Electronic Supplementary Material (ESI) for Green Chemistry.

Catalyst- and oxidant-free electrooxidative site-selective [3/4+2] annulation to fused polycyclic heteroaromatics

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Table of Contents

	Contents	Page
1	General Information	S2
2	General Material Information for Electrolysis Setup	S2
3	General Procedure for the Electrochemical Annulation	S3
4	Gram-Scale Synthesis of **3**	S3-S4
5	Mechanistic Studies	S4-S7
6	X-ray Crystallography Studies of Product **23**	S7-S8
7	Synthesis of Substrates	S8-S10
8	Characterization Data for Electrolysis Products	S10-S33
9	References	S34
10	NMR Spectra for Electrolysis Products and **50**	S35-S85

1、General Information

Commercially available reagents and solvents are of reagent grade quality without further purification. Flash column chromatography is performed using silicycle silica gel (200-300 mesh). Analytical thin-layer chromatography (TLC) is performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized using a UV lamp (254 nm). ^{1}H NMR and ^{13}C NMR are recorded on magnet system 400’54 ascend purchased from Bruker Biospin AG. HRMS (ESI) spectra are recorded on Agilent Q-TOF 6520.

Electrochemical oxidative [3+2] or [4+2] annulation was carried out in an undivided cell equipped with a carbon cloth anode and a platinum plate cathode under the open air. The carbon cloth, graphite rod (⌀ 6 mm) and platinum plate were purchased from Shanghai Jing Chong Electronic Technology Development Co., Ltd. Reticulated vitreous carbon (RVC) was purchased from Gaoss Union (Tianjin) Photoelectric Technology Co., Ltd. And, electrolysis was conducted under an AXIOMET AX3003P potentiostat in constant current mode. Cyclic voltammogram experiments were investigated using a Metrohm Autolab PGSTAT204 workstation and Nova 2.0 software.

2、General Material Information for Electrolysis setup

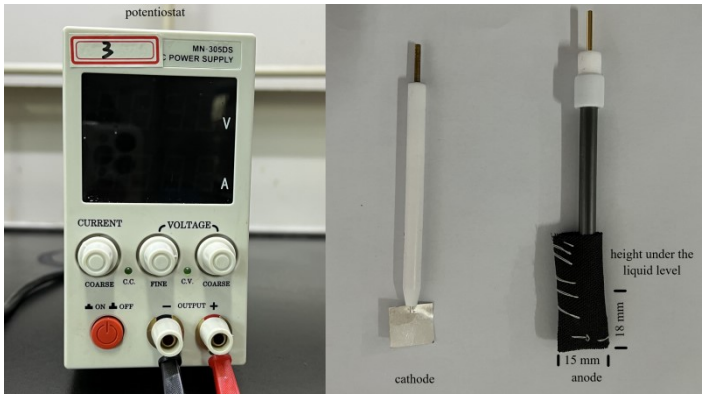
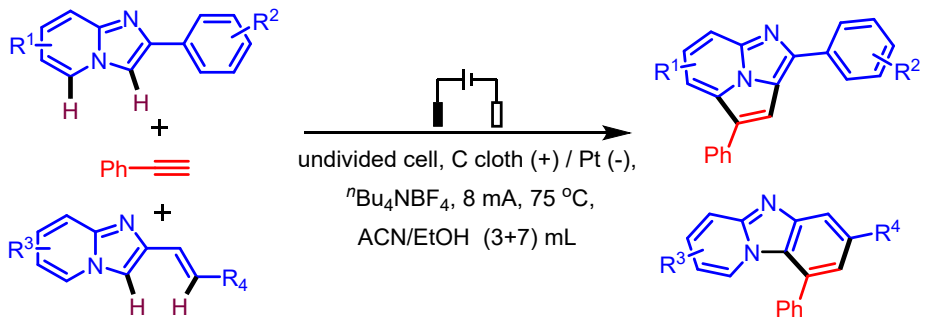


Figure S1 Picture of DIY electrolysis setup

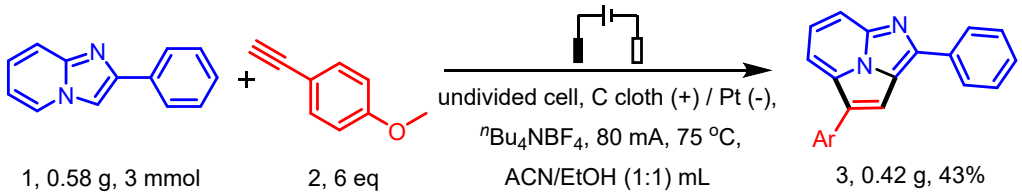
The DIY electrolysis setup used is shown in Fig. **S1**.

3、General Procedure for the Electrochemical Annulationlkynes



In an undivided cell equipped with a carbon cloth (35 mm x 15 mm) anode and a Pt (10 mm x 10 mm x 0.1 mm) cathode, imidazo[1,2-*a*]pyridine (0.2 mmol), ethynylbenzene (1.2 mmol), $^{n}Bu_4NBF_4$ (0.2 mmol, 65.8 mg) were dissolved in 3 mL ACN and 7 mL EtOH. The mixture above was stirred and electrolyzed at a constant current of 8 mA for 1.5-2 h under the open air. The reaction solution was diluted with ethyl acetate (50 mL) and washed with H_2O (50 mL). The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic separation (petroleum ether/ethyl acetate: 250/1 to 5/1) to obtain the desired product.

4、Gram-Scale Synthesis of 3



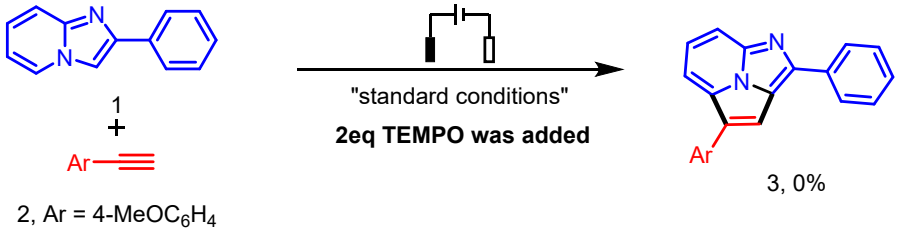
The imidazo[1,2-*a*]pyridine **1** (3 mmol, 0.58 g), $^{n}Bu_4NBF_4$ (2 mmol, 0.658 g), 1-ethynyl-4-methoxybenzene **2** (18 mmol, 2.38 g), ACN (50 mL) and EtOH (50 mL) was added in a 150 mL beaker, which was equipped with a stir bar, a carbon cloth (100 mm × 50 mm) anode and a platinum plate (20 mm × 20 mm × 0.1 mm) cathode. The solution was stirred and electrolyzed at a constant current of 80 mA for 4 h under the open air. The reaction solution was diluted with ethyl acetate (200 mL) and washed with brine (200 mL) and H_2O (200 mL). The separated organic

layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic separation (petroleum ether/ethyl acetate = 20/1, 0.42 g, 43%).

5、Mechanistic Studies

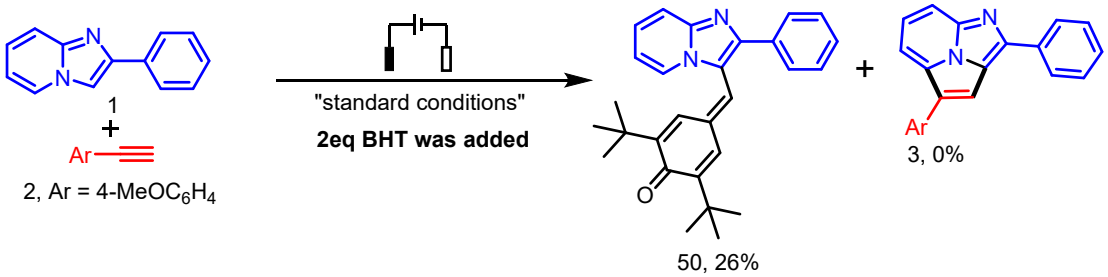
5-1、Radical-trapping experiments

5-1-1、TEMPO was added



In an undivided cell equipped with a carbon cloth (35 mm x 15 mm) anode and a Pt (10 mm x 10 mm x 0.1 mm) cathode, 2-phenylimidazo[1,2-*a*]pyridine **1** (0.2 mmol, 38.9 mg), 1-ethynyl-4-methoxybenzene **2** (1.2 mmol, 158.6 mg), $^{n}Bu_4NBF_4$ (0.2 mmol, 65.8 mg) and TEMPO (0.4 mmol, 62.5 mg) were dissolved in 3 mL ACN and 7 mL EtOH. The mixture above was stirred and electrolyzed at a constant current of 8 mA for 1.5 h under the open air. No desired product was detected.

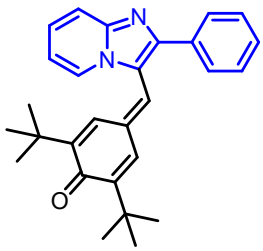
5-1-2、BHT was added



In an undivided cell equipped with a carbon cloth (35 mm x 15 mm) anode and a Pt (10 mm x 10 mm x 0.1 mm) cathode, 2-phenylimidazo[1,2-*a*]pyridine **1** (0.2 mmol, 38.9 mg), 1-ethynyl-4-methoxybenzene **2** (1.2 mmol, 158.6 mg), $^{n}Bu_4NBF_4$ (0.2 mmol, 65.8 mg) and BHT (0.4 mmol, 88.2 mg) were dissolved in 3 mL ACN and 7 mL EtOH. The mixture above was stirred and electrolyzed at a constant current of 8

mA for 2.5 h under the open air. No desired product was detected. Moreover, the corresponding radical trapping product **50** was generated.

The reaction solution was diluted with ethyl acetate (50 mL) and washed with brine (50 mL) and H_2O (50 mL). The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic separation (petroleum ether/ethyl acetate = 5/1) to obtain the radical trapping product **50** (21.4 mg, 26%).



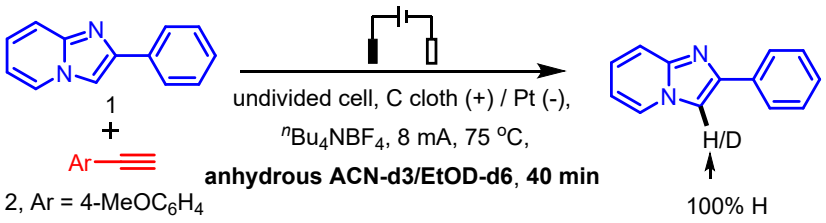
50

2,6-di-*tert*-butyl-4-((2-phenylimidazo[1,2-*a*]pyridin-3-yl)methylene)cyclohexa-2,5-dien-1-one (**50**):[1]

Orange oil; Eluent: petroleum ether/ethyl acetate 5:1; 21.4 mg, 26%;

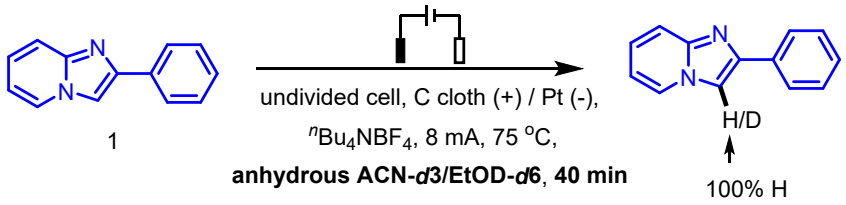
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 6.9 Hz, 1H), 7.81 (d, *J* = 7.0 Hz, 2H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.46 - 7.30 (m, 4H), 7.13 - 7.07 (m, 2H), 7.00 - 6.92 (m, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 1.35 (s, 9H), 0.95 (s, 9H); HRMS (ESI-TOF) Calcd for $C_{28}H_{31}N_2O$ $[M+H]^+$: 411.2431; found: 411.2422.

5-2、Isotope labeling experments:



In an undivided cell equipped with a carbon cloth (35 mm x 15 mm) anode and a Pt (10 mm x 10 mm x 0.1 mm) cathode, 2-phenylimidazo[1,2-*a*]pyridine **1** (0.2 mmol, 38.9 mg), 1-ethynyl-4-methoxybenzene **2** (1.2 mmol, 158.6 mg), ^{n}Bu$_4$NBF$_4$ (0.2

mmol, 65.8 mg) were dissolved in 3 mL CD_3CN-*d*3 and 7 mL EtOD-*d*6. The mixture above was stirred and electrolyzed at a constant current of 8 mA for 40 min under the N_2 atmosphere. No H/D change was detected.



In an undivided cell equipped with a carbon cloth (35 mm x 15 mm) anode and a Pt (10 mm x 10 mm x 0.1 mm) cathode, 2-phenylimidazo[1,2-*a*]pyridine **1** (0.2 mmol, 38.9 mg), ^{n}Bu$_4$NBF$_4$ (0.2 mmol, 65.8 mg) were dissolved in 3 mL CD_3CN-*d*3 and 7 mL EtOD-*d*6. The mixture above was stirred and electrolyzed at a constant current of 8 mA for 40 min under the N_2 atmosphere. No H/D change was detected.

5-3、Cyclic voltammetry experiments

The undivided cell was equipped with glassy-carbon disk working electrode (diameter, 3.0 mm) and Pt wire auxiliary electrode. The Ag/AgCl was used as reference electrode. The scan range was 0.0 V to 2 V. The scan rate was 100 mVs^{-1} (Fig. **S2**). ACN (3 mL) and EtOH (7 mL) containing ^{n}Bu$_4$NBF$_4$ (0.2 mmol, 65.8 mg) was poured into the electrochemical cell in all experiments.

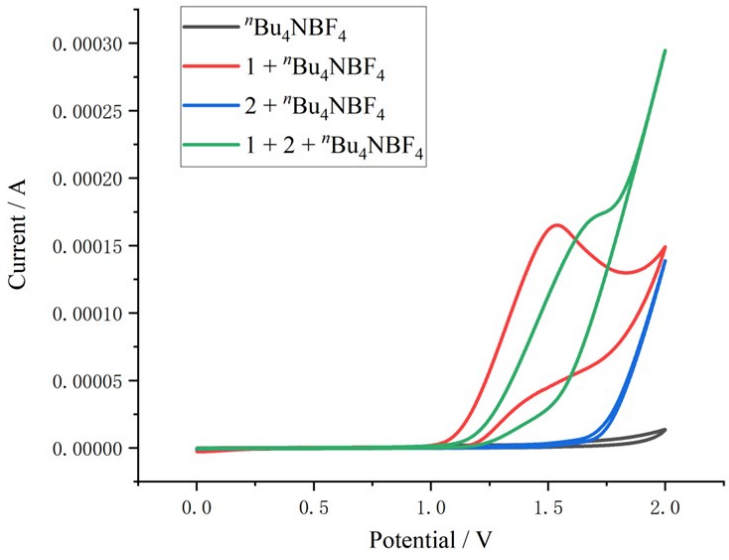


Figure S2 Cyclic voltammetry experiments of substrates

100 mVs-1: (black) blank; (red) 2-phenylimidazo[1,2-*a*]pyridine **1** (0.2 mmol, 38.9 mg); (blue) 1-ethynyl-4-methoxybenzene **2** (1.2 mmol, 158.6 mg); (green) 2-phenyl imidazo[1,2-a]pyridine **1** (0.2 mmol, 38.9 mg) and 1-ethynyl-4-methoxybenzene **2** (1.2 mmol, 158.6 mg).

6、X-ray Crystallography Studies of Product 23

Single crystal suitable for X-ray diffraction was obtained by slow evaporation of a saturated solution of compound **23** (cyclohexane/CH_2Cl_2) in a loosely capped vial.

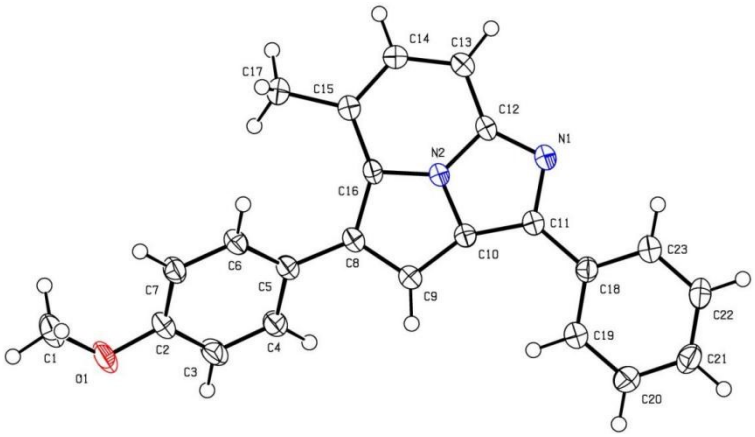


Figure S3 Structure of **23** by X-Ray crystallographic (CCDC = 2132237)

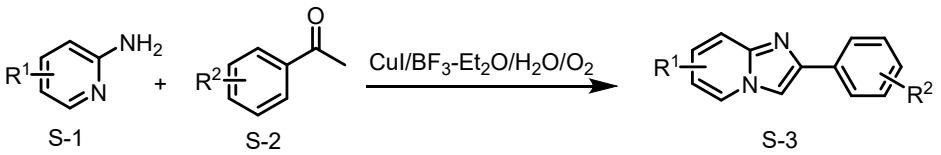
Table S1 Crystal data and structure refinement for **23**

Empirical formula	$C_{23}H_{18}N_2O$
Formula weight	338.39
Temperature/K	193
Crystal system	triclinic
Space group	P-1
a/Å	8.1325(4)
b/Å	9.3708(5)
c/Å	11.6459(7)
α/°	74.368(2)
β/°	81.158(2)

γ/°	83.467(2)
Volume/Å^3	842.08(8)
Z	2
ρcalcg/cm^3	1.335
μ/mm^{-1}	0.083
F(000)	356.0
Crystal size/mm^3	0.12 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.04 to 60.044
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 13, -14 ≤ l ≤ 16
Reflections collected	9842
Independent reflections	4853 [Rint = 0.0425, Rsigma = 0.0623]
Data/restraints/parameters	4853/0/237
Largest diff. peak/hole / e Å^{-3}	0.28/-0.21

7、Synthesis of Substrates

7-1

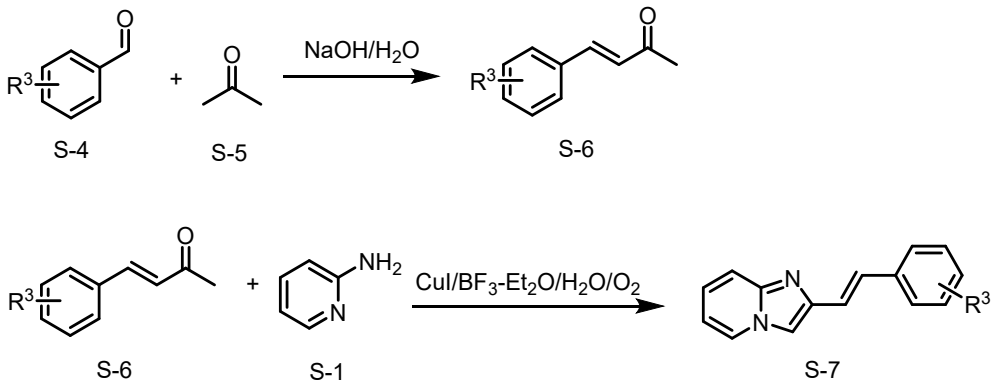


General procedure for the synthesis 2-phenylimidazo[1,2-*a*]pyridine (**S-3**):[2]

Substituted 2-aminopyridine (5 mmol, 1 eq), acetophenone (10 mmol, 2 eq), CuI (0.25 mmol, 5 mol%, 47 mg), $BF_3 \cdot Et_2O$ (0.5 mmol, 10 mol%, 70.96 mg) and H_2O (2 mL) was placed in an oven-dried round bottom flask equipped with a magnetic stir bar. The reaction mixture was stirred at 65 °C for 24 hours under O_2. After **S-1** was consumed, the reaction solution was diluted with ethyl acetate (150 mL) and washed

with brine (150 mL) and H_2O (150 mL). The separated organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to obtain a crude product, which was separated by column chromatography (eluent: petroleum ether = 3 : 1) to give the desired product **S-3**.

7-2



Step 1: General procedure for the synthesis of (*E*)-4-phenylbut-3-en-2-one (**S-6**):[3]

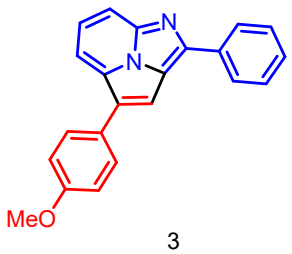
Substituted benzaldehyde (36 mmol, 1 eq), acetone (5 mL) and H_2O (5 mL) was placed in an oven-dried round bottom flask equipped with a magnetic stir bar, then add a 1% aqueous solution of sodium hydroxide (10 mL) slowly to the reaction mixture. The reaction mixture was stirred at 65 °C. After **S-6** was consumed, the reaction solution was diluted with ethyl acetate (150 mL) and washed with brine (150 mL) and H_2O (150 mL). The separated organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to obtain a crude product, which was separated by column chromatography (eluent: petroleum ether = 100 : 1) to give the desired product **S-6**.

Step 2: General procedure for the synthesis of substrates **S-7**:[2]

2-aminopyridine (5 mmol, 1 eq, 470 mg), (*E*)-4-phenylbut-3-en-2-one (10 mmol, 2 eq), CuI (0.25 mmol, 5 mol%, 47 mg), $BF_3 \cdot Et_2O$ (0.5 mmol, 10 mol%, 70.96 mg) and H_2O (2 mL) was placed in an oven-dried round bottom flask equipped with a magnetic stir bar. The reaction mixture was stirred at 65 °C for 24 hours under O_2. After **S-1** was consumed, the reaction solution was diluted with ethyl acetate (150 mL)

and washed with brine (150 mL) and H_2O (150 mL). The separated organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to obtain a crude product, which was separated by column chromatography (eluent: petroleum ether = 3 : 1) to give the desired product **S-7**.

8、Characterization Date for Electrolysis Products

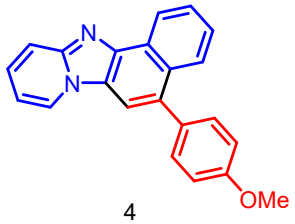


3

6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**3**):

Light yellow oil; Eluent:petroluem ether/ethyl acetate 25:1; 46.7 mg, 72%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (d, *J* = 7.1 Hz, 2H), 8.11 (d, *J* = 7.6 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.89 (s, 1H), 7.86 - 7.78 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.12 - 7.04 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.35, 149.35, 140.55, 134.06, 131.32, 130.89, 129.89, 129.21, 128.83, 128.25, 127.62, 126.96, 124.88, 114.83, 114.28, 113.63, 111.78, 55.55; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2O$ $[M+H]^+$: 325.1335; found: 325.1338.



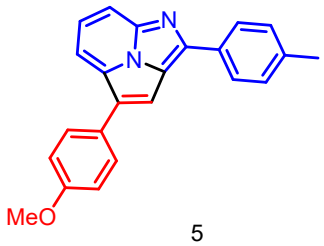
4

5-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**4**):

Brown solid; Eluent:petroluem ether/ethyl acetate 5:1; 20.8 mg, 8%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.94 (d, *J* = 8.1 Hz, 1H), 8.51 (d, *J* = 6.8 Hz, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 9.2 Hz, 1H), 7.84 (s, 1H), 7.76 - 7.70 (m,

1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.48 (dd, *J* = 9.0, 2.8 Hz, 3H), 7.16 -7.03 (m, 2H), 6.98 (t, *J* = 6.7 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.20, 146.86, 135.35, 133.30, 132.16, 131.53, 131.17, 130.11, 128.34, 127.97, 126.54, 126.32, 124.59, 123.86, 123.50, 117.75, 113.93, 111.95, 110.87, 55.54; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2O$ $[M+H]^+$: 325.1335; found: 325.1334.

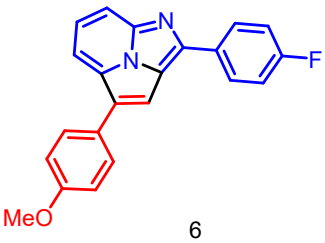


5

6-(4-methoxyphenyl)-1-(p-tolyl)imidazo[5,1,2-*cd*]indolizine (**5**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 55.5 mg, 82%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 7.8 Hz, 2H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.85 - 7.77 (m, 2H), 7.37 (d, *J* = 7.8 Hz, 2H), 7.11 - 7.03 (m, 2H), 3.90 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.31, 149.63, 140.58, 140.23, 131.27, 131.04, 130.77, 129.98, 128.83, 128.20, 127.72, 126.88, 124.71, 114.82, 114.26, 113.44, 111.42, 55.56, 21.70; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1429; found: 339.1500.



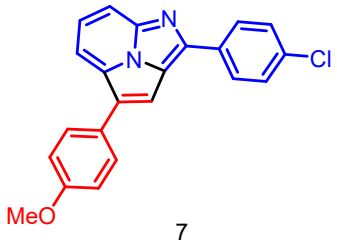
6

1-(4-fluorophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**6**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 40.4 mg, 59%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (t, *J* = 5.4 Hz, 2H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.89 (t, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 3H), 7.08 - 7.02 (m, 3H), 3.89 (s, 3H); ^{13}C NMR (101 MHz,

Chloroform-*d*) δ 165.10, 162.61, 159.35, 148.23, 140.48, 131.33, 130.83, 130.35, 129.99 (d, *J* = 9.1 Hz), 128.76, 127.50, 126.96, 124.51, 116.35, 116.13, 114.80, 113.92, 113.60, 111.68, 55.52; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -110.73; HRMS (EI-TOF) Calcd for $C_{22}H_{16}FN_2O$ $[M+H]^+$: 343.1241; found: 343.1250.

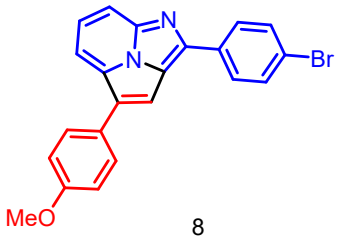


7

1-(4-chlorophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**7**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 55.3 mg, 77%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 - 8.26 (m, 2H), 8.10 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.83 (s, 1H), 7.80 (d, *J* = 8.7 Hz, 2H), 7.55 - 7.48 (m, 2H), 7.12 - 7.03 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.48, 147.75, 140.37, 135.84, 132.48, 131.79, 131.03, 129.47, 129.35, 128.87, 127.41, 127.28, 124.73, 114.87, 114.06, 113.91, 112.00, 55.57; HRMS (EI-TOF) Calcd for $C_{22}H_{16}ClN_2O$ $[M+H]^+$: 359.0946; found: 359.0953.



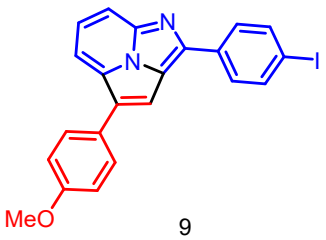
8

1-(4-bromophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**8**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 54.4 mg, 67%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.5 Hz, 2H), 8.12 (d, *J* = 7.6 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.96 (t, *J* = 7.8 Hz, 1H), 7.85 (s, 1H), 7.83 - 7.79 (m, 2H), 7.72 - 7.65 (m, 2H), 7.12 - 7.04 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.50, 147.83, 140.41, 132.97, 132.44, 131.84, 131.08, 129.60, 128.90, 127.43, 127.30, 124.77, 124.21, 114.89, 114.10, 113.95, 112.05, 55.59;

HRMS (EI-TOF) Calcd for $C_{22}H_{16}BrN_2O$ $[M+H]^+$: 403.0441; found: 403.0438

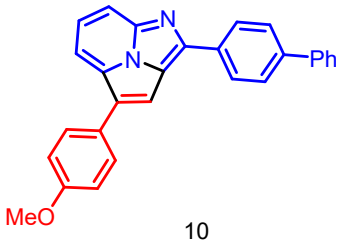


9

1-(4-iodophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**9**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 79.25 mg, 88%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 - 8.10 (m, 2H), 8.09 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.83 (s, 1H), 7.82 - 7.77 (m, 2H), 7.11 - 7.04 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.50, 147.89, 140.36, 138.37, 133.49, 131.84, 131.07, 129.68, 128.89, 127.41, 127.31, 124.78, 114.88, 114.08, 113.98, 112.07, 96.14, 55.59; HRMS (EI-TOF) Calcd for $C_{22}H_{16}IN_2O$ $[M+H]^+$: 451.0302; found: 451.0292.

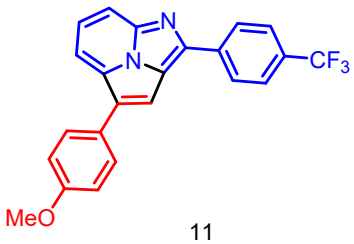


10

1-([1,1'-biphenyl]-4-yl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**10**):

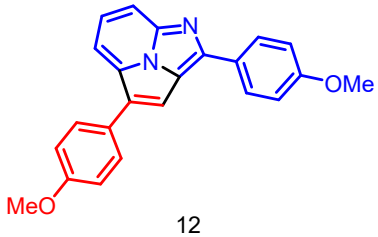
Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 44.85 mg, 56%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 6.9 Hz, 2H), 8.10 (d, *J* = 6.4 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.99 - 7.92 (m, 1H), 7.91 (s, 1H), 7.85 - 7.77 (m, 4H), 7.70 (d, *J* = 5.5 Hz, 2H), 7.54 - 7.44 (m, 2H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.11 - 7.05 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.44, 148.57, 142.66, 140.51, 140.35, 132.70, 131.60, 130.94, 129.05, 128.87, 128.69, 127.89, 127.76, 127.52, 127.23, 124.85, 114.86, 114.31, 113.76, 111.66, 55.57; HRMS (EI-TOF) Calcd for $C_{28}H_{21}N_2O$ $[M+H]^+$: 401.1648; found: 401.1676.



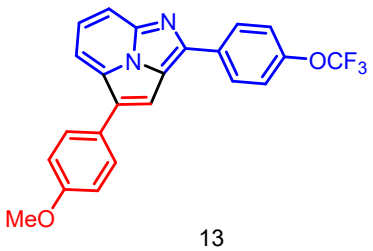
11

6-(4-methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)imidazo[5,1,2-*cd*]indolizine (**11**): Yellow solid; Eluent:petroluem ether/ethyl acetate 20:1; 42.4 mg, 54%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 (d, *J* = 8.0 Hz, 2H), 8.14 (d, *J* = 7.6 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.99 (t, *J* = 7.8 Hz, 1H), 7.88 (s, 1H), 7.85 - 7.78 (m, 4H), 7.13 - 7.06 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.64, 146.80, 137.29, 132.51, 131.32, 128.95, 128.32, 127.61, 127.21, 126.18 (q, *J* = 4.1 Hz), 125.16, 114.93, 114.34, 114.15, 112.63, 55.59; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.64; HRMS (EI-TOF) Calcd for $C_{23}H_{16}F_3N_2O$ $[M+H]^+$: 393.1209; found: 393.1210.



12

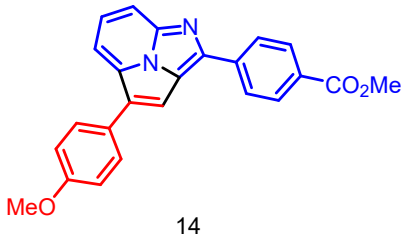
3-methoxy-5-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**12**): Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 34.75 mg, 49%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (d, *J* = 8.8 Hz, 2H), 8.07 (d, *J* = 7.5 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.85 (s, 1H), 7.83 - 7.78 (m, 2H), 7.08 (t, *J* = 8.3 Hz, 4H), 3.91 (s, 3H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.28, 159.28, 149.54, 140.66, 132.30, 130.79, 130.64, 129.78, 129.02, 128.80, 127.79, 126.83, 126.74, 124.39, 114.82, 114.71, 114.10, 113.24, 110.98, 55.57; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O_2$ $[M+H]^+$: 355.1441; found: 355.1446.



13

6-(4-methoxyphenyl)-1-(4-(trifluoromethoxy)phenyl)imidazo[5,1,2-*cd*]indolizine (**13**): Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 46.5 mg, 57%;

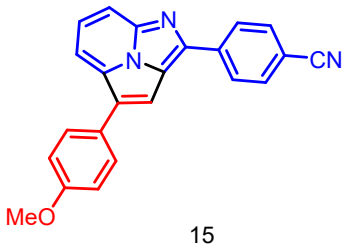
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 - 8.38 (m, 2H), 8.12 (d, *J* = 7.6 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.96 (t, *J* = 7.8 Hz, 1H), 7.85 (s, 1H), 7.84 - 7.78 (m, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.12 - 7.05 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.51, 150.31, 147.54, 140.45, 132.75, 131.89, 131.10, 129.63, 128.90, 127.34 (d, *J* = 14.2 Hz), 124.79, 121.93, 121.56, 114.89, 114.04, 113.96, 112.14, 55.58; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.60; HRMS (EI-TOF) Calcd for $C_{23}H_{16}F_3N_2O_2$ $[M+H]^+$: 409.1158; found: 409.1156.



14

methyl 4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzoate (**14**): Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 42.9 mg, 56%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 8.1 Hz, 2H), 8.21 (d, *J* = 8.0 Hz, 2H), 8.14 (d, *J* = 7.5 Hz, 1H), 8.08 (d, 1H), 7.99 (t, *J* = 7.8 Hz, 1H), 7.90 (s, 1H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 3.97 (s, 3H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.87, 159.63, 146.94, 140.11, 137.87, 132.57, 131.31, 130.96, 130.48, 128.95, 128.00, 127.72, 127.18, 126.40, 125.25, 114.92, 114.36, 112.51, 55.58, 52.42; HRMS (EI-TOF) Calcd for $C_{24}H_{19}N_2O_3$ $[M+H]^+$: 383.139; found: 383.1394.

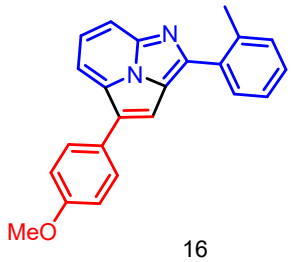


15

4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzonitrile (**15**):

Orange solid; Eluent: petroluem ether/ethyl acetate 15:1; 58.0 mg, 83%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (d, *J* = 8.3 Hz, 2H), 8.15 (d, *J* = 7.5 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.99 (t, *J* = 7.8 Hz, 1H), 7.85 (s, 1H), 7.81 (dd, *J* = 8.6, 1.8 Hz, 4H), 7.12 - 7.06 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.69, 146.18, 140.43, 138.38, 132.90, 132.79, 131.42, 128.95, 128.38, 127.71, 127.10, 125.43, 118.93, 114.95, 114.57, 113.97, 113.04, 112.67, 55.59; HRMS (EI-TOF) Calcd for $C_{23}H_{16}N_3O$ $[M+H]^+$: 372.1107; found: 372.1123.

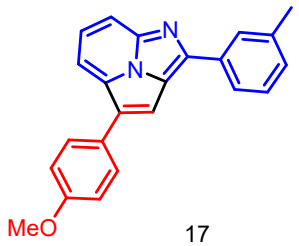


16

6-(4-methoxyphenyl)-1-(*o*-tolyl)imidazo[5,1,2-*cd*]indolizine (**16**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 31.2 mg, 23%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 6.9 Hz, 1H), 7.96 (d, *J* = 9.3 Hz, 1H), 7.87 (d, *J* = 8.9 Hz, 2H), 7.51 (d, *J* = 7.0 Hz, 1H), 7.50 - 7.45 (m, 2H), 7.45 - 7.40 (m, 2H), 7.10 - 7.03 (m, 2H), 6.96 (t, *J* = 6.8 Hz, 1H), 3.92 (s, 3H), 3.43 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.13, 146.17, 136.52, 135.65, 134.19, 132.34, 131.60, 128.83, 127.26, 126.28, 125.40, 124.81, 124.11, 118.41, 113.88, 111.52, 110.97, 55.55, 24.38; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1492; found: 339.1492.

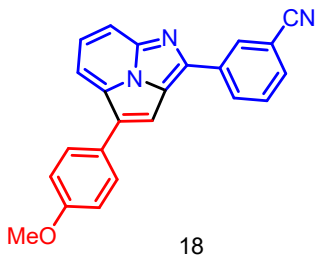


17

6-(4-methoxyphenyl)-1-(*m*-tolyl)imidazo[5,1,2-*cd*]indolizine (**17**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 48.8 mg, 72%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.96 (t, *J* = 7.8 Hz, 1H), 7.91 (s, 1H), 7.86 - 7.80 (m, 2H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.13 - 7.05 (m, 2H), 3.91 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.43, 140.30, 139.04, 131.52, 130.96, 130.91, 129.16, 128.90, 128.80, 127.59, 127.18, 125.60, 124.81, 114.87, 114.49, 113.72, 111.66, 55.58, 21.66; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1492; found: 339.1500.

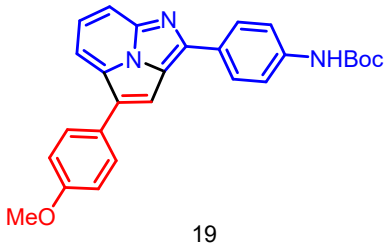


18

3-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzonitrile(**18**):

Orange solid; Eluent: petroluem ether/ethyl acetate 15:1; 47.6 mg, 68%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 - 8.58 (m, 2H), 8.16 (d, *J* = 7.5 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 8.00 (t, *J* = 7.8 Hz, 1H), 7.88 (s, 1H), 7.86 - 7.79 (m, 2H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.13 - 7.05 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.66, 140.31, 135.41, 132.72, 132.64, 132.05, 131.52, 131.37, 130.08, 128.94, 127.66, 127.13, 124.91, 118.72, 114.94, 114.46, 113.90, 113.52, 112.77, 55.59; HRMS (EI-TOF) Calcd for $C_{23}H_{16}N_3O$ $[M+H]^+$: 350.1288; found: 350.1292.

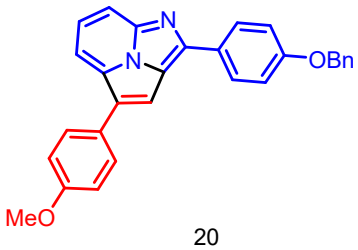


19

tert-butyl(4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)phenyl)carbamate (**19**)

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 34.3 mg, 39%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (d, *J* = 6.1 Hz, 2H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.97 (d, *J* = 22.1 Hz, 2H), 7.85 (s, 1H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.58 (s, 2H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.81 (s, 1H), 3.90 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.40, 152.63, 148.39, 140.34, 140.03, 131.44, 130.81, 129.22, 128.85, 128.05, 127.49, 127.33, 124.28, 118.80, 114.85, 114.32, 113.61, 111.16, 81.13, 55.56, 28.47; HRMS (EI-TOF) Calcd for $C_{27}H_{26}N_3O_3$ $[M+H]^+$: 440.1969; found: 440.1961.

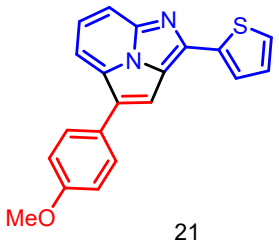


20

1-(4-(benzyloxy)phenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**20**)

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 38.8 mg, 45%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (s, 2H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.93 (d, *J* = 7.1 Hz, 1H), 7.79 (t, J = 10.6 Hz, 3H), 7.44 (d, J = 19.6 Hz, 4H), 7.36 (d, J = 7.3 Hz, 1H), 7.13 (d, *J* = 7.7 Hz, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 5.15 (s, 2H), 3.89 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.72, 159.47, 147.71, 139.36, 136.63, 131.72, 130.80, 129.99, 128.81, 128.29, 127.68, 127.26, 125.66, 123.81, 115.68, 114.85, 114.43, 113.73, 110.81, 70.28, 55.55; HRMS (EI-TOF) Calcd for $C_{29}H_{23}N_2O_2$ $[M+H]^+$: 431.1754; found: 431.1754.

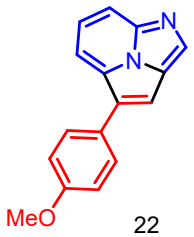


21

6-(4-methoxyphenyl)-1-(thiophen-2-yl)imidazo[5,1,2-*cd*]indolizine (**21**)

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 59.5 mg, 45%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 7.5 Hz, 1H), 8.01 - 7.95 (m, 2H), 7.92 (t, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 9.1 Hz, 3H), 7.53 (d, *J* = 5.0 Hz, 1H), 7.27 - 7.21 (m, 1H), 7.11 - 7.04 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.42, 140.42, 131.34, 130.93, 129.05, 128.86, 128.66, 128.60, 128.05, 127.55, 127.27, 123.98, 117.34, 114.86, 113.75, 113.29, 111.49, 55.57; HRMS (EI-TOF) Calcd for $C_{20}H_{15}N_2O_S$ $[M+H]^+$: 331.09; found: 331.0894.

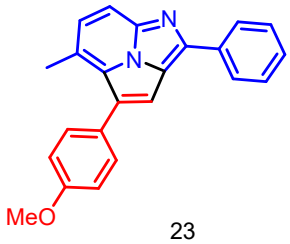


22

6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**22**)

Light yellow oil; Eluent: petroluem ether/ethyl acetate 10:1; 41.3 mg, 83%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 (s, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 8.1 Hz, 1H), 8.00 (t, *J* = 7.9 Hz, 1H), 7.84 - 7.76 (m, 2H), 7.73 (s, 1H), 7.12 - 7.04 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.41, 137.43, 133.12, 131.67, 131.36, 128.93, 127.58, 126.45, 114.85, 114.16, 113.87, 112.78, 55.57; HRMS (EI-TOF) Calcd for $C_{16}H_{13}N_2O$ $[M+H]^+$: 249.1022; found: 249.1022.

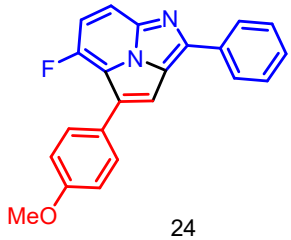


23

6-(4-methoxyphenyl)-5-methyl-1-phenylimidazo[5,1,2-*cd*]indolizine (**23**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 62.3 mg, 92%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 7.0 Hz, 2H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.63 (s, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.56 - 7.49 (m, 4H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.05 - 6.97 (m, 2H), 3.87 (s, 3H), 2.66 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.29, 148.32, 139.21, 134.28, 132.42, 131.23, 129.49, 129.46, 129.37, 129.07, 127.94, 127.88, 125.61, 124.55, 116.49, 113.86, 111.50, 55.42, 18.46; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1492; found: 399.1492.

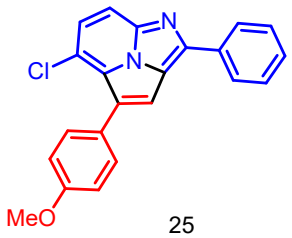


24

5-fluoro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**24**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 60:1; 58.9 mg, 86%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 6.9 Hz, 2H), 7.92 (dd, *J* = 8.5, 3.0 Hz, 1H), 7.86 - 7.79 (m, 3H), 7.66 (dd, *J* = 11.4, 8.5 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.09 - 7.02 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.54, 152.84, 150.53 (d, *J* = 5.1 Hz), 150.35, 138.02, 133.85, 131.16 (d, *J* = 5.1 Hz), 130.04, 129.67 (d, *J* = 4.1 Hz), 129.26, 128.09, 126.54 (d, *J* = 3.1 Hz), 119.10, 118.80, 115.13, 114.89, 114.54, 114.31 (d, *J* = 3.1 Hz), 112.12 (d, *J* = 8.1 Hz), 55.53; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -124.01; HRMS (EI-TOF) Calcd for $C_{22}H_{16}FN_2O$ $[M+H]^+$: 343.1241; found: 343.1249.

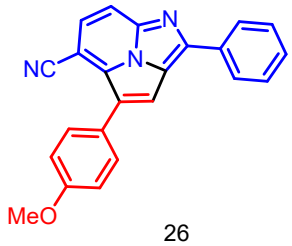


25

5-chloro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**25**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 40:1; 63.2 mg, 88%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 7.1 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.75 (s, 1H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 2H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.07 - 7.01 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.59, 150.19, 139.32, 133.52, 132.55, 131.63, 130.26, 129.29, 128.57, 128.24, 127.52, 126.31, 125.21, 121.39, 117.80, 113.82, 111.84, 55.50; HRMS (EI-TOF) Calcd for $C_{22}H_{16}ClN_2O$ $[M+H]^+$: 359.0946; found: 359.0941.

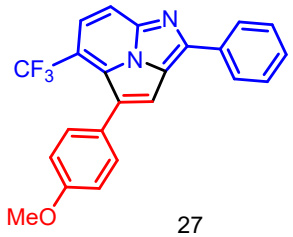


26

6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine-5-carbonitrile (**26**):

Orange solid; Eluent: petroluem ether/ethyl acetate 20:1; 45.5 mg, 65%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (d, *J* = 7.4 Hz, 2H), 8.19 (d, *J* = 7.2 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.94 (s, 1H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 2H), 7.57 - 7.52 (m, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.19, 153.46, 141.81, 132.86, 131.78, 131.26, 131.02, 130.96, 129.51, 128.81, 125.48, 124.94, 119.44, 116.82, 114.48, 111.52, 97.43, 55.55; HRMS (EI-TOF) Calcd for $C_{23}H_{16}N_3O$ $[M+H]^+$: 350.1288; found: 350.1292.

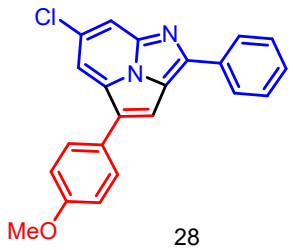


27

6-(4-methoxyphenyl)-1-phenyl-5-(trifluoromethyl)imidazo[5,1,2-*cd*]indolizine (**27**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 150:1; 55.8 mg, 71%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (d, *J* = 7.0 Hz, 2H), 8.18 (d, *J* = 8.3 Hz, 1H), 8.06 (d, *J* = 8.3 Hz, 1H), 7.83 (s, 1H), 7.57 (t, *J* = 7.4 Hz, 2H), 7.51 (d, *J* = 8.7 Hz, 3H), 7.02 (d, *J* = 8.3 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.63, 152.95, 141.84, 133.30, 132.44, 131.39, 130.79, 129.35, 128.57, 128.10, 127.82, 127.04, 125.24, 125.12, 124.52 (q, *J* = 5.1 Hz), 122.42, 120.80, 117.21, 116.86, 116.51, 113.58, 110.65, 55.45; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -55.05; HRMS (EI-TOF) Calcd for $C_{23}H_{16}F_3N_2O$ $[M+H]^+$: 393.1029; found: 393.1200.

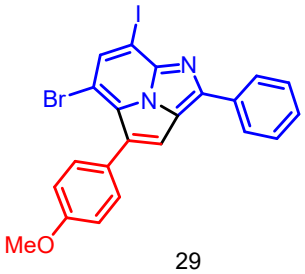


28

4-chloro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**28**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 40:1; 53.8 mg, 75%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 - 8.31 (m, 2H), 8.07 (s, 1H), 7.99 (s, 1H), 7.85 (s, 1H), 7.78 - 7.70 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.11 - 7.03 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.57, 150.90, 140.08, 133.47, 131.51, 130.36, 130.25, 129.28, 128.76, 128.32, 126.87, 124.96, 115.61, 114.91, 114.27, 111.95, 55.57; HRMS (EI-TOF) Calcd for $C_{22}H_{16}ClN_2O$ $[M+H]^+$: 359.0946; found: 359.0945.

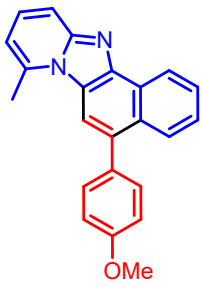


29

5-bromo-3-iodo-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**29**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 250:1; 64.6 mg, 61%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (d, *J* = 6.9 Hz, 2H), 8.31 (s, 1H), 7.65 (s, 1H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 14.5 Hz, 2H), 7.49 (d, *J* = 5.9 Hz, 1H), 7.02 (d, *J* = 1.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.74, 150.86, 141.43, 138.90, 133.47, 133.24, 132.08, 130.50, 129.21, 128.86, 128.56, 126.59, 125.70, 118.73, 113.68, 108.04, 55.50; HRMS (EI-TOF) Calcd for $C_{22}H_{15}BrIN_2O$ $[M+H]^+$:528.9407; found: 528.9406.

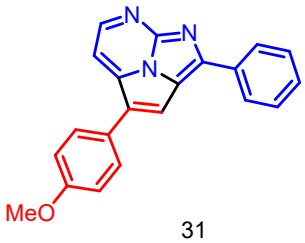


30

5-(4-methoxyphenyl)-8-methylnaphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**30**)

Brown solid; Eluent: petroluem ether/ethyl acetate 10:1; 43.4 mg, 64%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.97 (d, *J* = 8.2 Hz, 1H), 8.09 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 9.1 Hz, 1H), 7.74 - 7.66 (m, 1H), 7.59 - 7.51 (m, 1H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.32 (dd, *J* = 9.2, 6.8 Hz, 1H), 7.09 - 7.02 (m, 2H), 6.64 (d, *J* = 6.8 Hz, 1H), 3.93 (s, 3H), 3.03 (s, 5H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.07, 148.53, 141.14, 138.18, 133.96, 133.87, 131.57, 130.38, 127.92, 126.73, 126.66, 126.32, 126.18, 125.39, 123.51, 115.51, 115.07, 113.90, 112.12, 55.52, 21.63; HRMS (EI-TOF) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1492; found: 339.1492.

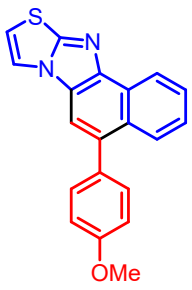


31

1-(4-methoxyphenyl)-3-phenyl-2a[1],4,5-triazacyclopenta[*cd*]indene (**31**):

Orange solid; Eluent: petroluem ether/ethyl acetate 15:1; 33.5mg, 76.8%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.88 (d, *J* = 5.4 Hz, 1H), 8.32 (d, *J* = 6.3 Hz, 2H), 7.83 (d, *J* = 5.4 Hz, 1H), 7.80 (s, 1H), 7.63 (d, *J* = 6.4 Hz, 2H), 7.53 - 7.42 (m, 3H), 6.99 - 6.92 (m, 2H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.47, 155.40, 148.00, 146.80, 133.69, 133.05, 131.14, 131.06, 129.11, 128.77, 128.22, 126.26, 123.26, 117.64, 114.76, 109.04, 55.45; HRMS (EI-TOF) Calcd for $C_{21}H_{16}N_3O$ $[M+H]^+$: 326.1288; found: 326.1286.

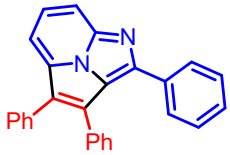


32

5-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[2,1-*b*]thiazole (**32**)

Brown solid; Eluent: petroluem ether/ethyl acetate 15:1; 59.5 mg, 90%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (d, *J* = 9.6 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.69 - 7.62 (m, 3H), 7.51 - 7.40 (m, 3H), 7.07 - 7.00 (m, 2H), 6.85 (d, *J* = 4.5 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.07, 154.24, 143.39, 134.39, 133.38, 131.50, 129.65, 127.04, 126.85, 126.51, 125.16, 122.52, 117.44, 113.84, 111.74, 111.43, 55.48; HRMS (EI-TOF) Calcd for $C_{20}H_{15}N_2OS$ $[M+H]^+$: 331.09; found: 331.0896.

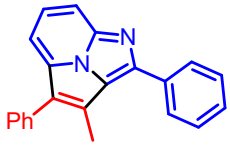


33

1,6,7-triphenylimidazo[5,1,2-*cd*]indolizine (**33**):[4]

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 37.1 mg, 50%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 - 8.03 (m, 1H), 8.00 - 7.95 (m, 2H), 7.86 - 7.80 (m, 2H), 7.49 - 7.45 (m, 2H), 7.43 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.41 - 7.31 (m, 7H), 7.31 - 7.27 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.14, 134.13, 134.04, 133.73, 131.83, 131.75, 131.15, 130.31, 129.82, 129.51, 128.77, 128.65, 128.48, 128.30, 127.46, 127.17, 127.14, 112.91, 111.48.; HRMS (EI-TOF) Calcd for: $C_{27}H_{19}N_2$ $[M+H]^+$: 371.1543; found: 371.1542.

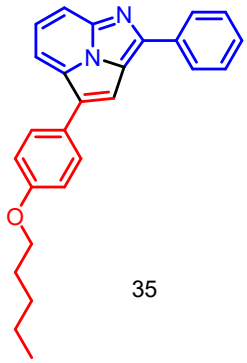


34

7-methyl-1,6-diphenylimidazo[5,1,2-*cd*]indolizine (**34**):[4]

Yellow solid; Eluent: petroluem ether/ethyl acetate 20:1; 35.6 mg, 58%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 7.3 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.63 (d, *J* = 7.9 Hz, 2H), 7.56 (dt, *J* = 11.5, 7.5 Hz, 4H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.4 Hz, 1H), 2.88 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.28, 139.80, 134.51, 134.15, 132.06, 130.08, 129.43, 129.18, 129.00, 128.92, 128.60, 127.48, 127.28, 126.74, 125.60, 111.36, 110.63, 14.06; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2$ $[M+H]^+$: 309.1386; found: 309.1389.

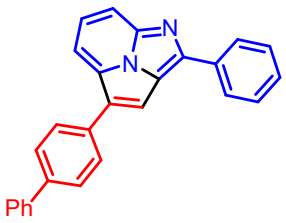


35

6-(4-(pentyloxy)phenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**35**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 25:1; 48.0 mg, 63%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 2H), 8.07 (d, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.90 (t, J = 7.8 Hz, 1H), 7.86 (s, 1H), 7.81 – 7.74 (m, 2H), 7.56 (t, J = 7.6 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.08 - 7.01 (m, 2H), 4.03 (t, *J* = 6.6 Hz, 2H), 1.90 - 1.80 (m, 2H), 1.55 - 1.36 (m, 4H), 0.97 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.93, 149.33, 140.57, 134.13, 131.36, 130.88, 129.83, 129.18, 128.76, 128.22, 127.39, 126.85, 124.89, 115.36, 114.16, 113.58, 111.72, 68.29, 29.12, 28.36, 22.61, 14.17; HRMS (EI-TOF) Calcd for $C_{26}H_{25}N_2O$ $[M+H]^+$: 381.1961; found: 381.1960.



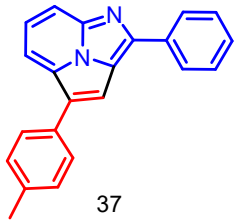
36

6-([1,1'-biphenyl]-4-yl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**36**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 41.5 mg, 28%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 7.3 Hz, 2H), 8.18 (d, *J* = 7.6 Hz, 1H), 8.07 - 8.01 (m, 2H), 7.97 (dd, *J* = 8.0, 4.2 Hz, 3H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 7.0 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 3H), 7.40 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.88, 140.67, 140.65, 140.35, 134.04, 133.95, 130.87, 130.82, 130.06, 129.26, 129.05, 128.32, 128.02, 127.98,

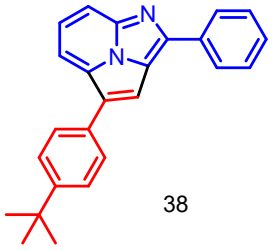
127.65, 127.25, 127.14, 124.99, 114.94, 113.86, 111.88; HRMS (EI-TOF) Calcd for $C_{27}H_{19}N_2$ $[M+H]^+$: 371.1543; found: 371.1534.



37

1-phenyl-6-(p-tolyl)imidazo[5,1,2-cd]indolizine (**37**):

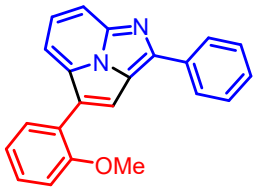
Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 32.1 mg, 52%; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.41 (d, J = 7.0 Hz, 2H), 8.13 (d, J = 7.6 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.98 - 7.90 (m, 2H), 7.79 (d, J = 6.3 Hz, 2H), 7.58 (t, J = 7.6 Hz, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.35 (d, J = 7.9 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.61, 140.61, 137.48, 134.05, 132.15, 131.45, 130.88, 130.06, 129.94, 129.22, 128.26, 127.55, 127.02, 124.90, 114.69, 113.75, 111.78, 21.40; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2$ $[M+H]^+$: 309.1386; found: 309.1388.



38

6-(4-(*ter*t-butyl)phenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**38**):

Yellow solid; Eluent: petroluem ether/ethyl acetate 15:1; 34.3 mg, 49%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (d, J = 7.0 Hz, 2H), 8.14 (d, J = 7.6 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.98 - 7.90 (m, 2H), 7.87 - 7.80 (m, 2H), 7.67 - 7.54 (m, 4H), 7.54 - 7.44 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.71, 149.57, 140.57, 134.03, 132.17, 131.36, 130.89, 129.93, 129.22, 128.26, 127.39, 127.03, 126.30, 124.90, 114.72, 113.78, 111.75, 34.81, 31.48; HRMS (EI-TOF) Calcd for $C_{25}H_{23}N_2$ $[M+H]^+$: 351.1856; found: 351.1858.

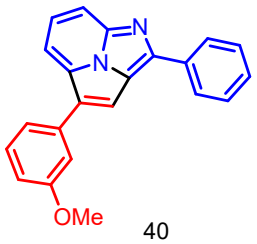


39

6-(2-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**39**):

Light yellow oil; Eluent: petroluem ether/ethyl acetate 30:1; 34.4 mg, 53%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 7.0, 1.5 Hz, 2H), 8.09 (s, 1H), 8.03 (dd, *J* = 7.8, 3.4 Hz, 2H), 7.92 (t, *J* = 7.9 Hz, 1H), 7.76 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.37 - 7.42 (m, 1H), 7.18 - 7.03 (m, 2H), 3.94 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.70, 149.62, 140.61, 134.15, 131.79, 131.08, 129.83, 129.17, 128.95, 128.31, 127.43, 126.81, 125.03, 123.74, 121.23, 117.97, 114.45, 111.60, 111.39, 55.65; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2O$ $[M+H]^+$: 325.1335; found: 325.1329.

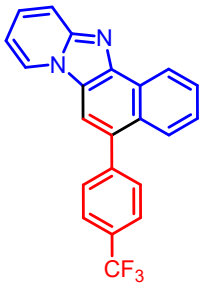


40

6-(3-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**40**):

Light yellow oil; Eluent: petroluem ether/ethyl acetate 30:1; 37.7 mg, 58%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 7.0 Hz, 2H), 8.16 (d, *J* = 7.6 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 8.01 - 7.90 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 2H), 7.52 - 7.45 (m, 3H), 7.43 (t, *J* = 2.0 Hz, 1H), 6.99 - 6.92 (m, 1H), 3.93 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.41, 149.98, 140.69, 136.39, 133.98, 131.16, 130.83, 130.39, 130.05, 129.26, 128.31, 127.20, 124.88, 120.24, 115.20, 113.83, 113.51, 112.86, 111.86, 55.54; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2O$ $[M+H]^+$: 325.1335; found: 325.1342.

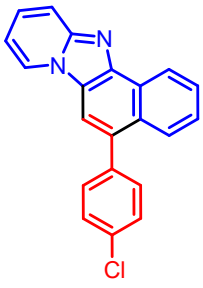


41

5-(4-(trifluoromethyl)phenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**41**):

Brown solid; Eluent: petroluem ether/ethyl acetate 3:1; 37.0 mg, 51%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.93 (d, *J* = 8.2 Hz, 1H), 8.45 (d, *J* = 6.8 Hz, 1H), 7.88 (t, *J* = 9.0 Hz, 2H), 7.82 - 7.75 (m, 3H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 7.9 Hz, 2H), 7.58 - 7.47 (m, 1H), 7.47 - 7.38 (m, 1H), 6.93 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.65, 144.89, 141.12, 133.46, 130.85, 130.34, 129.82, 129.50, 128.11, 127.02, 126.89, 126.64, 126.43, 125.80, 125.43 (q, *J* = 3.1 Hz), 124.49, 123.82, 123.52, 123.09, 118.09, 111.68, 111.27; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.30; HRMS (EI-TOF) Calcd for $C_{22}H_{14}F_3N_2$ $[M+H]^+$: 363.1104; found: 363.1117.

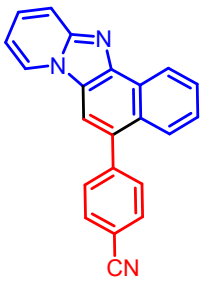


42

5-(4-chlorophenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**42**):

Brown solid; Eluent: petroluem ether/ethyl acetate 3:1; 46.7 mg, 71%;

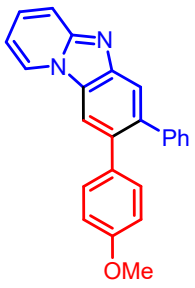
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, *J* = 8.1, 1.6 Hz, 1H), 8.47 (d, *J* = 6.9 Hz, 1H), 7.93 (d, *J* = 9.4 Hz, 1H), 7.87 (d, *J* = 9.2 Hz, 1H), 7.80 (s, 1H), 7.72 (t, *J* = 7.0 Hz, 1H), 7.54 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.48 (d, J = 1.0 Hz, 4H), 7.47 – 7.39 (m, 1H), 6.93 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.57, 141.04, 139.61, 133.77, 133.57, 131.80, 130.61, 128.68, 127.95, 127.09, 126.85, 126.80, 126.31, 124.51, 123.91, 123.47, 118.14, 111.59, 111.12; HRMS (EI-TOF) Calcd for $C_{21}H_{14}ClN_2$ $[M+H]^+$: 329.084; found: 329.0847.



43

4-(naphtho[1',2':4,5]imidazo[1,2-*a*]pyridin-5-*yl*)benzonitrile (**43**):

Green solid; Eluent: petroluem ether/ethyl acetate 5:1; 49.8 mg, 78%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.92 (d, *J* = 8.2 Hz, 1H), 8.49 (d, *J* = 6.8 Hz, 1H), 7.86 (d, *J* = 7.7 Hz, 2H), 7.82 (d, *J* = 4.5 Hz, 3H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 2H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.50 - 7.41 (m, 1H), 6.96 (d, *J* = 13.6 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.81, 146.08, 141.42, 132.80, 132.29, 131.26, 129.97, 128.27, 127.06, 126.99, 126.57, 126.33, 124.55, 123.81, 123.58, 119.04, 118.16, 111.77, 111.43, 111.21; HRMS (EI-TOF) Calcd for $C_{22}H_{14}N_3$ $[M+H]^+$: 320.1182; found: 320.1185.

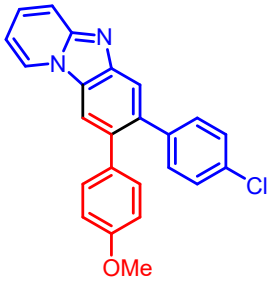


44

8-(4-methoxyphenyl)-7-phenylbenzo[4,5]imidazo[1,2-*a*]pyridine (**44**):

Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 65.2 mg, 93%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (d, *J* = 6.9 Hz, 1H), 7.96 (s, 1H), 7.87 (s, 1H), 7.72 (d, *J* = 9.3 Hz, 1H), 7.47 - 7.38 (m, 1H), 7.29 - 7.18 (m, 5H), 7.14 - 7.07 (m, 2H), 6.85 (t, *J* = 6.2 Hz, 1H), 6.82 - 6.74 (m, 2H), 3.78 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.39, 149.19, 143.58, 142.12, 139.53, 134.65, 134.37, 131.38, 130.38, 129.66, 128.31, 128.00, 126.49, 125.36, 121.21, 118.03, 113.49, 111.98, 110.72, 55.30; HRMS (EI-TOF) Calcd for $C_{24}H_{19}N_2O$ $[M+H]^+$: 351.1492; found: 351.1490.

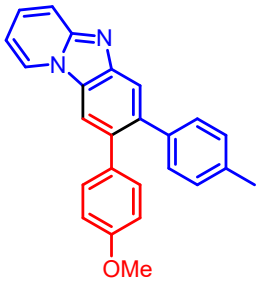


45

7-(4-chlorophenyl)-8-(4-methoxyphenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**45**):

Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 63.9 mg, 83%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 6.9 Hz, 1H), 7.89 (d, *J* = 13.8 Hz, 2H), 7.73 (d, *J* = 9.3 Hz, 1H), 7.50 - 7.41 (m, 1H), 7.26 - 7.19 (m, 2H), 7.15 (d, *J* = 6.6 Hz, 2H), 7.12 - 7.07 (m, 2H), 6.92 - 6.84 (m, 1H), 6.84 - 6.77 (m, 2H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.54, 149.45, 143.89, 140.70, 138.15, 134.48, 134.09, 132.62, 131.66, 131.42, 129.71, 128.57, 128.25, 125.38, 121.25, 118.23, 113.68, 112.14, 110.77, 55.37; HRMS (EI-TOF) Calcd for $C_{24}H_{18}ClN_2O$ $[M+H]^+$: 385.1102; found: 385.1096.

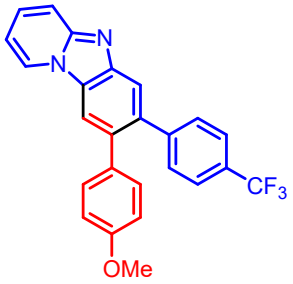


46

8-(4-methoxyphenyl)-7-(*p*-tolyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**46**):

Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 69.2 mg, 95%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (d, *J* = 6.9 Hz, 1H), 7.94 (s, 1H), 7.85 (s, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.46 - 7.38 (m, 1H), 7.12 (dd, *J* = 8.5, 2.7 Hz, 4H), 7.06 (d, *J* = 7.9 Hz, 2H), 6.85 (t, *J* = 6.7 Hz, 1H), 6.85 - 6.76 (m, 2H), 3.82 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.36, 149.23, 143.77, 139.48, 139.20, 136.08, 134.65, 134.60, 131.37, 130.23, 129.53, 128.76, 128.24, 125.34, 121.23, 118.09, 113.50, 111.96, 110.62, 55.32, 21.23; HRMS (EI-TOF) Calcd for $C_{25}H_{21}N_2O$ $[M+H]^+$: 365.1648; found: 365.1643.

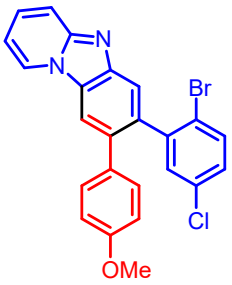


47

8-(4-methoxyphenyl)-7-(4-(trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**47**):

Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 45.3 mg, 55%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 6.8 Hz, 1H), 7.93 (d, *J* = 16.2 Hz, 2H), 7.77 (d, J = 9.2 Hz, 1H), 7.50 (t, *J* = 6.4 Hz, 3H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.12 - 7.05 (m, 2H), 6.91 (t, *J* = 6.7 Hz, 1H), 6.83 - 6.77 (m, 2H), 3.80 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.66, 149.27, 145.84, 143.26, 138.10, 134.64, 133.71, 132.04, 131.42, 130.62, 130.17, 128.81, 128.65, 128.49, 125.80, 125.44, 125.00 (q, *J* = 4.1 Hz), 123.10, 121.23, 118.09, 113.74, 112.33, 111.13, 55.36; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.29; HRMS (EI-TOF) Calcd for $C_{25}H_{18}F_3N_2O$ $[M+H]^+$: 419.1366; found: 419.1355.



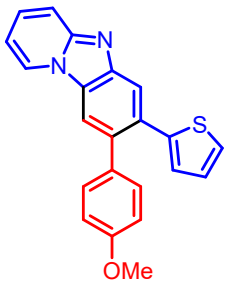
48

7-(2-bromo-5-chlorophenyl)-8-(4-methoxyphenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**48**):

Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 39.0 mg, 42%;

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 (d, *J* = 6.9 Hz, 1H), 7.90 (s, 1H), 7.82 (s, 1H), 7.74 (d, *J* = 9.3 Hz, 1H), 7.45 (dd, *J* = 15.9, 7.6 Hz, 2H), 7.24 (d, *J* = 2.6 Hz, 1H), 7.18 - 7.11 (m, 2H), 7.09 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.88 (t, *J* = 6.8 Hz, 1H), 6.81 - 6.75 (m, 2H), 3.79 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.60, 149.56,

144.53, 143.28, 137.21, 134.91, 133.68, 133.48, 132.82, 132.30, 131.10, 129.85, 128.99, 128.75, 125.42, 122.42, 121.47, 118.31, 113.48, 111.76, 110.83, 55.32; HRMS (EI-TOF) Calcd for $C_{24}H_{17}BrClN_2O$ $[M+H]^+$: 463.0207; found: 463.0189.



49

8-(4-methoxyphenyl)-7-(thiophen-2-yl)benzo[4,5]imidazo[1,2-*a*]pyridine (**49**): Colourless solid; Eluent: petroluem ether/ethyl acetate 3:1; 42.1 mg, 59%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 6.9 Hz, 1H), 8.08 (s, 1H), 7.82 (s, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.46 - 7.38 (m, 1H), 7.25 - 7.17 (m, 3H), 6.91 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.89 - 6.81 (m, 3H), 6.79 (dd, *J* = 3.6, 1.2 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.86, 149.44, 143.96, 143.73, 134.87, 134.29, 131.95, 131.24, 129.71, 128.52, 127.27, 127.00, 125.78, 125.35, 121.43, 118.15, 113.59, 112.26, 110.75, 55.36; HRMS (EI-TOF) Calcd for $C_{22}H_{17}N_2OS$ $[M+H]^+$: 357.1056; found: 357.1050.

9、Reference

1. Nipate, D. S., Sonam., Shinde, V. N., Rangan, K. & Kumar, A. Tempo-mediated synthesis of indolyl/imidazo 1,2-a pyridinyl-substituted para-quinone methides from butylated hydroxytoluene. *J. Org. Chem.* **2021,** *86* (23), 17090-17100.

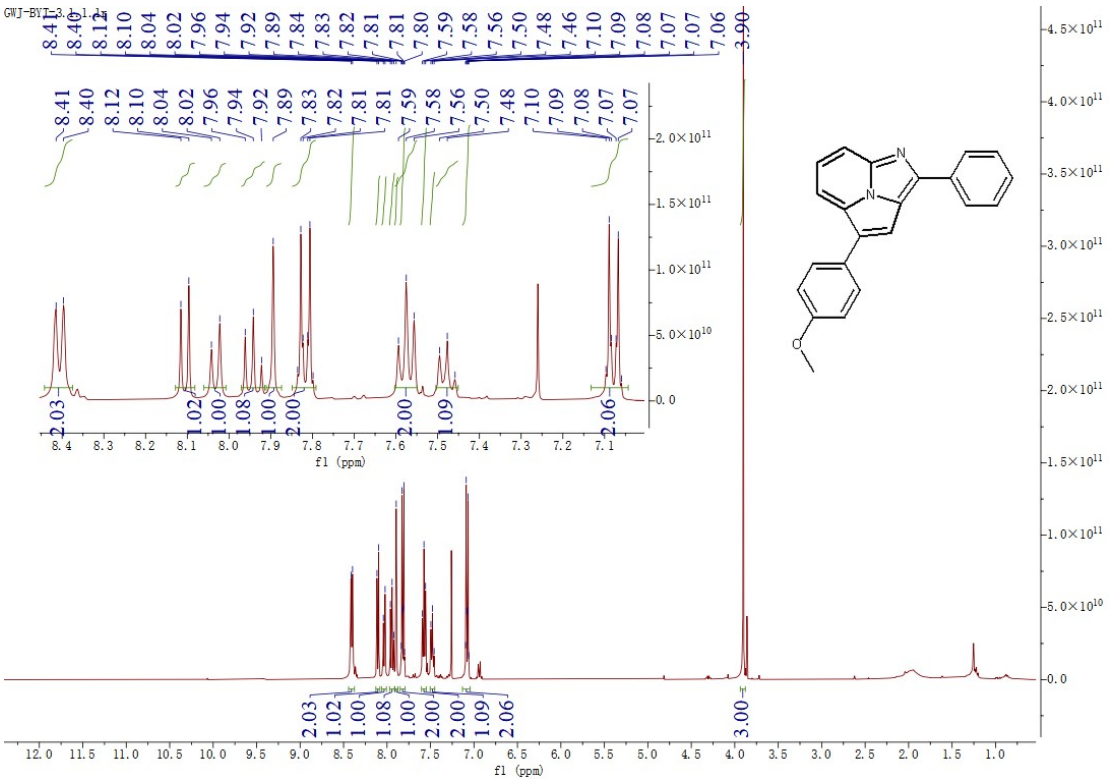
2. Mohan, D. C., Rao, S. N., Ravi, C. & Adimurthy, S. Copper(I) iodide catalyzed aerobic oxidative C-N and C-S bond formations through C-H activation: Synthesis of functionalized imidazo 1,2-a pyridines. *J. Org. Chem.* **2014,** *3* (5), 609-613.

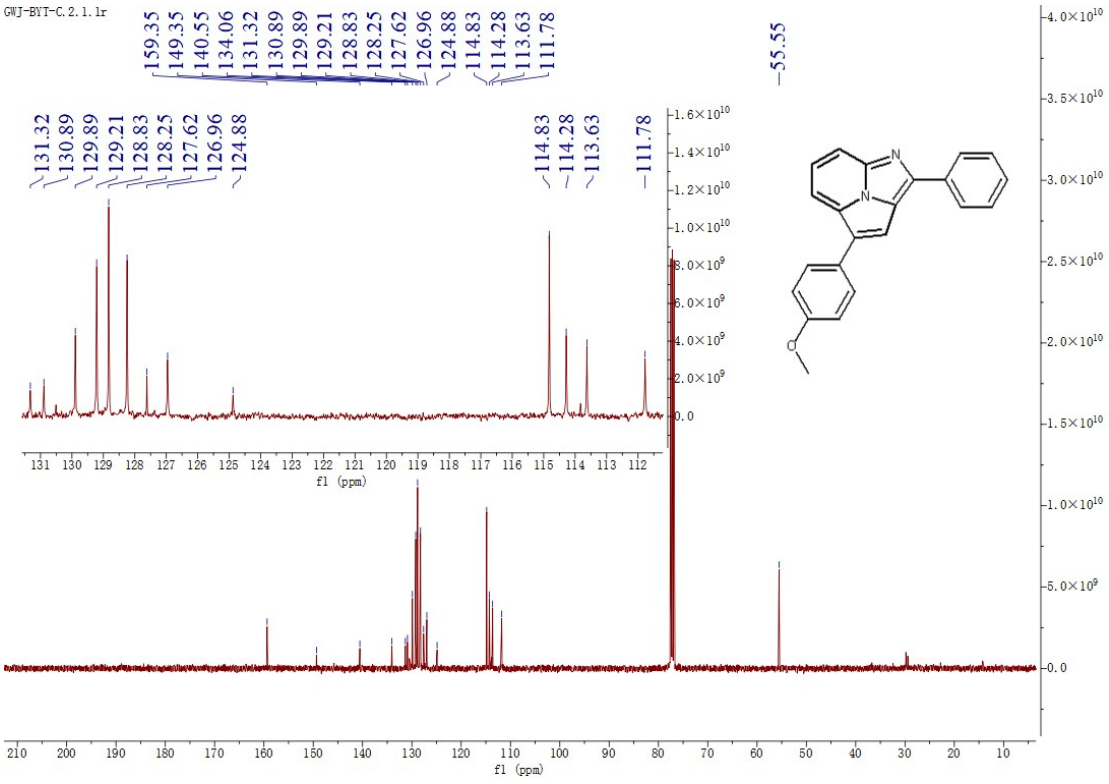
3. Hao, H.-Y., Mao, Y.-J., Xu, Z.-Y., Lou, S.-J. & Xu, D.-Q. Selective cross-dehydrogenative C(sp(3))-H arylation with arenes. *Org. Lett.* **2020,** *22* (6), 2396-2402.

4. Meena, N., Sharma, S., Bhatt, R., Shinde, V. N., Sunda, A. P., Bhuvanesh, N., Kumar, A. & Joshi, H. A selenium-coordinated palladium(ii)trans-dichloride molecular rotor as a catalyst for site-selective annulation of 2-arylimidazo 1,2-a pyridines. *Chem. Commun.* **2020,** *56* (70), 10223-10226.

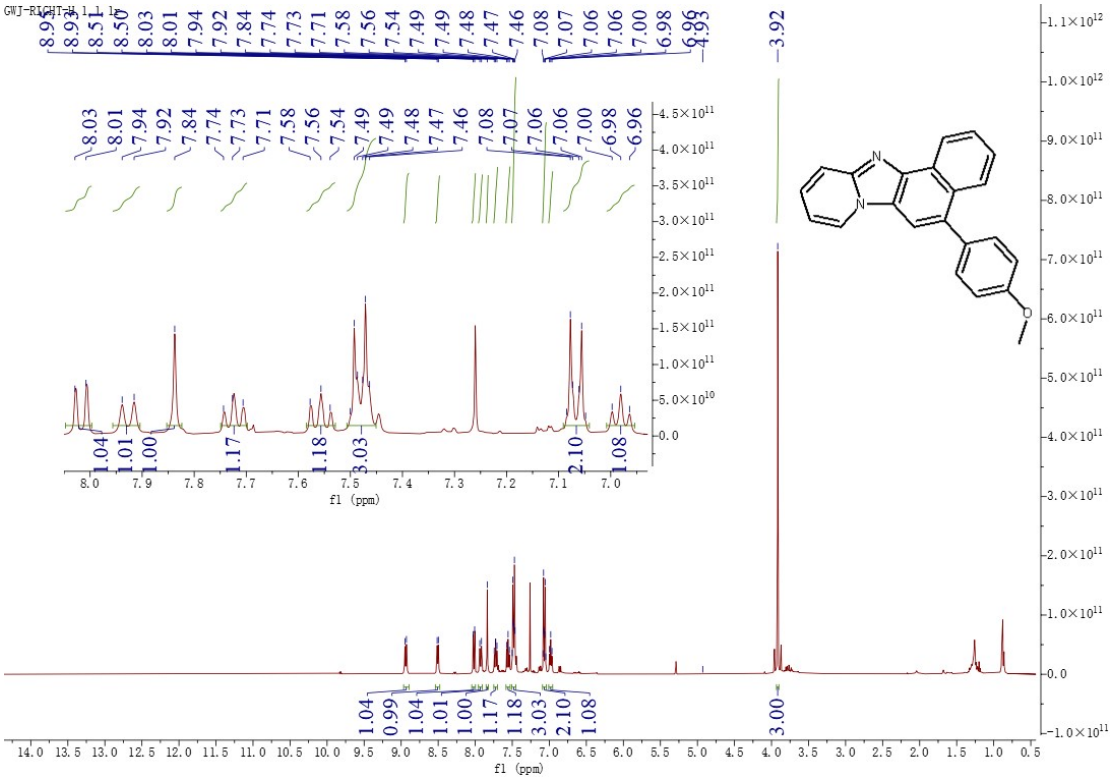
10、NMR Spectra for Electrolysis Products

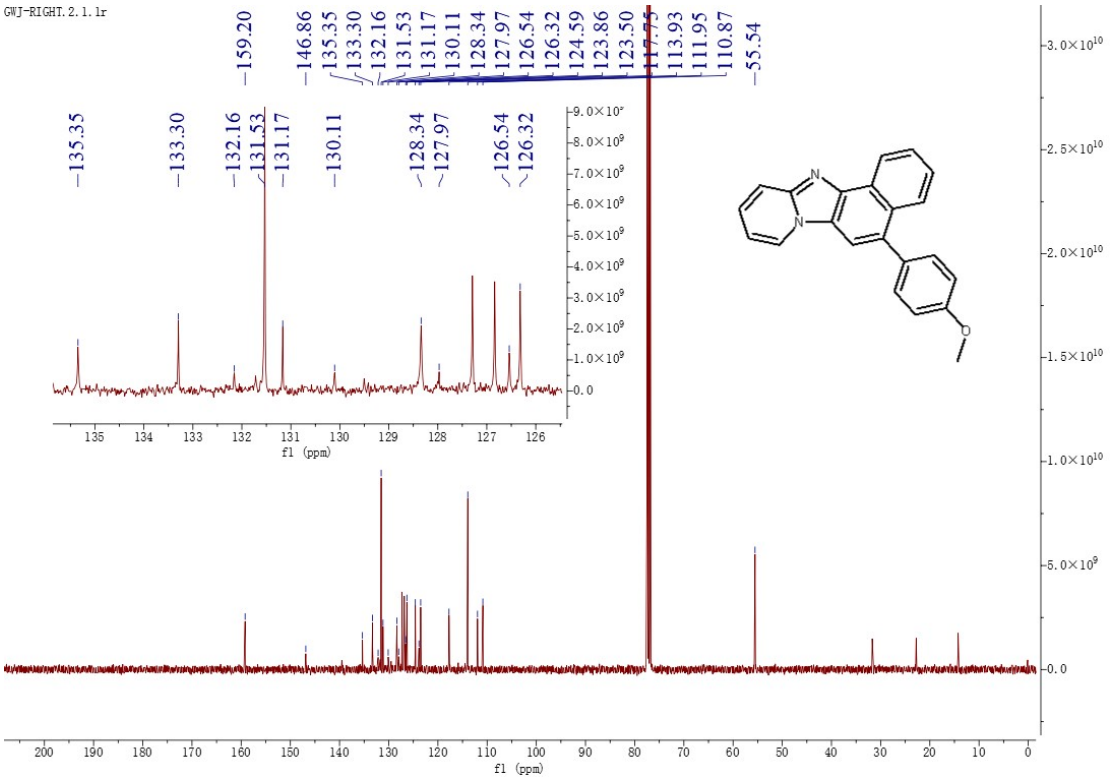
6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**3**):



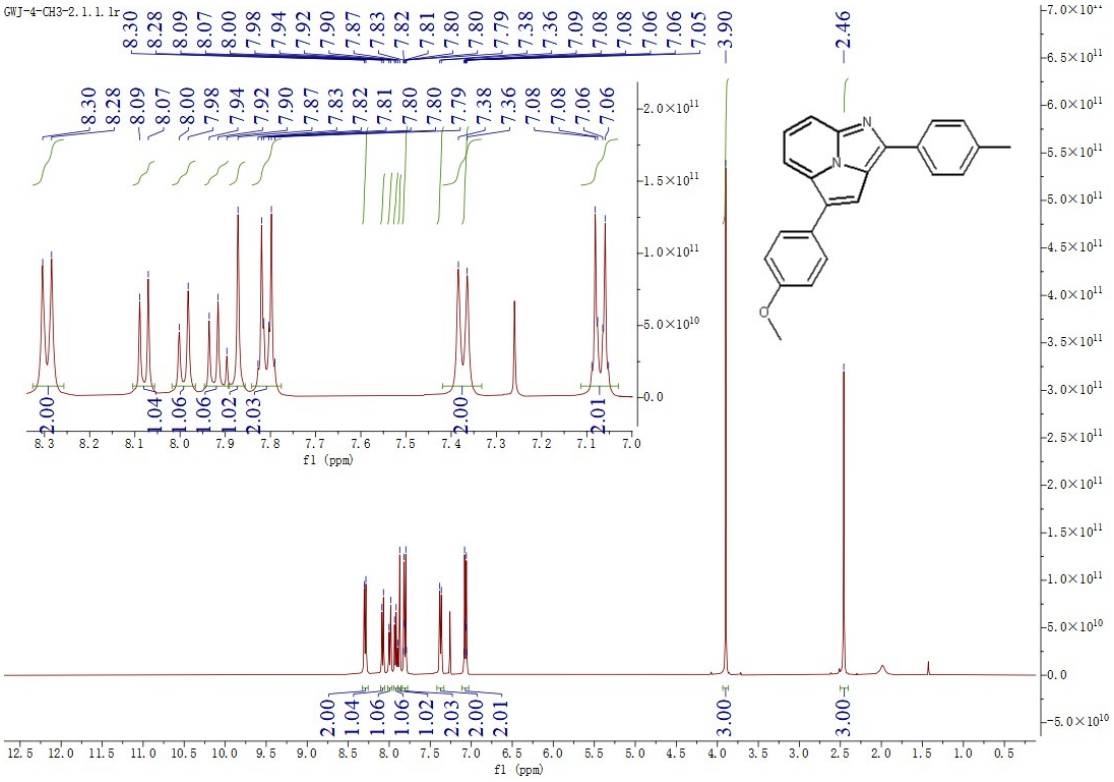


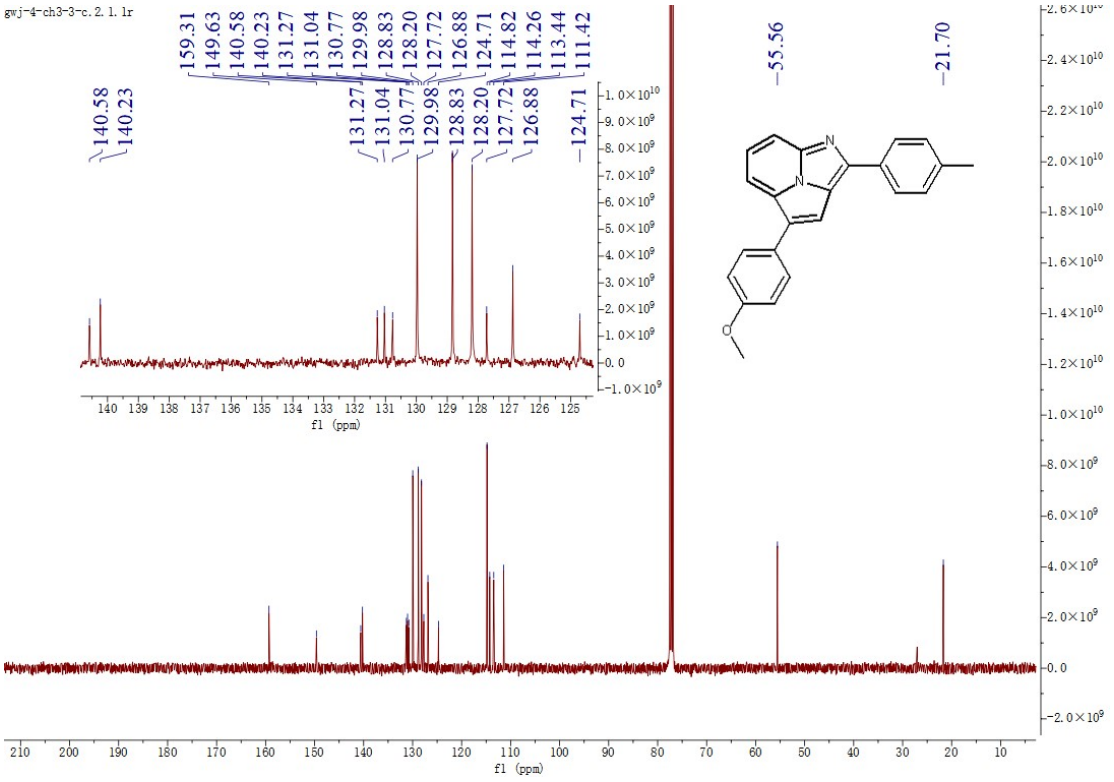
5-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**4**):



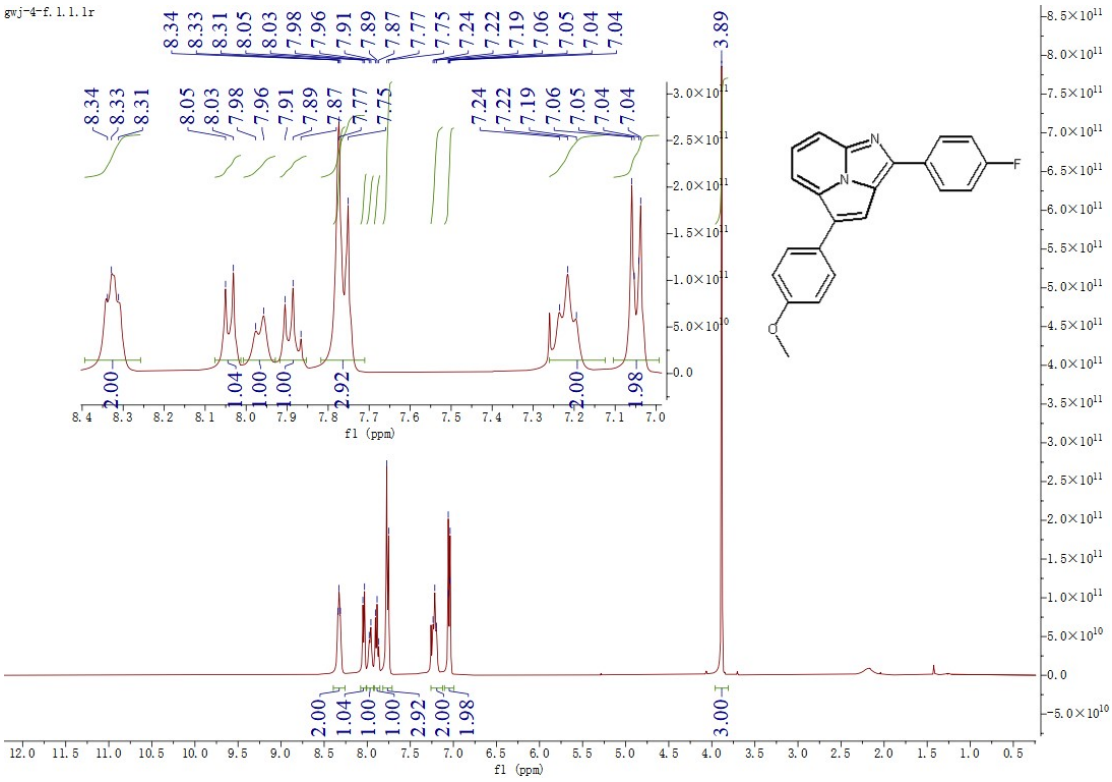


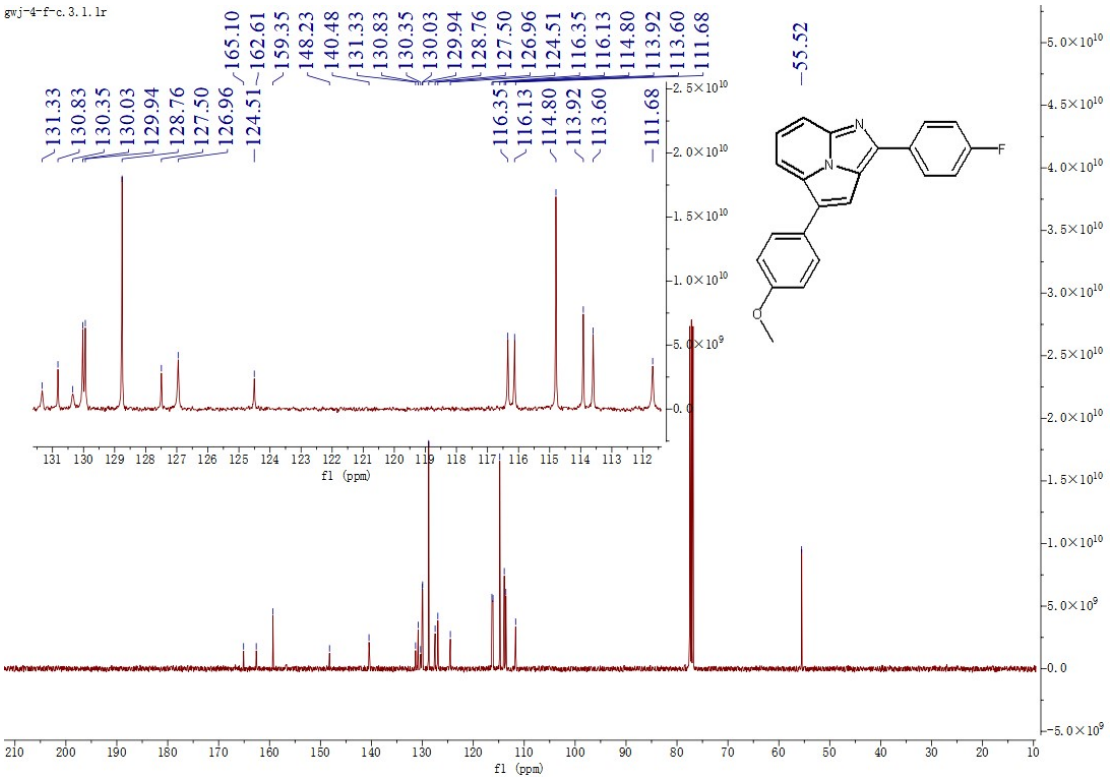
6-(4-methoxyphenyl)-1-(p-tolyl)imidazo[5,1,2-*cd*]indolizine (**5**):

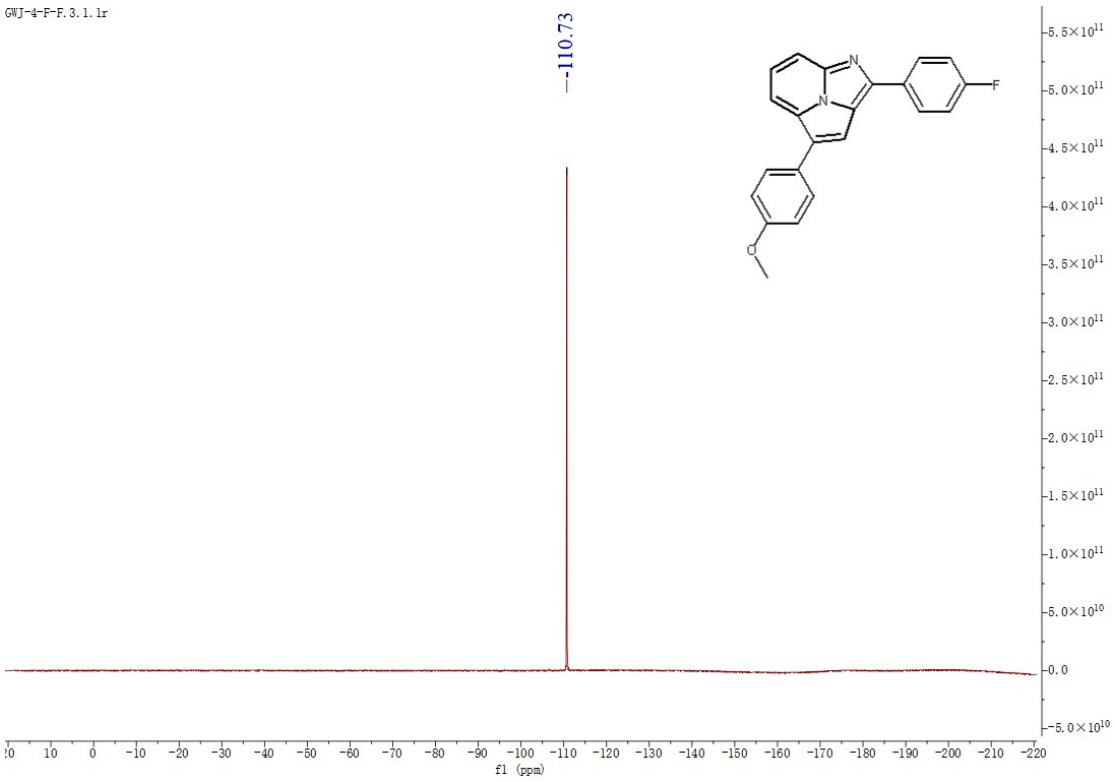




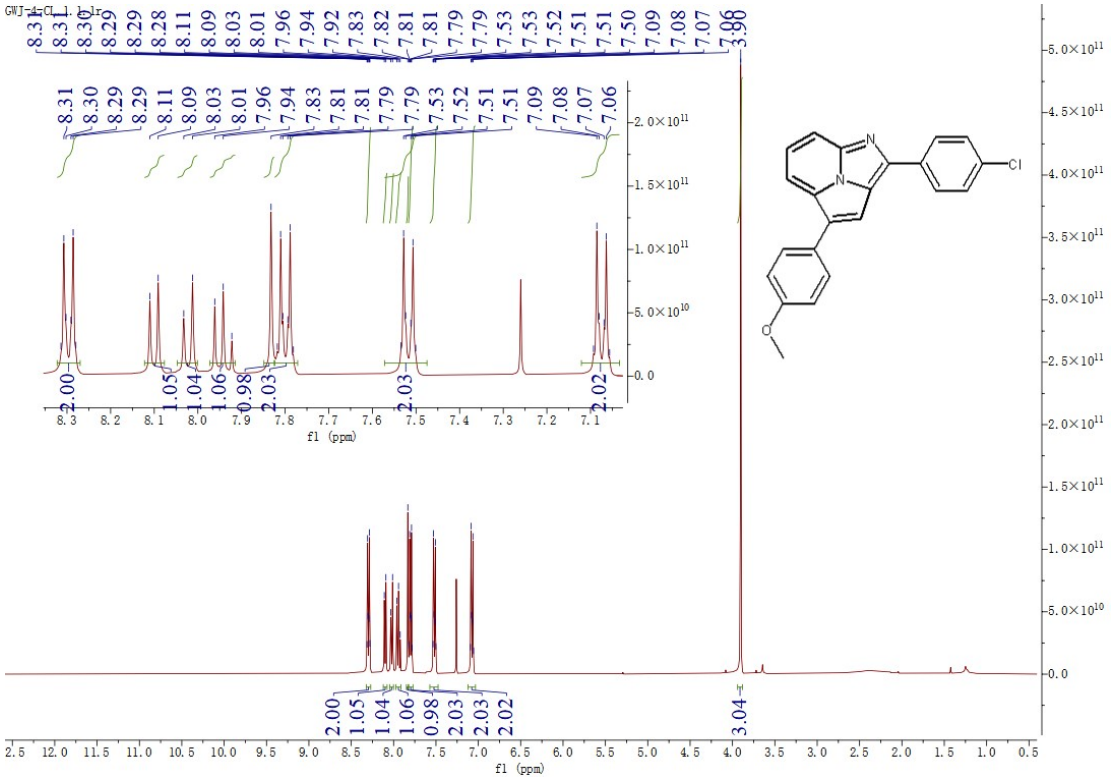
1-(4-fluorophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**6**):

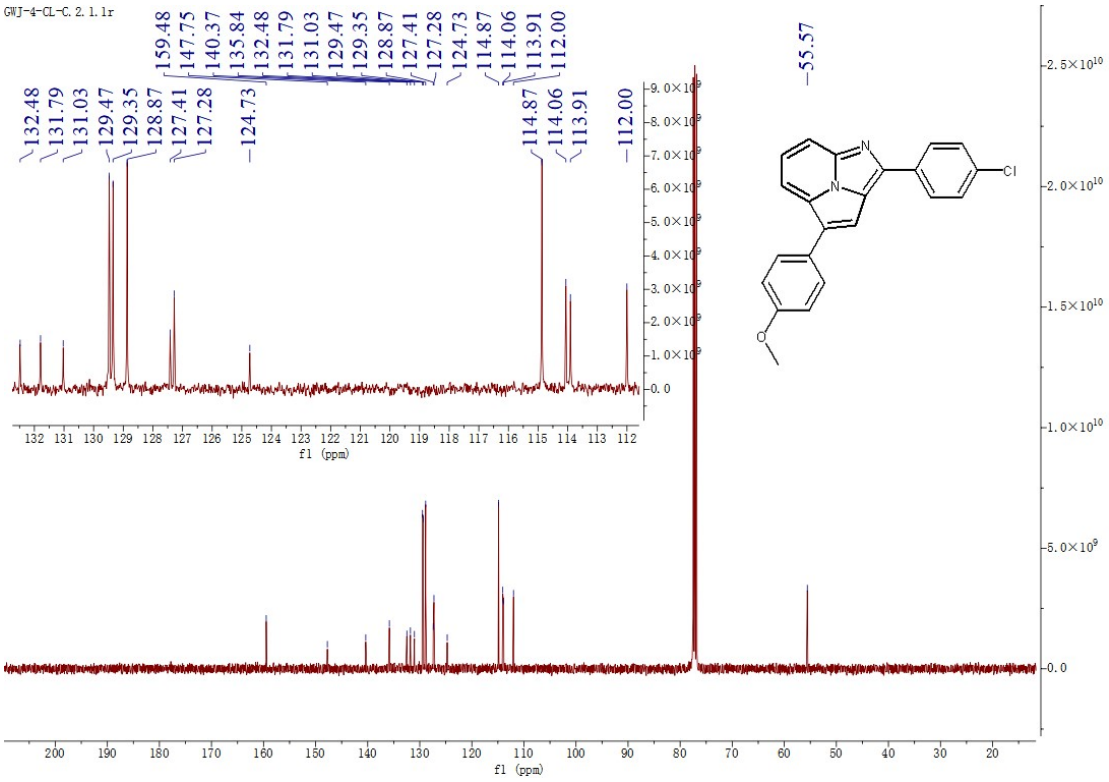




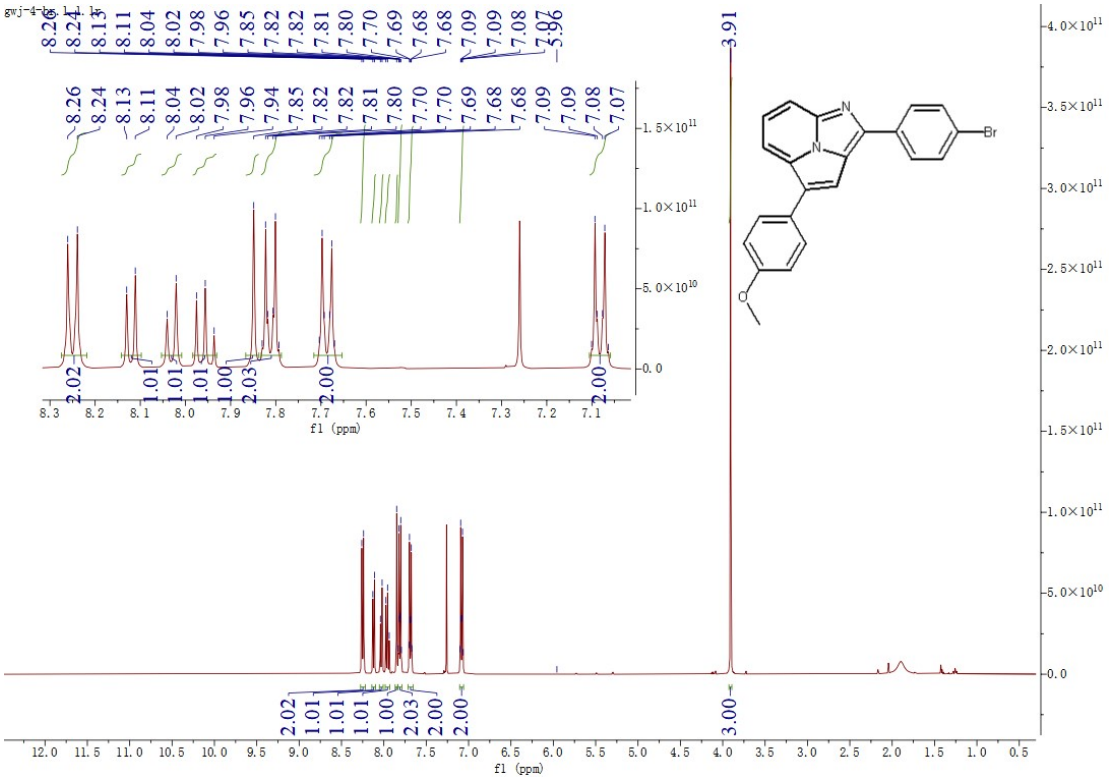


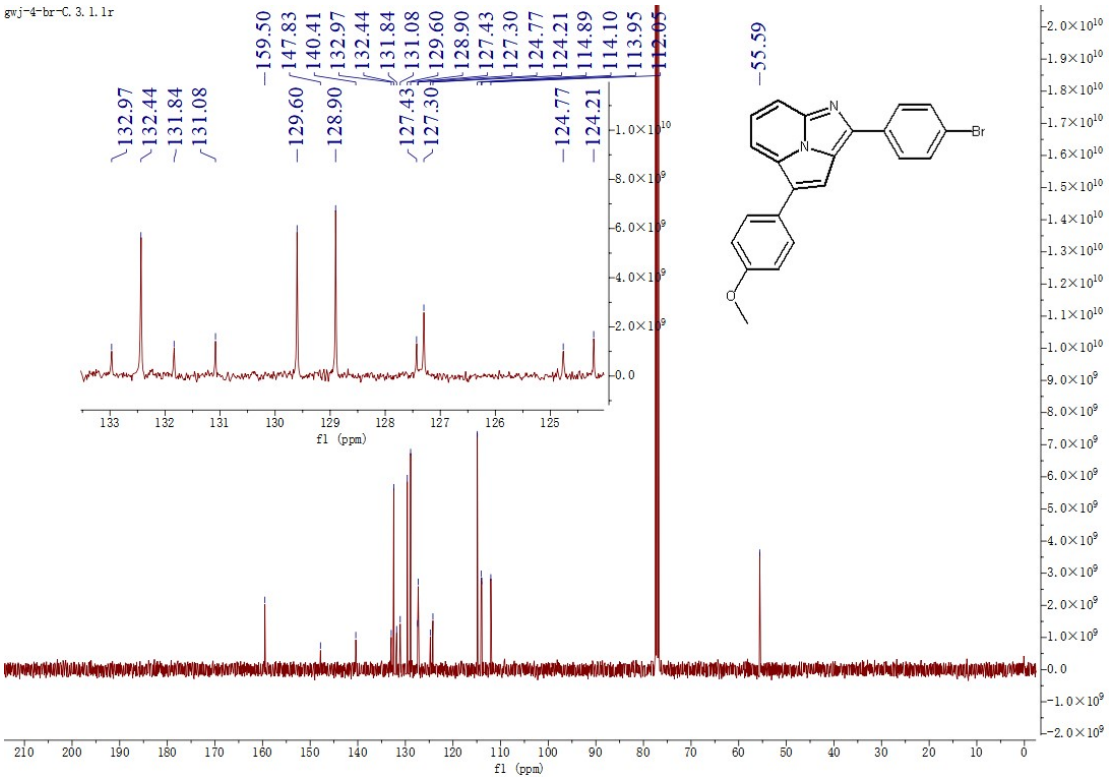
1-(4-chlorophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**7**):



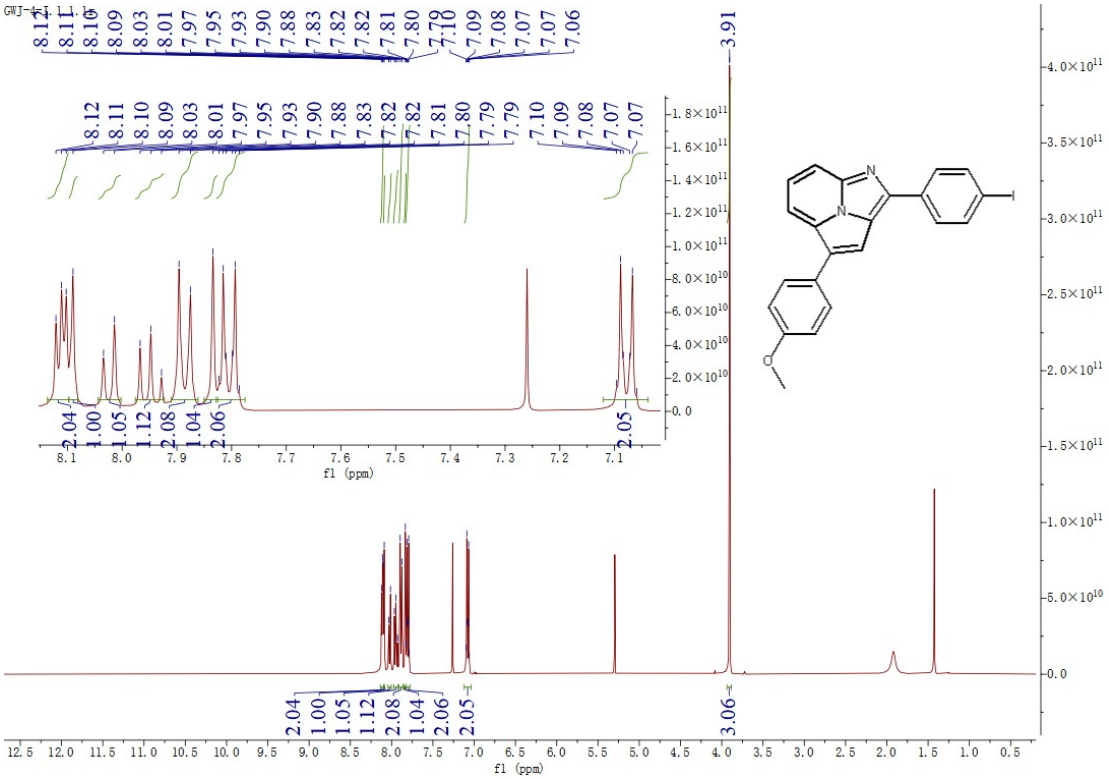


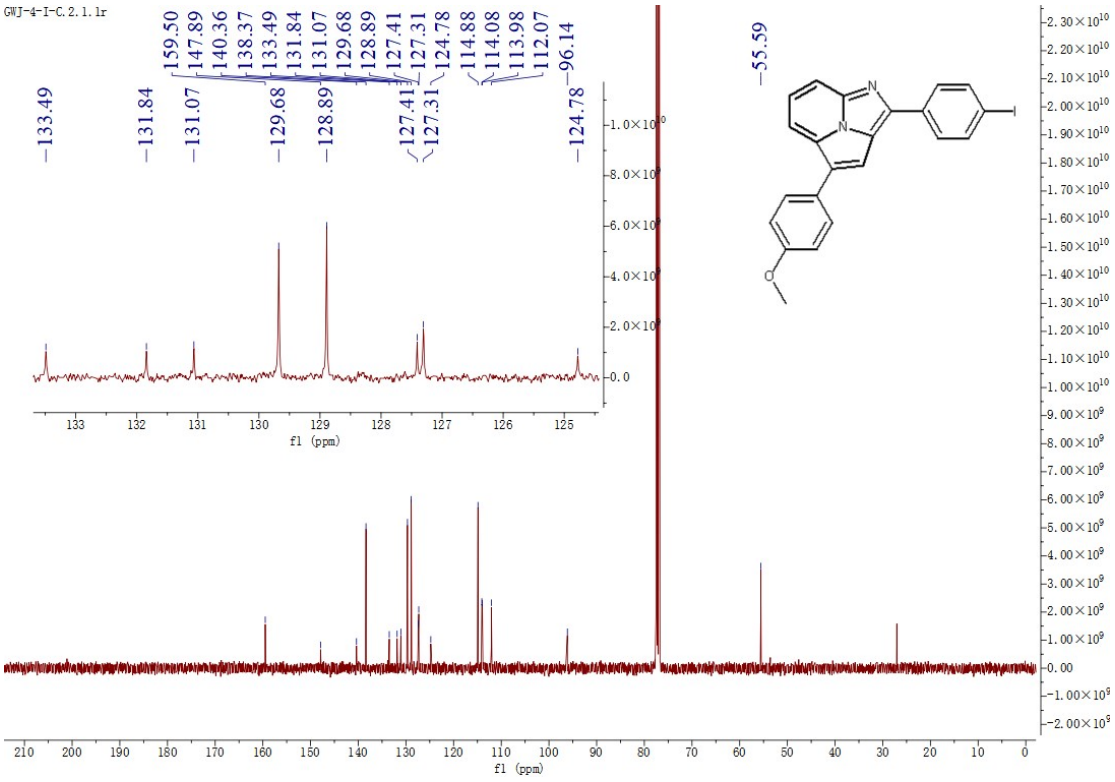
1-(4-bromophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**8**):



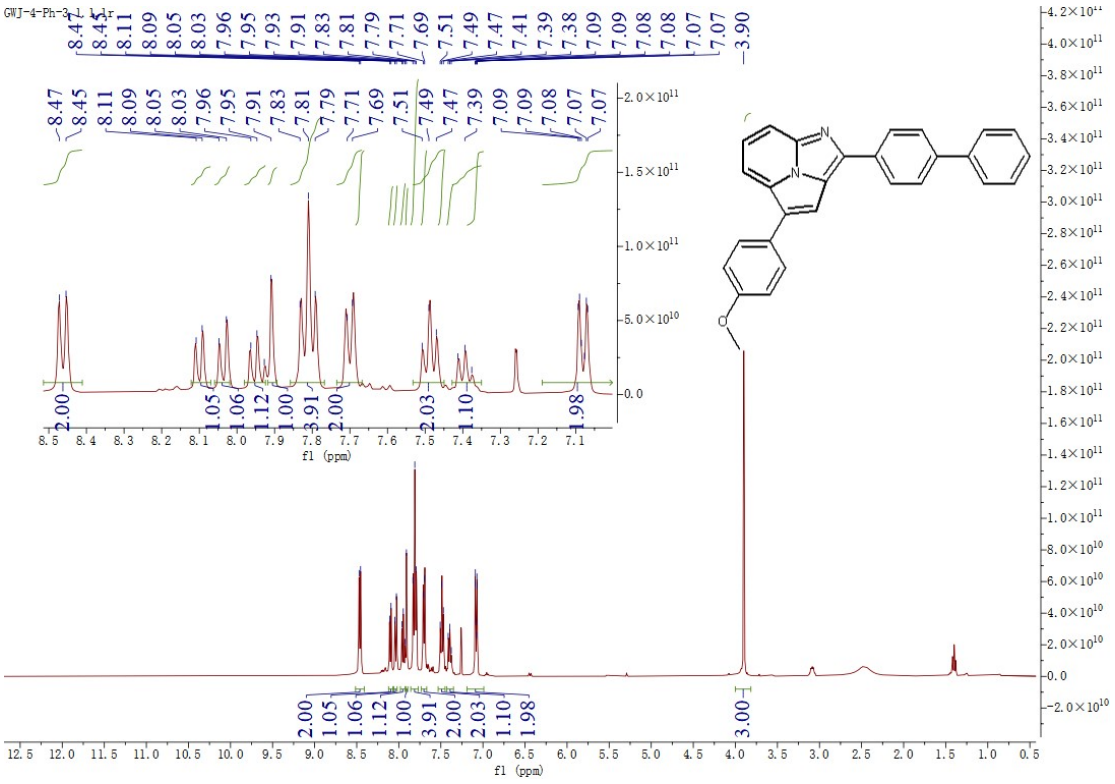


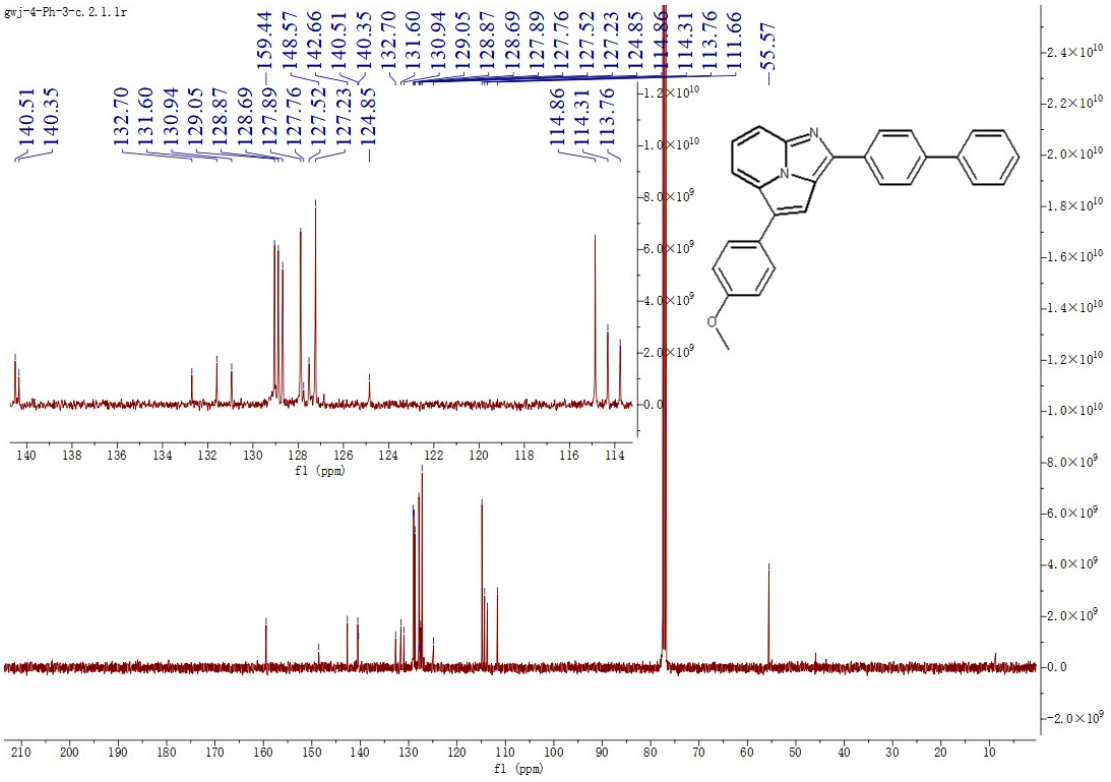
1-(4-iodophenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**9**):



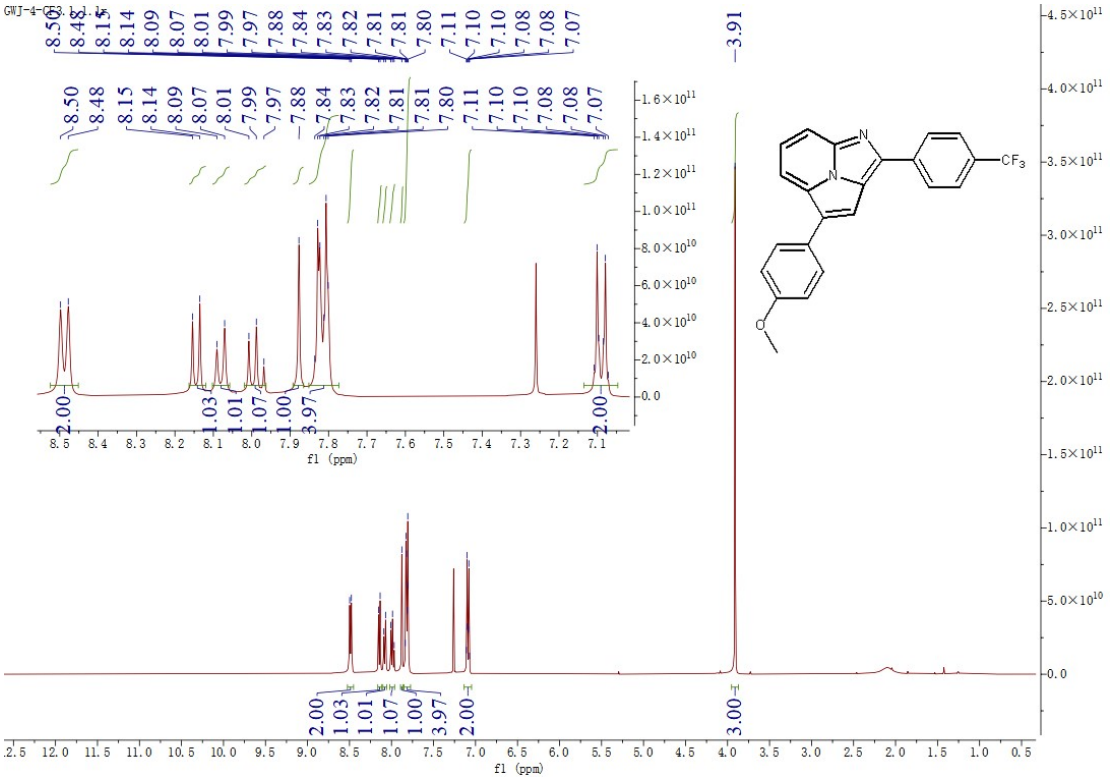


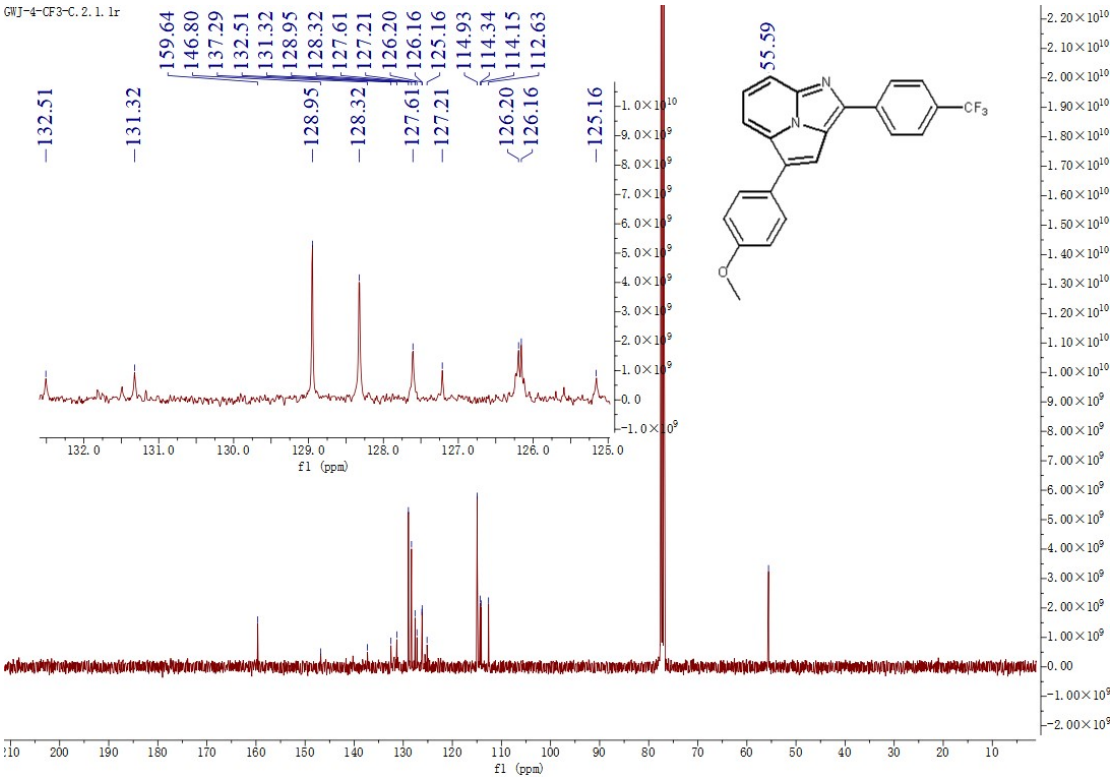
1-([1,1'-biphenyl]-4-yl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**10**):

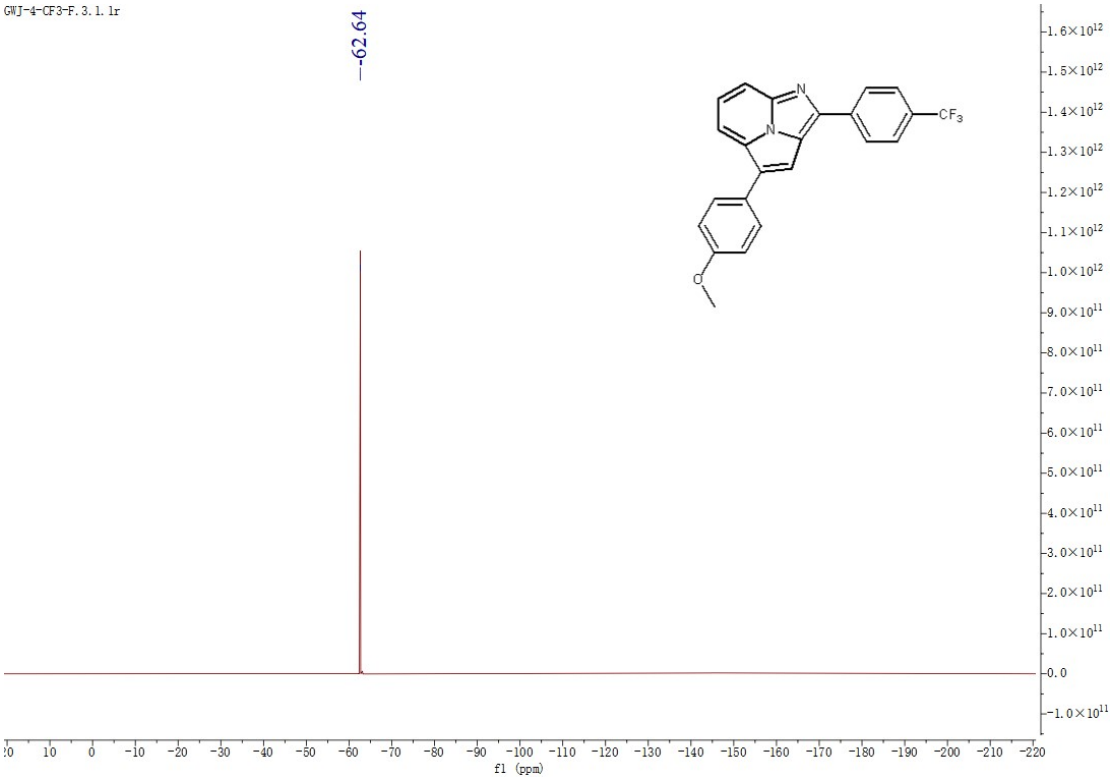




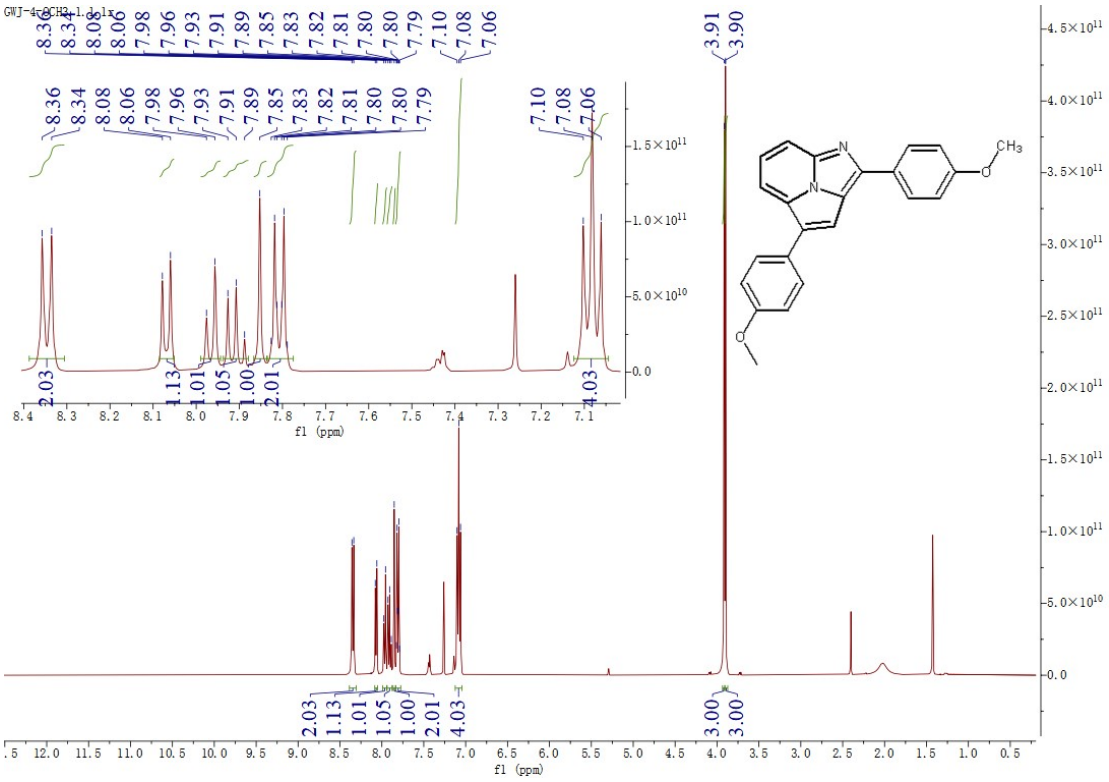
6-(4-methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)imidazo[5,1,2-*cd*]indolizine (**11**):

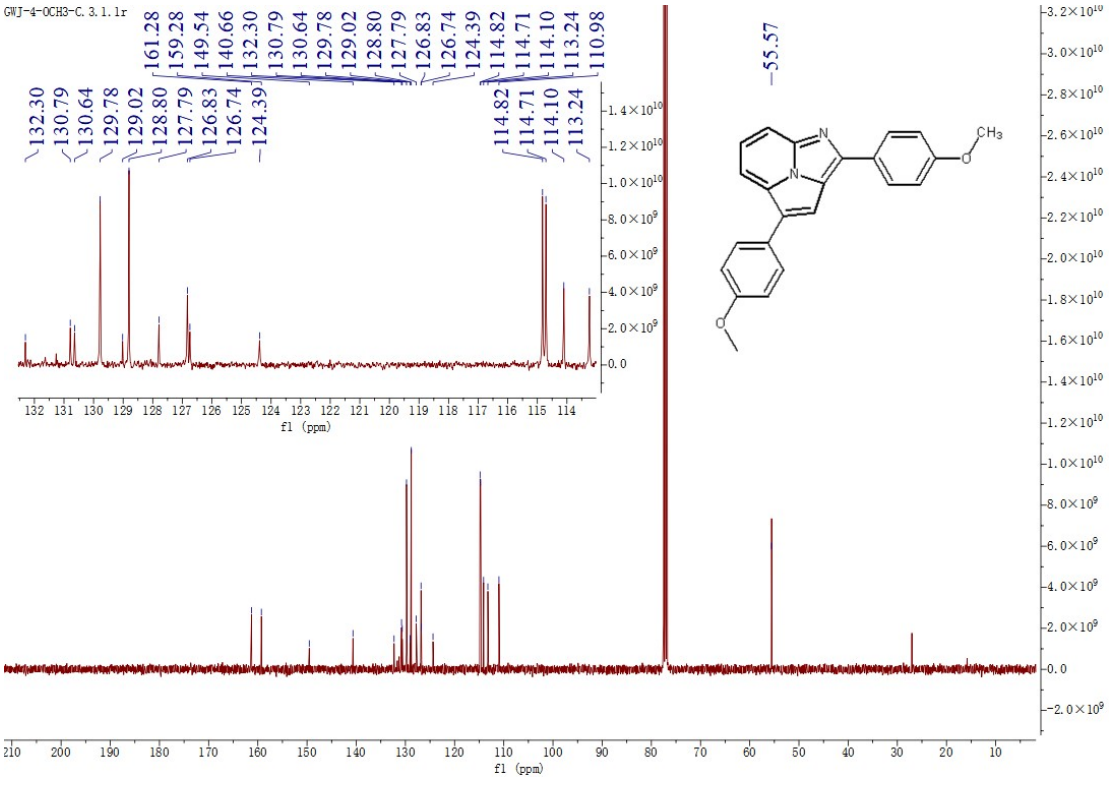



GWJ-4-CF3-C.2.1.1r
159.64
146.80
137.29
132.51
131.32
128.95
128.32
127.61
127.21
126.20
126.16
125.16
114.93
114.34
114.15
112.63
55.59
132.51
131.32
128.95
128.32
127.61
127.21
126.20
126.16
125.16
CF3
f1 (ppm)

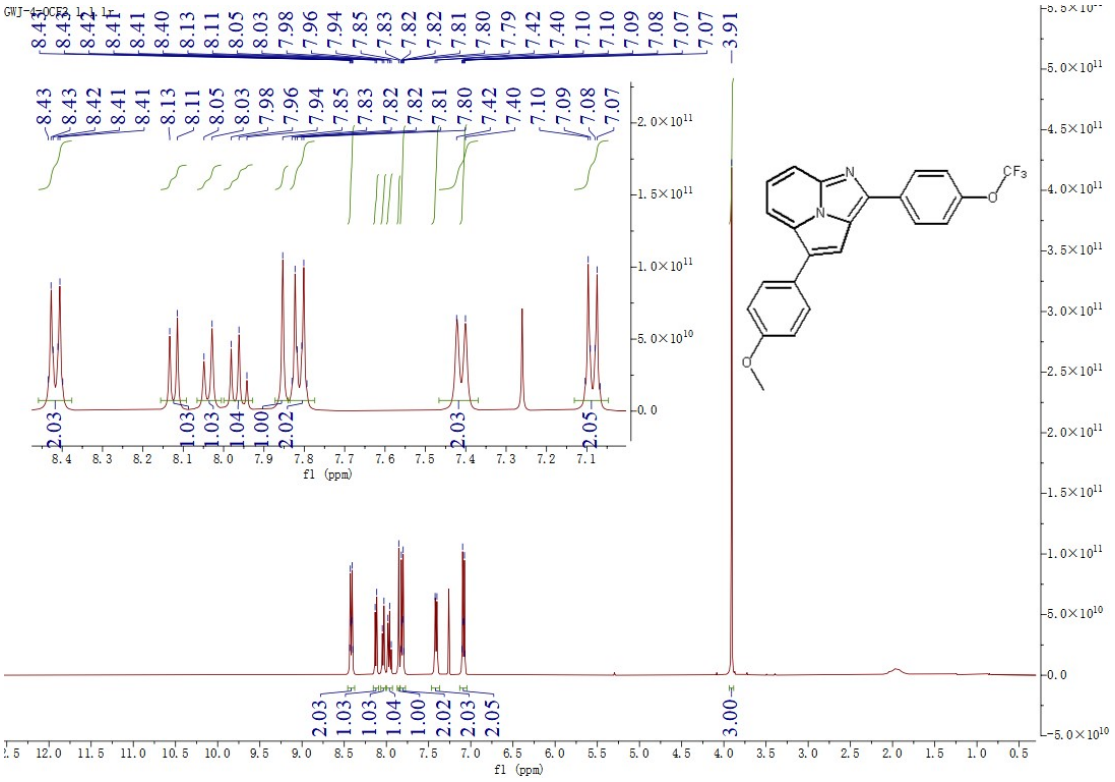

GWJ-4-CF3-F.3.1.1r
-62.64
CF3
f1 (ppm)

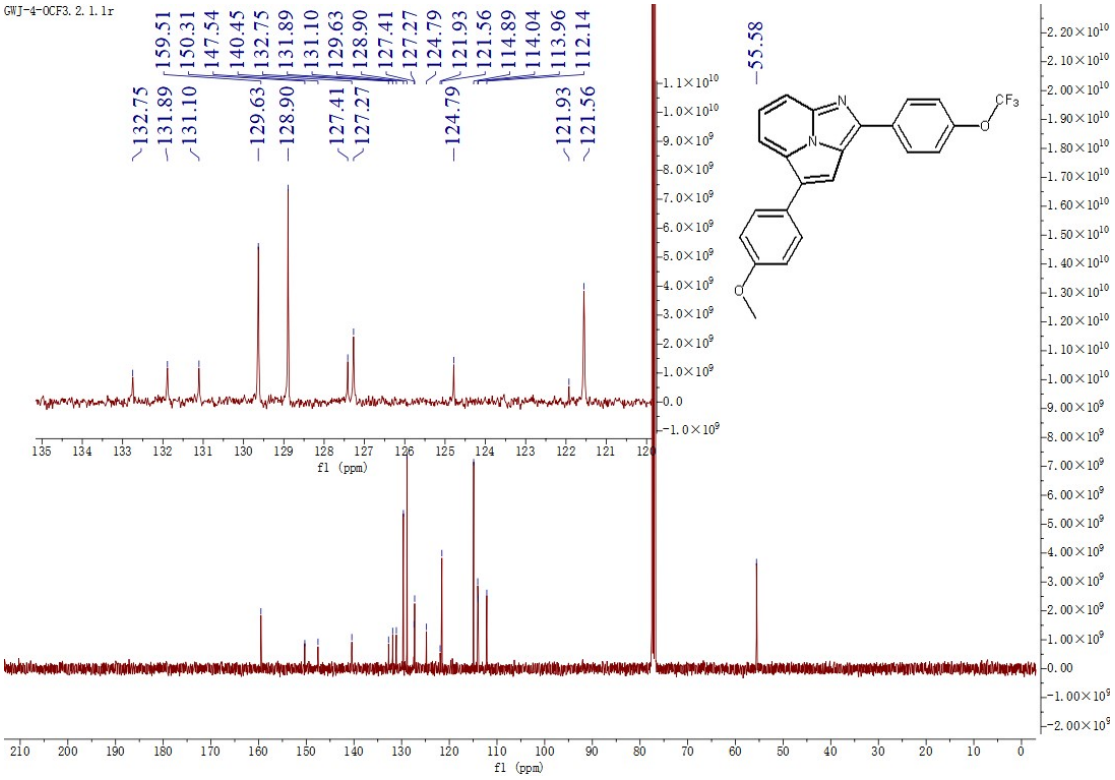
3-methoxy-5-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**12**):

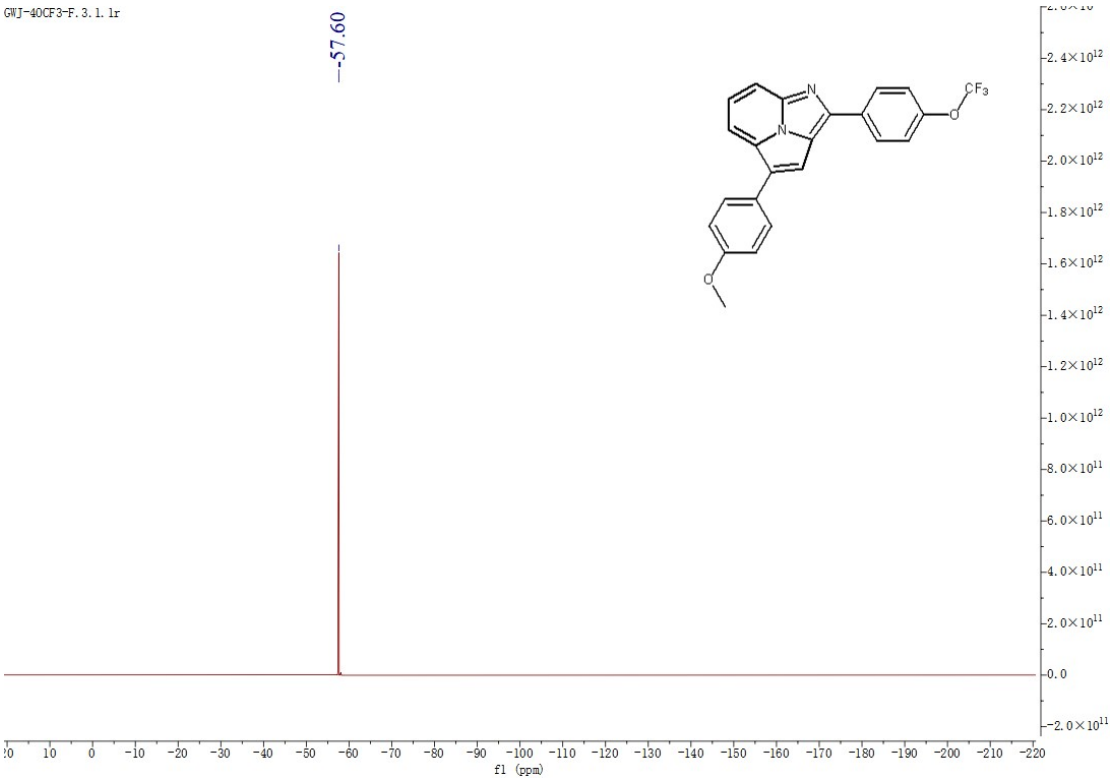




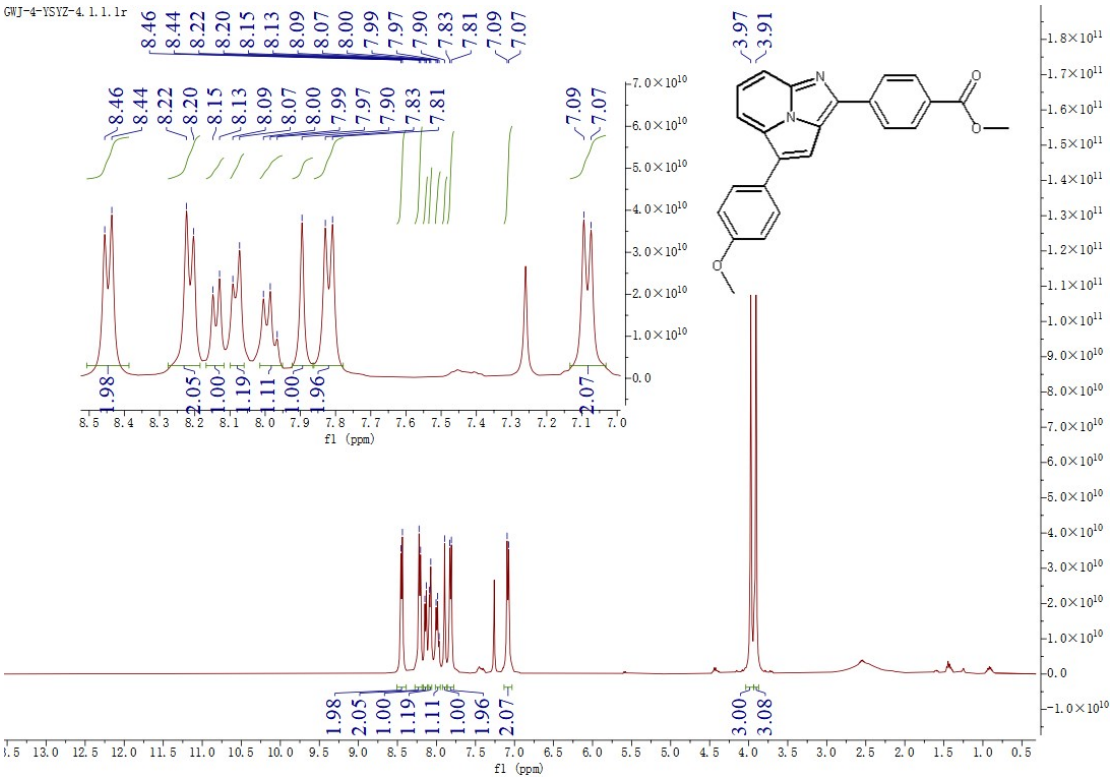
6-(4-methoxyphenyl)-1-(4-(trifluoromethoxy)phenyl)imidazo[5,1,2-*cd*]indolizine (**13**):

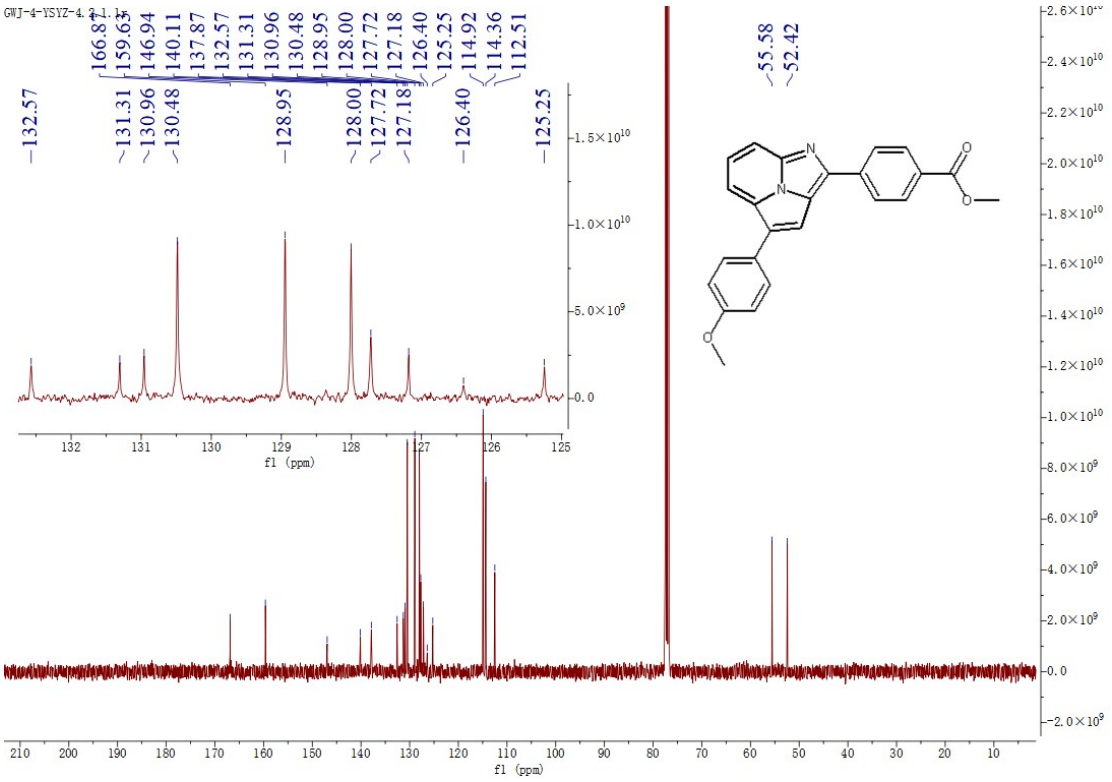




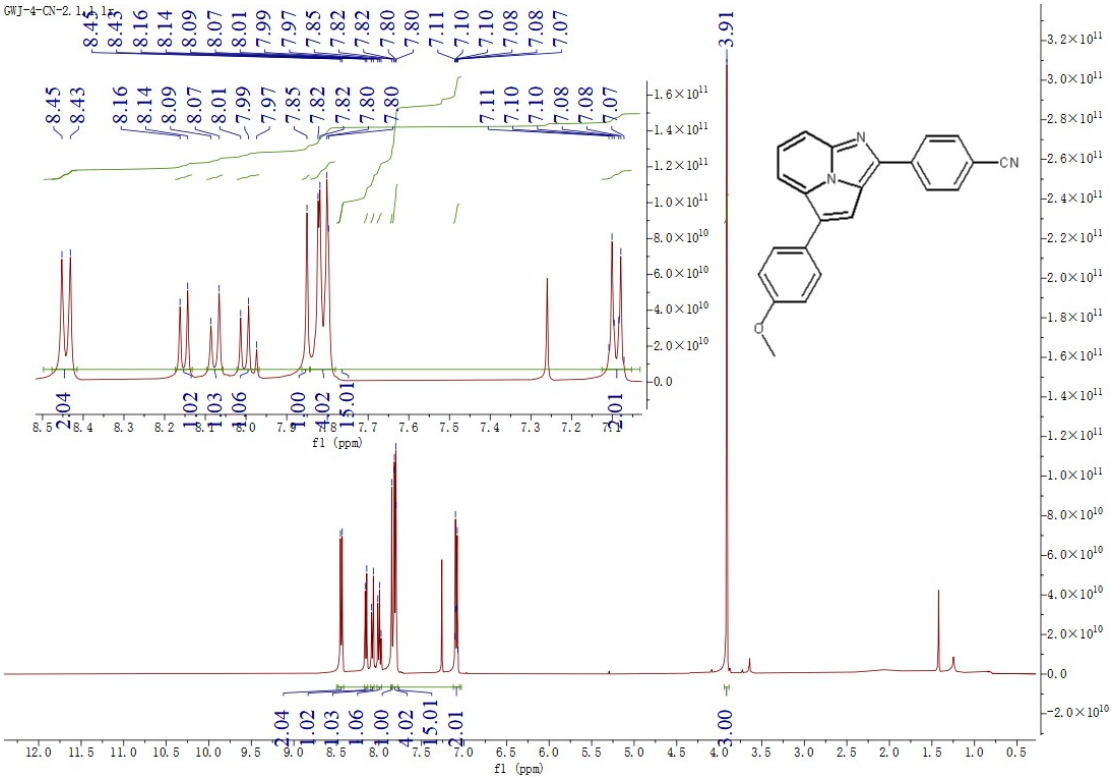


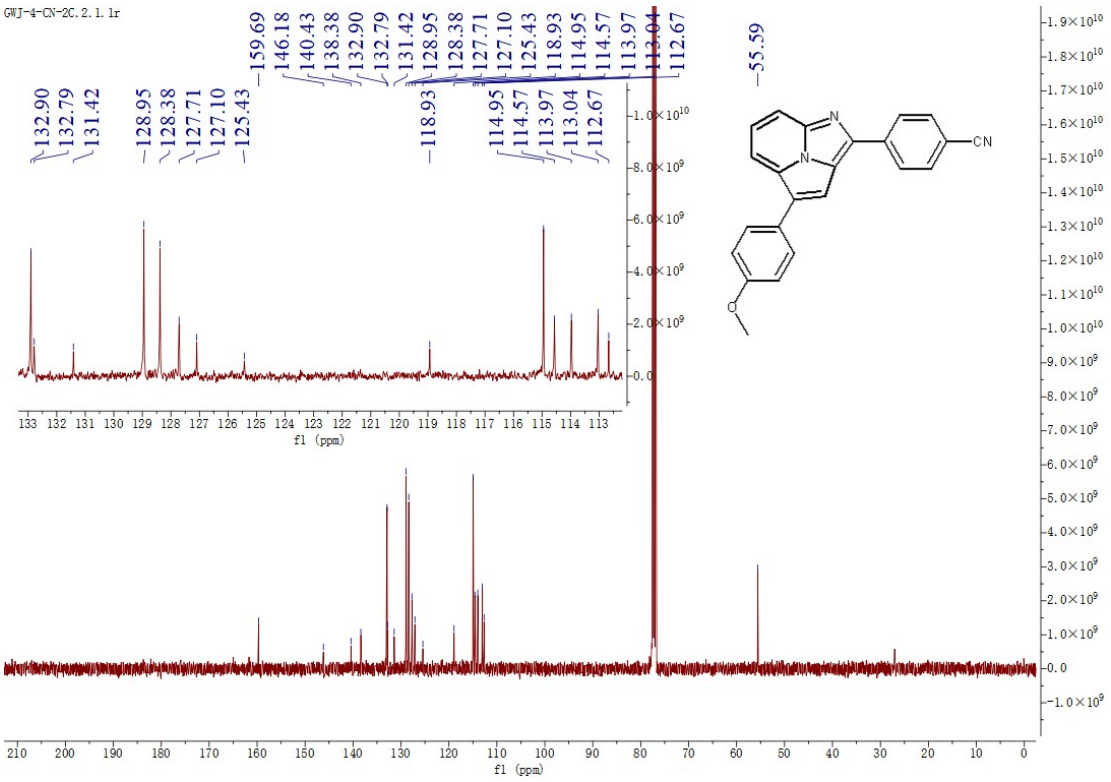
methyl 4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzoate (**14**):



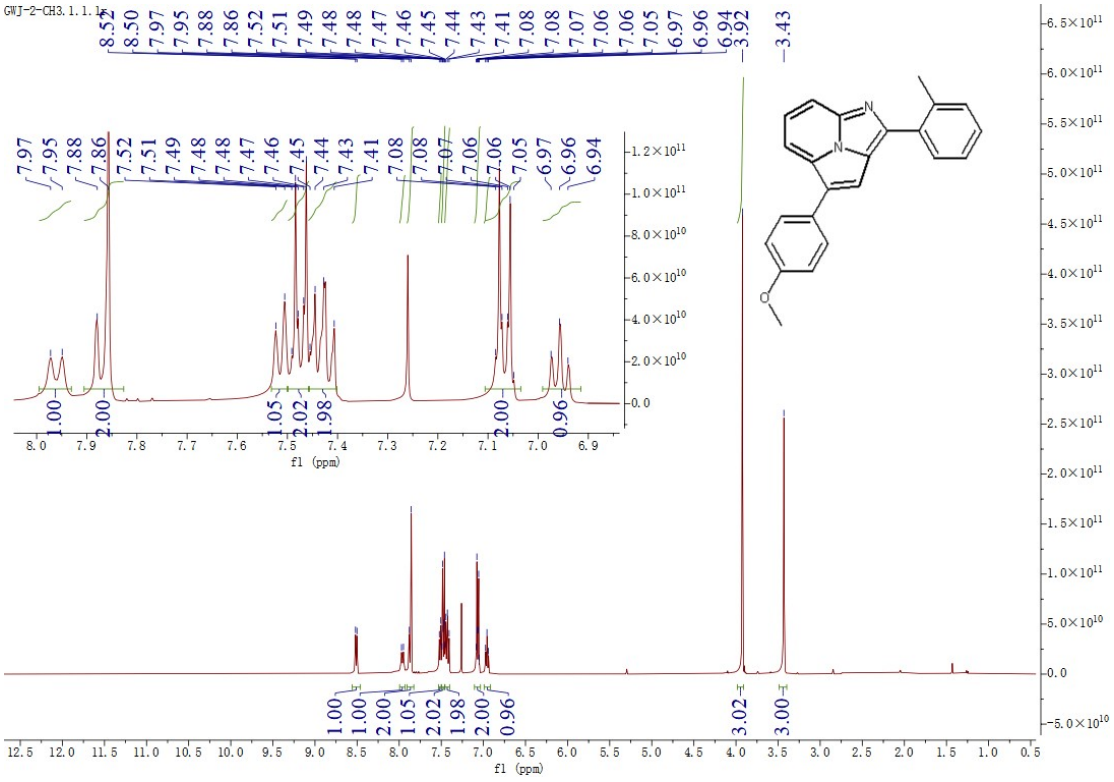


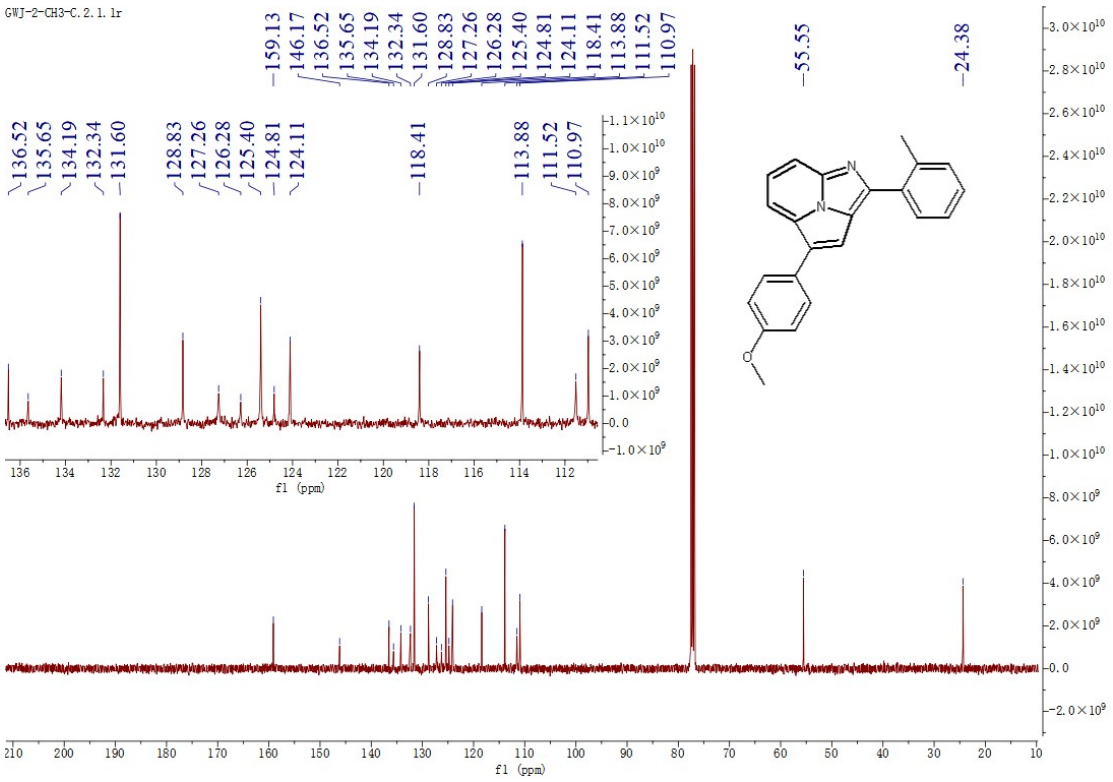
4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzonitrile (**15**):



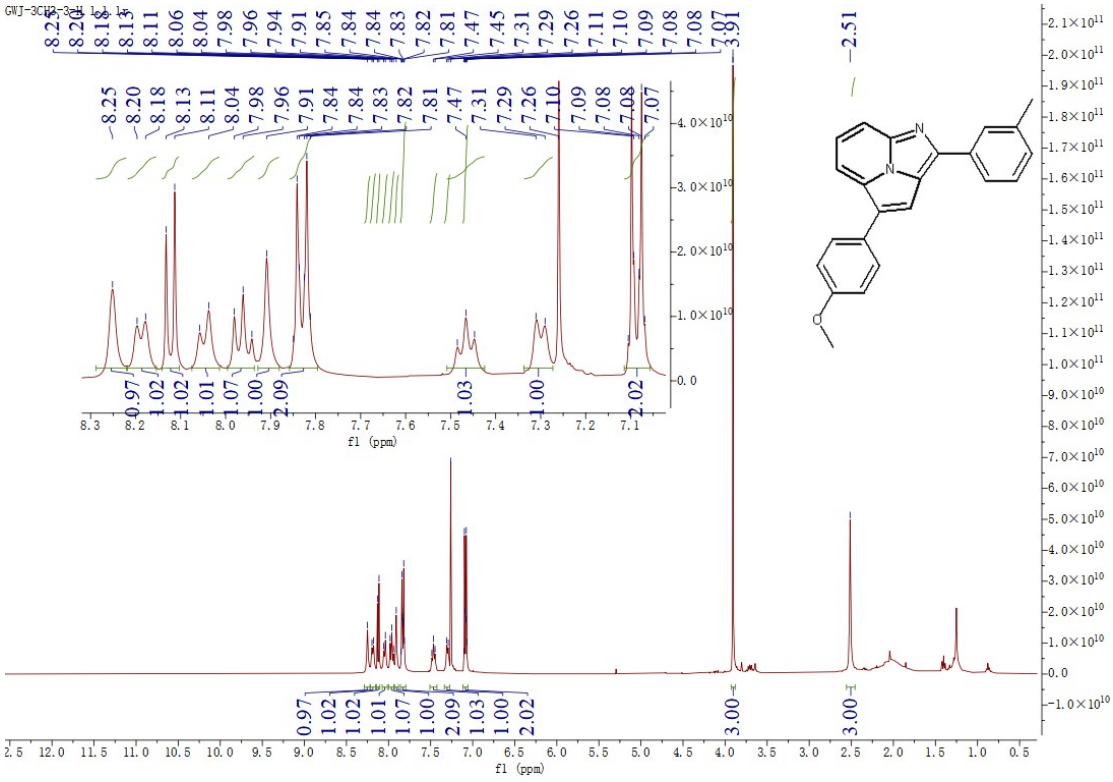


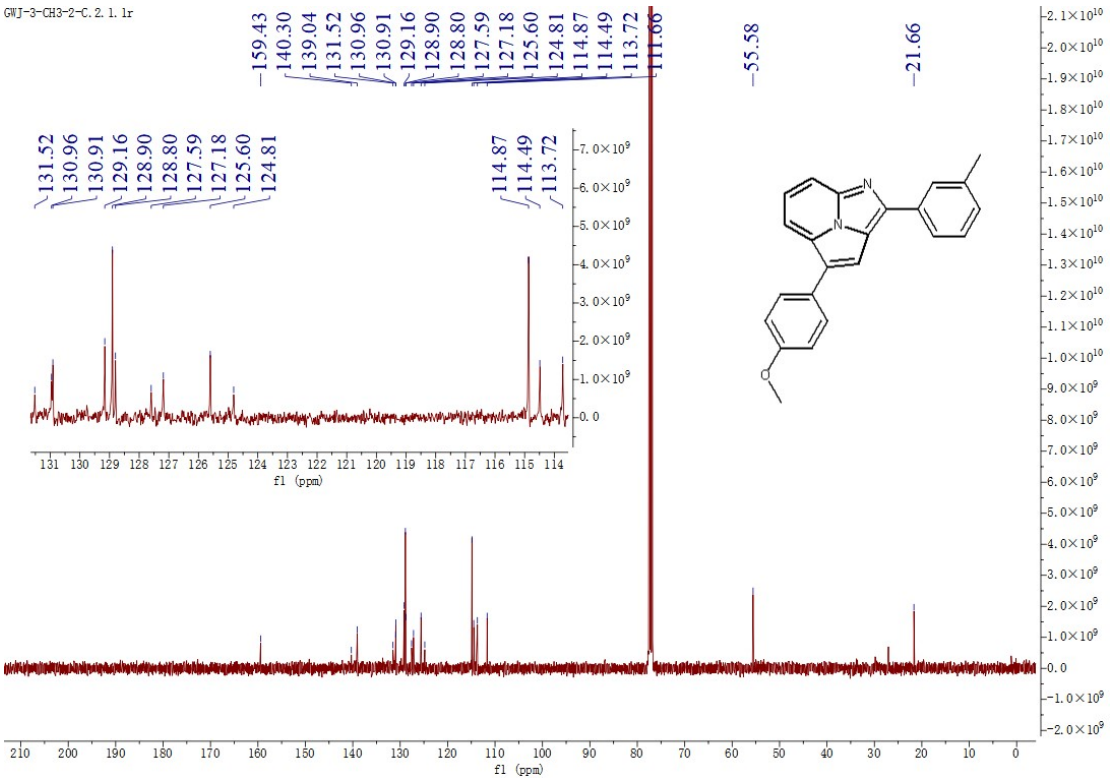
6-(4-methoxyphenyl)-1-(*o*-tolyl)imidazo[5,1,2-*cd*]indolizine (**16**):



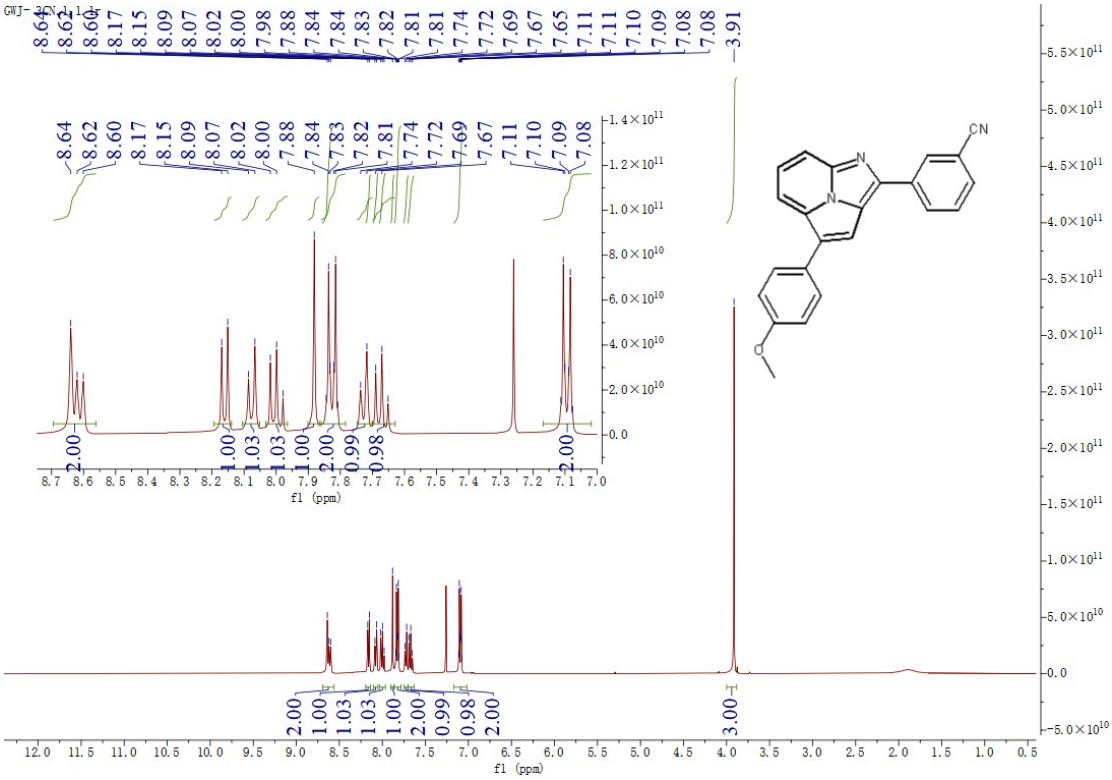


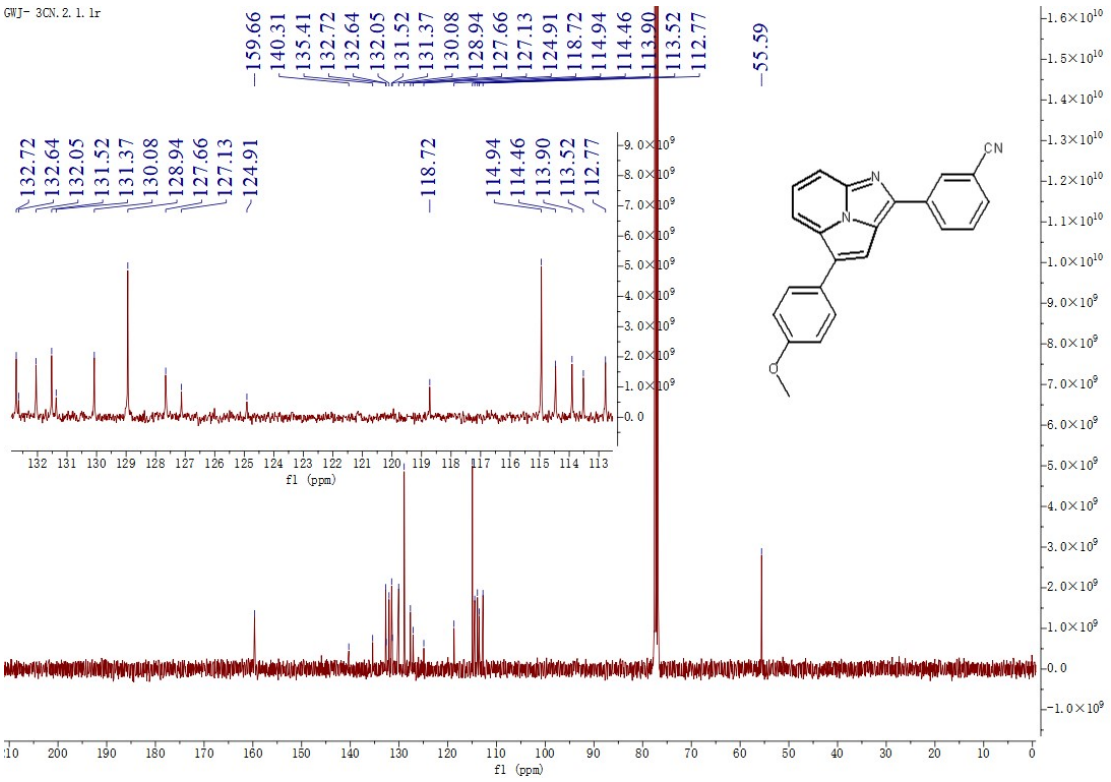
6-(4-methoxyphenyl)-1-(*m*-tolyl)imidazo[5,1,2-*cd*]indolizine (**17**):



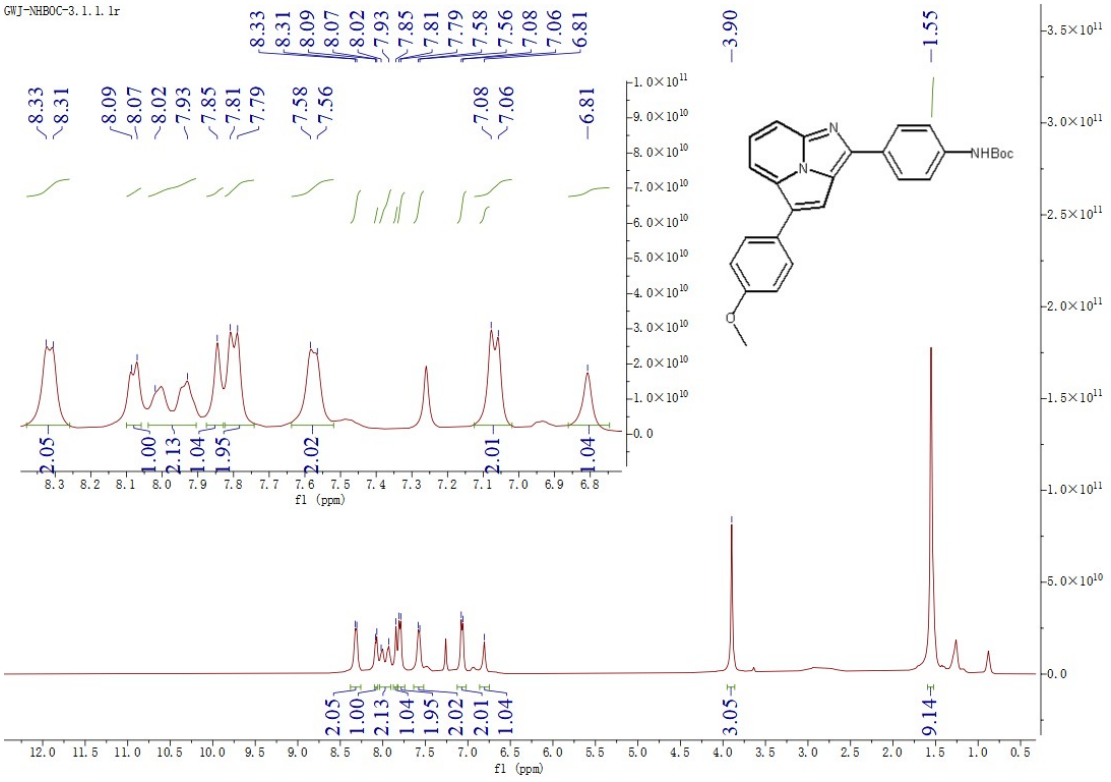


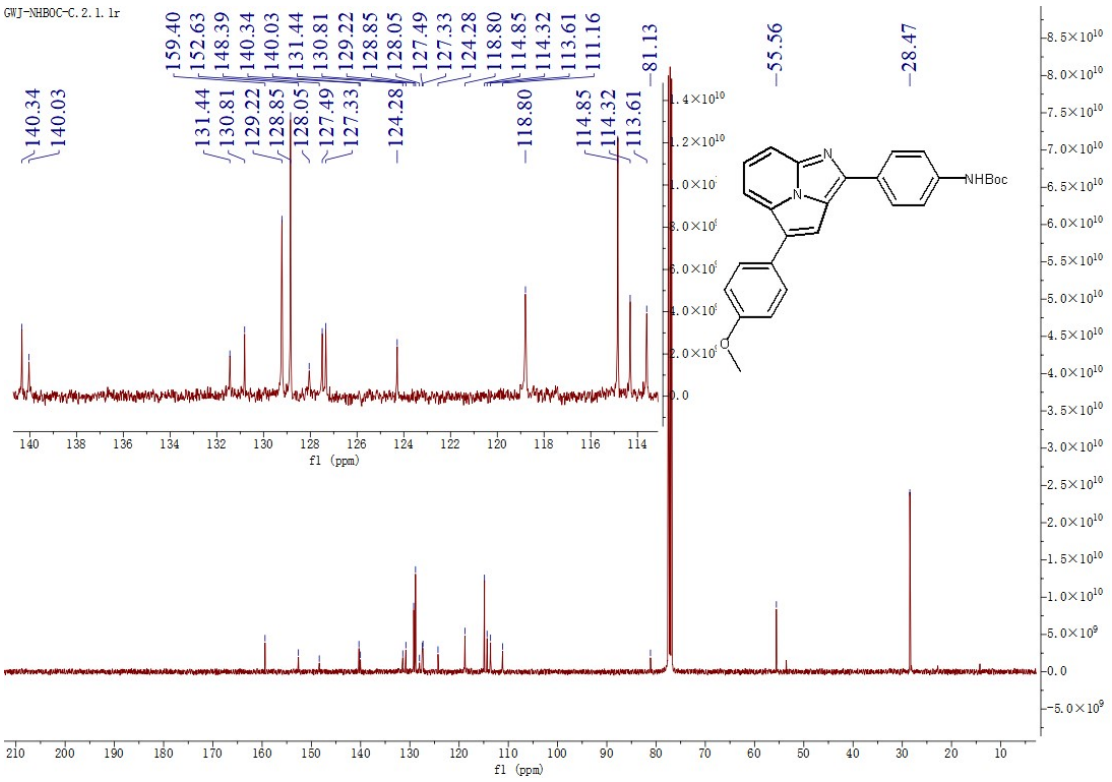
3-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)benzonitrile (**18**):



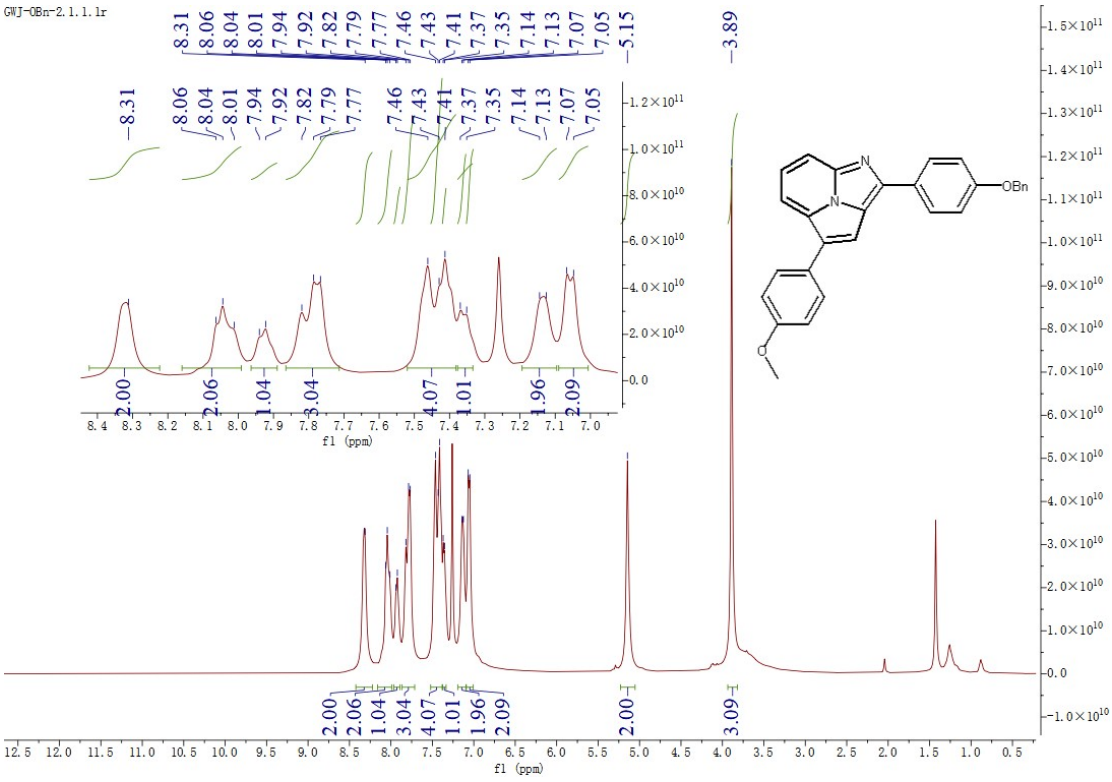


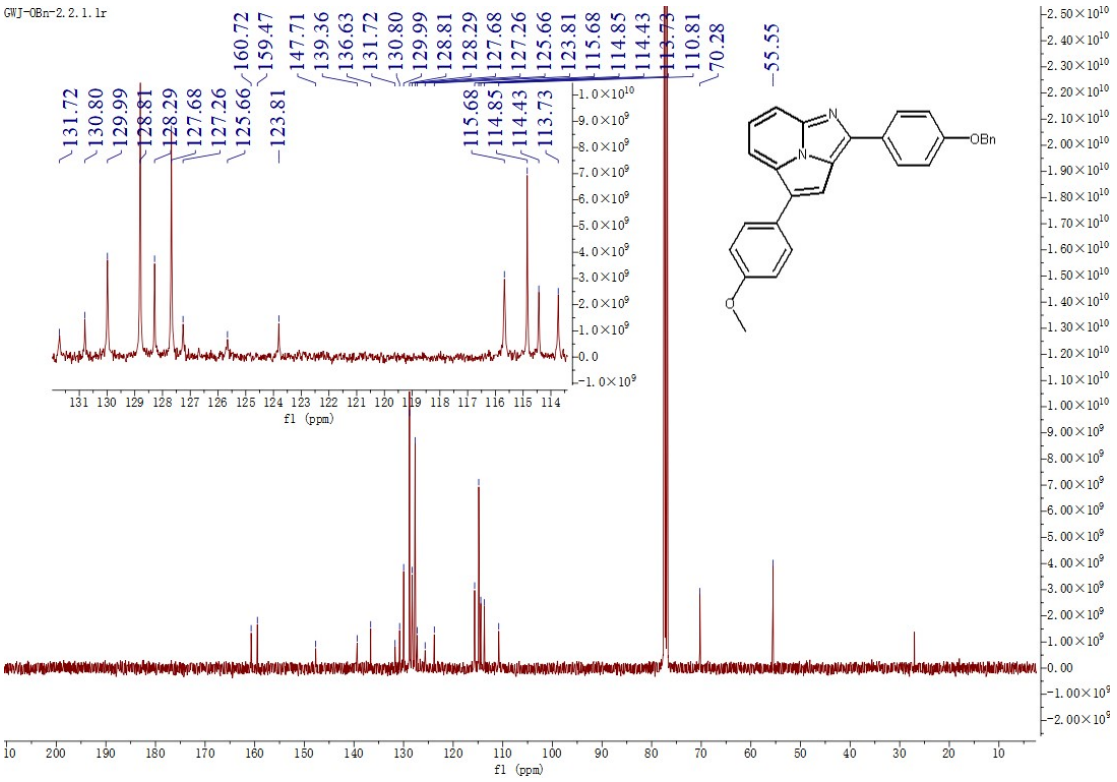
tert-butyl(4-(6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizin-1-yl)phenyl)carbamate (**19**)



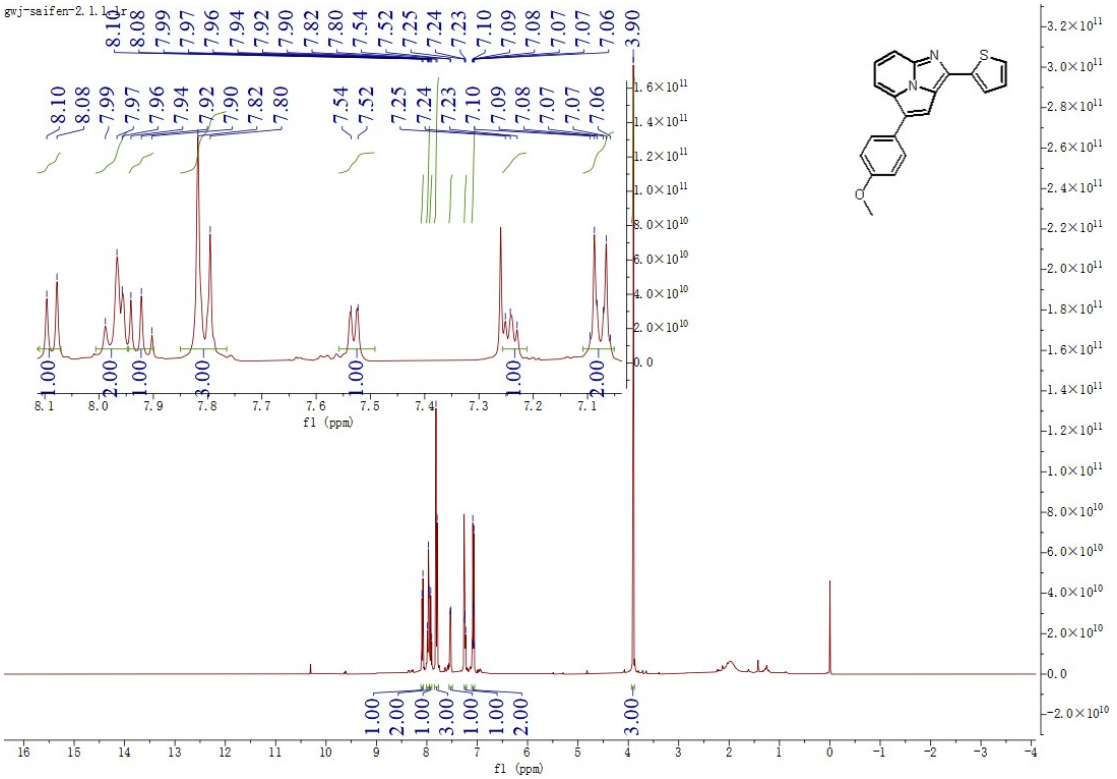


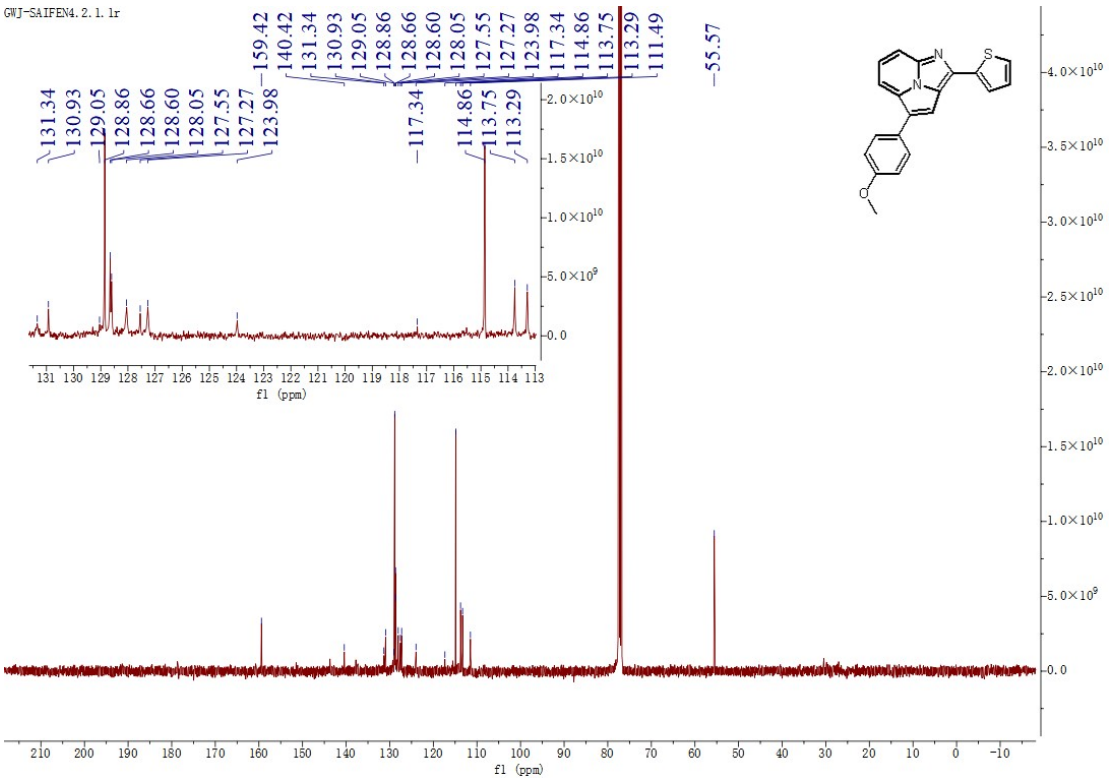
1-(4-(benzyloxy)phenyl)-6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**20**)



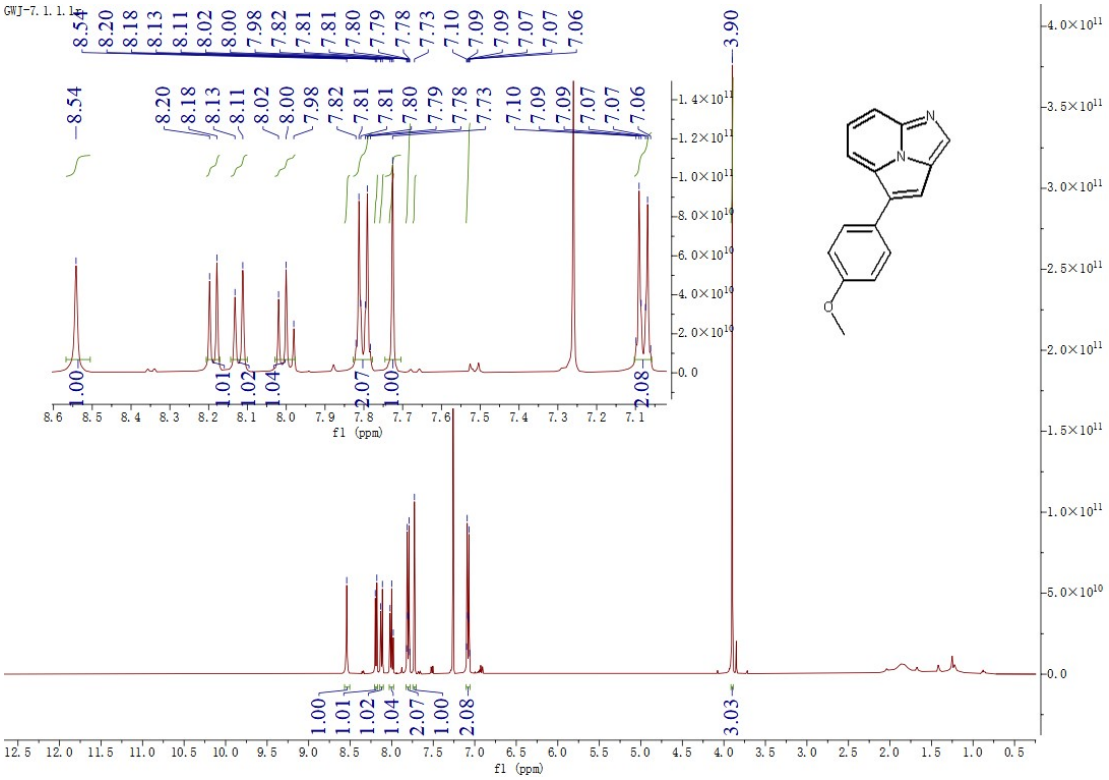


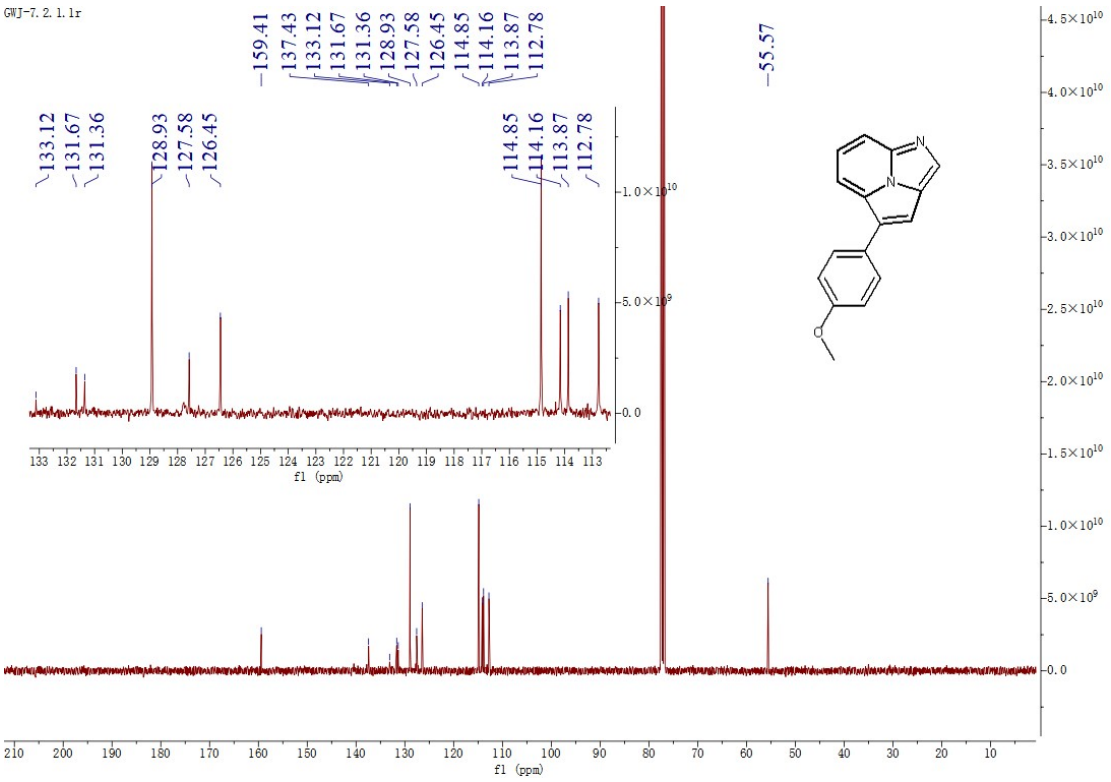
6-(4-methoxyphenyl)-1-(thiophen-2-yl)imidazo[5,1,2-*cd*]indolizine (**21**)



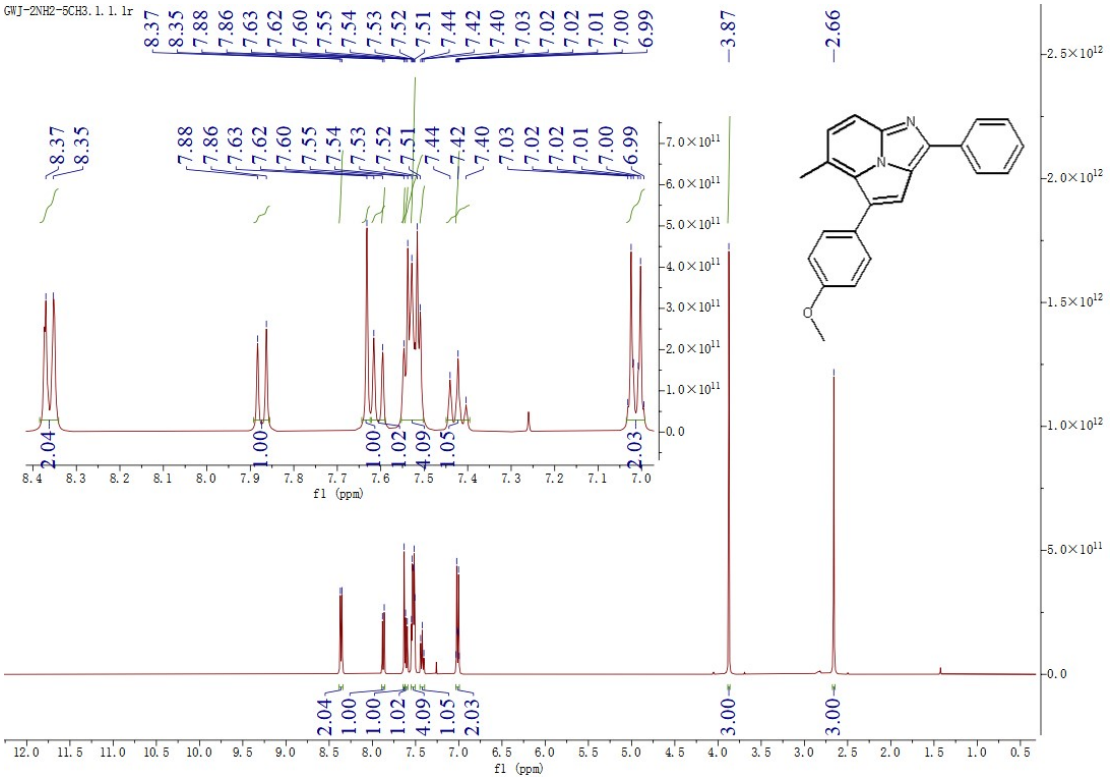


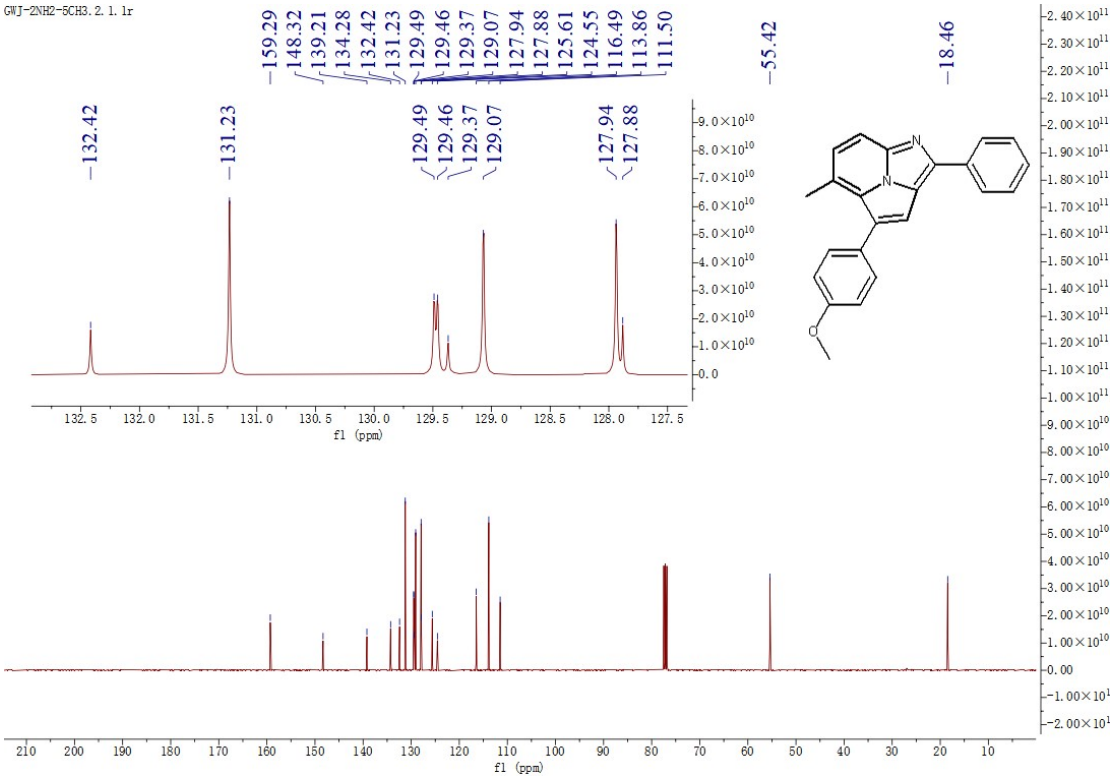
6-(4-methoxyphenyl)imidazo[5,1,2-*cd*]indolizine (**22**)



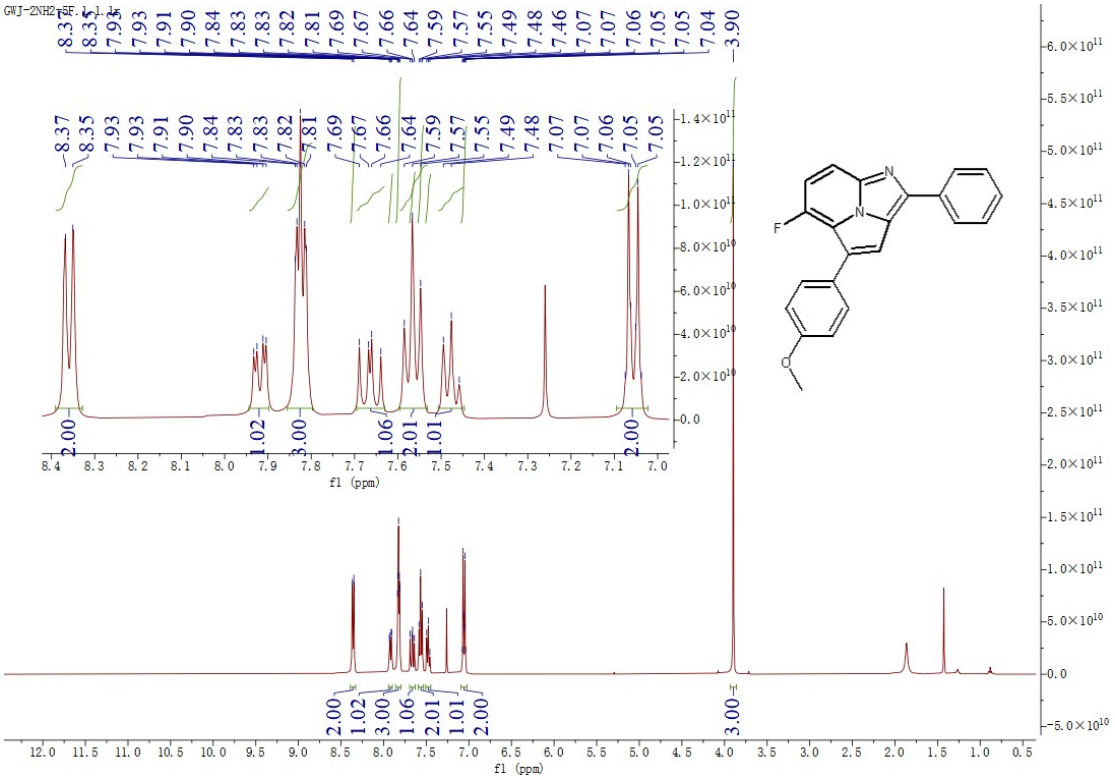


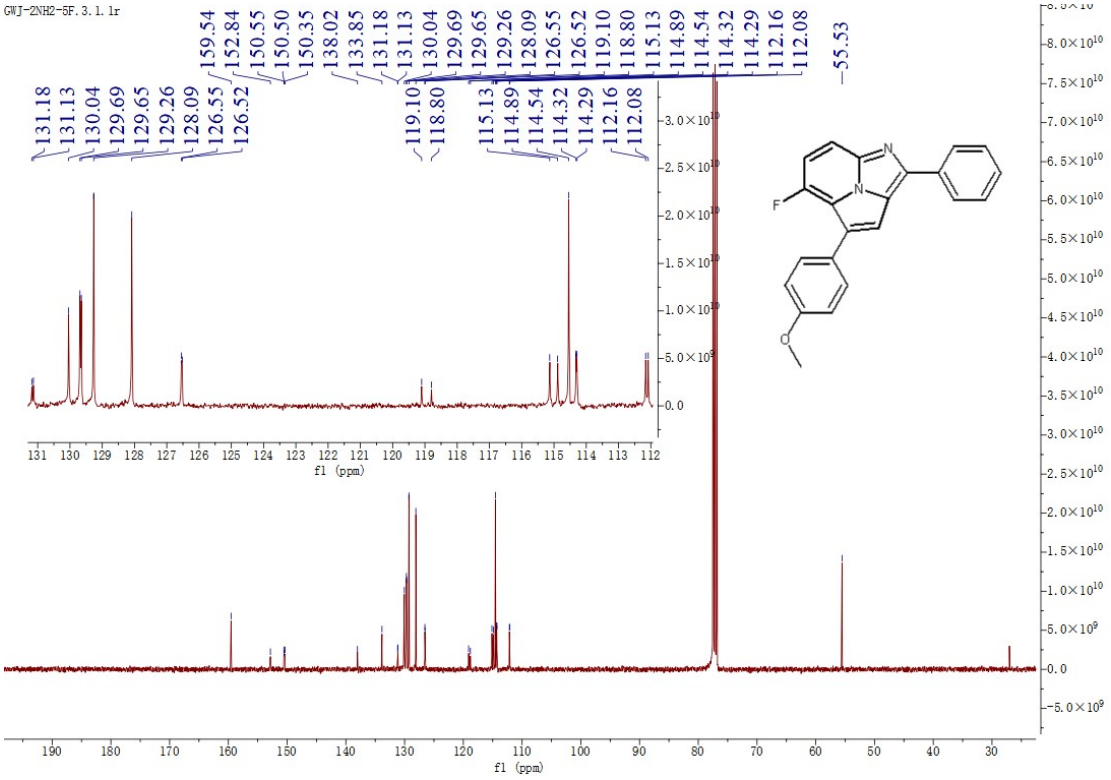
6-(4-methoxyphenyl)-5-methyl-1-phenylimidazo[5,1,2-*cd*]indolizine (**23**):

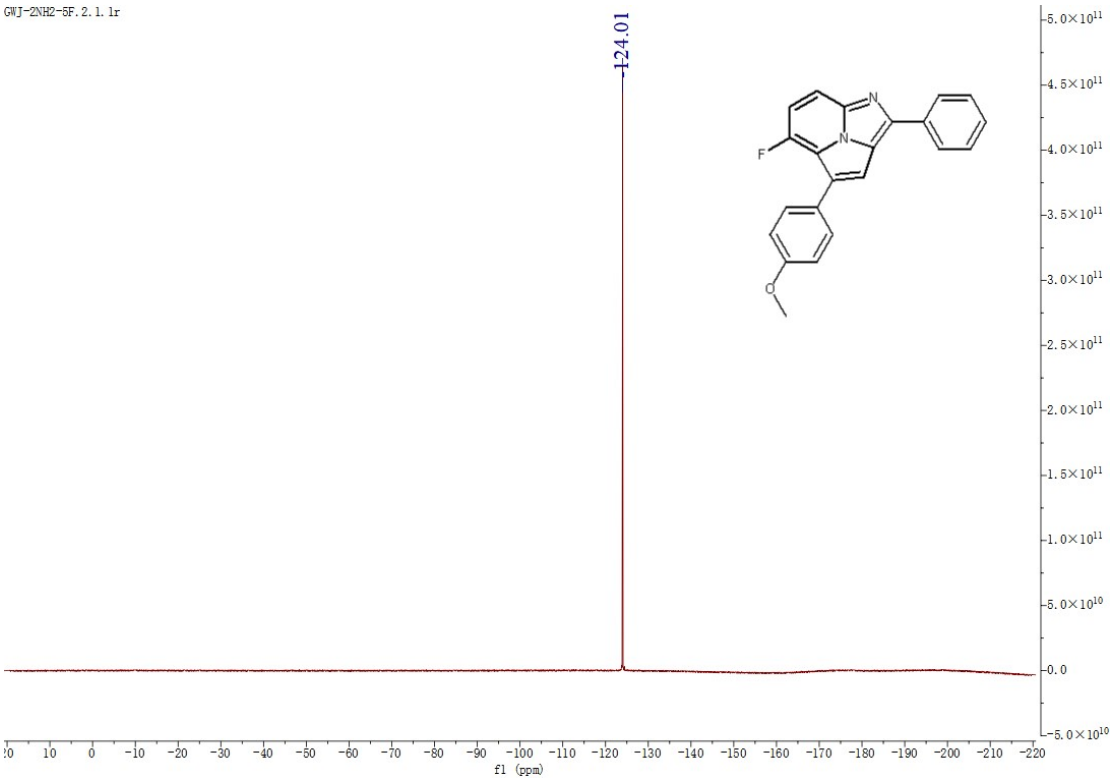




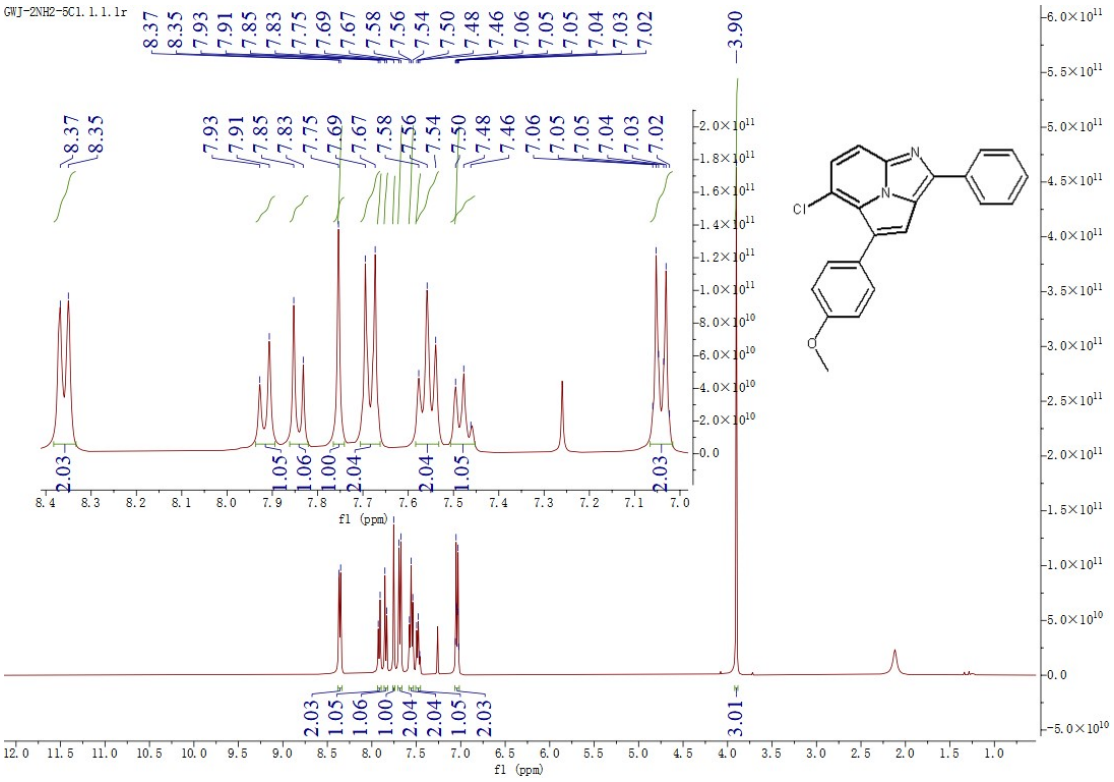
5-fluoro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**24**):

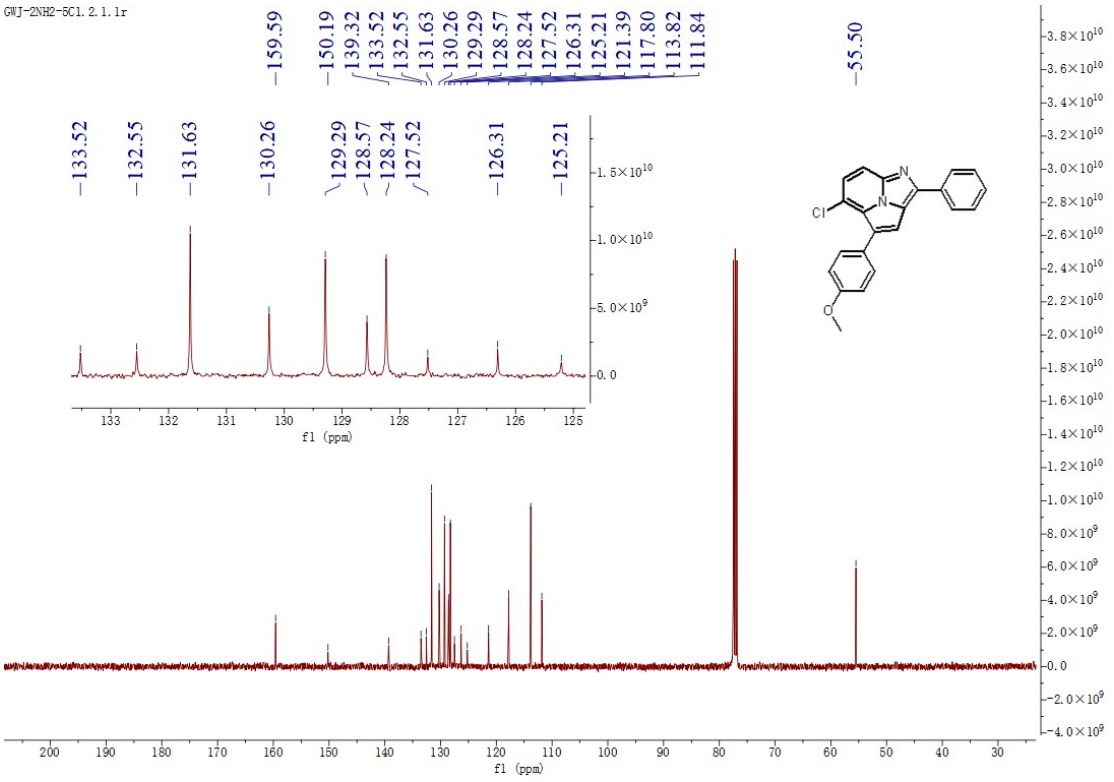



GWJ-2NH2-5F.3.1.1r
159.54
152.84
150.55
150.50
150.35
138.02
133.85
131.18
131.13
130.04
129.69
129.65
129.26
128.09
126.55
126.52
119.10
118.80
115.13
114.89
114.54
114.32
114.29
112.16
112.08
55.53
f1 (ppm)

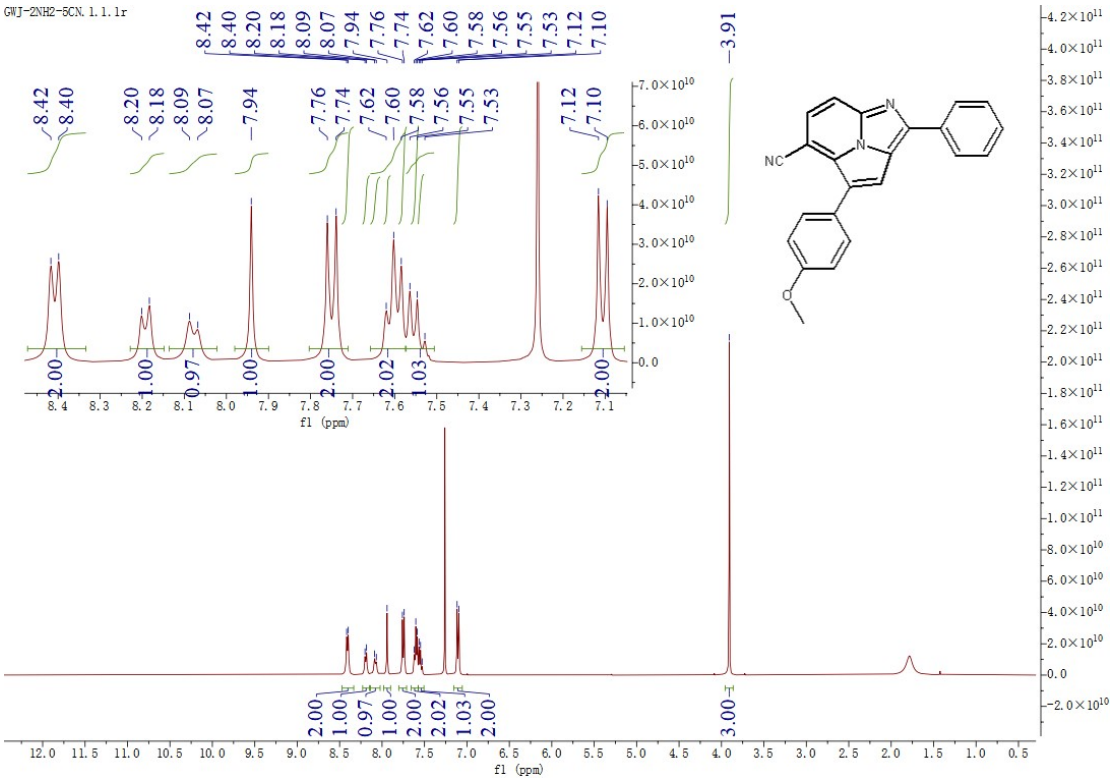

GWJ-2NH2-5F.2.1.1r
-124.01
f1 (ppm)

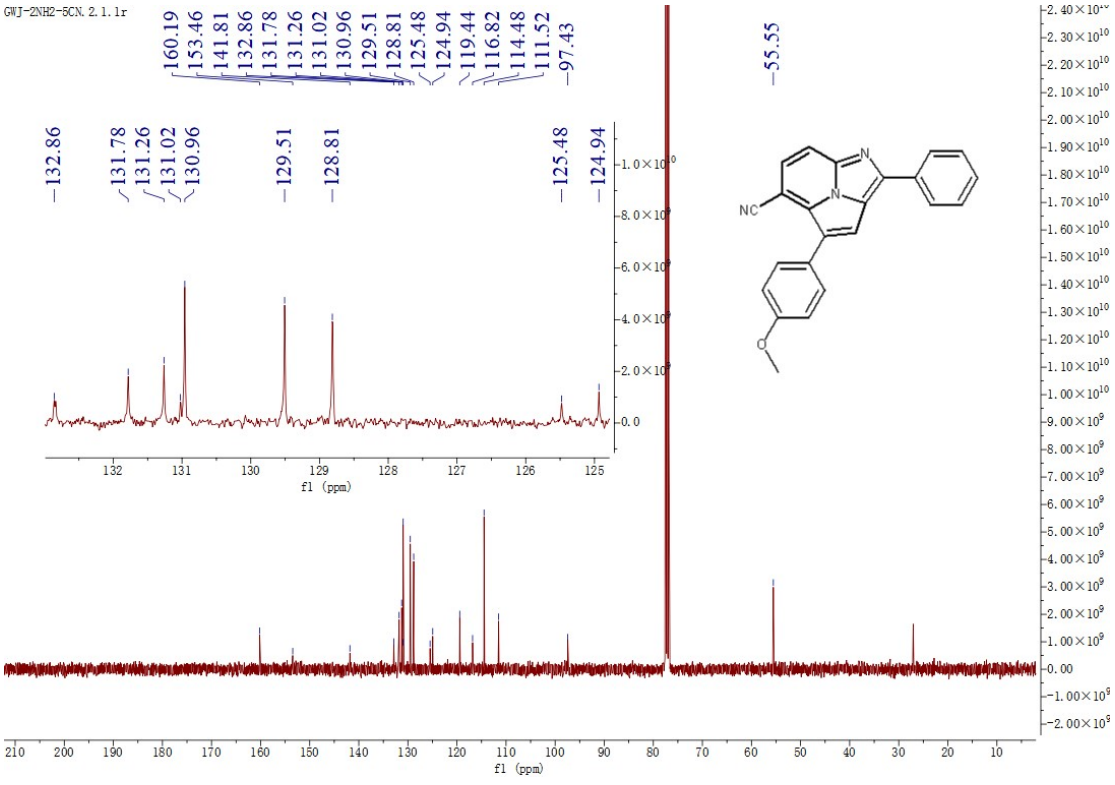
5-chloro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**25**):



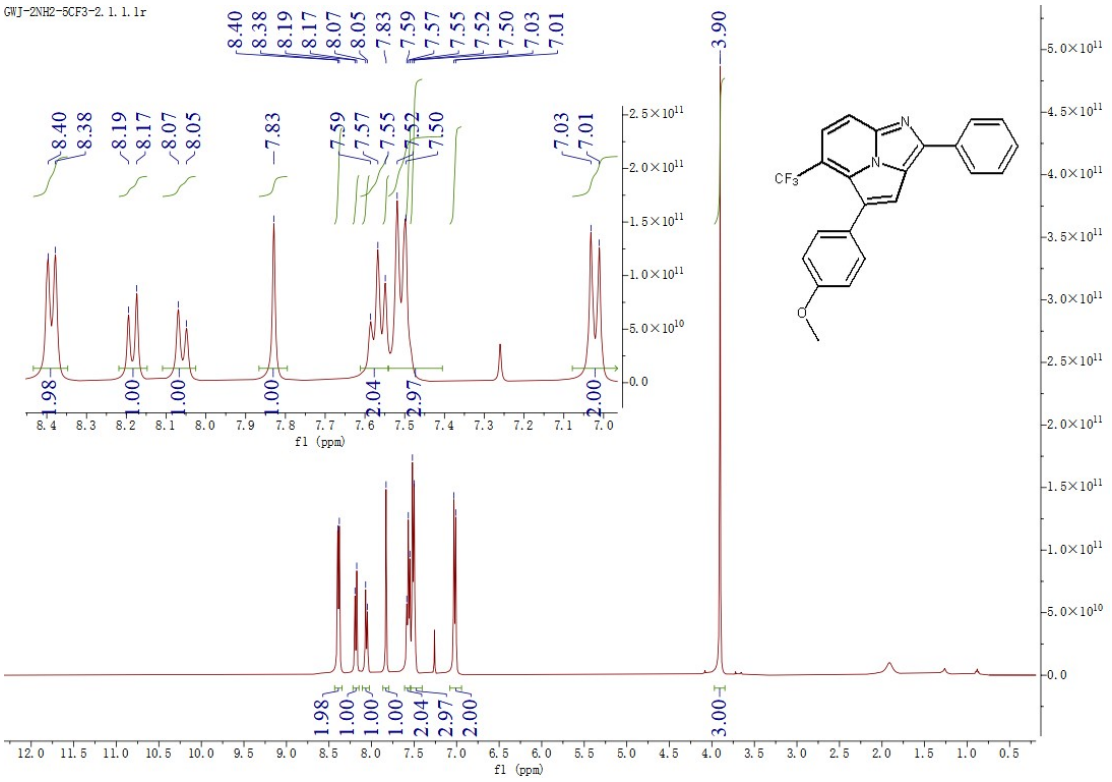


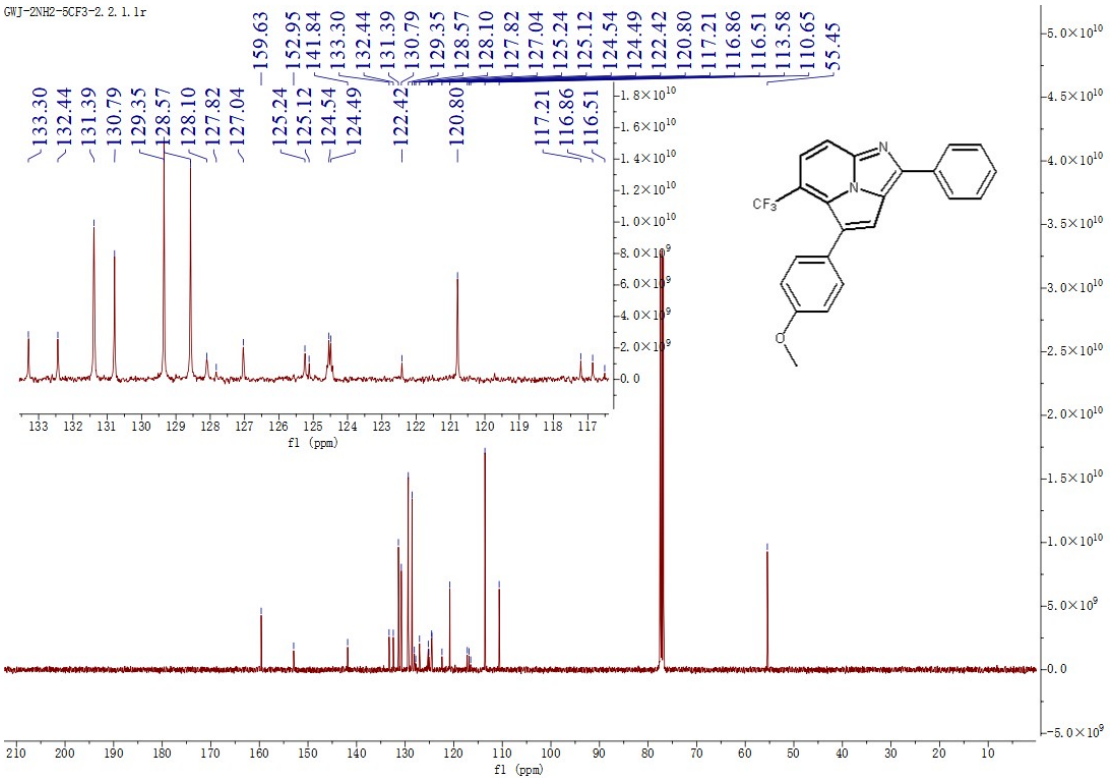
6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine-5-carbonitrile (**26**):

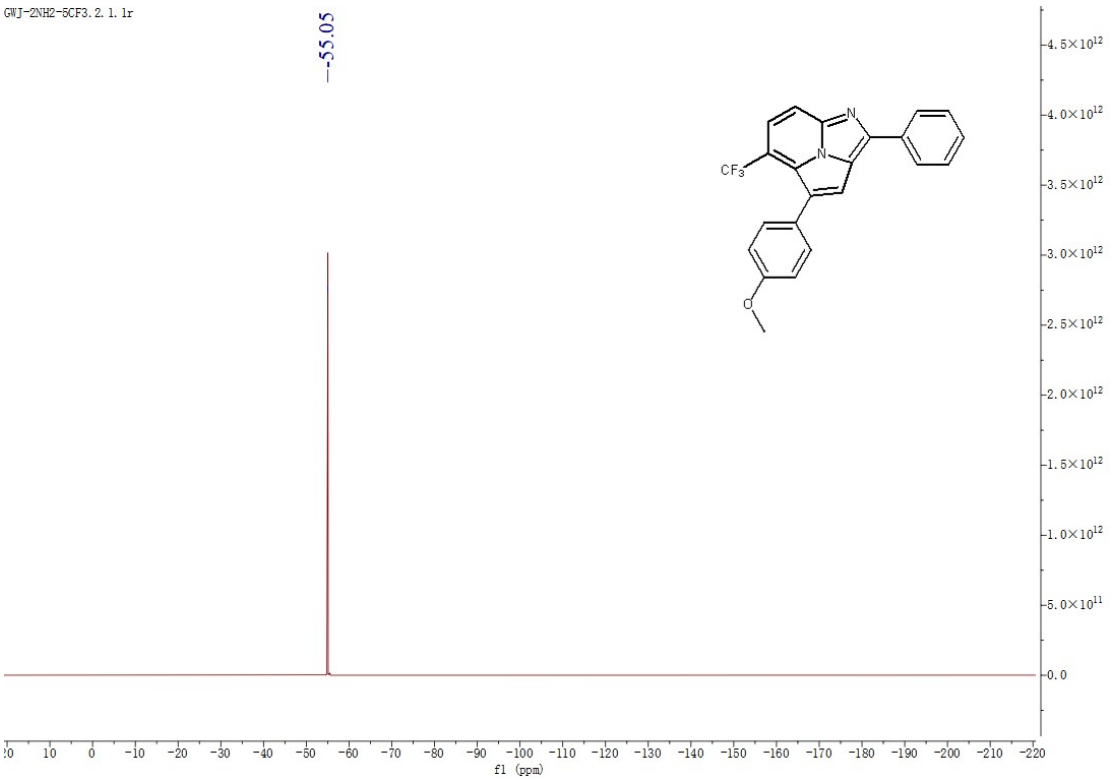




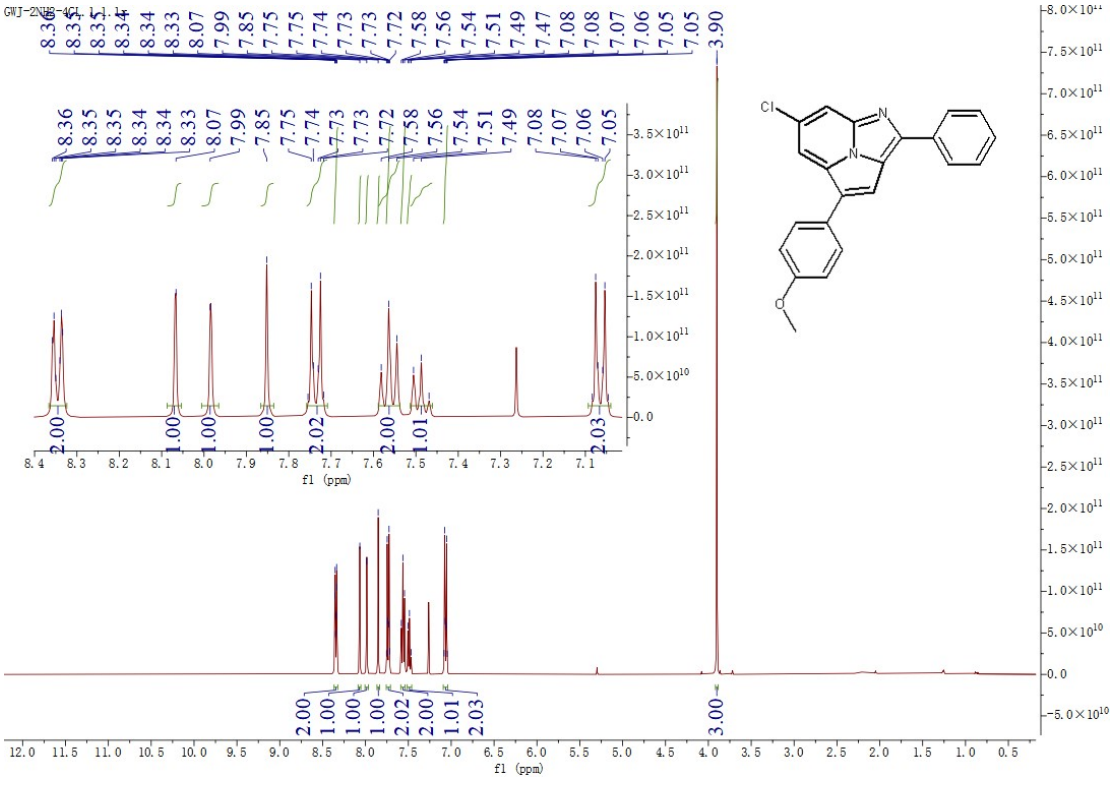
(4-methoxyphenyl)-1-phenyl-5-(trifluoromethyl)imidazo[5,1,2-*cd*]indolizine (**27**):

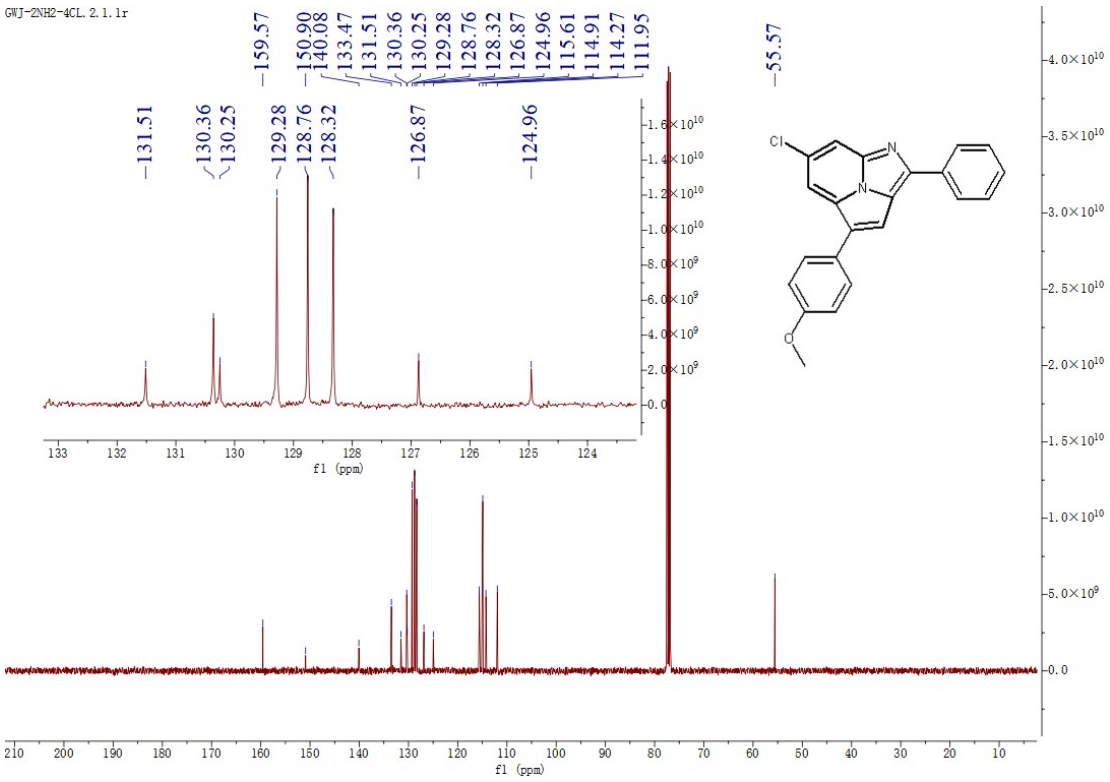




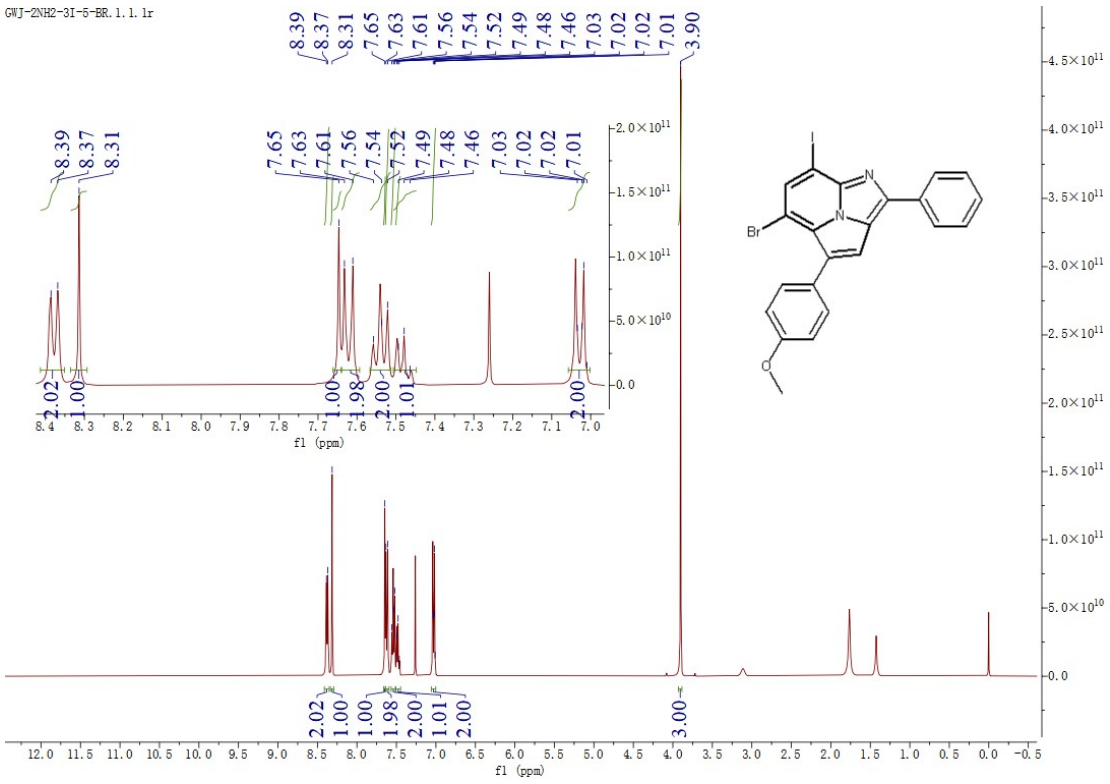


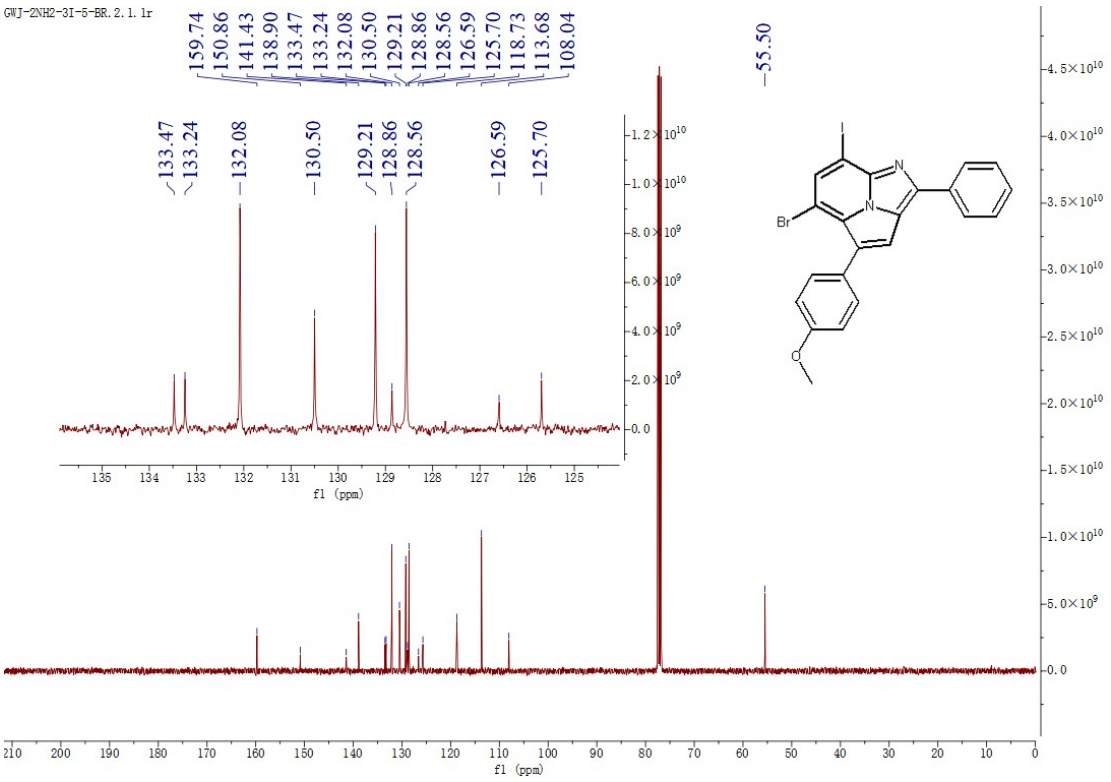
4-chloro-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**28**):



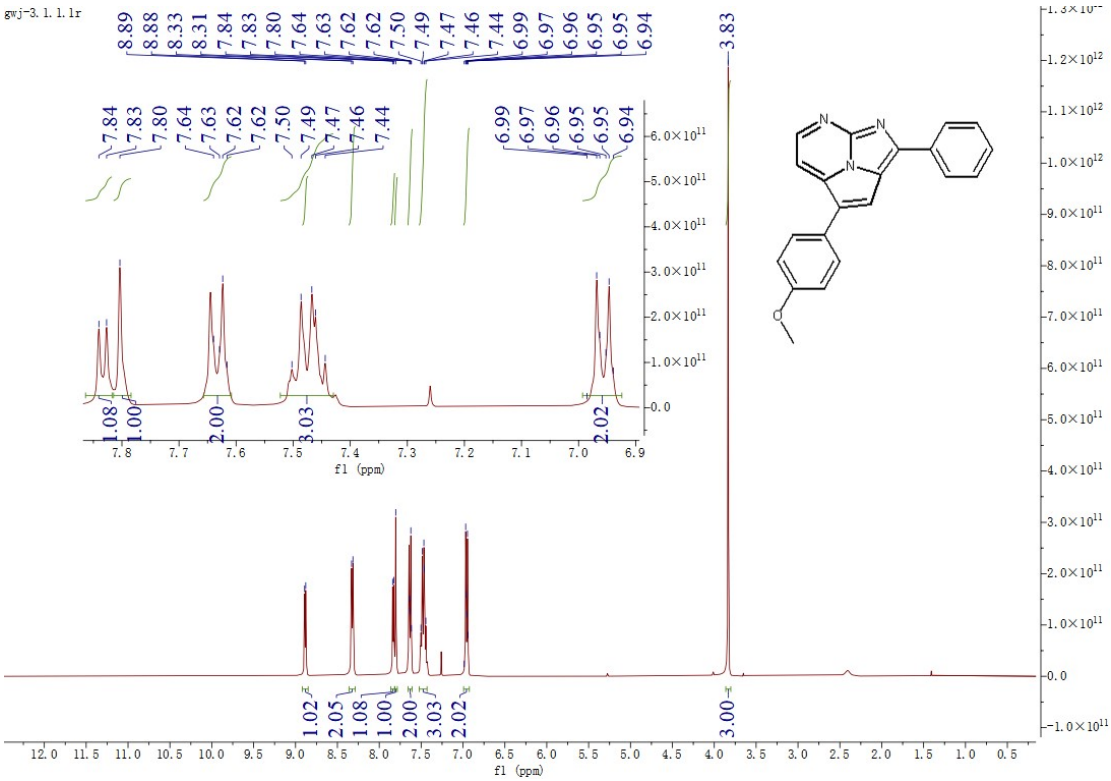


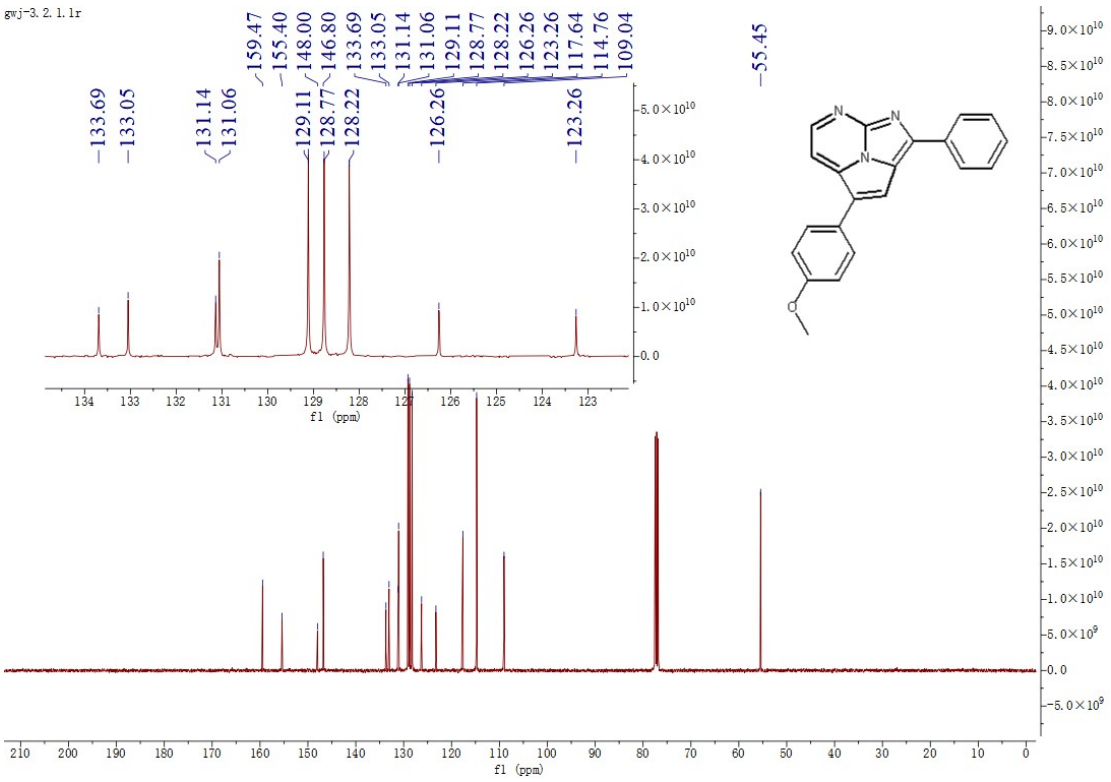
5-bromo-3-iodo-6-(4-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**29**):



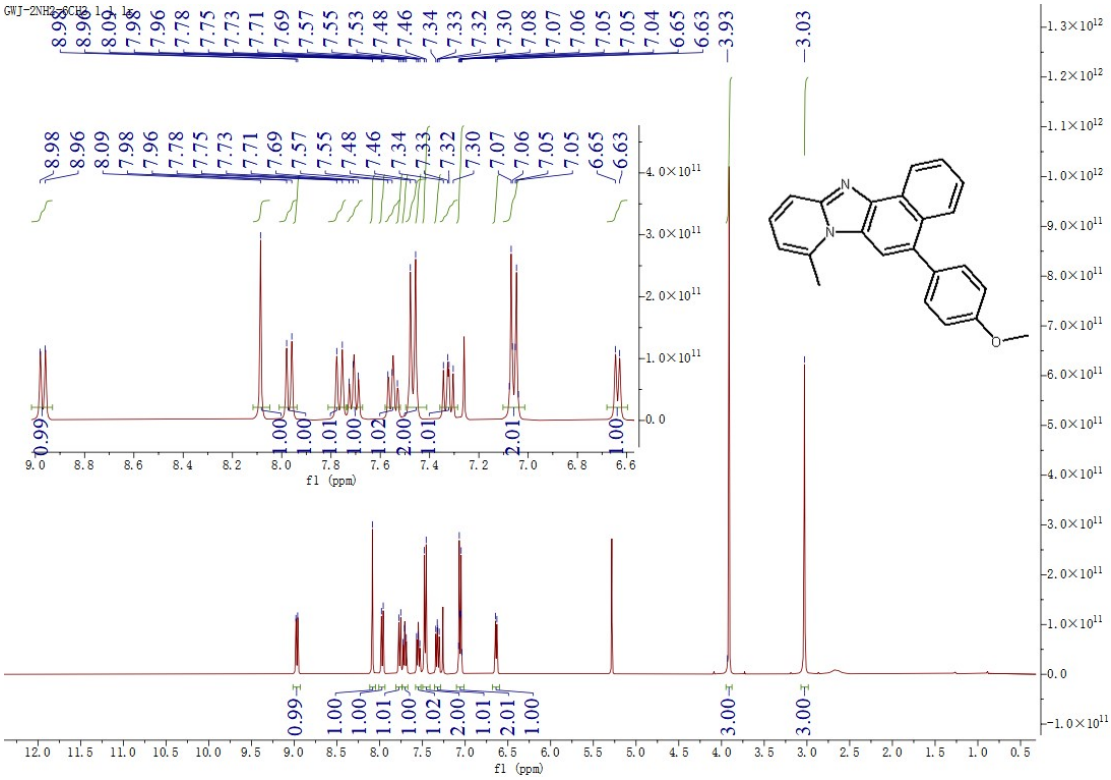


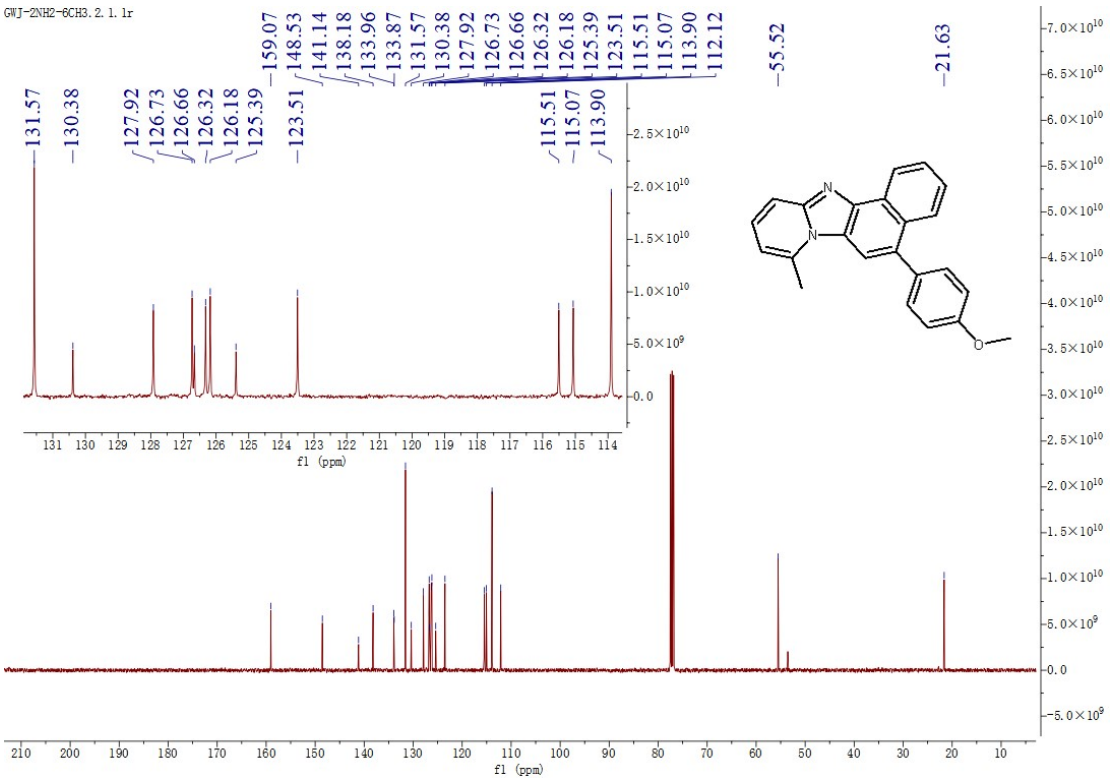
1-(4-methoxyphenyl)-3-phenyl-2a1,4,5-triazacyclopenta[*cd*]indene (**30**):



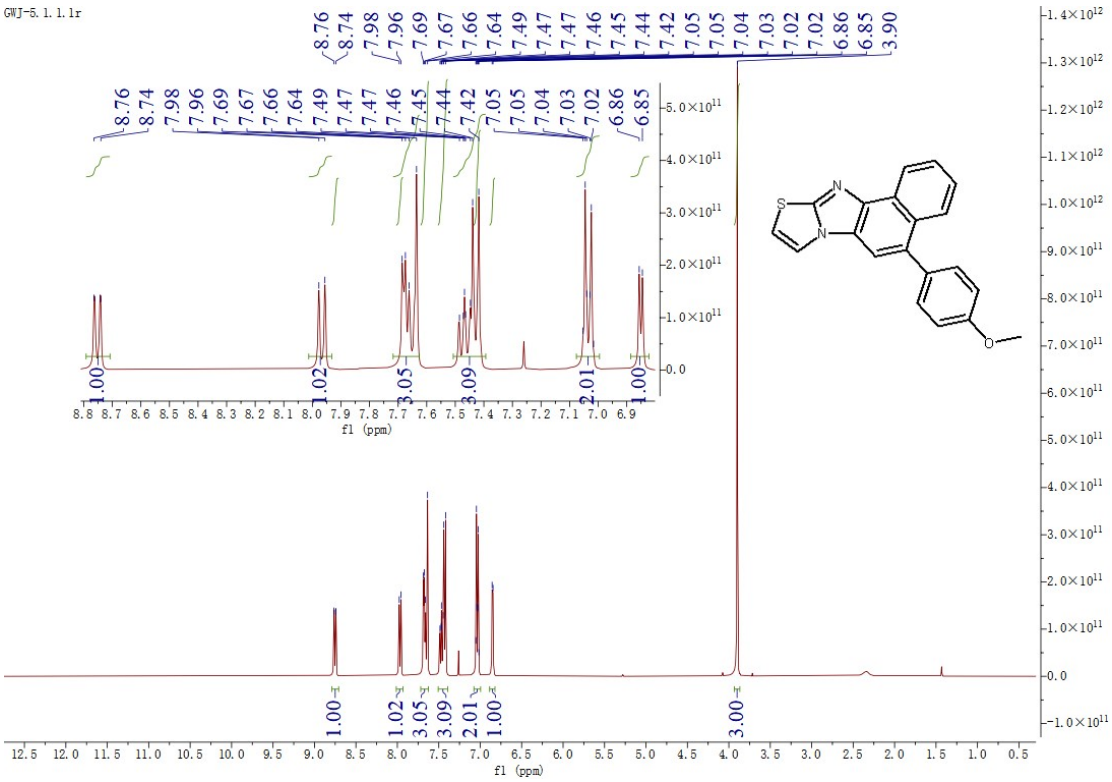


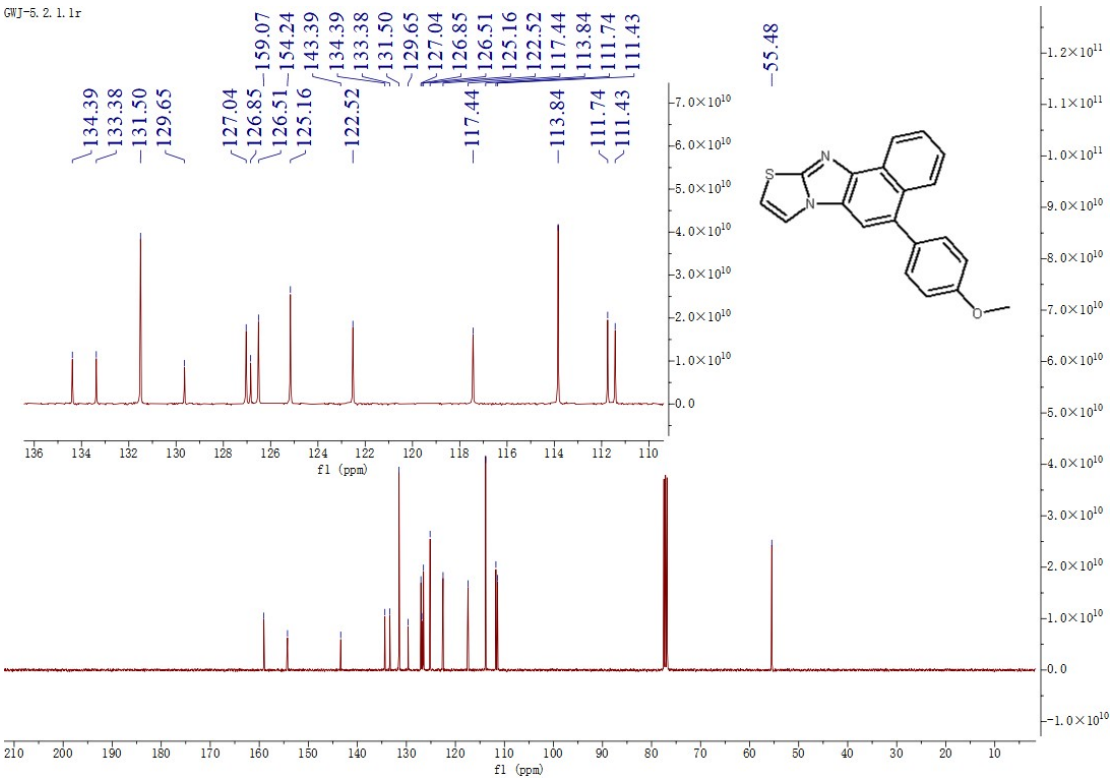
6-(4-methoxyphenyl)-8-methylnaphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**31**)



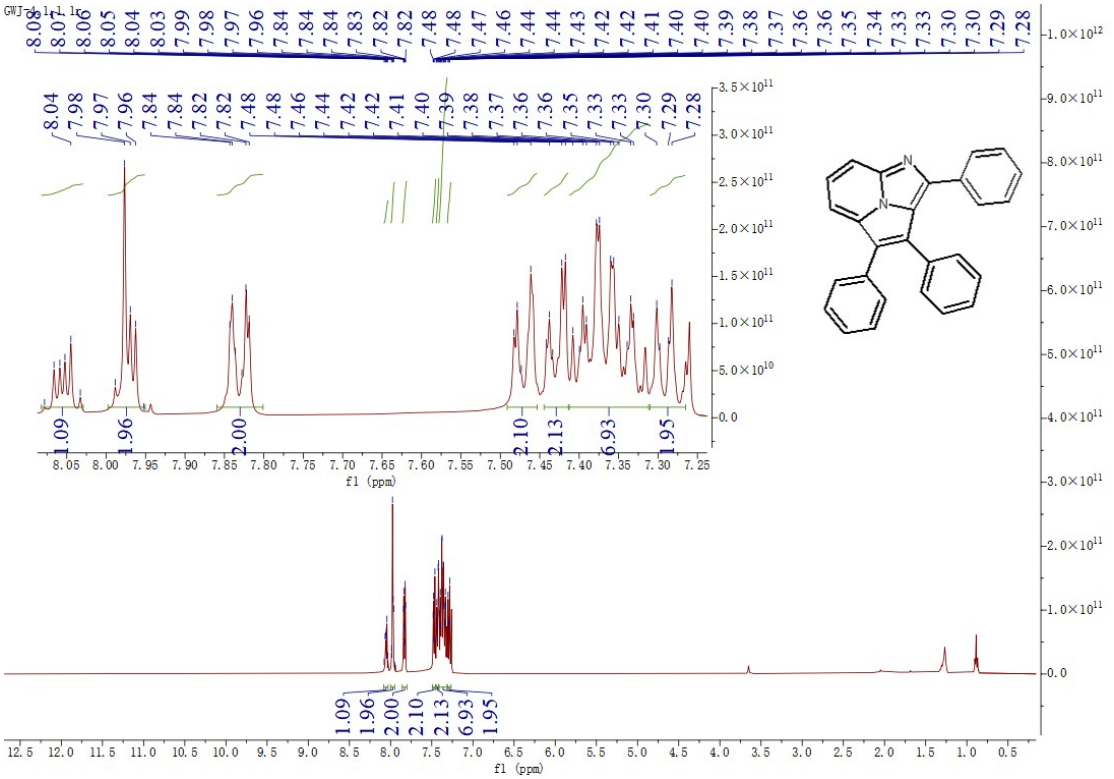


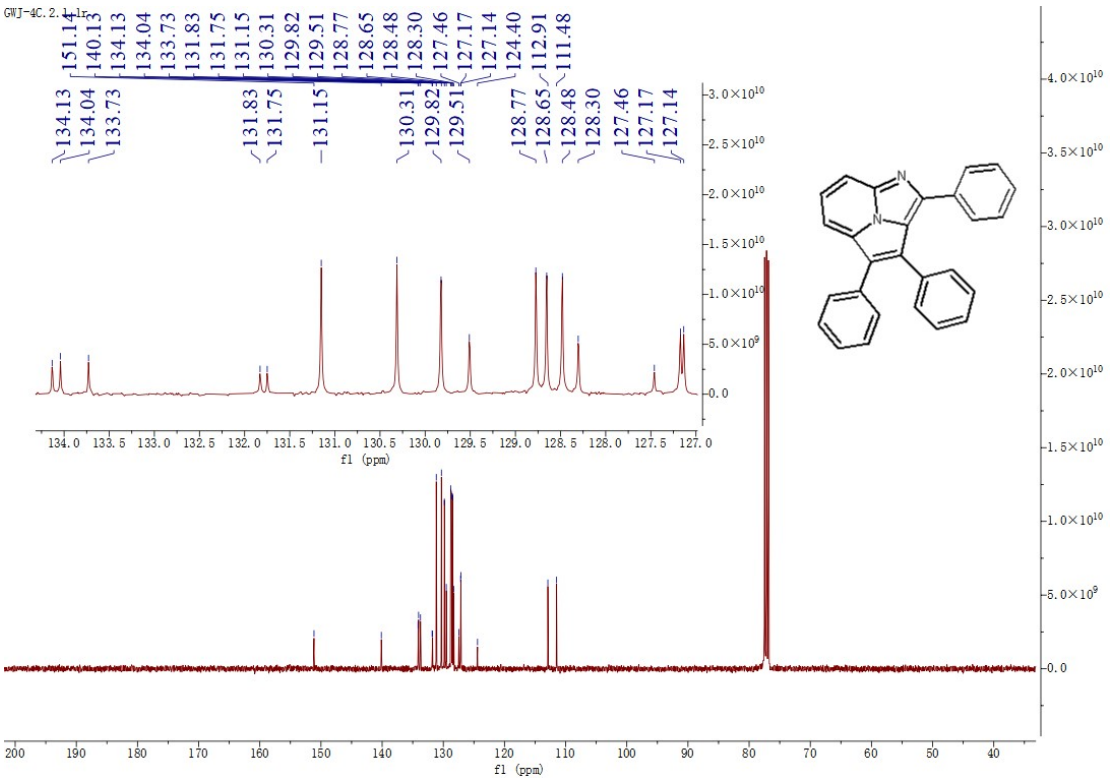
6-(4-methoxyphenyl)naphtho[1',2':4,5]imidazo[2,1-*b*]thiazole (**32**)



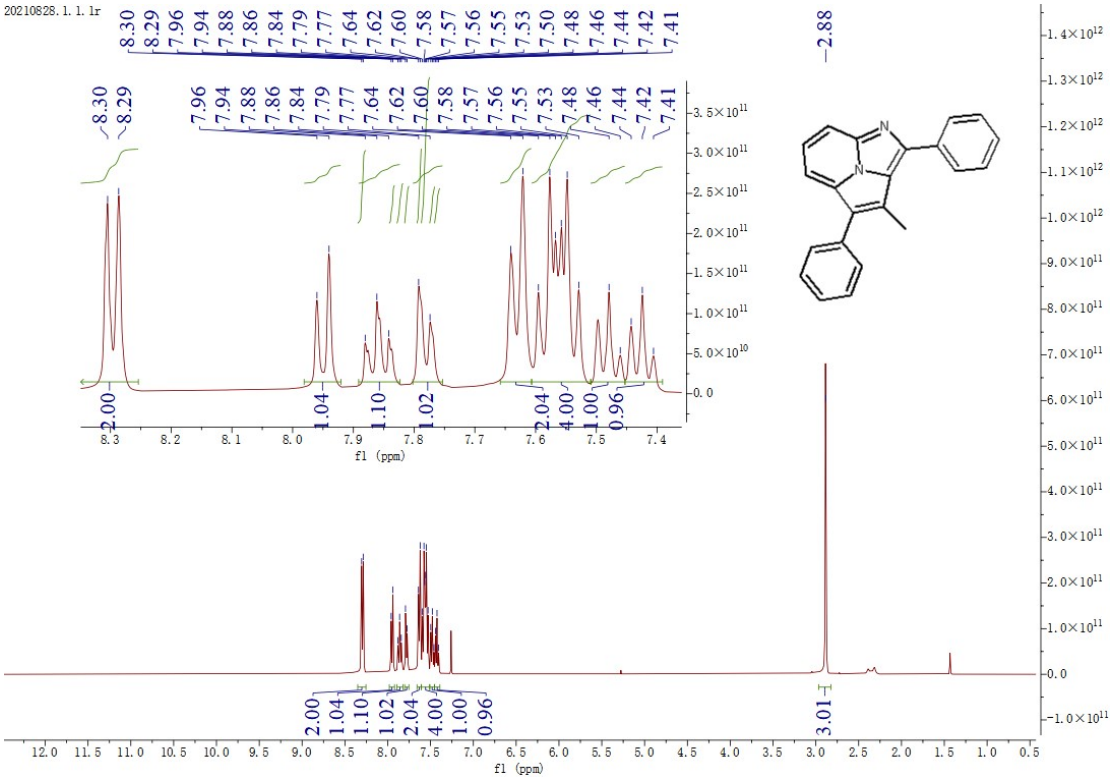


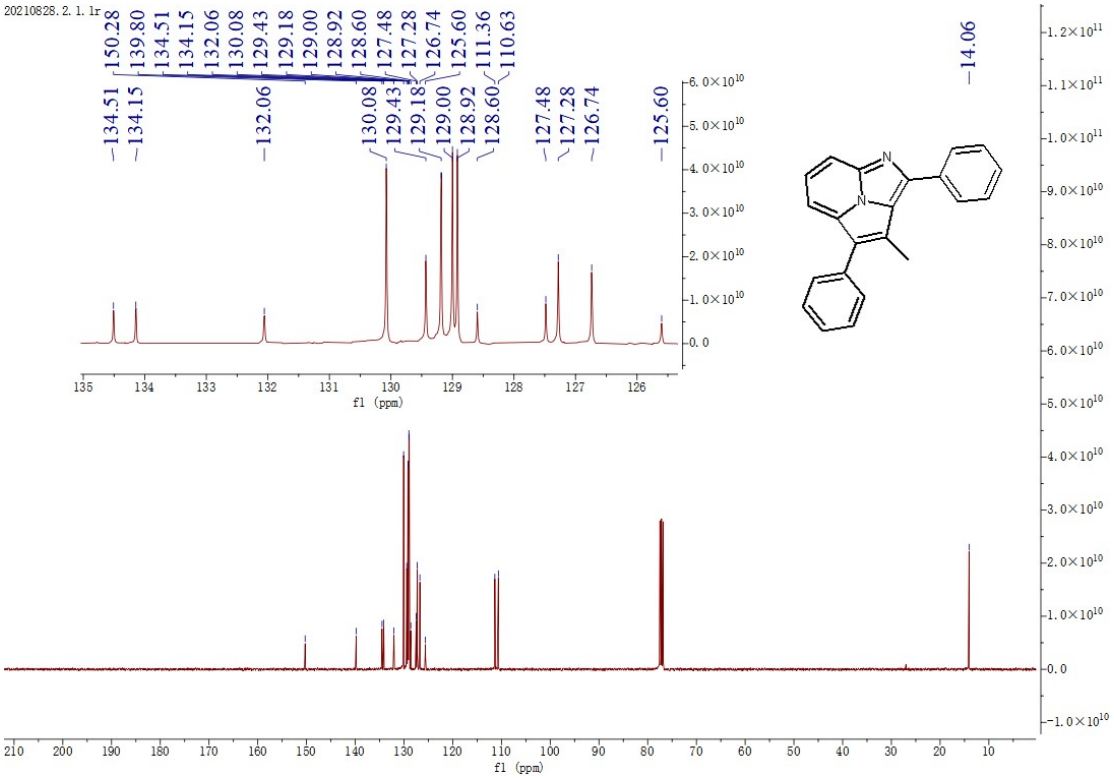
1,6,7-triphenylimidazo[5,1,2-*cd*]indolizine (**33**):



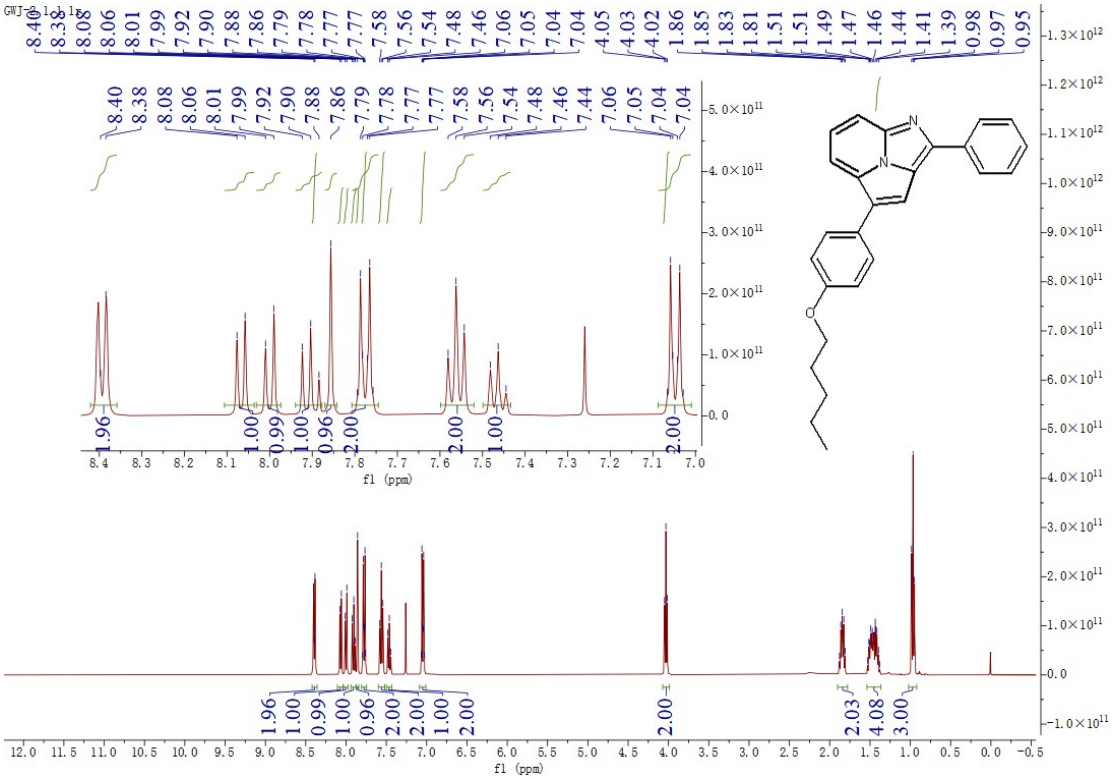


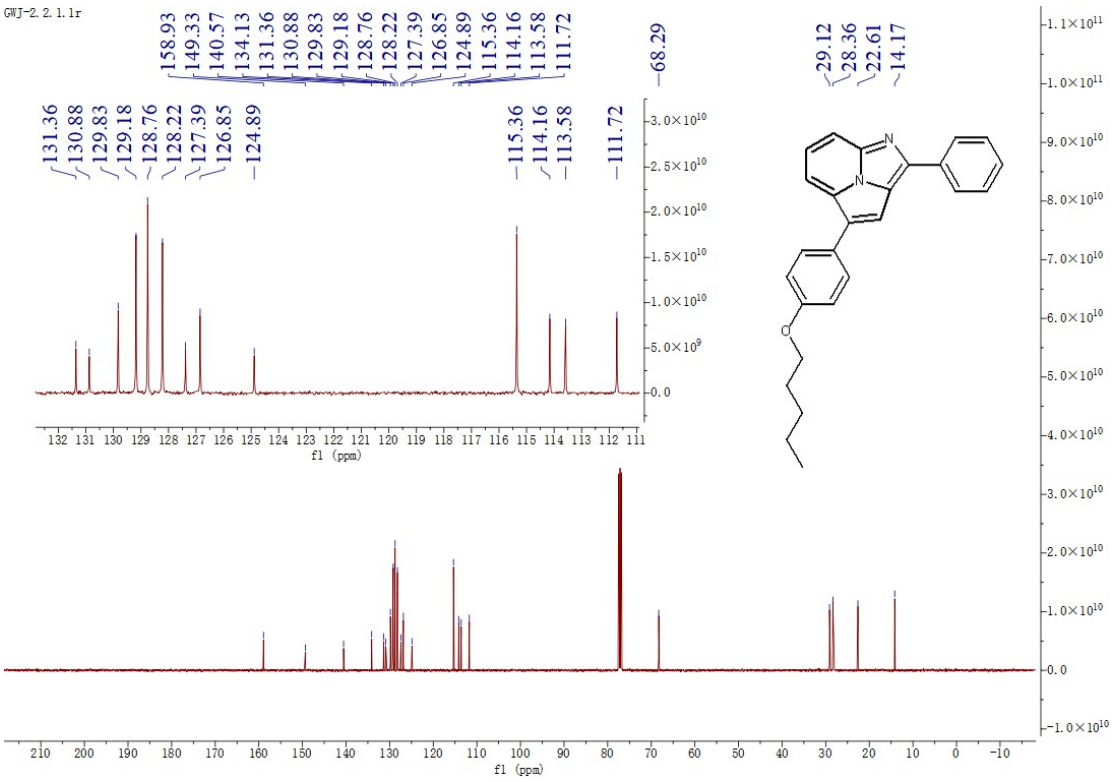
7-methyl-1,6-diphenylimidazo[5,1,2-*cd*]indolizine (**34**)



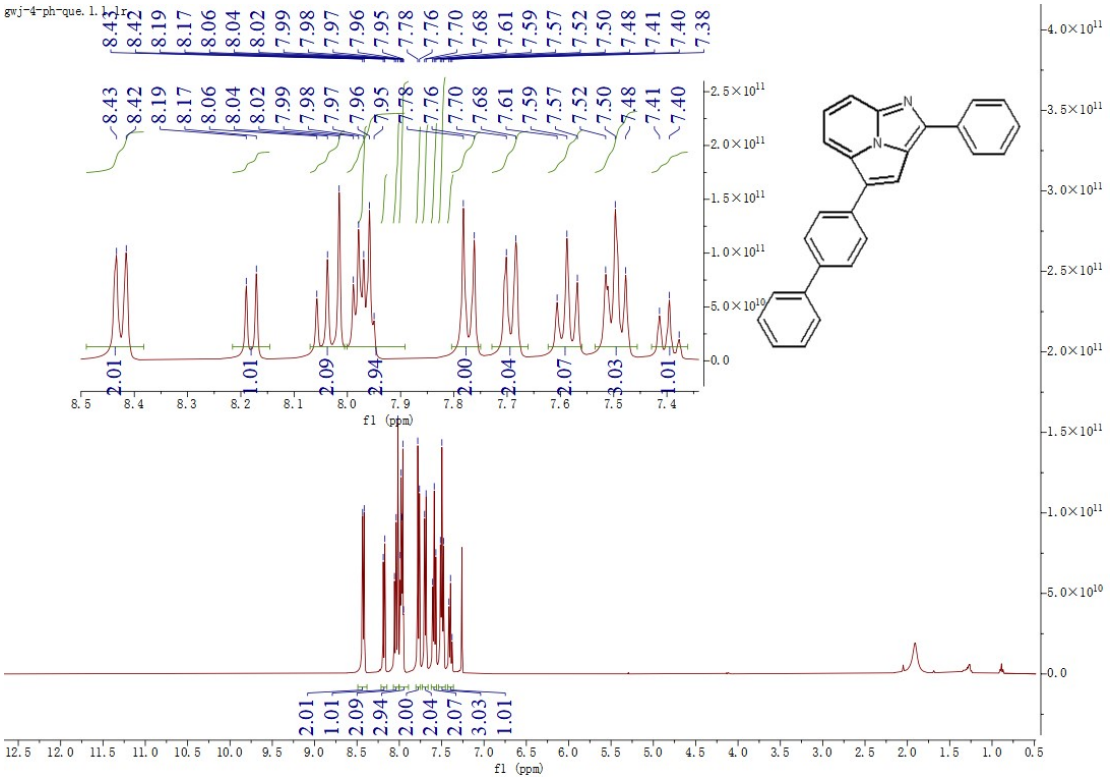


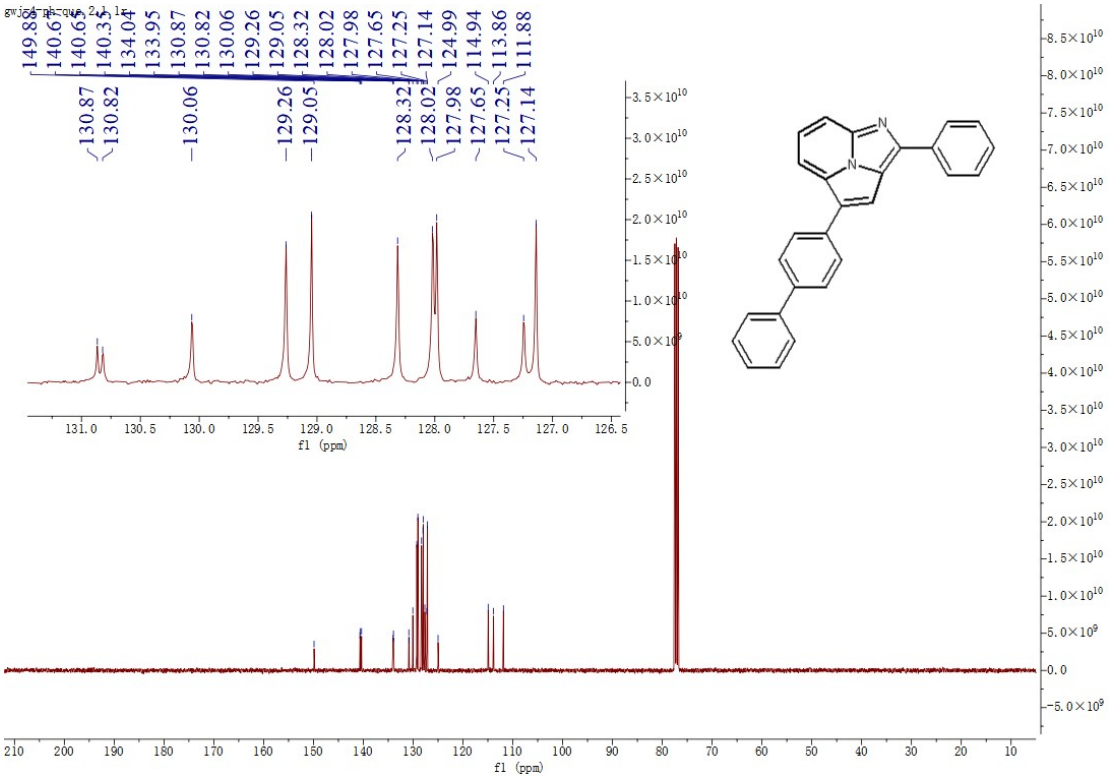
6-(4-(pentyloxy)phenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**35**):



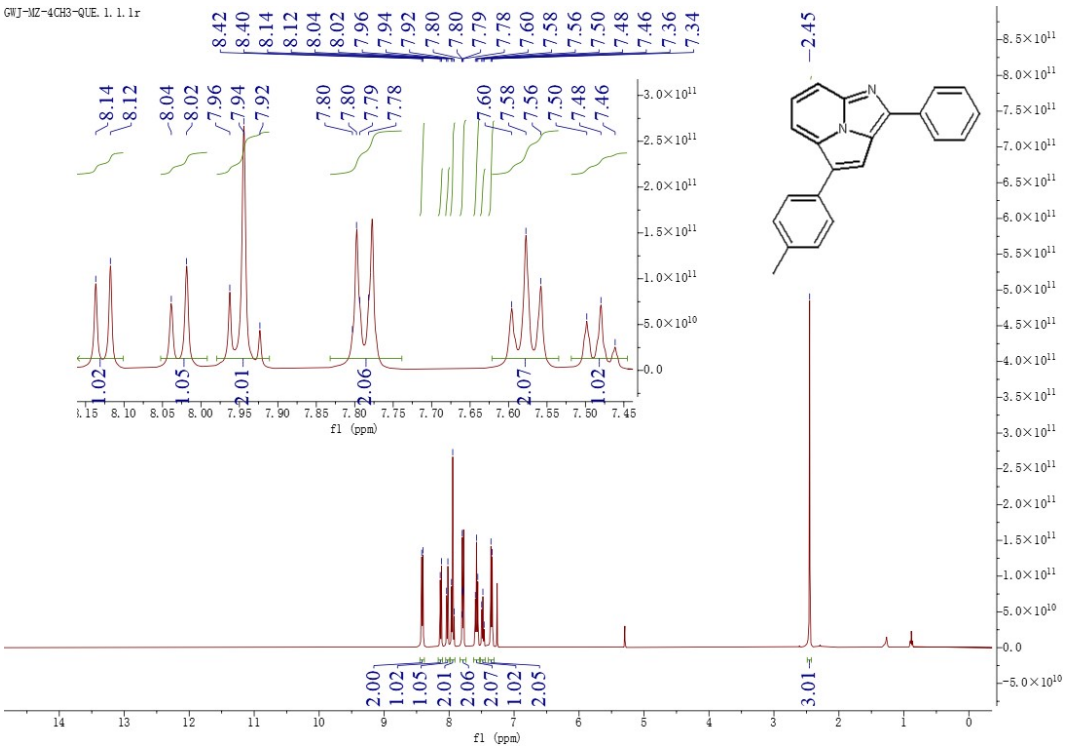


6-([1,1'-biphenyl]-4-yl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**36**):

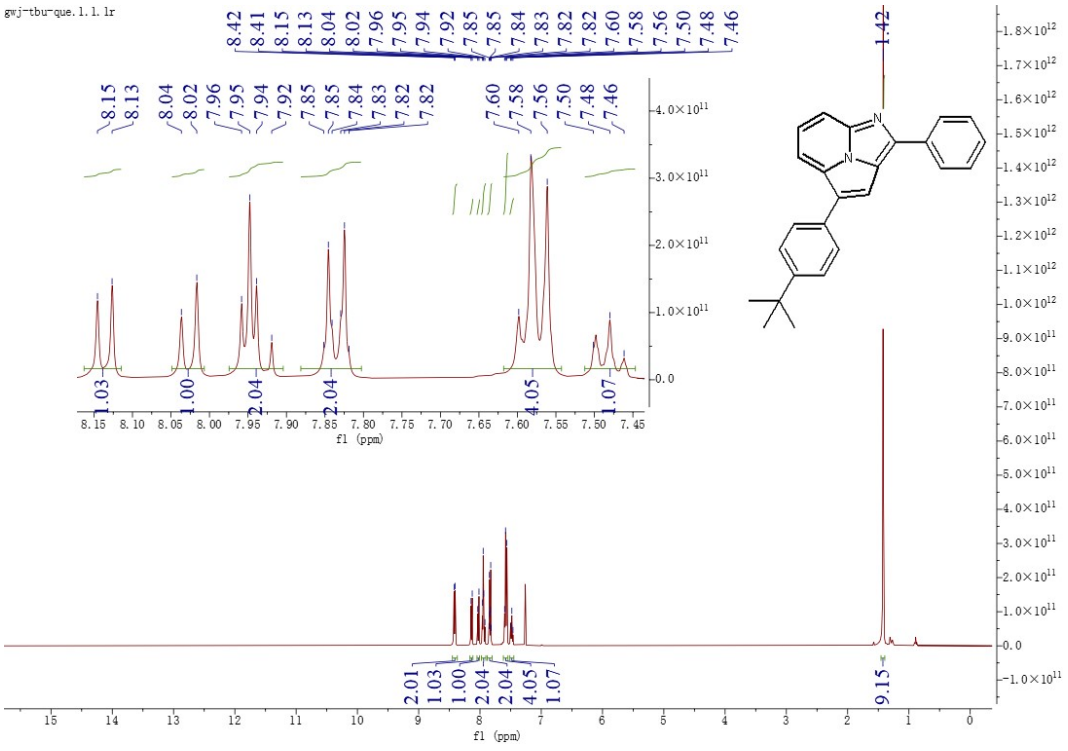


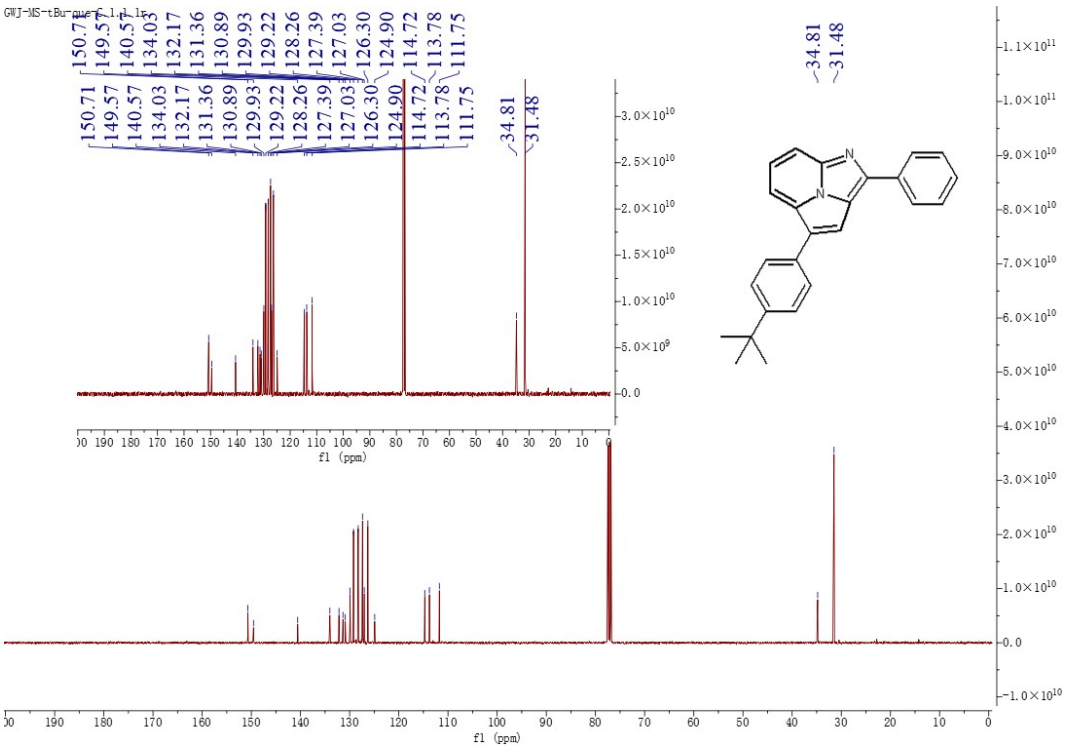


1-phenyl-6-(p-tolyl)imidazo[5,1,2-cd]indolizine (**37**):

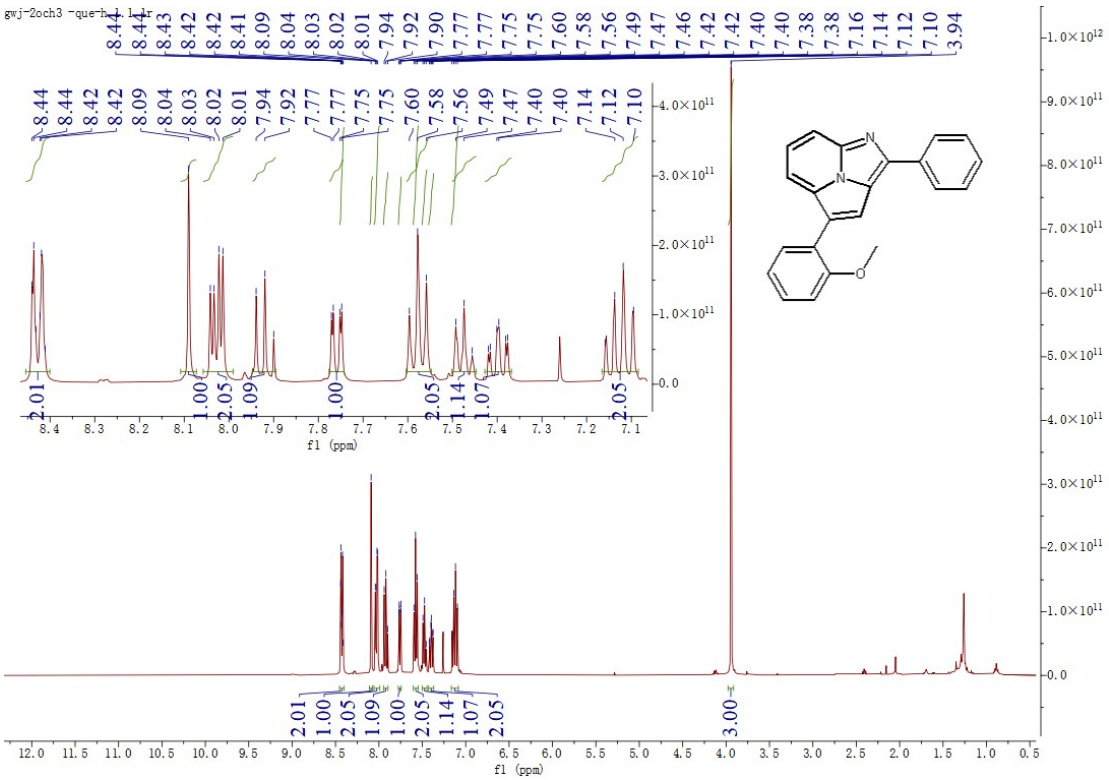


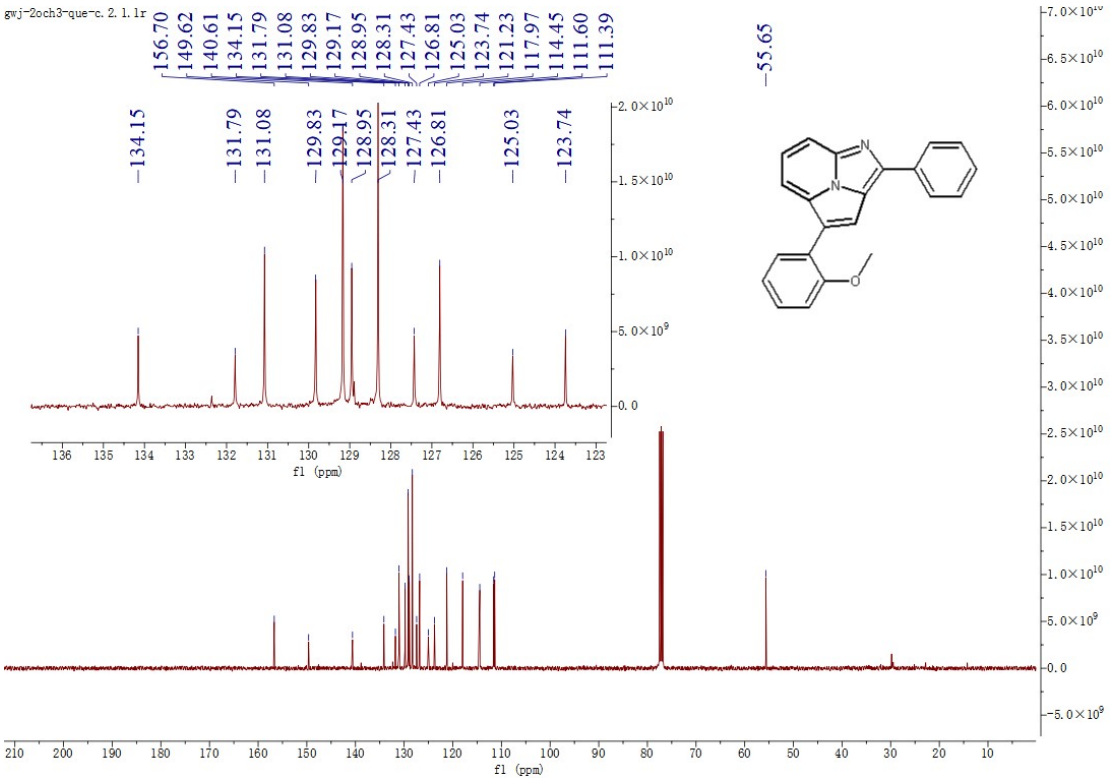
6-(4-(*ter*t-butyl)phenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**38**):



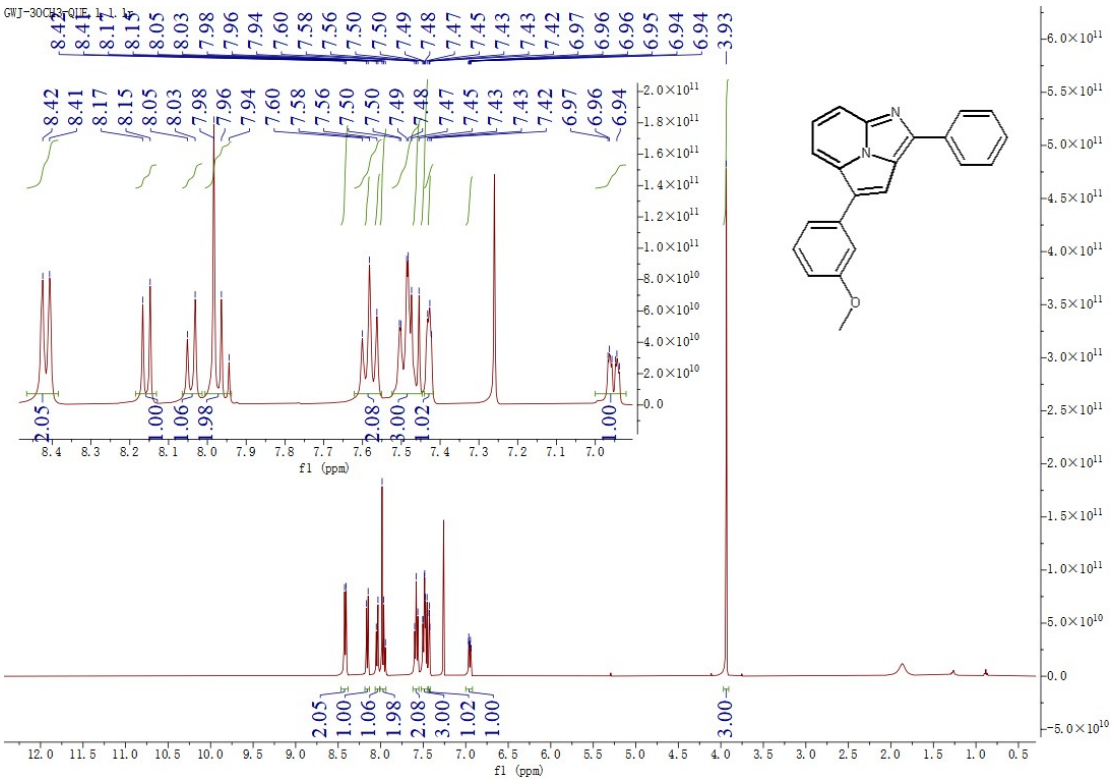


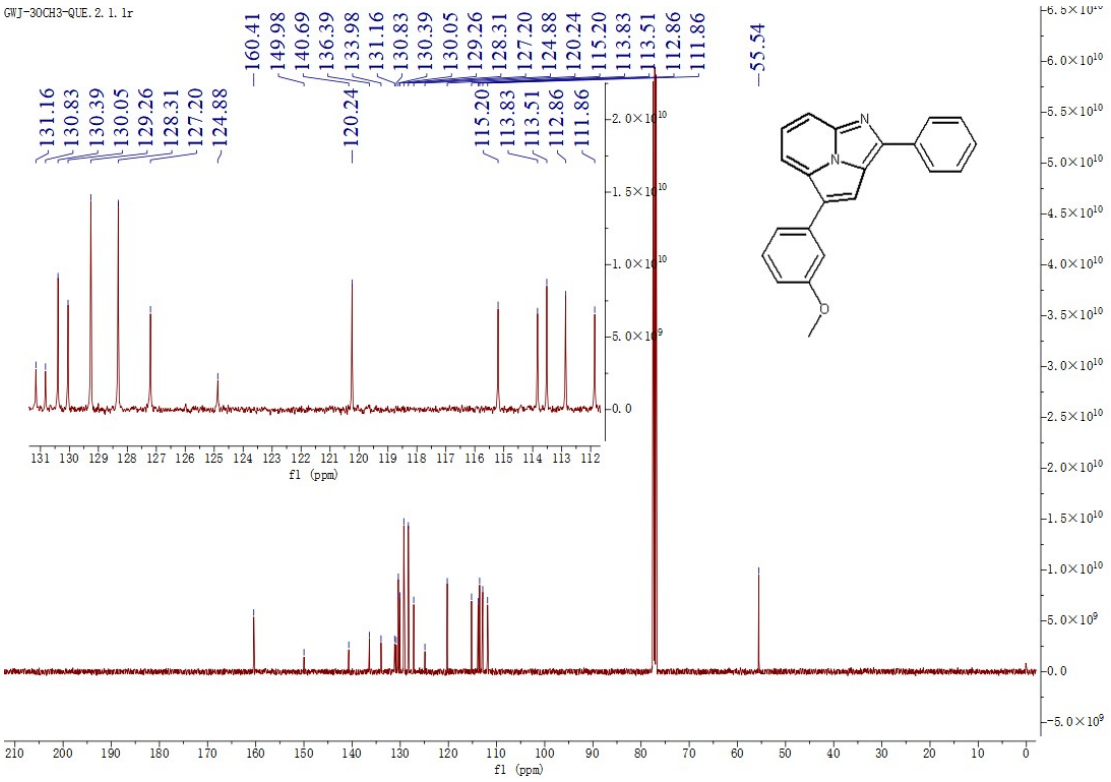
6-(2-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**39**):



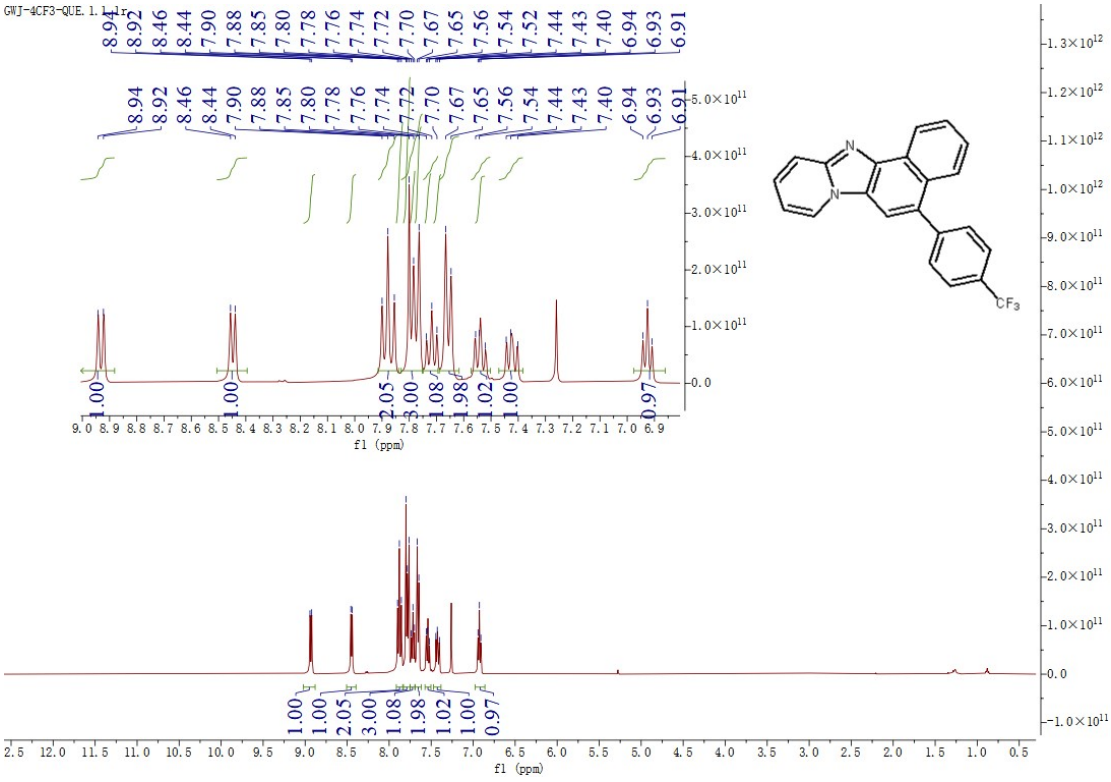


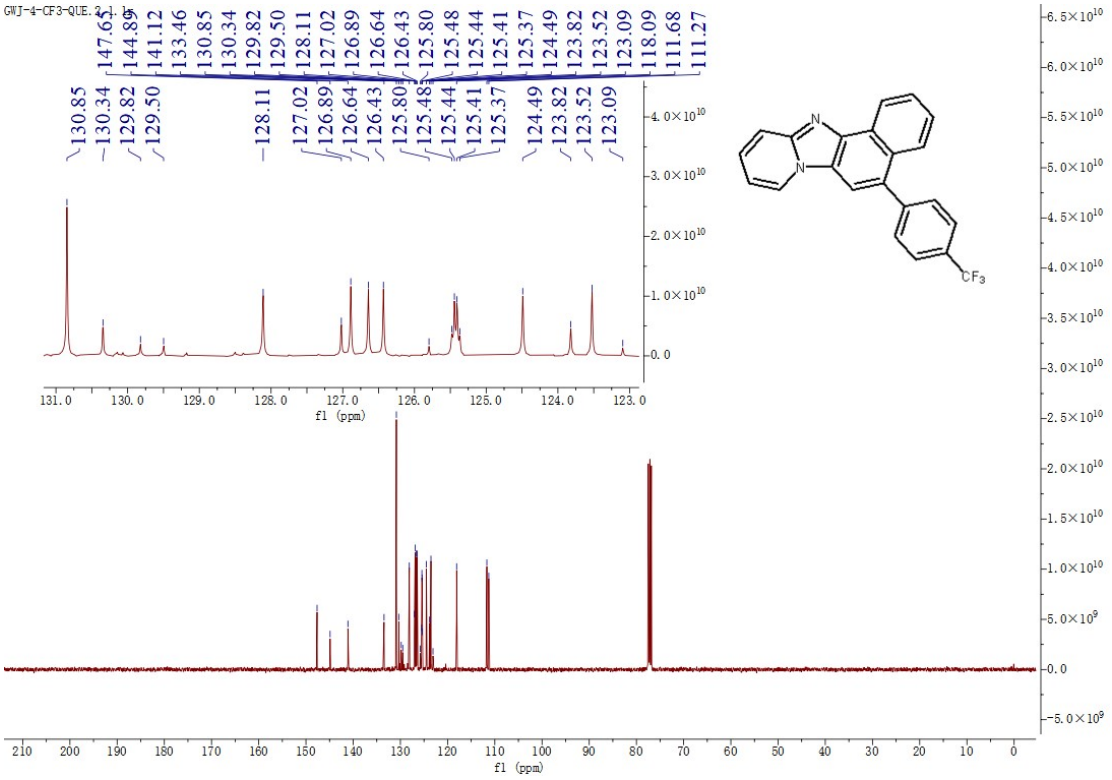
6-(3-methoxyphenyl)-1-phenylimidazo[5,1,2-*cd*]indolizine (**40**):

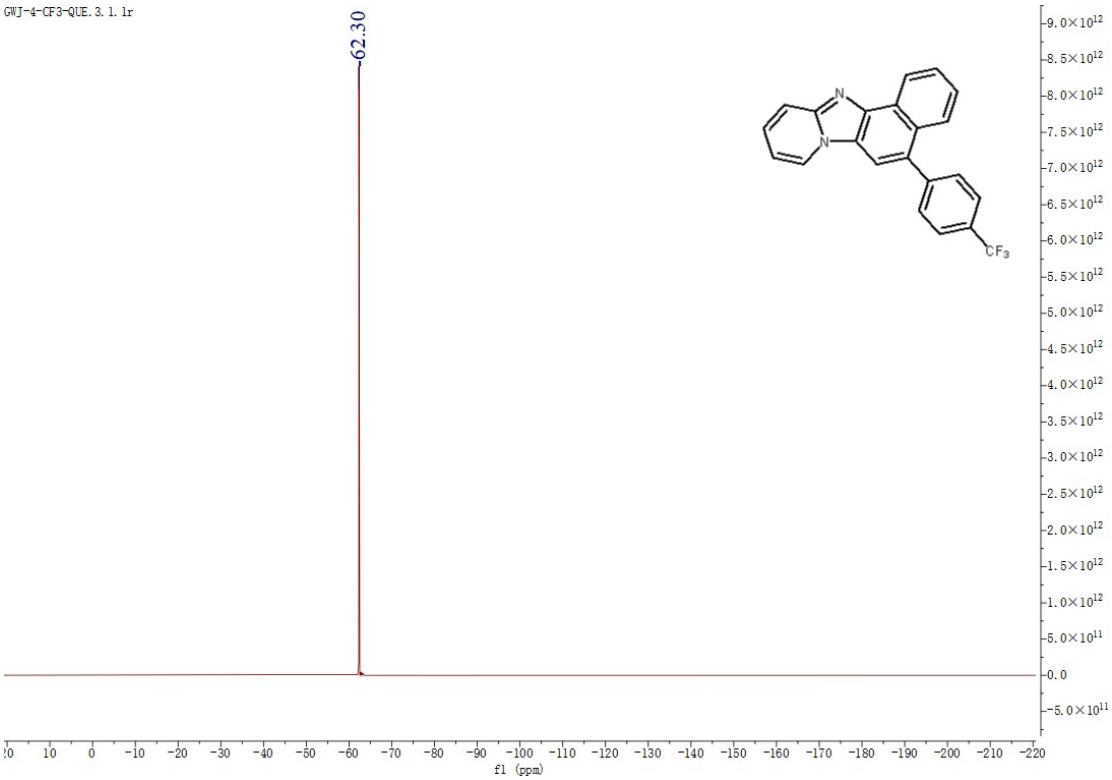




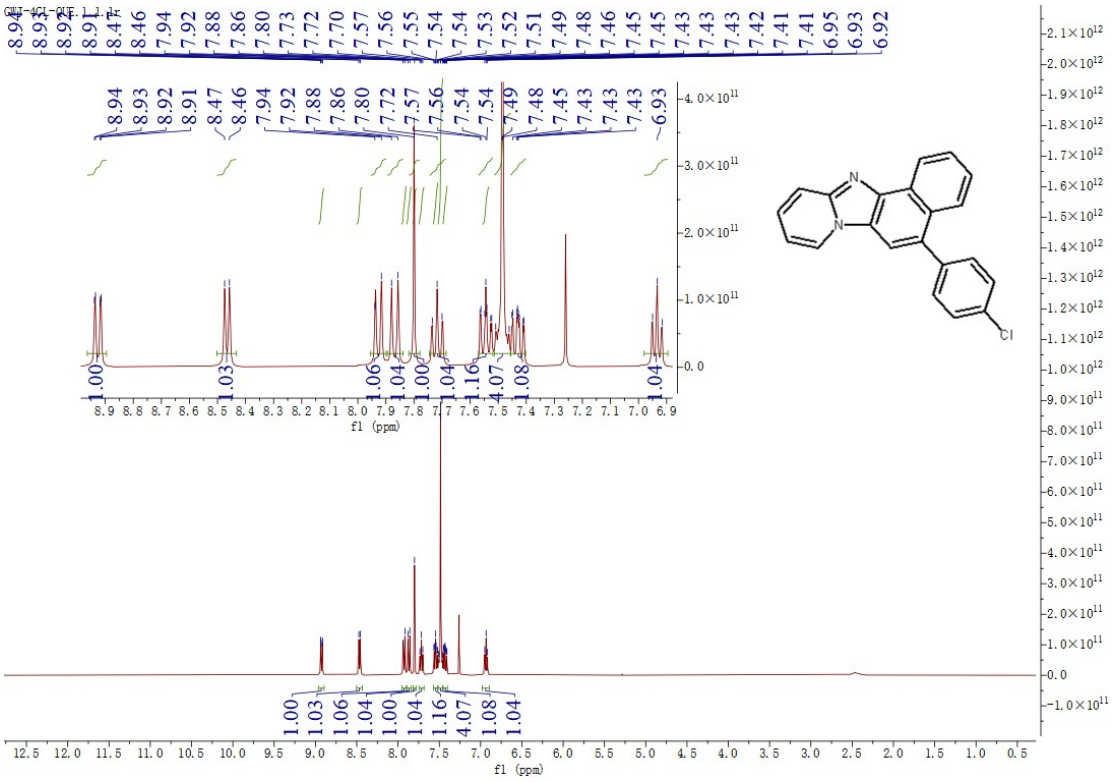
5-(4-(trifluoromethyl)phenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**41**):

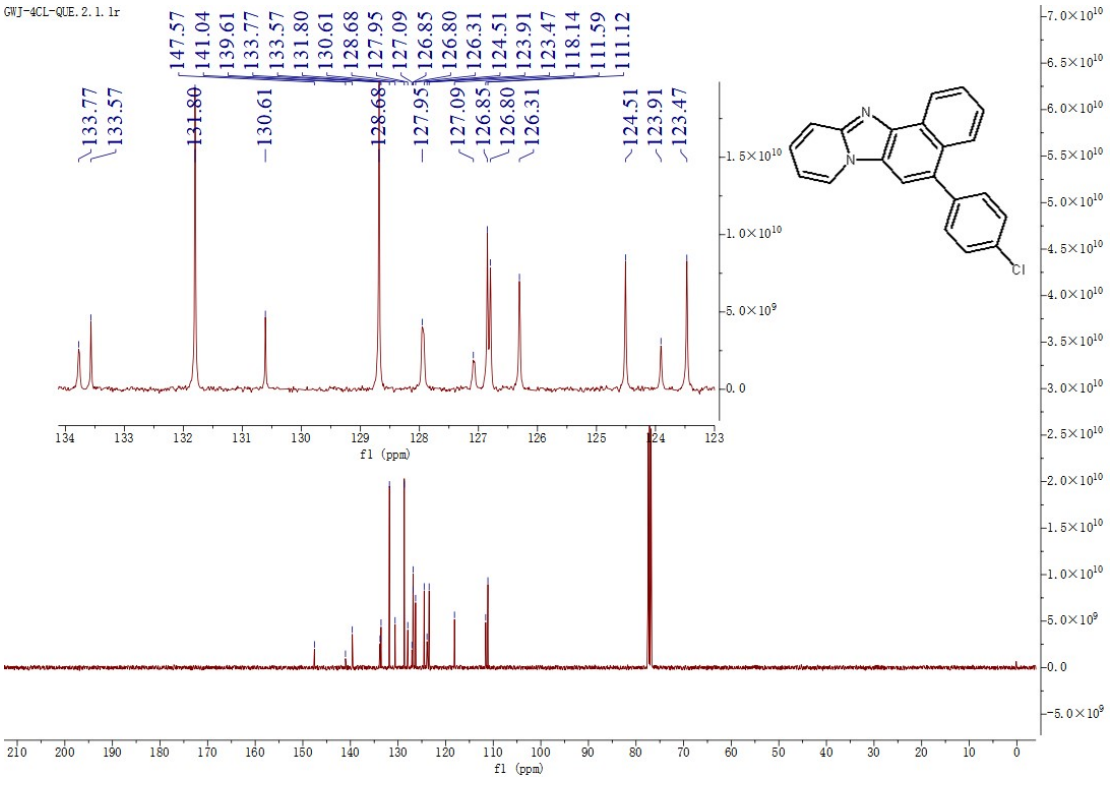



GWJ-4-CF3-QUE.2.1.1r
147.62
144.89
141.12
133.46
130.85
130.34
129.82
129.50
128.11
127.02
126.89
126.64
126.43
125.80
125.48
125.44
125.41
125.37
124.49
123.82
123.52
123.09
118.09
111.68
111.27
f1 (ppm)
f1 (ppm)
CF3

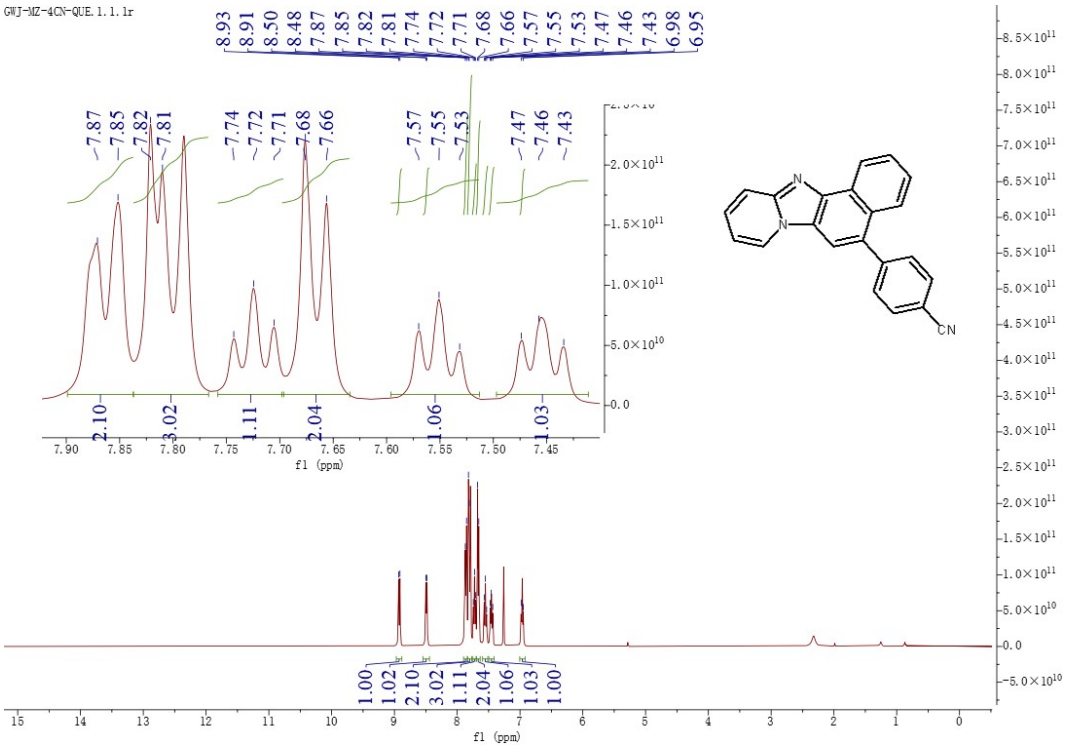

GWJ-4-CF3-QUE.3.1.1r
62.30
f1 (ppm)
CF3

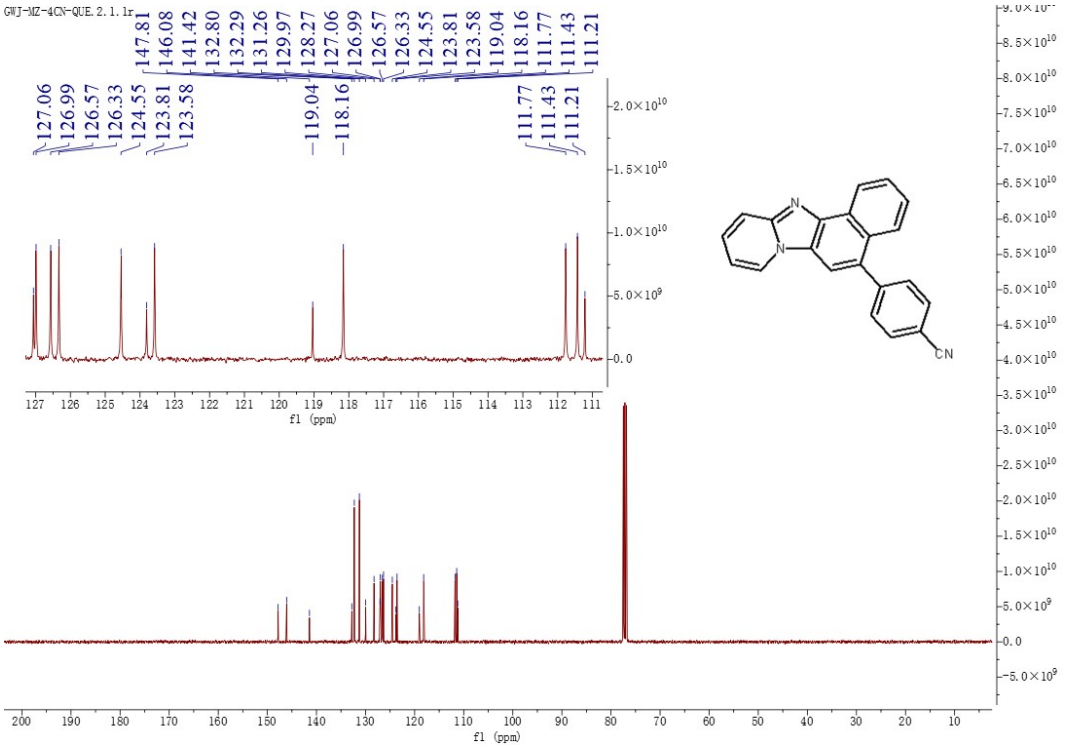
5-(4-chlorophenyl)naphtho[1',2':4,5]imidazo[1,2-*a*]pyridine (**42**):



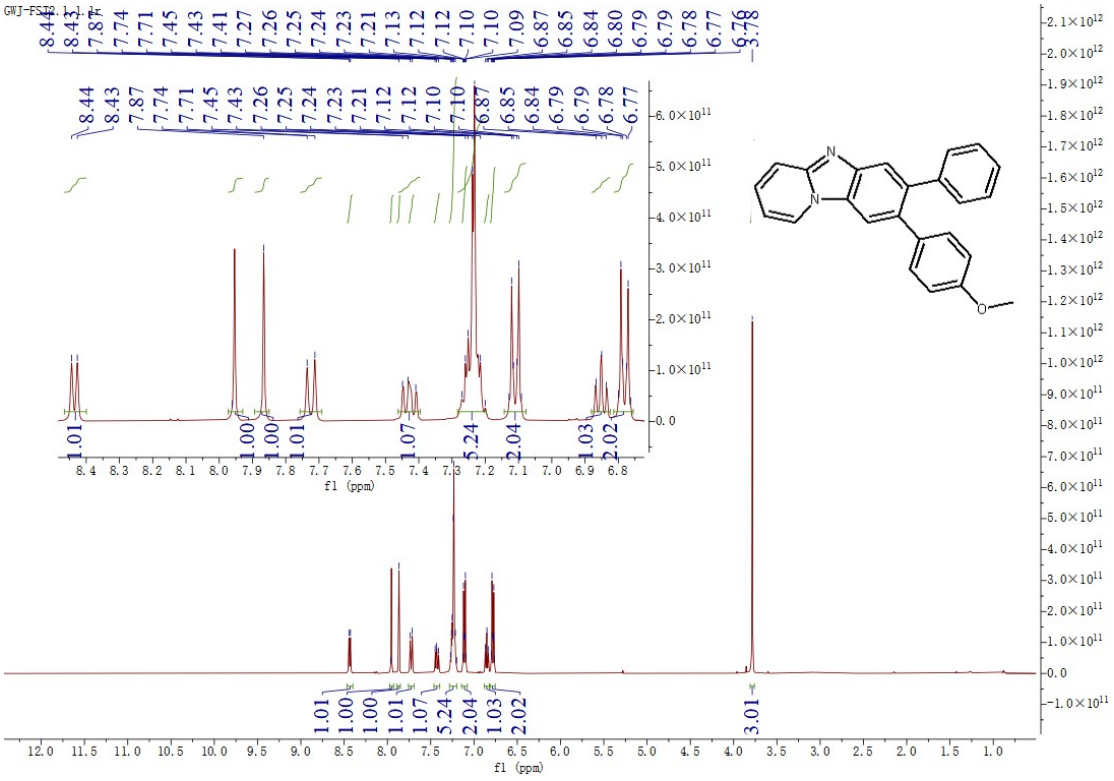


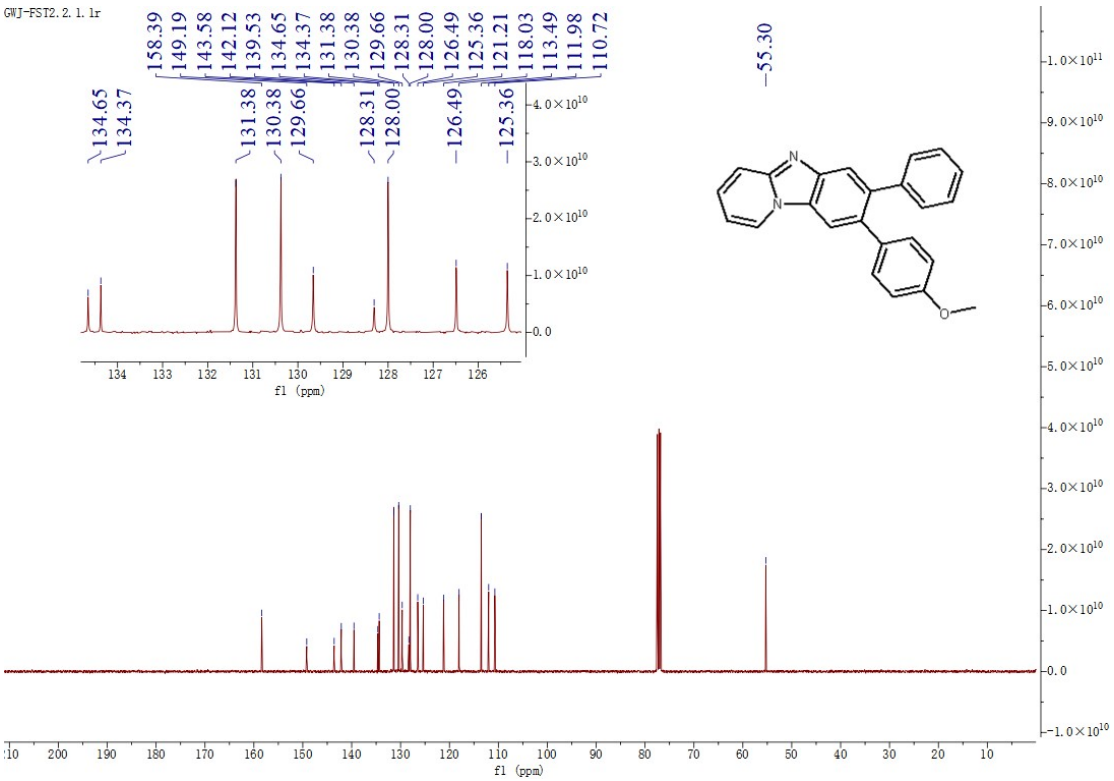
4-(naphtho[1',2':4,5]imidazo[1,2-*a*]pyridin-5-*yl*)benzonitrile (**43**):



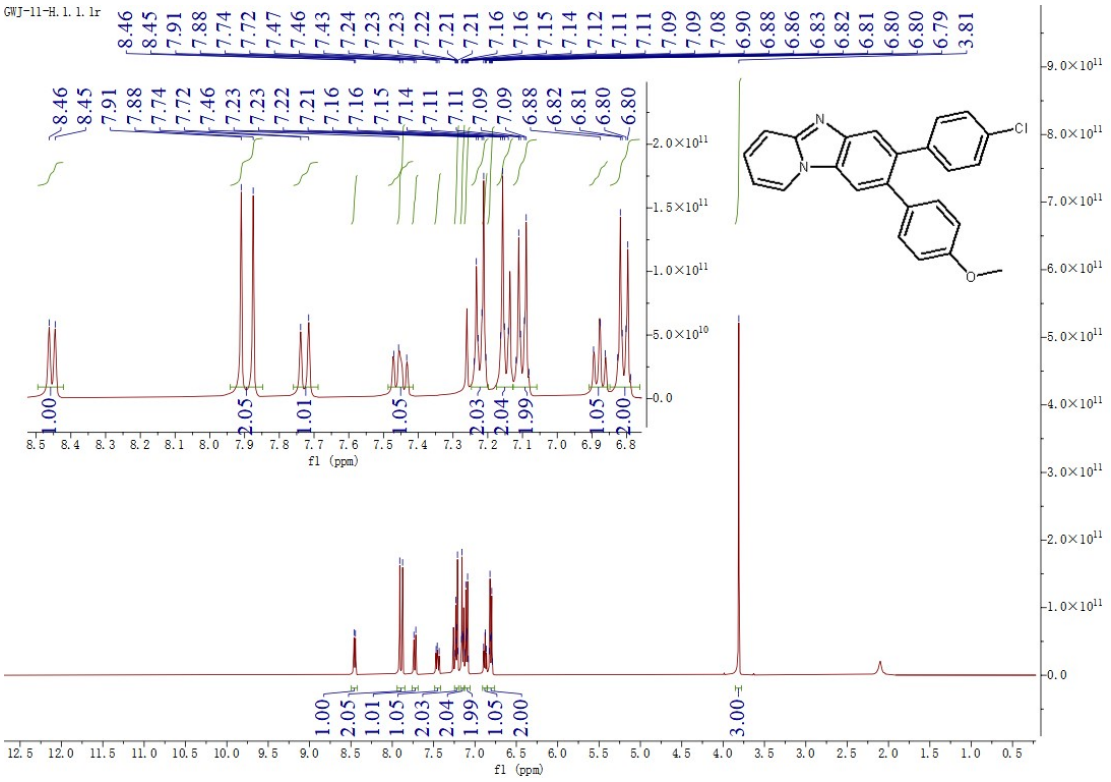


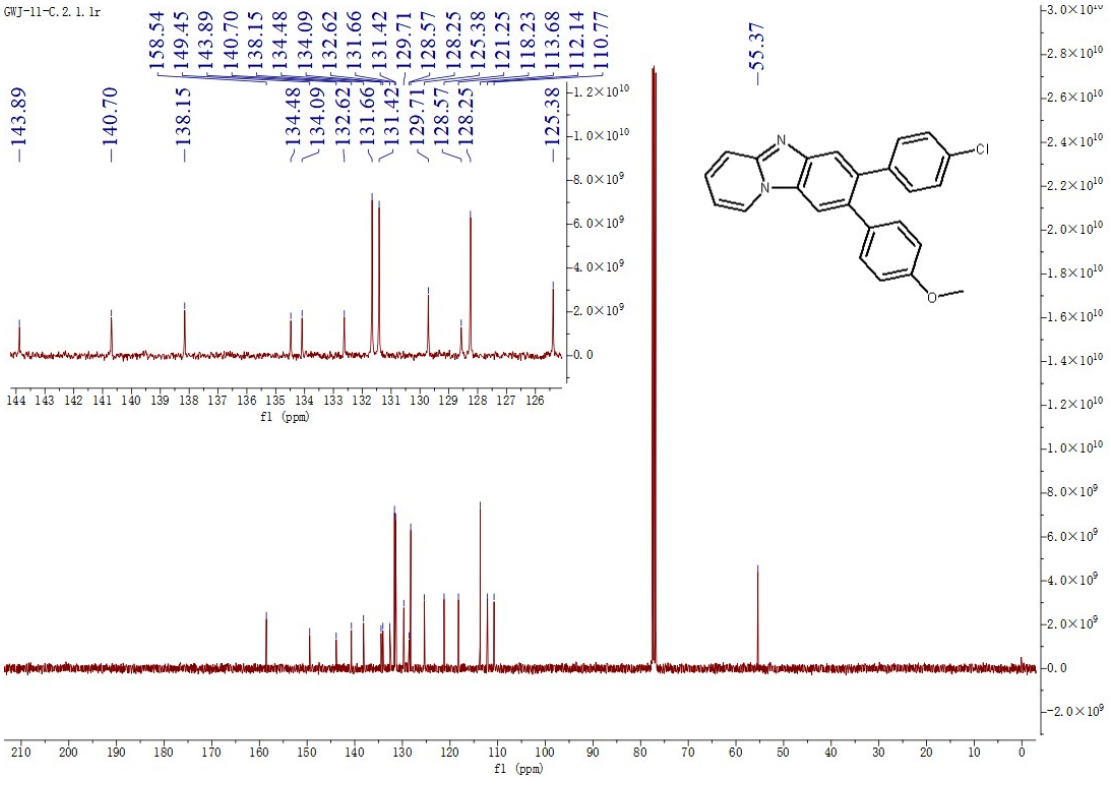
8-(4-methoxyphenyl)-7-phenylbenzo[4,5]imidazo[1,2-*a*]pyridine (**44**):



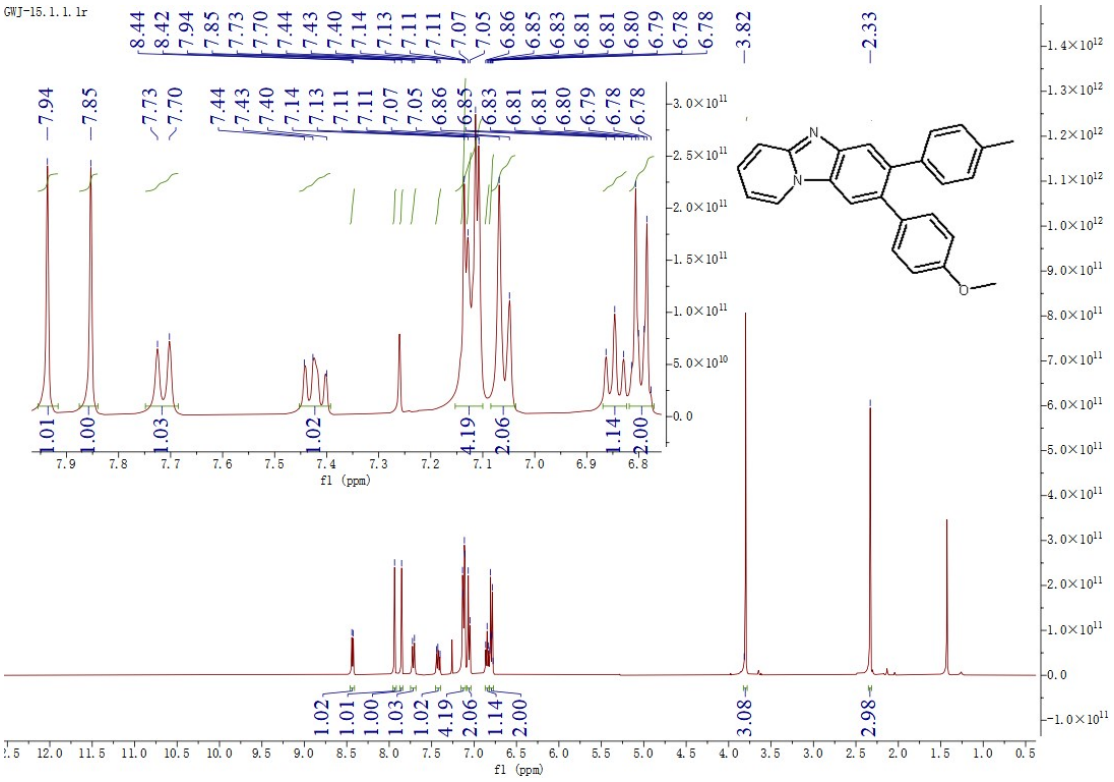


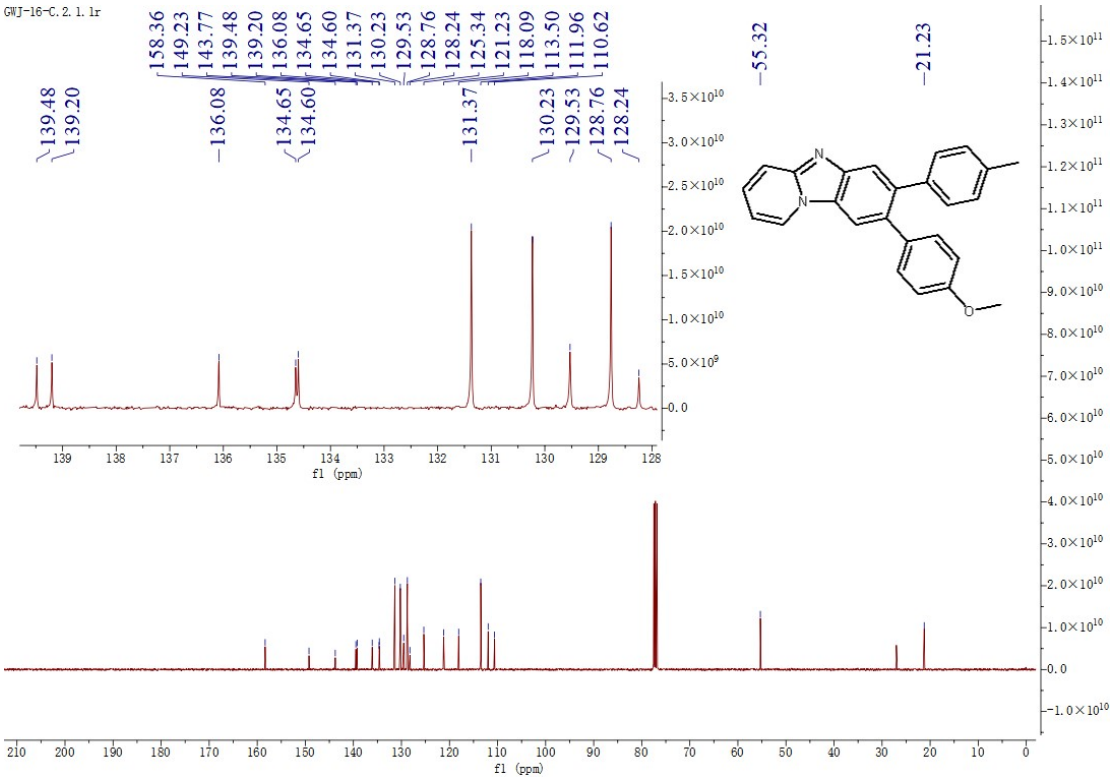
7-(4-chlorophenyl)-8-(4-methoxyphenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**45**):



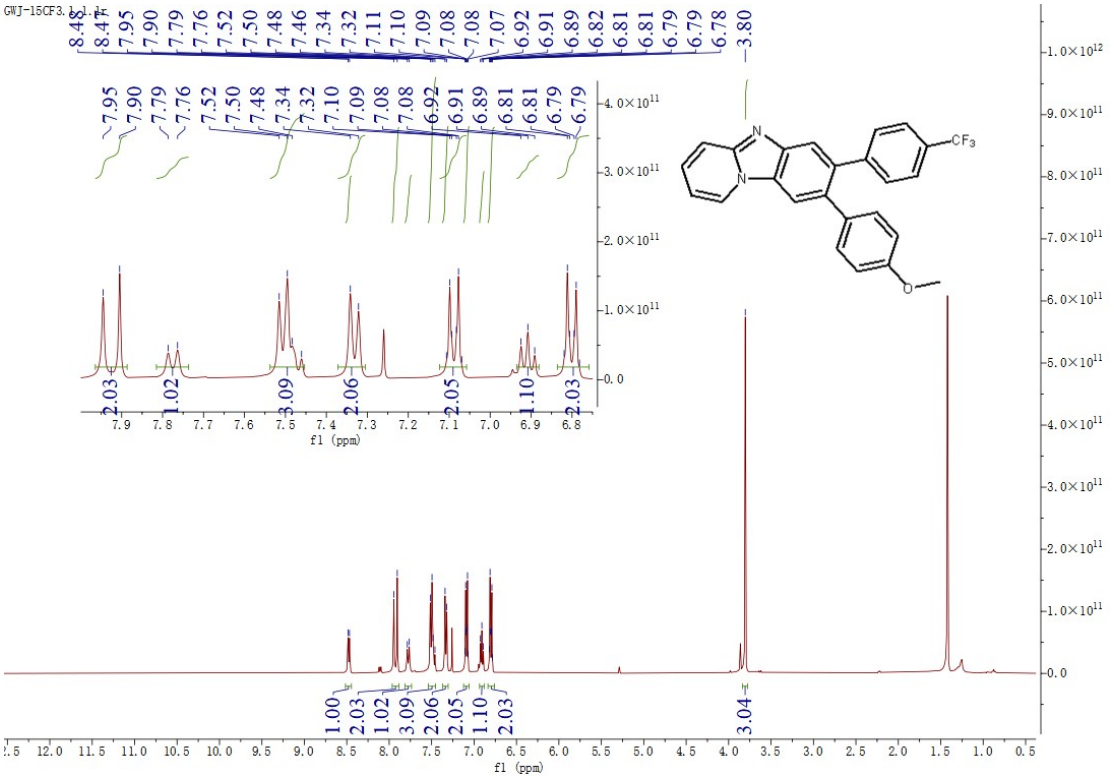


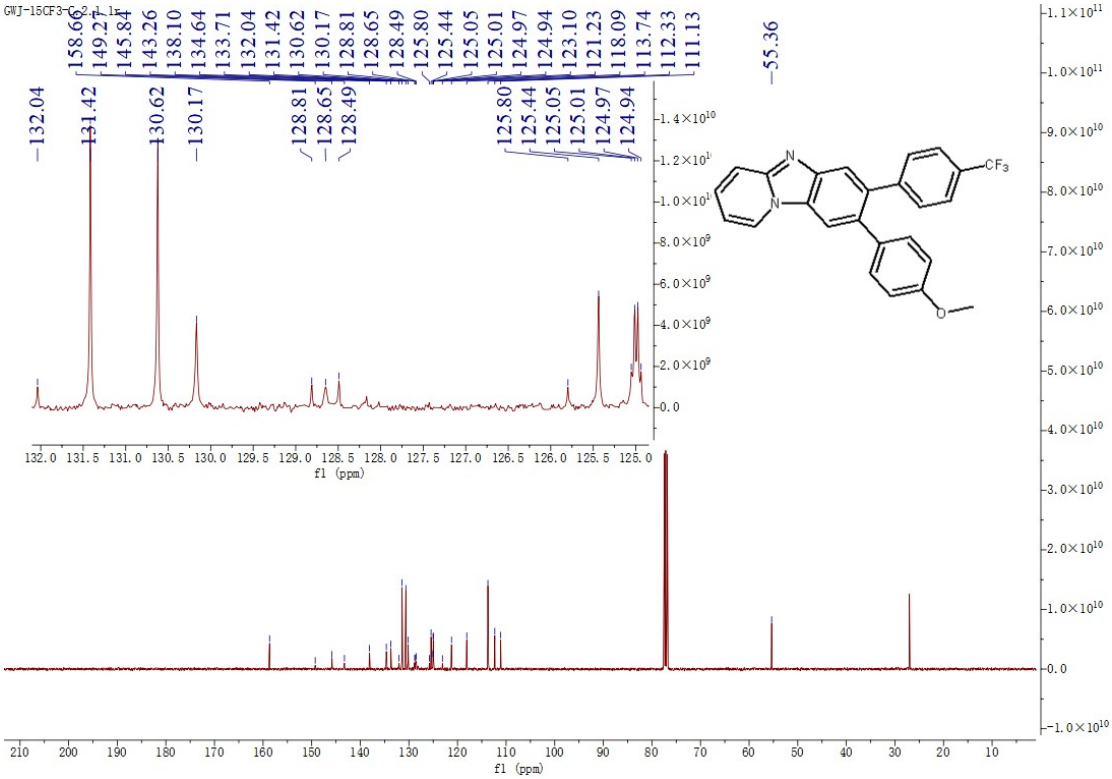
8-(4-methoxyphenyl)-7-(*p*-tolyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**46**):

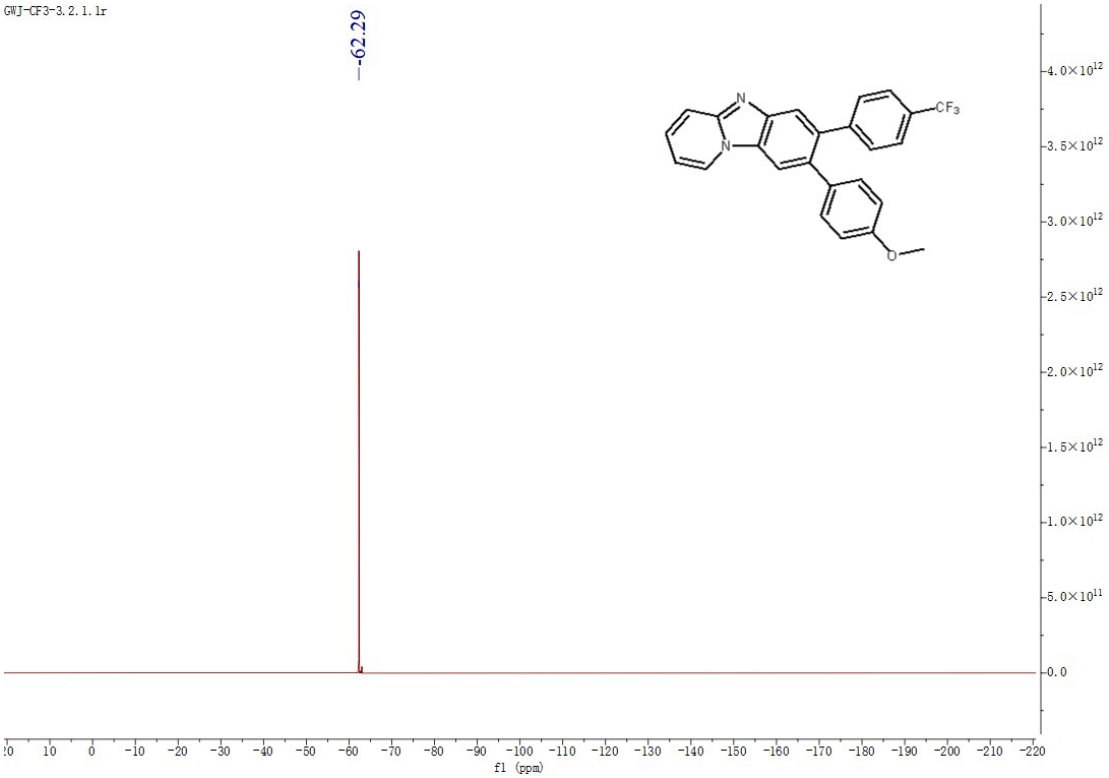




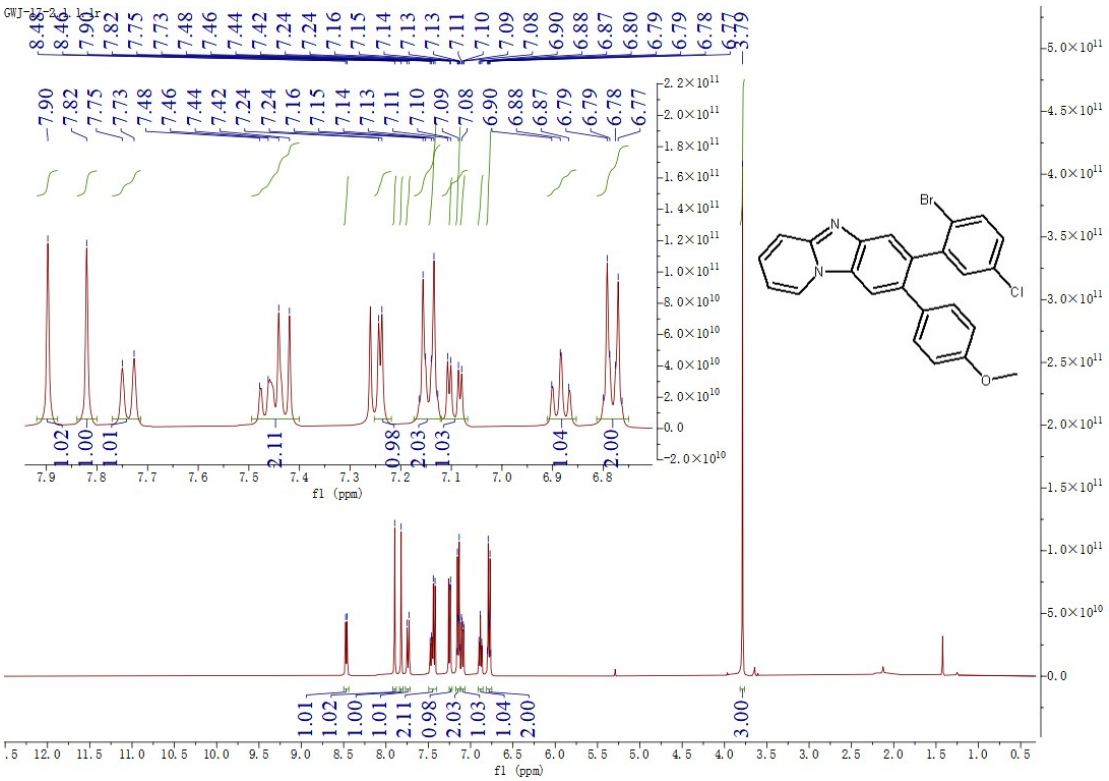
8-(4-methoxyphenyl)-7-(4-(trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**47**):

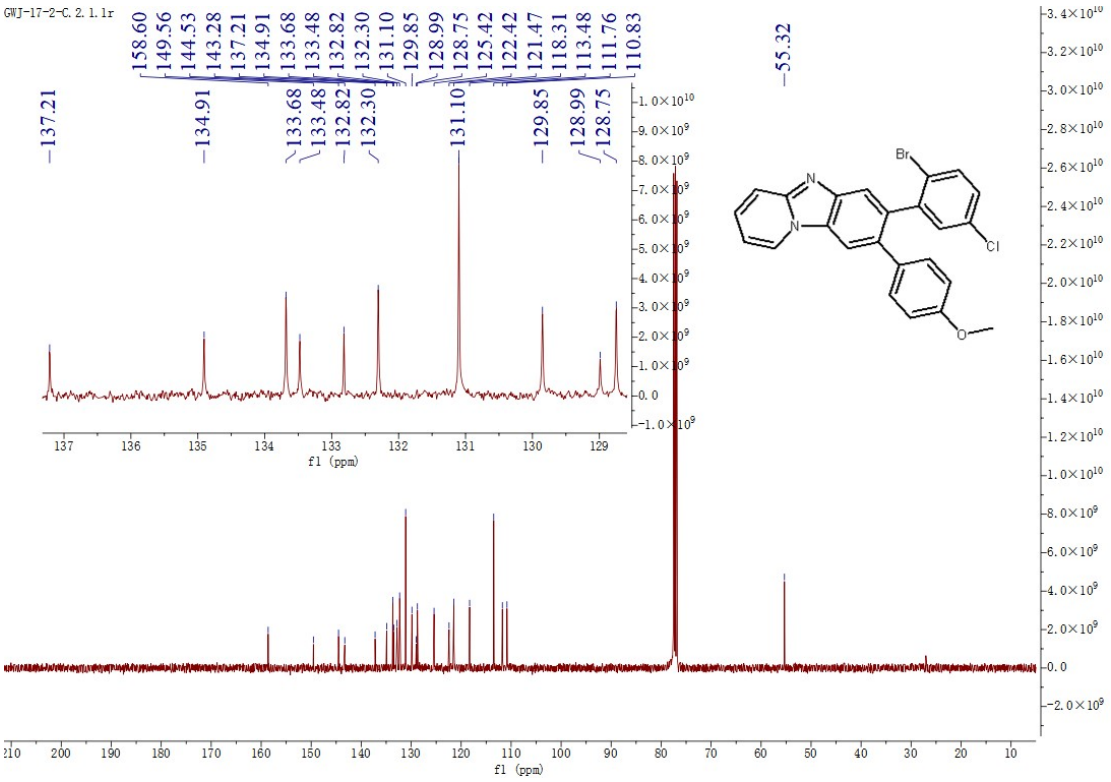




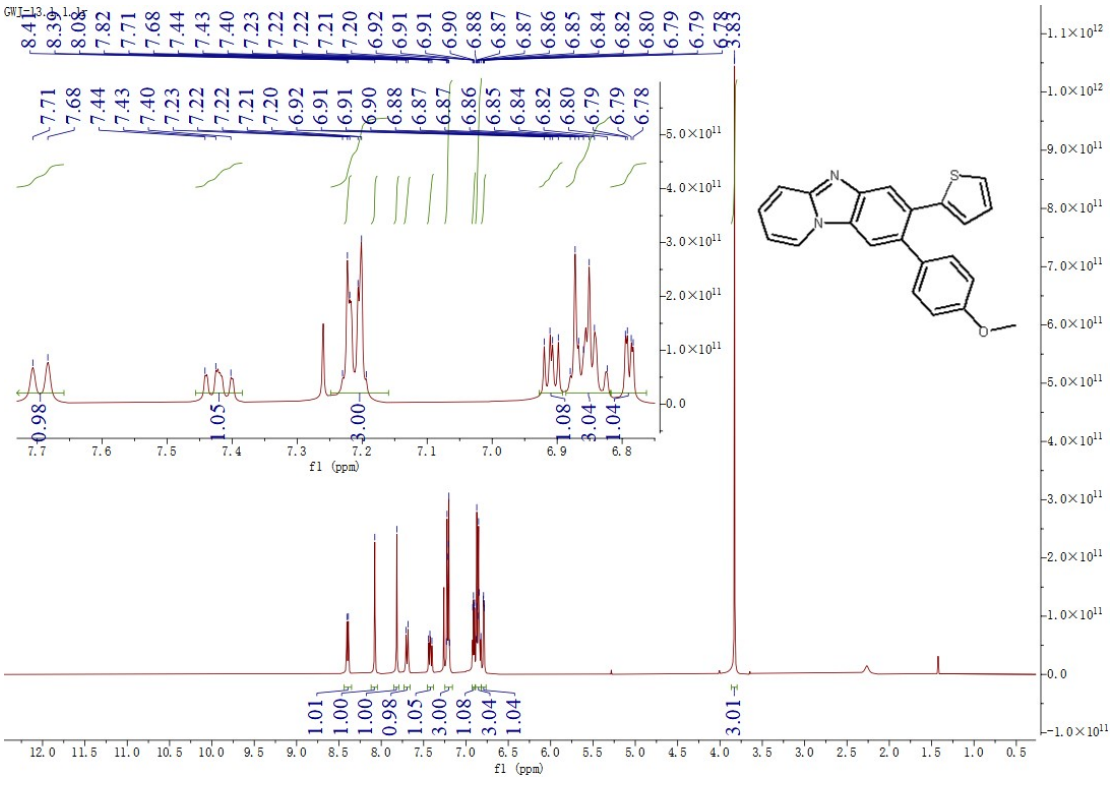


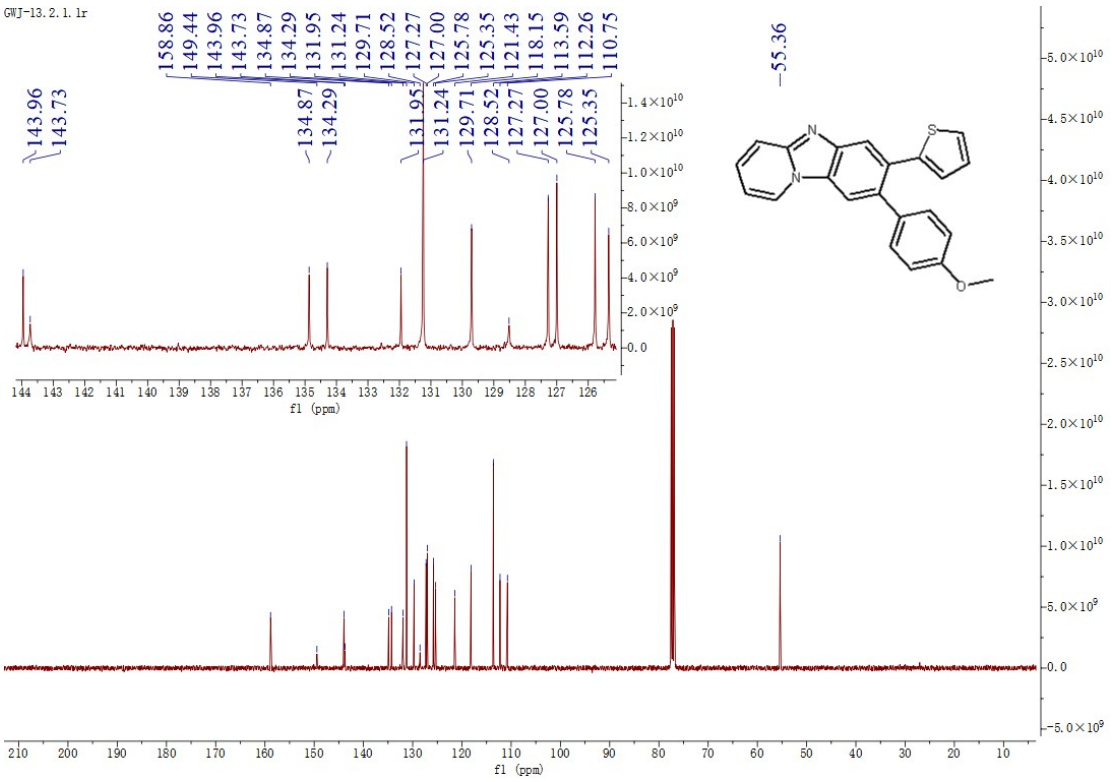
7-(2-bromo-5-chlorophenyl)-8-(4-methoxyphenyl)benzo[4,5]imidazo[1,2-*a*]pyridine (**48**):





8-(4-methoxyphenyl)-7-(thiophen-2-yl)benzo[4,5]imidazo[1,2-*a*]pyridine (**49**):





2,6-di-*tert*-butyl-4-((2-phenylimidazo[1,2-*a*]pyridin-3-yl)methylene)cyclohexa-2,5-dien-1-one (**50**):