Supporting Information for

Dearomative Cyclization of Pyridines/Isoquinolines with Cyclopropenones: Access to Indolizinones and Benzo-Fused Indolizinones

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1. General considerations

Unless otherwise noted, commercial reagents were purchased from Adamas, Alfa, Aladdin, TCI, *J&K* or Macklin and used without further purification. All reactions were carried out using oven-dried glassware and all reactions proceeded without special care. Column chromatography was performed on 200-300 mesh silica gel (Huanghai, China).

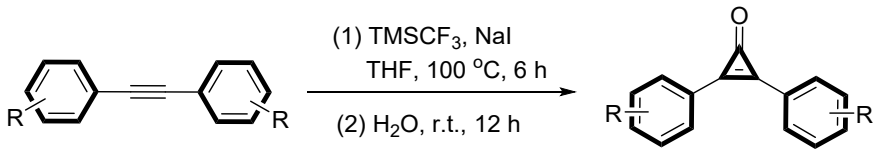
^{1}H, ^{19}F and $^{13}C\{^{1}H\}$ NMR spectra were recorded on an Bruker Ascend 400 MHz spectrometer at ambient temperature. ^{1}H NMR spectra are referred to the TMS signal (δ = 0 ppm) and ^{13}C NMR spectra are referred to the residual solvent signal (δ = 77.16 ppm). Data for ^{1}H NMR are reported as follows: chemical shifts (δ ppm), multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz), integration.

The data of HRMS was carried out on a waters G2-XS high-resolution mass spectrometer (HR-ESI-MS), or Thermo Fisher Scientific LTQ FTICR-MS, or Agilent 7250 GC/QTOF. Melting point were recorded using a SGW X-4 Melting Point Apparatus. X-ray diffraction data were collected on SuperNova, Dual, Cu at zero, AtlasS2.

2. Experimental procedures and characterization data

2.1 Experimental procedures

Synthesis of compounds 2 according to the following procedure[1]:

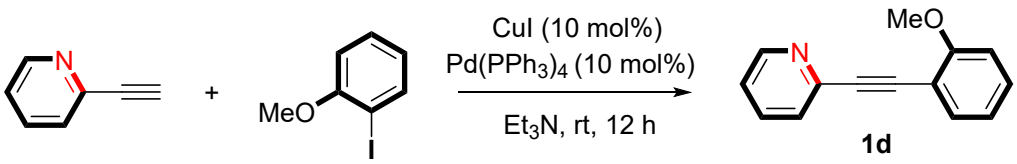


To an oven-dried Schlenk tube containing a stir bar was added NaI (1.65 g, 11 mmol, 2.2 equiv). A solution of diphenylacetylene (5.0 mmol, 1.0 equiv) in anhydrous THF (10.0 mL) was then added against positive N_2 flow. Trifluoromethyltrimethylsilane (1.42 g, 10.0 mmol, 2 equiv) was added, and the Schlenk tube was sealed. The reaction was stirred vigorously at 100 °C with a heating mantle for 6 h, then diluted with H_2O (10.0 mL) and stirred at room temperature for 12 h. The mixtures were extracted with CH_2Cl_2 (3 x 10 mL) and the combined organic layers were dried over $MgSO_4$ and filtered. The filtrate was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 5: 1) to give 2,3-diphenyl-2-cyclopropen-1-one as a yellow solid.

Compounds **2** were known compounds and synthesized according to the known procedures, and their NMR data were in agreement with those described in the literature.[1]

Synthesis of products 1 and 5 according to the following procedure[2]:

As exemplified for **1d**:

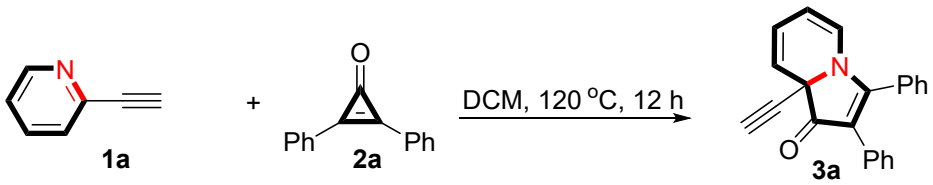


A pressure tube was charged with 2-ethynylpyridine (309.1 mg, 3.0 mmol, 1.0 equiv), 1-iodo-2-methoxybenzene (772.0 mg, 3.3 mmol, 1.1 equiv), CuI (57.0 mg, 0.3 mmol, 10 mol%), $Pd(PPh_3)_4$ (346.3 mg, 0.3 mmol, 10 mol%) and Et_3N (10.0 mL). The mixtures were stirred at room temperature for 12 h. The solution was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 20: 1) to give product **1d** in 78% yield (489.3 mg).

Compounds **1** and **5** were known compounds and synthesized according to the known procedures, and their NMR data were in agreement with those described in the literature.[2]

Synthesis of products 3 according to the following procedure:

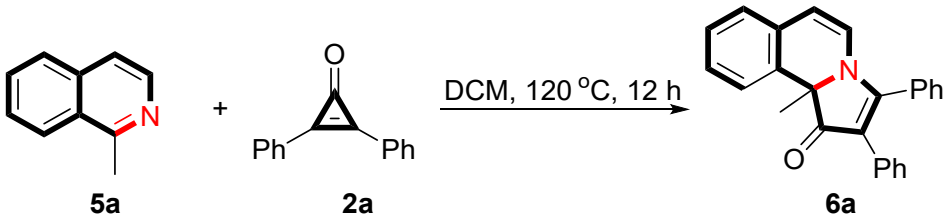
As exemplified for **3a**:



A pressure tube was charged with 2-ethynylpyridine (30.9 mg, 0.30 mmol, 1.0 equiv), 2,3-diphenyl-2-cyclopropen-1-one (61.8 mg, 0.30 mmol, 1.0 equiv) and DCM (3.0 mL). The mixtures were heated with a heating mantle at 120 °C for 12 h, then cooled to room temperature. The solution was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 7: 1) to give product **3a** in 80% yield (74.2 mg).

Synthesis of products 6 according to the following procedure:

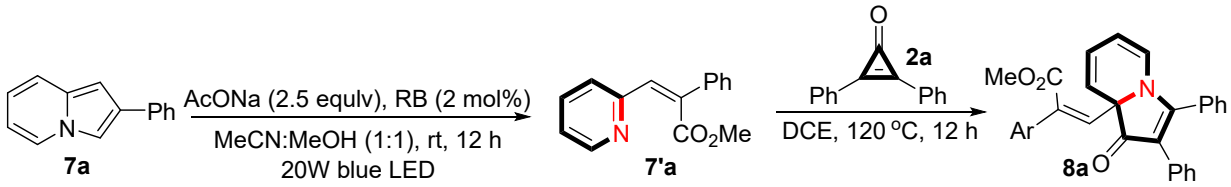
As exemplified for **6a**:



A pressure tube was charged with 1-methylisoquinoline (42.9 mg, 0.30 mmol, 1.0 equiv), 2,3-diphenyl-2-cyclopropen-1-one (61.8 mg, 0.30 mmol, 1.0 equiv) and DCM (3.0 mL). The mixtures were allowed to stir at 120 °C with a heating mantle for 12 h, then cooled to room temperature. The solution was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 1: 1) to give product **6a** in 78% yield (81.7 mg).

Synthesis of products 8 according to the following procedure:

As exemplified for **8a**:



A pressure tube was charged with a stirring bar, 2-phenylindolizine (57.9 mg, 0.30 mmol, 1.0 equiv), AcONa (61.5 mg, 075. mmol, 2.5 equiv), RB (6.1 mg, 0.006 mmol, 2 mol%) and MeCN (2.0 ml) : MeOH (2,0 ml) were added. The reaction was stirred at room temperature under irradiation of blue LED for 12 h. The solution was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 7: 1) to give product **7'a** in 75% yield.[3]

A pressure tube with 3.0 mL DCM was charged with a stirring bar, methyl (*Z*)-2-phenyl-3-(pyridin-2-yl)acrylate (71.1 mg, 0.30 mmol, 1.0 equiv), 2,3-diphenyl-2-cyclopropen-1-one (67.9 mg, 0.33 mmol, 1.1 equiv) were added. The reaction was heated with a heating mantle at 120 °C for 12 h, then cooled to room temperature. The solution was concentrated in vacuo, and the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 7: 1) to give product **8a** in 70% yield (85.7 mg).

2.2 Plausible mechanistic pathway

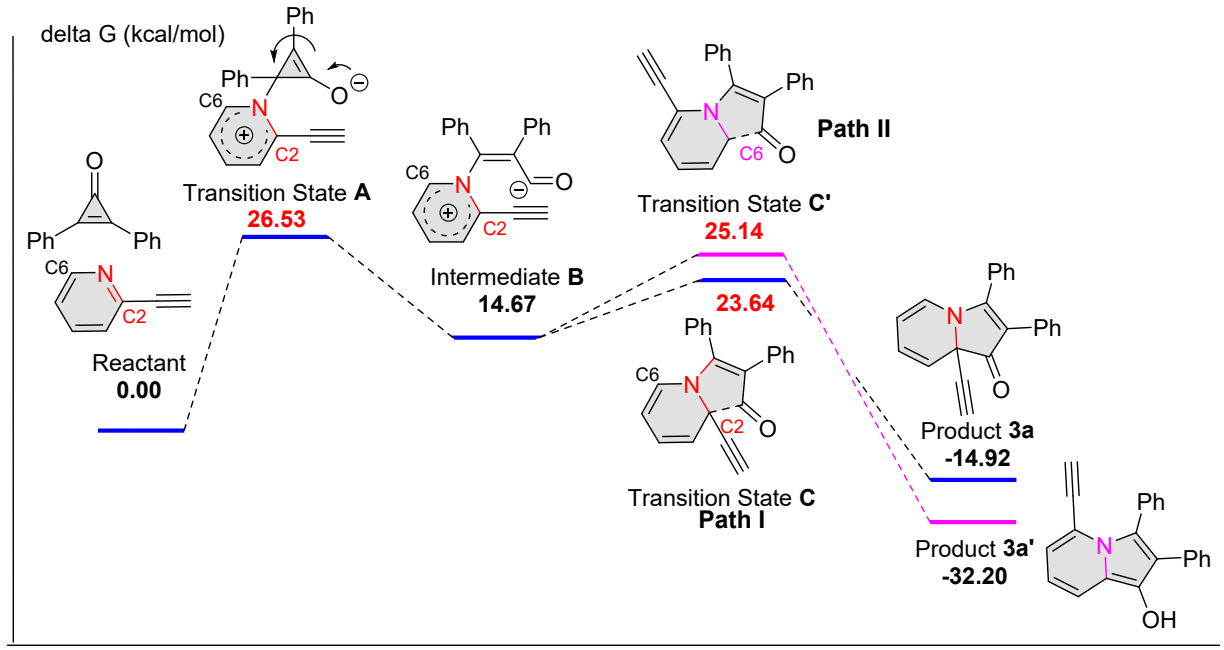


Figure S1 Plausible mechanistic pathway

2.3 DFT calculations

Computational methods

All calculations were conducted with Gaussian 03, Revision E.01 package.[4] Each structure was optimized in gas phase at the M062X/6-31G* level of theory. Analytical frequency calculations were performed at the same level of theory to ensure that all stationary points were either intermediates without any imaginary frequencies or transition states possessing only one

imaginary frequency. The Gibbs free energy was then refined based on single point calculations at the same functional, which was conducted in the presence of solvent through the SMD[5] method with dichloroethane. All listed energies are free energies at a concentration of 1 M. All three-dimensional structures of the species were generated using Molecular Operating Environment (MOE 2008.10) program.

Reactant

E = -976.554664 a.u.

C	0.04799900	-0.01846900	1.37979700
C	-1.25259000	0.34539500	1.23246000
C	-0.35765600	1.25854000	1.86766100
O	-0.10484400	2.32036600	2.39102200
C	1.10316600	-0.95023400	1.02927100
C	2.39179800	-0.73198000	1.52787400
C	3.43444100	-1.57155200	1.15179300
C	3.19681000	-2.62318400	0.26914800
C	1.91468300	-2.84027600	-0.23739600
C	0.86892300	-2.00857500	0.14099900
C	-2.54096200	-0.00127200	0.65897400
C	-3.43693700	1.01868000	0.32335500
C	-4.64627900	0.70571000	-0.28688900
C	-4.97622800	-0.62402700	-0.54367900
C	-4.09554200	-1.64591100	-0.18771400
C	-2.87895800	-1.33634500	0.40737900
H	2.56043700	0.10544400	2.19898900
H	4.43359900	-1.40305300	1.54153600
H	4.01265500	-3.27604200	-0.02667600
H	1.73504900	-3.65471400	-0.93243900
H	-0.12480000	-2.14144000	-0.27685700
H	-3.16185400	2.04915000	0.52658300
H	-5.33469300	1.49929800	-0.55975400

H	-5.92432400	-0.86555900	-1.01463200
H	-4.35900500	-2.68220400	-0.37595900
H	-2.18714100	-2.12406200	0.69287000
C	3.34368300	0.91487600	-1.39178100
C	2.19502500	0.36312700	-1.94334600
C	0.96033800	0.92443100	-1.60001700
N	0.83100600	1.97326600	-0.77575400
C	1.94254900	2.48370500	-0.24882900
C	3.21931000	1.99485800	-0.52382200
C	-0.26740900	0.33656500	-2.07697600
C	-1.30346200	-0.16873600	-2.43238500
H	4.31882000	0.49746100	-1.62420200
H	2.23225300	-0.49501100	-2.60515700
H	1.79580200	3.30823600	0.44435200
H	4.08847400	2.44818000	-0.05924100
H	-2.23976200	-0.59341200	-2.72258200

Transition State A (Transition State A')

E = -976.512380 a.u.

C	2.48589700	-3.47477100	-0.72358400
C	2.60469700	-2.99538800	0.57605400
C	1.93422400	-1.83443100	0.92748400
N	1.17565100	-1.16885200	0.03911700
C	1.03696600	-1.62133400	-1.22732600
C	1.69287700	-2.78449300	-1.63055700
C	-0.99546700	-0.03576100	0.95480900
C	0.42278400	0.10385800	0.61558500
C	-0.14199700	-0.21774200	1.98017100
O	0.26213100	-0.48931700	3.11409500
C	0.21028400	-0.90908700	-2.14885000
C	-0.46771600	-0.40352300	-3.00657300

C	-2.36260900	0.06194700	0.48732100
C	-3.39197200	-0.43344600	1.30553700
C	-4.72135900	-0.33759500	0.91585700
C	-5.06054400	0.24943600	-0.30250700
C	-4.04987800	0.74913800	-1.11993000
C	-2.71864600	0.66099900	-0.72893500
C	1.23280200	1.31184800	0.25008100
C	2.37011200	1.62207900	1.00553600
C	3.13059700	2.75046300	0.71540100
C	2.76035700	3.58937000	-0.33351000
C	1.62202000	3.29951600	-1.08085700
C	0.86503400	2.16827800	-0.78998600
H	2.99977400	-4.38025000	-1.02898300
H	3.20167100	-3.50851100	1.32027800
H	1.93164000	-1.42105600	1.93319600
H	1.56476700	-3.12337300	-2.65153600
H	-1.08872100	0.06031000	-3.74205600
H	-3.12639900	-0.89189200	2.25395700
H	-5.49937100	-0.72590000	1.56699900
H	-6.09995100	0.32272700	-0.60708100
H	-4.30140100	1.22368500	-2.06485800
H	-1.94079800	1.07484800	-1.36126000
H	2.63145200	0.98869400	1.84990200
H	4.00446000	2.98387900	1.31633100
H	3.35038400	4.47230600	-0.55997600
H	1.32051900	3.95783200	-1.89023300
H	-0.02542200	1.94704200	-1.36859400

Intermediate B (Intermediate B')

E = -976.531283 a.u.

C	4.21907900	-1.75707600	0.41386400

C	3.01419000	-2.37622300	0.68380300
C	1.79299200	-1.71780100	0.53630800
N	1.73881500	-0.41899200	0.01723000
C	2.95893700	0.19715800	-0.22597200
C	4.15889400	-0.42800100	-0.02922500
C	-0.57245300	-0.54726300	-0.80555900
C	0.55640500	0.23140100	-0.26877000
C	-0.27479700	-1.13815200	-1.96054200
O	0.06818900	-1.67260900	-2.93735400
C	0.59829700	-2.32130900	1.00798700
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C	-1.92707200	-0.62187400	-0.22336100
C	-2.16761900	-0.07459700	1.04102900
C	-3.43458800	-0.14892400	1.61099600
C	-4.47960800	-0.77325800	0.93516800
C	-4.24627200	-1.31909700	-0.32600300
C	-2.98549400	-1.23760900	-0.90325200
C	0.45144700	1.68369500	-0.16123800
C	1.18263200	2.42751000	0.78969000
C	0.99185000	3.79328900	0.93525100
C	0.05797600	4.46782200	0.14909800
C	-0.68795600	3.74628300	-0.77861600
C	-0.49810900	2.37829200	-0.93272300
H	5.16313300	-2.26959300	0.54776800
H	2.97084800	-3.38945500	1.06775600
H	2.88403000	1.19048800	-0.64390500
H	5.05908300	0.12747500	-0.26891300
H	-1.28169300	-3.28566500	1.85125300
H	-1.35124700	0.40213400	1.57557100
H	-3.60297400	0.28464900	2.59245100

H	-5.46657200	-0.83211100	1.38309300
H	-5.05173700	-1.80809300	-0.86592300
H	-2.82012400	-1.66002000	-1.89279700
H	1.89547000	1.92035000	1.43534600
H	1.56806400	4.33447000	1.68028400
H	-0.09091400	5.53638200	0.26622800
H	-1.42688700	4.25197100	-1.39333800
H	-1.09181200	1.82873600	-1.65661000

Transition State C

E = -976.516999 a.u.

C	4.42163700	0.19245700	-1.08791000
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C	2.62251900	-0.76729300	0.23648300
N	1.82436400	0.38830500	-0.01036700
C	2.50210900	1.54525800	-0.45398200
C	3.73150500	1.44097800	-1.00751800
C	-0.12577000	-1.01356100	-0.06028200
C	0.48962500	0.27906400	0.02393400
C	0.57536500	-2.16000000	-0.28273500
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C	2.36486200	-1.48309000	1.43599600
C	2.10920800	-2.11412700	2.43744600
C	-1.60446600	-1.21522700	-0.10065700
C	-2.41161800	-0.68089200	0.91155900
C	-3.78708600	-0.87537600	0.89017500
C	-4.37794000	-1.62372000	-0.12668300
C	-3.58096400	-2.17086500	-1.12699700
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C	-0.95359000	3.59652800	1.10819200
C	-1.90758500	3.81976600	0.11747800
C	-2.07532200	2.88997800	-0.90621200
C	-1.29560800	1.73949800	-0.94122800
H	5.37838400	0.11783400	-1.58895100
H	4.41579400	-1.79911700	-0.29077300
H	1.94604600	2.46940400	-0.39779600
H	4.19071400	2.34973600	-1.38250700
H	1.91691900	-2.65008200	3.33903100
H	-1.95157400	-0.10836000	1.71170500
H	-4.39978300	-0.44883300	1.67867600
H	-5.45214800	-1.77925500	-0.13683200
H	-4.03026000	-2.75447900	-1.92483000
H	-1.58854300	-2.37525900	-1.91379100
H	0.56719100	2.26148300	1.85125900
H	-0.82210000	4.31554400	1.91077900
H	-2.52004900	4.71563100	0.14435800
H	-2.81717600	3.05961500	-1.68010200
H	-1.43130000	1.00880200	-1.73280500

Product 3a

E = -976.578441 a.u.

C	3.99252000	-0.09430500	-1.37023900
C	3.27960800	-1.13721600	-0.93041100
C	2.21902400	-0.91482200	0.11837000
N	1.68213000	0.44914300	0.06115600
C	2.50412400	1.50658200	-0.32261900
C	3.66877000	1.26485200	-0.94952800
C	-0.19789100	-0.86915900	-0.02074100
C	0.30079000	0.40650000	0.01754600
C	0.94419700	-1.78382300	-0.09580500

O	0.98416600	-2.97907100	-0.27198300
C	2.74226100	-1.21179800	1.46484200
C	3.18016200	-1.48296000	2.55298700
C	-1.60103900	-1.30886400	-0.00576500
C	-2.56794500	-0.63902800	0.75771500
C	-3.88736800	-1.07421700	0.76836300
C	-4.26429200	-2.19297700	0.02798000
C	-3.30786100	-2.87529100	-0.71838700
C	-1.98627800	-2.44074100	-0.73689700
C	-0.46485500	1.66995900	-0.00432700
C	-0.25088200	2.64501400	0.97489700
C	-0.99837700	3.81860400	0.96404800
C	-1.95458200	4.02676200	-0.02742100
C	-2.16691300	3.05777900	-1.00610300
C	-1.42902900	1.87979100	-0.99403700
H	4.79036600	-0.24047400	-2.09209100
H	3.43463700	-2.16350400	-1.24675100
H	2.13582500	2.50148100	-0.10224700
H	4.31966600	2.09100300	-1.20665000
H	3.56685000	-1.72072800	3.51871000
H	-2.27761900	0.22086800	1.35422600
H	-4.62222200	-0.54341800	1.36631300
H	-5.29483800	-2.53446000	0.04074200
H	-3.58944500	-3.75351600	-1.29153600
H	-1.24051000	-2.98181600	-1.30824500
H	0.48852600	2.46925000	1.75227900
H	-0.83668800	4.56866800	1.73171900
H	-2.53669400	4.94294800	-0.03553200
H	-2.91293800	3.21734800	-1.77792800
H	-1.59799700	1.11106900	-1.74205300

Transition State C'

E = -976.514602 a.u.

C	-3.904714	-2.177852	-0.877354
C	-3.973711	-0.912860	-0.327297
C	-2.830292	-0.187570	0.042704
N	-1.542234	-0.698624	-0.251224
C	-1.488960	-2.010452	-0.736839
C	-2.614797	-2.714469	-1.065842
C	0.722420	-0.964212	0.430177
C	-0.354691	-0.050441	0.042931
C	0.235594	-2.044041	1.049227
O	-0.285079	-3.008285	1.462885
C	-2.974662	0.987284	0.810953
C	-3.195347	1.973202	1.481107
C	2.162631	-0.870469	0.095092
C	2.583357	-0.178711	-1.052936
C	3.935877	-0.115994	-1.382981
C	4.891981	-0.747926	-0.584815
C	4.482368	-1.437488	0.558075
C	3.133167	-1.487386	0.902792
C	-0.182646	1.395868	0.022416
C	-0.831957	2.212963	-0.931796
C	-0.562873	3.574816	-1.011694
C	0.359944	4.170628	-0.147062
C	1.012404	3.377854	0.800181
C	0.748929	2.014035	0.884928
H	-4.797372	-2.737713	-1.130083
H	-4.928118	-0.447865	-0.103389
H	-0.518289	-2.368414	-1.029256
H	-2.477393	-3.700912	-1.498192

H	-3.346094	2.839589	2.083690
H	1.845997	0.309295	-1.682060
H	4.242694	0.427199	-2.273048
H	5.945266	-0.696932	-0.846418
H	5.216248	-1.925977	1.193828
H	2.826362	-1.998086	1.812840
H	-1.541839	1.768644	-1.623645
H	-1.074968	4.175210	-1.759602
H	0.567904	5.235002	-0.212579
H	1.731186	3.824930	1.482434
H	1.260557	1.412001	1.629169

Product 3a'

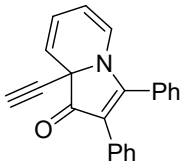
E = -976.584595 a.u.

C	-3.256246	-2.538664	1.006725
C	-3.731995	-1.285745	0.450680
C	-2.869782	-0.426332	-0.169763
N	-1.524969	-0.839928	-0.289962
C	-1.259956	-2.273370	-0.379017
C	-2.055296	-3.030177	0.643229
C	0.774030	-0.957107	-0.195483
C	-0.341867	-0.134668	-0.175322
C	0.317150	-2.342228	-0.261300
O	0.934669	-3.393682	-0.240669
C	-3.300498	0.805543	-0.739164
C	-3.724749	1.825284	-1.233799
C	2.195539	-0.594059	-0.030204
C	3.177002	-1.340692	-0.708900
C	4.530011	-1.037532	-0.568946
C	4.937126	0.013520	0.254343
C	3.975594	0.752377	0.946084

C	2.621941	0.449591	0.811324
C	-0.348867	1.341052	-0.032720
C	0.255401	2.143374	-1.010422
C	0.272404	3.529563	-0.867096
C	-0.298769	4.125623	0.259502
C	-0.890937	3.330579	1.242689
C	-0.921967	1.944681	1.096440
H	-3.891466	-3.073893	1.707396
H	-4.779954	-1.016674	0.515914
H	-1.496665	-2.631920	-1.397247
H	-1.647718	-3.964281	1.018489
H	-4.073939	2.735123	-1.666648
H	2.871543	-2.169877	-1.336882
H	5.268675	-1.627729	-1.105303
H	5.992604	0.248859	0.363200
H	4.279342	1.563327	1.603325
H	1.891059	1.020200	1.373956
H	0.708373	1.676026	-1.879324
H	0.737705	4.144121	-1.632764
H	-0.278027	5.206163	0.373087
H	-1.331410	3.789060	2.123732
H	-1.384306	1.326765	1.860886

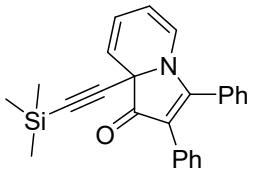
2.4 Characterization data

8A-ethynyl-2,3-diphenylindolizin-1(8a*H*)-one (3a)



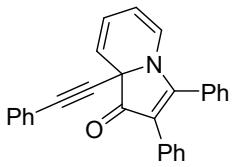
Flash column chromatography on silica gel (eluent: PE/EA = 7/1, v/v) to afford **3a**. Yellow solid (74.2 mg, 80%), mp 188.2-189.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.43 (m, 3H), 7.37 (d, *J* = 6.7 Hz, 2H), 7.19 – 7.09 (m, 5H), 6.38 (d, *J* = 7.3 Hz, 1H), 6.13 – 6.02 (m, 2H), 5.45 (ddd, *J* = 7.0, 5.4, 1.2 Hz, 1H), 2.62 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 169.2, 130.7, 130.1, 129.1, 128.9, 128.8, 128.5, 127.9, 126.3, 124.1, 123.6, 119.7, 110.4, 108.9, 79.8, 73.7, 62.3. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{22}H_{15}NO$, 309.1154; found 309.1146.

2,3-Diphenyl-8a-((trimethylsilyl)ethynyl)indolizin-1(8a*H*)-one (3b)



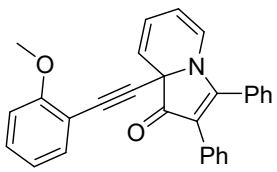
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3b**. Yellow solid (100.8 mg, 78%), mp 190.5-191.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, *J* = 9.1, 7.0 Hz, 3H), 7.22 (d, *J* = 6.5 Hz, 2H), 7.02 – 6.94 (m, 5H), 6.18 (d, *J* = 7.2 Hz, 1H), 5.91 – 5.84 (m, 2H), 5.26 (ddd, *J* = 6.9, 4.7, 2.0 Hz, 1H), -0.00 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 169.3, 130.7, 130.6, 129.2, 129.0, 128.9, 128.8, 128.0, 126.3, 123.8, 123.6, 120.5, 110.3, 109.1, 100.2, 90.7, 63.4. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{25}H_{23}NOSi$, 381.1549; found 381.1557.

2,3-Diphenyl-8a-(phenylethynyl)indolizin-1(8a*H*)-one (3c)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3c**. Yellow solid (88.1 mg, 77%), mp 198.3-198.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.39 (m, 7H), 7.27 (d, *J* = 6.7 Hz, 3H), 7.17 (d, *J* = 4.3 Hz, 4H), 7.13 – 7.09 (m, 1H), 6.40 (d, *J* = 7.2 Hz, 1H), 6.15 – 6.07 (m, 2H), 5.46 (ddd, *J* = 7.0, 4.3, 2.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 169.2, 132.1, 130.7, 130.4, 129.1, 128.9, 128.8, 128.7, 128.6, 128.1, 127.9, 126.2, 123.8, 123.7, 122.1, 120.1, 110.3, 109.1, 85.5, 85.1, 63.1. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{28}H_{19}NO$, 385.1467; found 385.1457.

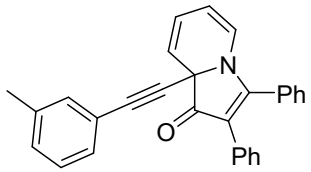
8A-((2-methoxyphenyl)ethynyl)-2,3-diphenylindolizin-1(8a*H*)-one (3d)



Flash column chromatography on silica gel (eluent: PE/EA = 8/1, v/v) to afford **3d**. Yellow solid (105.0 mg, 75%), mp 205.8-206.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.38 (m, 6H), 7.27 – 7.25 (m, 1H), 7.16 (d, *J* = 4.4 Hz, 4H), 7.12 – 7.09 (m,

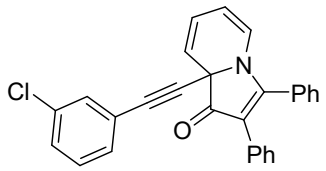
1H), 6.87 – 6.79 (m, 2H), 6.39 (d, *J* = 7.2 Hz, 1H), 6.18 – 6.06 (m, 2H), 5.46 (ddd, *J* = 6.8, 5.3, 1.3 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 169.0, 160.4, 134.0, 130.7, 130.6, 130.1, 129.1, 129.0, 128.9, 128.8, 128.7, 127.9, 126.1, 123.7, 120.3, 120.2, 111.5, 110.9, 110.2, 109.0, 88.9, 82.1, 63.3, 55.9. HRMS (GC/QTOF) m/z: [M] $^+$ calcd for $C_{29}H_{21}NO_2$, 415.1572; found 415.1572.

2,3-Diphenyl-8a-(*m*-tolylethynyl)indolizin-1(8a*H*)-one (3e)



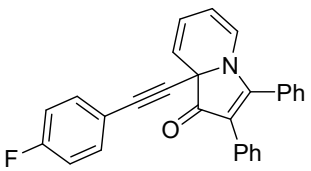
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3e**. Yellow solid (88.3 mg, 77%), mp 208.9-209.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.40 (m, 5H), 7.29 – 7.25 (m, 3H), 7.19 – 7.11 (m, 7H), 6.40 (d, *J* = 7.2 Hz, 1H), 6.11 (d, *J* = 3.5 Hz, 2H), 5.46 (ddd, *J* = 7.0, 4.1, 2.6 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 169.1, 137.8, 132.7, 130.6, 130.4, 129.5, 129.2, 129.1, 128.9, 128.8, 128.7, 128.0, 127.9, 126.2, 123.7, 121.9, 120.2, 110.2, 109.0, 85.6, 84.7, 63.1, 21.1. HRMS (GC/QTOF) m/z: [M] $^+$ calcd for $C_{29}H_{21}NO$, 399.1623; found 399.1617.

8A-((3-chlorophenyl)ethynyl)-2,3-diphenylindolizin-1(8a*H*)-one (3f)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3f**. Yellow solid (106.4 mg, 70%), mp 190.5-191.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.39 (m, 6H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.19 – 7.10 (m, 5H), 6.41 (d, *J* = 7.2 Hz, 1H), 6.11 (d, *J* = 5.0 Hz, 2H), 5.46 (ddd, *J* = 6.9, 4.7, 1.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6, 169.3, 134.0, 131.9, 130.7, 130.3, 130.2, 129.4, 129.1, 128.9, 128.8, 128.6, 127.9, 126.3, 124.0, 123.8, 123.7, 119.8, 110.4, 109.1, 86.3, 84.0, 62.9. HRMS (GC/QTOF) m/z: [M] $^+$ calcd for $C_{28}H_{18}ClNO$, 419.1077; found 419.1087.

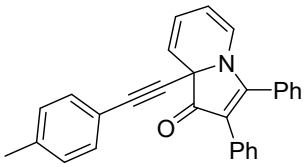
8A-((4-fluorophenyl)ethynyl)-2,3-diphenylindolizin-1(8a*H*)-one (3g)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3g**. Yellow solid (93.8 mg, 67%), mp 158.6-159.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.44 (m, 3H), 7.42 – 7.36 (m, 4H), 7.24 (d, *J* = 1.9 Hz, 1H), 7.18 – 7.12 (m, 5H), 6.41 (d, *J* = 7.2 Hz, 1H), 6.15 – 6.04 (m, 2H), 5.46 (ddd, *J* = 7.0, 4.3, 2.3 Hz, 1H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 194.7, 169.3, 134.7, 133.3, 130.7, 130.3, 129.1, 128.9, 128.8, 128.6, 128.5,

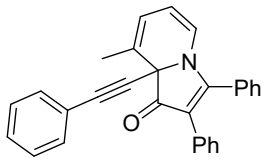
127.9, 126.3, 123.8 (d, J = 16.2 Hz), 120.6, 119.9, 110.3, 109.1, 86.0, 84.3, 63.0. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{28}H_{18}FNO$, 403.1372; found 403.1369.

2,3-Diphenyl-8a-(*p*-tolylethynyl)indolizin-1(8a*H*)-one (3h)



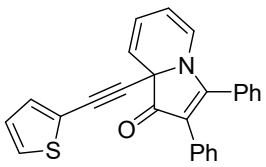
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3h**. Yellow solid (100.2 mg, 73%), mp 212.6-213.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.39 (m, 6H), 7.35 (d, J = 7.8 Hz, 2H), 7.19 – 7.16 (m, 4H), 7.08 (d, J = 8.0 Hz, 2H), 6.41 (d, J = 7.2 Hz, 1H), 6.11 (d, J = 4.7 Hz, 2H), 5.46 (ddd, J = 7.0, 4.6, 2.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 195.0, 169.2, 138.8, 132.0, 130.6, 130.5, 129.1, 128.9, 128.8, 128.7, 127.9, 126.2, 123.8, 123.7, 120.3, 119.0, 110.2, 109.1, 85.7, 84.4, 63.1, 21.5. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{29}H_{21}NO$, 399.1632; found 399.1629.

8-Methyl-2,3-diphenyl-8a-(phenylethynyl)indolizin-1(8a*H*)-one (3i)



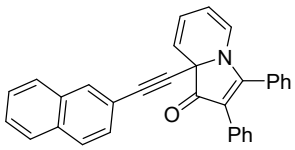
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3i**. Yellow solid (86.0 mg, 72%), mp 210.2-211.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.43 (m, 5H), 7.42 – 7.38 (m, 2H), 7.32 – 7.27 (m, 3H), 7.19 – 7.07 (m, 5H), 6.29 (d, J = 7.2 Hz, 1H), 5.76 (dd, J = 5.8, 1.7 Hz, 1H), 5.44 – 5.39 (m, 1H), 2.29 (d, J = 1.6 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.3, 168.4, 132.2, 131.7, 130.6, 130.5, 129.0, 128.9, 128.6, 128.1, 127.9, 126.1, 122.3, 121.5, 120.5, 110.3, 109.4, 85.4, 84.6, 65.2, 17.5. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{29}H_{21}NO$, 399.1623; found 399.1614.

2,3-Diphenyl-8a-(thiophen-2-ylethynyl)indolizin-1(8a*H*)-one (3j)



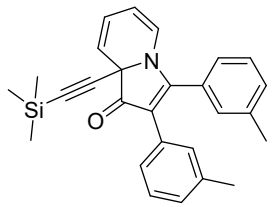
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3j**. Yellow solid (76.3 mg, 65%), mp 193.4-194.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (td, J = 8.5, 4.4 Hz, 3H), 7.39 (d, J = 7.2 Hz, 2H), 7.25 – 7.22 (m, 2H), 7.18 – 7.11 (m, 5H), 6.96 – 6.90 (m, 1H), 6.39 (d, J = 7.2 Hz, 1H), 6.14 – 6.06 (m, 2H), 5.45 (ddd, J = 7.0, 4.4, 2.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 169.3, 133.2, 130.7, 130.3, 129.1, 128.9, 128.8, 128.6, 127.9, 127.8, 126.9, 126.3, 124.0, 123.8, 122.0, 119.8, 110.3, 109.1, 88.7, 79.0, 63.2. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{26}H_{17}NOS$, 391.1031; found 391.1030.

8A-(naphthalen-2-ylethynyl)-2,3-diphenylindolizin-1(8a*H*)-one (3k)



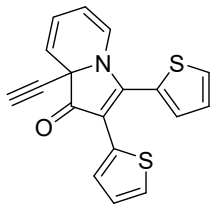
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3k**. Yellow solid (90.5 mg, 70%), mp 202.4-203.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.69 (d, *J* = 6.3 Hz, 1H), 7.56 – 7.39 (m, 9H), 7.20 (d, *J* = 4.3 Hz, 4H), 6.48 (d, *J* = 7.2 Hz, 1H), 6.25 – 6.15 (m, 2H), 5.53 (ddd, *J* = 7.0, 5.3, 1.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 169.1, 133.4, 133.0, 131.5, 130.9, 130.7, 130.4, 129.2, 129.1, 128.9, 128.7, 128.2, 128.0, 127.0, 126.4, 126.3, 126.1, 125.0, 124.0, 123.7, 120.2, 119.7, 110.5, 109.1, 90.0, 83.9, 63.4. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{32}H_{21}NO$, 435.1623; found 435.1632.

2,3-Di-*m*-tolyl-8a-((trimethylsilyl)ethynyl)indolizin-1(8a*H*)-one (3l)



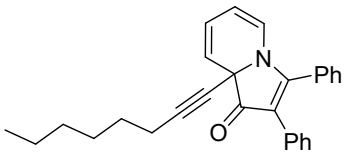
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3l**. Yellow solid (123.9 mg, 68%), mp 220.8-231.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 2H), 7.31 (s, 1H), 7.25 (s, 1H), 7.19 (d, *J* = 7.2 Hz, 1H), 7.14 (s, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.7 Hz, 1H), 6.40 (d, *J* = 7.2 Hz, 1H), 6.10 – 6.03 (m, 2H), 5.45 (t, *J* = 6.1 Hz, 1H), 2.42 (s, 3H), 2.27 (s, 3H), 0.21 (s, 9H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 194.9, 169.6, 139.0, 137.4, 131.4, 130.5, 129.5, 129.1, 129.0, 128.8, 127.8, 127.0, 126.1, 125.9, 123.9, 123.6, 120.5, 110.2, 108.9, 63.3, 21.5, 21.5, 0.0. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{27}H_{27}NOSi$, 409.1862; found 409.1864.

8A-ethynyl-2,3-di(thiophen-2-yl)indolizin-1(8a*H*)-one (3m)



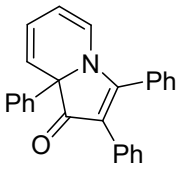
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3m**. Yellow solid (74.4 mg, 63%), mp 231.2-231.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 3.9 Hz, 1H), 7.35 (d, *J* = 3.7 Hz, 1H), 7.24 (dd, *J* = 5.0, 3.7 Hz, 1H), 7.17 (dd, *J* = 3.6, 1.1 Hz, 1H), 7.13 (d, *J* = 5.1 Hz, 1H), 6.94 – 6.91 (m, 1H), 6.46 (d, *J* = 7.2 Hz, 1H), 6.11 (dd, *J* = 9.0, 5.5 Hz, 1H), 6.02 (d, *J* = 9.1 Hz, 1H), 5.57 – 5.50 (m, 1H), 2.64 (s, 1H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 192.8, 160.5, 131.3, 131.2, 130.6, 128.1, 126.9, 126.6, 125.7, 124.5, 124.4, 123.5, 119.7, 109.6, 107.3, 79.2, 74.3, 62.1. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{18}H_{11}NOS_2$, 321.0282; found 321.0275.

8a-(oct-1-yn-1-yl)-2,3-diphenylindolizin-1(8a*H*)-one (3n)



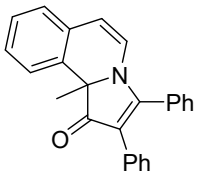
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **3n**. Yellow solid (96.6 mg, 82%), mp 221.2-225.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (q, *J* = 7.5, 6.2 Hz, 3H), 7.39 – 7.33 (m, 2H), 7.19 – 7.09 (m, 5H), 6.34 (d, *J* = 7.2 Hz, 1H), 6.03 (d, *J* = 3.3 Hz, 2H), 5.41 (dt, *J* = 6.9, 3.3 Hz, 1H), 2.21 (t, *J* = 7.2 Hz, 2H), 1.49 (q, *J* = 7.3 Hz, 2H), 1.33 – 1.22 (m, 6H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 195.5, 168.7, 130.6, 130.5, 129.1, 128.0, 128.9, 128.8, 127.9, 126.1, 123.5, 123.1, 120.8, 110.0, 108.8, 86.8, 62.8, 31.2, 28.4, 28.2, 22.5, 19.0, 14.0. HRMS (ESI): calculated $C_{28}H_{27}NaNO$ $[M+Na]^+$: 416.1990; found 416.1991.

2,3,8a-triphenylindolizin-1(8a*H*)-one (4a)



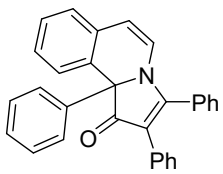
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **4a**. Yellow solid (21.6 mg, 20%), mp 243.2-244.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.6 Hz, 2H), 7.53 – 7.46 (m, 5H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.31 – 7.25 (m, 2H), 7.14 – 7.10 (m, 4H), 6.53 (d, *J* = 7.2 Hz, 1H), 6.42 (d, *J* = 9.2 Hz, 1H), 6.07 (dd, *J* = 9.2, 5.5 Hz, 1H), 5.34 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 198.8, 169.5, 140.6, 130.6, 129.2, 129.1, 128.9, 128.7, 127.9, 127.8, 126.0, 124.4, 124.2, 123.1, 122.9, 110.7, 109.1. HRMS (ESI): calculated $C_{26}H_{20}NO$ $[M+H]^+$: 362.1545; found 362.1541.

10B-methyl-2,3-diphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6a)



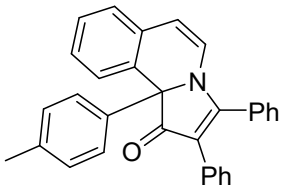
Flash column chromatography on silica gel (eluent: PE/EA = 1/1, v/v) to afford **6a**. Yellow solid (81.7mg, 78%), mp 206.7-207.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 – 8.24 (m, 1H), 7.48 – 7.42 (m, 3H), 7.34 (d, *J* = 6.2 Hz, 2H), 7.23 (dd, *J* = 5.2, 3.0 Hz, 2H), 7.16 (d, *J* = 4.4 Hz, 4H), 7.11 – 7.04 (m, 2H), 6.47 (d, *J* = 7.4 Hz, 1H), 5.88 (d, *J* = 7.4 Hz, 1H), 1.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 166.0, 133.2, 130.9, 130.8, 130.3, 129.2, 129.1, 128.9, 128.8, 127.9, 127.7, 126.8, 126.0, 125.8, 123.8, 122.2, 111.7, 110.9, 66.4, 28.5. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{25}H_{19}NO$, 349.1467; found 349.1474.

2,3,10B-triphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6b)



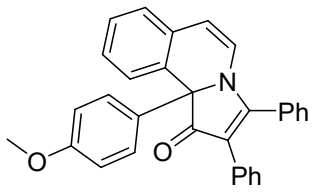
Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **6b**. Yellow solid (109.1 mg, 69%), mp 245.3-245.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.40 (m, 7H), 7.36 (d, *J* = 7.7 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 3H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.15 – 7.05 (m, 6H), 6.59 (d, *J* = 7.3 Hz, 1H), 5.85 (d, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.4, 167.6, 139.1, 132.0, 131.3, 130.7, 130.6, 129.2, 129.1, 128.9, 128.9, 128.6, 128.1, 127.9, 127.8, 126.6, 126.2, 126.1, 125.4, 125.3, 122.9, 112.0, 111.9, 70.8. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{30}H_{21}NO$, 411.1623; found 411.1631.

2,3-Diphenyl-10b-(*p*-tolyl)pyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6c)



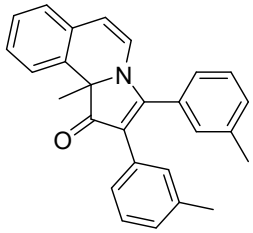
Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **6c**. Yellow solid (114.4 mg, 67%), mp 245.3-245.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.42 (m, 5H), 7.32 – 7.26 (m, 3H), 7.14 – 7.05 (m, 7H), 6.58 (d, *J* = 7.3 Hz, 1H), 5.85 (d, *J* = 7.3 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 167.5, 137.6, 136.3, 132.0, 131.5, 130.6, 130.5, 129.3, 129.2, 129.1, 129.0, 128.9, 128.1, 127.9, 126.6, 126.2, 126.1, 125.3, 125.2, 122.8, 111.9, 70.7, 21.0. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{31}H_{23}NO$, 425.1780; found 425.1789.

10B-(4-methoxyphenyl)-2,3-diphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6d)



Flash column chromatography on silica gel (eluent: PE/EA= 5/1, v/v) to afford **6d**. Yellow solid (121.2 mg, 62%), mp 243.2-244.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.7 Hz, 1H), 7.52 – 7.42 (m, 5H), 7.35 – 7.26 (m, 4H), 7.16 – 7.05 (m, 6H), 6.85 – 6.78 (m, 2H), 6.57 (d, *J* = 7.3 Hz, 1H), 5.86 (d, *J* = 7.3 Hz, 1H), 3.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 167.5, 159.2, 132.0, 131.5, 131.4, 130.7, 130.6, 129.2, 129.1, 128.9, 128.1, 127.9, 126.7, 126.6, 126.2, 126.1, 125.2, 122.8, 114.0, 112.0, 111.9, 70.4, 55.3. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{31}H_{23}NO_2$, 441.1729; found 441.1738.

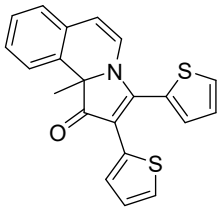
10B-methyl-2,3-di-*m*-tolylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6e)



Flash column chromatography on silica gel (eluent: PE/EA= 5/1, v/v) to afford **6e**. Yellow solid (99.6 mg, 65%), mp 243.2-244.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ

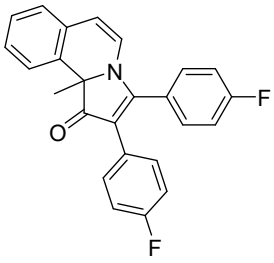
8.28 (d, *J* = 3.6 Hz, 1H), 7.30 (dd, *J* = 14.8, 7.5 Hz, 2H), 7.23 – 7.20 (m, 2H), 7.15 (d, *J* = 5.7 Hz, 2H), 7.11 (d, *J* = 7.2 Hz, 1H), 7.06 – 6.99 (m, 2H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.46 (d, *J* = 7.4 Hz, 1H), 5.86 (d, *J* = 7.4 Hz, 1H), 2.35 (s, 3H), 2.22 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.1, 166.3, 138.9, 137.3, 133.3, 131.1, 130.9, 130.8, 129.5, 129.2, 129.1, 129.0, 127.8, 127.7, 127.5, 126.9, 126.8, 126.0, 125.8, 125.7, 123.8, 122.4, 111.6, 110.7, 66.3, 28.6, 21.5. HRMS (ESI): calculated $C_{27}H_{24}NO$ $[M+H]^+$: 377.1780, found 378.1855.

10B-methyl-2,3-di(thiophen-2-yl)pyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6f)



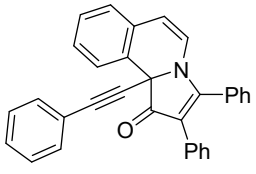
Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **6f**. Yellow solid (78.9 mg, 60%), mp 234.8-235.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 5.0 Hz, 1H), 7.46 (d, *J* = 3.8 Hz, 1H), 7.24 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.21 – 7.15 (m, 2H), 7.10 – 7.04 (m, 2H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.92 – 6.85 (m, 2H), 6.79 (d, *J* = 7.8 Hz, 1H), 6.12 (d, *J* = 7.3 Hz, 1H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 167.3, 149.0, 137.9, 136.1, 133.9, 132.9, 131.8, 131.1, 130.8, 130.7, 130.0, 129.8, 129.5, 129.1, 128.9, 128.6, 125.3, 122.8, 115.0, 67.4, 29.2. HRMS GC/QTOF (m/z): $[M]^+$ calcd for $C_{21}H_{15}NOS_2$, 361.0595; found: 361.0599.

2,3-Bis(4-fluorophenyl)-10b-methylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6g)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **6g**. Yellow solid (112.0 mg, 57%), mp 243.4-244.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 – 8.17 (m, 1H), 7.34 (dd, *J* = 8.3, 5.3 Hz, 2H), 7.27 – 7.23 (m, 3H), 7.17 (t, *J* = 8.4 Hz, 2H), 7.13 – 7.04 (m, 3H), 6.94 – 6.84 (m, 2H), 6.45 (d, *J* = 7.3 Hz, 1H), 5.92 (d, *J* = 7.4 Hz, 1H), 1.70 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 198.7, 164.8, 133.2, 131.0 (d, *J* = 8.6 Hz), 130.6, 130.5, 130.4, 127.8, 127.0, 125.9, 123.7, 121.9, 116.6 (d, *J* = 21.9 Hz), 115.1 (d, *J* = 21.3 Hz), 111.4, 111.1, 66.6, 28.4. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{25}H_{17}F_2NO$, 385.1278; found 385.1268.

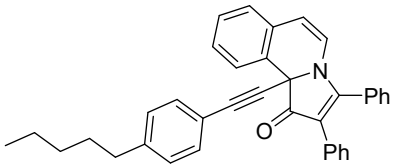
2,3-Diphenyl-10b-(phenylethynyl)pyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6h)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **6h**. Yellow solid (103.7 mg, 73%), mp 252.3-253.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.37 (m, 1H), 7.46 – 7.31 (m, 7H), 7.30 – 7.24 (m, 2H), 7.22 –

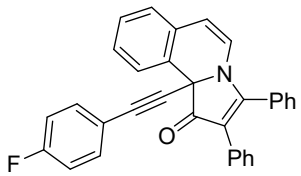
7.12 (m, 7H), 7.12 – 7.06 (m, 2H), 6.48 (d, *J* = 7.3 Hz, 1H), 5.98 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.1, 167.7, 132.2, 131.2, 130.7, 130.5, 130.3, 129.2, 129.1, 128.9, 128.8, 128.7, 128.2, 128.0, 127.4, 126.4, 126.2, 124.5, 122.7, 122.1, 112.1, 111.7, 86.6, 84.7, 62.2. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{32}H_{21}NO$, 435.1623; found 435.1618.

10B-((4-pentylphenyl)ethynyl)-2,3-diphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6i)



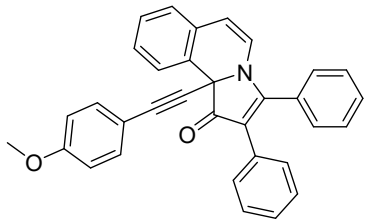
Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **6i**. Yellow solid (92.3 mg, 65%), mp 265.2-266.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.35 (m, 1H), 7.47 (q, *J* = 7.3, 6.1 Hz, 3H), 7.40 (d, *J* = 7.1 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 4H), 7.19 (d, *J* = 4.3 Hz, 4H), 7.15 – 7.11 (m, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 6.52 (d, *J* = 7.4 Hz, 1H), 6.01 (d, *J* = 7.4 Hz, 1H), 2.55 (t, *J* = 7.7 Hz, 2H), 1.60 – 1.51 (m, 2H), 1.32 – 1.24 (m, 4H), 0.87 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.2, 167.5, 143.8, 132.0, 131.1, 130.6, 130.5, 130.4, 129.1, 129.0, 128.9, 128.8, 128.5, 128.2, 127.9, 127.3, 126.2, 126.0, 124.5, 122.6, 119.2, 111.9, 111.6, 85.8, 77.2, 62.2, 35.8, 31.3, 30.9, 22.5, 14.0. HRMS (ESI): calculated $C_{37}H_{32}NO$ $[M+H]^+$: 506.2485, found 506.2481.

10b-((4-fluorophenyl)ethynyl)-2,3-diphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6j)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **6j**. Yellow solid (112.5 mg, 70%), mp 220.4-221.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.36 (m, 1H), 7.48 (q, *J* = 7.2, 6.1 Hz, 3H), 7.42 – 7.36 (m, 4H), 7.34 – 7.30 (m, 2H), 7.19 (d, *J* = 4.3 Hz, 4H), 7.16 – 7.12 (m, 2H), 6.94 (t, *J* = 8.5 Hz, 2H), 6.53 (d, *J* = 7.3 Hz, 1H), 6.02 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.0, 167.7, 134.1 (d, *J* = 8.5 Hz), 131.1, 130.7, 130.4, 130.1, 129.1, 129.0, 128.9, 128.7, 128.6, 128.0, 127.4, 126.2 (d, *J* = 19.4 Hz), 124.4, 122.6, 115.5, 115.3, 112.0, 111.6, 86.2, 83.5, 62.0. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{32}H_{20}FNO$, 435.1529; found 435.1519.

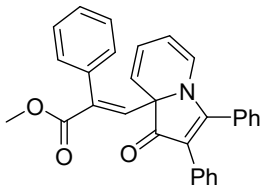
10B-((4-methoxyphenyl)ethynyl)-2,3-diphenylpyrrolo[2,1-*a*]isoquinolin-1(10b*H*)-one (6k)



Flash column chromatography on silica gel (eluent: PE/EA = 10/1, v/v) to afford **6k**. Yellow solid (103.6 mg, 68%), mp 245.2-246.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.0 Hz, 1H), 7.52 – 7.46 (m, 3H), 7.43 (d,

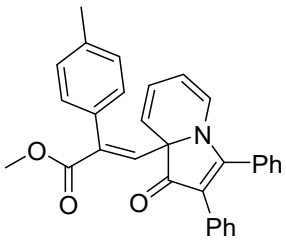
J = 7.1 Hz, 2H), 7.39 – 7.33 (m, 4H), 7.30 – 7.21 (m, 5H), 7.18 (d, *J* = 6.6 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 6.57 (d, *J* = 7.4 Hz, 1H), 6.06 (d, *J* = 7.4 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.3, 167.6, 133.7, 131.1, 130.6, 130.5, 130.4, 129.1, 129.0, 128.9, 128.8, 128.5, 128.0, 127.3, 126.3, 126.1, 124.5, 122.7, 114.2, 113.7, 112.0, 111.5, 85.2, 84.6, 55.3. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{33}H_{23}NO_2$, 465.1729; found 465.1725.

Methyl (*E*)-3-(1-oxo-2,3-diphenylindolizin-8a(1*H*)-yl)-2-phenylacrylate (8a)



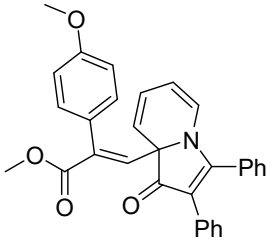
Flash column chromatography on silica gel (eluent: PE/EA = 7/1, v/v) to afford **8a**. Yellow solid (85.7 mg, 70%), mp 234.8-235.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 2H), 7.37 (dd, *J* = 18.8, 7.5 Hz, 3H), 7.20 – 7.11 (m, 5H), 7.09 – 7.03 (m, 2H), 6.91 (s, 1H), 6.72 (d, *J* = 7.6 Hz, 2H), 6.02 – 5.88 (m, 3H), 5.35 (ddd, *J* = 6.8, 5.2, 1.3 Hz, 1H), 3.68 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 170.1, 166.9, 140.7, 133.7, 131.6, 131.5, 130.7, 130.6, 130.3, 129.0, 128.9, 128.8, 128.0, 126.3, 124.9, 123.4, 122.3, 121.4, 110.8, 110.0, 70.6, 52.6. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{30}H_{23}NO_3$, 445.1678; found 445.1684.

Methyl (*E*)-3-(1-oxo-2,3-diphenylindolizin-8a(1*H*)-yl)-2-(*p*-tolyl)acrylate (8b)



Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **8b**. Yellow solid (114.1 mg, 65%), mp 234.8-235.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 1H), 7.25 (d, *J* = 1.6 Hz, 2H), 7.14 (ddd, *J* = 17.4, 7.4, 2.3 Hz, 7H), 7.08 – 7.04 (m, 2H), 6.88 (s, 1H), 6.66 (d, *J* = 7.6 Hz, 2H), 6.00 – 5.90 (m, 3H), 5.37 – 5.31 (m, 1H), 3.67 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.4, 170.2, 167.6, 139.4, 137.6, 132.3, 131.7, 131.5, 130.6, 130.4, 129.7, 129.1, 128.8, 128.4, 128.3, 128.2, 127.9, 126.2, 125.0, 123.3, 121.7, 110.5, 110.0, 70.7, 52.5, 21.3. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{31}H_{25}NO_3$, 459.1834; found 459.1836.

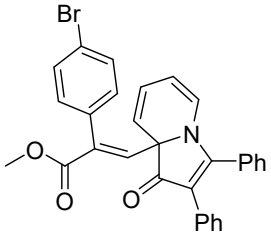
Methyl (*E*)-2-(4-methoxyphenyl)-3-(1-oxo-2,3-diphenylindolizin-8a(1*H*)-yl)acrylate (8c)



Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **8c**. Brown solid (95.3 mg, 64%), mp 247.5-247.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 2H), 7.20 – 7.04 (m, 8H), 6.90 – 6.85

(m, 3H), 6.84 – 6.78 (m, 2H), 5.99 (d, *J* = 7.2 Hz, 1H), 5.91 (d, *J* = 4.6 Hz, 2H), 5.33 (ddd, *J* = 6.9, 4.5, 2.0 Hz, 1H), 3.83 (s, 3H), 3.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 168.9, 166.6, 158.3, 139.1, 131.7, 130.0, 129.5, 129.4, 128.0, 127.9, 127.7, 127.5, 127.2, 126.9, 125.8, 125.1, 123.7, 122.1, 120.7, 111.9, 109.7, 108.9, 69.7, 54.2, 51.4. HRMS (GC/QTOF) m/z: $[M]^+$ calcd for $C_{31}H_{25}NO_4$, 475.1784; found 475.1781.

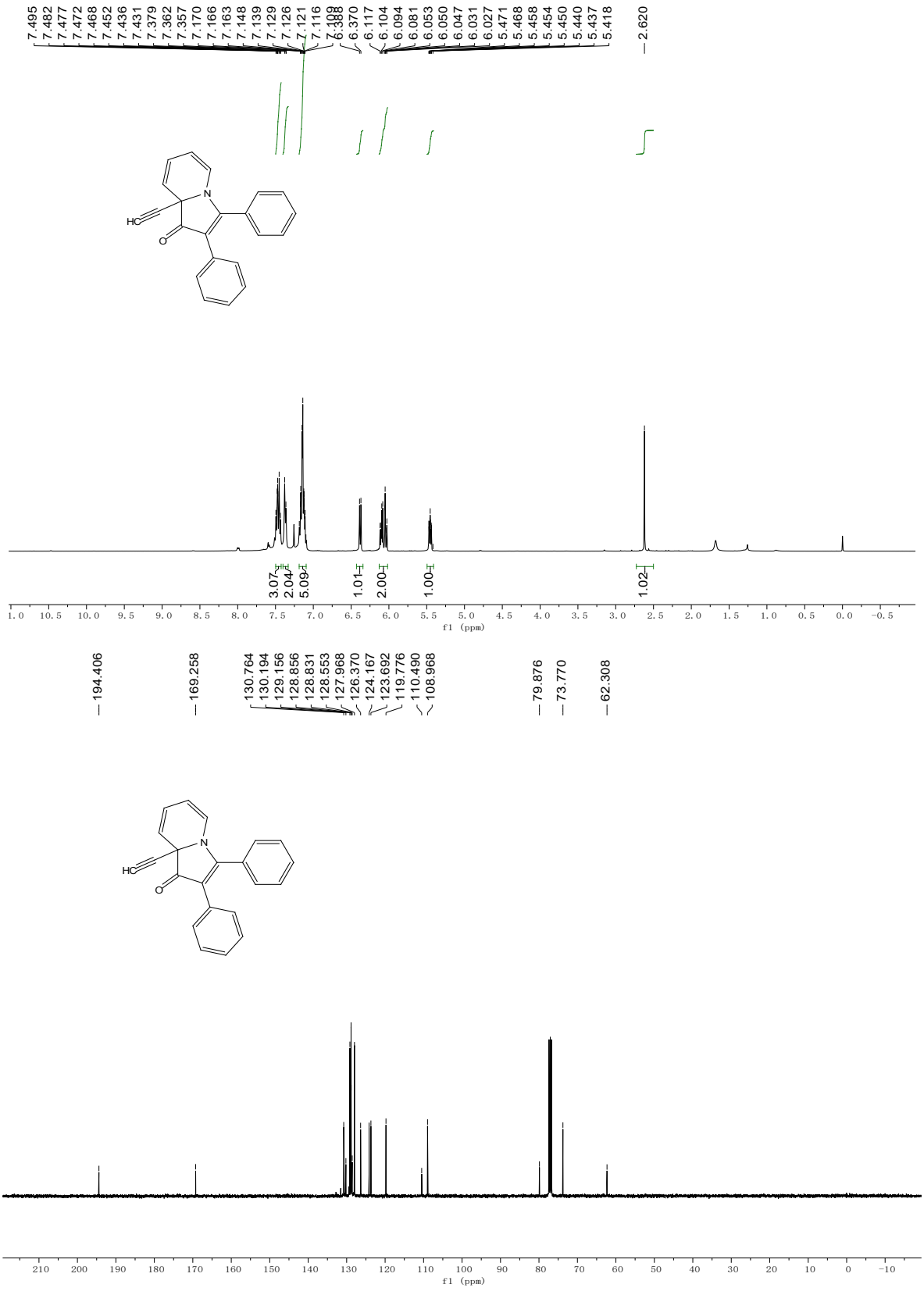
Methyl (*E*)-2-(4-bromophenyl)-3-(1-oxo-2,3-diphenylindolizin-8a(1*H*)-yl)acrylate (8d)



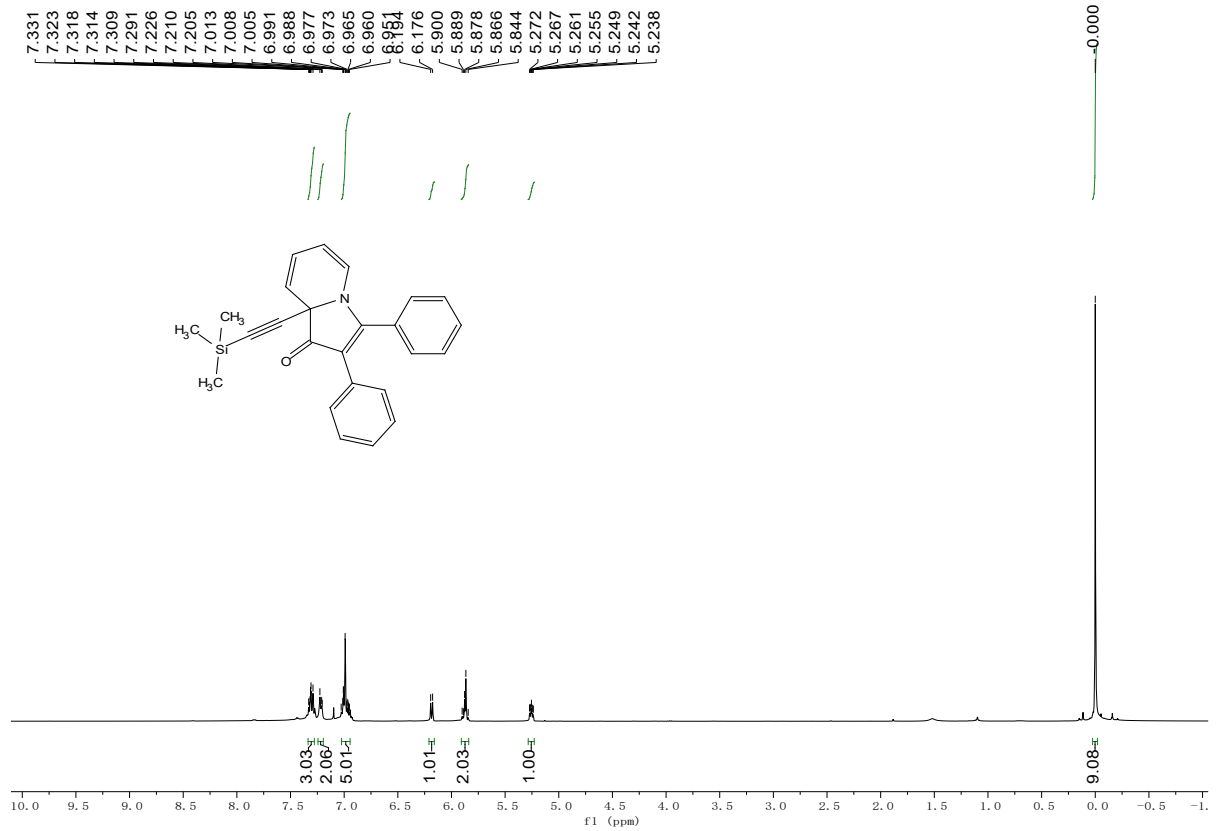
Flash column chromatography on silica gel (eluent: PE/EA = 5/1, v/v) to afford **8d**. Brown solid (115.8 mg, 62%), mp 252.3-253.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 2H), 7.42 – 7.31 (m, 4H), 7.20 – 7.11 (m, 6H), 7.08 – 7.04 (m, 2H), 6.91 (s, 1H), 6.72 (d, *J* = 7.6 Hz, 2H), 5.99 – 5.88 (m, 3H), 5.35 (dd, *J* = 7.0, 5.4 Hz, 1H), 3.68 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 170.1, 166.9, 140.7, 133.6, 131.6, 131.5, 130.7, 130.6, 130.3, 128.9, 128.9, 128.8, 128.1, 128.0, 127.9, 126.3, 124.9, 123.5, 122.3, 121.4, 110.8, 110.0, 70.7, 52.6. HRMS (ESI): calculated $C_{30}H_{22}BrNaNO_3$ $[M+Na]^+$: 546.0681, found 546.0676.

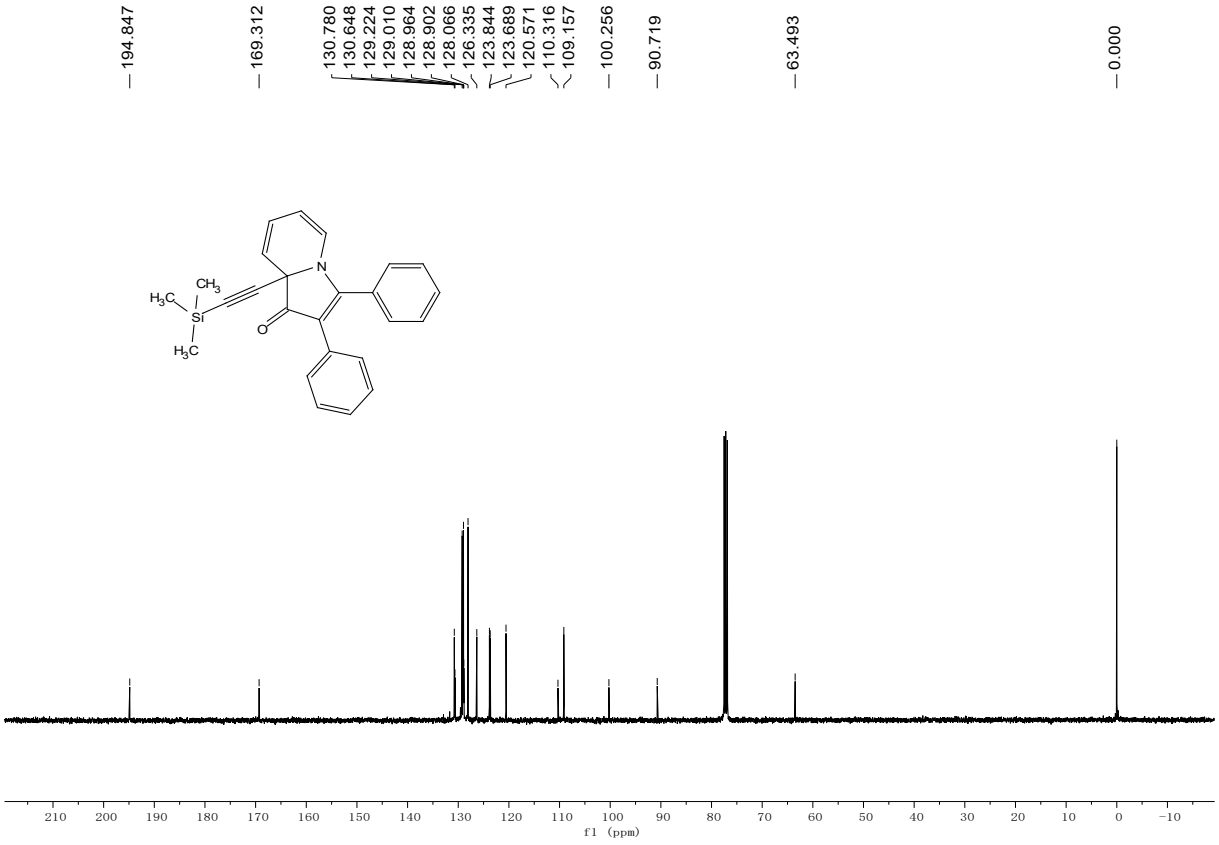
3. NMR spectra for new compounds

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3a**

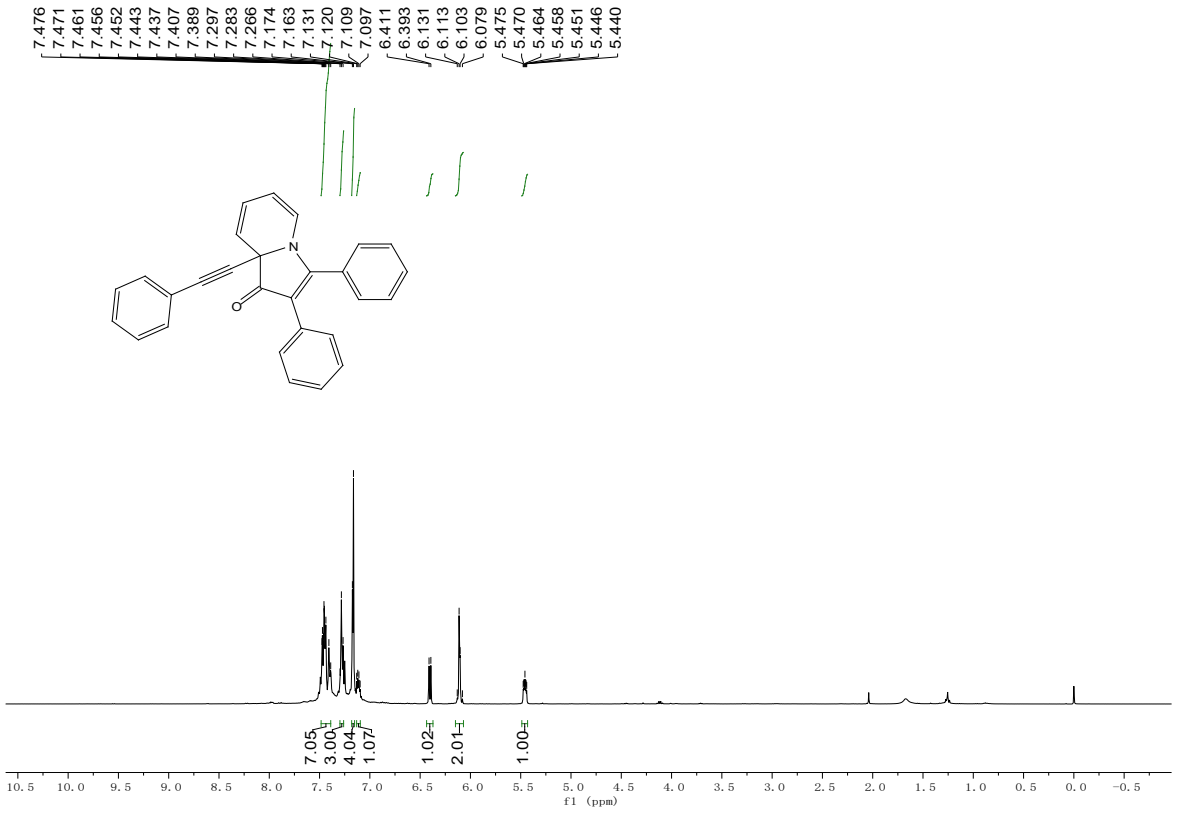


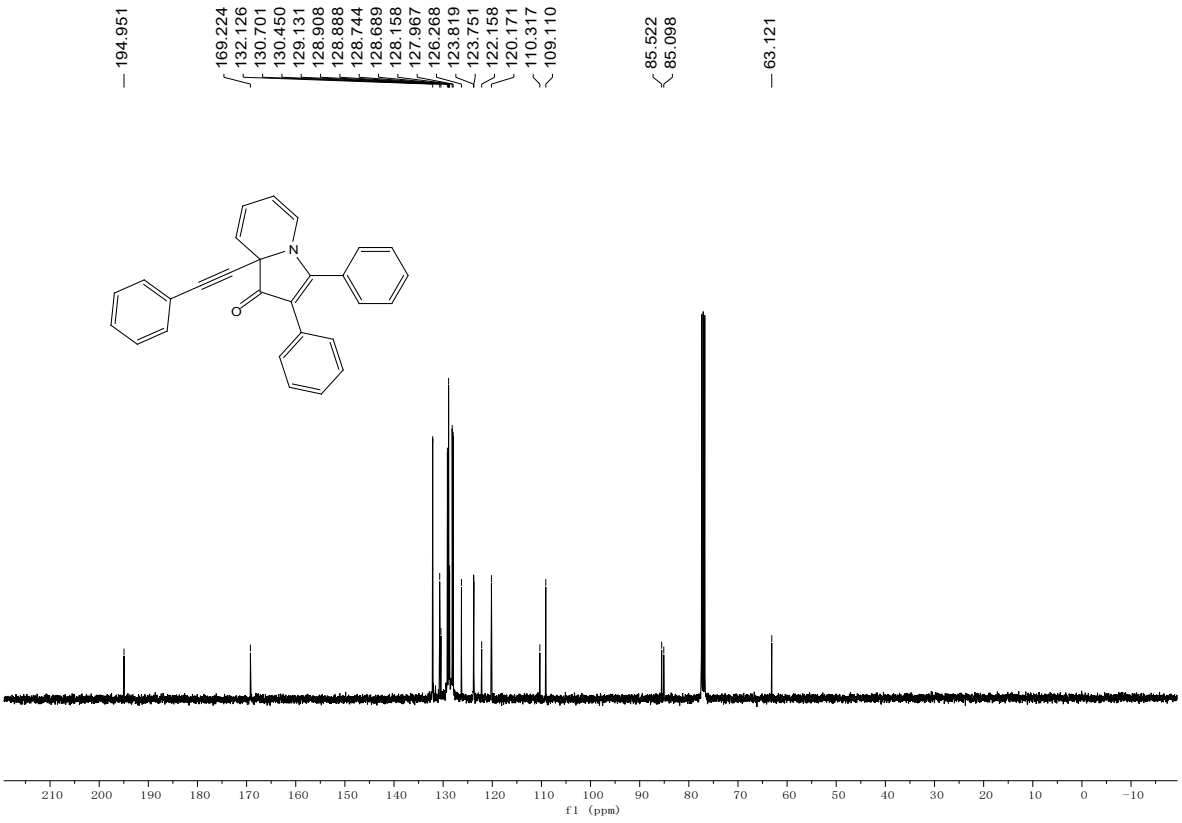
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3b**



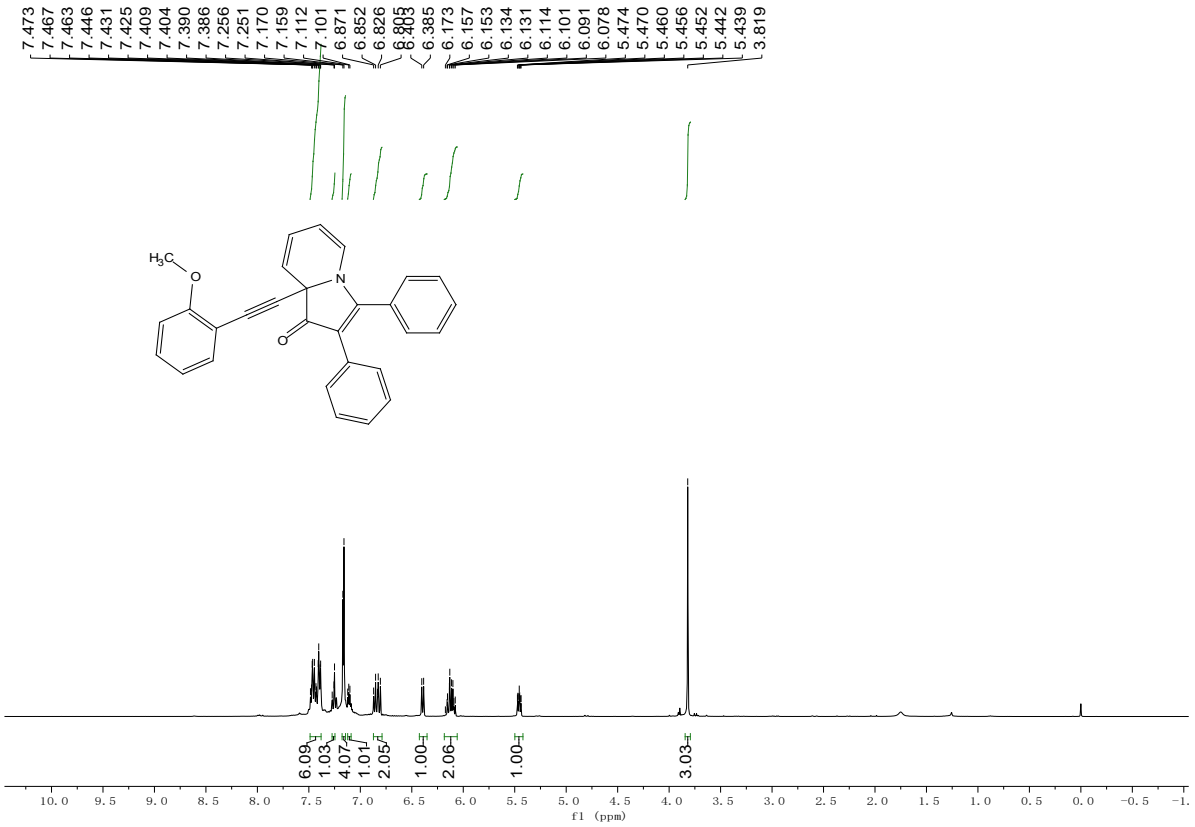


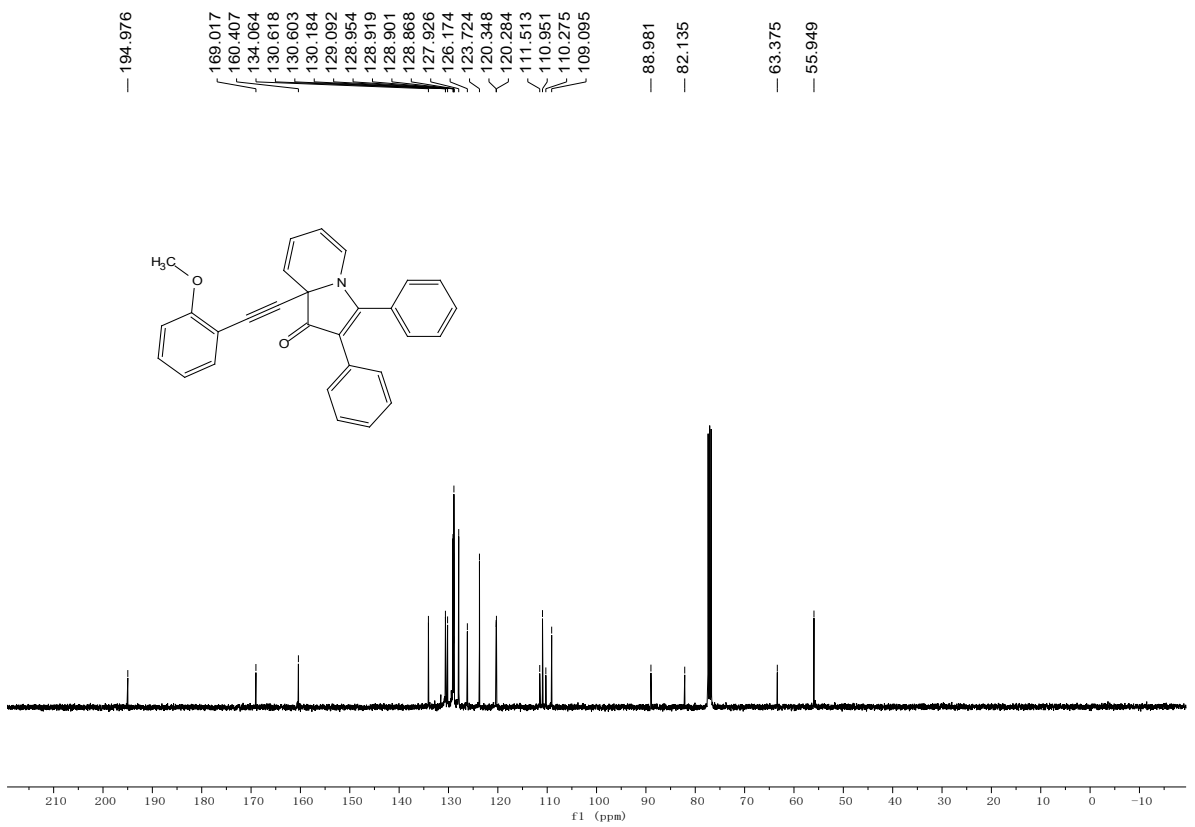
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3c**



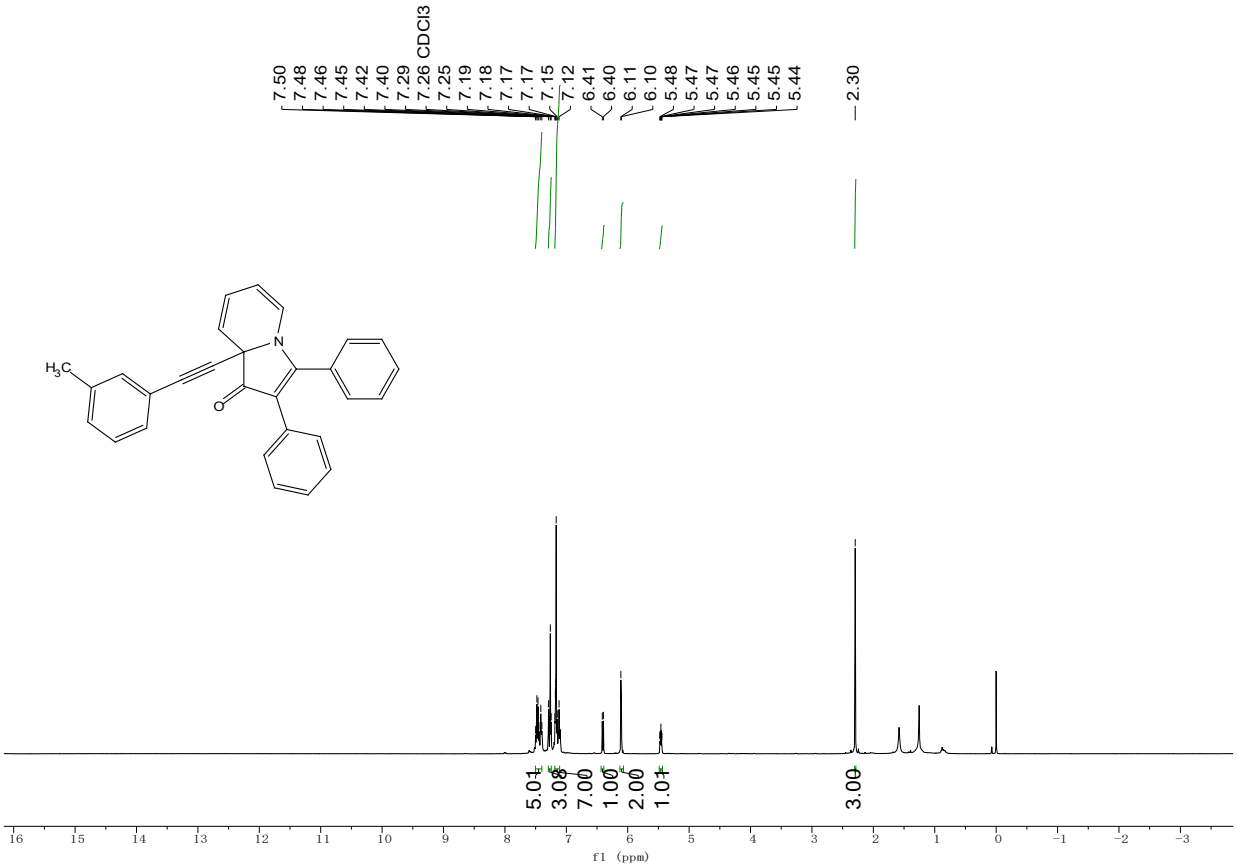


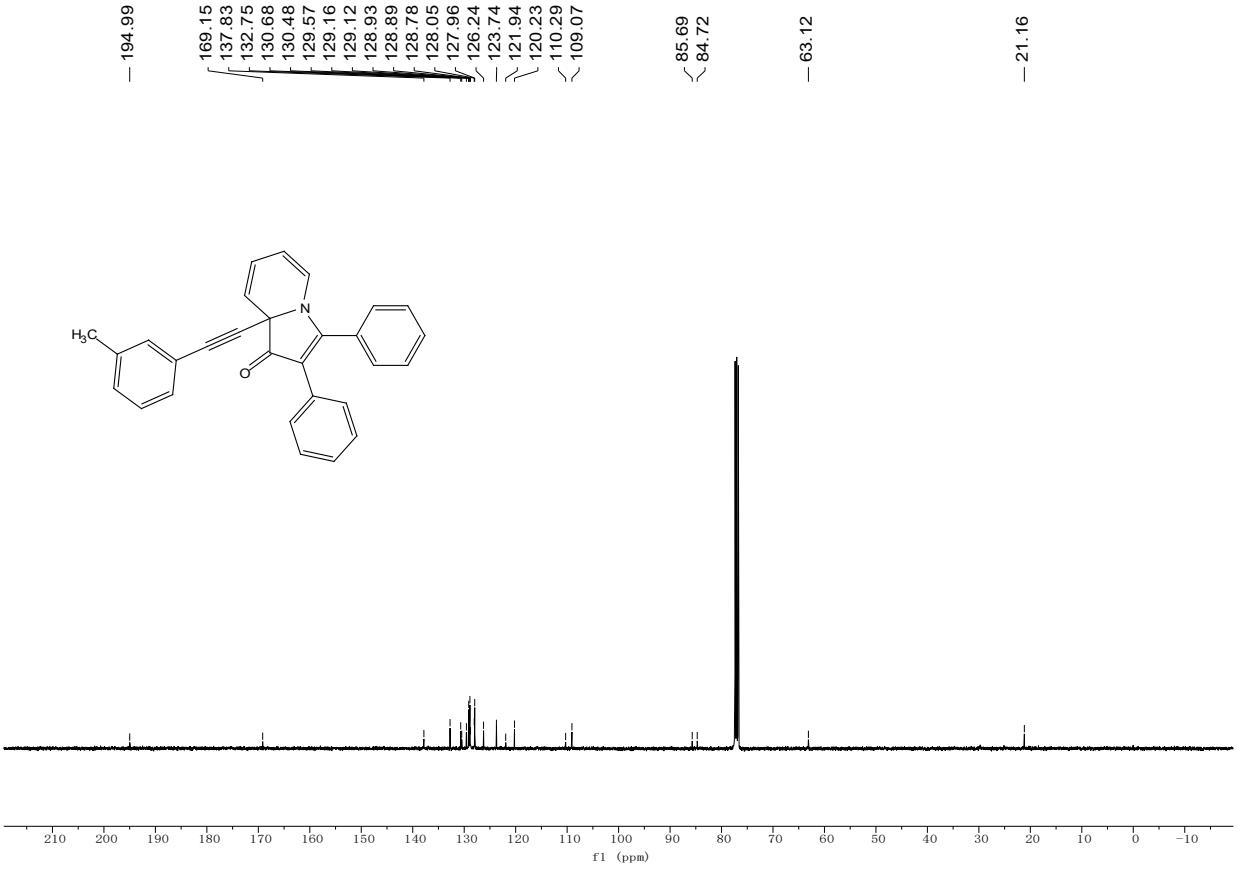
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3d**



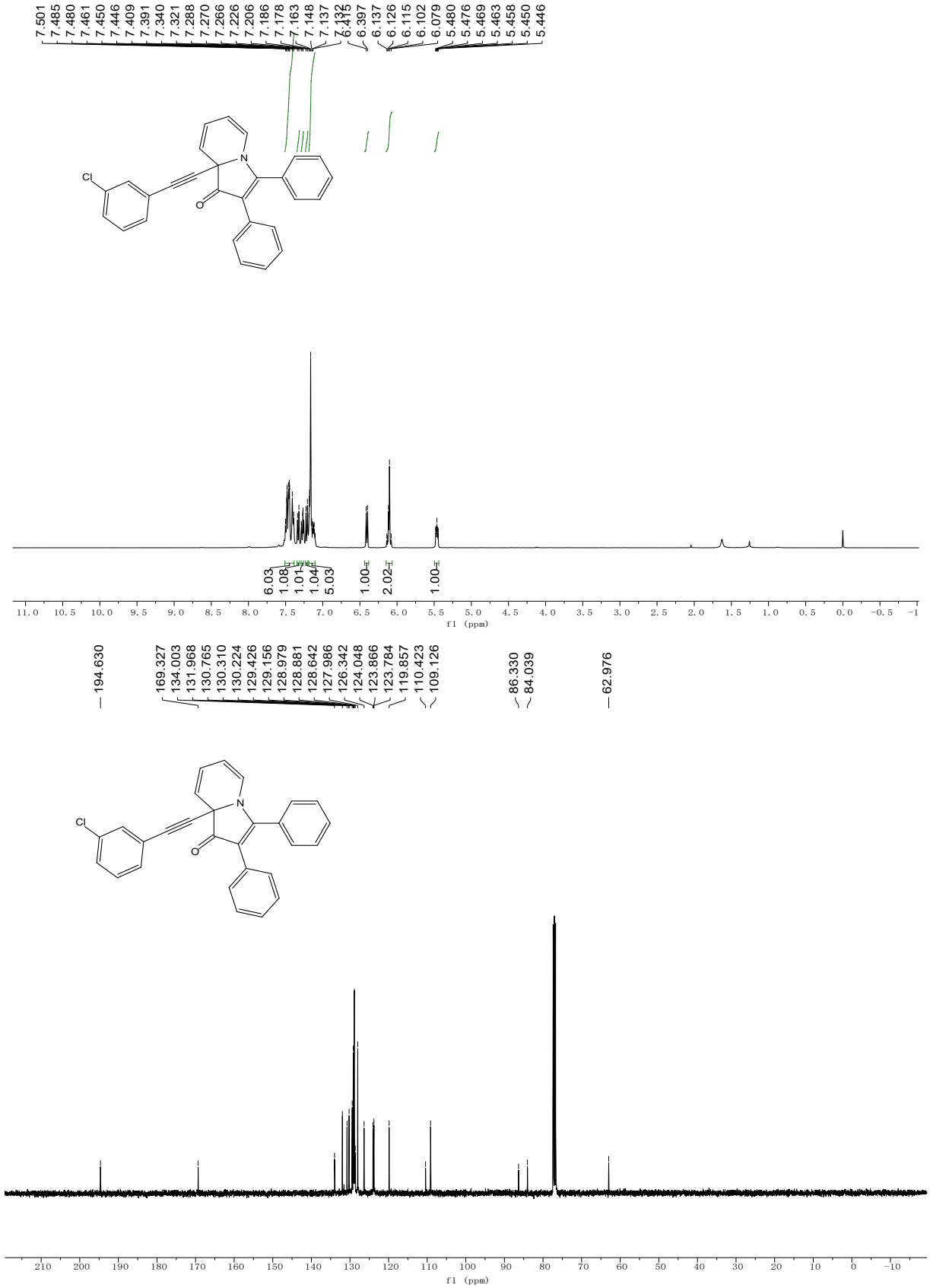


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3e**

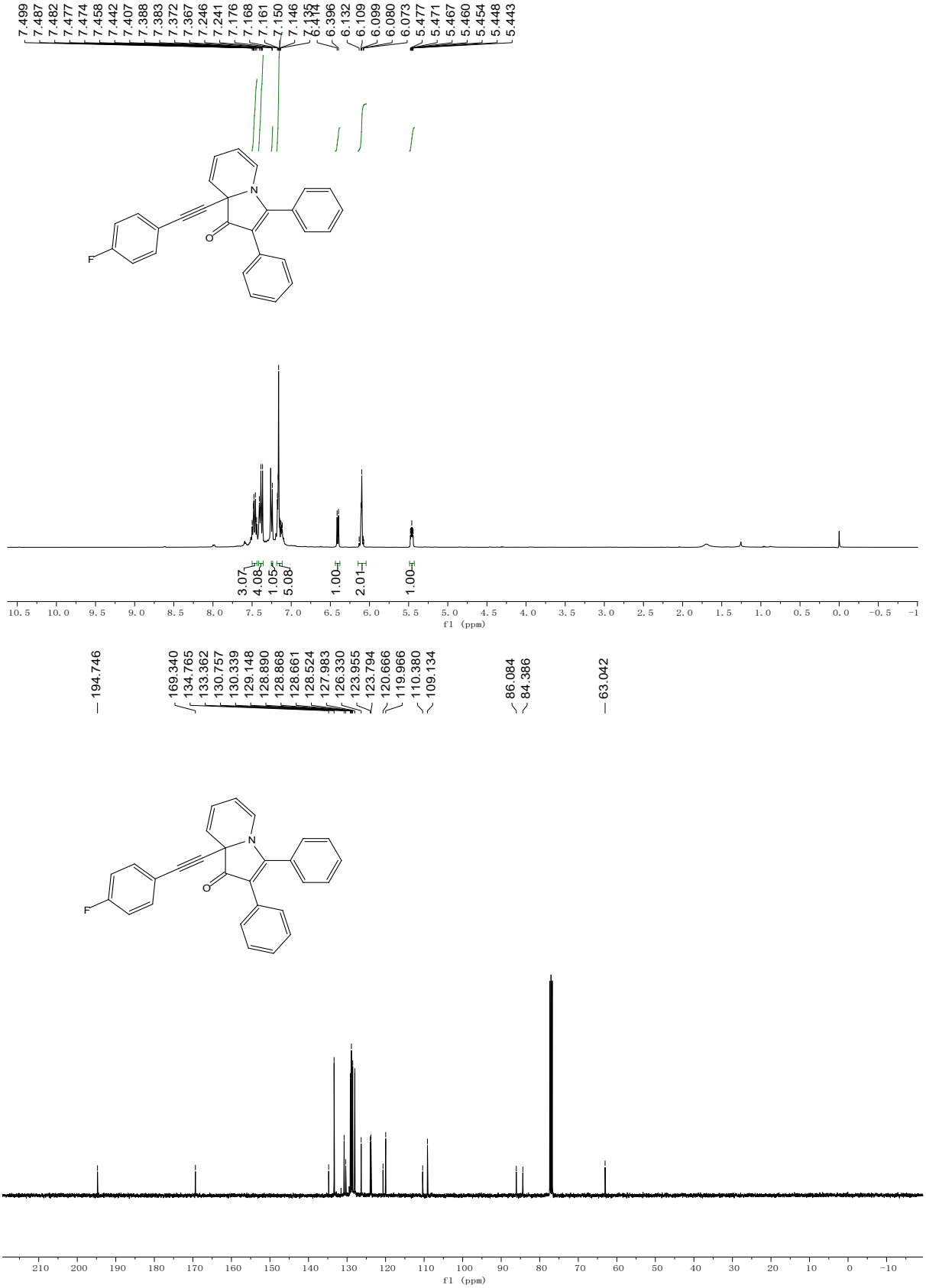




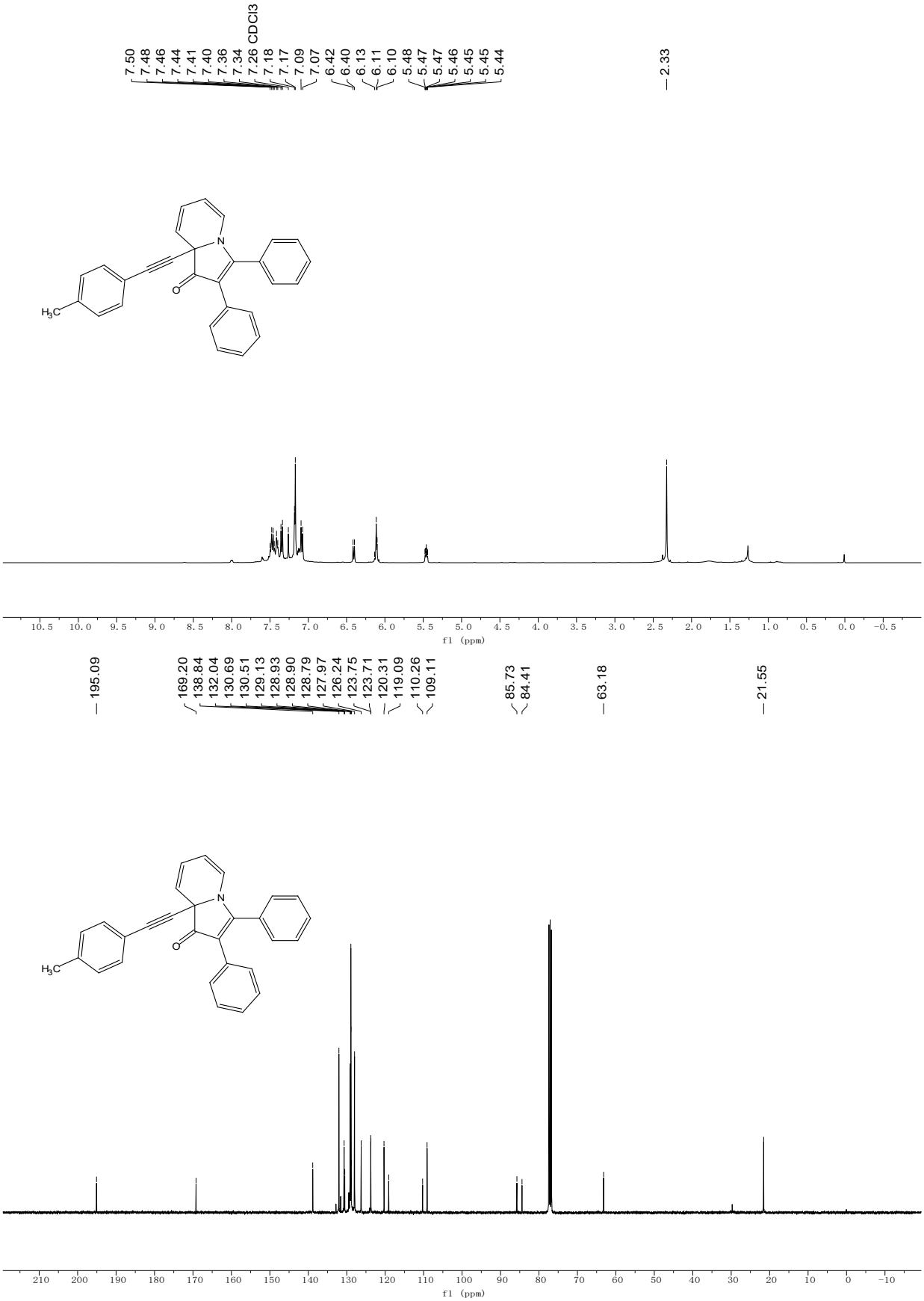
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3f**



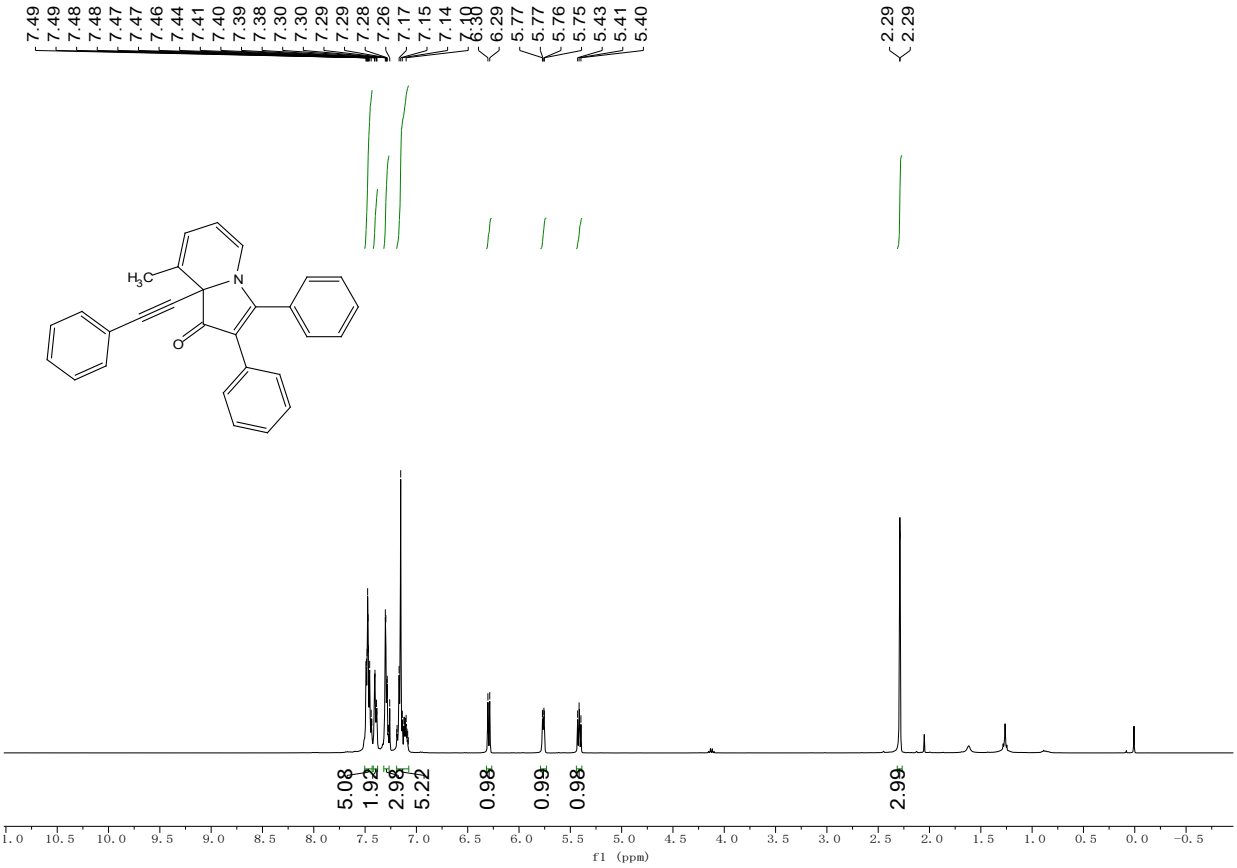
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3g**

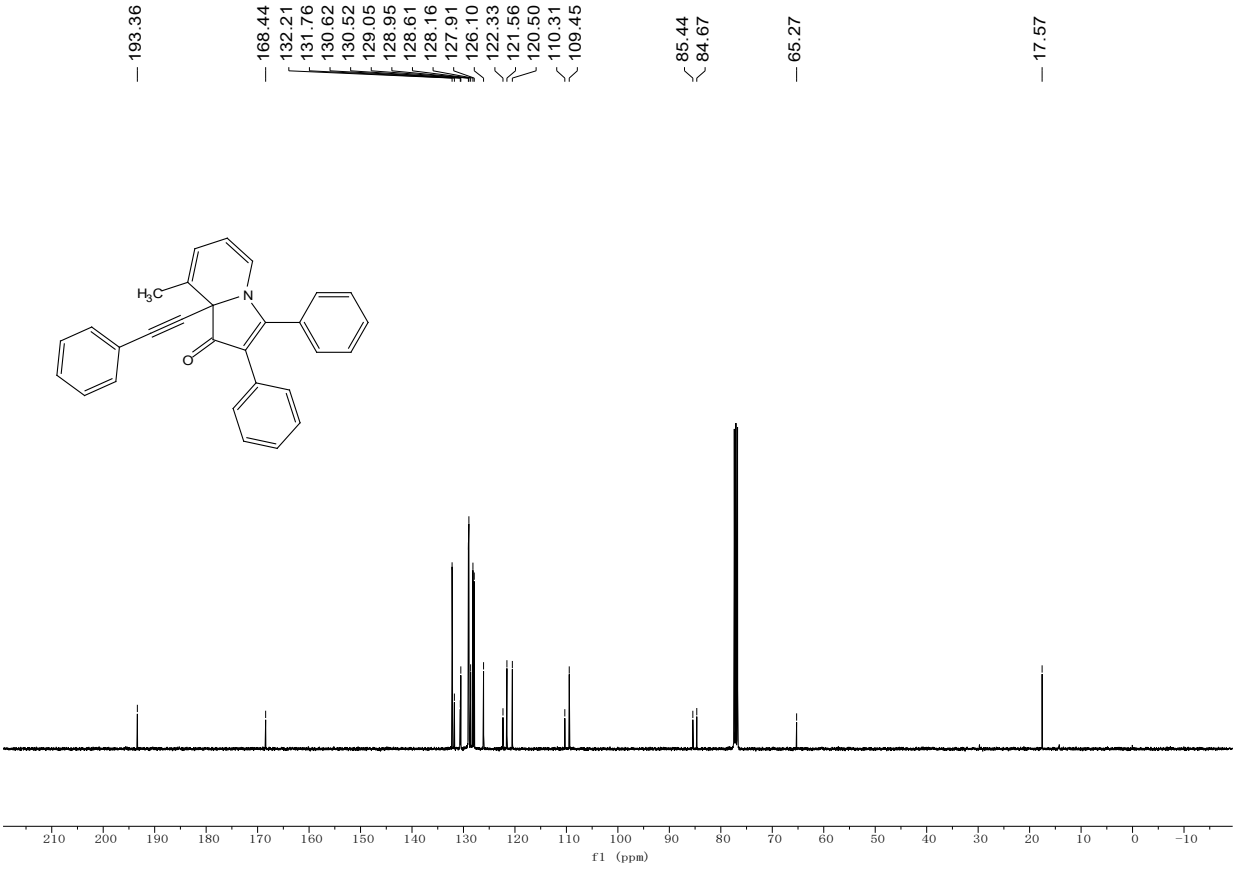


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3h**

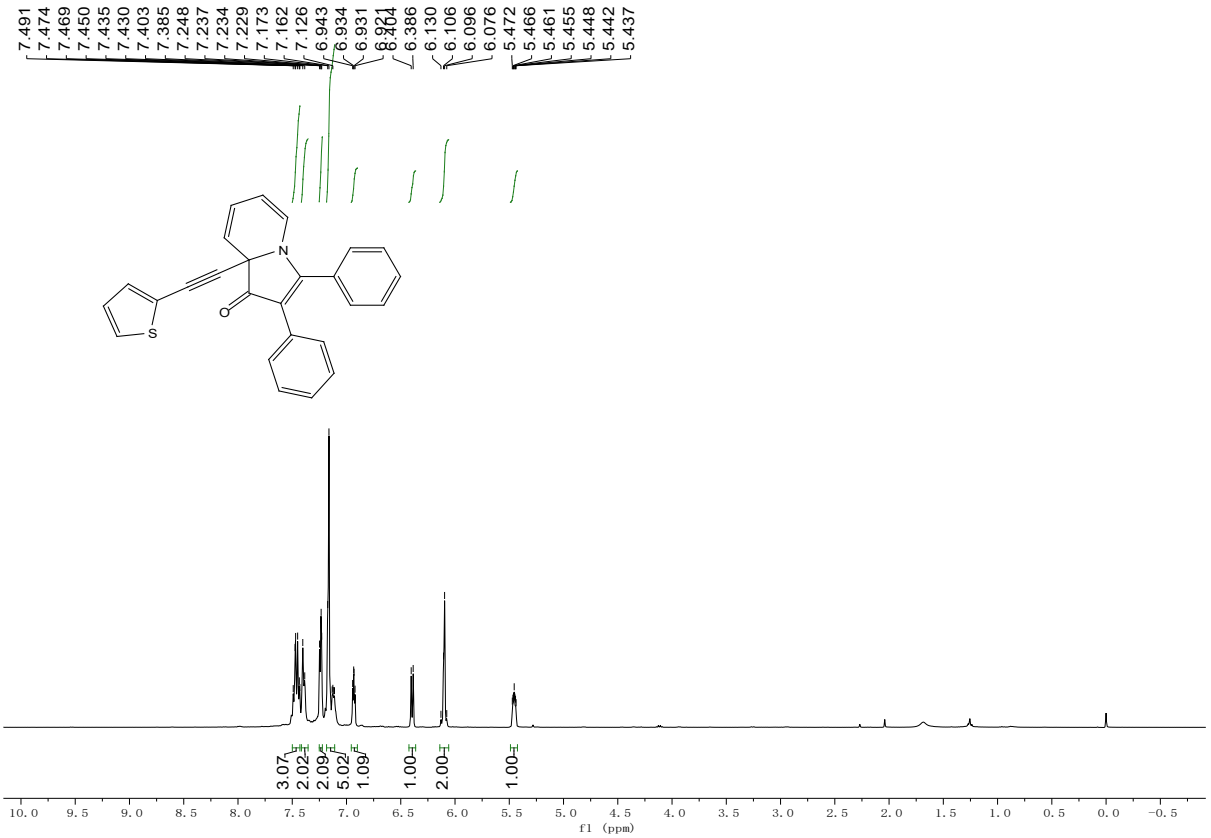


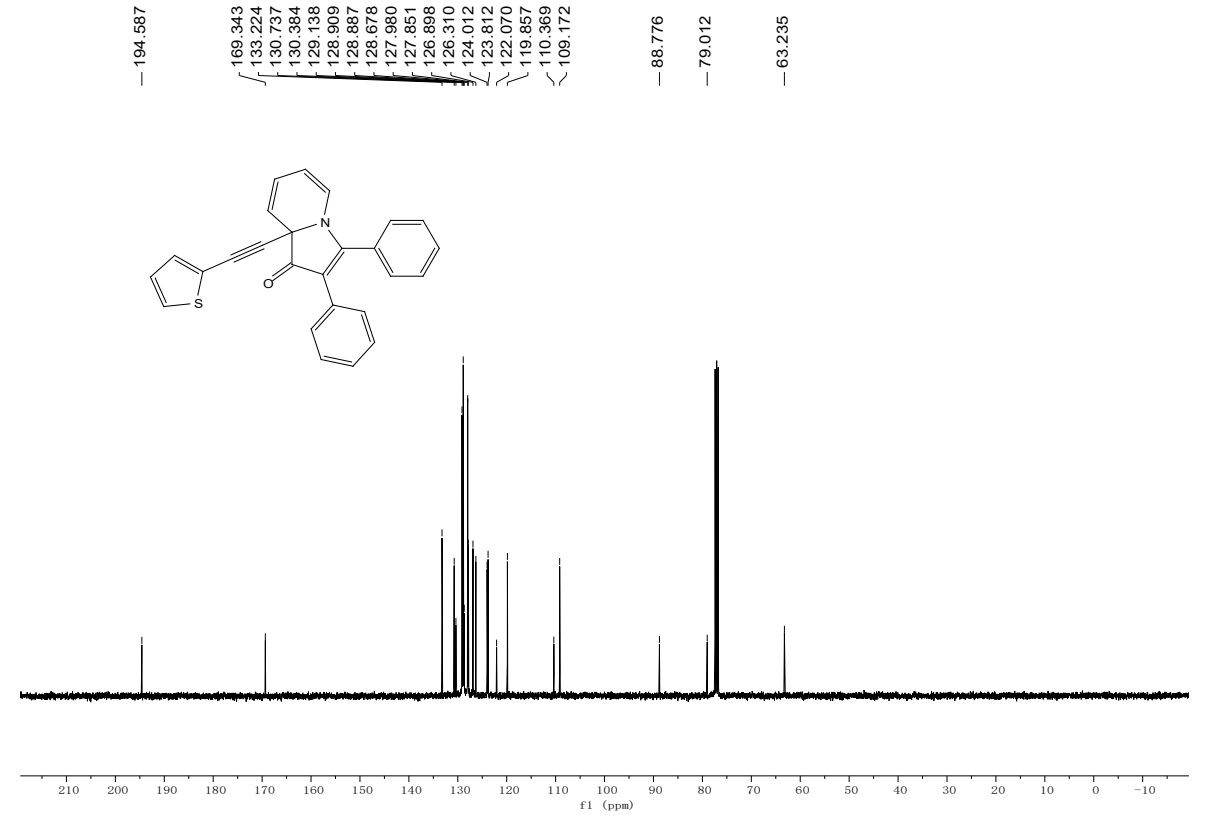
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3i**



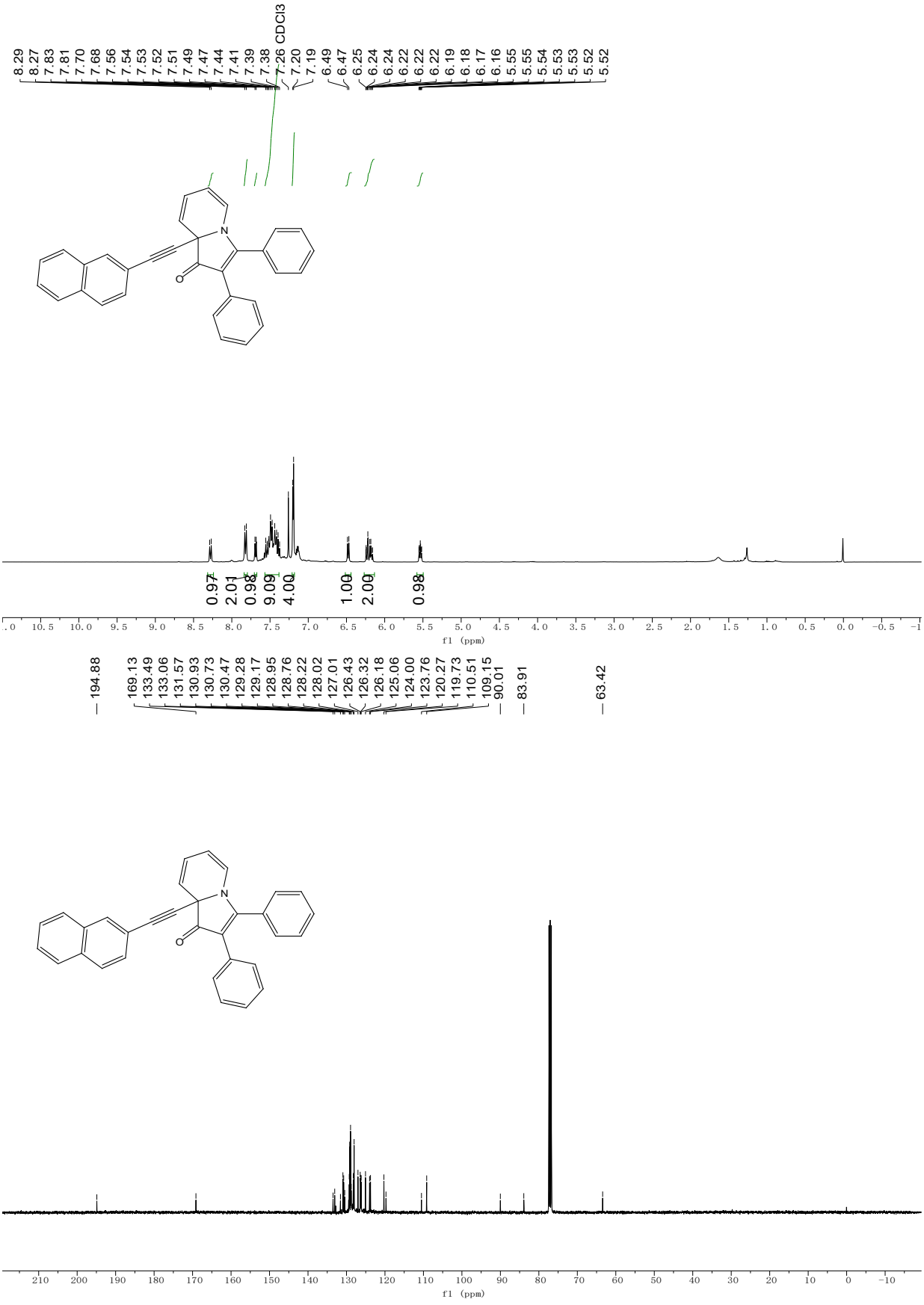


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3j**

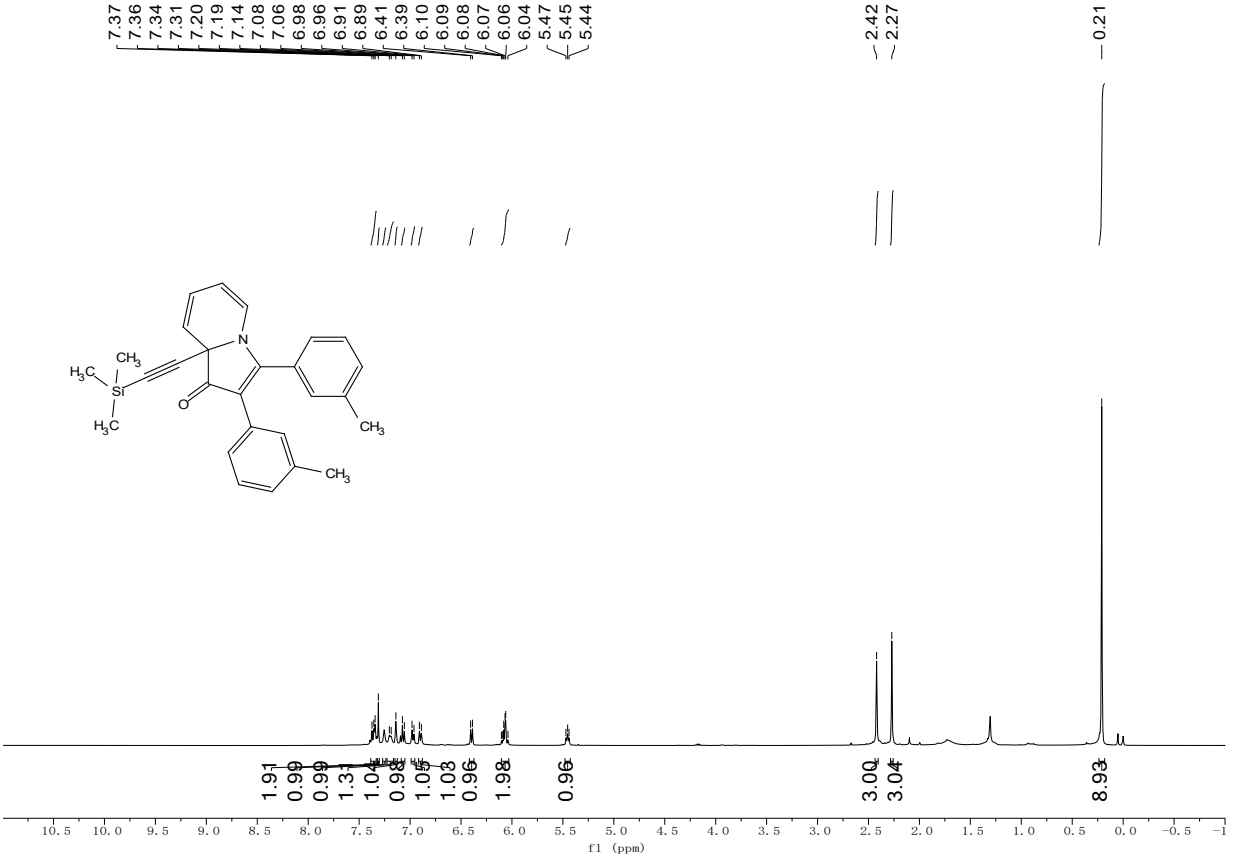


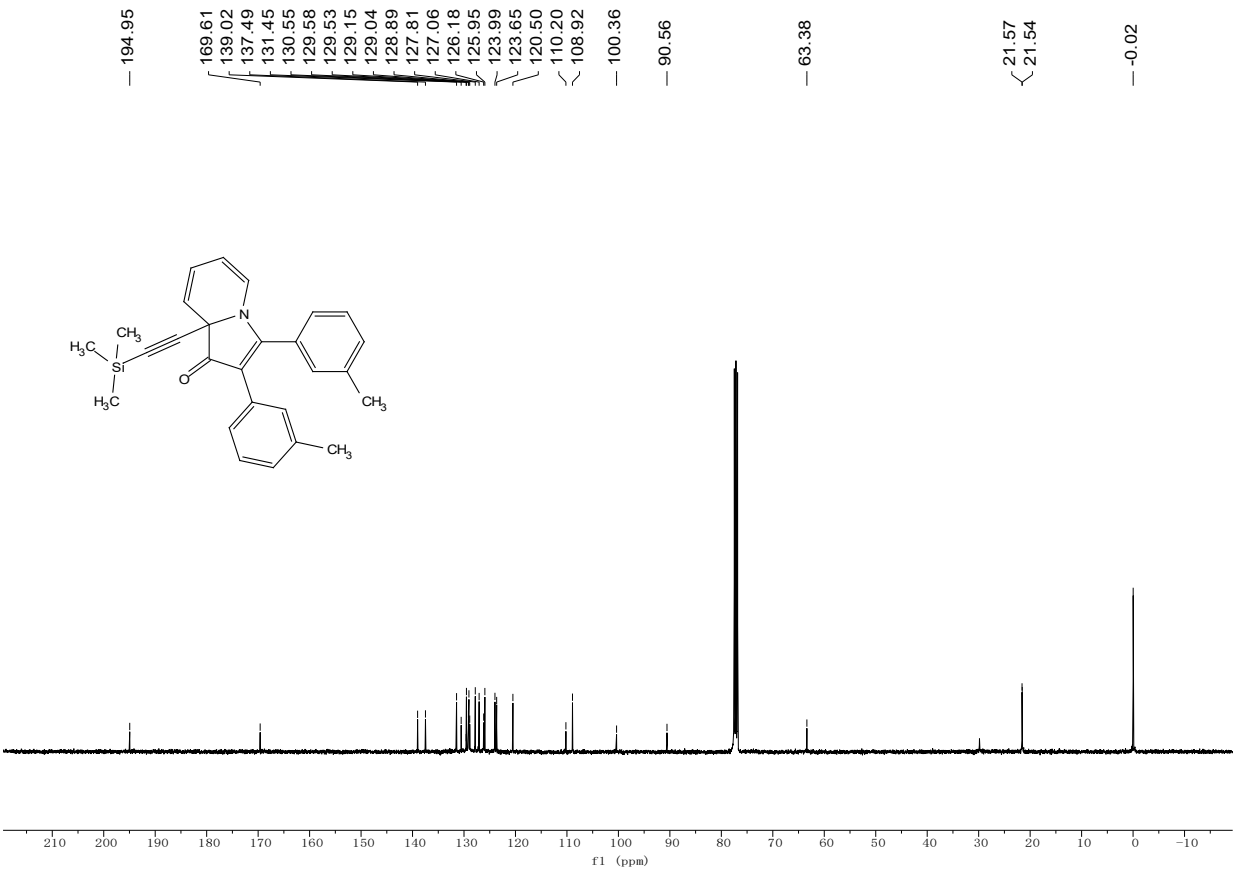


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3k**

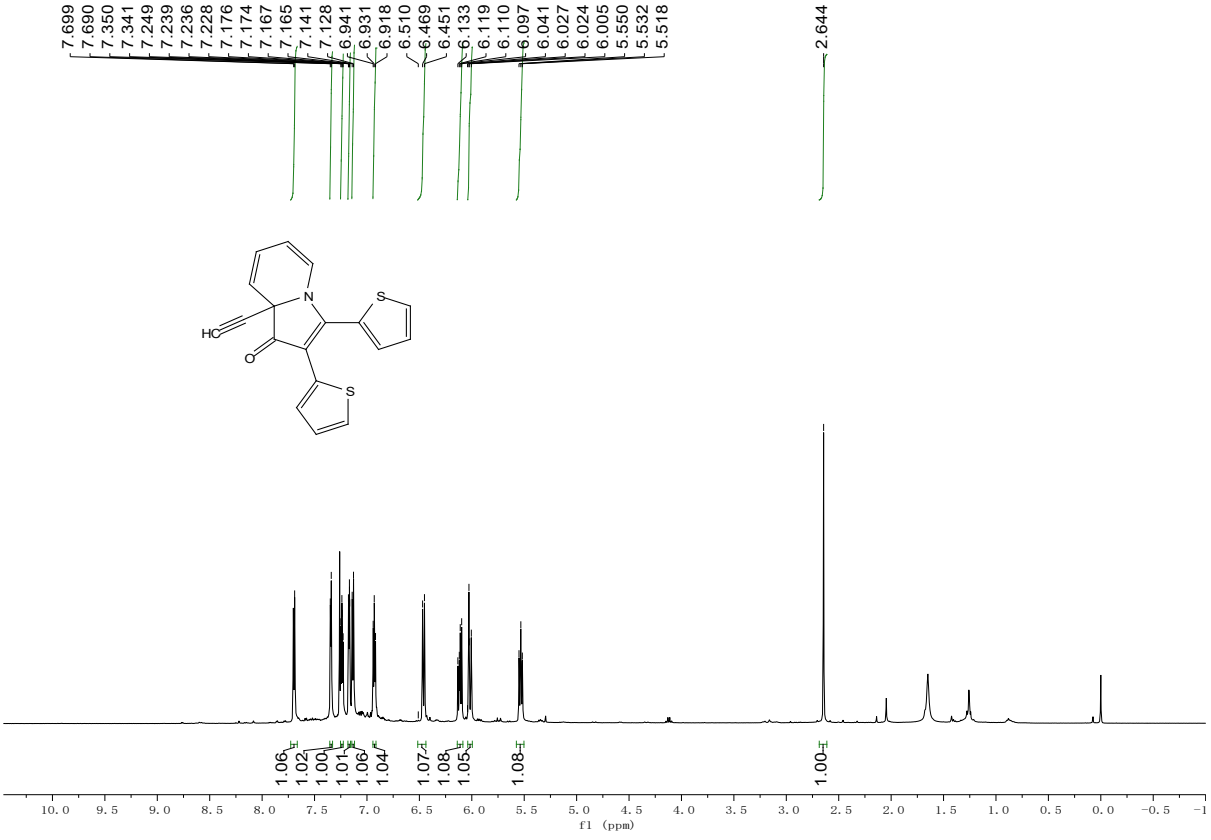


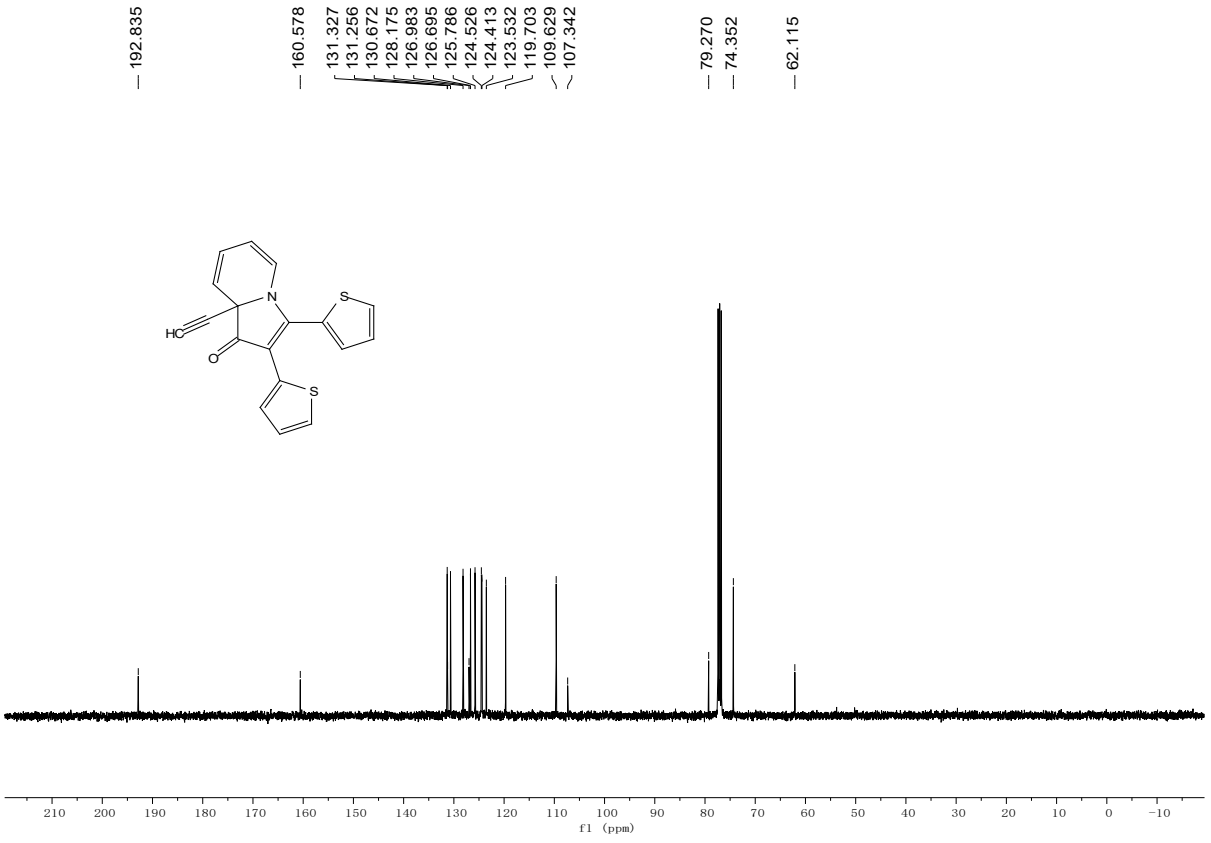
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3l**



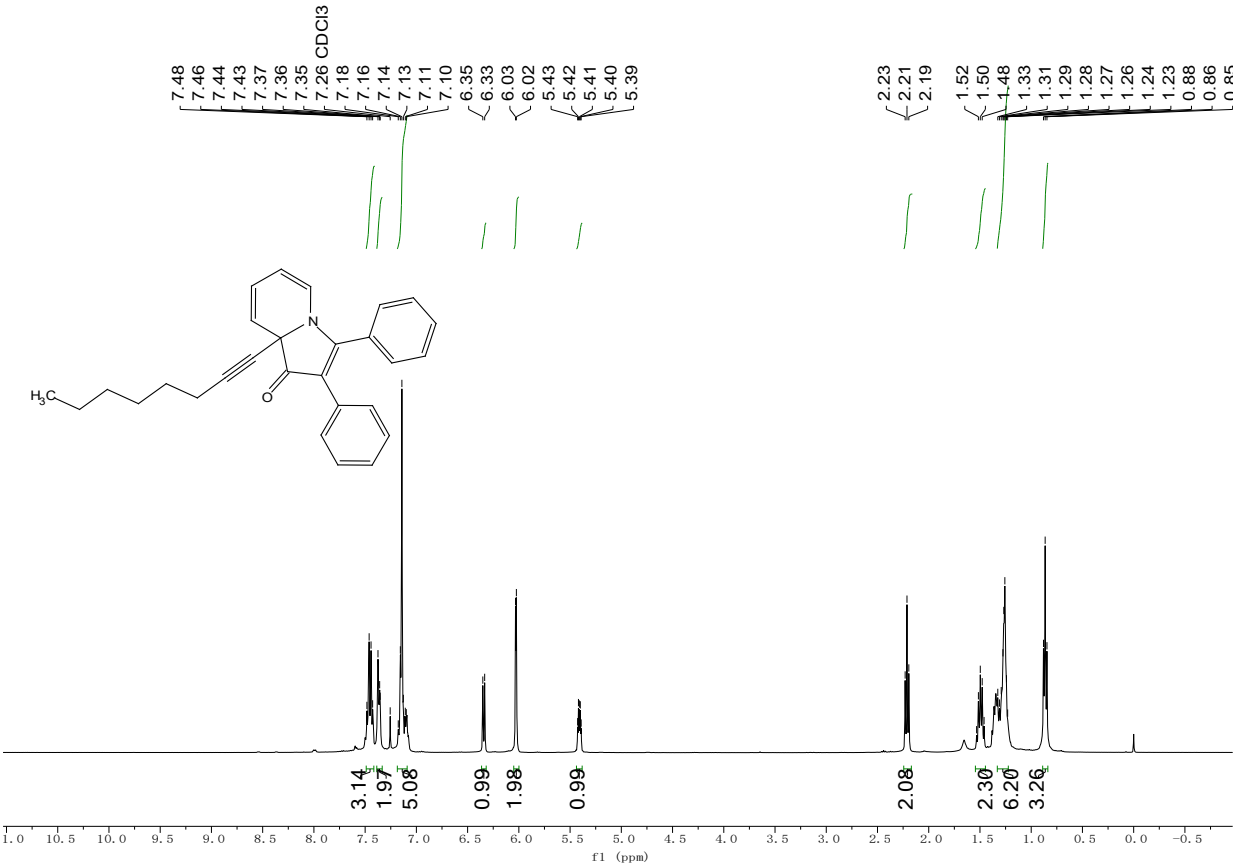


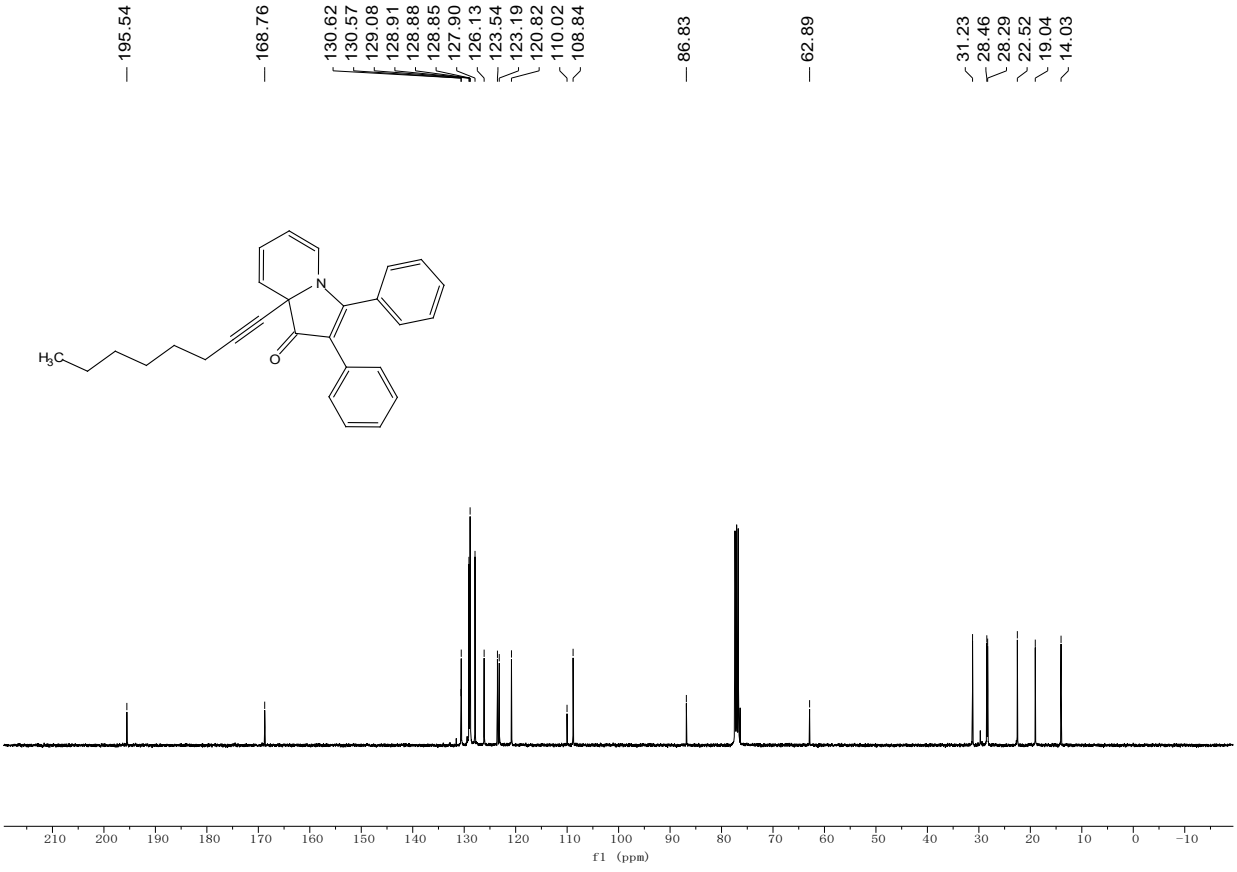
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3m**



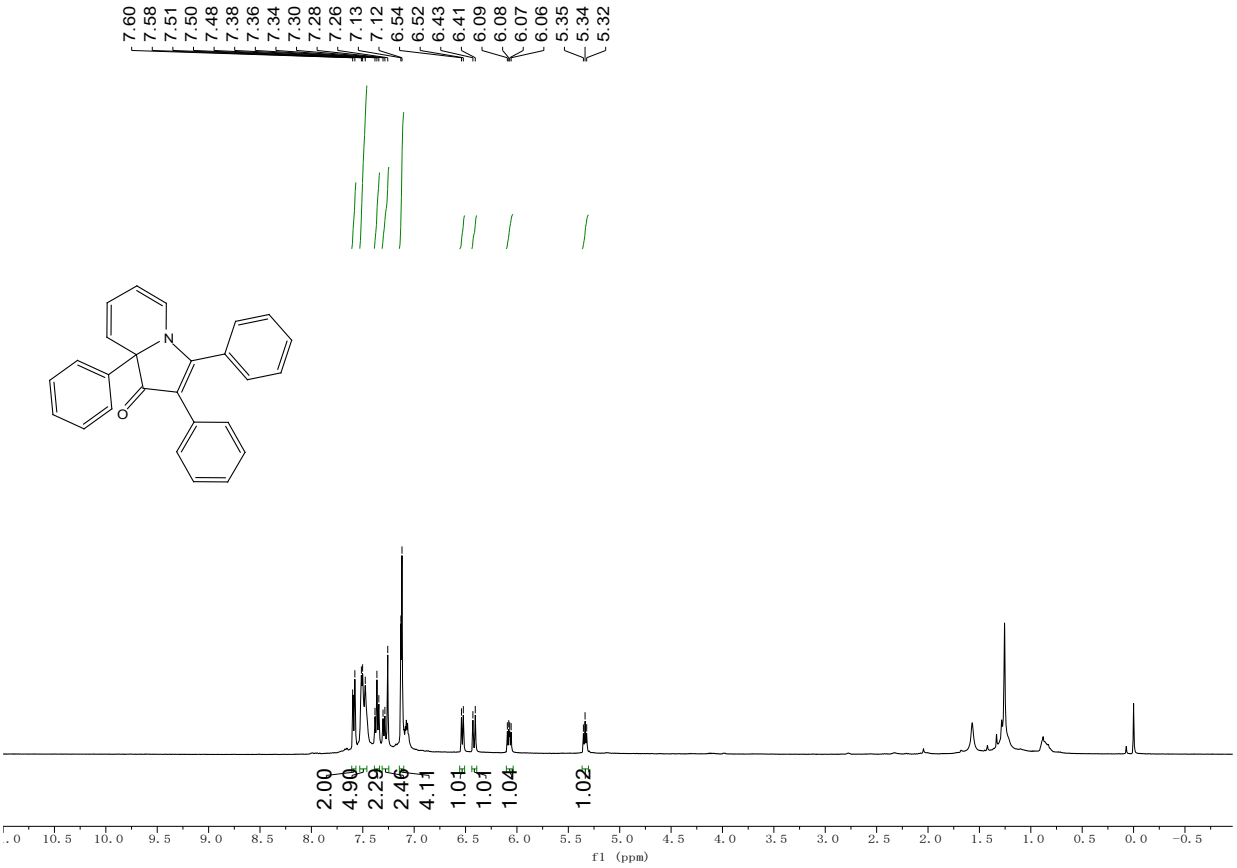


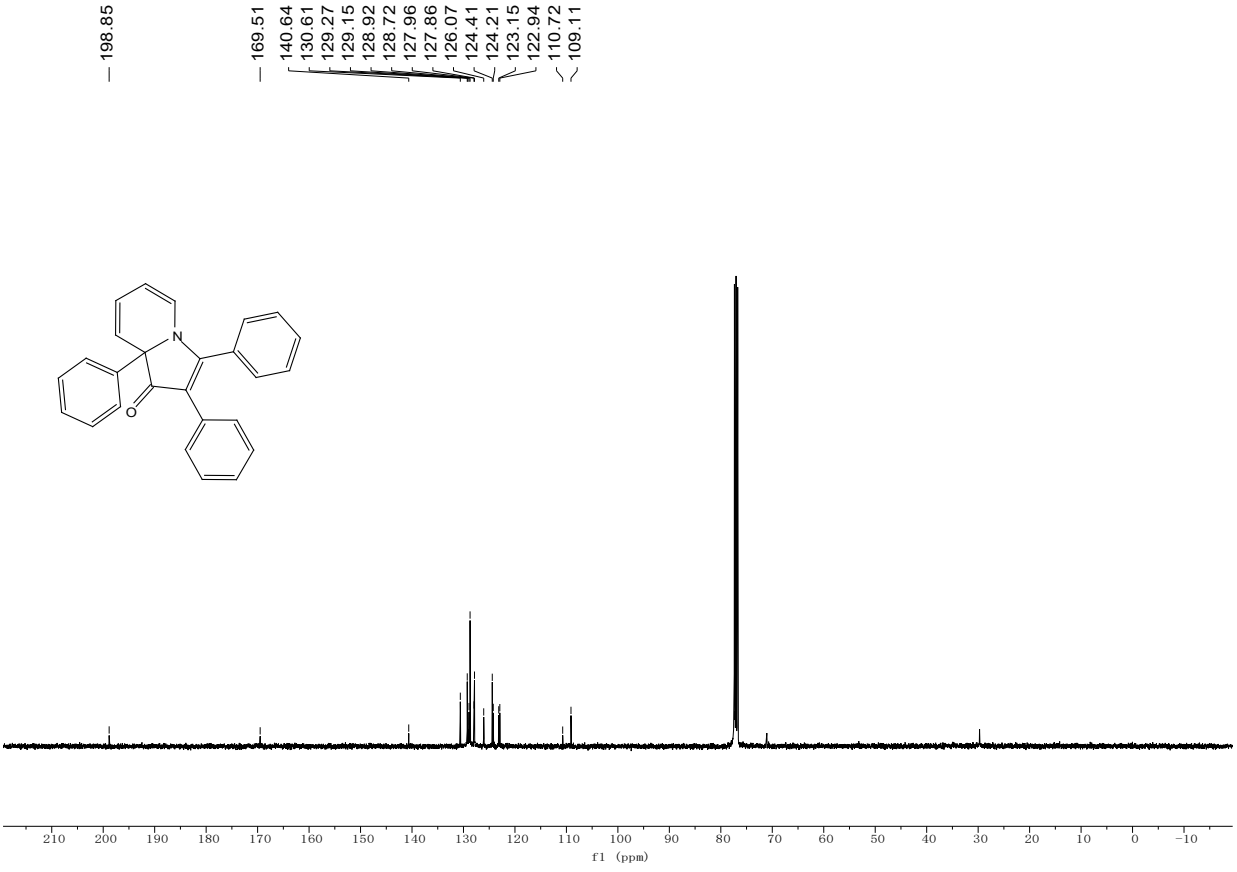
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3n**



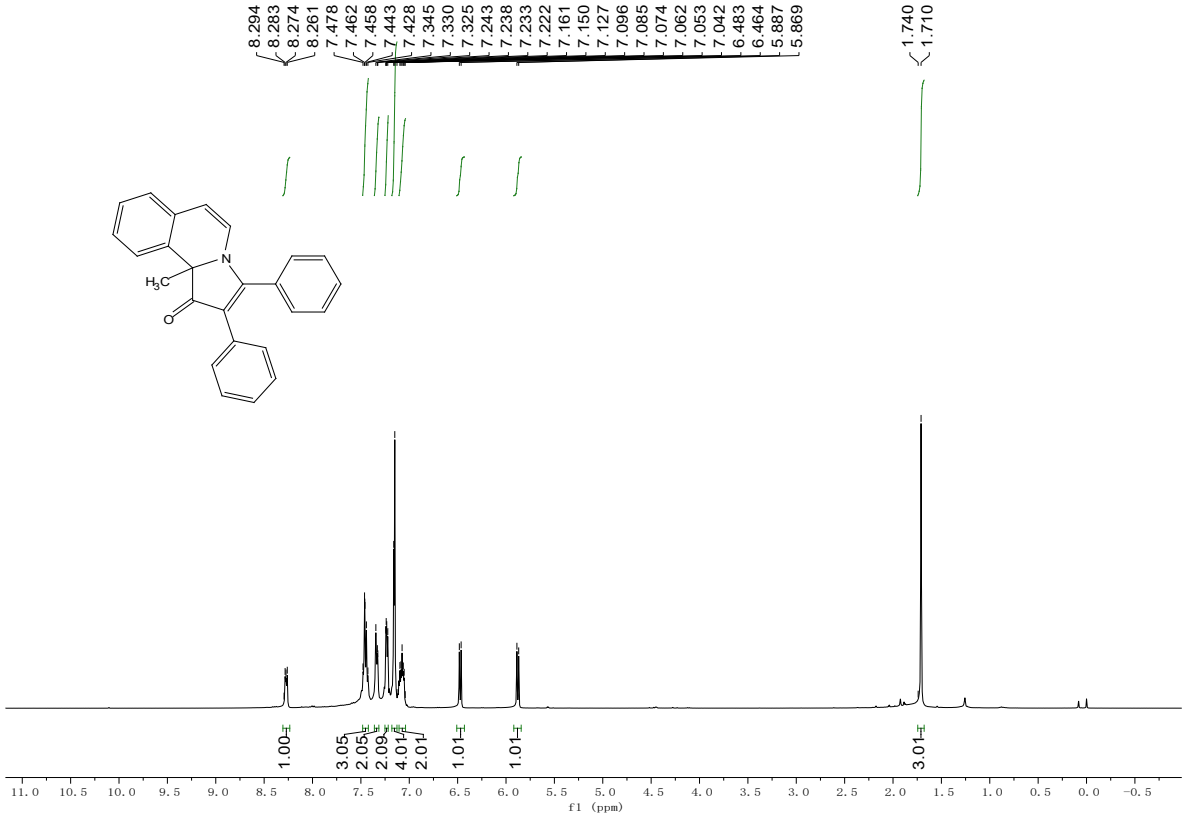


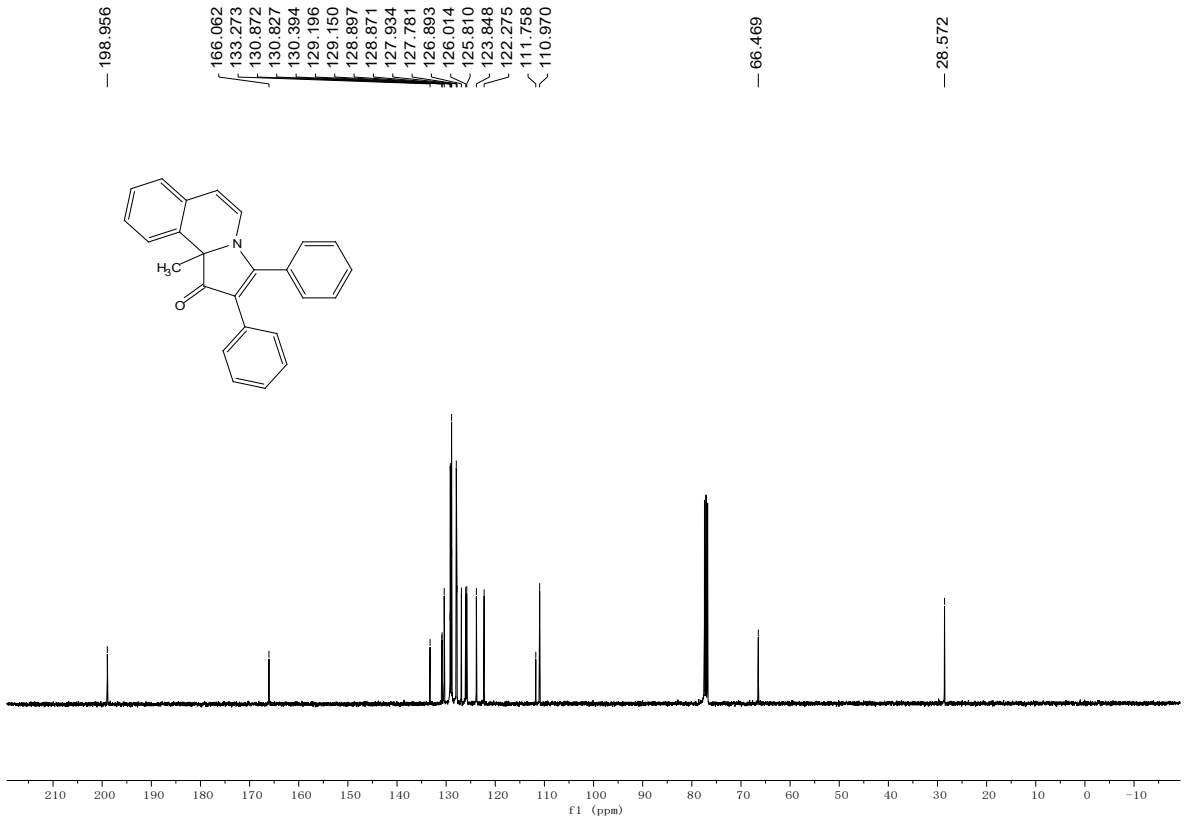
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4a**



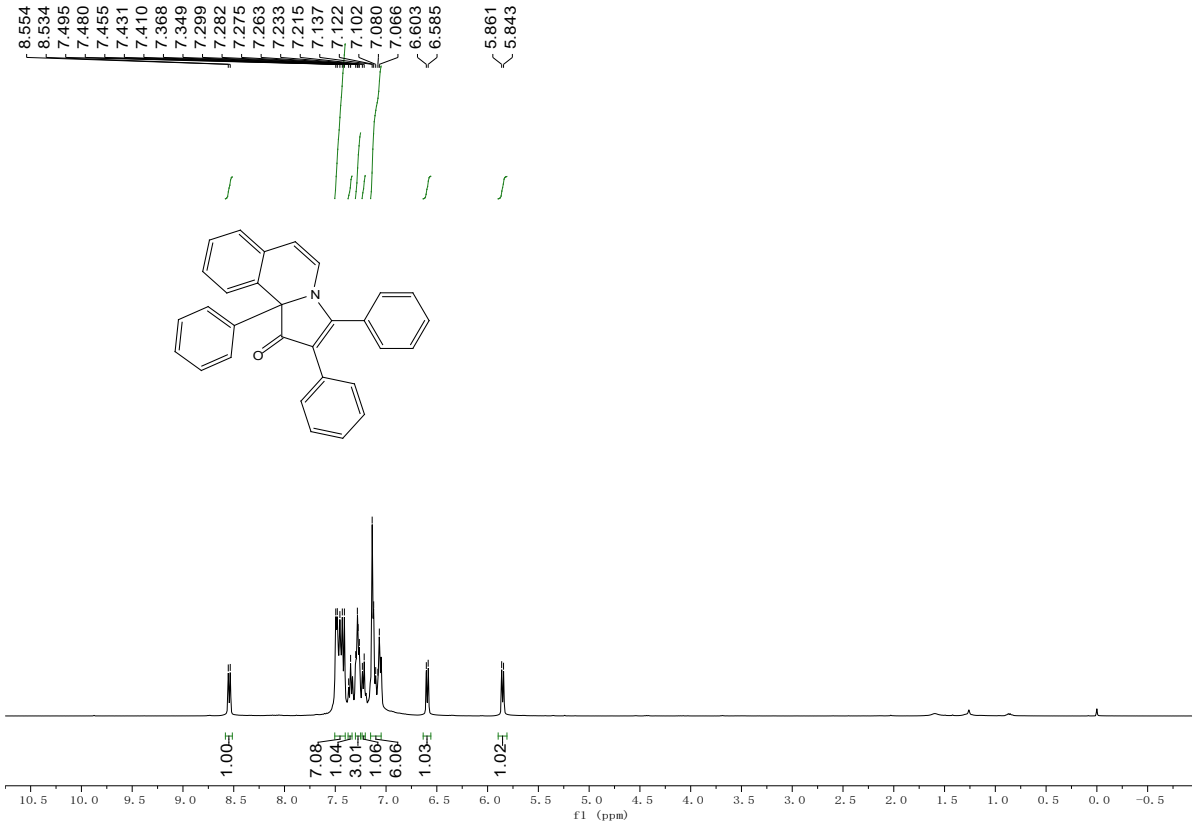


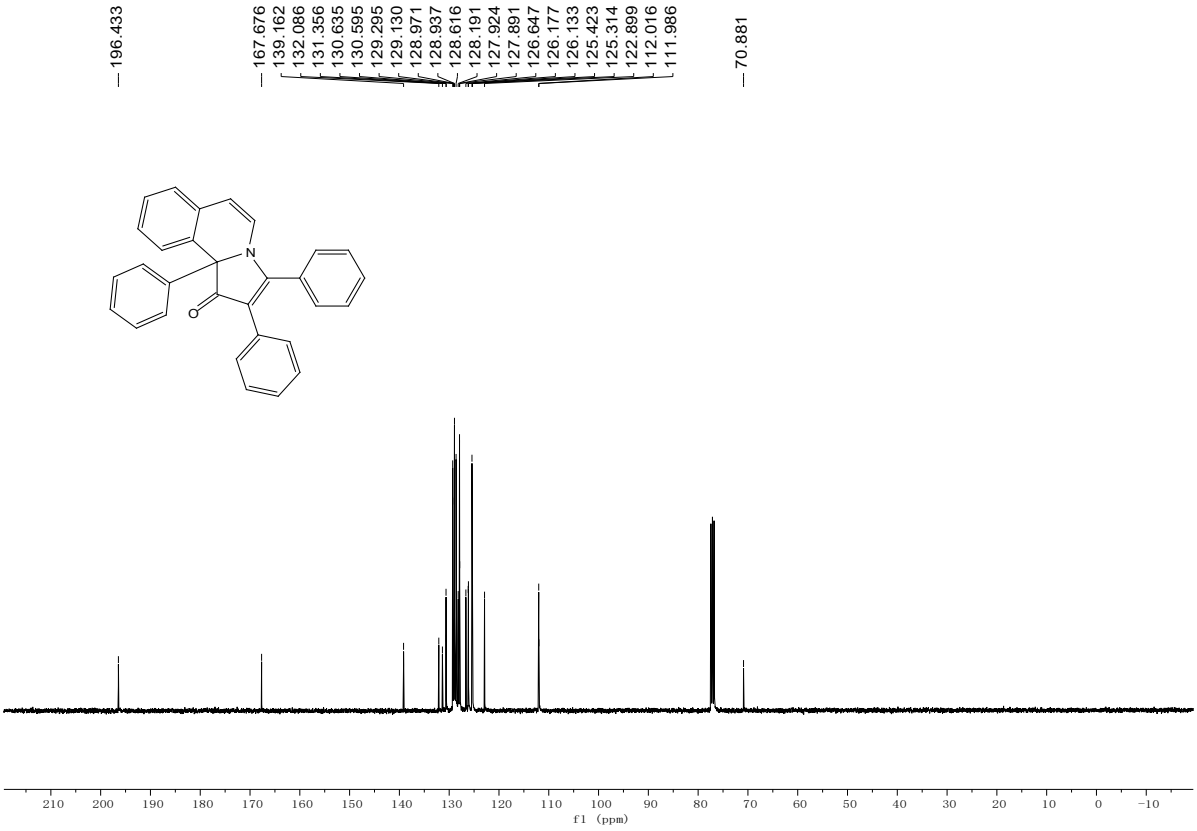
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6a**



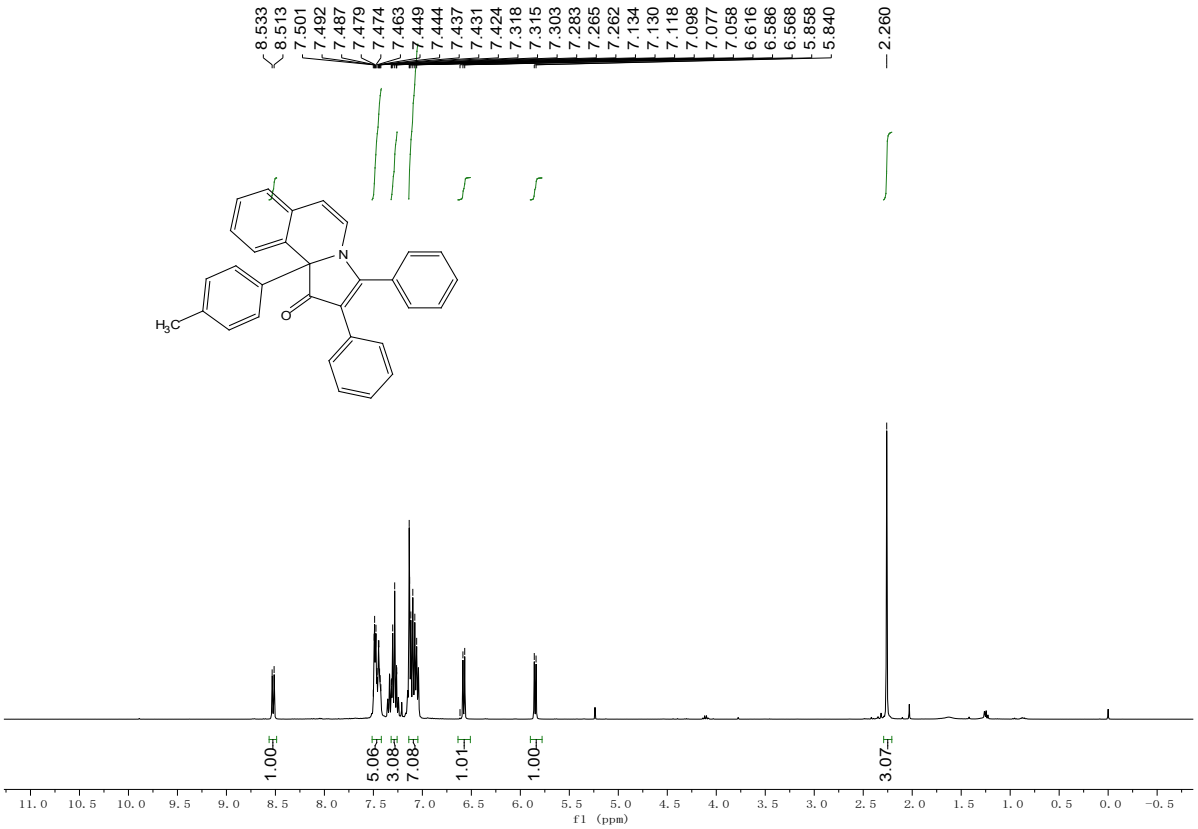


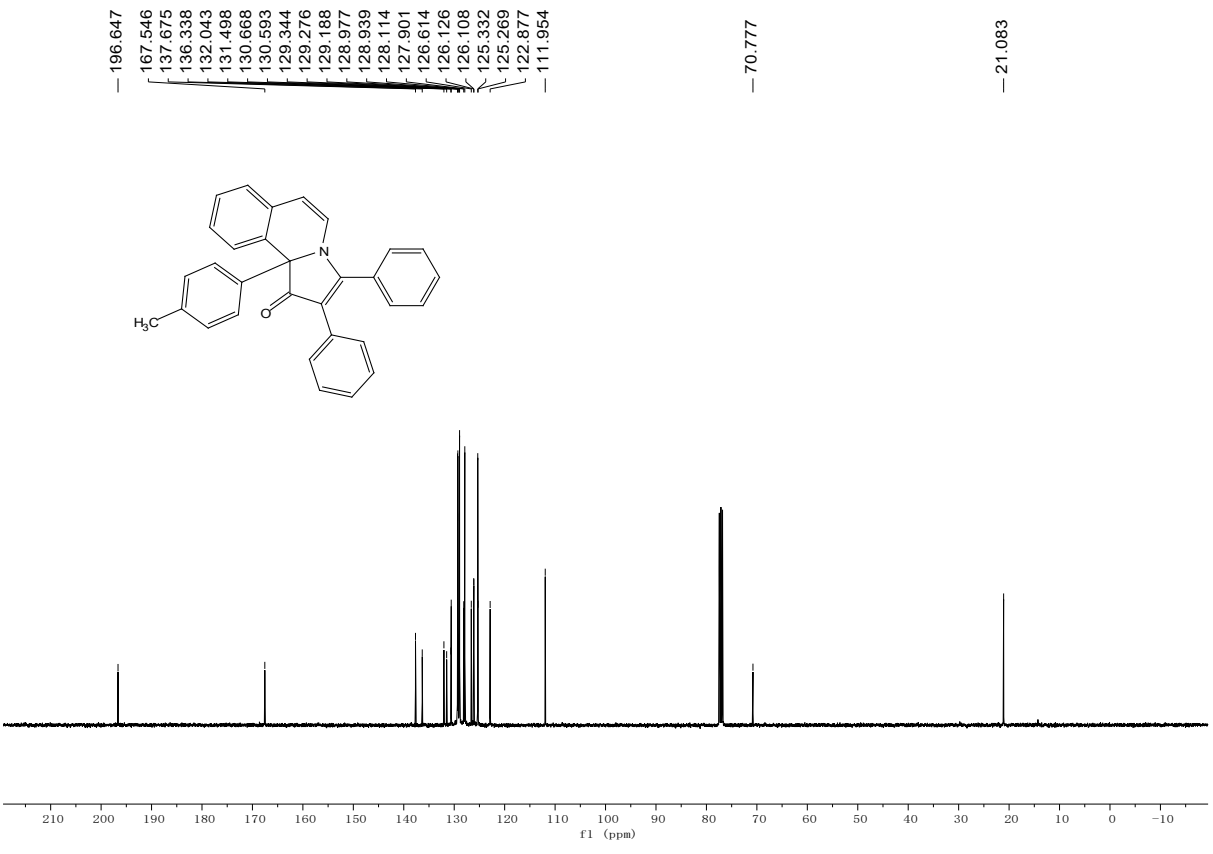
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6b**



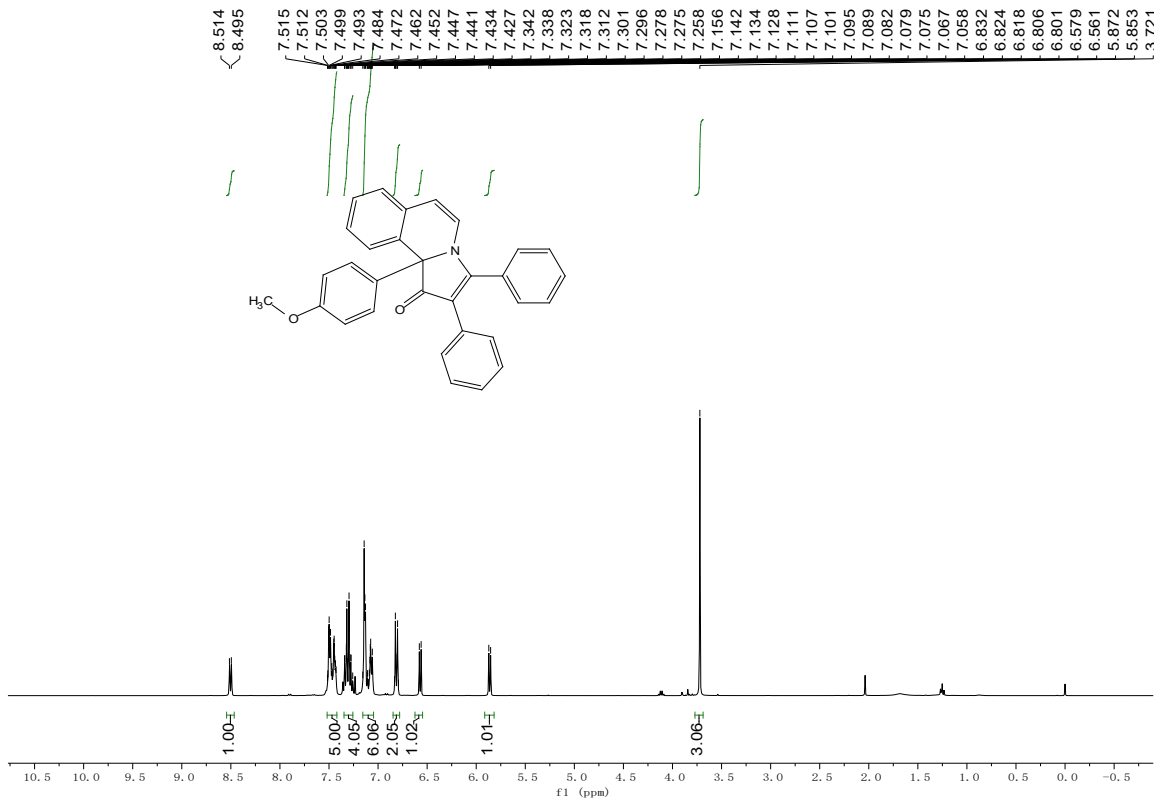


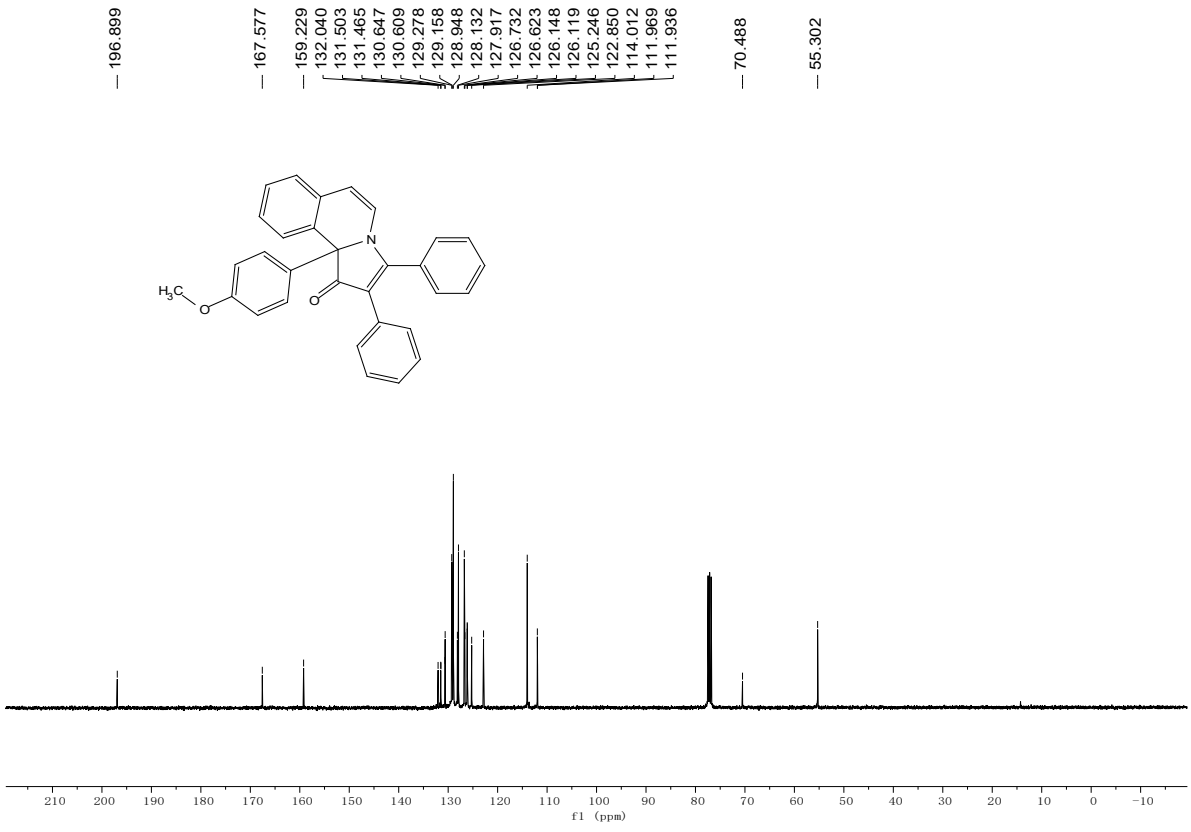
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6c**



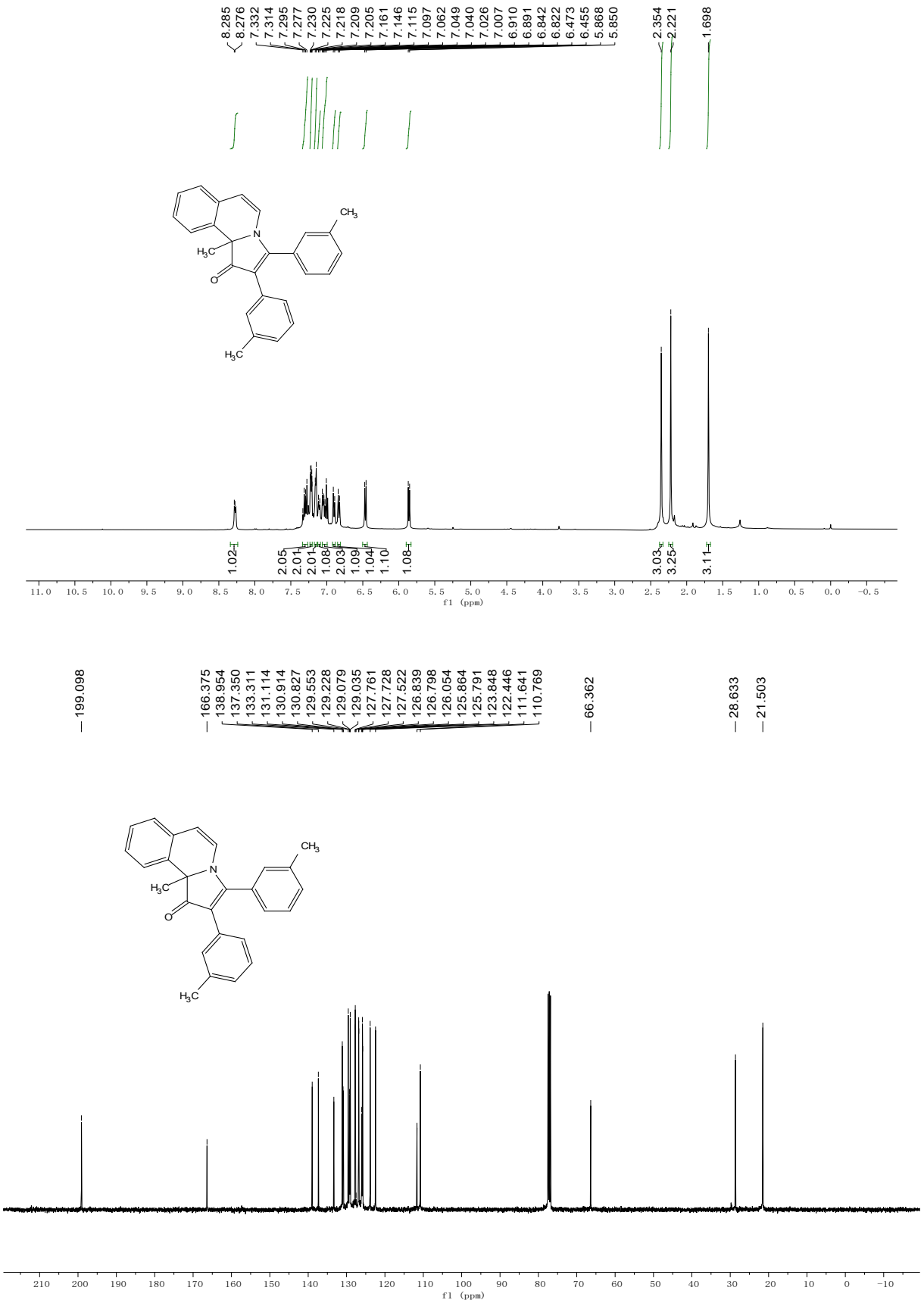


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6d**

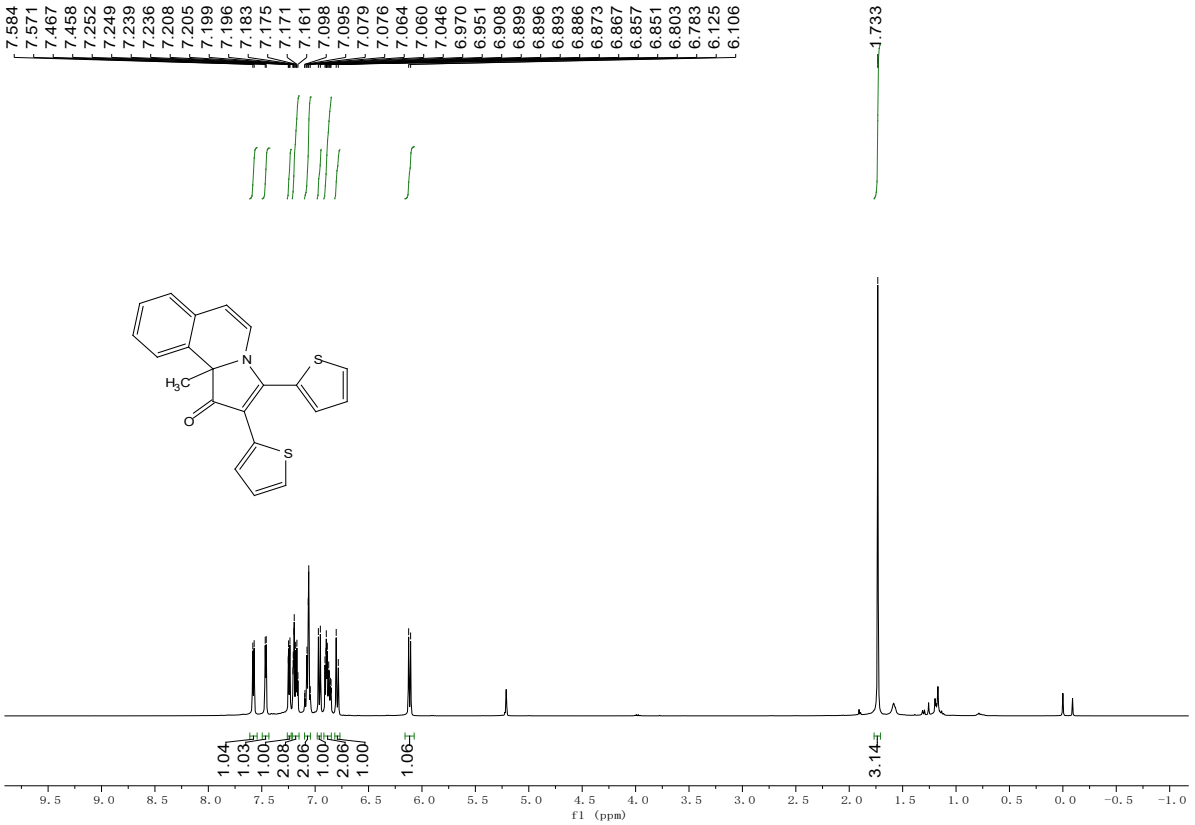


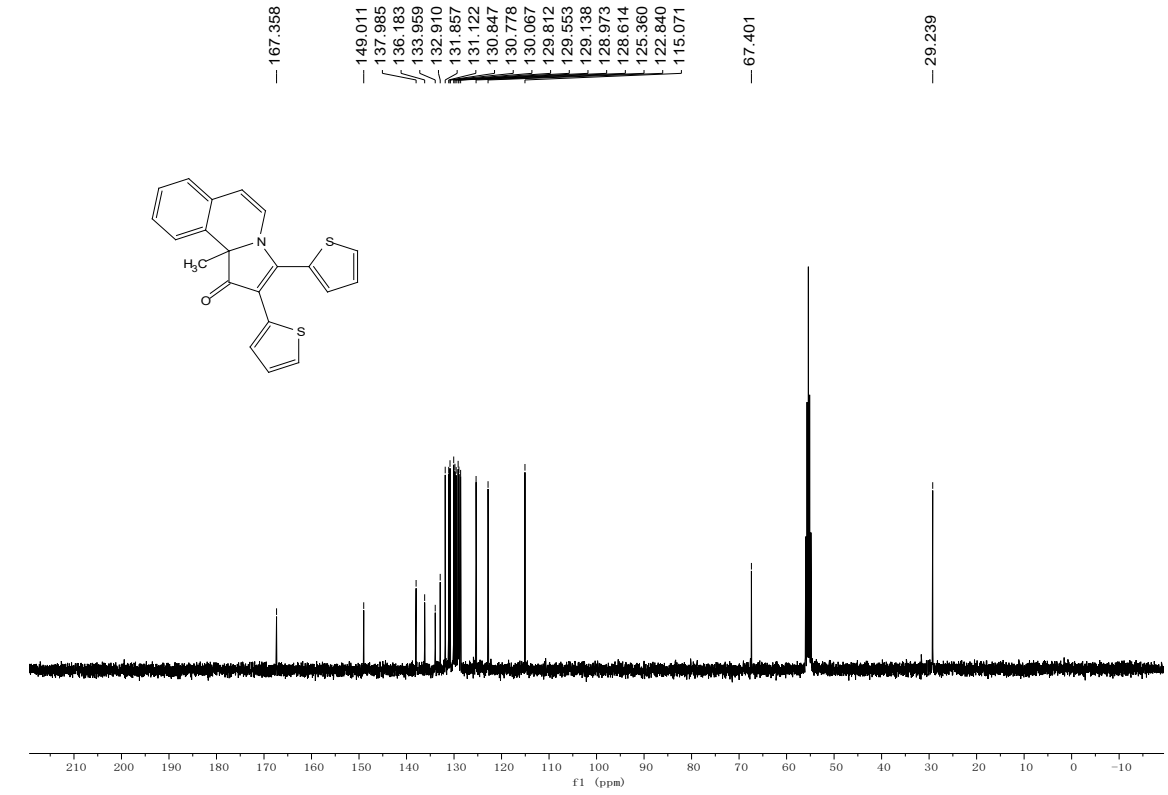


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6e**

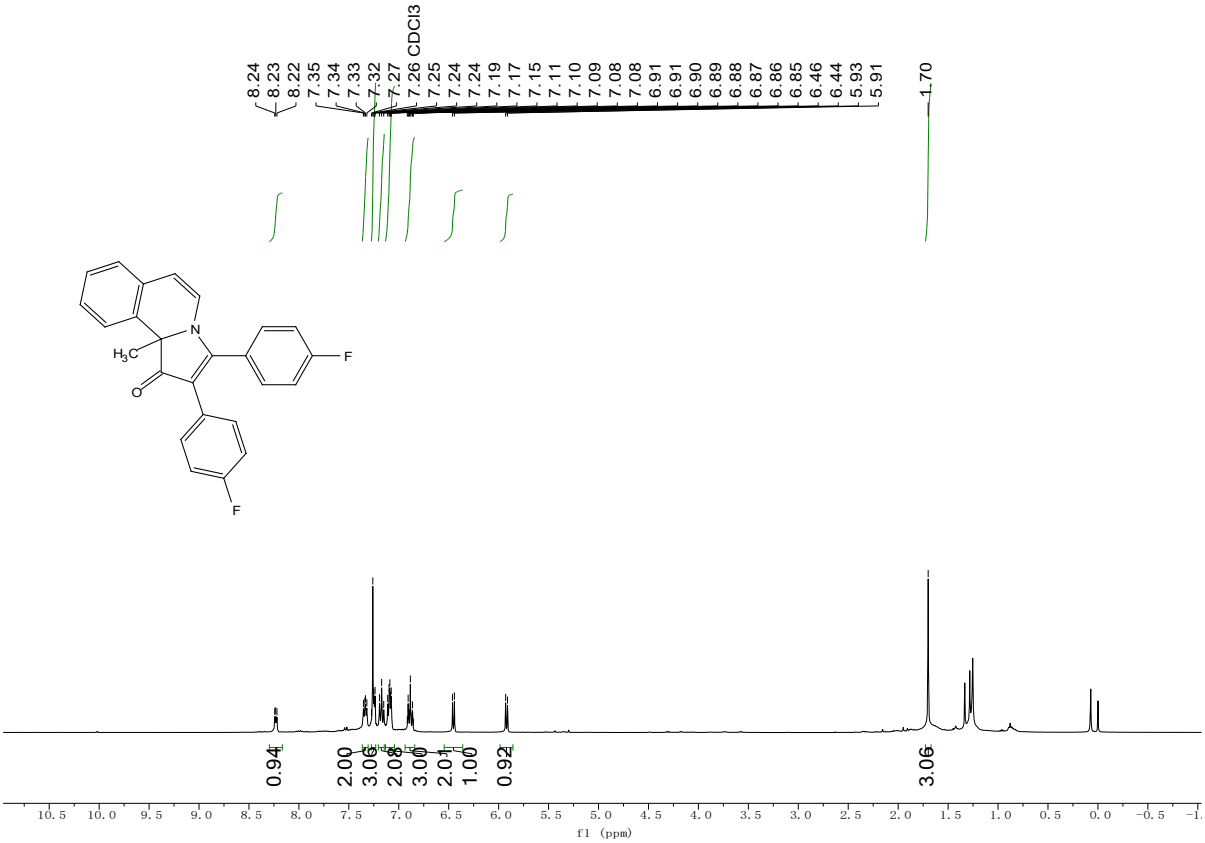


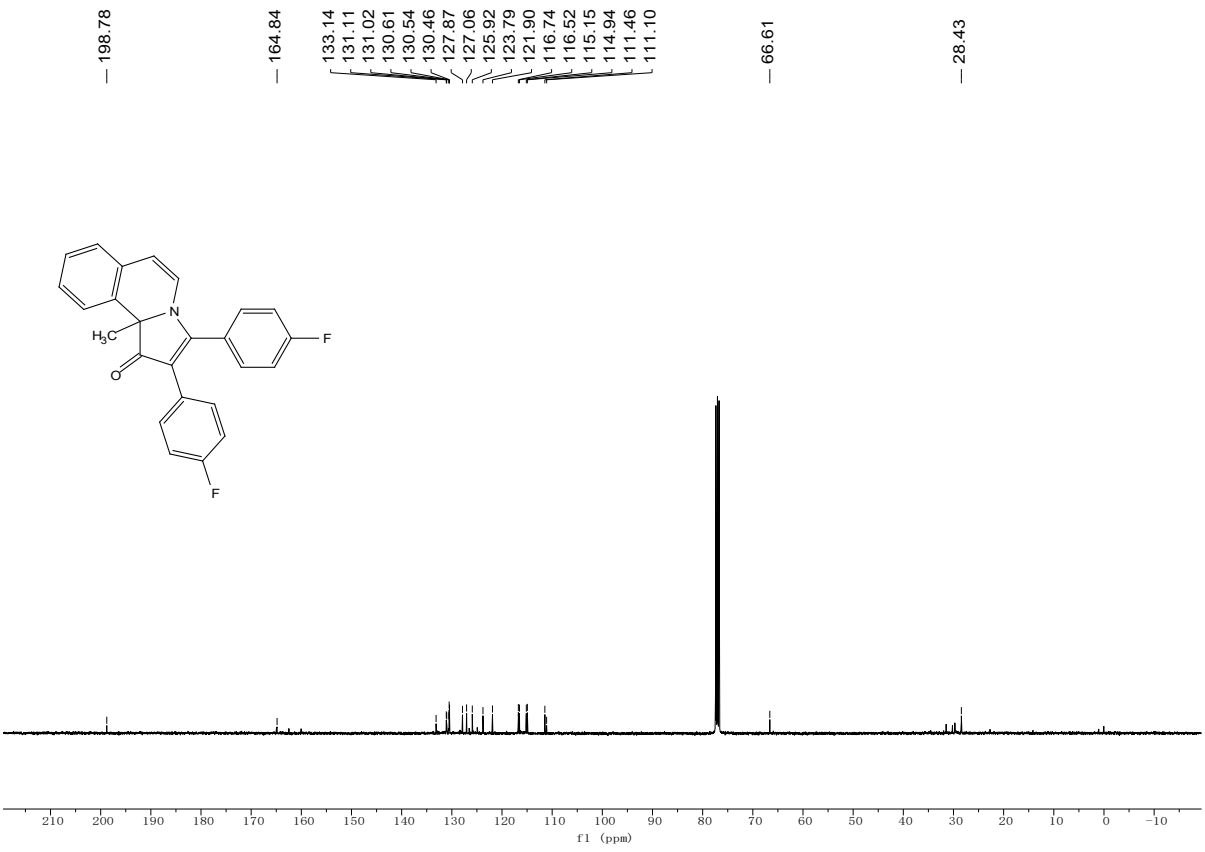
^{1}H NMR (400 MHz, CD_2Cl_2) and ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of compound **6f**



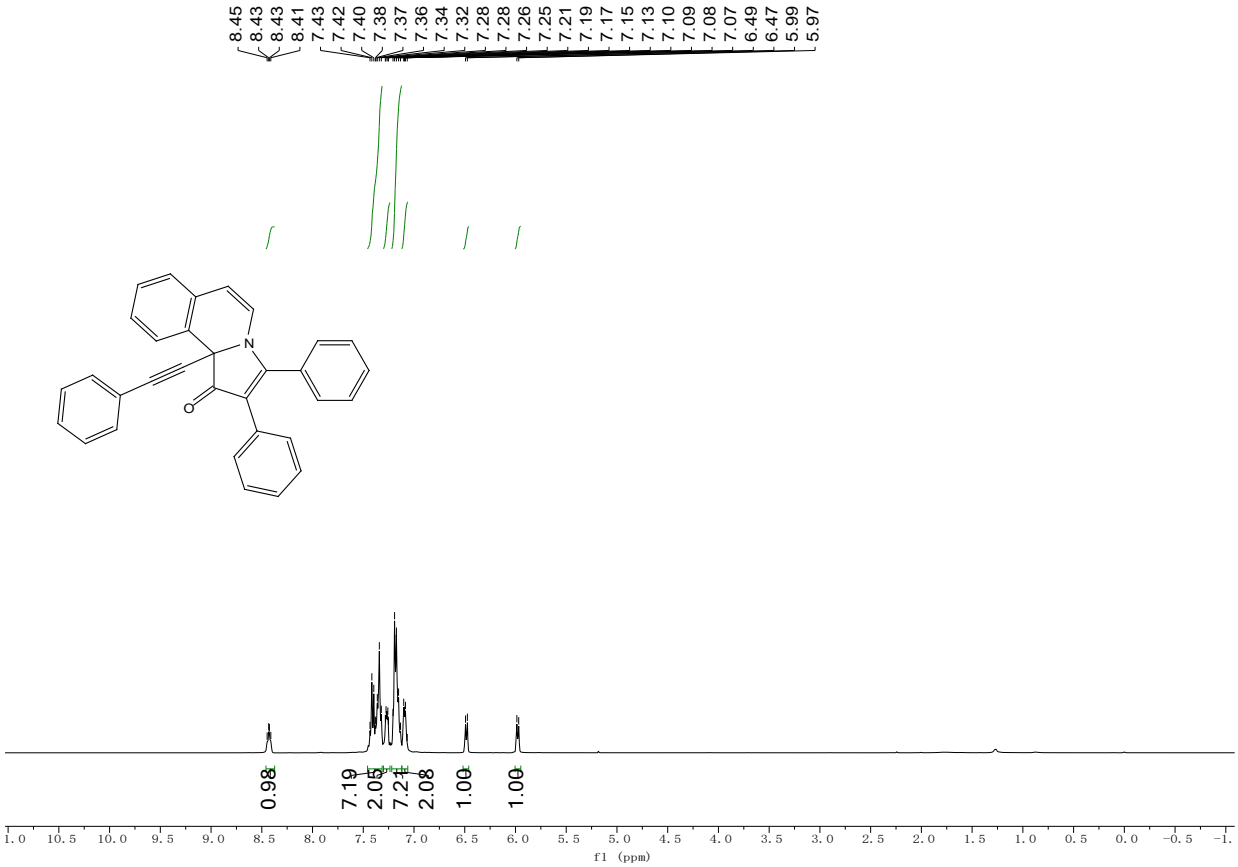


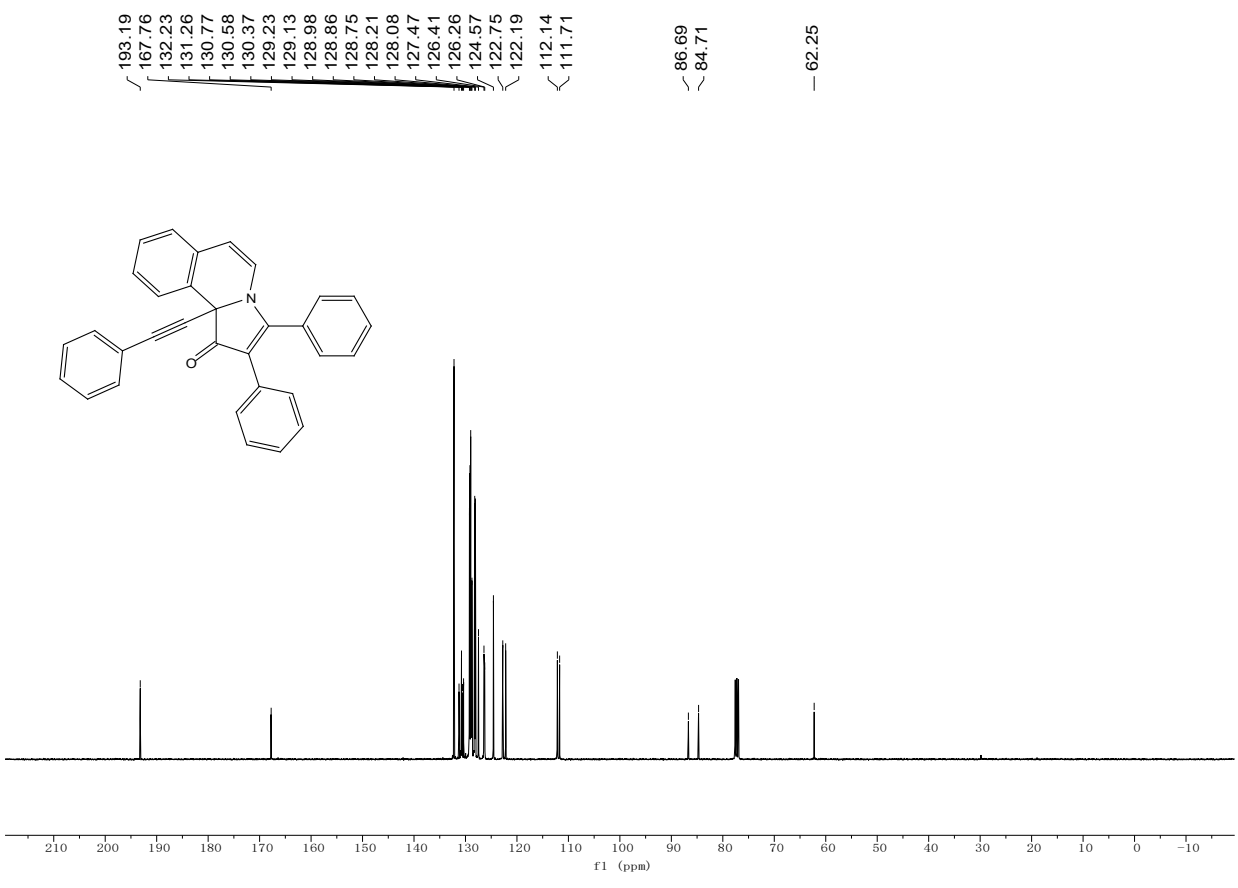
^{1}H NMR (400 MHz, CD_2Cl_2) and ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of compound **6g**



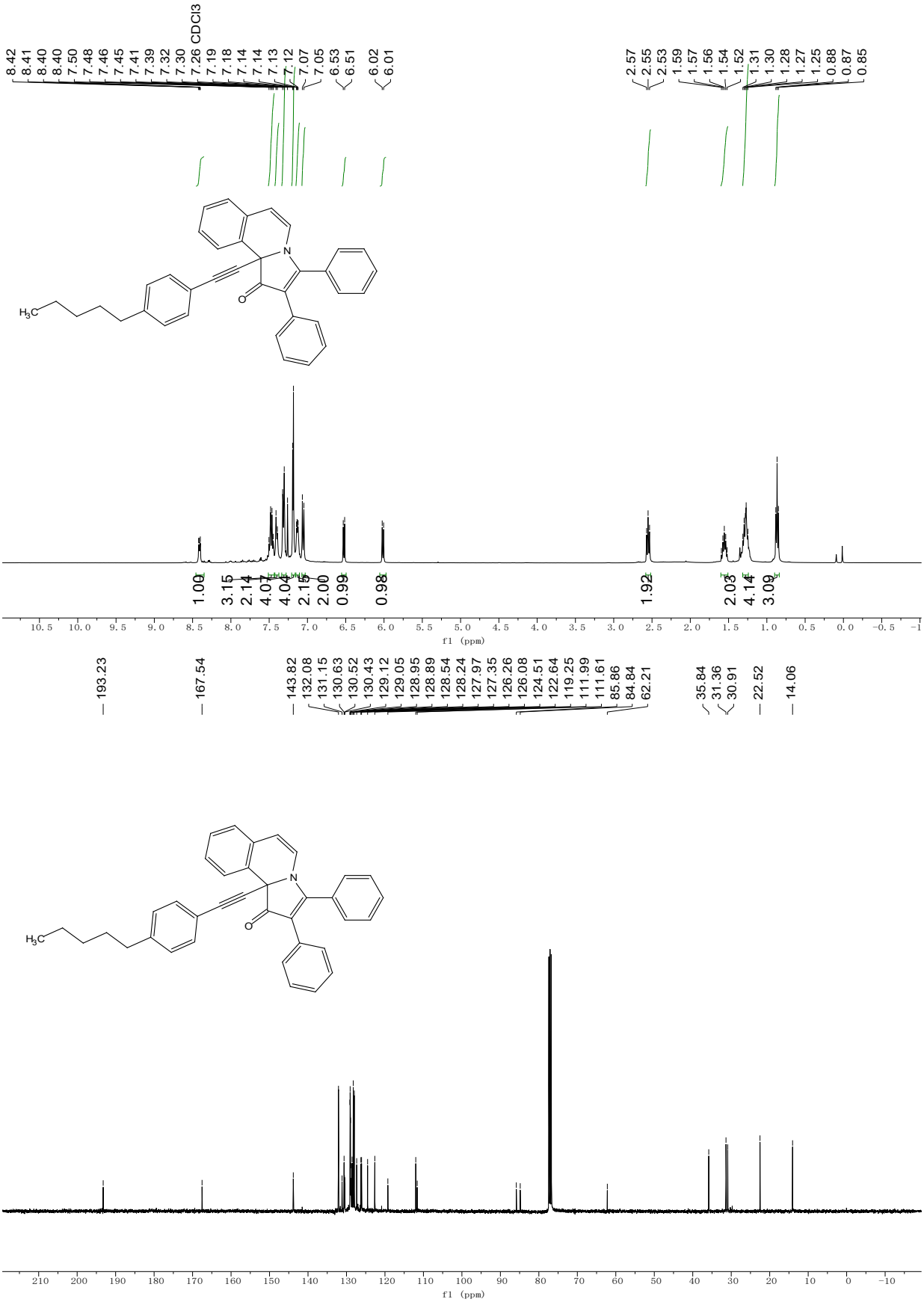


^{1}H NMR (400 MHz, CD_2Cl_2) and ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of compound **6h**

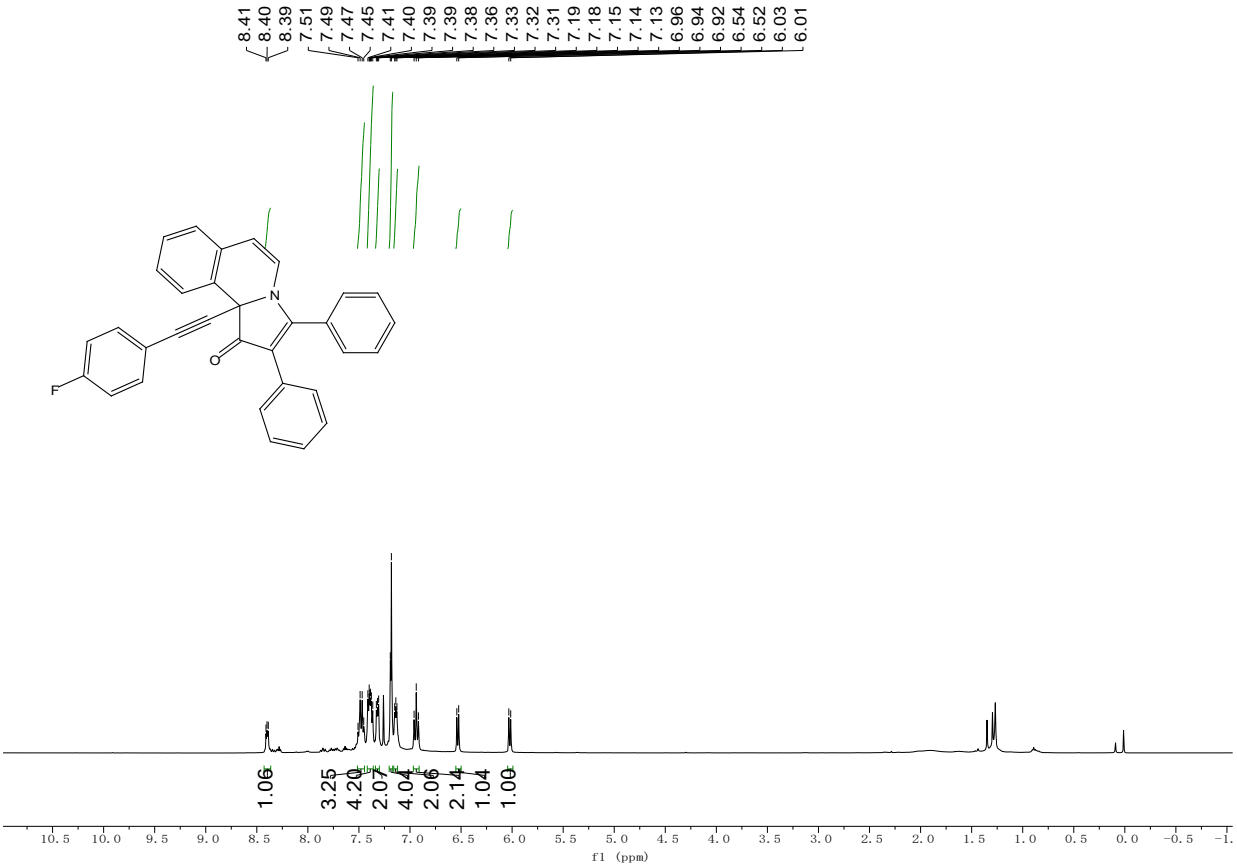


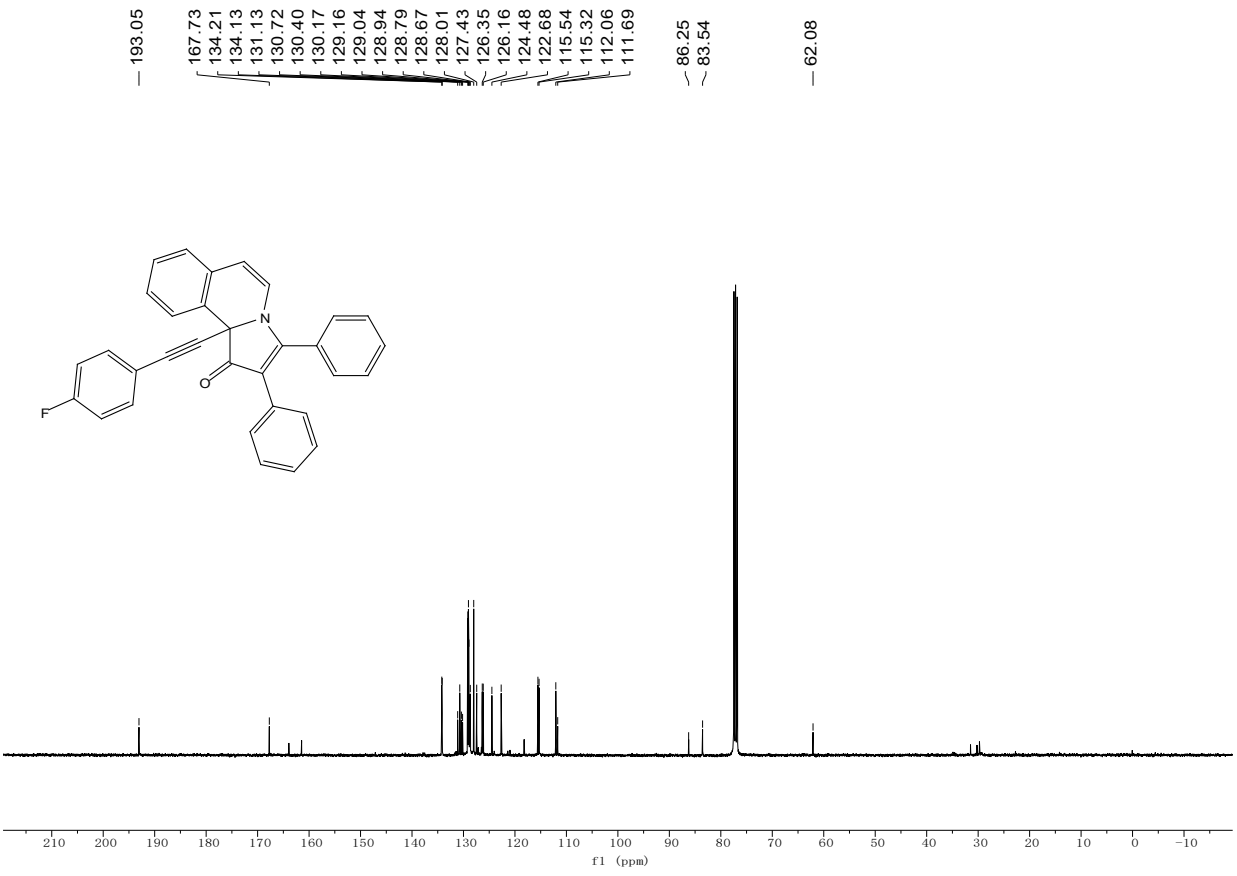


^{1}H NMR (400 MHz, CD_2Cl_2) and ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of compound **6i**

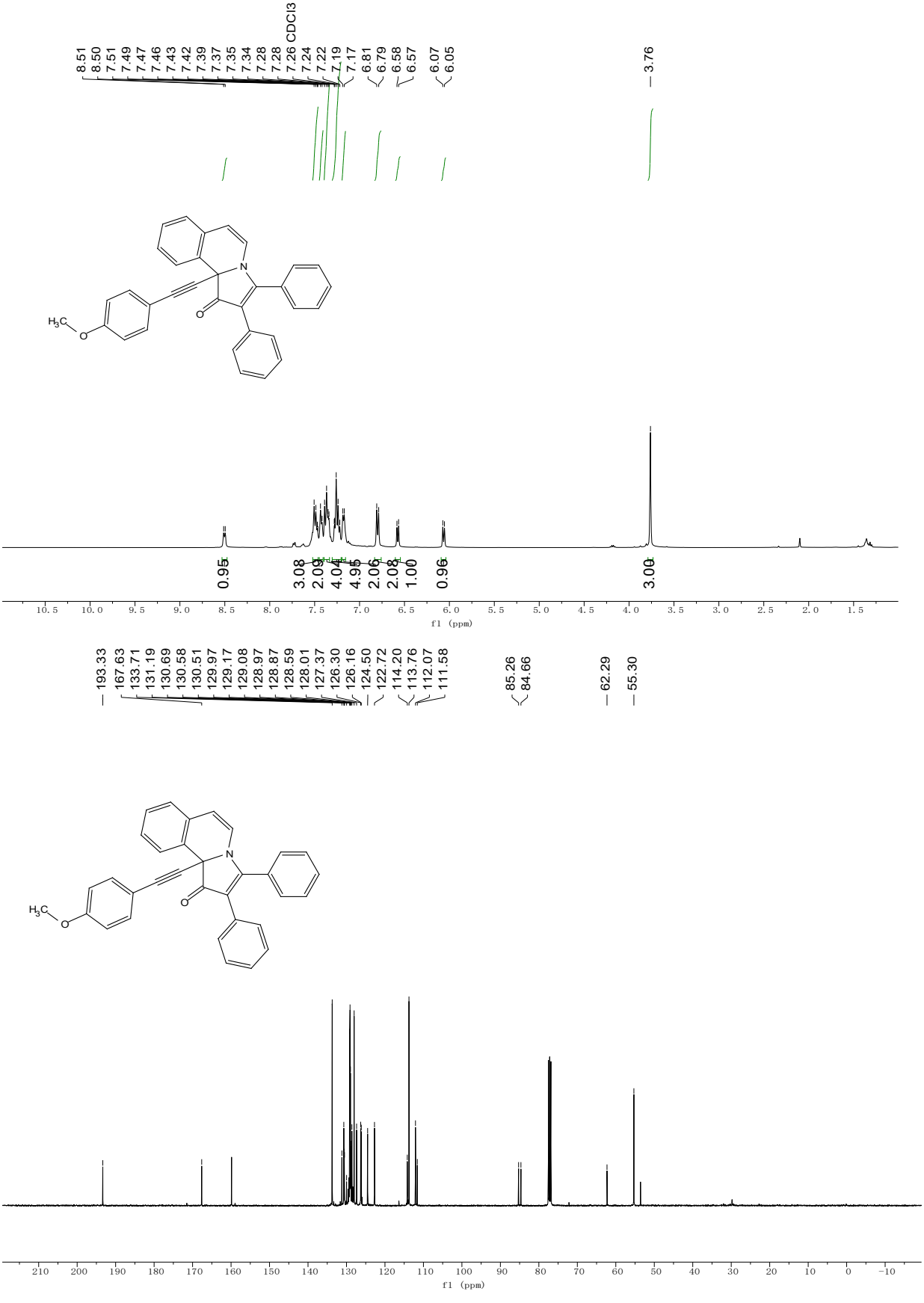


^{1}H NMR (400 MHz, CD_2Cl_2) and ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of compound **6j**

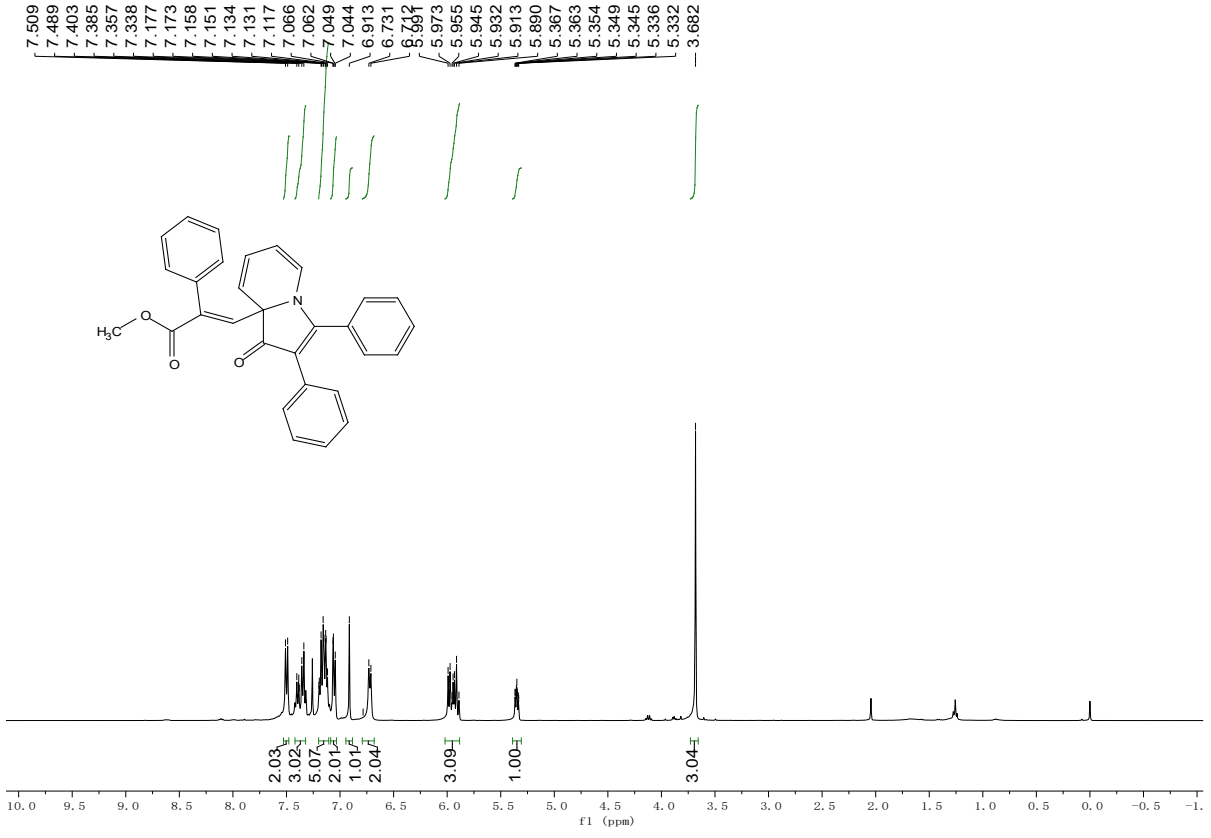


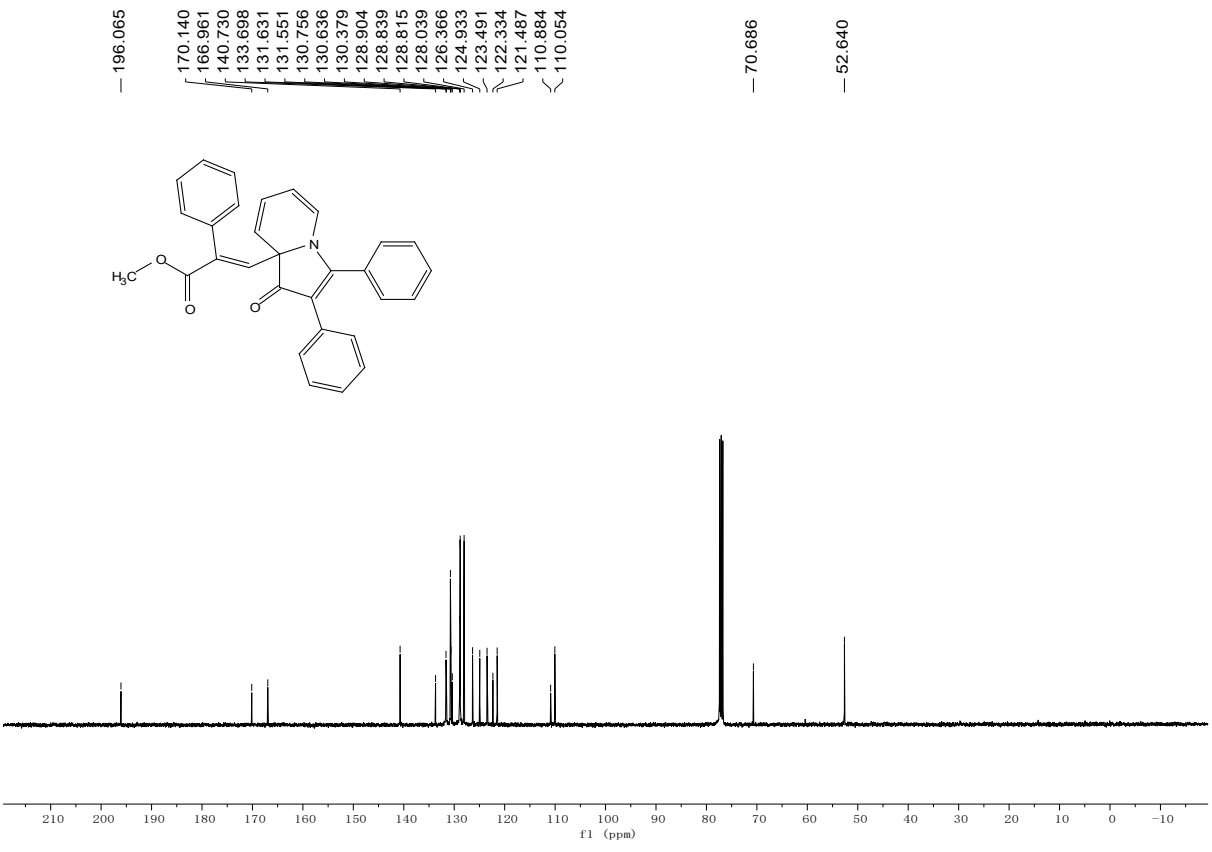


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6k**

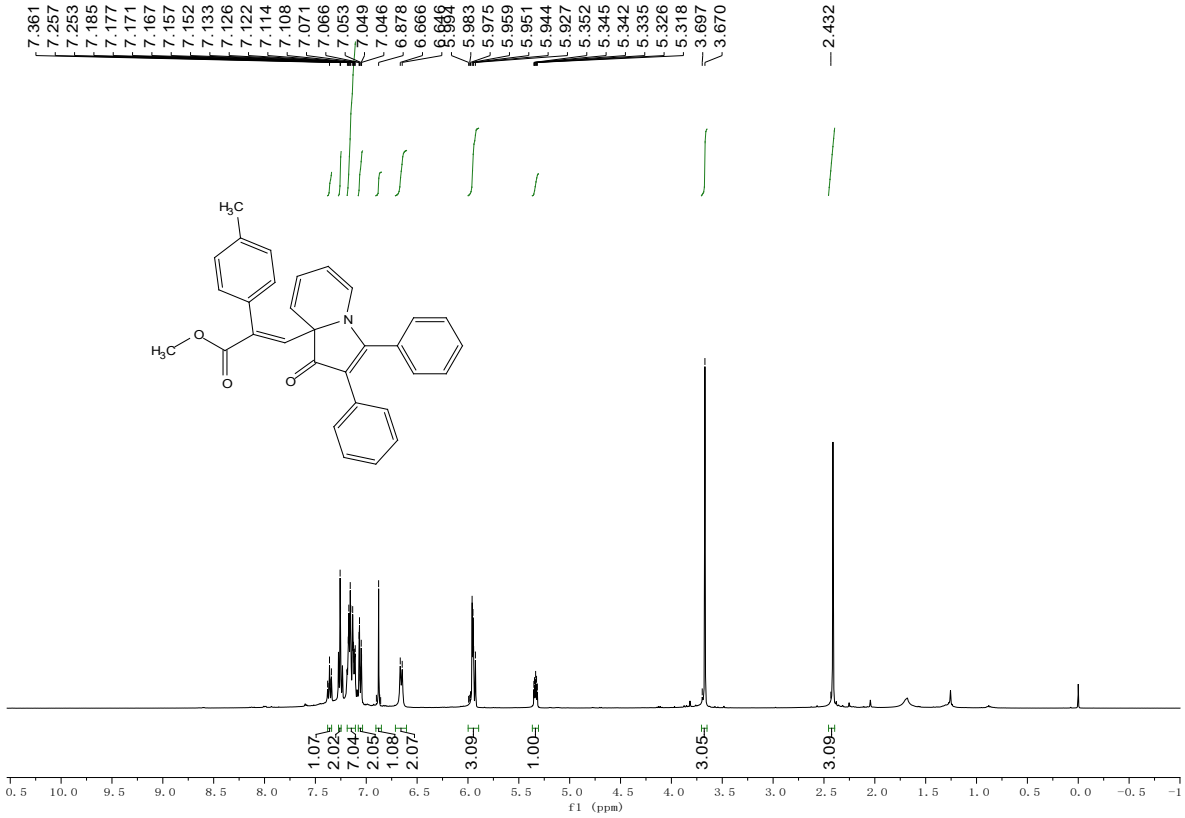


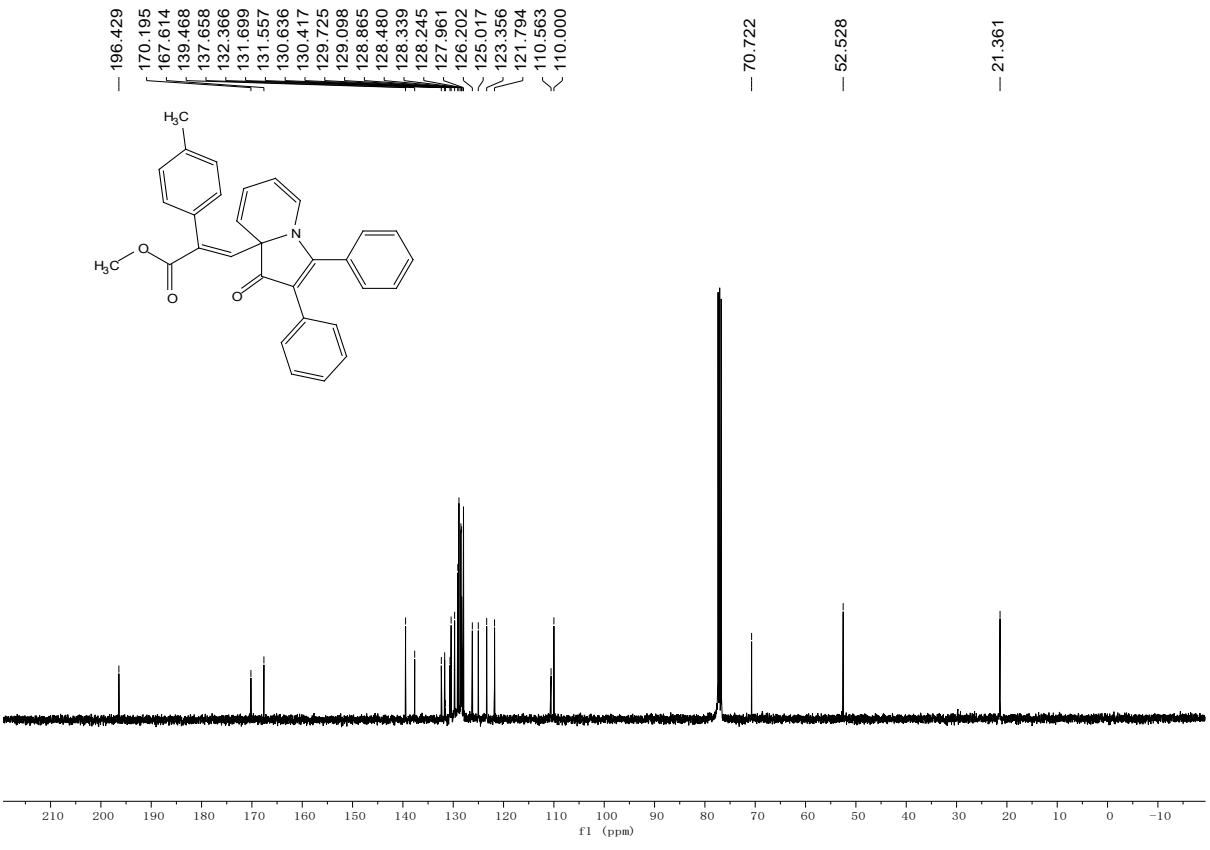
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8a**



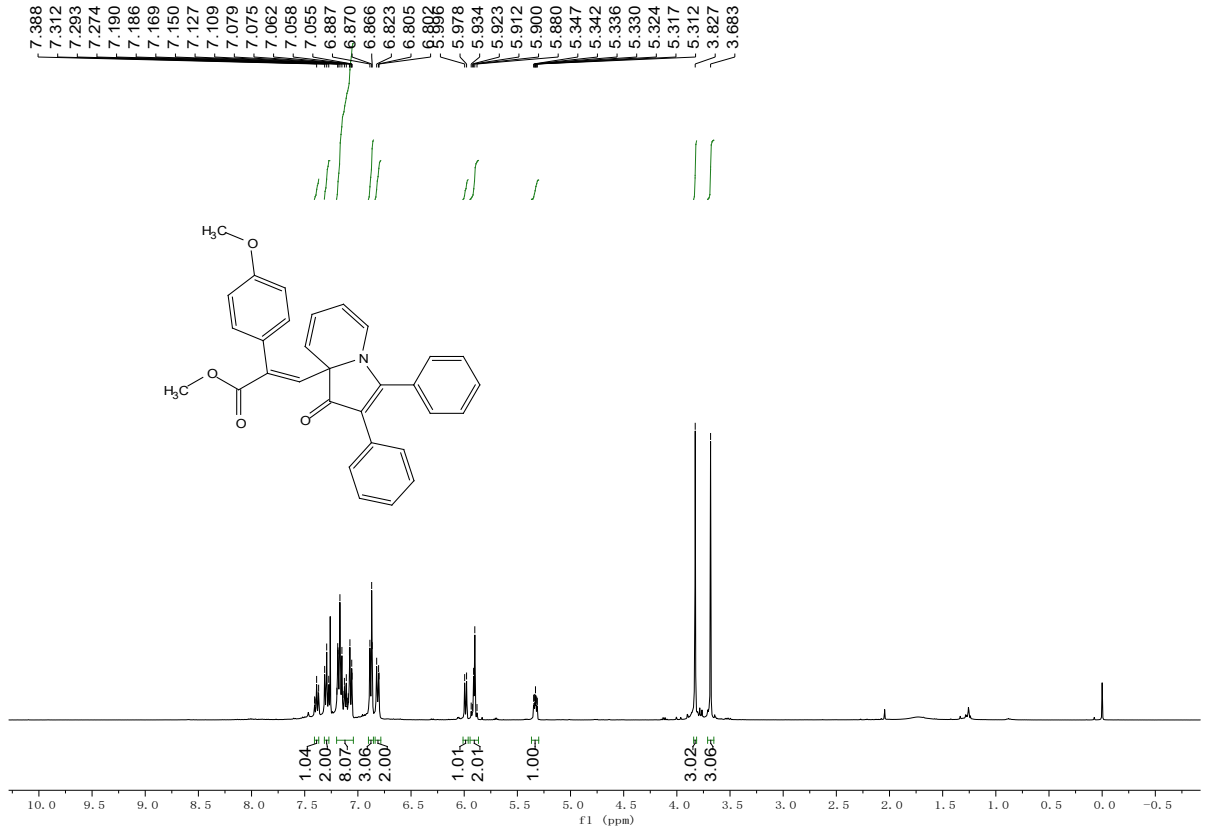


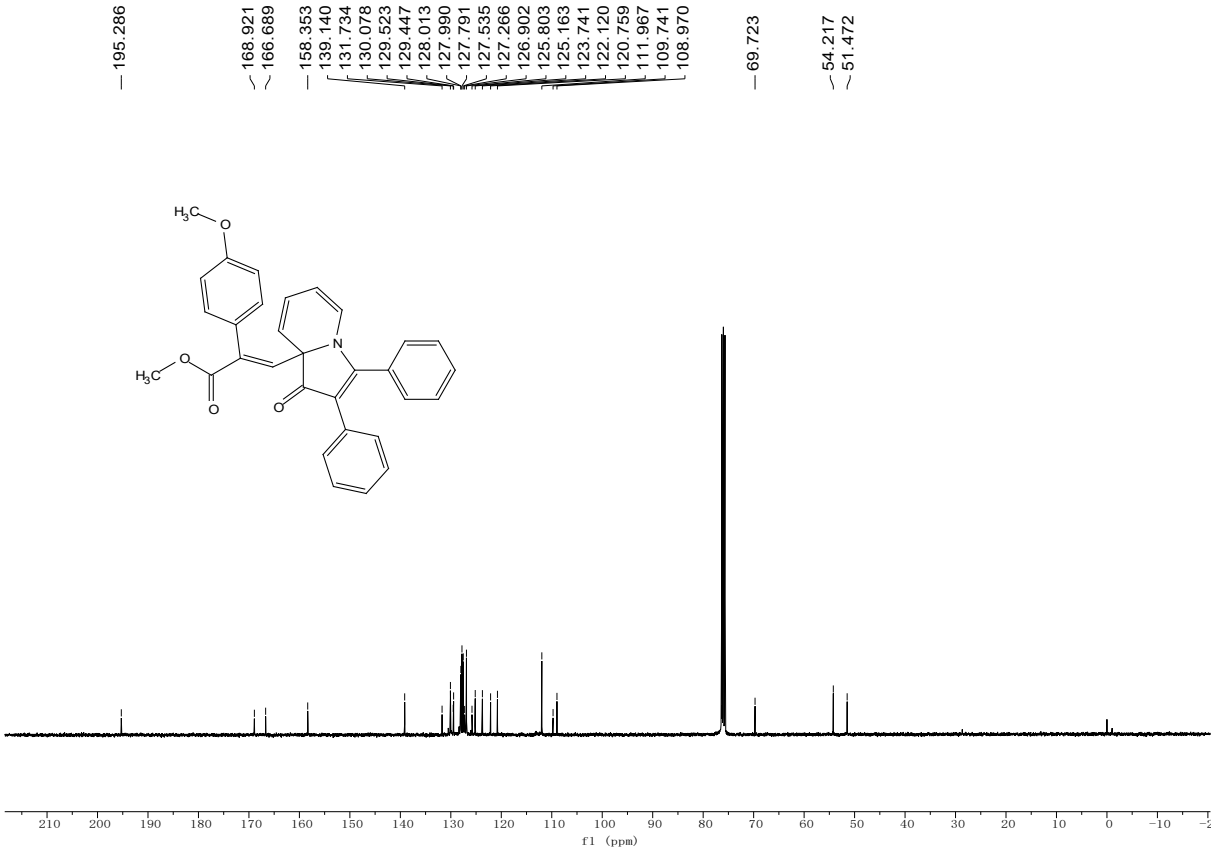
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8b**



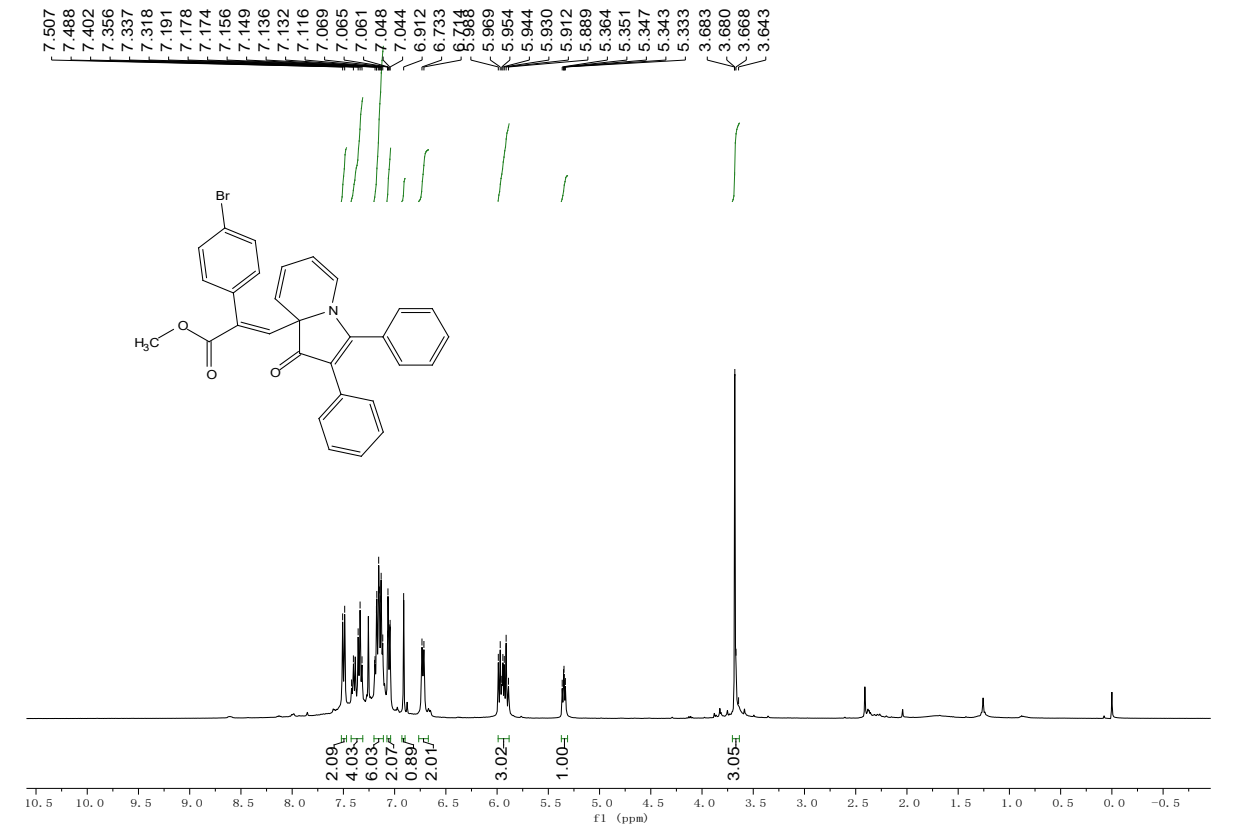


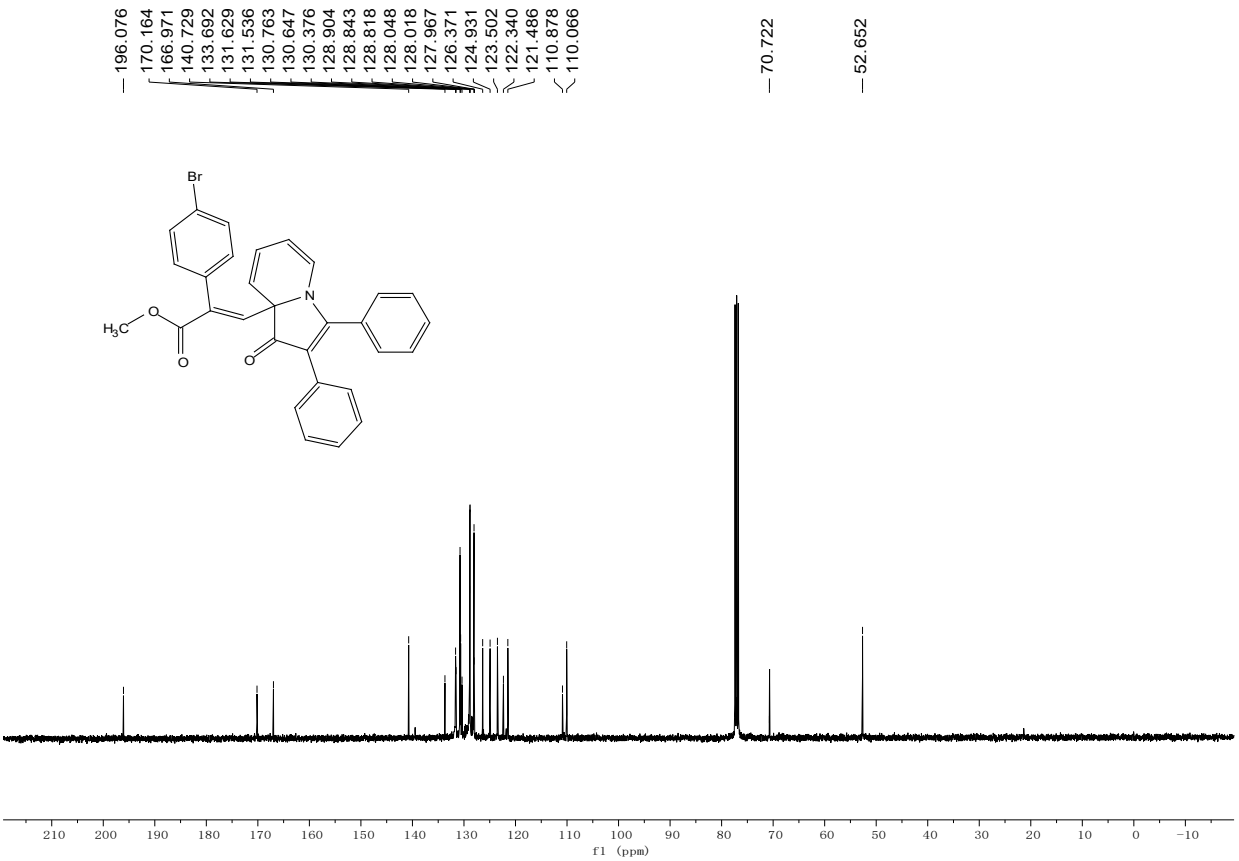
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8c**





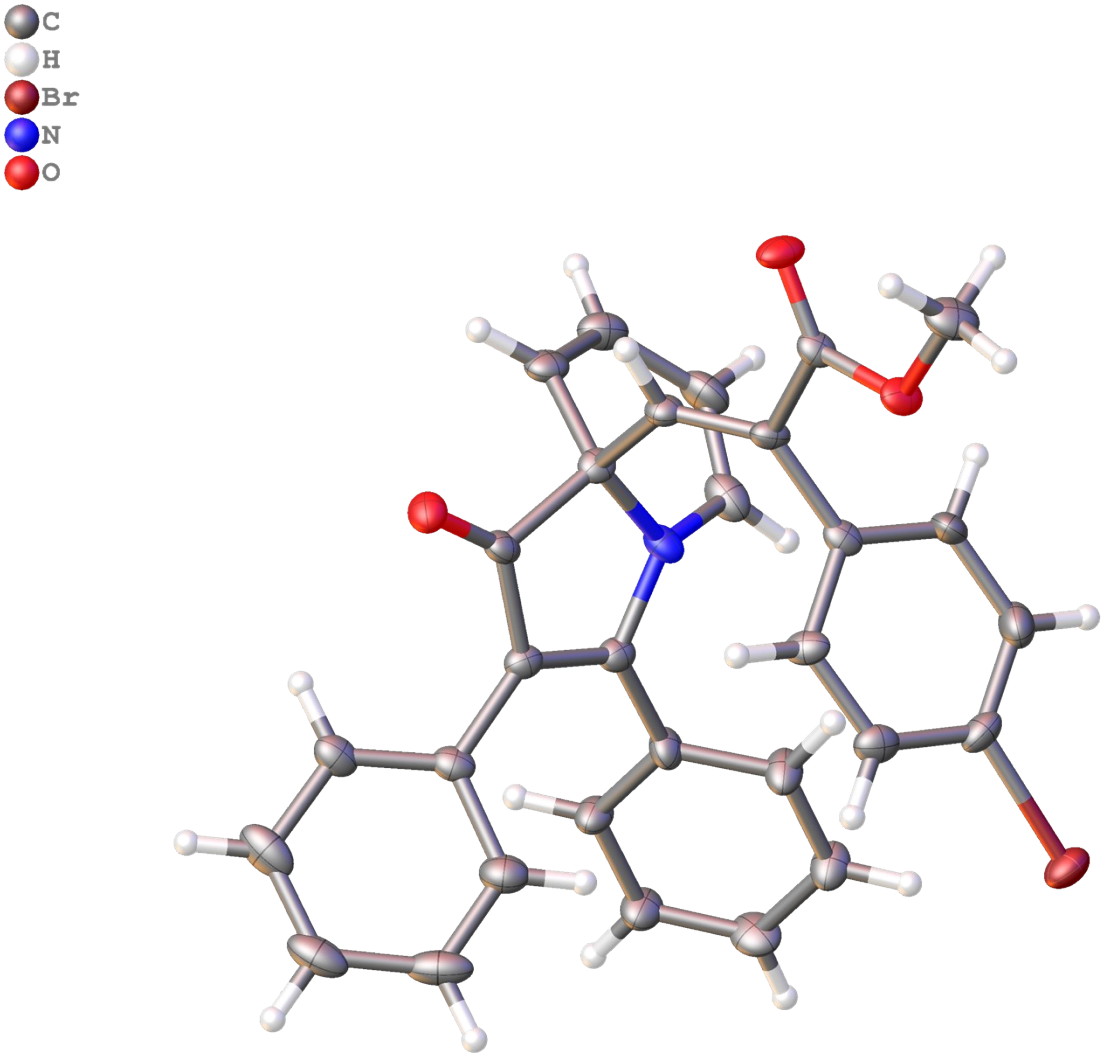
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8d**





4. X-ray crystallographic data

Figure S2 X-ray single crystal structure of **8d** (displacement ellipsoids are drawn at the 50% probability level)



Single crystals of **8d** were grown by slow evaporation of its EA/PE solution. The crystal was kept at 149.99 K during data collection. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2227171).

Table S1 Crystal data and structure refinement for **8d.**

Identification code	2-297
Empirical formula	$C_{30}H_{22}BrNO_3$
Formula weight	524.39
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.5059(4)
b/Å	10.6245(4)

c/Å	24.3428(16)
α/°	90
β/°	100.388(5)
γ/°	90
Volume/Å^3	2418.2(2)
Z	4
ρ_{calc}g/cm^3	1.440
μ/mm^{-1}	2.580
F(000)	1072.0
Crystal size/mm^3	0.14 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.384 to 133.178
Index ranges	-10 ≤ h ≤ 11, -8 ≤ k ≤ 12, -28 ≤ l ≤ 28
Reflections collected	8406
Independent reflections	4271 [R_{int} = 0.0495, R_{sigma} = 0.0584]
Data/restraints/parameters	4271/9/328
Goodness-of-fit on F^2	1.165
Final R indexes [I>=2σ (I)]	R_1 = 0.1253, wR_2 = 0.2837
Final R indexes [all data]	R_1 = 0.1331, wR_2 = 0.2876
Largest diff. peak/hole / e Å-3	1.28/-0.89

Table S2 Bond Lengths for **8d**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C24	1.900(6)	C9	C27	1.505(8)
Br2	C24	1.946(10)	C10	C11	1.466(8)
O1	C8	1.213(6)	C11	C12	1.383(8)
O2	C19	1.201(7)	C11	C16	1.394(8)
O3	C19	1.335(7)	C12	C13	1.382(8)
O3	C20	1.449(7)	C13	C14	1.414(9)
N1	C9	1.468(6)	C14	C15	1.342(9)
N1	C10	1.388(7)	C15	C16	1.396(8)
N1	C30	1.394(7)	C17	C18	1.345(8)
C1	C2	1.367(8)	C18	C19	1.520(7)
C1	C6	1.414(9)	C18	C21	1.482(7)
C1	C7	1.458(8)	C21	C22	1.371(7)
C2	C3	1.406(9)	C21	C26	1.408(8)
C3	C4	1.355(11)	C22	C23	1.378(9)
C4	C5	1.417(10)	C23	C24	1.362(9)
C5	C6	1.362(9)	C24	C25	1.376(8)
C7	C8	1.444(8)	C25	C26	1.388(8)
C7	C10	1.387(7)	C27	C28	1.337(8)
C8	C9	1.548(7)	C28	C29	1.453(9)
C9	C17	1.517(7)	C29	C30	1.317(10)

Table S3 Bond Angles for **8d**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C19	O3	C20	114.3(5)	C16	C11	C10	119.8(5)
C10	N1	C9	110.3(4)	C13	C12	C11	121.7(6)
C10	N1	C30	125.1(5)	C12	C13	C14	118.1(6)
C30	N1	C9	119.3(5)	C15	C14	C13	120.2(6)
C2	C1	C6	116.9(5)	C14	C15	C16	121.9(6)
C2	C1	C7	121.1(5)	C11	C16	C15	118.7(5)

C6	C1	C7	121.9(5)	C18	C17	C9	130.7(5)
C1	C2	C3	122.6(6)	C17	C18	C19	115.6(5)
C4	C3	C2	119.1(6)	C17	C18	C21	127.5(5)
C3	C4	C5	120.2(6)	C21	C18	C19	116.9(4)
C6	C5	C4	119.4(7)	O2	C19	O3	124.8(5)
C5	C6	C1	121.8(6)	O2	C19	C18	124.0(5)
C8	C7	C1	124.5(4)	O3	C19	C18	111.2(5)
C10	C7	C1	127.7(5)	C22	C21	C18	122.1(5)
C10	C7	C8	107.8(5)	C22	C21	C26	118.5(5)
O1	C8	C7	130.6(5)	C26	C21	C18	119.2(4)
O1	C8	C9	121.8(5)	C21	C22	C23	120.9(5)
C7	C8	C9	107.7(4)	C24	C23	C22	120.7(5)
N1	C9	C8	102.2(4)	C23	C24	Br1	121.4(4)
N1	C9	C17	115.6(4)	C23	C24	Br2	103.9(5)
N1	C9	C27	111.0(4)	C23	C24	C25	119.9(6)
C17	C9	C8	110.2(4)	C25	C24	Br1	118.4(5)
C27	C9	C8	112.3(4)	C25	C24	Br2	136.2(6)
C27	C9	C17	105.7(5)	C24	C25	C26	120.1(6)
N1	C10	C11	120.9(4)	C25	C26	C21	119.8(5)
C7	C10	N1	111.9(5)	C28	C27	C9	118.2(5)
C7	C10	C11	127.2(5)	C27	C28	C29	121.4(6)
C12	C11	C10	121.1(5)	C30	C29	C28	119.5(6)
C12	C11	C16	119.1(5)	C29	C30	N1	120.4(6)

5. References

1. a) C. M. Vanos, T. H. Lambert, *Angew. Chem. Int. Ed.,* 2011, **50**, 12222-12226. b) A. P. Patricia, J. D, Tovar, *J. Org. Chem*., 2010, **75**, 5689-5696.

2. S. Prateeptongkum, K. Driller, R. Jackstell, A. Spannenberg, M. Beller, Efficient Synthesis of Biologically Interesting 3,4-Diaryl-Substituted Succinimides and Maleimides: Application of Iron-Catalyzed Carbonylations., *Chem. Eur. J.,* 2010, **16**, 9606-9615.
3. J. Tian, Z. Zhang, X. Yang, H. Fun, J. Xu, *J. Org. Chem*., 2001, **66**, 8230-8235.
4. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, O.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision E.01; Gaussian, Inc.: Pittsburgh PA, 2004.
5. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem., B* 2009, **113**, 6378-6396.