Supporting Information

Electrochemically Enabled Synthesis of Sulfide Imidazopyridines via a Radical Cyclization Cascade

Ping-Fu Zhong, Hong-Min Lin, Lin-Wei Wang, Zu-Yu Mo, Xiu-Jin Meng, Hai-Tao Tang* and Ying-Ming Pan*

State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmaceutical Sciences of Guangxi Normal University, Guilin 541004, People's Republic of China.

panym@mailbox.gxnu.edu.cn;

httang@gxnu.edu.cn

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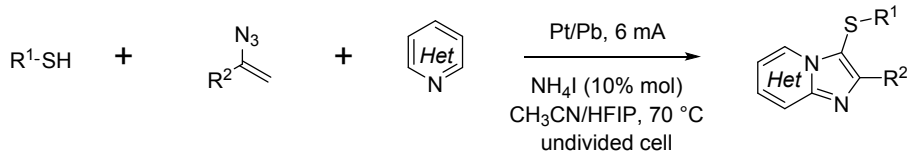
General Information

Without special instructions, all reagents and solvents were commercially available and were not further purified. Column chromatography was carried out using silica gel (300-400 mesh). NMR spectroscopy was performed on Bruker AV-400 instruments. Chemical shifts were reported in ppm. ^{1}H NMR spectra were referenced to $CDCl_3$ (7.26 ppm) or DMSO-d_6 (2.50 ppm) or CD_3OD (3.31 ppm), and ^{13}C-NMR spectra were referenced to $CDCl_3$ (77.0 ppm) or DMSO-d_6 (39.5 ppm) or CD_3OD (49.15 ppm). Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet; brs, broad singlet and *J*, coupling constant in Hz. The HRMS spectrum was measured by micromass QTOF2 Quadrupole/Time of Flight Tandem mass spectrometer with electron spray ionization. Cyclic voltammograms were recorded on a CHI 660E potentiostat.

1. Procedures for the Electrolysis



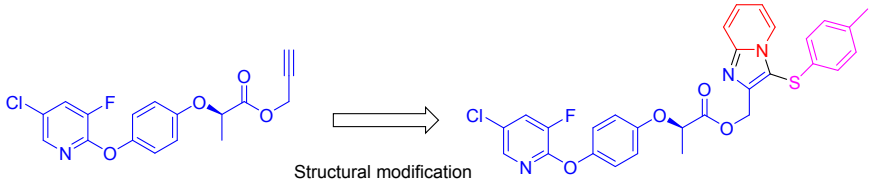
A 10 ml three-necked round bottom flask was charged with thiophenol compound (0.24 mmol, 1.2 equiv), vinyl azide (0.2 mmol, 1.0 equiv), NH_4I (0.02 mmol, 10 mol%) and pyridine (0.8 mmol, 4 equiv).The flask was equipped with a platinum plate (1 cm x 1 cm x 0.1 cm) anode and a lead plate (1 cm x 1 cm x 0.1 cm) cathode. CH_3CN (5 mL) and HFIP (3 mL) were added. Electrolysis was carried out at 70 °C (oil bath temperature), which using a constant current until the substrate was completely consumed (monitored by TLC, about 2 hours). After the reaction was completed, the solvent was concentrated under reduced pressure. Purification with silica gel column chromatography using ethyl acetate/petroleum ether to afford the desired products.

Figure S1. reaction setup

2. Study on Anti-tumor Activity

2.1 MTT assay

Table S1. IC_{50} (μM) values for 4bl and 4bl'.



4bl' **4bl**

Compounds	MGC-803	T-24	HeLa	HpeG-2	HL-7402
4bl	7.2 ± 0.6	1.5 ± 1.1	2.7 ± 0.9	5.7 ± 0.4	15.6 ± 1.3
4bl'	34.6 ± 0.9	>40	>40	37.2 ± 0.3	>40
5-FU	36.4 ± 1.4	38.9 ± 0.9	>40	>40	>40

2.2 Anticancer activity assay

The 180 μL cell suspensions (4500-5000 cells/mL) was seeded in 96-well plates and incubated for 24 h. All compounds and 5-FU were dissolved in the Phosphate Buffered Saline (PBS) with 1% DMSO to give various concentrations (2.5, 5, 10, 20, and 40 μM,

respectively) to 96-well plates and control wells contained supplemented media with 1% DMSO. Continue incubating for 48 h at 37 ^{o}C in 5% CO_2 atmosphere and then the MTT solution (10 μL, 5 mg/mL) was added into each well and the cultures were incubated further for 4~6 h. After removal of the supernatant, DMSO (100 μL) was added to dissolve the formazan crystals. The absorbance was read by enzyme labeling instrument with 570/630 nm double wavelength measurement. The cytotoxicity was estimated based on the percentage cell survival in a dose dependent manner relative to the negative control. The final IC_{50} (a drug concentration killing 50% cells) values were calculated by the Bliss method. All the tests were repeated in at least three independent experiments.

2.3 Cells morphological analysis

The T-24 cells was seeded in 6-well plates and incubated for 24 h. Then, the cells were treated with different concentrations (0, 1.5 and 3 μM) of the compound **4bl** and incubated for 12 h. Finally, control and treated cells were observed with fluorescence microscope (Cytation 5 Cell Imaging Multi-Mode Reader, BioTek Instruments, Inc., USA.). The results shown that the cells were shrink, round and even die after treament with compound **4bl**, which revealed that the compound **4bl** has a good inhibitory effect on T-24 cells.

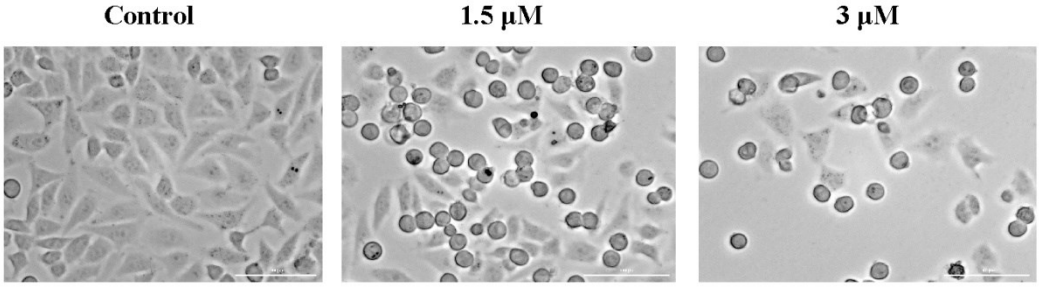


Figure S2. Changes of T-24 cell morphology after 12 h with treatment of compound **4bl.**

2.4 Hoechst 33342nucleic acid staining

Nuclear morphological changes were observed through Hoechst 33342 staining. After treatment with compound **4bl** for 24 h in T-24 cells, cells were washed with PBS and permeabilized with 0.1% Tween 20 for 10 min followed by staining with Hoechst

33342 (2.5 μg/mL). Control and treated cells were observed with fluorescence microscope (Cytation 5 Cell Imaging Multi-Mode Reader, BioTek Instruments, Inc., USA.). The results from Fig. S3-2 illustrated that the nuclear structure of untreated cells was intact whereas compound **4bl** treated cells exhibitedcondensed, or fragmented nuclei.

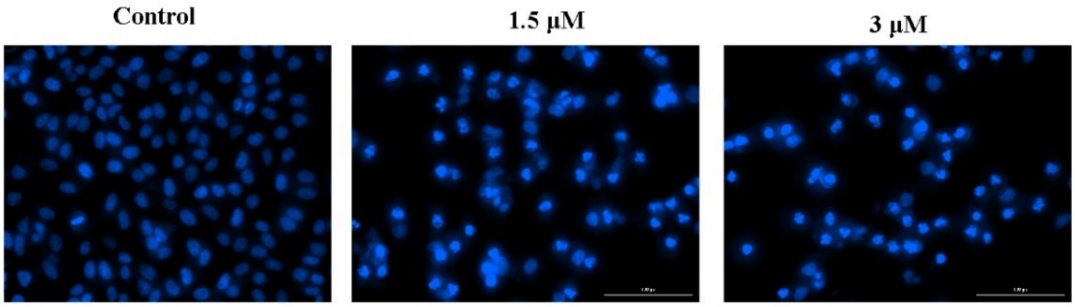


Figure S3. Assessment of nuclear morphological changes by Hoechst 33342 staining in T-24 cells after 24 h.

2.5 Measurement of intracellular reactive oxygen species

Intracellular reactive oxygen species (ROS) was detected by using fluorescence microscope by with 2′,7′-dichlorofluorescein diacetate (DCHF-DA) staining kit. T-24 cells were seeded at 2×10^6/well in 10% FBS/DMEM into 6-well plates and treated with different concentrations of compound **4bl** (0 and 3 μM) for 24 h, then cells were washed twice with serum free DMEM and incubated with DCHF-DA for 30 minutes at 37 ^oC in dark. The fluorescence microscope was used to measure the enhanced green flourescent intensity in cells, the intensity of the microscope is 488 nm, and the emission wavelength is 525 nm. As shown in Figure S3-3, after treatment with compound **3ag** (0 and 3 μM) for 24 h, the green fluorescence in T-24 cells were enhanced compared with that in the untreated controls. Hence, compound **3ag** can increase the level of ROS in T-24 cells, respectively.

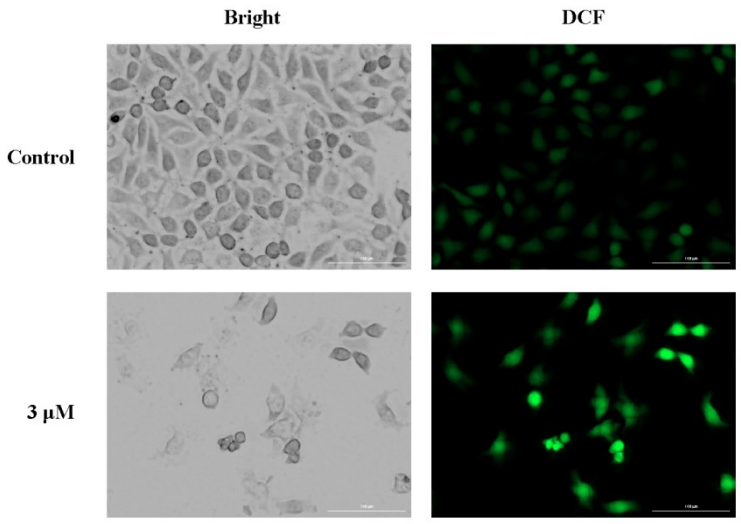


Figure S4. Changes in ROS concentration in T-24 cells treated with compound **4bl** determined with a DCFH-DA staining kit under a fluorescence microscope. Scale bar: 100 μm.

2.6 Measurement of intracellular Ca^{2+} levels

The intracellular Ca^{2+} levels were determined by fluorescent with Fluo-3 AM staining kit, which could pass through the cell membrane and be cut into Fluo-3 by the esterase. The Fluo-3 could bind with calcium ions to produce strong green fluorescence. T-24 cells were seeded at 2×10^6/well in 10% FBS/DMEM into 6-well plates and incubation for 24 hours. After the cells were treated with compound **4bl** (0 and 3 μM) for 24 h, the Fluo-3 AM (5.0 μM) was added and incubated for 30 min at 37 ^{o}C. The fluorescence microscope was used to measure the enhanced green flourescent intensity in cells, the intensity of the microscope is 506 nm, and the emission wavelength is 526 nm. As shown in Fig. S3-4, after treatment with compound **4bl** (0 and 3 μM) , the green fluorescence intensity increased significantly in T-24 cells. Hence, compound **4bl** can increase the intracellular levels of Ca^{2+}.

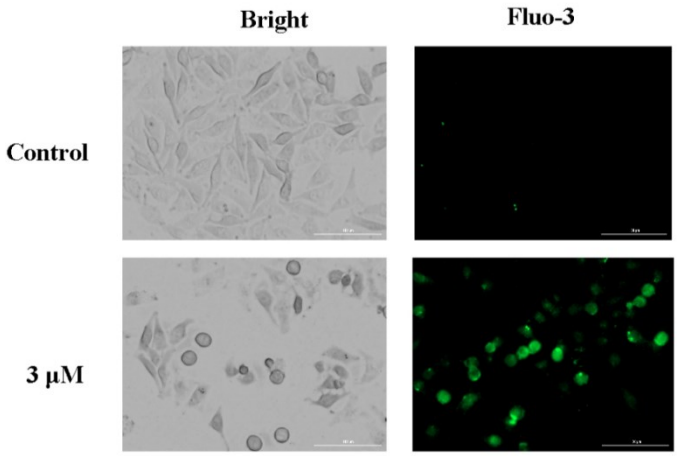


Figure S5. Changes in Ca^{2+} concentration in T-24 cells treated with compound **4bl** determined with a DCFH-DA staining kit under a fluorescence microscope. Scale bar: 100 μm.

2.7 Wound healing assay

T-24 cells (5×10^5 cells/well) were grown in petridishes for 24 h. Scratches were made in confluent monolayers using 200 mL pipette tip. Then, wounds were washed twice with PBS to remove non-adherent cell debris. The media containing different concentrations (0, 1.5 and 3 μM) of the compound **4bl** were added to the petridishes. Cells which migrated across the wound area were photographed under the fluorescence microscope (Cytation 5 Cell Imaging Multi-Mode Reader, BioTek Instruments, Inc., USA) after 0 and 24 h treatment. As shown in Fig. S3-5, the compound **4bl** treatment resulted in significant inhibition of migration capacity of T-24 cells and the effect was more prominent after 24 h. For instance, compound **4bl** treatment at 1.5 and 3 μM concentration led to strong inhibition of migration in to the scratch area in relative comparison to control after 24 h. It can be inferred from the results that the compound **4bl** suppresses the migration potential of the T-24 cells in dose dependent manner.

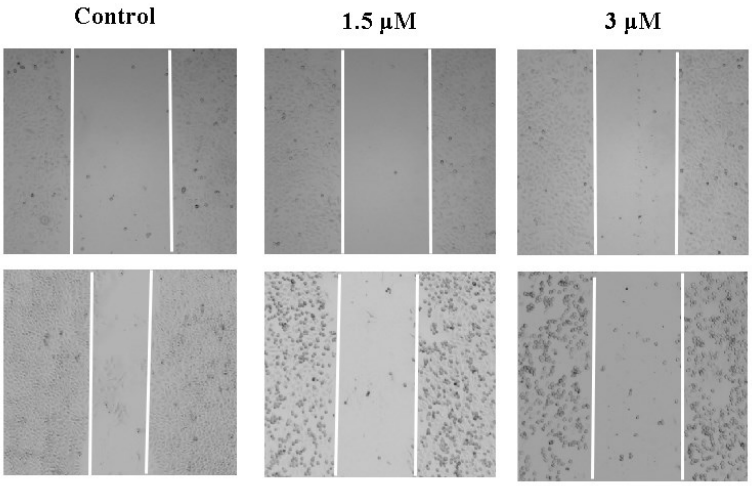
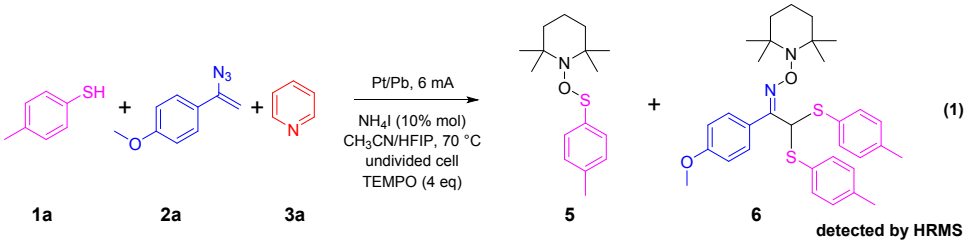


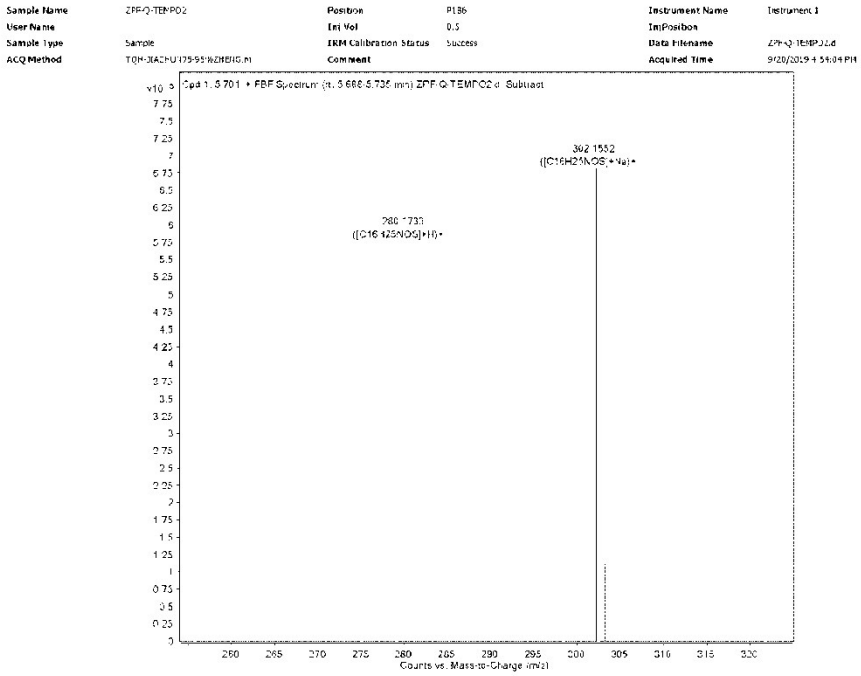
Figure S6. Effect of compound **4bl** on in vitro migration potential of T-24 cells

3. Mechanistic Experiments

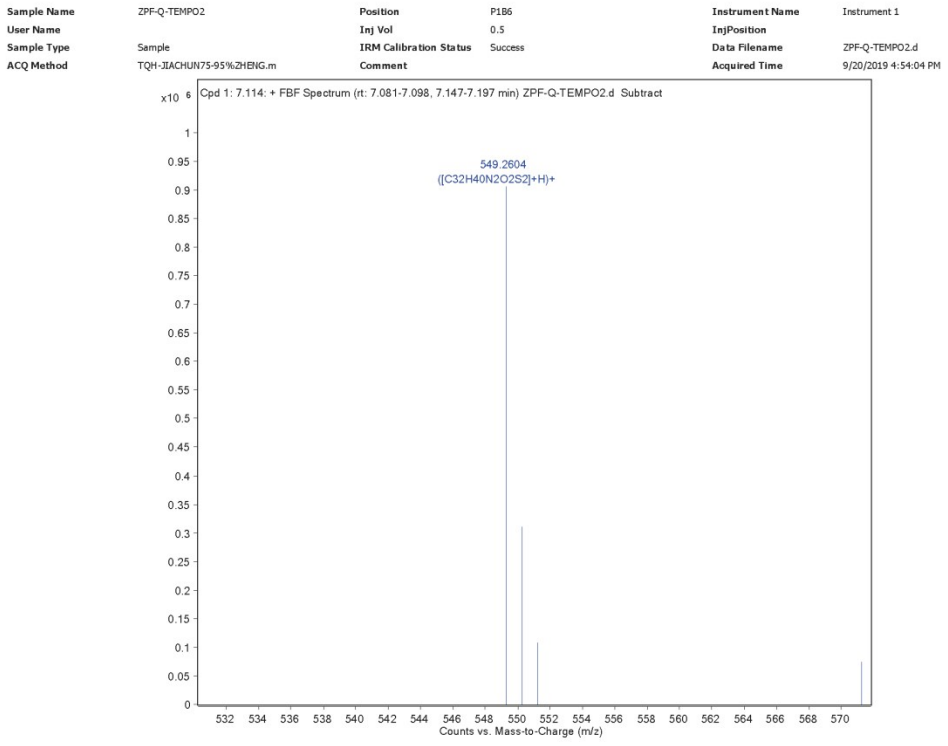
3.1 The HRMS spectra of compounds 5, 6 and 7



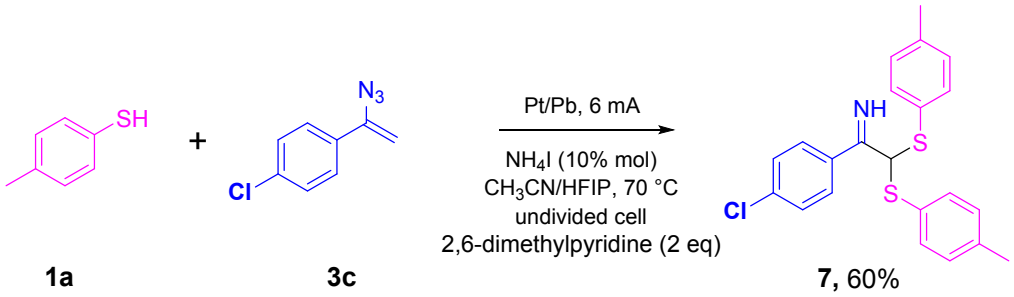
Compound **5**：**HRMS** (m/z) [ESI]: calculated for $C_{16}H_{26}NOS^{+}[M+H]^{+}$: 280.1730, found 280.1733.



Compound **6**：**HRMS** (m/z) [ESI]: calculated for $C_{32}H_{41}N_2O_2S_2^+[M+H]^+$: 549.2604, found 549.2604.



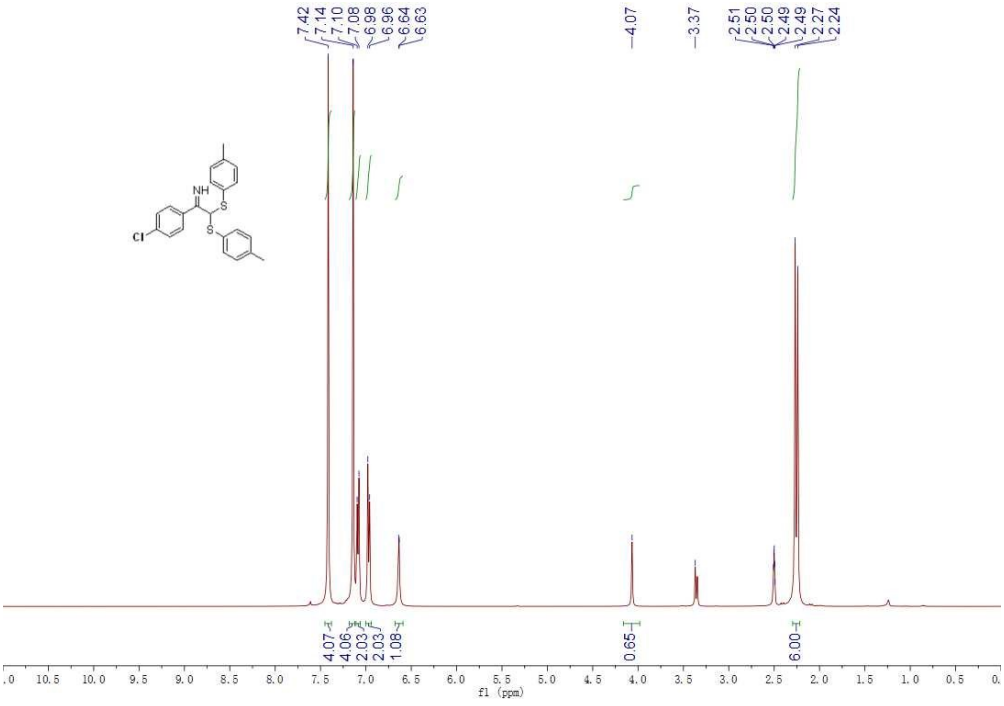
3.2 The ^{1}H NMR and ^{13}C NMR of compounds 7

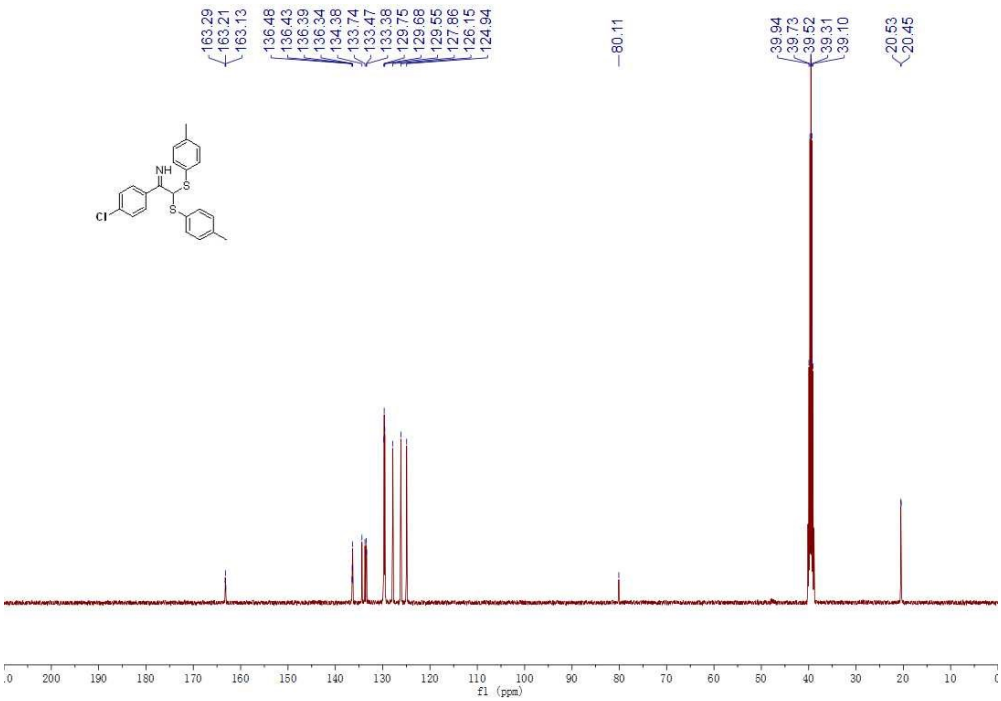


1a **3c** **7,** 60%

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.42 (s, 4H), 7.14 (s, 4H), 7.09 (d, J = 7.9 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 6.68 – 6.59 (m, 1H), 4.07 (s, 1H), 2.27 (s, 3H), 2.24 (s, 3H).

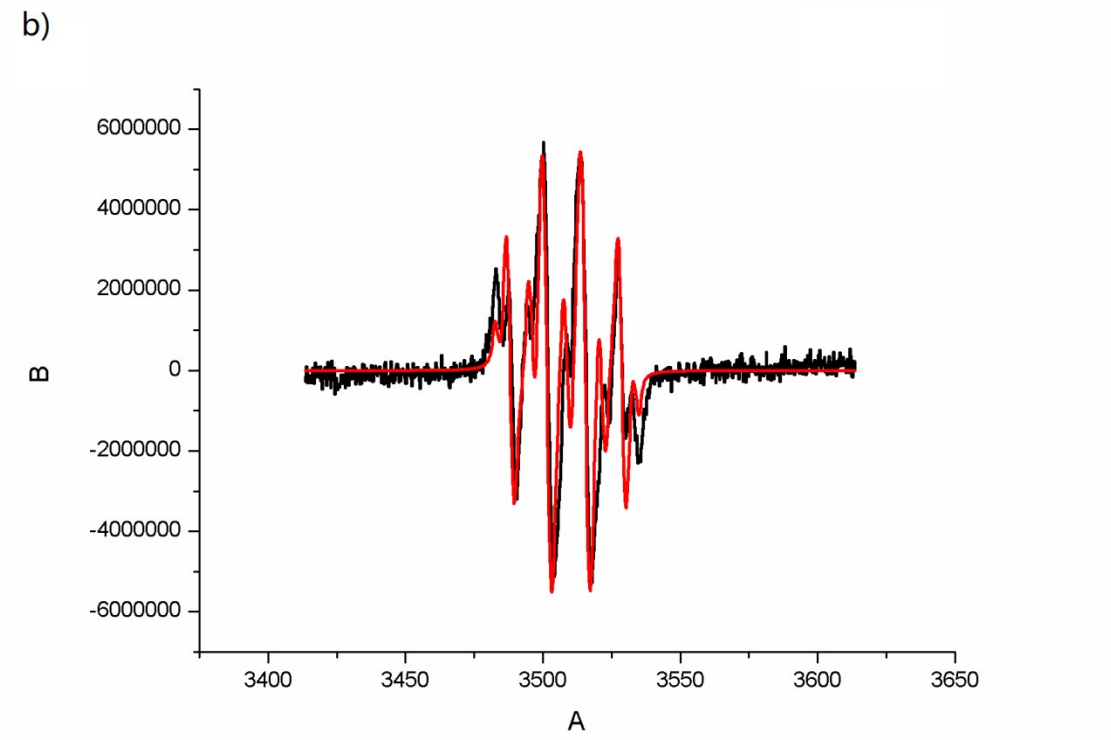
^{13}C NMR (101 MHz, DMSO-d_6) δ 163.2 (t, J = 8.0 Hz), 136.4 (t, J = 5.0 Hz), 136.3, 134.4, 133.7, 133.5, 133.4, 129.8, 129.7, 129.6, 127.9, 126.2, 124.9, 80.1, 20.5, 20.4.

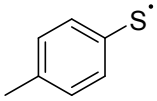


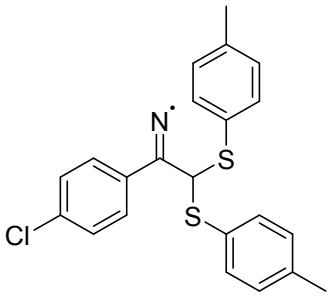


3.3 General procedure for EPR studies

A 10 ml three-necked round bottom flask was charged with thiophenol compound (1.8 mmol, 1.2 equiv), vinyl azide (1.5 mmol, 1.0 equiv), NH_4I (0.3 mmol, 10 mol%) and pyridine (6.0 mmol, 4 equiv). The flask was equipped with a platinum plate (1 cm x 1 cm x 0.1 cm) anode and a lead plate (1 cm x 1 cm x 0.1 cm) cathode. CH_3CN (5 mL) and HFIP (3 mL) were added. Electrolysis was carried out at 70 °C (oil bath temperature), which using a constant current for 0.5 h. Add DMPO (15 mmol) to the reaction bottle and continue stirring for 10min, The solution sample was taken out into a small tube for EPR test. EPR spectra was recorded at room temperature on EPR spectrometer operated at 9.851 GHz. Typical spectrometer parameters were shown as follows, sweep width: 200.00 G; center field set: 3513.50 G; time constant: 20.48 ms; sweep time: 40.96 s; modulation amplitude: 3.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^5; microwave power: 2.20 mW.





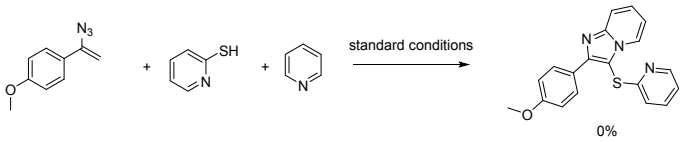


g=2.0062, A_N=14.01, A_H=12.6

g=2.0060, A_N=13.01, A_H=11.98

3.4 Special substrate research

As shown in the figure below heterocyclic thiols and benzyl mercaptan could not react with pyridine and p-methoxystyryl azide in our conditions, the main reason may be that these sulfur compounds were easy to dimer into disulfide compounds. These results have been added to the manuscript and supporting information.



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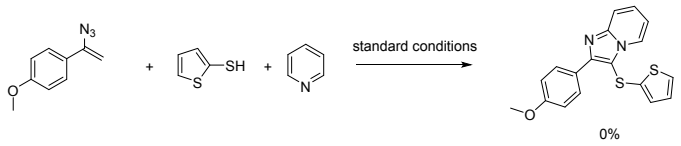

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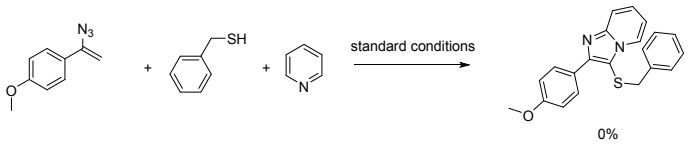

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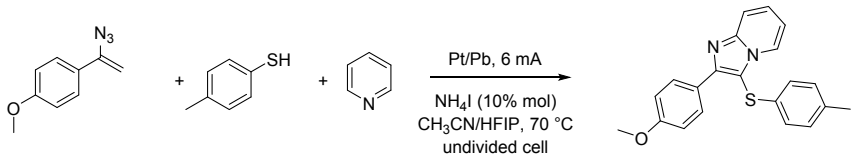
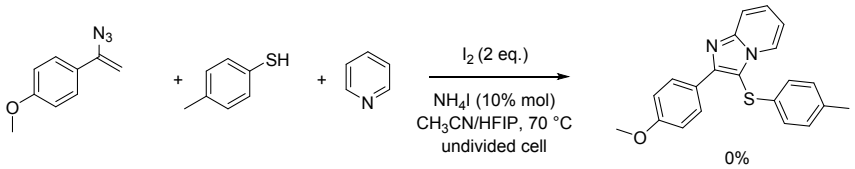
3.5 Control experiments.



Ar: 24% yield

O_2: 47% yield



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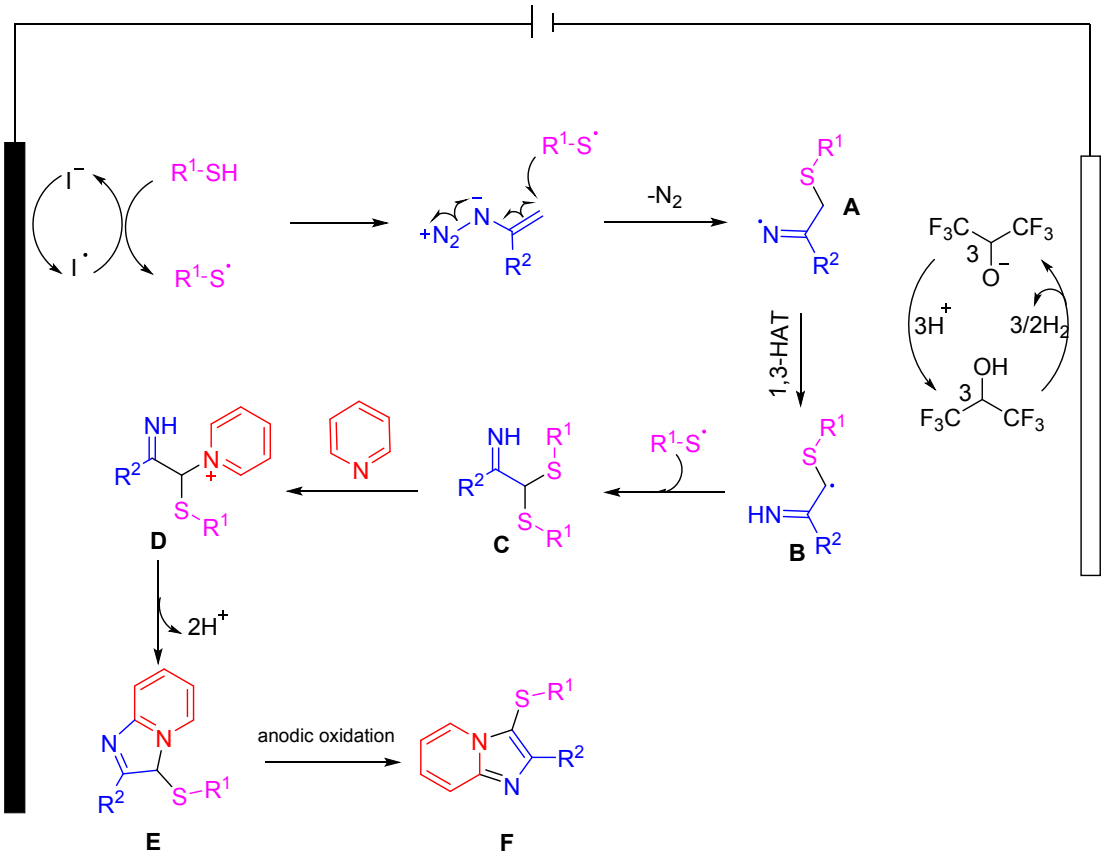
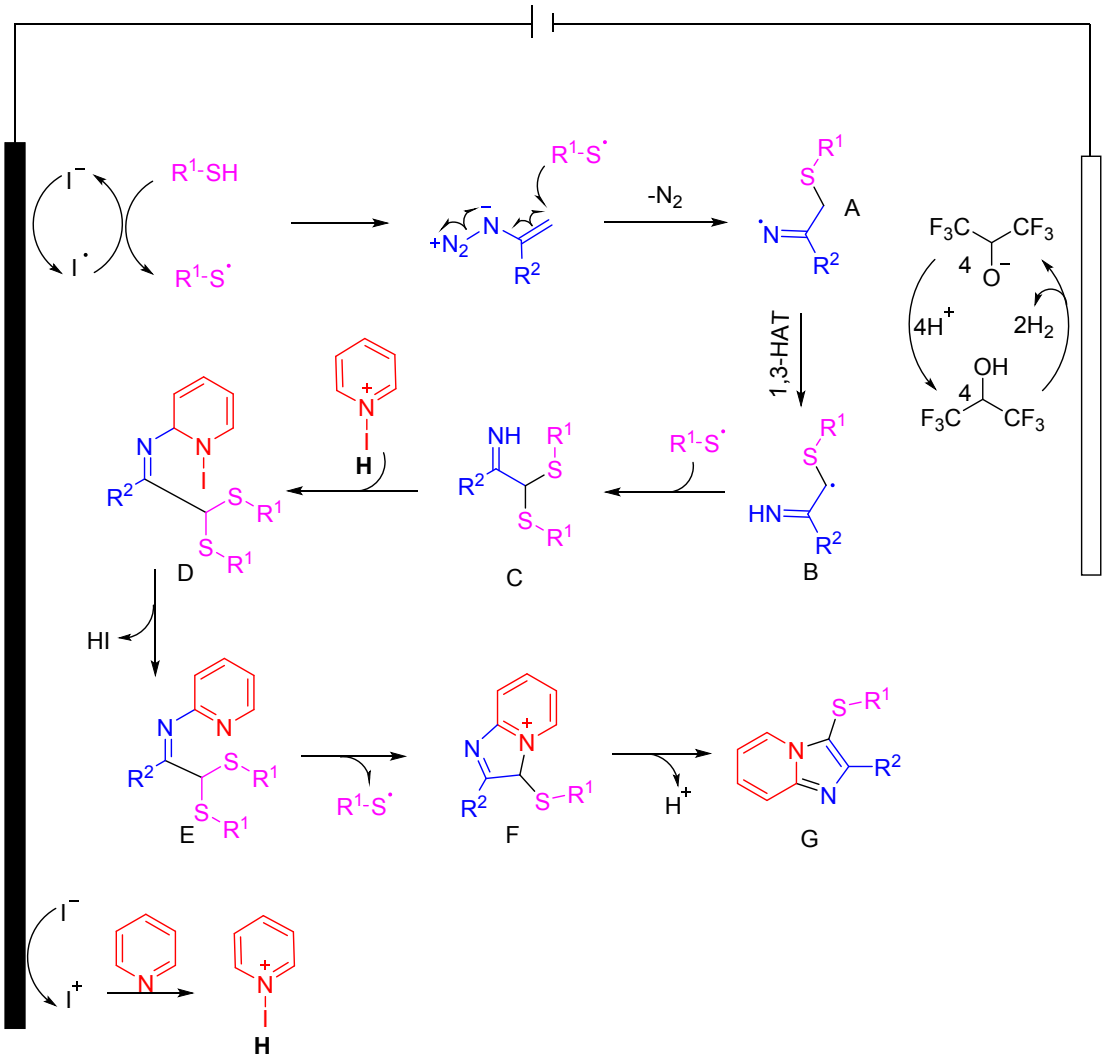
4. Mechanism Study

4.1 Possible reaction path

path a



path b


I⁻
I•
R1-SH
R1-S•
+N2
-N2
A
R2
1,3-HAT
F3C
CF3
4
O⁻
4H+
2H2
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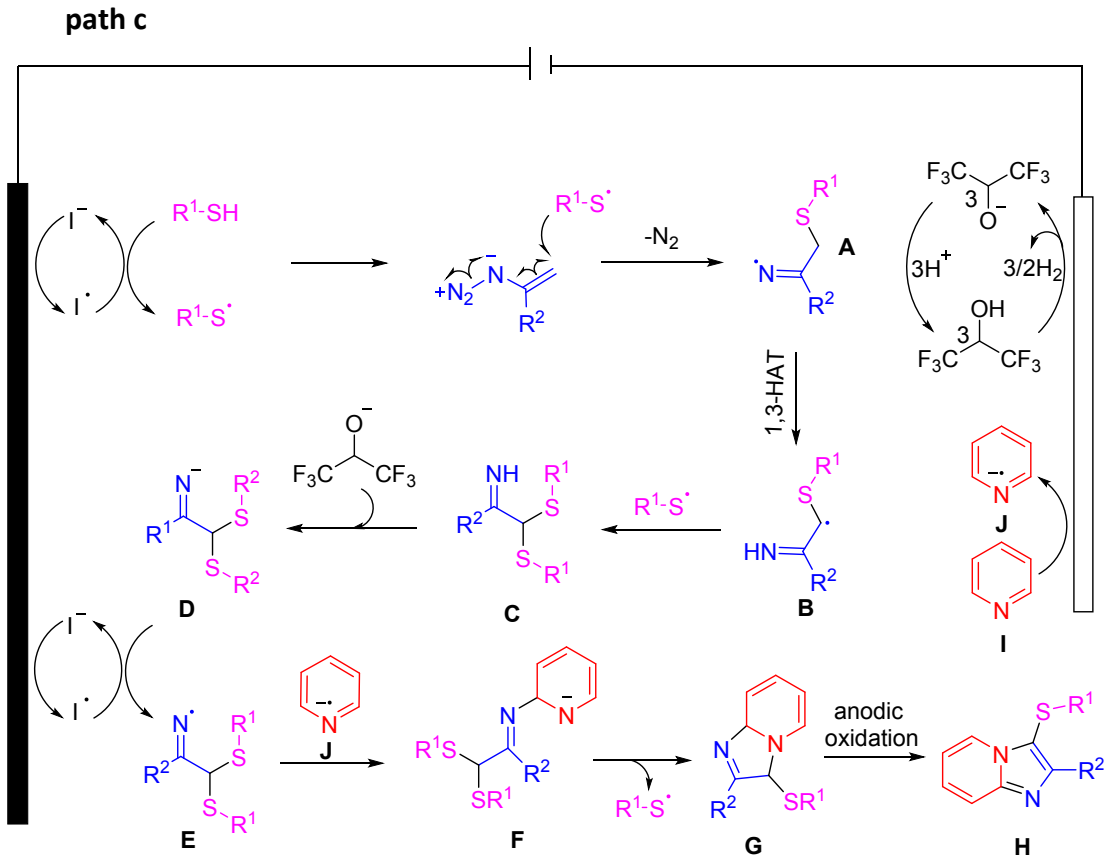
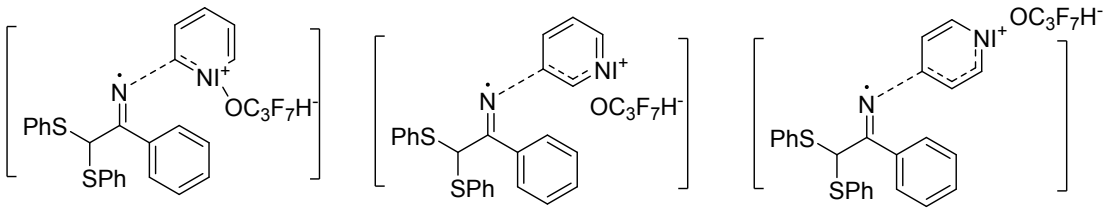
NH
HN
H
B
C
D
HI
E
F
G
I+



4.2 Selectivity



TS_PylAdd_radical	TS_PylAdd_radical_m	TS_PylAdd_radical_p
0.0	2.0	0.2

Relative Gibbs Free Energies of the transition states to different regioisomers

4.3 General Computational Calculation Details

Gaussian 09 program[1] was employed for DFT calculations. Geometry optimization was performed at M06-2X/def2-SVP[2-4]. The IEFPCM model[5] was used and the dielectric constant was set to 30.5 to simulate the mixed solvent used experimentally.

1. Frisch, M.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.; Others, Gaussian 09, revision D. 01. In Gaussian, Inc., Wallingford CT: 2009.
2. Zhao, Y.; Schultz, N. E.; Truhlar, D. G., Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for

Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation* **2006,** 2, (2), 364.

3. Zhao, Y. A. T. D., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theoretical Chemistry Accounts* **2008,** 120, (1), 215.
4. Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. Phys. Chem. Chem. Phys. 2005, 7,3297−3305.
5. M. Cossi, V. Barone, R. Cammi, and J. Tomasi, "Ab initio study of solvated molecules: A new implementation of the polarizable continuum model," Chem. Phys. Lett., 255 (1996) 327-35.

5. X-ray Crystallography Data

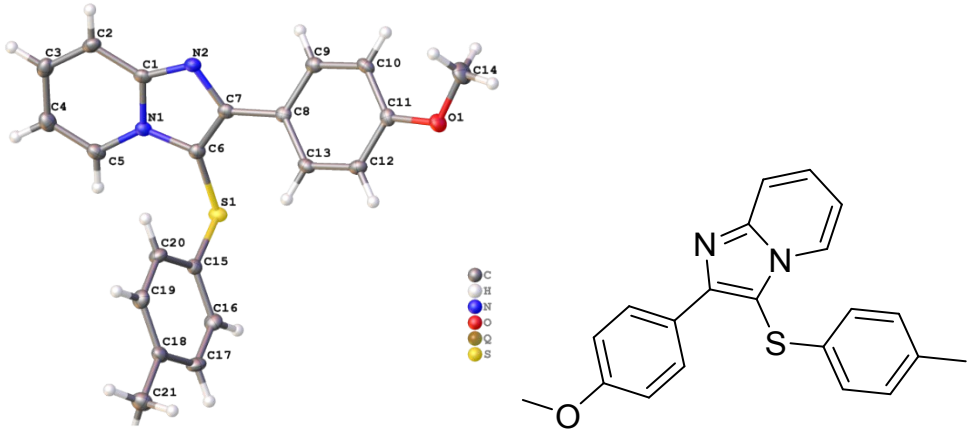


Figure S7. X-ray Structure of 4ab, CCDC number: 1960709

Table S2 Crystal data and structure refinement for 4ab.	
Identification code	4aa
Empirical formula	$C_{21}H_{18}N_2OS$
Formula weight	346.43
Temperature/K	100.00(10)

Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.3700(4)
b/Å	10.2878(4)
c/Å	14.5801(6)
α/°	90
β/°	97.519(4)
γ/°	90
Volume/Å^3	1690.80(11)
Z	4
ρ_{calc}g/cm^3	1.361
μ/mm^{-1}	0.203
F(000)	728.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.282 to 49.986
Index ranges	$-8 \le h \le 13$, $-12 \le k \le 10$, $-15 \le l \le 17$
Reflections collected	7544
Independent reflections	2978 [R_{int} = 0.0269, R_{sigma} = 0.0406]
Data/restraints/parameters	2978/0/228
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0382, wR_2 = 0.0847
Final R indexes [all data]	R_1 = 0.0462, wR_2 = 0.0901
Largest diff. peak/hole / e Å^{-3}	0.23/-0.27

Crystal structure determination of 4ab

Crystal Data for $C_{21}H_{18}N_2OS$ (M =346.43 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 11.3700(4) Å, b = 10.2878(4) Å, c = 14.5801(6) Å, β = 97.519(4)°, V = 1690.80(11) Å^3, Z = 4, T = 100.00(10) K, μ(MoKα) = 0.203 mm^{-1}, *Dcalc* = 1.361 g/cm^3, 7544 reflections measured (4.282° ≤ 2Θ ≤ 49.986°), 2978 unique (R_{int} = 0.0269, R_{sigma} = 0.0406) which were used in all calculations. The final R_1 was 0.0382 (I > 2σ(I)) and wR_2 was 0.0901 (all data).

Refinement model description

Table S3 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4ab. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	2413.6(4)	2231.8(4)	2265.6(3)	16.30(14)
O1	6662.2(11)	6771.1(12)	1487.7(9)	20.2(3)
N1	3349.5(13)	1540.3(14)	4025.2(10)	14.3(3)
N2	4821.7(13)	2957.7(14)	4441.9(10)	15.4(3)
C8	4859.8(15)	4182.7(16)	2998.6(12)	13.0(4)

C7	4342.1(15)	3187.4(17)	3543.3(13)	14.1(4)
C11	6074.6(15)	5963.7(17)	2022.1(13)	15.1(4)
C1	4214.7(16)	1953.3(17)	4722.8(13)	15.2(4)
C15	3023.6(15)	984.9(17)	1618.6(13)	14.5(4)
C6	3423.1(16)	2335.9(17)	3264.0(13)	15.1(4)
C10	6016.8(16)	6151.8(17)	2955.7(13)	16.3(4)
C9	5401.8(15)	5271.7(17)	3434.6(13)	16.0(4)
C13	4922.2(15)	4015.0(17)	2052.8(13)	15.1(4)
C2	4348.2(17)	1270.6(18)	5567.9(13)	17.8(4)
C16	2511.9(16)	821.5(18)	704.6(13)	18.9(4)
C12	5515.6(15)	4897.1(17)	1569.1(13)	15.8(4)
C20	3939.7(16)	172.4(18)	1978.8(13)	18.4(4)
C18	3847.6(16)	-962.2(17)	517.4(13)	17.9(4)
C3	3633.7(17)	231.8(18)	5668.5(14)	20.7(4)
C5	2637.3(16)	482.7(18)	4123.1(13)	18.4(4)
C19	4339.5(17)	-792.8(18)	1431.1(13)	19.9(4)
C17	2931.9(17)	-136.8(18)	171.4(13)	20.3(4)
C4	2772.1(17)	-167.6(18)	4933.0(14)	21.5(5)
C21	4287.8(18)	-1999.4(19)	-82.5(15)	24.9(5)
C14	7505.3(18)	7652.3(19)	1957.2(15)	26.6(5)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 4ab. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	12.5(2)	18.5(3)	17.1(3)	-3.2(2)	-0.80(19)	1.35(17)
O1	19.6(7)	19.1(7)	22.4(7)	-0.2(6)	4.1(6)	-6.1(5)
N1	12.9(8)	15.8(8)	14.6(8)	-2.5(7)	2.8(6)	-0.4(6)
N2	15.9(8)	15.8(8)	14.2(8)	-2.6(7)	0.9(6)	0.3(6)
C8	7.9(9)	15.1(9)	15.8(10)	-0.1(8)	0.7(7)	2.8(7)
C7	12.8(9)	14.5(9)	15.2(10)	-2.7(8)	2.7(7)	2.3(7)
C11	11.0(9)	14.3(9)	20.2(10)	1.4(8)	2.3(8)	2.0(7)
C1	15.0(10)	15.2(9)	15.7(10)	-5.2(8)	3.0(8)	1.9(7)
C15	12.2(9)	14.9(9)	16.5(10)	-0.3(8)	2.5(7)	-2.4(7)
C6	14.2(10)	16.7(9)	14.8(10)	-1.8(8)	3.6(8)	0.8(7)
C10	14.0(9)	12.9(9)	21.6(11)	-4.7(8)	0.8(8)	0.1(7)
C9	14.0(10)	17.1(9)	16.6(10)	-2.0(8)	0.9(8)	3.1(7)
C13	12.2(9)	14.1(9)	18.4(10)	-3.2(8)	-0.5(8)	0.3(7)
C2	20.7(10)	20.2(10)	12.8(10)	-2.9(8)	3.0(8)	3.5(8)
C16	15.3(10)	21.3(10)	18.9(10)	0.7(9)	-2.1(8)	1.0(8)

C12	14.5(10)	18.9(10)	14.0(10)	-3.2(8)	1.8(8)	2.6(7)
C20	19.3(10)	21.7(10)	13.3(10)	-0.7(8)	-1.1(8)	0.8(8)
C18	19.9(10)	16.0(9)	18.4(10)	-1.8(8)	4.6(8)	-4.6(7)
C3	24.7(11)	20.6(10)	18.2(11)	1.9(9)	8.6(8)	3.0(8)
C5	16.8(10)	18.9(10)	20.2(11)	-5.1(9)	4.9(8)	-3.2(8)
C19	19.6(10)	18.4(10)	21.1(11)	2.2(9)	0.7(8)	4.5(8)
C17	19.9(11)	25.8(11)	14.2(10)	-3.3(9)	-2.0(8)	-2.9(8)
C4	21.9(11)	18.9(10)	25.4(12)	-0.9(9)	9.6(9)	-2.7(8)
C21	27.3(11)	23.1(11)	24.7(12)	-5.3(9)	4.8(9)	0.2(8)
C14	22.4(11)	23.9(11)	34.0(13)	0.7(10)	5.0(9)	-10.4(8)

Table S5 Bond Lengths for 4ab.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C15	1.7854(18)	C11	C12	1.391(2)
S1	C6	1.7351(19)	C1	C2	1.409(3)
O1	C11	1.371(2)	C15	C16	1.393(3)
O1	C14	1.427(2)	C15	C20	1.384(3)
N1	C1	1.386(2)	C10	C9	1.387(3)
N1	C6	1.390(2)	C13	C12	1.379(3)
N1	C5	1.375(2)	C2	C3	1.362(3)
N2	C7	1.372(2)	C16	C17	1.379(3)
N2	C1	1.336(2)	C20	C19	1.388(3)
C8	C7	1.466(2)	C18	C19	1.387(3)
C8	C9	1.392(2)	C18	C17	1.386(3)
C8	C13	1.401(3)	C18	C21	1.506(3)
C7	C6	1.383(2)	C3	C4	1.415(3)
C11	C10	1.385(3)	C5	C4	1.348(3)

Table S6 Bond Angles for 4ab.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	S1	C15	103.15(8)	C20	C15	C16	119.31(17)
C11	O1	C14	117.31(15)	N1	C6	S1	122.08(13)
C1	N1	C6	107.11(14)	C7	C6	S1	132.63(15)
C5	N1	C1	122.51(16)	C7	C6	N1	105.06(15)
C5	N1	C6	130.29(16)	C11	C10	C9	119.70(17)
C1	N2	C7	105.61(15)	C10	C9	C8	121.19(17)
C9	C8	C7	120.01(16)	C12	C13	C8	120.92(17)

C9	C8	C13	118.20(16)	C3	C2	C1	119.20(18)
C13	C8	C7	121.54(16)	C17	C16	C15	119.57(17)
N2	C7	C8	120.01(16)	C13	C12	C11	120.01(17)
N2	C7	C6	111.26(16)	C15	C20	C19	120.05(17)
C6	C7	C8	128.64(17)	C19	C18	C17	117.51(17)
O1	C11	C10	124.28(16)	C19	C18	C21	121.60(17)
O1	C11	C12	115.76(16)	C17	C18	C21	120.89(17)
C10	C11	C12	119.96(17)	C2	C3	C4	120.64(18)
N1	C1	C2	118.28(16)	C4	C5	N1	118.86(18)
N2	C1	N1	110.95(16)	C18	C19	C20	121.43(17)
N2	C1	C2	130.73(17)	C16	C17	C18	122.12(18)
C16	C15	S1	116.72(14)	C5	C4	C3	120.50(18)
C20	C15	S1	123.95(14)				

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4ab.

Atom	*x*	*y*	*z*	U(eq)
H10	6388.7	6864.85	3260.2	20
H9	5350.69	5411.96	4058.29	19
H13	4558.38	3298.6	1746.94	18
H2	4917.25	1526.39	6051.07	21
H16	1890.82	1355.24	455.54	23
H12	5542.02	4778.89	939.71	19
H20	4287.44	273.51	2588.26	22
H3	3712.62	-219.49	6225.88	25
H5	2072.29	220.33	3639.12	22
H19	4950.67	-1337.96	1682.3	24
H17	2589.97	-232.42	-440.04	24
H4	2295.42	-883.95	5008.99	26
H21A	4768.78	-1608.75	-501.65	37
H21B	3623.28	-2429.79	-428.43	37
H21C	4751.95	-2620.85	300.32	37
H14A	7961.39	8040.9	1520.03	40
H14B	8025.11	7189.47	2416.89	40
H14C	7096.28	8319.06	2250.42	40

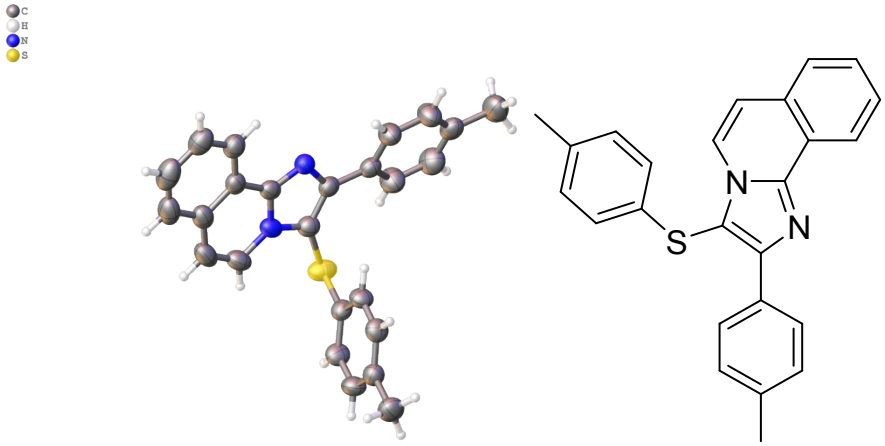


Figure S8. X-ray Structure of 4cj, CCDC number: 1960714

Table S8 Crystal data and structure refinement for 4cj.

Identification code	4cj
Empirical formula	$C_{25}H_{21}N_2S$
Formula weight	380.517
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.6915(2)
b/Å	12.7636(7)
c/Å	26.8264(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1948.80(15)
Z	4
ρ_{calc}g/cm^3	1.297
μ/mm^{-1}	0.179
F(000)	800.8
Crystal size/mm^3	0.41 × 0.28 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.86 to 52.74
Index ranges	$-6 \le h \le 7$, $-16 \le k \le 14$, $-34 \le l \le 35$
Reflections collected	7649
Independent reflections	3830 [R_{int} = 0.0291, R_{sigma} = 0.0645]
Data/restraints/parameters	3830/0/255
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0537, wR_2 = 0.1132
Final R indexes [all data]	R_1 = 0.0823, wR_2 = 0.1335
Largest diff. peak/hole / e Å^{-3}	0.25/-0.34

Flack parameter	0.10(12)

Table S9 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 4cj. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	8499.0(14)	5461.7(7)	1532.6(4)	60.3(3)
N1	4907(4)	4890(2)	2141.6(10)	48.0(7)
N2	3805(4)	3308(2)	1909.7(9)	46.7(7)
C1	8524(7)	841(3)	21.3(14)	82.0(13)
C2	7853(6)	1555(3)	442.3(13)	60.4(10)
C3	5724(6)	1444(3)	685.7(15)	66.2(10)
C4	5046(6)	2117(3)	1067.0(14)	59.3(9)
C5	6492(5)	2925(3)	1221.1(11)	45.5(7)
C6	8662(6)	3016(3)	986.9(14)	66.2(10)
C7	9291(7)	2353(3)	603.9(16)	69.6(11)
C8	5671(5)	3613(3)	1618.6(12)	44.8(8)
C9	6396(5)	4603(3)	1756.2(12)	49.0(8)
C10	3357(5)	4082(2)	2219.0(11)	44.3(7)
C11	1552(6)	4183(3)	2588.4(11)	47.0(8)
C12	-105(6)	3403(3)	2666.0(12)	56.3(9)
C13	-1841(6)	3537(4)	3014.3(14)	67.6(11)
C14	-1932(7)	4463(4)	3291.6(14)	77.8(13)
C15	-294(7)	5230(3)	3222.5(14)	69.5(11)
C16	1469(6)	5127(3)	2863.4(13)	54.5(9)
C17	3155(7)	5918(3)	2767.6(13)	63.0(10)
C18	4802(7)	5812(3)	2415.5(14)	57.0(9)
C19	2755(6)	8596(3)	338.2(14)	68.5(11)
C20	4136(5)	7820(3)	636.2(12)	49.5(8)
C21	3373(6)	6806(3)	698.6(12)	52.5(9)
C22	4642(5)	6080(3)	968.0(13)	51.9(9)
C23	6716(5)	6362(3)	1191.8(11)	45.9(8)
C24	7510(6)	7383(3)	1139.4(12)	54.5(9)
C25	6242(6)	8087(3)	863.9(13)	54.2(8)

Table S10 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 4cj. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	47.7(4)	53.7(6)	79.6(6)	-9.7(4)	-12.8(5)	15.6(5)
N1	55.6(15)	38.8(16)	49.7(16)	-1.3(13)	-14.1(14)	0.2(14)
N2	54.8(15)	37.9(15)	47.5(15)	-5.4(14)	-2.1(13)	0.2(14)
C1	102(3)	72(3)	72(3)	23(3)	13(2)	-5(2)
C2	74(2)	52(2)	56(2)	14(2)	5.5(18)	10(2)
C3	74(2)	56(2)	68(2)	-12(2)	9.5(19)	-10(2)
C4	66(2)	55(2)	57(2)	-8(2)	13.3(18)	-4(2)
C5	49.1(17)	44.5(19)	42.9(17)	0.5(17)	-1.6(15)	8.4(16)
C6	60(2)	68(3)	70(2)	-11(2)	8.9(19)	-4(2)
C7	62(2)	74(3)	72(3)	2(2)	14(2)	1(2)
C8	47.4(16)	47.3(19)	39.8(17)	-2.7(15)	-4.3(14)	7.7(16)
C9	50.2(17)	46.2(19)	50.6(18)	-2.0(18)	-5.9(16)	3.5(17)
C10	51.7(17)	37.7(17)	43.4(17)	2.8(16)	-11.6(16)	2.0(15)
C11	54.4(18)	47.4(19)	39.2(16)	7.3(18)	-6.2(15)	2.9(16)
C12	62(2)	60(2)	47(2)	6(2)	-2.1(17)	4.6(19)
C13	64(2)	77(3)	61(2)	10(2)	2.9(19)	15(2)
C14	72(2)	106(4)	56(2)	30(3)	7(2)	9(3)
C15	84(2)	71(3)	54(2)	24(2)	-3(2)	-7(2)
C16	63.7(19)	54(2)	46.4(19)	13.4(19)	-10.0(18)	-2.7(18)
C17	84(2)	49(2)	56(2)	10(2)	-17(2)	-13.4(19)
C18	67(2)	39(2)	64(2)	-1.2(18)	-17.3(19)	-3.6(19)
C19	79(2)	62(2)	65(2)	9(2)	-12.1(19)	9(2)
C20	52.7(19)	48(2)	47.8(19)	3.7(17)	0.7(15)	-0.0(17)
C21	45.2(17)	58(2)	54.0(19)	-2.1(18)	-9.0(16)	-3.1(18)
C22	54.2(18)	43(2)	58(2)	-10.8(17)	-4.9(16)	-0.3(18)
C23	44.8(17)	49(2)	43.9(18)	-9.1(16)	0.7(14)	3.7(16)
C24	49.3(18)	55(2)	59(2)	-12.4(17)	-12.1(16)	1(2)
C25	61(2)	38.7(18)	63(2)	-5.4(18)	-0.4(19)	3.1(18)

Table S11 Bond Lengths for 4cj.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C9	1.731(3)	C10	C11	1.433(4)
S1	C23	1.785(3)	C11	C12	1.387(5)
N1	C9	1.386(4)	C11	C16	1.414(4)
N1	C10	1.373(4)	C12	C13	1.371(5)
N1	C18	1.389(4)	C13	C14	1.398(6)
N2	C8	1.374(4)	C14	C15	1.364(5)
N2	C10	1.314(4)	C15	C16	1.397(5)

C1	C2	1.500(5)	C16	C17	1.416(5)
C2	C3	1.384(5)	C17	C18	1.337(5)
C2	C7	1.376(5)	C19	C20	1.496(4)
C3	C4	1.390(5)	C20	C21	1.376(4)
C4	C5	1.383(4)	C20	C25	1.388(4)
C5	C6	1.390(4)	C21	C22	1.379(4)
C5	C8	1.459(4)	C22	C23	1.372(4)
C6	C7	1.378(5)	C23	C24	1.387(4)
C8	C9	1.379(4)	C24	C25	1.369(4)

Table S12 Bond Angles for 4cj.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C23	S1	C9	101.07(14)	C11	C10	N2	130.0(3)
C10	N1	C9	107.9(3)	C12	C11	C10	121.8(3)
C18	N1	C9	130.1(3)	C16	C11	C10	117.5(3)
C18	N1	C10	121.9(3)	C16	C11	C12	120.7(3)
C10	N2	C8	107.2(3)	C13	C12	C11	120.2(4)
C3	C2	C1	121.1(4)	C14	C13	C12	119.7(4)
C7	C2	C1	122.3(4)	C15	C14	C13	120.6(4)
C7	C2	C3	116.6(4)	C16	C15	C14	121.2(4)
C4	C3	C2	121.8(4)	C15	C16	C11	117.6(4)
C5	C4	C3	121.0(3)	C17	C16	C11	119.3(3)
C6	C5	C4	117.1(3)	C17	C16	C15	123.1(4)
C8	C5	C4	118.5(3)	C18	C17	C16	122.1(4)
C8	C5	C6	124.4(3)	C17	C18	N1	119.3(4)
C7	C6	C5	121.1(4)	C21	C20	C19	121.5(3)
C6	C7	C2	122.3(4)	C25	C20	C19	121.8(3)
C5	C8	N2	119.5(3)	C25	C20	C21	116.7(3)
C9	C8	N2	109.8(3)	C22	C21	C20	122.1(3)
C9	C8	C5	130.7(3)	C23	C22	C21	120.3(3)
N1	C9	S1	120.9(2)	C22	C23	S1	123.0(3)
C8	C9	S1	134.0(3)	C24	C23	S1	118.1(2)
C8	C9	N1	105.0(3)	C24	C23	C22	118.8(3)
N2	C10	N1	110.1(3)	C25	C24	C23	119.9(3)
C11	C10	N1	119.8(3)	C24	C25	C20	122.2(3)

Table S13 Torsion Angles for 4cj.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C9	N1	C10	176.6(2)	C3	C4	C5	C6	-1.5(4)
S1	C9	N1	C18	-1.7(3)	C3	C4	C5	C8	179.2(3)
S1	C9	C8	N2	-176.4(3)	C4	C5	C6	C7	2.6(4)
S1	C9	C8	C5	0.6(4)	C4	C5	C8	C9	-161.0(3)
S1	C23	C22	C21	-178.3(3)	C10	C11	C12	C13	-178.4(3)
S1	C23	C24	C25	177.4(3)	C10	C11	C16	C15	179.8(3)
N1	C9	C8	N2	0.1(3)	C10	C11	C16	C17	-0.6(3)
N1	C9	C8	C5	177.0(2)	C11	C12	C13	C14	-0.1(4)
N1	C10	N2	C8	-0.6(3)	C11	C16	C15	C14	-2.5(4)
N1	C10	C11	C12	177.5(3)	C11	C16	C17	C18	1.6(4)
N1	C10	C11	C16	-0.5(3)	C12	C13	C14	C15	-0.7(4)
N1	C18	C17	C16	-1.6(4)	C13	C14	C15	C16	2.1(4)
N2	C8	C5	C4	15.7(3)	C14	C15	C16	C17	177.8(3)
N2	C8	C5	C6	-163.5(3)	C15	C16	C17	C18	-178.7(3)
N2	C10	C11	C12	-0.7(4)	C19	C20	C21	C22	179.3(3)
N2	C10	C11	C16	-178.7(3)	C19	C20	C25	C24	179.7(3)
C1	C2	C3	C4	-178.1(4)	C20	C21	C22	C23	1.1(4)
C1	C2	C7	C6	179.2(4)	C20	C25	C24	C23	1.0(4)
C2	C3	C4	C5	-0.5(5)	C21	C22	C23	C24	-0.3(4)
C2	C7	C6	C5	-1.8(5)	C22	C23	C24	C25	-0.7(4)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4cj.

Atom	*x*	*y*	*z*	U(eq)
H1a	9230(40)	217(10)	153.0(15)	123.0(19)
H1b	7147(11)	659(17)	-166(6)	123.0(19)
H1c	9620(40)	1192(9)	-193(6)	123.0(19)
H3	4720(6)	904(3)	591.7(15)	79.4(12)
H4	3597(6)	2022(3)	1220.8(14)	71.1(11)
H6	9706(6)	3533(3)	1090.4(14)	79.5(12)
H7	10737(7)	2448(3)	449.2(16)	83.6(14)
H12	-38(6)	2787(3)	2481.1(12)	67.6(11)
H13	-2953(6)	3014(4)	3065.9(14)	81.1(13)
H14	-3120(7)	4558(4)	3525.4(14)	93.4(15)
H15	-352(7)	5831(3)	3417.8(14)	83.4(13)
H17	3117(7)	6530(3)	2955.5(13)	75.6(12)
H18	5865(7)	6350(3)	2354.7(14)	68.4(11)
H19a	1700(30)	8967(14)	554(2)	102.8(16)

H19b	3810(7)	9085(12)	183(8)	102.8(16)
H19c	1870(30)	8236(4)	86(6)	102.8(16)
H21	1958(6)	6603(3)	554.6(12)	62.9(10)
H22	4089(5)	5398(3)	998.2(13)	62.3(10)
H24	8904(6)	7590(3)	1291.4(12)	65.4(11)
H25	6810(6)	8766(3)	828.2(13)	65.1(10)
H2	3068(4)	2721(2)	1892.6(9)	56.1(8)

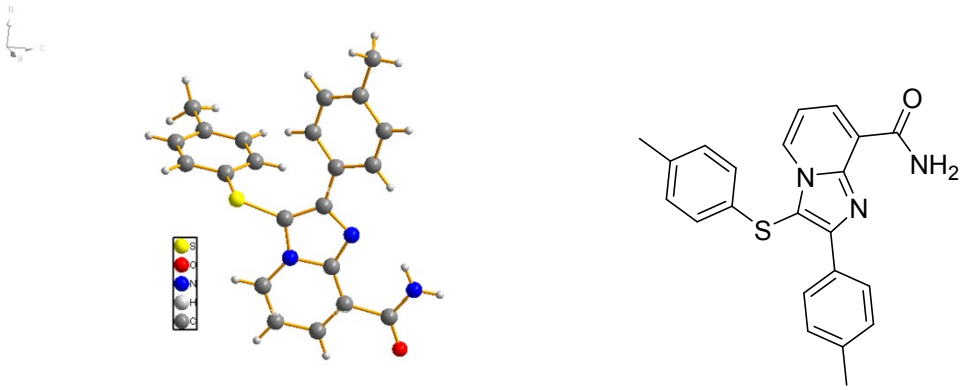


Figure S9. X-ray Structure of 4ci, CCDC number: 1970761

Table S15 Crystal data and structure refinement for 4ci.

Identification code	**4ci**
Empirical formula	$C_{22.75}H_{22}N_3O_{1.75}S$
Formula weight	397.49
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	4.9241(18)
b/Å	14.209(4)
c/Å	15.2990(16)
α/°	90.853(15)
β/°	96.934(19)
γ/°	99.10(3)
Volume/Å^3	1048.6(5)
Z	2
ρ_{calc}g/cm^3	1.259
μ/mm^{-1}	0.176
F(000)	419.0
Crystal size/mm^3	0.41 × 0.28 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.776 to 49.426
Index ranges	-5 ≤ h ≤ 5, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17
Reflections collected	10064

Independent reflections	3555 [R_{int} = 0.2226, R_{sigma} = 0.2078]
Data/restraints/parameters	3555/12/266
Goodness-of-fit on F^2	0.890
Final R indexes [I>=2σ (I)]	R_1 = 0.1070, wR_2 = 0.2312
Final R indexes [all data]	R_1 = 0.2222, wR_2 = 0.3136
Largest diff. peak/hole / e $Å^{-3}$	0.38/-0.40

Table S16 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 4ci. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	-183(4)	6605.5(13)	5740.9(10)	71.8(7)
O1	9483(13)	4361(4)	8908(3)	104.3(19)
N1	3478(10)	5706(4)	6740(3)	57.6(14)
N2	3955(11)	6369(4)	8098(3)	64.9(15)
N3	7379(12)	5538(4)	9339(4)	87.6(19)
C1	7931(17)	4936(5)	8747(4)	75(2)
C2	6429(14)	5011(5)	7826(4)	67.3(18)
C3	6834(15)	4393(5)	7198(4)	76(2)
C4	5474(15)	4412(5)	6330(4)	76(2)
C5	3857(14)	5056(5)	6117(4)	67.1(18)
C6	4698(13)	5683(5)	7615(4)	59.6(17)
C7	2313(13)	6837(5)	7546(4)	62.7(17)
C8	1922(13)	6444(5)	6691(4)	62.7(18)
C9	1048(13)	7615(5)	7885(4)	60.3(17)
C10	824(16)	7700(5)	8790(5)	84(2)
C11	-438(17)	8378(6)	9118(5)	92(2)
C12	-1530(16)	9050(6)	8577(6)	89(2)
C13	-1241(15)	8981(6)	7699(5)	83(2)
C14	20(14)	8295(5)	7359(4)	69.1(19)
C15	-3028(16)	9771(6)	8947(6)	115(3)
C16	1994(14)	7435(5)	5147(4)	59.6(17)
C17	4313(14)	7998(5)	5549(4)	70.0(19)
C18	5844(16)	8640(6)	5029(5)	85(2)
C19	5090(17)	8737(6)	4151(5)	73(2)
C20	2729(19)	8171(6)	3786(5)	83(2)
C21	1128(15)	7517(5)	4261(5)	79(2)

C22	6787(16)	9431(6)	3619(6)	109(3)
O2	410(30)	2489(9)	8438(9)	200(5)
C23	3130(30)	2420(11)	8590(10)	153(6)

Table S17 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4ci. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	82.8(14)	84.4(14)	42.7(11)	-3.0(9)	-5.5(9)	6.6(10)
O1	158(5)	94(4)	62(3)	-7(3)	-27(3)	55(4)
N1	70(4)	65(4)	34(3)	-4(2)	3(3)	5(3)
N2	76(4)	74(4)	42(3)	-1(3)	4(3)	8(3)
N3	121(5)	97(5)	42(3)	1(3)	-19(3)	32(4)
C1	108(6)	70(5)	41(4)	-15(4)	3(4)	1(4)
C2	86(5)	76(5)	36(4)	-1(3)	1(4)	6(4)
C3	96(5)	83(5)	52(4)	6(4)	9(4)	29(4)
C4	113(6)	68(5)	51(4)	-5(4)	12(4)	21(4)
C5	87(5)	74(5)	36(4)	-13(3)	-1(4)	8(4)
C6	70(5)	66(4)	40(4)	-2(3)	4(3)	4(3)
C7	70(5)	69(4)	46(4)	-2(3)	2(4)	6(4)
C8	64(4)	78(5)	39(4)	-7(3)	-9(3)	3(4)
C9	60(4)	77(5)	42(4)	-5(3)	11(3)	4(3)
C10	114(6)	86(6)	47(4)	-7(4)	12(4)	7(4)
C11	122(7)	95(6)	58(5)	-22(5)	28(5)	5(5)
C12	79(5)	107(7)	77(6)	-28(5)	4(5)	10(5)
C13	92(6)	104(6)	56(5)	-18(4)	3(4)	29(5)
C14	79(5)	82(5)	47(4)	-3(4)	10(4)	14(4)
C15	103(6)	137(8)	107(7)	-50(6)	18(6)	27(6)
C16	82(5)	66(4)	31(3)	-7(3)	-6(3)	22(4)
C17	72(5)	95(5)	41(4)	-2(4)	1(4)	14(4)
C18	87(5)	96(6)	65(5)	-9(4)	-2(4)	3(4)
C19	81(6)	88(6)	57(5)	6(4)	6(4)	31(4)
C20	119(7)	95(6)	45(4)	20(4)	20(5)	41(5)
C21	85(5)	90(6)	57(5)	-13(4)	-14(4)	21(4)
C22	124(7)	109(7)	106(7)	46(6)	43(6)	28(6)
O2	236(11)	163(10)	192(11)	-45(8)	-40(9)	61(9)
C23	155(11)	173(13)	137(12)	22(10)	29(10)	38(10)

Table S18 Bond Lengths for 4ci.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C8	1.721(6)	C9	C10	1.407(8)
S1	C16	1.797(7)	C9	C14	1.384(9)
O1	C1	1.212(8)	C10	C11	1.349(9)
N1	C5	1.366(7)	C11	C12	1.401(10)
N1	C6	1.403(7)	C12	C13	1.371(10)
N1	C8	1.390(7)	C12	C15	1.496(9)
N2	C6	1.337(7)	C13	C14	1.364(8)
N2	C7	1.353(7)	C16	C17	1.360(9)
N3	C1	1.317(8)	C16	C21	1.384(8)
C1	C2	1.525(9)	C17	C18	1.408(9)
C2	C3	1.345(9)	C18	C19	1.366(9)
C2	C6	1.394(8)	C19	C20	1.358(10)
C3	C4	1.417(9)	C19	C22	1.503(9)
C4	C5	1.324(8)	C20	C21	1.392(10)
C7	C8	1.395(8)	O2	C23	1.349(14)
C7	C9	1.469(8)			

Table S19 Bond Angles for 4ci.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8	S1	C16	103.8(3)	C7	C8	S1	134.5(5)
C5	N1	C6	121.0(5)	C10	C9	C7	120.1(6)
C5	N1	C8	131.4(5)	C14	C9	C7	123.7(6)
C8	N1	C6	107.6(5)	C14	C9	C10	116.2(6)
C6	N2	C7	106.8(5)	C11	C10	C9	121.7(7)
O1	C1	N3	123.9(7)	C10	C11	C12	121.6(8)
O1	C1	C2	121.8(6)	C11	C12	C15	120.7(8)
N3	C1	C2	114.3(7)	C13	C12	C11	116.5(7)
C3	C2	C1	117.2(6)	C13	C12	C15	122.7(9)
C3	C2	C6	119.7(6)	C14	C13	C12	122.5(8)
C6	C2	C1	123.1(6)	C13	C14	C9	121.5(7)
C2	C3	C4	120.3(6)	C17	C16	S1	122.3(5)
C5	C4	C3	120.6(6)	C17	C16	C21	120.7(7)
C4	C5	N1	119.9(6)	C21	C16	S1	116.9(6)
N2	C6	N1	109.6(5)	C16	C17	C18	117.9(6)
N2	C6	C2	132.1(6)	C19	C18	C17	123.4(8)
C2	C6	N1	118.3(6)	C18	C19	C22	121.7(8)
N2	C7	C8	111.6(6)	C20	C19	C18	116.2(8)

N2	C7	C9	120.4(6)	C20	C19	C22	122.0(7)
C8	C7	C9	127.9(6)	C19	C20	C21	123.3(7)
N1	C8	S1	120.7(5)	C16	C21	C20	118.4(7)
N1	C8	C7	104.3(5)				

Table S20 Torsion Angles for 4ci.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C16	C17	C18	-178.6(5)	C7	C9	C10	C11	-176.9(7)
S1	C16	C21	C20	178.4(5)	C7	C9	C14	C13	177.2(6)
O1	C1	C2	C3	1.8(11)	C8	S1	C16	C17	-19.6(6)
O1	C1	C2	C6	-178.0(7)	C8	S1	C16	C21	163.8(5)
N2	C7	C8	S1	171.1(5)	C8	N1	C5	C4	179.9(6)
N2	C7	C8	N1	-1.1(7)	C8	N1	C6	N2	0.0(7)
N2	C7	C9	C10	-18.9(10)	C8	N1	C6	C2	-178.5(6)
N2	C7	C9	C14	161.1(6)	C8	C7	C9	C10	156.7(7)
N3	C1	C2	C3	-177.8(7)	C8	C7	C9	C14	-23.2(11)
N3	C1	C2	C6	2.3(10)	C9	C7	C8	S1	-4.9(12)
C1	C2	C3	C4	179.1(6)	C9	C7	C8	N1	-177.1(6)
C1	C2	C6	N1	178.3(6)	C9	C10	C11	C12	-1.7(13)
C1	C2	C6	N2	0.2(12)	C10	C9	C14	C13	-2.7(11)
C2	C3	C4	C5	2.0(11)	C10	C11	C12	C13	-0.1(13)
C3	C2	C6	N1	1.6(10)	C10	C11	C12	C15	177.4(7)
C3	C2	C6	N2	-179.7(7)	C11	C12	C13	C14	0.4(12)
C3	C4	C5	N1	-0.3(11)	C12	C13	C14	C9	1.1(12)
C5	N1	C6	N2	-178.2(5)	C14	C9	C10	C11	3.0(11)
C5	N1	C6	C2	3.3(9)	C15	C12	C13	C14	-177.1(7)
C5	N1	C8	S1	5.0(9)	C16	S1	C8	N1	-92.3(5)
C5	N1	C8	C7	178.6(6)	C16	S1	C8	C7	96.5(7)
C6	N1	C5	C4	-2.4(10)	C16	C17	C18	C19	1.2(11)
C6	N1	C8	S1	-172.9(4)	C17	C16	C21	C20	1.7(10)
C6	N1	C8	C7	0.6(7)	C17	C18	C19	C20	0.0(11)
C6	N2	C7	C8	1.1(7)	C17	C18	C19	C22	-179.9(6)
C6	N2	C7	C9	177.4(6)	C18	C19	C20	C21	-0.4(11)
C6	C2	C3	C4	-1.0(11)	C19	C20	C21	C16	-0.4(11)
C7	N2	C6	N1	-0.7(7)	C21	C16	C17	C18	-2.1(10)
C7	N2	C6	C2	177.5(7)	C22	C19	C20	C21	179.5(6)

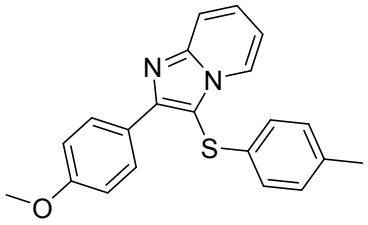
Table S21 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4ci.

Atom	*x*	*y*	*z*	U(eq)
H3A	8138	5538	9875	105
H3B	6260	5931	9188	105
H3	8012	3950	7335	91
H4	5720	3969	5905	92
H5	2979	5065	5545	81
H10	1567	7277	9172	100
H11	-588	8401	9718	110
H13	-1931	9418	7322	100
H14	193	8284	6760	83
H15A	-4914	9677	8672	172
H15B	-2135	10401	8834	172
H15C	-2995	9699	9571	172
H17	4871	7959	6148	84
H18	7453	9018	5298	102
H20	2152	8223	3190	99
H21	-485	7145	3989	95
H22A	7027	9121	3078	164
H22B	8568	9648	3949	164
H22C	5851	9965	3490	164
H2	127	2967	8697	300
H23A	4048	2682	8109	229
H23B	3329	1761	8642	229
H23C	3933	2766	9126	229

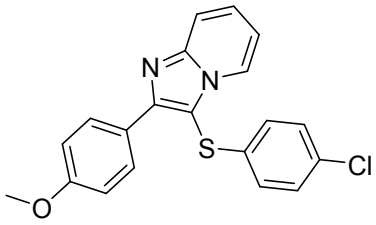
Table S22 Atomic Occupancy for 4ci.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O2	0.75	H2	0.75	C23	0.75
H23A	0.75	H23B	0.75	H23C	0.75

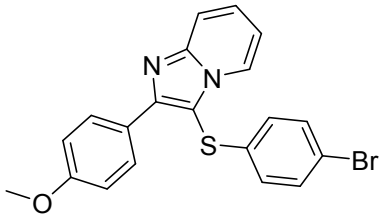
6. Characterization Data for the Electrolysis Products



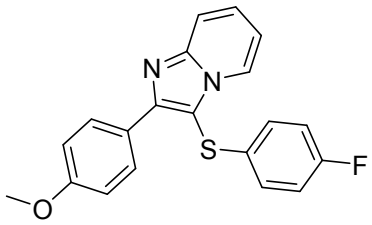
2-(4-methoxyphenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4aa** was obtained in 87% yield (60.2 mg) according to the general procedure (0.2 mmol). Yellow solid. mp: 157 -158 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (d, J = 6.8 Hz, 1H), 8.15 – 8.12 (m, 2H), 7.72 (d, J = 9.2 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.11 – 6.96 (m, 5H), 6.87 (d, J = 8.0 Hz, 2H), 3.78 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.6, 149.8, 146.4, 135.8, 131.2, 130.3, 129.1, 127.2, 125.7, 125.5, 124.5, 117.0, 113.9, 113.5, 104.9, 55.2, 20.4. HR-MS (ESI) m/z calc. for $C_{21}H_{19}N_2OS$ $[M+H]^+$: 347.1213, found: 347.1216.



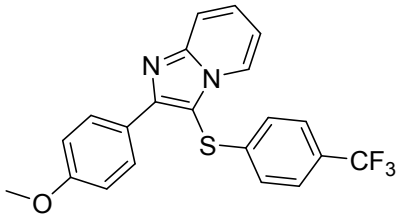
3-((4-chlorophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine, Compound **4ab** was obtained in 84% yield (61.5 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 142 -143 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (dt, J = 6.8, 1.2 Hz, 1H), 8.11 – 8.08 (m, 2H), 7.74 (dt, J = 9.2, 1.2 Hz, 1H), 7.49 –7.45 (m, 1H), 7.35 – 7.32 (m, 2H), 7.07 – 6.96 (m, 5H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.70, 150.22, 146.62, 134.03, 130.90, 129.64, 129.12, 127.46, 126.92, 125.50, 124.54, 117.11, 113.99, 113.73, 103.78, 55.18. HR-MS (ESI) m/z calc. for $C_{20}H_{16}ClN_2OS$ $[M+H]^+$: 367.0666, found: 367.0672.



3-((4-bromophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine, Compound **4ac** was obtained in 67% yield (55.1 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 145 -146 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (dt, J = 6.9, 1.1 Hz, 1H), 8.12 – 8.07 (m, 2H), 7.75 (dt, J = 8.9, 1.1 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.09 – 7.01 (m, 3H), 6.94 – 6.89 (m, 2H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.7, 150.2, 146.6, 134.6, 132.5, 129.1, 127.5, 127.2, 125.5, 124.6, 119.1, 117.1, 114.0, 113.7, 103.6, 55.2. HR-MS (ESI) m/z calc. for $C_{20}H_{16}BrN_2OS$ $[M+H]^+$: 411.0161, found: 411.0165.

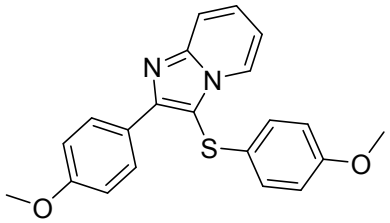


3-((4-fluorophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine, Compound **4ad** was obtained in 82% yield (57.4 mg) according to the general procedure (0.2 mmol). Yellow solid. mp: 103 -105 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.41 (dt, J = 6.8, 1.2 Hz, 1H), 8.17 – 8.10 (m, 2H), 7.73 (dt, J = 9.2, 0.8 Hz, 1H), 7.50 –7.41 (m, 1H), 7.17 – 7.08 (m, 2H), 7.07 – 7.00 (m, 5H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.9 (d, J = 242.1 Hz), 159.7, 150.0, 146.5, 130.3 (d, J = 2.9 Hz), 129.1, 127.6 (d, J = 8.1 Hz), 127.3, 125.6, 124.5, 117.1, 116.9 (d, J = 22.2 Hz), 114.0, 113.6, 104.7, 55.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ -116.2. HR-MS (ESI) m/z calc. for $C_{20}H_{16}FN_2OS$ $[M+H]^+$: 351.0962, found: 351.0972.



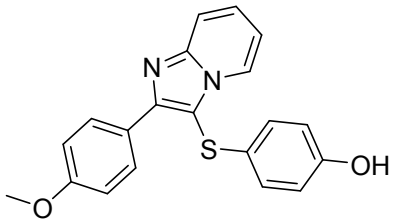
2-(4-methoxyphenyl)-3-((4-(trifluoromethyl)phenyl)thio)imidazo[1,2-a]pyridine,

Compound **4ae** was obtained in 59% yield (47.3 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 98 -99 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (dt, J = 6.8, 1.2 Hz, 1H), 8.10 – 8.06 (m, 2H), 7.78 (dt, J = 8.9, 1.1 Hz, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.49 (ddd, J = 9.0, 6.8, 1.3 Hz, 1H), 7.17 – 7.12 (m, 2H), 7.06 (td, J = 6.8, 1.2 Hz, 1H), 7.04 – 7.00 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.2, 151.1, 147.3, 141.4, 129.6, 128.1, 127.0 (q, J = 30.9 Hz), 126.9 (q, J = 3.8 Hz), 125.9, 125.8, 125.5 (q, J = 270.3 Hz), 125.1, 117.6, 114.5, 114.3, 103.1, 55.6. ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.9. HR-MS (ESI) m/z calc. for $C_{21}H_{16}F_3N_2OS$ $[M+H]^+$: 401.0930, found: 401.0936.

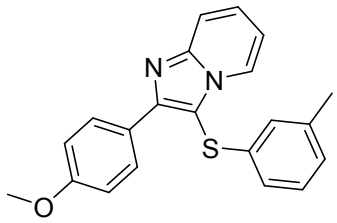


2-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)imidazo[1,2-a]pyridine，

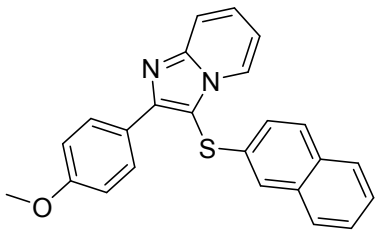
Compound **4af** was obtained in 56% yield (40.7 mg) according to the general procedure (0.2 mmol). Yellow oily. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.29 (dt, J = 6.8, 1.2 Hz, 1H), 8.12 – 8.19 (m, 2H), 7.69 (dt, J = 9.2, 0.8 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.00–6.97 (m, 4H), 6.84 (td, J = 6.8, 1.2 Hz, 1H), 6.77 – 6.73 (m, 2H), 3.84 (s, 3H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 160.1 , 158.6, 151.0, 146.9 , 129.8, 128.0, 126.6, 126.1, 125.7, 124.5, 117.4, 115.2, 114.0, 112.9, 107.0, 55.5, 55.4. HR-MS (ESI) m/z calc. for $C_{21}H_{19}N_2O_2S$ $[M+H]^+$: 363.1162, found: 363.1170.



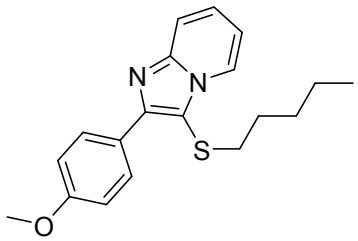
4-((2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)thio)phenol, Compound **4ag** was obtained in 47% yield (32.8 mg) according to the general procedure (0.2 mmol). white soild. mp: 214 -215 °C ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.57 (s, 1H), 8.45 (dt, J = 6.8, 1.2 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.70 (dt, J = 8.8, 1.2 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.06 – 7.02 (m, 3H), 6.93 – 6.91 (m, 2H), 6.69 – 6.67 (m, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.6, 156.7, 149.1, 146.1, 129.2, 128.5, 127.0, 125.8, 124.5, 122.6, 117.0, 116.8, 113.9, 113.4, 106.6, 55.2. HR-MS (ESI) m/z calc. for $C_{20}H_{17}N_2O_2S$ $[M+H]^+$: 349.1006, found: 349.1014.



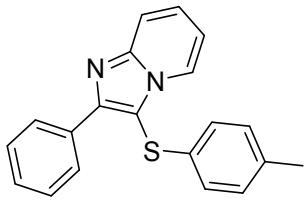
2-(4-methoxyphenyl)-3-(m-tolylthio)imidazo[1,2-a]pyridine, Compound **4ah** was obtained in 79% yield (54.9 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 156 -157 °C. ^{1}H NMR (400 MHz, Chloroform-d)δ 8.37 (dt, J = 6.9, 1.2 Hz, 1H), 8.16 – 8.08 (m, 2H), 7.74 (dt, J = 9.0, 1.1 Hz, 1H), 7.46 (ddd, J = 9.0, 6.8, 1.3 Hz, 1H), 7.13 (t, J = 7.7 Hz, 1H), 7.07 – 7.00 (m, 3H), 6.98 (d, J = 7.3 Hz, 1H), 6.89 (d, J = 2.0 Hz, 1H), 6.68 – 6.62 (m, 1H), 3.78 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 159.6, 150.0, 146.5, 139.2, 134.6, 129.6, 129.1, 127.3, 127.1, 125.7, 125.6, 124.5, 122.1, 117.1, 113.9, 113.6, 104.3, 55.2, 20.9. HR-MS (ESI) m/z calc. for $C_{21}H_{19}N_2OS$ $[M+H]^+$: 347.1213, found: 347.1219.



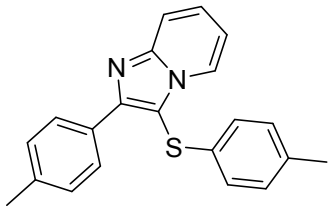
2-(4-methoxyphenyl)-3-(naphthalen-2-ylthio)imidazo[1,2-a]pyridine, Compound **4ai** was obtained in 37% yield (28.4 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 124 -126 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 6.8 Hz, 1H), 8.22 – 8.20 (m, 2H), 7.76 – 7.70 (m, 3H), 7.60 – 7.57 (m, 1H), 7.43 – 7.37 (m, 3H), 7.34 – 7.30 (m, 1H), 7.17 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.98 – 6.95 (m, 2H), 6.84 – 6.81 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.1, 151.5, 147.2, 133.9, 132.8, 131.8, 129.7, 129.3, 127.8, 127.0, 126.8, 126.7, 125.9, 125.7, 124.5, 123.8, 123.4, 117.5, 113.9, 113.0, 105.2, 55.28. HR-MS (ESI) m/z calc. for $C_{24}H_{19}N_2OS$ $[M+H]^+$: 383.1208, found: 383.1217.



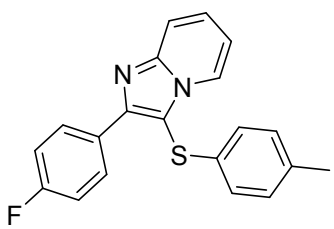
2-(4-methoxyphenyl)-3-(pentylthio)imidazo[1,2-a]pyridine, Compound **4aj** was obtained in 39% yield (25.5 mg) according to the general procedure (0.2 mmol). Yellow oily. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.65 (dt, *J* = 6.9, 1.2 Hz, 1H), 8.12 – 8.06 (m, 2H), 7.60 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.44 (ddd, *J* = 9.0, 6.8, 1.3 Hz, 1H), 7.09 (td, *J* = 6.8, 1.2 Hz, 1H), 7.06 – 7.02 (m, 2H), 3.86 (s, 3H), 2.65 (t, *J* = 6.9 Hz, 2H), 1.26 – 1.20 (m, 2H), 1.13 – 1.05 (m, 2H), 0.98 – 0.87 (m, 2H), 0.74 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.0, 149.5, 146.5, 129.8, 126.8, 126.7, 125.8, 124.4, 117.4, 113.8, 112.5, 109.6, 55.4, 35.8, 30.8, 39.3, 22.3, 14.0. HR-MS (ESI) m/z calc. for $C_{19}H_{23}N_2OS$ $[M+H]^+$: 327.1526, found: 327.1529.



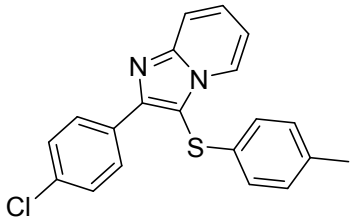
2-phenyl-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4ba** was obtained in 82% yield (52.1 mg) according to the general procedure (0.2 mmol). white soild. mp: 133 - 134 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (dt, *J* = 6.9, 1.2 Hz, 1H), 8.24 – 8.21 (m, 2H), 7.73 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.39 – 7.35 (m, 1H), 7.34 – 7.30 (m, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.92 – 6.90 (m, 2H), 6.85 (tt, *J* = 6.8, 1.1 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.2, 147.1, 136.1, 133.5, 131.6, 130.3, 128.7 , 128.5, 128.5, 126.7, 126.0, 124.6, 117.7, 113.1, 107.0, 21.0. HR-MS (ESI) m/z calc. for $C_{20}H_{17}N_2S$ $[M+H]^+$: 317.1107, found: 317.1113.



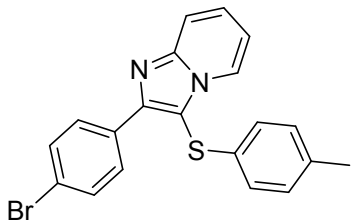
2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bb** was obtained in 83% yield (55.0 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 127 -128 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 – 8.18 (m, 1H), 8.05 – 8.03 (m, 2H), 7.64 (d, *J* = 9.2 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.84 – 6.82 (m, 2H), 6.77 (td, *J* = 6.8, 0.8 Hz, 1H), 2.30 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.3, 147.0, 138.6, 136.1, 131.7, 130.6, 130.3, 129.3, 128.4, 126.7, 125.9, 124.6, 117.6, 113.1, 106.6, 21.48 , 21.0. HR-MS (ESI) m/z calc. for $C_{21}H_{19}N_2S$ $[M+H]^+$: 331.1264, found: 331.1272.



2-(4-fluorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bc** was obtained in 85% yield (57.0 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 94 -95 °C. ^{1}H NMR (400 MHz, Methanol-d_4) δ 8.30 (dt, J = 6.8, 1.2 Hz, 1H), 8.09 – 8.03 (m, 2H), 7.64 (dt, J = 8.8, 1.2 Hz, 1H), 7.42 (ddd, J = 8.8, 6.8, 1.2 Hz, 1H), 7.16 – 7.11 (m, 2H), 6.99 – 6.94 (m, 3H), 6.84 – 6.81 (m, 2H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, Methanol-d_4) δ 164.5 (d, J = 248.6 Hz), 150.8, 148.1, 137.8, 132.2, 131.5(d, J = 8.3 Hz), 131.3, 130.5 (d, J = 3.2 Hz), 129.1, 127.1, 125.9, 117.7, 116.3 (d, J = 21.9 Hz), 114.9, 108.9, 20.9. ^{19}F NMR (376 MHz, Methanol-d_4) δ -114.5. HR-MS (ESI) m/z calc. for $C_{20}H_{16}N_2FS$ $[M+H]^+$: 335.1013, found: 335.1015.

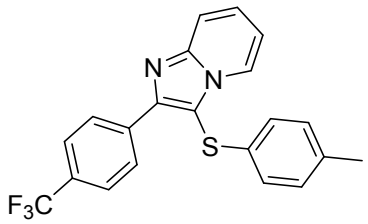


2-(3-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bd** was obtained in 88% yield (61.8 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 118 -119 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.42 – 8.38 (m, 1H), 8.22 – 8.18 (m, 1H), 7.77 (dd, J = 9.0, 1.0 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.51 – 7.46 (m, 1H), 7.10 – 7.06 (m, 1H), 6.89 (d, J = 1.7 Hz, 1H), 2.20 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 148.4, 146.5, 136.0, 133.4, 132.1, 130.7, 130.4, 129.4, 128.6, 127.6, 125.7, 124.7, 117.4, 114.0, 106.3, 21.0. HR-MS (ESI) m/z calc. for $C_{20}H_{16}N_2ClS$ $[M+H]^+$: 351.0718, found: 351.0726.

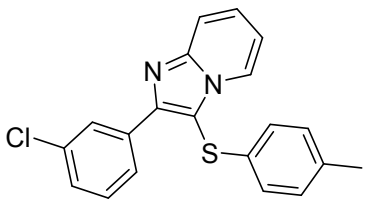


2-(4-bromophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4be** was obtained in 71% yield (56.1 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 123 -124 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.39 (dt, J = 6.8, 1.2 Hz,

1H), 8.18 – 8.13 (m, 2H), 7.76 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.48 (ddd, *J* = 9.2, 6.8, 1.3 Hz, 1H), 7.10 – 7.06 (m, 3H), 6.90 – 6.88 (m, 2H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 148.5, 146.4, 136.1, 132.5, 131.5, 130.6, 130.4, 129.7, 127.6, 125.8, 124.7, 122.1, 117.3, 113.9, 106.4, 20.4. HR-MS (ESI) m/z calc. for $C_{20}H_{16}N_2BrS$ $[M+H]^+$: 395.0213, found: 395.0219.

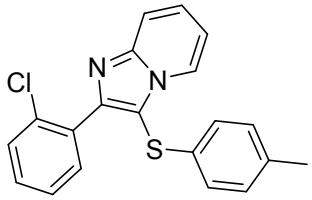


3-(p-tolylthio)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine, Compound **4bf** was obtained in 67% yield (51.6 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 109 -110 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.43 – 8.40 (m, 3H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.79 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.50 (ddd, *J* = 9.0, 6.8, 1.2 Hz, 1H), 7.12 – 7.07 (m, 3H), 6.92 – 6.89 (m, 2H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 147.9, 146.5, 137.2, 136.2, 130.5, 130.4, 128.6 (q, *J* = 31.7 Hz), 128.3, 127.8, 125.9, 125.4(q, *J* = 7.7 Hz), 124.8, 124.2 (q, *J* = 270.4 Hz), 117.5, 114.2, 107.4, 20.4. ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.1. HR-MS (ESI) m/z calc. for $C_{21}H_{16}N_2F_3S$ $[M+H]^+$: 385.0981, found: 385.0985.

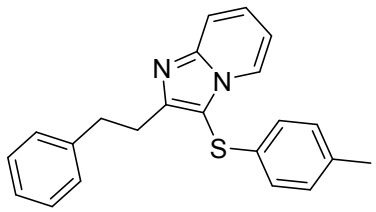


2-(3-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bg** was obtained in 87% yield (61.1 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 118 -119 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.19 (t, *J* = 1.8 Hz, 1H), 8.16 (dt, *J* = 7.6, 1.5 Hz, 1H), 7.77 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.10 – 7.06 (m, 3H), 6.90 – 6.88 (m, 2H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 147.9, 146.4, 136.1, 135.3, 133.3, 130.6, 130.5, 130.4, 128.4, 127.7, 127.3, 126.2, 125.8, 124.7,

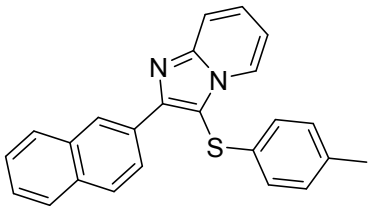
117.4, 114.1, 106.9, 20.4. HR-MS (ESI) m/z calc. for $C_{20}H_{16}N_2ClS$ $[M+H]^+$: 351.0718, found: 351.0722.



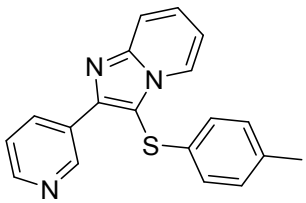
2-(2-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bh** was obtained in 42% yield (29.5 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 117 -118 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (dt, J = 6.8, 1.2 Hz, 1H), 7.78 (dt, J = 9.0, 1.1 Hz, 1H), 7.59 (dd, J = 7.8, 1.4 Hz, 1H), 7.53 – 7.40 (m, 4H), 7.10 (td, J = 6.8, 1.2 Hz, 1H), 7.06 – 7.04 (m, 2H), 6.84 – 6.82 (m, 2H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 150.0, 146.2, 135.9, 133.0, 132.8, 132.4, 130.5, 130.3, 130.2, 129.5, 127.1, 126.9, 126.1, 124.7, 117.5, 113.9, 108.7, 20.4. HR-MS (ESI) m/z calc. for $C_{20}H_{16}N_2ClS$ $[M+H]^+$: 351.0718, found: 351.0724.



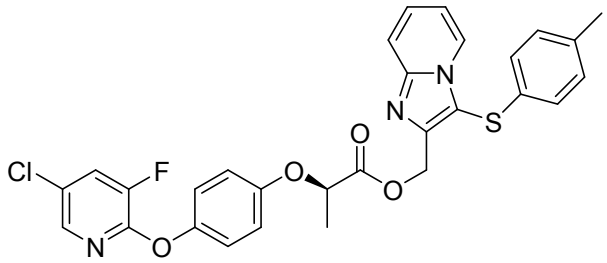
2-phenethyl-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bi** was obtained in 85% yield (58.7 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 144 -145 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (dt, J = 6.9, 1.2 Hz, 1H), 7.41 (dd, J = 9.0, 1.2 Hz, 1H), 7.05 – 6.98 (m, 5H), 6.92 (q, J = 8.4 Hz, 1H), 6.72 (d, J = 8.0 Hz, 2H), 6.59 – 6.46 (m, 3H), 3.08 – 2.96 (m, 2H), 2.92 – 2.83 (m, 2H), 2.00 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.2, 147.0, 141.8, 136.1, 131.8, 130.1, 128.6, 128.4, 126.2, 126.1, 126.0, 124.5, 117.2, 112.8, 108.2, 35.9, 30.3, 21.0. HR-MS (ESI) m/z calc. for $C_{22}H_{21}N_2S$ $[M+H]^+$: 345.1415, found: 345.1423.



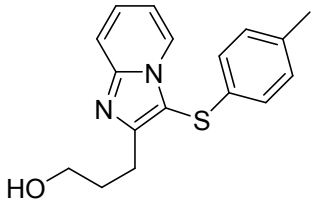
2-(naphthalen-2-yl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bj** was obtained in 42% yield (30.8 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 171 -172 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 – 8.73 (m, 1H), 8.41 (dd, *J* = 8.6, 1.8 Hz, 1H), 8.34 (dt, *J* = 6.7, 1.2 Hz, 1H), 7.91 (dd, *J* = 7.2, 2.7 Hz, 2H), 7.86 – 7.83 (m, 1H), 7.77 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.35 (ddd, *J* = 9.0, 6.8, 1.3 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.99 – 6.94 (m, 2H), 6.89 (td, *J* = 6.8, 1.1 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.0, 147.2, 136.3, 133.5, 131.6, 130.9, 130.4, 128.9, 128.1, 128.0, 127.7, 126.9, 126.5, 126.2, 126.2, 126.1, 124.7, 117.7, 113.2, 107.6, 21.04 . HR-MS (ESI) m/z calc. for $C_{24}H_{19}N_2S$ $[M+H]^+$: 367.1258, found: 367.1271.



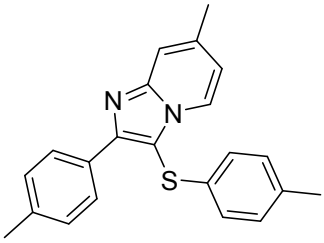
2-(pyridin-3-yl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4bk** was obtained in 41% yield (26.1 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 115 -116 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.43 (dd, *J* = 2.2, 0.8 Hz, 1H), 8.59 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.48 (dt, *J* = 8.0, 2.0 Hz, 1H), 8.30 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.72 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.05 – 6.98 (m, 2H), 6.92 – 6.86 (m, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.6, 149.5, 148.4, 147.4, 136.5, 135.6, 131.1, 130.4, 129.6, 127.1, 126.0, 124.7, 123.4, 117.9, 113.5, 108.0, 21.0. HR-MS (ESI) m/z calc. for $C_{19}H_{16}N_3S$ $[M+H]^+$: 318.1060, found: 318.1067.



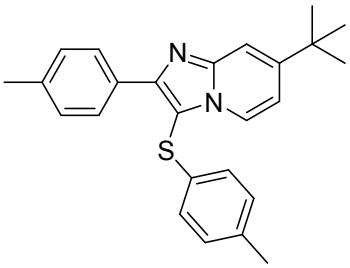
(3-(p-tolylthio)imidazo[1,2-a]pyridin-2-yl)methyl (R)-2-(4-((5-chloro-3-fluoropyridin-2-yl)oxy)phenoxy)propanoate, Compound **4bl** was obtained in 17% yield (19.2 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 101 -102 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 9.2 Hz, 1H), 7.48 (dd, *J* = 9.1, 2.2 Hz, 1H), 7.34 (ddd, *J* = 9.1, 6.8, 1.3 Hz, 1H), 7.01 – 6.95 (m, 4H), 6.92 – 6.85 (m, 5H), 5.59 – 5.43 (m, 2H), 4.73 (q, *J* = 6.8 Hz, 1H), 2.24 (s, 3H), 1.58 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.9, 155.0, 151.5 (d, *J* = 11.1 Hz), 148.4, 147.4, 147.2, 147.1, 145.8, 140.3 (d, *J* = 6.0 Hz), 136.7, 130.9, 130.3, 127.0 (d, *J* = 221.2 Hz), 126.8, 125.1(d, *J* = 9.3 Hz), 125.0 (d, *J* = 0.4 Hz), 122.3, 118.2, 116.3, 113.6, 111.2, 73.1, 60.4, 21.0, 18.7. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -134.4. HR-MS (ESI) m/z calc. for $C_{29}H_{24}N_3FClO_4S$ $[M+H]^+$: 564.1150, found: 564.1158.



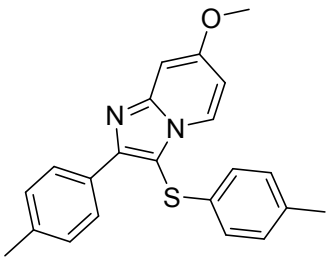
3-(3-(p-tolylthio)imidazo[1,2-a]pyridin-2-yl)propan-1-ol, Compound **4bm** was obtained in 42% yield (25.1 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.61 (dt, *J* = 9.0, 1.1 Hz, 1H), 7.30 (ddd, *J* = 9.0, 6.8, 1.3 Hz, 1H), 7.04 – 6.99 (m, 2H), 6.88 – 6.80 (m, 3H), 3.77 (t, *J* = 5.7 Hz, 2H), 3.10 (dd, *J* = 7.3, 6.1 Hz, 2H), 2.26 (s, 3H), 2.03 – 1.98 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.5, 146.7, 136.3, 131.8, 130.2, 126.6, 126.1, 124.6, 117.1, 113.1, 108.2, 62.9, 31.7, 29.9, 25.7. HR-MS (ESI) m/z calc. for $C_{17}H_{19}N_2OS$ $[M+H]^+$: 299.1213, found: 299.1215.



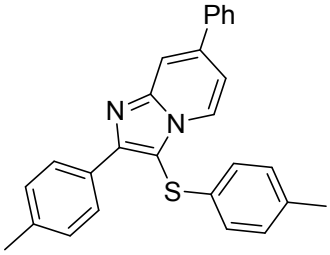
7-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4ca** was obtained in 89% yield (61.4 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 125 -126 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (dd, *J* = 7.4, 4.7 Hz, 3H), 7.50 (s, 1H), 7.30 – 7.24 (m, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.98 – 6.88 (m, 2H), 6.68 (dd, *J* = 7.0, 1.6 Hz, 1H), 2.44 (s, 3H), 2.40 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.2, 147.4, 138.4, 137.8, 135.9, 132.0, 130.8, 130.2, 129.2, 128.3, 125.8, 123.7, 116.1, 115.6, 105.7, 21.5, 21.4, 21.0. HR-MS (ESI) m/z calc. for $C_{22}H_{21}N_2S$ $[M+H]^+$: 345.1420, found: 345.1426.



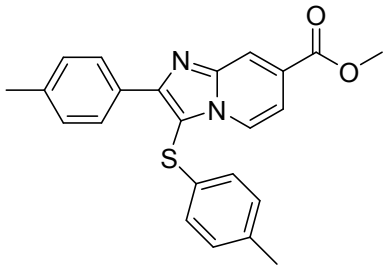
7-(tert-butyl)-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4cb** was obtained in 72% yield (55.6 mg) according to the general procedure (0.2 mmol). Yellow oily. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 7.2, 0.8 Hz, 1H), 8.09 – 8.03 (m, 2H), 7.57 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.14 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.92 – 6.84 (m, 2H), 2.32 (s, 3H), 2.18 (s, 3H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 150.6, 150.0, 146.6, 137.9, 135.8, 131.3, 130.6, 130.3, 129.0, 127.5, 125.6, 123.7, 112.6, 111.8, 104.7, 34.7, 30.1, 20.8, 20.4. HR-MS (ESI) m/z calc. for $C_{25}H_{27}N_2S$ $[M+H]^+$: 387.1890, found: 387.1891.



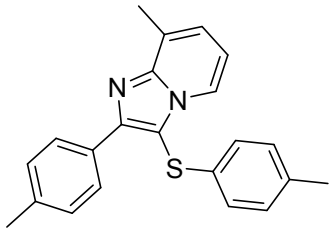
7-methoxy-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4cc** was obtained in 70% yield (50.9 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 102 -103 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.3 Hz, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 6.56 (dd, *J* = 7.4, 2.5 Hz, 1H), 2.38 (s, 1H), 2.26 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.7, 150.9, 148.4, 138.5, 136.1, 132.1, 130.6, 130.3, 129.3, 128.1, 125.9, 125.0, 107.9, 105.2, 95.2, 55.9, 21.5, 21.0. HR-MS (ESI) m/z calc. for $C_{22}H_{21}N_2OS$ $[M+H]^+$: 361.1370, found: 361.1375.



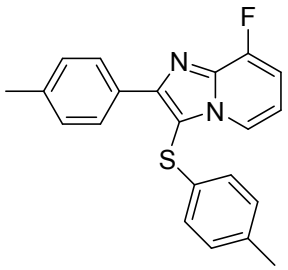
7-phenyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4cd** was obtained in 67% yield (54.3 mg) according to the general procedure (0.2 mmol). White soild. mp: 196 -197 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 7.2 Hz, 1H), 8.07 – 7.99 (m, 2H), 7.81 (d, *J* = 1.6 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.38 – 7.32 (m, 2H), 7.31 – 7.25 (m, 1H), 7.15 – 7.11 (m, 2H), 7.00 (dd, *J* = 7.1, 1.8 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.86 – 6.78 (m, 2H), 2.27 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.9, 147.4, 139.7, 138.7, 138.5, 136.2, 131.8, 130.6, 130.3, 129.3, 129.2, 128.6, 128.3, 126.9, 126.0, 124.4, 114.3, 112.9, 106.5, 21.5, 21.0. HR-MS (ESI) m/z calc. for $C_{27}H_{23}N_2S$ $[M+H]^+$: 407.1577, found: 407.1587.



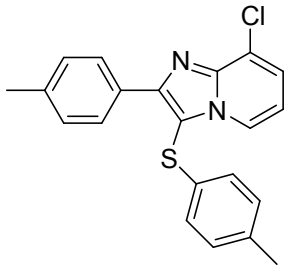
methyl 2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine-7-carboxylate, Compound **4ce** was obtained in 62% yield (48.5 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 162 -163 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (s, 1H), 8.28 (d, *J* = 7.2 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.43 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 3.95 (s, 3H), 2.38 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.6, 153.1, 145.9, 139.1, 136.6, 130.9, 130.5, 130.2, 129.4, 128.5, 128.0, 126.3, 124.3, 119.9, 112.4, 109.2, 52.8, 21.5, 21.0. HR-MS (ESI) m/z calc. for $C_{23}H_{21}N_2O_2S$ $[M+H]^+$: 389.1319, found: 389.1326.



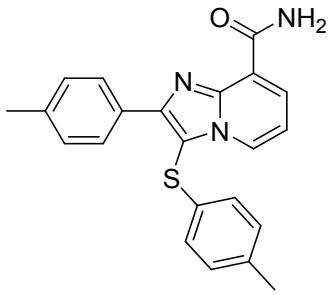
8-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4cf** was obtained in 59% yield (40.8 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 133 -134 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (d, *J* = 6.8 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 3H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.97 (t, *J* = 6.8 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 2H), 2.60 (s, 3H), 2.34 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.4, 146.6, 137.9, 135.8, 131.2, 130.6, 130.3, 129.0, 127.7, 126.8, 125.8, 125.6, 122.3, 113.5, 105.9, 20.9, 20.4, 16.3. HR-MS (ESI) m/z calc. for $C_{22}H_{21}N_2S$ $[M+H]^+$: 345.1420, found: 345.1421.



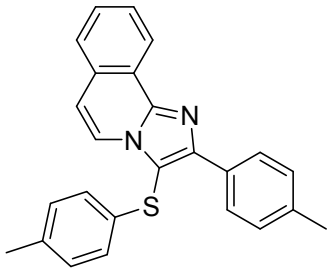
8-fluoro-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4cg** was obtained in 54% yield (37.7 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 128 -129 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 – 8.05 (m, 2H), 8.01 (dd, *J* = 6.8, 1.0 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.89 (m, 3H), 6.85 – 6.79 (m, 2H), 6.67 (td, *J* = 7.2, 4.4 Hz, 1H), 2.30 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.6, 151.6 (d, *J* = 252.6 Hz), 139.5 (d, *J* = 27.7 Hz), 138.9, 136.39 , 131.2, 130.4, 130.2, 129.3, 128.5, 126.1, 120.9 (d, *J* = 4.8 Hz), 111.9 (d, *J* = 6.5 Hz), 109.3 (d, *J* = 16.3 Hz), 108.7, 21.5, 21.0. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -130.3. HR-MS (ESI) m/z calc. for $C_{21}H_{18}FN_2S$ $[M+H]^+$: 349.1170, found: 349.1179.



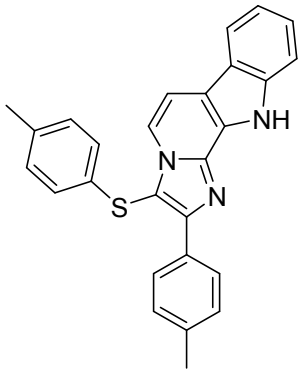
8-chloro-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine, Compound **4ch** was obtained in 52% yield (38.0 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 143 -144 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 6.8 Hz, 1H), 8.07 (d, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.18 – 7.15 (m, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.73 – 6.66 (m, 1H), 2.30 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.0, 144.3, 138.9, 136.4, 131.2, 130.4, 130.3, 129.2, 128.6, 126.1, 125.5, 123.5, 123.4, 112.5, 108.8, 21.5, 21.0. HR-MS (ESI) m/z calc. for $C_{21}H_{18}ClN_2S$ $[M+H]^+$: 365.0874, found: 365.0882.



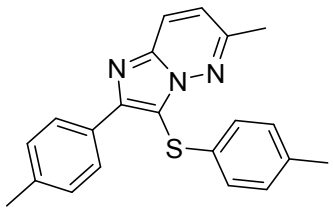
2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine-8-carboxamide, Compound **4ci** was obtained in 40% yield (30.0 mg) according to the general procedure (0.2 mmol). Yellow soild. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.48 (d, J = 3.2 Hz, 1H), 8.60 (dd, J = 6.9, 1.4 Hz, 1H), 8.18 (dd, J = 7.3, 1.2 Hz, 1H), 8.14 (d, J = 3.2 Hz, 1H), 8.10 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.22 (t, J = 6.8 Hz, 1H), 7.08 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 8.0 Hz, 2H), 2.34 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.4, 149.1, 144.4, 138.6, 136.1, 130.5, 130.4, 130.1, 129.5, 129.2, 127.8, 127.7, 125.9, 120.8, 113.5, 107.2, 20.9, 20.4. HR-MS (ESI) m/z calc. for $C_{22}H_{20}N_3OS$ $[M+H]^+$: 374.1317, found: 374.1325.



2-(p-tolyl)-3-(p-tolylthio)imidazo[2,1-a]isoquinoline, Compound **4cj** was obtained in 83% yield (63.5 mg) according to the general procedure (0.2 mmol). white soild. mp: 220 – 221 °C.^{1}H NMR (400 MHz, Chloroform-d) δ 8.73 (dd, J = 8.1, 1.2 Hz, 1H), 8.13–8.05 (m, 2H), 8.00 (d, J = 7.3 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.51 (td, J = 7.5, 1.4 Hz, 1H), 7.19 – 7.15 (m, 2H), 6.98 (d, J = 7.3 Hz, 1H), 6.91 (d, J = 8.1 Hz, 2H), 6.87– 6.81 (d, 2H), 2.30 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 149.7, 144.9, 138.2, 136.0, 132.3, 130.8, 130.4, 130.3, 129.3, 128.9, 128.3, 128.2, 127.1, 126.0, 123.8, 123.6, 121.3, 113.5,108.7, 21.5, 21.0. HR-MS (ESI) m/z calc. for $C_{25}H_{21}N_2S$ $[M+H]^+$: 381.1420, found: 381.1428.



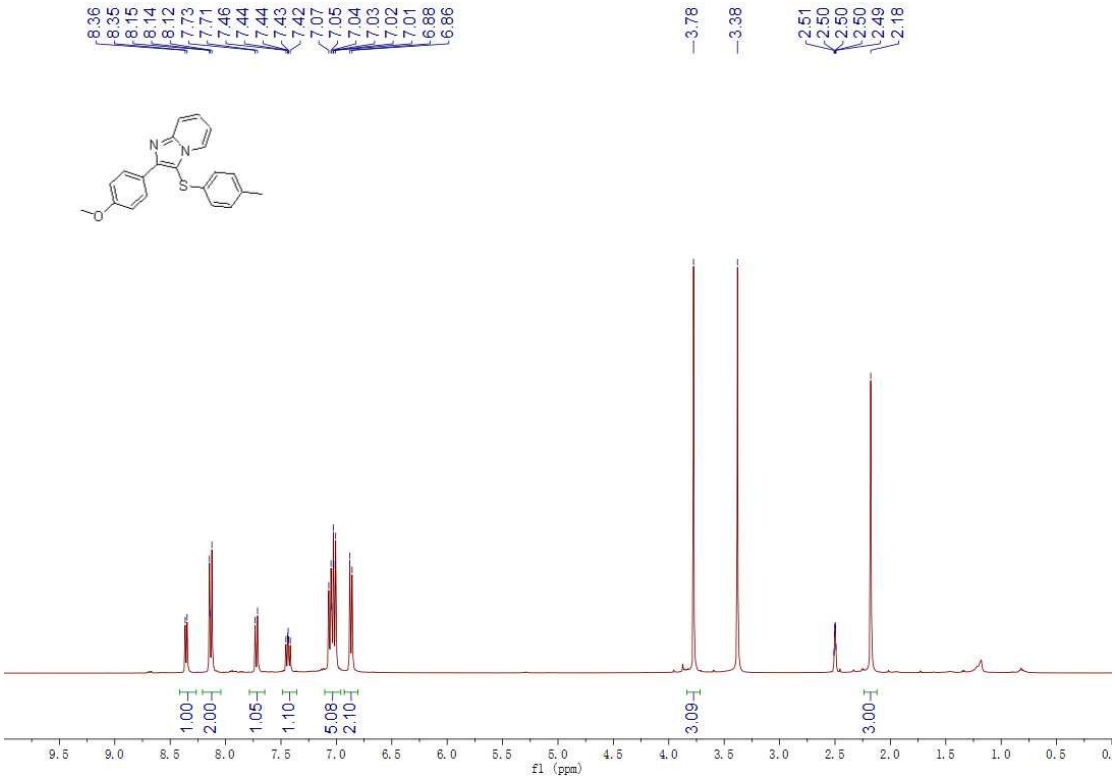
2-(p-tolyl)-3-(p-tolylthio)-10H-imidazo[1',2':1,6]pyrido[4,3-b]indole, Compound **4ck** was obtained in 53% yield (44.2 mg) according to the general procedure (0.2 mmol). Yellow soild. mp: 216 -217 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 11.48 (s, 1H), 8.20 (d, *J* = 1.9 Hz, 1H), 8.14 (d, *J* = 6.5 Hz, 1H), 7.96 (d, *J* = 1.5 Hz, 1H), 7.53 (s, 1H), 7.29 – 7.26 (m, 1H), 7.22 (t, *J* = 2.8 Hz, 1H), 7.05 (d, *J* = 1.9 Hz, 1H), 7.00 (d, *J* = 5.2 Hz, 1H), 2.34 (s, 1H), 2.28 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.6, 139.2, 138.6, 138.6, 136.1, 132.1, 130.5, 130.3, 129.4, 128.4, 126.7, 126.0, 125.8, 122.9, 120.4, 119.9, 118.2, 116.8, 112.3, 108.2, 107.6 , 21.5, 21.1. HR-MS (ESI) m/z calc. for $C_{27}H_{22}N_3S$ $[M+H]^+$: 420.1529, found: 420.1537.

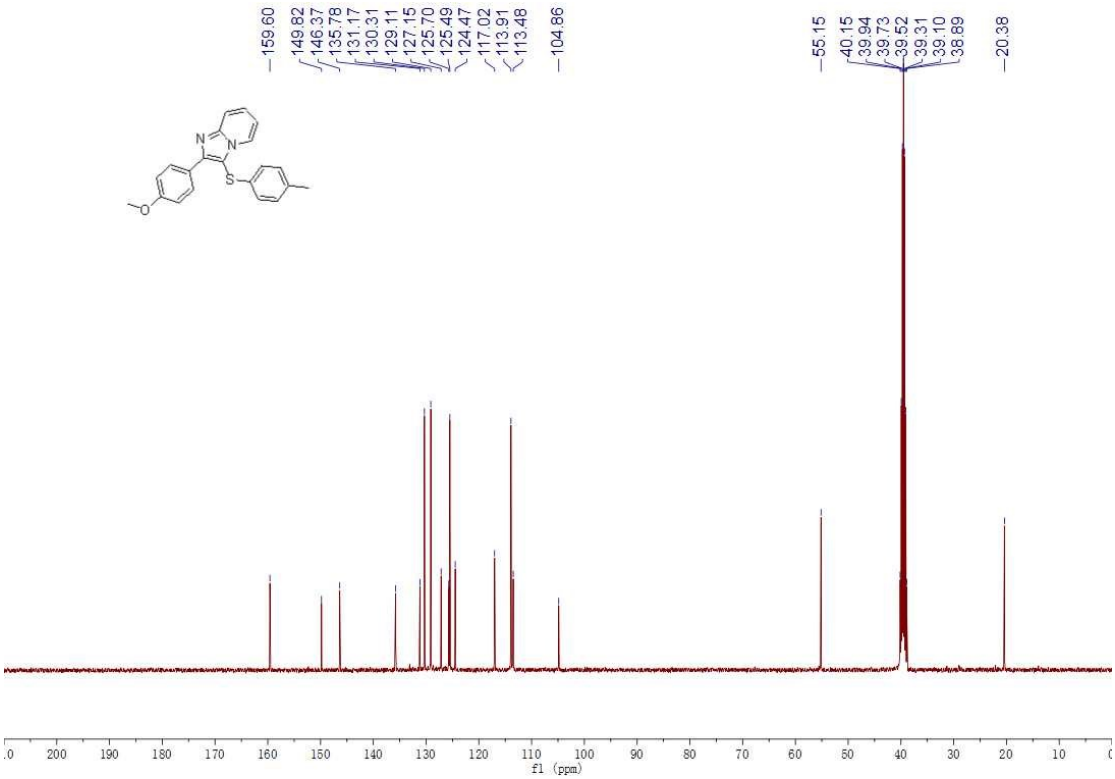


6-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-b]pyridazine, Compound **4cl** was obtained in 45% yield (31.4 mg) according to the general procedure (0.2 mmol). white solid. mp: 167 -168 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 – 8.07 (m, 2H), 7.89 (dd, *J* = 9.2, 1.6 Hz, 1H), 7.26 – 7.23 (m, 2H), 7.09 – 6.95 (m, 5H), 2.59 (d, *J* = 1.5 Hz, 3H), 2.38 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.6, 149.9, 134.0, 138.7, 136.2, 132.2, 130.5, 129.9, 129.3, 128.3, 127.4, 124.8, 120.7, 113.1, 22.1, 21.5, 21.1. HR-MS (ESI) m/z calc. for $C_{21}H_{20}N_3S$ $[M+H]^+$: 346.1373, found: 346.1377.

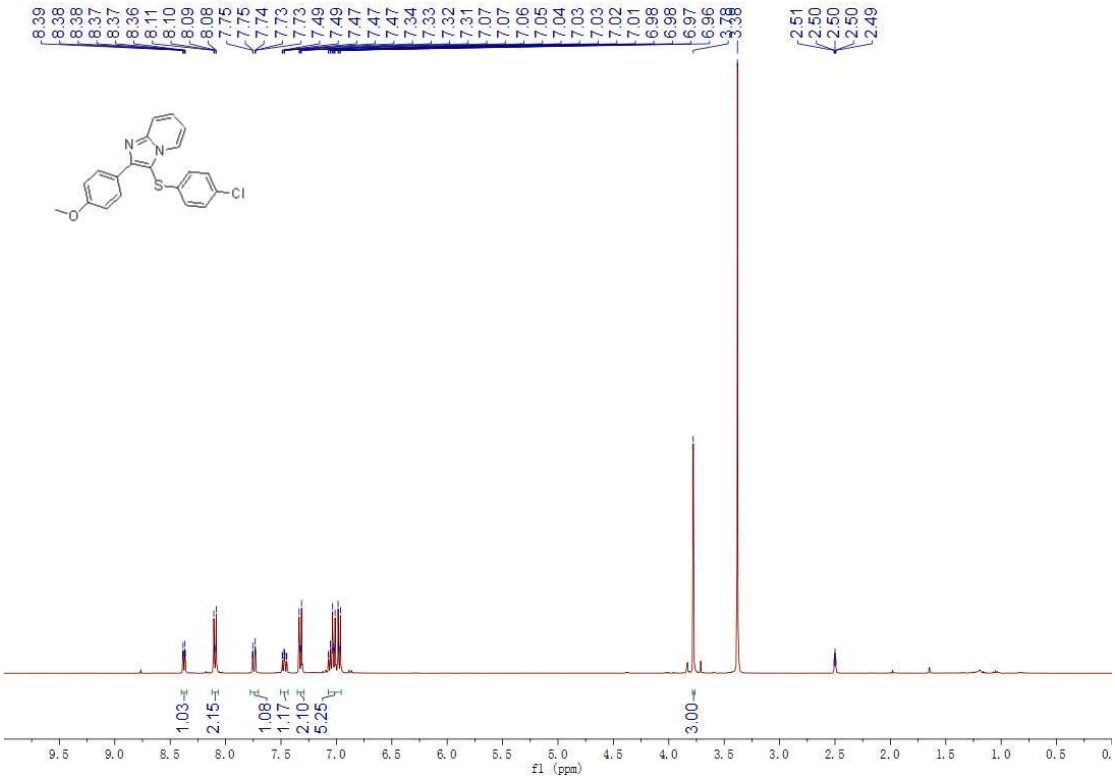
7. Copies of ^{1}H NMR and ^{13}C NMR for the Products

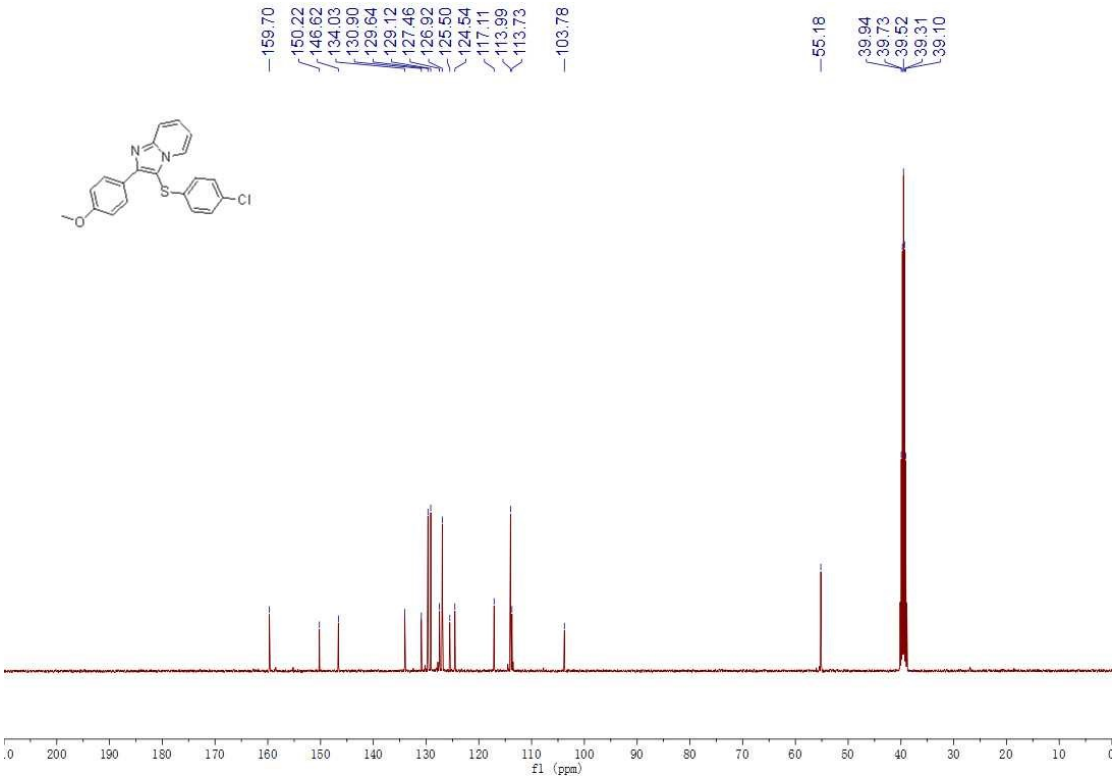
2-(4-methoxyphenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4aa）



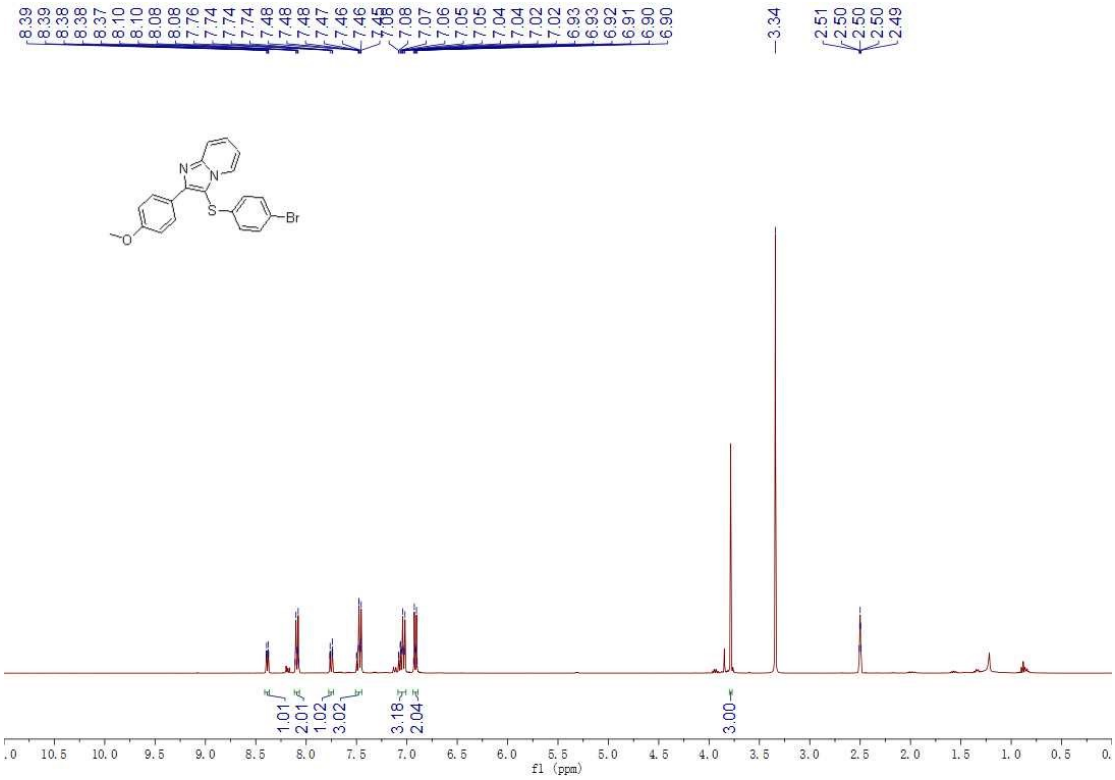


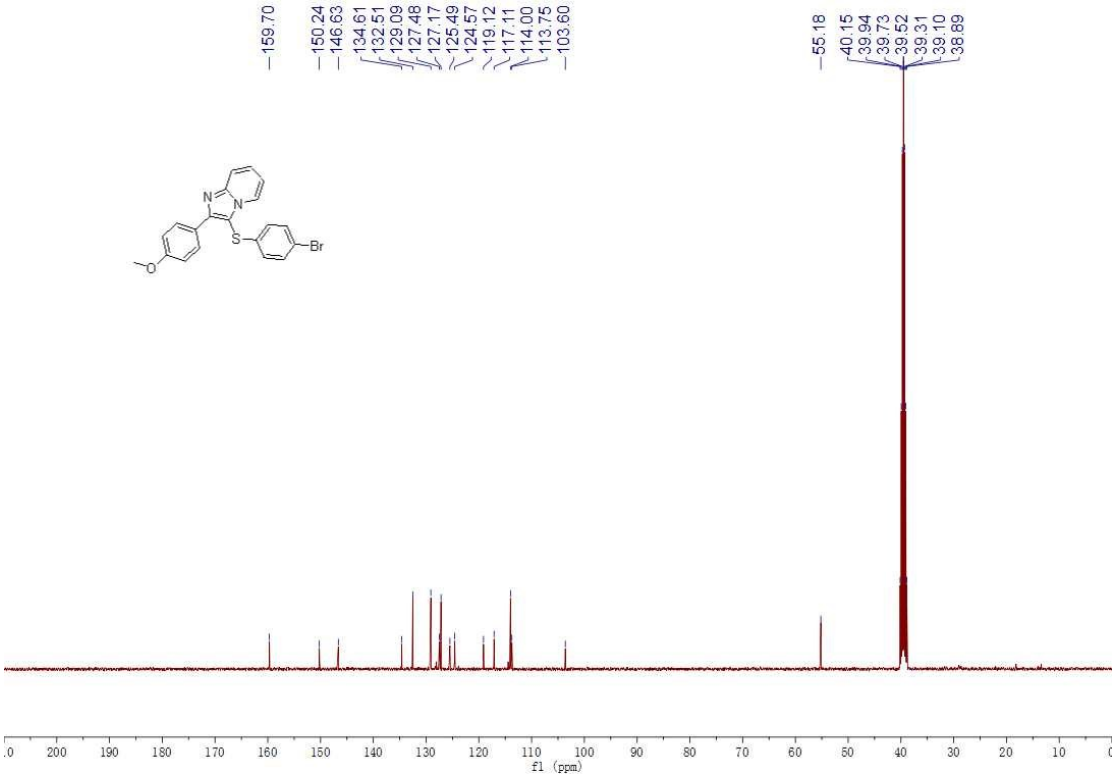
3-((4-chlorophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine（4ab）



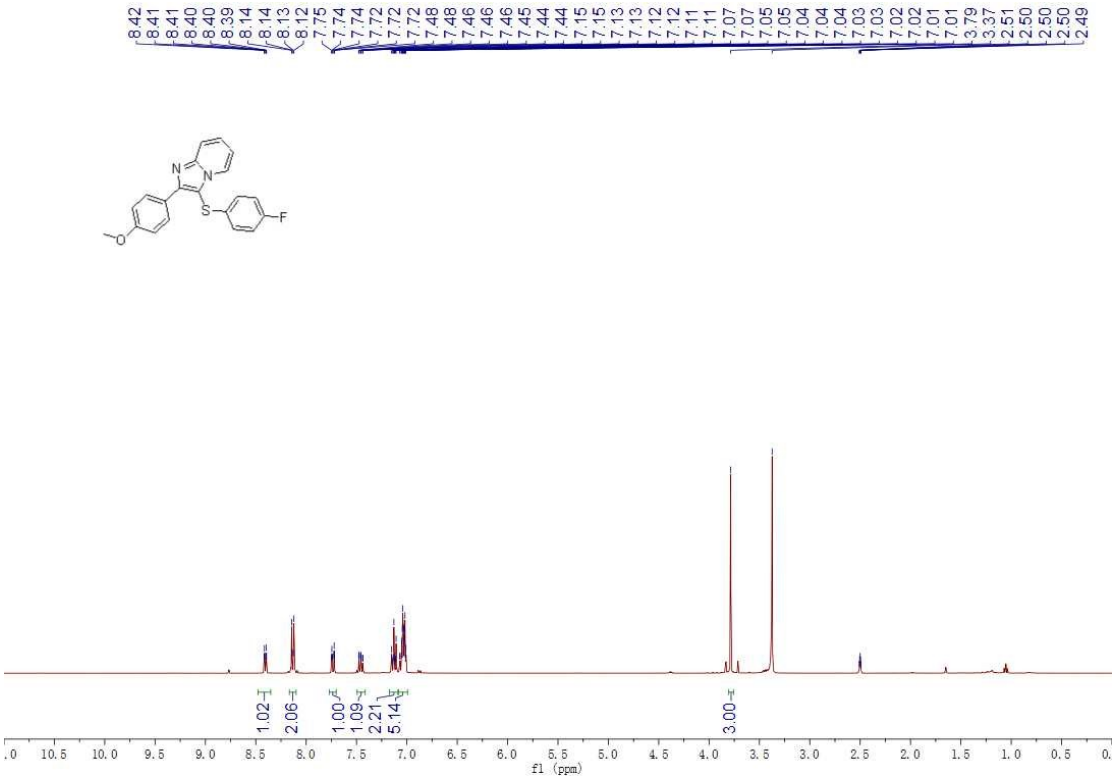


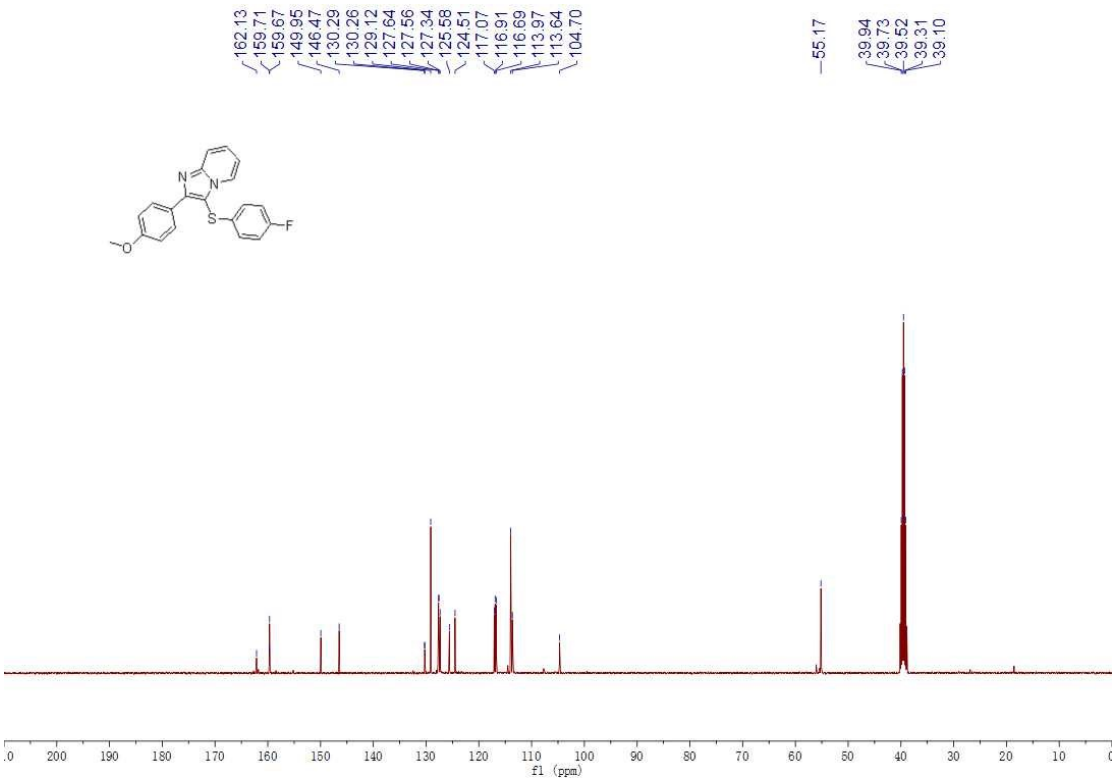
3-((4-bromophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine（4ac）

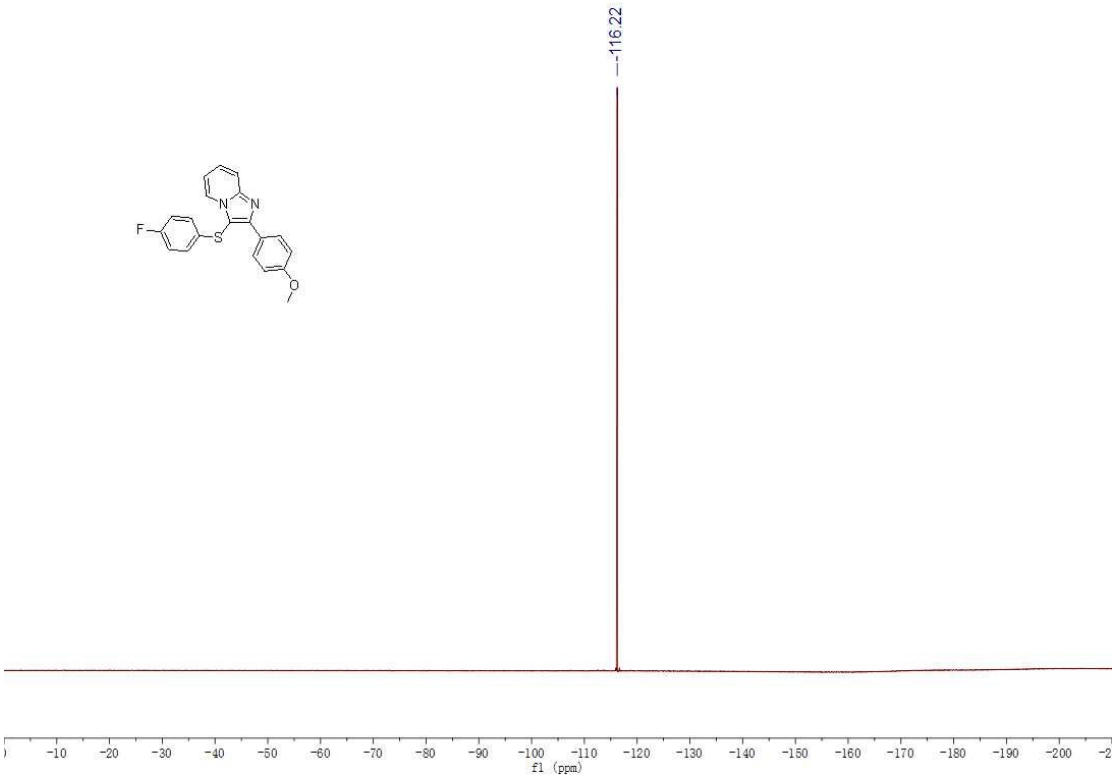




3-((4-fluorophenyl)thio)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine（4ad）



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F
S
N
O
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-110
-120
-130
-140
-150
-160
-170
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-190
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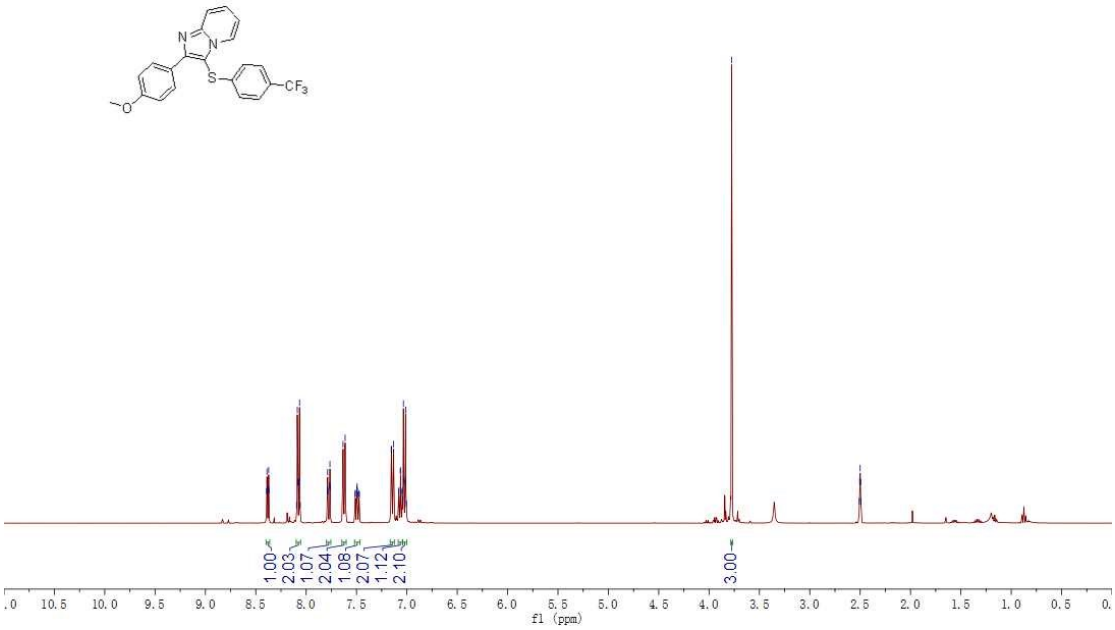
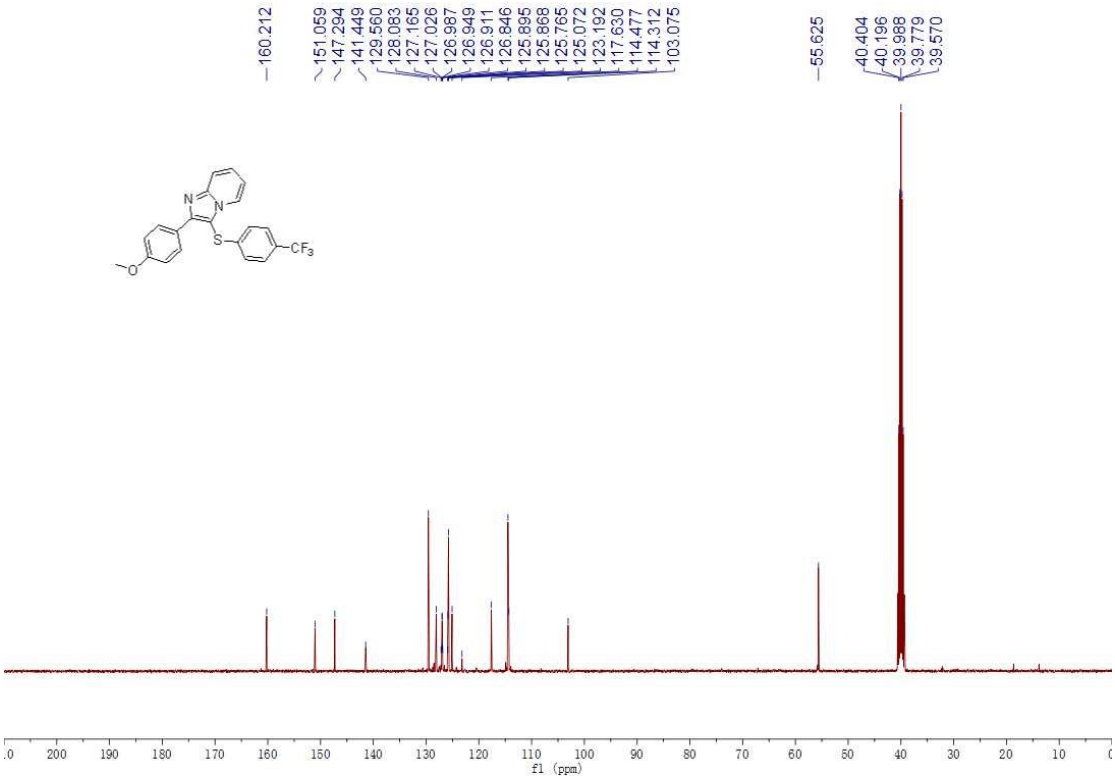
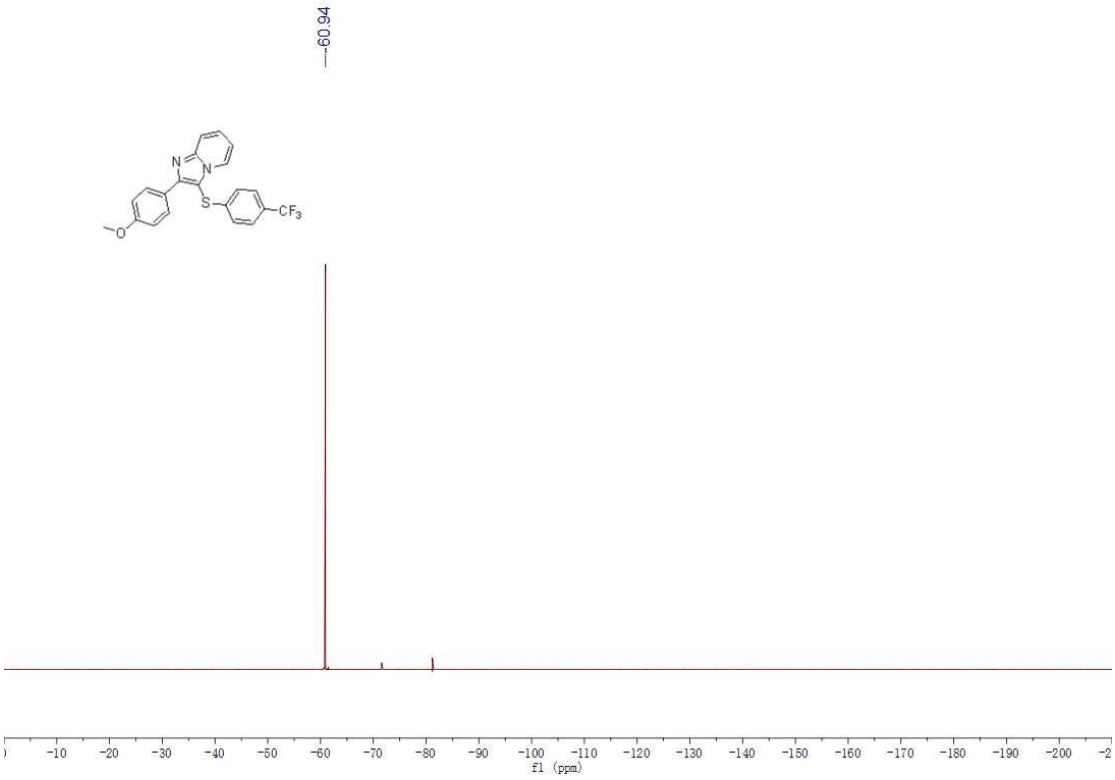
f1 (ppm)

2-(4-methoxyphenyl)-3-((4-(trifluoromethyl)phenyl)thio)imidazo[1,2-a]pyridine（4ae）



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N
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S
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O
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-130
-140
-150
-160
-170
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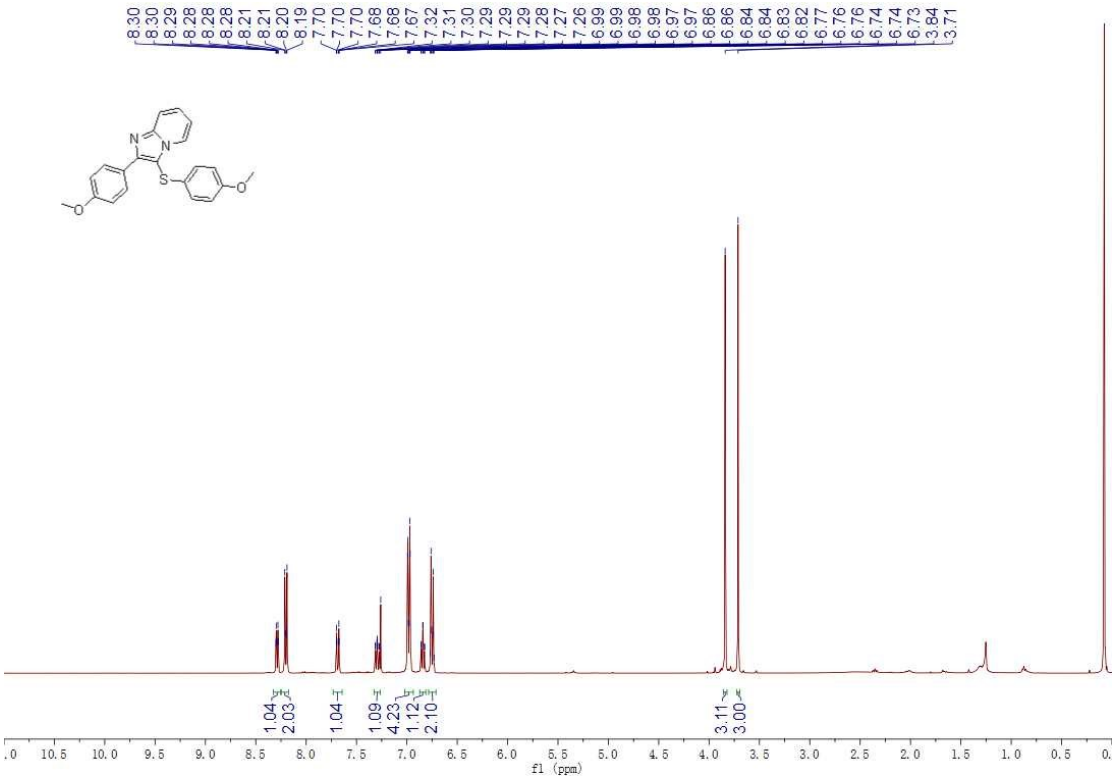
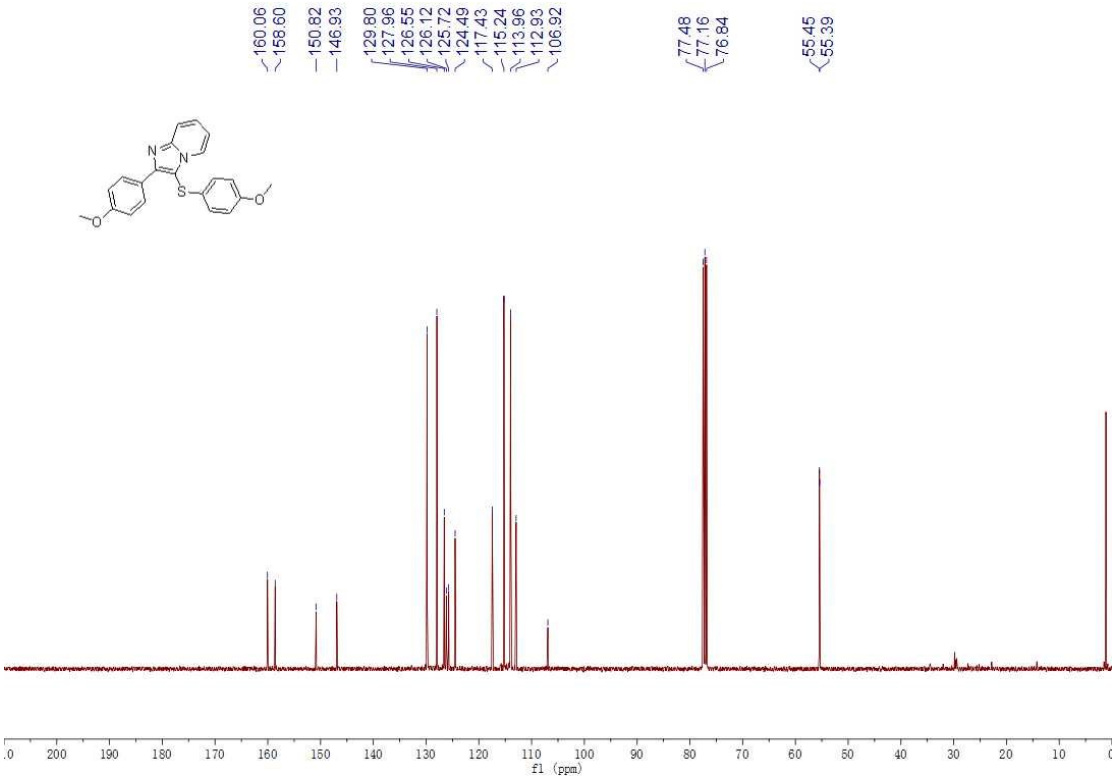
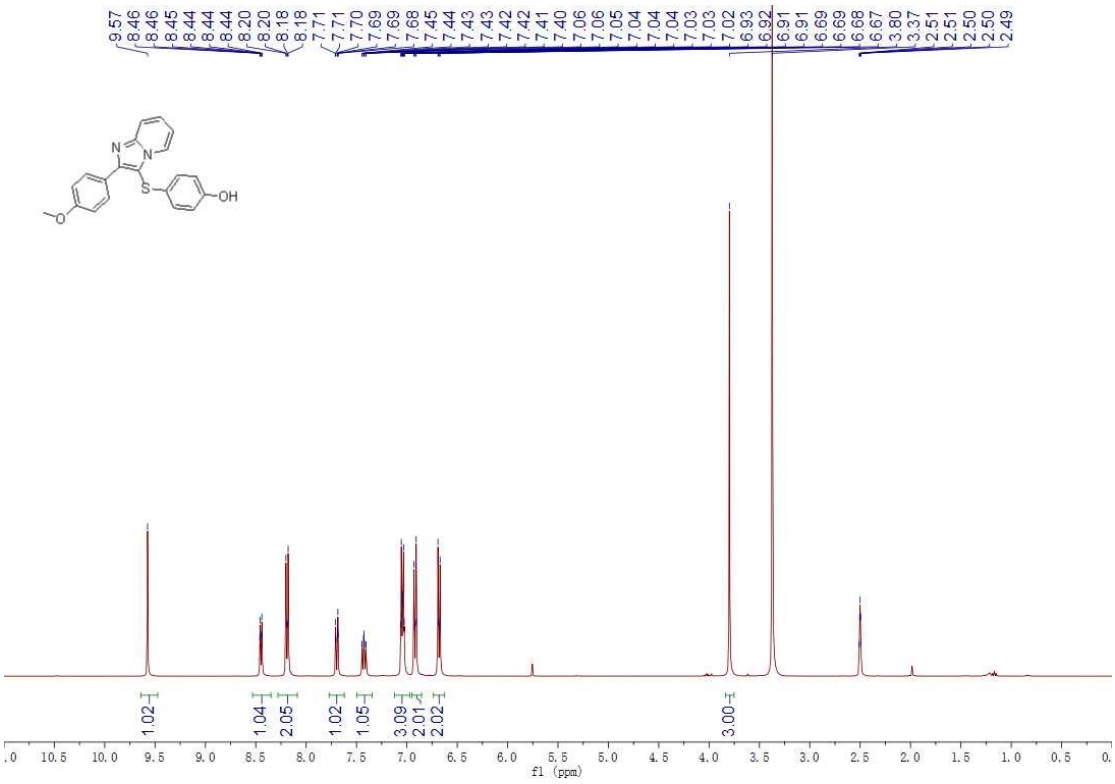
f1 (ppm)

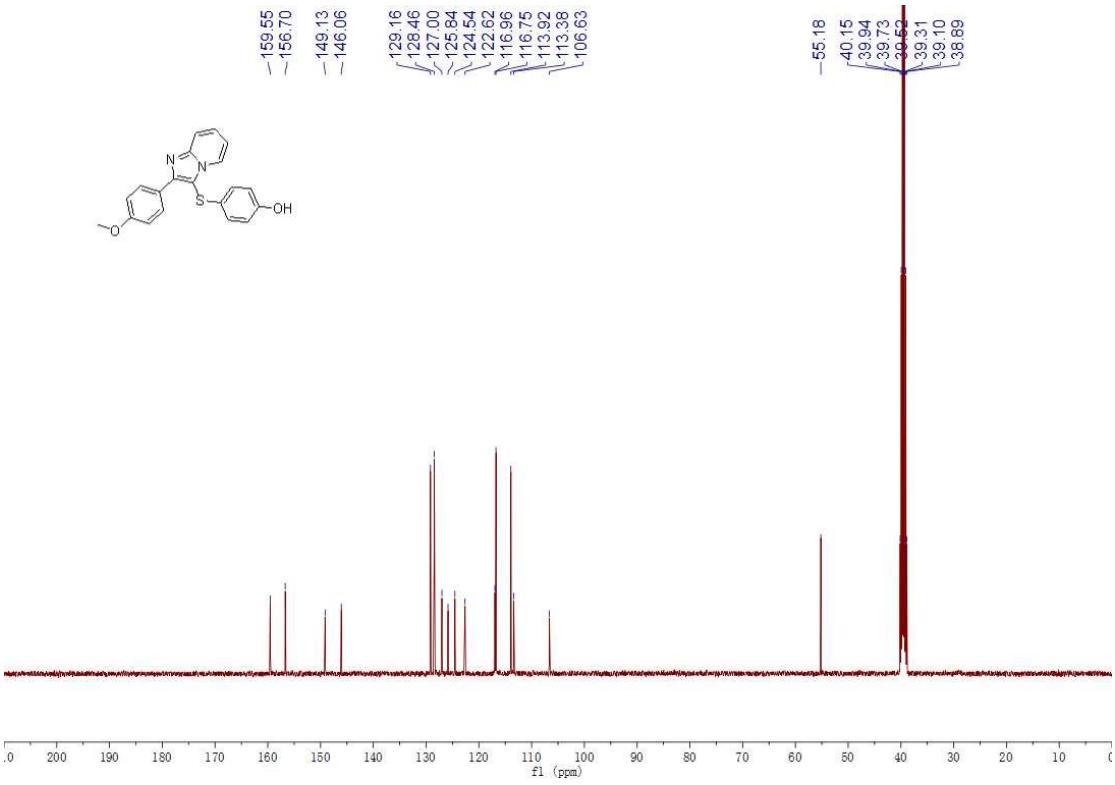
2-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)imidazo[1,2-a]pyridine(4af)



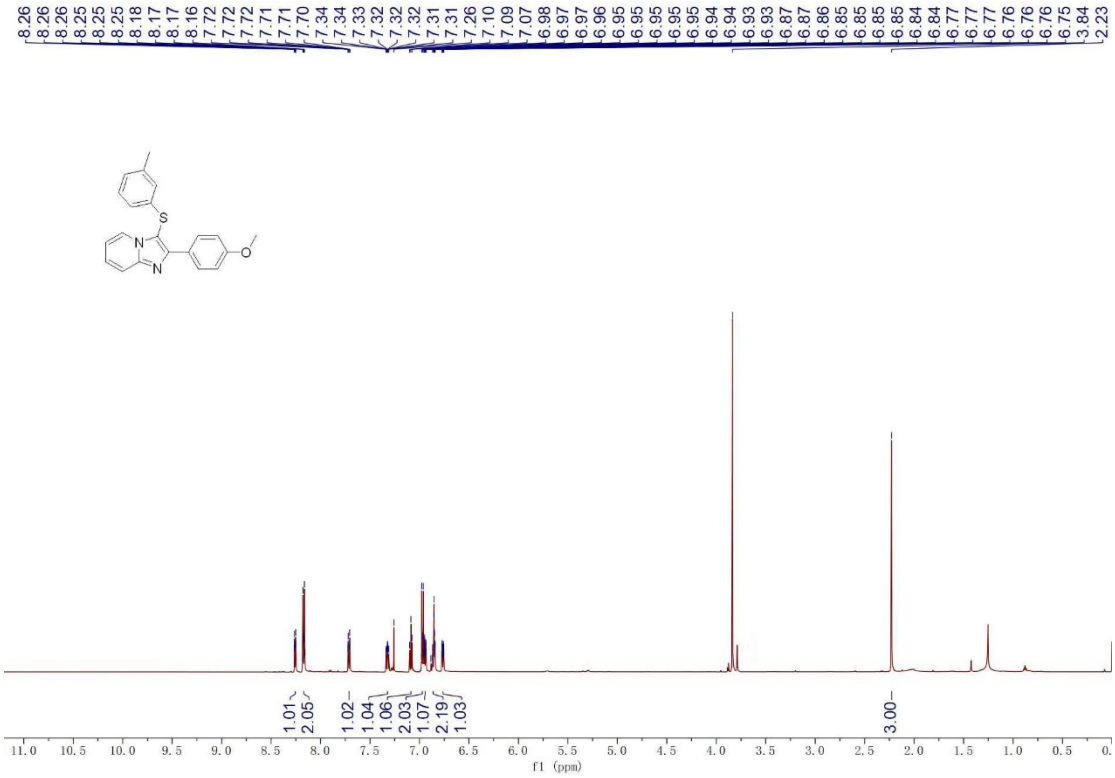


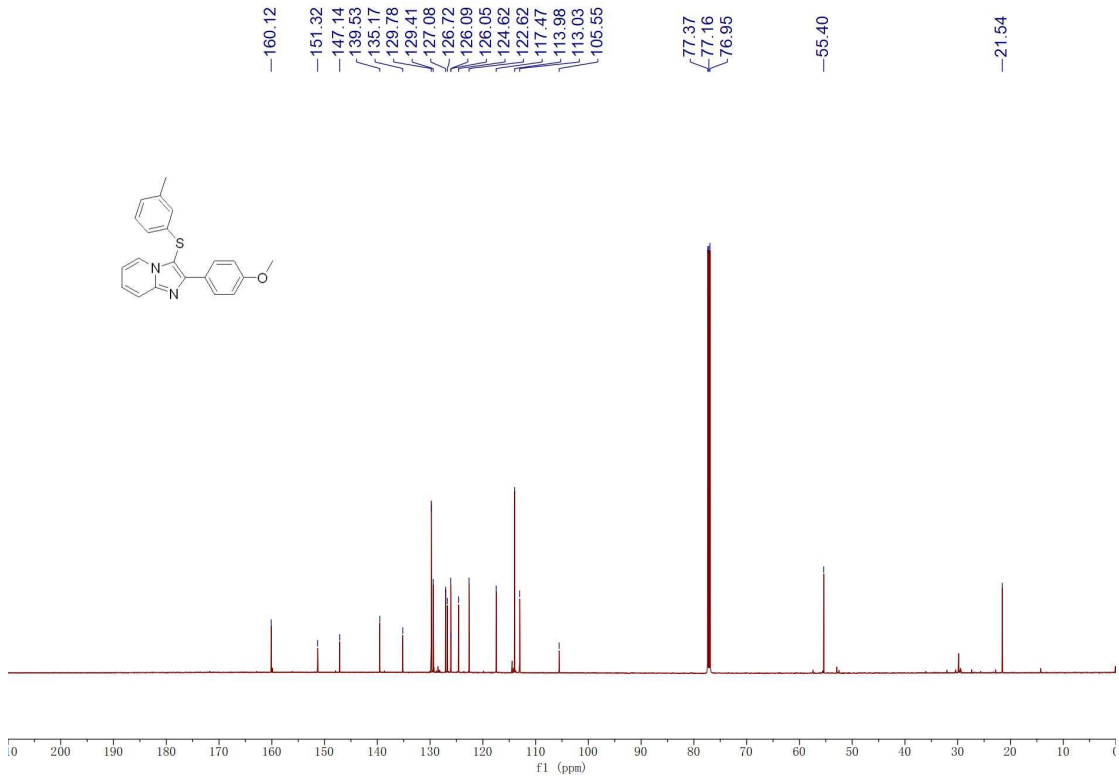
4-((2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)thio)phenol（4ag）



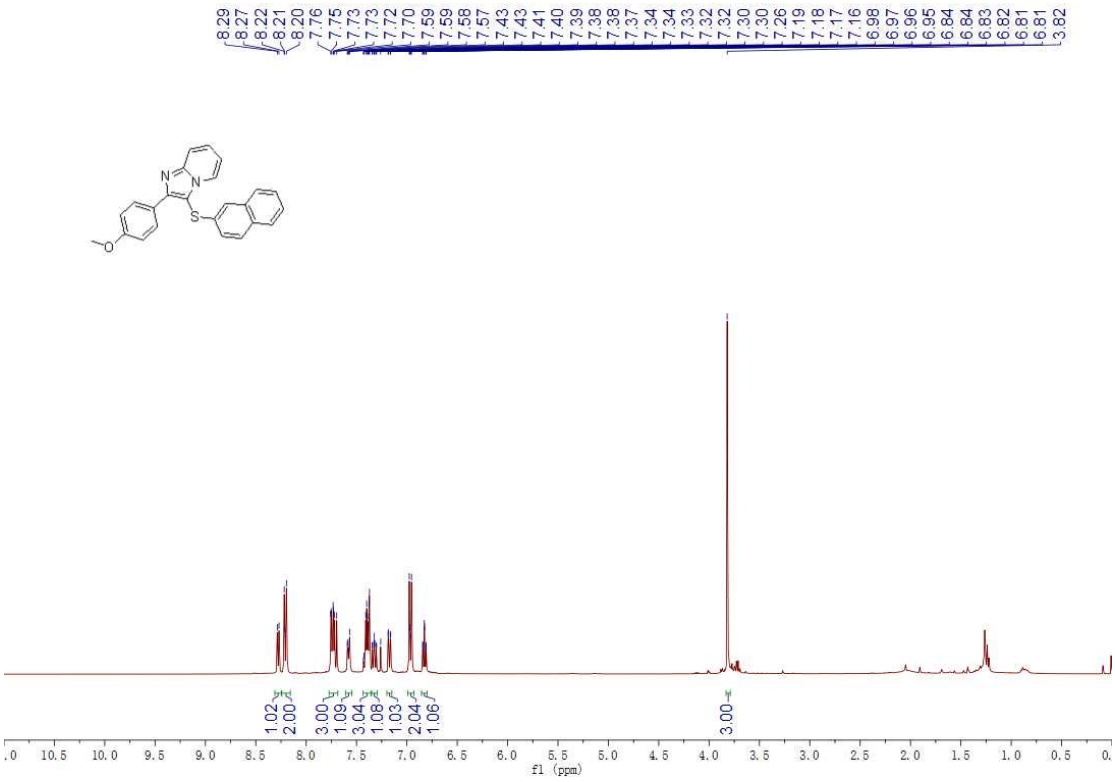


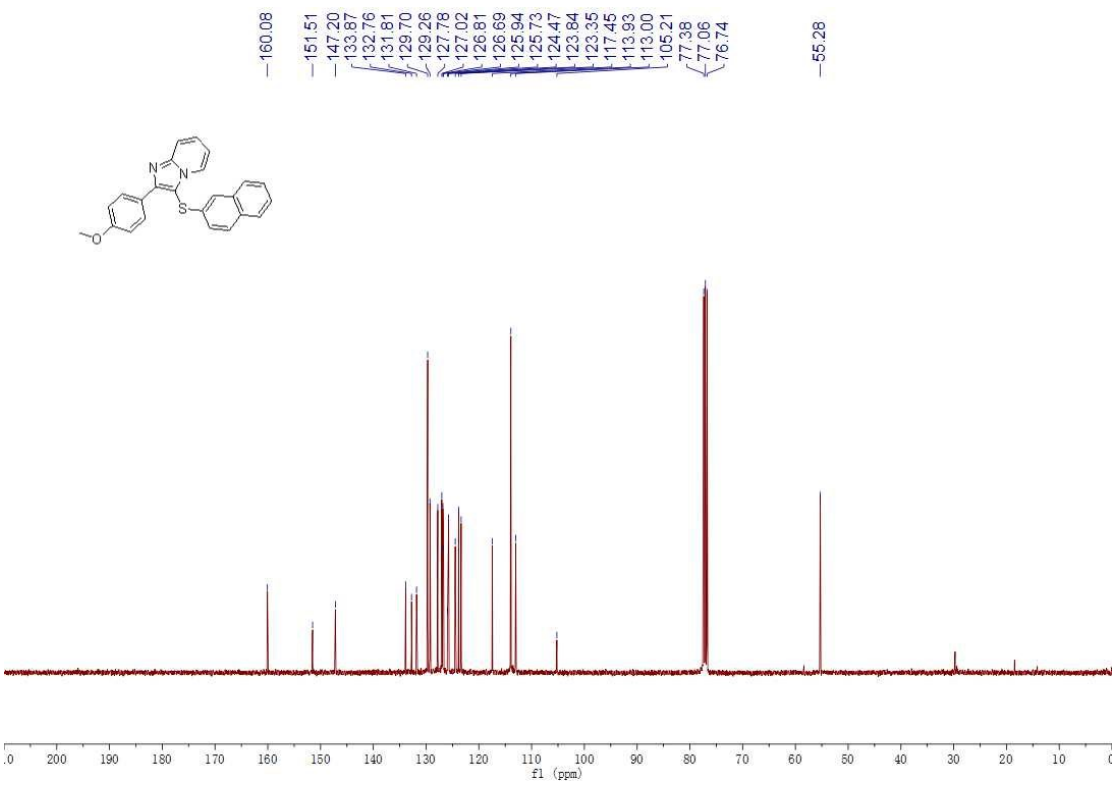
2-(4-methoxyphenyl)-3-(m-tolylthio)imidazo[1,2-a]pyridine（4ah）



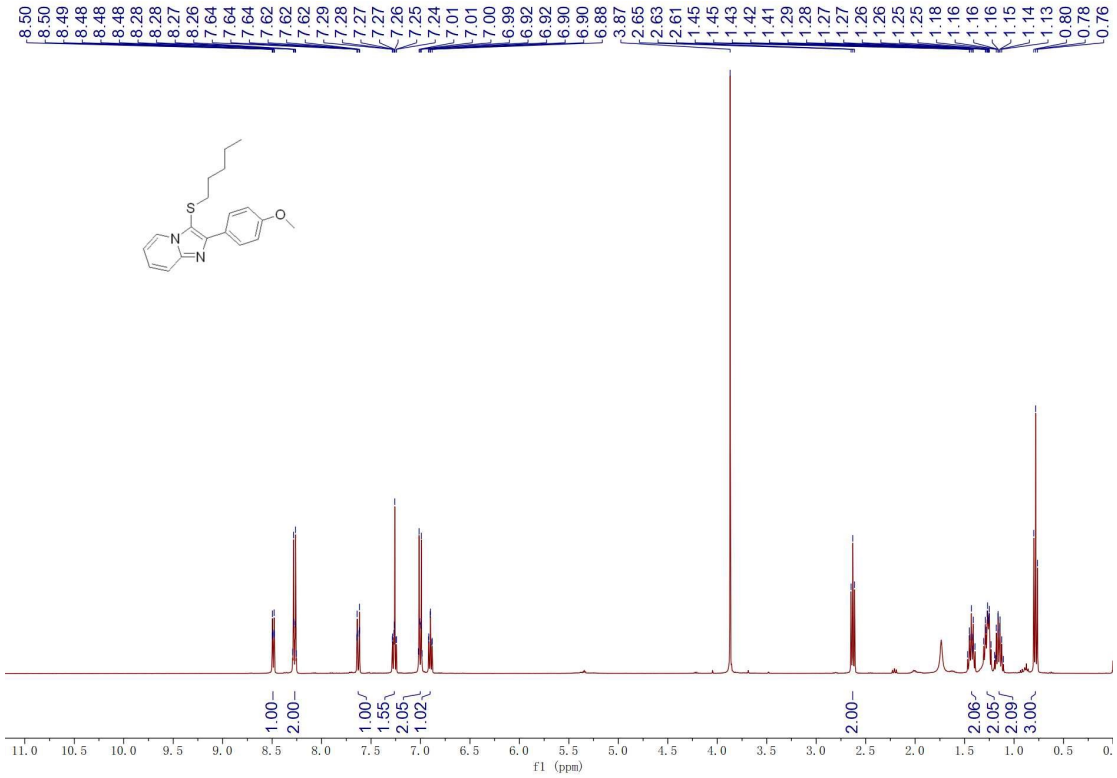


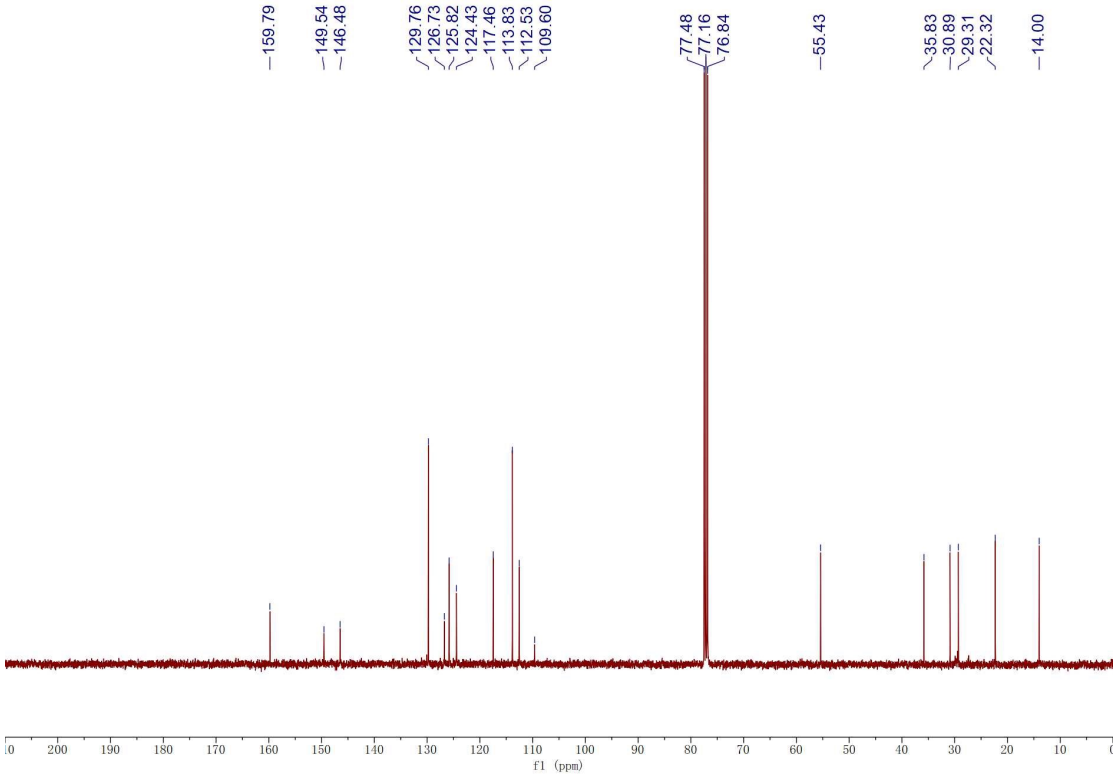
2-(4-methoxyphenyl)-3-(naphthalen-2-ylthio)imidazo[1,2-a]pyridine（4ai）



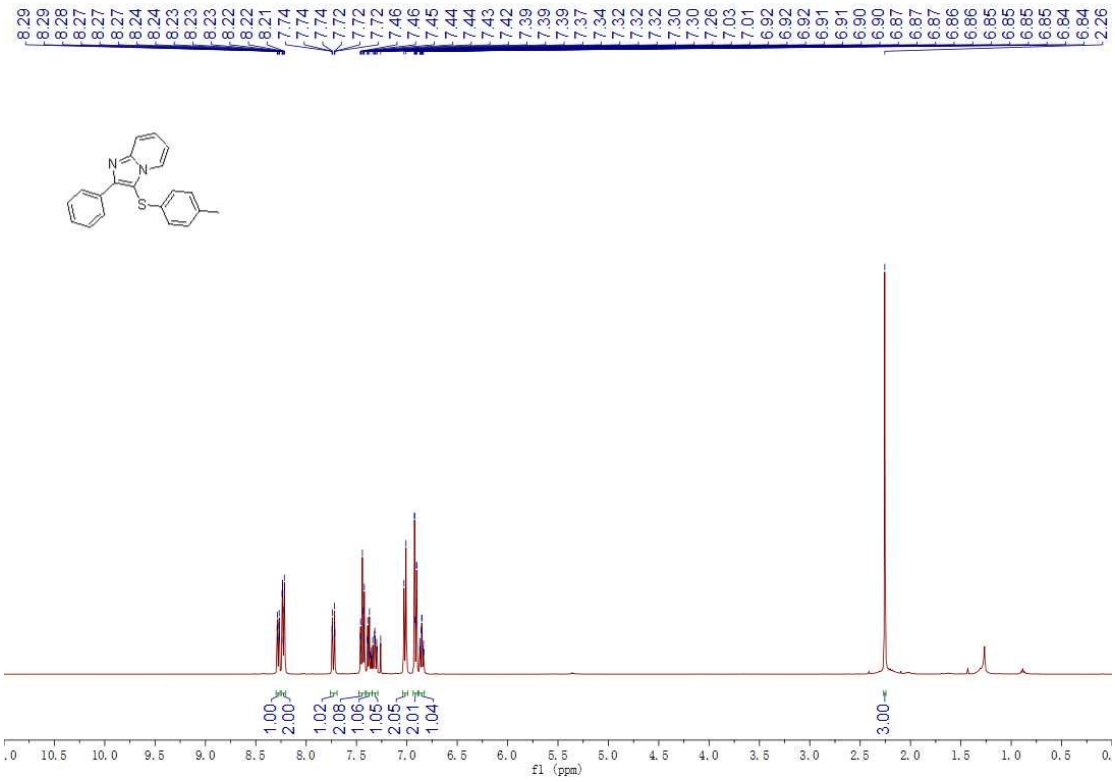


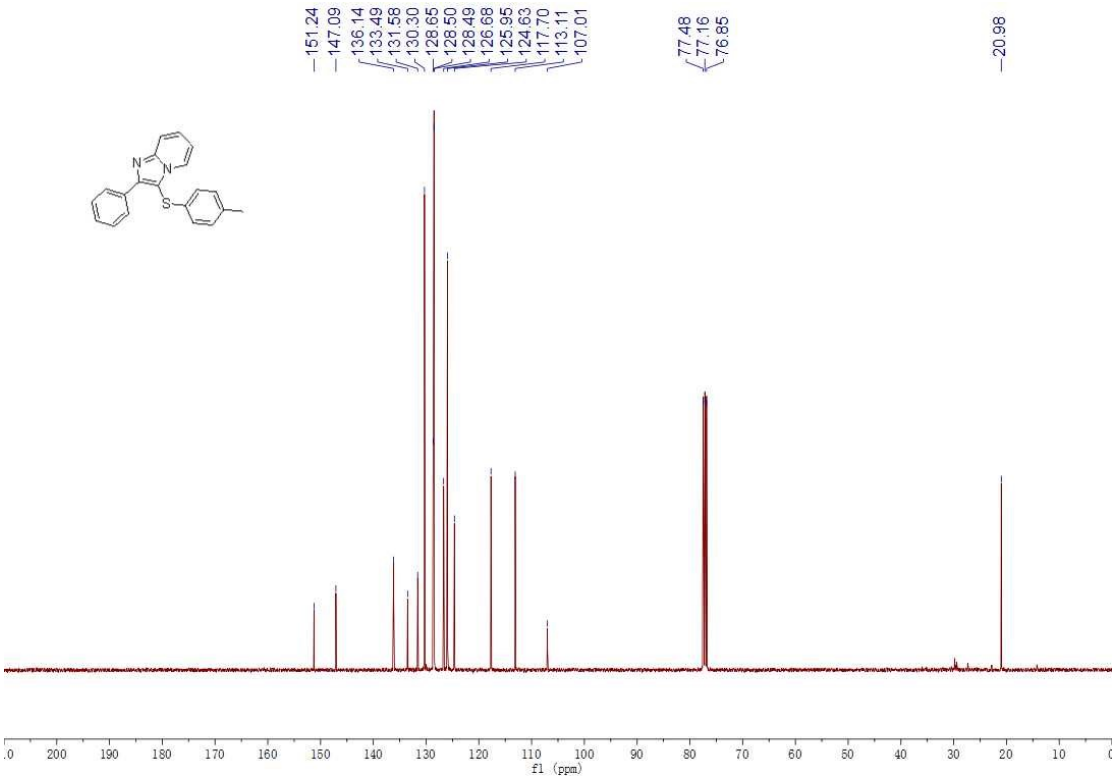
2-(4-methoxyphenyl)-3-(pentylthio)imidazo[1,2-a]pyridine（4aj）



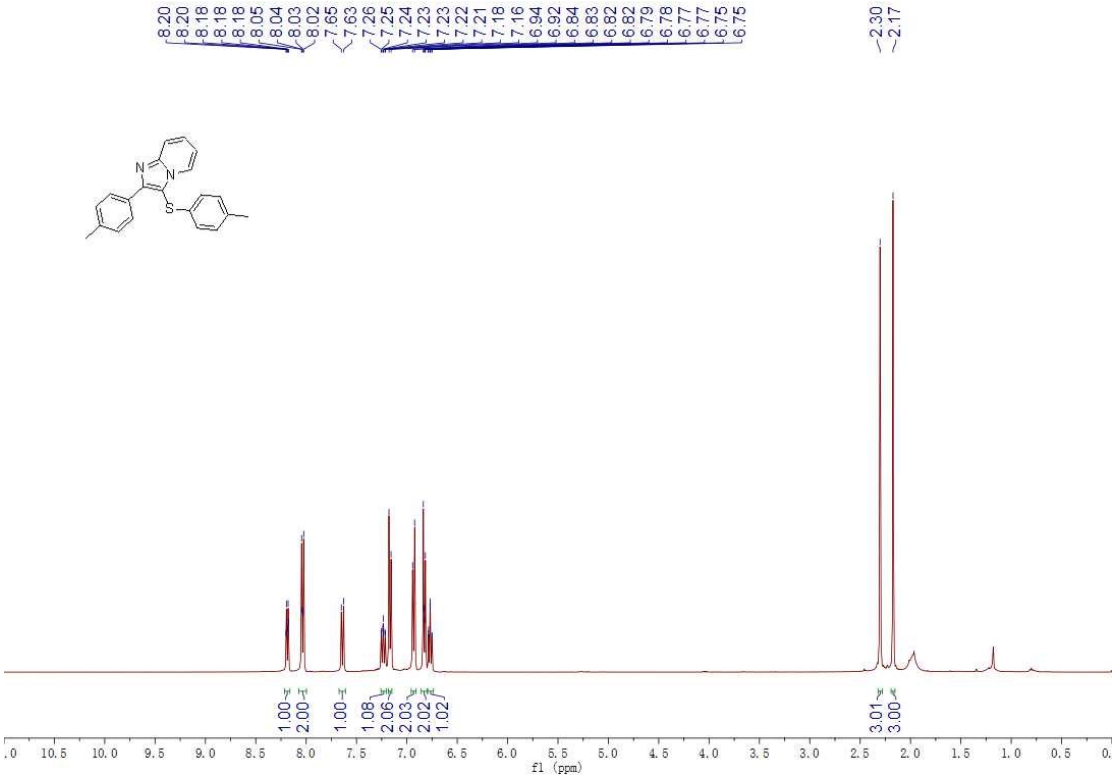


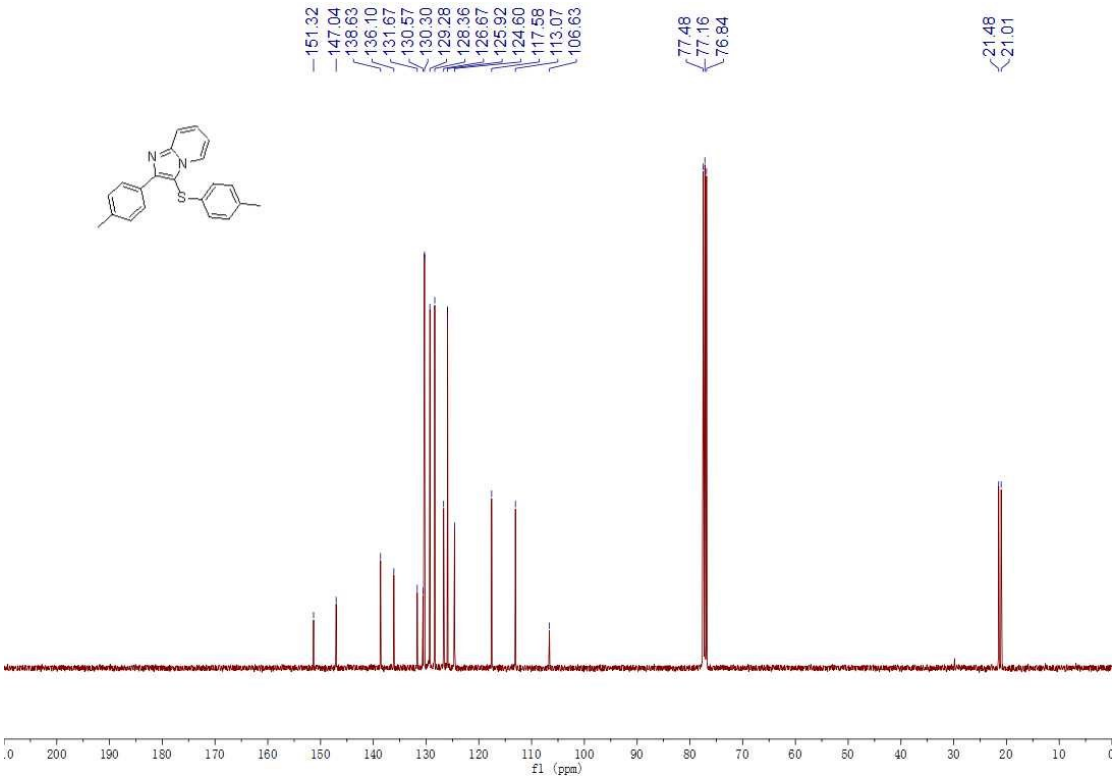
2-phenyl-3-(p-tolylthio)imidazo[1,2-a]pyridine（4ba）



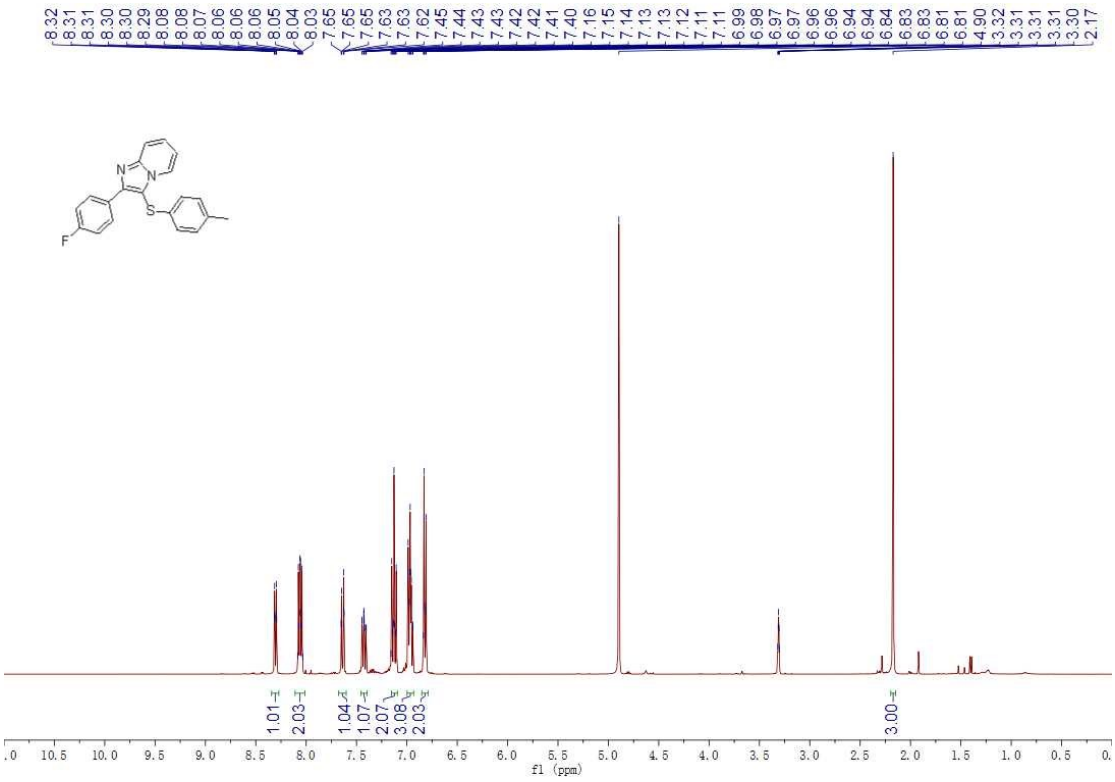


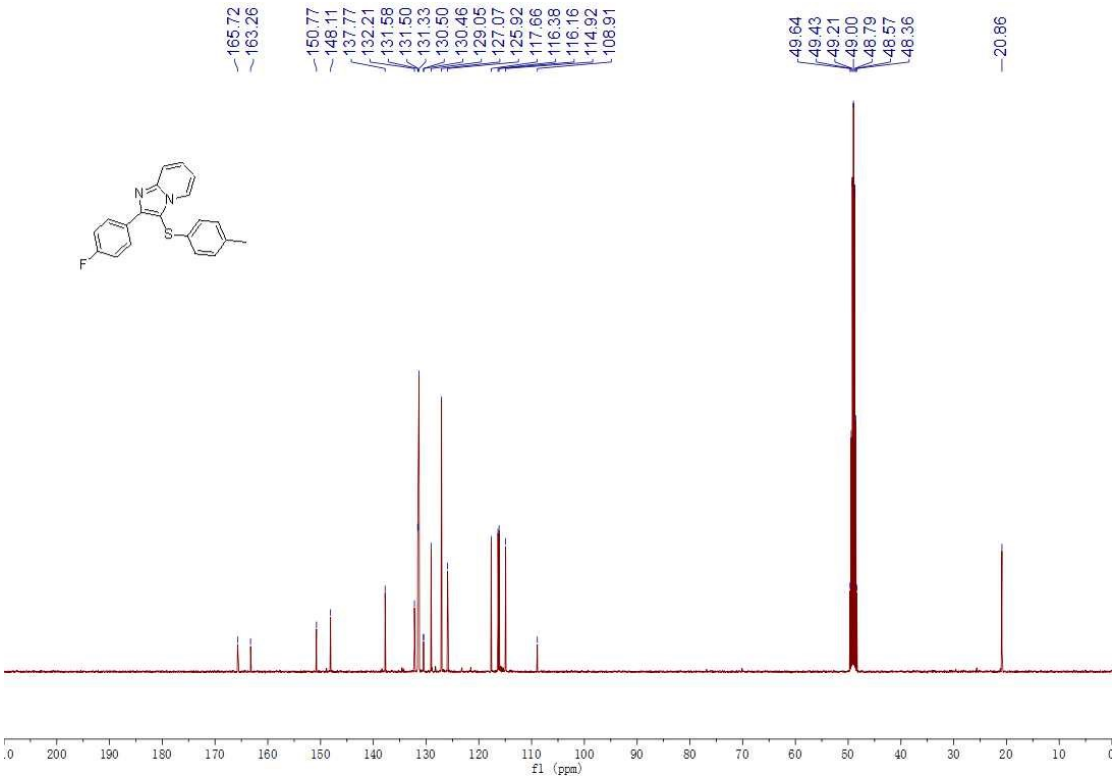
2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bb）

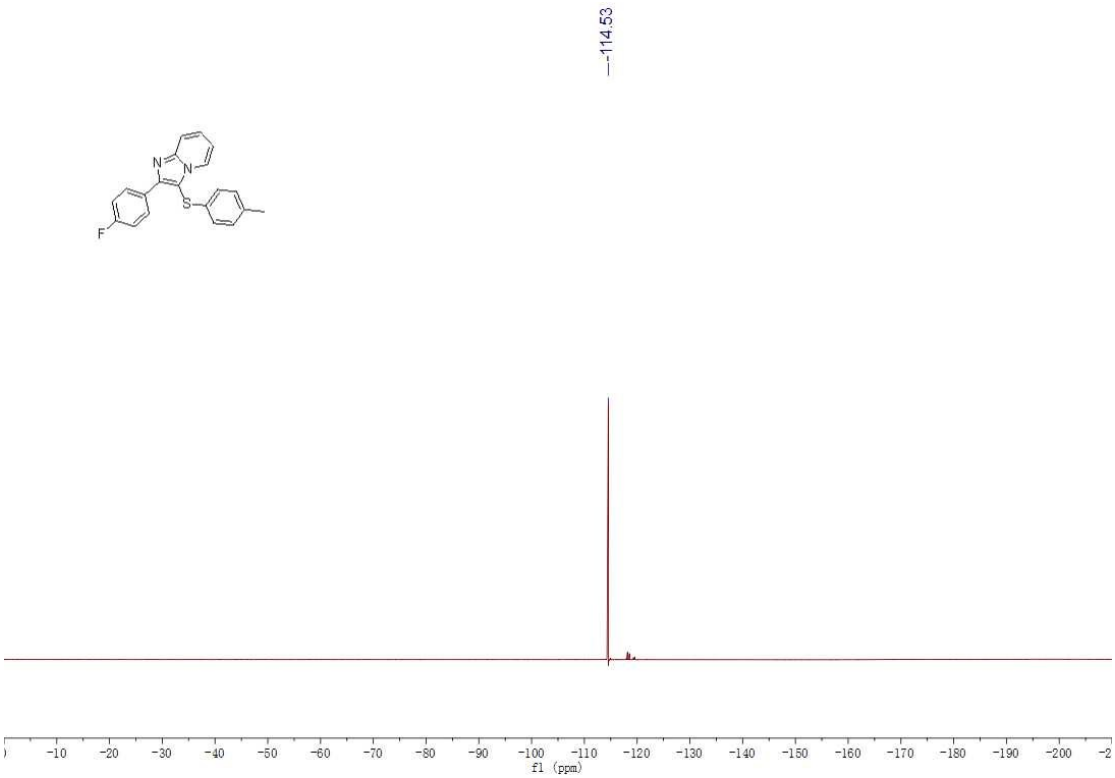




2-(4-fluorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bc）






-114.53
N
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S
F
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-140
-150
-160
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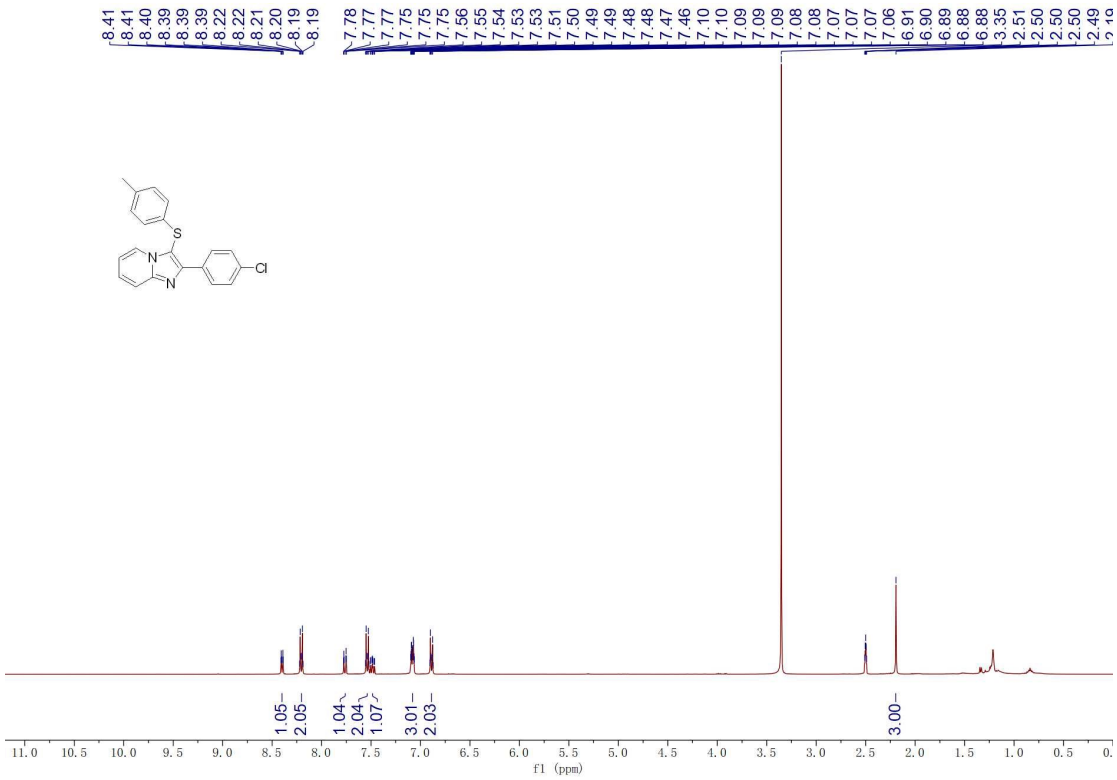
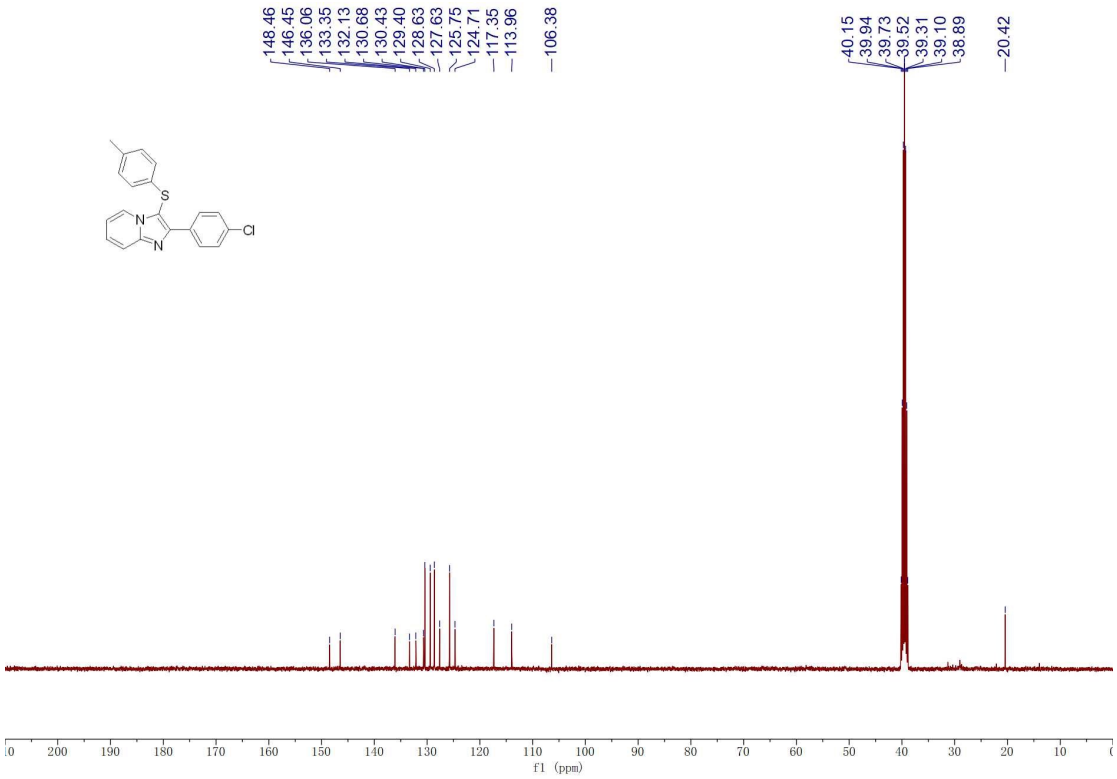
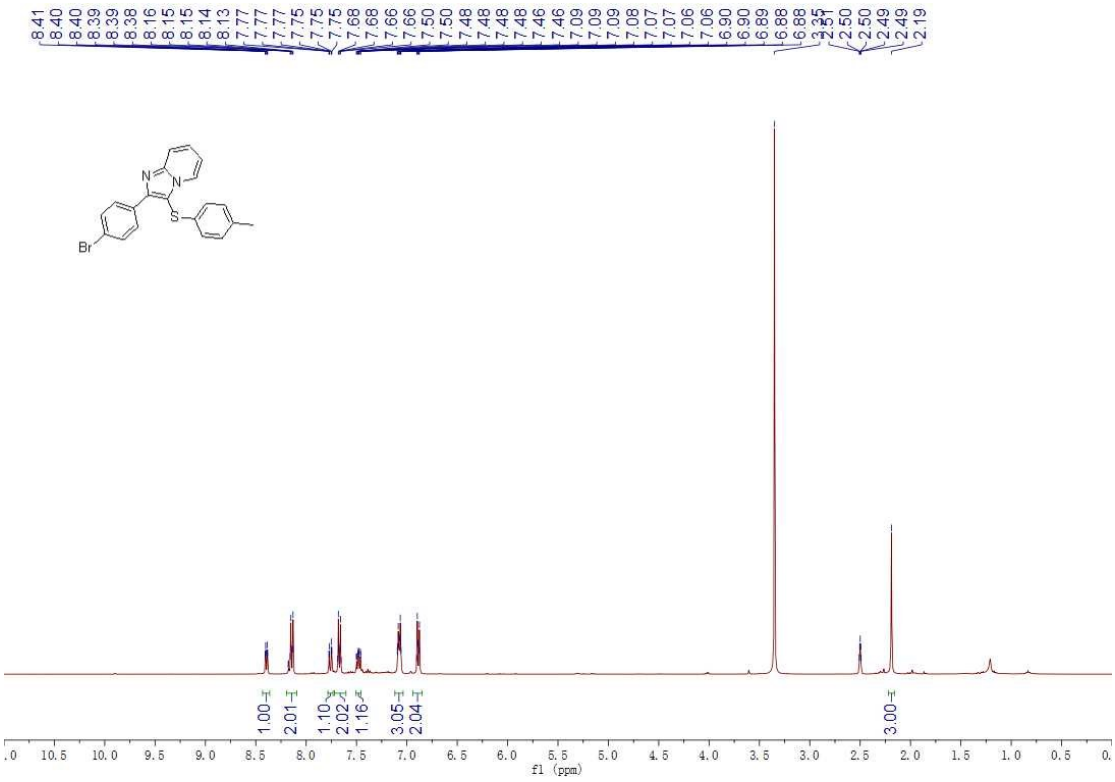
-190
-200
f1 (ppm)

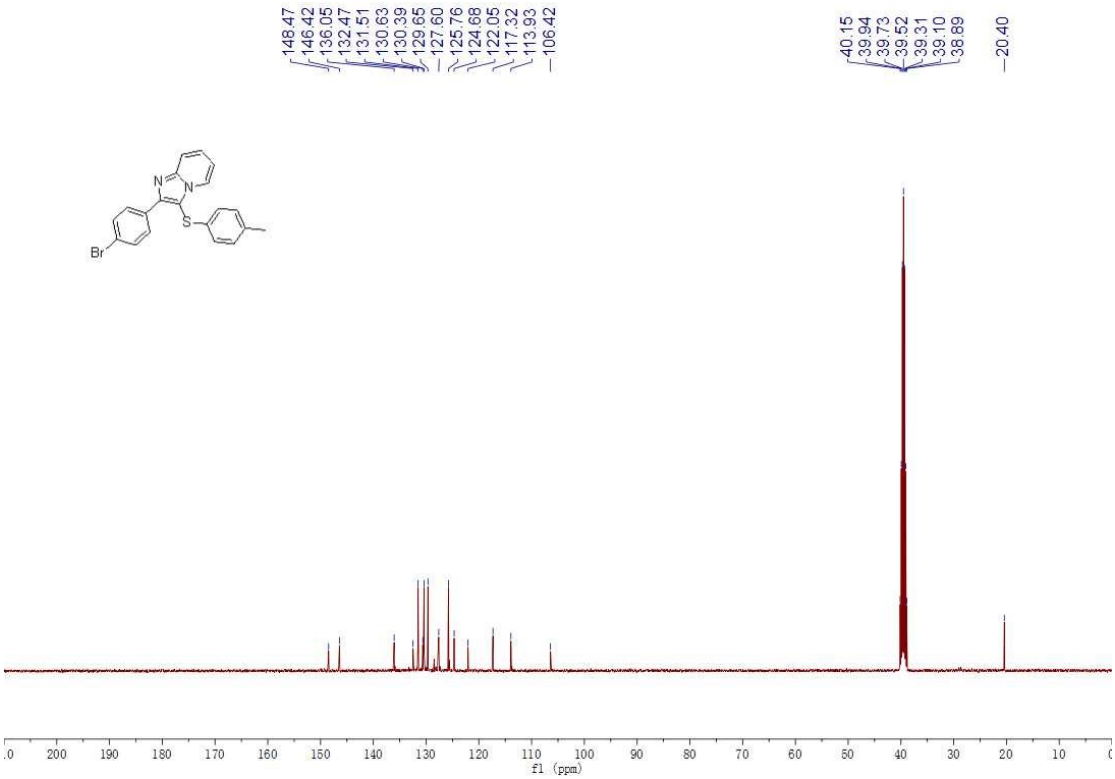
2-(3-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bd）



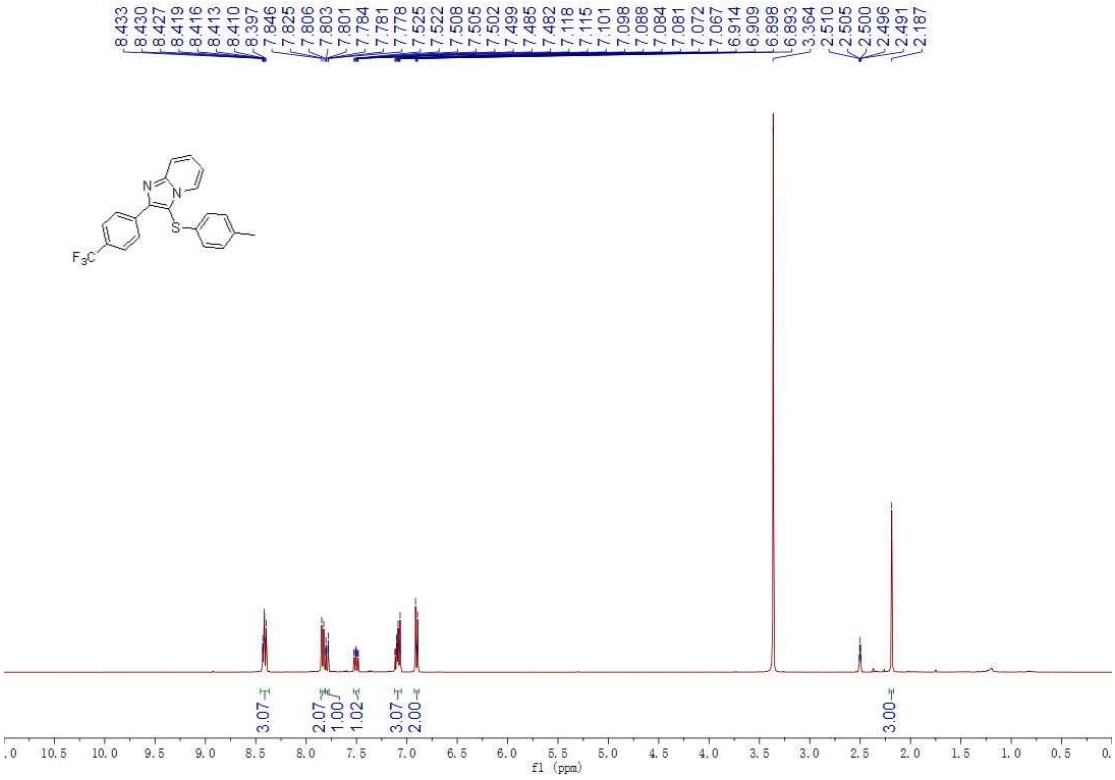


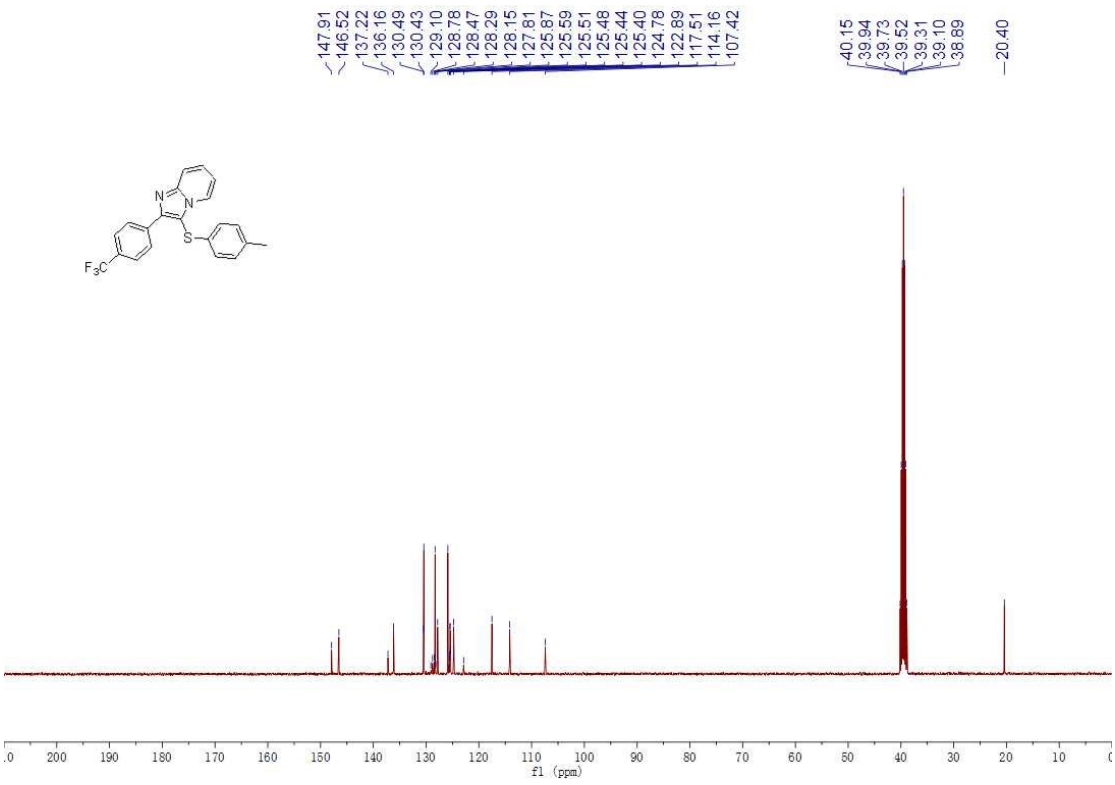
2-(4-bromophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4be）

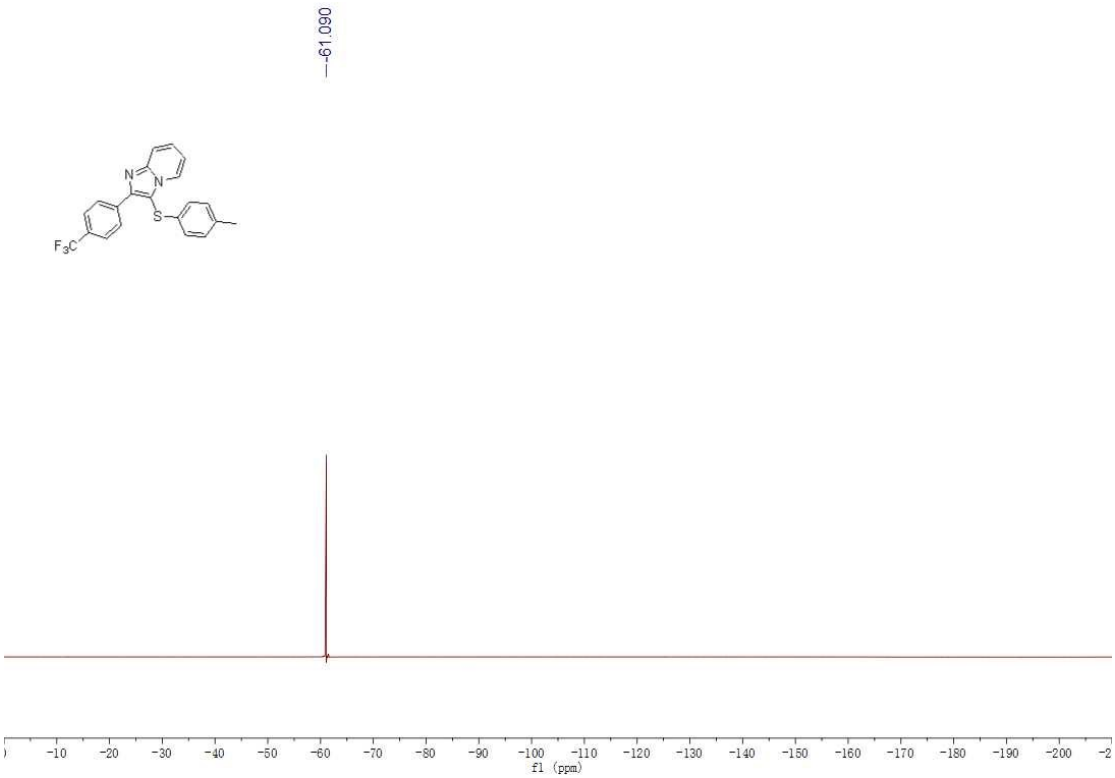




3-(p-tolylthio)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine（4bf）






-61.090
N
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S
F3C
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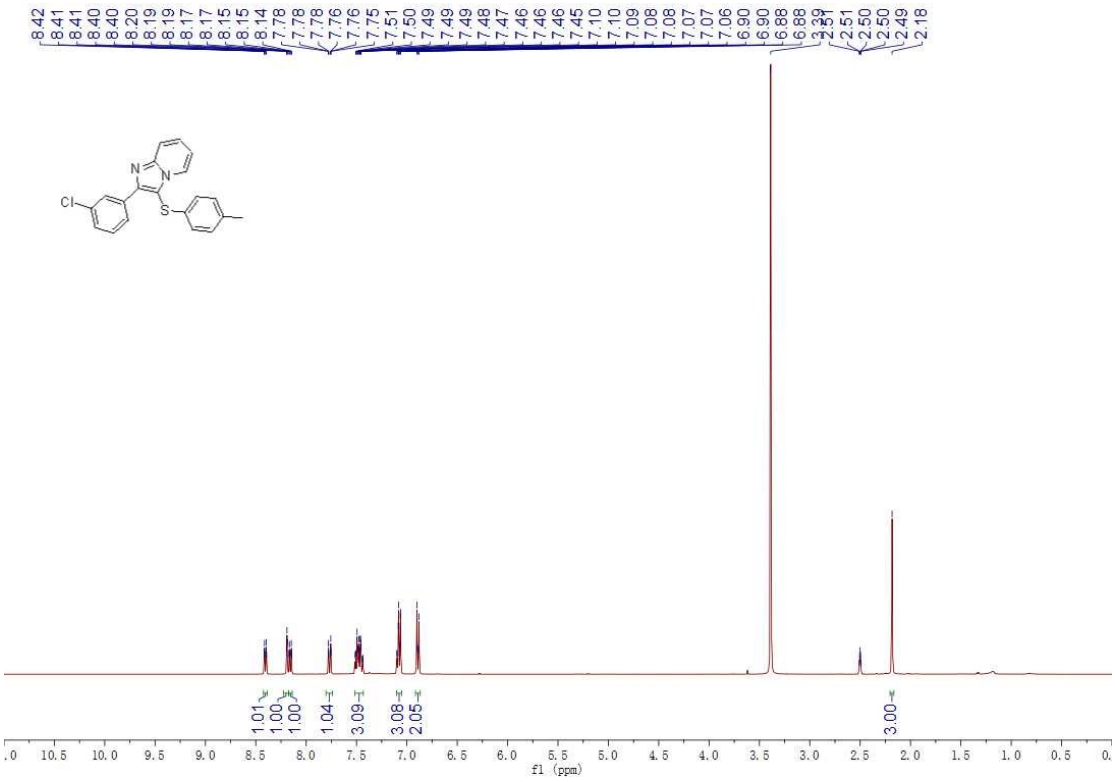
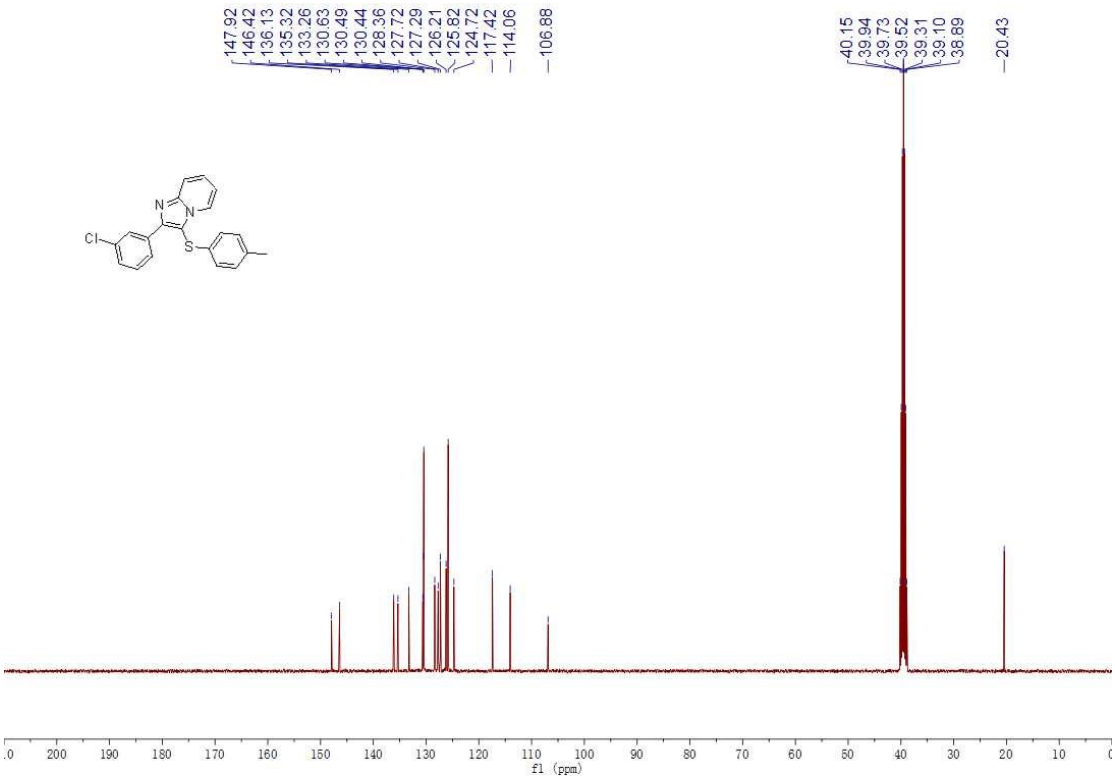
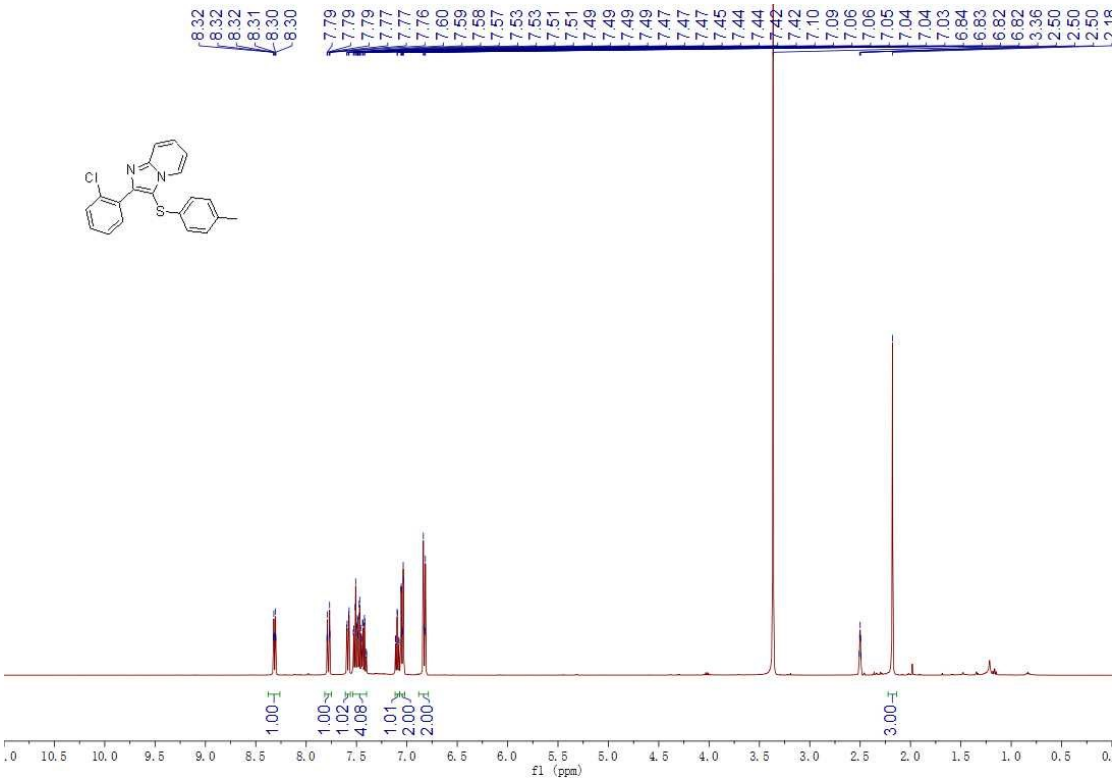
-120
-130
-140
-150
-160
-170
-180
-190
-200
-2
f1 (ppm)

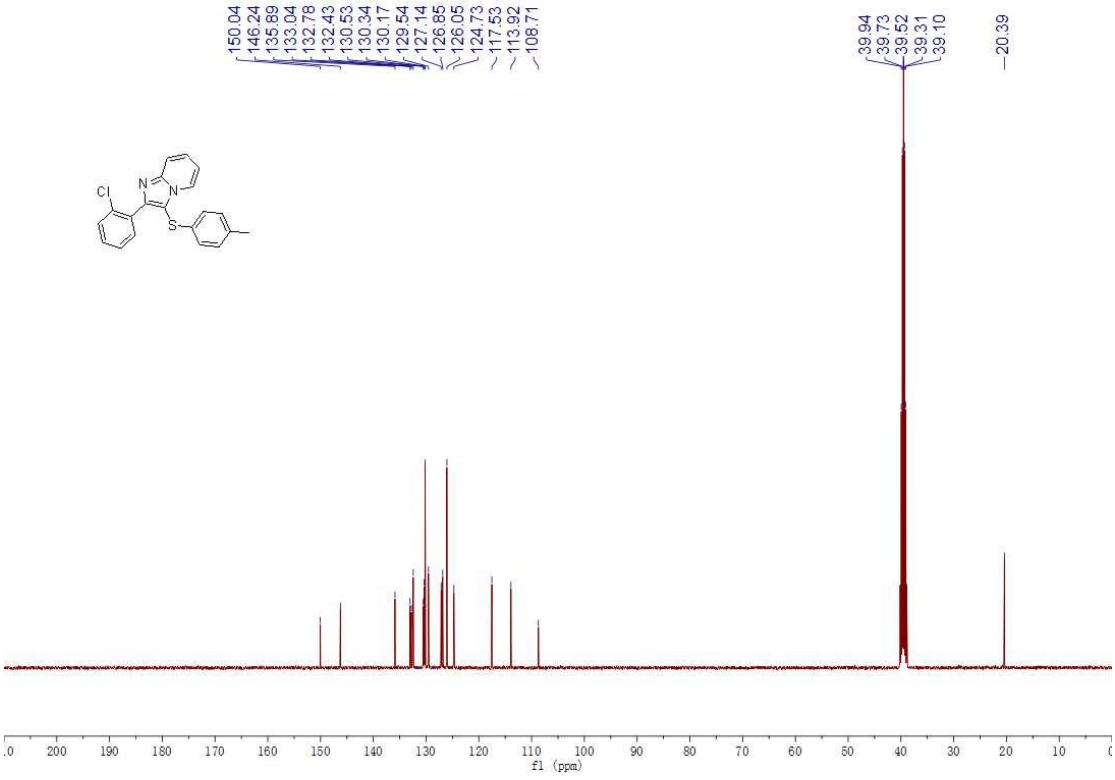
2-(3-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bg）



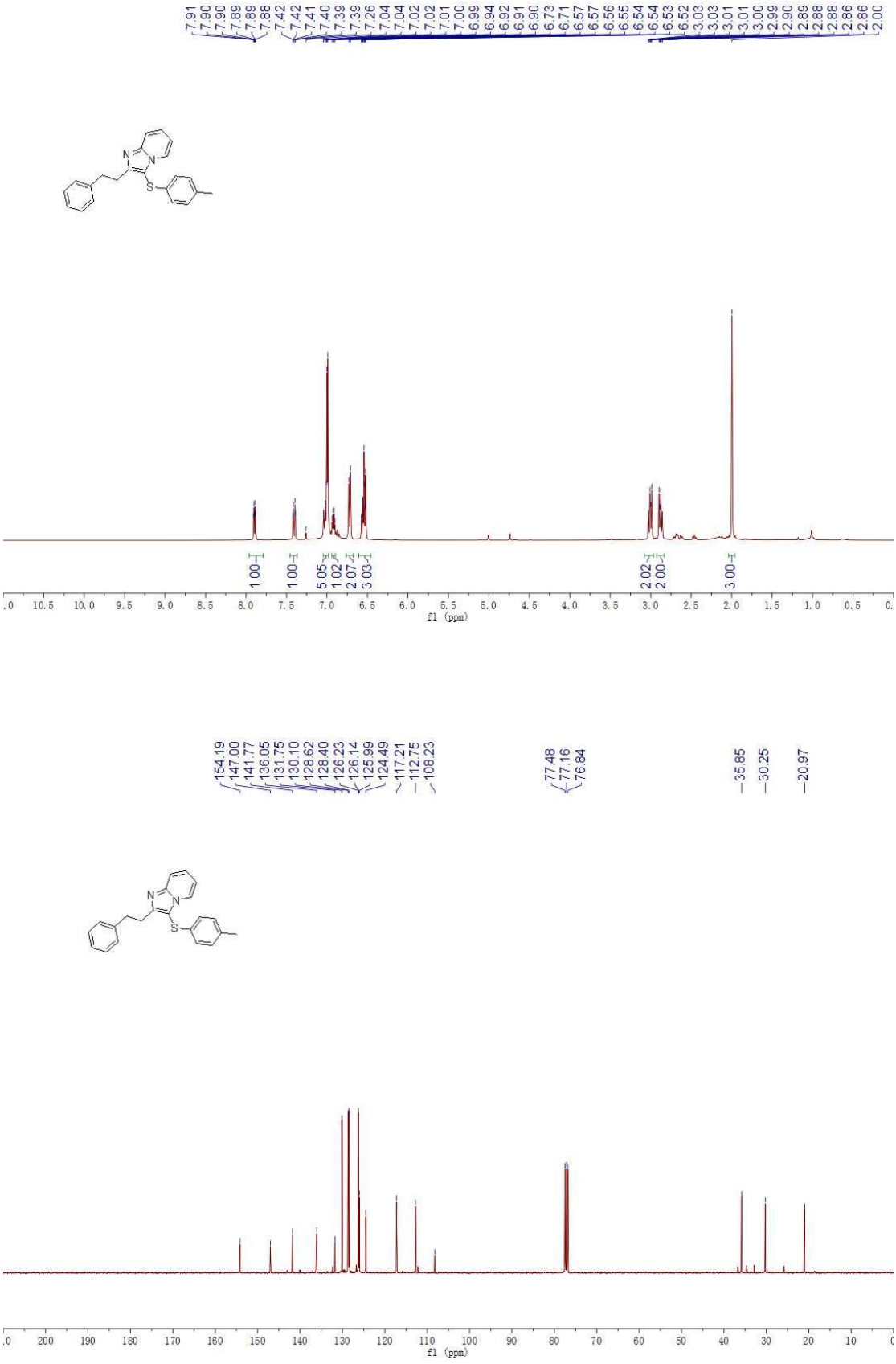


2-(2-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bh）

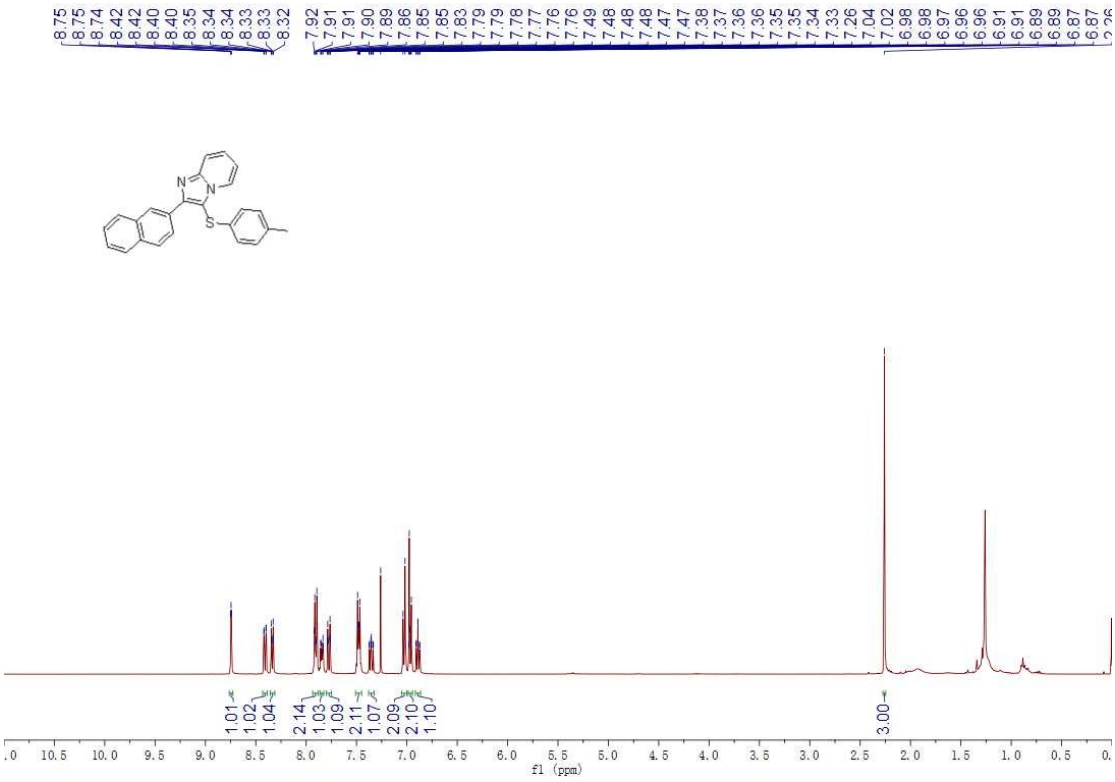


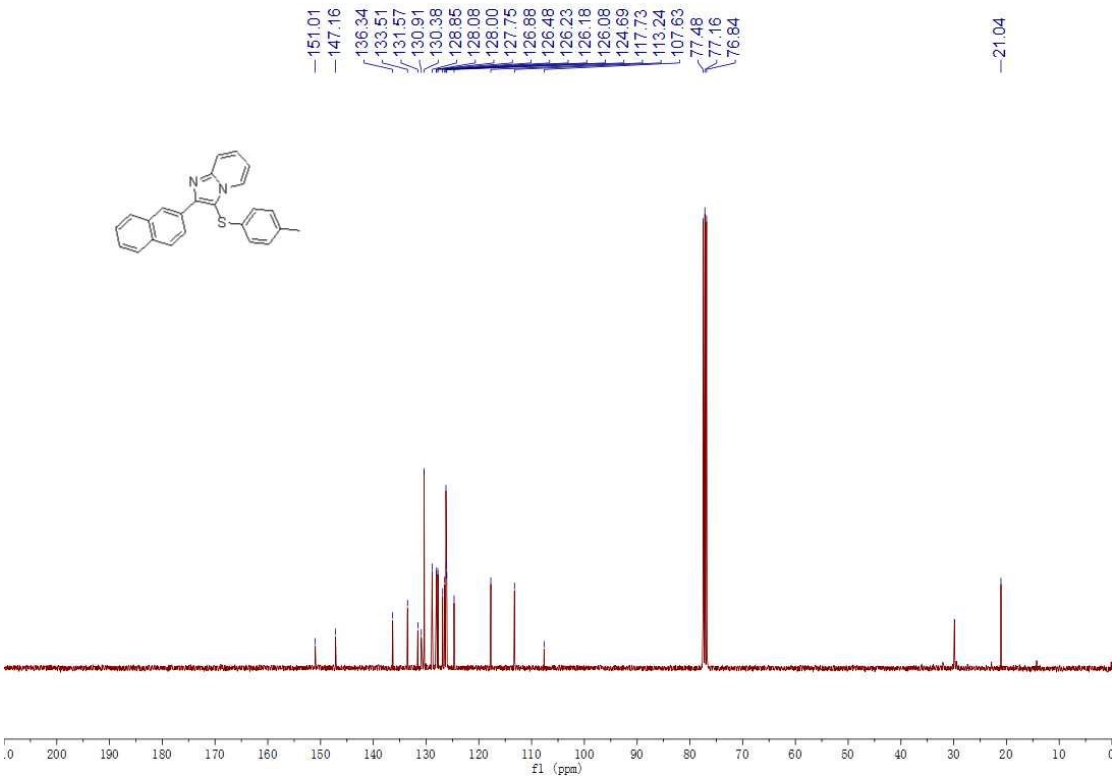


2-phenethyl-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bi）

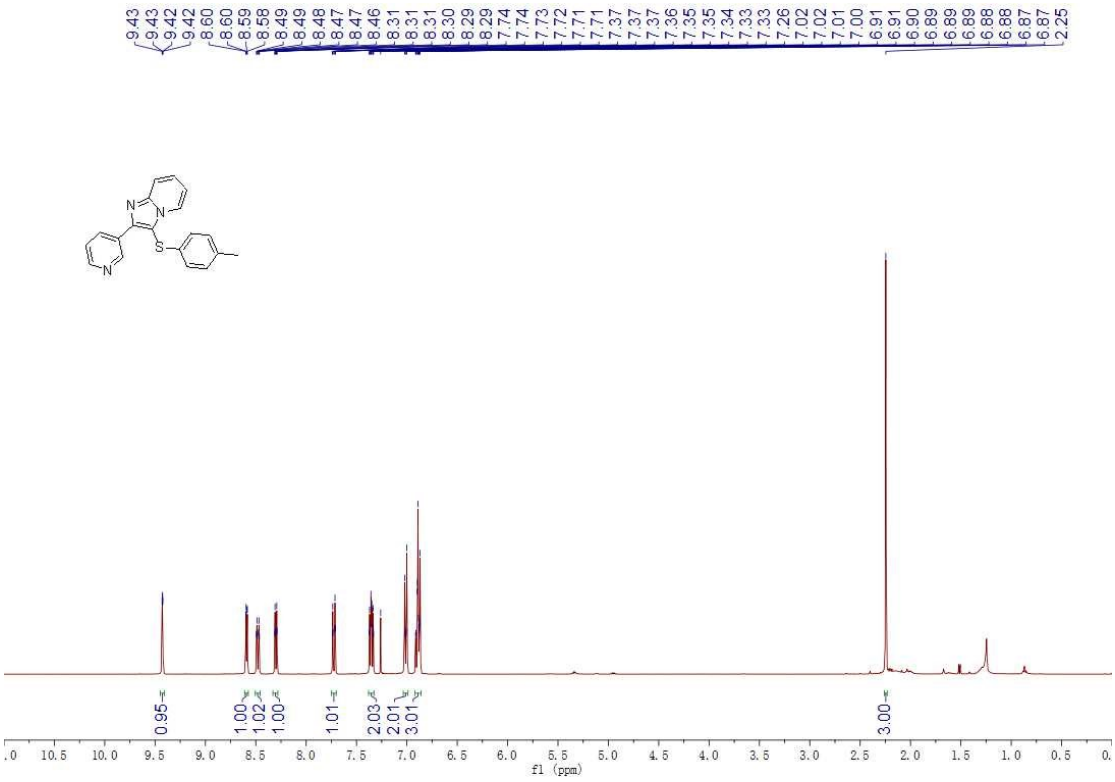


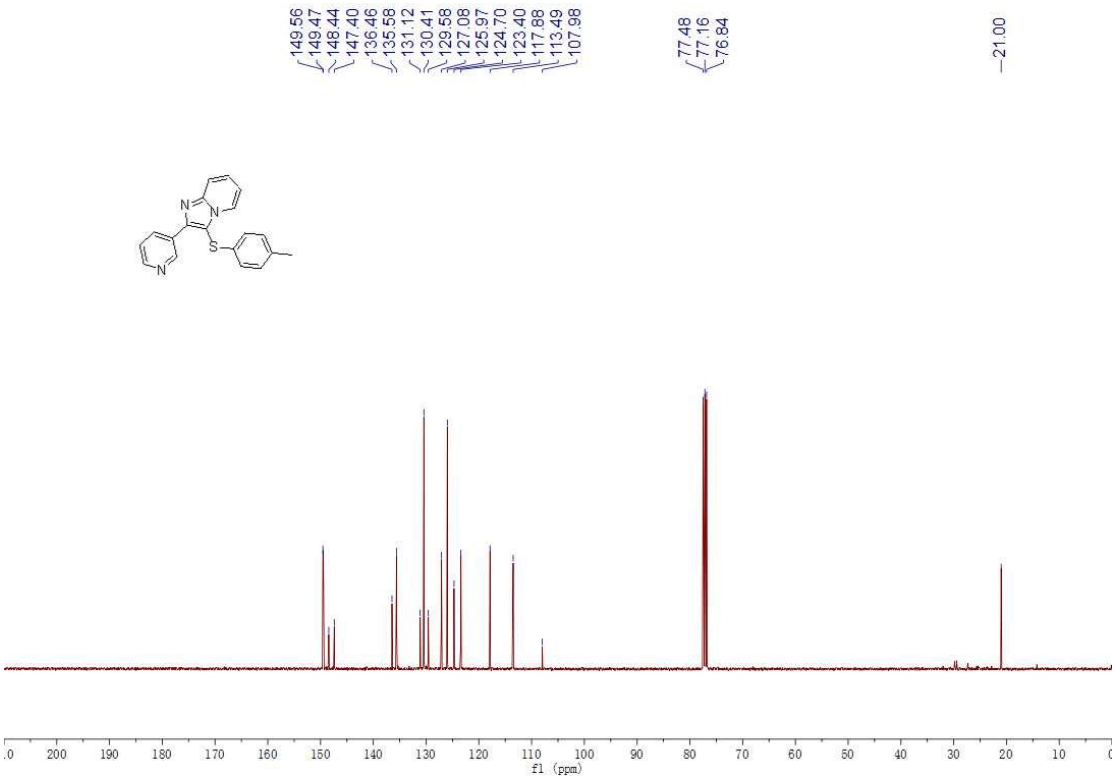
2-(naphthalen-2-yl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bj）



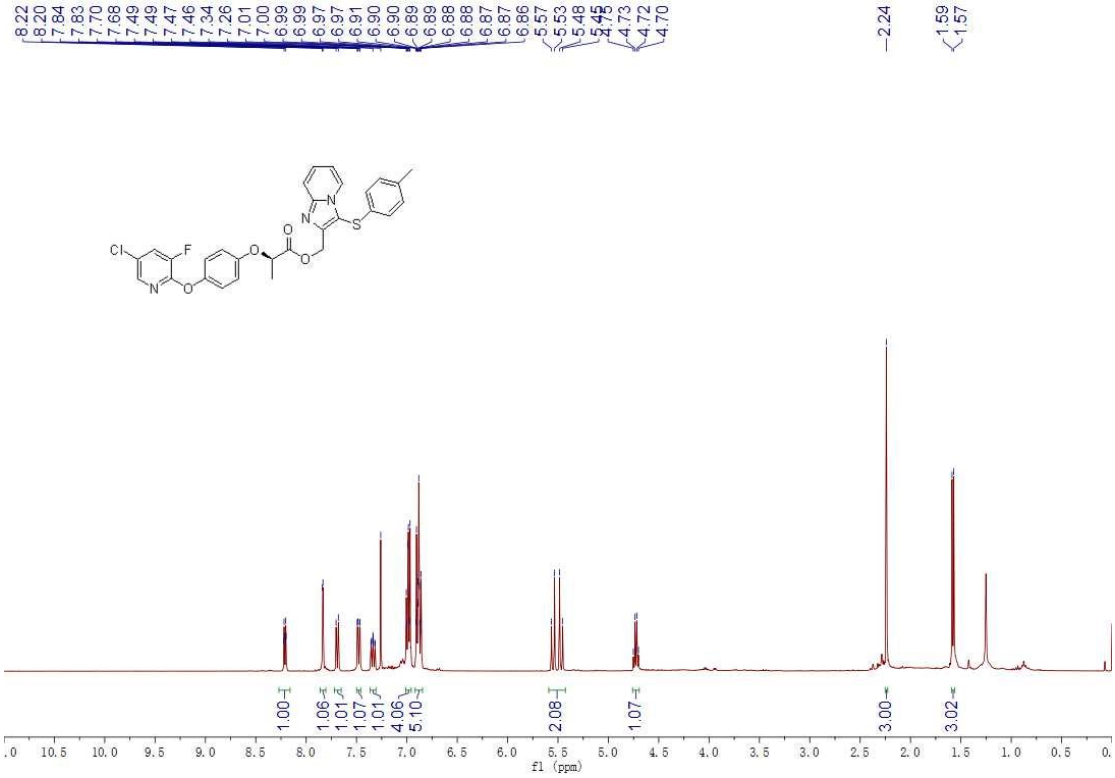


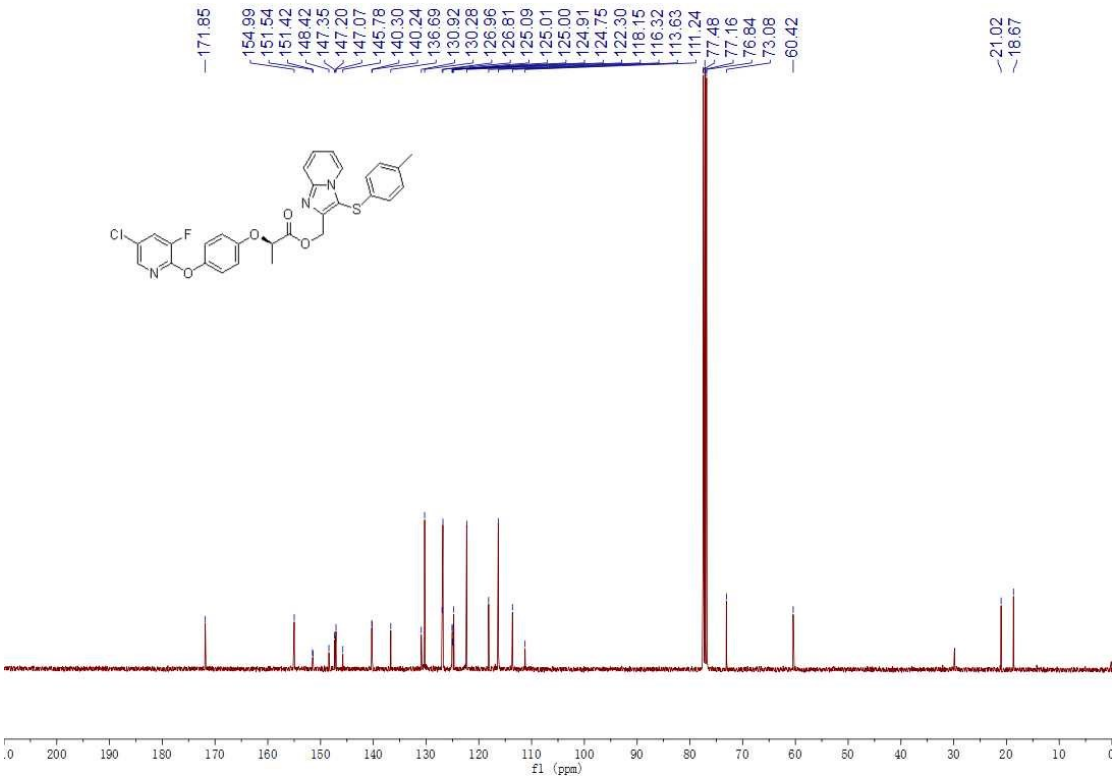
2-(pyridin-3-yl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4bk）

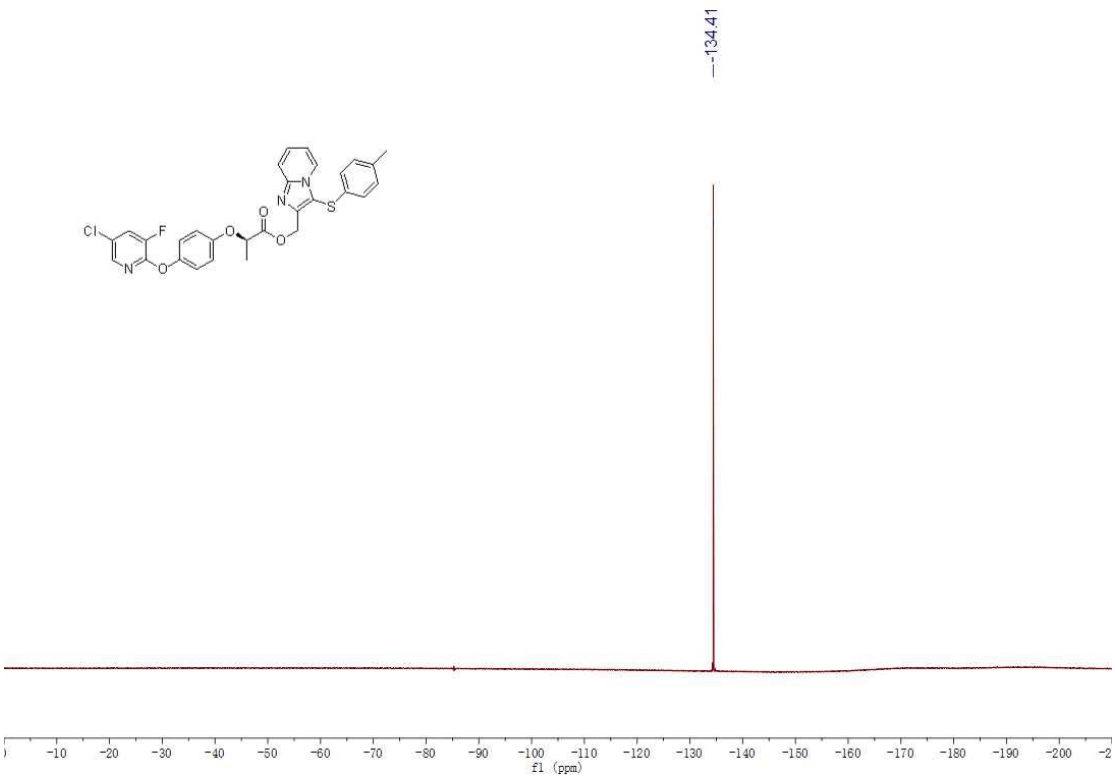




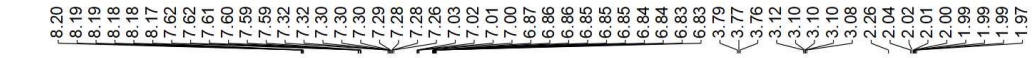
(3-(p-tolylthio)imidazo[1,2-a]pyridin-2-yl)methyl (R)-2-(4-((5-chloro-3-fluoropyridin-2-yl)oxy)phenoxy)propanoate（4bl）

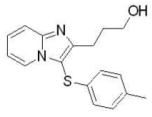


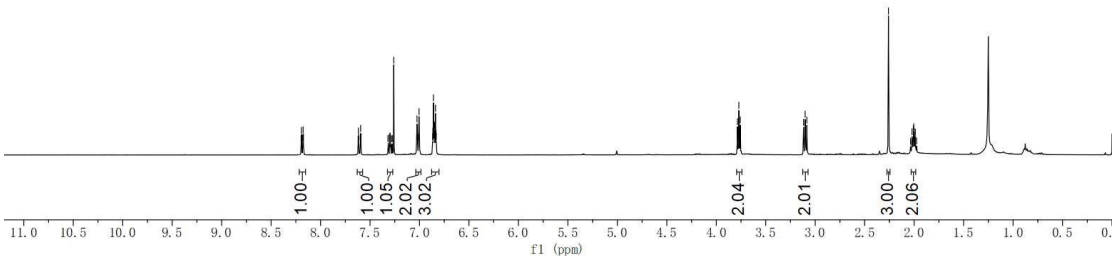


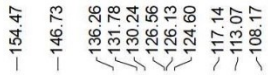

-134.41
Cl
F
N
O
O
O
N
N
S
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

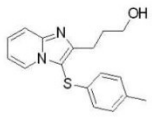
3-(3-(p-tolylthio)imidazo[1,2-a]pyridin-2-yl)propan-1-ol （4bm）



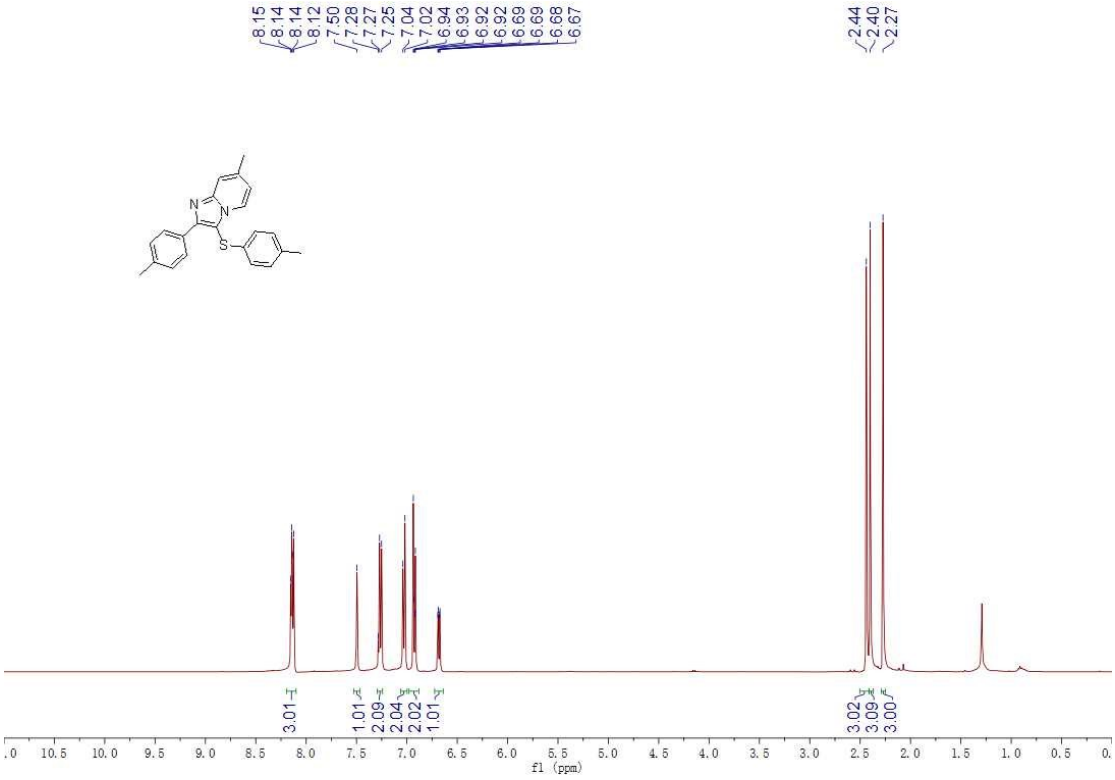


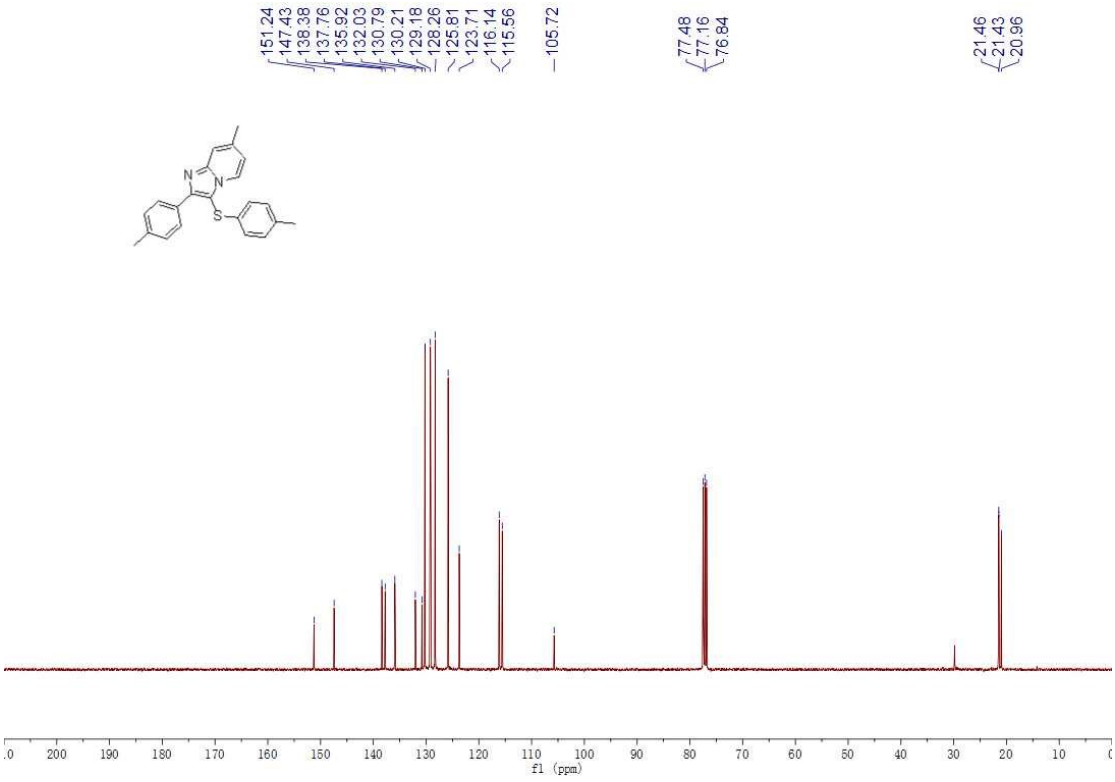




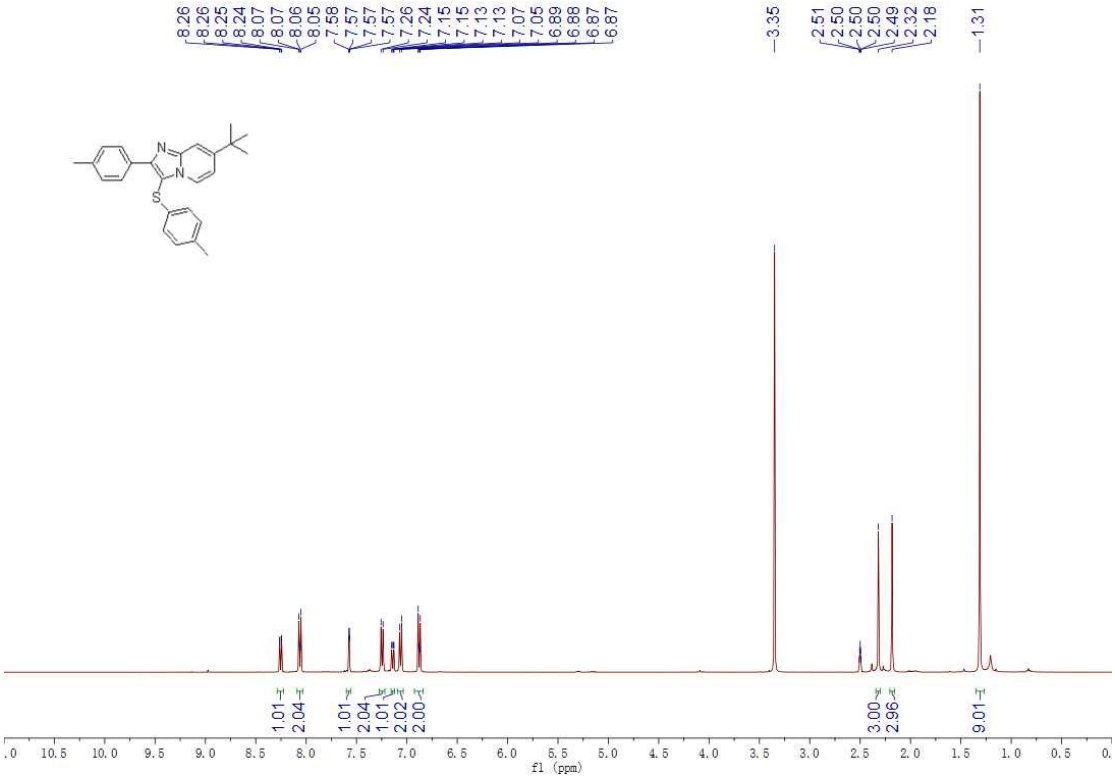


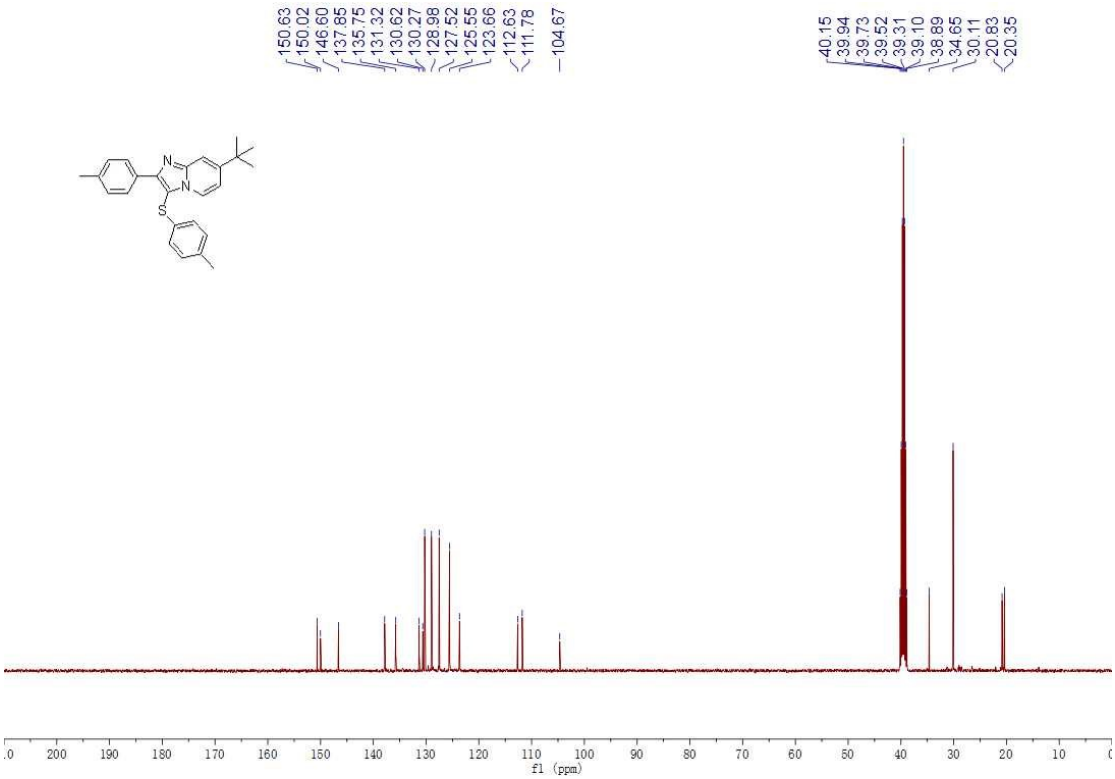
7-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4ca）



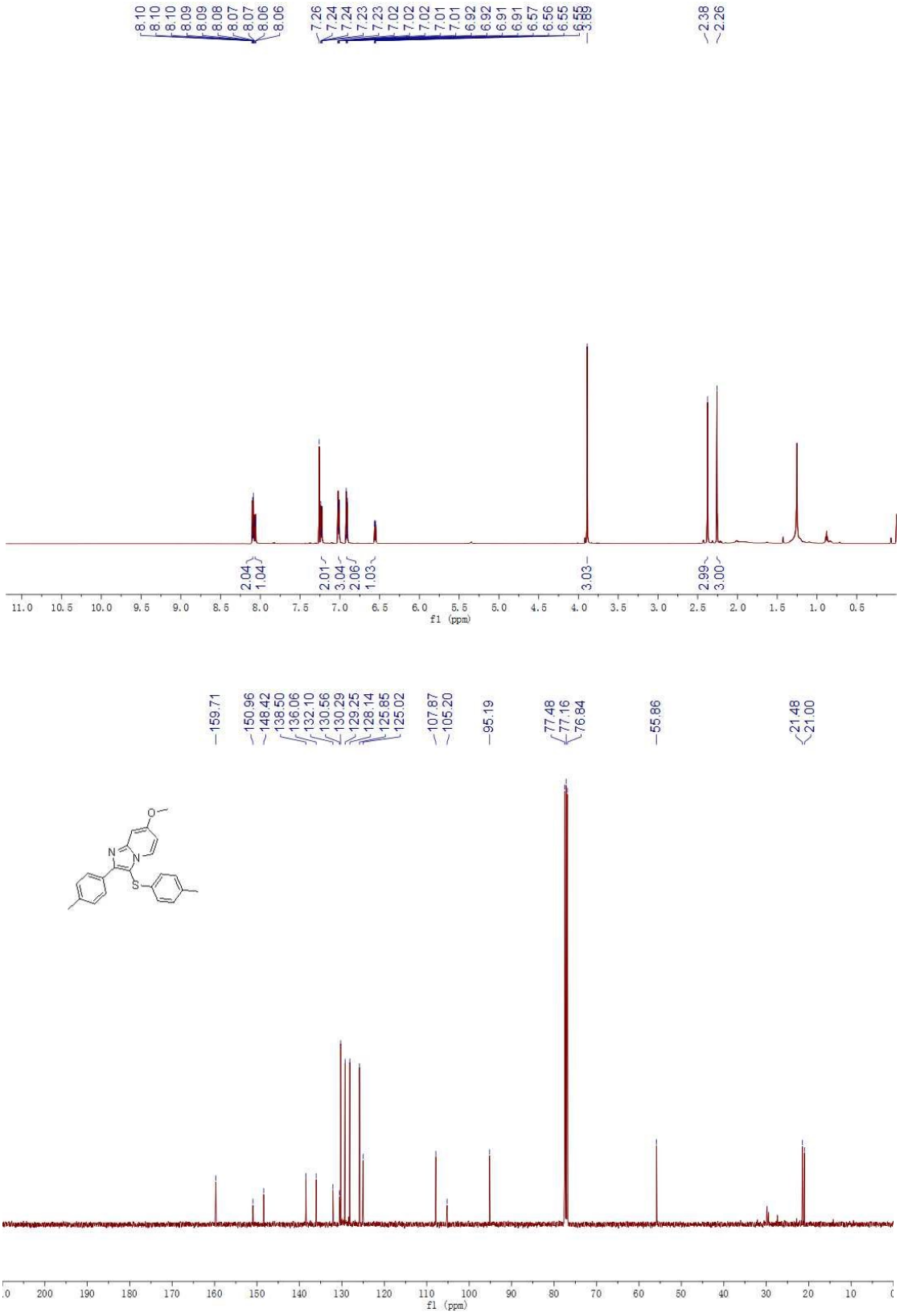


7-(tert-butyl)-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4cb）

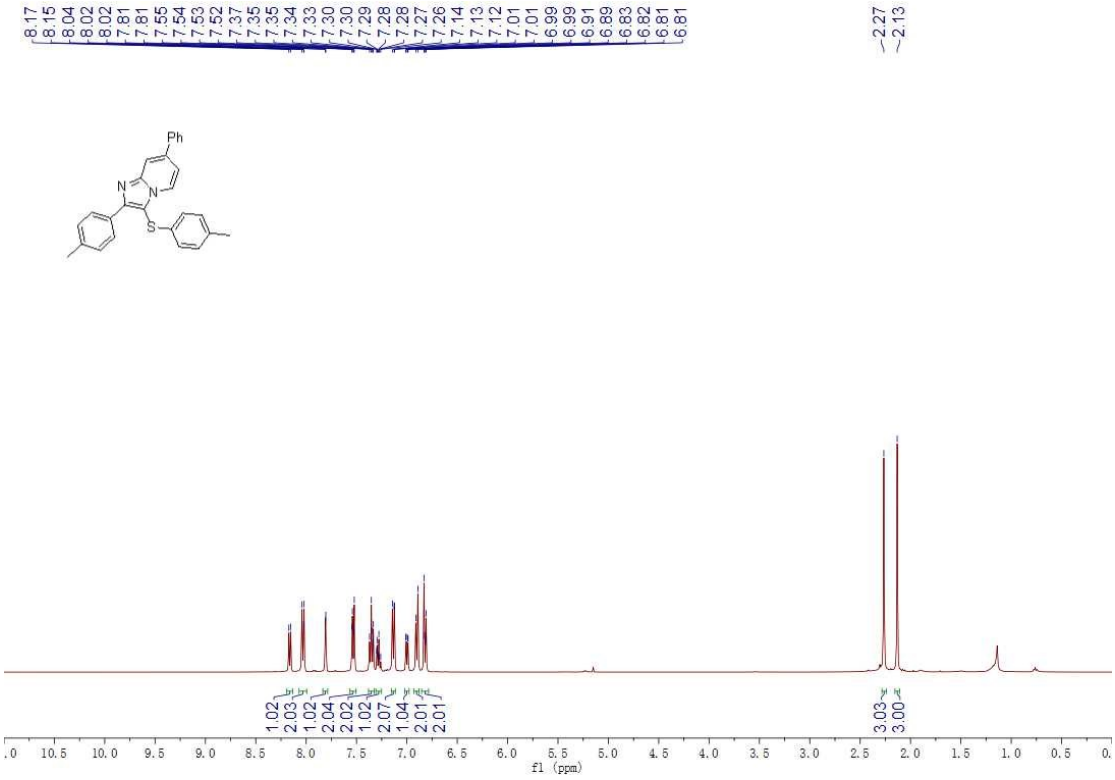


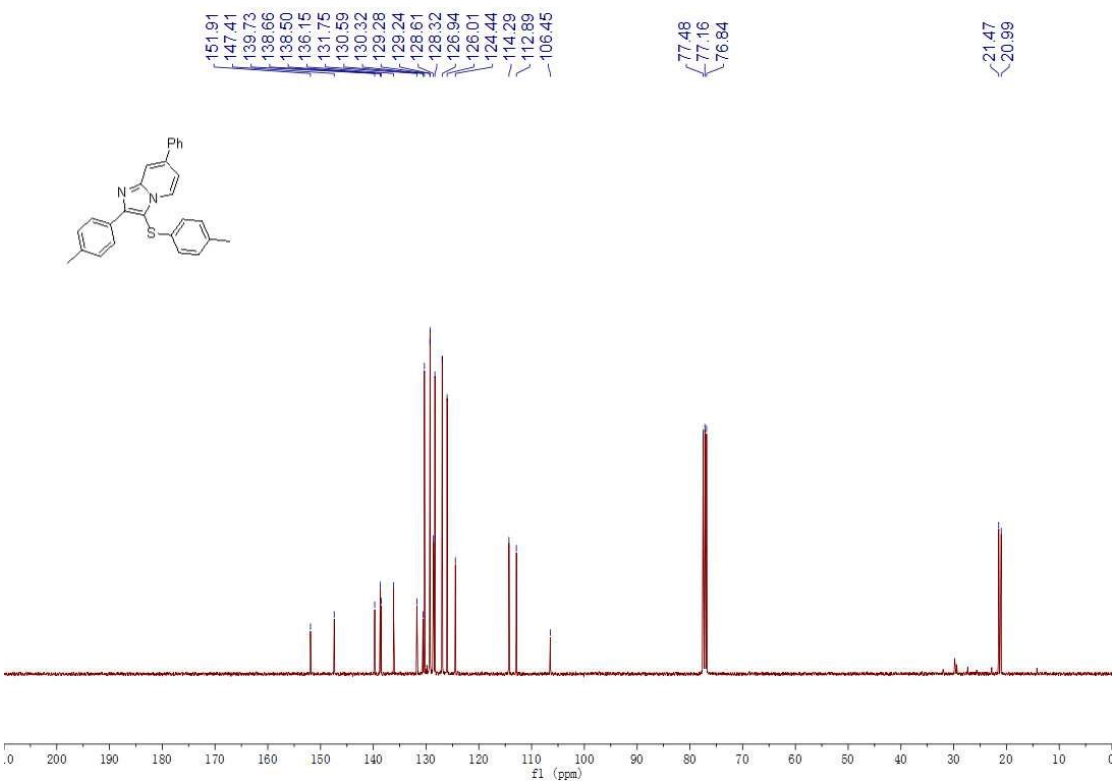


7-methoxy-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4cc）

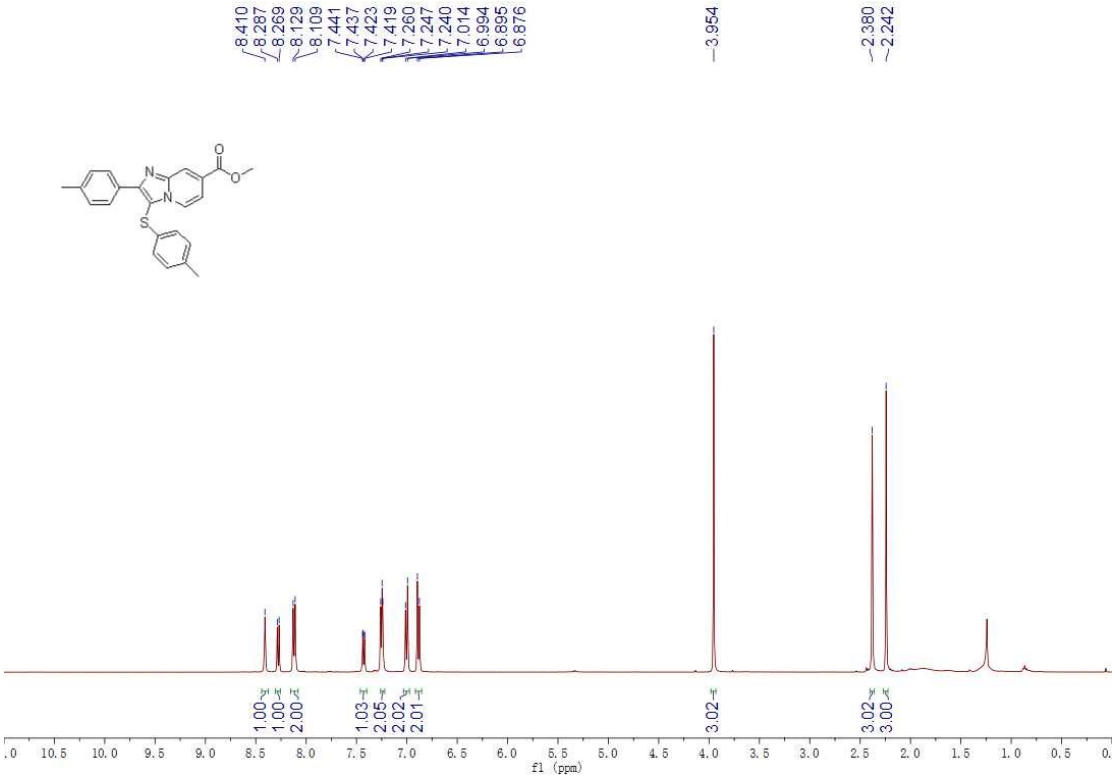


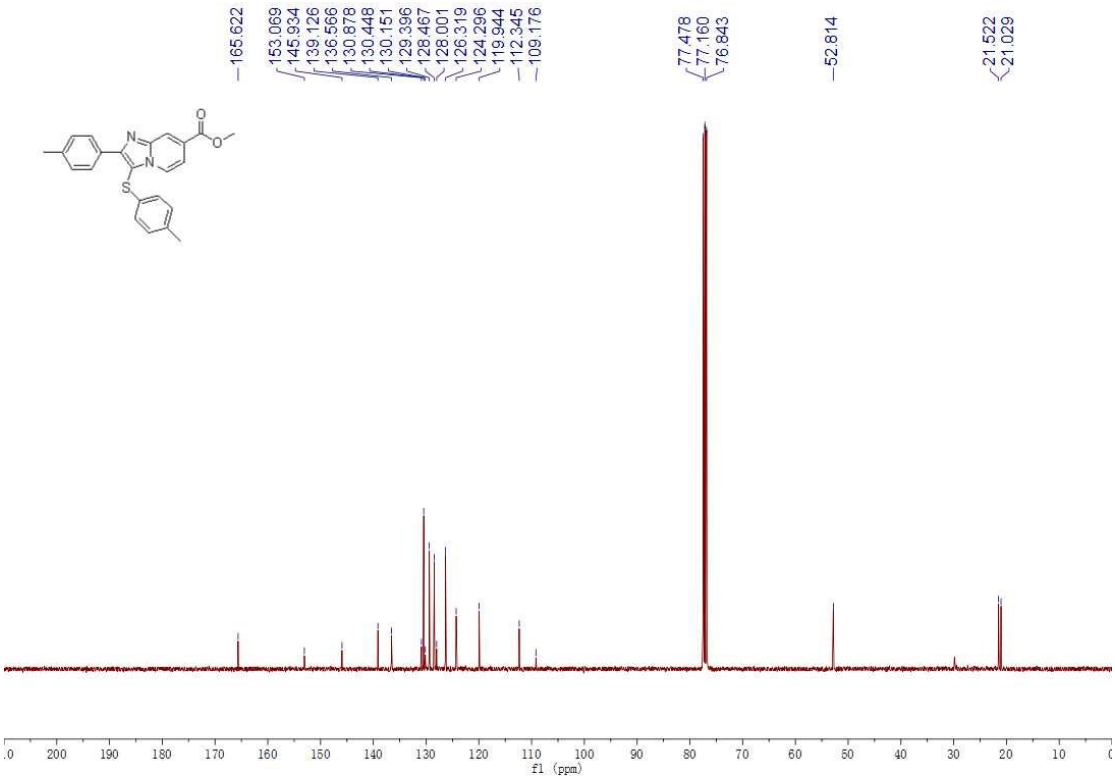
7-phenyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4cd）



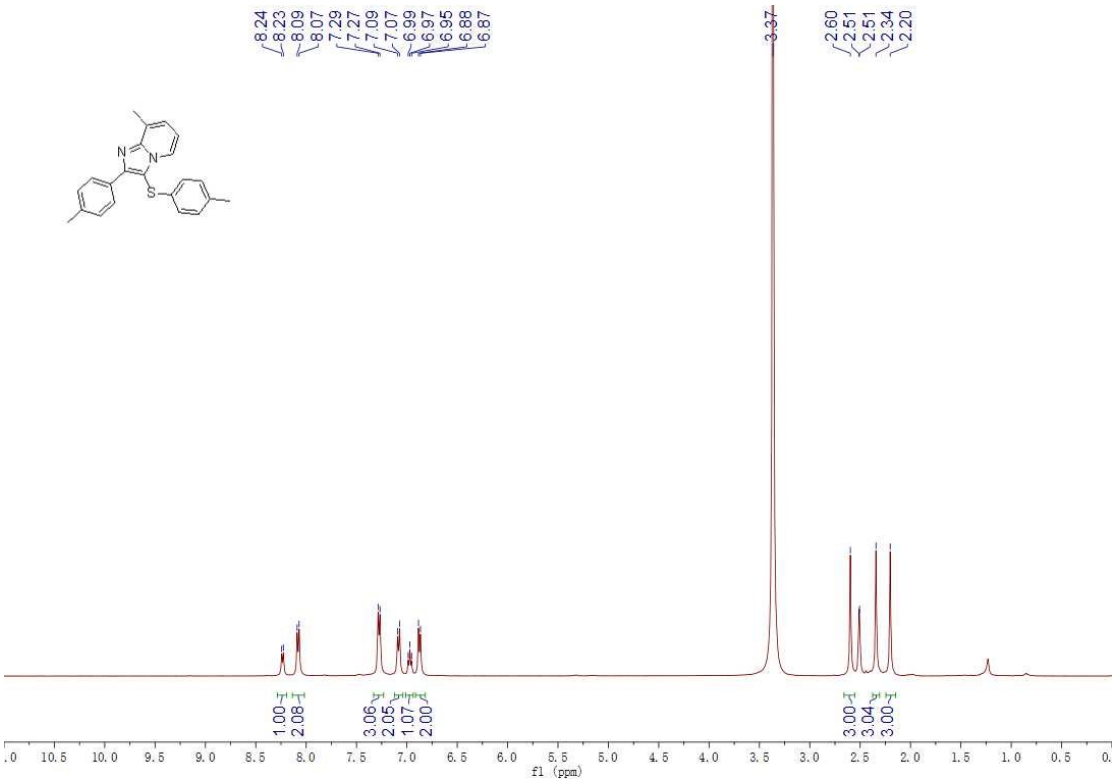


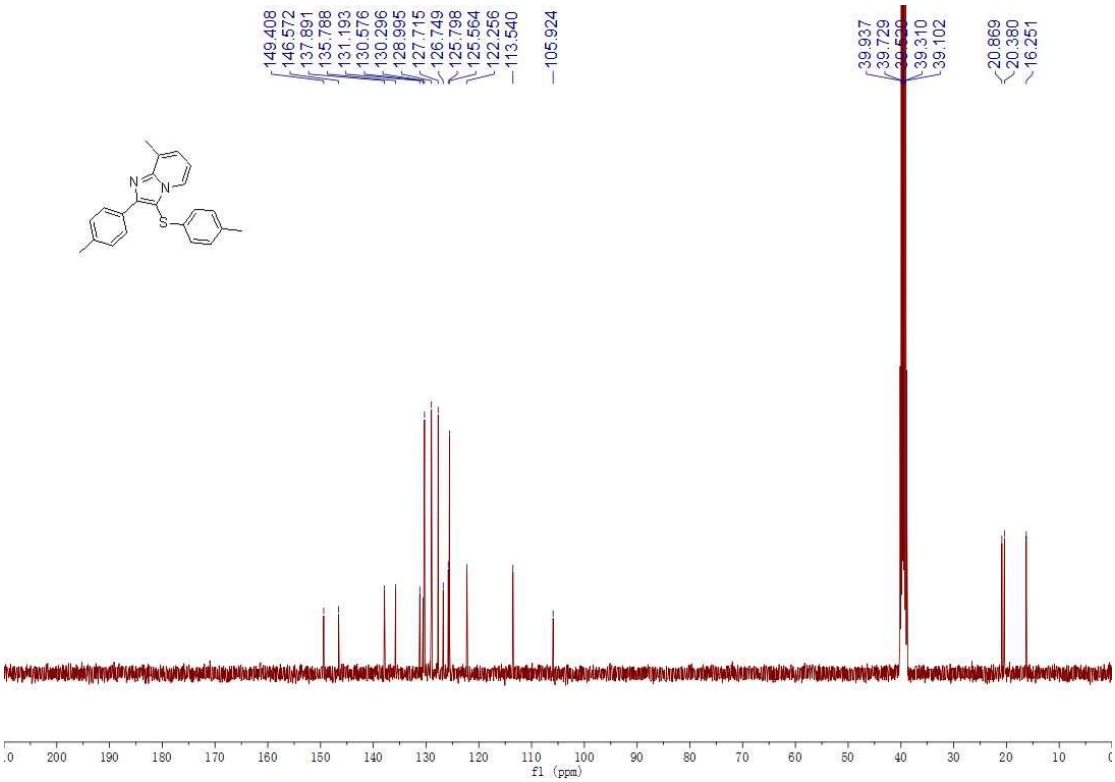
methyl 2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine-7-carboxylate（4ce）



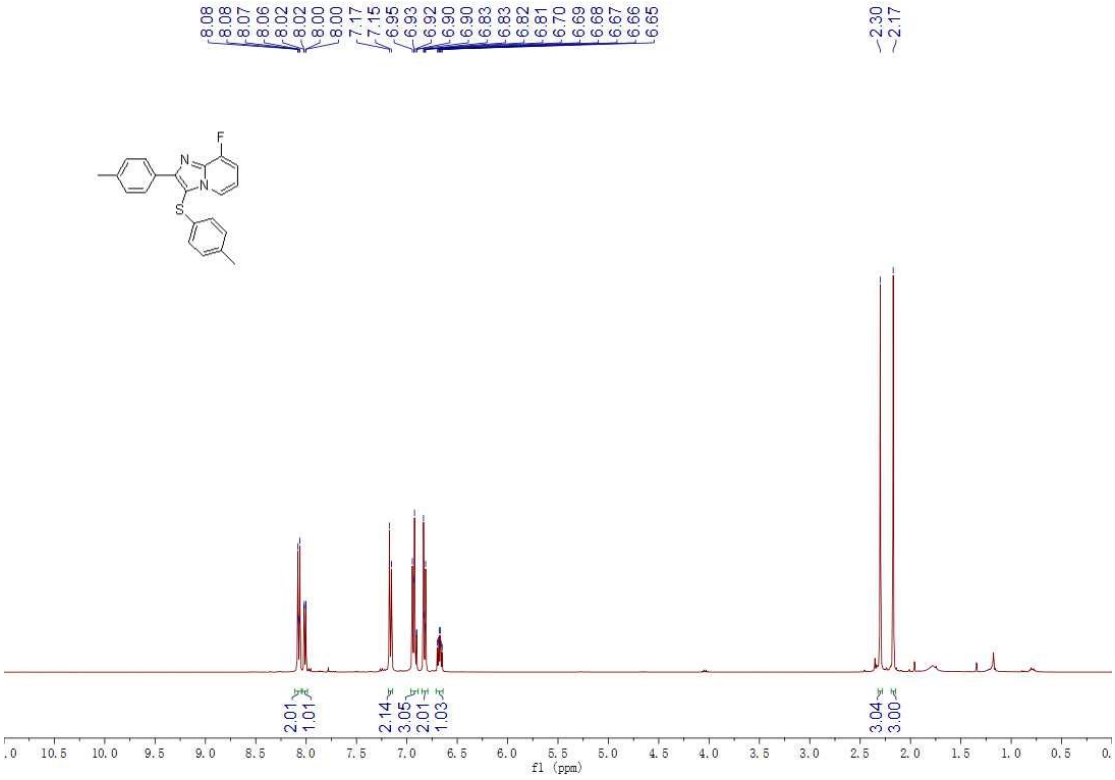


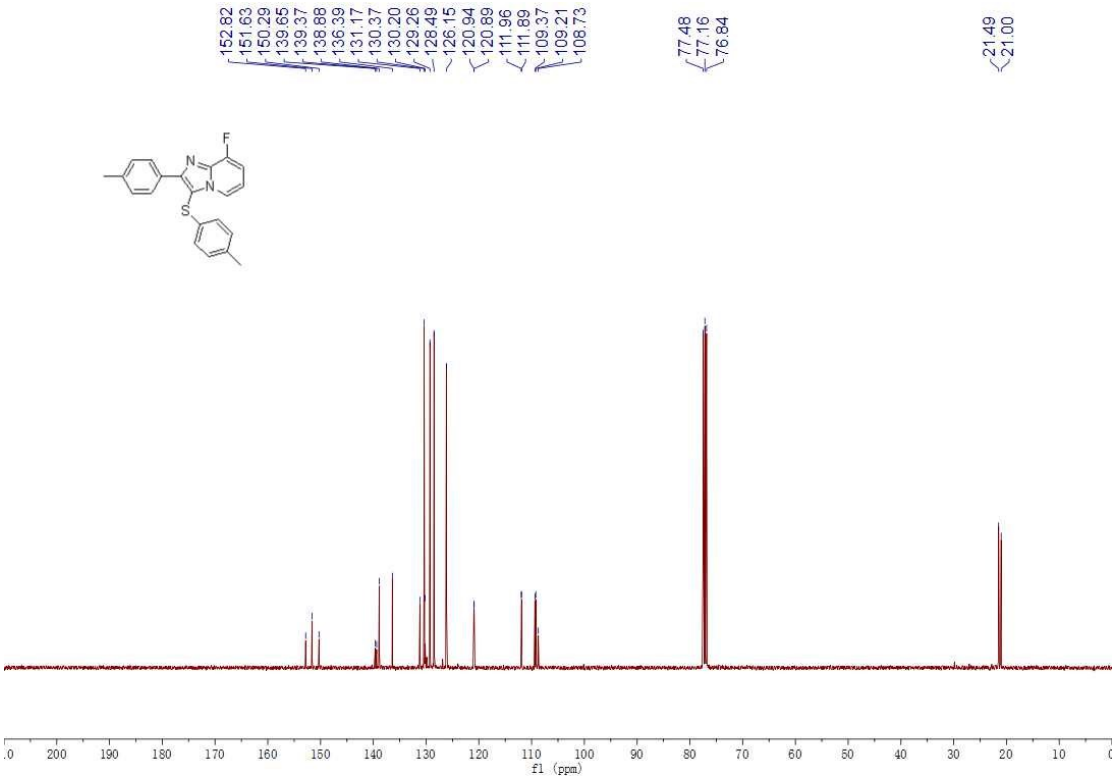
8-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4cf）

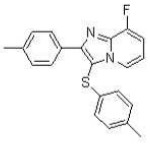




8-fluoro-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4cg）

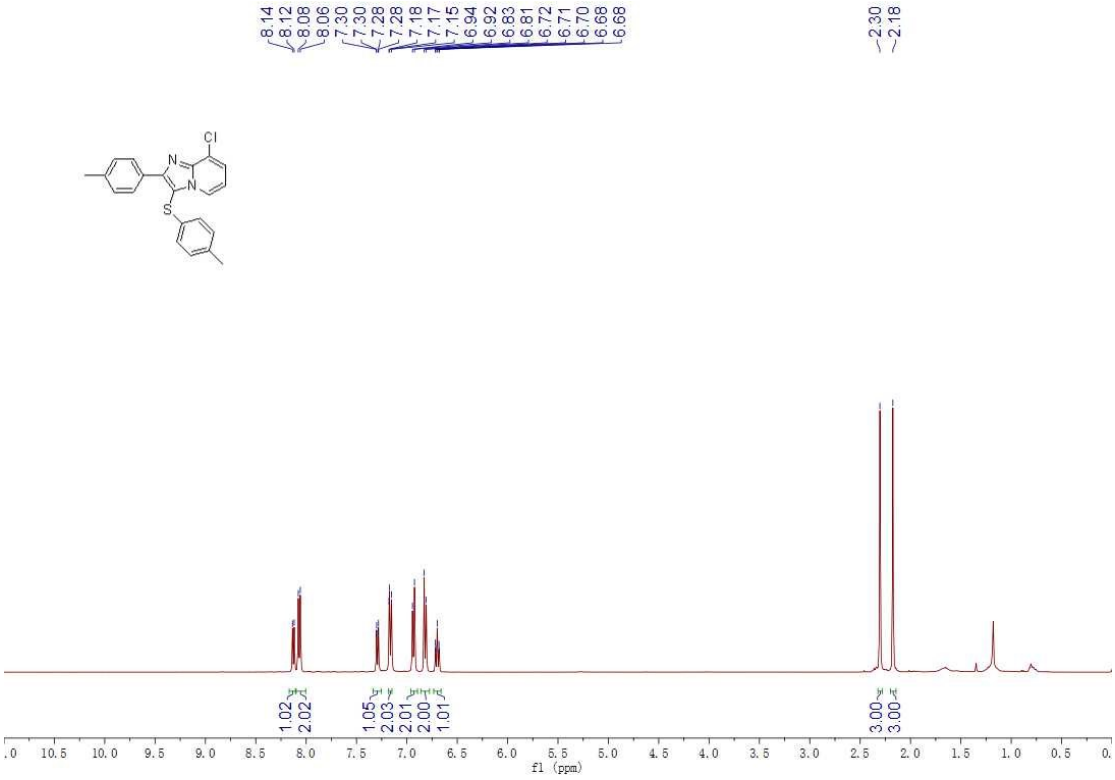


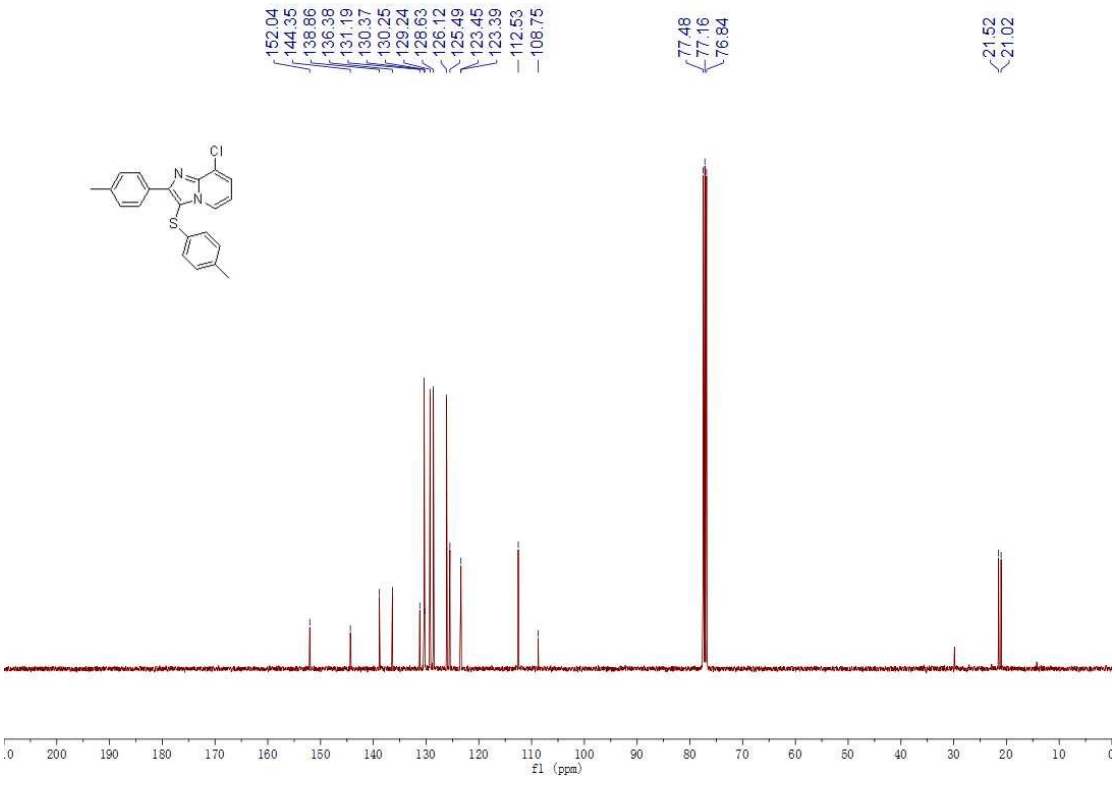



F
N
N
S

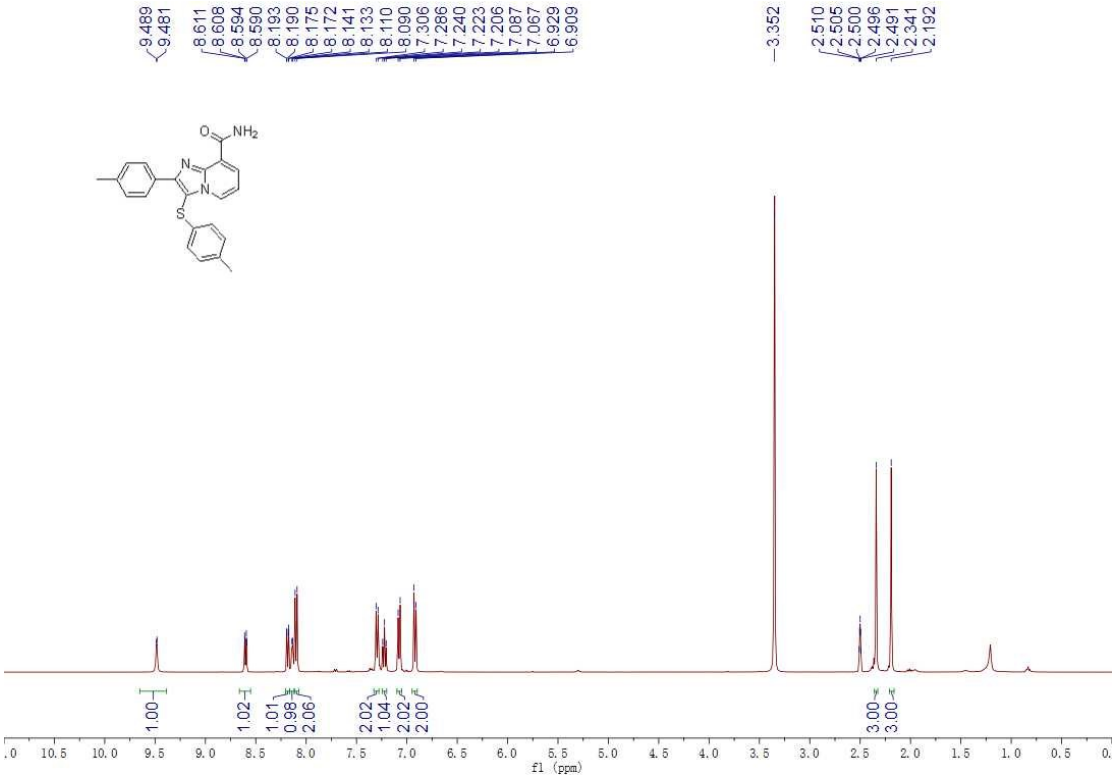
-130.30
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-2
f1 (ppm)

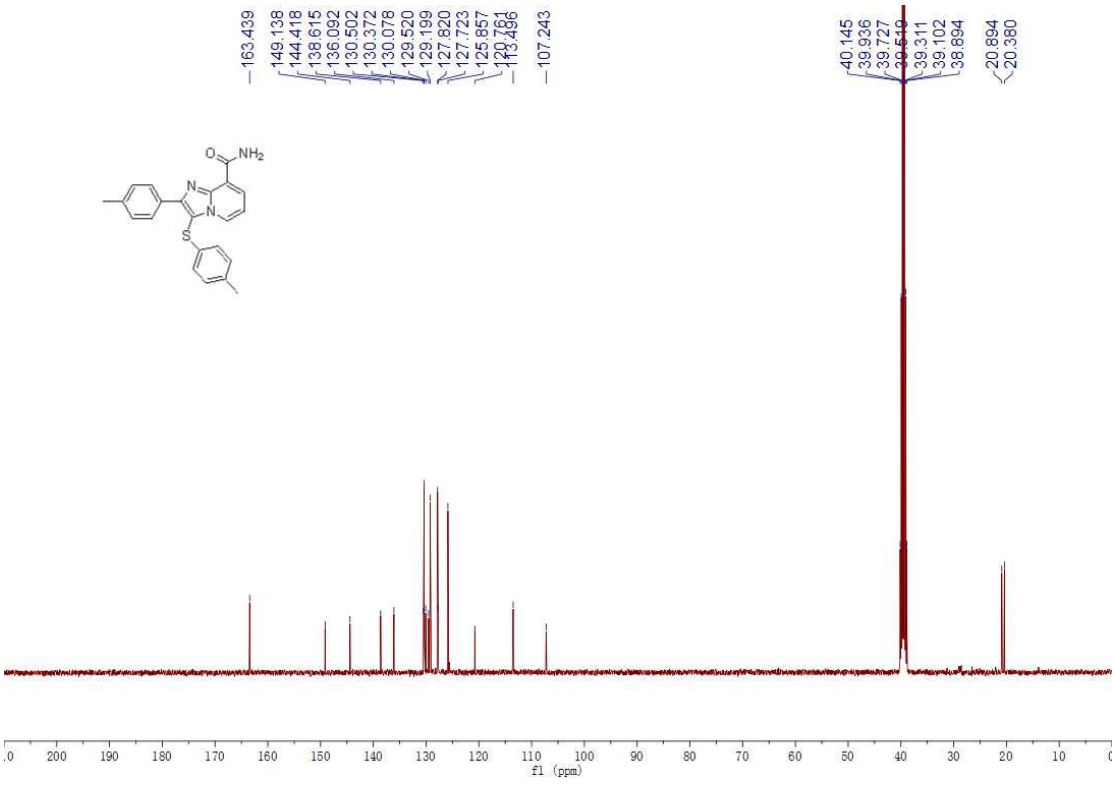
8-chloro-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine（4ch）



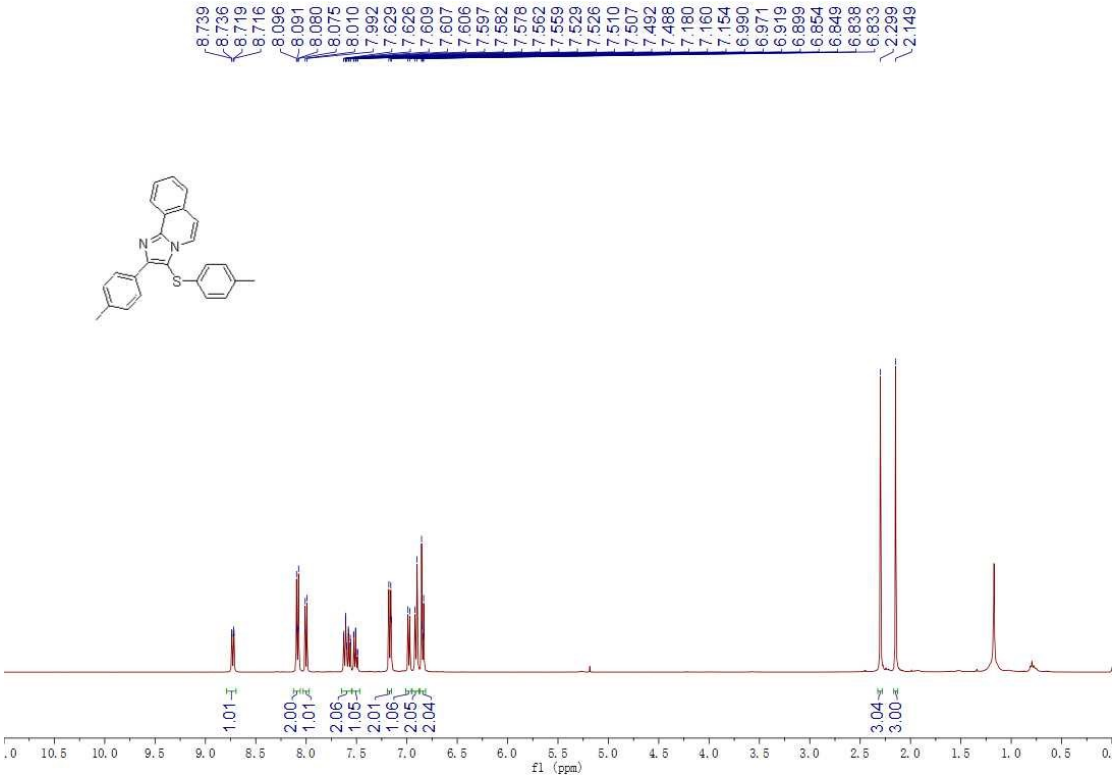


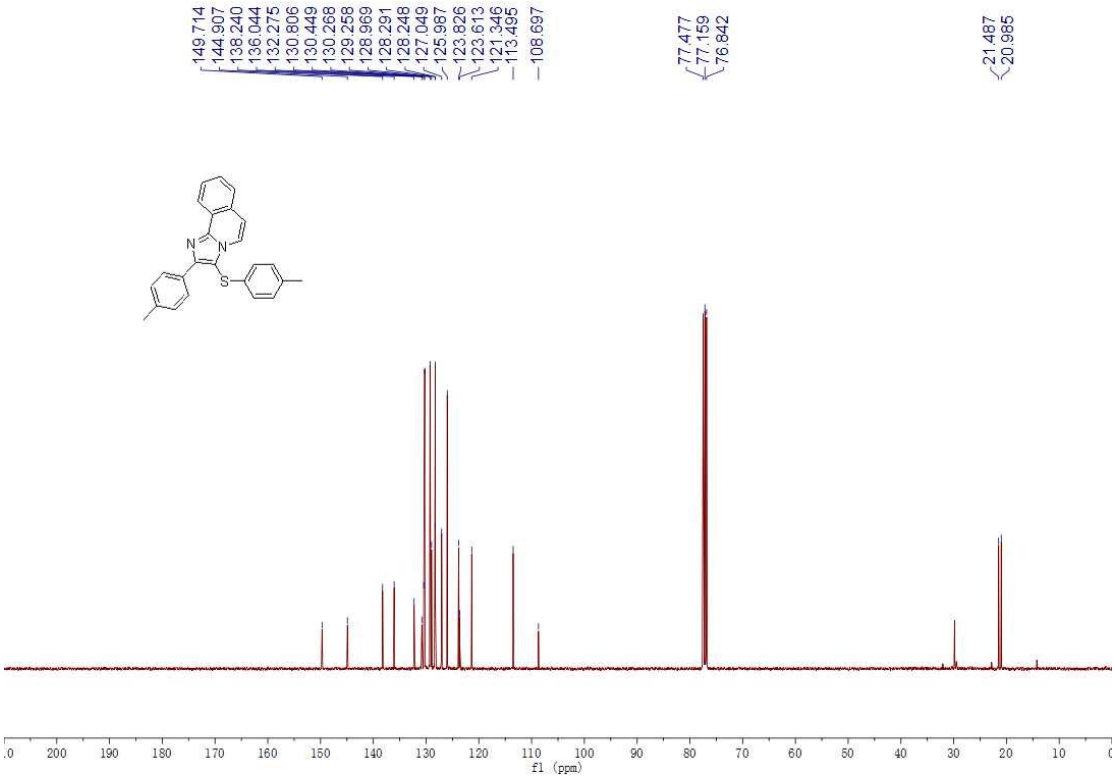
2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-a]pyridine-8-carboxamide（4ci）



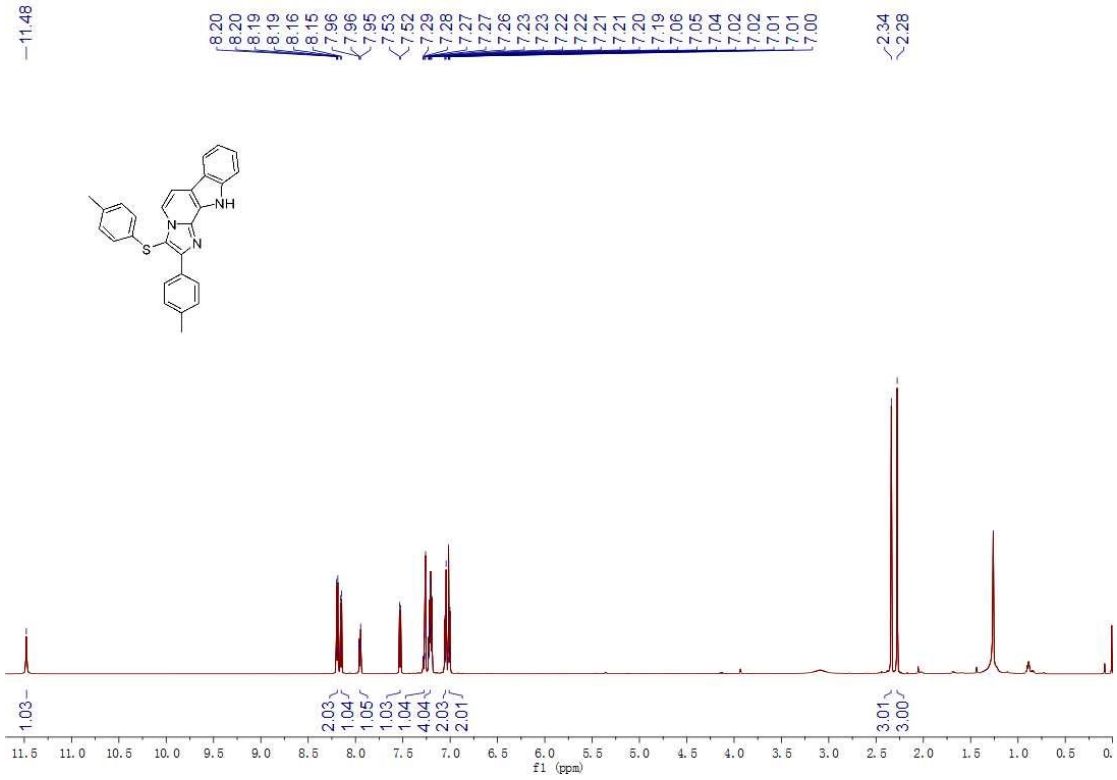


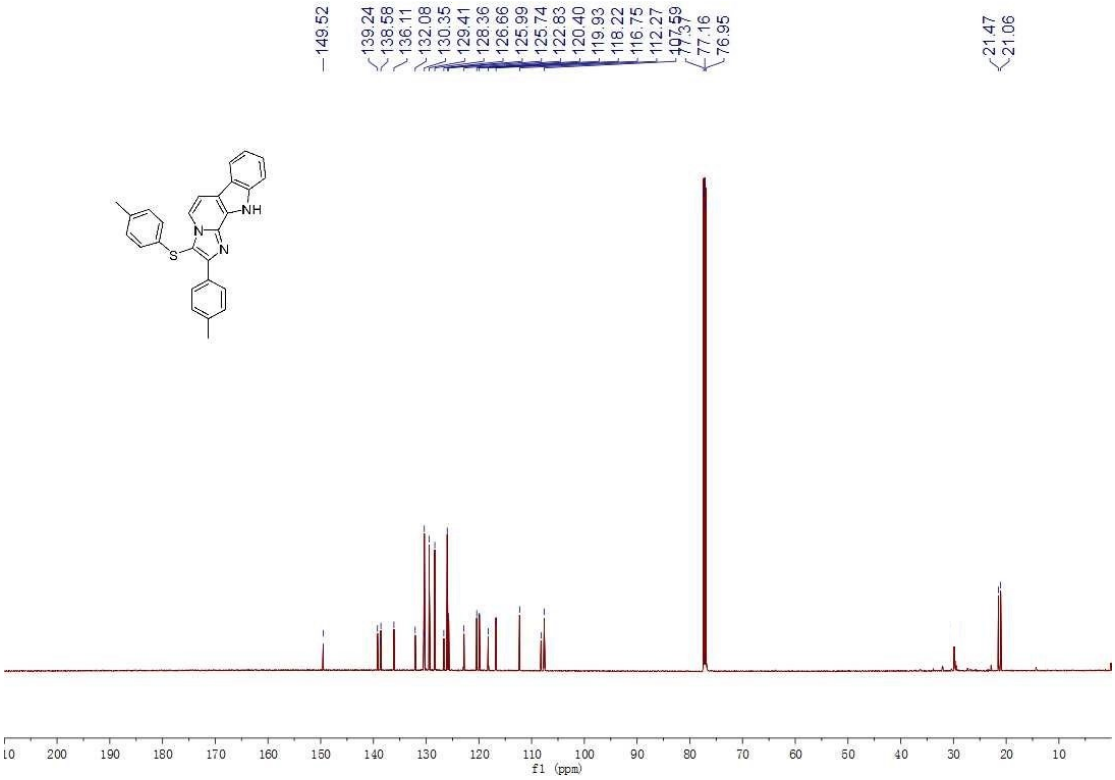
2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-b]isoquinoline（4cj）





2-(p-tolyl)-3-(p-tolylthio)-10H-imidazo[1',2':1,6]pyrido[4,3-b]indole（4ck）





6-methyl-2-(p-tolyl)-3-(p-tolylthio)imidazo[1,2-b]pyridazine（4cl）