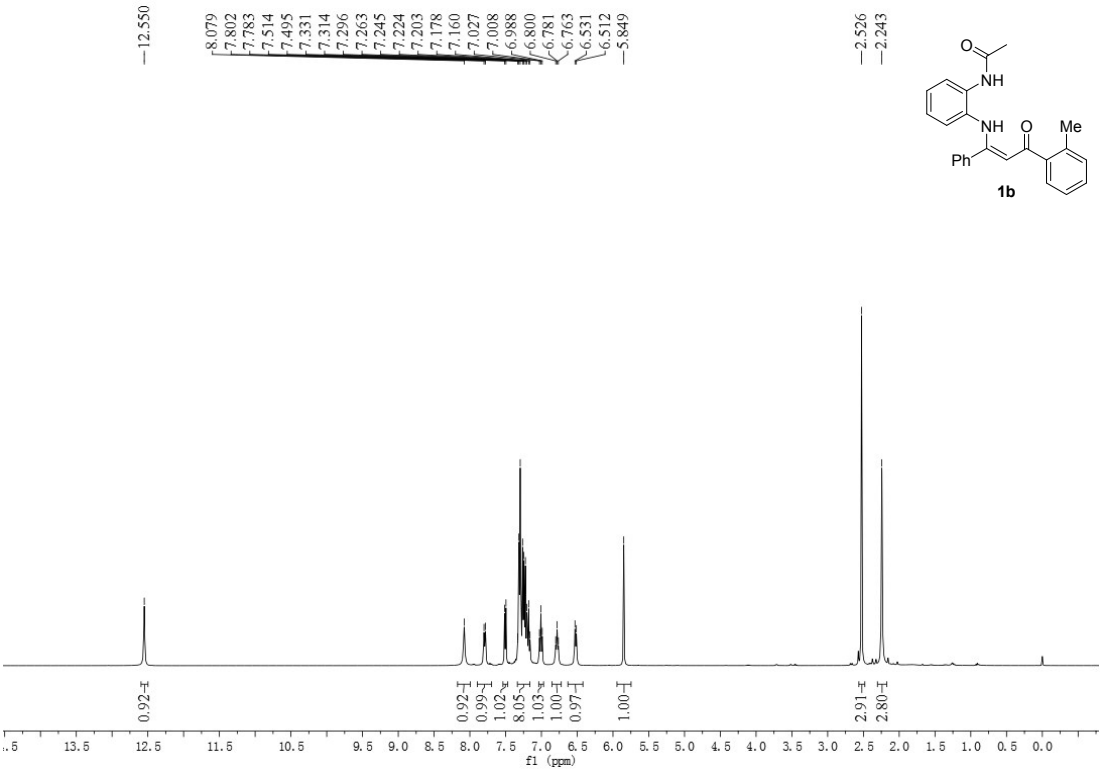
1-(2-benzoyl-3-phenylquinoxalin-1(2*H*)-yl)ethan-1-one (**5a**)

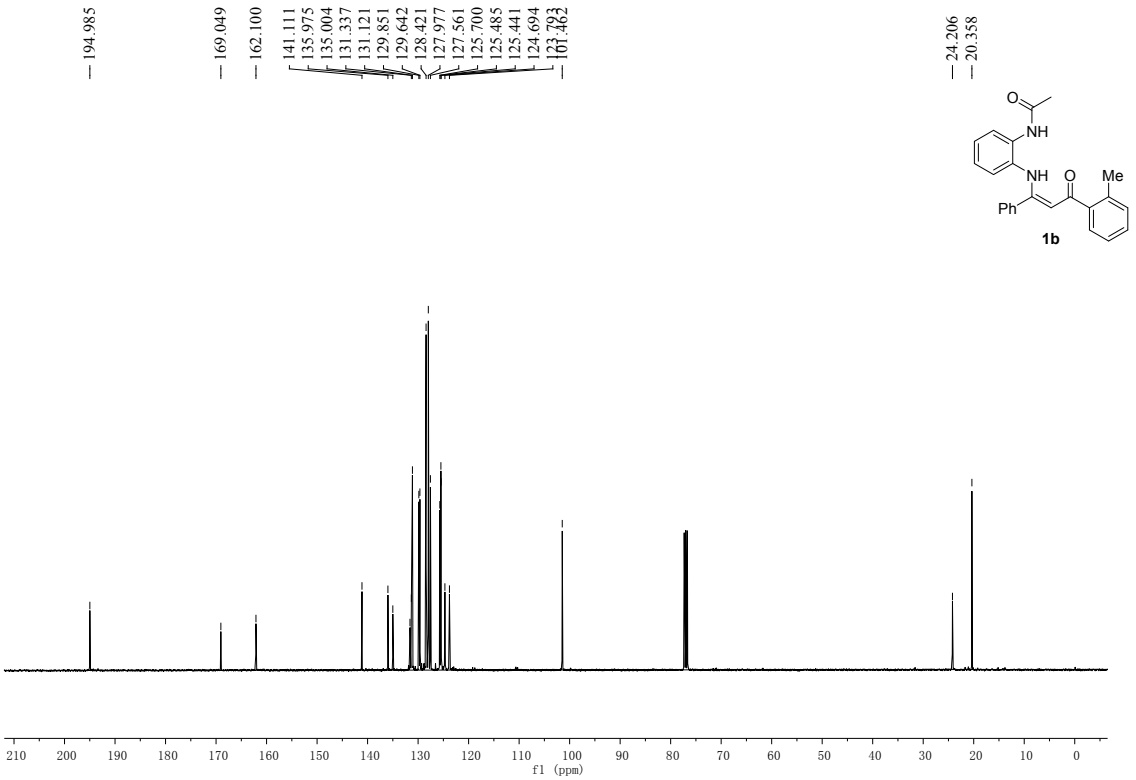
56.6 mg, 32% yield; Yellow solid; mp: 56-58 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.05 (m, 2H), 8.02 (d, *J* = 7.4 Hz, 2H), 7.67 – 7.57 (m, 2H), 7.56 (s, 1H), 7.53 – 7.43 (m, 5H), 7.31 (td, *J* = 7.8, 1.0 Hz, 1H), 7.13 (td, *J* = 7.8, 1.3 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.3, 169.8, 164.3, 139.9, 136.5, 134.2, 133.8, 131.4, 128.8, 128.7, 128.7, 127.9, 127.3, 127.3, 127.2, 126.8, 123.7, 53.6, 21.9. HRMS m/z (ESI) calcd for $C_{23}H_{19}N_2O_2$ $(M + H)^+$ 355.1441, found 355.1440.

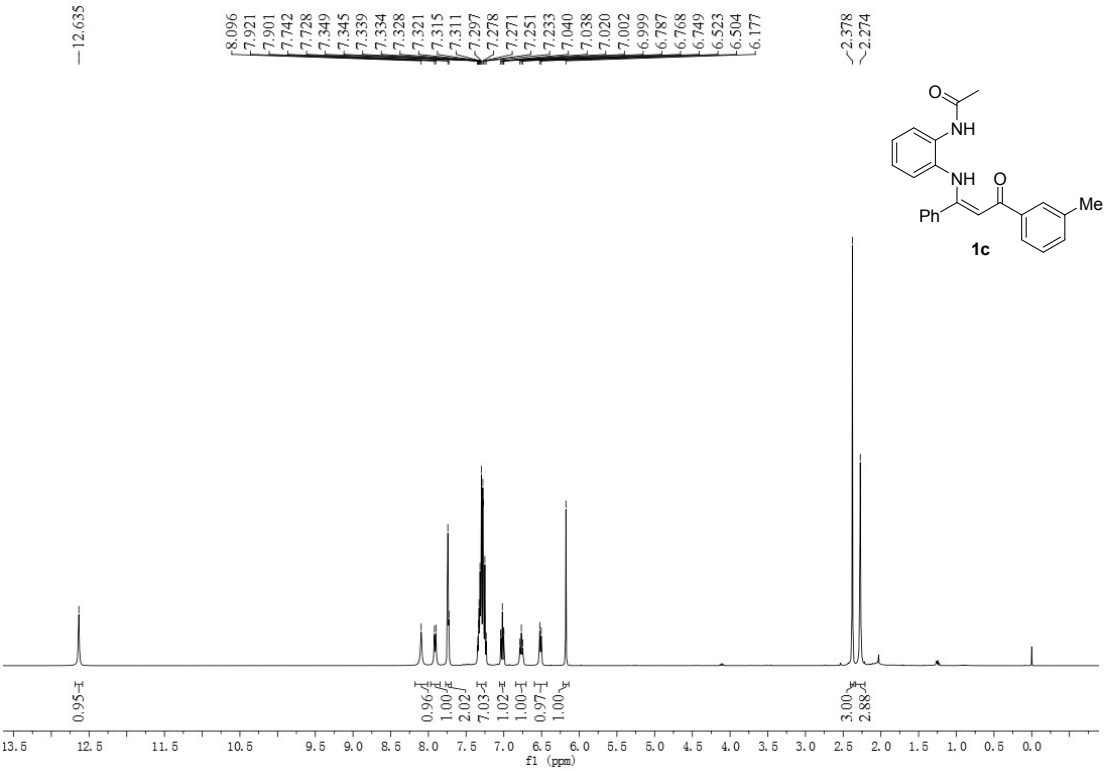
6. NMR Spectra of compounds **1a-1s**, **2a-2s**, **3a**, **4a, 5a**:

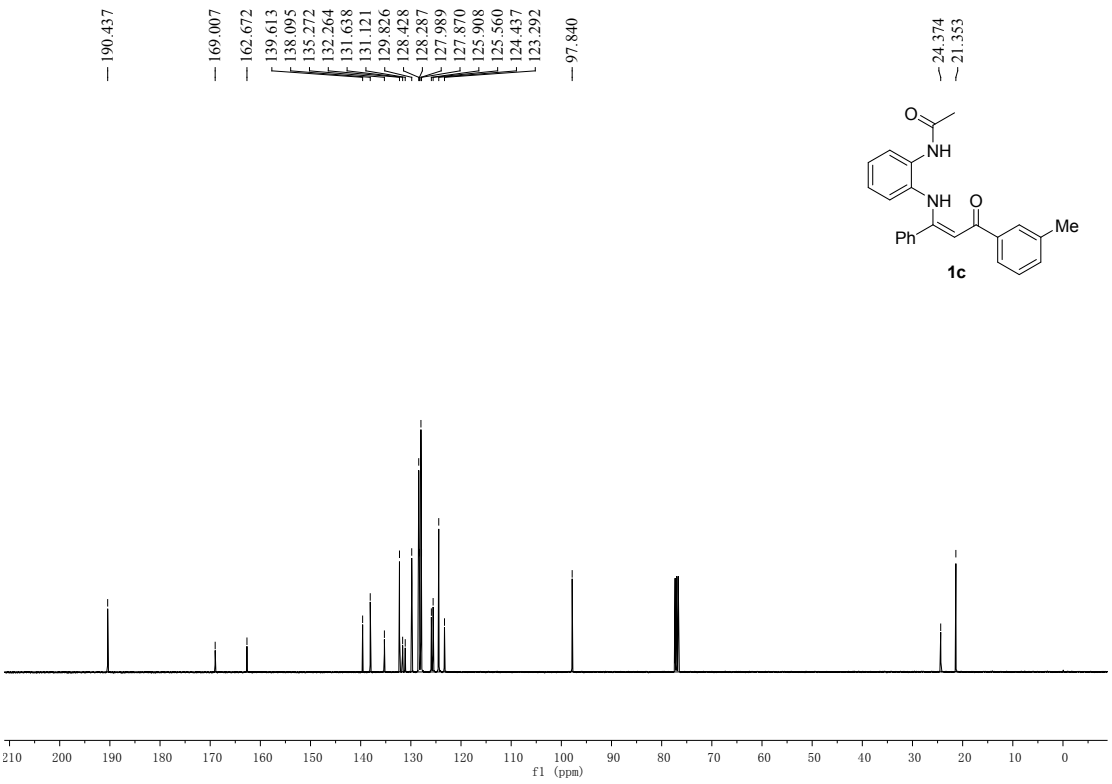


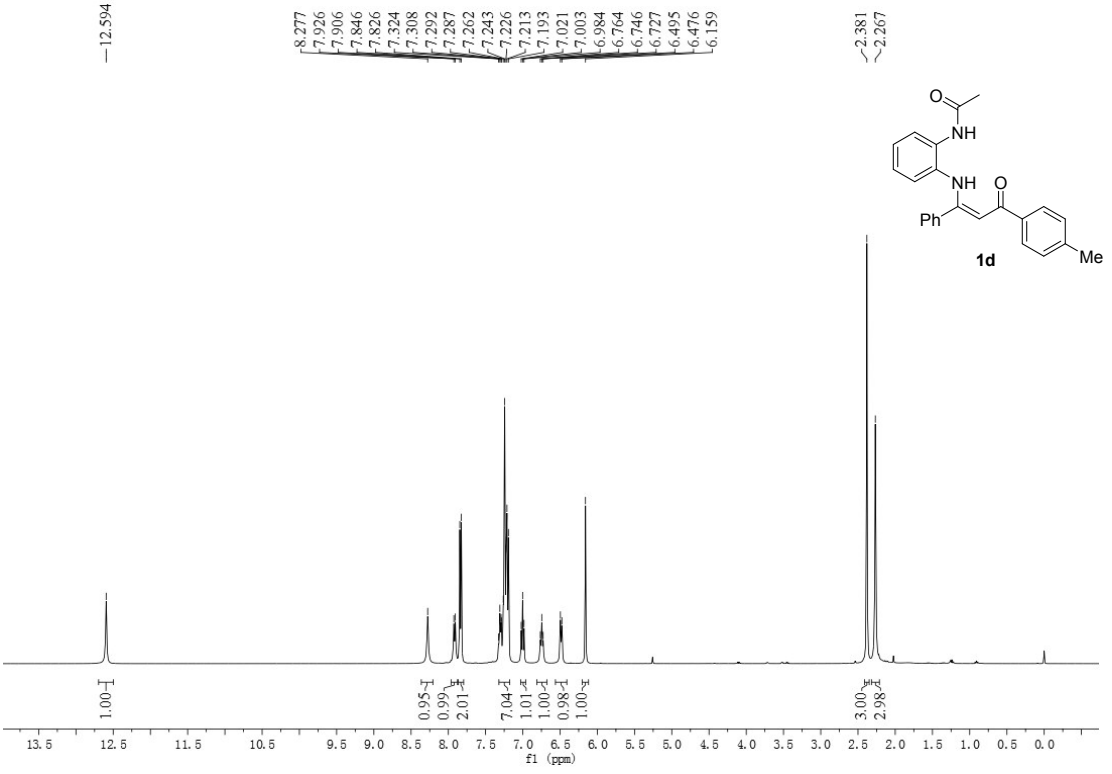


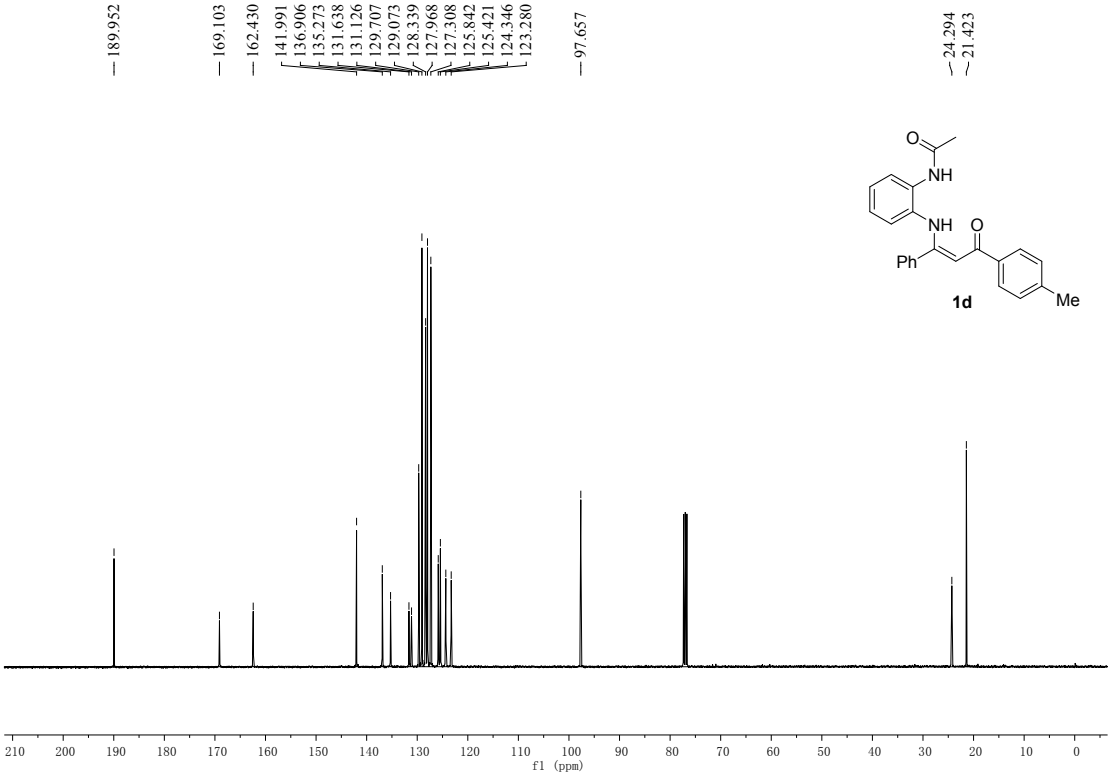

12.550
8.079
7.802
7.783
7.514
7.495
7.331
7.314
7.296
7.263
7.245
7.224
7.203
7.178
7.160
7.027
7.008
6.988
6.800
6.781
6.763
6.531
6.512
5.849
2.526
2.243
O
NH
NH
O
Me
Ph
1b
0.92
0.92
0.99
1.02
8.05
1.03
1.00
0.97
1.00
2.91
2.80
f1 (ppm)

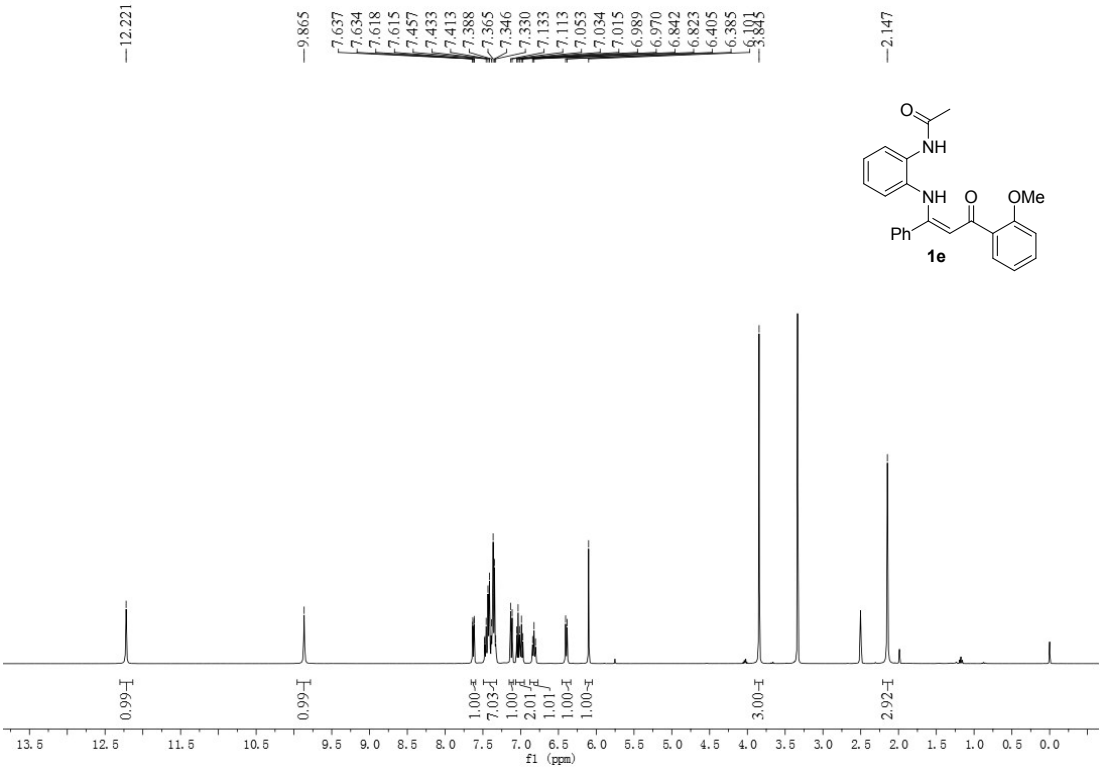

194.985
169.049
162.100
141.111
135.975
135.004
131.337
131.121
129.851
129.642
128.421
127.977
127.561
125.700
125.485
125.441
124.694
123.793
101.462
24.206
20.358
O
NH
NH
O
Me
Ph
1b
f1 (ppm)

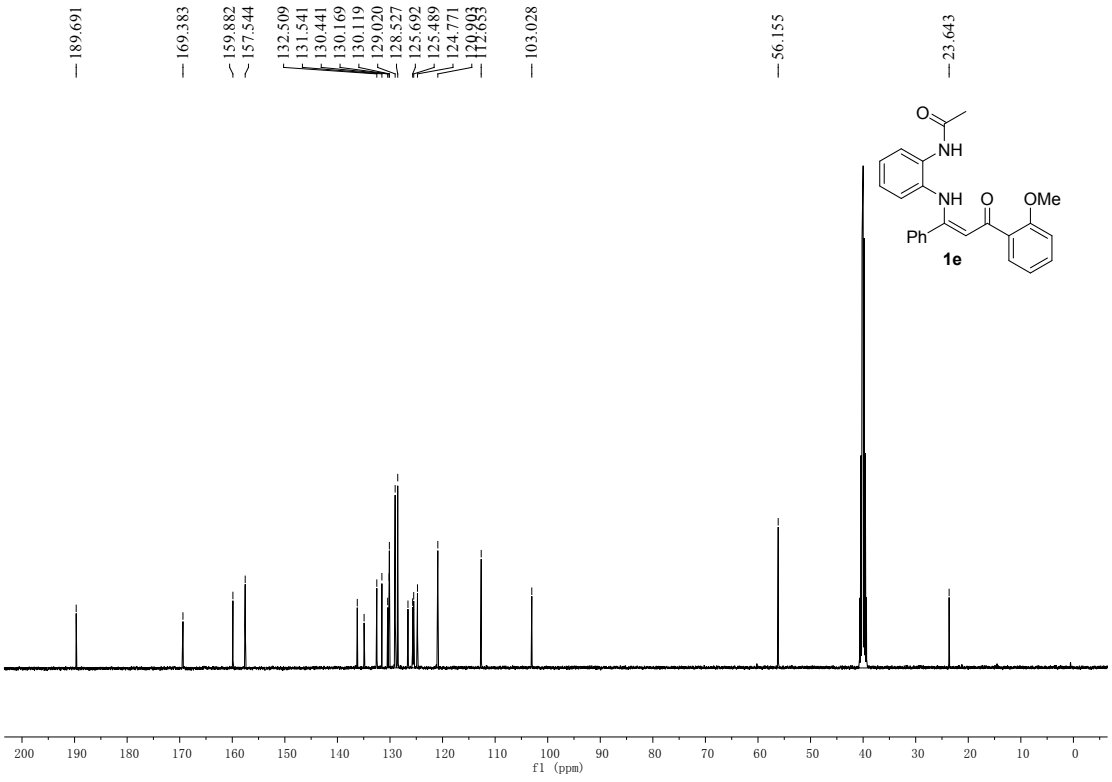

12.635
8.096
7.921
7.901
7.742
7.728
7.349
7.345
7.339
7.334
7.328
7.321
7.315
7.311
7.297
7.278
7.271
7.251
7.233
7.040
7.038
7.020
7.002
6.999
6.787
6.768
6.749
6.523
6.504
6.177
2.378
2.274
O
NH
NH
O
Ph
Me
1c
0.95
0.96
1.00
2.02
7.03
1.02
1.00
0.97
1.00
3.00
2.88
f1 (ppm)

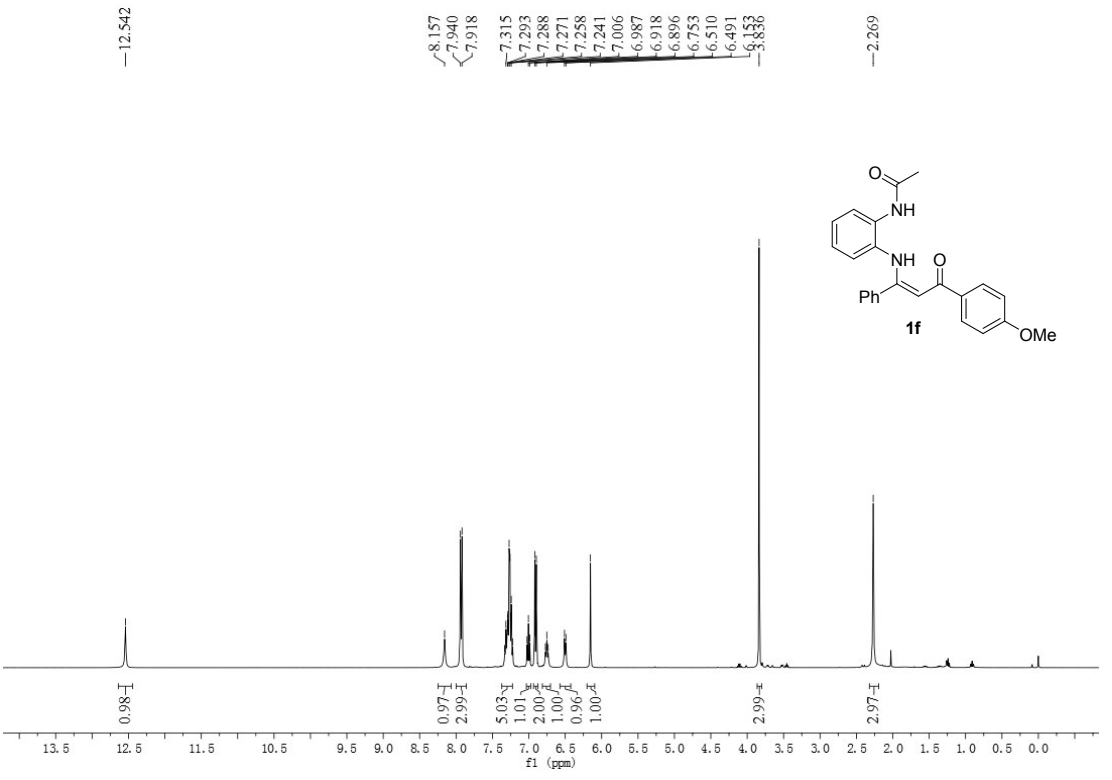

190.437
169.007
162.672
139.613
138.095
135.272
132.264
131.638
131.121
129.826
128.428
128.287
127.989
127.870
125.908
125.560
124.437
123.292
97.840
24.374
21.353
O
NH
NH
O
Ph
Me
1c
f1 (ppm)

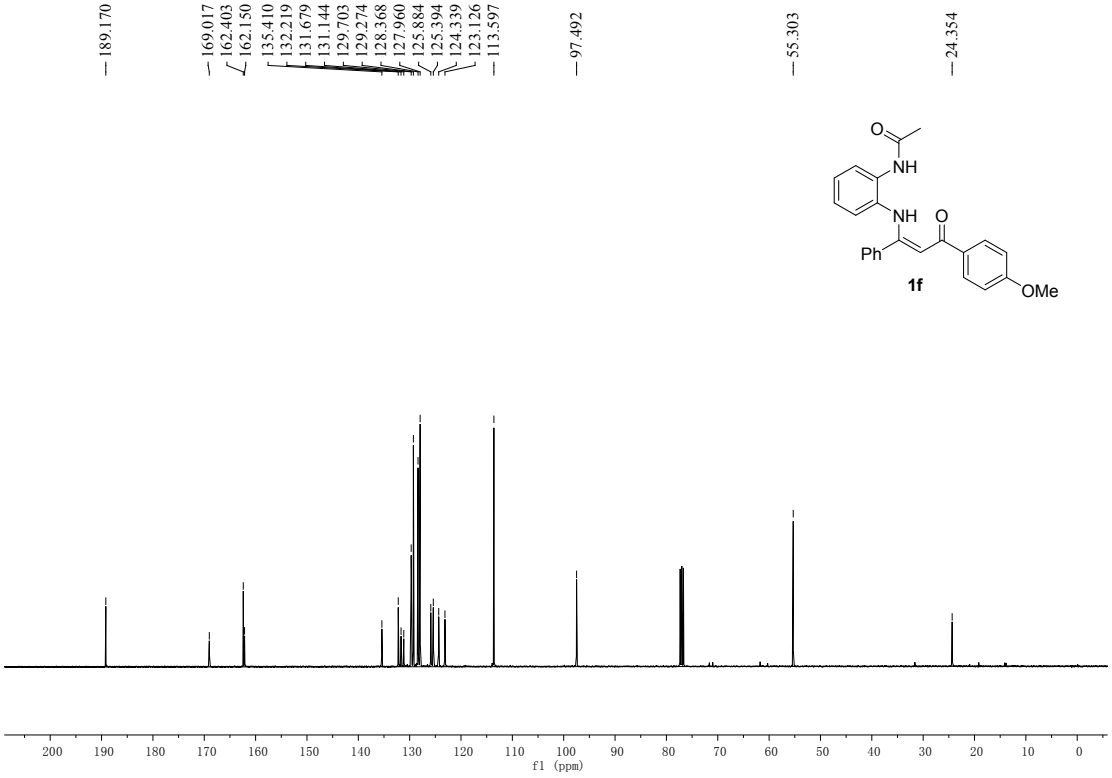

12.594
8.277
7.926
7.906
7.846
7.826
7.324
7.308
7.292
7.287
7.262
7.243
7.226
7.213
7.193
7.021
7.003
6.984
6.764
6.746
6.727
6.495
6.476
6.159
2.381
2.267
1.00
0.95
0.99
2.01
7.04
1.01
1.00
0.98
1.00
3.00
2.98
f1 (ppm)
1d

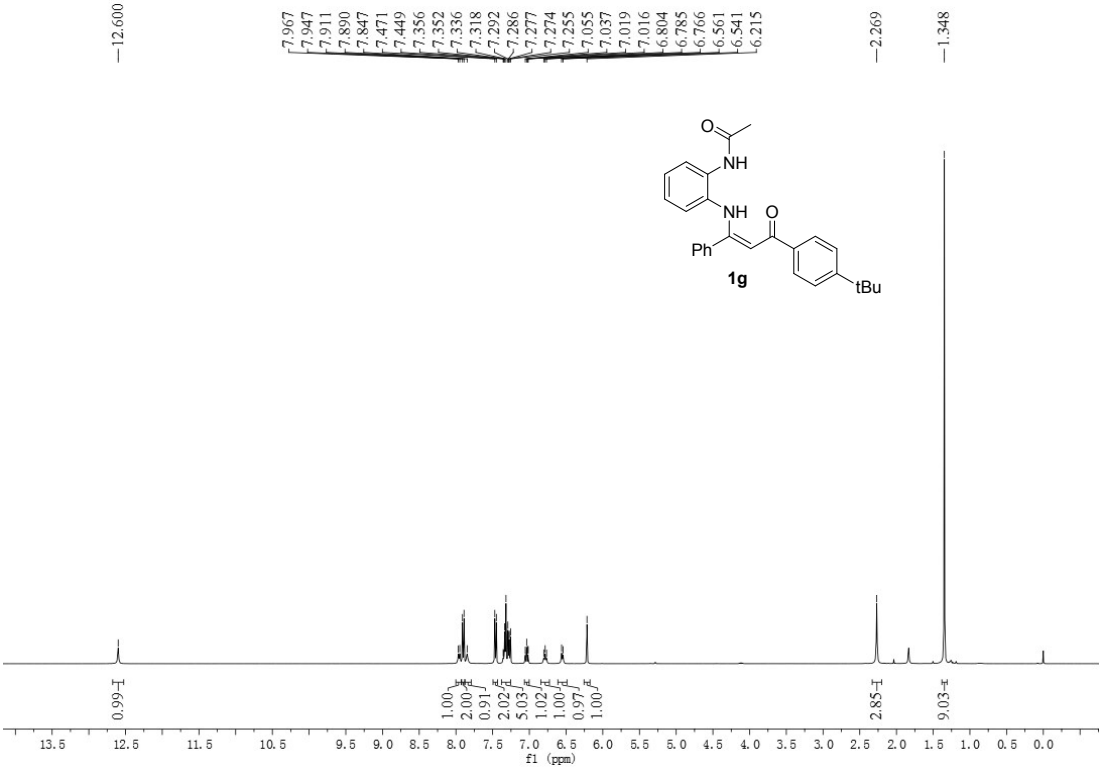

189.952
169.103
162.430
141.991
136.906
135.273
131.638
131.126
129.707
129.073
128.339
127.968
127.308
125.842
125.421
124.346
123.280
97.657
24.294
21.423
f1 (ppm)
1d

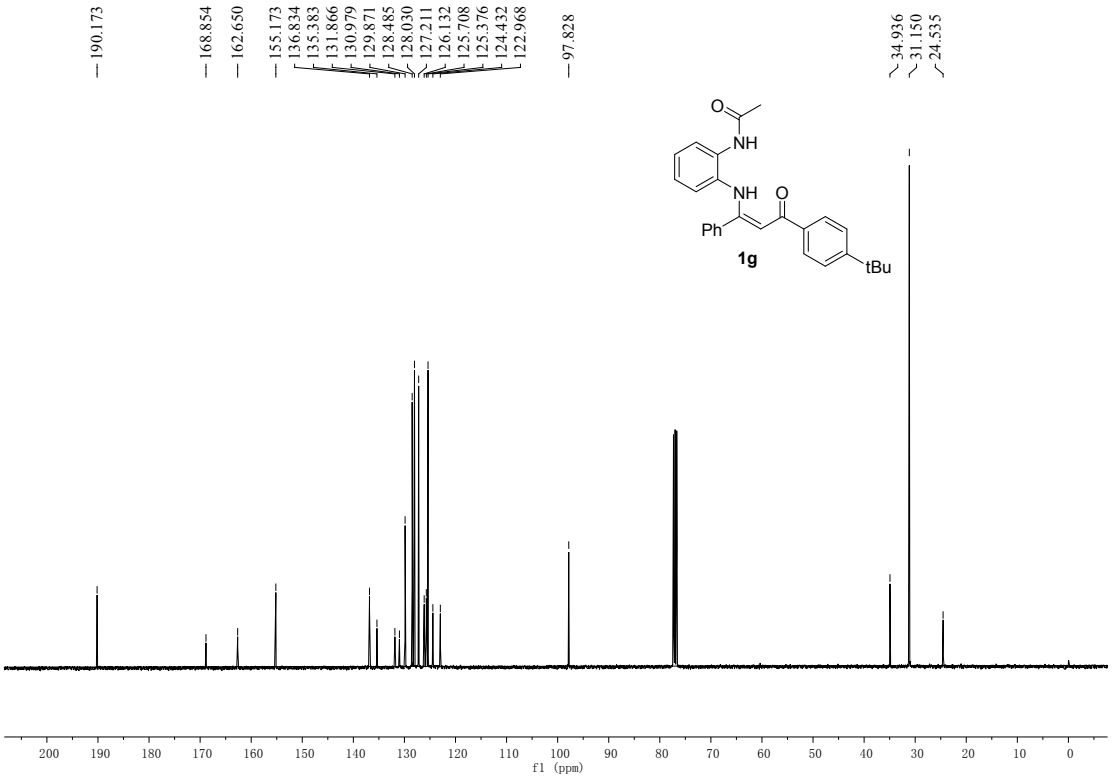

12.221
9.865
7.637
7.634
7.618
7.615
7.457
7.433
7.413
7.388
7.365
7.346
7.330
7.133
7.113
7.053
7.034
7.015
6.989
6.970
6.842
6.823
6.405
6.385
6.101
3.845
2.147
O
NH
NH
O
OMe
Ph
1e
0.99
0.99
1.00
7.03
1.00
2.01
1.01
1.00
1.00
3.00
2.92
f1 (ppm)

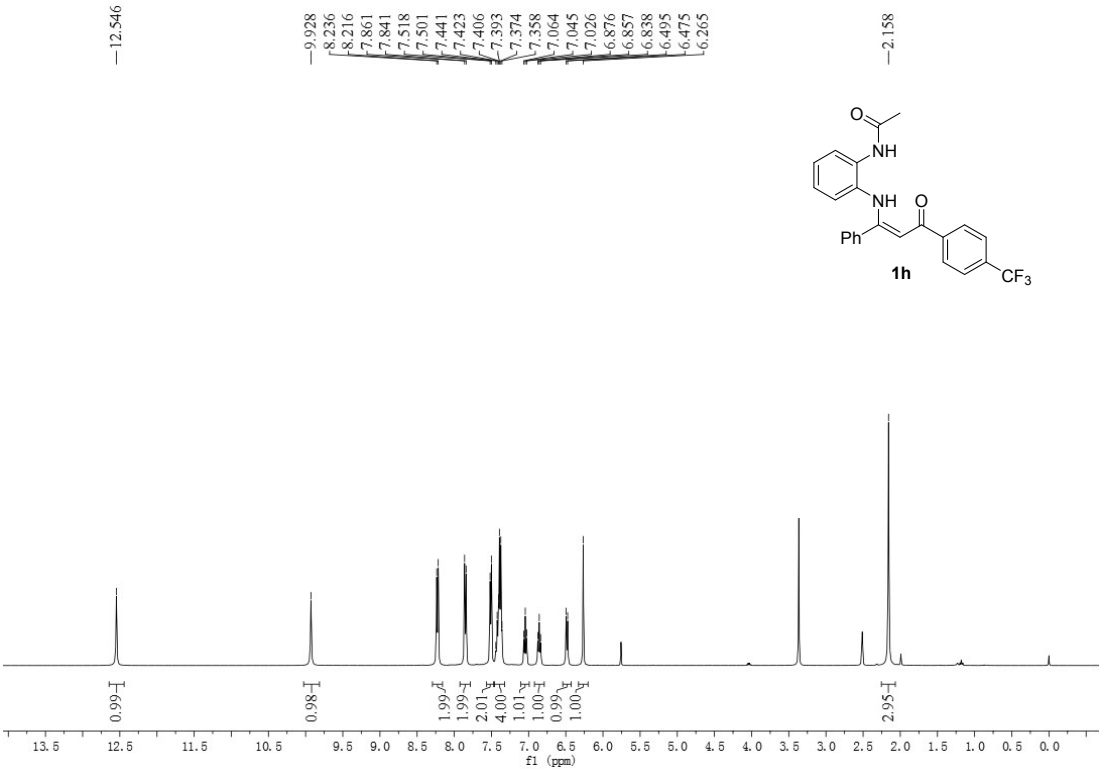

189.691
169.383
159.882
157.544
132.509
131.541
130.441
130.169
130.119
129.020
128.527
125.692
125.489
124.771
120.903
112.653
103.028
56.155
23.643
O
NH
NH
O
OMe
Ph
1e
f1 (ppm)

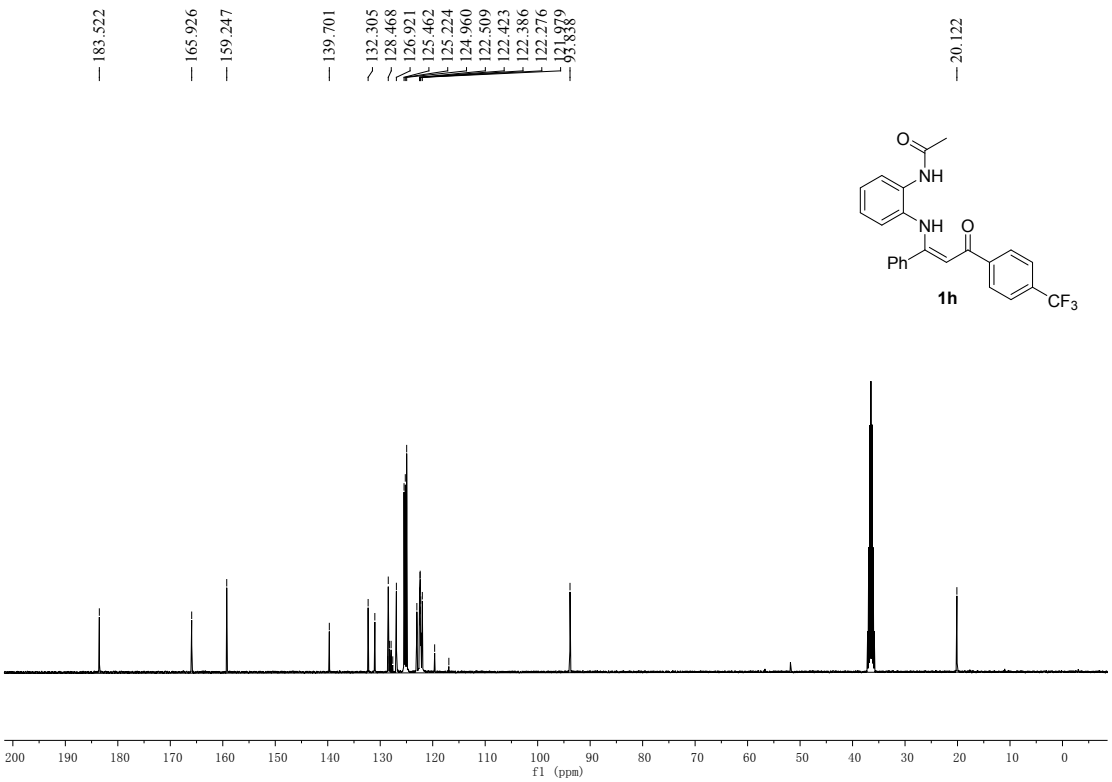

12.542
8.157
7.940
7.918
7.315
7.293
7.288
7.271
7.258
7.241
7.006
6.987
6.918
6.896
6.753
6.510
6.491
6.153
3.836
2.269
O
NH
NH
O
Ph
1f
OMe
0.98
0.97
2.99
5.03
1.01
2.00
1.00
0.96
1.00
2.99
2.97
f1 (ppm)

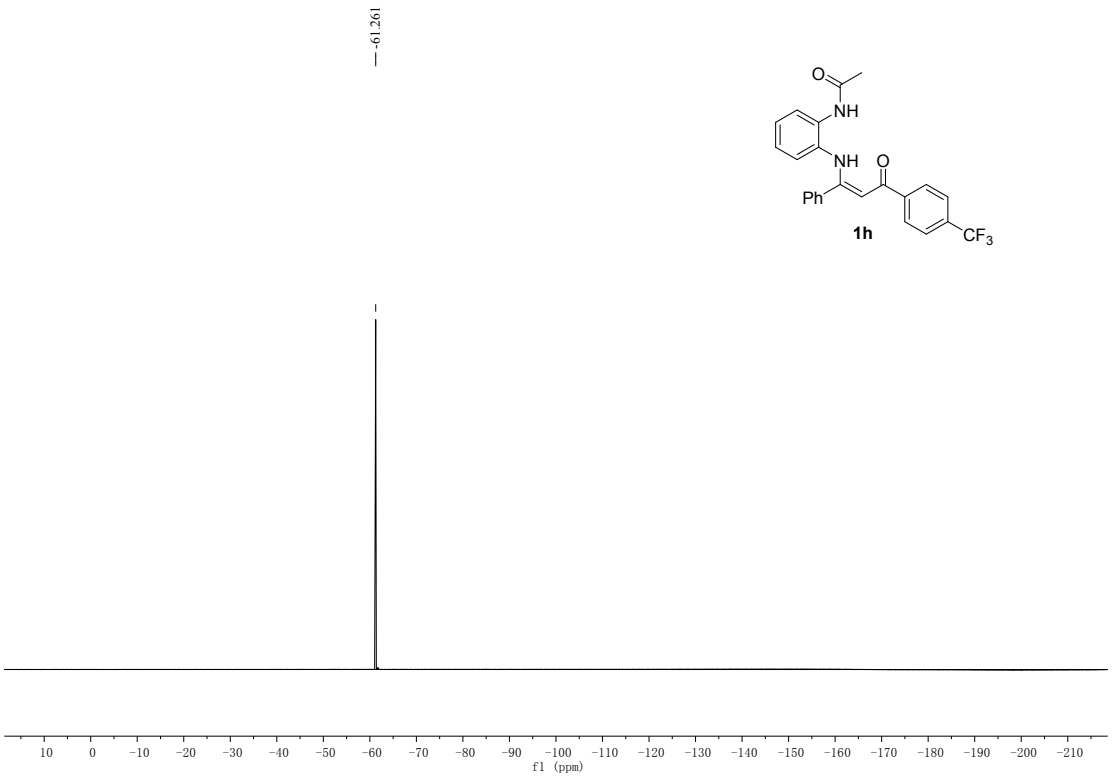

189.170
169.017
162.403
162.150
135.410
132.219
131.679
131.144
129.703
129.274
128.368
127.960
125.884
125.394
124.339
123.126
113.597
97.492
55.303
24.354
O
NH
NH
O
Ph
1f
OMe
f1 (ppm)

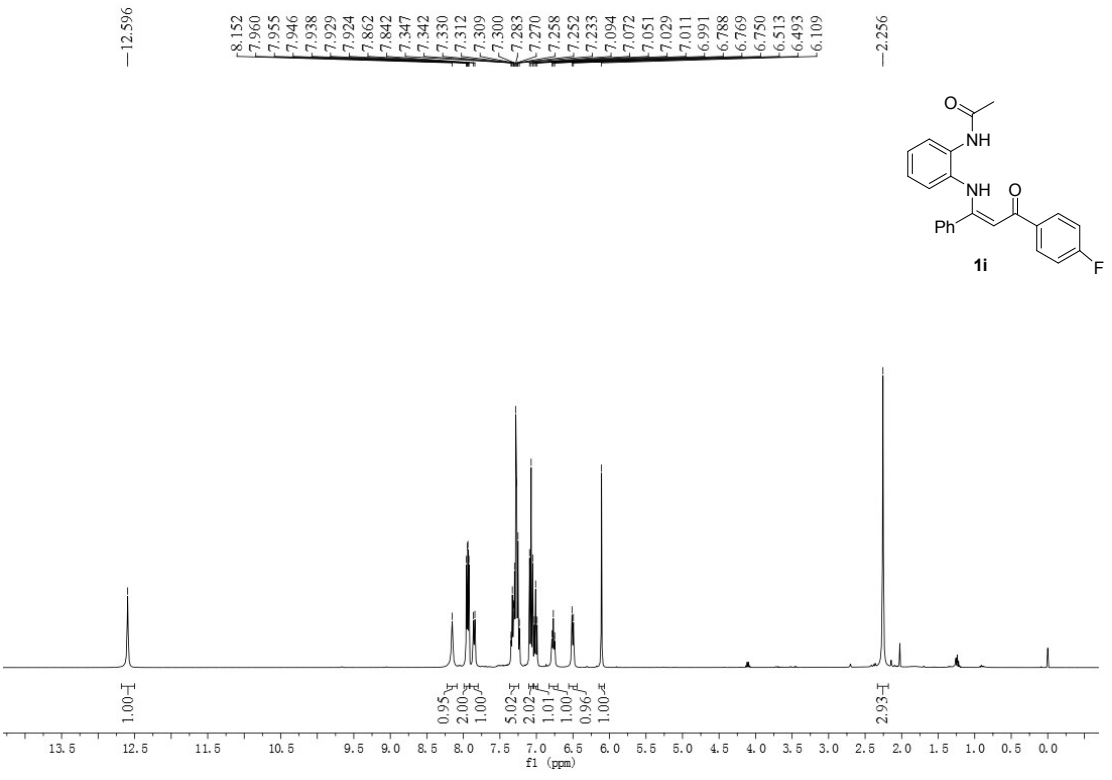

12.600
7.967
7.947
7.911
7.890
7.847
7.471
7.449
7.356
7.352
7.336
7.318
7.292
7.286
7.277
7.274
7.255
7.055
7.037
7.019
7.016
6.804
6.785
6.766
6.561
6.541
6.215
2.269
1.348
O
NH
NH
O
Ph
1g
tBu
0.99
1.00
2.00
0.91
2.02
5.03
1.02
1.00
0.97
1.00
2.85
9.03
f1 (ppm)

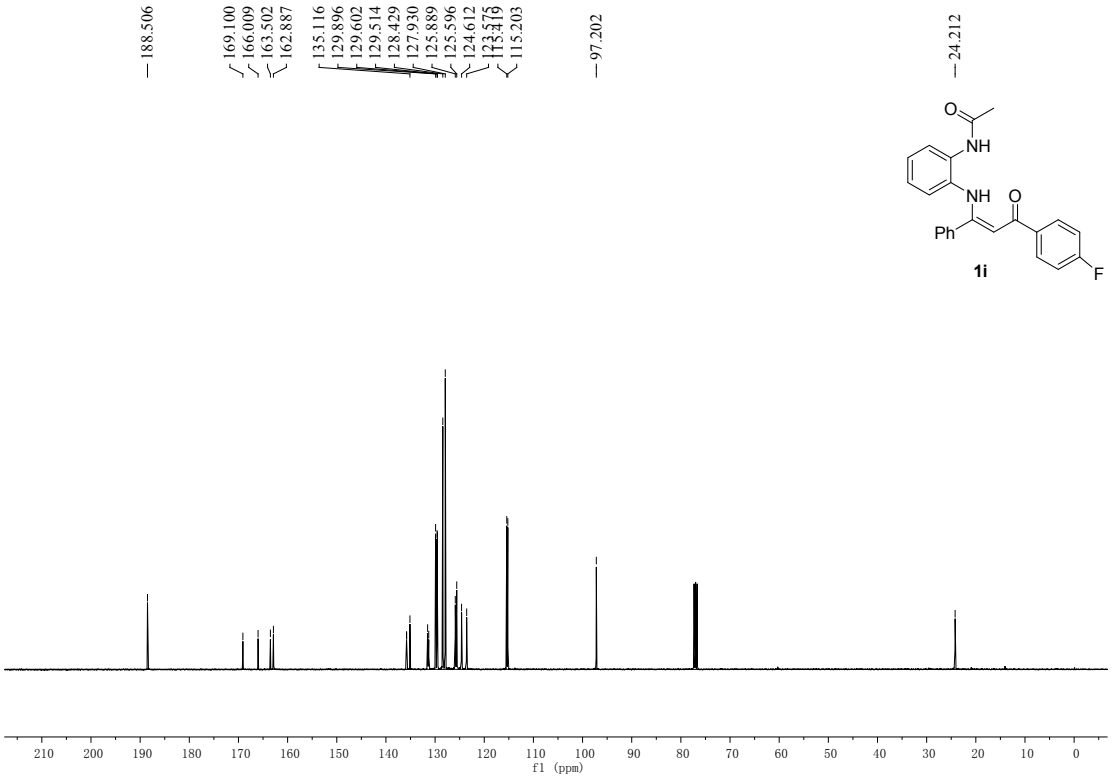

190.173
168.854
162.650
155.173
136.834
135.383
131.866
130.979
129.871
128.485
128.030
127.211
126.132
125.708
125.376
124.432
122.968
97.828
34.936
31.150
24.535
O
NH
NH
O
Ph
1g
tBu
f1 (ppm)

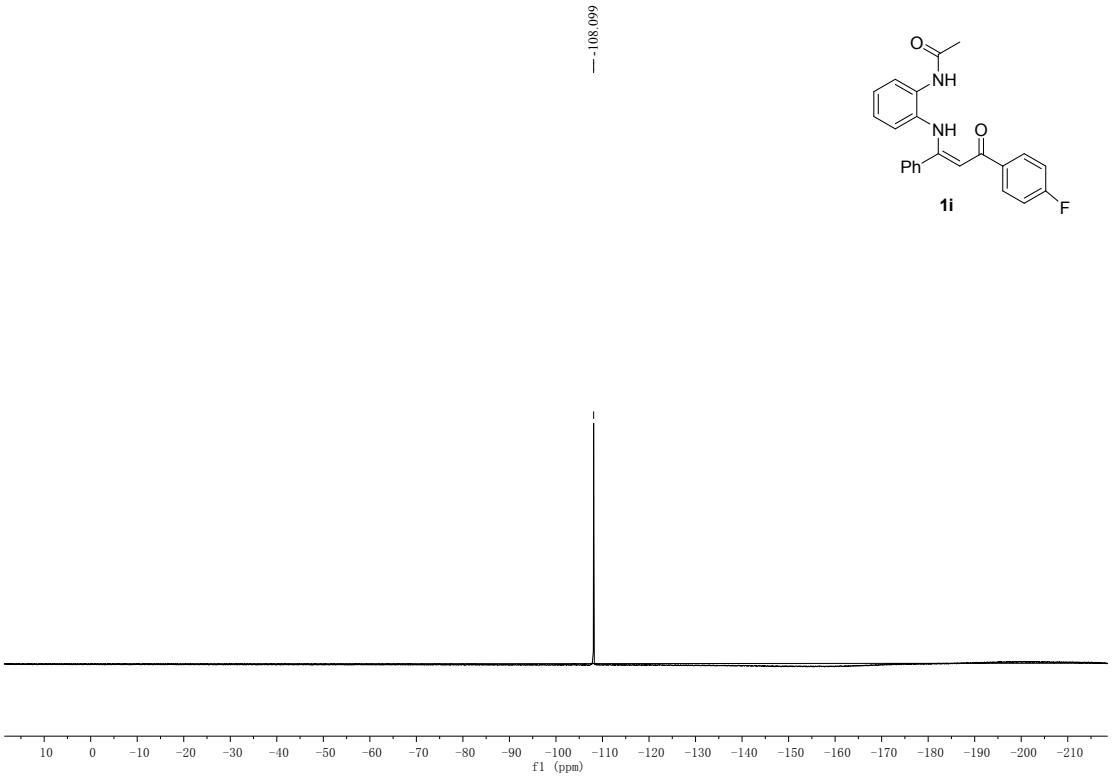

12.546
9.928
8.236
8.216
7.861
7.841
7.518
7.501
7.441
7.423
7.406
7.393
7.374
7.358
7.064
7.045
7.026
6.876
6.857
6.838
6.495
6.475
6.265
2.158
O
NH
NH
O
Ph
1h
CF3
0.99
0.98
1.99
1.99
2.01
4.00
1.01
1.00
0.99
1.00
2.95
f1 (ppm)

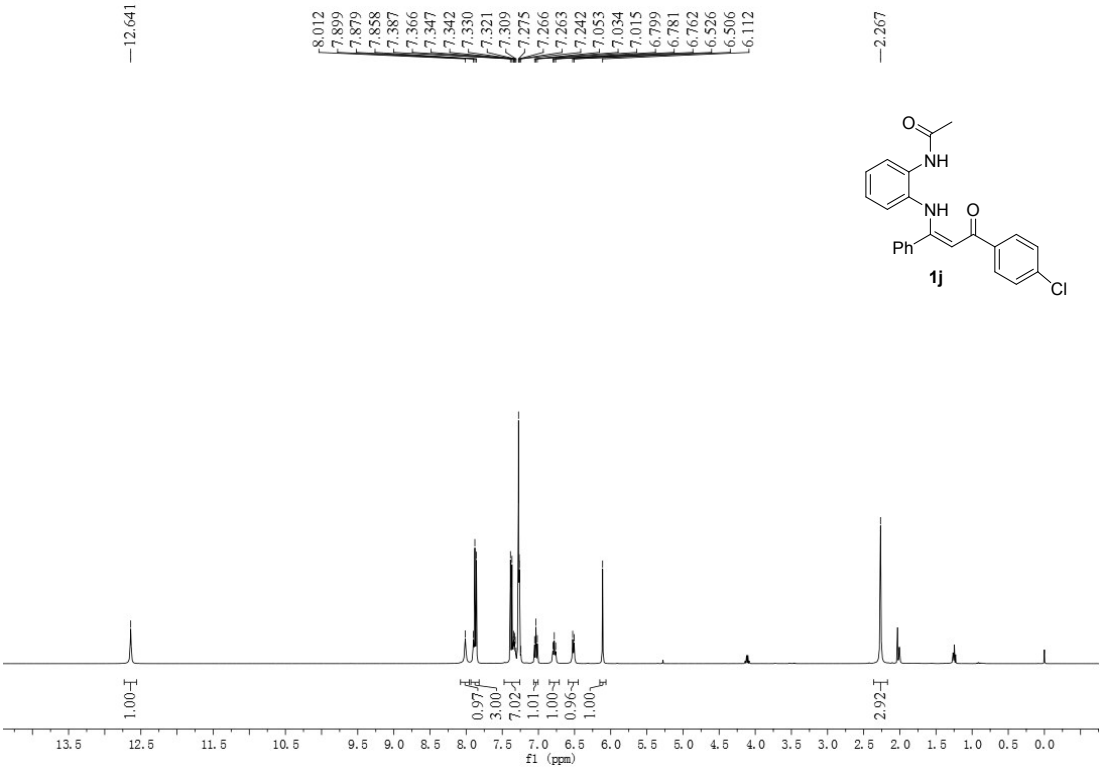

183.522
165.926
159.247
139.701
132.305
128.468
126.921
125.462
125.224
124.960
122.509
122.423
122.386
122.276
121.879
93.838
20.122
O
NH
NH
O
Ph
1h
CF3
f1 (ppm)

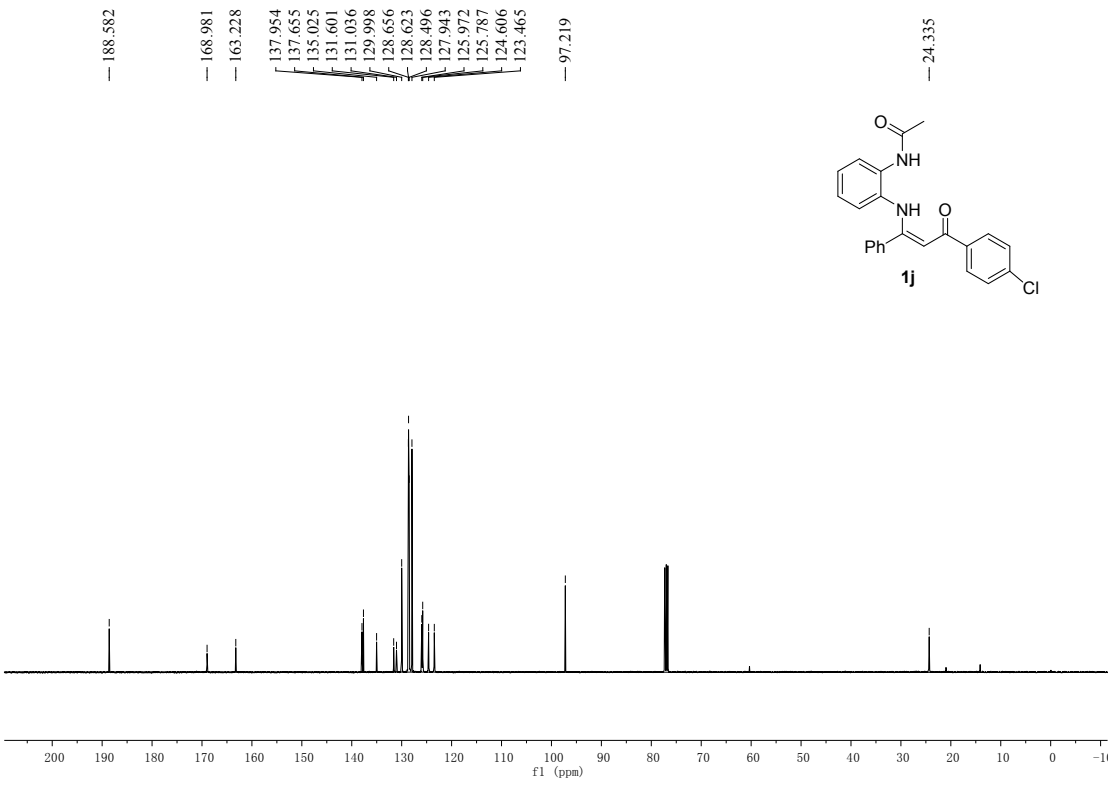

-61.261
O
NH
NH
O
Ph
CF3
1h
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

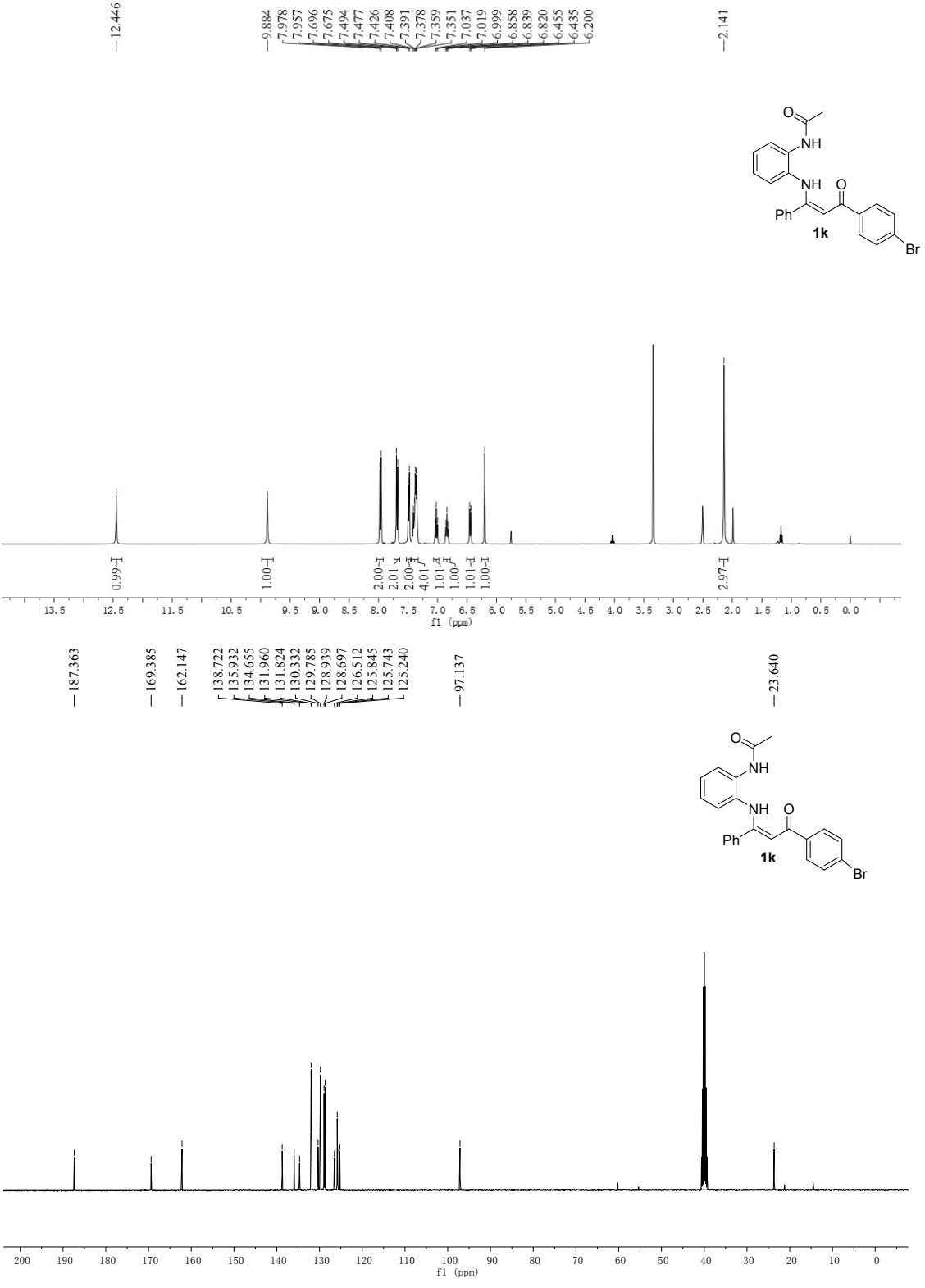

12.596
8.152
7.960
7.955
7.946
7.938
7.929
7.924
7.862
7.842
7.347
7.342
7.330
7.312
7.309
7.300
7.283
7.270
7.258
7.252
7.233
7.094
7.072
7.051
7.029
7.011
6.991
6.788
6.769
6.750
6.513
6.493
6.109
2.256
O
NH
NH
O
Ph
F
1i
1.00
0.95
2.00
1.00
5.02
2.02
1.01
1.00
0.96
1.00
2.93
f1 (ppm)

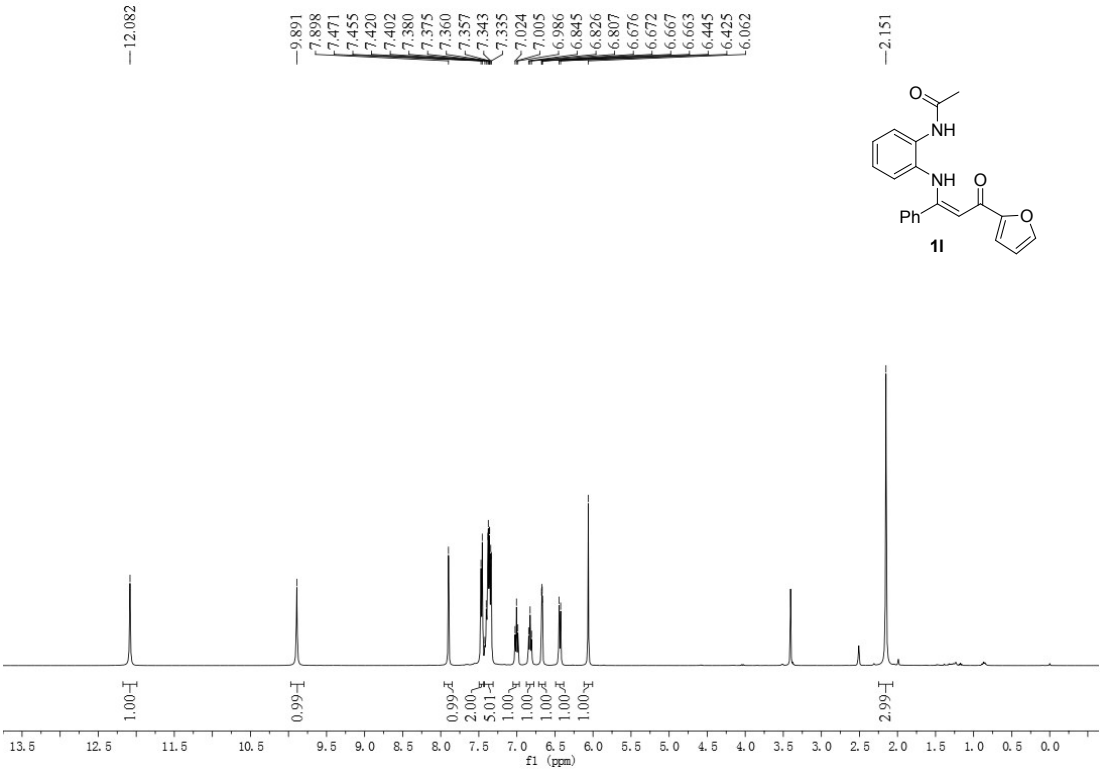

188.506
169.100
166.009
163.502
162.887
135.116
129.896
129.602
129.514
128.429
127.930
125.889
125.596
124.612
123.575
115.419
115.203
97.202
24.212
O
NH
NH
O
Ph
F
1i
f1 (ppm)

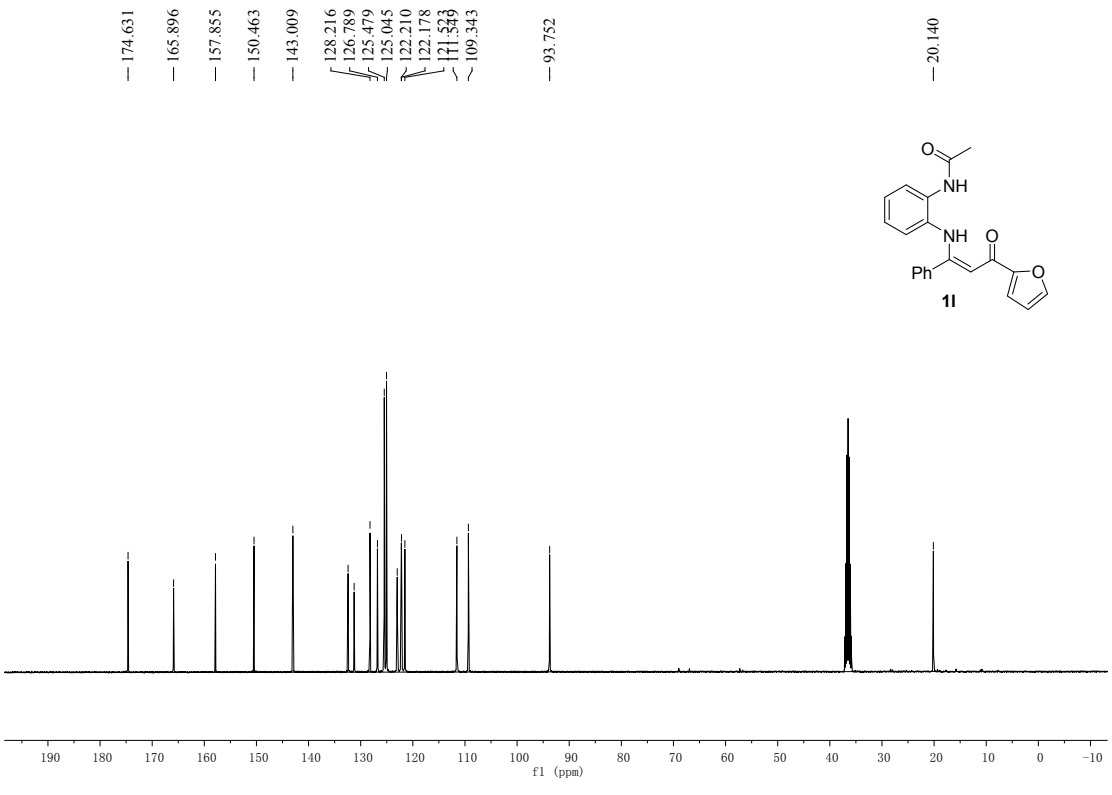

-108.099
O
NH
NH
O
Ph
F
1i
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

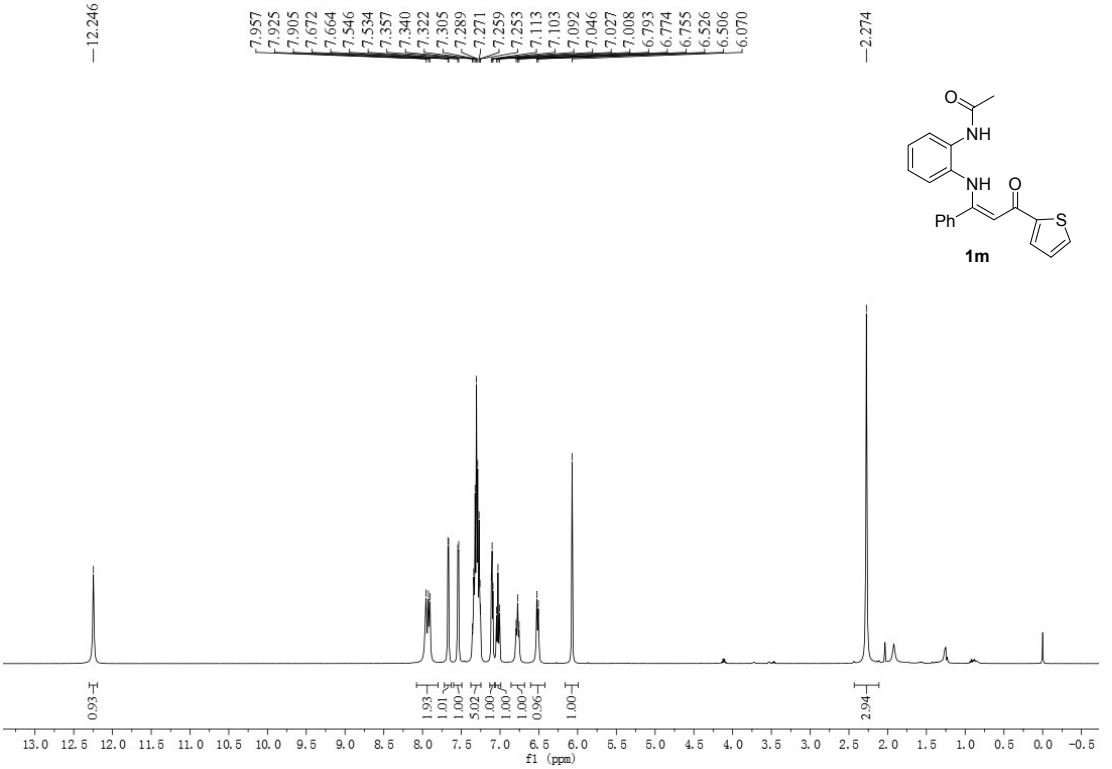

12.641
8.012
7.899
7.879
7.858
7.387
7.366
7.347
7.342
7.330
7.321
7.309
7.275
7.266
7.263
7.242
7.053
7.034
7.015
6.799
6.781
6.762
6.526
6.506
6.112
2.267
O
NH
NH
O
Ph
1j
Cl
1.00
0.97
3.00
7.02
1.01
1.00
0.96
1.00
2.92
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

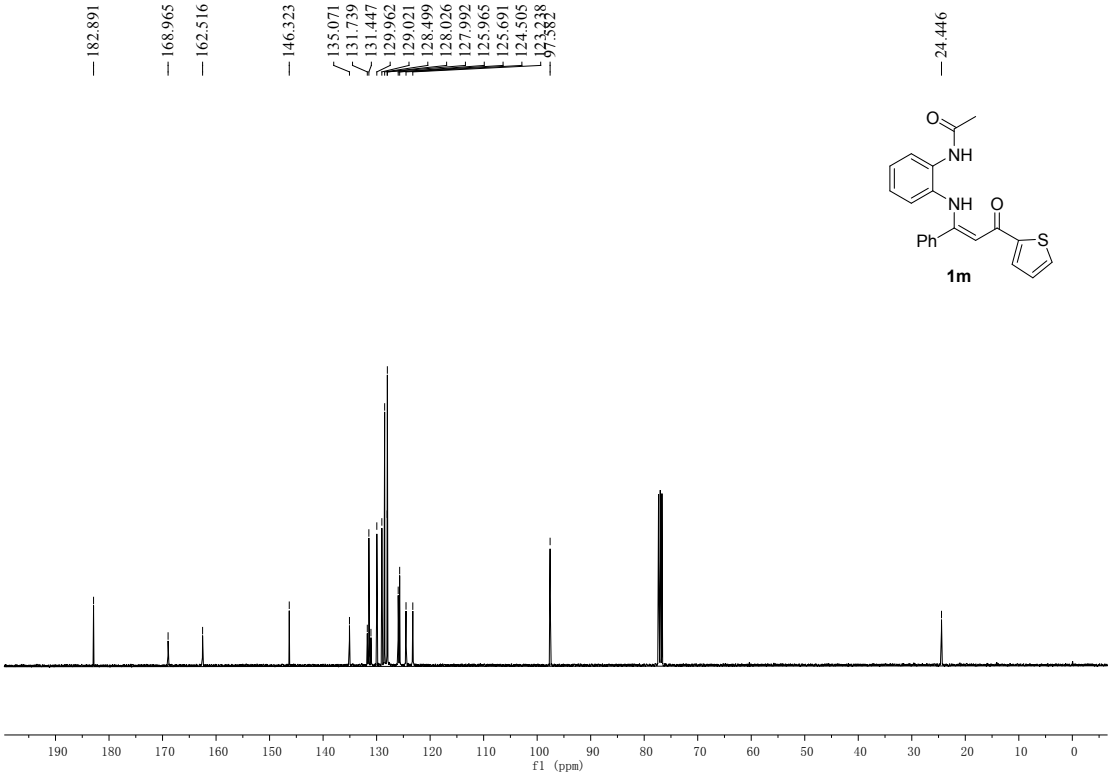

188.582
168.981
163.228
137.954
137.655
135.025
131.601
131.036
129.998
128.656
128.623
128.496
127.943
125.972
125.787
124.606
123.465
97.219
24.335
O
NH
NH
O
Ph
1j
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

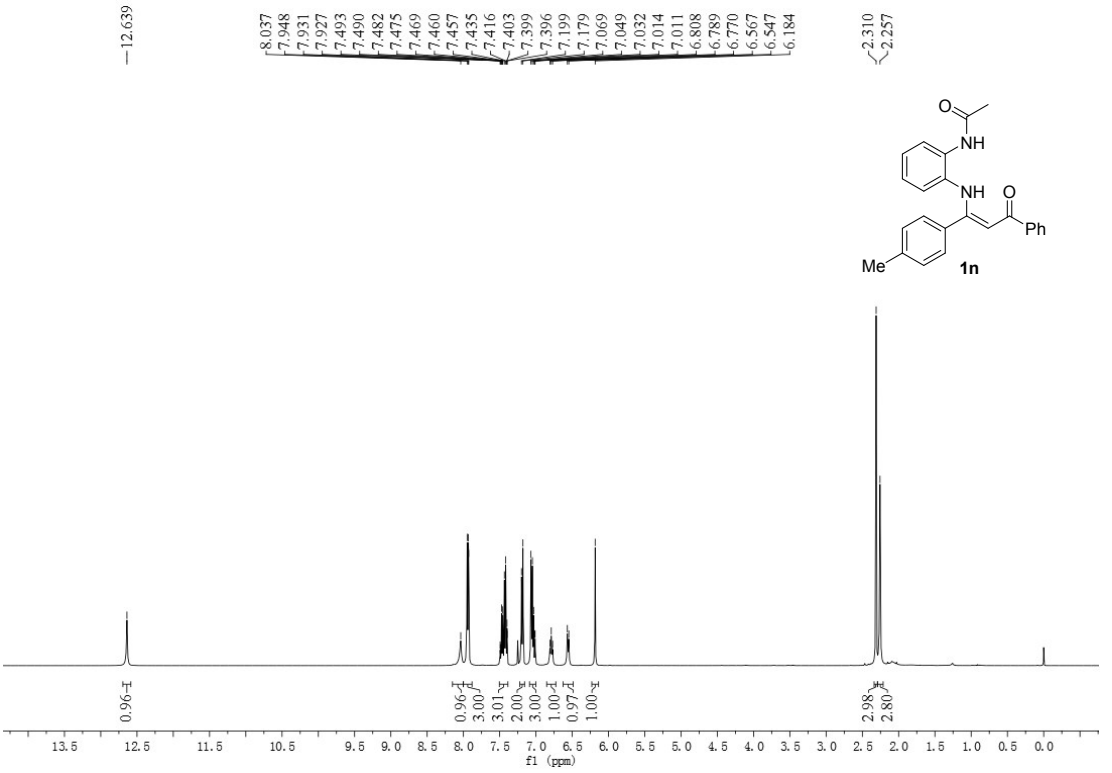

12.446
9.884
7.978
7.957
7.696
7.675
7.494
7.477
7.426
7.408
7.391
7.378
7.359
7.351
7.037
7.019
6.999
6.858
6.839
6.820
6.455
6.435
6.200
2.141
O
NH
NH
O
Ph
1k
Br
0.99
1.00
2.00
2.01
2.00
4.01
1.01
1.00
1.01
1.00
2.97
f1 (ppm)
187.363
169.385
162.147
138.722
135.932
134.655
131.960
131.824
130.332
129.785
128.939
128.697
126.512
125.845
125.743
125.240
97.137
23.640
f1 (ppm)

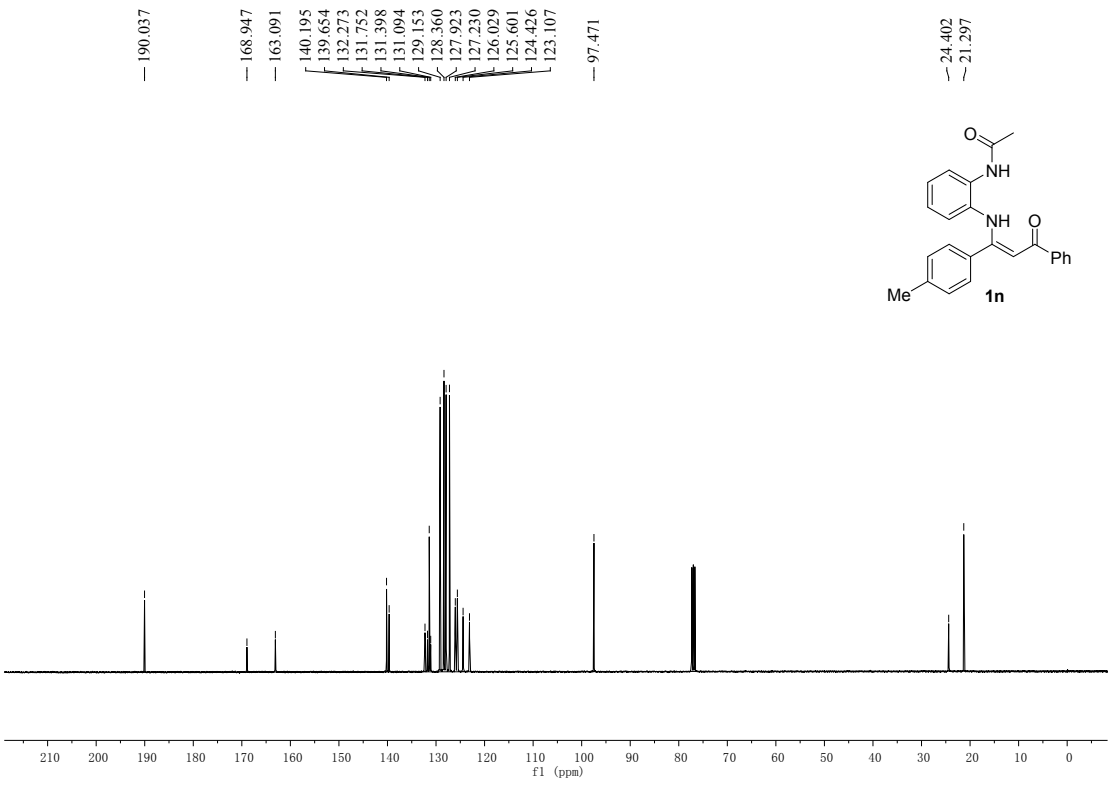

12.082
9.891
7.898
7.471
7.455
7.420
7.402
7.380
7.375
7.360
7.357
7.343
7.335
7.024
7.005
6.986
6.845
6.826
6.807
6.676
6.672
6.667
6.663
6.445
6.425
6.062
2.151
NH
NH
O
O
Ph
O
1l
1.00
0.99
0.99
2.00
5.01
1.00
1.00
1.00
1.00
2.99
f1 (ppm)

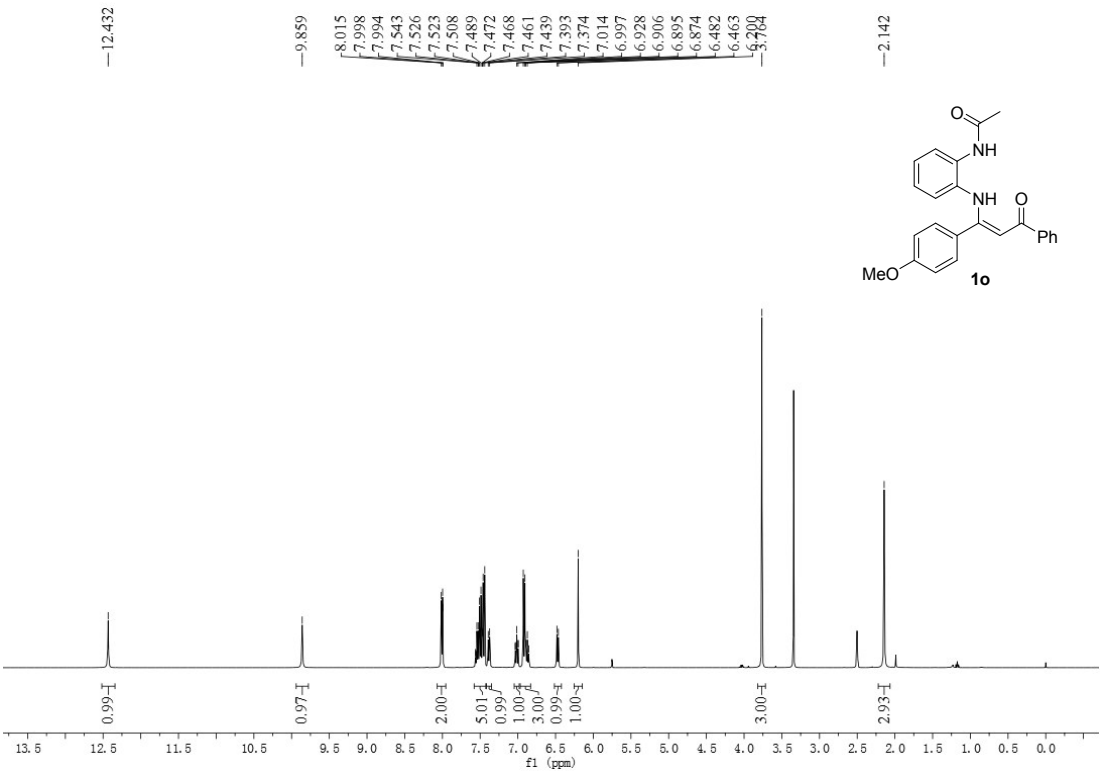

174.631
165.896
157.855
150.463
143.009
128.216
126.789
125.479
125.045
122.210
122.178
111.523
111.349
109.343
93.752
20.140
NH
NH
O
O
Ph
O
1l
f1 (ppm)

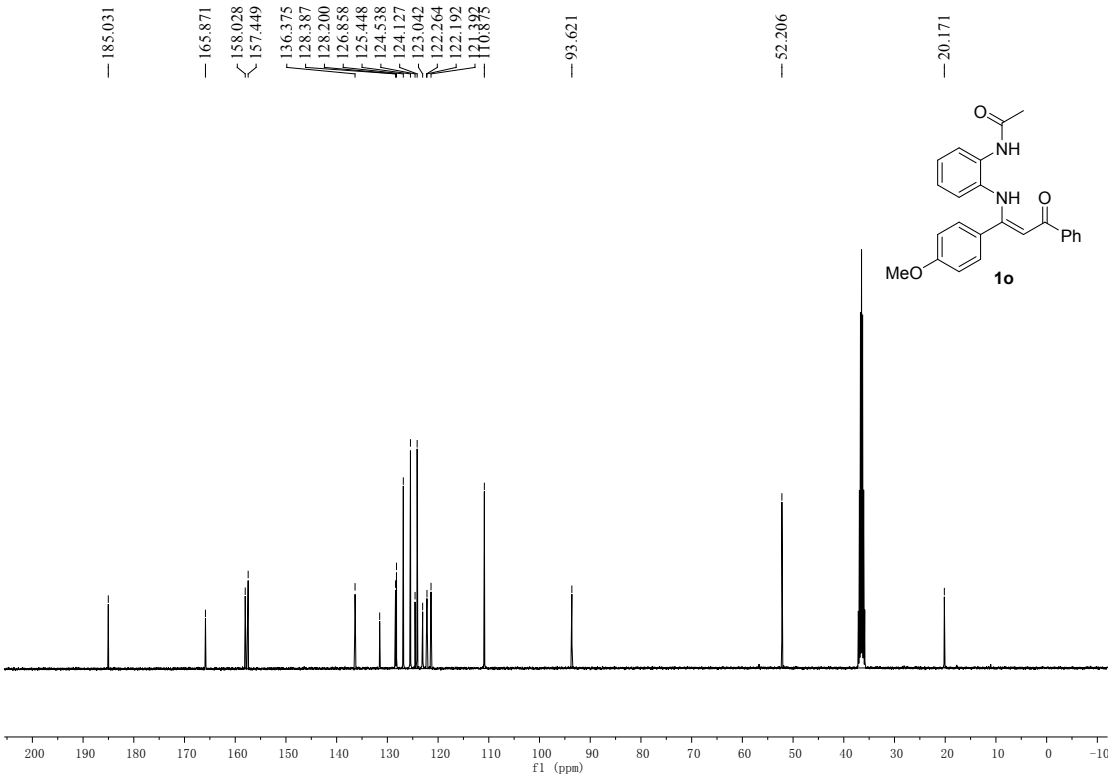

12.246
7.957
7.925
7.905
7.672
7.664
7.546
7.534
7.357
7.340
7.322
7.305
7.289
7.271
7.259
7.253
7.113
7.103
7.092
7.046
7.027
7.008
6.793
6.774
6.755
6.526
6.506
6.070
2.274
O
NH
NH
O
Ph
S
1m
0.93
1.93
1.01
1.00
5.02
1.00
1.00
1.00
0.96
1.00
2.94
f1 (ppm)

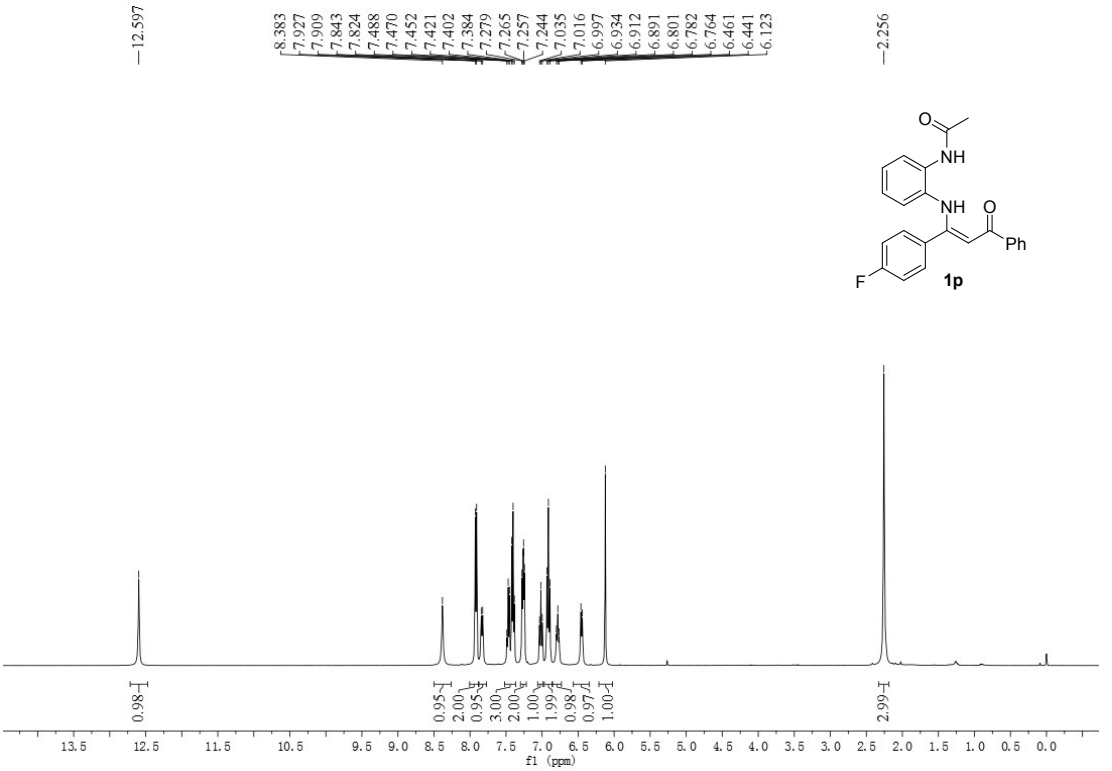

182.891
168.965
162.516
146.323
135.071
131.739
131.447
129.962
129.021
128.499
128.026
127.992
125.965
125.691
124.505
123.238
97.382
24.446
O
NH
NH
O
Ph
S
1m
f1 (ppm)

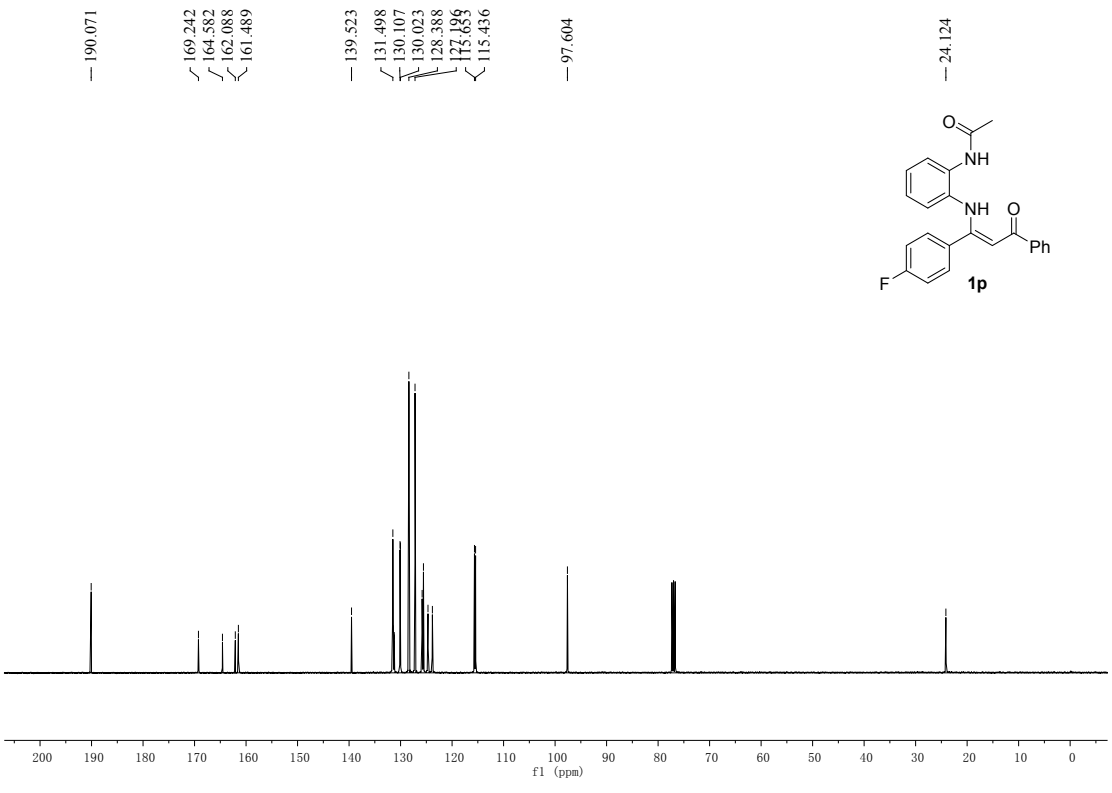

12.639
8.037
7.948
7.931
7.927
7.493
7.490
7.482
7.475
7.469
7.460
7.457
7.435
7.416
7.403
7.399
7.396
7.199
7.179
7.069
7.049
7.032
7.014
7.011
6.808
6.789
6.770
6.567
6.547
6.184
2.310
2.257
O
NH
NH
O
Ph
Me
1n
0.96
3.00
3.01
2.00
3.00
1.00
0.97
1.00
2.98
2.80
f1 (ppm)

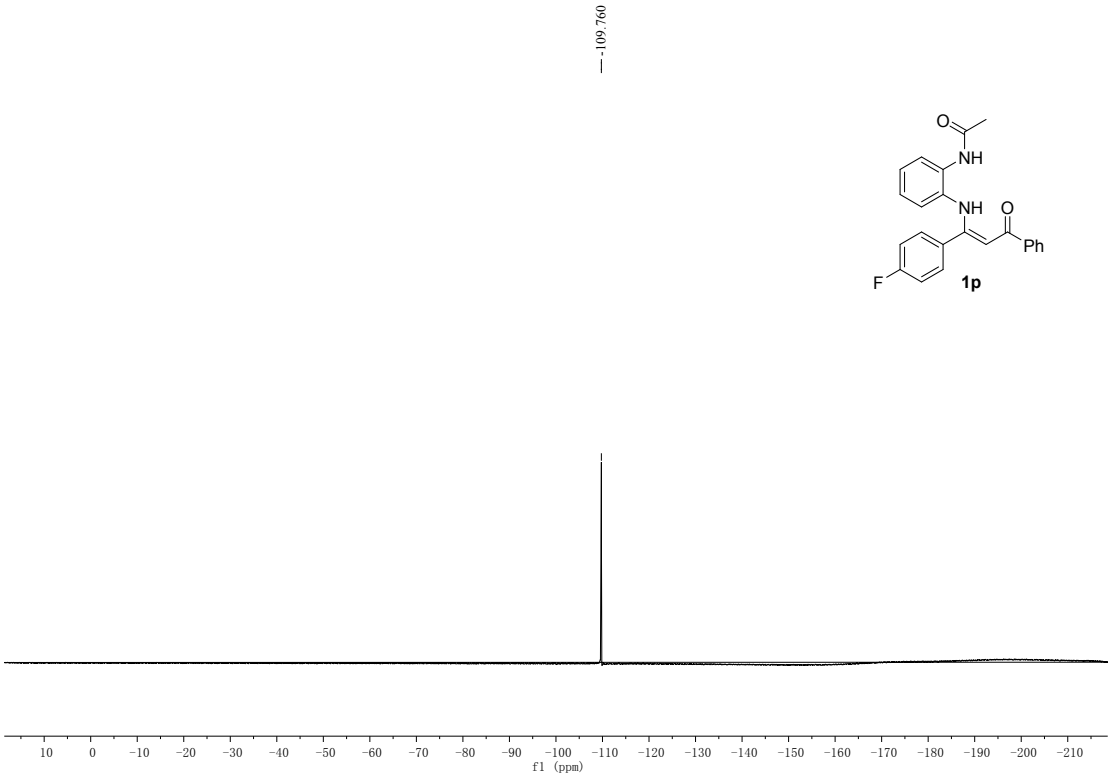

190.037
168.947
163.091
140.195
139.654
132.273
131.752
131.398
131.094
129.153
128.360
127.923
127.230
126.029
125.601
124.426
123.107
97.471
24.402
21.297
O
NH
NH
O
Ph
Me
1n
f1 (ppm)

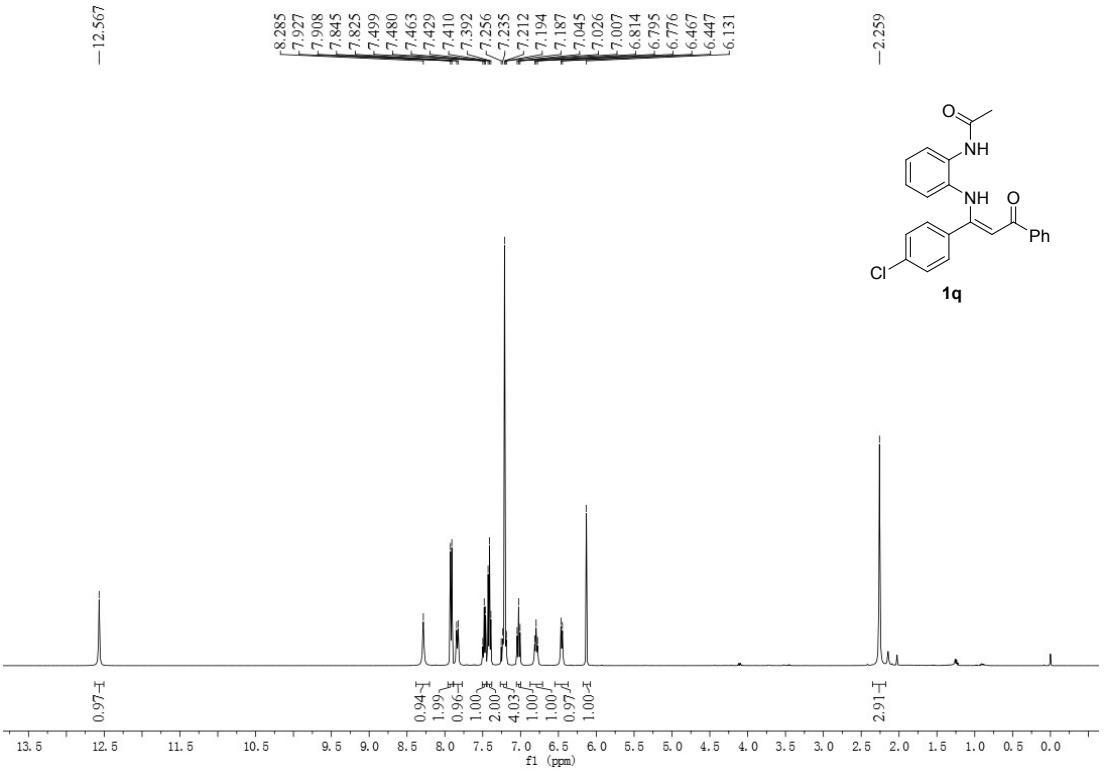

12.432
9.859
8.015
7.998
7.994
7.543
7.526
7.523
7.508
7.489
7.472
7.468
7.461
7.439
7.393
7.374
7.014
6.997
6.928
6.906
6.895
6.874
6.482
6.463
6.200
3.764
2.142
O
NH
NH
O
Ph
MeO
1o
0.99
0.97
2.00
5.01
0.99
1.00
3.00
0.99
1.00
3.00
2.93
f1 (ppm)

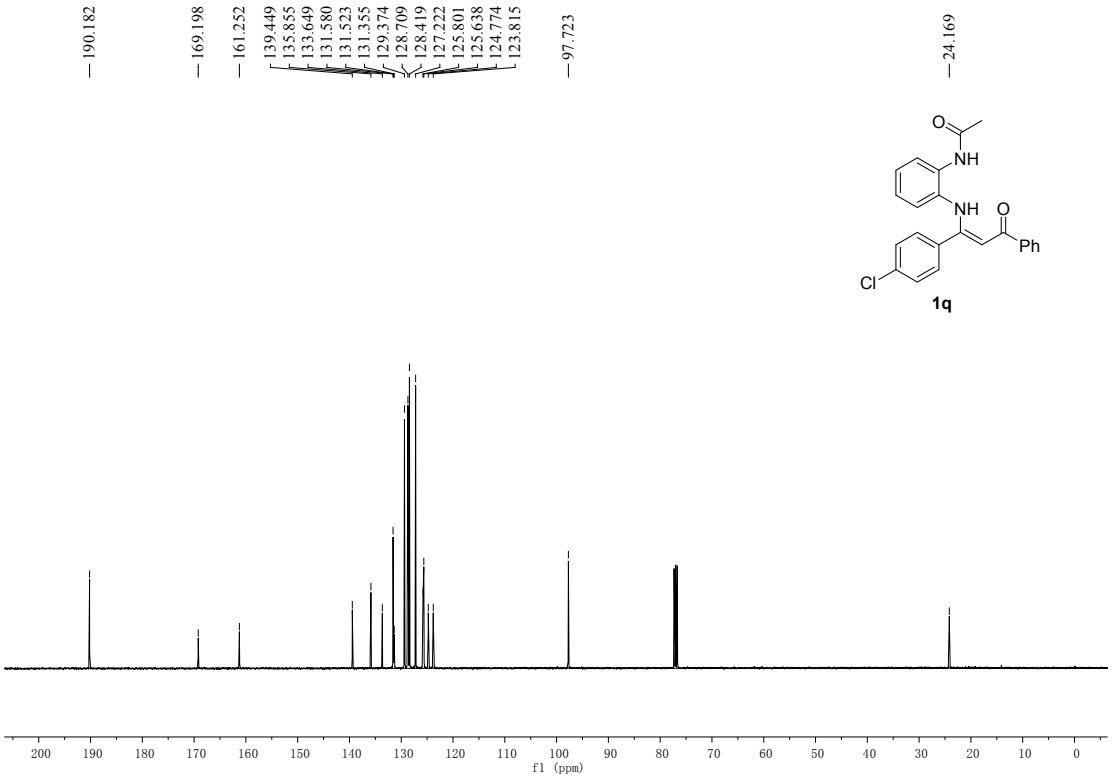

185.031
165.871
158.028
157.449
136.375
128.387
128.200
126.858
125.448
124.538
124.127
123.042
122.264
122.192
121.392
110.875
93.621
52.206
20.171
O
NH
NH
O
Ph
MeO
1o
f1 (ppm)

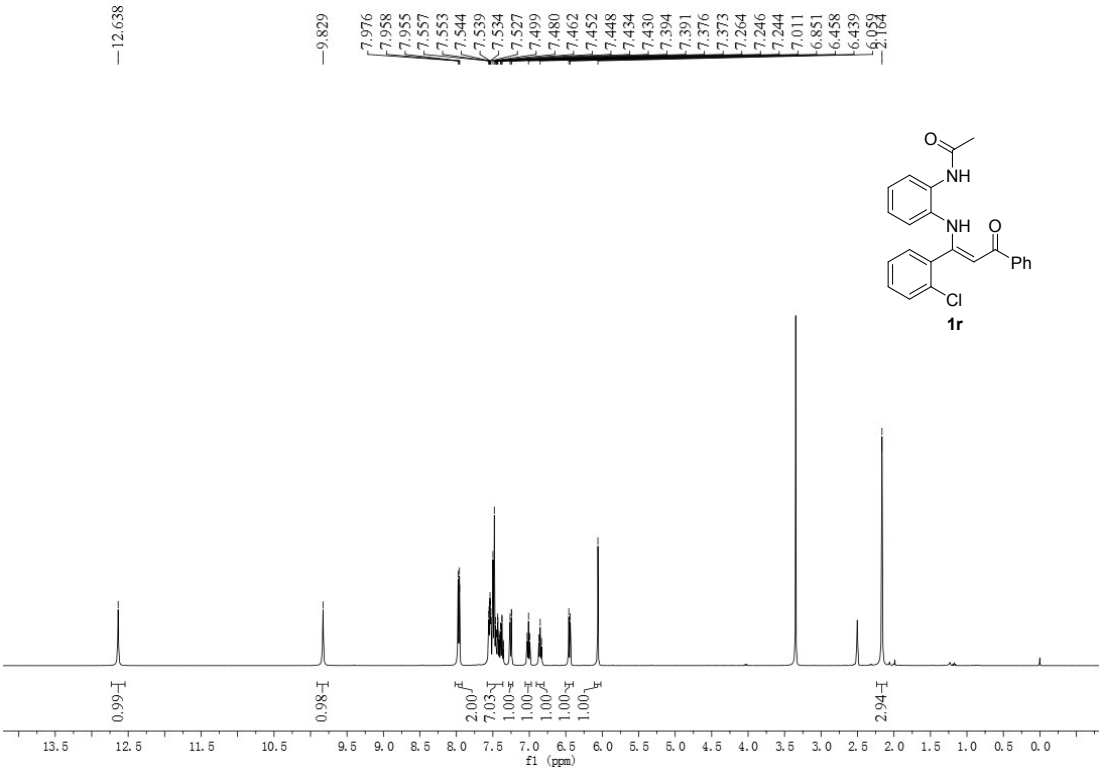

12.597
8.383
7.927
7.909
7.843
7.824
7.488
7.470
7.452
7.421
7.402
7.384
7.279
7.265
7.257
7.244
7.035
7.016
6.997
6.934
6.912
6.891
6.801
6.782
6.764
6.461
6.441
6.123
2.256
O
NH
NH
O
Ph
F
1p
0.98
0.95
2.00
0.95
3.00
2.00
1.00
1.99
0.98
0.97
1.00
2.99
f1 (ppm)

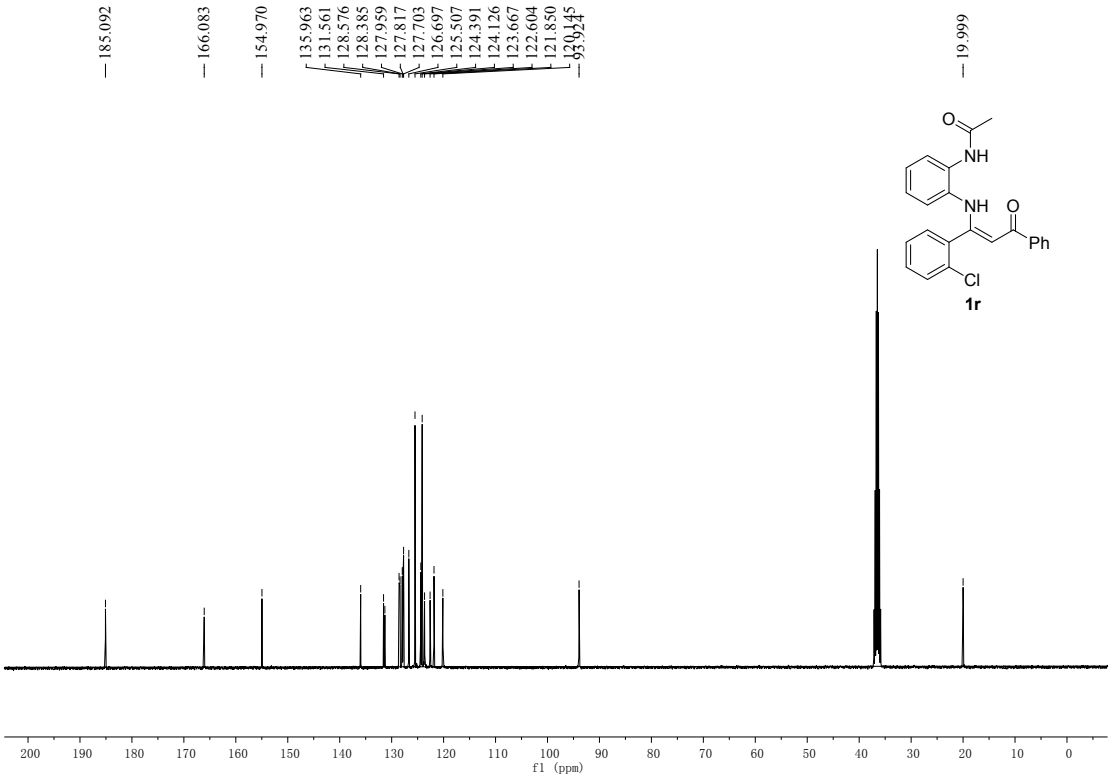

190.071
169.242
164.582
162.088
161.489
139.523
131.498
130.107
130.023
128.388
127.196
115.653
115.436
97.604
24.124
O
NH
NH
O
Ph
F
1p
f1 (ppm)

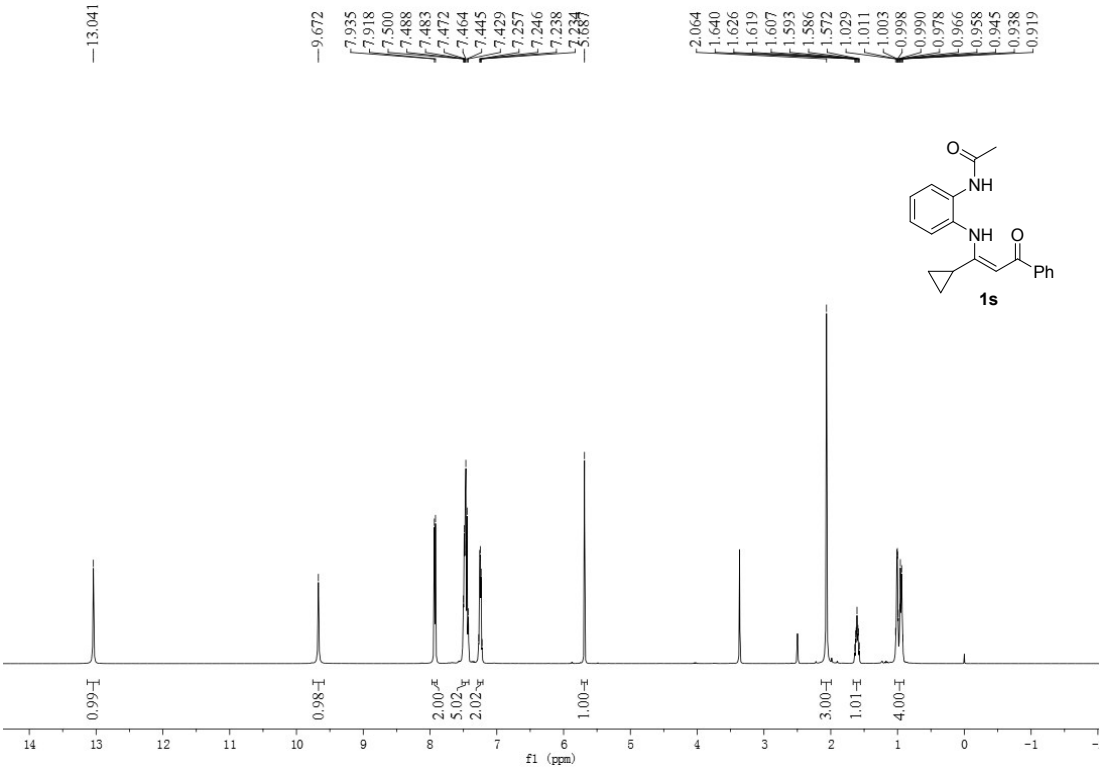

-109.760
O
NH
NH
O
Ph
F
1p
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

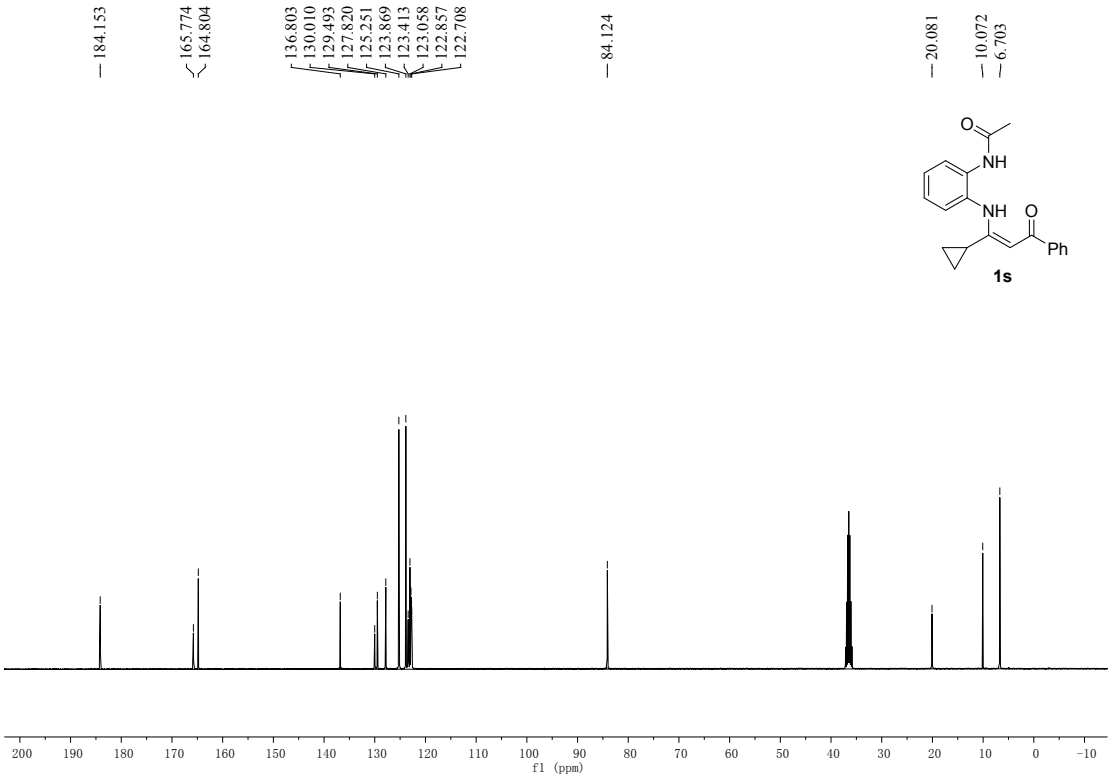

12.567
8.285
7.927
7.908
7.845
7.825
7.499
7.480
7.463
7.429
7.410
7.392
7.256
7.235
7.212
7.194
7.187
7.045
7.026
7.007
6.814
6.795
6.776
6.467
6.447
6.131
2.259
O
NH
NH
O
Ph
Cl
1q
0.97
0.94
1.99
0.96
1.00
2.00
4.03
1.00
1.00
0.97
1.00
2.91
f1 (ppm)


190.182
169.198
161.252
139.449
135.855
133.649
131.580
131.523
131.355
129.374
128.709
128.419
127.222
125.801
125.638
124.774
123.815
97.723
24.169
O
NH
NH
O
Ph
Cl
1q
f1 (ppm)

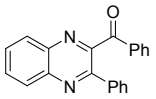

12.638
9.829
7.976
7.958
7.955
7.557
7.553
7.544
7.539
7.534
7.527
7.499
7.480
7.462
7.452
7.448
7.434
7.430
7.394
7.391
7.376
7.373
7.264
7.246
7.244
7.011
6.851
6.458
6.439
6.053
2.164
O
NH
NH
O
Ph
Cl
1r
0.99
0.98
2.00
7.03
1.00
1.00
1.00
1.00
2.94
f1 (ppm)


185.092
166.083
154.970
135.963
131.561
128.576
128.385
127.959
127.817
127.703
126.697
125.507
124.391
124.126
123.667
122.604
121.850
120.145
93.924
19.999
O
NH
NH
O
Ph
Cl
1r
f1 (ppm)

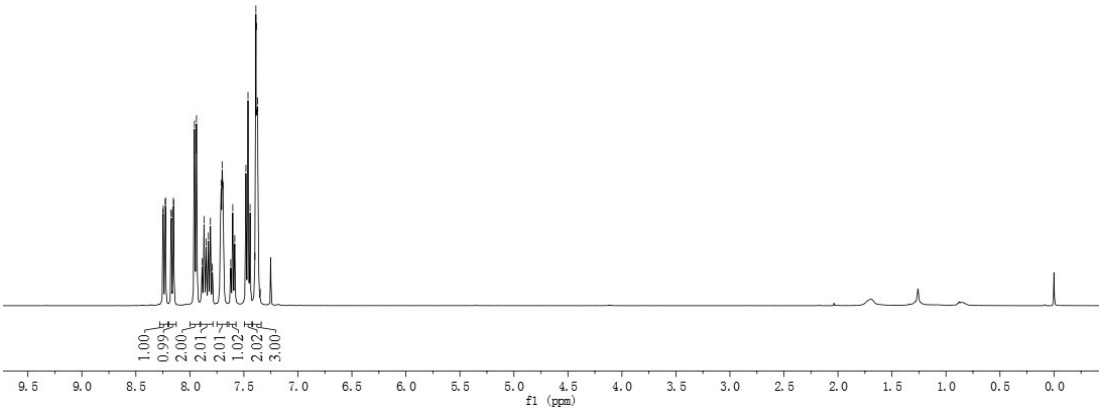

13.041
9.672
7.935
7.918
7.500
7.488
7.483
7.472
7.464
7.445
7.429
7.257
7.246
7.238
7.234
5.687
2.064
1.640
1.626
1.619
1.607
1.593
1.586
1.572
1.029
1.011
1.003
0.998
0.990
0.978
0.966
0.958
0.945
0.938
0.919
O
NH
NH
O
Ph
1s
0.99
0.98
2.00
5.02
2.02
1.00
3.00
1.01
4.00
f1 (ppm)

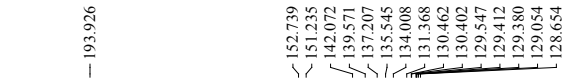

184.153
165.774
164.804
136.803
130.010
129.493
127.820
125.251
123.869
123.413
123.058
122.857
122.708
84.124
20.081
10.072
6.703
O
NH
NH
O
Ph
1s
f1 (ppm)

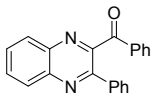

8.249
8.246
8.228
8.226
8.173
8.171
8.153
8.150
7.958
7.939
7.887
7.869
7.850
7.829
7.810
7.792
7.710
7.702
7.699
7.693
7.621
7.603
7.584
7.481
7.462
7.443
7.398
7.389
7.382
7.373
7.348


O
N
Ph
N
Ph

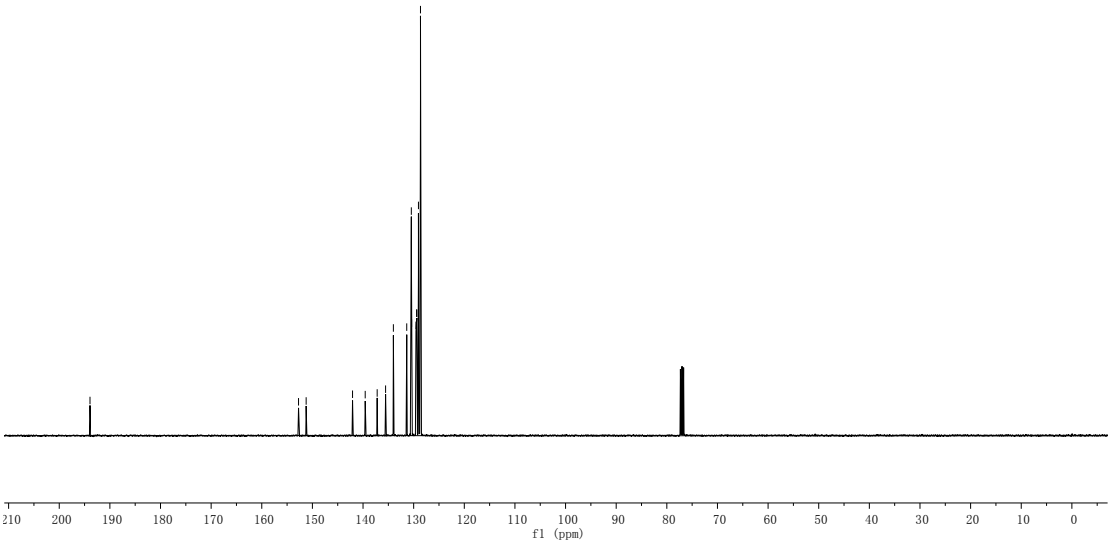
2a

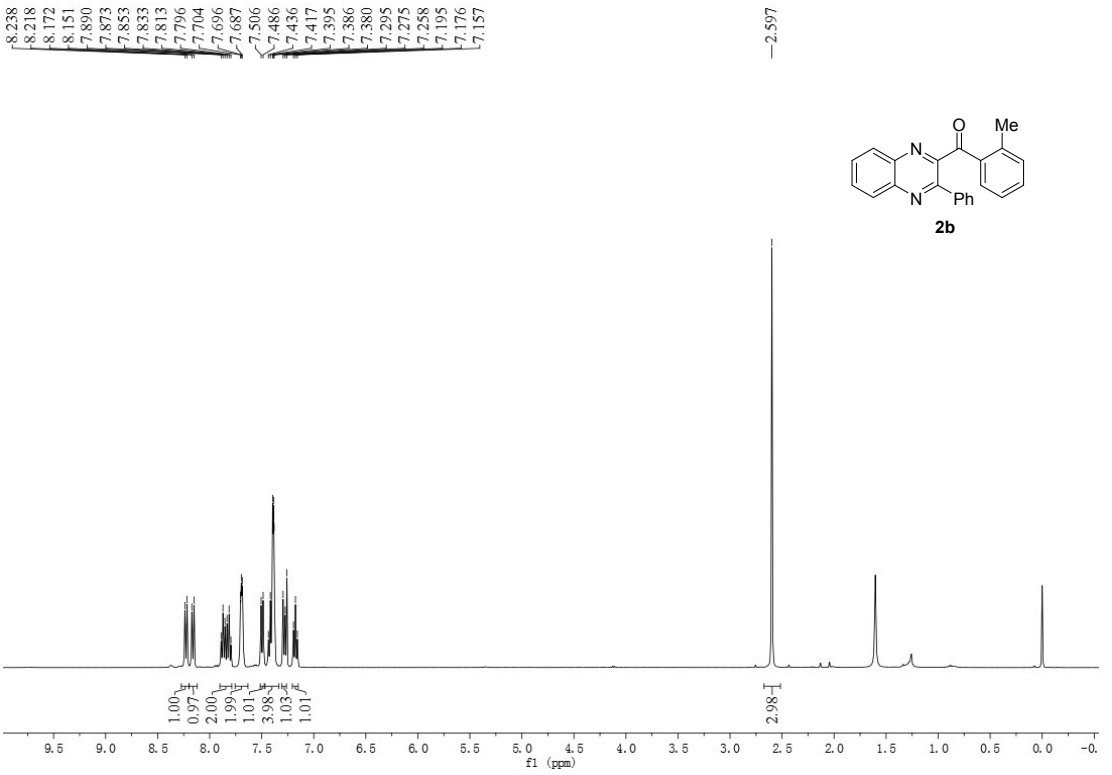

1.00
0.99
2.00
2.01
2.01
1.02
2.02
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

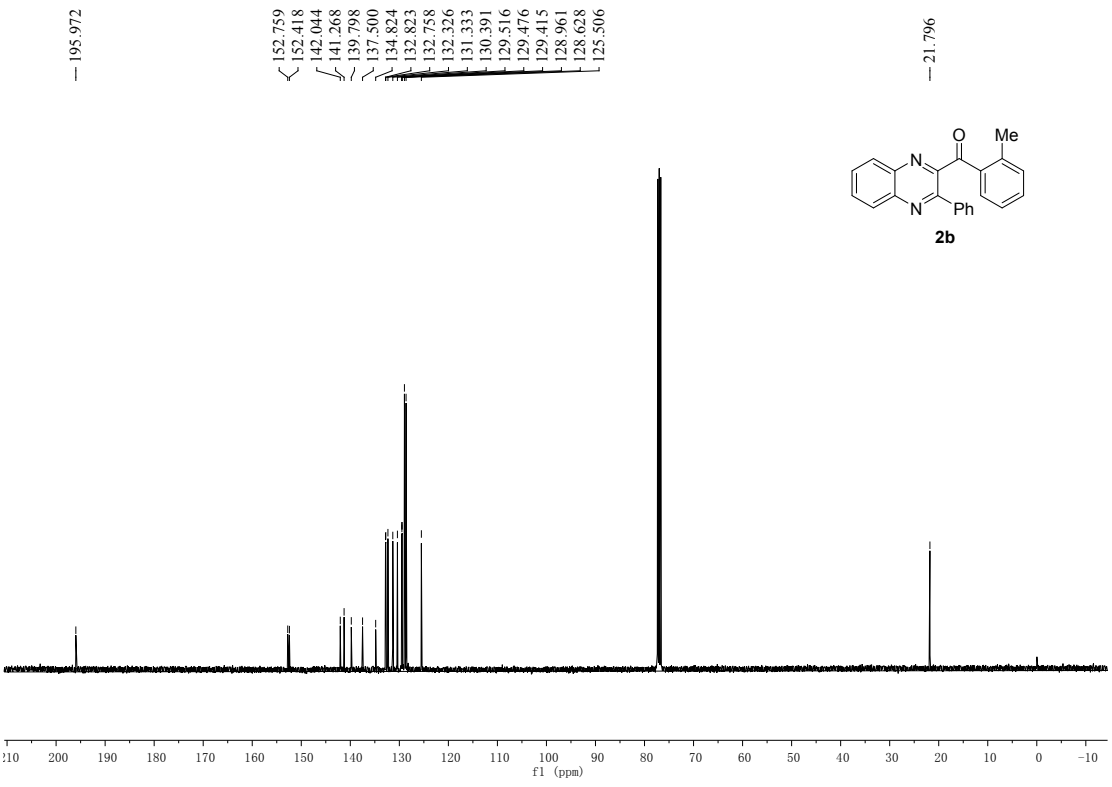

193.926
152.739
151.235
142.072
139.571
137.207
135.545
134.008
131.368
130.462
130.402
129.547
129.412
129.380
129.054
128.654

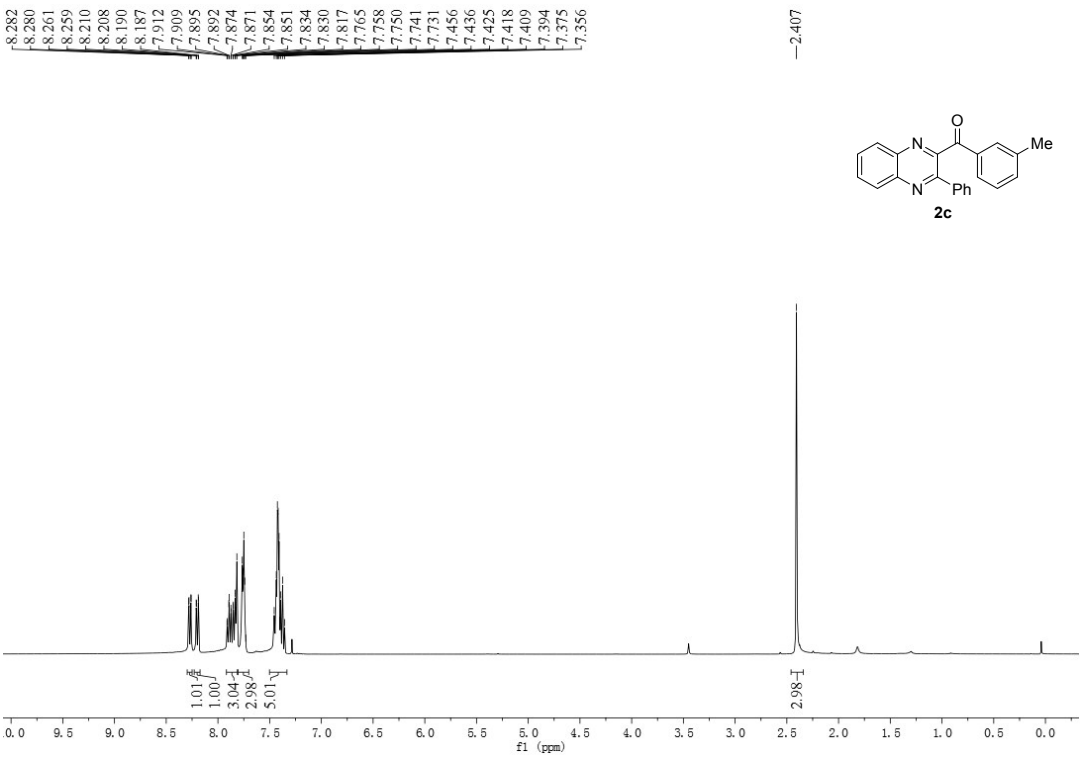

O
N
Ph
N
Ph

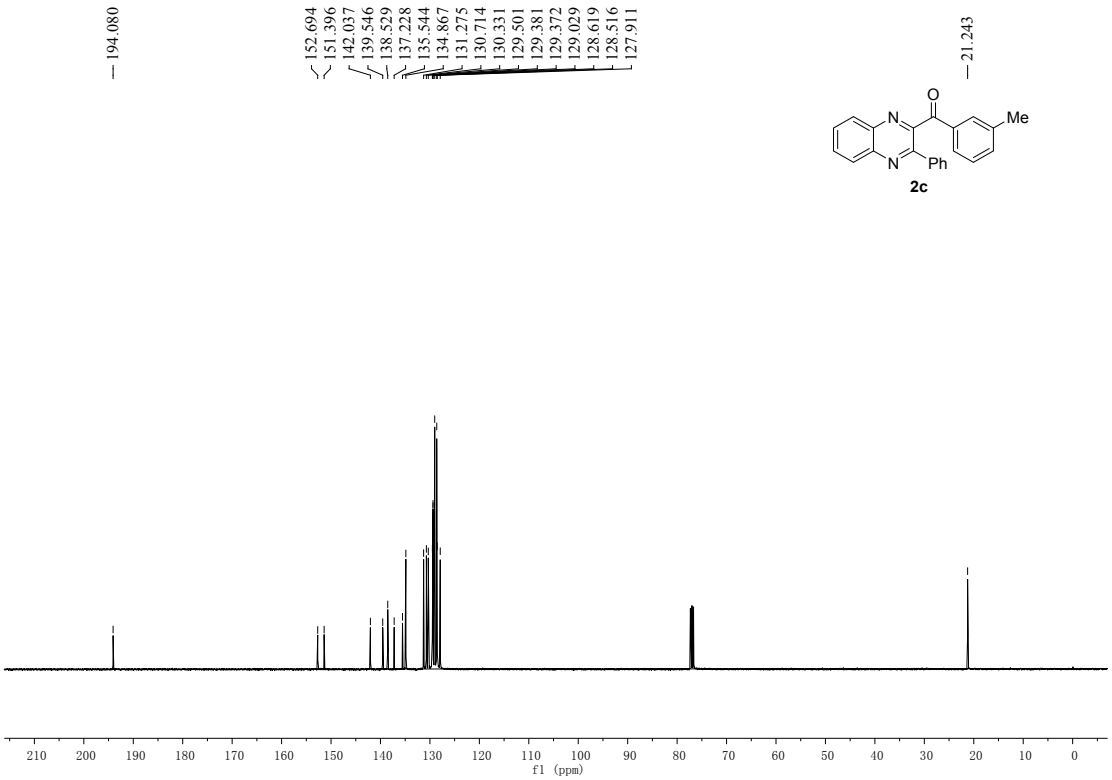
2a

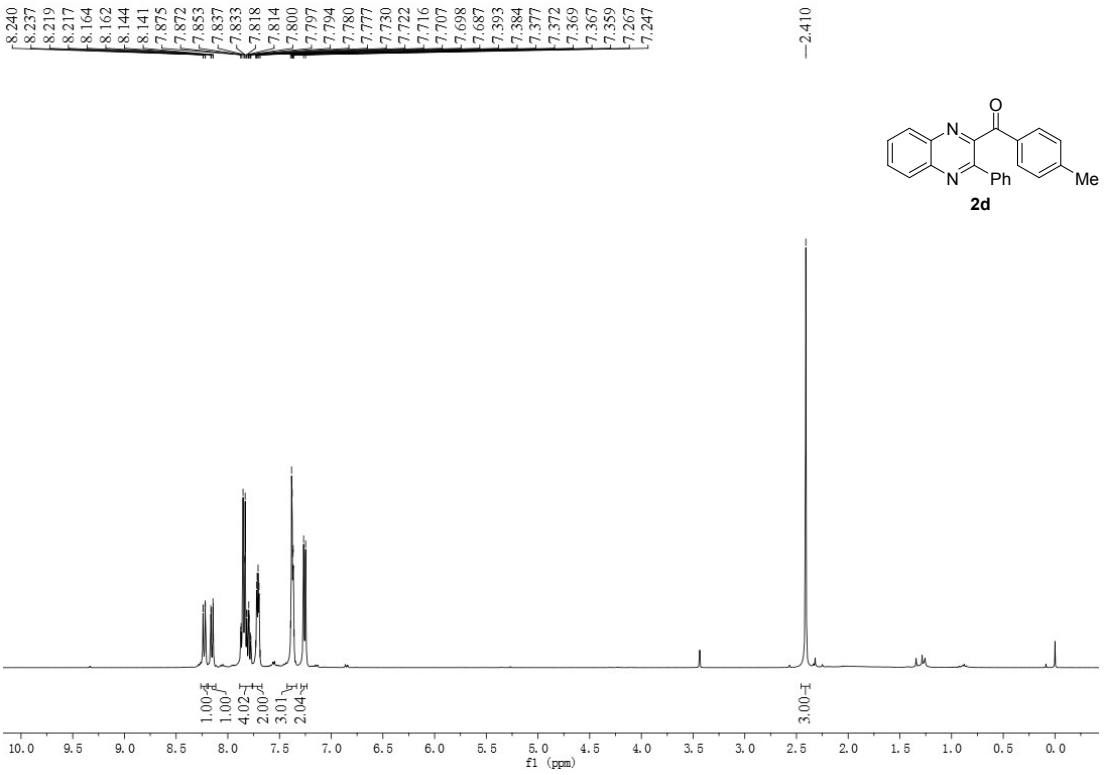

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

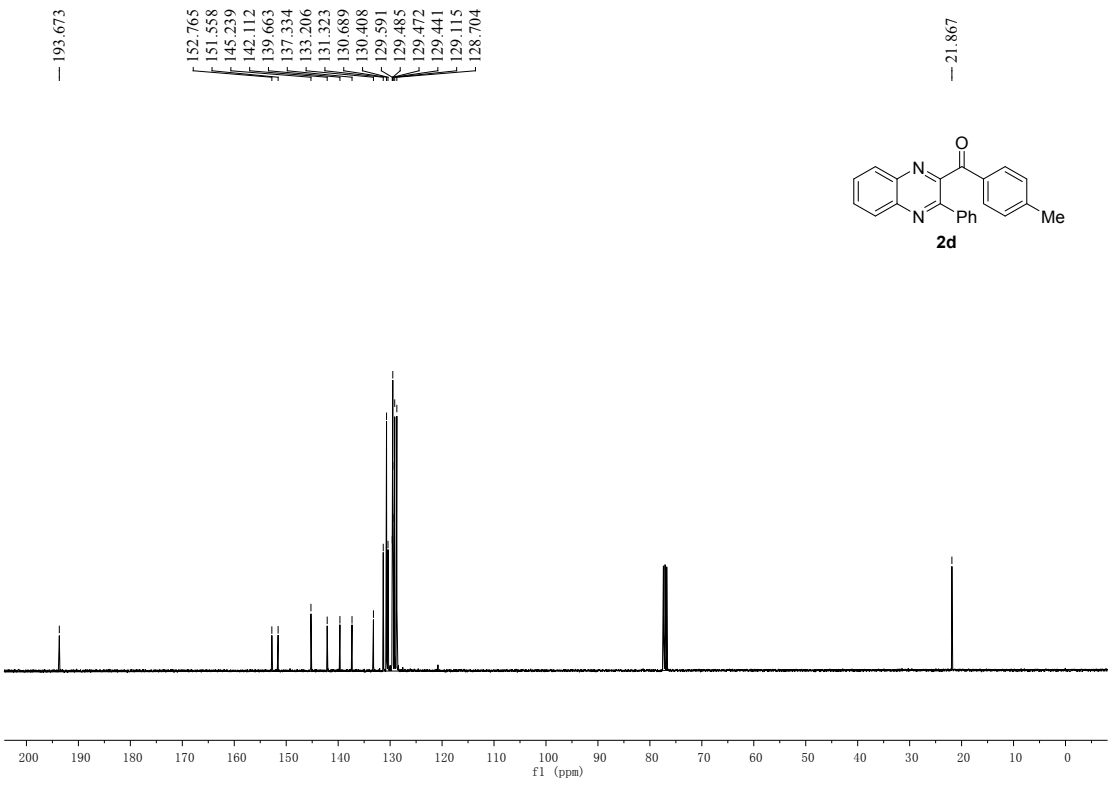

8.238
8.218
8.172
8.151
7.890
7.873
7.853
7.833
7.813
7.796
7.704
7.696
7.687
7.506
7.486
7.436
7.417
7.395
7.386
7.380
7.295
7.275
7.258
7.195
7.176
7.157
2.597
O
Me
N
N
Ph
2b
1.00
0.97
2.00
1.99
1.01
3.98
1.03
1.01
2.98
f1 (ppm)


195.972
152.759
152.418
142.044
141.268
139.798
137.500
134.824
132.823
132.758
132.326
131.333
130.391
129.516
129.476
129.415
128.961
128.628
125.506
21.796
O
Me
N
N
Ph
2b
f1 (ppm)

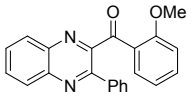

8.282
8.280
8.261
8.259
8.210
8.208
8.190
8.187
7.912
7.909
7.895
7.892
7.874
7.871
7.854
7.851
7.834
7.830
7.817
7.765
7.758
7.750
7.741
7.731
7.456
7.436
7.425
7.418
7.409
7.394
7.375
7.356
2.407
O
N
N
Me
Ph
2c
1.01
1.00
3.04
2.98
5.01
2.98
f1 (ppm)


194.080
152.694
151.396
142.037
139.546
138.529
137.228
135.544
134.867
131.275
130.714
130.331
129.501
129.381
129.372
129.029
128.619
128.516
127.911
21.243
O
N
N
Me
Ph
2c
f1 (ppm)

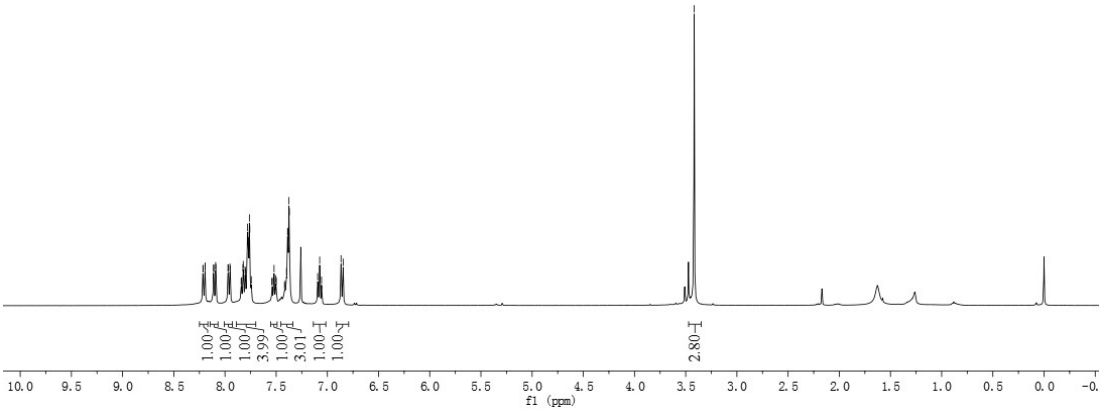

8.240
8.237
8.219
8.217
8.164
8.162
8.144
8.141
7.875
7.872
7.853
7.837
7.833
7.818
7.814
7.800
7.797
7.794
7.780
7.777
7.730
7.722
7.716
7.707
7.698
7.687
7.393
7.384
7.377
7.372
7.369
7.367
7.359
7.267
7.247
2.410
O
N
N
Ph
Me
2d
1.00
1.00
4.02
2.00
3.01
2.04
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.673
152.765
151.558
145.239
142.112
139.663
137.334
133.206
131.323
130.689
130.408
129.591
129.485
129.472
129.441
129.115
128.704
21.867
O
N
N
Ph
Me
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.215
8.213
8.194
8.193
8.112
8.110
8.091
8.089
7.971
7.967
7.951
7.947
7.839
7.825
7.822
7.804
7.801
7.781
7.777
7.771
7.762
7.757
7.743
7.521
7.503
7.499
7.399
7.388
7.384
7.376
7.371
7.094
7.075
7.057
6.867
6.846
3.447

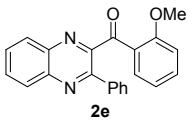

O
OMe
N
N
Ph

2e

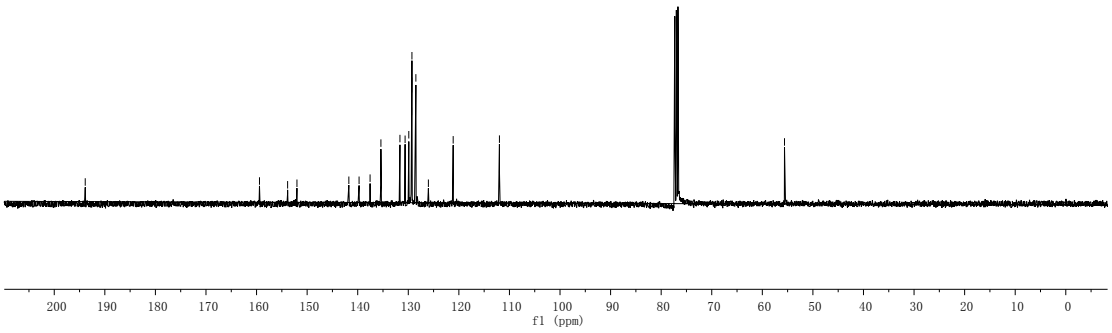

1.00
1.00
1.00
3.99
1.00
3.01
1.00
1.00
2.80
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

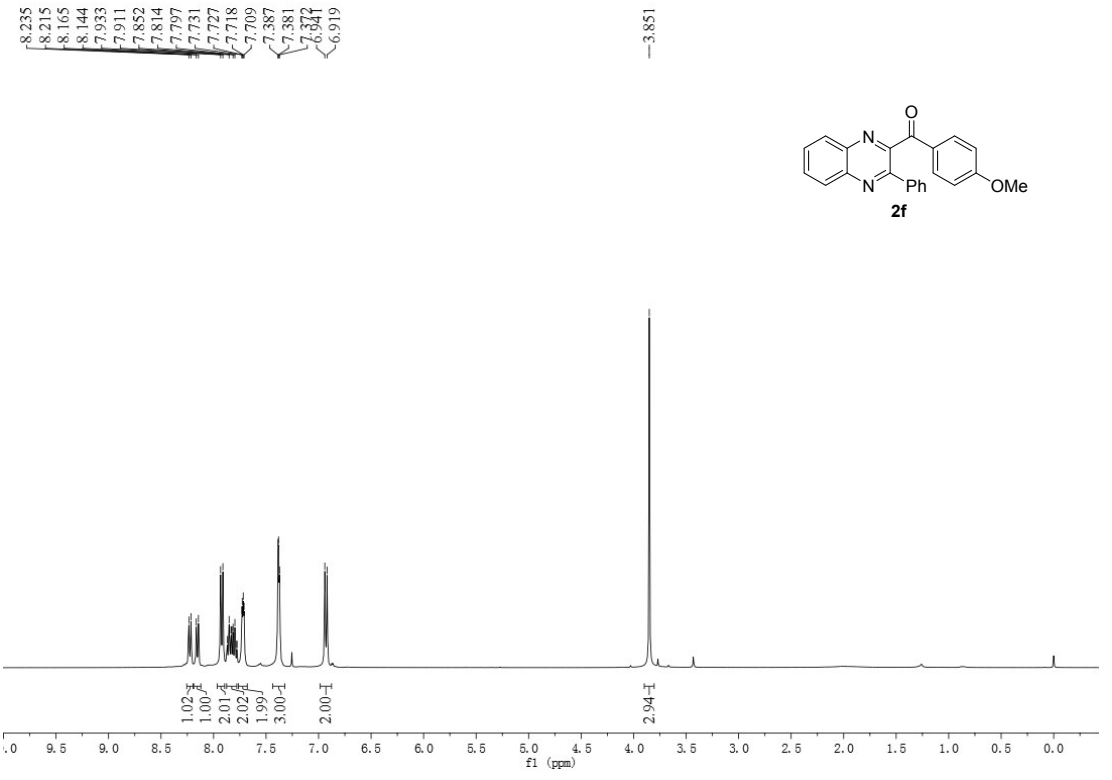

193.874
159.421
153.860
152.014
131.650
130.631
129.900
129.336
129.303
129.293
129.279
128.500
121.125
111.978

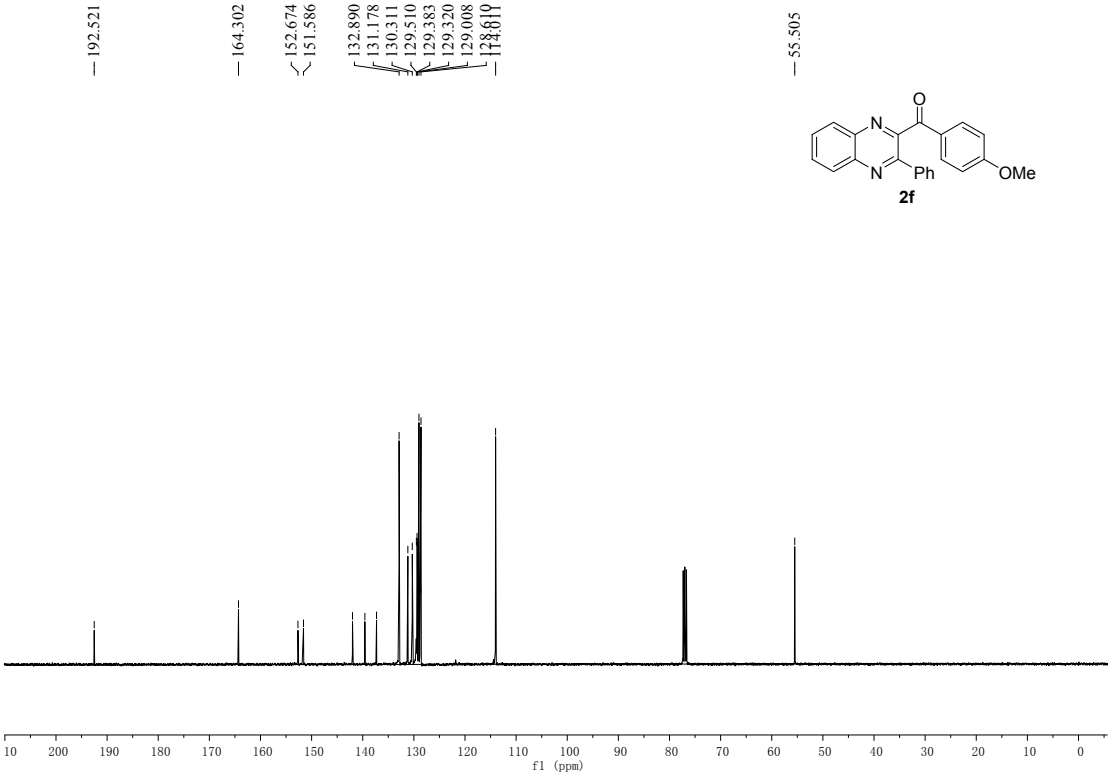
55.615

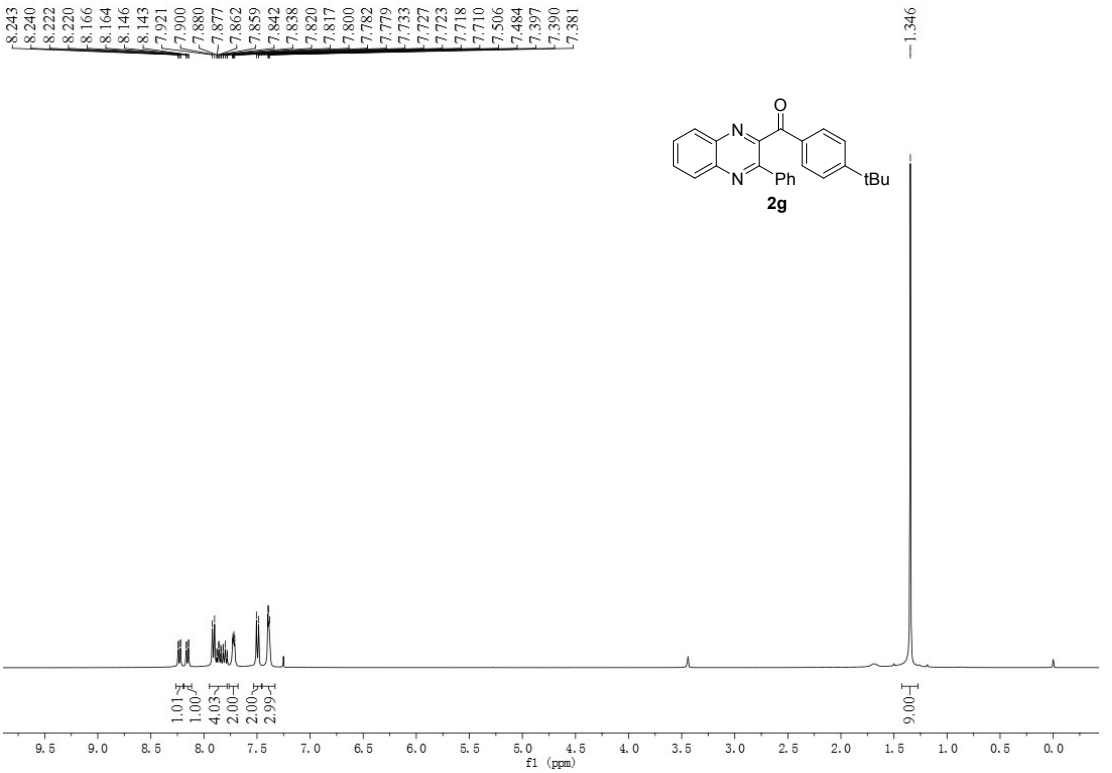

O
OMe
N
N
Ph

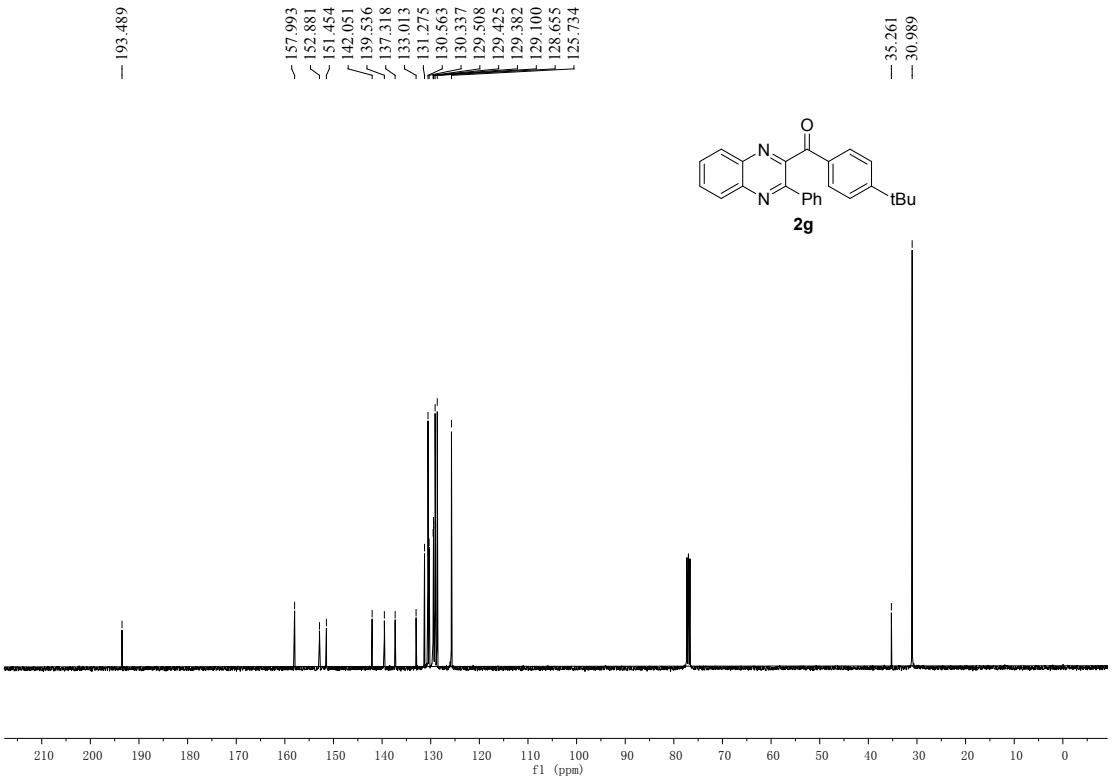
2e


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

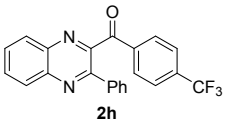

8.235
8.215
8.165
8.144
7.933
7.911
7.852
7.814
7.797
7.731
7.727
7.718
7.709
7.387
7.381
7.372
6.941
6.919
3.851
O
N
N
Ph
OMe
2f
1.02
1.00
2.01
2.02
1.99
3.00
2.00
2.94
f1 (ppm)


192.521
164.302
152.674
151.586
132.890
131.178
130.311
129.510
129.383
129.320
129.008
55.505
O
N
N
Ph
OMe
2f
f1 (ppm)

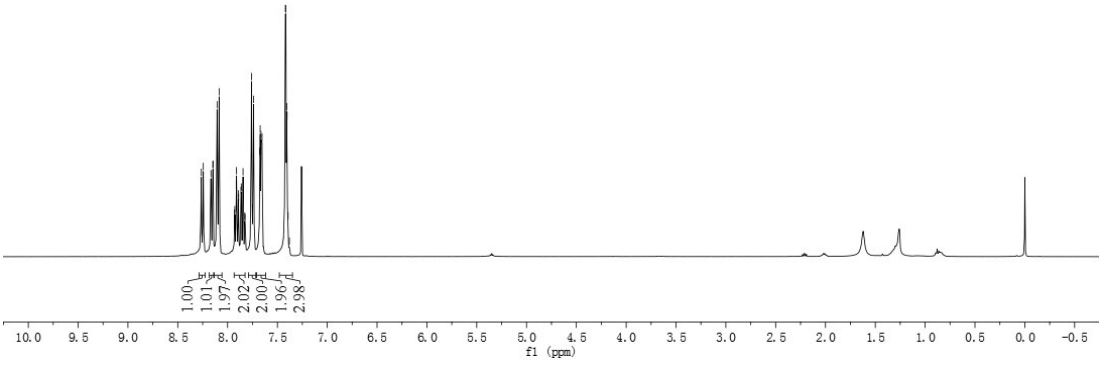

8.243
8.240
8.222
8.220
8.166
8.164
8.146
8.143
7.921
7.900
7.880
7.877
7.862
7.859
7.842
7.838
7.820
7.817
7.800
7.782
7.779
7.733
7.727
7.723
7.718
7.710
7.506
7.484
7.397
7.390
7.381
1.346
O
N
N
Ph
tBu
2g
1.01
1.00
4.03
2.00
2.00
2.99
9.00
f1 (ppm)


193.489
157.993
152.881
151.454
142.051
139.536
137.318
133.013
131.275
130.563
130.337
129.508
129.425
129.382
129.100
128.655
125.734
35.261
30.989
O
N
N
Ph
tBu
2g
f1 (ppm)

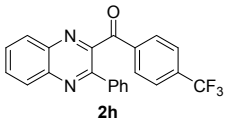

8.263
8.244
8.167
8.148
8.146
8.105
8.085
7.931
7.927
7.913
7.910
7.893
7.889
7.866
7.862
7.845
7.828
7.825
7.760
7.739
7.678
7.673
7.664
7.654
7.420
7.415
7.407
7.403
7.393
7.380


O
N
N
Ph
CF3

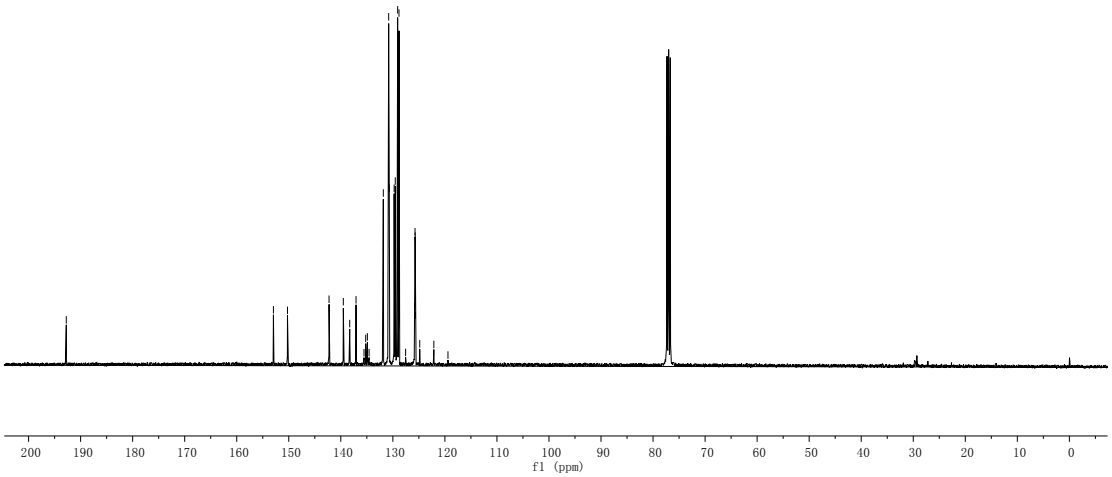
2h


1.00
1.01
1.97
2.02
2.00
1.96
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

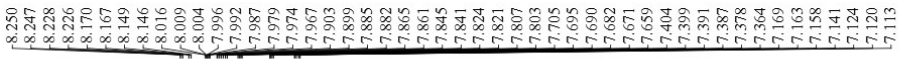

192.753
152.950
150.248
142.261
139.517
138.289
137.073
135.545
135.220
134.894
134.568
131.835
130.802
130.682
129.753
129.537
129.463
129.078
128.821
127.546
125.778
125.742
125.705
125.668
124.834
122.121
119.409

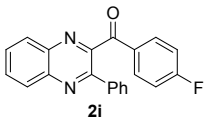

O
N
N
Ph
CF3

2h

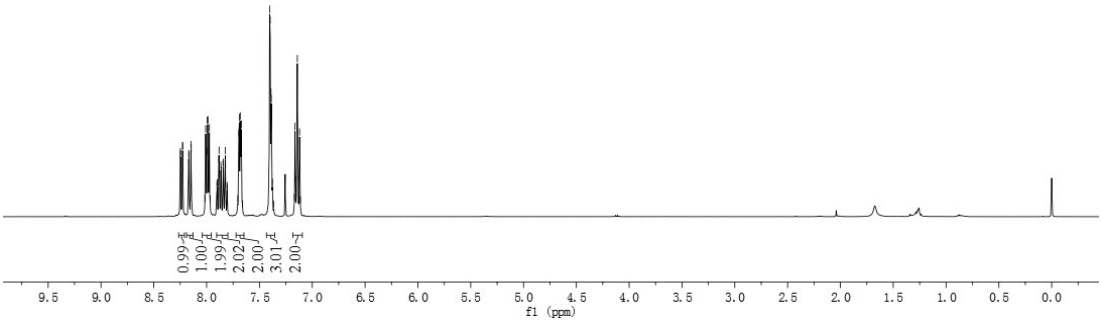

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

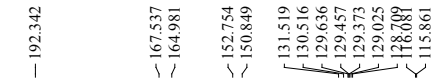

-63.195
O
N
N
Ph
CF3
2h
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

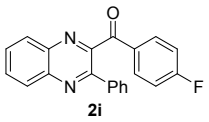

8.250
8.247
8.228
8.226
8.170
8.167
8.149
8.146
8.016
8.009
8.004
7.996
7.992
7.987
7.979
7.974
7.967
7.903
7.899
7.885
7.882
7.865
7.861
7.845
7.841
7.824
7.821
7.807
7.803
7.705
7.695
7.690
7.682
7.671
7.659
7.404
7.399
7.391
7.387
7.378
7.364
7.169
7.163
7.158
7.141
7.124
7.120
7.113


O
N
N
Ph
F

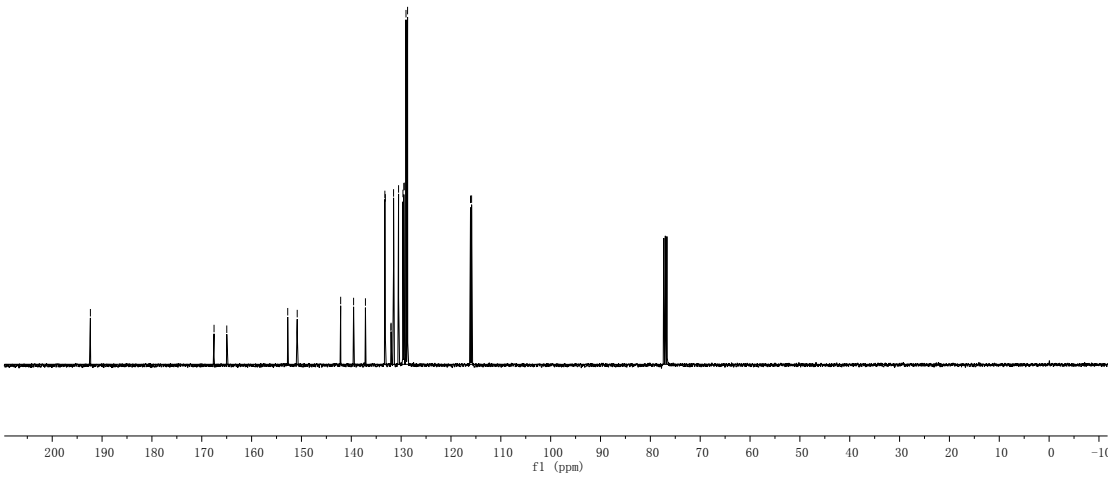
2i

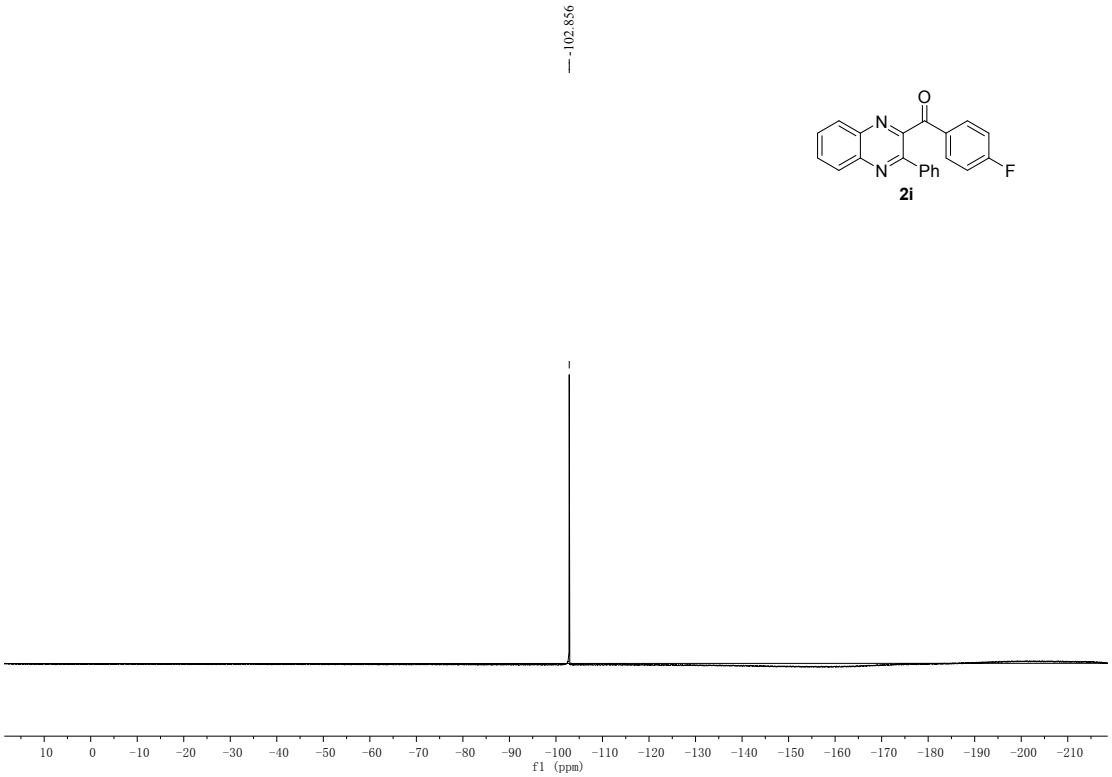

0.99
1.00
1.99
2.02
2.00
3.01
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


192.342
167.537
164.981
152.754
150.849
131.519
130.516
129.636
129.457
129.373
129.025
128.709
116.081
115.861


O
N
N
Ph
F

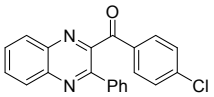
2i


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

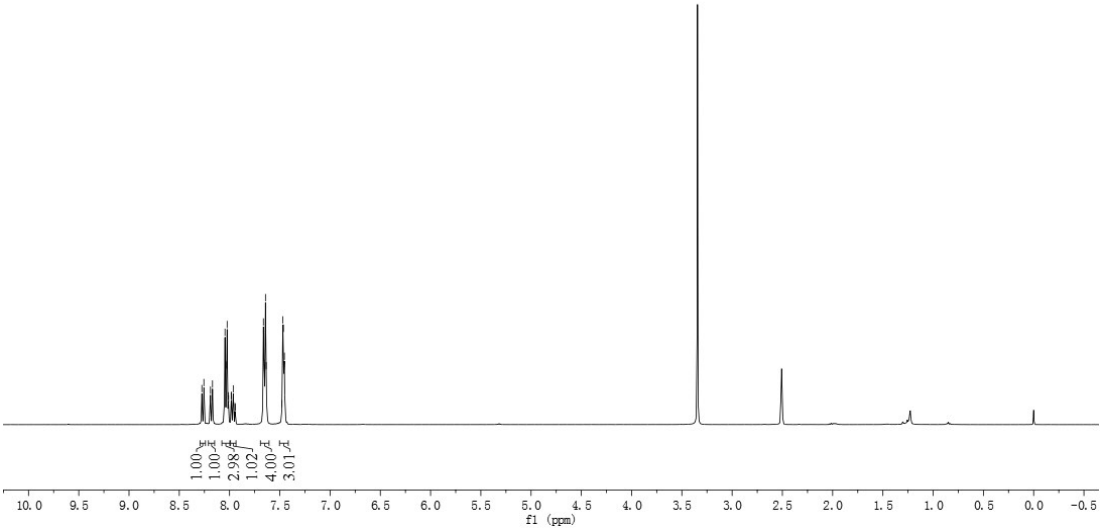

-102.856
O
N
N
Ph
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

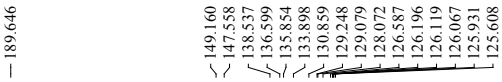
2i

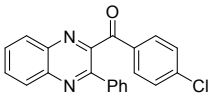

8.275
8.255
8.190
8.170
8.045
8.029
8.024
8.013
8.009
7.984
7.981
7.963
7.946
7.943
7.663
7.659
7.653
7.642
7.635
7.479
7.470
7.464
7.454


O
N
N
Ph
Cl

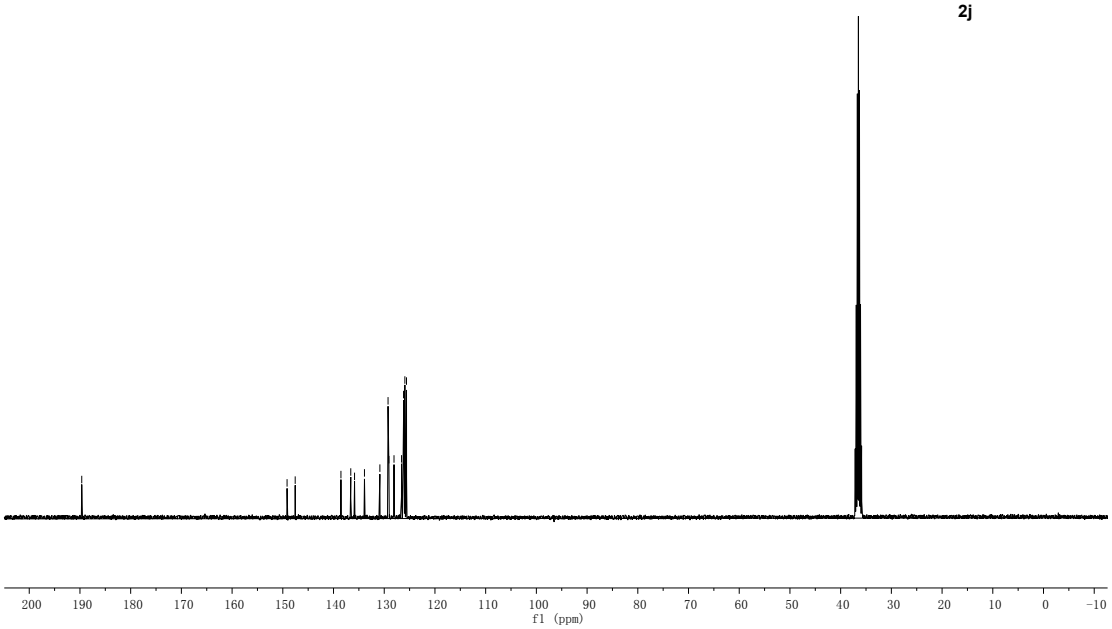
2j

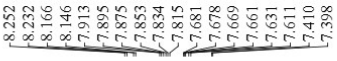

1.00
1.00
2.98
1.02
4.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

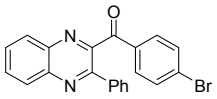

189.646
149.160
147.558
138.537
136.599
135.854
133.898
130.859
129.248
129.079
128.072
126.587
126.196
126.119
126.067
125.931
125.608


O
N
N
Ph
Cl

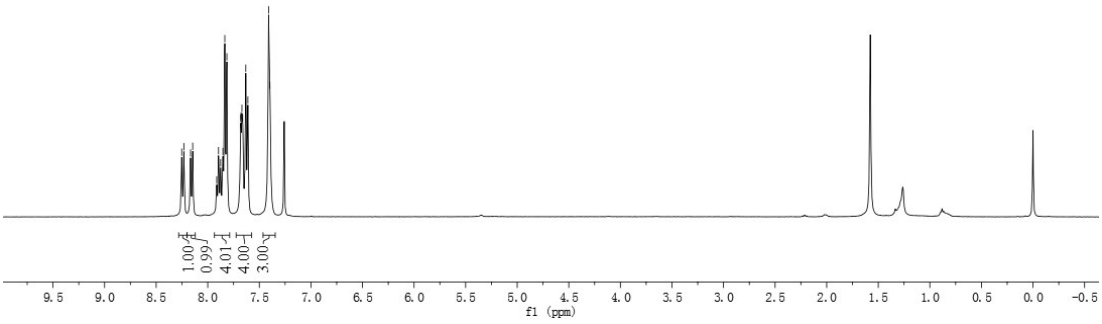
2j


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

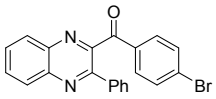

8.252
8.232
8.166
8.146
7.913
7.895
7.875
7.853
7.834
7.815
7.681
7.678
7.669
7.661
7.631
7.611
7.410
7.398


O
N
N
Ph
Br

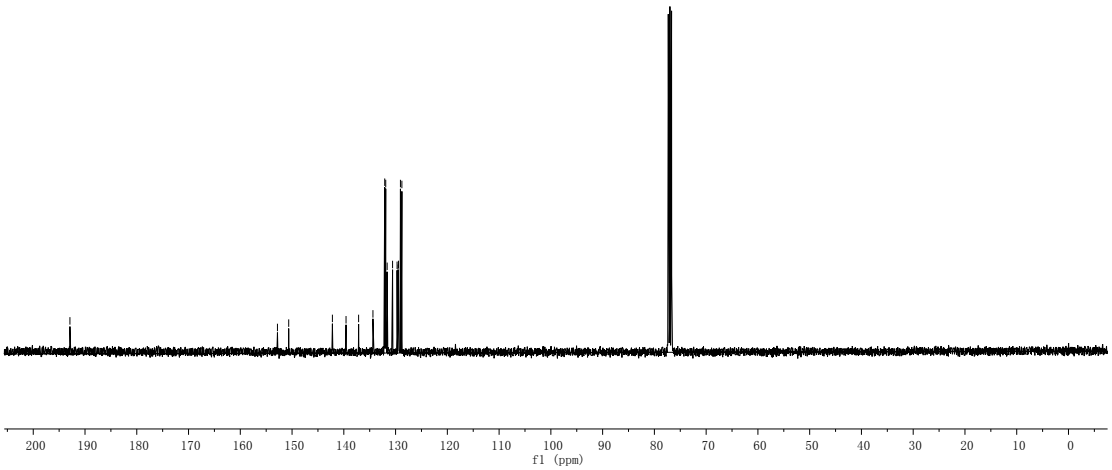
2k


1.00
0.99
4.01
4.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

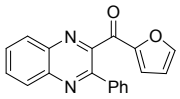

192.913
152.821
150.646
142.206
139.572
137.142
134.374
132.098
131.902
131.627
130.581
129.711
129.593
129.516
129.444
129.062
128.782


O
N
N
Ph
Br

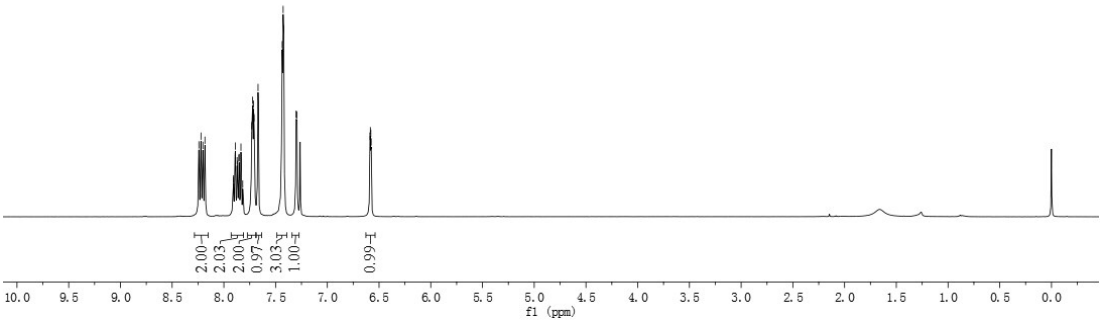
2k

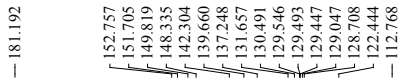

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

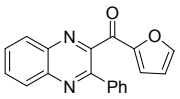

8.241
8.221
8.203
8.183
7.890
7.852
7.835
7.731
7.722
7.713
7.708
7.670
7.436
7.427
7.421
7.302
7.293
6.588
6.584
6.580
6.576


O
N
O
N
Ph

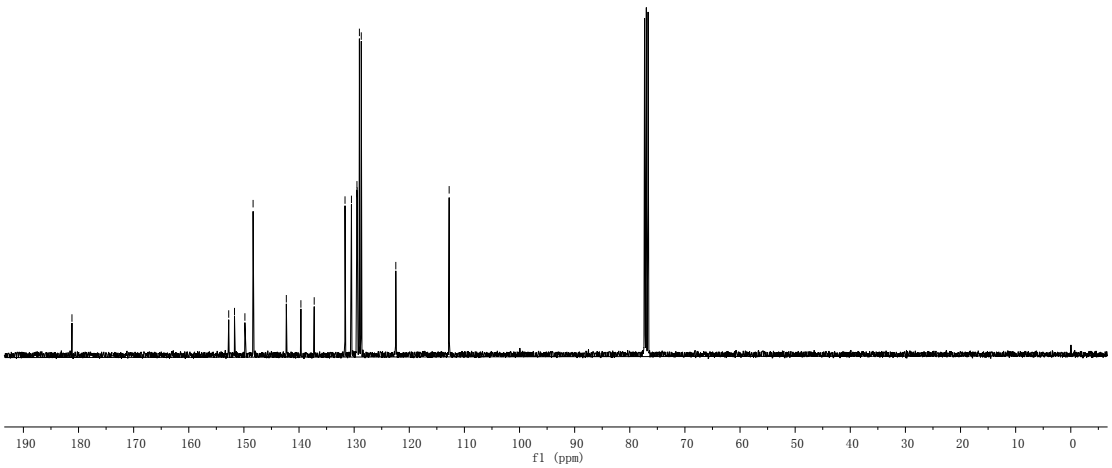
2l

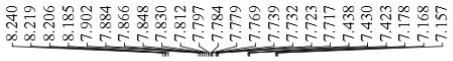

2.00
2.03
2.00
0.97
3.03
1.00
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

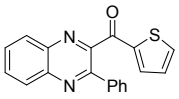

181.192
152.757
151.705
149.819
148.335
142.304
139.660
137.248
131.657
130.491
129.546
129.493
129.447
129.047
128.708
122.444
112.768


O
N
O
N
Ph

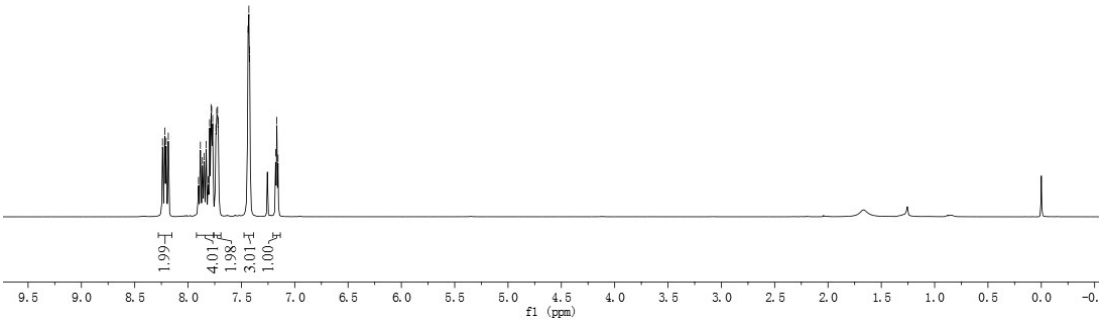
2l

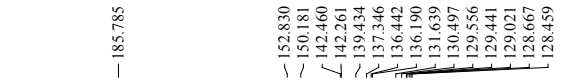

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

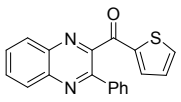

8.240
8.219
8.206
8.185
7.902
7.884
7.866
7.848
7.830
7.812
7.797
7.784
7.779
7.769
7.739
7.732
7.723
7.717
7.438
7.430
7.423
7.178
7.168
7.157


O
N
S
N
Ph

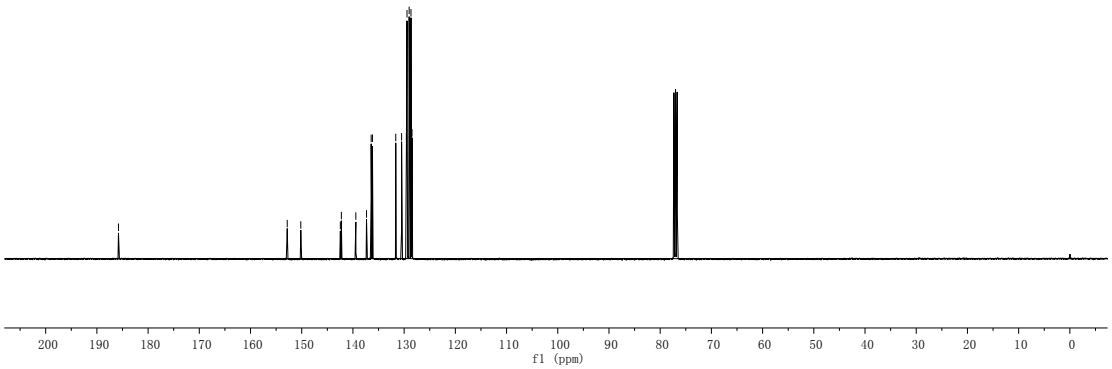
2m

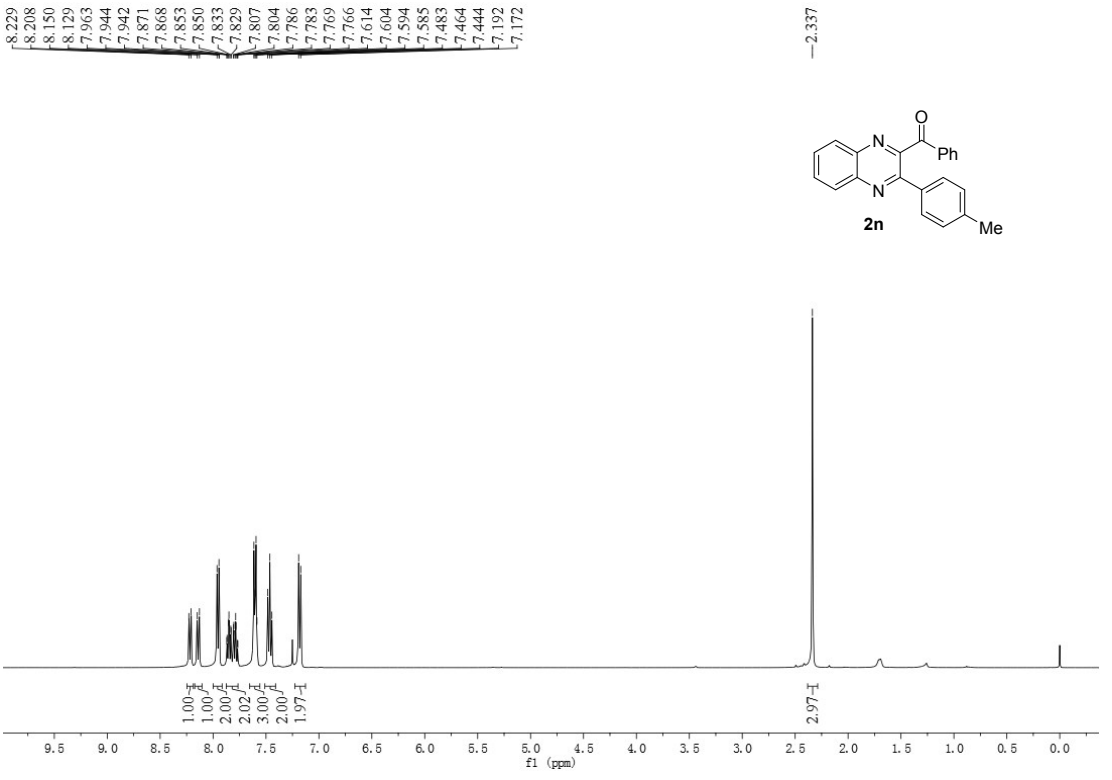

1.99
4.01
1.98
3.01
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

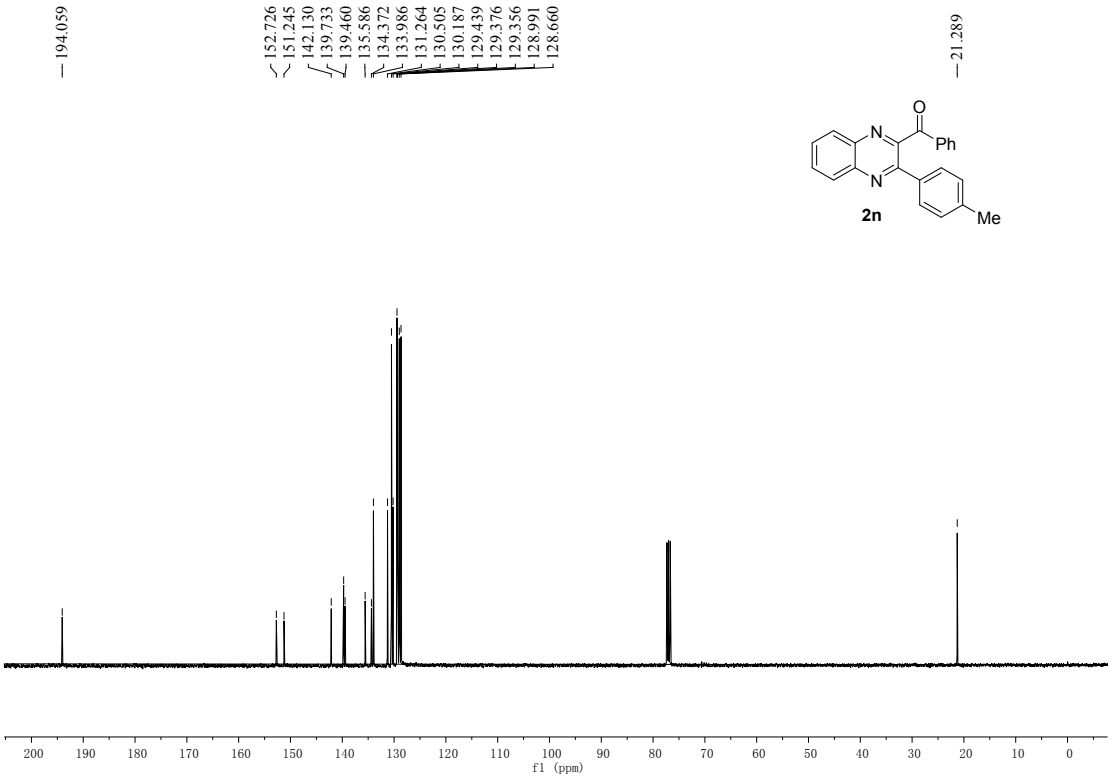

185.785
152.830
150.181
142.460
142.261
139.434
137.346
136.442
136.190
131.639
130.497
129.556
129.441
129.021
128.667
128.459

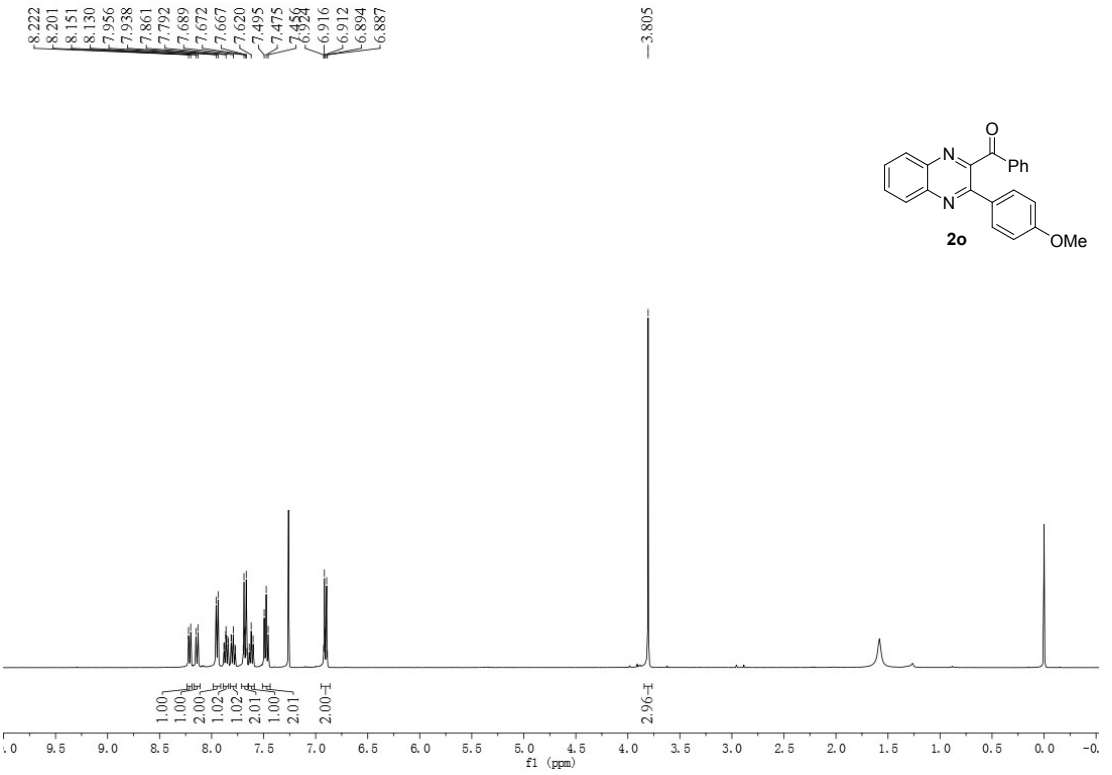

O
N
S
N
Ph

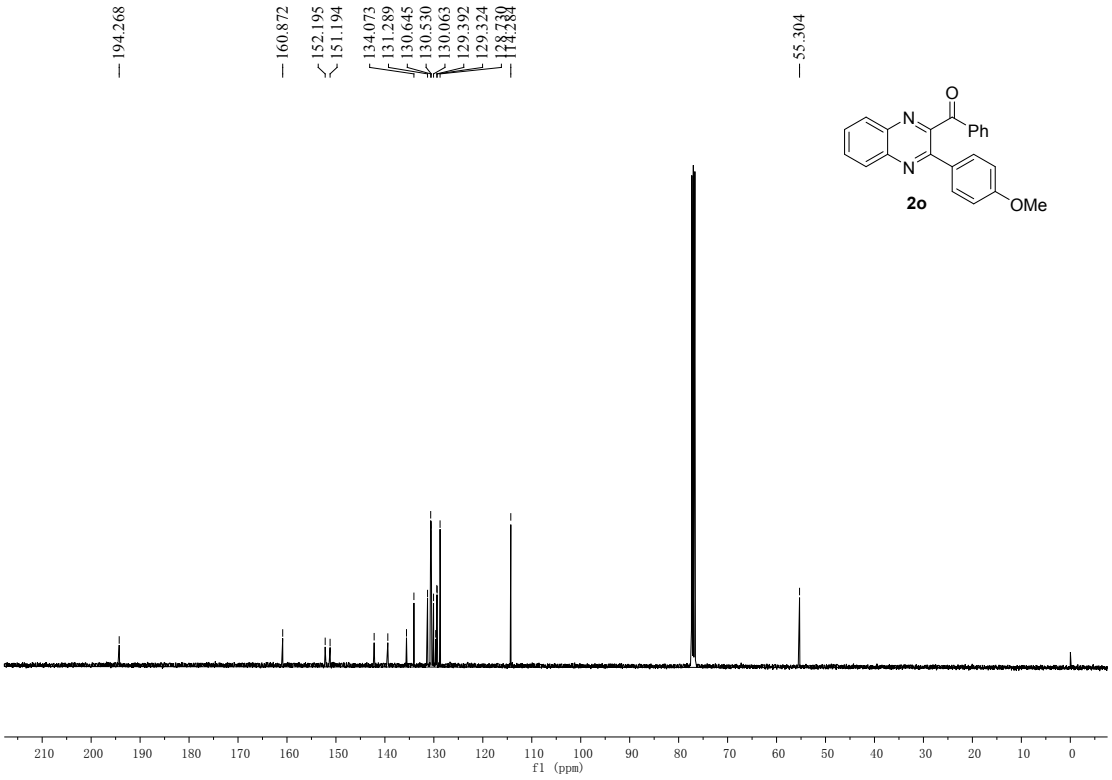
2m


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

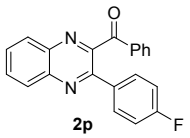

8.229
8.208
8.150
8.129
7.963
7.944
7.942
7.871
7.868
7.853
7.850
7.833
7.829
7.807
7.804
7.786
7.783
7.769
7.766
7.614
7.604
7.594
7.585
7.483
7.464
7.444
7.192
7.172
2.337
O
Ph
N
N
Me
2n
1.00
1.00
2.00
2.02
3.00
2.00
1.97
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.059
152.726
151.245
142.130
139.733
139.460
135.586
134.372
133.986
131.264
130.505
130.187
129.439
129.376
129.356
128.991
128.660
21.289
O
Ph
N
N
Me
2n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

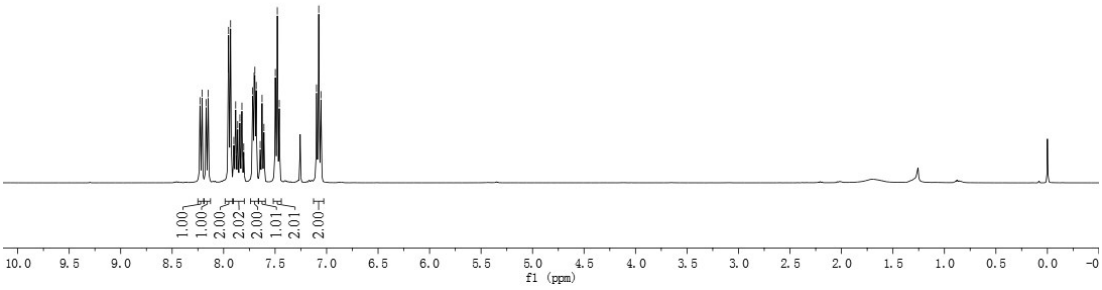

8.222
8.201
8.151
8.130
7.956
7.938
7.861
7.792
7.689
7.672
7.667
7.620
7.495
7.475
6.916
6.912
6.894
6.887
3.805
O
Ph
N
N
OMe
2o
1.00
1.00
2.00
1.02
1.02
2.01
1.00
2.01
2.00
2.96
f1 (ppm)

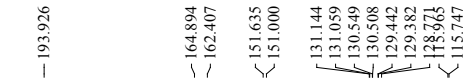

194.268
160.872
152.195
151.194
134.073
131.289
130.645
130.530
130.063
129.392
129.324
128.730
114.284
55.304
O
Ph
N
N
OMe
2o
f1 (ppm)

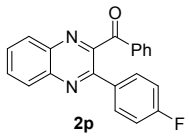

8.230
8.209
8.170
8.150
7.952
7.933
7.901
7.883
7.863
7.842
7.822
7.805
7.718
7.704
7.697
7.683
7.645
7.627
7.609
7.498
7.479
7.460
7.098
7.077
7.055


O
Ph
N
N
F

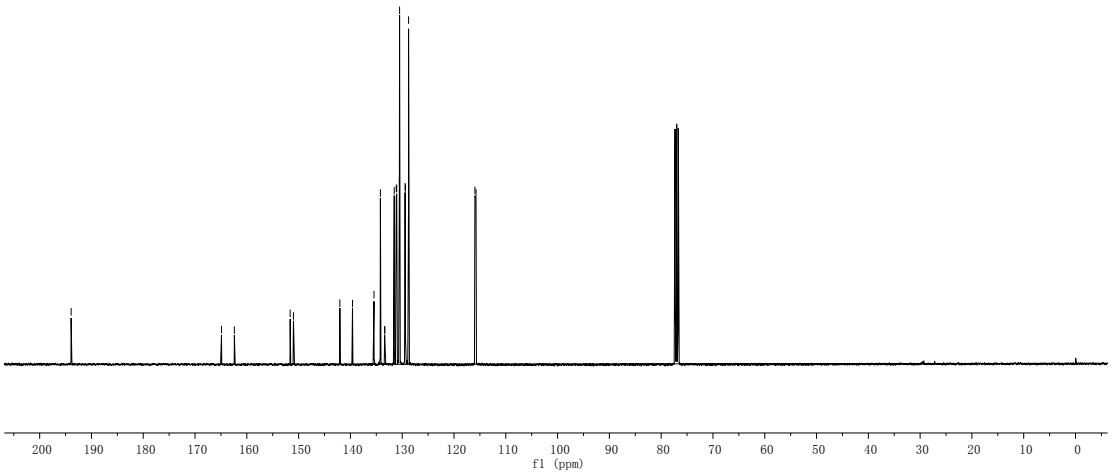
2p

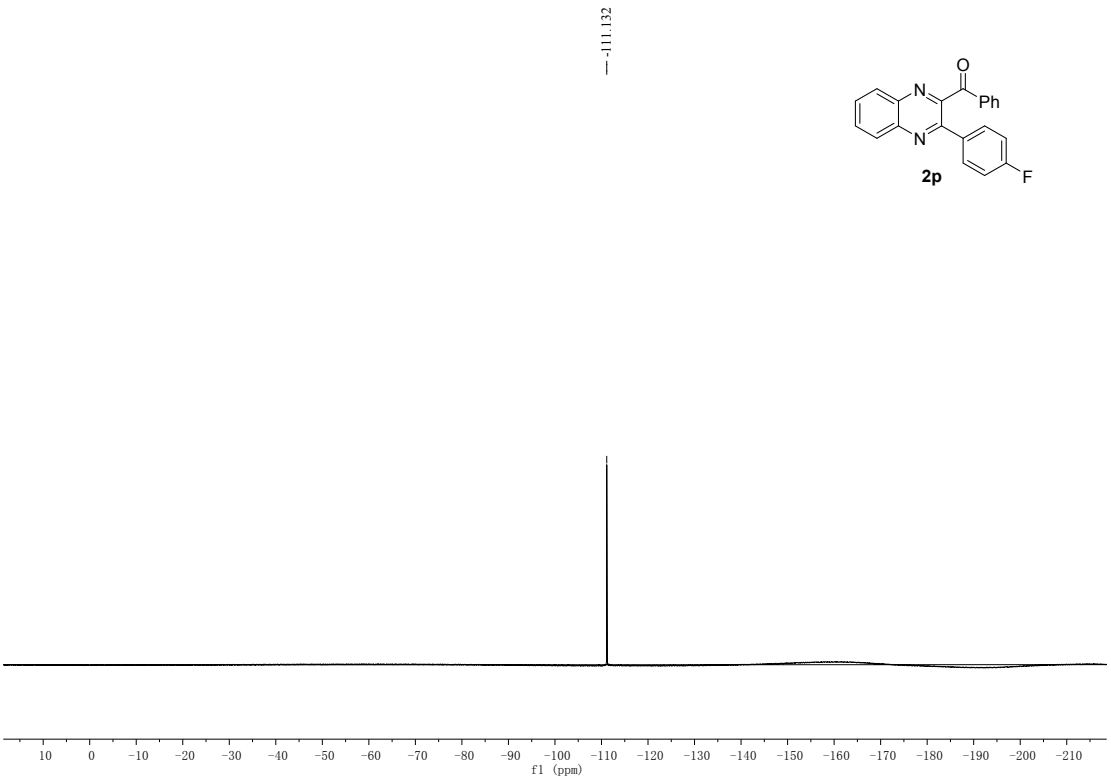

1.00
1.00
2.00
2.02
2.00
1.01
2.01
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


193.926
164.894
162.407
151.635
151.000
131.144
131.059
130.549
130.508
129.442
129.382
128.771
115.965
115.747

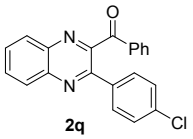

O
Ph
N
N
F

2p

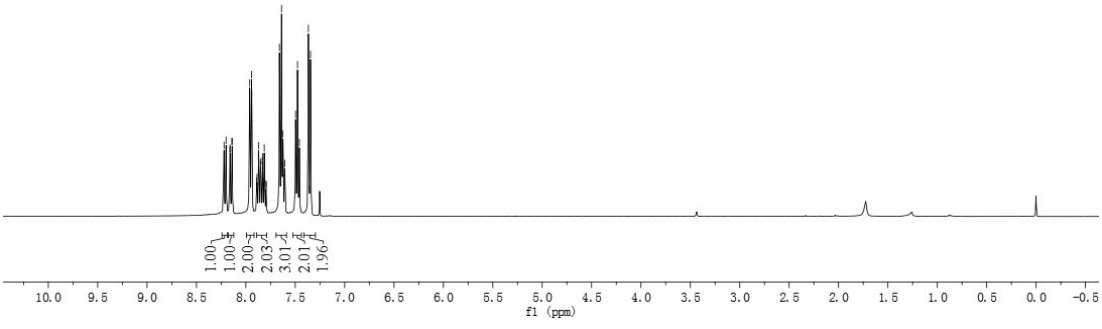

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

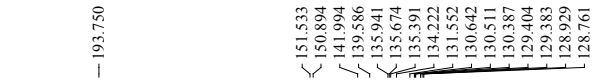

-111.132
O
Ph
N
N
F
2p
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

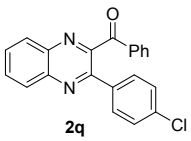

8.221
8.200
8.162
8.160
8.142
8.139
7.961
7.943
7.940
7.891
7.887
7.873
7.870
7.853
7.849
7.834
7.831
7.814
7.796
7.793
7.660
7.639
7.625
7.606
7.497
7.477
7.458
7.367
7.346


O
Ph
N
N
Cl

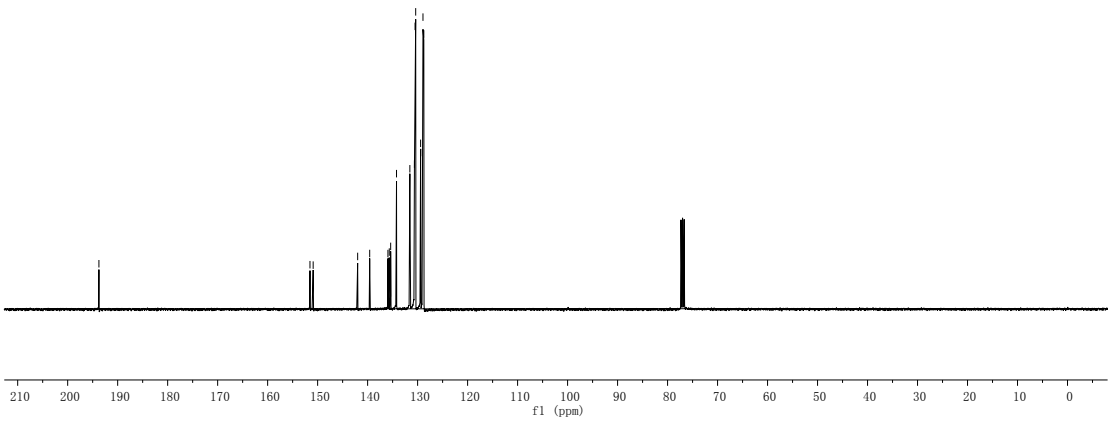
2q

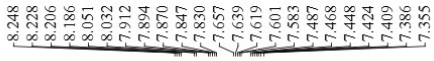

1.00
1.00
2.00
2.03
3.01
2.01
1.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

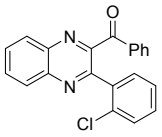

193.750
151.533
150.894
141.994
139.586
135.941
135.674
135.391
134.222
131.552
130.642
130.511
130.387
129.404
129.383
128.929
128.761


O
Ph
N
N
Cl

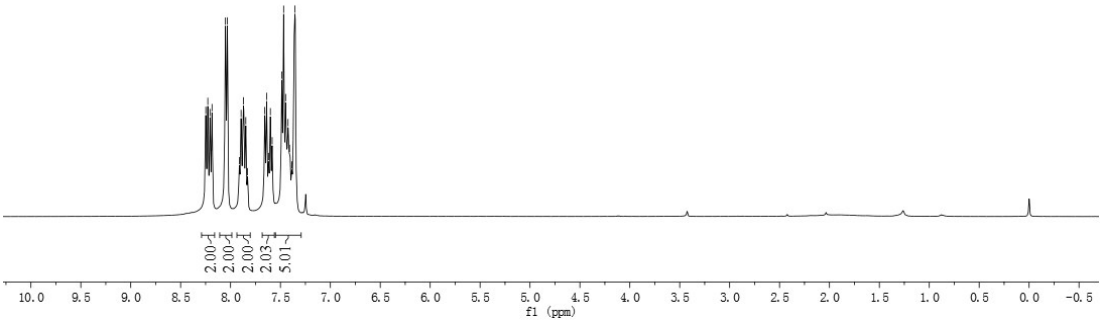
2q

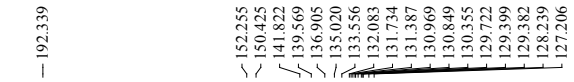

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

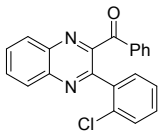

8.248
8.228
8.206
8.186
8.051
8.032
7.912
7.894
7.870
7.847
7.830
7.657
7.639
7.619
7.601
7.583
7.487
7.468
7.448
7.424
7.409
7.386
7.355


O
N
Ph
N
Cl

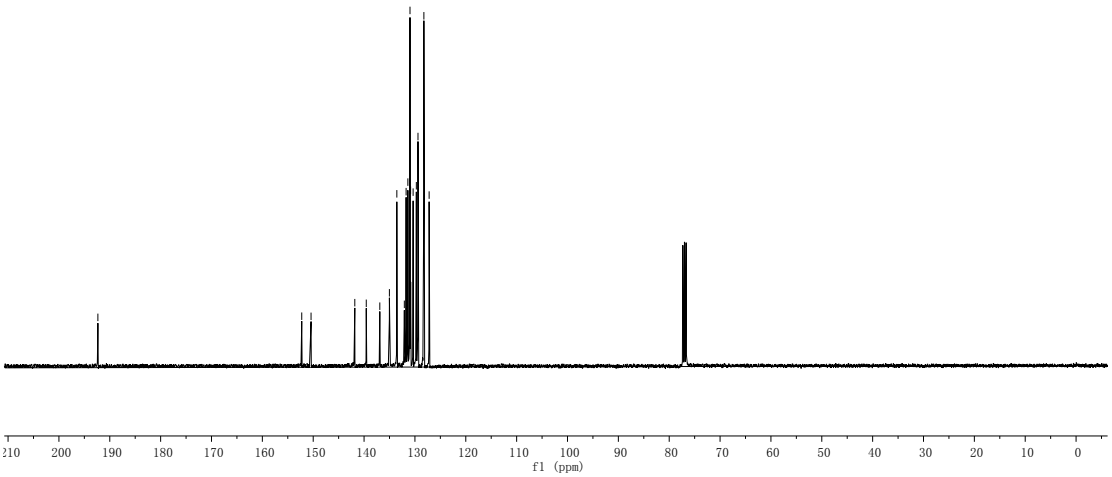
2r

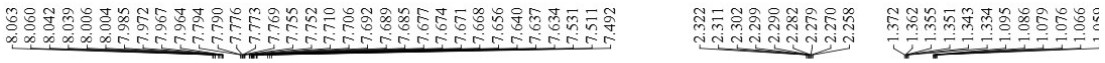

2.00
2.00
2.00
2.03
5.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

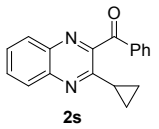

192.339
152.255
150.425
141.822
139.569
136.905
135.020
133.556
132.083
131.734
131.387
130.969
130.849
130.355
129.722
129.399
129.382
128.239
127.206


O
N
Ph
N
Cl

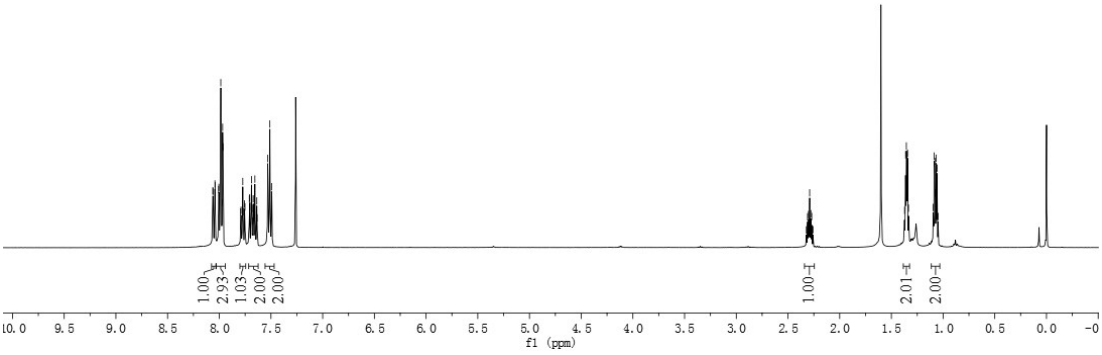
2r


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

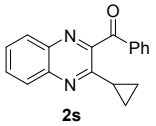

8.063
8.060
8.042
8.039
8.006
8.004
7.985
7.972
7.967
7.964
7.794
7.790
7.776
7.773
7.769
7.755
7.752
7.710
7.706
7.692
7.689
7.685
7.677
7.674
7.671
7.668
7.656
7.640
7.637
7.634
7.531
7.511
7.492
2.322
2.311
2.302
2.299
2.290
2.282
2.279
2.270
2.258
1.372
1.362
1.355
1.351
1.343
1.334
1.095
1.086
1.079
1.076
1.066


O
Ph
N
N

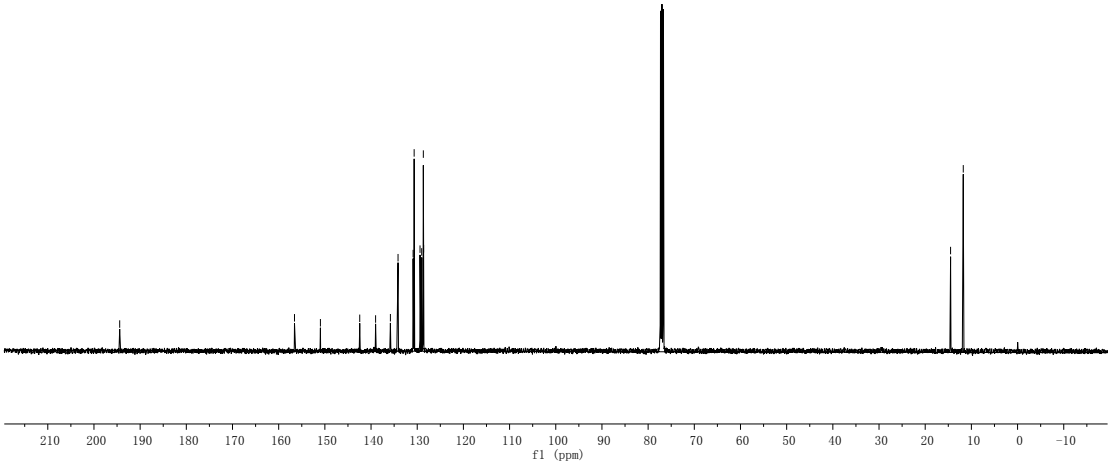
2s


1.00
2.93
1.03
2.00
2.00
1.00
2.01
2.00
f1 (ppm)

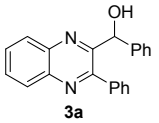

194.428
156.576
150.965
142.448
139.014
135.808
134.154
130.891
130.666
129.394
129.029
128.677
128.615
14.505
11.758


O
Ph
N
N

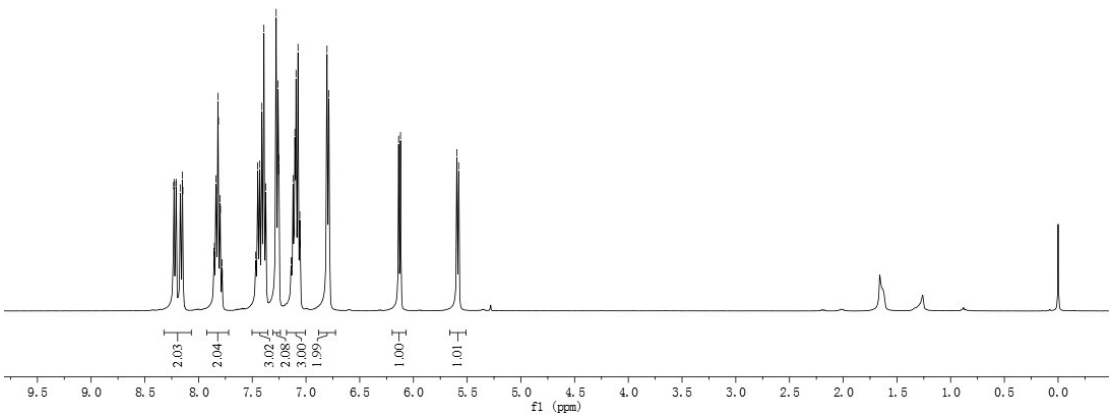
2s

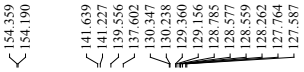

f1 (ppm)


8.232
8.228
8.211
8.209
8.170
8.150
8.146
7.852
7.838
7.835
7.820
7.815
7.800
7.796
7.411
7.392
7.278
7.260
7.103
7.093
7.074
6.805
6.120
5.596
5.579

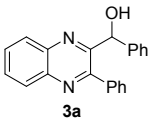

OH
N
Ph
N
Ph

3a

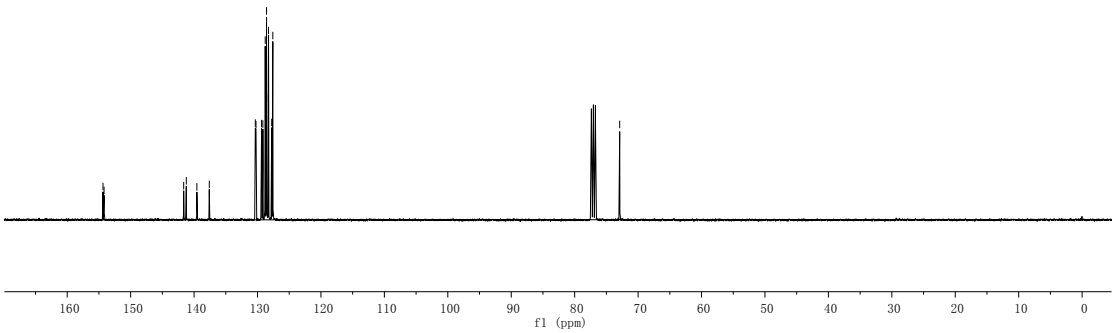

2.03
2.04
3.02
2.08
3.00
1.99
1.00
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


154.359
154.190
141.639
141.227
139.556
137.602
130.347
130.238
129.360
129.156
128.785
128.577
128.559
128.262
127.764
127.587

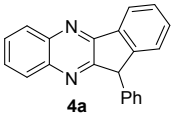

72.901


OH
N
Ph
N
Ph

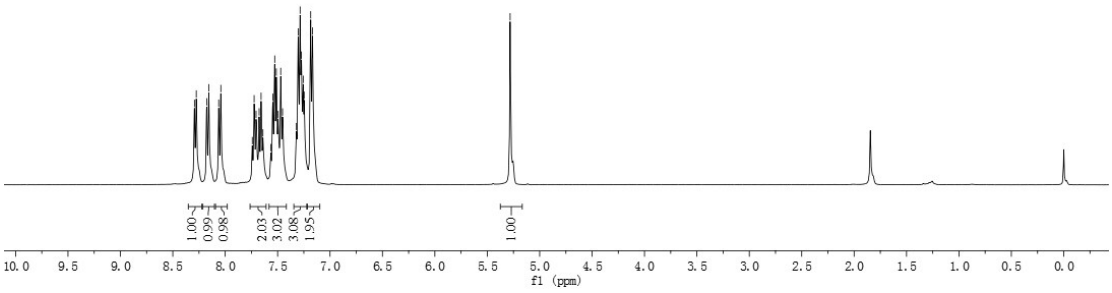
3a

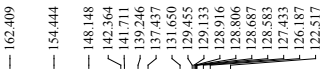

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.293
8.276
8.177
8.156
8.062
8.042
7.742
7.724
7.706
7.676
7.658
7.640
7.564
7.546
7.528
7.512
7.495
7.471
7.453
7.320
7.304
7.285
7.273
7.256
7.247
7.184
7.167
5.282

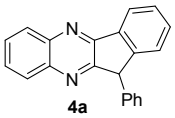

N
N
Ph

4a

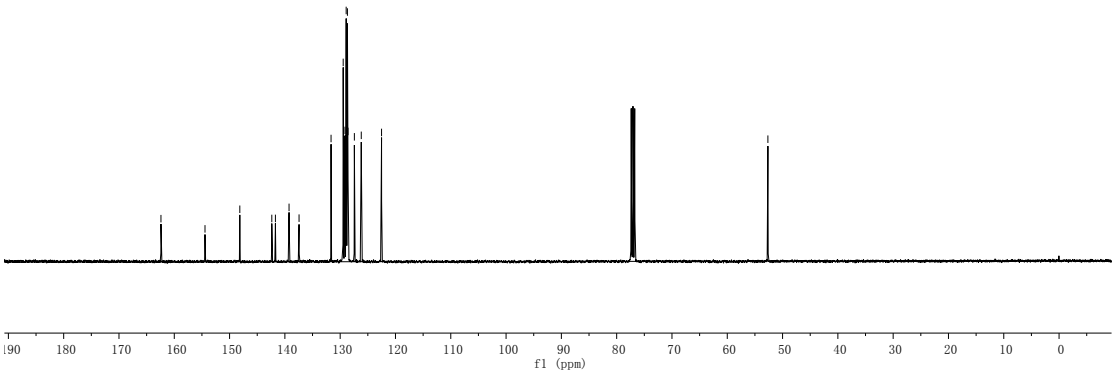

1.00
0.99
0.98
2.03
3.02
3.08
1.95
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.409
154.444
148.148
142.364
141.711
139.246
137.437
131.650
129.455
129.133
128.916
128.806
128.687
128.583
127.433
126.187
122.517

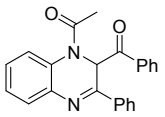

52.653


N
N
Ph

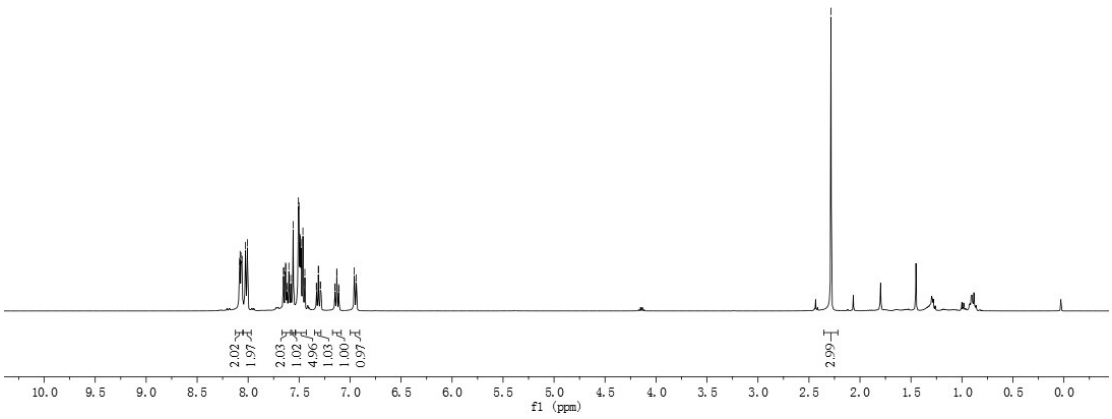
4a

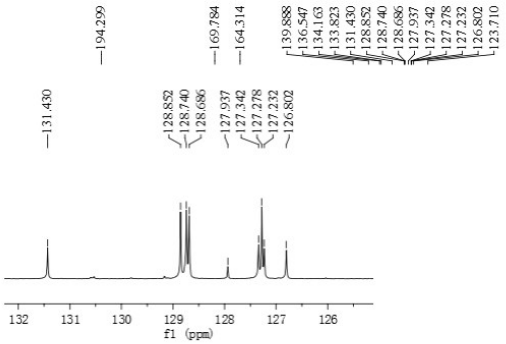

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

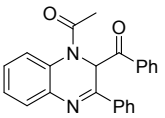

8.084
8.079
8.070
8.060
8.026
8.008
7.653
7.650
7.634
7.631
7.619
7.601
7.582
7.559
7.507
7.501
7.493
7.489
7.482
7.463
7.444
7.331
7.329
7.312
7.310
7.293
7.290
7.151
7.148
7.131
7.128
7.112
7.109
6.959
6.939
2.284


O
N
O
Ph
N
Ph

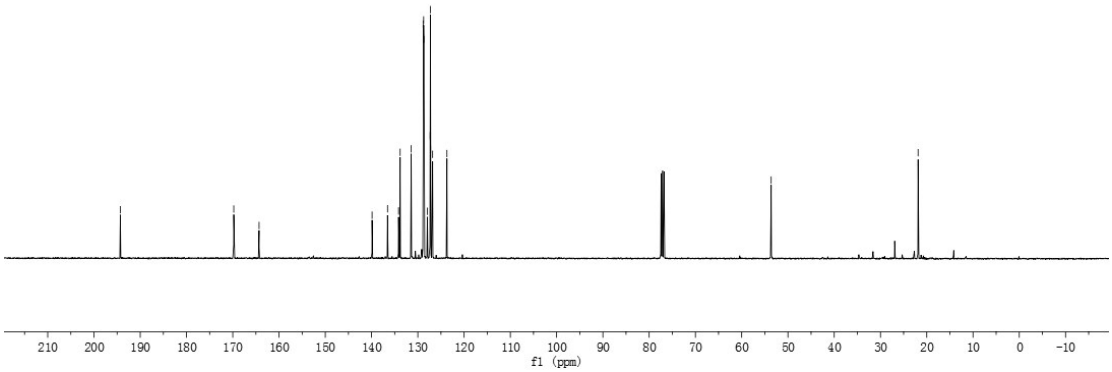
5a


2.02
1.97
2.03
1.02
4.96
1.03
1.00
0.97
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.299
169.784
164.314
139.888
136.547
134.163
133.823
131.430
128.852
128.740
128.686
127.937
127.342
127.278
127.232
126.802
123.710
53.625
21.870
131.430
128.852
128.740
128.686
127.937
127.342
127.278
127.232
126.802
132 131 130 129 128 127 126
f1 (ppm)


O
N
O
Ph
N
Ph

5a


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

7. HRMS spectrum of intermediate C

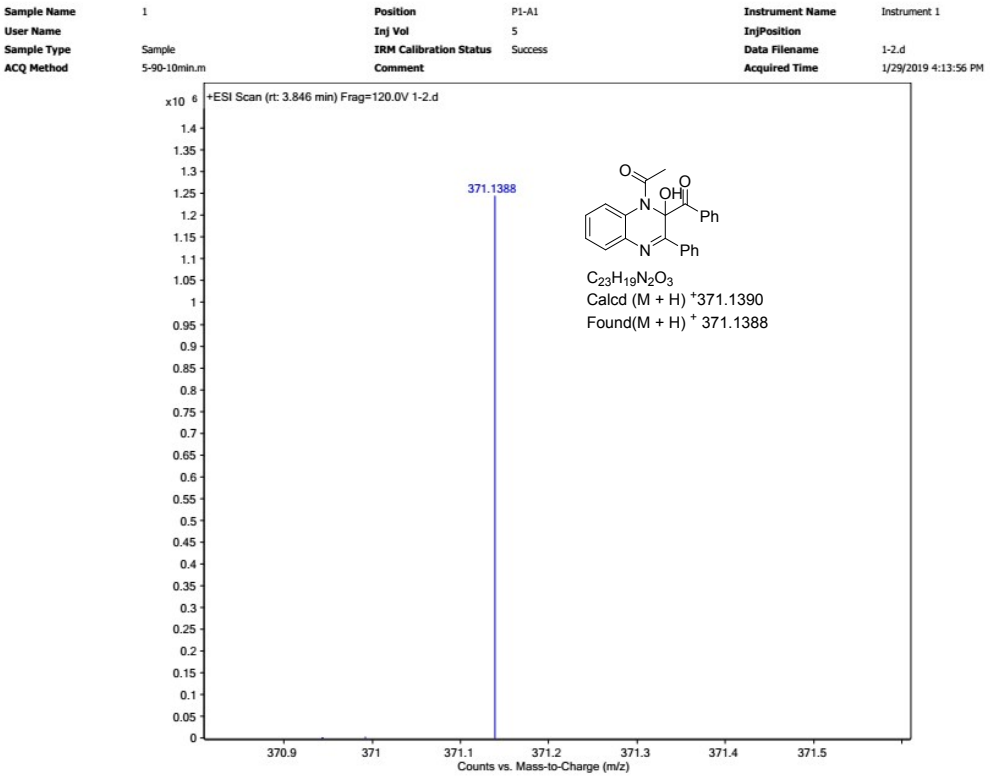


Figure S1 HRMS spectrum of 1-(2-benzoyl-2-hydroxy-3-phenylquinoxalin-1(2*H*)-yl)ethan-1-one