

Supporting Information

Catalyst-free Synthesis of Pyrazolo[5,1-*a*]isoquinolines from Hydrazine Hydrate

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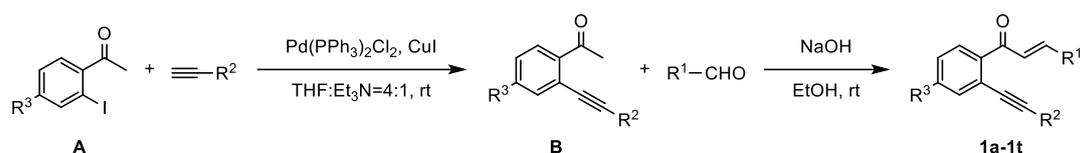
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1. Experimental procedures and spectroscopic data

1.1 General information

All reactions were carried out in 25 mL reaction vial, solvents were purified by standard method. ^1H , ^{13}C , ^{19}F NMR spectra were recorded on a Bruker AVANCE 400 (400 MHz for ^1H ; 101 MHz for ^{13}C ; 376 MHz for ^{19}F), ^1H NMR and ^{13}C NMR chemical shifts were determined relative to internal standard TMS at δ 0.0 and ^{19}F NMR chemical shifts were determined relative to CFCl_3 as external standard. Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = single, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Mass spectra (MS) were acquired using an Waters G₂-S Qtof ESI/TOF mass spectrometer. Melting points were determined using a hot stage apparatus. X-ray crystallography analysis was performed on Bruker D8 QUEST X-ray diffractionmeter. All reagents were used as received from commercial sources, unless specified otherwise, or prepared as described in the literature.

1.2 Typical procedure for the synthesis of 1

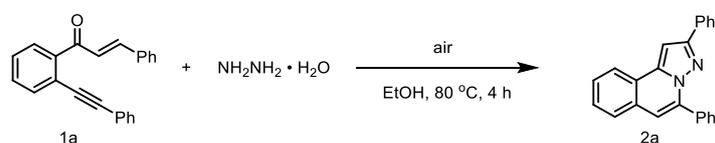


Procedure for the synthesis of **1a-1s** was similar to our previous reported procedures¹: In a Schlenk tube with a magnetic bar under nitrogen atmosphere, **A** (1 equiv), phenylacetylene (1.2 equiv), CuI (5 mol%) and $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (3 mol%) were added in a mixed solution of THF (0.125 M) and Et_3N (0.2 M). The mixture was stirred at room temperature until the **A** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc /petroleum ether as eluent to afford the product **B** (68 % - 93 %).

A solution of NaOH (20 mol%) in ethanol (10 mL) was cooled to $0\text{ }^\circ\text{C}$ and **B** (1 equiv) and benzaldehyde (1 equiv) were slowly added successively. The reaction mixture was allowed to warm to room temperature until the **B** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc /petroleum ether as eluent to afford the product **1a-1t** (28% - 99%).

Product information **1a-t**, please refer to our previous report for all data information.^{1,2}

1.3 Typical procedure for the synthesis of 2

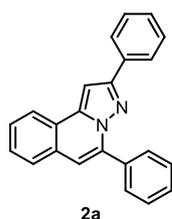


In a reaction vial with a magnetic bar, EtOH (4.0 mL), the substrate of **1a** (61.6 mg, 0.2 mmol) and

$\text{NH}_2\text{NH}_2\cdot\text{H}_2\text{O}$ (50%, 20 mg, 0.4 mmol) were added. The mixture was stirred at 80 °C in oil bath until the substrate **1a** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **2a** (73 mg, 0.15 mmol).

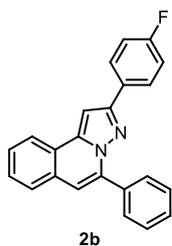
The procedures of other substrates **1** were similar with that mentioned above.

2,5-diphenylpyrazolo[5,1-a]isoquinoline



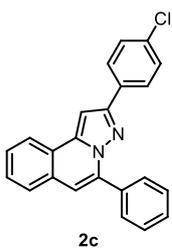
Known compound, the spectral datas were consistent with reported literature values³. Yield 73% (47 mg, 0.15 mmol), yellow solid, m. p. 70-71 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.16 (dd, $J = 7.1$, 2.0 Hz, 1H), 8.08 - 8.01 (m, 4H), 7.76 - 7.73 (m, 1H), 7.61 - 7.52 (m, 5H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.41 (s, 1H), 7.39 - 7.34 (m, 1H), 7.08 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.3, 140.8, 138.5, 133.8, 133.4, 129.7, 129.33, 129.27, 128.7, 128.24, 128.21, 128.0, 127.34, 127.27, 126.5, 124.0, 123.5, 112.5, 94.8.

2-(4-fluorophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline



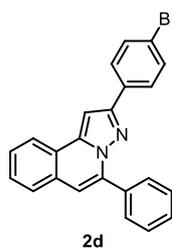
Known compound, the spectral datas were consistent with reported literature values³. Yield 74% (50 mg, 0.15 mmol), yellow solid, m. p. 114-115 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (dd, $J = 6.8$, 2.2 Hz, 1H), 8.01 (dd, $J = 8.0$, 1.7 Hz, 2H), 7.97 - 7.90 (m, 2H), 7.72 (dd, $J = 6.7$, 2.3 Hz, 1H), 7.58 - 7.48 (m, 5H), 7.31 (s, 1H), 7.14 - 7.07 (m, 2H), 7.05 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 163.0 (d, $^1J_{\text{C-F}} = 247.5$ Hz), 151.4, 140.9, 138.4, 133.7, 129.7, 129.6, 129.34, 129.30, 128.22, 128.16, 128.1 (d, $^4J_{\text{C-F}} = 2.0$ Hz), 127.3 (d, $^3J_{\text{C-F}} = 10.1$ Hz), 123.9, 123.5, 115.6 (d, $^2J_{\text{C-F}} = 21.2$ Hz), 112.6, 94.6. ; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -113.87.

2-(4-chlorophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline



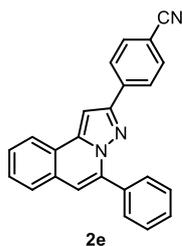
Known compound, the spectral datas were consistent with reported literature values³. Yield 56% (40 mg, 0.11 mmol), yellow solid, m. p. 147-148 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (dd, $J = 6.8$, 2.2 Hz, 1H), 8.00 (dd, $J = 8.0$, 1.8 Hz, 2H), 7.91 (d, $J = 8.5$ Hz, 2H), 7.73 (dd, $J = 6.7$, 2.2 Hz, 1H), 7.59 - 7.49 (m, 5H), 7.38 (d, $J = 8.6$ Hz, 2H), 7.34 (s, 1H), 7.07 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 151.1, 140.9, 138.4, 134.0, 133.7, 132.0, 129.7, 129.3, 128.8, 128.2, 128.1, 127.7, 127.4, 127.3, 123.9, 123.5, 112.8, 94.8.

2-(4-bromophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline



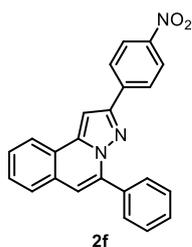
Known compound, the spectral datas were consistent with reported literature values³. Yield 77% (61 mg, 0.15 mmol), yellow solid, m. p. 152-153 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (dd, $J = 7.7$, 1.5 Hz, 1H), 8.01 (dd, $J = 8.0$, 1.7 Hz, 2H), 7.88 - 7.83 (m, 2H), 7.74 (dd, $J = 6.7$, 2.6 Hz, 1H), 7.58 - 7.51 (m, 7H), 7.35 (s, 1H), 7.08 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 1151.1, 140.9, 138.4, 133.7, 132.4, 131.8, 129.6, 129.3, 128.2, 128.1, 128.0, 127.5, 127.3, 123.9, 123.5, 122.2, 112.8, 94.8.

4-(5-phenylpyrazolo[5,1-a]isoquinolin-2-yl)benzonitrile



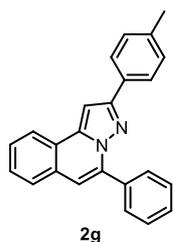
New compound, Yield 62% (43 mg, 0.12 mmol), orange solid, m. p. 148-149 °C, R_f = 0.5 (EtOAc/petroleum ether = 1/10); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.15 (dd, J = 6.8, 2.7 Hz, 1H), 8.09 – 8.05 (m, 2H), 7.99 (dd, J = 7.8, 1.8 Hz, 2H), 7.76 (dd, J = 6.5, 2.7 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.62 – 7.53 (m, 5H), 7.42 (s, 1H), 7.12 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 150.1, 141.1, 138.3, 137.8, 133.4, 132.5, 129.6, 129.5, 129.3, 128.4, 128.3, 127.7, 127.4, 126.8, 123.8, 123.5, 119.1, 113.5, 111.4, 95.5.; HRMS (ESI) Calcd for $\text{C}_{24}\text{H}_{16}\text{N}_3$ ($\text{M}+\text{H}$) $^+$ 346.1339, found 346.1347.

2-(4-nitrophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline



New compound, Yield 65% (47 mg, 0.13 mmol), brown solid, m.p. 251-252 °C, R_f = 0.5 (EtOAc/petroleum ether = 1/10); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.30 – 8.25 (m, 2H), 8.18 – 8.12 (m, 3H), 8.00 (dd, J = 7.9, 1.7 Hz, 2H), 7.78 (dd, J = 6.6, 2.5 Hz, 1H), 7.64 – 7.54 (m, 5H), 7.47 (s, 1H), 7.15 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 149.8, 147.4, 141.2, 139.7, 138.3, 133.4, 129.6, 129.5, 129.3, 128.5, 128.3, 127.7, 127.5, 126.8, 124.1, 123.8, 123.5, 113.6, 95.8.; HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{16}\text{N}_3\text{O}_2$ ($\text{M}+\text{H}$) $^+$ 366.1237, found 366.1246.

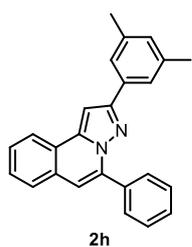
5-phenyl-2-(p-tolyl)pyrazolo[5,1-a]isoquinoline



Known compound, the spectral datas were consistent with reported literature values³. Yield 60% (40 mg, 0.12 mmol), yellow solid, m. p. 132-133 °C, R_f = 0.6 (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (dd, J = 7.5, 2.0 Hz, 1H), 8.04 (dd, J = 8.1, 1.6 Hz, 2H), 7.91 – 7.87 (m, 2H), 7.72 (dd, J = 6.9, 2.3 Hz, 1H), 7.57 – 7.49 (m, 5H), 7.35 (s, 1H), 7.23 (d, J = 7.5 Hz, 2H), 7.04 (s, 1H), 2.38 (s, 3H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.4, 140.7, 138.5, 138.1, 133.8, 130.6, 129.7, 129.4, 129.3, 129.2, 128.2, 127.9, 127.3, 127.2, 126.3, 124.0, 123.5, 112.4, 94.6,

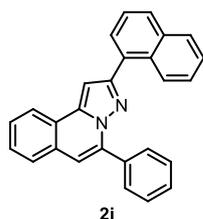
21.4.

2-(3,5-dimethylphenyl)-5-phenylpyrazolo[5,1-a]isoquinoline



New compound, Yield 69% (48 mg, 0.14 mmol), yellow solid, m. p. 133-134 °C, R_f = 0.5 (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (dd, J = 7.5, 1.9 Hz, 1H), 8.06 – 8.01 (m, 2H), 7.72 (dd, J = 7.0, 2.3 Hz, 1H), 7.61 (s, 2H), 7.57 – 7.50 (m, 5H), 7.37 (s, 1H), 7.04 (s, 1H), 6.98 (s, 1H), 2.38 (s, 6H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.6, 140.7, 138.5, 138.1, 133.9, 133.2, 130.0, 129.7, 129.3, 129.2, 128.3, 127.9, 127.3, 127.2, 124.3, 124.0, 123.5, 112.5, 95.0, 21.4.; HRMS (ESI) Calcd for $\text{C}_{25}\text{H}_{21}\text{N}_2$ ($\text{M}+\text{H}$) $^+$ 349.1699, found 349.1708.

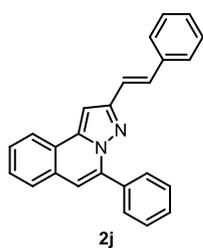
2-(naphthalen-1-yl)-5-phenylpyrazolo[5,1-a]isoquinoline



Known compound, the spectral datas were consistent with reported literature values³. Yield 65% (48 mg, 0.13 mmol), yellow solid, m. p. 122-123 °C, R_f = 0.4 (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.74 – 8.66 (m, 1H), 8.21 – 8.17 (m, 1H), 8.08 – 8.04 (m, 2H), 7.91 – 7.85 (m, 3H), 7.79 (dd, J = 6.4, 2.9 Hz, 1H), 7.61 – 7.47 (m, 8H), 7.42 (s, 1H), 7.13 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.4, 140.0, 138.5, 134.0, 133.8, 131.6, 131.5, 129.6, 129.4, 129.3, 128.7, 128.33, 128.28, 128.1, 128.0, 127.4, 127.3, 126.4, 125.8, 125.4,

124.0, 123.6, 112.6, 98.9.

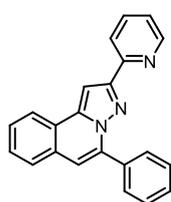
5-phenyl-2-styrylpyrazolo[5,1-a]isoquinoline



2j

New compound, Yield 57% (39 mg, 0.11 mmol), yellow solid, m. p. 133-134 °C, $R_f = 0.4$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.95 (dd, $J = 8.0, 1.6$ Hz, 2H), 7.72 (dd, $J = 6.6, 2.6$ Hz, 1H), 7.57 - 7.50 (m, 7H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.33 (s, 2H), 7.30 (s, 1H), 7.29 - 7.25 (m, 1H), 7.01 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 151.7, 140.5, 138.3, 137.1, 133.8, 131.6, 129.6, 129.39, 129.36, 128.7, 128.4, 128.1, 127.9, 127.4, 127.2, 126.7, 123.8, 123.6, 121.2, 112.5, 94.8.; HRMS (ESI) Calcd for $\text{C}_{25}\text{H}_{19}\text{N}_2$ ($\text{M}+\text{H}$) $^+$ 347.1543, found 347.1550.

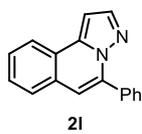
5-phenyl-2-(pyridin-2-yl)pyrazolo[5,1-a]isoquinoline



2k

Known compound, the spectral datas were consistent with reported literature values⁴. Yield 41% (26 mg, 0.08 mmol), orange solid, m. p. 204-205 °C, $R_f = 0.4$ (EtOAc/petroleum ether = 1/10); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.69 (dd, $J = 4.9, 0.9$ Hz, 1H), 8.21 - 8.15 (m, 2H), 8.06 - 8.00 (m, 2H), 7.81 (s, 1H), 7.77 - 7.71 (m, 2H), 7.62 - 7.52 (m, 5H), 7.26 - 7.23 (m, 1H), 7.12 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.4, 149.4, 140.9, 138.4, 136.6, 133.7, 129.7, 129.3, 129.2, 128.2, 128.1, 127.6, 127.2, 124.3, 123.7, 122.9, 121.0, 113.2, 96.6.

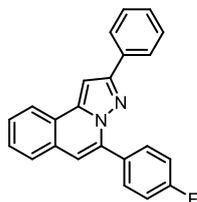
5-phenylpyrazolo[5,1-a]isoquinoline



2l

Known compound, the spectral datas were consistent with reported literature values⁵. Yield 18% (9 mg, 0.04 mmol), yellow solid, m. p. 103-104 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.14 (dd, 1H), 8.01 (d, $J = 2.1$ Hz, 1H), 7.92 - 7.86 (m, 2H), 7.76 (dd, $J = 6.5, 2.7$ Hz, 1H), 7.59 - 7.50 (m, 5H), 7.10 (d, $J = 2.2$ Hz, 1H), 7.06 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 140.9, 133.9, 129.5, 129.3, 129.2, 128.4, 128.0, 127.4, 127.2, 124.1, 123.6, 112.6, 97.9.

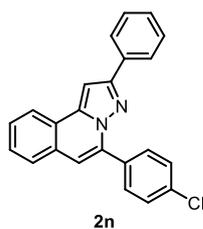
5-(4-fluorophenyl)-2-phenylpyrazolo[5,1-a]isoquinoline



2m

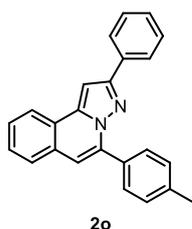
New compound, Yield 63% (43 mg, 0.12 mmol), white solid, m. p. 128-129 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.13 (dd, $J = 7.4, 2.0$ Hz, 1H), 8.04 - 7.96 (m, 4H), 7.71 (dd, $J = 7.0, 2.2$ Hz, 1H), 7.58 - 7.51 (m, 2H), 7.43 (t, $J = 7.5$ Hz, 2H), 7.38 - 7.32 (m, 2H), 7.24 - 7.19 (m, 2H), 7.01 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 163.3 (d, $^1J_{\text{C-F}} = 249.5$ Hz), 152.35, 140.78, 137.42, 133.32, 131.6 (d, $^3J_{\text{C-F}} = 8.1$ Hz), 129.8 (d, $^4J_{\text{C-F}} = 3.0$ Hz), 129.23, 128.69, 128.32, 128.05, 127.43, 127.23, 126.41, 123.95, 123.56, 115.2 (d, $^2J_{\text{C-F}} = 21.2$ Hz), 112.39, 94.91.; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -111.74; HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{16}\text{N}_2\text{F}$ ($\text{M}+\text{H}$) $^+$ 339.1292, found 339.1295.

5-(4-chlorophenyl)-2-phenylpyrazolo[5,1-a]isoquinoline



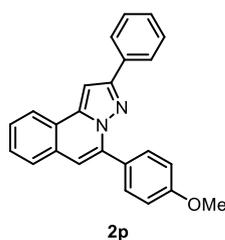
Known compound, the spectral datas were consistent with reported literature values³. Yield 51% (36 mg, 0.10 mmol), yellow solid, m. p. 142-143 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (dd, $J = 7.5$, 1.7 Hz, 1H), 8.01 - 7.95 (m, 4H), 7.72 (dd, $J = 7.2$, 2.1 Hz, 1H), 7.59 - 7.53 (m, 2H), 7.52 - 7.49 (m, 2H), 7.45 - 7.41 (m, 2H), 7.37 - 7.32 (m, 2H), 7.03 (s, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.4, 140.8, 137.3, 135.2, 133.3, 132.2, 131.0, 129.1, 128.7, 128.4, 128.3, 128.1, 127.6, 127.3, 126.4, 124.0, 123.6, 112.5, 94.9.

2-phenyl-5-(p-tolyl)pyrazolo[5,1-a]isoquinoline



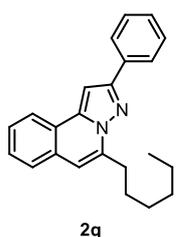
Known compound, the spectral datas were consistent with reported literature values⁶. Yield 70% (46 mg, 0.14 mmol), yellow solid, m. p. 100-101 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (dd, $J = 7.7$, 1.7 Hz, 1H), 8.00 (dd, $J = 8.3$, 1.3 Hz, 2H), 7.95 - 7.91 (m, 2H), 7.73 - 7.70 (m, 1H), 7.56 - 7.50 (m, 2H), 7.45 - 7.40 (m, 2H), 7.37 (s, 1H), 7.37 - 7.32 (m, 3H), 7.03 (s, 1H), 2.46 (s, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.2, 140.8, 139.3, 138.5, 133.5, 130.9, 129.6, 129.4, 128.9, 128.6, 128.2, 127.9, 127.2, 126.5, 123.9, 123.5, 112.1, 94.8, 21.5.

5-(4-methoxyphenyl)-2-phenylpyrazolo[5,1-a]isoquinoline



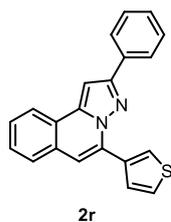
New compound, Yield 79% (55 mg, 0.16 mmol), yellow solid, 123-124 °C $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.17 - 8.11 (m, 1H), 8.04 - 7.98 (m, 4H), 7.72 (dd, $J = 6.1$, 3.0 Hz, 1H), 7.57 - 7.51 (m, 2H), 7.46 - 7.41 (m, 2H), 7.39 (s, 1H), 7.36 - 7.32 (m, 1H), 7.10 - 7.05 (m, 2H), 7.03 (s, 1H), 3.91 (s, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 160.4, 152.2, 140.8, 138.2, 133.5, 131.1, 129.5, 128.6, 128.2, 127.9, 127.09, 127.05, 126.4, 126.2, 123.7, 123.5, 113.6, 111.7, 94.8, 55.4; HRMS (ESI) Calcd for $\text{C}_{24}\text{H}_{19}\text{N}_2\text{O}$ ($\text{M}+\text{H}$)⁺ 351.1492, found 351.1499.

5-hexyl-2-phenylpyrazolo[5,1-a]isoquinoline



Known compound, the spectral datas were consistent with reported literature values³. Yield 52% (34 mg, 0.10 mmol), brown solid, m. p. 67-68 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 - 8.08 (m, 1H), 8.07 - 8.03 (m, 2H), 7.69 - 7.64 (m, 1H), 7.52 - 7.45 (m, 4H), 7.39 - 7.34 (m, 1H), 7.32 (s, 1H), 6.82 (s, 1H), 3.26 - 3.20 (m, 2H), 1.98 - 1.91 (m, 2H), 1.56 - 1.48 (m, 2H), 1.43 - 1.35 (m, 4H), 0.92 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.0, 140.1, 139.8, 133.7, 129.3, 128.7, 128.1, 127.7, 126.6, 126.5, 126.4, 123.5, 109.4, 94.6, 31.7, 30.9, 29.2, 26.8, 22.7, 14.1.

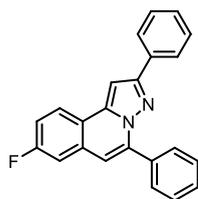
2-phenyl-5-(thiophen-3-yl)pyrazolo[5,1-a]isoquinoline



2r

Known compound, the spectral datas were consistent with reported literature values³. Yield 74% (48 mg, 0.15 mmol), green solid, m. p. 204-205 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/20); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.70 (dd, $J = 3.1, 1.3$ Hz, 1H), 8.12 (dd, $J = 7.2, 2.2$ Hz, 1H), 8.08 – 8.03 (m, 2H), 7.83 (dd, $J = 5.1, 1.3$ Hz, 1H), 7.75 – 7.71 (m, 1H), 7.57 – 7.51 (m, 2H), 7.50 – 7.44 (m, 3H), 7.40 – 7.36 (m, 2H), 7.28 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.2, 141.0, 133.5, 133.4, 133.3, 129.1, 128.7, 128.3, 127.99, 127.95, 127.3, 127.3, 127.2, 126.4, 125.0, 123.6, 123.5, 111.2, 94.7.

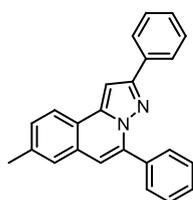
8-fluoro-2,5-diphenylpyrazolo[5,1-a]isoquinoline



2s

Known compound, the spectral datas were consistent with reported literature values⁶. Yield 82% (55 mg, 0.16 mmol), yellow oil, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.10 (dd, $J = 8.8, 5.4$ Hz, 1H), 8.02 – 7.96 (m, 4H), 7.56 – 7.50 (m, 3H), 7.42 (dd, $J = 8.2, 6.6$ Hz, 2H), 7.38 – 7.33 (m, 2H), 7.31 (s, 1H), 7.27 (dd, $J = 8.6, 2.6$ Hz, 1H), 6.98 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 162.1 (d, $^1J_{\text{C-F}} = 248.5$ Hz), 152.6, 140.5, 139.5, 133.4, 133.2, 131.0 (d, $^3J_{\text{C-F}} = 9.1$ Hz), 129.7, 129.5, 128.7, 128.4, 128.2, 126.5, 125.8 (d, $^3J_{\text{C-F}} = 9.1$ Hz), 120.6 (d, $^4J_{\text{C-F}} = 2.0$ Hz), 116.1, 115.9, 112.0 (d, $^2J_{\text{C-F}} = 22.2$ Hz), 111.7 (d, $^2J_{\text{C-F}} = 3.0$ Hz), 94.6.; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -112.21.

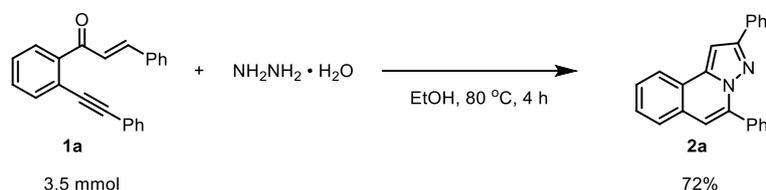
8-methyl-2,5-diphenylpyrazolo[5,1-a]isoquinoline



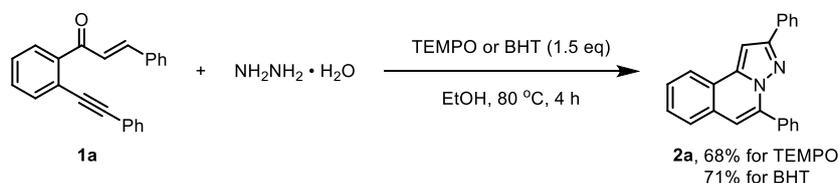
2t

Known compound, the spectral datas were consistent with reported literature values⁶. Yield 63% (42 mg, 0.13 mmol), yellow solid, m. p. 107-108 °C, $R_f = 0.5$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05 – 7.97 (m, 5H), 7.56 – 7.49 (m, 4H), 7.45 – 7.37 (m, 3H), 7.35 – 7.30 (m, 2H), 6.99 (s, 1H), 2.51 (s, 3H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 152.2, 140.9, 138.4, 138.0, 133.9, 133.5, 129.7, 129.5, 129.2, 129.0, 128.6, 128.17, 128.15, 127.0, 126.4, 123.4, 121.8, 112.4, 94.3, 21.7.

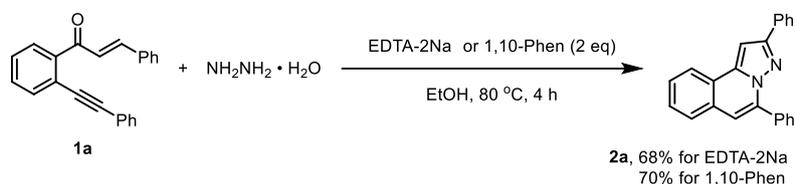
1.4 Gram-scale reaction of 2a



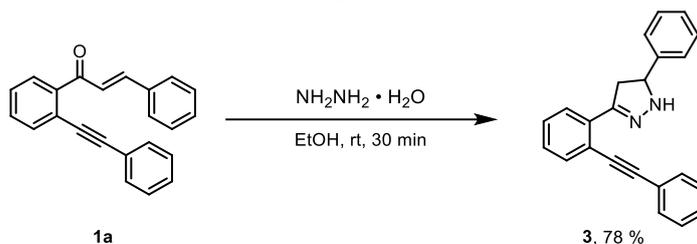
1.5 Control Reactions



In a reaction vial with a magnetic bar, EtOH (4.0 mL), TEMPO (1.5 eq) or BHT (1.5 eq), the substrate of **1a** (61.6 mg, 0.2 mmol) and $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ (50%, 20 mg, 0.4 mmol) were added. The mixture was stirred at 80 °C in oil bath until the substrate **1a** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **2a**.



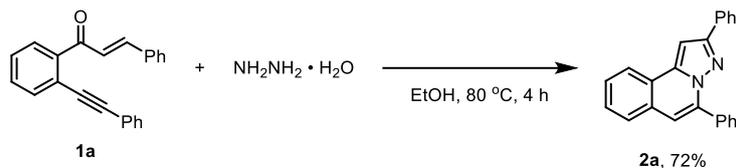
In reaction tubes with magnetic stir bars, EtOH (4.0 mL), EDTA - 2Na (1 eq) or 1,10 - Phen (1 eq) respectively, the substrate of **1a** (61.6 mg, 0.2 mmol) was added, and the mixture was stirred at room temperature for 2 h. The same operation was performed with $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ (50%, 20 mg, 0.4 mmol) simultaneously. After that, mixture of **1a** and $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ was combined to the vial together and stirred at 80 °C in an oil bath for more 4 h. After rapid filtration through silica gel, the solvent was evaporated by a rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as the eluent to afford the product **2a**.



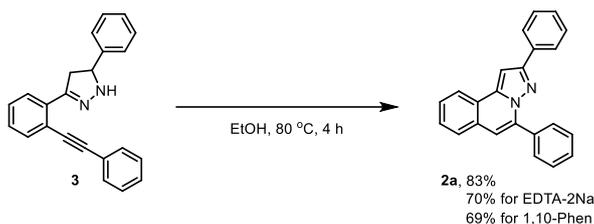
In a reaction vial with a magnetic bar, EtOH (4.0 mL), the substrate of **1a** and $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ were added. The mixture was stirred at room temperature using a magnetic stirrer until the substrate **1a** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, to afford the product **3**. (note: NMR yield, unstable and will partially decompose when purified by flash column chromatography on silica gel).



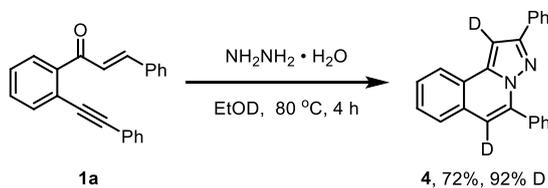
Equipment cleaning using aqua regia (for 7 h)^a Tube and magnetic stir after aqua regia cleaning
^aMix concentrated HNO_3 and HCl in a volume ratio of 1:3 slowly in a fume hood, prepare fresh and use immediately. The prepared aqua regia is transferred into a reaction tube with a magnetic stir bar. A balloon is attached to the side arm to collect exhaust gas. After soaking the reaction tube and stir bar for 7 hours, they are rinsed repeatedly with deionized water and dried for later use.



In reaction tubes with magnetic stir bars (cleaned with aqua regia), EtOH (4.0 mL), the substrate of **1a** (61.6 mg, 0.2 mmol) and $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ (50%, 20 mg, 0.4 mmol) were added. The mixture was stirred at 80 °C in oil bath for 4 h. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **2a**.

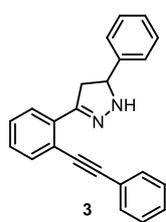


In reaction tubes with magnetic stir bars, EtOH (4.0 mL), the substrate of **3** (none; with EDTA - 2Na (2 eq) or 1,10 - Phen (2 eq)) were added. The mixture was stirred using a magnetic stirrer at 80 °C for 4 h. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **2a**.



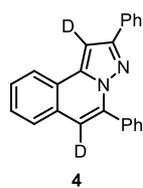
In reaction tubes with magnetic stir bars, EtOD (4.0 mL, 99% D), substrate of **1a** (61.6 mg, 0.2 mmol) and $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$ (50%, 20 mg, 0.4 mmol) were added. The mixture was stirred at 80 °C in oil bath for 4 h. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **4**.

5-phenyl-3-(2-(phenylethynyl)phenyl)-4,5-dihydro-1H-pyrazole



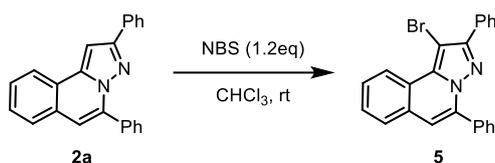
New compound, Yield 83% (53 mg, 0.16 mmol), yellow oil, $R_f = 0.4$ (EtOAc/petroleum ether = 1/20); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 (dd, $J = 7.6, 1.7$ Hz, 1H), 7.56 (dd, $J = 6.9, 2.4$ Hz, 1H), 7.41 - 7.38 (m, 2H), 7.37 - 7.31 (m, 6H), 7.31 - 7.26 (m, 5H), 4.96 (dd, $J = 10.6, 7.8$ Hz, 1H), 3.80 (dd, $J = 16.7, 10.6$ Hz, 1H), 3.51 (dd, $J = 16.7, 7.9$ Hz, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 151.7, 142.8, 135.0, 133.7, 131.2, 128.9, 128.43, 128.41, 128.39, 128.3, 128.2, 127.8, 126.3, 123.2, 121.1, 93.9, 89.2, 65.1, 43.3. HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{17}\text{N}_2$ (M-H) $^-$ 321.1397, found 321.1396.

2,5-diphenylpyrazolo[5,1-a]isoquinoline-1,6-d₂



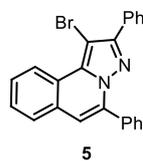
New compound, Yield 72%, 92% D, (46 mg, 0.14 mmol), yellow oil, $R_f = 0.6$ (EtOAc/petroleum ether = 1/20); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.16 (dd, $J = 7.3, 1.8$ Hz, 1H), 8.08 – 8.00 (m, 4H), 7.75 (dd, $J = 6.9, 2.3$ Hz, 1H), 7.60 – 7.51 (m, 5H), 7.48 – 7.43 (m, 2H), 7.38 – 7.34 (m, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ , 129.7, 129.3, 128.7, 128.24, 128.21, 128.0, 127.3, 127.2, 126.5, 124.0, 123.6. HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{15}\text{D}_2\text{N}_2$ ($\text{M}+\text{H}$) $^+$ 323.1512, found 323.1518.

1.6 Experimental procedures for the synthesis of compounds 5 – 6

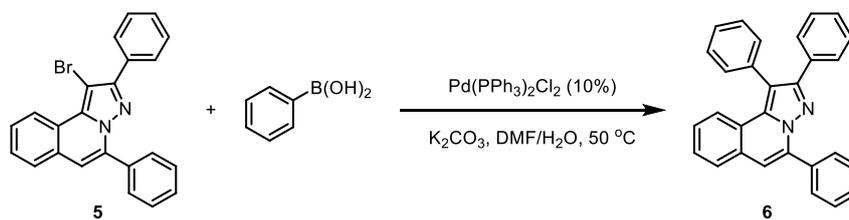


In a reaction vial with a magnetic bar, the substrate of **2a** (64 mg, 0.2 mmol) and NBS (42.7 mg, 0.24 mmol) were added, followed by addition of CHCl_3 (4 mL). The resulting mixture was stirred at room temperature using a magnetic stirrer until the substrate **2a** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **5**.

1-bromo-2,5-diphenylpyrazolo[5,1-a]isoquinoline

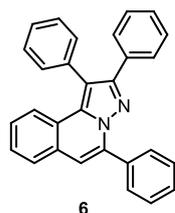


Known compound, the spectral datas were consistent with reported literature values³. Yield 80% (64 mg, 0.16 mmol), yellow solid, m. p. 154-155 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/40); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.26 (dd, $J = 7.6, 1.8$ Hz, 1H), 7.98 (dd, 2H), 7.93 (dd, $J = 7.9, 1.8$ Hz, 2H), 7.75 (dd, $J = 7.7, 1.6$ Hz, 1H), 7.61 (td, $J = 6.9, 1.8$ Hz, 2H), 7.55 – 7.47 (m, 4H), 7.45 – 7.38 (m, 2H), 7.09 (s, 1H).; $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 150.4, 138.3, 135.3, 133.2, 132.2, 130.0, 129.7, 129.4, 129.0, 128.6, 128.4, 128.30, 128.28, 127.3, 127.2, 124.1, 123.1, 113.7, 86.2.



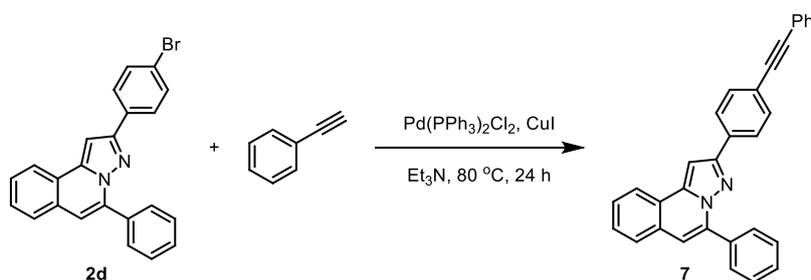
In a Schlenk tube with a magnetic bar under nitrogen atmosphere, $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (14 mg, 2 mol%), K_2CO_3 (55 mg, 0.4 mmol), the substrate of **4** (79.8 mg, 0.2 mmol) and Phenylboronic acid (29 mg, 0.24 mmol) were added in 1.0 mL of $\text{DMF-H}_2\text{O}$ (5 : 1, v/v). The resulting mixture was stirred at 50 °C in oil bath until the substrate **5** was completely consumed. The mixture was cooled to room temperature and water (10 mL) was added. The mixture was extracted with ethyl acetate (5.0 mL \times 3) and the organic layer was combined, which was then washed with brine, dried over Na_2SO_4 , and purified by column chromatography on silica gel to afford the desired product **6**.

1,2,5-triphenylpyrazolo[5,1-a]isoquinoline



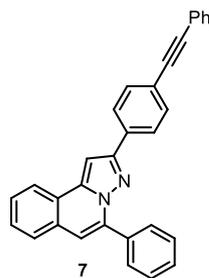
New compound, Yield 83% (66 mg, 0.17 mmol), white solid, m. p. 214-215 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/20); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05 (dd, 2H), 7.70 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.59 (d, $J = 8.3$ Hz, 1H), 7.57 - 7.48 (m, 10H), 7.45 - 7.41 (m, 1H), 7.24 - 7.19 (m, 4H), 7.07 (s, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 150.1, 138.3, 136.6, 134.9, 133.9, 133.4, 131.3, 129.9, 129.7, 129.24, 129.22, 128.4, 128.2, 128.1, 127.8, 127.63, 127.56, 127.3, 126.9, 124.7, 123.2, 114.4, 113.0.; HRMS (ESI) Calcd for $\text{C}_{29}\text{H}_{21}\text{N}_2$ ($\text{M}+\text{H}$) $^+$ 397.1699, found 397.1708.

1.7 Experimental procedures for the synthesis of compounds 7



In a Schlenk tube with a magnetic bar under nitrogen atmosphere, $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (4.2 mg, 0.6 mol%), CuI (1.9 mg, 1 mmol%), the substrate of **2d** (79.8 mg, 0.2 mmol) and phenylacetylene (24.4 mg, 0.24 mmol) were added in Et_3N (4 mL). The resulting mixture was stirred at 80 °C in oil bath until the substrate **2d** was completely consumed. After rapid filtration of silica gel, the solvent was evaporated by rotary evaporator, and the residue was purified by flash column chromatography on silica gel using EtOAc/petroleum ether as eluent to afford the product **7**.

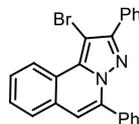
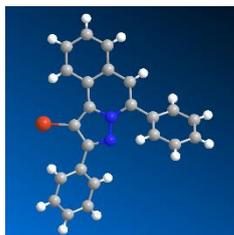
5-phenyl-2-(4-(phenylethynyl)phenyl)pyrazolo[5,1-a]isoquinoline



New compound, Yield 71% (59 mg, 0.14 mmol), white solid, m. p. 193-194 °C, $R_f = 0.6$ (EtOAc/petroleum ether = 1/20); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.15 (dd, $J = 7.0, 2.0$ Hz, 1H), 8.04 (dd, $J = 8.1, 1.6$ Hz, 2H), 8.02 - 7.98 (m, 2H), 7.75 (dd, $J = 6.8, 2.4$ Hz, 1H), 7.62 - 7.53 (m, 9H), 7.41 (s, 1H), 7.39 - 7.34 (m, 3H), 7.09 (s, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 151.5, 140.9, 138.4, 133.7, 133.3, 131.9, 131.7, 129.7, 129.3, 128.4, 128.29, 128.25, 128.1, 127.4, 127.3, 126.3, 123.9, 123.5, 123.4, 122.9, 112.8, 95.0, 90.2, 89.7.; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{21}\text{N}_2$ ($\text{M}+\text{H}$) $^+$ 421.1699, found 421.1707.

2. X-Ray diffraction analysis

2.1 Crystal data and structure refinement for 5



CCDC	2520091
Identification code	Z20251224D
Empirical formula	C ₂₃ H ₁₅ BrN ₂
Formula weight	399.28
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	7.9816(4)
b/Å	10.6623(5)
c/Å	11.8043(5)
α /°	106.078(2)
β /°	109.297(2)
γ /°	96.220(2)
Volume/Å ³	888.65(7)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.492
μ/mm^{-1}	2.321
F(000)	404.0
Crystal size/mm ³	0.32 × 0.24 × 0.12
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	4.076 to 50.018
Index ranges	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	19450
Independent reflections	3112 [Rint = 0.0581, Rsigma = 0.0341]
Data/restraints/parameters	3112/0/235
Goodness-of-fit on F ²	1.049
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0332, wR ₂ = 0.0845
Final R indexes [all data]	R ₁ = 0.0407, wR ₂ = 0.0883
Largest diff. peak/hole / e Å ⁻³	0.58/-0.75

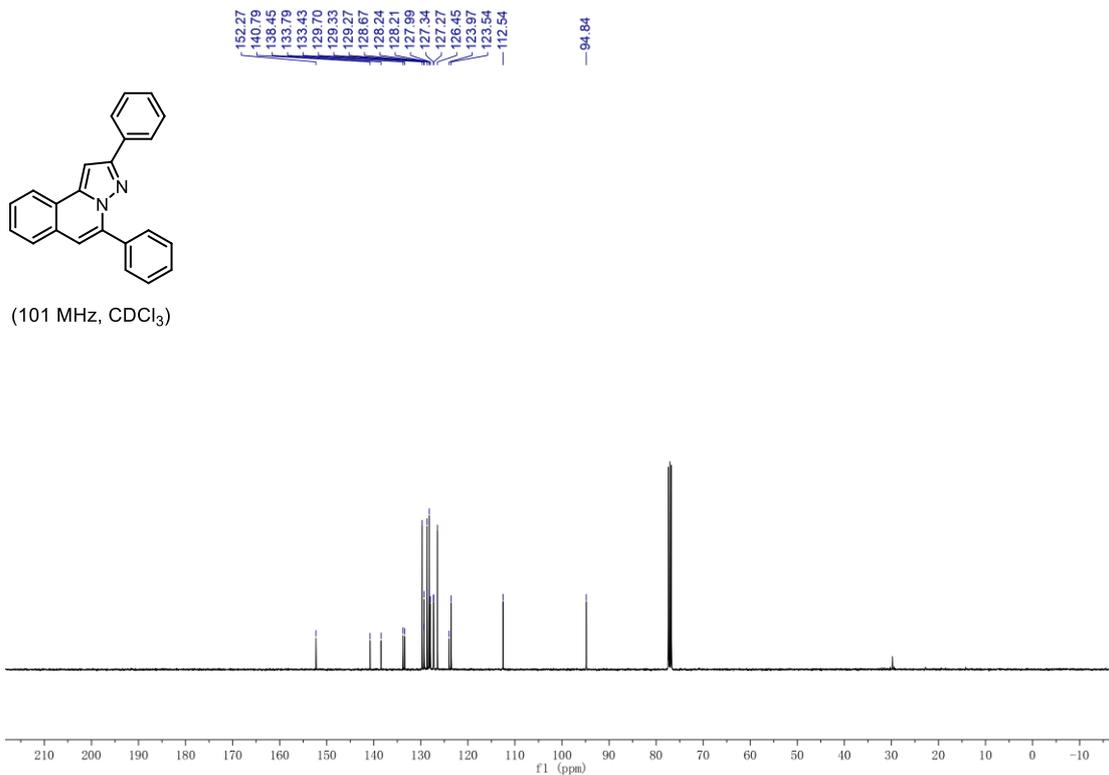
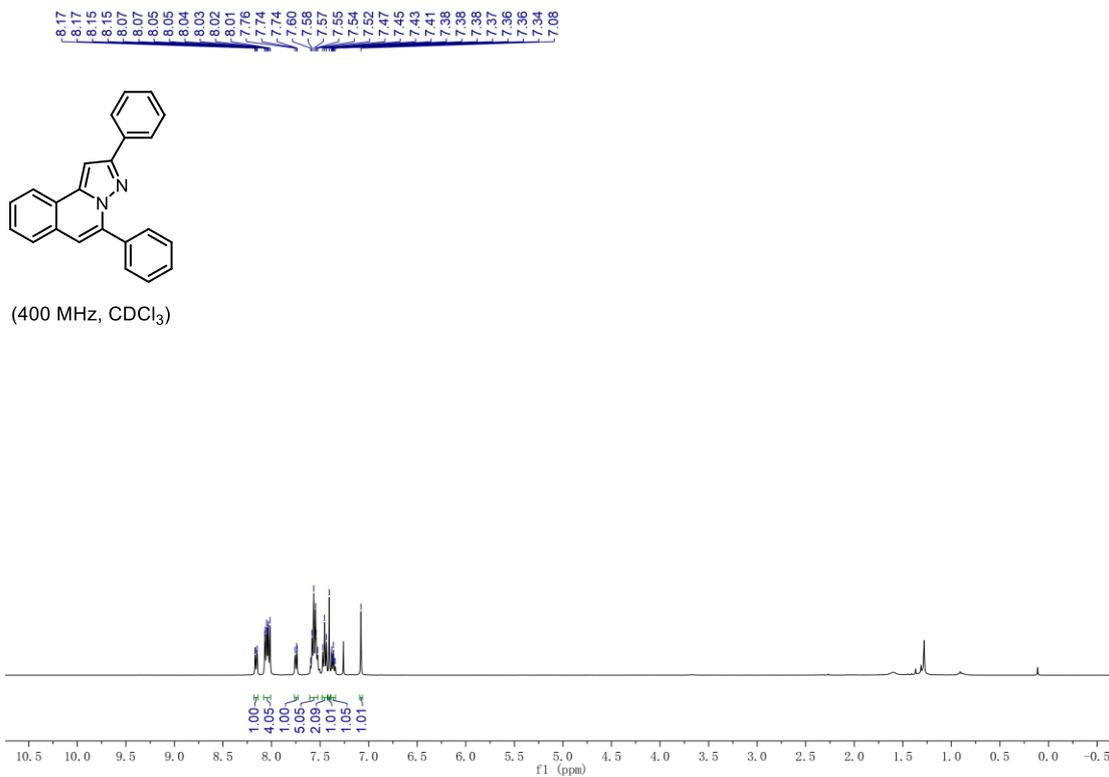
3. References

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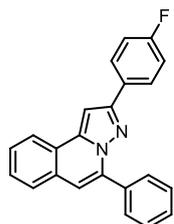
4. Copies of NMR spectrum

2,5-diphenylpyrazolo[5,1-a]isoquinoline (2a)

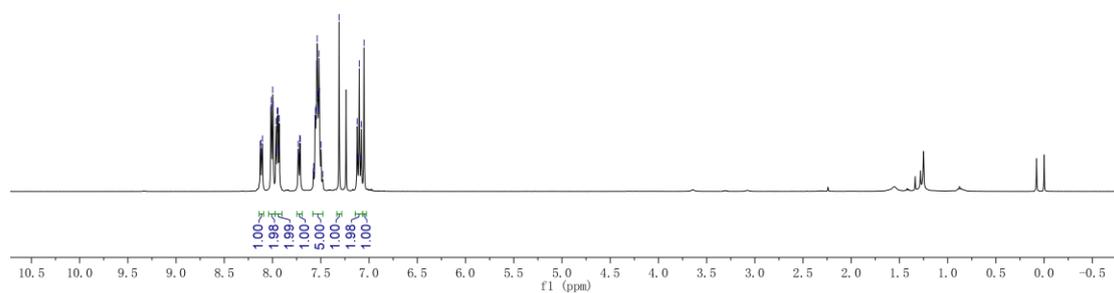


2-(4-fluorophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline (2b)

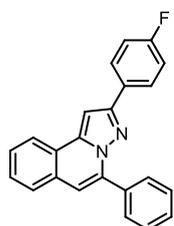
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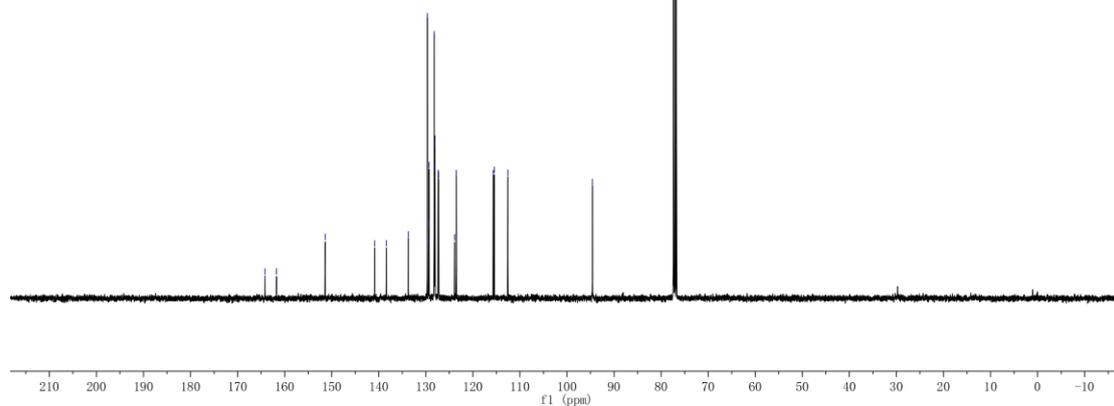
(400 MHz, CDCl₃)

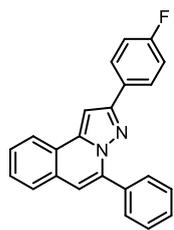


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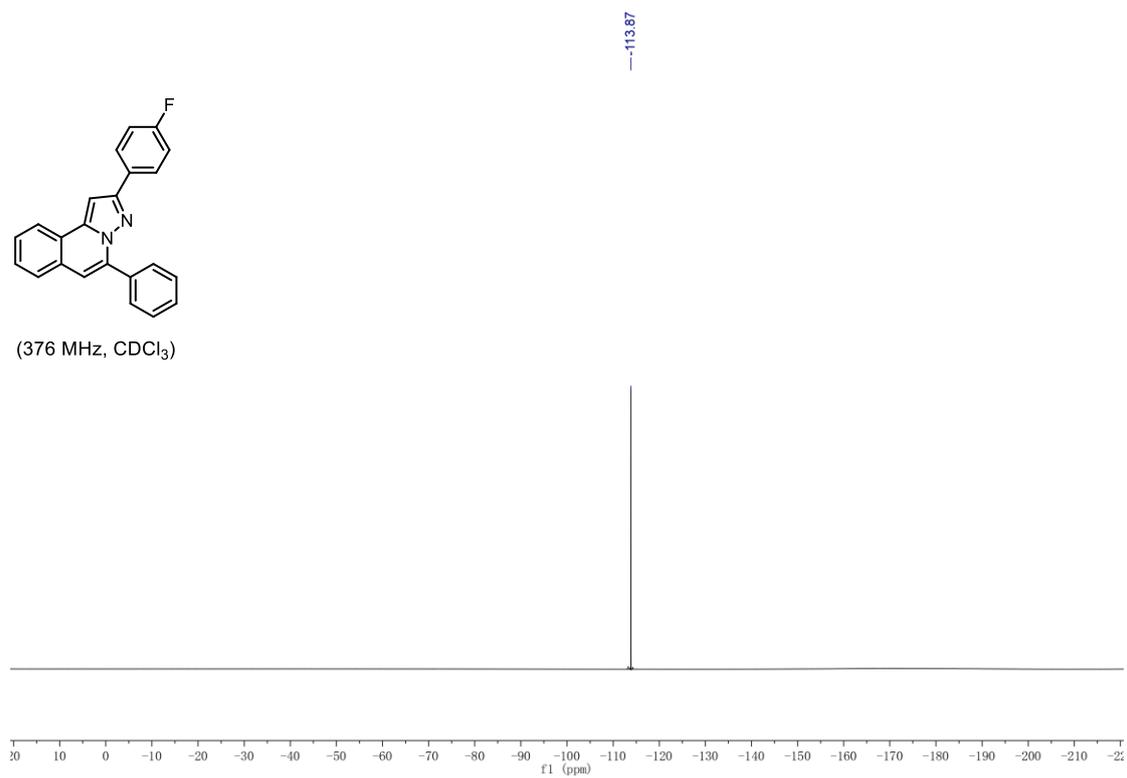


(101 MHz, CDCl₃)

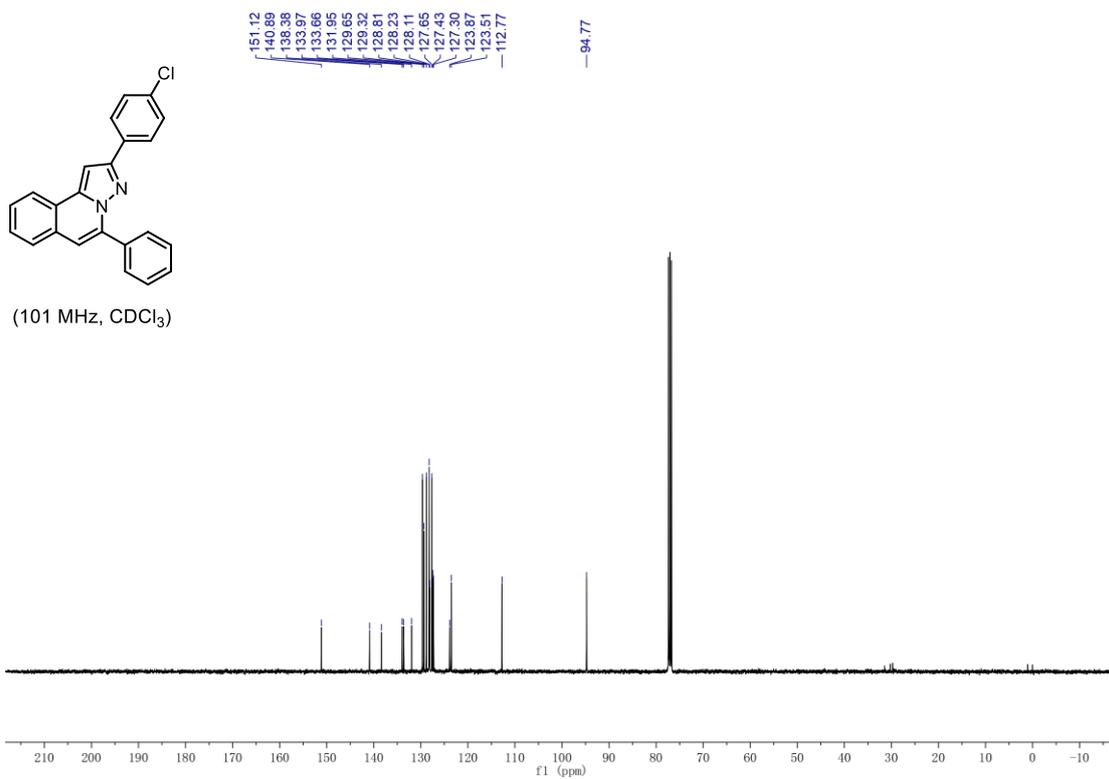
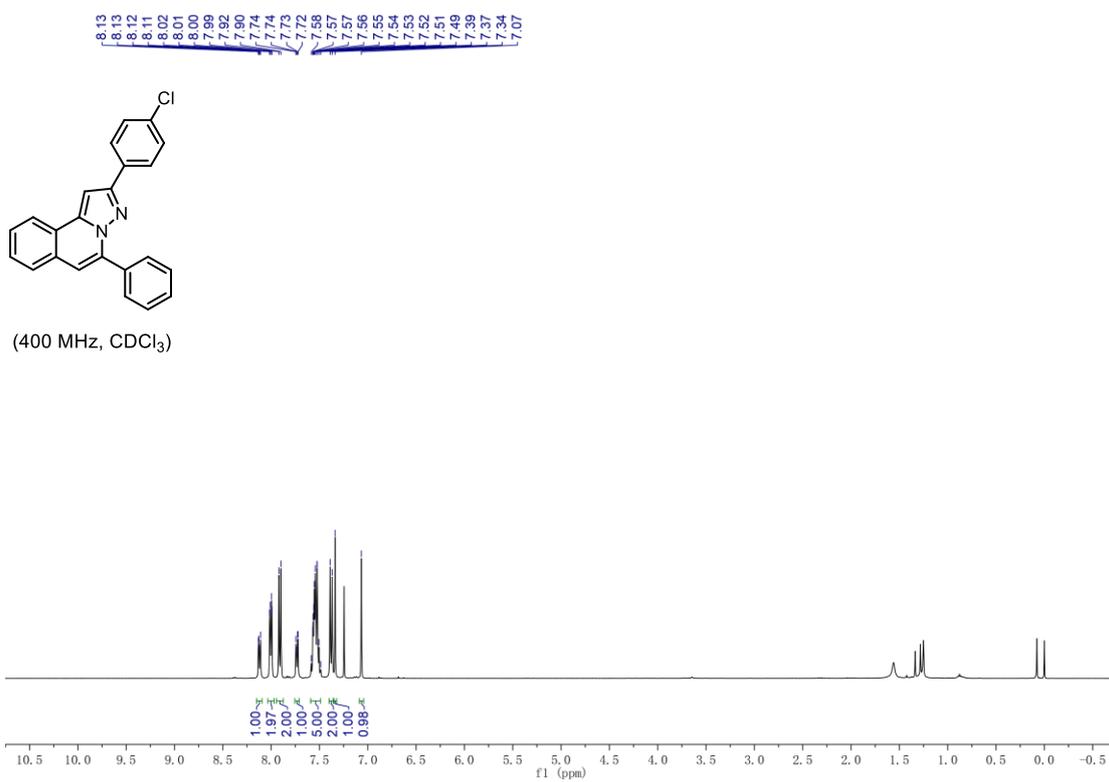




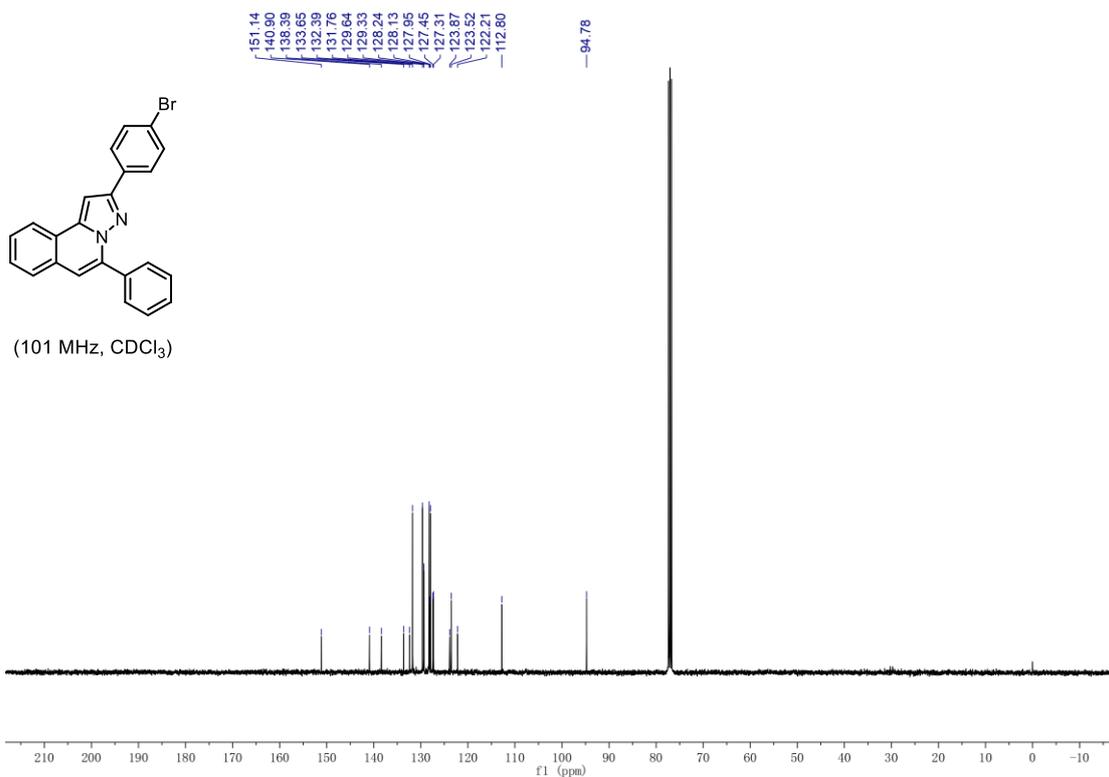
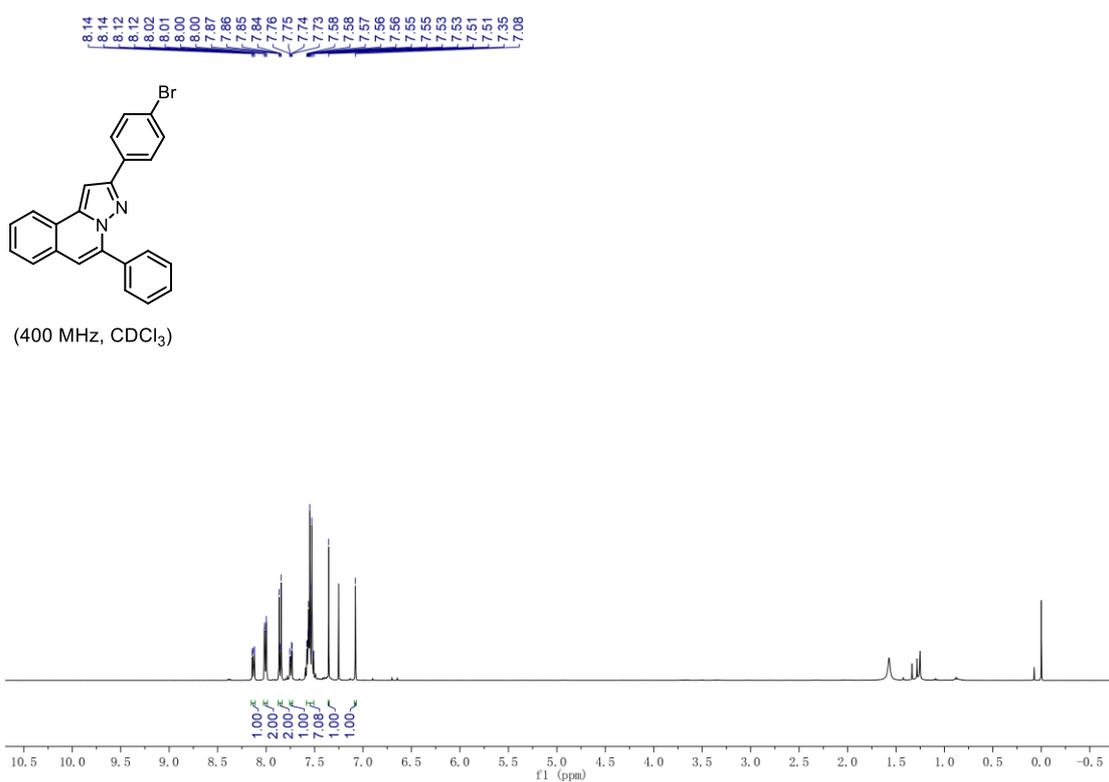
(376 MHz, CDCl₃)



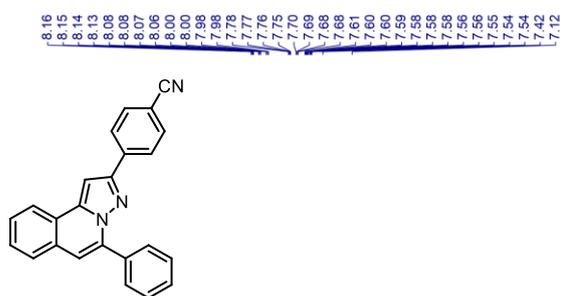
2-(4-chlorophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline (2c)



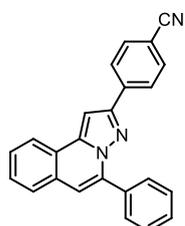
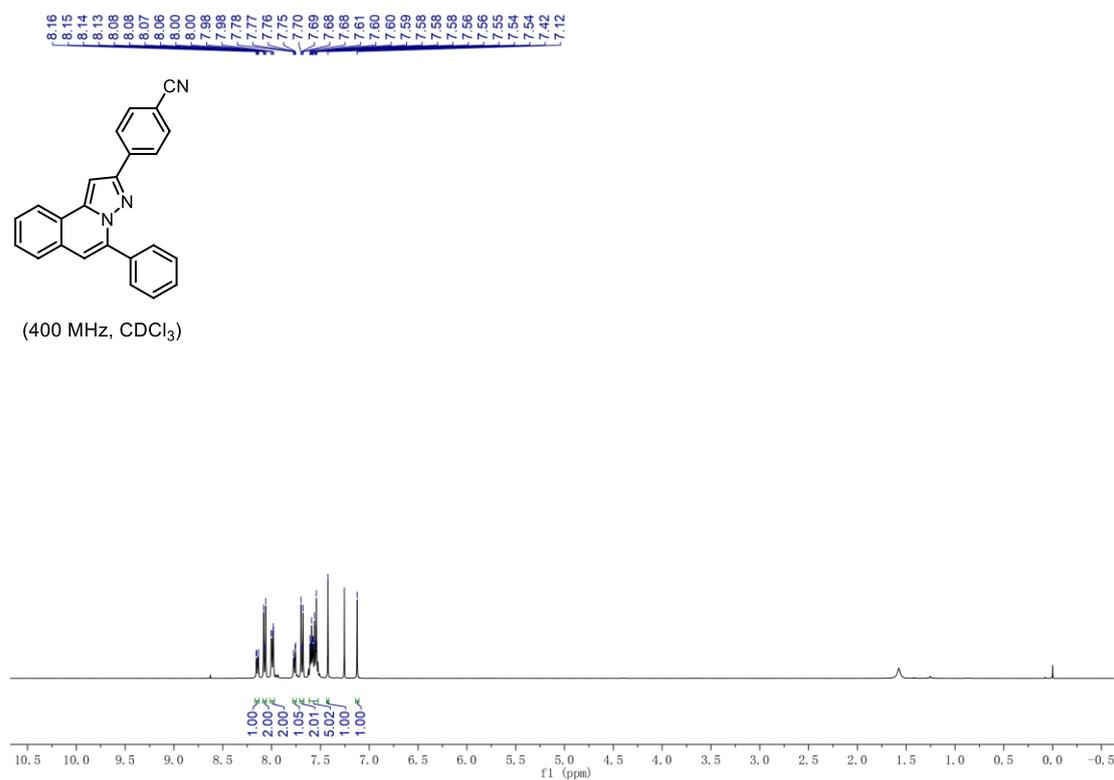
2-(4-bromophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline (2d)



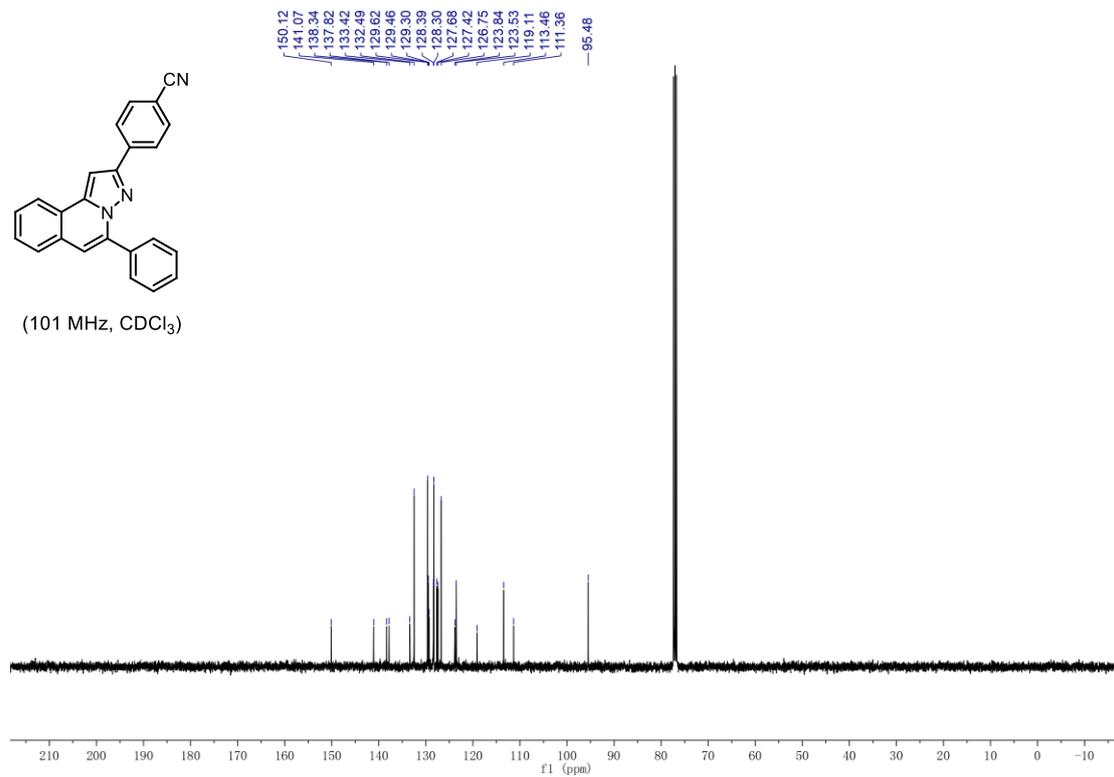
4-(5-phenylpyrazolo[5,1-a]isoquinolin-2-yl)benzotrile (2e)



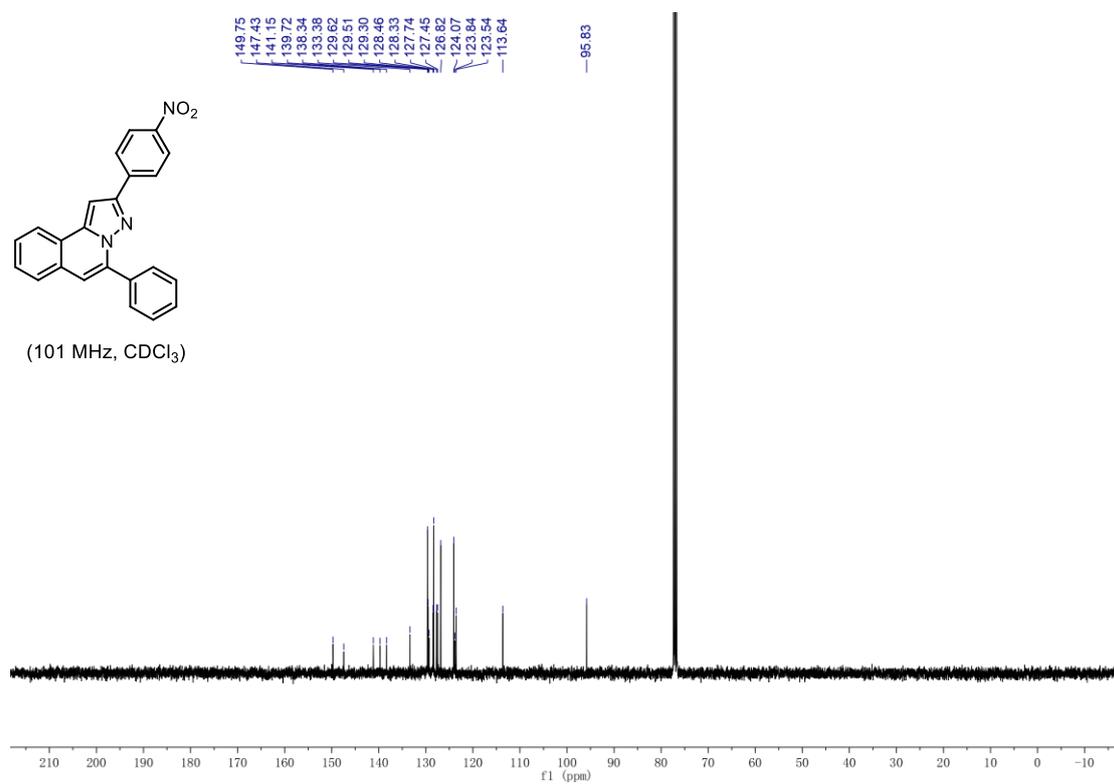
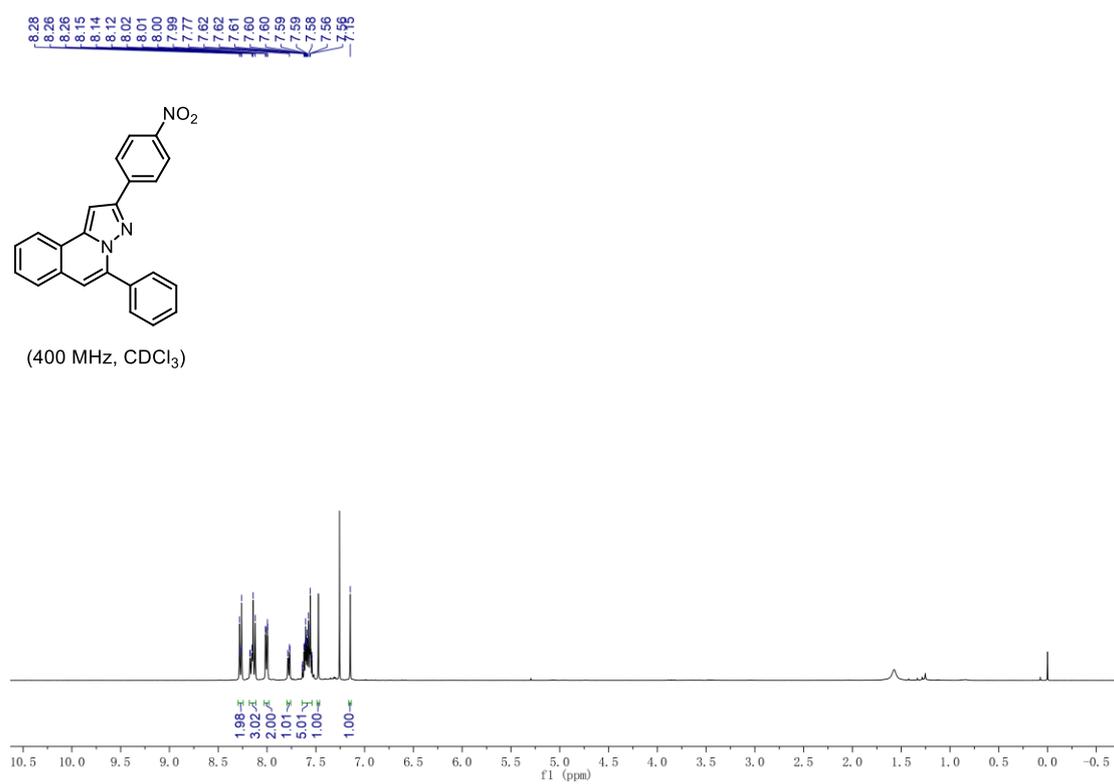
(400 MHz, CDCl₃)



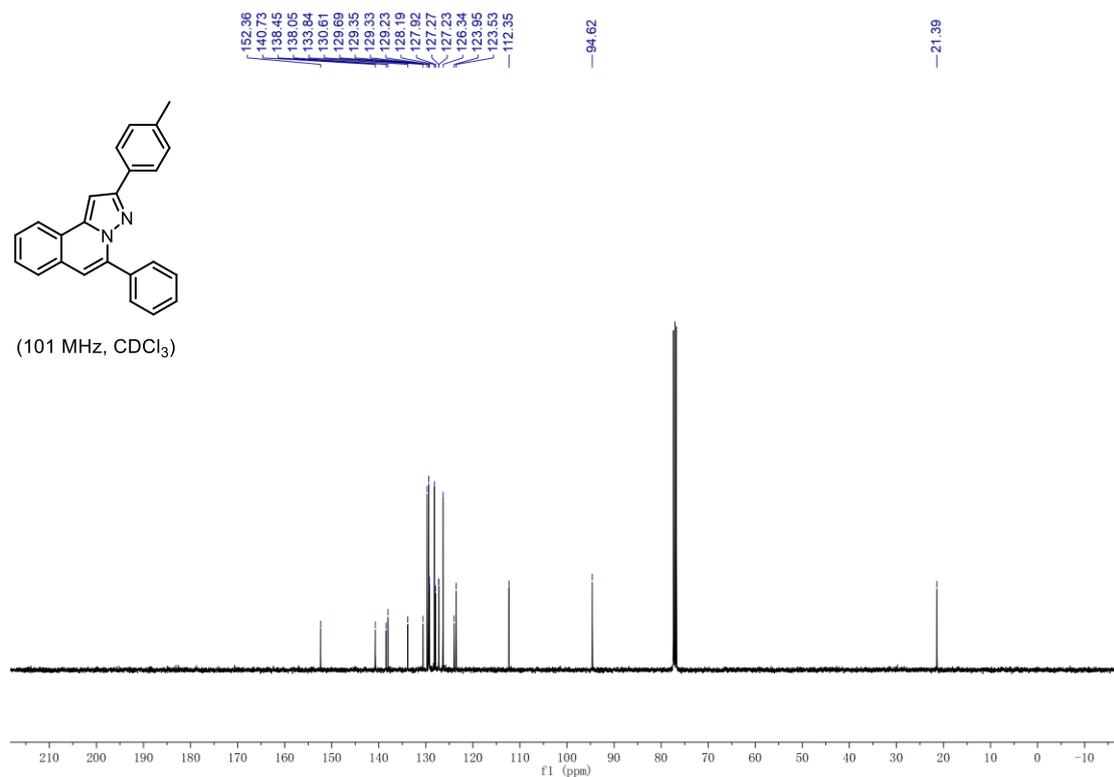
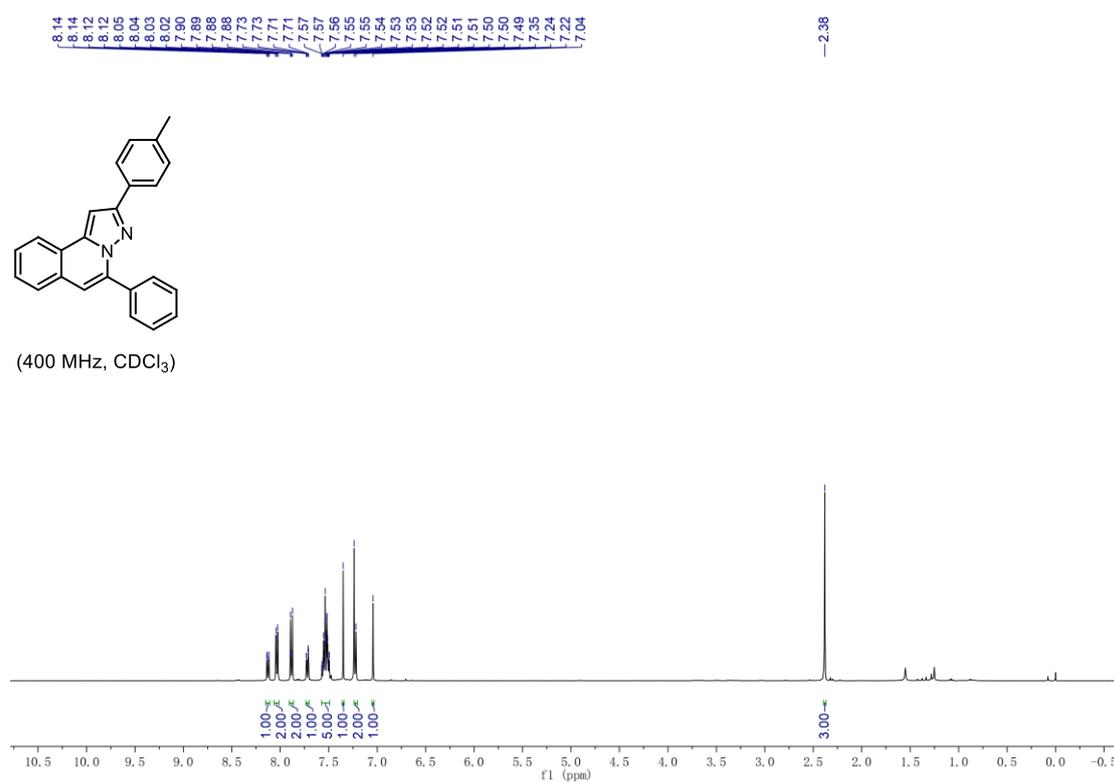
(101 MHz, CDCl₃)



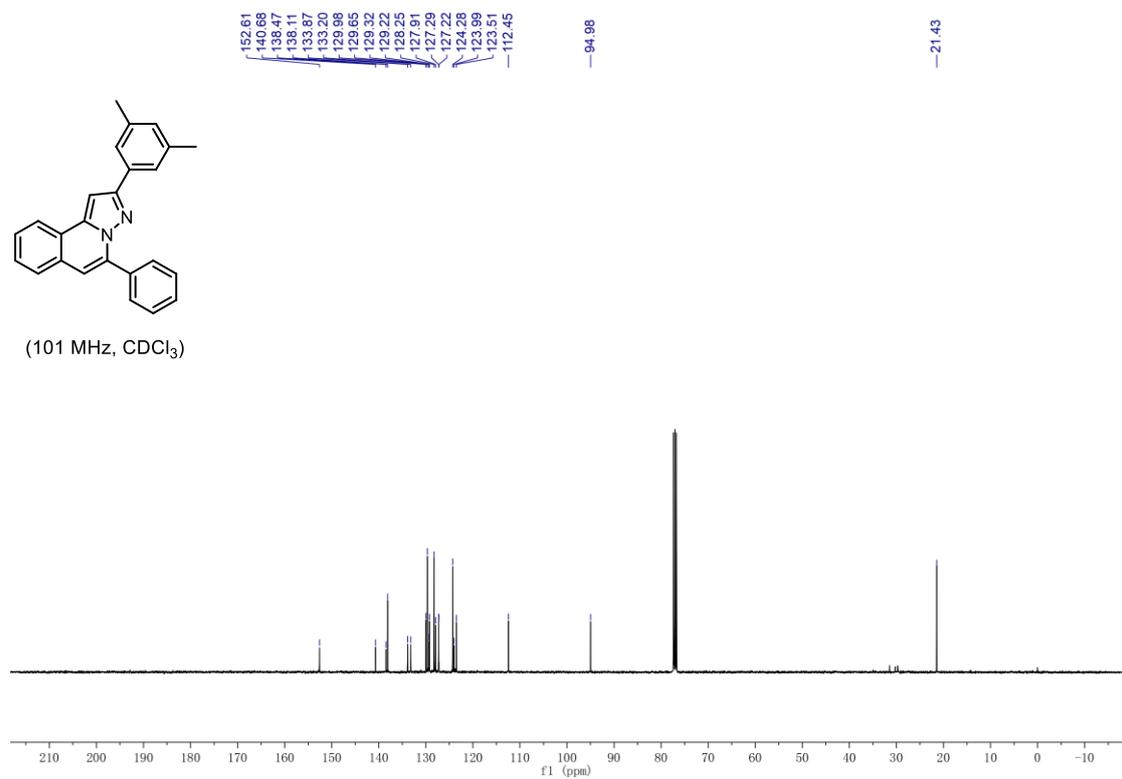
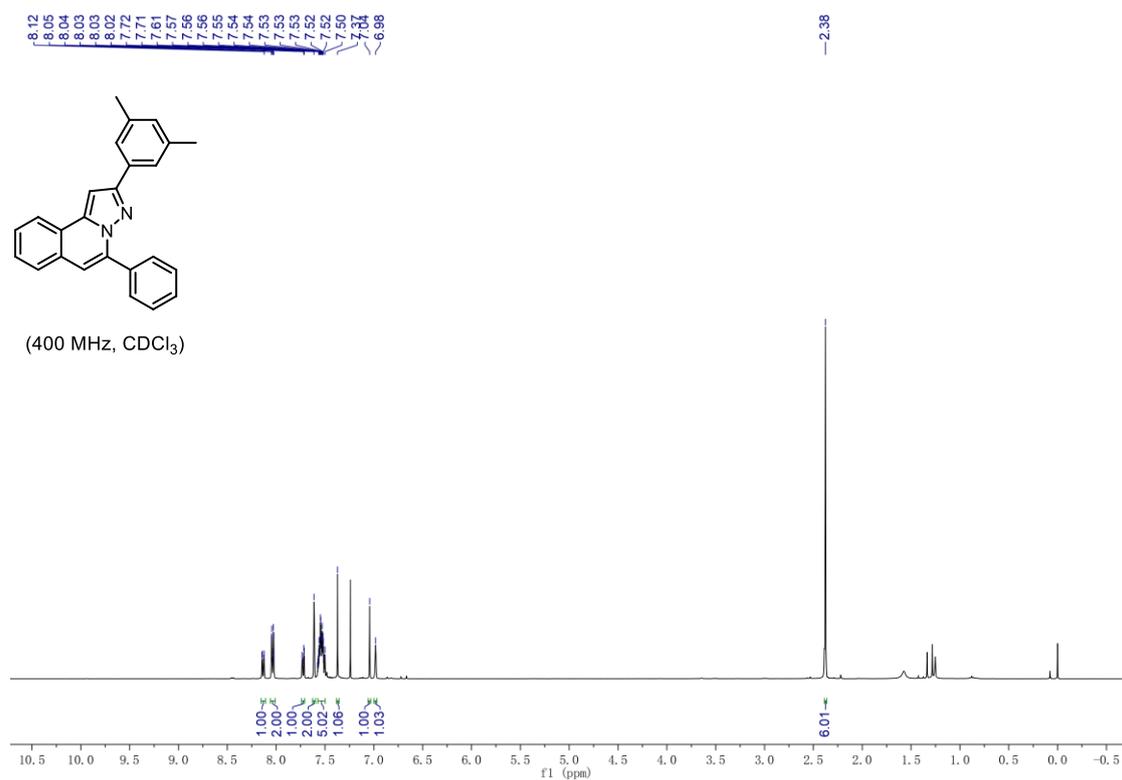
2-(4-nitrophenyl)-5-phenylpyrazolo[5,1-a]isoquinoline (2f)



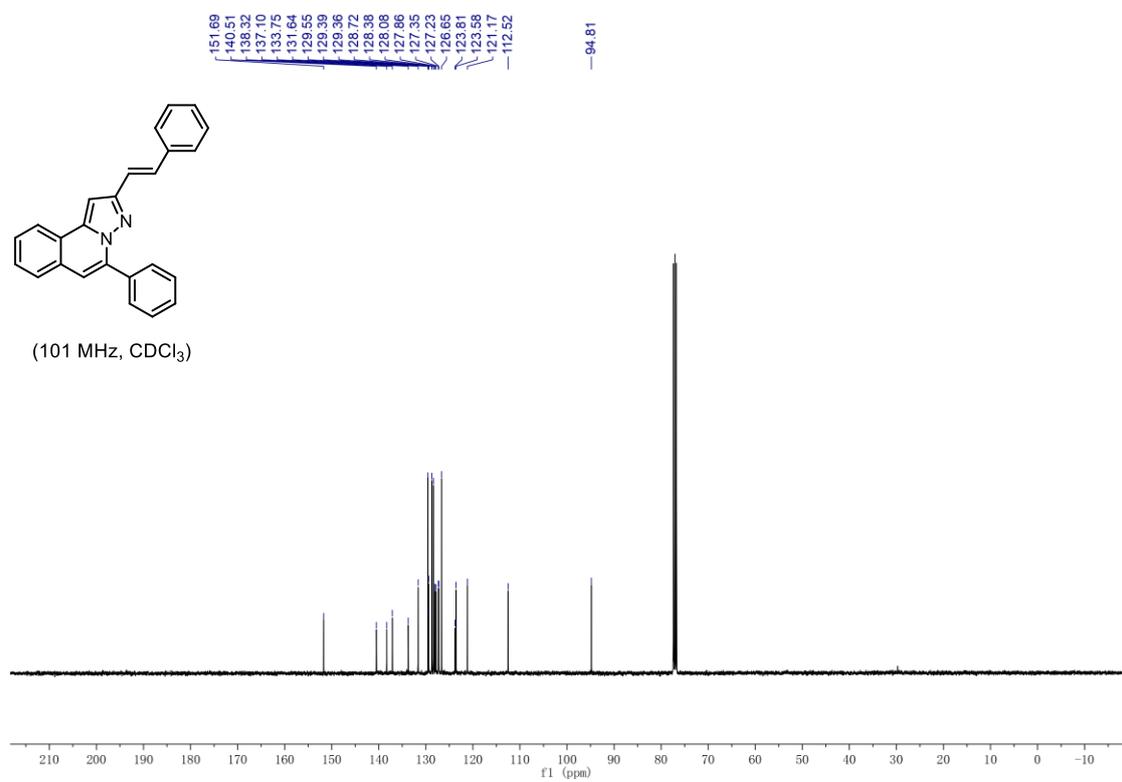
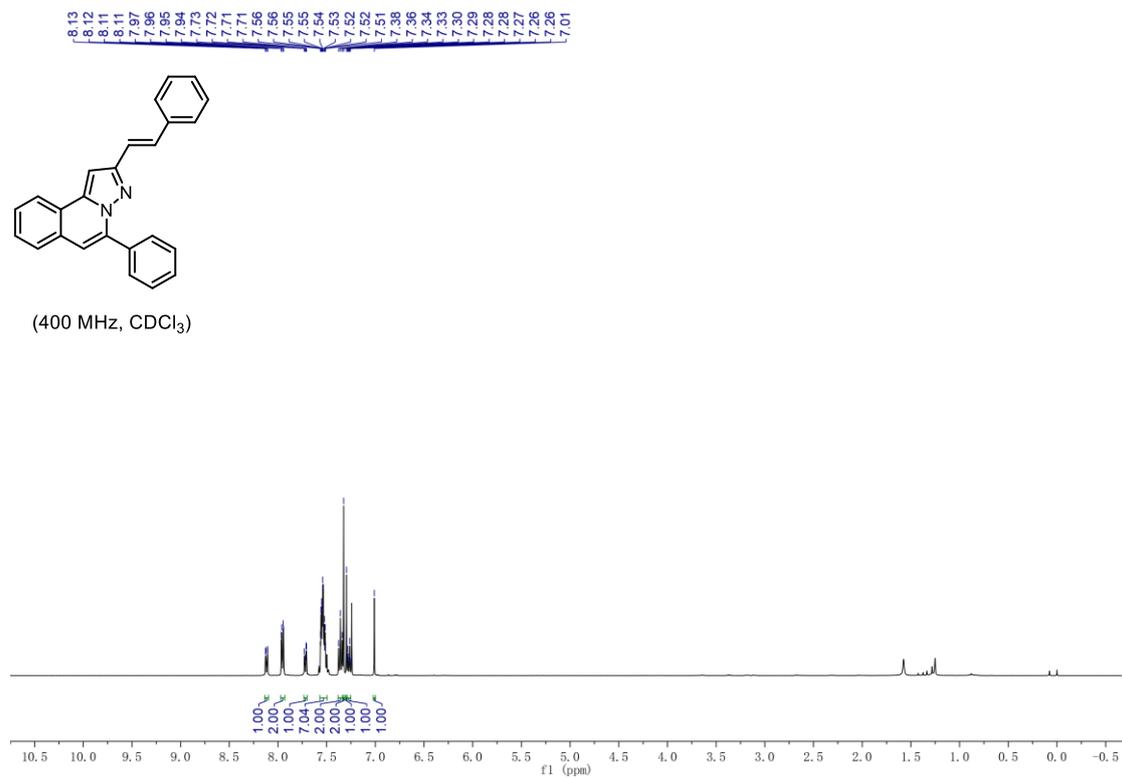
5-phenyl-2-(p-tolyl)pyrazolo[5,1-a]isoquinoline (2g)



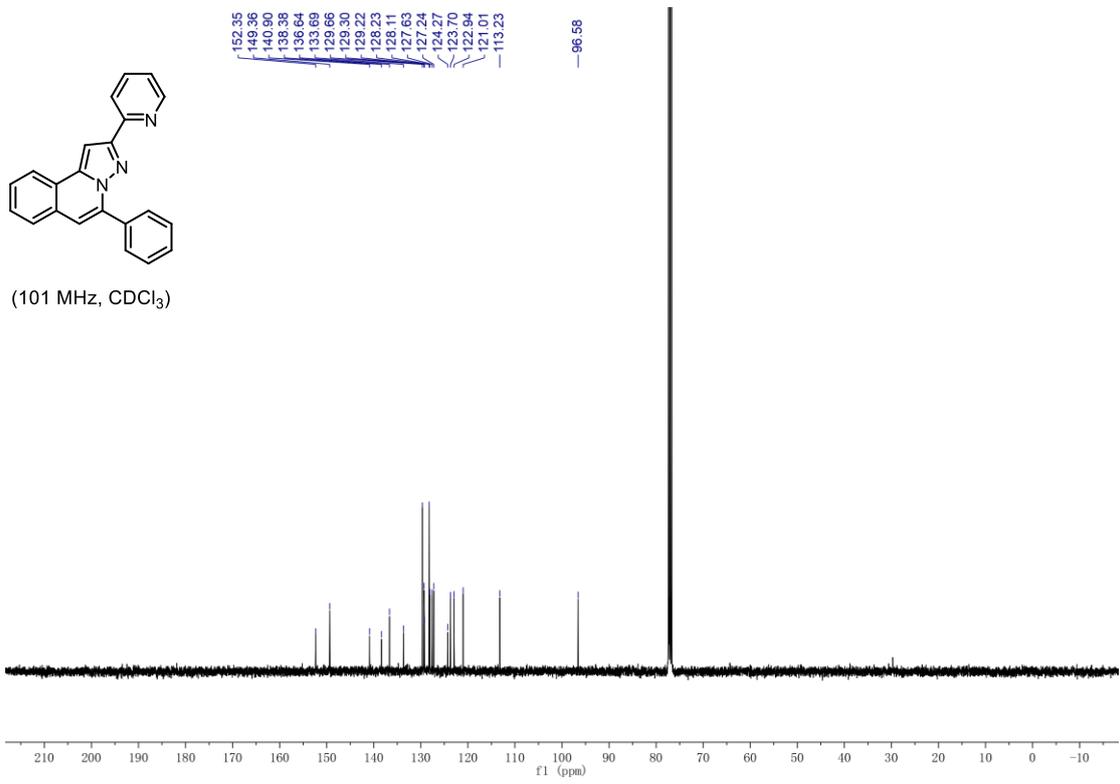
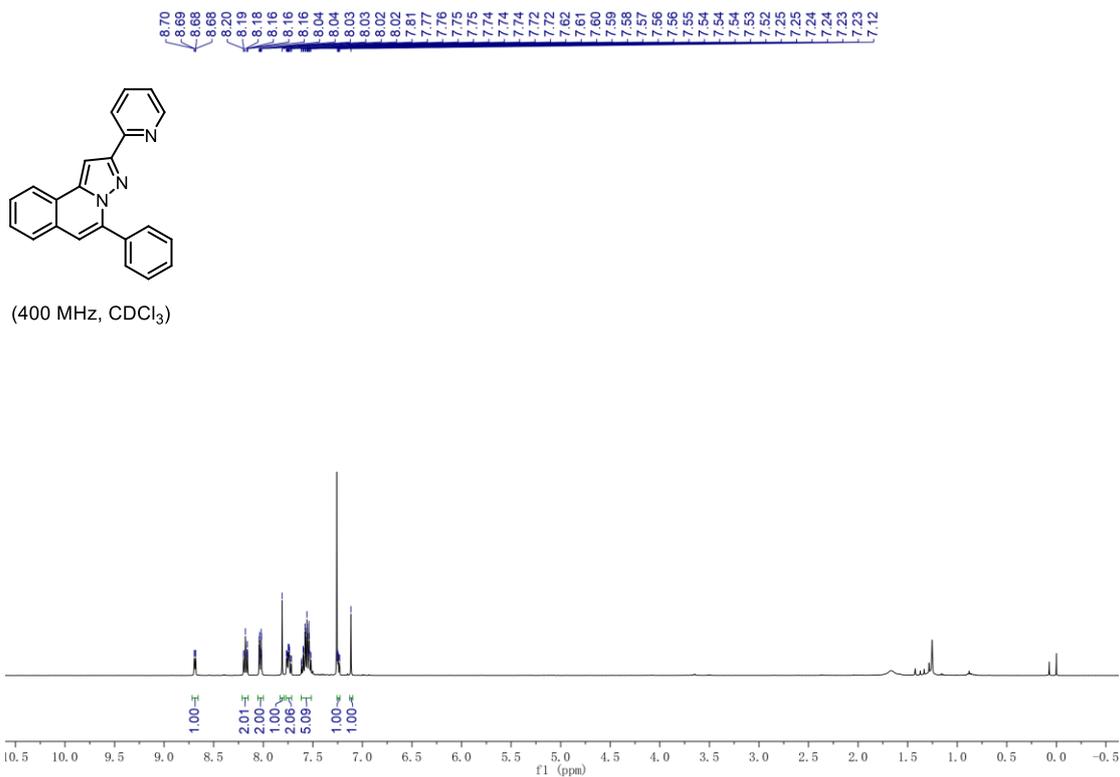
2-(3,5-dimethylphenyl)-5-phenylpyrazolo[5,1-a]isoquinoline (2h)



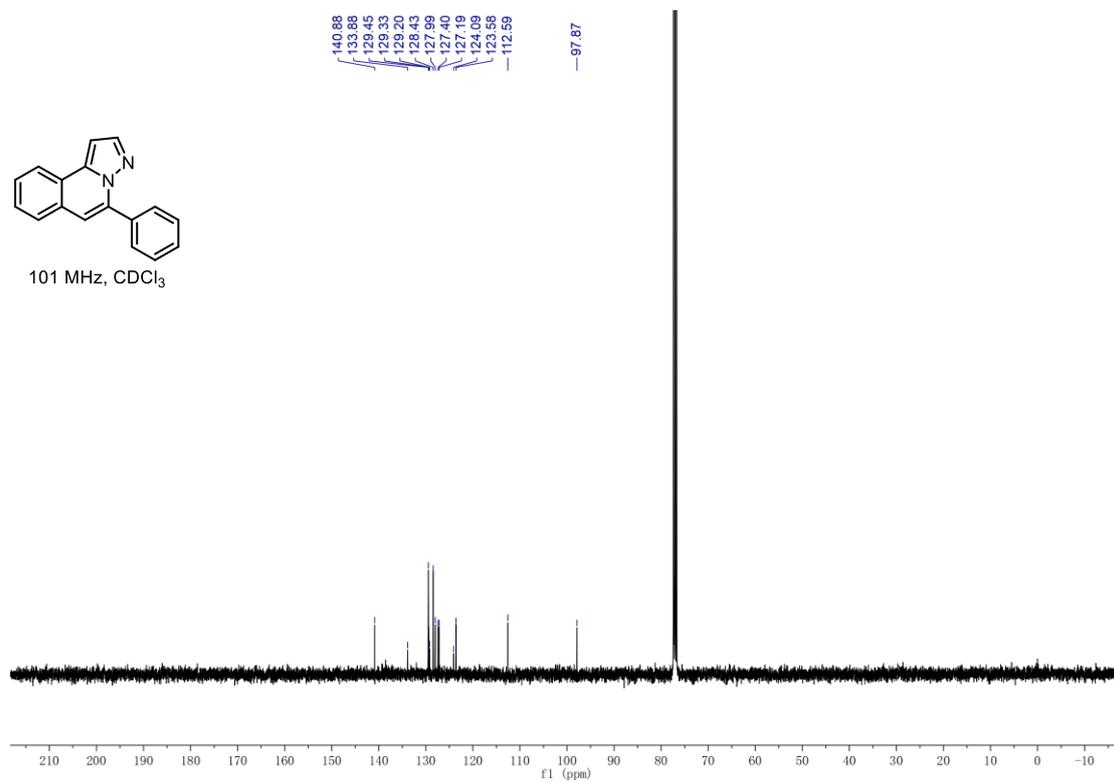
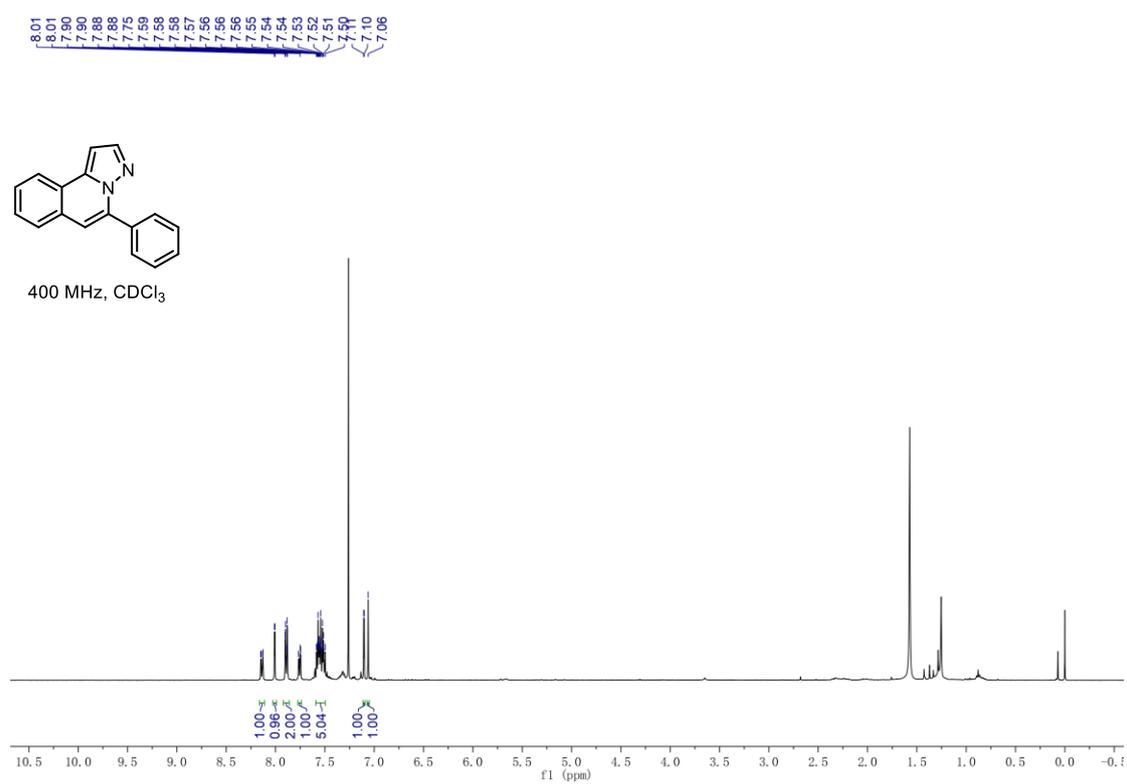
5-phenyl-2-styrylpyrazolo[5,1-a]isoquinoline (2j)



5-phenyl-2-(pyridin-2-yl)pyrazolo[5,1-a]isoquinoline (2k)

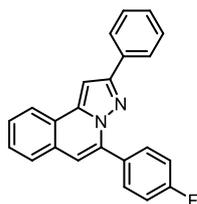


5-phenylpyrazolo[5,1-a]isoquinoline (21)

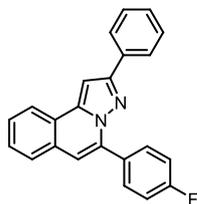
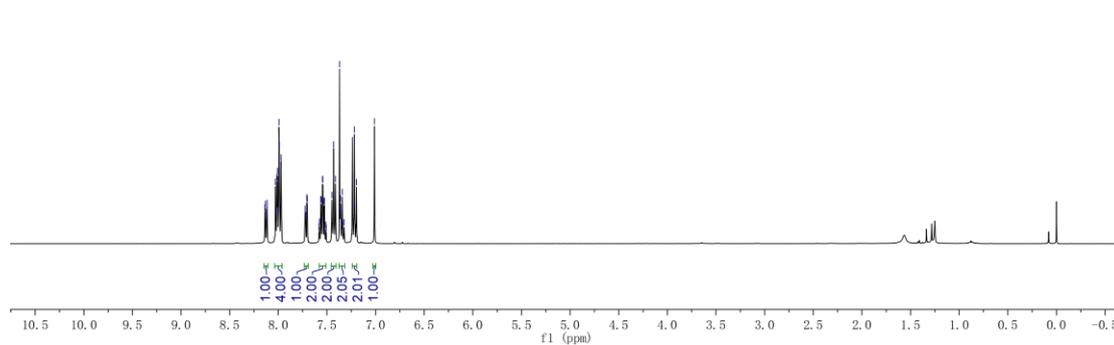


5-(4-fluorophenyl)-2-phenylpyrazolo[5,1-a]isoquinoline (2m)

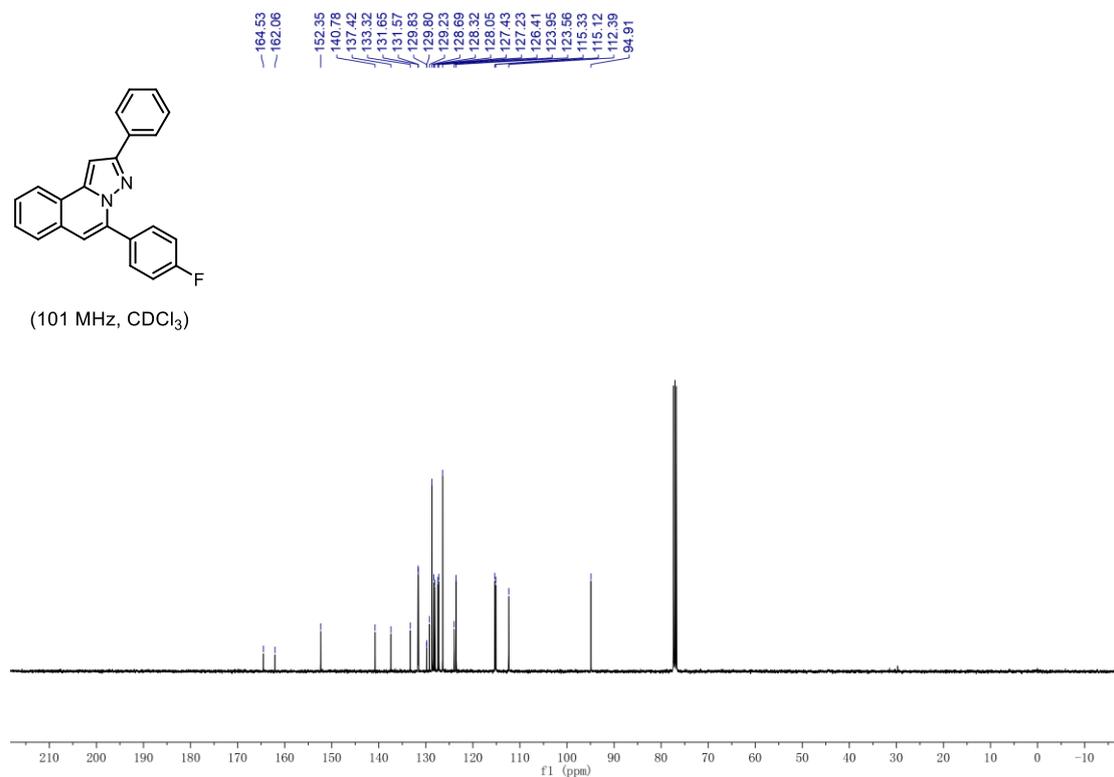
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7.01

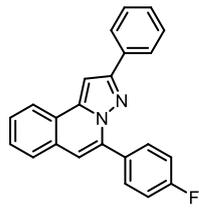


(400 MHz, CDCl₃)

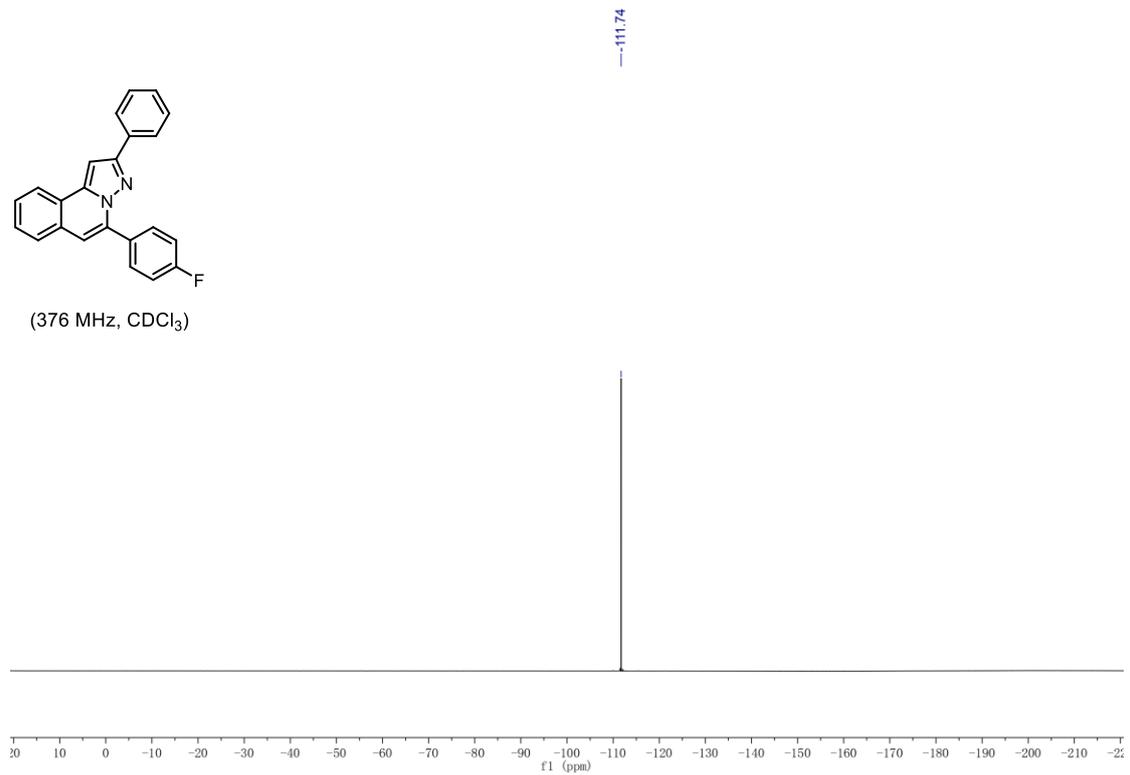


(101 MHz, CDCl₃)



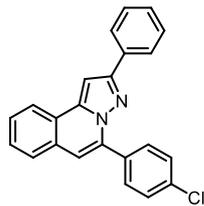


(376 MHz, CDCl₃)

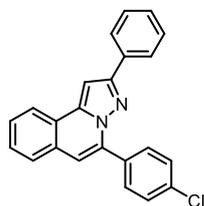
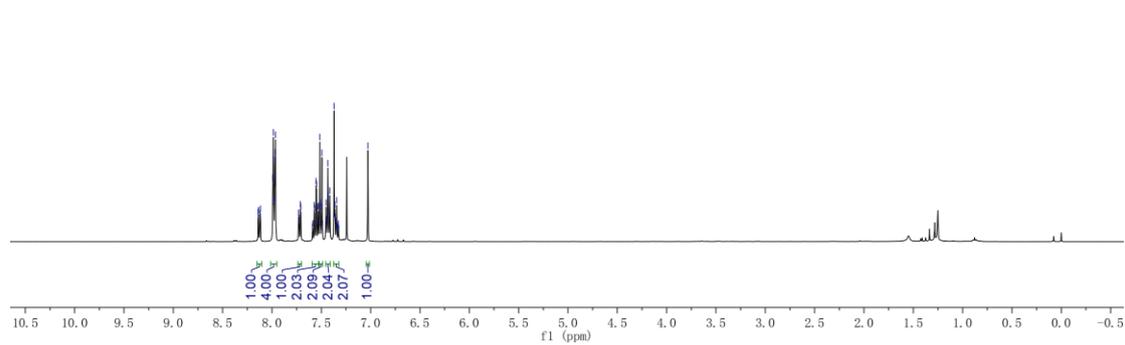


5-(4-chlorophenyl)-2-phenylpyrazolo[5,1-a]isoquinoline (2n)

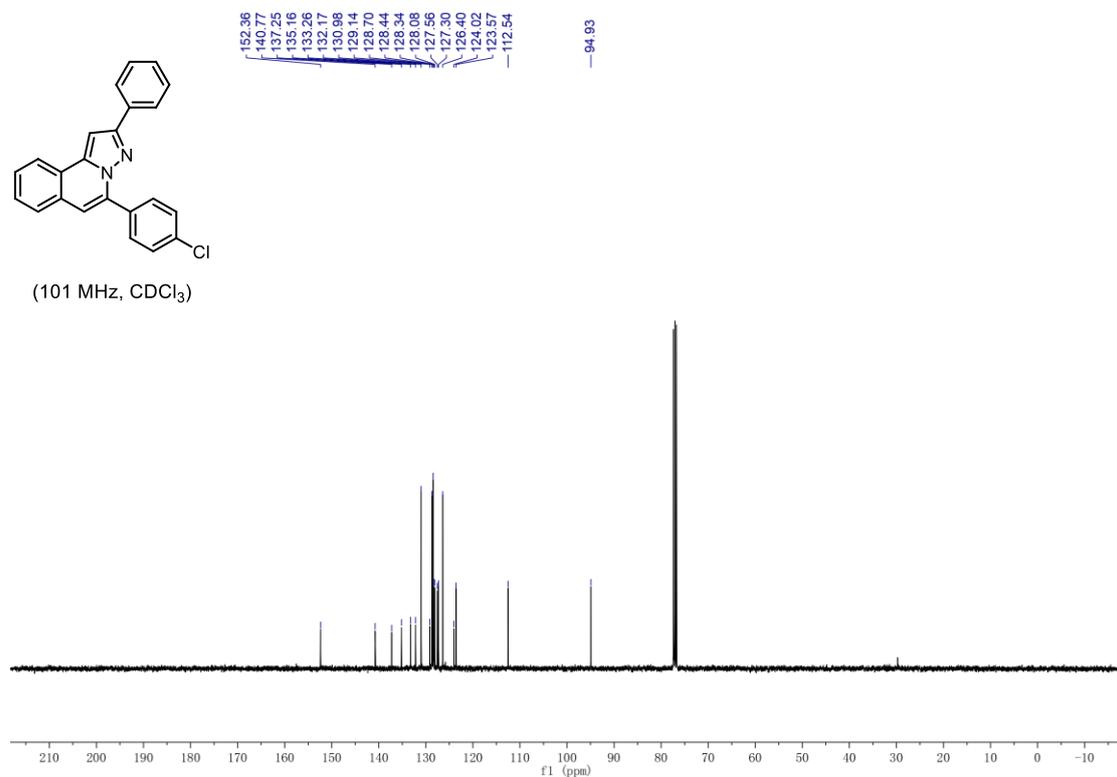
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8.12
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7.32
7.03



(400 MHz, CDCl₃)



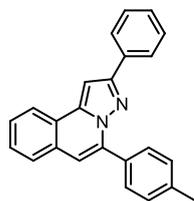
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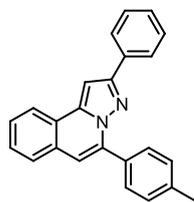
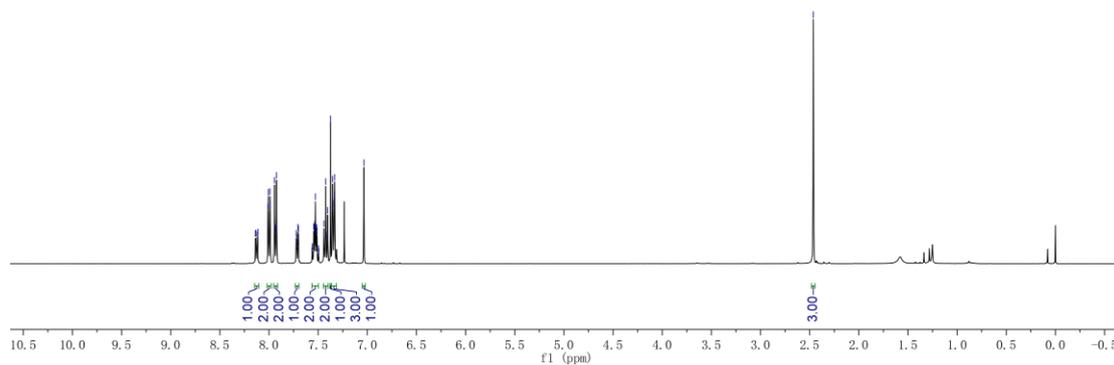
2-phenyl-5-(p-tolyl)pyrazolo[5,1-a]isoquinoline (2o)

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7.53
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7.51
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7.33
7.03

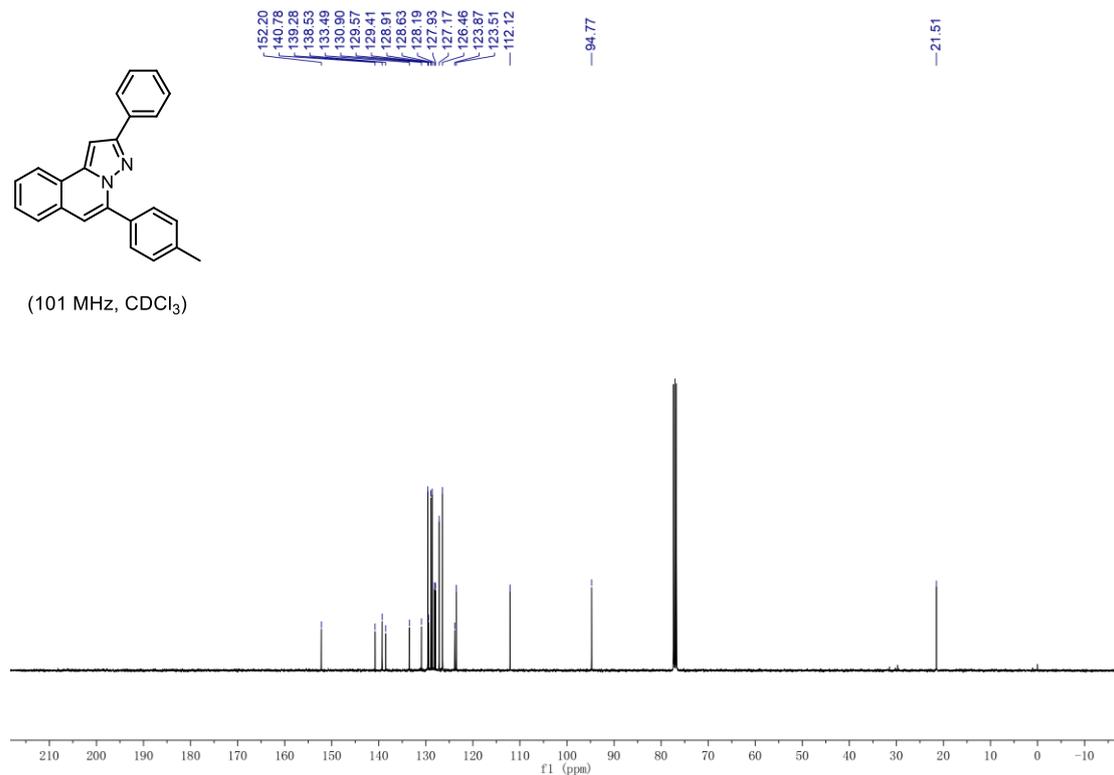
— 2.46



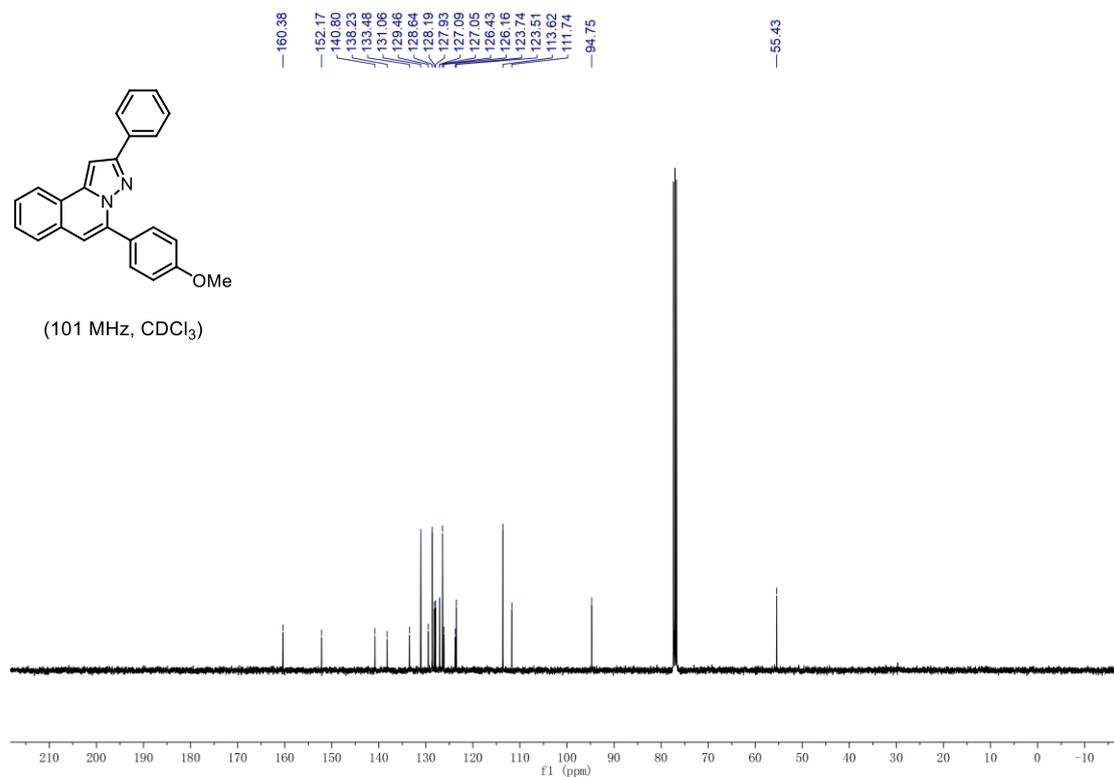
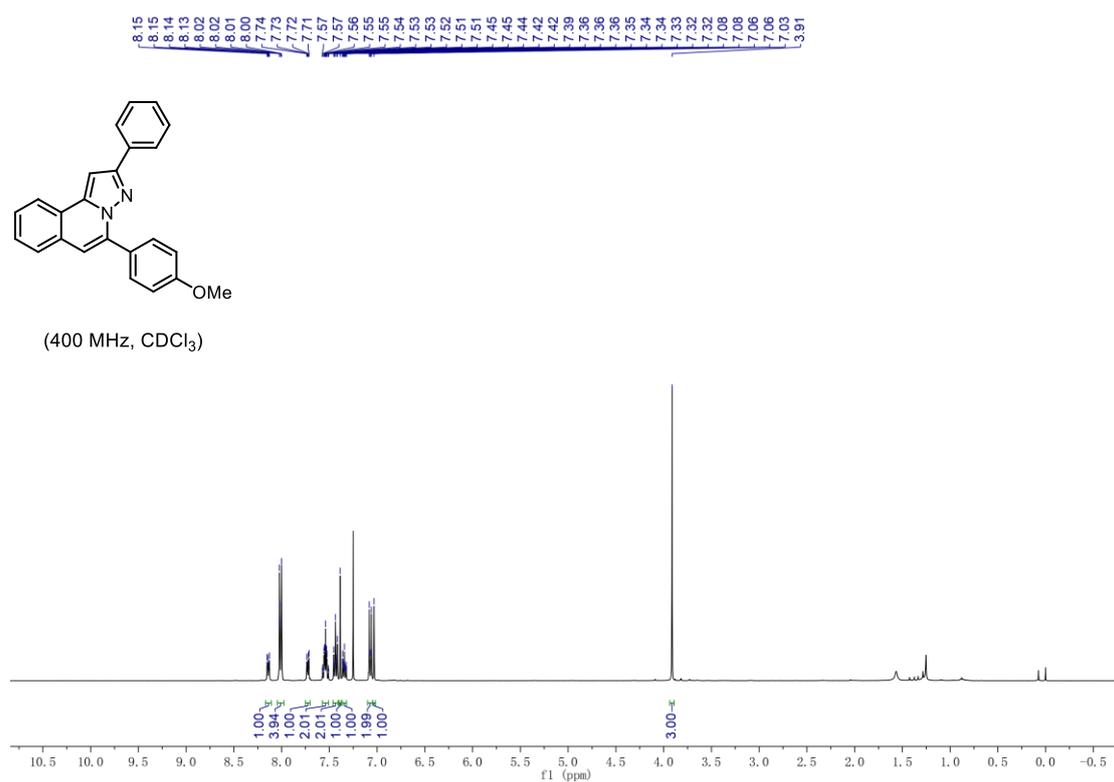
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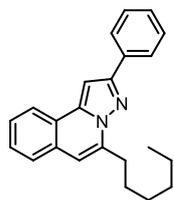
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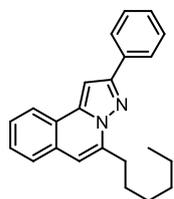
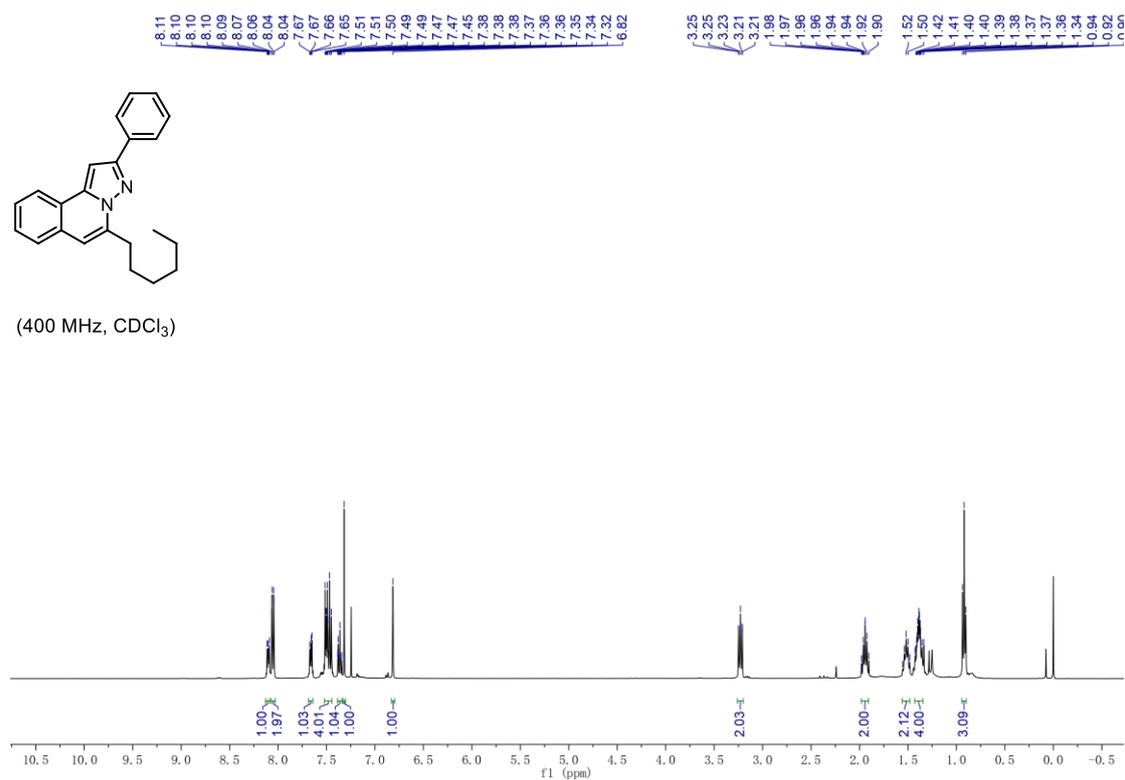
5-(4-methoxyphenyl)-2-phenylpyrazolo[5,1-a]isoquinoline (2p)



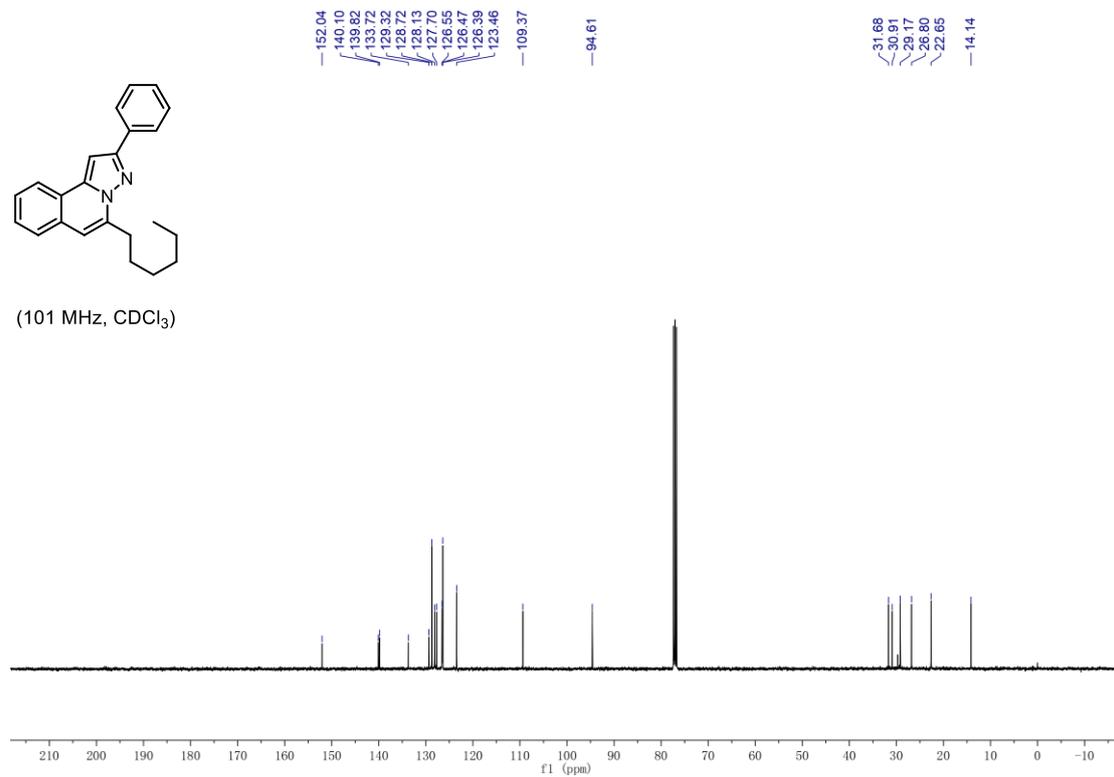
5-hexyl-2-phenylpyrazolo[5,1-a]isoquinoline (2q)



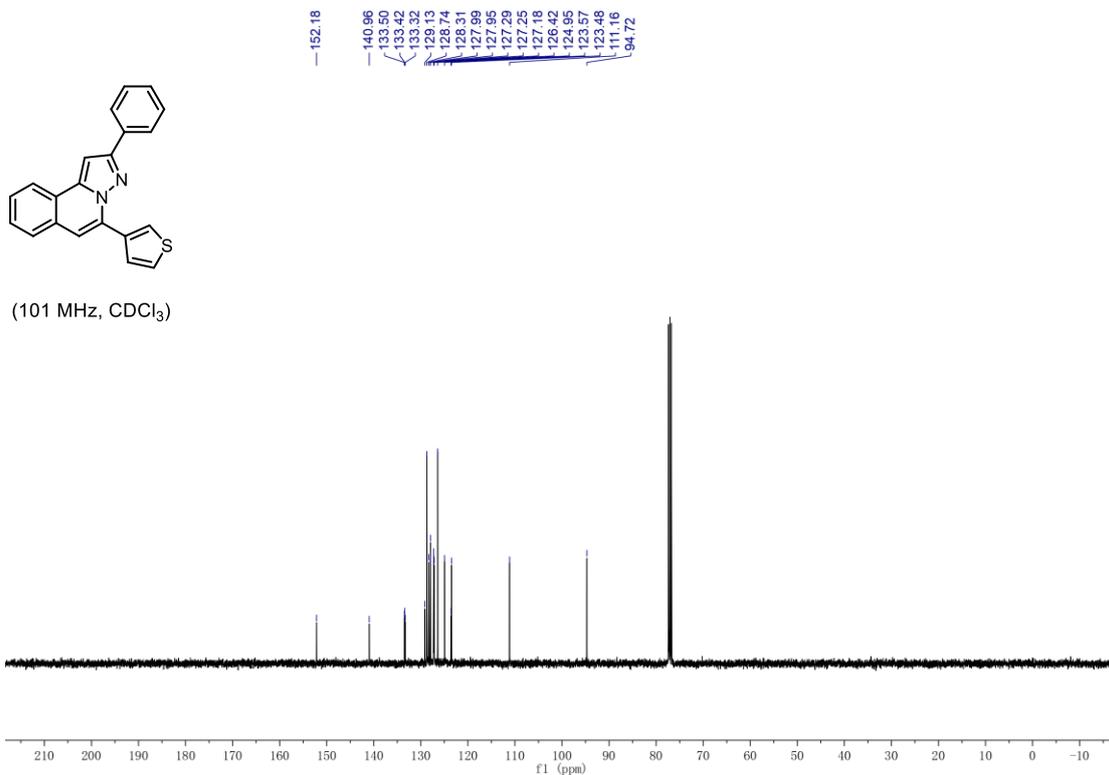
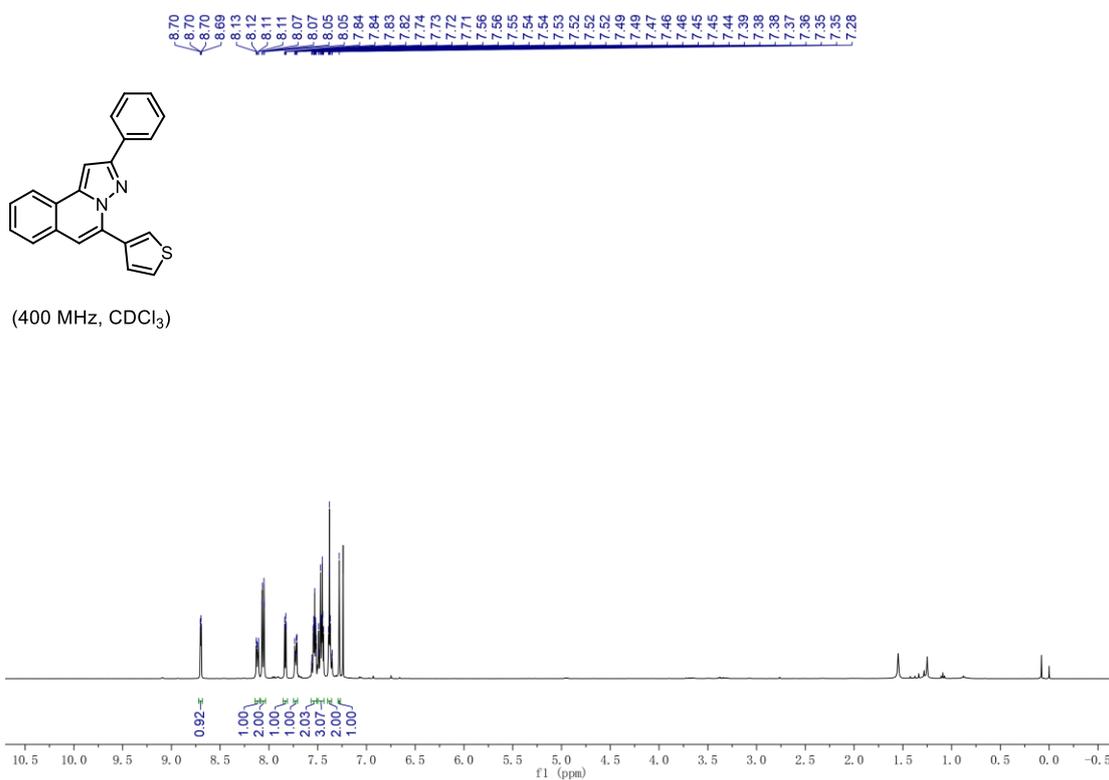
(400 MHz, CDCl₃)

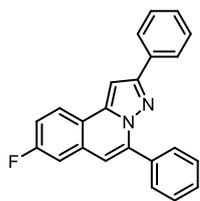


(101 MHz, CDCl₃)

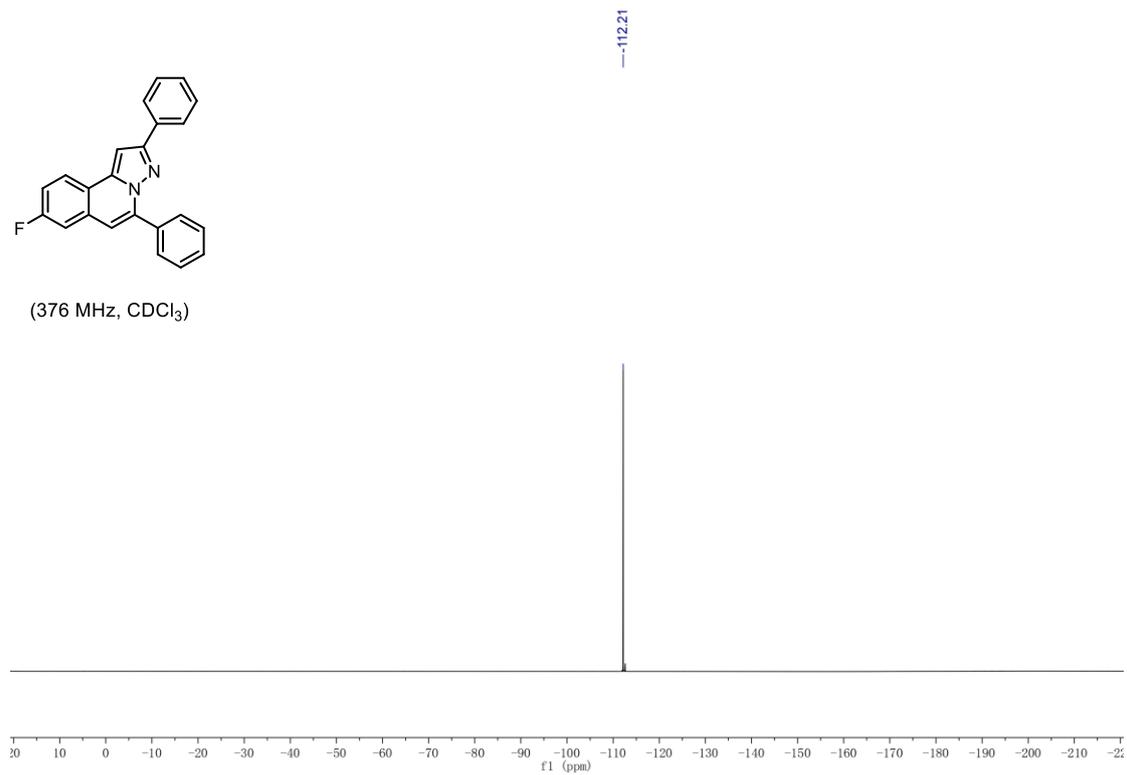


2-phenyl-5-(thiophen-3-yl)pyrazolo[5,1-a]isoquinoline (2r)

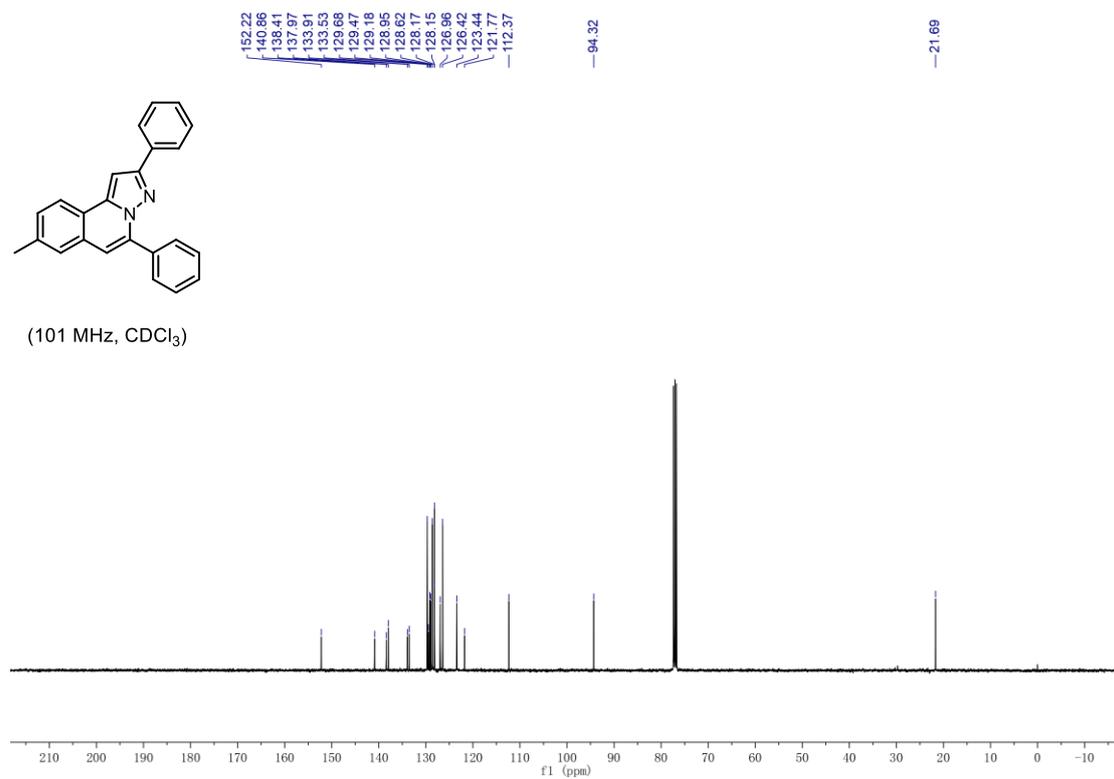
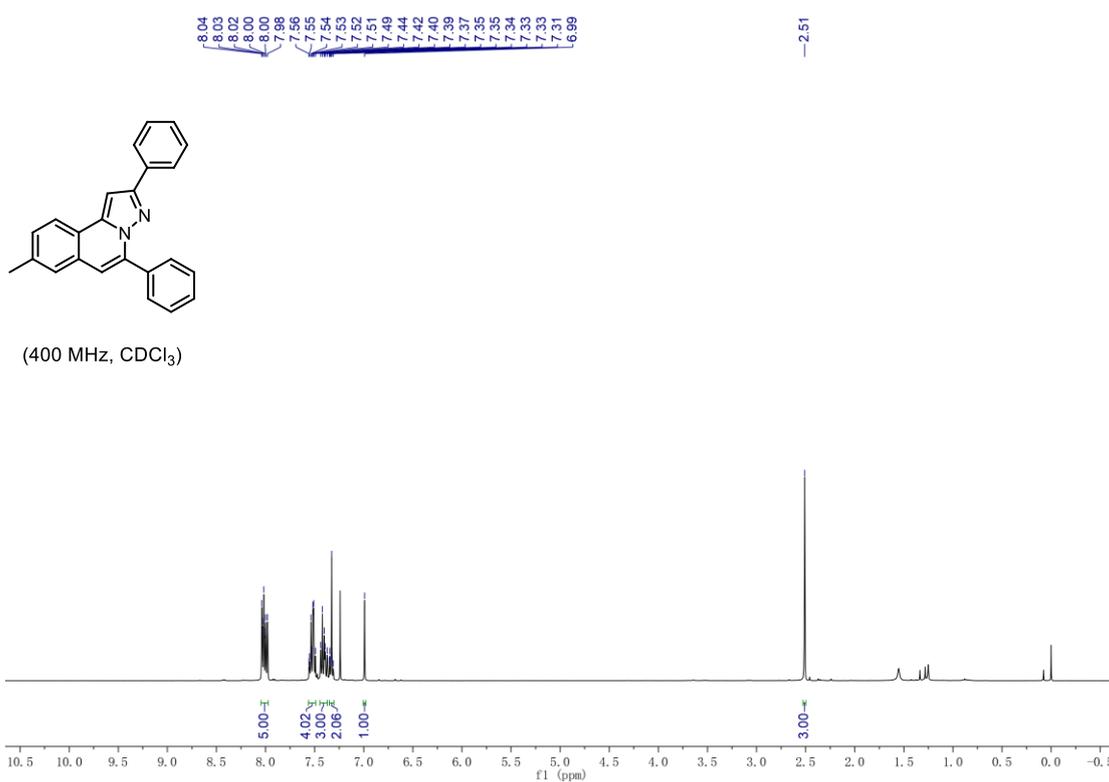




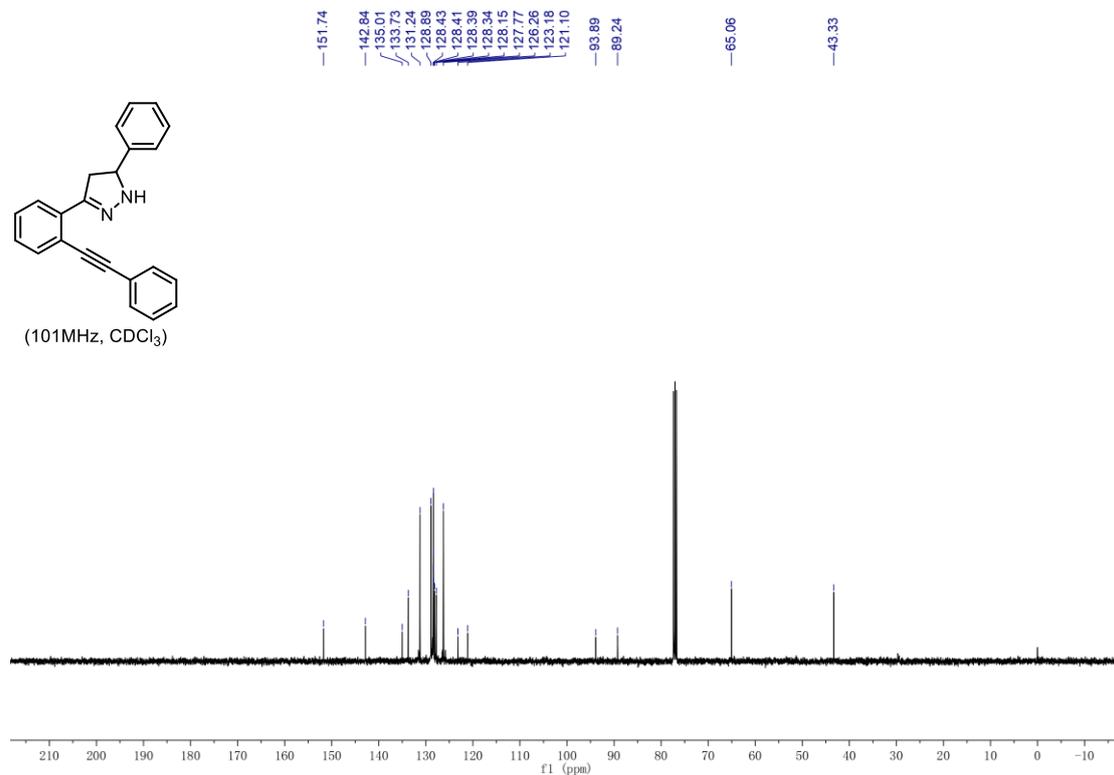
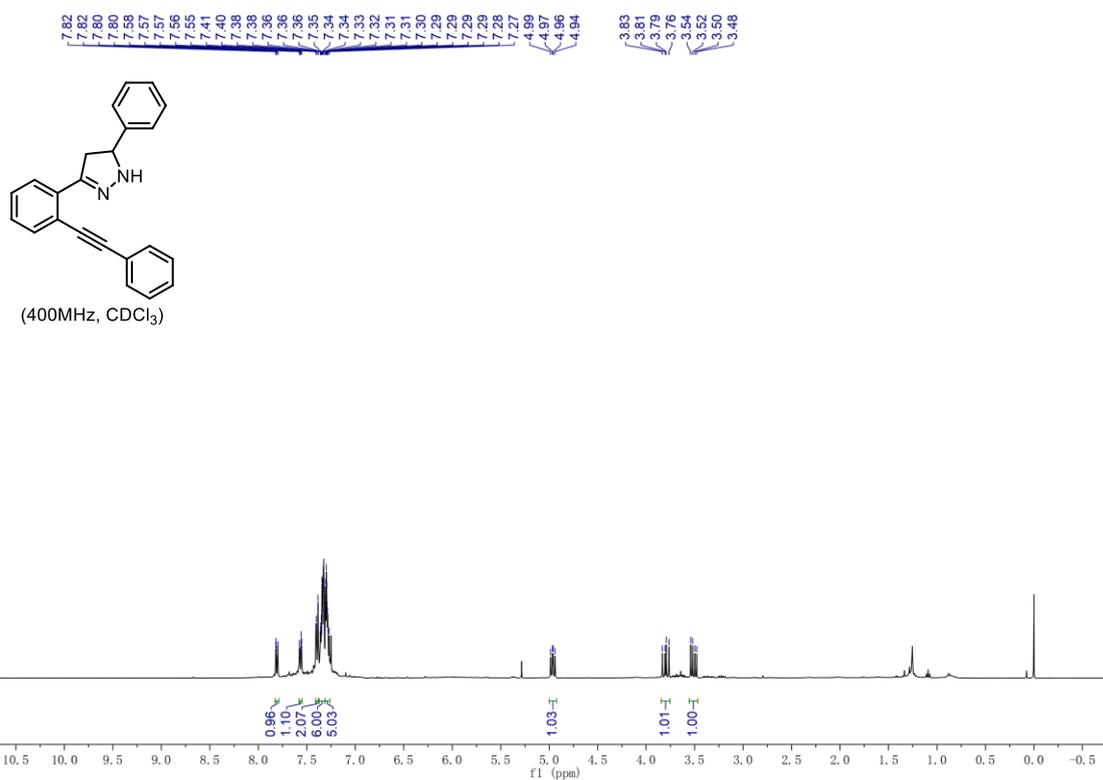
(376 MHz, CDCl₃)



8-methyl-2,5-diphenylpyrazolo[5,1-a]isoquinoline (2t)

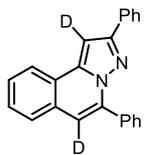


5-phenyl-3-(2-(phenylethynyl)phenyl)-4,5-dihydro-1H-pyrazole (3)

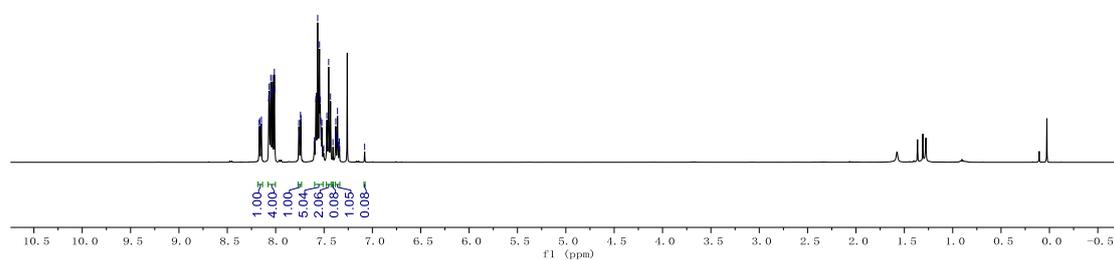


2,5-diphenylpyrazolo[5,1-a]isoquinoline-1,6-d₂ (4)

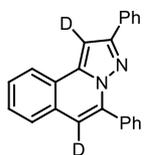
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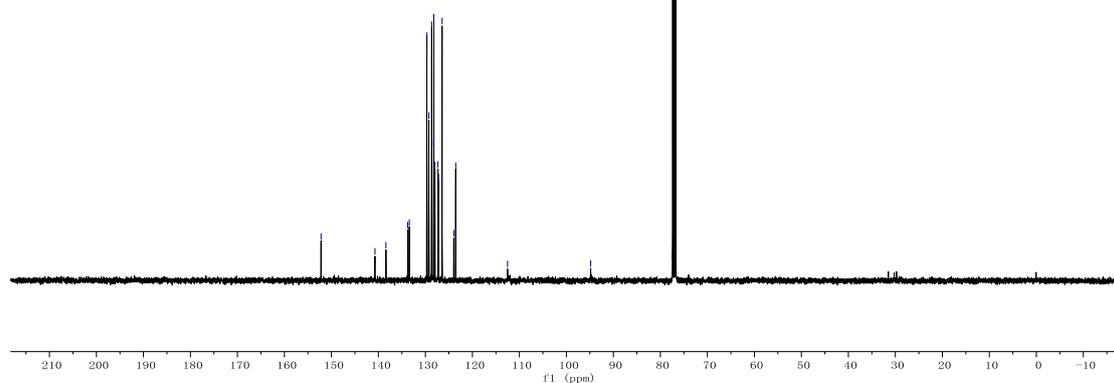
400 MHz, CDCl₃



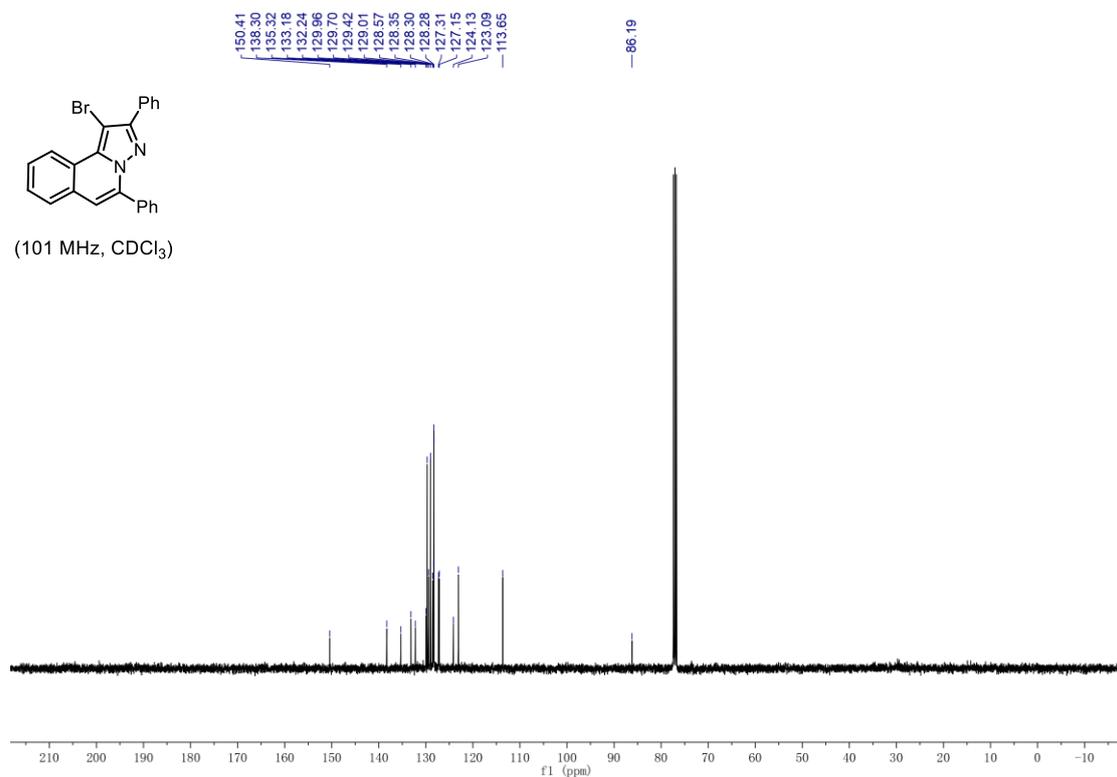
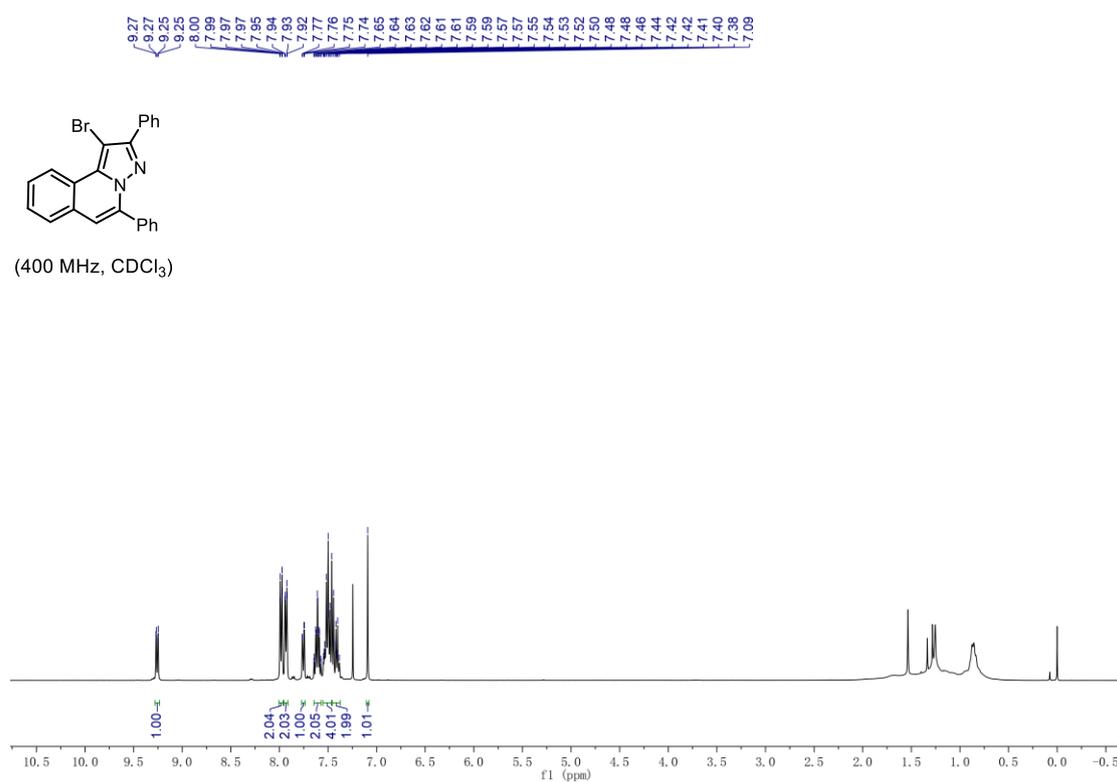
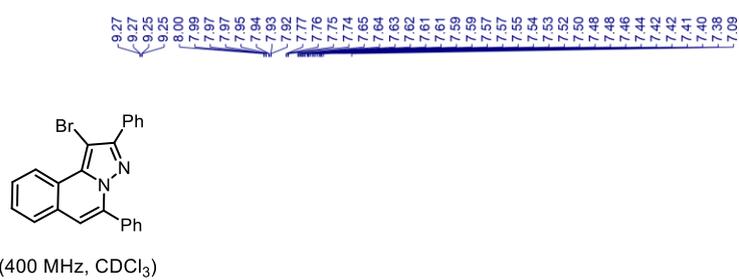
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94.83



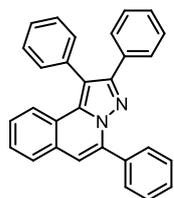
101 MHz, CDCl₃



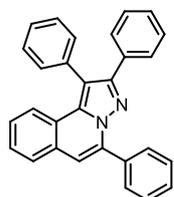
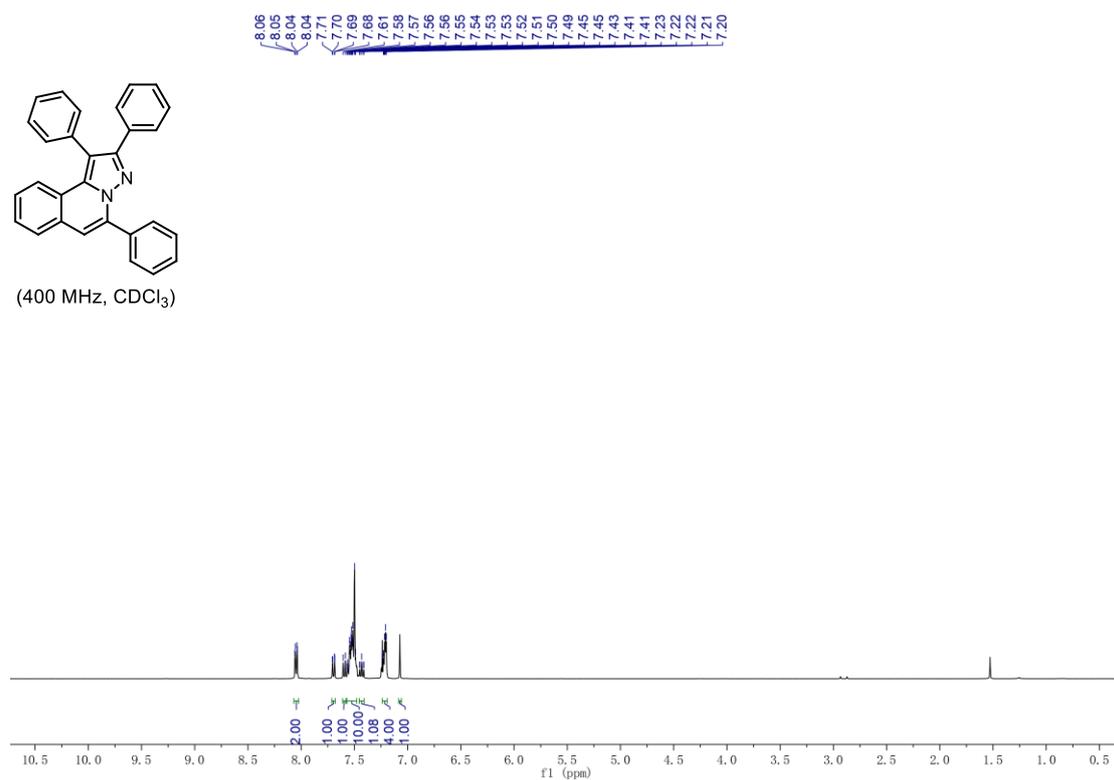
1-bromo-2,5-diphenylpyrazolo[5,1-a]isoquinoline (5)



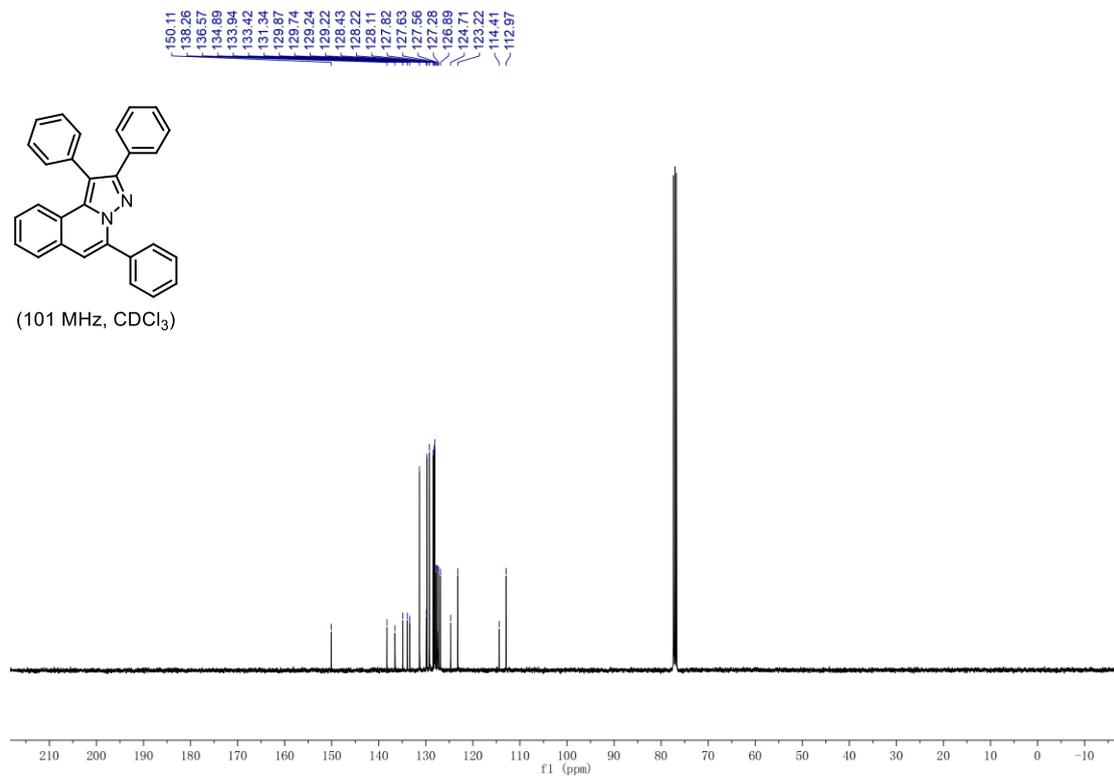
1,2,5-triphenylpyrazolo[5,1-a]isoquinoline (6)



(400 MHz, CDCl₃)



(101 MHz, CDCl₃)



5-phenyl-2-(4-(phenylethynyl)phenyl)pyrazolo[5,1-a]isoquinoline (7)

